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(54)名稱

介白素—２３受體之雙環肽抑制劑

(57)摘要

本發明關於介白素-23 受體(IL-23R)之新穎雙環肽抑制劑或其醫藥上可接受之鹽、對應之醫藥組成物、用於治療自體免疫發炎及相關疾病與病症之方法及/或用途。

The present invention relates to novel bicyclic peptide inhibitors of the interleukin-23 receptor (IL-23R) or pharmaceutically acceptable salt thereof, corresponding pharmaceutical compositions, methods and/or uses for treatment of autoimmune inflammation and related diseases and disorders.

特徵化學式：

R1-X4-X5-T-X7-X8-X9-AEF-2Nal-X12-X13-N-X15-meG-R2 (I')

【發明摘要】

【中文發明名稱】　介白素-23受體之雙環肽抑制劑

【英文發明名稱】　BICYCLIC PEPTIDE INHIBITORS OF INTERLEUKIN-23 RECEPTOR

【中文】

本發明關於介白素-23受體(IL-23R)之新穎雙環肽抑制劑或其醫藥上可接受之鹽、對應之醫藥組成物、用於治療自體免疫發炎及相關疾病與病症之方法及/或用途。

【英文】

The present invention relates to novel bicyclic peptide inhibitors of the interleukin-23 receptor (IL-23R) or pharmaceutically acceptable salt thereof, corresponding pharmaceutical compositions, methods and/or uses for treatment of autoimmune inflammation and related diseases and disorders.

【指定代表圖】無

【代表圖之符號簡單說明】無

【特徵化學式】

R1-X4-X5-T-X7-X8-X9-AEF-2Nal-X12-X13-N-X15-meG-R2 (I')

【發明說明書】

【中文發明名稱】　介白素-23受體之雙環肽抑制劑

【英文發明名稱】　BICYCLIC PEPTIDE INHIBITORS OF INTERLEUKIN-23 RECEPTOR

【技術領域】

【0001】　本發明關於介白素-23受體(IL-23R)之新穎雙環肽抑制劑或其醫藥上可接受之鹽、溶劑合物及/或其他形式，發明關於相應之醫藥組成物、IL-23R抑制劑用於治療自體免疫發炎疾病及/或相關病症之方法及/或用途。

【先前技術】

【0002】　介白素-23 (IL-23)細胞介素已涉及在自體免疫發炎與相關疾病及病症之發病機制中扮演關鍵角色，諸如多發性硬化症、氣喘、類風濕性關節炎、牛皮癬、及發炎性腸疾(IBD)（例如，潰瘍性結腸炎及Crohn氏症）。IBD之急性及慢性小鼠模型顯露了介白素-23受體(IL-23R)及下游效應細胞介素在疾病發病機制中之主要角色。IL-23R會在各種適應性及先天性免疫細胞中表現，包括Th17細胞、γδ T細胞、自然殺手(NK)細胞、樹突細胞、巨噬細胞、及先天性淋巴細胞，其等在腸內大量發現。在腸黏膜表面，發現IL-23R之基因表現及蛋白水準在IBD患者中有所升高。據信IL-23會促進生產IL-6、IL-17、及腫瘤壞死因子(TNF)之病原性$CD4^+$ T細胞群的發育而介導了此效應。

【0003】　IL-23之生產在腸內是更豐富的，據信此在透過腸發炎之T細胞依賴性及T細胞非依賴性途徑而調控耐受性與免疫性之間的平衡上扮演關鍵角色，其係透過對於T輔助1 (Th1)及Th17相關細胞介素之效應，以及限制調控性T

細胞反應（從而有利於發炎）。此外，IL-23受體(IL-23R)之多型性已與易遭受發炎性腸疾(IBD)相關聯，此進一步證實IL-23途徑在腸恆定中之關鍵角色。

【0004】　牛皮癬（一種影響一般群體約2%至3%的慢性皮膚病）已顯示係由身體的T細胞發炎性反應機制所介導。IL-23為數種涉及在牛皮癬發病機制中扮演關鍵角色的介白素其中之一，其發病機制據信為經由引入介白素-17、調控T記憶細胞、及活化巨噬細胞而維持慢性自體免疫發炎。IL-23及IL-23R之表現已顯示在患有牛皮癬之患者的組織中有所增加，並且中和IL-23之抗體在牛皮癬動物模型中顯示牛皮癬發展之IL-23依賴性抑制。

【0005】　IL-23是一種雜二聚體，其包含獨特的p19次單元及與IL-12共有之p40次單元，其為涉及生產干擾素-γ (IFN-γ)之T輔助1 (T_H1)細胞發育的細胞介素。雖然IL-23及IL-12皆含有p40次單元，但其等具有不同的表型性質。例如缺乏IL-12之動物容易遭受發炎性自體免疫疾病，而缺乏IL-23之動物則具有抵抗性，據推測是由於在缺乏IL-23動物之CNS中生產IL-6、IL-17、及TNF的$CD4^+$ T細胞數目降低所致。IL-23會結合IL-23R，其為包含IL-12Rβ1及IL-23R次單元之雜二聚體受體。IL-23對IL-23R之結合會活化Jak-Stat傳訊分子Jak2、Tyk2、及Stat1、Stat 3、Stat 4、及Stat 5，雖然Stat4活化實質上較弱且不同的DNA結合Stat複合物回應於IL-23（相較於IL-12）而形成。IL-23R與Jak2構成性地締合且以配體依賴性方式與Stat3締合。相比於IL-12（其主要作用在初始CD4(+) T細胞上），IL-23會優先作用在記憶CD4(+) T細胞上。

【0006】　已開發抑制IL-23路徑之治療部份(moiety)用於治療IL-23相關疾病及病症。已識別出多種結合至IL-23或IL-23R之抗體（包括優特克單抗

(ustekinumab)），其等已證明可用於治療中度至嚴重斑塊型牛皮癬(PSO)、活動性牛皮癬性關節炎(PSA)、中度至嚴重活動性Crohn氏症(CD)、及中度至嚴重活動性潰瘍性結腸炎(UC)。此類已識別抗體之實例包括：替拉珠單抗（Tildrakizumab，一種核可用於治療斑塊型牛皮癬之抗IL23抗體）、鼓賽庫單抗（Guselkumab，一種核可用於治療牛皮癬性關節炎之抗IL23抗體）、及里森基單抗（Risankizumab，一種在美國核可用於治療斑塊型牛皮癬且在日本核可用於治療廣泛性化膿性牛皮癬、紅皮性牛皮癬、及牛皮癬性關節炎之抗IL23抗體）。

【0007】　雖然已在臨床上使用靶向IL-23抗體治療劑，但還沒有選擇性抑制IL-23傳訊之小分子治療劑。已識別出一些結合至IL-23R且抑制IL-23結合至IL-23R之多肽抑制劑（參見例如美國專利申請公開案第US2013/0029907號）。

【0008】　因此，在所屬技術領域中對於用以治療及/或預防IL-23相關及/或IL23R相關疾病及病症之有效小分子及/或多肽治療劑仍有顯著需求，包括但不限於牛皮癬、牛皮癬性關節炎、發炎性腸疾、潰瘍性結腸炎、及Crohn氏症。特定而言：

- 用於特異性靶向來自腸之腔側的 IL-23R 之化合物及方法可對遭受腸組織之局部發炎的 IBD 患者提供治療效益；及/或
- 口服生體可用之 IL-23 的小分子及/或多肽抑制劑可對患有輕度至中度牛皮癬之患者提供非類固醇型治療選項及對不需要輸注遞送之中度至嚴重牛皮癬提供治療。

【0009】　用於特異性靶向來自腸之腔側的IL-23R之化合物及方法可對遭受腸組織之局部發炎的IBD患者提供治療效益。此外，口服生體可用之IL-23的小分子及/或多肽抑制劑可對患有輕度至中度牛皮癬之患者提供非類固醇型治療選項及對不需要輸注遞送之中度至嚴重牛皮癬提供治療。

【0010】　本發明係關於藉由提供結合IL-23R以抑制IL-23結合及傳訊的雙環肽抑制劑或其醫藥上可接受之鹽、溶劑合物、及/或其他形式來處理這些需求，其經由不同合適的投予途徑，可包括但不限於口服投予。

【發明內容】

【0011】　一般而言，本發明關於介白素-23受體(IL-23R)之新穎雙環肽抑制劑或其醫藥上可接受之鹽、溶劑合物及/或其他形式，對應之醫藥組成物、IL-23R抑制劑用於治療自體免疫發炎疾病及/或相關病症之方法及/或用途。

【0012】　特定而言，本發明關於式(I')、(I)至(III)之化合物、或其醫藥上可接受之鹽、溶劑合物、及/或其他形式、對應之醫藥組成物、用於治療自體免疫發炎疾病及相關病症之方法及/或用途。

【0013】　本發明的IL-23R之雙環肽抑制劑係由式(I')之線性形式結構所代表：

R1-X3-X4-X5-X6-X7-X8-X9-X10-X11-X12-X13-X14-X15-X16-X17-R2　(I')

式(I')之線性形式結構係意欲用於例示性及非限制性目的，其將因本說明書各處中所提出及例示之實例而清楚易見，亦即例如其中各結構可長於或短於十八個胺基酸之長度及/或如本文中所定義之其他對應化學部份或官能基取代基。

【0014】 具體而言在式(I')中：

- X3 至 X17 各別且個別代表個別胺基酸(aa)殘基或如下所述及本說明書中之其他對應化學部份或官能基取代基；
- R1 代表 N 端末端，其可係例如氫或在胺基上取代之化學部份或官能基；
- 同樣地，R2 代表羧基末端，其可係例如該羧基之 OH 或附接至或取代該 OH 基之化學部份或官能基（例如，胺基以給出末端醯胺，例如-$C(O)HN_2$）；。
- 如線性形式結構中所示之任何殘基可存在或不存在，例如 X3 及/或 X16-X18 可不存在；
- 肽抑制劑可在位置 X4 與 X9（例如，一對 Pen 殘基或 Abu 與 Cys 殘基）之間具有鍵結而形成雙硫鍵或硫醚鍵，從而導致形成雙環環結構之第一個環，然而形成雙環結構之第一個環的鍵可位於 X4 及 X9 以外的其他胺基酸或化學部份之間；且/或
- 形成雙環環結構之第二個環的鍵可導致橋聯第一個環結構之環或將藉由分子之中介部分連結的環結構分開。

【0015】 在其他態樣中，雙環結構之第二個環可藉由X3與X10、X13、X15、X16、或X17中一者之間的鍵結而形成。在進一步態樣中，肽可具有雙環

結構之第二個環，其藉由X5與X10之間的鍵而提供。雙環結構之第二個環亦可藉由X8與X12之間的鍵而提供。亦包括具有雙環結構之第二個環的雙環肽，其藉由X10與X13、X15、X16、R2、或R3中一者之間的鍵而提供。在多個態樣中，X13與X15或X16中任一者之間的鍵形成雙環結構之第二個環。在一進一步態樣中，雙環結構之第二個環藉由R1與R2之間的鍵而提供。進一步細節係提供於下。

【0016】　本發明關於式(I')、(I)至(XX)之化合物、其鹽、溶劑合物、或形式、對應之醫藥組成物、及用於治療自體免疫發炎疾病及相關病症之方法及/或用途。

【0017】　特定而言，本發明關於IL-23R之肽抑制劑或其醫藥上可接受之鹽、溶劑合物、及/或其他形式、對應之醫藥組成物、用於治療疾病（包括自體免疫發炎疾病及相關病症）之方法及/或用途；其中：

- 本發明的 IL-23R 之抑制劑係藉由下列來識別：式(I')、(I)至(XX)；或
- 分別於本說明書之表 1A、表 1B、表 1C、表 1D、表 1E、表 1F、表 1G、及表 1H 中者。

【0018】　本發明關於係為IL-23受體之雙環抑制劑的化合物，其包含式XIX之胺基酸序列

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-X12-X13-X14-X15-X16-X17-R2　(XIX)

其中：

R1係7Ahp、6Ahx、5Ava、PEG2、AEEP、AEEP(Ns)、GABA、pFS、bAla、PEG2PEGE2gEC16OH、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、5cpaCO、cPEG3aCO、或-H

X3係dR、R、G、R5H、R6H、R7H、S5H、S6H、S7H、K、dK、Orn、dOrn、Dap、dDap、Dab、dDab、Dab(COCH2)、dDab(COCH2)、hE、dhE、hK、dhK,dK(Me)3、K(Me)3、dK(PEG2PEG2gEC18OH)、K(PEG2PEG2gEC18OH)、或不存在；

X4係Pen、Abu、或C；

X5係N、Q、N(N(Me)2)、或K(PEG2PEG2gEC18OH)；

X7係W、或7MeW，

X8係K(Ac)、dK(Ac)、Q、dQ、K(NMeAc)、dK(NMeAc)、K(PEG2PEG2gEC18OH)、或dK(PEG2PEG2gEC18OH)；

X9係Pen、Abu、或C；

X10係AEF、或TMAPF；

X11為2Nal；

X12係THP、Acpx、或aMeK；

X13係E、dE、hE、dhE、aMeE、d-aMeE、D、dD、Aad、dAad、K(Ac)、dK(Ac)、K、dK、hSer、dhSer、Dap(pF)、R5H、R6H、R7H、S5H、S6H、S7H、C、dC、K(NMe)、或dK(NMe)，

X14係N；

X15係3Pal、H、dH、3MeH、3MedH、F、dF、aMeF、aMedF、THP、bAla、NMeTyr、NMedY、K、dK；

X16係meG、NMedY、NMeK(PEG2PEG2gEC18OH)、NMedK(PEG2PEG2gEC18OH)、或不存在

X17係不存在或K(PEG2PEG2gEC18OH)；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及R1與X13之間或X3與X13之間的第二醯胺、脂族（由環合歧化「RCM」反應而產生）、烷基胺、或硫醚鍵聯而環化。

【0019】　本發明亦關於式XIX之化合物、其鹽、溶劑合物、或形式、對應之醫藥組成物、及用於治療自體免疫發炎疾病及相關病症之方法及/或用途。

【0020】　本發明關於係為IL-23受體之雙環抑制劑的化合物，其包含式XX之胺基酸序列

R1-X3-X4-X5-X6-X7-X8-X9-X10-X11-X12-X13-X14-X15-X16-R2 (XX)

其中：

R1係選自CF3CO、5cpaCO、cPEG3aCO、-H、C1至C4烷基C(O)-、或經氰基、Cl、或F所取代之C1至C4烷基C(O)-；

X3係R、dR、K、dK、K(Me)3、dK(Me)3、hK(Me)3、dhK(Me)3、或不存在

X4係Pen、Abu、或C；

X5係選自E、D、K、K(Ac)、Dap、或K(NMe)、K(NNs)；

X6係選自T、L；

X7係選自W、7MeW、7PhW；

X8係選自K(Ac)、dK(Ac)、hK(Me)3、dhK(Me)3、K(Me)3、dK(Me)3、K(NMeAc)、dK(NMeAc)、Q(N(Me)2)、KPeg12、dKPeg12、KAcMor、A、Q、dKacMor、dQ(N(Me)2)、K(mPEG12)、dA、dQ、或dK(mPEG12)；

X9係Pen、Abu、或C；

X10係選自AEF、AEF(NMe)、F4CONH2、或F4OMe；

X11係2Nal；

X12係選自THP、aMeLeu、或A；，

X13係選自E、dE、K(Ac)、dK(Ac)、K(Me)3、dK(Me)3、K(NMeAc)、dK(NMeAc)、Q(N(Me)2)、dQ(N(Me)2)、A、dA、L、或dL；

X14係選自L、N、或S；

X15係選自3Pal、L、dL、或Aib

X16係選自meG；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X5與X10之間的第二醯胺或烷基胺鍵聯而環化。

【0021】 本發明亦關於式XX之化合物、其鹽、溶劑合物、或形式、對應之醫藥組成物、及用於治療自體免疫發炎疾病及相關病症之方法及/或用途。

【0022】 本發明關於係為IL-23受體之雙環抑制劑的化合物，其包含式I之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-X11-X12-X13-N-X15-meG-R2 (I)

其中：

R1係7Ahp、6Ahx、5Ava、PEG2、AEEP、或AEEP(Ns)；

X4係Pen、Abu、aMeC、hC、或**C**；

X5係N或K(PEG2PEG2gEC18OH)；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K(Ac)、Q、K(NMeAc)、K(PEG2PEG2gEC18OH)、dK(Ac)、dQ、dK(NMeAc)、或dK(PEG2PEG2gEC18OH)；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP或aMeK；

X13係E、dE、hE、dhR、D、dD、hSer、或dhSer；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；

R2係-NH_2、N(H)C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及R1與X13之間的第二醯胺鍵或硫醚鍵（在pFS與Dap(pF)之間）而環化。

【0023】　本發明亦關於式I之化合物、其鹽、溶劑合物、或形式、對應之醫藥組成物、及用於治療自體免疫發炎疾病及相關病症之方法及/或用途。

【0024】　本發明關於係為IL-23受體之雙環抑制劑的化合物，其包含式II-XVIII之胺基酸序列。

【0025】　本發明亦關於式II-XVIII之化合物、其鹽、溶劑合物、或形式、對應之醫藥組成物、及用於治療自體免疫發炎疾病及相關病症之方法及/或用途。

【0026】　本發明關於係為IL-23受體之雙環抑制劑的化合物，其包含式III之胺基酸序列。

【0027】　除了前述者外，本發明關於製造式(I)至(XX)或表1A至1H之化合物之方法或程序。

【0028】　本發明亦關於醫藥組成物，其包含本文中所述的IL-23R之雙環肽抑制劑化合物或如本文中所述的其醫藥上可接受之鹽、溶劑合物、或形式、及醫藥上可接受之載劑、賦形劑、或稀釋劑。醫藥組成物可包含或可排除吸收增強劑，取決於預期之遞送途徑或其用於治療特定適應症之用途。吸收增強劑可滲透增強劑或腸滲透增強劑。在一態樣中，吸收增強劑會改善口服生體可用性。

【0029】　本發明關於用於治療對象中之發炎性疾病之方法及/或用途，其包含分別投予治療有效量的一或多種本文中所述的IL-23R之雙環肽抑制劑化合物或其醫藥上可接受之鹽、或溶劑合物、或如本文中所述的對應之醫藥組成物至有需要之對象中。此類發炎性疾病及相關病症可包括但不限於發炎性腸疾(IBD)、Crohn氏症(CD)、潰瘍性結腸炎(UC)、牛皮癬(PsO)、或牛皮癬性關節炎(PsA)、及類似者。

【0030】　本發明提供一或多種本文中所述的化合物（例如，式(I)至(XX)或表1A至1H之化合物）用於製備用於治療發炎性疾病及相關病症之醫藥組成物之用途，包括但不限於發炎性腸疾(IBD)、Crohn氏症(CD)、潰瘍性結腸炎(UC)、牛皮癬(PsO)、及牛皮癬性關節炎(PsA)。

【0031】　本發明提供一或多種本文中所述的式(I)至(XX)之化合物）用於治療發炎性疾病及相關病症之用途，包括但不限於發炎性腸疾(IBD)、Crohn氏症(CD)、潰瘍性結腸炎(UC)、牛皮癬(PsO)、及牛皮癬性關節炎(PsA)。

【0032】　本發明提供套組，其包含一或多種本文中所述的式(I)至(XX)之化合物及對於治療患者中之疾病之使用說明。該疾病可係發炎性疾病或相關病症，包括但不限於發炎性腸疾(IBD)、Crohn氏症(CD)、潰瘍性結腸炎(UC)、牛皮癬(PsO)、及牛皮癬性關節炎(PsA)。

【圖式簡單說明】

【實施方式】

I.　一般

【0033】　本發明關於介白素-23受體(IL-23R)之新穎雙環肽抑制劑或其醫藥上可接受之鹽、溶劑合物及/或其他形式、對應之醫藥組成物、IL-23R抑制劑用於治療自體免疫發炎疾病及/或相關病症之方法及/或用途。

【0034】　本發明關於IL-23R之雙環環狀肽抑制劑。本發明之雙環肽抑制劑可展現增強之性質，諸如更長之體內半衰期（相較於對應的IL-23R之單環肽抑制劑）。

II.　定義

【0035】　除非在本文中另有定義，否則本申請案中所使用之科學及技術用語均具有所屬技術領域中具有通常知識者所通常理解的含義。

【0036】 「約(about)」當指涉數值時，其包括所陳述數值+/−所陳述數值之10%。例如，約50%包括45%至55%之範圍，而約20莫耳當量包括18至22莫耳當量之範圍。因此，當指涉範圍時，「約」係指該範圍各端之各所陳述數值+/−所陳述數值之10%。例如，約1至約3之比率（重量/重量）包括0.9至3.3之範圍。

【0037】 「患者(patient)」或「對象(subject)」（其等可互換使用）係指活生物體，其包括但不限於罹患或易患可藉由投予如本文中所提供之醫藥組成物來治療的疾病或病況之人類對象。進一步非限制性實例可包括但不限於包括但不限於、其他哺乳動物、牛、大鼠、小鼠、狗、猴、山羊、綿羊、乳牛、鹿、馬、及其他哺乳類動物與類似者。在一些態樣中，患者係人類。

【0038】 除非另有指明，本文中所使用之天然出現及非天然出現胺醯殘基遵循IUPAC有機化學命名法委員會及IUPAC-IUB生物化學命名法委員會所建議之命名規約，如「Nomenclature of α-Amino Acids (Recommendations, 1974)」Biochemistry, 14(2), (1975)中所提出。倘若本說明書及隨附申請專利範圍中所採用之胺基酸及胺醯殘基與那些建議不同，其等將對讀者清楚表明。在代表IL-23抑制劑之胺基酸的序列中，個別胺基酸係由連字號「-」或括號所分開，例如離胺酸係顯示為[K]。

【0039】 在本說明書各處中，除非天然出現胺基酸係以其全名（例如，丙胺酸、精胺酸等）來指稱，否則其等係以其常規三字母或單字母縮寫（例如，針對丙胺酸為Ala或A，針對精胺酸為Arg或R等）來標示。除非另有指明，胺基酸之三字母及單字母縮寫係指所提及胺基酸之L-異構形式。如本文中所使

用，用語「L-胺基酸(L-amino acid)」係指肽之「L」異構形式，而用語「D-胺基酸」相反地係指肽之「D」異構形式（例如，(D)Asp或D-Asp；(D)Phe或D-Phe）。可將D異構形式中之胺基酸殘基取代為任何L-胺基酸殘基，只要肽保留所欲之功能。當使用單字母縮寫來指稱時，D-胺基酸可依慣例以小寫標示。例如，L-精胺酸可表示為「Arg」或「R」，而D-精胺酸可表示為「arg」或「r」。同樣地，L-離胺酸可表示為「Lys」或「K」，而D-離胺酸可表示為「lys」或「k」。替代地，胺基酸前面的小寫「d」可用來指示其具有D異構形式，例如D-離胺酸可表示為dK。

【0040】　在較不常見或非天然出現胺基酸的情況下，除非其等係以其全名來指稱（例如肌胺酸、鳥胺酸等），否則針對其殘基採用常用的三或四字母代碼，包括Sar或Sarc（肌胺酸，即N-甲甘胺酸）、Aib（α-胺異丁酸）、Dab（2,4-二胺丁酸）、Dapa（2,3-二胺丙酸）、γ-Glu（γ-麩胺酸）、Gaba（γ-胺丁酸）、β-Pro（吡咯啶-3-羧酸）、及Abu（2-胺丁酸）。

【0041】　D-異構形式之胺基酸可位於本文中所陳述的IL-23R抑制劑之任何位置（出現在分子中之X1至X18中任一者）。在一態樣中，D-異構形式之胺基酸可僅位於X3、X5、X6、X8、X13、X16之任一或多者、及可選地一個額外位置。在其他態樣中，D-異構形式之胺基酸可僅位於X3、X8、X13、X16之任一或多者、及可選地一個額外位置。在其他態樣中，D-異構形式之胺基酸可僅位於X8、X13（例如，X8係dK(Ac)且x13係dE）之任一或多者、及可選地一個額外位置。在一態樣中，D-異構形式之胺基酸可僅位於X3、及可選地一個額外位置。在其他態樣中，D-異構形式之胺基酸可僅位於X3、及可選地二或三個額

外位置。在其他態樣中，D-異構形式之胺基酸可位於出現在本文中所陳述之IL-23R抑制劑的位置X1至X18之僅一或二者。在其他態樣中，D-異構形式之胺基酸可位於出現在本文中所陳述之IL-23R抑制劑的位置X1至X18之僅三或四者。例如，僅具有位置X3至X15存在的本文中所陳述之IL-23R抑制劑可具有存在於這些位置之3或4者的D-形式之胺基酸。在其他態樣中，D-異構形式之胺基酸可位於出現在本文中所陳述之IL-23R抑制劑的位置X1至X18之僅五或六者。

【0042】　如所屬技術領域中或對具有通常知識者而言所習知理解，本文中所揭示之肽序列係顯示為由左至右前進，並且序列左端係肽之N-端而序列右端係肽之C-端。在本文中所揭示之序列中，有序列是在序列之羧基端（C-端）結合「-OH」部份或「$-NH_2$」部份。在此類情況下，且除非另有指明，在序列之C-端的「-OH」或「$–NH_2$」部份表示羥基或胺基，分別對應於在C-端存在羧酸(COOH)或醯胺基($CONH_2$)。在本發明之各序列中，可將C-端「–OH」部份取代為C-端「$–NH_2$」部份，反之亦然。

【0043】　所屬技術領域中具有通常知識者將理解，某些胺基酸及其他化學部份在結合至另一個分子時會有所改變。例如，胺基酸側鏈在其與另一個胺基酸側鏈形成分子內橋聯時可有所改變，例如一或多個氫可遭到移除或由該鍵所置換。

【0044】　「本發明之化合物」、「本發明之抑制劑」、「本發明之IL-23R抑制劑」、「本文中所述之化合物」、及「本文中所述的化合物」包括本文中所揭示的新穎化合物，例如任何實例之化合物，包括式(I)至(XX)之化合物，諸如見於表1A、表1B、表1C、表1D、表1E、表1F、表1G、或表1H中者。

【0045】 「醫藥有效量(pharmaceutically effective amount)」係指本發明之化合物在組成物或其組合中的量，其提供所欲的治療或醫藥結果。

【0046】 所謂「醫藥上可接受(pharmaceutically acceptable)」，其意指本發明之組成物的載劑、稀釋劑、鹽、或賦形劑必須與其他組分或成分相容，亦即其等對於醫藥用途係可用、安全、無毒性而可接受的。根據本發明，醫藥上可接受意指已核可或可核可，如列於美國藥典(U.S. Pharmacopoeia)或其他廣獲認可用於動物（且更特定而言人類）之藥典中者。

【0047】 「醫藥上可接受之賦形劑(pharmaceutically acceptable excipient)」包括但不限於任何佐劑、載劑、賦形劑、助滑劑、增甜劑、稀釋劑、保存劑、染料/著色劑、增味劑、界面活性劑、潤濕劑、分散劑、懸浮劑、穩定劑、等張劑、溶劑、或乳化劑，其已由美國食藥署核可為對於在人類或家畜中使用係可接受的。

【0048】 「吸收增強劑」係指改善或促進藥物在胃腸道中之黏膜吸收的組分，諸如滲透增強劑或腸滲透增強劑。如所屬技術領域中所習知理解，滲透增強劑(PE)係意欲改善生體可用性不佳之治療藥物的口服遞送之藥劑。PE能夠增加藥物之細胞旁(paracellular)及/或跨細胞通過。

【0049】 已將可增加滲透之醫藥賦形劑視為「吸收改良賦形劑」(AME)。AME可用於口服組成物中，例如作為潤濕劑（十二基硫酸鈉）、抗氧化劑（例如EDTA）、及乳化劑（例如聚乙烯二醇甘油酯(macrogol glyceride)），並且可專門包括於組成物中作為PE以改善生體可用性。PE可依其如何經由細胞旁或跨細胞途徑來改變障壁完整性而分類。

【0050】 「腸滲透增強劑(IPE)」係指改善組分之生體可用性的組分。適用於本發明之代表性IPE包括但不限於各種界面活性劑、脂肪酸、中鏈甘油酯、類固醇型清潔劑、醯肉鹼、及烷醯膽鹼、*N*-乙醯化α-胺基酸及*N*-乙醯化非α-胺基酸、及幾丁聚醣、其他黏膜黏著性(mucoadhesive)聚合物、及類似者。例如，適用於本發明之IPE可係癸酸鈉。

【0051】 如本文中所使用，「組成物(Composition)」或「醫藥組成物(Pharmaceutical Composition)」係意欲涵蓋包含指定活性產物成分(API)之發明或產物，其可包括如本文中所述的醫藥上可接受之賦形劑、載劑、或稀釋劑，諸如以本發明各處中所定義之指定量。組成物或醫藥組成物來自特定組分之組合，諸如以如本文中所述的指定量組合指定成分。

【0052】 本發明之組成物或醫藥組成物可呈不同的醫藥上可接受之形式，其可包括但不限於液體組成物、錠劑或基質組成物(matrix composition)、膠囊組成物等、及類似者。當組成物係錠劑組成物時，錠劑可包括但不限於二或更多種不同相之不同層，包括內部相及外部相（可包含核心）。錠劑組成物亦可包括但不限於一或多種塗層。

【0053】 如本文中所使用，「溶劑合物(solvate)」意指本發明之化合物與一或多種溶劑分子的物理性締合。此物理性締合涉及不同程度的鍵結，包括氫鍵結。在某些情況下，溶劑合物將能夠單離。用語「溶劑合物」意欲涵括溶液相和可單離之溶劑合物兩者。合適溶劑合物之非限制性實例包括水合物。

【0054】 亦提供本文中所述之化合物的醫藥上可接受之鹽及互變異構形式。「醫藥上可接受」或「生理上可接受(physiologically acceptable)」係指可用

於製備適用於獸醫或人類醫藥用途之醫藥組成物的化合物、鹽、組成物、劑型、及其他材料。

【0055】 本發明之IL-23R抑制劑、或其醫藥上可接受之鹽或溶劑合物可含有一或多個非對稱中心，因而可產生鏡像異構物、非鏡像異構物、及其他立體異構形式，其等在絕對立體化學上可定義為(*R*)-或(*S*)-，或針對胺基酸可定義為(D)-或(L)-。本發明意欲包括本發明之IL-23R抑制劑的所有此類可能異構物，以及其等之外消旋及光學上純形式。光學活性(+)及(-)、(*R*)-及(*S*)-、或(D)-及(L)-異構物可使用掌性合成組元s或掌性試劑來製備，或使用習知技術來解析，例如層析法及分段結晶。用於製備/單離個別鏡像異構物之習知技術包括由合適的光學上純前驅物進行掌性合成，或使用例如掌性高壓液相層析法(HPLC)進行外消旋物（或鹽或衍生物之外消旋物）解析。當本文中所述的化合物含有烯雙鍵或其他幾何非對稱中心時，除非另有指明，意欲使化合物同時包括E及Z幾何異構物。同樣地，亦意欲包括所有互變異構形式。若化合物係以其掌性形式來代表時，應理解為該態樣涵蓋但不限於特定非鏡像異構或鏡像異構濃化形式。若掌性未指明但存在時，應理解為該態樣係關於此類化合物之特定非鏡像異構或鏡像異構濃化形式；或外消旋或比例混合物(scalemic mixture)。如本文中所使用，「比例混合物」係立體異構物鏡像異構物以非為1:1之比率的混合物

【0056】 「外消旋物(racemate)」係指鏡像異構物之混合物。此種混合物可包括等量或不等量的各鏡像異構物。

【0057】 「立體異構物(stereoisomer/stereoisomers)」係指在一或多個立體中心之掌性有所不同的化合物。立體異構物包括鏡像異構物及非鏡像異構

物。如果化合物擁有一或多個非對稱中心或具有非對稱取代之雙鍵，則其可以立體異構形式存在，並因此可作為個別立體異構物或作為混合物而生產。除非另有指明，此描述係意欲包括個別立體異構物以及混合物。用於判定立體化學及分離立體異構物之方法在所屬技術領域中係熟知的（參見例如Chapter 4 of Advanced Organic Chemistry, 4th ed., J. March, John Wiley and Sons, New York, 1992）。

【0058】 「互變異構物(tautomer)」係指質子位置有所不同之化合物交替形式，諸如烯醇-酮及亞胺-烯胺互變異構物、或含有附接至環-NH-及環=N-之雜芳基的互變異構形式，諸如吡唑、咪唑、苯并咪唑、三唑、及四唑。

【0059】 除非另有定義，本文中所使用之所有技術與科學用語的意義，均與所屬技術領域中具有通常知識者所通常或習知理解的意義相同。在化學技術領域中，化學基團前面或末端之虛線是為了方便；化學基團可繪示為具有或不具有一或多個虛線而不失去其原始意義。穿過結構中線條的波形線指示基團之附接點。虛線指示可選的鍵結。除非化學上或結構上需要，書寫化學基團或其對分子其餘部分之附接點的順序不指示或暗示方向性。例如，基團「-SO_2CH_2-」等同於「-CH_2SO_2-」且兩者皆可在任一方向連接。同樣地，「芳基烷基」例如可在基團之芳基或烷基部分附接至分子之其餘部分。諸如「C_{u-v}」或(C_u-C_v)之前綴詞指示其後之基團具有u至v個。例如，「C_{1-6}烷基」及「C_1-C_6烷基」皆指示烷基具有1至6個碳原子。

【0060】 如本文中所使用，「治療(treatment/treat/treating)」係指獲得有益或所欲結果之方法。為本發明之目的，有益或所欲結果包括但不限於減輕症狀及/或減低症狀之程度及/或預防與疾病或病況之相關聯之症狀的惡化。在一

個態樣中，「治療」包括下列一或多者：(a)抑制疾病或病況（例如，降低因疾病或病況而產生之一或多種症狀、及/或減低疾病或病況之程度）；(b)減緩或遏止一或多種與疾病或病況相關聯之症狀的發展（例如，穩定疾病或病況、延緩疾病或病況之惡化或進展）；及(c)緩解疾病或病況，例如造成臨床症狀之減退、改善疾病狀態、延緩疾病之進展、增加生活品質、及/或延長存活期。

【0061】 如本文中所使用，「治療有效量(therapeutically effective amount)」或「有效量(effective amount)」係指有效引發所欲生物或醫學反應之量，包括化合物當投予至對象以治療疾病時足以使此疾病治療生效的量。有效量將隨化合物、疾病、及其嚴重性，以及所要治療之對象的年齡、體重等而有所變化。有效量可包括一個範圍的量。如所屬技術領域中所理解，有效量可呈一或多個劑量，亦即可能需要單個劑量或多個劑量以達到所欲治療終點。可在投予一或多種治療劑之背景下考慮有效量，並且如果單種藥劑在與一或多種其他藥劑結合時可達到或已達到所欲或有益結果，則可將單種藥劑認為是以有效量給予。任何共投予化合物之合適劑量可選地可因為化合物之組合作用（例如，加成性或協同性效應）而降低。

【0062】 如本文中所使用，「共投予(co-administration)」係指在投予單位劑量的一或多種額外治療劑之前或之後投予單位劑量的本文中所揭示的化合物，諸如在投予該一或多種額外治療劑的數秒、數分鐘、或數小時內投予本文中所揭示的化合物。例如，在一些態樣中，先投予單位劑量的本發明之化合物，接著在數秒或數分鐘內投予單位劑量的一或多種額外治療劑。替代地，在其他態樣中，先投予單位劑量的一或多種額外治療劑，接著在數秒或數分鐘內

投予單位劑量的本發明之化合物。在一些態樣中，先投予單位劑量的本發明之化合物，接著在數小時（例如，1至12小時）之期間後投予單位劑量的一或多種額外治療劑。在其他態樣中，先投予單位劑量的一或多種額外治療劑，接著在數小時（例如，1至12小時）之期間後投予單位劑量的本發明之化合物。本文中所揭示的化合物與一或多種額外治療劑之共投予一般係指同時或依序投予本文中所揭示的化合物及一或多種額外治療劑，使得治療有效量的各藥劑存在於患者體內。

【0063】　縮寫「(V/V)」係指詞組「體積對體積」，亦即特定物質在混合物中之比例，如藉由本文中所揭示的組成物之組分體積或體積量相對於組成物總體積所測量。因此，該量係無單位的且代表組分相對於組成物總體積之體積百分比量。例如，2% (V/V)溶劑混合物可表示2 mL的一種溶劑存在於100 mL的溶劑混合物中。

【0064】　縮寫「(w/w)」係指詞組「重量對重量」，亦即特定物質在混合物中之比例，如藉由本文中所揭示的組成物之組分的質量或重量相對於組成物總重量所測量。因此，該量係無單位的且代表組分相對於組成物的總重量之重量百分比量。例如，2% (w/w)溶液可表示2克的溶質溶於100克的溶液中。

【0065】　如醫療或醫藥技術領域中所習知理解，全身性投予途徑係指或係定義為藥物、醫藥組成物或配方、或其他物質投予至循環系統中而使得各種身體組織及器官暴露於該藥物、配方、或其他物質之途徑。如所屬技術領域中所習知理解，投予可口服投予（其中藥物或口服製劑係以口攝取並經由胃腸道

吸收）、經由腸道投予（藥物之吸收亦透過胃腸道發生）或腸胃外投予（一般為注射、輸注、或植入等）。

【0066】 「全身性活性(systemically active)」肽藥物療法當其關於本發明時，一般係指藉由包含肽活性成分之醫藥組成物的治療，其中該肽會抵抗立即代謝及/或排出，從而導致其在各種身體組織及器官中之暴露，諸如心血管、呼吸、胃腸、神經、或免疫系統。

【0067】 全身性藥物活性在本發明中亦指使用行經血流之物質的治療，從而到達並影響各種身體組織及器官中之細胞。全身性活性藥物會運輸至其作用部位，並在全身發揮作用以攻擊造成發炎性疾病之生理過程。

【0068】 「生體可用性(bioavailability)」係指活性部份（藥物或代謝物）進入全身性循環，藉以觸及作用部位之程度及速率。藥物之生體可用性會受到劑型之性質所影響，其部分取決於其設計及製造。

【0069】 如本文中所使用，「消化道組織(digestive tract tissue)」係指包含消化管之器官的所有組織。以下僅作為範例且不造成限制，「消化道組織」包括口部、食道、胃部、小腸、大腸、十二指腸、及肛門之組織。

III. 化合物

【0070】 本發明關於介白素-23受體(IL-23R)之新穎雙環肽抑制劑或其醫藥上可接受之鹽。

【0071】 特定而言，本發明關於介白素-23受體(IL-23R)之雙環肽抑制劑或其醫藥上可接受之鹽、包括結構係如表1A、表1B、表1C、表1D、表1E、表1F、表1G、及表1H中所標示者。

【0072】 在一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1A中之化合物的結構。

【0073】 在另一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1B中之化合物的結構。

【0074】 在另一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1C中之化合物的結構。

【0075】 在另一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1D中之化合物的結構。

【0076】 在另一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1E中之化合物的結構。

【0077】 在另一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1F中之化合物的結構。

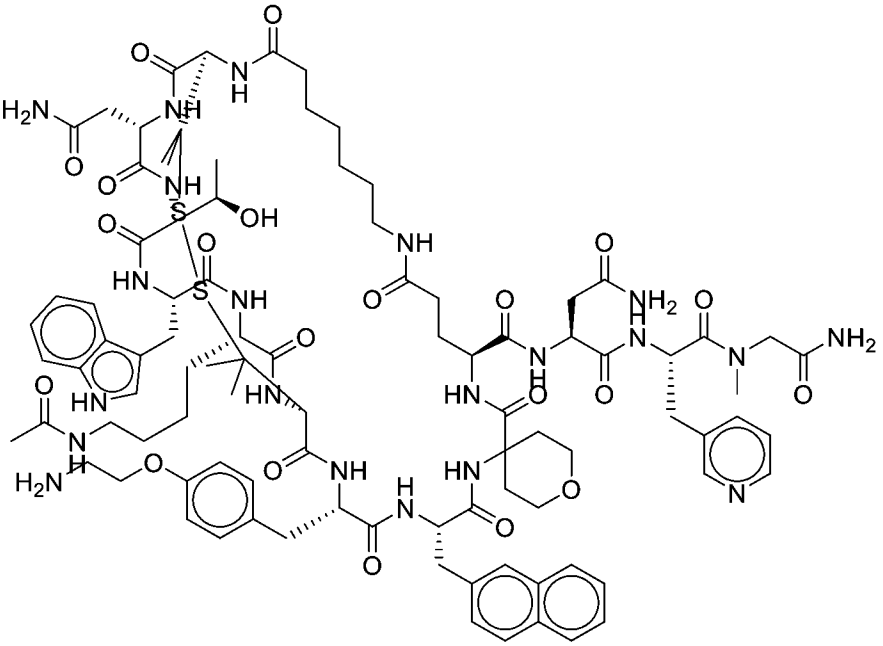
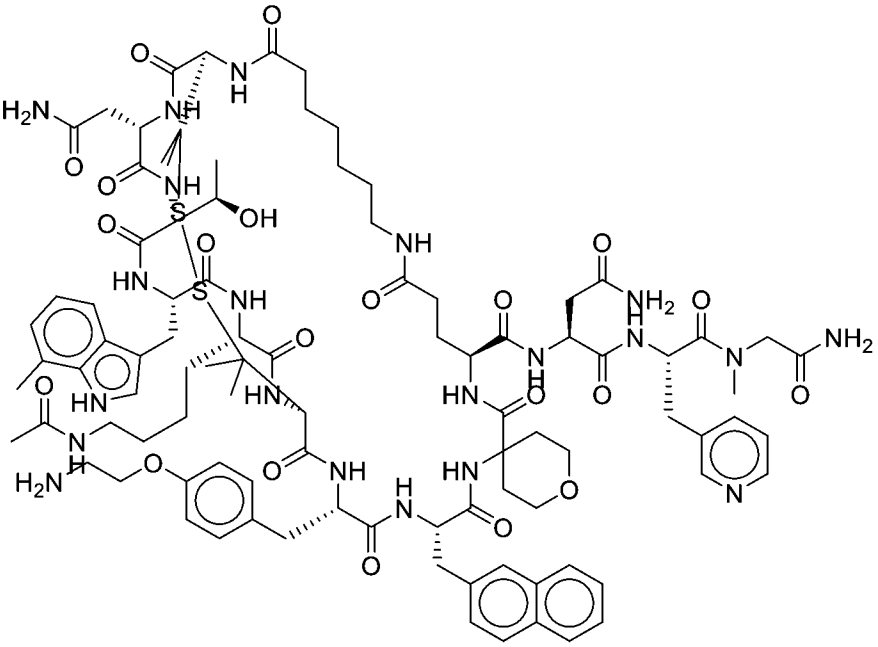
【0078】 在另一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1G中之化合物的結構。

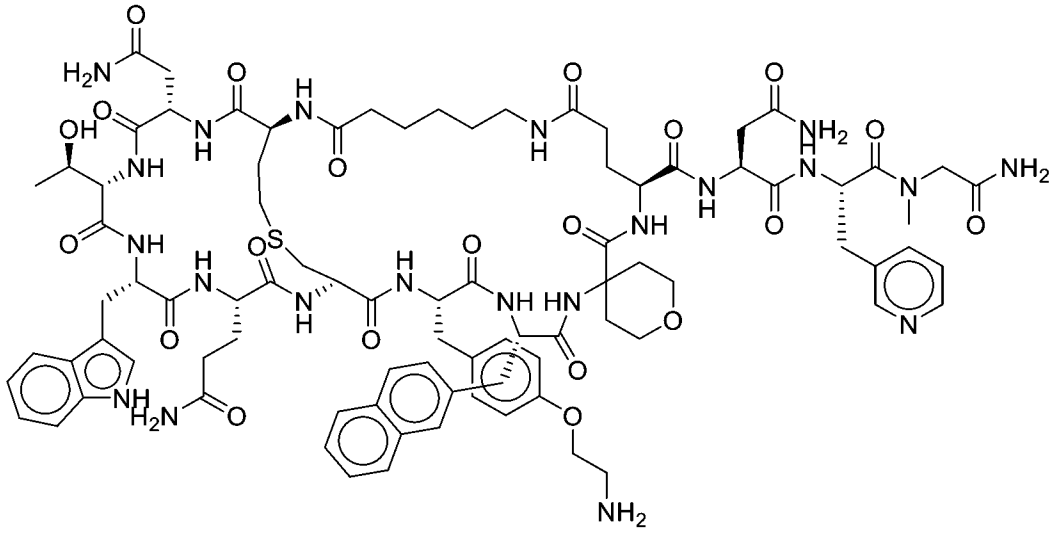
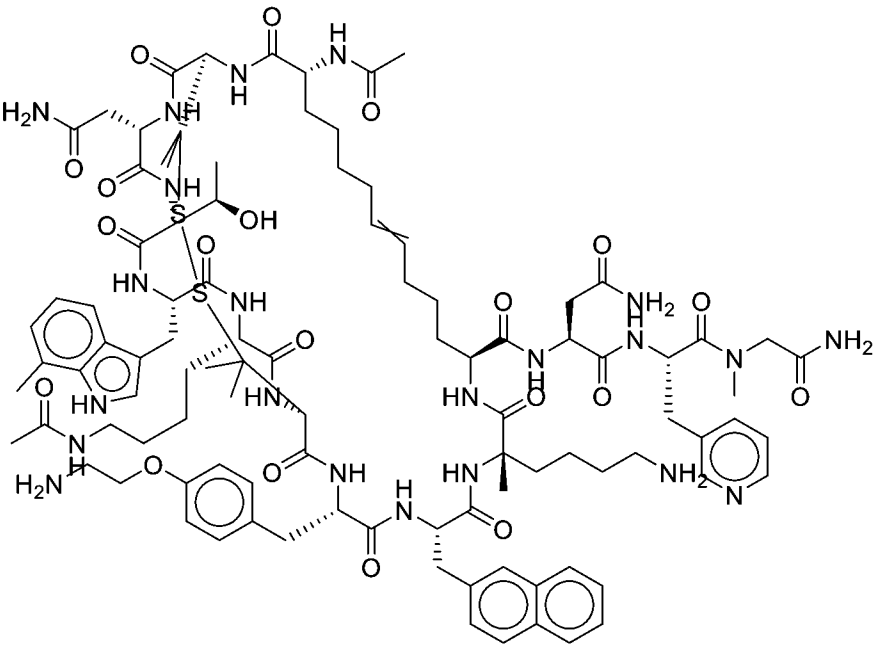
【0079】 在另一個態樣中，介白素-23受體(IL-23R)化合物之雙環肽抑制劑化合物、或其醫藥上可接受之鹽具有表1H中之化合物的結構。

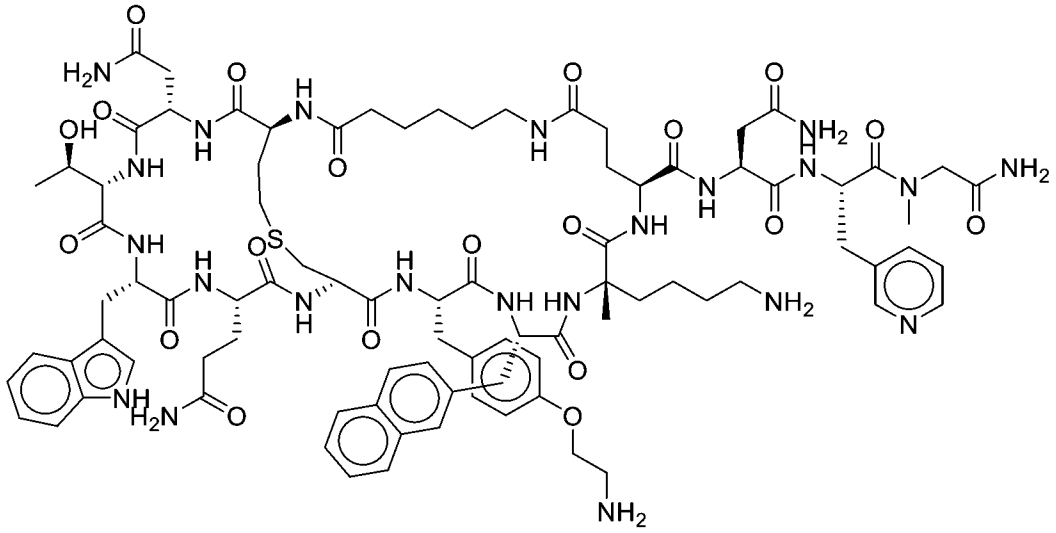
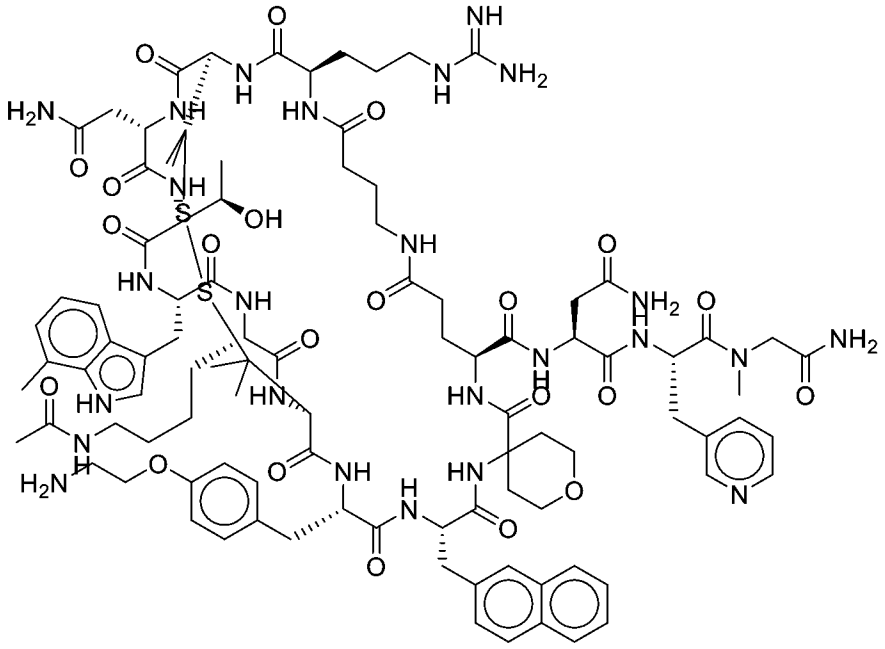
【0080】

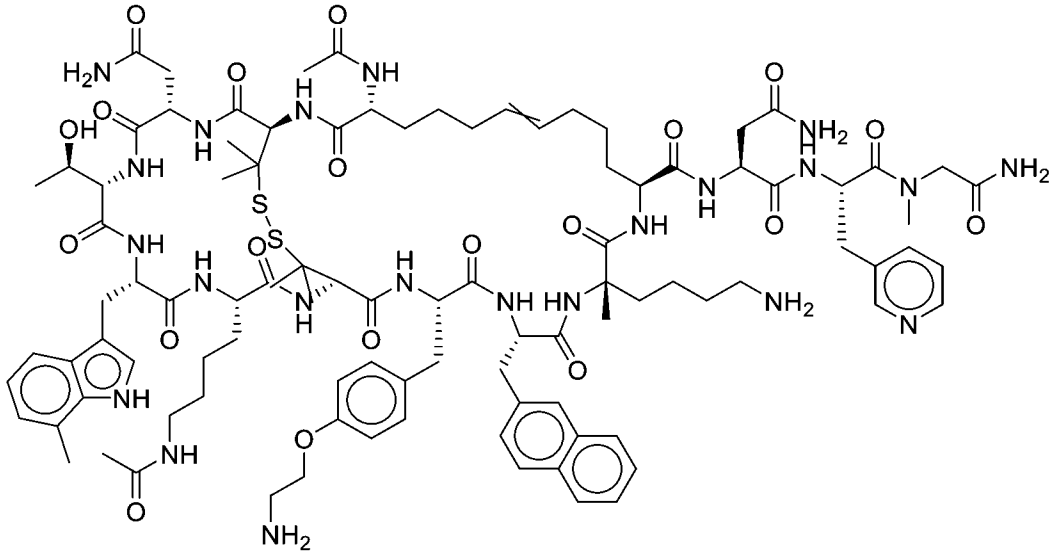
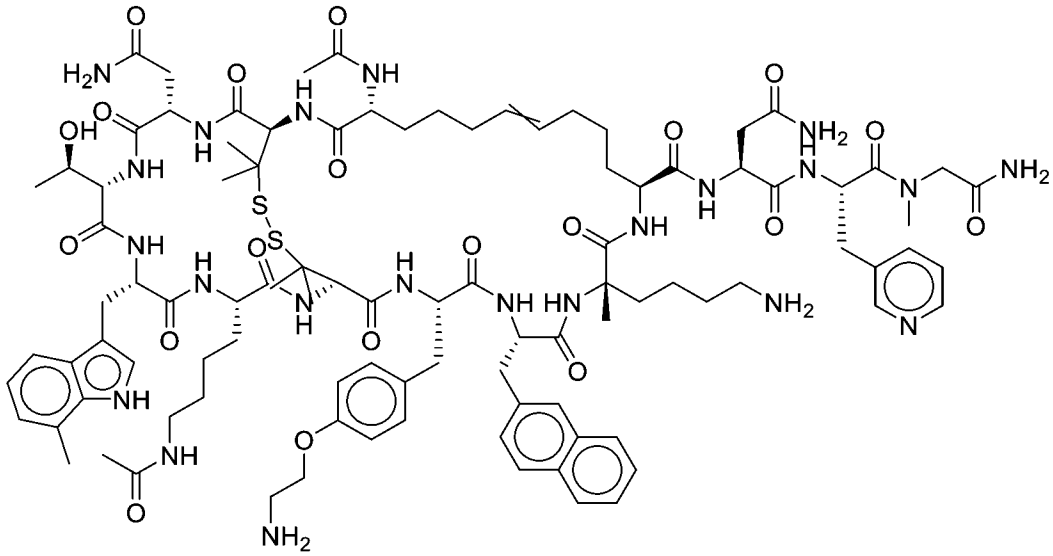
表1A.化合物

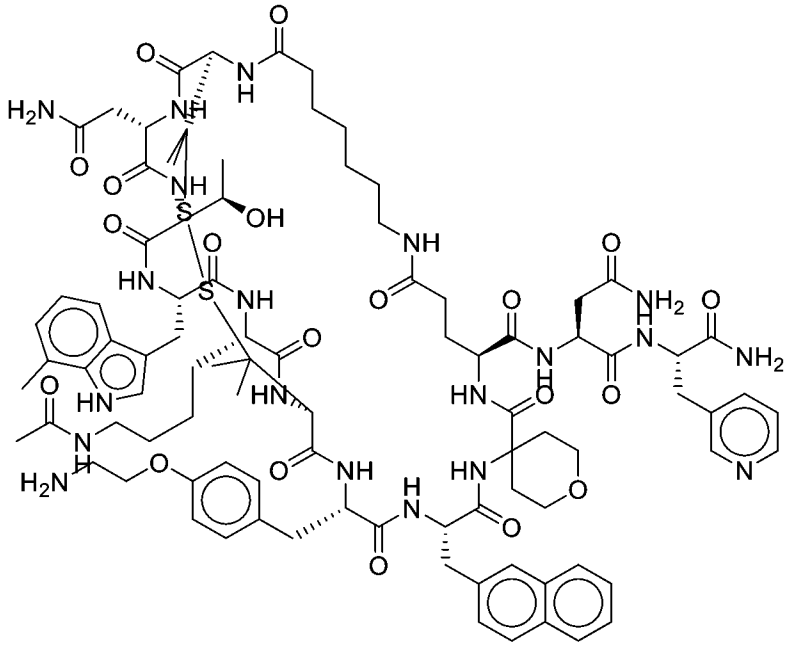
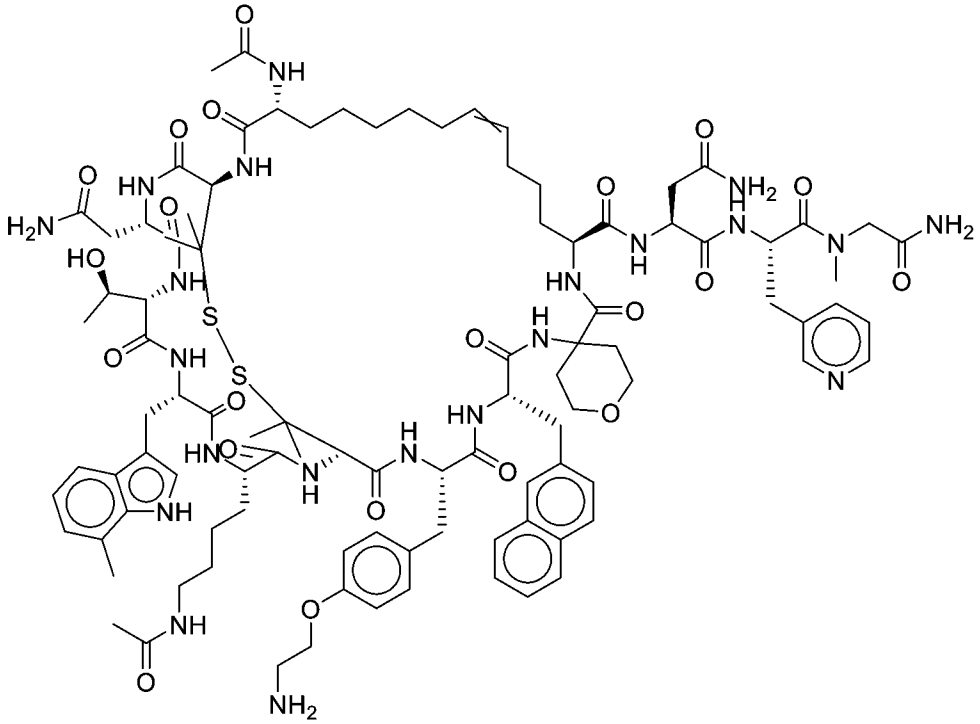
表1A

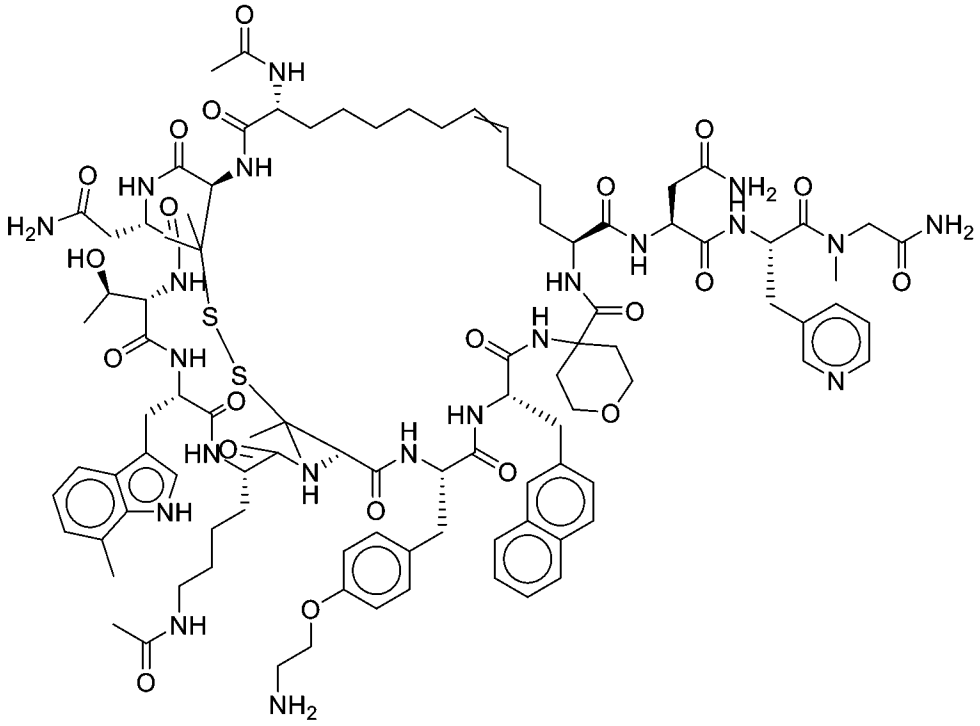
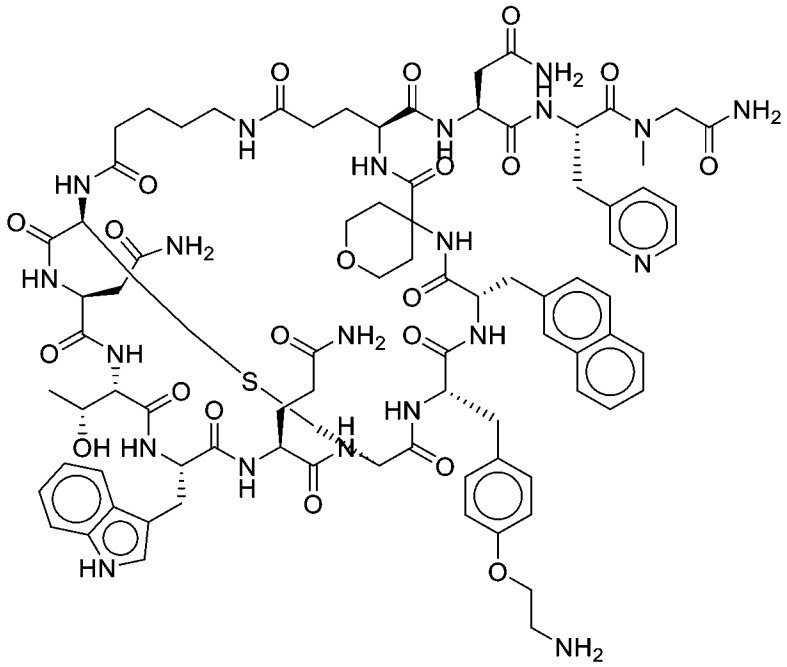
SEQ ID	化合物	序列/結構
1	201	7Ahp(2)--Pen(3)-N-T-W-K(Ac)-Pen(3)-AEF-2Nal-THP-E(2)-N-3Pya-Sar--CONH2 
2	202	7Ahp(2)--Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-E(2)-N-3Pya-Sar—CONH2 

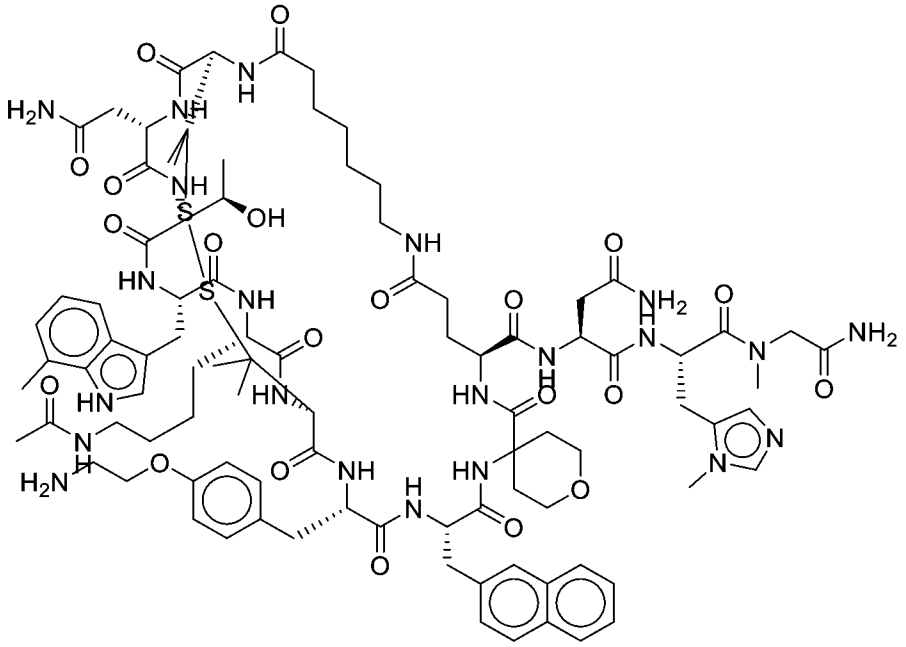
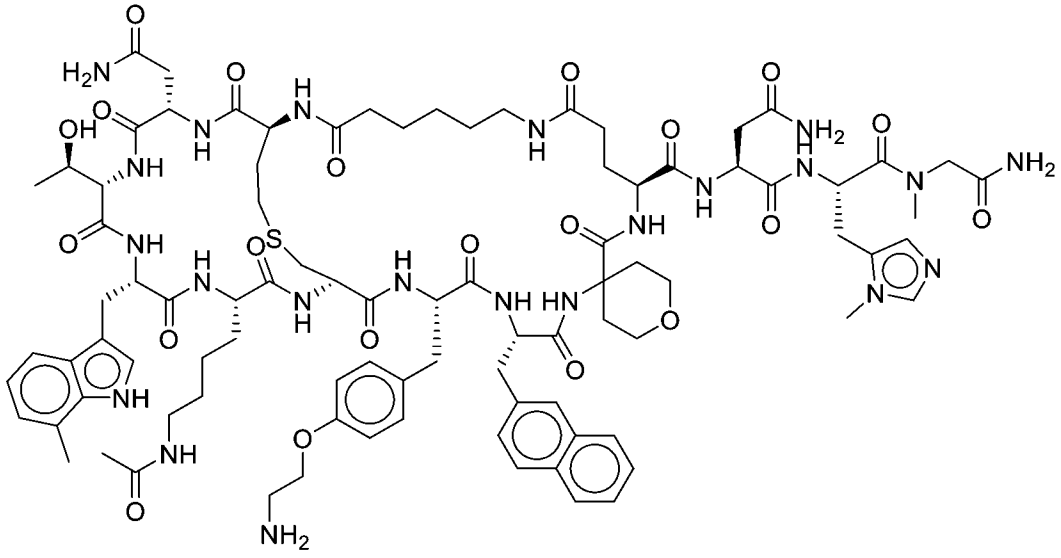
SEQ ID	化合物	序列/結構
3	203	6Ahx(2)--Abu(1)-N-T-W-Q-C(1)-AEF-2Nal-THP-E(2)-N-3Pya-Sar--CONH2 
4	204	MeCO-R6H(4)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-aMeK-S5H(4)-N-3Pya-Sar--CONH2 

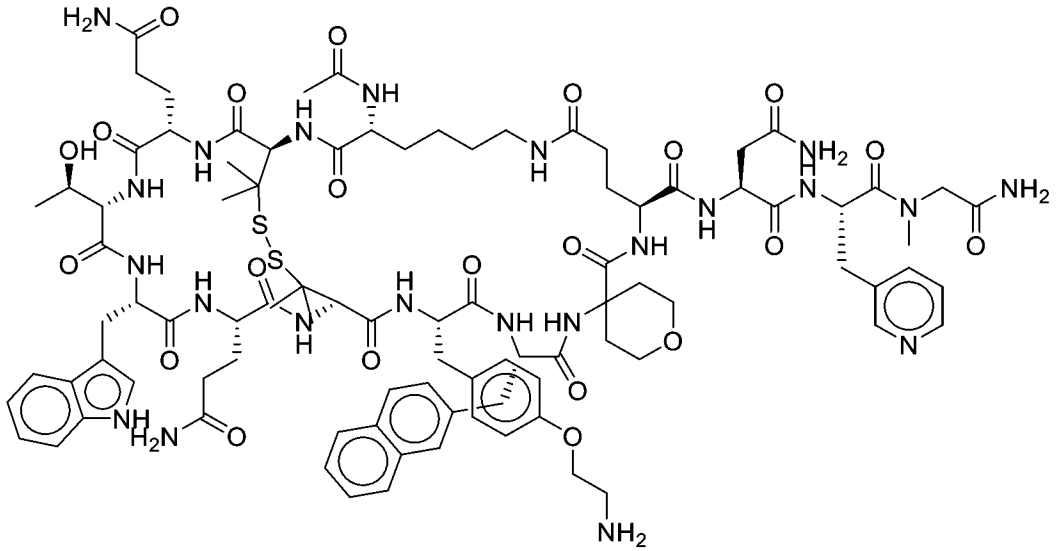
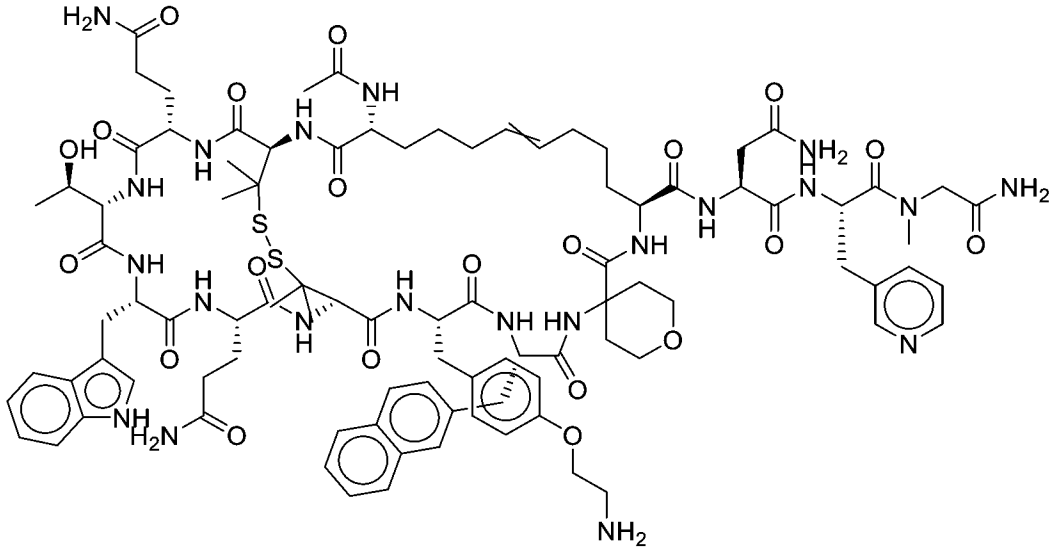
SEQ ID	化合物	序列/結構
5	205	6Ahx(2)--Abu(1)-N-T-W-Q-C(1)-AEF-2Nal-aMeK-E(2)-N-3Pya-Sar--CONH2 
6	206	GABA(2)-r-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-E(2)-N-3Pya-Sar--CONH2 

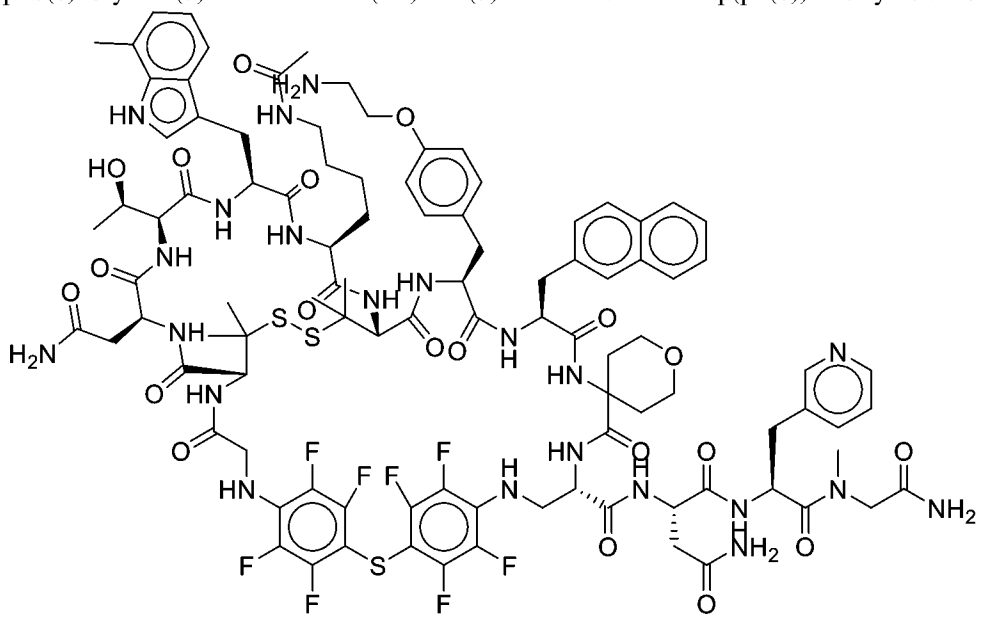
SEQ ID	化合物	序列/結構
7	207	MeCO-R5H(4)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-aMeK-S5H(4)-N-3Pya-Sar-CONH2 
8	208	MeCO-R5H(4)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-aMeK-S5H(4)-N-3Pya-Sar-CONH2 

SEQ ID	化合物	序列/結構
9	209	7Ahp(2)--Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-E(2)-N-3Pya---CONH2 
10	210	MeCO-R7H(4)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-S5H(4)-N-3Pya-Sar-CONH2 

SEQ ID	化合物	序列/結構
11	211	MeCO-R7H(4)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-S5H(4)-N-3Pya-Sar-CONH2 
12	212	5Ava(2)--Abu(1)-N-T-W-Q-C(1)-AEF-2Nal-THP-E(2)-N-3Pya-Sar--CONH2 

SEQ ID	化合物	序列/結構
13	213	7AHP(2)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-E(2)-N-3MeH-Sar-CONH2 
14	214	-6Ahx(2)-Abu(1)-N-T-7MeW-K(Ac)-C(1)-AEF-2Nal-THP-E(2)-N-3MeH-Sar-CONH2 

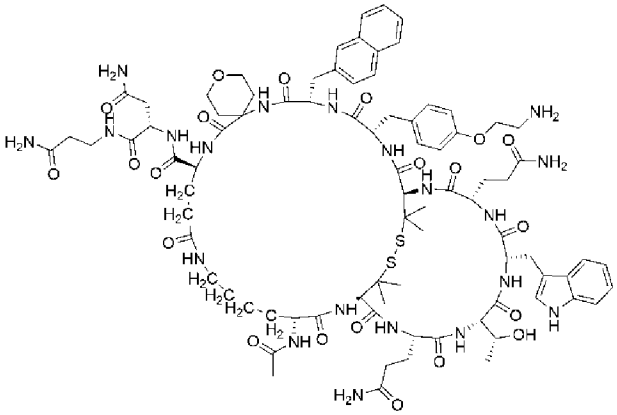
SEQ ID	化合物	序列/結構
15	215	MeCO-lys(2)-Pen(3)-Q-T-W-Q-Pen(3)-AEF-2Nal-THP-E(2)-N-3Pya-Sar-CONH2 
16	216	MeCO-R5H(4)-Pen(3)-Q-T-W-Q-Pen(3)-AEF-2Nal-THP-S5H(4)-N-3Pya-Sar-CONH2 

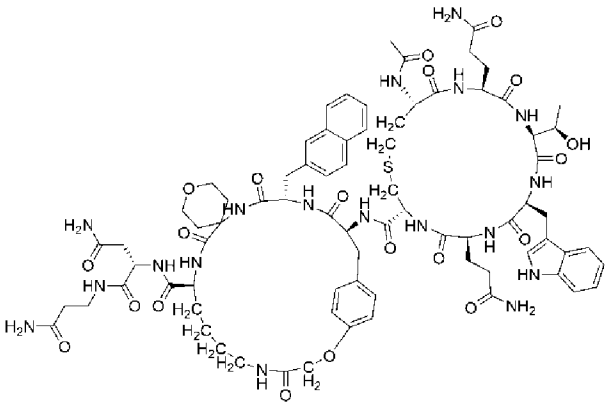
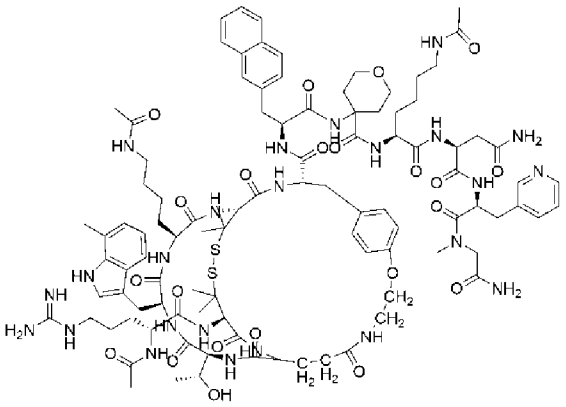
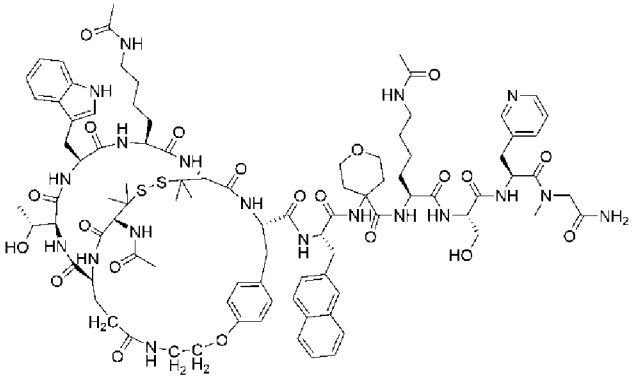
SEQ ID	化合物	序列/結構
17	217	pFS(6)-Gly-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-Dap(pF(6))-N-3Pya-Sar--CONH2 

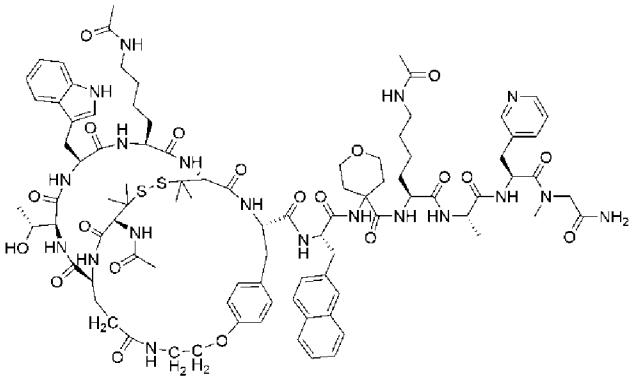
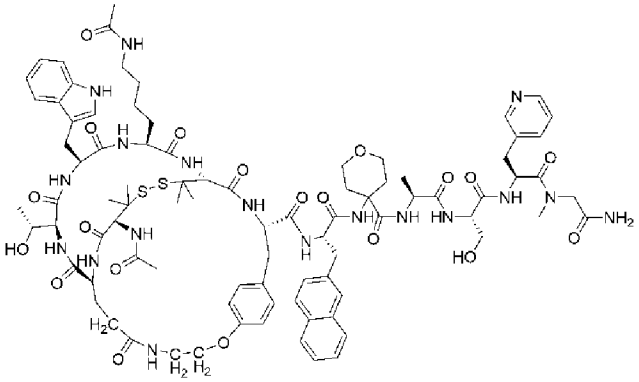
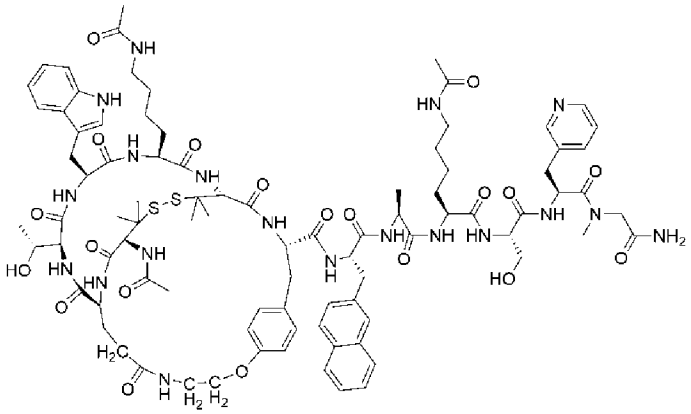
其中例如，Pen-Pen形成雙硫鍵，或Abu-C形成硫醚鍵。

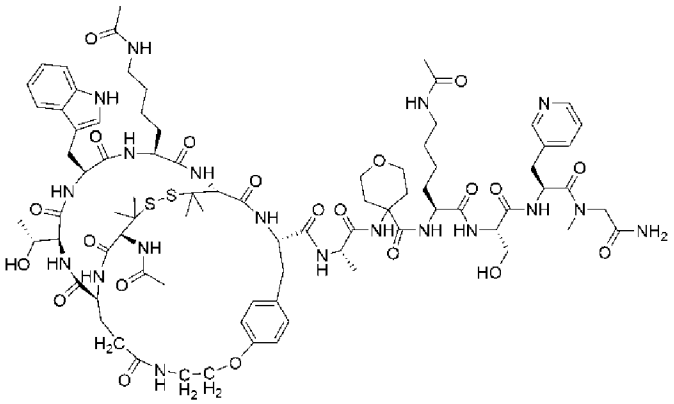
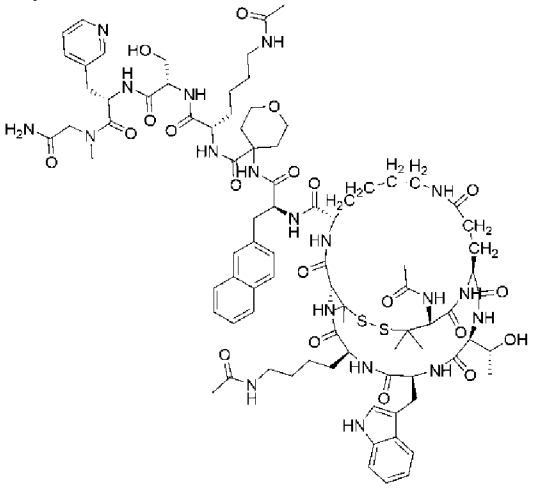
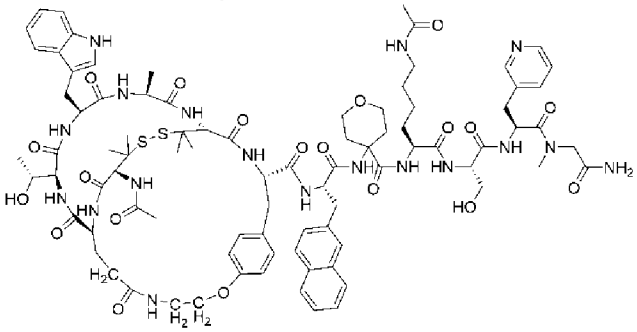
【0081】

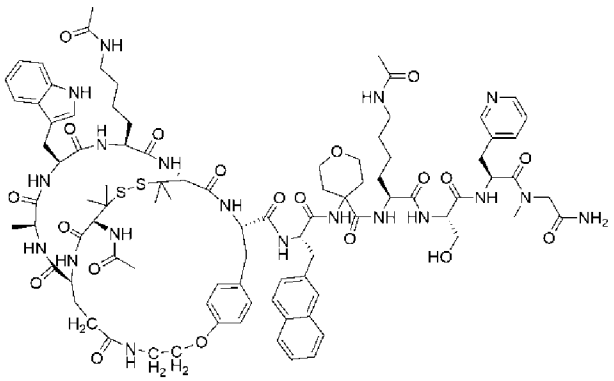
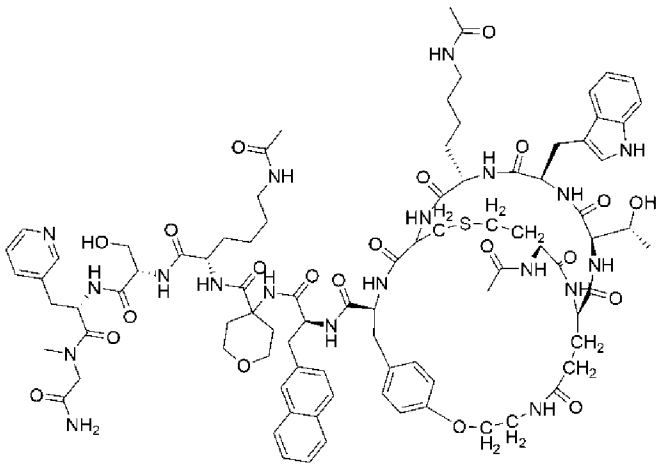
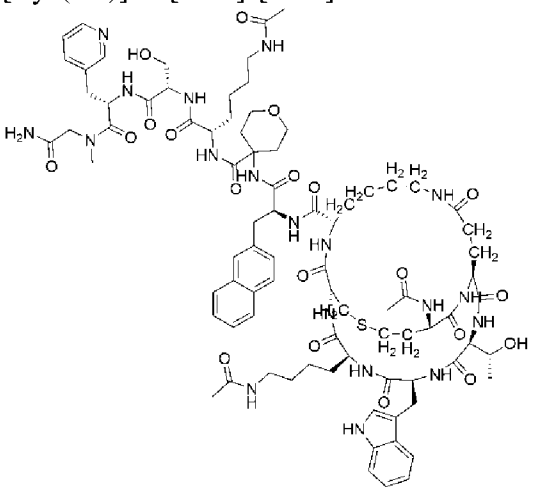
表1B.化合物

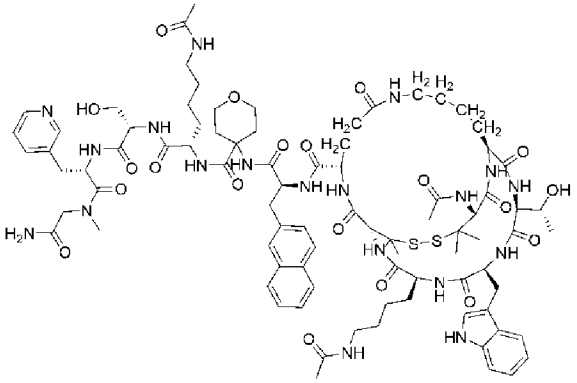
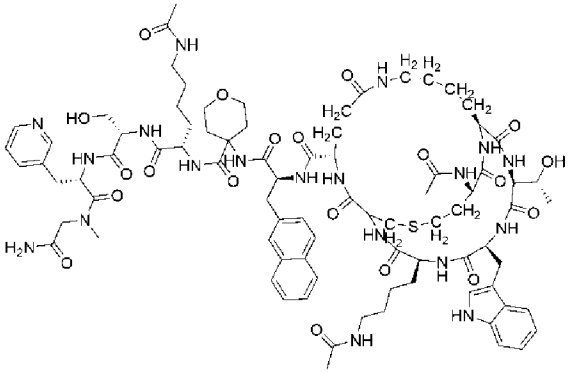
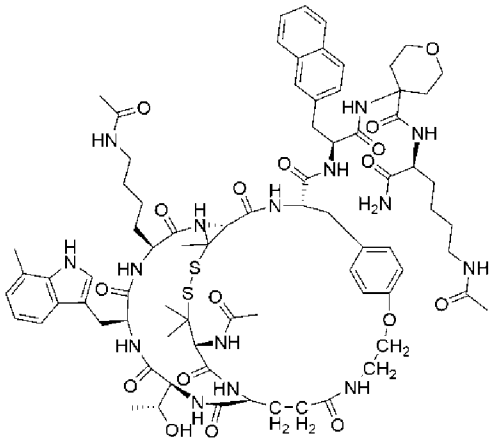
SEQ ID.	化合物	序列/結構	註
18	1	Ac-[(D)Lys]-[Pen]-Q-T-W-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[bAla]-NH2 	#N/A

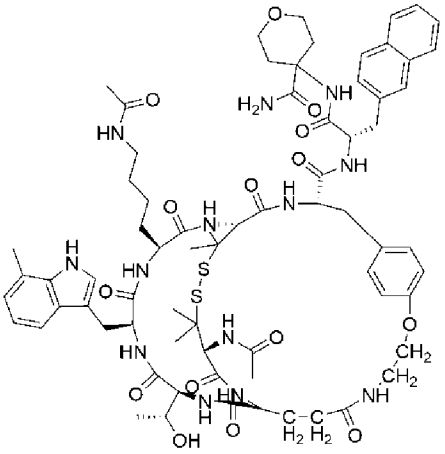
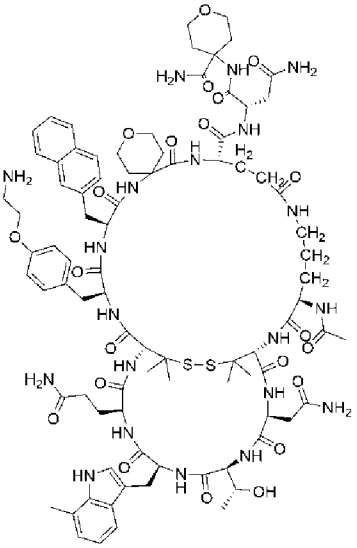
SEQ ID.	化合物	序列/結構	註
19	2	Ac-[Abu]-Q-T-W-Q-C-[Phe(4-OCH2COOH)]-[2Nal]-[THP]-K-N-[bAla]-NH2 	AEF 之 Glu C(O)及 NH 形成內醯胺
20	3	Ac-[(D)Arg]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
21	4	Ac-[Pen]-E-T-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺異構物 1

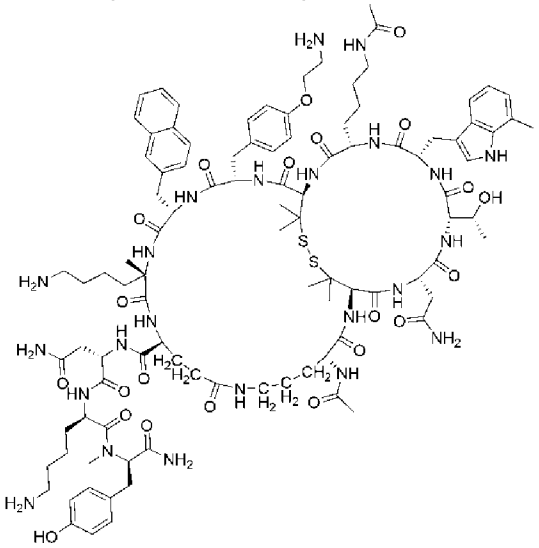
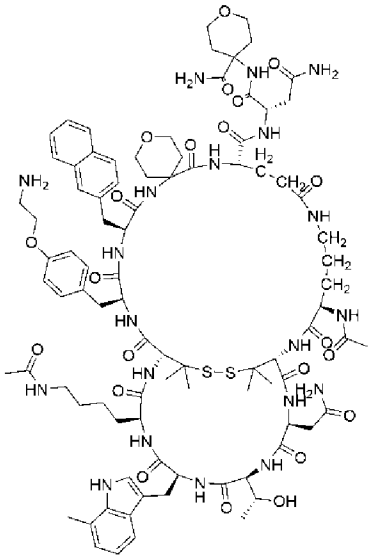
SEQ ID.	化合物	序列/結構	註
22	5	Ac-[Pen]-E-T-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-A-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺異構物 1
23	6	Ac-[Pen]-E-T-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-A-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
24	7	Ac-[Pen]-E-T-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-A-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺異構物 1

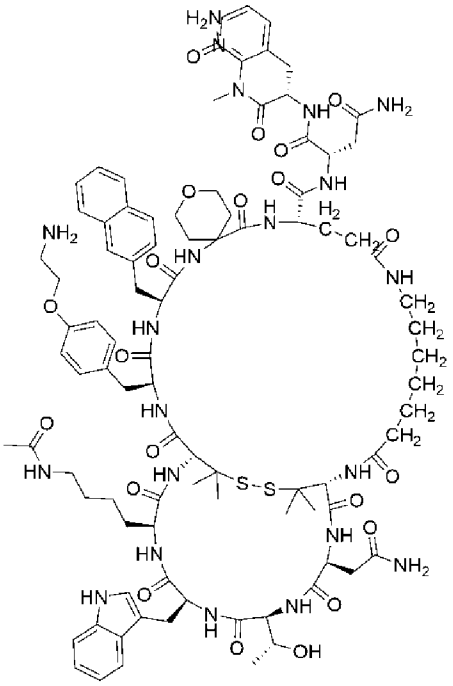
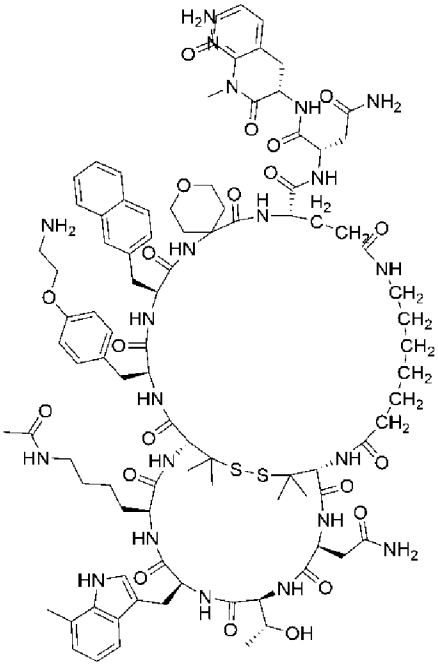
SEQ ID.	化合物	序列/結構	註
25	8	Ac-[Pen]-E-T-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-A-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺異構物 1
26	9	Ac-[Pen]-E-T-W-[Lys(Ac)]-[Pen]-K-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Lys 之 NH 及 Glu 之 C(O)形成內醯胺
27	10	Ac-[Pen]-E-T-W-A-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺異構物 1

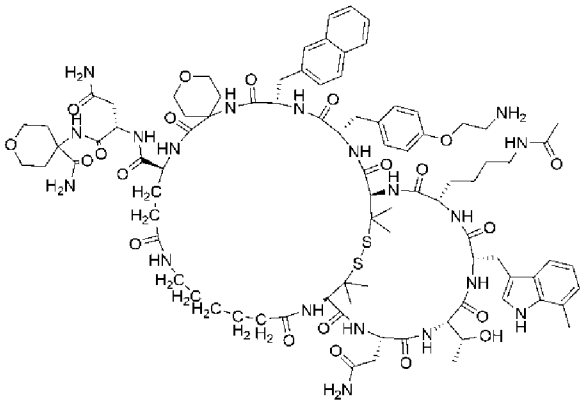
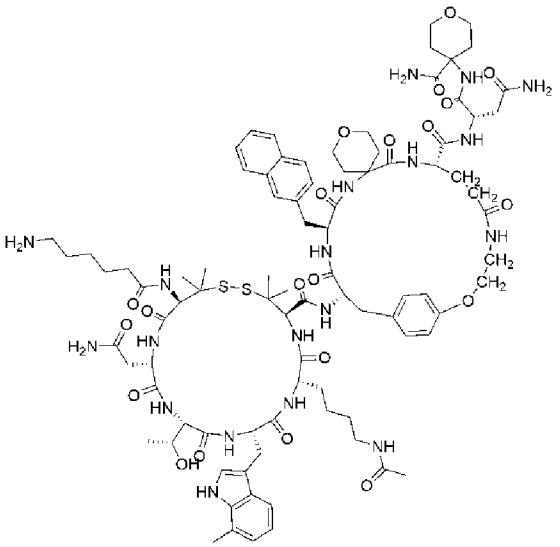
SEQ ID.	化合物	序列/結構	註
28	11	Ac-[Pen]-E-A-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
29	12	Ac-[Abu]-E-T-W-[Lys(Ac)]-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
30	13	Ac-[Abu]-E-T-W-[Lys(Ac)]-C-K-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Lys 之 NH 及 Glu 之 C(O)形成內醯胺

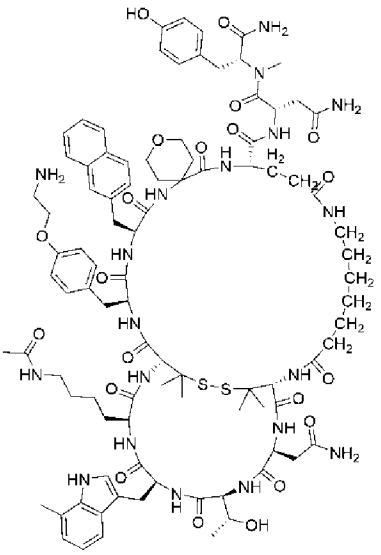
SEQ ID.	化合物	序列/結構	註
31	14	Ac-[Pen]-K-T-W-[Lys(Ac)]-[Pen]-E-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Lys 之 NH 及 Glu 之 C(O)形成內醯胺
32	15	Ac-[Abu]-K-T-W-[Lys(Ac)]-C-E-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Lys 之 NH 及 Glu 之 C(O)形成內醯胺
33	16	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺

SEQ ID.	化合物	序列/結構	註
34	17	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
35	18	Ac-[(D)Orn]-[Pen]-N-T-[W(7-Me)]-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	(D)Orn 之 NH 及 Glu 之 C(O)形成內醯胺

SEQ ID.	化合物	序列/結構	註
36	19	Ac-[(D)Orn]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLys]-E-N-[(D)Lys]-[(D)NMeTyr]-NH2 	(D)Orn 之 NH 及 Glu 之 C(O) 形成內醯胺
37	20	Ac-[(D)Orn]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	(D)Orn 之 NH 及 Glu 之 C(O) 形成內醯胺

SEQ ID.	化合物	序列/結構	註
38	21	[7 胺基庚酸]-[Pen]-N-T-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[3Pal]-[Sarc]-NH2 	7 胺基庚酸之 NH 及 Glu 之 C(O)形成內醯胺
39	22	[7 胺基庚酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[3Pal]-[Sarc]-NH2 	7 胺基庚酸之 NH 及 Glu 之 C(O)形成內醯胺

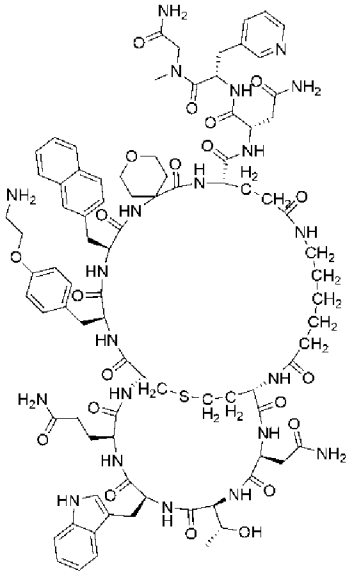
SEQ ID.	化合物	序列/結構	註
40	23	[Ahx]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	Ahx 之 NH 及 Glu 之 C(O)形成內醯胺
41	24	[6 胺基己酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺

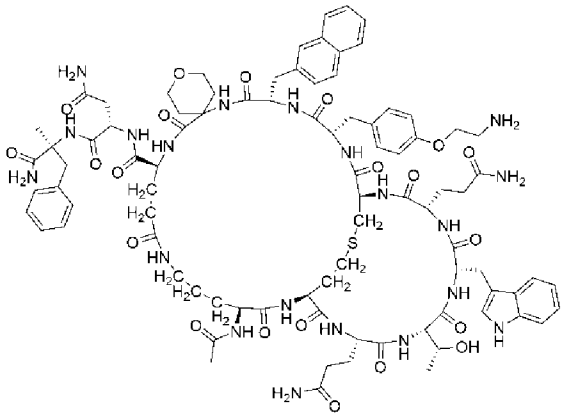
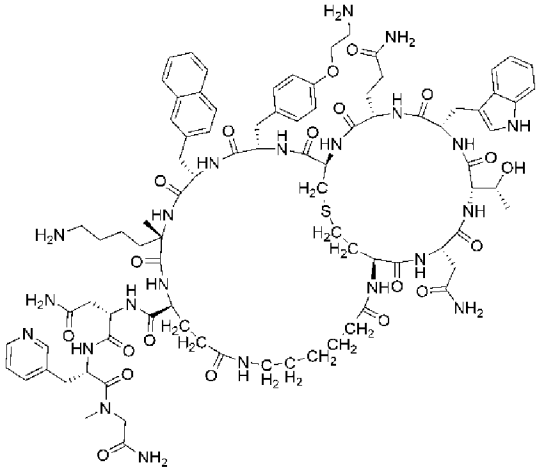
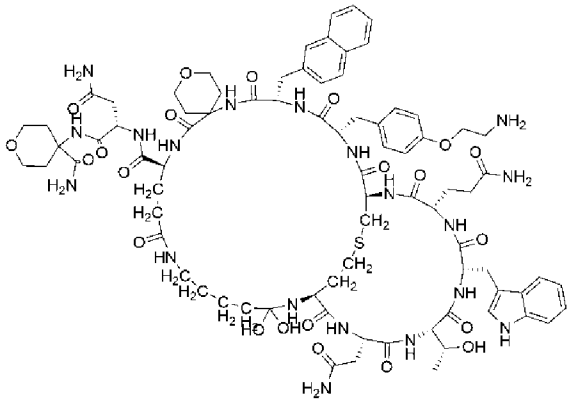
SEQ ID.	化合物	序列/結構	註
42	25	[7 胺基庚酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[(D)NMeTyr]-NH2 	7 胺基庚酸之 NH 及 Glu 之 C(O)形成內醯胺

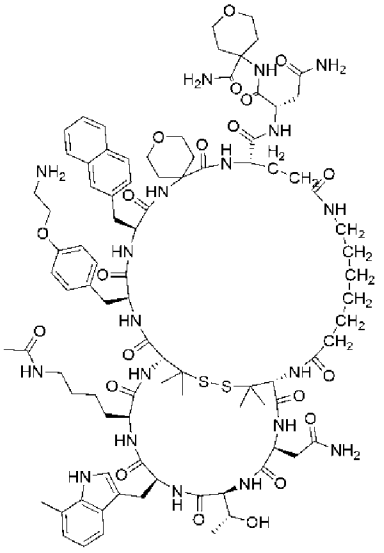
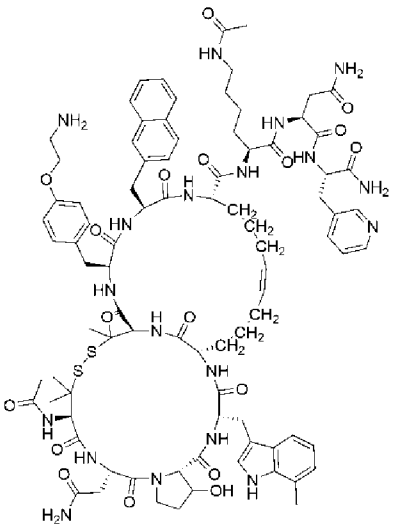
其中Pen-Pen形成雙硫鍵，或Abu-Cys形成硫醚鍵。

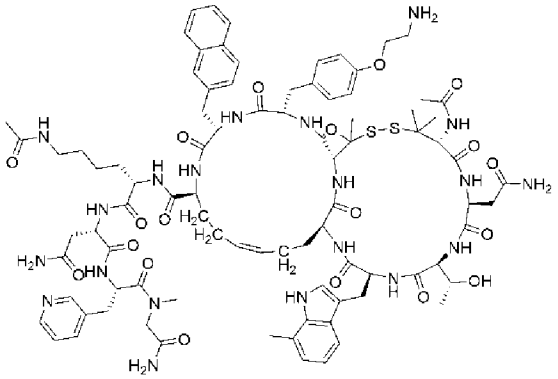
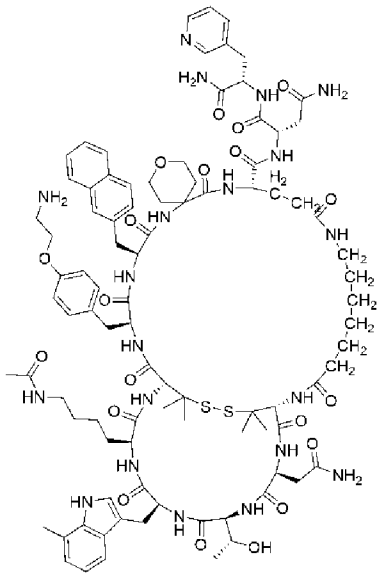
【0082】

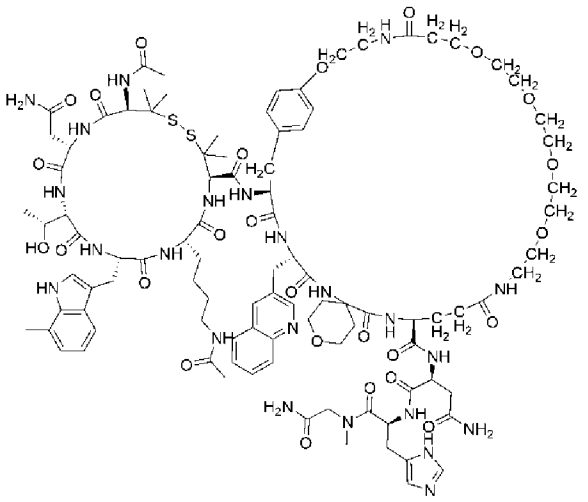
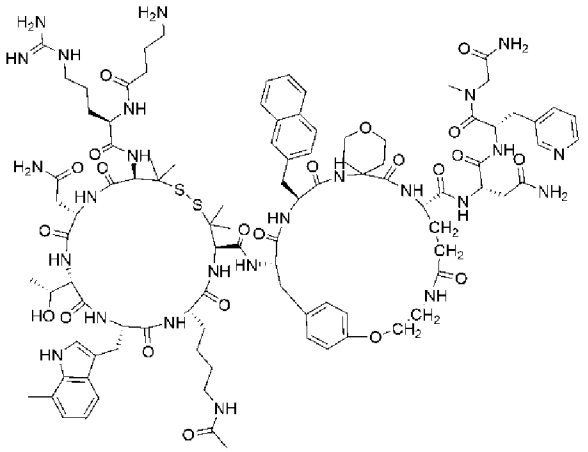
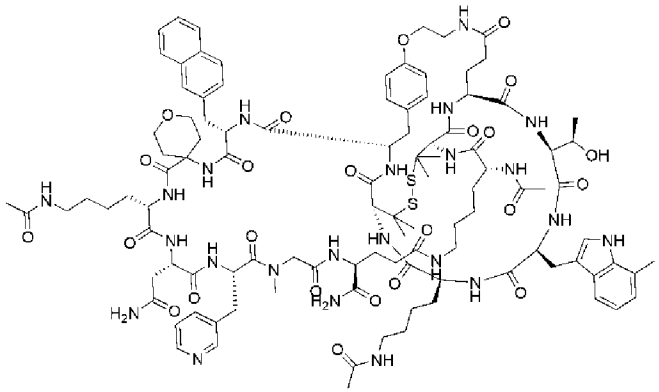
表1C.化合物

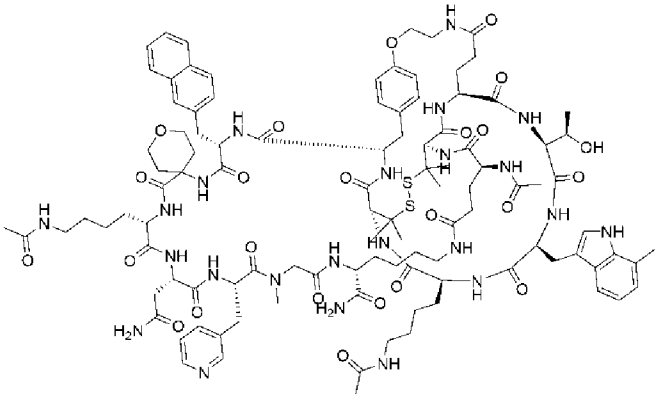
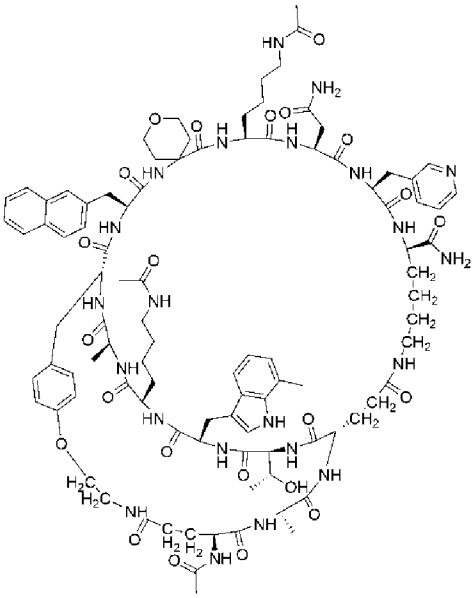
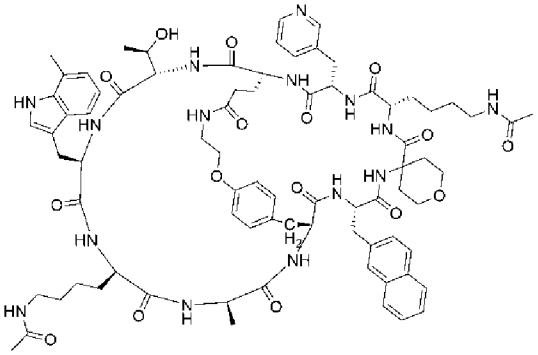
SEQ ID.	化合物	序列/結構	註
43	26	[Ahx]-[Abu]-N-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[3Pal]-[Sarc]-NH2 	Ahx 之 NH 及 Glu 之 C(O)形成內醯胺

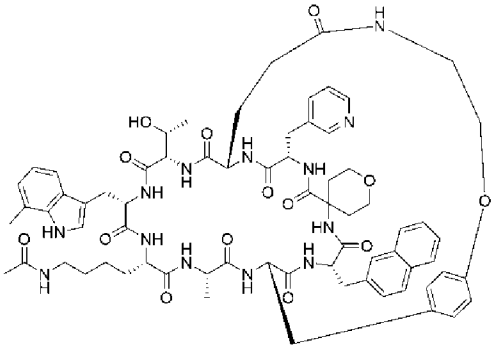
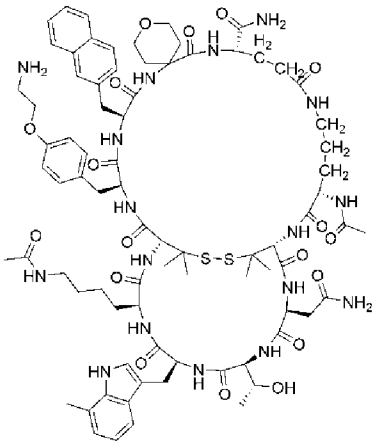
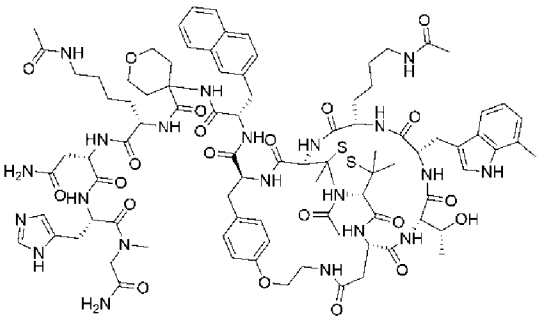
SEQ ID.	化合物	序列/結構	註
44	27	Ac-[Orn]-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[aMePhe]-NH2 	#N/A
45	28	[Ahx]-[Abu]-N-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLys]-E-N-[3Pal]-[Sarc]-NH2 	Ahx 之 NH 及 Glu 之 C(O)形成內醯胺
46	29	[5 胺基戊酸]-[Abu]-N-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	7 胺基戊酸之 NH 及 Glu 之 C(O)形成內醯胺

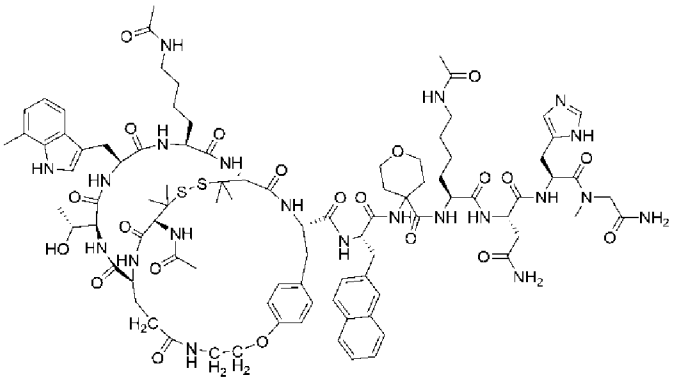
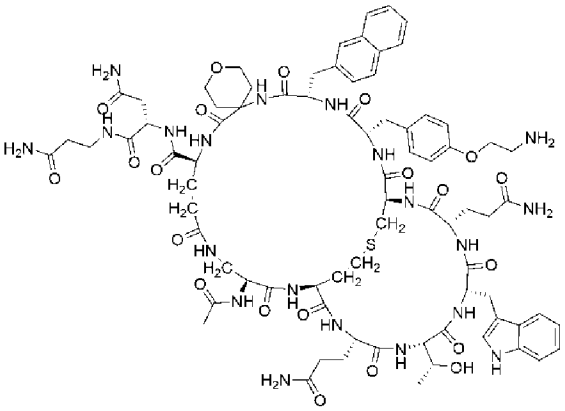
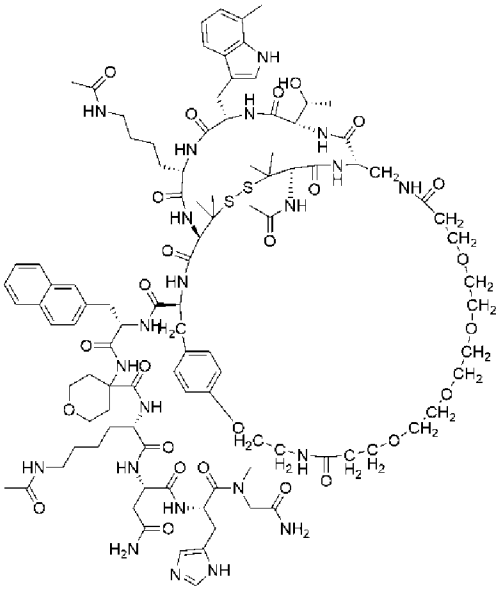
SEQ ID.	化合物	序列/結構	註
47	30	[7 胺基庚酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	7 胺基庚酸之 NH 及 Glu 之 C(O)形成內醯胺
48	31	Ac-[Pen]-N-[Pro(3-OH)]-[W(7-Me)]-[O3S]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[O3S]-[Lys(Ac)]-N-[3Pal]-NH2 	(D)Ala(X8)之側鏈 C 及 (D)Ala(X12)之側鏈 C 經由-CH2-CH2-CH=CH-CH2-CH2-異構物 1 而環化

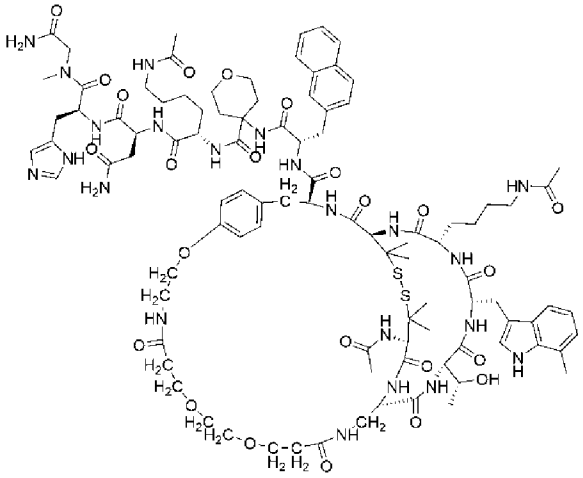
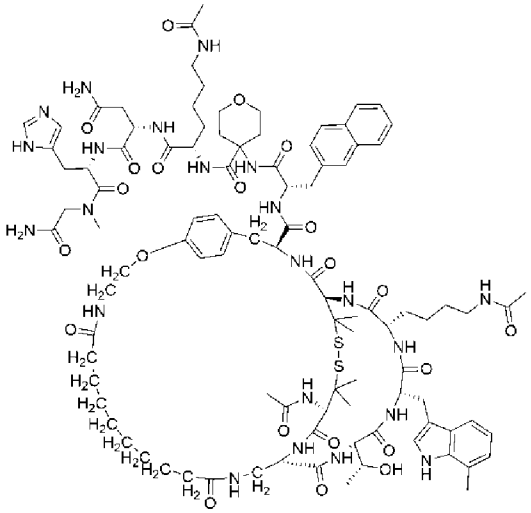
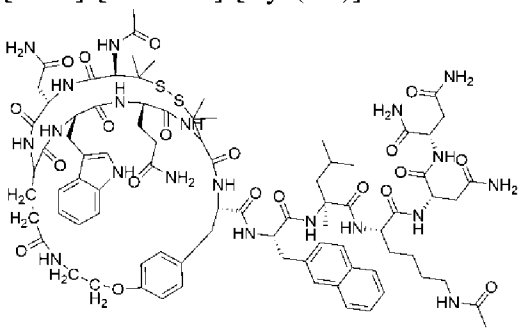
SEQ ID.	化合物	序列/結構	註
49	32	Ac-[Pen]-N-T-[W(7-Me)]-[O3S]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[O3S]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	(D)Ala(X8)之側鏈 C 及 (D)Ala(X12)之側鏈 C 經由-CH2-CH2-CH=CH-CH2-CH2-異構物 2 而環化
50	33	[7 胺基庚酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[3Pal]-NH2 	7 胺基庚酸之 NH 及 Glu 之 C(O)形成內醯胺

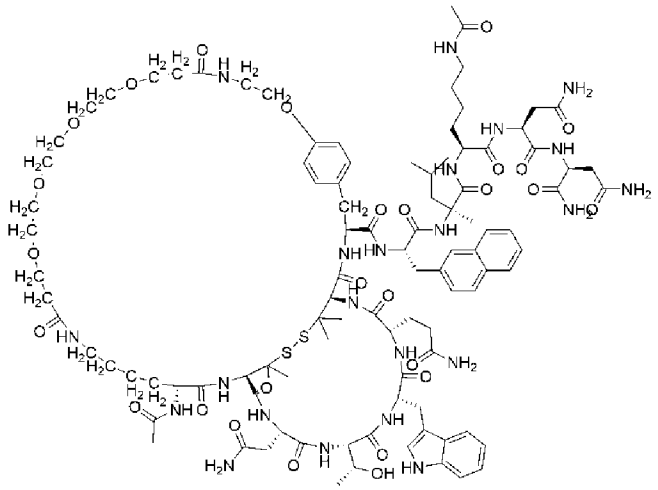
SEQ ID.	化合物	序列/結構	註
51	34	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[3Quin]-[THP]-E-N-H-[Sarc]-[NH2]-[PEG4] 	#N/A
52	35	[Gaba]-[(D)Arg]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
53	36	Ac-[(D)Lys]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-E-NH2 	(D)Lys 之 NH 及 Glu 之 C(O) (X17)形成內醯胺；且(Phe2ae)之 NH 及 Glu 之 C(O) (X5)形成內醯胺異構物 1

SEQ ID.	化合物	序列/結構	註
54	37	Ac-E-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-[(D)Lys]-NH2 	(D)Lys 之 NH 及 Glu 之 C(O) (X3)形成內醯胺；且(Phe2ae)之 NH 及 Glu 之 C(O) (X5)形成內醯胺異構物 1
55	38	Ac-E-A-E-T-[W(7-Me)]-[Lys(Ac)]-A-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-NH2 	Phe(4(2ae))之-NH 及 Glu 之 C(O) (X3)形成內醯胺；且(D)Lys 之-NH 及 Glu 之 C(O) (X5)形成內醯胺
56	39	E-T-[W(7-Me)]-[Lys(Ac)]-A-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-[3Pal] 	E 之 α 胺基與 Pal 之羧基末端形成醯胺且 E 之側鏈羧基與 Phe(4-(2-胺基乙氧基)形成醯胺

SEQ ID.	化合物	序列/結構	註
57	40	E-T-[W(7-Me)]-[Lys(Ac)]-A-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[3Pal] 	E 之 α 胺基與 Pal 之羧基末端形成醯胺且 E 之側鏈羧基與 Phe(4-(2-胺基乙氧基)形成醯胺
58	41	Ac-[Orn]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-NH2 	Orn 之 NH 及 Glu 之 C(O)形成內醯胺異構物 1
59	42	Ac-[Pen]-D-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-H-[Sarc]-NH2 	#N/A

SEQ ID.	化合物	序列/結構	註
60	43	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-H-[Sarc]-NH2 	#N/A
61	44	Ac-[Dap]-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[bAla]-NH2 	#N/A
62	45	Ac-[Pen]-[Dap]-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-H-[Sarc]-[NH2]-[PEG4DA] 	#N/A

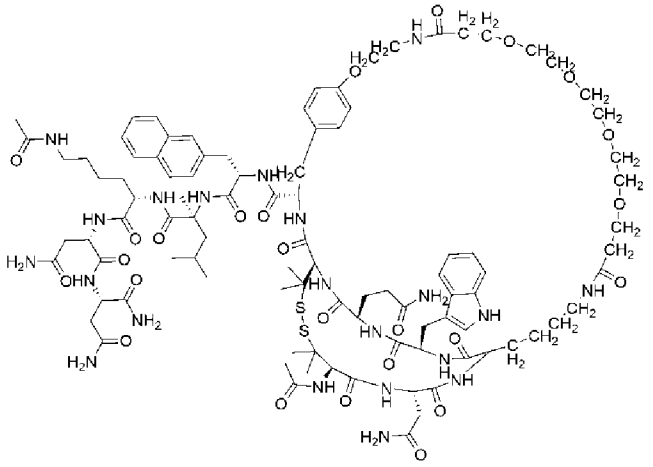
SEQ ID.	化合物	序列/結構	註
63	46	Ac-[Pen]-[Dap]-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-H-[Sarc]-[NH2]-[PEG2DA] 	#N/A
64	47	Ac-[Pen]-[Dap]-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-H-[Sarc]-[NH2]-[癸二酸] 	#N/A
65	48	Ac-[Pen]-N-E-W-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-N-NH2 	#N/A

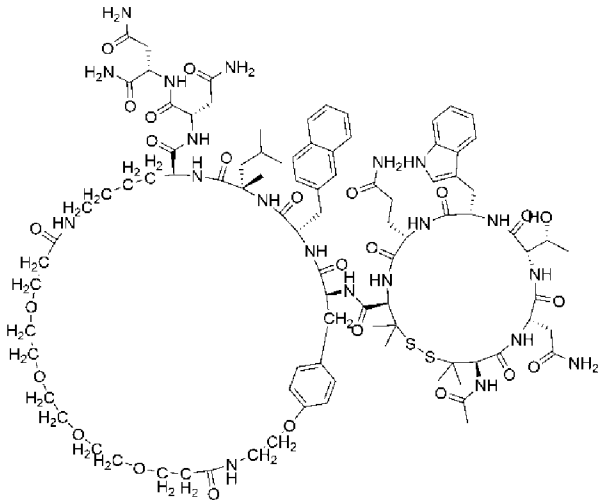
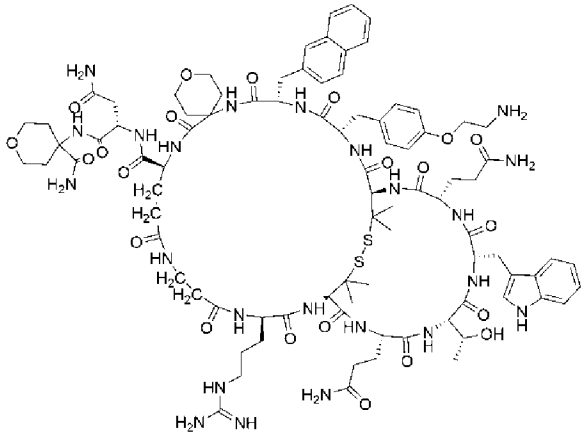
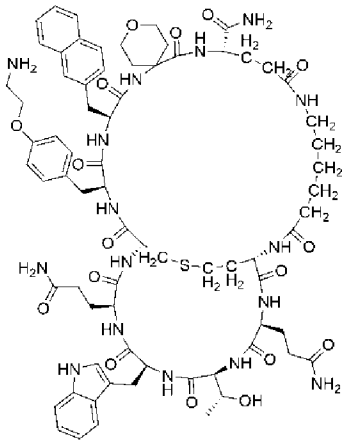
SEQ ID.	化合物	序列/結構	註
66	49	Ac-[(D)Lys]-[Pen]-N-T-W-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-N-[NH2]-[PEG4DA] 	(D)Lys 之-NH 及 Phe(4-胺基乙氧基)之-NH 經由-C(O)-(CH2CH2O)4-CH2-CH2-C(O)-鍵聯物而環化

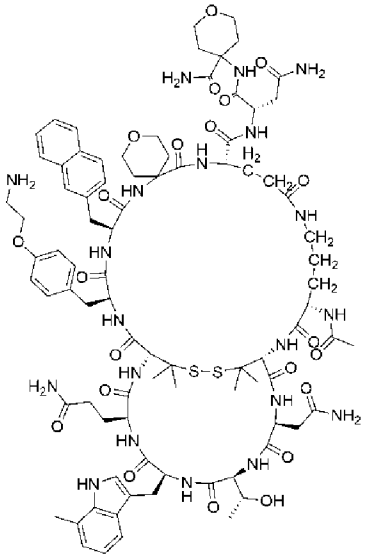
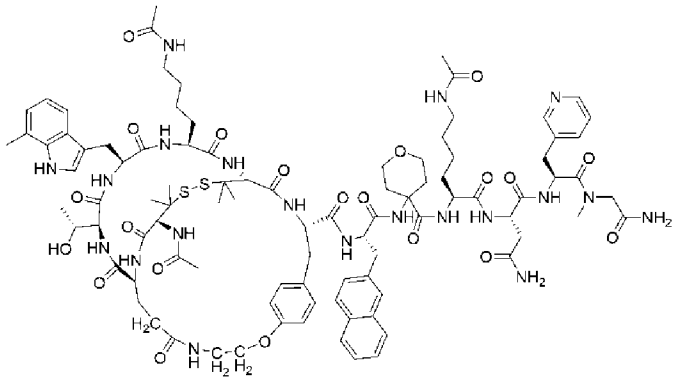
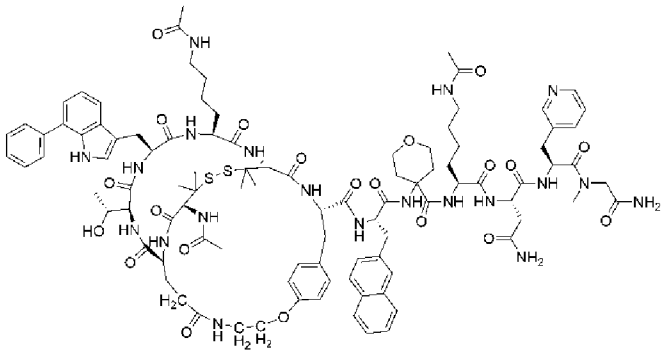
其中Pen-Pen形成雙硫鍵，或Abu-C形成硫醚鍵。

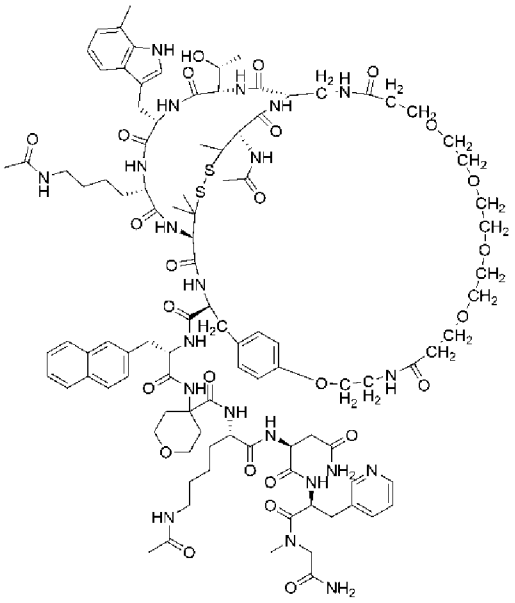
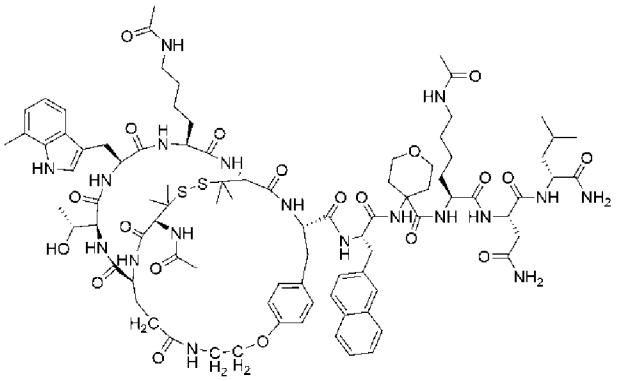
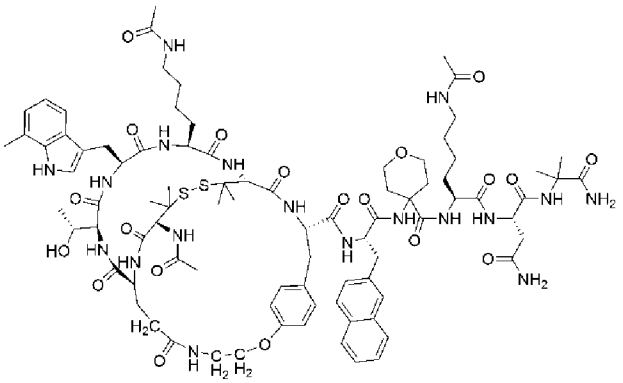
【0083】

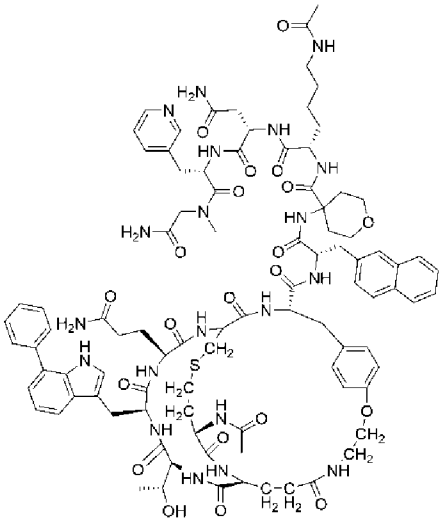
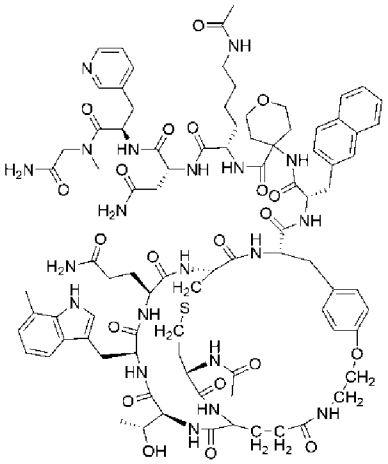
表1D.化合物

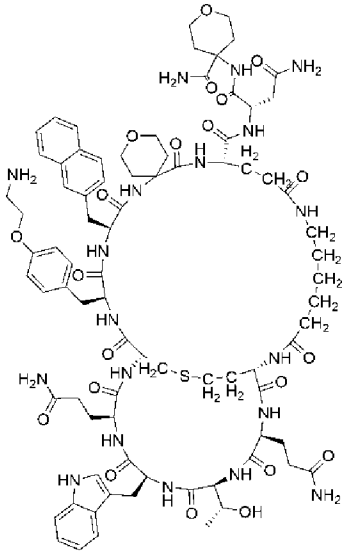
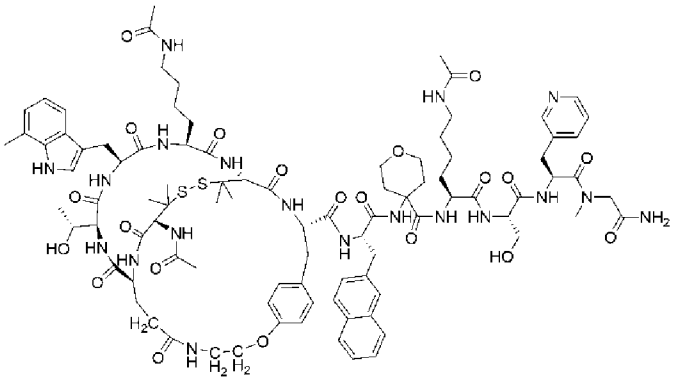
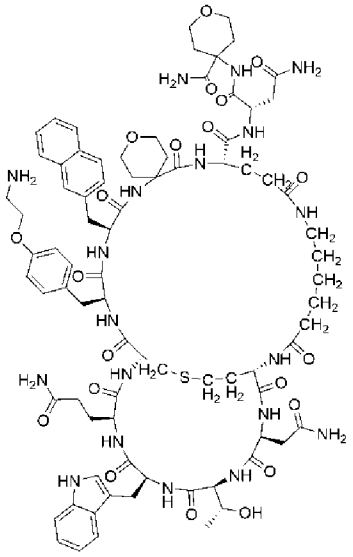
SEQ ID.	化合物	序列/結構	註
67	50	Ac-[Pen]-N-K-W-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-N-[NH2]-[PEG4DA] 	Phe[4-(2-胺基乙氧基)]之-NH 及 Lys 之-NH 經由-C(O)-(CH2CH2O)4-CH2-CH2-C(O)-鍵聯物而環化

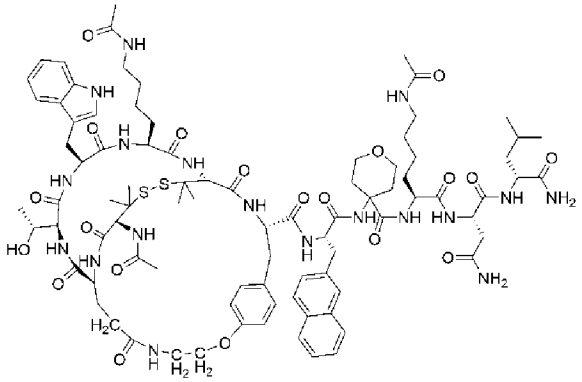
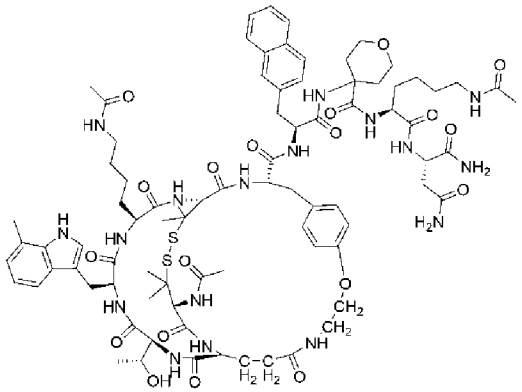
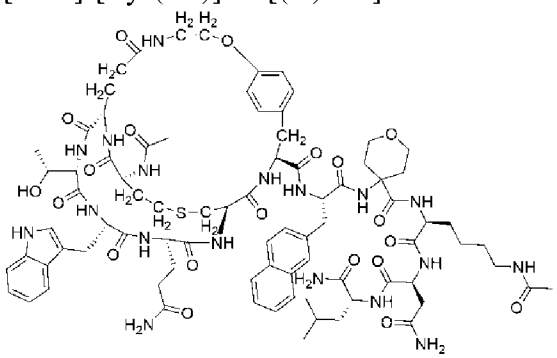
SEQ ID.	化合物	序列/結構	註
68	51	Ac-[Pen]-N-T-W-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-K-N-N-[NH2]-[PEG4DA] 	Phe[4-(2-胺基乙氧基)]之-NH 及 Lys 之-NH 經由-C(O)-(CH2CH2O)4-CH2-CH2-C(O)-鍵聯物而環化
69	52	[bAla]-[(D)Arg]-[Pen]-Q-T-W-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	bAla 之-NH 及 Glu 之 C(O)形成內醯胺
70	53	[Ahx]-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-NH2 	#N/A

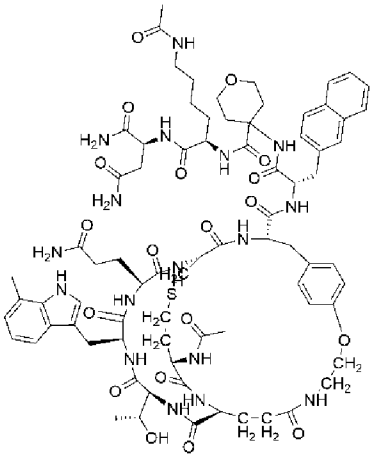
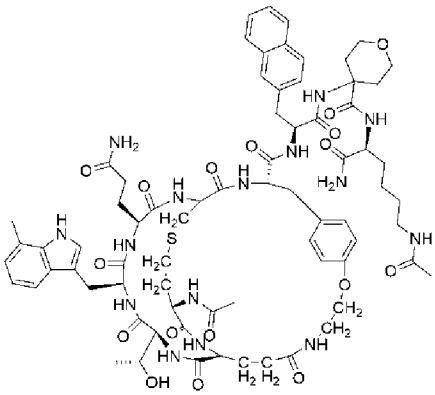
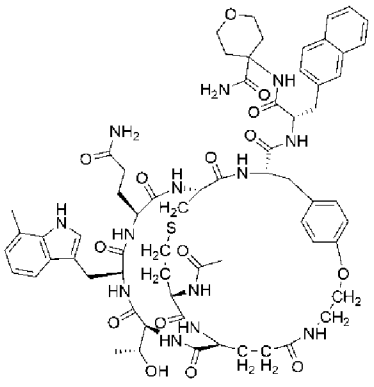
SEQ ID.	化合物	序列/結構	註
71	54	Ac-[Orn]-[Pen]-N-T-[W(7-Me)]-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	Orn 之-NH 及 Glu 之 C(O)形成內醯胺
72	55	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺異構物 1
73	56	Ac-[Pen]-E-T-[W(7-Ph)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺，異構物 1

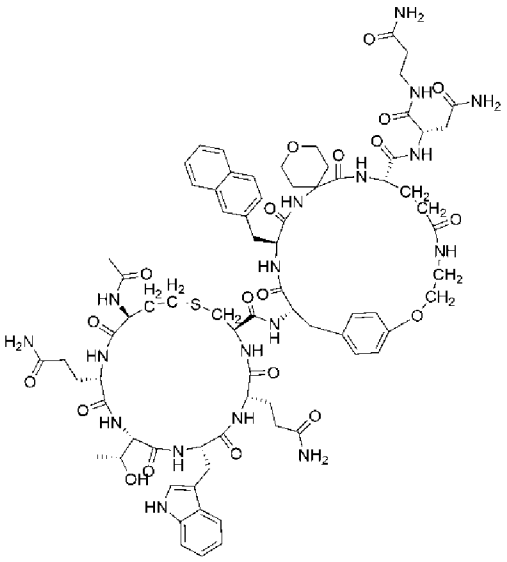
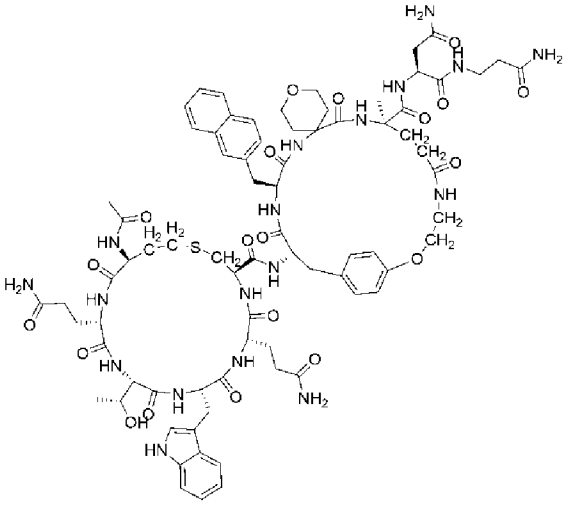
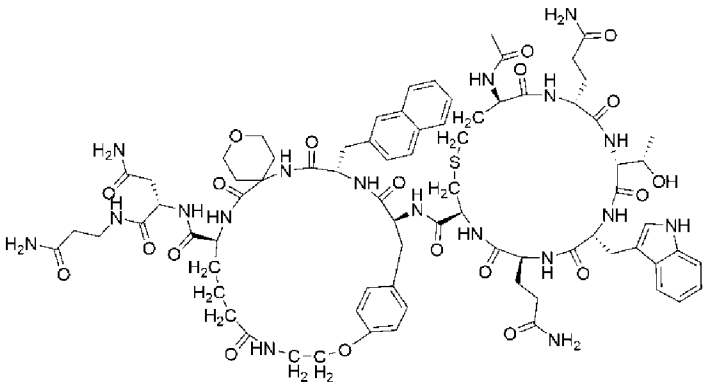
SEQ ID.	化合物	序列/結構	註
74	57	Ac-[Pen]-[Dap]-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-[NH2]-[PEG4DA] 	Phe[4-(2-胺基乙氧基)]之-NH 及 Dap 之-NH 形成內醯胺
75	58	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[(D)Leu]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
76	59	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[Aib]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺

SEQ ID.	化合物	序列/結構	註
77	60	Ac-[Abu]-E-T-[W(7-Ph)]-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
78	61	Ac-[Abu]-E-T-[W(7-Me)]-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺

SEQ ID.	化合物	序列/結構	註
79	62	[Ahx]-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	#N/A
80	63	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-S-[3Pal]-[Sarc]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
81	64	[Ahx]-[Abu]-N-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 	Ahx 之-NH 及 Glu 之 C(O)形成內醯胺

SEQ ID.	化合物	序列/結構	註
82	65	Ac-[Pen]-E-T-W-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[(D)Leu]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
83	66	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
84	67	Ac-[Abu]-E-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[(D)Leu]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺

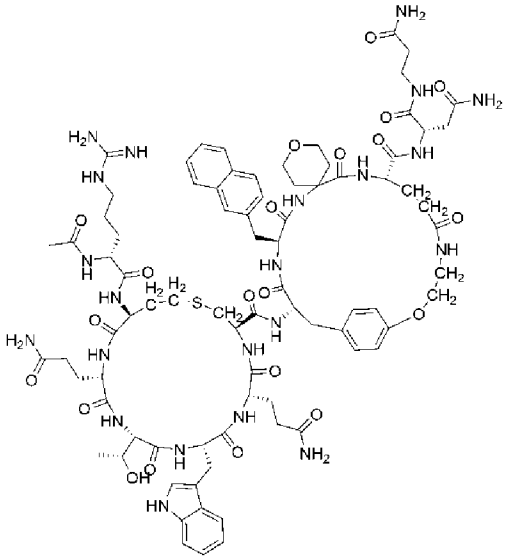
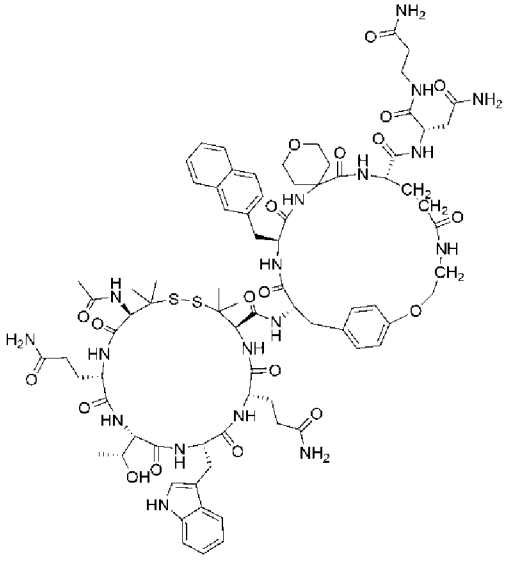
SEQ ID.	化合物	序列/結構	註
85	68	Ac-[Abu]-E-T-[W(7-Me)]-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
86	69	Ac-[Abu]-E-T-[W(7-Me)]-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺
87	70	Ac-[Abu]-E-T-[W(7-Me)]-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-NH2 	Phe[4-(2-胺基乙氧基)]之-NH 及 Glu 之 C(O)形成內醯胺

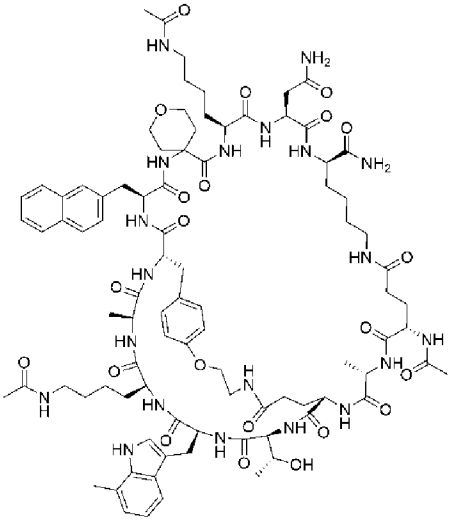
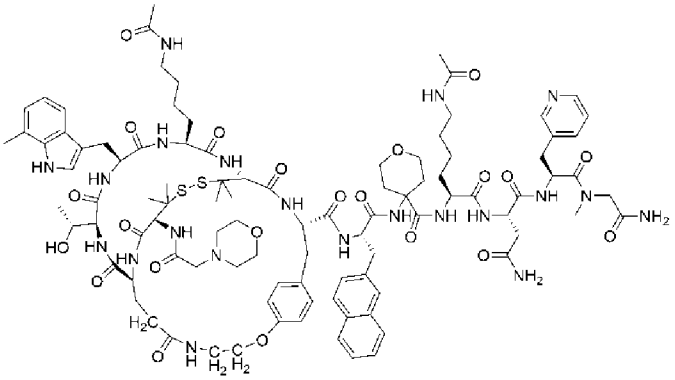
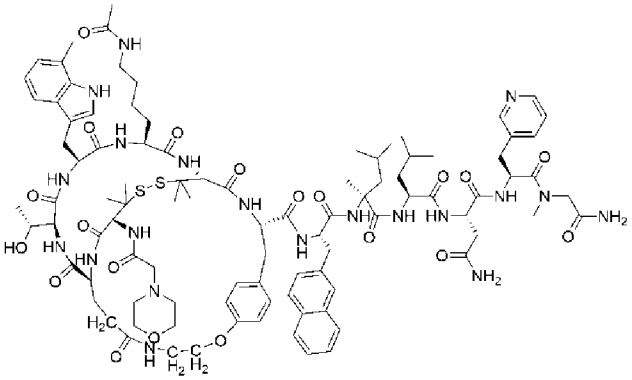
SEQ ID.	化合物	序列/結構	註
88	71	Ac-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[bAla]-NH2 	#N/A
89	72	Ac-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[aMeGlu]-N-[bAla]-NH2 	#N/A
90	73	Ac-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Aad]-N-[bAla]-NH2 	#N/A

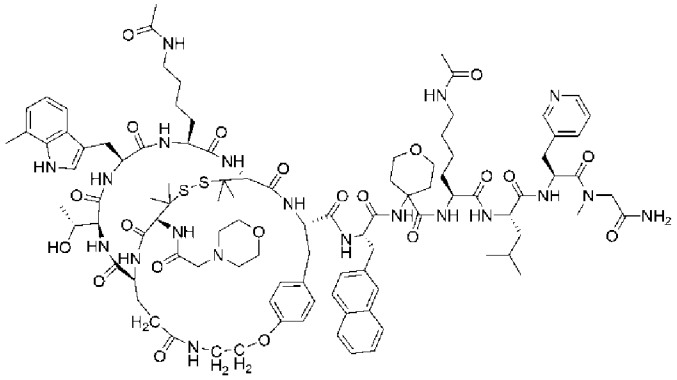
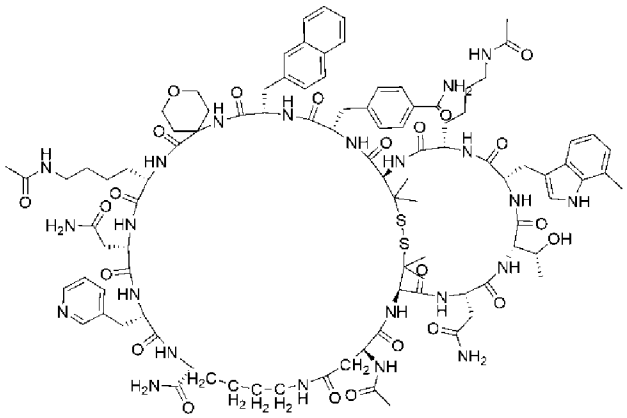
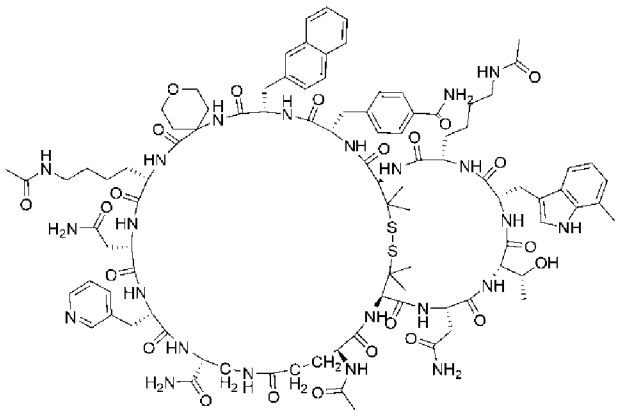
其中Pen-Pen形成雙硫鍵，或Abu-C形成硫醚鍵。

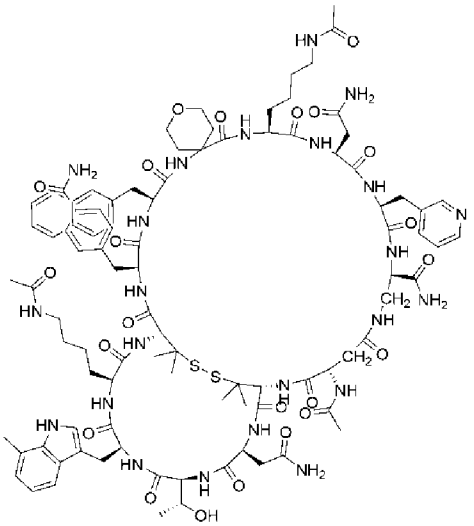
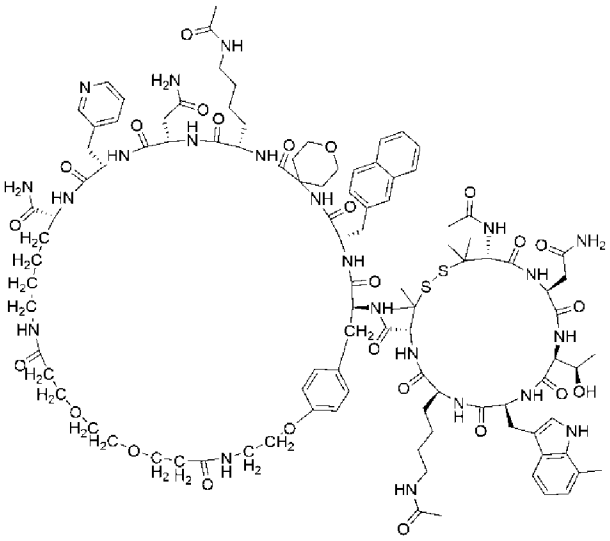
【0084】

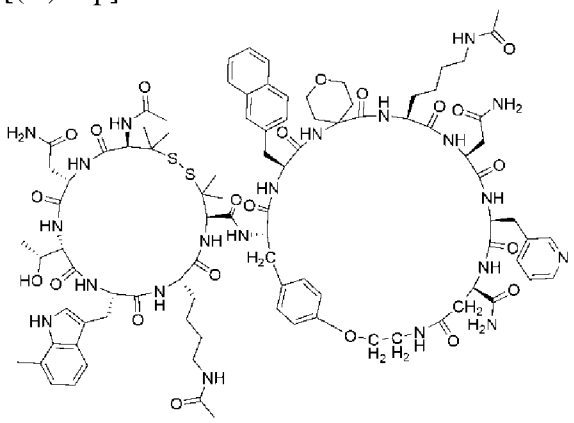
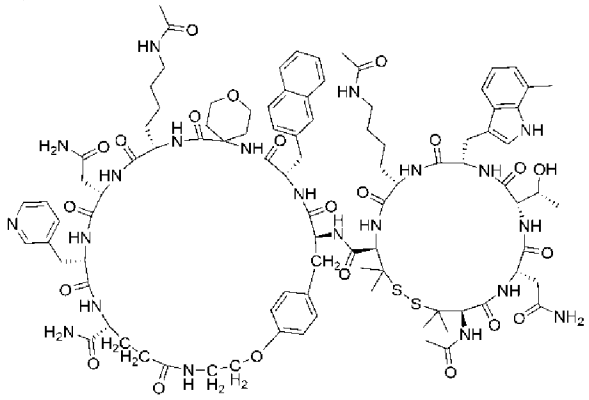
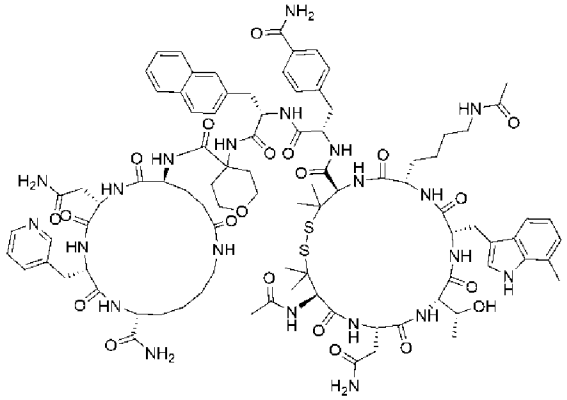
表1E.化合物

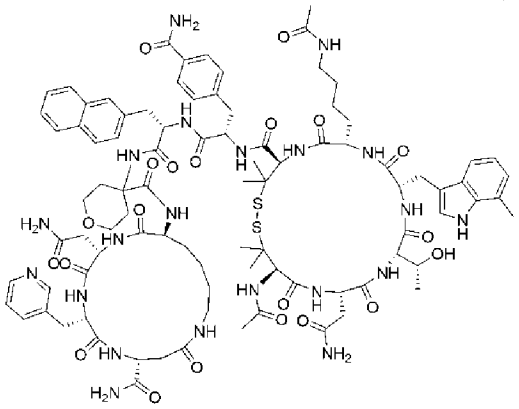
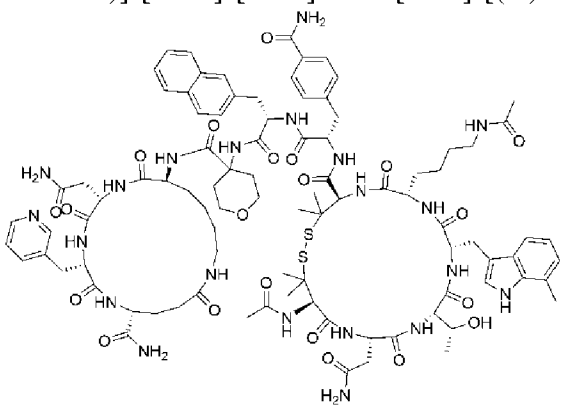
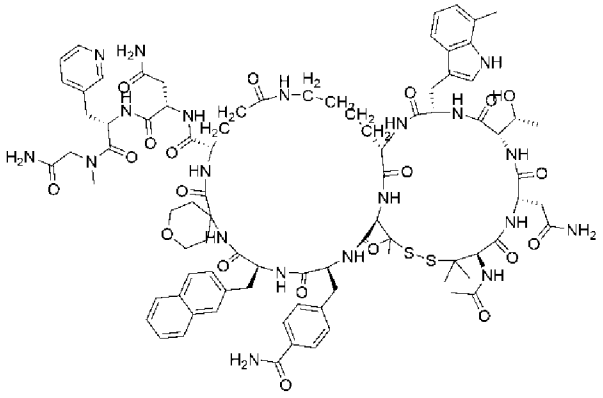
SEQ ID.	化合物	序列/結構
91	74	Ac-[(D)Arg]-[Abu]-Q-T-W-Q-C-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[bAla]-NH2 
92	75	Ac-[Pen]-Q-T-W-Q-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[bAla]-NH2 

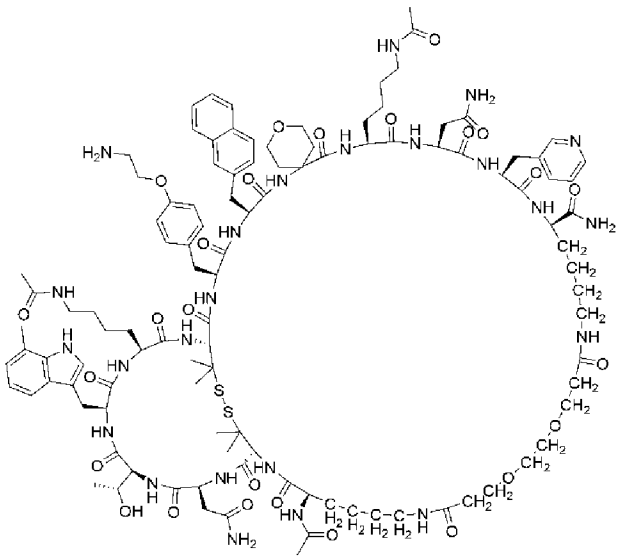
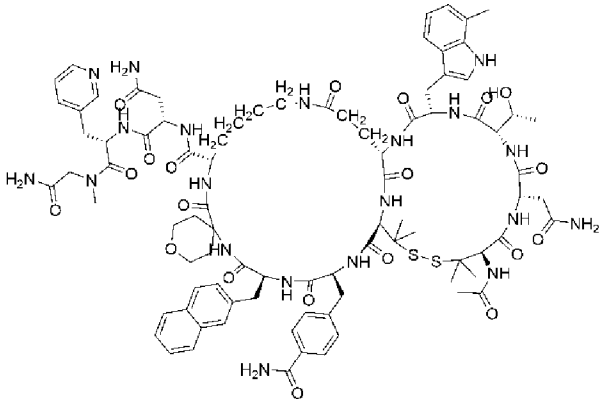
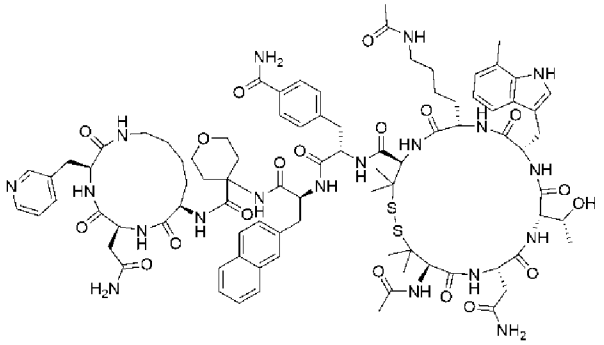
SEQ ID.	化合物	序列/結構
93	76	Ac-E-A-E-T-[W(7-Me)]-[Lys(Ac)]-A-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[(D)Lys]-NH2 
94	77	[Ac_Morph]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 
95	78	[Ac_Morph]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 

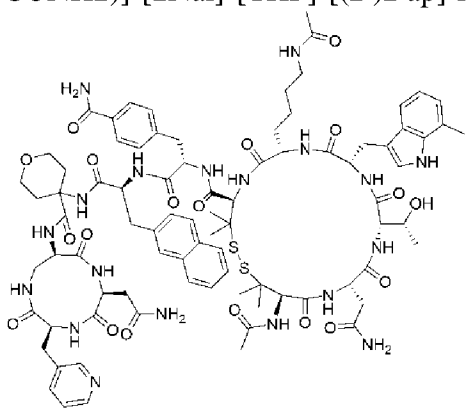
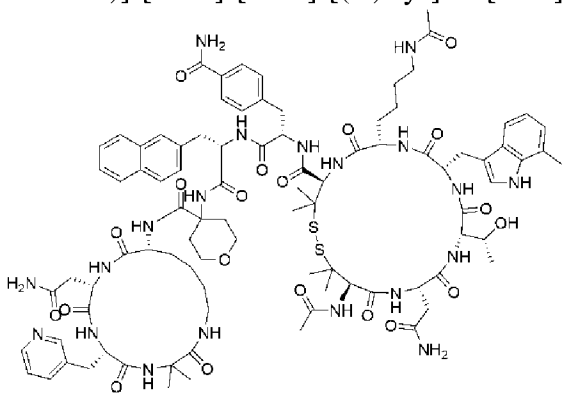
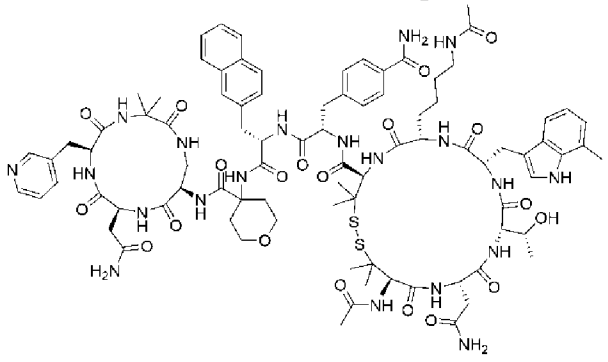
SEQ ID.	化合物	序列/結構
96	79	[Ac_Morph]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 
97	80	Ac-D-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-NH2 
98	81	Ac-E-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Dap]-NH2 

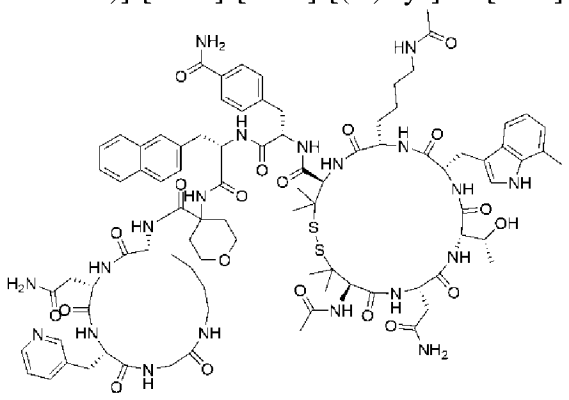
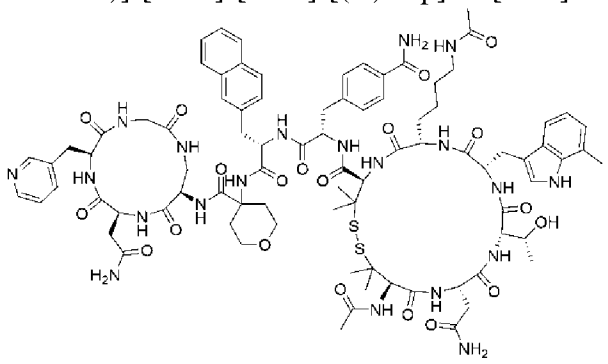
SEQ ID.	化合物	序列/結構
99	82	Ac-D-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Dap]-NH2 
100	83	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-[NH2]-[PEG2_二酸] 

SEQ ID.	化合物	序列/結構
101	84	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Asp]-NH2 
102	85	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Glu]-NH2 
103	86	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-E-N-[3Pal]-[(D)Lys]-NH2 

SEQ ID.	化合物	序列/結構
104	87	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-K-N-[3Pal]-[(D)Asp]-NH2 
105	88	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-K-N-[3Pal]-[(D)Glu]-NH2 
106	89	Ac-[Pen]-N-T-[W(7-Me)]-K-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-E-N-[3Pal]-[Sarc]-NH2 

SEQ ID.	化合物	序列/結構
107	90	Ac-[(D)Lys]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-[NH2]-[PEG2_二酸] 
108	91	Ac-[Pen]-N-T-[W(7-Me)]-E-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-K-N-[3Pal]-[Sarc]-NH2 
109	92	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Lys]-N-[3Pal] 

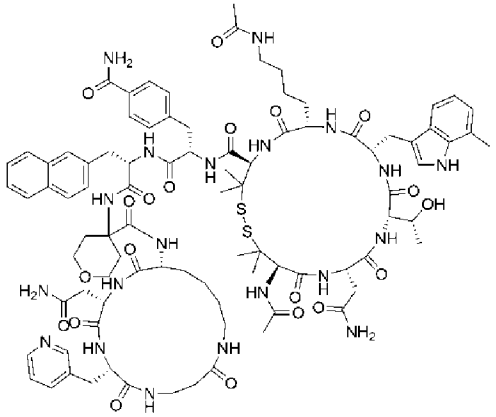
SEQ ID.	化合物	序列/結構
110	93	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Dap]-N-[3Pal] 
111	94	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Lys]-N-[3Pal]-[Aib] 
112	95	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Dap]-N-[3Pal]-[Aib] 

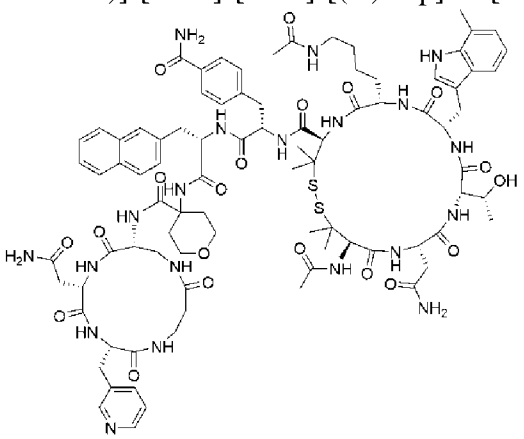
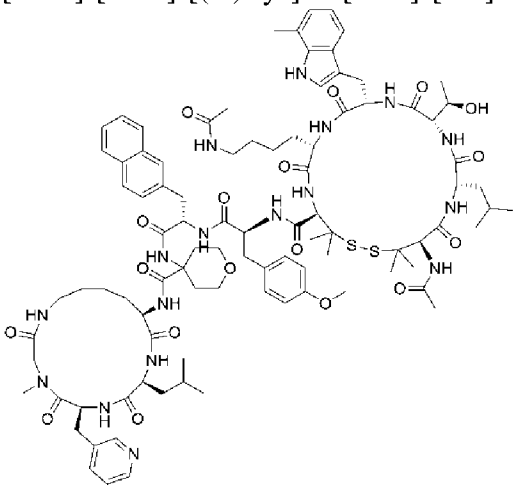
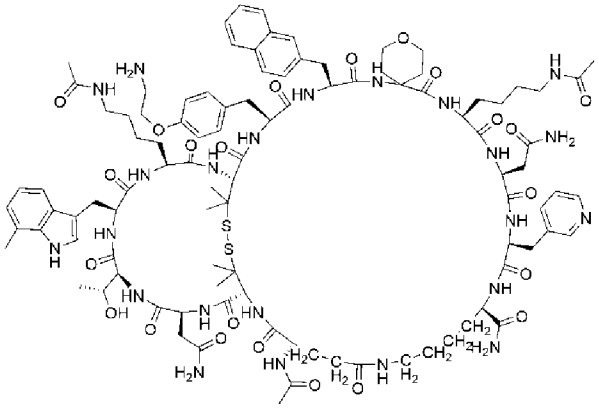
SEQ ID.	化合物	序列/結構
113	96	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Lys]-N-[3Pal]-G 
114	97	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Dap]-N-[3Pal]-G 

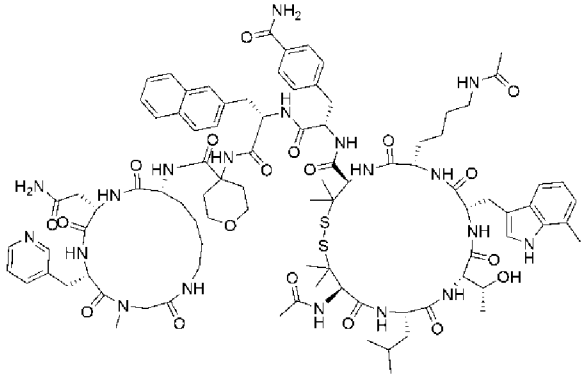
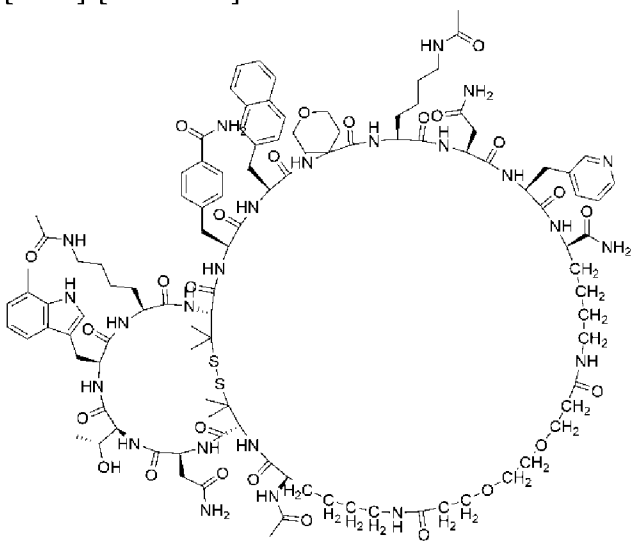
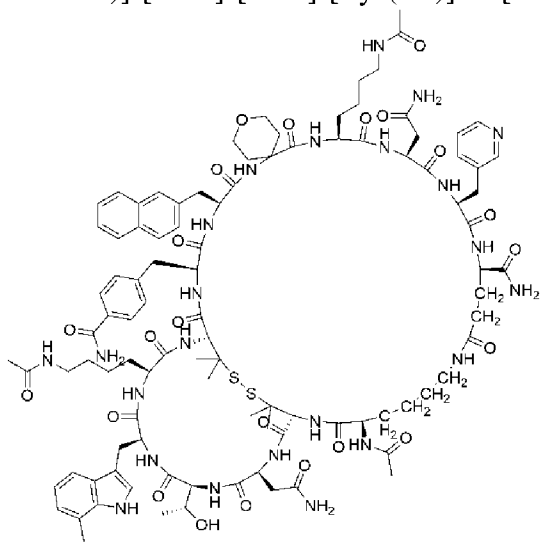
其中Pen-Pen形成雙硫鍵，或Abu-C形成硫醚鍵。

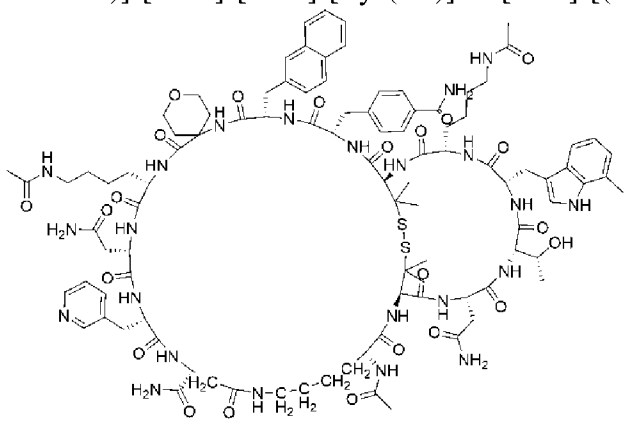
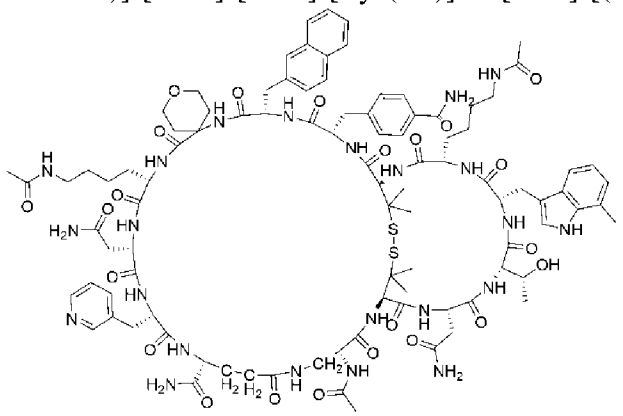
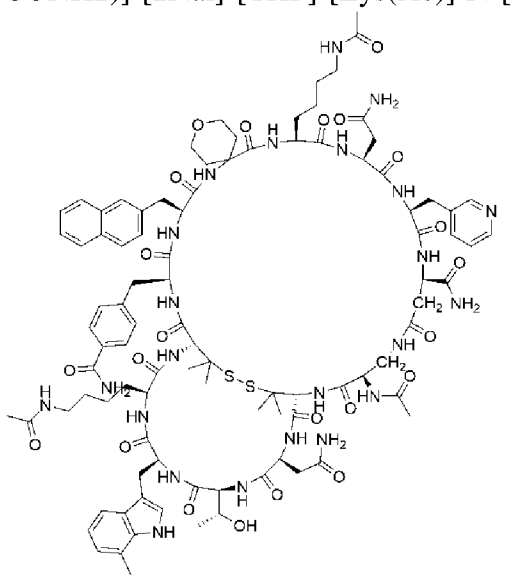
【0085】

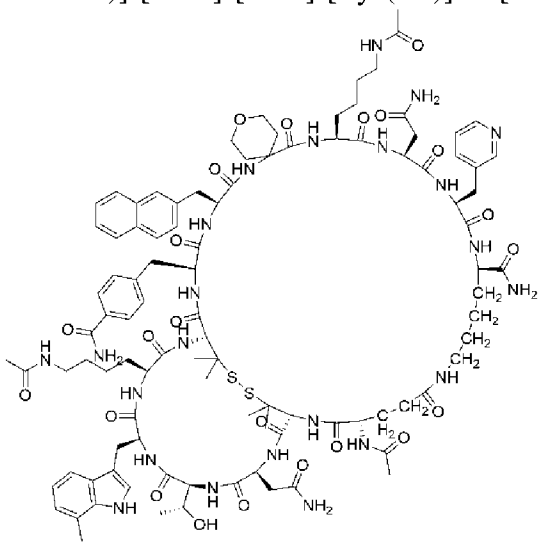
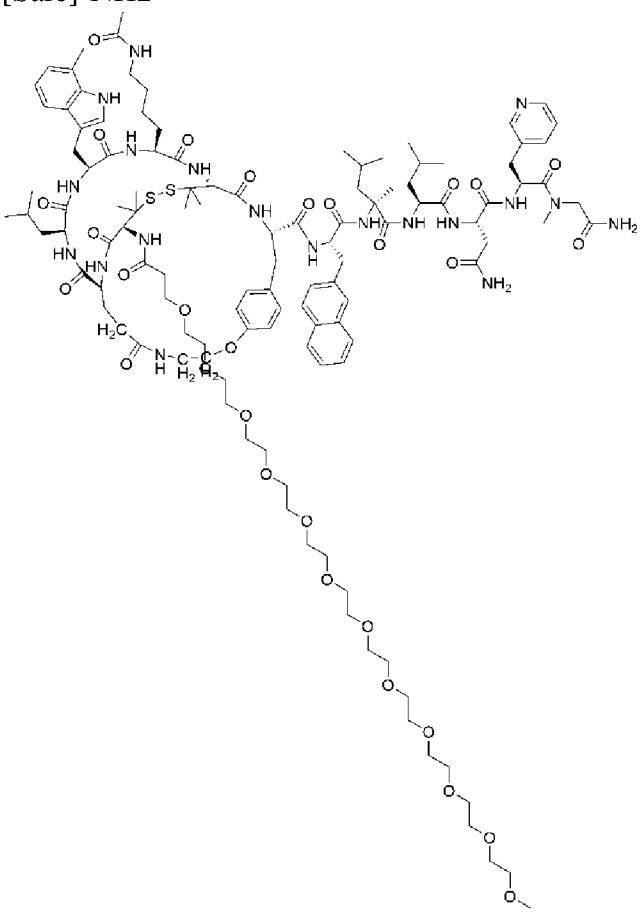
表1F.化合物

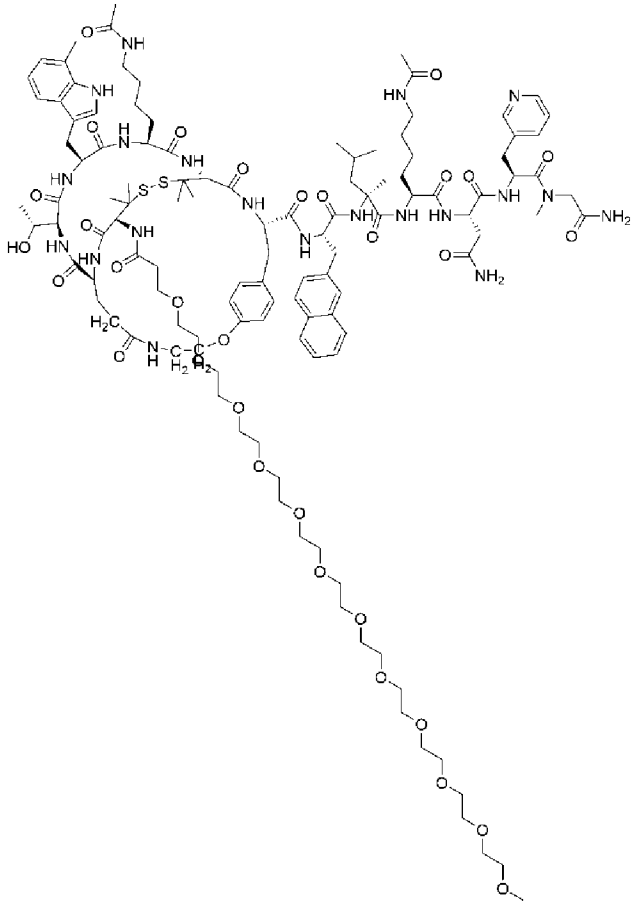
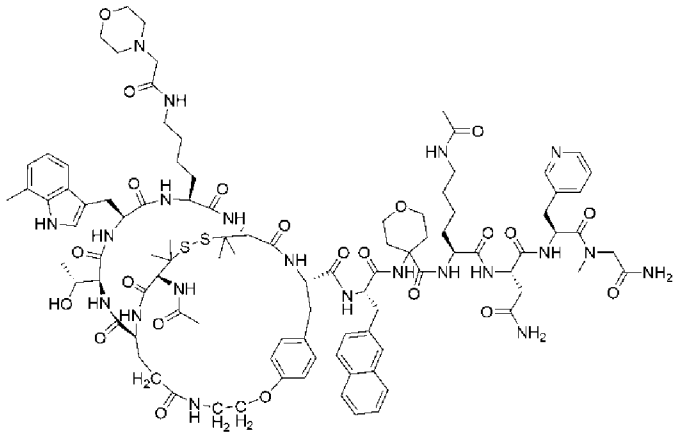
	化合物	序列/結構	註
115	98	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Lys]-N-[3Pal]-[bAla] 	#N/A

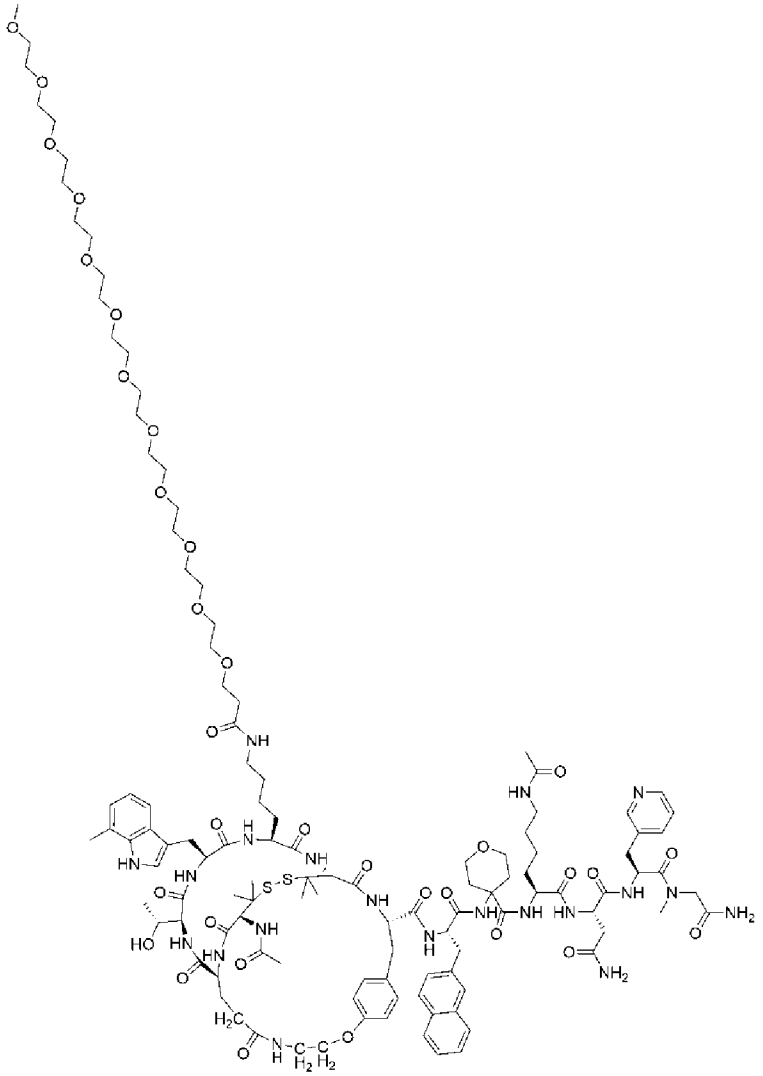
	化合物	序列/結構	註
116	99	Ac-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Dap]-N-[3Pal]-[bAla] 	#N/A
117	100	Ac-[Pen]-L-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-OMe)]-[2Nal]-[THP]-[(D)Lys]-L-[3Pal]-[Sar] 	#N/A
118	101	Ac-E-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-NH2 	#N/A

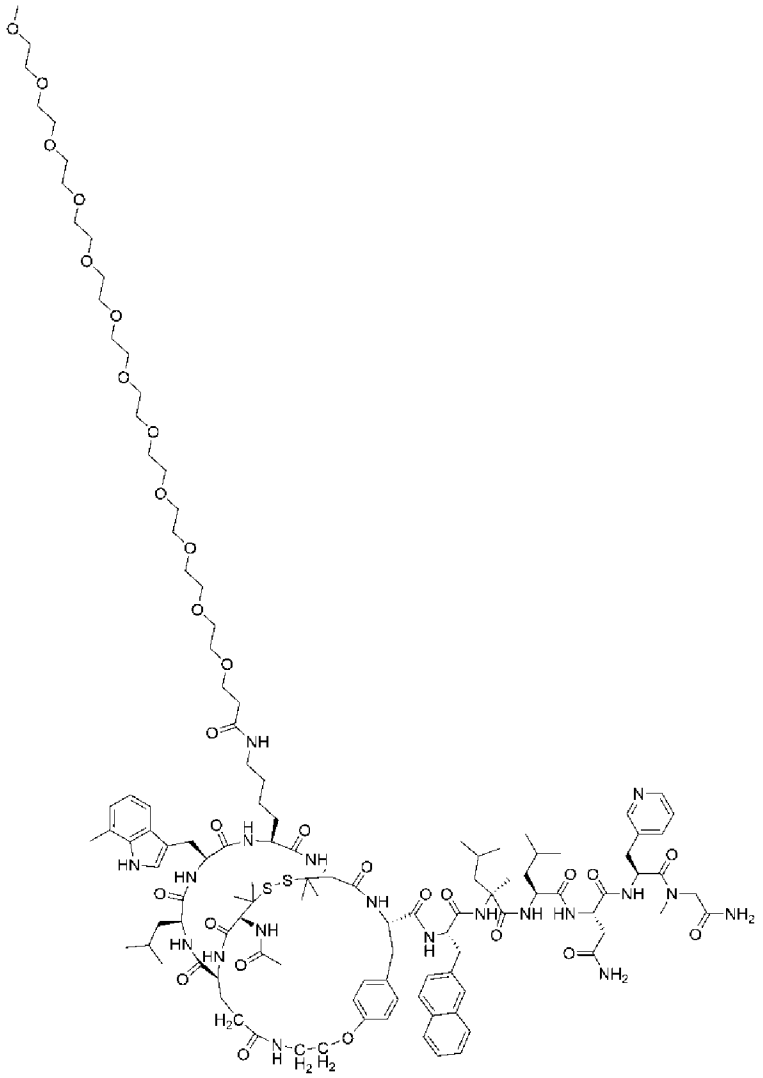
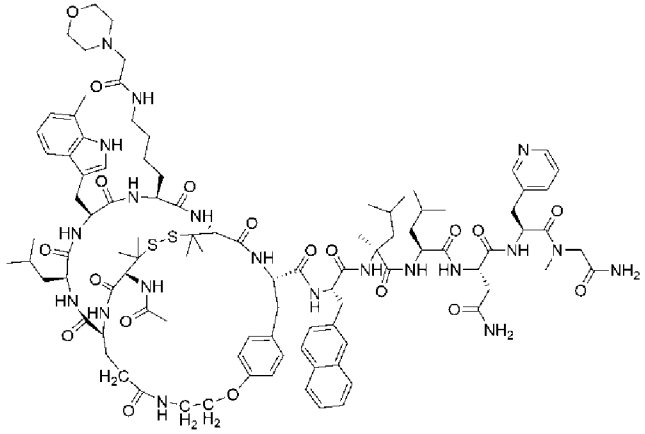
	化合物	序列/結構	註
119	102	Ac-[Pen]-L-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[(D)Lys]-N-[3Pal]-[Sar] 	#N/A
120	103	Ac-[(D)Lys]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-[NH2]-[PEG2DA] 	#N/A
121	104	Ac-[(D)Lys]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Glu]-NH2 	#N/A

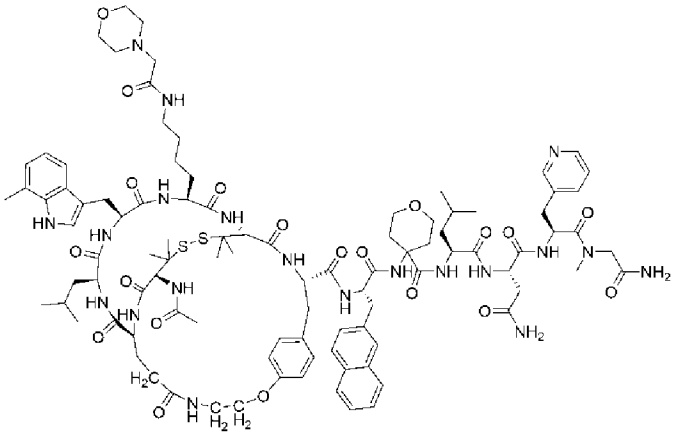
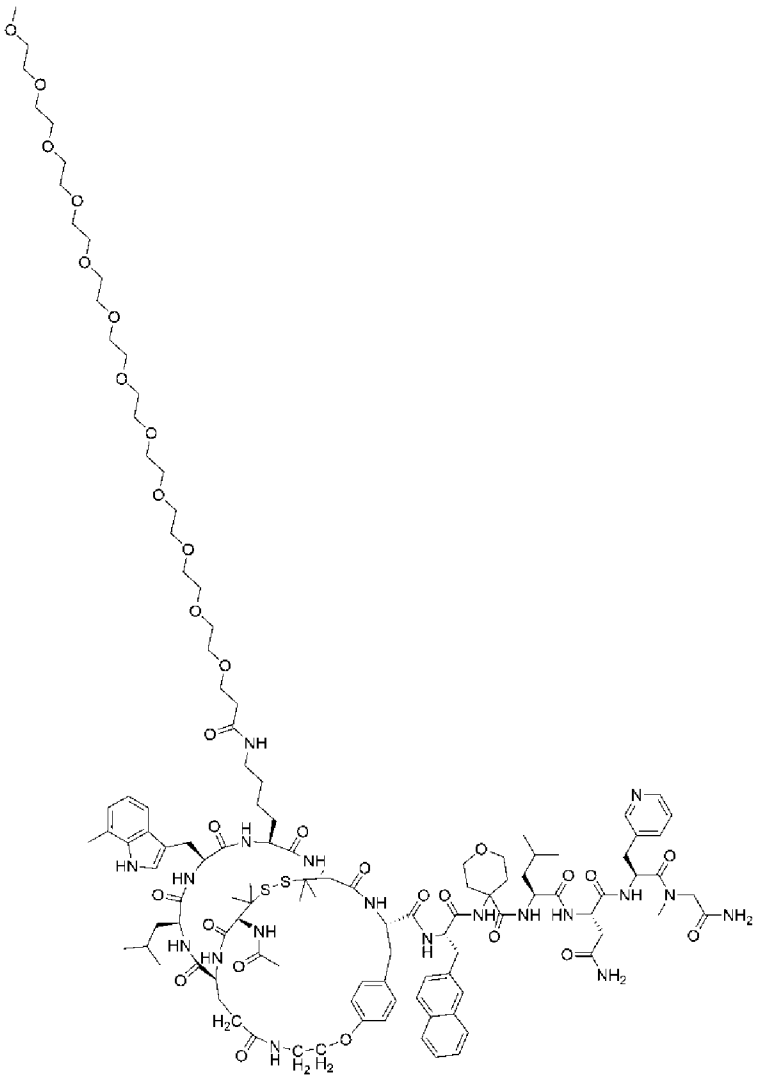
	化合物	序列/結構	註
122	105	Ac-[(D)Lys]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Asp]-NH2 	#N/A
123	106	Ac-[(D)Dap]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Glu]-NH2 	#N/A
124	107	Ac-[(D)Dap]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Asp]-NH2 	#N/A

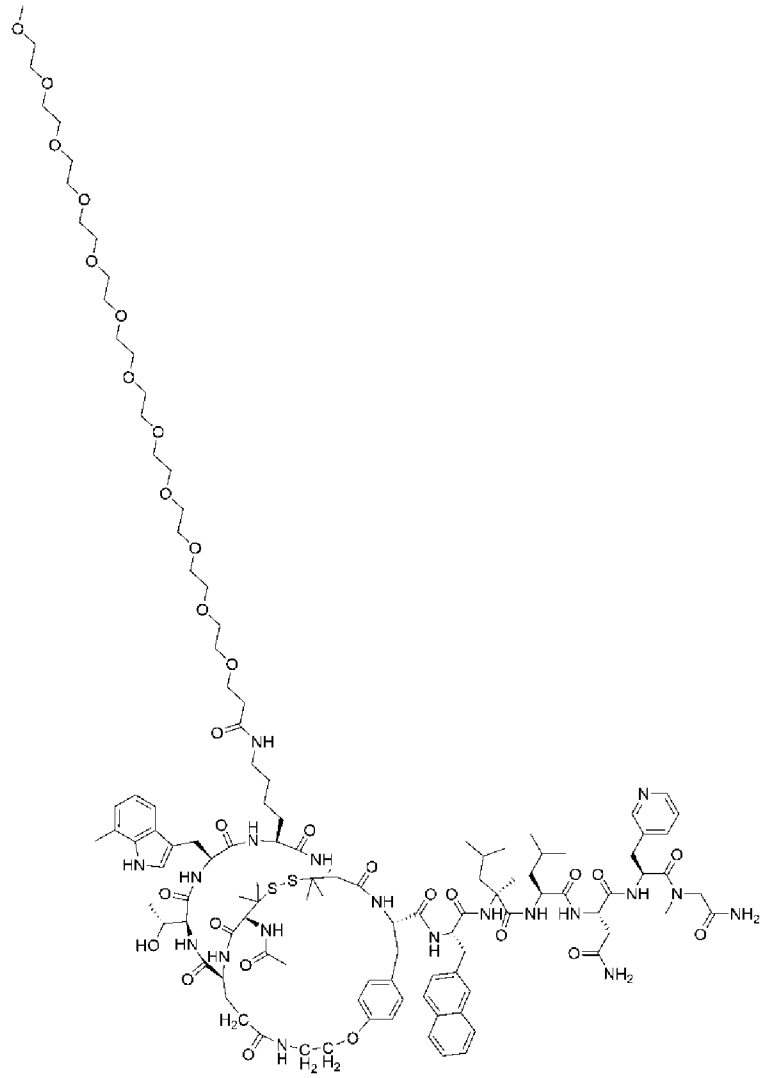
	化合物	序列/結構	註
125	108	Ac-E-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-CONH2)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-NH2 	#N/A
126	109	[PEG12_OMe]-[Pen]-E-L-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 	#N/A

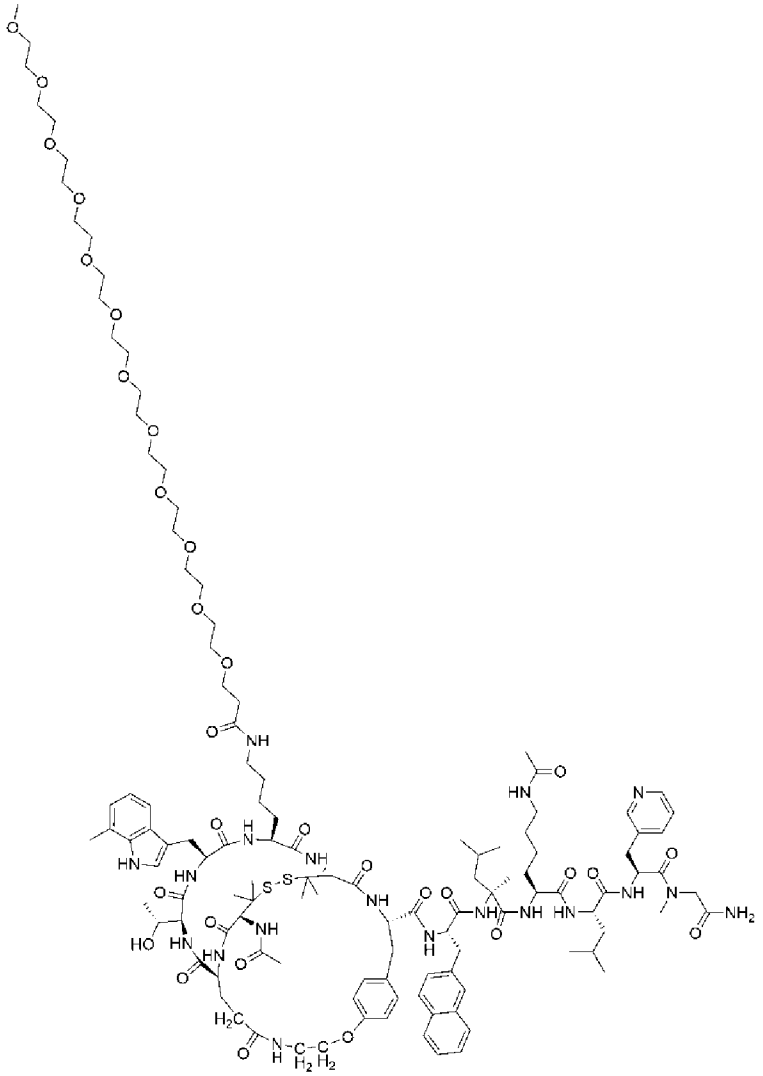
	化合物	序列/結構	註
127	110	[PEG12_OMe]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	#N/A
128	111	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	#N/A

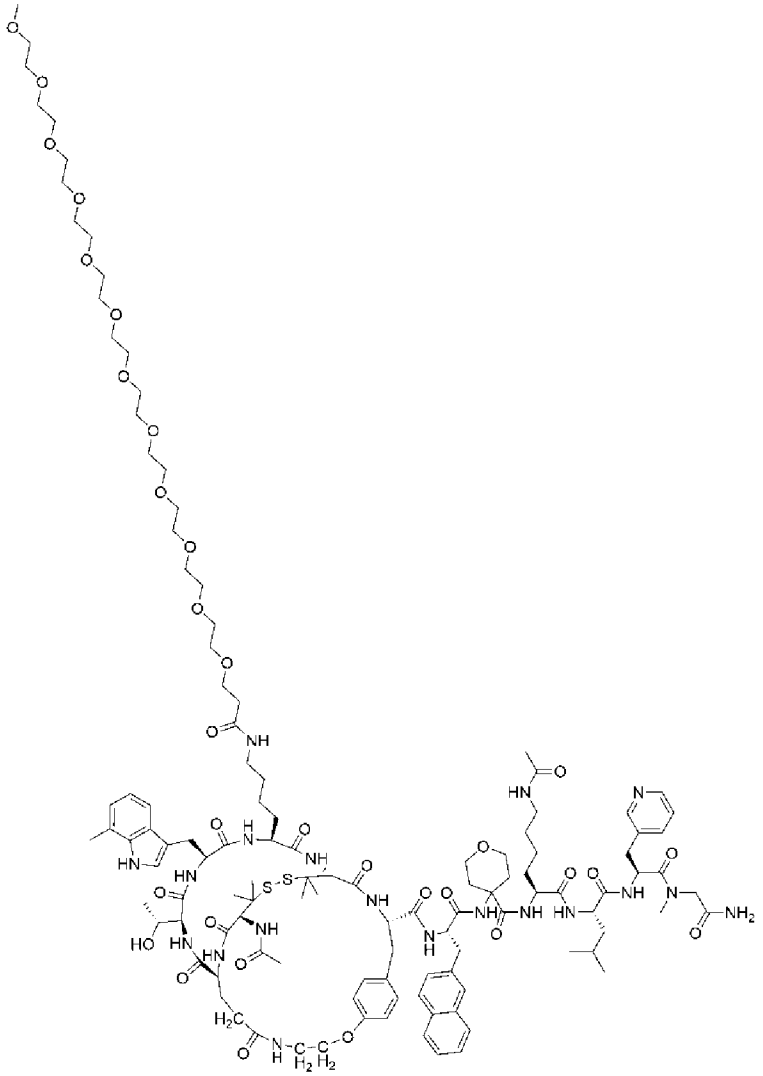
	化合物	序列/結構	註
129	112	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	#N/A

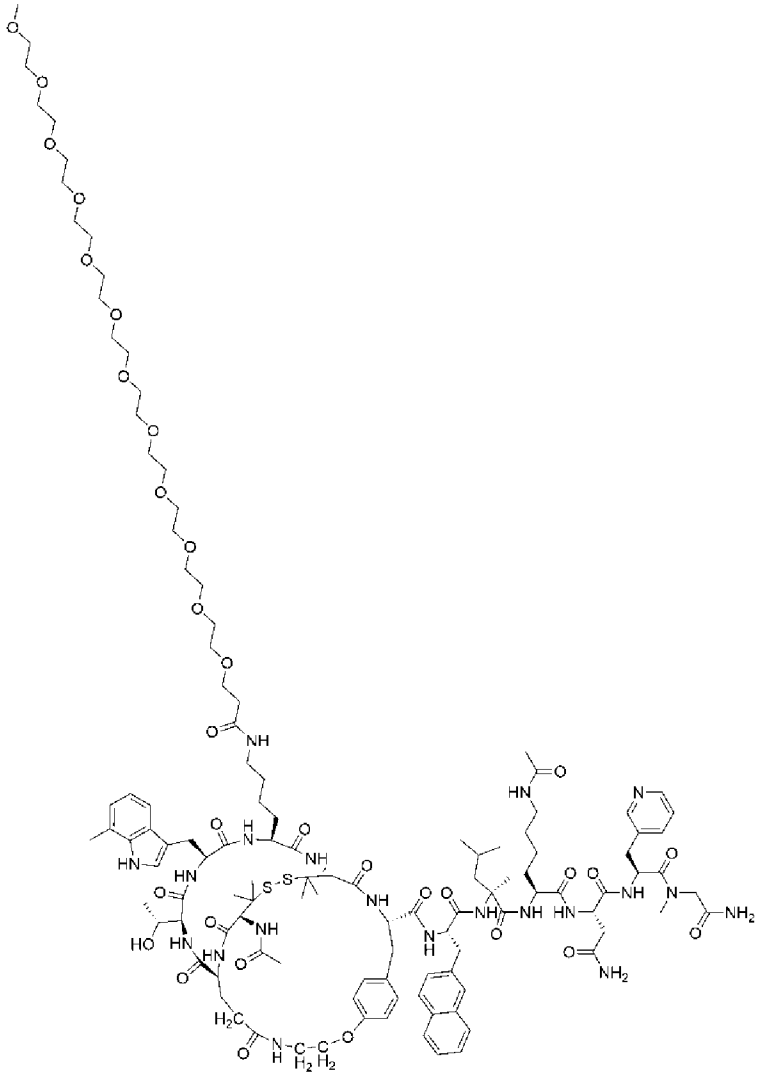
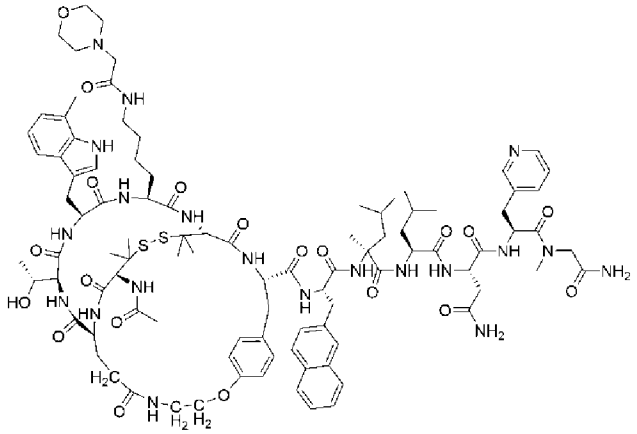
	化合物	序列/結構	註
130	113	Ac-[Pen]-E-L-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 	#N/A
131	114	Ac-[Pen]-E-L-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 	#N/A

	化合物	序列/結構	註
132	115	Ac-[Pen]-E-L-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-L-N-[3Pal]-[Sarc]-NH2 	#N/A
133	116	Ac-[Pen]-E-L-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-L-N-[3Pal]-[Sarc]-NH2 	#N/A

	化合物	序列/結構	註
134	117	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 	#N/A

	化合物	序列/結構	註
135	118	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 	#N/A

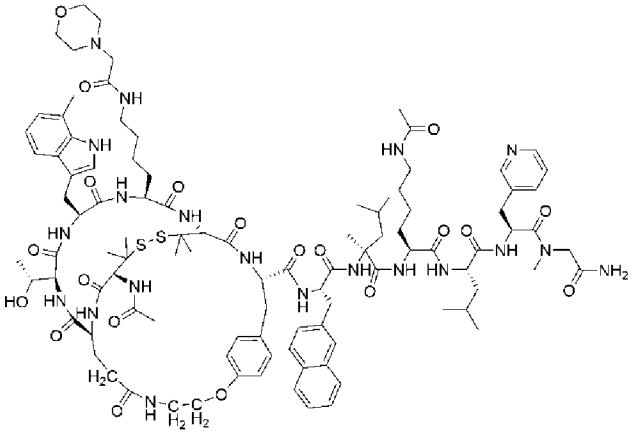
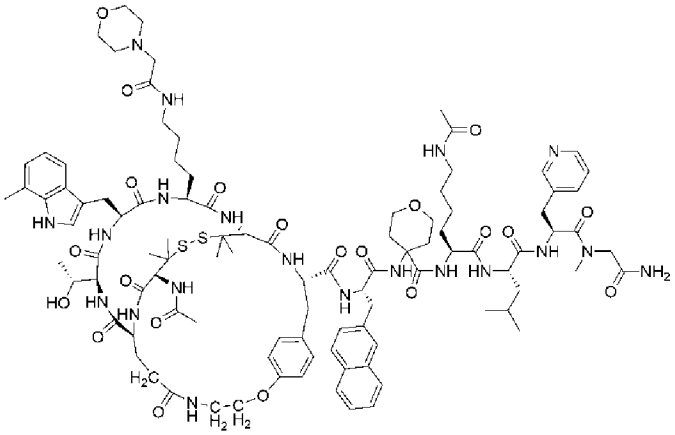
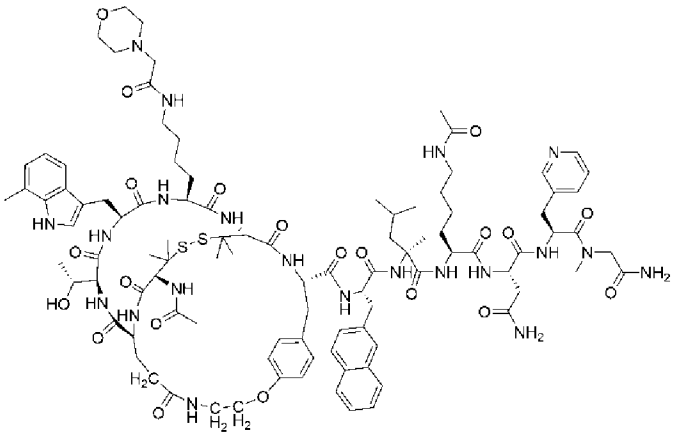
	化合物	序列/結構	註
136	119	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 	#N/A

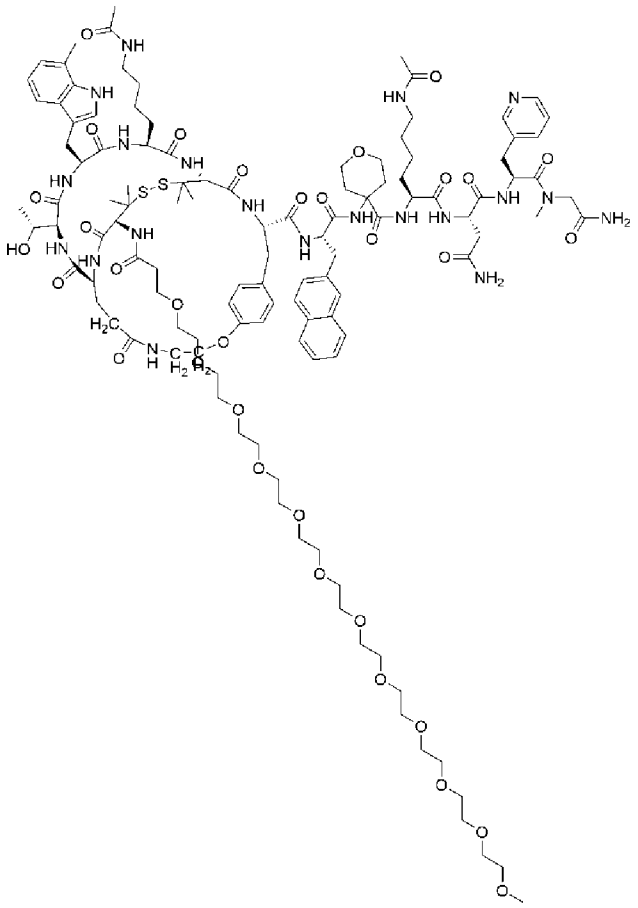
	化合物	序列/結構	註
137	120	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 	#N/A
138	121	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 	#N/A

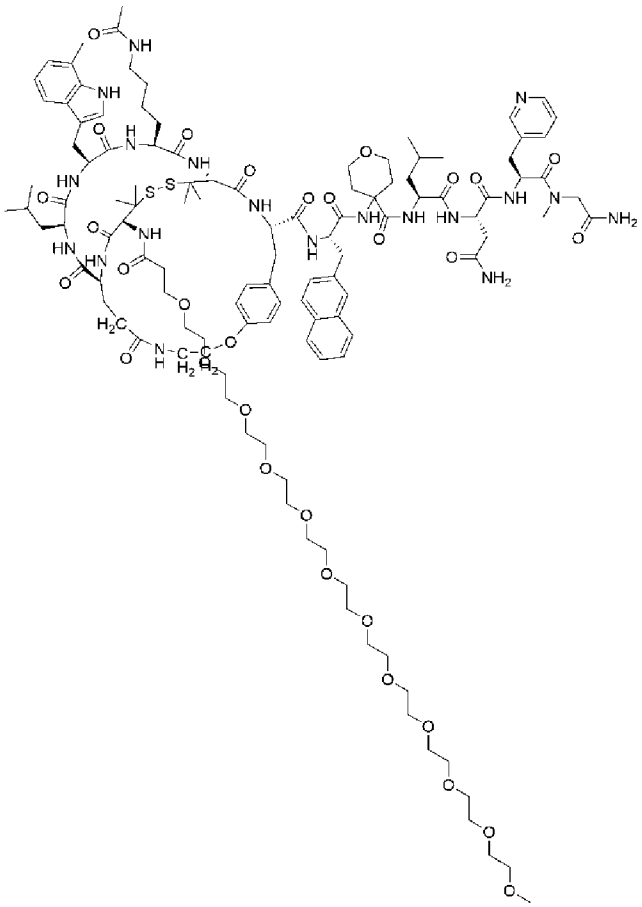
其中Pen-Pen形成雙硫鍵，或Abu-C形成硫醚鍵。

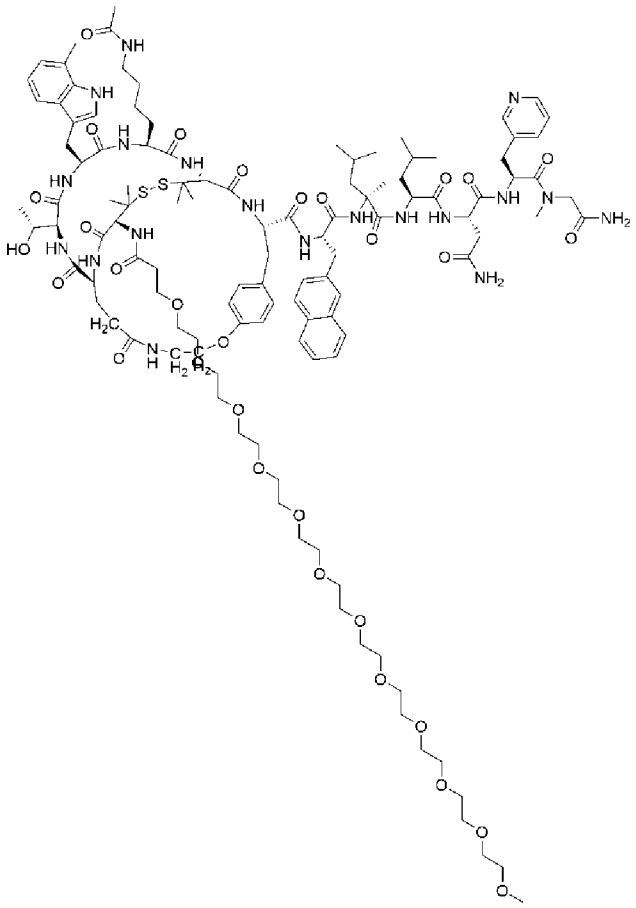
【0086】

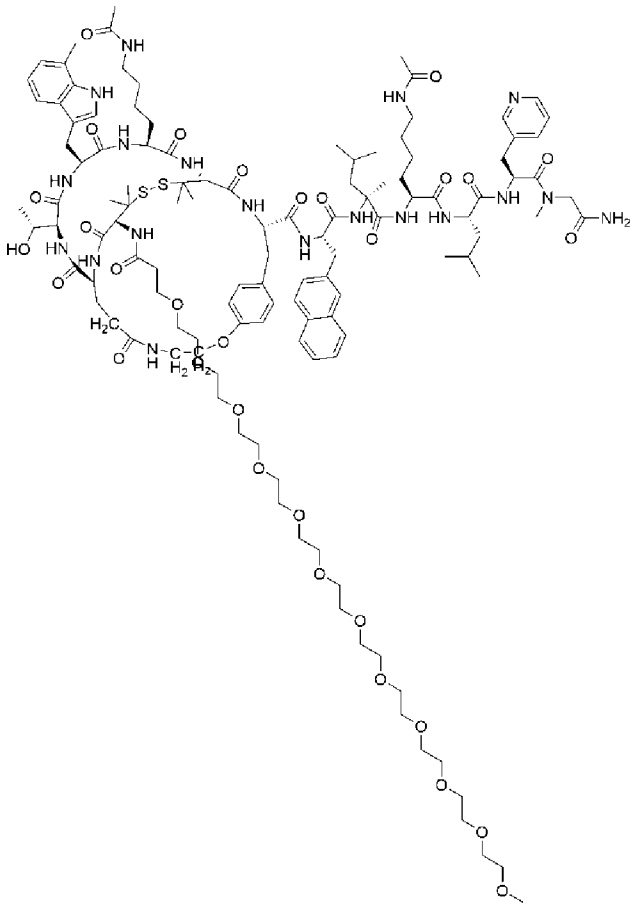
表1G.化合物

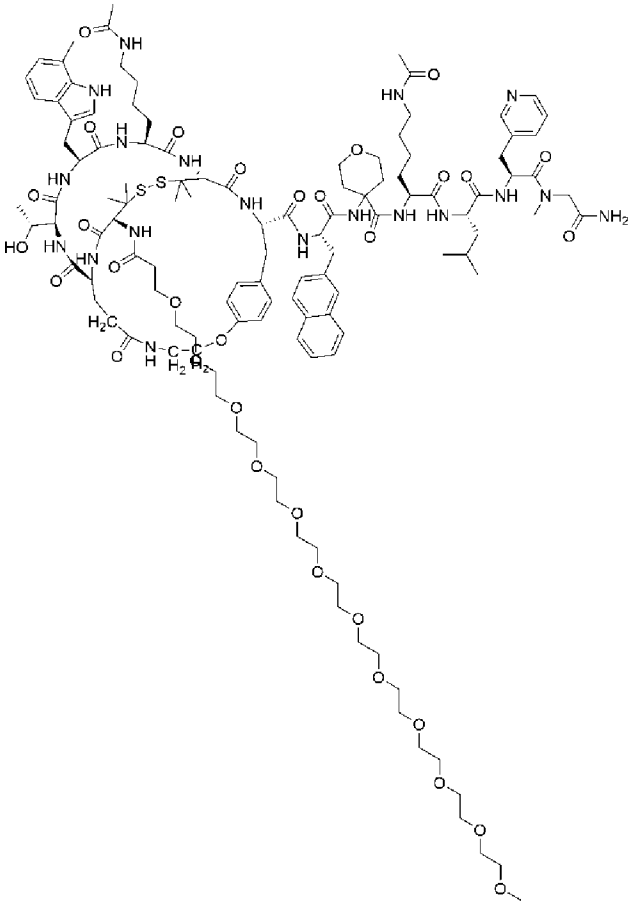
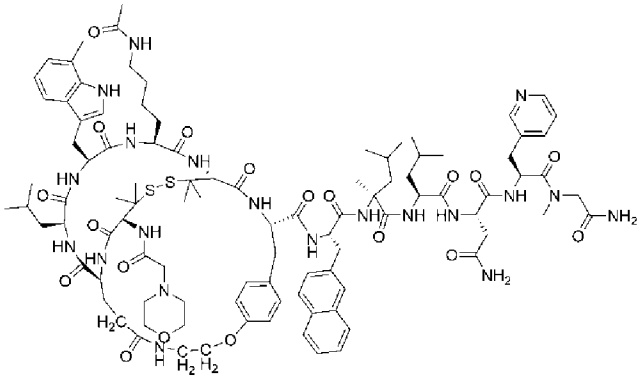
SEQ ID.	化合物	序列/結構
139	122	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 
140	123	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 
141	124	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 

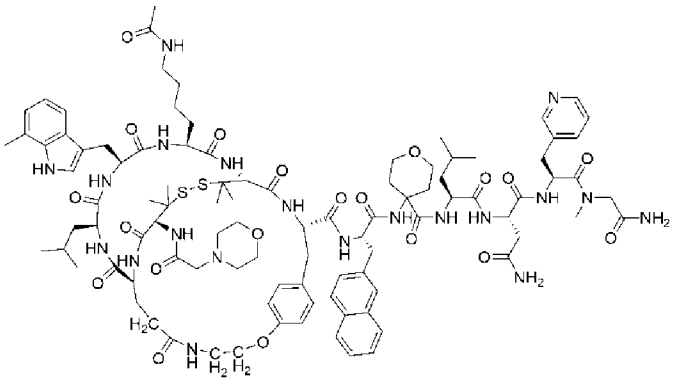
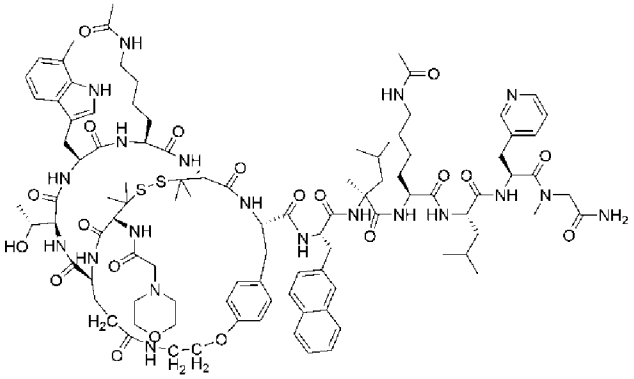
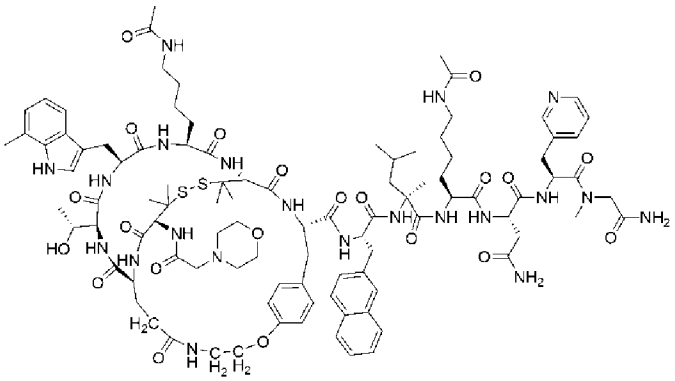
SEQ ID.	化合物	序列/結構
142	125	[PEG12_OMe]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 

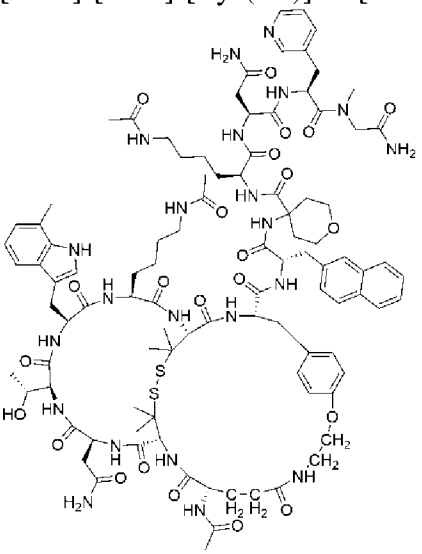
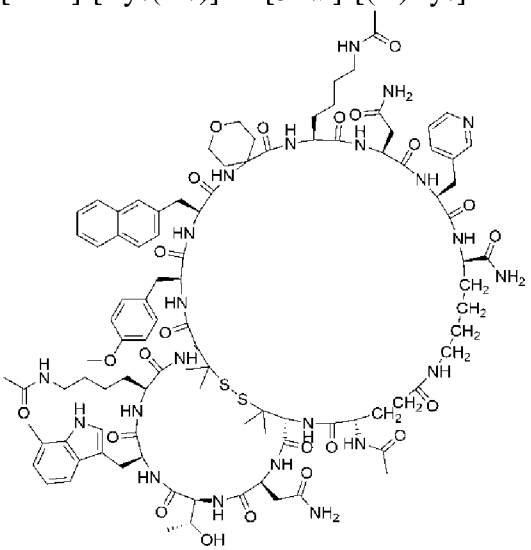
SEQ ID.	化合物	序列/結構
143	126	[PEG12_OMe]-[Pen]-E-L-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-L-N-[3Pal]-[Sarc]-NH2 

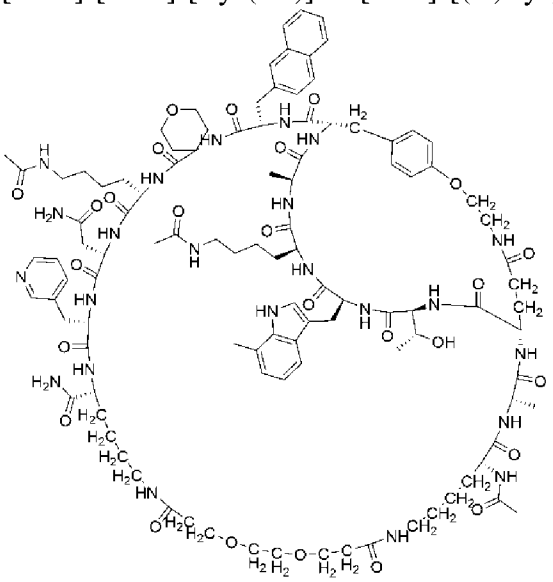
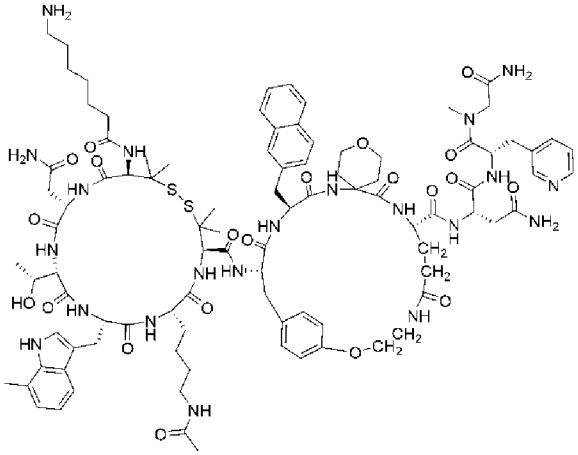
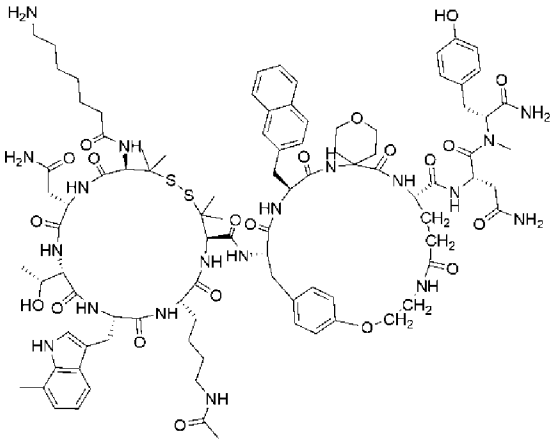
SEQ ID.	化合物	序列/結構
144	127	[PEG12_OMe]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 

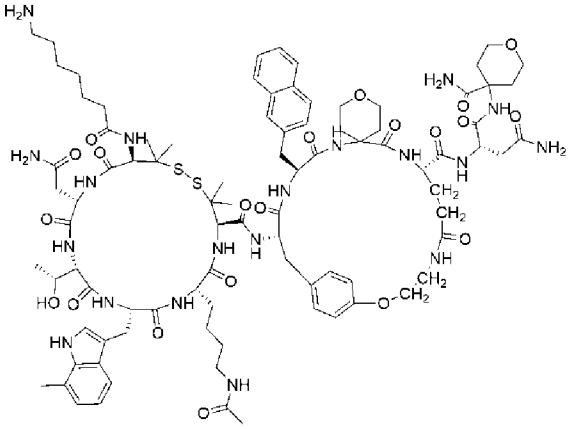
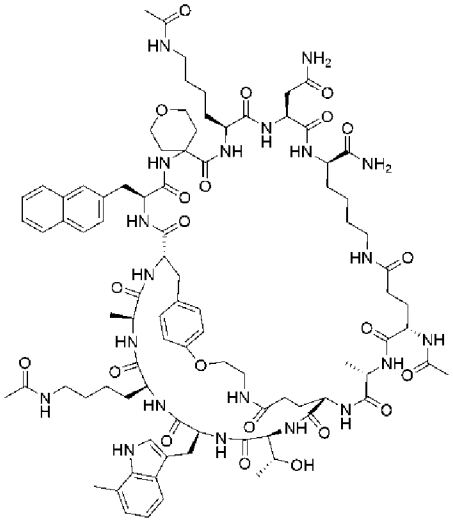
SEQ ID.	化合物	序列/結構
145	128	[PEG12_OMe]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 

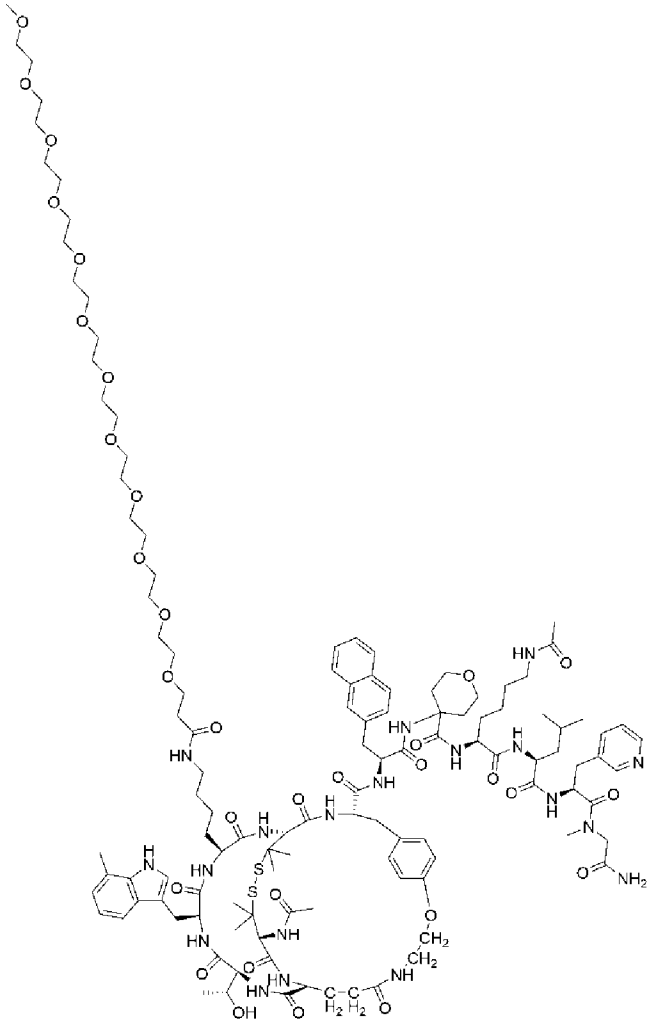
SEQ ID.	化合物	序列/結構
146	129	[PEG12_OMe]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 
147	130	[Ac_Morph]-[Pen]-E-L-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-L-N-[3Pal]-[Sarc]-NH2 

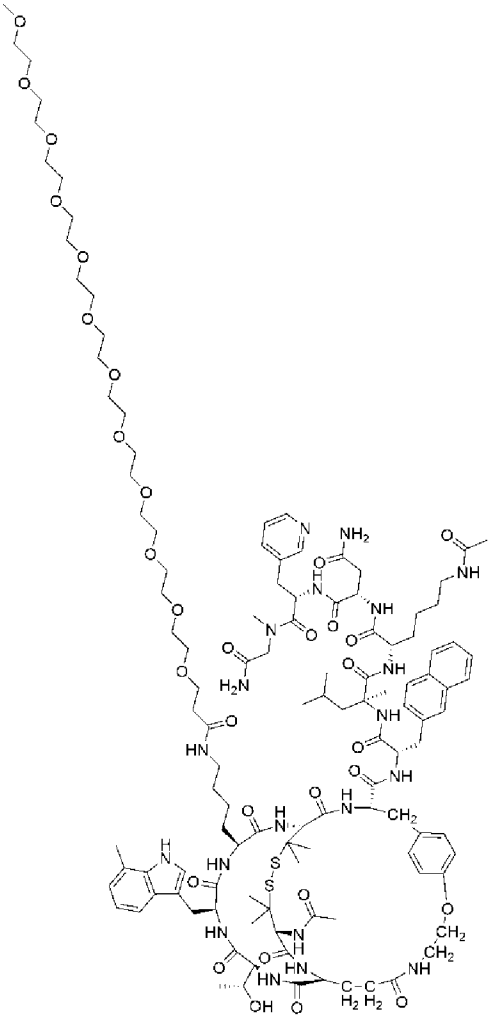
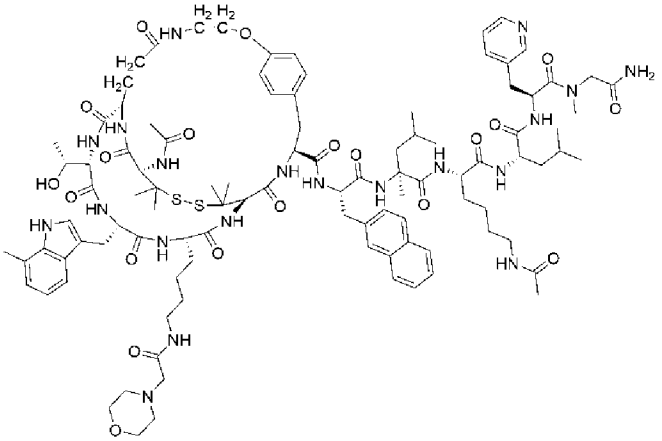
SEQ ID.	化合物	序列/結構
148	131	[Ac_Morph]-[Pen]-E-L-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-L-N-[3Pal]-[Sarc]-NH2 
149	132	[Ac_Morph]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 
150	133	[Ac_Morph]-[Pen]-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 

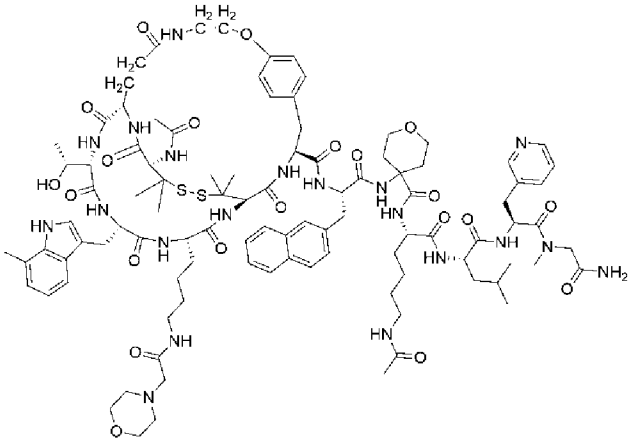
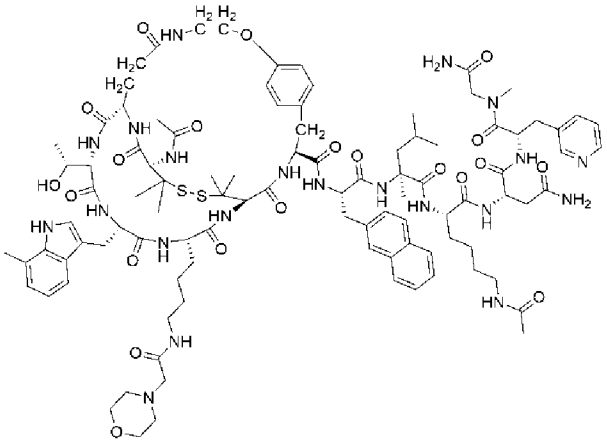
SEQ ID.	化合物	序列/結構
151	134	Ac-E-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 
152	135	Ac-E-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-OMe)]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-NH2 

SEQ ID.	化合物	序列/結構
153	136	Ac-[(D)Lys]-A-E-T-[W(7-Me)]-[Lys(Ac)]-A-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[3Pal]-[(D)Lys]-[NH2]-[PEG2DA] 
154	137	[7 胺基庚酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[3Pal]-[Sarc]-NH2 
155	138	[7 胺基庚酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[(D)NMeTyr]-NH2 

SEQ ID.	化合物	序列/結構
156	139	[7 胺基庚酸]-[Pen]-N-T-[W(7-Me)]-[Lys(Ac)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-E-N-[THP]-NH2 
157	140	Ac-E-A-E-T-[W(7-Me)]-[Lys(Ac)]-A-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-N-[(D)Lys]-NH2 

SEQ ID.	化合物	序列/結構
158	141	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 

SEQ ID.	化合物	序列/結構
159	142	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(PEG12_OMe)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 
160	143	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 

SEQ ID.	化合物	序列/結構
161	144	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[THP]-[Lys(Ac)]-L-[3Pal]-[Sarc]-NH2 
162	145	Ac-[Pen]-E-T-[W(7-Me)]-[Lys(Ac_Morph)]-[Pen]-[Phe(4-(2-胺基乙氧基))]-[2Nal]-[aMeLeu]-[Lys(Ac)]-N-[3Pal]-[Sarc]-NH2 

插入額外化合物之表1H

合成

【0087】 本文中所述的化合物可藉由所屬技術領域中具有通常知識者已知之許多技術來合成。在某些態樣中，單體次單元係使用隨附實例中所述之技術來合成及純化。在一些態樣中，本發明提供一種生產本發明之化合物（或其單體次單元）之方法，其包含化學合成本文中所述的胺基酸序列之肽，包括但不限於式(I)至(XX)、本文中表1A、表1B、表1C、表1D、表1E、表1F、表1G、及表1H之化合物中所陳述的任何胺基酸序列。在一些態樣中，肽之一部分係重

組合成的，而不是化學合成的。在一些態樣中，生產化合物之方法進一步包括在組成次單元已附接後環化化合物前驅物。在特定態樣中，環化係經由本文中所述的任何各種方法來達成。

【0088】 本發明進一步描述本文中所述的化合物之合成，諸如式(I)至(XX)之化合物及表1A、表1B、表1C、表1D、表1E、表1F、表1G、及表1H之化合物。在一些態樣中，將一或多個胺基酸殘基或胺基酸單體脂化然後共價附接至另一個而形成本發明之化合物。在一些態樣中，將一或多個胺基酸殘基或胺基酸單體共價附接至另一個並在中間寡聚物階段脂化，之後附接額外胺基酸並環化而形成本發明之化合物。在一些態樣中，合成環狀肽然後脂化而形成本發明之化合物。說明性合成方法係描述於實例中。

【0089】 本發明進一步描述本文中所述的化合物之合成，諸如式(I)至(XX)之化合物及表1A、表1B、表1C、表1D、表1E、表1F、表1G、及表1H之化合物。說明性合成方法係描述於實例中。

IV. 醫藥組成物

【0090】 本發明關於包含本發明之IL-23R抑制劑的醫藥組成物。

【0091】 本發明包括包含本發明之一或多種抑制劑及醫藥上可接受之載劑、稀釋劑、或賦形劑的醫藥組成物。

【0092】 醫藥上可接受之載劑、稀釋劑、或賦形劑可係任何類型之固體、半固體或液體填料、稀釋劑、包封材料、或配方輔助劑。微生物作用之預防可藉由納入各種抗細菌及抗真菌劑（例如，對羥基苯甲酸酯、氯丁醇、苯

酚、山梨酸、及類似者）來確保。所欲的亦可是包括等張劑，諸如糖、氯化鈉、及類似者。

【0093】 醫藥組成物可口服、腸胃外、腦池內、陰道內、腹膜內、直腸內、局部（如藉由粉劑、軟膏劑、滴劑、栓劑、或經皮貼片劑）、藉由吸入（諸如鼻內噴劑）、經眼（諸如眼內）、或口頰投予。如本文中所使用，用語「腸胃外(parenteral)」係指包括靜脈內、肌內、腹膜內、胸骨內、皮下、皮內、及關節內注射與輸注之投予模式。因此，在某些實施例中，組成物係針對藉由任何這些投予途徑遞送而調配。醫藥組成物可針對口服投予而調配。醫藥組成物可針對腸胃外投予而調配。

【0094】 在特定態樣中，本發明之IL-23R抑制劑係懸浮於持續釋放基質中。如本文中所使用，持續釋放基質是一種以通常為聚合物之材料製成的基質，其可藉由酶或酸鹼水解或藉由溶解而降解。一旦進入體內，基質會藉由酶及體液而發揮作用。持續釋放基質所欲地係選自生物相容性材料，諸如微脂體、聚乳酸(polylactic acid)、聚乙交酯（乙醇酸之聚合物）、聚乳酸共乙交酯（乳酸及乙醇酸之共聚物）聚酐、聚(原)酯、多肽、玻尿酸、膠原蛋白、硫酸軟骨素、羧酸、脂肪酸、磷脂、多醣、核酸、聚胺基酸、胺基酸（諸如苯丙胺酸、酪胺酸、異白胺酸）、多核苷酸、聚乙烯丙烯、聚乙烯吡咯啶酮、及聚矽氧。可生物降解基質之一個實施例係聚乳酸、聚乙交酯、或聚乳酸共乙交酯（乳酸及乙醇酸之共聚物）中一者之基質。

【0095】 本發明之IL-23R抑制劑可製備及/或調配為醫藥上可接受之鹽或呈中性形式（適當時）。醫藥上可接受之鹽係化合物中性形式之無毒性鹽，其

擁有該中性形式之所欲醫藥活性。這些鹽可衍生自無機或有機酸或鹼。例如，含有鹼性氮之化合物可藉由使該化合物與無機或有機酸接觸而製備為醫藥上可接受之鹽。醫藥上可接受之鹽的非限制性實例包括硫酸鹽、焦硫酸鹽、硫酸氫鹽、亞硫酸鹽、亞硫酸氫鹽、磷酸鹽、磷酸氫鹽、磷酸二氫鹽、偏磷酸鹽、焦磷酸鹽、氯化物、溴化物、碘化物、乙酸鹽、丙酸鹽、癸酸鹽、辛酸鹽、丙烯酸酯、甲酸酯、異丁酸鹽、己酸鹽、庚酸鹽、丙炔酸鹽、草酸鹽、丙二酸鹽、琥珀酸鹽、栓酸鹽、癸二酸鹽、反丁烯二酸鹽、順丁烯二酸鹽、丁炔-1,4-二酸、己炔-1,6-二酸、苯甲酸、氯苯甲酸、苯甲酸甲酯、二硝基苯甲酸、羥苯甲酸、甲氧苯甲酸、鄰苯二甲酸鹽、磺酸鹽、甲磺酸鹽、丙磺酸鹽、苯磺酸鹽、二甲苯磺酸鹽、萘-1-磺酸鹽、萘-2-磺酸鹽、苯乙酸鹽、苯丙酸鹽、苯丁酸鹽、檸檬酸、乳酸鹽、γ-羥丁酸鹽、甘醇酸鹽、酒石酸鹽、及苯乙醇酸鹽。其他合適的醫藥上可接受之鹽的清單係見於Remington: The Science and Practice of Pharmacy, 21st Edition, Lippincott Wiliams and Wilkins, Philadelphia, Pa., 2006。

【0096】　本文中所揭示的化合物之「醫藥上可接受之鹽」的實例亦包括衍生自適當的鹼之鹽，諸如鹼金屬（例如，鈉、鉀）、鹼土金屬（例如，鎂）、銨、及NX_4^+（其中X係C_1-C_4烷基）。亦包括鹼加成鹽，諸如鈉或鉀鹽。

【0097】　本發明關於醫藥組成物，其包含本發明之IL-23R抑制劑或其醫藥上可接受之鹽、異構物、或混合物，其中附接至碳原子之1至n個氫原子可經氘原子或D所置換，其中n係分子中之氫原子數。如所屬技術領域中已知，氘原子係氫原子之非放射性同位素。此等化合物可增加對代謝之抗性，因而可用於延長本文中所述的化合物或其醫藥上可接受之鹽、異構物、或混合物當投予至

哺乳動物時之半衰期。參見例如Foster,「Deuterium Isotope Effects in Studies of Drug Metabolism,」Trends Pharmacol.Sci., 5(12):524-527 (1984)。此類化合物係藉由所屬技術領域中所熟知之手段來合成，例如藉由採用一或多個氫原子已由氘所置換之起始材料。

【0098】　可結合至所揭示化合物中之同位素的實例亦包括氫、碳、氮、氮、磷、氟、氯、及碘之同位素，諸如分別為^{2}H、^{3}H、^{11}C、^{13}C、^{14}C、^{13}N、^{15}N、^{15}O、^{17}O、^{18}O、^{31}P、^{32}P、^{35}S、^{18}F、^{36}Cl、^{123}I、及^{125}I。用正子放射性同位素（諸如^{11}C、^{18}F、^{15}O、及^{13}N）進行取代可用於正子放射斷層攝影(Positron Emission Topography, PET)研究中以檢驗受質受體佔用。同位素標記的式(I)之化合物一般可藉由所屬技術領域中具有通常知識者已知之習知技術或藉由類似於如以下所提出之實例中所述者的程序，使用適當的同位素標記試劑代替先前所採用之未標記試劑來製備。

【0099】　在一些態樣中，用於腸胃外注射之醫藥組成物包含醫藥上可接受之無菌水性或非水性溶液、分散液、懸浮液、或乳液、或無菌粉劑，以用於剛在使用之前重組為無菌可注射溶液或分散液。合適的水性及非水性載劑、稀釋劑、溶劑、或媒劑之實例包括水、乙醇、多元醇（諸如甘油、丙二醇、聚乙二醇、及類似者）、羧甲纖維素及其合適的混合物、β-環糊精、植物油（諸如橄欖油）、及可注射有機酯（諸如油酸乙酯）。適當流動性可例如藉由下列方式來維持：使用塗層材料（諸如卵磷脂）、保持所需粒徑（在分散液的情況下）、及使用界面活性劑。這些組成物亦可含有佐劑，諸如保存劑、潤濕劑、

乳化劑、及分散劑。可注射醫藥形式之延長吸收可藉由納入延緩吸收之藥劑來達成，諸如單硬脂酸鋁及明膠。

【0100】　可注射貯存形式包括藉由在一或多種可生物降解聚合物中形成肽抑制劑之微包封基質來製造，可生物降解聚合物諸如聚乳酸-聚乙交酯、聚(原酯)、聚(酐)、及(聚)二醇（諸如PEG）。取決於肽對聚合物之比率及所採用特定聚合物之本質，可控制肽抑制劑之釋放速率。貯存可注射配方亦藉由將肽抑制劑陷捕於與身體組織相容之微脂體或微乳液中而製備。

【0101】　可注射配方可經滅菌，例如藉由通過擋菌過濾器過濾、或藉由結合呈無菌固體組成物形式之滅菌劑（其剛在使用之前可溶於或分散於無菌水或其他無菌可注射介質中）。

【0102】　局部投予包括投予至皮膚或黏膜，包括肺臟及眼睛之表面。用於局部肺投予之組成物（包括用於吸入及鼻內者）可涉及在水性及非水性配方中之溶液及懸浮液，並且可製備為乾粉劑（其可經加壓或未經加壓）。在未經加壓粉劑組成物中，活性成分可係細分形式，其可用於與大尺寸醫藥上可接受之惰性載劑混摻，該惰性載劑包含具有例如至多100微米直徑之粒徑的粒子。合適的惰性載劑包括糖，諸如乳糖。

【0103】　替代地，本發明之醫藥組成物可經加壓且含有壓縮氣體，諸如氮或液化氣體推進劑。液化推進劑介質及實際上整體組成物可係使得活性成分不會以任何實質程度溶於其中。經加壓組成物亦可含有表面活性劑，諸如液體或固體非離子性表面活性劑，或可係固體陰離子表面活性劑。較佳的是使用呈鈉鹽形式之固體陰離子表面活性劑。

【0104】 局部投予之進一步形式係投予至眼睛。本發明之肽抑制劑可在醫藥上可接受之眼用媒劑中遞送，使得該肽抑制劑維持與眼睛表面接觸一段足夠期間，而讓該肽抑制劑滲入眼睛之角膜及內部區域，如例如前房、後房、玻璃狀體、房水、玻璃狀液、角膜、虹膜/睫狀體、水晶體、脈絡膜/視網膜、及鞏膜。醫藥上可接受之眼用媒劑可例如係軟膏劑、植物油、或包封材料。替代地，本發明之肽抑制劑可直接注射至玻璃狀液及房水中。

【0105】 用於直腸或陰道投予之組成物包括栓劑，其可藉由將本發明之肽抑制劑與合適的無刺激性賦形劑或載劑混合而製備，無刺激性賦形劑或載劑諸如可可脂、聚乙二醇、或栓劑臘，其在室溫下為固體但在體溫下為液體，因而會在直腸或陰道空腔中融化並釋放活性化合物。

【0106】 本發明之肽抑制劑亦可在微脂體或其他基於脂質之載劑中投予。如所屬技術領域中已知，微脂體通常衍生自磷脂或其他脂質物質。微脂體係以分散於水性介質中之單層或多層狀水合液晶來形成。可使用能夠形成微脂體的任何無毒性、生理上可接受且可代謝之脂質。呈微脂體形式之本案組成物除了本發明之肽抑制劑，還含有穩定劑、保存劑、賦形劑、及類似者。在某些實施例中，脂質包含磷脂，包括磷脂膽鹼（卵磷脂）及絲胺酸，兩者可係天然及合成的。形成微脂體之方法在所屬技術領域中係已知的。

【0107】 適用於在本文中所述的方法或用途中腸胃外投予之醫藥組成物可包含IL-23R抑制劑之無菌水性溶液及/或懸浮液，其與接受者之血液等張，一般使用氯化鈉、甘油、葡萄糖、甘露醇、山梨醇、及類似者。

【0108】　本發明提供一種用於口服遞送之醫藥組成物。本發明之組成物及肽抑制劑可針對口服投予根據本文中所述的任何方法、技術、及/或遞送媒劑來製備。再者，所屬技術領域中具有通常知識者將認知到，本發明之肽抑制劑可經修飾或結合至非本文中所揭示、但在所屬技術領域中係熟知且相容於在肽之口服遞送中使用的系統或遞送媒劑。

【0109】　用於口服投予之配方可包含佐劑（例如間苯二酚s及/或非離子界面活性劑，諸如聚氧乙烯油醚及正十六基聚乙烯醚）以人工增加對腸壁之滲透性，及/或酶抑制劑（例如胰蛋白酶抑制劑、氟磷酸二異丙酯(DFF)或抑肽酶(trasylol)）以抑制酵素性降解。在某些實施例中，用於口服投予之固體型劑型肽抑制劑可與至少一種添加劑混合，諸如蔗糖、乳糖、纖維素、甘露醇、繭糖、棉子糖、氫化麥芽糖、葡聚醣、澱粉、瓊脂、藻酸鹽、幾丁質、幾丁聚醣、果膠、黃蓍膠、阿拉伯膠、明膠、膠原蛋白、酪蛋白、白蛋白、合成或半合成聚合物、或甘油酯。這些用於口服投予之配方亦可含有其他類型的添加劑，例如非活性稀釋劑、潤滑劑（諸如硬脂酸鎂、對羥基苯甲酸酯）、保存劑（諸如山梨酸、抗壞血酸、α-生育酚）、抗氧化劑（諸如半胱胺酸）、崩解劑、黏合劑、增稠劑、緩衝劑、pH調整劑、增甜劑、調味劑、或增香劑。

【0110】　在特定態樣中，相容於與本發明之肽抑制劑搭配使用的口服劑型或單位劑型可包括肽抑制劑與非藥物組分或賦形劑，以及其他非可再用材料（可將其視為成分或包裝）之混合物。口服組成物可包括液體劑型、固體劑型、及半固體劑型中之至少一者。在一些實施例中，提供一種口服劑型，包含有效量的肽抑制劑，其中該劑型包含丸劑、錠劑、膠囊、凝膠、糊劑、飲料、

糖漿、軟膏劑、及栓劑中之至少一者。在一些情況下，提供一種口服劑型，其係經設計及配置以達到肽抑制劑在對象小腸及/或大腸中之延緩釋放。

【0111】 錠劑可含有賦形劑、助滑劑、填料、黏合劑、及類似者。水性組成物係製備為無菌形式，且當意欲用於藉由口服投予以外之方式遞送時一般將係等張的。組成物可選地可含有賦形劑，諸如「Handbook of Pharmaceutical Excipients」(1986)中所提出者。賦形劑包括抗壞血酸及其他抗氧化劑、螯合劑（諸如EDTA）、碳水化合物（諸如葡聚醣、羥烷基纖維素、羥烷基甲基纖維素）、硬脂酸、及類似者。組成物之pH在例如約3至約11範圍中。組成物之pH可例如在約5至約7或約7至約10範圍中。

【0112】 本發明之口服醫藥組成物可包含本發明之IL-23R抑制劑，其可包含經設計以延緩IL-23R抑制劑在小腸中之釋放的腸溶衣(enteric coating)。本發明關於一種醫藥組成物，其包含本發明之IL-23R抑制劑及蛋白酶抑制劑（諸如抑肽酶(aprotinin)）在延緩釋放醫藥配方中。醫藥組成物（例如，口服醫藥組成物）可包含可溶於pH約5.0或更高之胃液中的腸溶衣。此類腸溶衣可包含具有可解離羧基之聚合物，諸如纖維素之衍生物，包括羥丙基甲基苯二甲酸纖維素、乙酸苯二甲酸纖維素、及乙酸偏苯三酸纖維素(cellulose acetate trimellitate)，以及類似的纖維素衍生物及其他碳水化合物聚合物。

【0113】 包含本發明之IL-23R抑制劑的口服醫藥組成物包含IL-23R抑制劑，其可包含經設計以保護該醫藥組成物及在對象之下胃腸系統中以受控方式釋放該醫藥組成物的腸溶衣，以避免全身性副作用。除了腸溶衣外，本發明之肽抑制劑可經包封、塗佈、接合、或以其他方式締合在任何口服藥物遞送系統

或組分內。例如在一些實施例中，本發明之IL-23R抑制劑係在脂質載劑系統中提供，該脂質載劑系統包含聚合物水凝膠、奈米粒子、微球、微胞、及其他脂質系統中之至少一者。

【0114】 為了克服本發明之IL-23R抑制劑在小腸中的肽降解，醫藥組成物可包含水凝膠聚合物載劑系統，其中含有本發明之肽抑制劑，藉此水凝膠聚合物保護IL-23R抑制劑免於在小腸及/或大腸中蛋白分解。IL-23R抑制劑可經進一步調配以相容於與載劑系統搭配使用，該載劑系統係經設計以增加溶解動力學及增強肽之腸吸收。這些方法包括使用微脂體、微胞、及奈米粒子以增加肽之胃腸道滲透。

【0115】 各種生物響應性(bioresponsive)系統亦可與一或多種本發明之IL-23R抑制劑組合以提供用於口服遞送之醫藥劑。例如，本發明之IL-23R抑制劑可與生物響應性系統組合使用以提供用於口服投予之治療劑，該生物響應性系統諸如水凝膠及具有氫鍵結基團之黏膜黏著性聚合物（例如，PEG、聚(甲基丙烯)酸[PMAA]、纖維素、Eudragit®、幾丁聚醣及藻酸鹽）。

【0116】 在某些態樣中，醫藥組成物及配方可包括本發明之IL-23R抑制劑及一或多種吸收增強劑、酶抑制劑、或黏膜黏著性聚合物。在一實施例中，吸收增強劑可係腸滲透增強劑。

【0117】 本發明之IL-23R抑制劑可調配於配方媒劑中，諸如例如乳液、微脂體、微球、或奈米粒子。

【0118】 本發明提供一種用於使用本發明之IL-23R抑制劑來治療對象之方法，該IL-23R抑制劑具有延長之半衰期。在一個態樣中，本發明提供一種肽

抑制劑，其具有足以用於每天一次(q.d.)或每天兩次(b.i.d.)給藥治療有效量之至少數小時至一天體外或體內半衰期（例如，當投予至人類對象時）。在某些實施例中，IL-23R抑制劑具有足以用於每週一次(q.w.)給藥治療有效量之三天或更長半衰期。在某些實施例中，IL-23R抑制劑具有足以用於每兩週一次(b.i.w.)或每月一次給藥治療有效量之八天或更長半衰期。在某些實施例中，IL-23R抑制劑係經衍生化或修飾而使得其具有比未經衍生化或未經修飾肽抑制劑長之半衰期。在某些實施例中，IL-23R抑制劑含有一或多個化學修飾以增加血清半衰期。

【0119】 當用於本文中所述的治療或遞送系統中之至少一者中時，可採用呈純形式的本發明之肽抑制劑，其中此類形式存在為醫藥上可接受之鹽形式。

【0120】 本發明之IL-23R抑制劑及組成物的每天總用量可由主治醫師在合理醫療判斷之範疇內決定。針對任何特定對象之特定治療有效劑量水準將取決於各種因素，包括：a)所要治療之病症及病症之嚴重性；b)所採用之特定化合物的活性；c)所採用之組成物、患者之年齡、體重、一般健康狀況、性別、及飲食；d)投予時間、投予途徑、及所採用之肽抑制劑的排出速率；e)治療之持續期間；f)與所採用之特定肽抑制劑組合或同時使用的藥物、及醫療技術領域中熟知之類似因素。

【0121】 在特定實施例中，本發明之IL-23R抑制劑以單次或分次劑量投予至人類或其他哺乳動物主體的每日總劑量可為例如每天0.0001至300 mg/kg體重或每天1至300 mg/kg體重。

【0122】 組成物可便利地以單位劑型存在，且可藉由藥學技術領域中熟知之任何方法來製備。技術及組成一般係見於Remington's Pharmaceutical Sciences (Mack Publishing Co., Easton, PA)。此類方法包括使活性成分與構成一或多種輔助成分之載劑締合的步驟。一般而言，組成物係藉由使活性成分與液體載劑或細分固體載劑或兩者均勻且緊密地締合，接著若有需要則將產物成形來製備。

【0123】 適用於口服投予之組成物可存在為分離之單元，諸如膠囊、藥包、或錠劑，其各含有預定量的活性成分；存在為粉劑或粒劑；存在為水性或非水性液體中之溶液或懸浮液；或存在為水包油液體乳液或油包水液體乳液。活性成分亦可投予為推注、舐劑、或糊劑。活性成分亦可投予為口頰或舌下配方。口頰或舌下配方可包含基質中之活性成分，其釋放活性成分以傳輸穿過口頰及/或舌下膜。口頰或舌下配方可進一步包括速率控制基質，其以預定速率釋放活性化合物以傳輸穿過口頰及/或舌下膜。口頰或舌下配方可進一步包括一或多種選自由下列所組成之群組的化合物：(i)掩味劑、(ii)增強劑、(iii)複合劑、及其混合物；以及(iv)其他醫藥上可接受之載劑及/或賦形劑。增強劑可係滲透增強劑。

【0124】 錠劑係藉由壓製或模製來製造，可選地與一或多種輔助成分一起壓製或模製。壓製錠劑可藉由在合適的機器中壓製呈自由流動形式（諸如粉劑或粒劑）之活性成分來製備，可選地與黏合劑、潤滑劑、惰性稀釋劑、保存劑、表面活性劑或分散劑一起混合。模製錠劑可藉由在合適的機器中模製經惰

性液體稀釋劑潤濕之粉狀活性的混合物來製造。錠劑可選地可經塗佈或刻劃且可選地經調配以提供活性成分自其中緩慢或受控釋放。

V. 腸發炎之非侵入性偵測

【0125】 本發明之IL-23R抑制劑可用於藉由microPET造影來偵測、評估、及診斷腸發炎（其中該肽抑制劑係經螯合基團或可偵測標示標記）而為非侵入性診斷程序之一部分。在某些實施例中，本發明之IL-23R抑制劑係與雙官能性螯合劑偶聯。在某些實施例中，本發明之IL-23R抑制劑係經放射標記的。接著將經標記IL-23R抑制劑口服或經直腸投予至對象。在某些實施例中，IL-23R抑制劑係包括於飲用水中。在攝取IL-23R抑制劑之後，可使用microPET造影來視覺化對象腸道及消化道之發炎。

VI. 治療方法及/或用途

【0126】 本發明關於用於治療罹患與IL-23或IL-23R相關聯之病況或適應症（例如，IL-23/IL-23R傳訊路徑之活化）的對象之方法，其中該方法包含向該對象投予本文中所揭示的IL-23R抑制劑。在一個態樣中，本發明關於一種用於治療罹患特徵在於不適當、失調控、或增加之IL-23或IL-23活性或傳訊之病況或適應症的對象之方法，其包含以足以（部分或完全）抑制該對象中IL-23與IL-23R之結合的量向該個體投予本發明之肽抑制劑。對IL-23與IL-23R之結合的抑制可發生在對象之特定器官或組織中，例如胃部、小腸、大腸/大腸、腸黏膜、固有層、派亞氏斑(Peyer's Patch)、腸繫膜淋巴結、或淋巴管。

【0127】 本發明關於包含提供本文中所述的肽抑制劑至有需要之對象中之方法。有需要之對象可係已遭診斷患有與IL-23/IL-23R相關聯之疾病或病症或已遭判定有發展與IL-23/IL-23R相關聯之疾病或病症的風險之對象。對象可係哺乳動物。對象可尤其係人類。

【0128】 要藉由使用本發明之IL-23R抑制劑的治療來治療之疾病或病症可係自體免疫發炎及相關疾病與病症，諸如多發性硬化症、氣喘、類風濕性關節炎、腸道發炎、發炎性腸疾(IBD)、幼年型IBD、青年期IBD、Crohn氏症、潰瘍性結腸炎、肉瘤病、全身性紅斑性狼瘡、關節黏連性脊椎炎（中軸性脊椎關節炎(axial spondyloarthritis)）、牛皮癬性關節炎、或牛皮癬。特定而言，疾病或病症可係牛皮癬（例如，斑塊型牛皮癬、滴狀牛皮癬、反轉型牛皮癬、膿疱性牛皮癬、掌蹠膿疱症、尋常牛皮癬、或紅皮性牛皮癬）、異位性皮膚炎、痤瘡異位(acne ectopica)、潰瘍性結腸炎、Crohn氏症、乳糜瀉（非熱帶性口瘡）、與血清反應陰性關節病變相關聯之腸病變、顯微鏡性結腸炎、膠原性結腸炎、嗜伊紅性胃腸炎/食道炎、與放射或化學療法相關聯之結腸炎、與如在白血球黏附分子缺乏症-1中的先天免疫性病症相關聯之結腸炎、慢性肉芽腫疾病、肝糖貯積病第1b型、Hermansky-Pudlak氏症候群、Chediak-Higashi氏症候群、Wiskott-Aldrich氏症候群、囊炎、直腸結腸切除術及回腸肛管吻合術後產生之囊炎(pouchitis resulting after proctocolectomy and ileoanal anastomosis)、胃腸癌、胰臟炎、胰島素依賴性糖尿病、乳腺炎、膽囊炎、膽管炎、原發性膽汁性肝硬化、病毒相關腸病變、膽管週圍炎、慢性支氣管炎、慢性竇炎、氣喘、眼色素層炎、或移植物抗宿主疾病。

【0129】 本發明關於一種IL-23R抑制劑用於治療對象中之發炎性疾病之方法或用途，其包括向該對象投予治療有效量的本發明之IL-23R抑制劑或其醫藥上可接受之溶劑合物或鹽、或本文中所揭示的包含本發明之IL-23抑制劑的組成物。在一些態樣中，本發明提供一種治療對象中之發炎性疾病之方法，其包括向該對象投予治療有效量的本發明之IL-23R抑制劑或其醫藥上可接受之溶劑合物或鹽、或本發明之組成物。適用於使用本發明之化合物或其醫藥上可接受之鹽、或組成物來治療的發炎性疾病可包括但不限於發炎性腸疾(IBD)、Crohn氏症(CD)、潰瘍性結腸炎(UC)、牛皮癬(PsO)、或牛皮癬性關節炎(PsA)、及類似者。所要治療之發炎性疾病可係發炎性腸疾(IBD)、Crohn氏症、或潰瘍性結腸炎。所要治療之發炎性疾病可選自牛皮癬、或牛皮癬性關節炎。所要治療之發炎性疾病可係牛皮癬。所要治療之發炎性疾病可係牛皮癬性關節炎。所要治療之發炎性疾病可係IBD。

【0130】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予本文中所揭示的IL-23R抑制劑（例如，式(I)至(XX)或表1A至1H中任一者之肽抑制劑或IL-23R）。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0131】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式(I)之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係

Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0132】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式I之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0133】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式II之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0134】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式III之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0135】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式IV之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係

Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0136】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式V之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0137】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式VI之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0138】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式VII之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0139】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式VIII之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係

Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0140】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式IX之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0141】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式X之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0142】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XI之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0143】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XII之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係

Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0144】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XIII之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0145】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XIV之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0146】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XV之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0147】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XVI之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係

Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0148】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XVII之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0149】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XVIII之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0150】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XIX之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0151】 本發明關於用於治療有需要之對象中的發炎性疾病之方法，其包含向該對象投予式XX之IL-23R抑制劑。發炎性疾病可係IBD、Crohn氏症、或潰瘍性結腸炎。在態樣中，IBD可係潰瘍性結腸炎。在一態樣中，IBD可係

Crohn氏症。在一態樣中，發炎性疾病可係牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0152】 本發明關於抑制IL-23結合至細胞上之IL-23R之方法，其包含使該IL-23R與本文中所揭示的受體之肽抑制劑接觸。細胞可係哺乳動物細胞。方法可在體外或體內執行。對結合之抑制可藉由所屬技術領域中已知之各種常規實驗方法及檢定來判定。

【0153】 本發明關於一種選擇性抑制對象中（例如，有需要之對象中）的IL-23或IL-23R傳訊（IL-23與IL-23R之結合）之方法，其包含向該對象提供本文中所述的IL-23R之肽抑制劑。本發明包括及提供一種選擇性抑制對象（例如，有需要之對象）之胃腸道中的IL-23或IL-23R傳訊（或IL-23與IL-23R之結合）之方法，其包含藉由口服投予向該對象提供本發明的IL-23R之肽抑制劑。胃腸組織（例如，小腸或大腸）對所投予肽抑制劑之暴露可比血中暴露（水準）大上至少10倍、至少20倍、至少50倍、或至少100倍。在特定實施例中，本發明包括一種選擇性抑制對象（例如，有需要之對象）之胃腸道中的IL23或IL23R傳訊（或IL23與IL23R之結合）之方法，其包含向該對象提供肽抑制劑，其中該肽抑制劑不會阻斷IL-6與IL-6R之間的交互作用或拮抗IL-12傳訊路徑。在一進一步相關實施例中，本發明包括一種抑制胃腸發炎及/或嗜中性球浸潤至胃腸之方法，其包含向有需要之對象提供本發明之肽抑制劑。在一些實施例中，本發明包含方法向對象（例如，有需要之對象）提供本發明之肽抑制劑（亦即，第一治療劑）與第二治療劑之組合。在某些實施例中，第二治療劑係在肽抑制劑投予至對象之前/同時/之後向對象提供。在特定實施例中，第二治

療劑係消炎劑。在某些實施例中，第二治療劑係非類固醇型消炎藥物、類固醇、或免疫調節劑。在某些實施例中，方法包含向對象投予第三治療劑。在某些實施例中，第二治療劑係結合IL-23或IL-23R之抗體。

【0154】 本發明關於抑制細胞之IL-23傳訊之方法，其包含使IL-23R與本文中所述的肽抑制劑接觸。在某些實施例中，細胞係哺乳動物細胞。在特定實施例中，方法係在體外或體內進行。在特定實施例中，IL-23傳訊之抑制可藉由測量細胞中之phospho-STAT3水準變化來判定。

【0155】 在任何前述方法中，向對象之IL-23R抑制劑投予可口服進行，但不排除其他投予途徑。其他投予途徑包括但不限於腸胃外、皮下、靜脈內、肌內、腹膜內、經皮、局部、口頰、或經眼途徑。本文中所述的肽抑制劑或IL-23R（例如，式(I)至式(XX)或任何表1A至1H之化合物、或其鹽或溶劑合物）投予至對象之劑量可由所屬技術領域中具有通常知識者考量所要治療之疾病或病況（包括其嚴重性）、及多種因素（包括年齡體重、性別、及類似者）來決定。例示性劑量範圍包括但不限於約1 mg至約1000 mg、或約1 mg至約500 mg、約1 mg至約100 mg、約10 mg至約50 mg、約20 mg至約40 mg、或約20 mg至約30 mg。本文中所述的肽抑制劑或IL-23R之劑量範圍可係約600 mg至約1000 mg。本文中所述的肽抑制劑或IL-23R之劑量範圍可係約300 mg至約600 mg。本文中所述的肽抑制劑或IL-23R之劑量範圍可係約5 mg至約300 mg。本文中所述的肽抑制劑或IL-23R之劑量範圍可係約25 mg至約150 mg。本文中所述的肽抑制劑或IL-23R之劑量範圍可係約25 mg至約100 mg。本文中所述的肽抑制劑或IL-23R可以約1 mg至約100 mg之劑量範圍存在。本文中所述的肽抑制劑

或IL-23R可以約20 mg至約40 mg之劑量範圍存在。本文中所述的肽抑制劑或IL-23R可以約20 mg至約30 mg之劑量範圍存在。

VII. 某些態樣

【0156】 下列態樣說明本發明。這些態樣不意欲限制本發明之範疇，而是對所屬技術領域中具有通常知識者提供指引以製備及使用本發明之化合物、組成物、及方法。雖然描述了本發明之特定態樣，所屬技術領域中具有通常知識者將認知到，可作出各種改變及修改而不偏離本發明之精神與範疇。

【0157】 1.一種介白素-23受體之雙環肽抑制劑，其包含式I之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-X11-X12-X13-N-X15-meG-R2 (I)

其中：

R1係7Ahp、6Ahx、5Ava、PEG2、AEEP、或AEEP(Ns)；

X4係Pen、Abu、aMeC、hC、或C；

X5係N或K(PEG2PEG2gEC18OH)；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、

7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K(Ac)、Q、K(NMeAc)、K(PEG2PEG2gEC18OH)、dK(Ac)、dQ、dK(NMeAc)、或dK(PEG2PEG2gEC18OH)；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP或aMeK；

X13係E、dE、hE、dhR、D、dD、hSer、或dhSer；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；及

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及R1與X13之間的第二醯胺鍵或硫醚鍵（在pFS與Dap(pF)之間）而環化。

【0158】 2.如態樣1所述之雙環肽抑制劑，其中X11係2Nal。

【0159】 3.如態樣1至2中任一者所述之雙環肽抑制劑，其中X7 W或7MeW。

【0160】 4.如態樣1至3中任一者所述之雙環肽抑制劑，其中X15係3Pya、H、3MeH、或F。

【0161】 5.一種介白素-23受體之雙環肽抑制劑，其包含式II之胺基酸序列

R1- X3-X4-X5-T-X7-K(Ac)-X9-AEF-X11-THP-X13-N-X15-X16-R2 (II)

其中：

R1係GABA、pFS、bAla、或(HOC16gEPEG2PEG2)orn；

X3係dR、G、dK(PEG2PEG2gEC18OH) R、或K(PEG2PEG2gEC18OH)；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、或Q；

X7係7MeW、或W；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、dD、Dap(pF(6))、或dDap(pF(6))；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、

5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedYK、dK、NMeY、NMedY、N、dH、dN、dL、Aib、L、或不存在；

X16係meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、D、dD、或不存在；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及R1與X13之間的第二醯胺或硫醚（在pFS與Dap(pF(6)之間）鍵而環化。

【0162】 6.如態樣5所述之雙環肽抑制劑，其中X11係2Nal。

【0163】 7.如態樣5至6中任一者所述之雙環肽抑制劑，其中X15係3Pya或THP。

【0164】 8.如態樣5至7中任一者所述之雙環肽抑制劑，其中X16係meG或不存在。

【0165】 9.一種介白素-23受體之雙環肽抑制劑，其包含式III之胺基酸序列

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-X12-X13-N-X15-X16-R2 (III)

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、5cpa、cPEG3aCO、或-H；

X3係R5H、S5H、R6H、S6H、R7H、S7H、K、dK、Orn、d-Orn、Dap、dDap、Dab(COCH2)、dDab(COCH2)、dhE、hE、hK、dhK；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、Q、或N(N(Me)2)，

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K(Ac)、Q、K(NMeAc)、dK(Ac)、dQ、或dK(NMeAc)；

X9係Pen、Abu、aMeC、hC、或C；

X10係AEF或TMAPF；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP、Acpx、或aMeK；

X13係R5H、R6H、R7H、S5H、S6H、S7H,C、E、hE、KNMe、dC、dE、dhE、或dKNMe；

X15係3Pya、bAla、THP、dK、或aMePhe；

X16係meG、NMedY、或不存在；

R2係-NH_2、N(H)C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X3與X13之間的第二醯胺、硫醚、或脂族（由環合歧化「RCM」反應而產生）鍵而環化。

【0166】 10.如態樣9所述之雙環肽抑制劑，其中X11係2Nal。

【0167】 11.如態樣9至10中任一者所述之雙環肽抑制劑，其中：X7係W或7MeW。

【0168】 12.一種介白素-23受體之雙環肽抑制劑，其包含式IV之胺基酸序列

R1-X3-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-X16- R2 (IV)

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、-H、7Ahp、6Ahx、5Ava、或GABA；

X3係dR、R、d-Orn、Orn、或不存在；

X4係Pen、Abu、aMeC、hC、或C；

X5係Q、或N；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係Q、K(Ac)、dQ、dK(Ac)；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、aMeE、Aad、hE、K、dE、dAad、dhE、或dK；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；

X16係meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、D、dD、或不存在；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及AEF與X13之間的第二醯胺鍵而環化。

【0169】 13.如態樣12所述之雙環肽抑制劑，其中X11係2Nal。

【0170】 14.如態樣12至13中任一者所述之雙環肽抑制劑，其中X15係bAla、3Pya、THP、或NMedY。

【0171】 15.如態樣12至14中任一者所述之雙環肽抑制劑，其中X16係meG或不存在。

【0172】 16.一種介白素-23受體之雙環肽抑制劑，其包含式V之胺基酸序列

R1-X4-N-T-X7-X8-X9-F4CONH2-X11-THP-X13-N-3Pya-meG-R2 (V)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X4係Pen、Abu、aMeC、hC、或C；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K或dK；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、dD；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X8與X13之間的第二醯胺鍵而環化。

【0173】 17.如態樣16所述之雙環肽抑制劑，其中X11係2Nal。

【0174】 18.如態樣16至17中任一者所述之雙環肽抑制劑，其中X7係W或7MeW。

【0175】 19.一種介白素-23受體之雙環肽抑制劑，其包含式VI之胺基酸序列

R1-X3-A-X5-T-X7-X8-A-AEF-X11-THP-X13-N-X15-R2 (VI)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係K、dK、hdK、E、dE、D、dD；

X5係E、dE、D、dD；

X7係W或7MeW；

X8係K(Ac)或dK(Ac)；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係K(Ac)或dK(Ac)；

X15係K、dK、dH、hdK E、dE、D、dD；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X5與X10之間的第一醯胺鍵、及X3及X15之間的第二醯胺鍵而環化。

【0176】 20.如態樣19所述之雙環肽抑制劑，其中X11係2Nal。

【0177】 21.如態樣19至20中任一者所述之雙環肽抑制劑，其中X7係W或7MeW。

【0178】 22.如態樣19至21中任一者所述之雙環肽抑制劑，其中X15係K或dK。

【0179】 23.一種介白素-23受體之雙環肽抑制劑，其包含式VII之胺基酸序列

R1-X3-X4-N-T-X7-K(Ac)-X9-X10-X11-THP-X13-N-3Pya-X16-R2 (VII)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係D、dK、E、dDap、dD、K、dE、或Dap；

X4係Pen、Abu、aMeC、hC、或C；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X9係Pen、Abu、aMeC、hC、或C；

X10係AEF、F4CONH2、或F4OMe；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係K(Ac)或dK(Ac)；

X16係K、dK、E、dE、R、dR、D、dD、或不存在；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X3與X16之間的第二醯胺鍵而環化。

【0180】 24.如態樣23所述之雙環肽抑制劑，其中X11係2Nal。

【0181】 25.如態樣23至24中任一者所述之雙環肽抑制劑，其中X7係W或7MeW。

【0182】 26.如態樣23至25中任一者所述之雙環肽抑制劑，其中X16係K、dK、E、dE、R、dR、D、或dD。

【0183】 27.一種介白素-23受體之雙環肽抑制劑，其包含式VIII之胺基酸序列

R1-X4-X5-X6-X7-X8-X9-X10-X11-X12-X13-X14-3Pya-meG-R2 (VIII)

其中：

R1係選自-H、CF3CO、5cpaCO、cPEG3aCO、C_1至C_4烷基C(O)-、或經氰基、Cl、F所取代之C_1至C_4烷基C(O)-、AcMorph、或PEG12OMe；

X4係Pen、Abu、aMeC、hC、或C；

X5係選自E、K、Dap、或K(NMe),；

X6係選自T、L、I；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係選自K(Ac)、KPeg12、KAcMor、Q(N(Me)2)、K(Me)3、hK(Me)3；K(NMeAc)、K(mPEG12)、A、或Q、dKAc、dKPeg12、dKacMor、dQ(N(Me)2)、dK(Me)3、dhK(Me)3、dK(NMeAc)、dK(mPEG12)、dA、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X10係選自AEF、AEF(NMe)、K、或E；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係選自THP、aMeLeu、或A；

X13係選自K(Ac)、A、L、K(NMeAc)、Q(N(Me)2))、K(Me)3、E、dK(Ac)、dA；dL、dK(NMeAc)、dQ(N(Me)2))、dK(Me)3、或dE；

X14係選自A、L、N或S；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X5與X10之間的第二醯胺或烷基胺（在K(NMe)及AEF之間）鍵而環化。

【0184】 28.如態樣27所述之雙環肽抑制劑，其中X11係2Nal。

【0185】 29.如態樣27至28中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、7PhW、dW、d7MeW、或d7PhW。

【0186】 30.一種介白素-23受體之雙環肽抑制劑，其包含式IX之胺基酸序列

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-THP-X13-X14-3Pya-meG-R2 (IX)

其中

R1係選自-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、或HOC18gEPEG2PEG2CO；

X3係R、dR、K、dK、dK(Me)3、K(Me)3、dK(PEG2PEG2gEC18OH)、或K(PEG2PEG2gEC18OH)；

X4係Pen、Abu、aMeC、hC、或C；

X5係選自E；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係選自K(Ac)或dK(Ac)；

X9係Pen、Abu、aMeC、hC、或C；

X10係選自AEF或AEF(NMe)；X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係選自K(Ac)、E、dK(Ac)、或dE；

X14係選自N；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X5與X10之間的第二醯胺鍵而環化。

【0187】 31.如態樣30所述之雙環肽抑制劑，其中X11係2Nal。

【0188】 32.如態樣30至31中任一者所述之雙環肽抑制劑，其中X7係W或7MeW。

【0189】 33.一種介白素-23受體之雙環肽抑制劑，其包含式X之胺基酸序列

X5-T-X7-X8-A-AEF-X11-THP-X13-3Pya (X)

其中：

X5係E、dE、D、或dD；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K(Ac)或dK(Ac)；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；且

X13係K(Ac)、dK(Ac)、或不存在；且

其中該介白素-23受體之雙環肽抑制劑係藉由X5與AEF之間的第一醯胺鍵、及X5之胺基端與3Pya之羧基端之間的第二環化而環化。

【0190】 34.如態樣33所述之雙環肽抑制劑，其中X11係2Nal。

【0191】 35.如態樣33至34中任一者所述之雙環肽抑制劑，其中X7係W或7MeW。

【0192】 36.一種介白素-23受體之雙環肽抑制劑，其包含式XI之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-R2 (XI)

其中：

R1係7Ahp、6Ahx、5Ava、或AEEP；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、或Q、

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K(Ac)、Q、dK(Ac)、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、或dD；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及R1與X13之間的第二醯胺鍵而環化。

【0193】 37.如態樣36所述之雙環肽抑制劑，其中X11係2Nal。

【0194】 38.如態樣36至37中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、dW、或d7MeW。

【0195】 39.如態樣36至38中任一者所述之雙環肽抑制劑，其中X15係3Pya THP、NMeY、或NMedY。

【0196】 40.一種介白素-23受體之雙環肽抑制劑，其包含式XII之胺基酸序列

R1-X4-N-T-X7-X8-X9-AEF-2Nal-X12-X13-N-3Pya-X16-R2 (XII)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X4係Pen、Abu、aMeC、hC、或C；

X6係3Hyp、T、或3OHPro；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係R5H、R6H、R7H、S5H、S6H、或S7H；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係R5H、R6H、R7H、S5H、S6H、或S7H；

X13係K、dK、KAc、dKAc、E、dE、D、或dD；

X16係meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、D、dD、或不存在；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X8與X12之間的第二醯胺或脂族（由環合歧化「RCM」反應而產生）鍵而環化。

【0197】 41.如態樣40所述之雙環肽抑制劑，其中X11係2Nal。

【0198】 42.如態樣40至41中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、dW、或d7MeW。

【0199】 43.如態樣36至39中任一者所述之雙環肽抑制劑，其中X16係meG或不存在。

【0200】 44.一種介白素-23受體之雙環肽抑制劑，其包含式XIII之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-2Nal-THP-X13-N-X15-X16-X17-R2 (XIII)

其中：

R1係7Ahp、6Ahx、5Ava、或AEEP；

X4係Pen、Abu、aMeC、hC、或C；，

X5係N，

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K(Ac)、Q、dK(Ac)、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、或dD；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、L、或不存在；

X16係meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、

R、dR、D、dD、NMeK(PEG2PEG2gEC18OH)、

dNMeK(PEG2PEG2gEC18OH)、或不存在；

X17係不存在、K(PEG2PEG2gEC18OH)、或dK(PEG2PEG2gEC18OH)，且

R2係-NH_2、N(H)C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及R1與X13之間的第二醯胺鍵而環化。

【0201】 45.如態樣44所述之雙環肽抑制劑，其中X11係2Nal。

【0202】 46.如態樣44至45中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、dW、或d7MeW。

【0203】 47.如態樣44至46中任一者所述之雙環肽抑制劑，其中X15係3Pya、THP、NMeY、或NMedY。

【0204】 48.如態樣44至47中任一者所述之雙環肽抑制劑，其中X16係meG或不存在。

【0205】 49.一種介白素-23受體之雙環肽抑制劑，其包含式XIV之胺基酸序列

R1-X3-X4-X5-X6-X7-X8-X9-AEF-X11-X12-X13-N-X15-X16-R2-R3 (XIV)

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係dK、或K；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、Q、或Dap，

X6係T或K；

X7係W、7MeW、dW、或d7MeW；

X8係K(Ac)、Q、dK(Ac)、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP、或aMeL；

X13係E、K(Ac)、dE、D、dD、或dK(Ac)；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；

X16係meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、D、dD、或不存在；

R2係-NH2、或–NH-R3；且

R3係PEG4 (-HN[(CH2)2O]4(CH2)2CO-)、PEG4DA (-OC[(CH2)2O]4(CH2)2CO-)、或C6-C20飽和或不飽和二羧酸（例如，1,10-癸二酸、1,12-十二烷二酸、1,14-十四烷二酸、或1,16-十六烷二酸）

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及AEF與R3之間的第二醯胺鍵而環化。

【0206】 50.如態樣49所述之雙環肽抑制劑，其中X11係2Nal或3Quin或X11係2 Nal。

【0207】 51.如態樣49至50中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、dW、或d7MeW。

【0208】 52.如態樣49至51中任一者所述之雙環肽抑制劑，其中X15係H、N、dH、或dN。

【0209】 53.一種介白素-23受體之雙環肽抑制劑，其包含式XV之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-R2 (XV)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X4係Pen、Abu、aMeC、hC、或C；

X5係E、dE、D、或dD；

X7係W、7MeW、dW、或d7MeW；

X8係K(Ac)、Q、dK(Ac)、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、K(Ac)、dE、D dDor dK(Ac)；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及AEF與X5之間的第二醯胺鍵而環化。

【0210】 54.如態樣53所述之雙環肽抑制劑，其中X11係2Nal。

【0211】 55.如態樣53至54中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、dW、或d7MeW。

【0212】 56.如態樣53至55中任一者所述之雙環肽抑制劑，其中X15係dL、Aib、或L。一種介白素-23受體之雙環肽抑制劑，其包含式XVI之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-X16-R2 (XVI)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X4係Pen、Abu、aMeC、hC、或C；

X5係N、或L；

X7係W、7MeW、dW、或d7MeW；

X8係K(Ac)、或dK(Ac)；

X9係Pen、Abu、aMeC、hC、或C；

X10係F4CONH2、4AmF、或F4OMe；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dK、dDap、K、Dap、dE；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；

X16係dK、dD、dE、Aib、G、bAla、meG、K、D、E、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、R、dR、或不存在且

R2係不存在或-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X13與X15、X16、R2、或當R2係不存在時X15或X16之羧基端之間的第二醯胺鍵而環化。

【0213】 57.如態樣56所述之雙環肽抑制劑，其中X11係2Nal。

【0214】 58.如態樣56至57中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、dW、或d7MeW。

【0215】 59.如態樣56至58中任一者所述之雙環肽抑制劑，其中X15係dL、Aib、或L及/或X16係dK、dD、dE、Aib、G、bAla、meG或dK。

【0216】 60.一種介白素-23受體之雙環肽抑制劑，其包含式XVII之胺基酸序列

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-THP-X13-X14-X15-X16-R2 (XVII)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係Orn、E、dOrn、或dE；

X4係Pen、Abu、aMeC、hC、或C；

X5係N；

X7係W、7MeW、dW、或d7MeW；

X8係K(Ac)、或dK(Ac)；

X9係Pen、Abu、aMeC、hC、或C；

X10係F4CONH2或AEF；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、K(Ac)、dK(Ac)、或dE；，

X14係N或不存在；

X15係3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、d3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、N、dH、dN、dL、Aib、L、或不存在；

X16係4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、D、dD、dDap、meG、Dap、或不存在；且

R2係不存在或-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X3與X10、X13、或X16中之一者之間的第二醯胺鍵而環化。

【0217】 61.如態樣60所述之雙環肽抑制劑，其中X11係2Nal。

【0218】 62.如態樣60至61中任一者所述之雙環肽抑制劑，其中X7係W、7MeW、dW、或d7MeW。

【0219】 63.如態樣60至62中任一者所述之雙環肽抑制劑，其中X15係3Pya或不存在。

如態樣60至63中任一者所述之雙環肽抑制劑，其中X16係dDap、meG、Dap、或dMeG。

【0220】 64.一種介白素-23受體之三環肽抑制劑，其包含式XVIII之胺基酸序列

R1-X3-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-3Pya-meG-X17-R2 (XVIII)

其中：

R1係-H、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係K、dK、E、dE；

X4係Pen、Abu、aMeC、hC、或C；

X5係E、dE、D、或dD；

X7係W或7MeW；

X8係K(Ac)或dK(Ac)；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係K(Ac)或dK(Ac)；

X17係E、dE、K、dK、D、或dD；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之三環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、第二醯胺鍵之間的X3及X17、及X5與AEF之間的第三醯胺鍵而環化。

【0221】 65.如態樣64所述之雙環肽抑制劑，其中X11係2Nal。

【0222】 66.如態樣64至65中任一者所述之雙環肽抑制劑，其中X7係W或7MeW。

【0223】 67.一種介白素-23受體之雙環肽抑制劑，其包含式XIX之胺基酸序列

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-X12-X13-X14-X15-X16-X17-R2 (XIX)

其中：

R1係7Ahp、6Ahx、5Ava、PEG2、AEEP、AEEP(Ns)、GABA、pFS、bAla、PEG2PEGE2gEC16OH、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、5cpaCO、cPEG3aCO、或-H

X3係dR、R、G、R5H、R6H、R7H、S5H、S6H、S7H、K、dK、Orn、dOrn、Dap、dDap、Dab、dDab、Dab(COCH2)、dDab(COCH2)、hE、dhE、hK、dhK,dK(Me)3、K(Me)3、dK(PEG2PEG2gEC18OH)、K(PEG2PEG2gEC18OH)、或不存在；

X4係Pen、Abu、aMeC、或C；

X5係N、Q、N(N(Me)2)、或K(PEG2PEG2gEC18OH)；

X7係W、7PhW、或7MeW；

X8係K(Ac)、dK(Ac)、Q、dQ、K(NMeAc)、dK(NmeAc)、K(PEG2PEG2gEC18OH)、或dK(PEG2PEG2gEC18OH)；

X9係Pen、Abu、aMeC、或C；

X10係AEF、或TMAPF；

X11係2Nal；

X12係THP、Acpx、或aMeK；

X13係E、dE、hE、dhE、aMeE、d-aMeE、D、dD、Aad、dAadK、dK、hSer、dhSer、Dap(pF)、R5H、R6H、R7H、S5H、S6H、S7H、C、dC、K(NMe)、或dK(NMe)；

X14係N或不存在；

X15係3Pal、H、dH、3MeH、3MedH、F、dF、aMeF、aMedF、THP、bAla、NMeTyr、NMedY、K、dK；

X16係meG、NMedY、NMeK(PEG2PEG2gEC18OH)、NMedK(PEG2PEG2gEC18OH)、或不存在；

X17係不存在或K(PEG2PEG2gEC18OH)；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及R1與X13之間或X3與X13之間的第二醯胺、脂族（由環合歧化「RCM」反應而產生）、烷基胺、或硫醚鍵聯而環化。

【0224】 68.一種介白素-23受體之雙環肽抑制劑，其包含式XX之胺基酸序列

R1-X3-X4-X5-X6-X7-X8-X9-X10-X11-X12-X13-X14-X15-X16-R2 (XX)

其中：

R1係選自CF3CO、5cpaCO、cPEG3aCO、-H、C1至C4烷基C(O)-、或經氰基、Cl、或F所取代之C1至C4烷基C(O)-；

X3係R、dR、K、dK、K(Me)3、dK(Me)3、hK(Me)3、dhK(Me)3、或不存在

X4係Pen、Abu、或C；

X5係選自E、D、K、K(Ac)、Dap、或K(NMe)、K(NNs)；

X6係選自T、L；

X7係選自W、7MeW、7PhW；

X8係選自K(Ac)、dK(Ac)、hK(Me)3、dhK(Me)3、K(Me)3、dK(Me)3、K(NMeAc)、dK(NMeAc)、Q(N(Me)2)、KPeg12、dKPeg12、KAcMor、A、Q、dKacMor、dQ(N(Me)2)、K(mPEG12)、dA、dQ、或dK(mPEG12)；

X9係Pen、Abu、或C；

X10係選自AEF、AEF(NMe)、F4CONH2、或F4OMe；

X11係2Nal、或A；

X12係選自THP、aMeLeu、或A；，

X13係選自E、dE、K(Ac)、dK(Ac)、K(Me)3、dK(Me)3、K(NMeAc)、dK(NMeAc)、Q(N(Me)2)、dQ(N(Me)2)、A、dA、L、或dL；

X14係選自L、N、或S；

X15係選自3Pal、L、dL、或Aib

X16係選自meG；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C1-C_4烷基)、-N(C_1-C_4烷基)$_2$，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及X5與X10之間的第二醯胺或烷基胺鍵聯而環化。

【0225】 69.如態樣1至68中任一者所述之介白素-23受體之肽抑制劑，其中當：X4係Pen、aMeC、hC、或C時，且當X9係Pen、aMeC、hC、或C時，則X4及X9形成雙硫鍵。

【0226】 70.如態樣1至68中任一者所述之介白素-23受體之肽抑制劑，其中當：X4係Pen或C時，且當X9係Pen或C時，則X4及X9形成雙硫鍵。

【0227】 71.如態樣1至68中任一者所述之介白素-23受體之肽抑制劑，其中當：X4係Abu時且當X9係Pen、aMeC、hC、或C時，則X4及X9形成硫醚鍵。

【0228】 72.如態樣1至68中任一者所述之介白素-23受體之肽抑制劑，其中當：X4係Pen、aMeC、hC、或C時，且當X9係Abu時，則X4及X9形成硫醚鍵。

【0229】 73.如態樣1至72中任一者所述之介白素-23受體之肽抑制劑，其中X7係W。

【0230】 74.如態樣1至72中任一者所述之介白素-23受體之肽抑制劑，其中X7係7MeW。

【0231】 75.如態樣1至74中任一者所述之介白素-23受體之肽抑制劑，其中X11係2Nal。

【0232】 76.如態樣1至75中任一者所述之介白素-23受體之肽抑制劑，其中當X15係存在時，其係3Pya。

【0233】 77.如態樣1至76中任一者所述之介白素-23受體之肽抑制劑，其中當X16係存在時其係meG。

【0234】 78.如態樣1至77中任一者所述之介白素-23受體之肽抑制劑，其中D胺基酸僅存在於

(i) 存在於該抑制劑中的位置 X3、X5、X6、X8 及 X13 中之一或多者、及可選地位置 X1 至 X2、X4、X7、X9 至 X12、X14 至 X18 中之一者；或

(ii) 存在於該抑制劑中的位置 X3、X8 及 X13 中之一或多者、及可選地位置 X1 至 X2、X4 至 X7、X9 至 X12、X14 至 X18 中之一者。

【0235】 79.如態樣1至77中任一者所述之介白素-23受體之肽抑制劑，其中D胺基酸僅存在於

(i) 存在於該抑制劑中的 X3、及可選地位置 X1 至 X2、X4 至 X18 中之一者；或

(ii) 存在於該抑制劑中的位置 X3、及 X8 中之一者、及可選地位置 X1 至 X2、X4 至 X7、X9 至 X18 中之一者。

【0236】 80.如態樣1至77中任一者所述之介白素-23受體之肽抑制劑，其中該抑制劑僅在出現於本文中所陳述的IL-23R抑制劑之位置X1至X18中之一或二者包含該D-異構形式之胺基酸。

【0237】 81.如態樣1至77中任一者所述之介白素-23受體之肽抑制劑，其中該抑制劑僅在出現於本文中所陳述的IL-23R抑制劑之位置X1至X18中之三或四者包含該D-異構形式之胺基酸。

【0238】 82.如態樣1至77中任一者所述之介白素-23受體之肽抑制劑，其中該抑制劑僅在出現於本文中所陳述的IL-23R抑制劑之位置X1至X18中之五或六者包含該D-異構形式之胺基酸。

【0239】 83.一種介白素-23受體之肽抑制劑、或其醫藥上可接受之鹽、溶劑合物、或形式，其具有表1A、表1B、表1C、表1D、表1E、表1F、表1G、或表1H中之化合物的結構。

【0240】 84.一種介白素-23受體之肽抑制劑、或其醫藥上可接受之鹽、溶劑合物、或形式，其具有表1A或表B中之化合物的結構。

【0241】 85.一種介白素-23受體之肽抑制劑、或其醫藥上可接受之鹽、溶劑合物、或形式，其具有表1C或表1D中之化合物的結構。

【0242】 86.一種介白素-23受體之肽抑制劑、或其醫藥上可接受之鹽、溶劑合物、或形式，其具有表1E或表1F中之化合物的結構。

【0243】 87.一種介白素-23受體之肽抑制劑、或其醫藥上可接受之鹽、溶劑合物、或形式，其具有表1G或表1H中之化合物的結構。

【0244】 88.任何前述態樣所述之介白素-23受體之肽抑制劑，其中該介白素-23受體係人類介白素受體，例如NCBI參考序列：NP_653302.2。

【0245】 89.一種醫藥組成物，其包含：

(i) 根據態樣 1 至 88 中任一者之介白素-23 受體之肽抑制劑介白素-23 受體或其醫藥上可接受之鹽、溶劑合物、或形式，及

(ii) 醫藥上可接受之載劑、賦形劑、或稀釋劑。

【0246】 90.一種醫藥組成物，其包含：

(i) 根據態樣 1 至 79 中任一者之介白素-23 受體之肽抑制劑介白素-23 受體或其醫藥上可接受之鹽、溶劑合物、或形式，及

(ii) 醫藥上可接受之載劑、賦形劑、或稀釋劑。

【0247】 91.一種醫藥組成物，其包含：

(i) 根據態樣 80 或 81 中任一者之介白素-23 受體之肽抑制劑介白素-23 受體或其醫藥上可接受之鹽、溶劑合物、或形式，及

(ii) 醫藥上可接受之載劑、賦形劑、或稀釋劑。

【0248】 92.一種醫藥組成物，其包含：

(i) 根據態樣 82 或 83 中任一者之介白素-23 受體之肽抑制劑介白素-23 受體或其醫藥上可接受之鹽、溶劑合物、或形式，及

(ii) 醫藥上可接受之載劑、賦形劑、或稀釋劑。

【0249】 93.一種醫藥組成物，其包含：

(i) 根據態樣 84 或 85 中任一者之介白素-23 受體之肽抑制劑介白素-23 受體或其醫藥上可接受之鹽、溶劑合物、或形式，及

(ii) 醫藥上可接受之載劑、賦形劑、或稀釋劑。

【0250】 94.一種醫藥組成物，其包含：

(i) 根據態樣 86 或 87 中任一者之介白素-23 受體之肽抑制劑介白素-23 受體或其醫藥上可接受之鹽、溶劑合物、或形式，及

(ii) 醫藥上可接受之載劑、賦形劑、或稀釋劑。

【0251】 95.一種根據態樣1至88中任一者之介白素-23受體之肽抑制劑用於製備藥劑之用途。

【0252】 96.一種根據態樣1至88中任一者之介白素-23受體之肽抑制劑、或根據態樣89至94中任一者之醫藥組成物用於製備用於治療發炎性病症或自體免疫發炎性病症之藥劑之用途。

【0253】 97.如請求項18所述用於製備用於治療自體免疫發炎及相關疾病與病症之藥劑之用途，該等疾病與病症包括但不限於：多發性硬化症、氣喘、類風濕性關節炎、腸道發炎、發炎性腸疾(IBD)、幼年型IBD、青年期IBD、

Crohn氏症、潰瘍性結腸炎、乳糜瀉(非熱帶性口瘡)、顯微鏡性結腸炎、膠原性結腸炎、嗜伊紅性胃腸炎/食道炎、與放射或化學療法相關聯之結腸炎、與如在白血球黏附分子缺乏症-1中的先天免疫性病症相關聯之結腸炎、肉瘤病、全身性紅斑性狼瘡、關節黏連性脊椎炎（中軸性脊椎關節炎）、牛皮癬性關節炎、牛皮癬（例如，斑塊型牛皮癬、滴狀牛皮癬、反轉型牛皮癬、膿疱性牛皮癬、掌蹠膿疱症、尋常牛皮癬、或紅皮性牛皮癬）、異位性皮膚炎、痤瘡異位、與血清反應陰性關節病變相關聯之腸病變、慢性肉芽腫疾病、肝糖貯積病第1b型、Hermansky-Pudlak氏症候群、Chediak-Higashi氏症候群、Wiskott-Aldrich氏症候群、囊炎、直腸結腸切除術及回腸肛管吻合術後產生之囊炎、胃腸癌、胰臟炎、胰島素依賴性糖尿病、乳腺炎、膽囊炎、膽管炎、原發性膽汁性肝硬化、病毒相關腸病變、膽管週圍炎、慢性支氣管炎、慢性竇炎、氣喘、眼色素層炎、或移植物抗宿主疾病。

【0254】 98.如態樣97所述之用途，其中該等疾病或病症係選自發炎性腸疾(IBD)、潰瘍性結腸炎(UC)、Crohn氏症(CD)、牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0255】 99.一種用於治療與介白素23 (IL-23)/介白素23受體(IL-23R)相關聯之疾病或病症之方法，其包含投予：

(i) 有效量的根據態樣 1 至 88 中任一者之介白素-23 受體之肽抑制劑、或其醫藥上可接受之鹽、溶劑合物、或形式；

或

(ii) 根據態樣 89 至 94 中任一者之醫藥組成物分別至有需要之患者。

【0256】 100.如態樣99所述之方法，其中該疾病或病症係與自體免疫發炎相關聯。

【0257】 101.如態樣99所述之方法，其中該疾病或病症係與下列相關聯：多發性硬化症、氣喘、類風濕性關節炎、腸道發炎、發炎性腸疾(IBD)、幼年型IBD、青年期IBD、Crohn氏症、潰瘍性結腸炎、肉瘤病、全身性紅斑性狼瘡、關節黏連性脊椎炎（中軸性脊椎關節炎）、牛皮癬性關節炎、或牛皮癬。特定而言，該疾病或病症可係牛皮癬（例如，斑塊型牛皮癬、滴狀牛皮癬、反轉型牛皮癬、膿疱性牛皮癬、掌蹠膿疱症、尋常牛皮癬、或紅皮性牛皮癬）、異位性皮膚炎、痤瘡異位、潰瘍性結腸炎、Crohn氏症、乳糜瀉（非熱帶性口瘡）、與血清反應陰性關節病變相關聯之腸病變、顯微鏡性結腸炎、膠原性結腸炎、嗜伊紅性胃腸炎/食道炎、與放射或化學療法相關聯之結腸炎、與如在白血球黏附分子缺乏症-1中的先天免疫性病症相關聯之結腸炎、慢性肉芽腫疾病、肝糖貯積病第1b型、Hermansky-Pudlak氏症候群、Chediak-Higashi氏症候群、Wiskott-Aldrich氏症候群、囊炎、直腸結腸切除術及回腸肛管吻合術後產生之囊炎、胃腸癌、胰臟炎、胰島素依賴性糖尿病、乳腺炎、膽囊炎、膽管炎、原發性膽汁性肝硬化、病毒相關腸病變、膽管週圍炎、慢性支氣管炎、慢性竇炎、氣喘、眼色素層炎、或移植物抗宿主疾病

【0258】 102.如態樣99所述之方法，其中該疾病或病症係與下列相關聯：潰瘍性結腸炎(UC)、Crohn氏症(CD)、牛皮癬(PsO)、或牛皮癬性關節炎(PsA)。

【0259】 103.如態樣99所述之方法，其中該疾病或病症係潰瘍性結腸炎(UC)。

【0260】 104.如態樣99所述之方法，其中該疾病或病症係Crohn氏症(CD)。

【0261】 105.如態樣99所述之方法，其中該疾病或病症係牛皮癬(PsO)。

【0262】 106.如態樣99所述之方法，其中該疾病或病症係牛皮癬牛皮癬性關節炎(PsA)。

【0263】 107.一種套組，其包含如態樣1至88所述之介白素-23受體之肽抑制劑、或根據態樣89至94中任一者之醫藥組成物、及對於該介白素-23受體之抑制劑或醫藥組成物之使用說明。

【0264】 108.如態樣107所述之套組，其中該說明係關於發炎性疾病或病症之治療。

【0265】 109.如態樣108所述之套組，其中該疾病係發炎性腸疾(IBD)、Crohn氏症(CD)、潰瘍性結腸炎(UC)、牛皮癬(PsO)、及牛皮癬性關節炎(PsA)。

【0266】 110.製備如態樣1至88中任一者所述之化合物之方法，其包含鍵聯一或多種單體及造成第一鍵及第二鍵之形成，從而產生雙環結構。

【0267】 111.一種介白素-23受體之雙環肽抑制劑，其包含式XXI之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-X11-X12-X13-N-X15-meG-R2 (A)

其中：

R1係7Ahp、6Ahx、5Ava、Peg2、AEEP、或AEEP(Ns)；

X4係Pen、Abu、aMeC、hC、或C；

X5係N或K(PEG2PEG2gEC18OH)；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(6(2OxdeQuin8Me))W、7(6(2OxIquin))W、7(7(124TAZP))W、7(7(2OMeQuin))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、D7MeW、或在位置7經C1至C7烷基、鹵基、鹵基烷基、OH、CN、C1至C7烷氧基、含有1至2個氮、及/或硫、及/或氧之5至7員雜芳基所取代的Trp。

X8係K-Ac、Q、K(NMeAc)、K(PEG2PEG2gEC18OH)、dK-Ac、dQ、dK(NMeAc)、或dK(PEG2PEG2gEC18OH)；

X9係Pen、Abu、aMeC、hC、或C；

X12係THP、aMeK、Aib、Acpx、Achx、4diFAchx、aMeL、Pip(NMe)、Pip(NMe2)、或α、α-經二取代（C1-C5烷基及C1至C5烷基、鹵基烷基、烷氧基、羧基、烷基胺、或3至7員碳環或含有1至2個氮、硫、及/或氧之雜環）甘胺酸。

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp、及其含有1至2個氮、硫、及/或氧之雜芳族類似物。

X13係E、dE、hE、dhE、D、dD、或hSer、dhSer；

X15係3pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NmeDTyr、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、L、經C1至C7烷基、鹵基、鹵基烷基、OH、CN、C1至C7烷氧基所取代之3pya、經C1至C7烷基、鹵基、鹵基烷基、OH、CN、C1至C7烷氧基、含有1至2個氮、硫、及/或氧之5至7員雜芳族、含有1至2個氮、硫、及/或氧且經C1至C7烷基、鹵基、鹵基烷基、OH、CN、C1至C7烷氧基所取代之5至7員雜芳族所取代的H、或不存在；

R2係-NH2、N(H)C_1至C_4烷基、-H(C_1-C_4烷基、-N(C_1至C_4烷基)2，各烷基可選地經Cl、F、或氰基所取代；且

其中該介白素-23受體之雙環肽抑制劑係藉由X4與X9之間的第一雙硫鍵或硫醚鍵、及-R1與X13之間的第二醯胺鍵或硫醚鍵（在pFS與Dap(pF)之間）、或具有10至18個共價鍵之合併長度的任何脂族鍵聯物組成、或在X4與X13之α碳之間具有相等長度的任何脂族及/或芳族鍵聯物組成而環化。

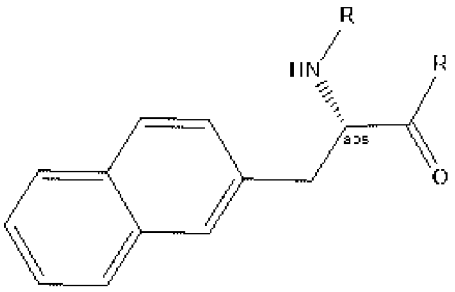
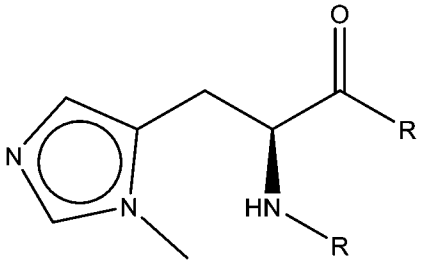
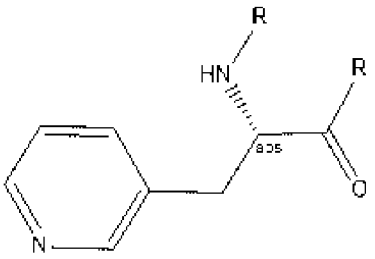
【0268】 112.一種醫藥組成物，其包含如態樣111所述之介白素-23受體之抑制劑、及醫藥上可接受之賦形劑。

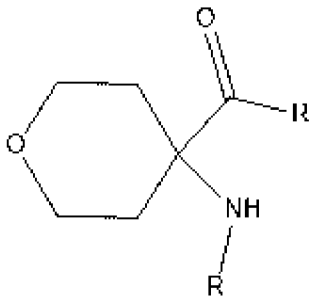
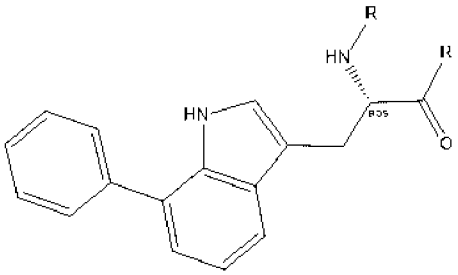
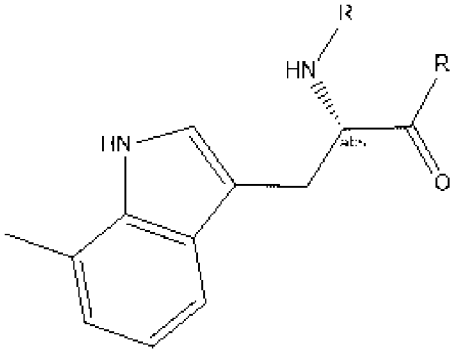
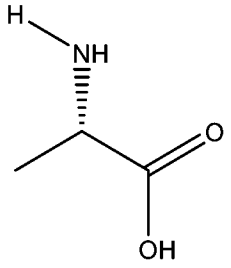
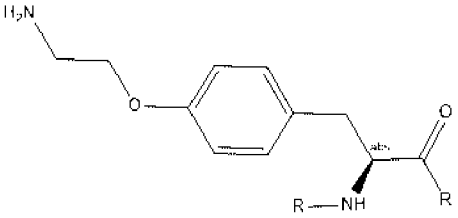
【0269】 113.一種治療方法，其包含投予如態樣111所述之介白素-23受體之抑制劑或如態樣112所述之醫藥組成物至有需要之患者

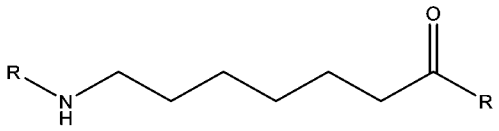
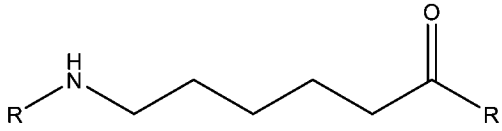
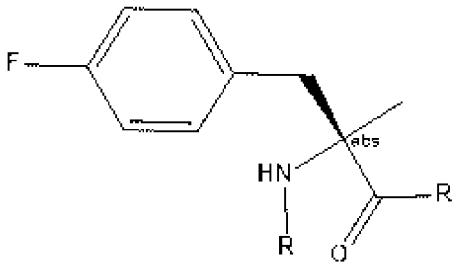
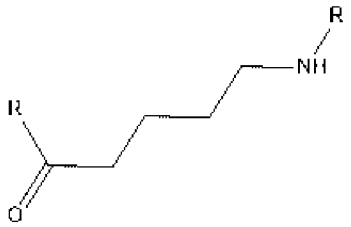
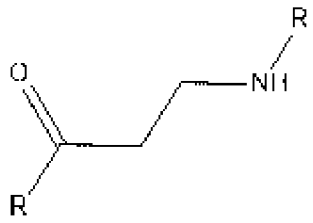
【0270】 可用於描述本發明之一些縮寫係定義於下列表2A及表2B中。

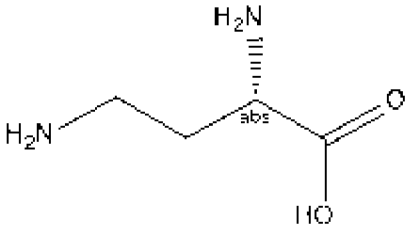
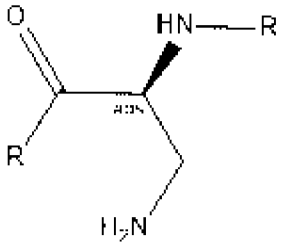
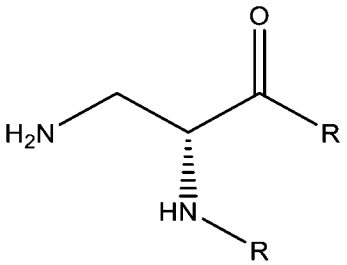
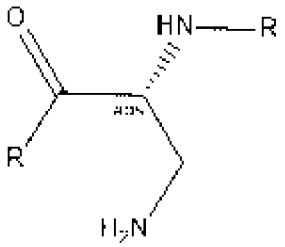
【0271】

表2A.胺基酸縮寫

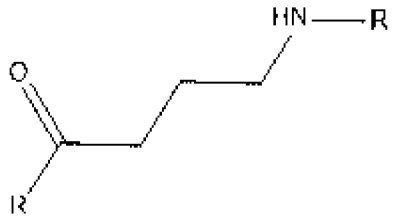
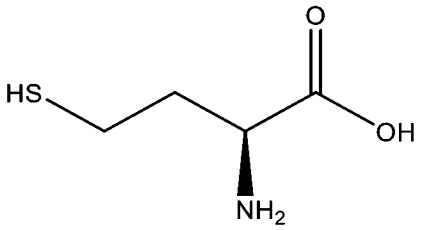
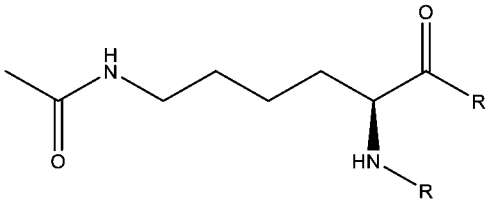
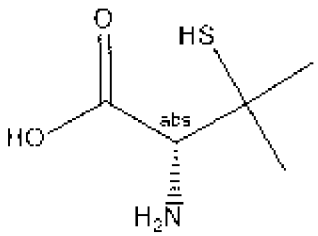
縮寫	定義	Smiles
dR、arg、或 r	D-精胺酸	
dK、(D)Lys、(D)-Lys、lys、或 k	D-離胺酸	
5Apa	5 胺基戊酸	
2-Nal 或 2Nal	 $C_{13}H_{11}NOR_2$	O=C([C@H](Cc1 cc2 ccccc2 cc1)N[R])[R]
3MeH	 3-甲基-L-組胺酸	Cn1cncc1C[C@H](N[R])C([R])=O
3Pya、3Pal、3-(2-吡啶基)-丙胺酸		O=C([C@H](Cc1cnccc1)N[R])[R]

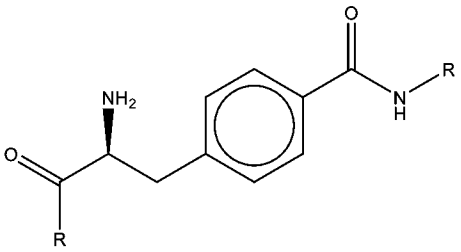
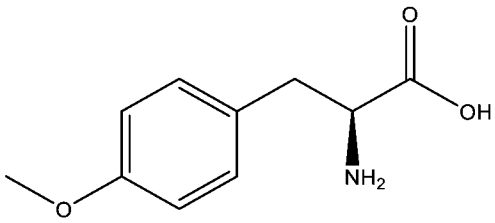
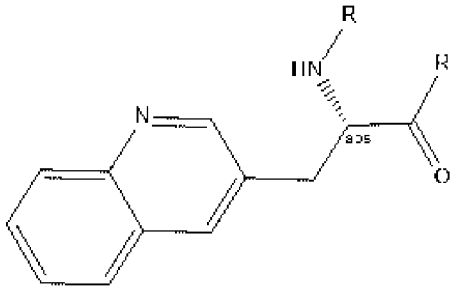
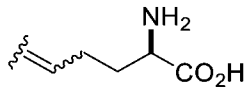
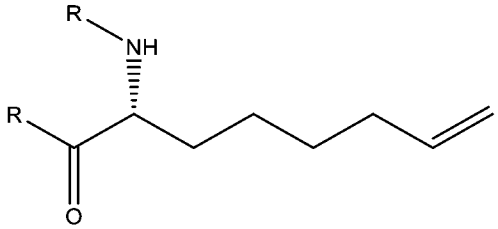
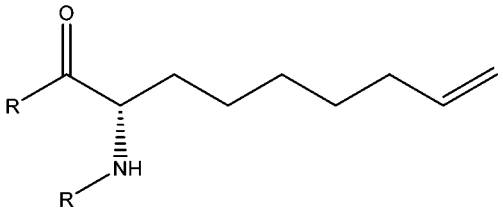
THP、4-胺基四氫-2H-哌喃-4-羧酸	 4-胺基-4-羧基-四氫哌喃	O=C(C1(CCOCC1)N[R])[R]
7PhW、7PhTrp、或 W(7-Ph)	 7-苯基-L-色胺酸	O=C([C@H](Cc1c[nH]c2c1 cccc2-c1 ccccc1)N[R])[R]
7MeW、7(MeW)、7MeTrp、7-甲基-L-色胺酸	 7-甲基-L-色胺酸	Cc1 cccc2c1[nH]cc2C[C@@H](C([R])=O)N[R]
Abu	 2-胺基丁酸	C[C@@H](C=O)N
AEF、Phe(4-(2-胺基乙氧基))、或 F(4-2ae)	 4-(2-胺基乙氧基)-L-苯基丙胺酸	NCCOc1 ccc(C[C@@H](C([R])=O)N[R])cc1

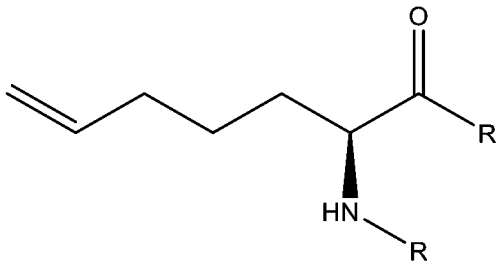
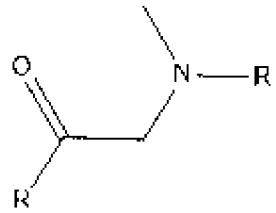
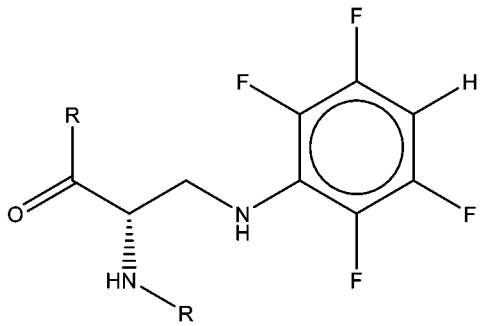
Ahp、7Ahp、7AHP、或 7AHP(2)	 7-胺基庚酸	O=C([R])CCCCCCN[R]
Ahx 或 6Ahx、6Ahx、6Ahx(2)、6-胺基己酸	 6-胺基己酸	O=C(CCCCCN[R])[R]
aMeF、aMePhe、或 aMe-Phe	 α-甲基 L-苯基丙胺酸	C[C@](Cc(cc1)ccc1F)(C([R])=O)N[R]
aMeK、aMeLys、或 aMe-Lys	α-甲基 L-離胺酸	
Arg 或 R	L-精胺酸	
dR、arg、r 或 (D)Arg	D-精胺酸	
Asn 或 N	L-天冬醯胺酸	
Ava、5Ava(2)、或 5Ava	 5-胺基戊酸	O=C(CCCCN[R])[R]
bAla、b-ALA、β-丙胺酸、bA	 β-丙胺酸	O=C(CCN[R])[R]
雙-胺基-PEG2	1,2-雙(2-胺基乙氧基)乙烷	
Cys 或 C	L-半胱胺酸	

Dbu、Dab、(*S*)-2,4-二胺基丁酸、或DAB	 L-2,4-二胺基丁酸	NCC[C@@H](C(O)=O)N
Dap、Dap、DAP、Dpr、或(S)-2,3-二胺基丙酸	 L-2,3-二胺基丙酸	NC[C@@H](C([R])=O)N[R]
dDab、D(Dab)、dDpr、(R)-2,3-二胺基丙酸	 D-2,4-二胺基丁酸	NC[C@H](C([R])=O)N[R]
dDap、D(Dap)、dDap、dap、dDbu、(R)-2,3-二胺基丙酸	 D-2,3-二胺基丙酸	NC[C@H](C([R])=O)N[R]
Fmoc-2Nal	2-((((9H-芴-9-基)甲氧基)羰基)胺基)-3-(萘-2-基)丙酸	
Fmoc-3Pya	(S)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)-4-(吡啶-3-基)丁酸	
Fmoc-7MeW	(S)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)-3-(7-甲基-1H-吲哚-3-基)丙酸	
Fmoc-AEF	(S)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)-3-(4-(2-((三級丁氧基羰基)胺基)乙氧基)苯基)丙酸	
Fmoc-aMePhe	(((9H-芴-9-基)甲氧基)羰基)-α甲基-L-苯基丙胺酸	

Fmoc-arg 或 Fmoc-r	N-α-(9-芴基甲基氧基羰基)-N'-2,2,4,6,7-五甲基二氫苯并呋喃-5-磺醯基-D-精胺酸	
Fmoc-Asn 或 Fmoc-N	N^2-(((9H-芴-9-基)甲氧基)羰基)-N4-三苯甲基-L-天冬醯胺酸	
Fmoc-Dap(DDe)	N2-(Fmoc)-N6-(1-(4,4-二甲基-3,5-二側氧基亞環己基)乙基)-L-Dap	
Fmoc-DDe-Lys(Fmoc)-OH	N6-(((9H-芴-9-基)甲氧基)羰基)-N2-(1-(4,4-二甲基-3,5-二側氧基亞環己基)乙基)-L-離胺酸	
Fmoc-Glu 或 Fmoc-E	(S)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)-5-(三級丁氧基)-2-甲基-5-側氧基戊酸	
Fmoc-Lys(Ac)或 Fmoc-K(Ac)	N2-(((9H-芴-9-基)甲氧基)羰基)-N6-乙醯基-L-離胺酸	
Fmoc-Lys(DDe)或 Fmoc-K(DDe)	N2-(Fmoc)-N6-(1-(4,4-二甲基-3,5-二側氧基亞環己基)乙基)-L-離胺酸	
Fmoc-Lys(NMeAc)或 Fmoc-K(NMeAc)	N2-(((9H-芴-9-基)甲氧基)羰基)-N6-乙醯基-N6-甲基-L-離胺酸	
Fmoc-NMeLys(DDe)或 Fmoc-NMeK(DDe)	(1-胺基-6-((1-(4,4-二甲基-3,5-二側氧基亞環己基)乙基)胺基)-1-側氧基己-2-基)(甲基)胺甲酸(9H-芴-9-基)甲酯	
Fmoc-Pen-Trt	(R)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)-3-甲基-3-(三苯甲基硫)丁酸	
Fmoc-Pro 或 Fmoc-P	Fmoc-脯胺酸-OH	
Fmoc-pro 或 Fmoc-p	Fmoc-D-脯胺酸-OH	
Fmoc-R5H	(R)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)庚-6-烯酸	
Fmoc-Sar 或 Fmoc-Sarc	N-(((9H-芴-9-基)甲氧基)羰基)-N-甲基甘胺酸	
Fmoc-THP	4-((((9H-芴-9-基)甲氧基)羰基)胺基)四氫-2H-哌喃-4-羧酸	
Fmoc-Thr 或 Fmoc-T	N-(((9H-芴-9-基)甲氧基)羰基)-O-(三級丁基)-L-蘇胺酸	

GABA、Gaba、Gaba(2)、Gaba2、或 4Abu	 4-胺基丁酸	O=C(CCCN[R])[R]
Glu 或 E	L-麩胺酸	
glu 或 e 或 D(Glu)	D-麩胺酸	
His 或 H	L-組胺酸	
Lys 或 K	L-離胺酸	
lys 或 k 或(D)Lys	D-離胺酸	
hCys、hC	 L-升半胱胺酸	C(CS)[C@@H](C(=O)O)N
KAc、Lys(Ac)、K(Ac)、K(COMe)、或 K-Ac	 N-ε-乙醯基-L-離胺酸 N6-乙醯基-L-離胺酸	CC(NCCCC[C@@H](C([R])=O)N[R])=O
MeK、N-MeLys、NMeLys、NMeK、或 MeLys	N-甲基-離胺酸 (2S)-2-胺基-6-(甲基胺基)己酸	
Pen	 L-青黴胺、3-巰基-L-纈胺酸 (R)-2-胺基-3-巰基-3-甲基丁酸	CC(C)([C@@H](C(O)=O)N)S

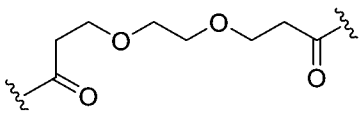
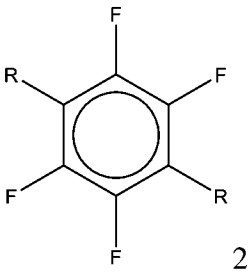
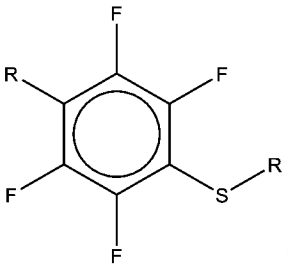
F4CONH2、Phe(4-CONH$_2$)或 Phe(4-CONH2)或 Phe(Cmd)或 Phe_4Ad	 4-胺甲醯基-L-苯基丙胺酸(S)-2-胺基-3-(4-胺甲醯基苯基)丙酸	N[C@H](C([R])=O)Cc1ccc(C(N[R])=O)cc1
F4OMe、Phe(4-OMe)、或 Phe_4OMe	 4-甲氧基-L-苯基丙胺酸	N[C@@H](CC1=CC=C(OC)C=C1)C(O)=O
Quin、3Quin、3-Quin、3QuinolAla、或 3QuinA	 (S)-2-胺基-3-(喹啉-3-基)丙酸	O=C([C@H](Cc1 cc2ccccc2nc1)N[R])[R]
R5H	 (R)-2-胺基戊酸 5-二基	
R6H、(R,E)-2-胺基-8-羥基辛-7-烯酸	 (R)-2-胺基己酸 6-二基	C=CCCCC[C@H](C([R])=O)N[R]
R7H、(R,E)-2-胺基-9-羥基壬-8-烯酸	 (R)-2-胺基庚酸 7-二基	C=CCCCCC[C@H](C([R])=O)N[R]

S5H	 (S)-2-胺基戊酸 5-二基	C=CCCC[C@H](N[R])C([R])=O
meG、Sarc、MeGly、Sar、Sarc、MeGly、肌胺酸、甲基胺基-乙酸、N-甲基甘胺酸	 肌胺酸或 N-甲基甘胺酸	CN(CC([R])=O)[R]
Thr 或 T	L-蘇胺酸	
nFEtOH、Phe(4-OCH2COOH、或 2-胺基-2-[4-(羧基甲氧基)苯基]乙酸	Fc1c(F)c([H])c(F)c(F)c1NC[C@@H](C([R])=O)N[R] (R)-2-胺基-2-(4-(羧基甲氧基)苯基)乙酸	N[C@@H](C=O)c(cc1)ccc1OCC=O
DappF6 Dap(pF(6))	 四-氟-苯基丙胺酸	Fc1c(F)c([H])c(F)c(F)c1NC[C@@H](C([R])=O)N[R]

【0272】

表2B.取代基、試劑、及溶劑之縮寫

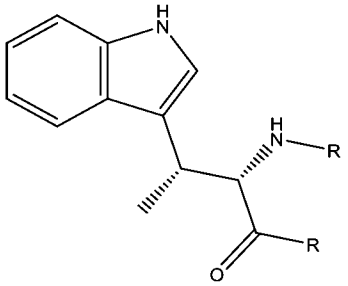
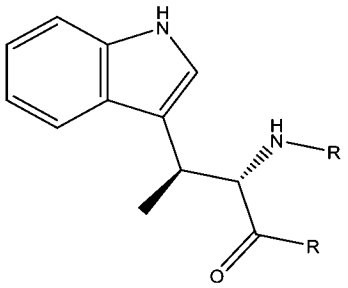
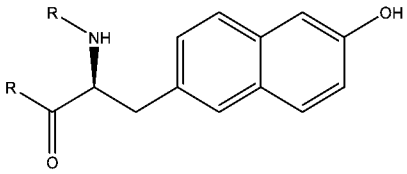
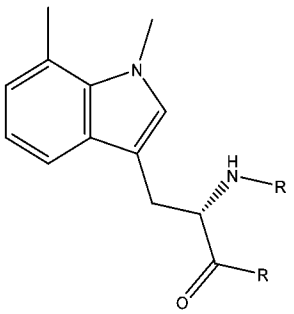
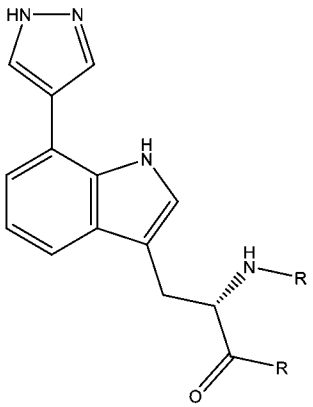
縮寫	定義
Ac 或 MeCO	乙醯基
ACN	乙腈
Boc	三級丁氧基-羰基
$CONH_2$	羧醯胺
COOH	羧酸
DCM	二氯甲烷
Dde	N-(1-(4,4-二甲基-2,6-二側氧基亞環己基)乙基

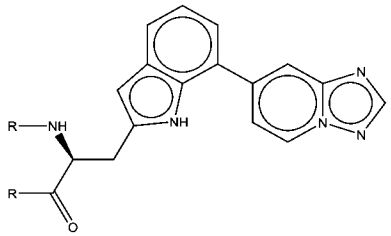
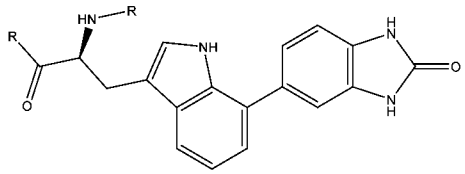
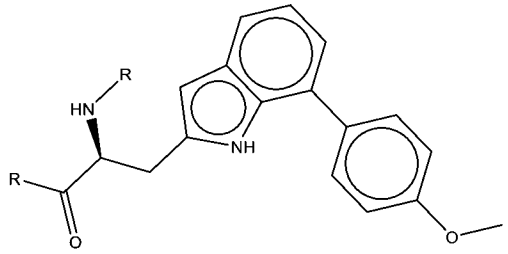
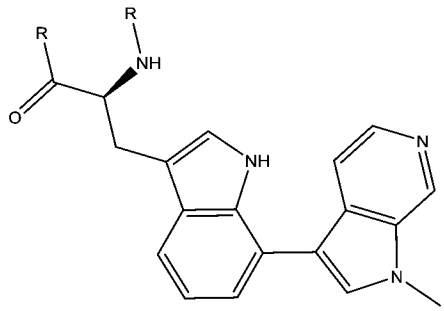
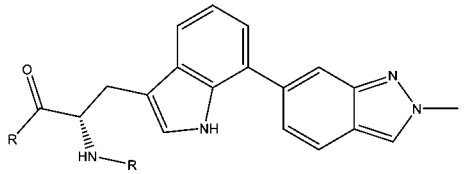
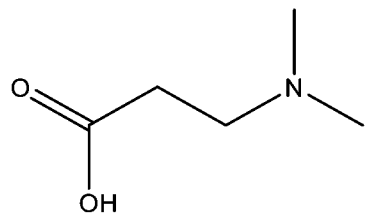
縮寫	定義
DIC	N,N'-二異丙基碳二亞胺
DMF	N,N-二甲基甲醯胺
Et_2O	二乙醚
FMOC 或 Fmoc	((9H-芴-9-基)甲氧基)羰基
HOAT 或 HOAt	1-羥基-7-吖苯并三唑
MeOH	甲醇
MTBE	甲基三級丁醚
MW	微波
Oxyma	氰基羥基亞胺基乙酸乙酯
PEG2_DiAcid 或 PEG2DA	 3,3'-(乙烷-1,2-二基雙(氧基))二丙烷羰基
pF	 2,3,5,6-四氟苯-1,4-二基鍵聯物 Fc1c(F)c([R])c(F)c(F)c1[R]
pFS	 2,3,5,6-tetra 氟-4-巰基酚 Fc(c(S[R])c(c(F)c1[R])F)c1F
RT	室溫
TFA	三氟乙酸
TIPS	三異丙基矽烷

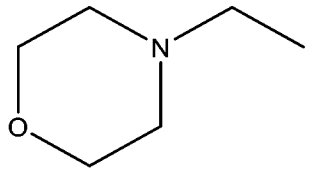
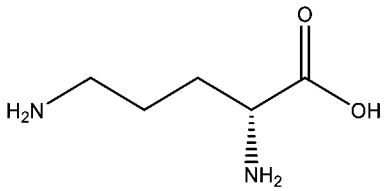
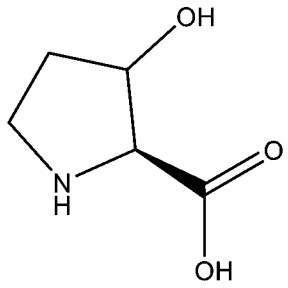
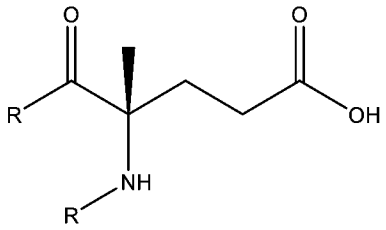
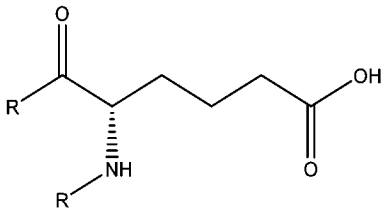
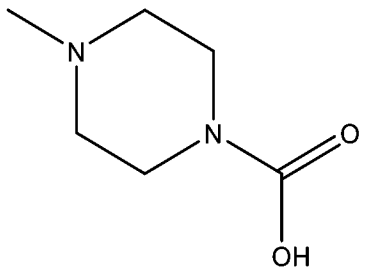
【0273】

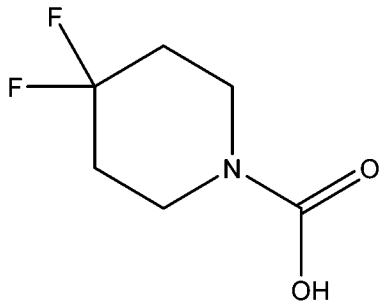
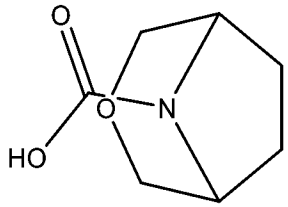
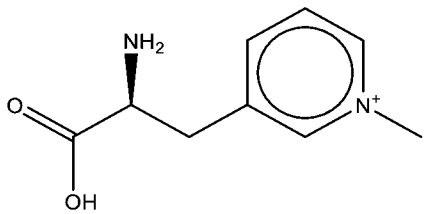
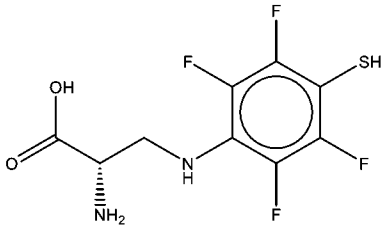
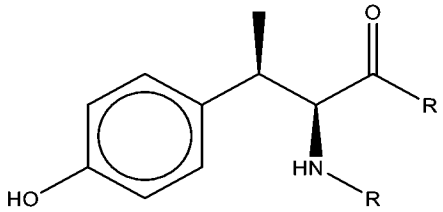
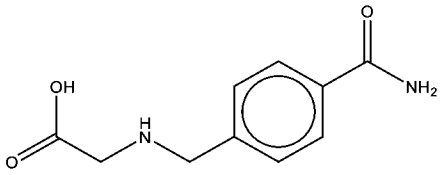
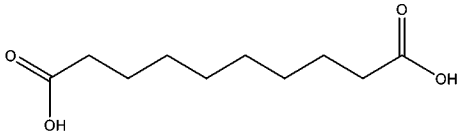
表2C單體及結構

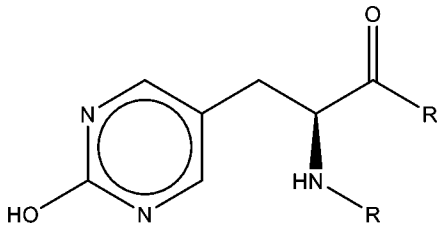
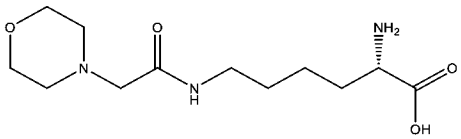
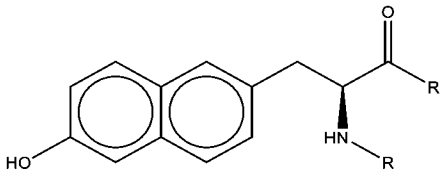
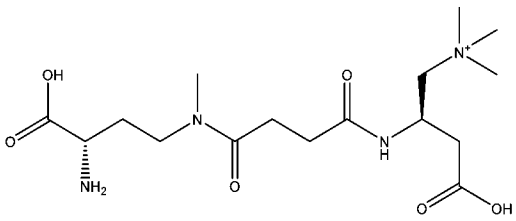
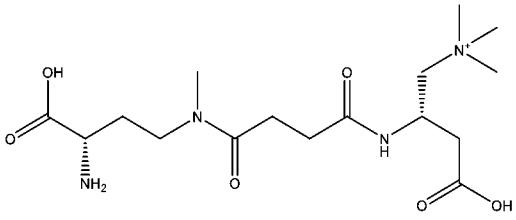
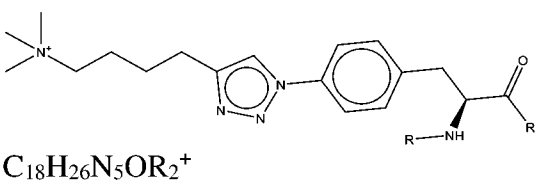
#	符號/名稱	結構	Smiles

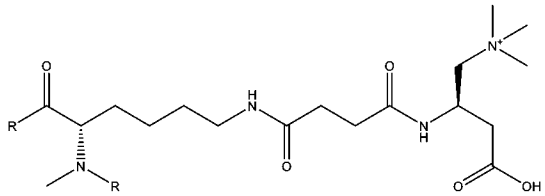
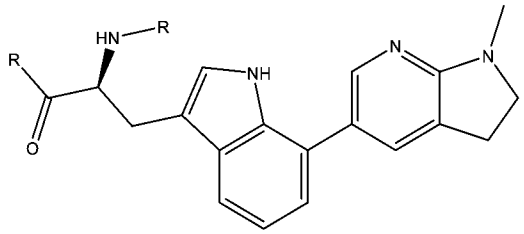
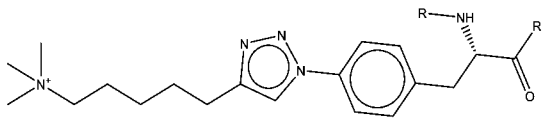
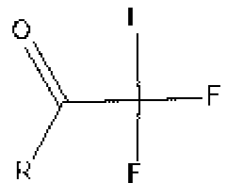
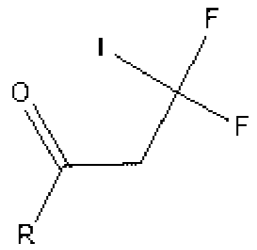
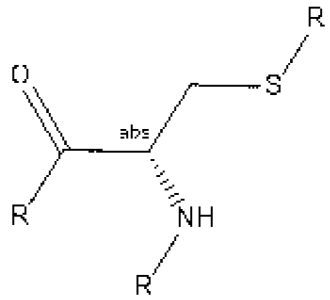
1	bMeW(2S3R) bMeW(2S,3R)	 $C_{12}H_{12}N_2OR_2$	C[C@H](C1=CNC2=C1C=CC=C2)[C@H](N[R])C([R])=O
2	bMeW(2S3S)、 bMeW(2S,3S)	 $C_{12}H_{12}N_2OR_2$	C[C@@H](C1=CNC2=C1C=CC=C2)[C@H](N[R])C([R])=O
3	6OH2Nal	 (*S*)-2-胺基-3-(6-羥基萘-2-基)丙酸	[R]C([C@H](CC1=CC=C(C=C(O)C=C2)C2=C1)N[R])=O
4	NMe7MeW	 $C_{13}H_{14}N_2OR_2$	[R]C([C@@H](N[R])CC1=CN(C)C2=C1C=CC=C2C)=O
5	7(4Paz)W	 $C_{14}H_{12}N_4OR_2$	[R]C([C@@H](N[R])CC1=CNC2=C1C=CC=C2C3=CNN=C3)=O

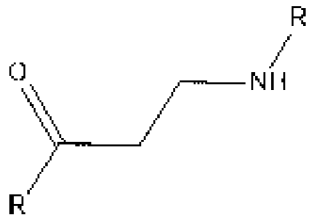
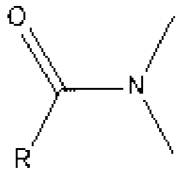
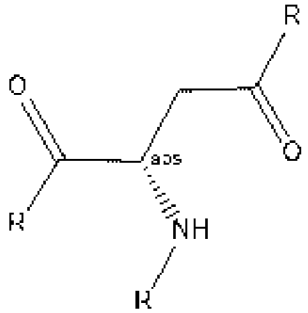
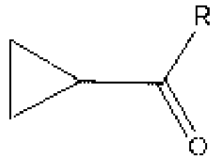
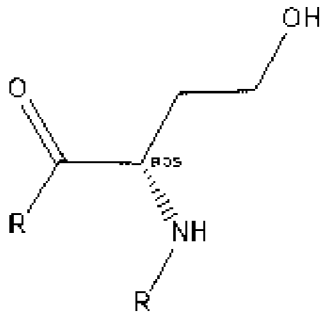
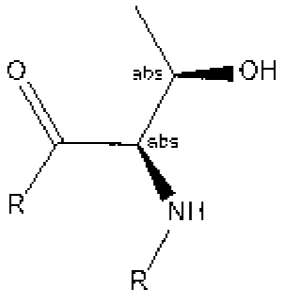
6	7(7(124TAZP))W	 $C_{17}H_{13}N_5OR_2$	O=C([R])[C@@H](N[R])Cc1[nH]c2c(c(c3)ccn4c3ncn4)cccc2c1
7	7(3UrPh)W	 $C_{18}H_{14}N_4O_2R_2$	[R]C([C@@H](N[R])CC1=CNC2=C1C=CC=C2C3=CC(NC(N4)=O)=C4C=C3)=O
8	7(7Imzpy)W	$C_{18}H_{14}N_4OR_2$	[R]C([C@@H](N[R])CC1=CNC2=C1C=CC=C2C3=CC4=NC=CN4C=C3)=O]
9	7(4OMePh)W	 $C_{18}H_{16}N_2O_2R_2$	[R]C([C@@H](N[R])CC1=CNC2=C1C=CC=C2C3=CC=C(OC)C=C3)=O
10	7(3(6AzaInd1Me))W	 $C_{19}H_{16}N_4OR_2$	[R]C([C@@H](N[R])CC1=CNC2=C1C=CC=C2C3=CN(C)C4=C3C=CN=C4)=O
11	7(6(2MeNDAZ))W	 $C_{19}H_{16}N_4OR_2$	[R]C([C@@H](N[R])CC1=CNC2=C1C=CC=C2C3=CC4=NN(C)C=C4C=C3)=O
12	NMebAla	 $C_5H_{11}NO$	CN(C)CCC=O

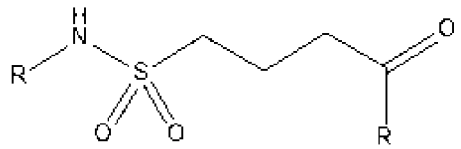
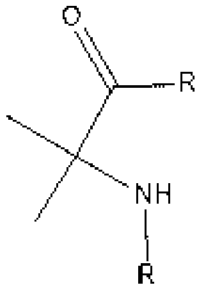
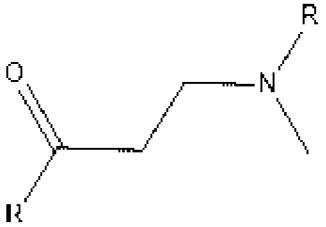
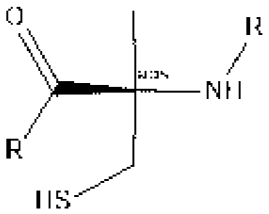
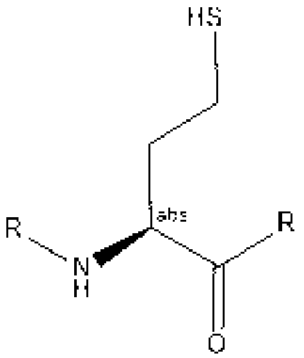
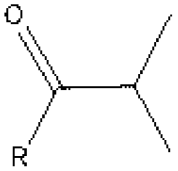
13	AcMorp、乙基-N-味啉基	 $C_5H_{11}NO$	CN1CCOCC1
14	dOrn、D-Orn D-鳥胺酸	 $C_5H_{12}N_2O$	NCCC[C@H](C(O)=O)N
15	3Hyp、3-羥基-L-脯胺酸	 $C_5H_9NO_2$	OC1[C@@H](C=O)NCC1
16	aMeE aMeGlu、α-甲基麩胺酸	 $C_6H_{11}NO_2$	C[C@](CCC(O)=O)(C([R])=O)N[R] C[C@](CCC(O)=O)(C=O)N
17	hGlu、(S)-2-胺基己二酸	 $C_6H_{11}NO_2$	N[C@@H](CCCC=O)C=O OC(CCC[C@@H](C([R])=O)N[R])=O
18	CON(NMePip)	 $C_6H_{12}N_2O$	CN(CC1)CCN1C=O

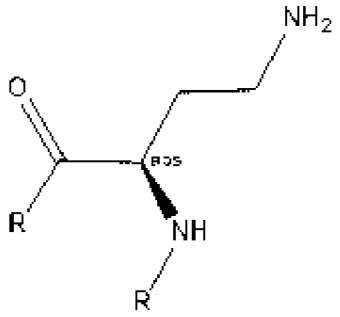
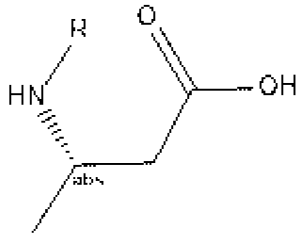
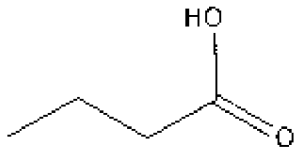
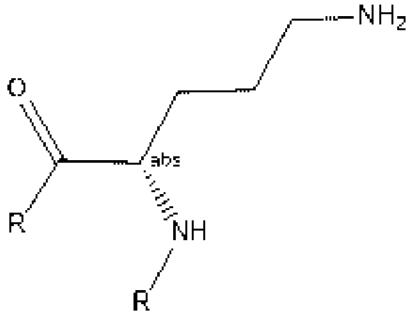
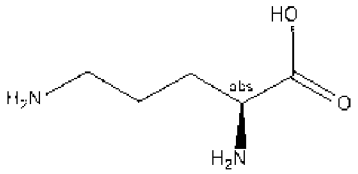
19	-CODiFPip、CO(二 FPip)	 $C_6H_9F_2NO$	O=CN(CC1)CCC1(F)F
20	CO(OAZBO)	 $C_8H_{13}NO_2$	CC(N1C2COCC1CC2)=O
21	Me1Pya、(S)-3-(2-胺基-2-羧基乙基)-1-甲基吡啶-1-鎓	 $C_9H_{13}N_2O^+$	C[n+]1cccc(C[C@@H](C=O)N)c1
22	DappF6、四-氟-苯基丙胺酸	 $C_9H_8F_4N_2O$	N[C@@H](CNc(c(F)c(c(S)c1F)F)c1F)C=O
23	bMePhe(2S,3R) bMePhe(SR)、bMePhe(2S,3R)	 $C_{10}H_{11}NOR_2$	C[C@@H]([C@@H](C([R])=O)N[R])c1 ccccc1
24	N4Am 苄基 Gly、N(4Am 苄基)Gly	 $C_{10}H_{12}N_2O_2$	NC(c1ccc(CNCC=O)cc1)=O
25	-Dec、1,10-癸二酸	 $C_{10}H_{18}O_3$	OC(CCCCCCCCC=O)=O

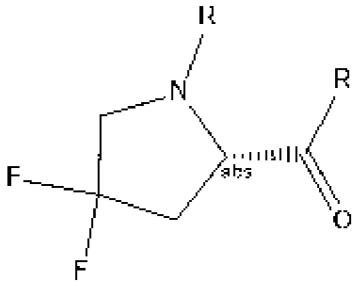
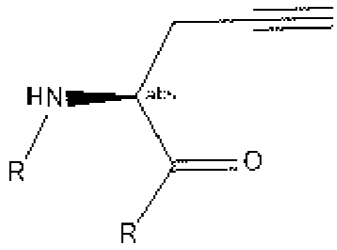
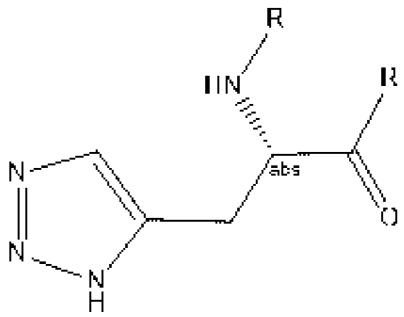
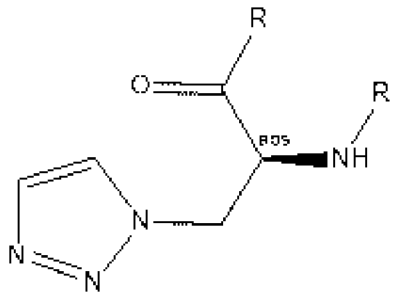
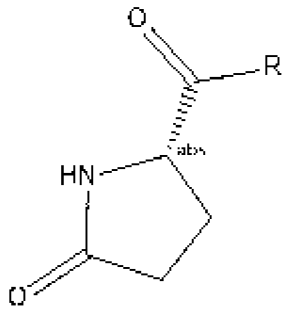
26	2OH3Pyrimid5Ala	 $C_{11}H_{15}N_3O_2R_2$	CC(C)(C)Oc1nc c(C[C@@H](C([R])=O)N[R])cn1
27	KacMorph、 K(AcMorph)、 KAcMorph、L-離 胺酸(ac-N-味啉基	 $C_{12}H_{23}N_3O_3$	N[C@@H](CCC CNC(CN1CCOC C1)=O)C=O
28	6OH2Nal	 $C_{13}H_{13}NO$	N[C@@H](Cc1 cc2 ccccc2 cc1)C=O N[C@@H](Cc1 cc2 ccccc2 cc1)C=O Oc1 ccc(cc(C[C@@ H](C([R])=O)N[R])cc2)c2c1
29	DabNMecarn、 Dab(NMecarn)	 $C_{16}H_{31}N_4O_4^+$	CN(CC[C@@H] (C=O)N)C(CCC(N[C@H](CC=O) C[N+](C)(C)C)= O)=O CN(CC[C@@H] (C=O)N)C(CCC(N[C@H](CC=O) C[N+](C)(C)C)= O)=O CN(CC[C@@H] (C=O)N)C(CCC(N[C@H](CC(O) =O)C[N+](C)(C) C)=O)=O
30	DabNMeCarn、 Dab(NMeCarn)	 $C_{16}H_{31}N_4O_5^+$	CN(CC[C@@H] (C=O)N)C(CCC(N[C@@H](CC(O)=O)C[N+](C)(C)C)=O)=O
31	F(4TzlTMA4)	 $C_{18}H_{26}N_5OR_2^+$	C[N+](C)(C)CC CCc1cn(-c2 ccc(C[C@@H](C([R])=O)N[R]) cc2)nn1

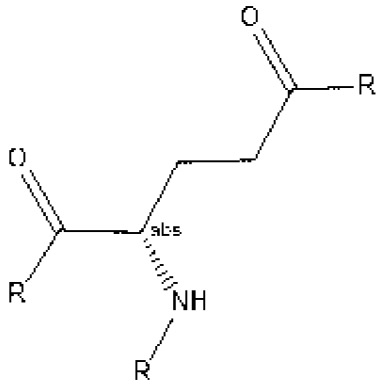
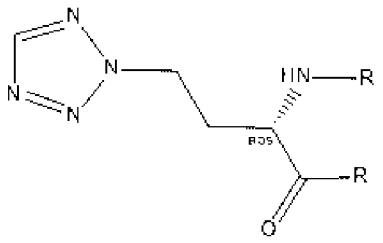
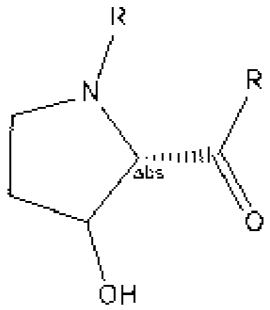
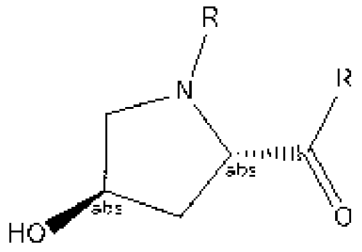
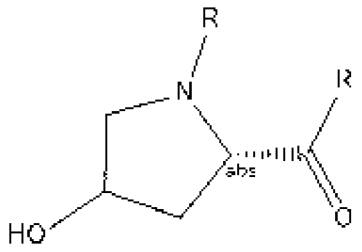
32	NMeK(d)、NMeKdCar	 $C_{18}H_{33}N_4O_5R_2^+$	CN([C@@H](CCCCNC(CCC(N[C@H](CC(O)=O)C[N+](C)(C)C)=O)=O)C([R])=O)[R]
33	7(5(Ina7Pyr))W	 $C_{19}H_{18}N_4OR_2$	[R]C([C@@H](N[R])CC1=CNC2=C1C=CC=C2C3=CN=C(N(C)CC4)C4=C3)=O
34	F(4TzlTMA5)	 $C_{19}H_{28}N_5OR_2^+$	C[N+](C)(C)CCCCCc1cn(-c2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1
35	CF3CO F3CO	 C_2F_3OR	O=C(C(F)(F)F)[R]
36	CF3 丙醯胺	 $C_3H_2F_3OR$	O=C(CC(F)(F)F)[R]
37	C(1*)（*純的但組態未知）	 $C_3H_4NOSR_3$	O=C([C@H](CS[R])N[R])[R]

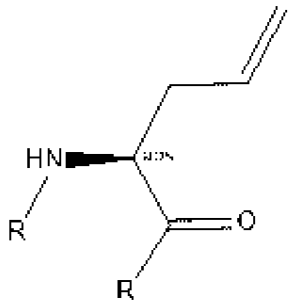
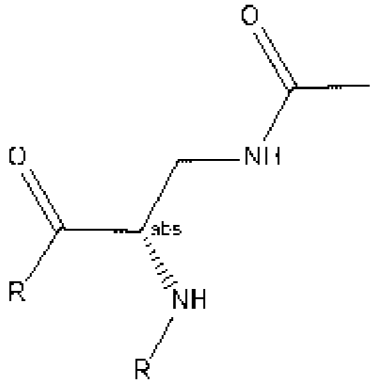
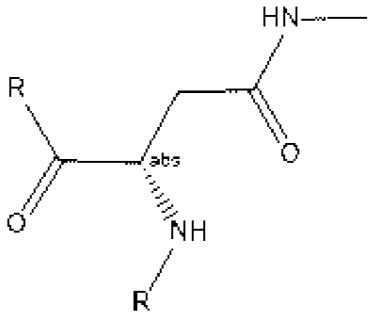
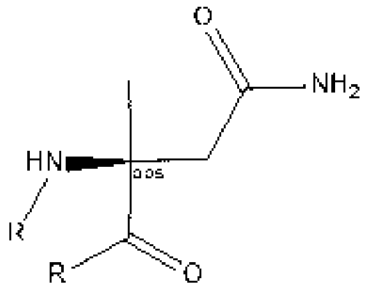
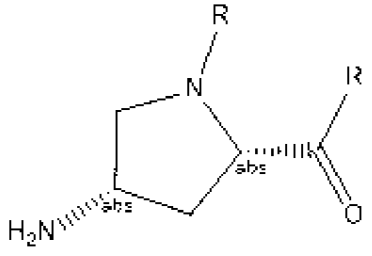
38	bAla、b-ALA、β-丙胺酸、bA	 $C_3H_5NOR_2$	O=C(CCN[R])[R]
39	CON(Me)2	 C_3H_6NOR	CN(C)C([R])=O
40	D(2)	 $C_4H_4NO_2R_3$	O=C(C[C@@H](C([R])=O)N[R])[R]
41	cPrCO	 C_4H_5OR	O=C(C1CC1)[R]
42	hS、hS、Hse、L-升絲胺酸、homoS、或homoSer	 $C_4H_7NO_2R_2$	OCC[C@@H](C([R])=O)N[R]
43	T、dThr、dT	 $C_4H_7NO_2R_2$	C[C@H]([C@H](C([R])=O)N[R])O

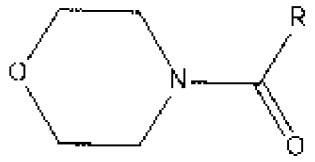
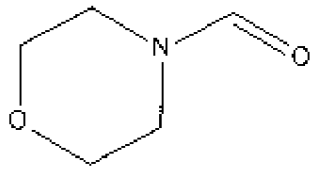
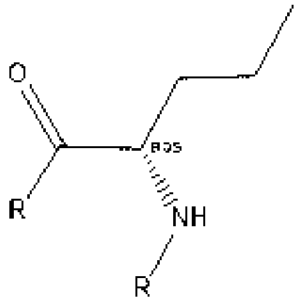
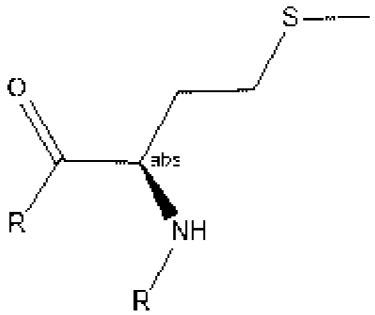
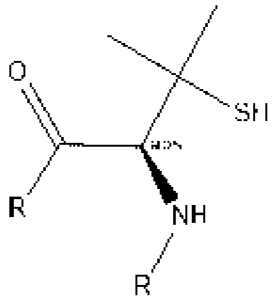
44	4sb、4SB	 $C_4H_7NO_3SR_2$	O=C([R])CCCS(=O)(N[R])=O
45	Aib、AIB、2-胺基異丁酸、α-胺基異丁酸、(2-胺基丙胺酸)	 $C_4H_7NOR_2$	CC(C)(C([R])=O)N[R]
46			
47	NMebAla	 $C_4H_7NOR_2$	CN(CCC([R])=O)[R]
48	aMeC	 $C_4H_7NOSR_2$	C[C@](CS)(C([R])=O)N[R] C[C@](CS)(C=O)N
49	hC、hCys、homoC、或homoCys	 $C_4H_7NOSR_2$	O=C([C@H](CCS)N[R])[R]
50	iPrCO	 C_4H_7OR	CC(C)C([R])=O

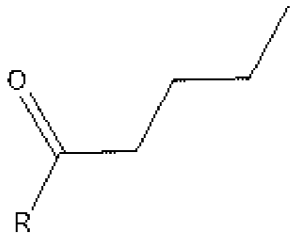
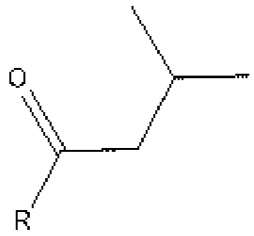
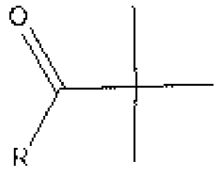
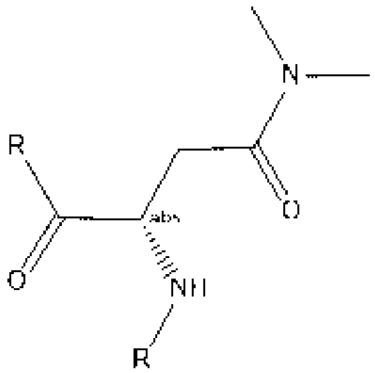
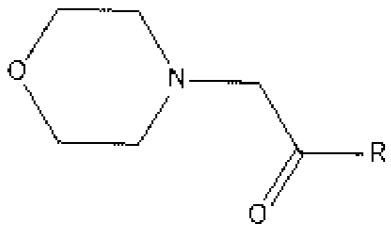
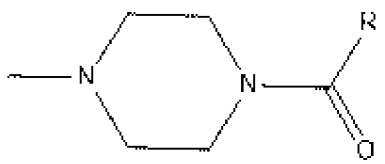
51	dDab、dab、(R)-2,4-二胺基丁酸	 $C_4H_8N_2OR_2$	NCC[C@H](C([R])=O)N[R]
52	homobAla	 $C_4H_8NO_2R$	C[C@@H](CC(O)=O)N[R]
53	Bua、丁酸	 $C_4H_8O_2$	CCCC(O)=O
54	Orn、ORN、鳥胺酸	 $C_5H_{10}N_2OR_2$	NCCC[C@@H](C([R])=O)N[R]
55			
56	Orn、L-鳥胺酸	 $C_5H_{12}N_2O_2$	NCCC[C@@H](C(O)=O)N

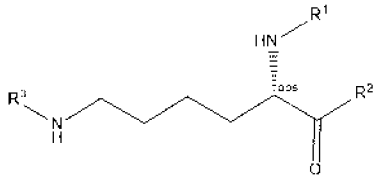
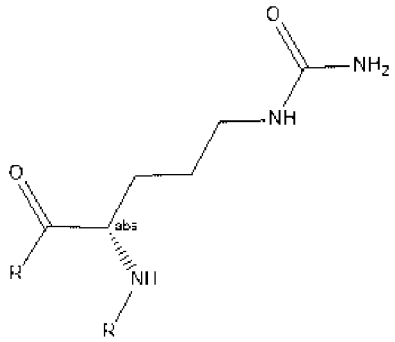
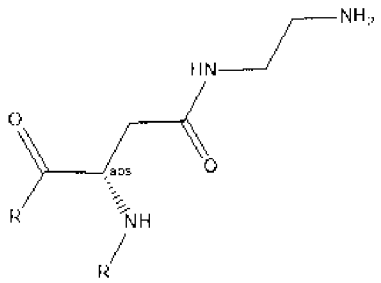
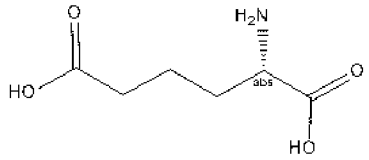
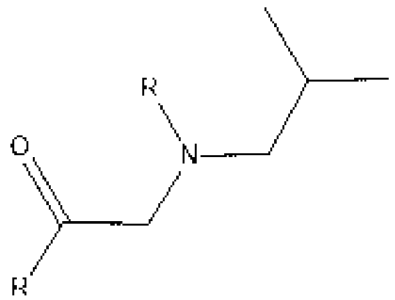
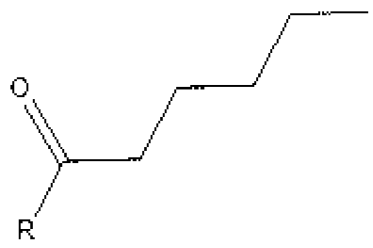
57	4diFPro	 $C_5H_5F_2NOR_2$	O=C([C@H](CC(C1)(F)F)N1[R])[R] O=C[C@H](C1)NCC1(F)F
58	prG、prG、Fmoc-L-炔丙基-Gly-OH、Pra	 $C_5H_5NOR_2$	C#CC[C@@H](C([R])=O)N[R]
59	4TriazolAla	 $C_5H_6N_4OR_2$	O=C([C@H](Cc1cnn[nH]1)N[R])[R]
60	Tzl	 $C_5H_6N_4OR_2$	O=C([C@H](Cn1nncc1)N[R])[R]
61	PyE、PyE (S)-5-側氧基吡咯啶-2-羧酸	 $C_5H_6NO_2R$	O=C([C@H](CC1)NC1=O)[R] O=C[C@H](CC1)NC1=O

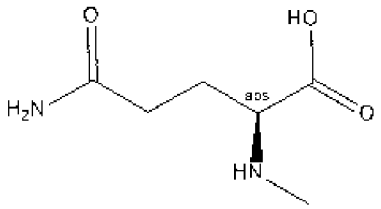
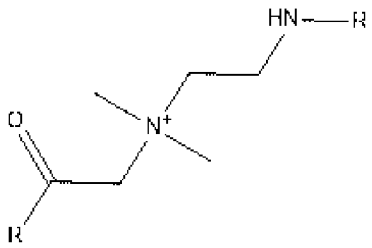
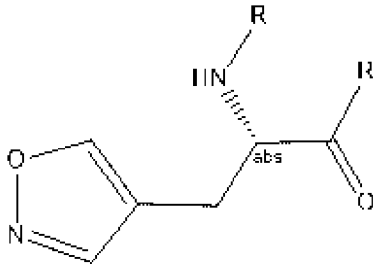
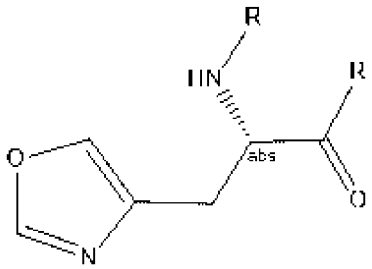
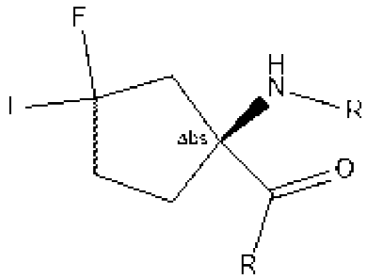
62	E(2)	 $C_5H_6NO_2R_3$	O=C(CC[C@@H](C([R])=O)N[R])[R]
63	四唑	 $C_5H_7N_5OR_2$	O=C([C@H](CCn1nncn1)N[R])[R] N[C@@H](CCn1nncn1)C=O
64	3OHPro	 $C_5H_7NO_2R_2$	OC(CC1)[C@@H](C([R])=O)N1[R]
65	4(R)羥基 Pro	 $C_5H_7NO_2R_2$	O[C@H](C[C@H]1C([R])=O)CN1[R]
66	Hyp	 $C_5H_7NO_2R_2$	OC(C[C@H]1C([R])=O)CN1[R]

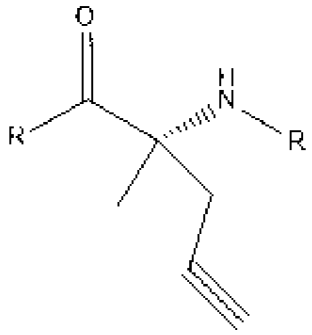
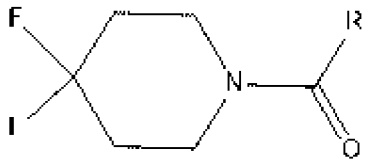
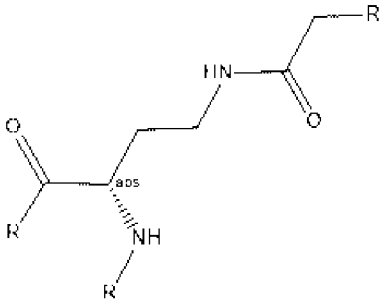
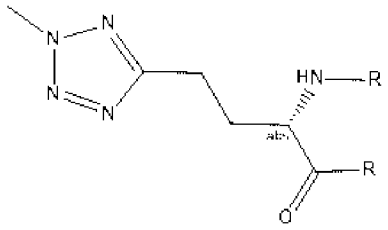
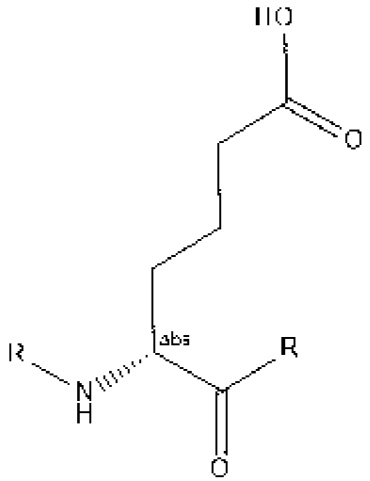
67	AllylGly	 $C_5H_7NOR_2$	C=CC[C@@H](C([R])=O)N[R]
68	Dap(Ac)	 $C_5H_8N_2O_2R_2$	CC(NC[C@@H](C([R])=O)N[R])=O
69	N(NMe)、NNMe、NMeAsn	 $C_5H_8N_2O_2R_2$	CNC(C[C@@H](C([R])=O)N[R])=O
70	aMeN. aMeAsn	 $C_5H_8N_2O_2R_2$	C[C@](CC(N)=O)(C([R])=O)N[R]
71	4(S)胺基 Pro	 $C_5H_8N_2OR_2$	N[C@@H](C[C@H]1C([R])=O)CN1[R]

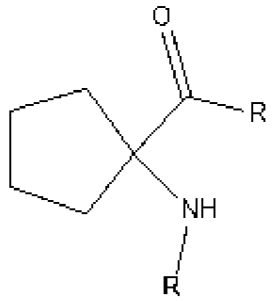
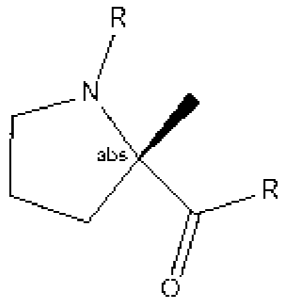
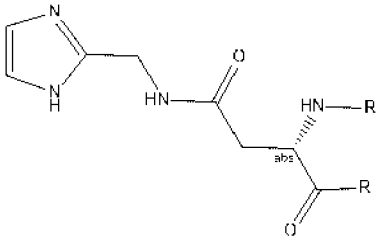
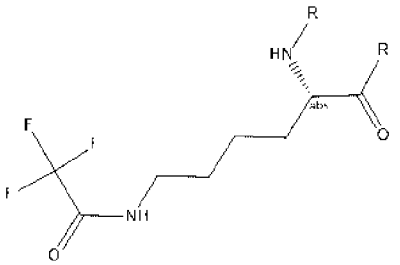
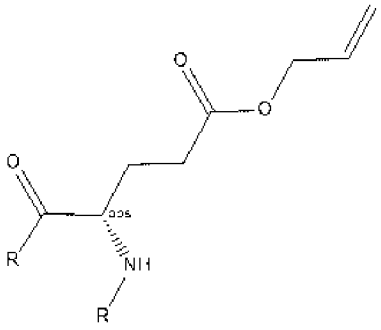
72	CO(Morph)	 $C_5H_8NO_2R$	O=C(N1CCOCC1)[R]
73	-COMorph、CO(Morph)	 $C_5H_9NO_2$	O=CN1CCOCC1
74			
75	Nva	 $C_5H_9NOR_2$	CCC[C@@H](C([R])=O)N[R]
76	dM、dMet、D-甲硫胺酸	 $C_5H_9NOSR_2$	CSCC[C@H](C([R])=O)N[R]
77	dPen、pen	 $C_5H_9NOSR_2$	CC(C)([C@H](C([R])=O)N[R])S

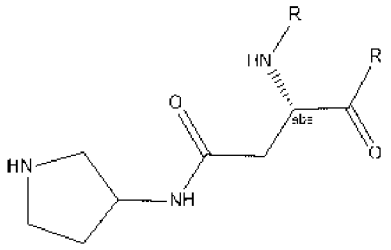
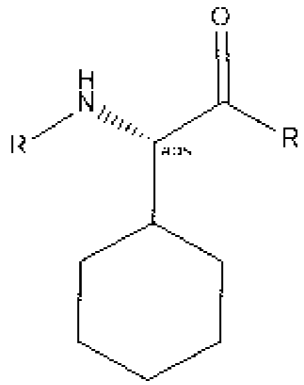
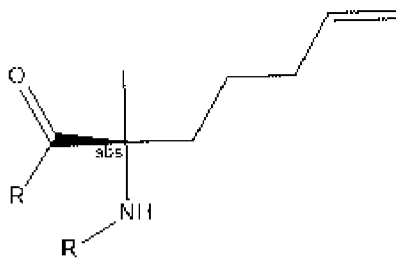
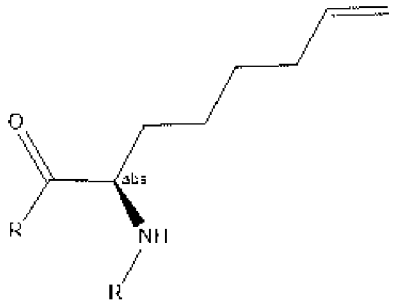
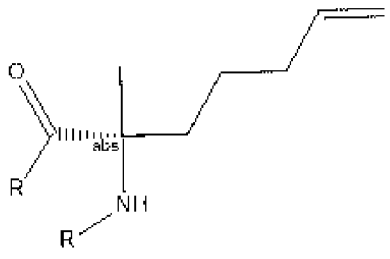
78	BuCO	 C_5H_9OR	CCCCC([R])=O
79	iBuCO	 C_5H_9OR	CC(C)CC([R])=O CC[C@H](C)C([R])=O
80	tBuCO	 C_5H_9OR	CC(C)(C)C([R])=O
81	N(N(Me)2)、NNMe2	 $C_6H_{10}N_2O_2R_2$	CN(C)C(C[C@@H](C([R])=O)N[R])=O
82	MorphCO、2-N-味啉基乙酸	 $C_6H_{10}NO_2R$	O=C(CN1CCOCC1)[R]
83	CON(NMePip)	 $C_6H_{11}N_2OR$	CN(CC1)CCN1C([R])=O

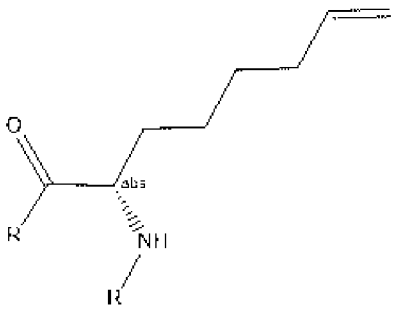
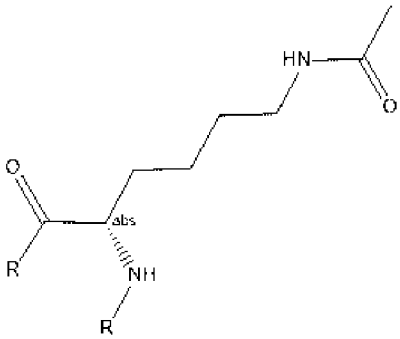
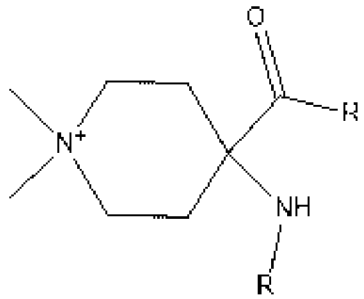
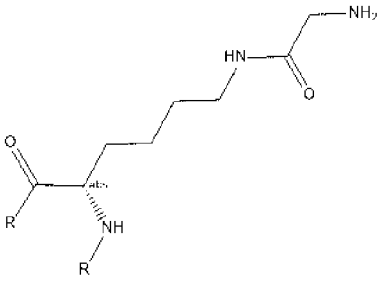
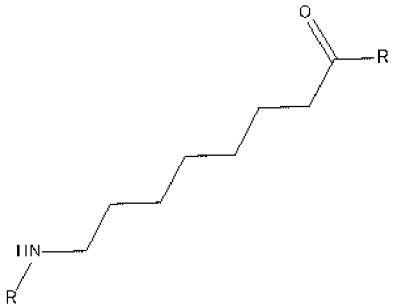
84	eK	 $C_6H_{11}N_2OR_3$	O=C(O)[C@@H](N[R])CCCCN[R]
85	Cit、瓜胺酸	 $C_6H_{11}N_3O_2R_2$	NC(NCCC[C@@H](C([R])=O)N[R])=O N[C@@H](CCCNC(N)=O)C(O)=O
86	D(NEtNH2)	 $C_6H_{11}N_3O_2R_2$	NCCNC(C[C@@H](C([R])=O)N[R])=O
87	Aad、2-胺基己二酸	 $C_6H_{11}NO_4$	N[C@@H](CCCC(O)=O)C(O)=O
88	N(異丁基)Gly	 $C_6H_{11}NOR_2$	CC(C)CN(CC([R])=O)[R]
89	PentCO	 $C_6H_{11}OR$	CCCCCC([R])=O

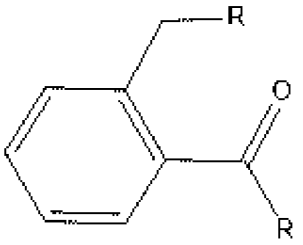
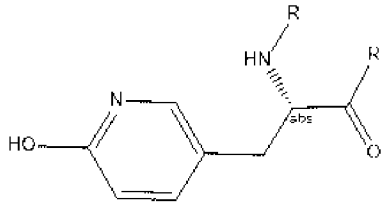
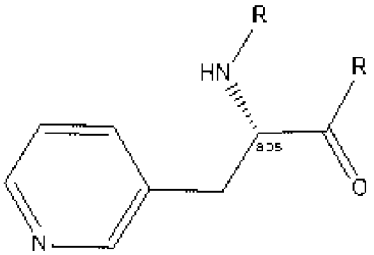
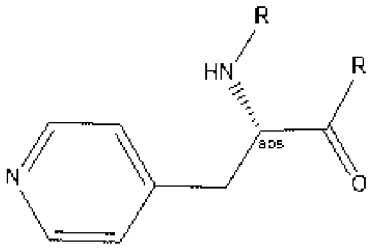
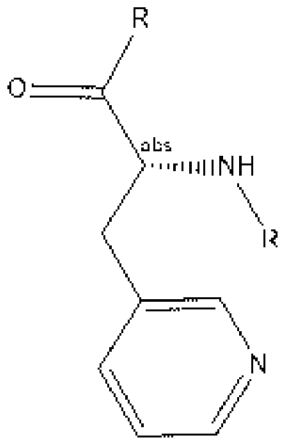
90	NMeQ、NMeGln、N-甲基-麩醯胺酸	 $C_6H_{12}N_2O_3$	CN[C@@H](CCC(N)=O)C(O)=O
91	SP6	 $C_6H_{13}N_2OR_2^+$	C[N+](C)(CCN[R])CC([R])=O C[N+](C)(CCN)CC=O
92	3IOxa4Ala	 $C_6H_6N_2O_2R_2$	O=C([C@H](Cc1conc1)N[R])[R]
93	3Oxa4Ala	 $C_6H_6N_2O_2R_2$	O=C([C@H](Cc1cocn1)N[R])[R]
94	diFCpx	 $C_6H_7F_2NOR_2$	O=C([C@](CC1)(CC1(F)F)N[R])[R]

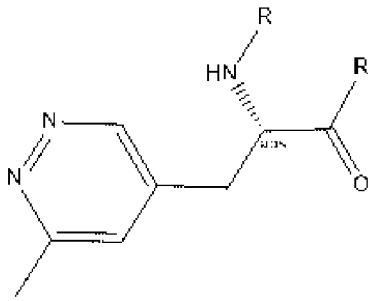
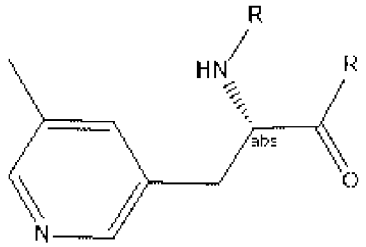
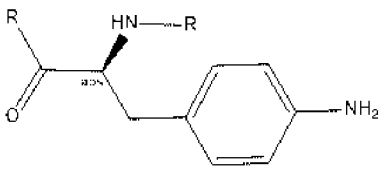
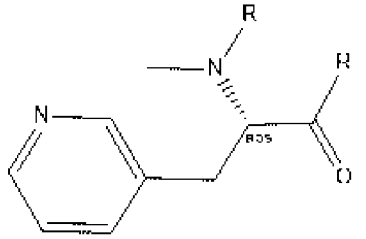
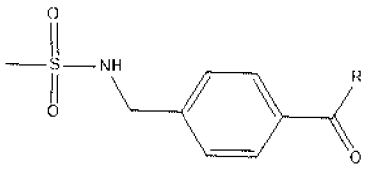
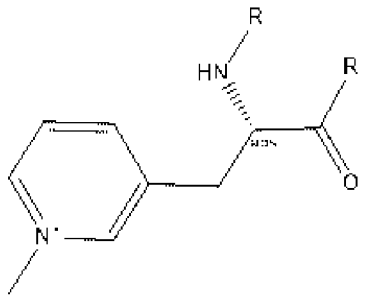
95	aMePra	 $C_6H_7NOR_2$	C[C@](CC#C)(C([R])=O)N[R]
96	CO(二 FPip)	 $C_6H_8F_2NOR$	O=C(N(CC1)CCC1(F)F)[R]
97	dab(COCH2(1*)) dab(COCH2)(1*)	 $C_6H_9N_2O_2R_3$	O=C(C[R])NCC[C@@H](C([R])=O)N[R]
98	四唑(NMe)	 $C_6H_9N_5OR_2$	Cn1nnc(CC[C@@H](C([R])=O)N[R])n1
99			
100	dhE	 $C_6H_9NO_3R_2$	OC(CCC[C@H](C([R])=O)N[R])=O

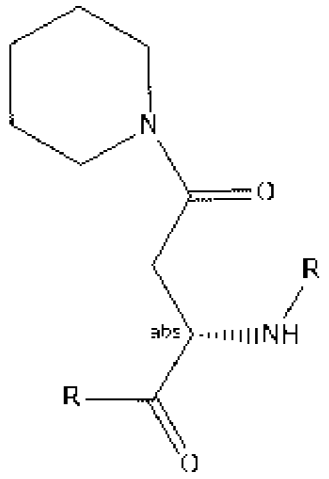
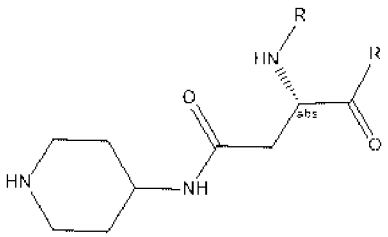
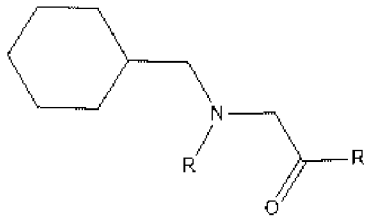
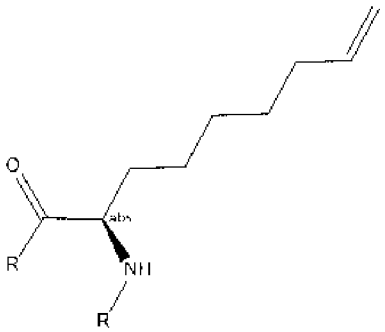
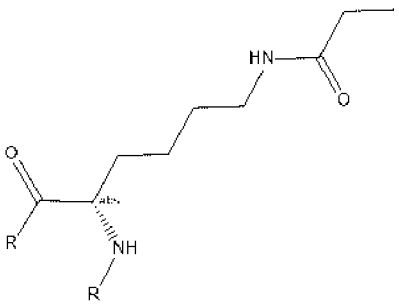
101	Acpx	 $C_6H_9NOR_2$	O=C(C1(CCCC1)N[R])[R] NC1(CCCC1)C=O
102	aMeP、aMePro	 $C_6H_9NOR_2$	C[C@](CCC1)(C([R])=O)N1[R]
103	D(N2AmIm)	 $C_8H_{10}N_4O_2R_2$	O=C(C[C@@H](C([R])=O)N[R])NCc1ncc[nH]1
104	KTfa、K(Tfa)、L-Lys(Tfa)	 $C_8H_{11}F_3N_2O_2R_2$	O=C([C@H](CCCCNC(C(F)(F)F)=O)N[R])[R]
105	E(OAll)	 $C_8H_{11}NO_3R_2$	C=CCOC(CC[C@@H](C([R])=O)N[R])=O

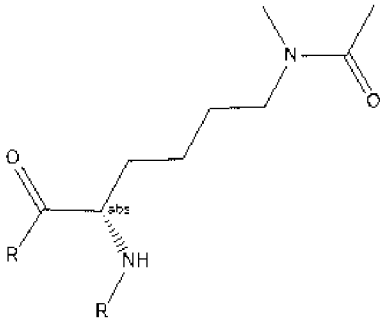
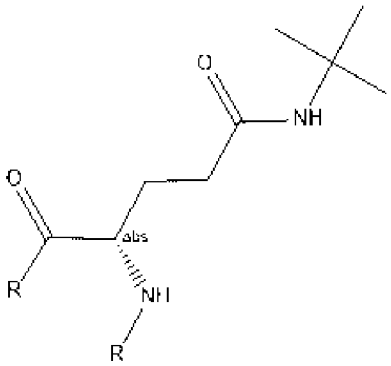
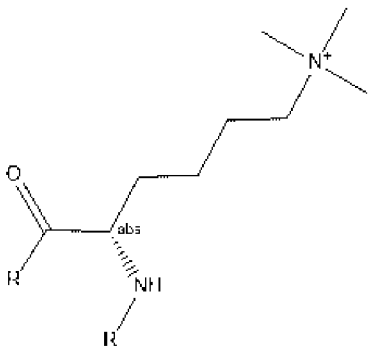
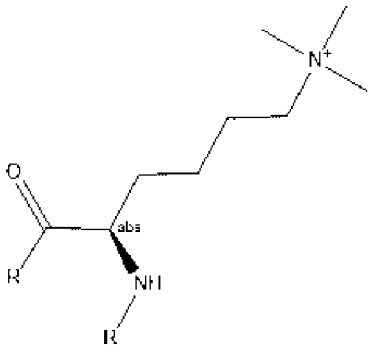
106	D(NPyr)	 $C_8H_{13}N_3O_2R_2$	O=C(C[C@@H](C([R])=O)N[R])NC1CNCC1
107	Chg	 $C_8H_{13}NOR_2$	O=C([C@H](C1CCCCC1)N[R])[R]
108	R5Me、aMeR5H	 $C_8H_{13}NOR_2$	C[C@@](CCCC=C)(C([R])=O)N[R]
109	R6H、(R,E)-2-胺基-8-羥基辛-7-烯酸	 $C_8H_{13}NOR_2$	C=CCCCC[C@H](C([R])=O)N[R]C=CCCCC[C@H](C=O)N
110	S5Me aMeS5H	 $C_8H_{13}NOR_2$	C[C@](CCCC=C)(C([R])=O)N[R]

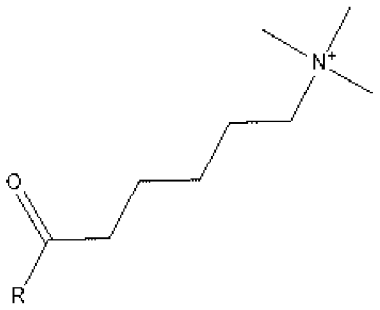
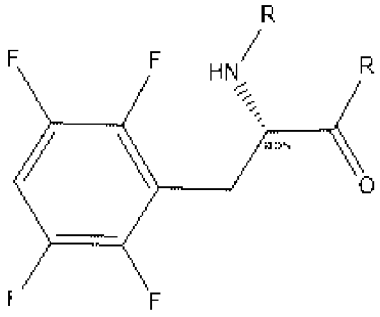
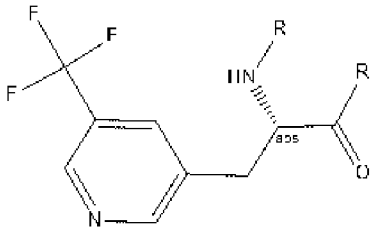
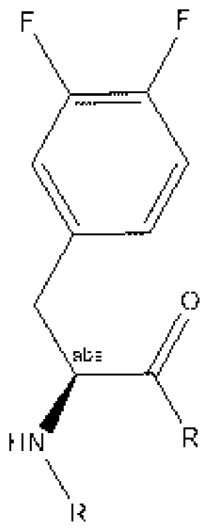
111	S6H	 $C_8H_{13}NOR_2$	C=CCCCC[C@@H](C([R])=O)N[R]
112	KAc、K(Ac)、K(COMe)、K-Ac、N6-乙醯基-L-離胺酸	 $C_8H_{14}N_2O_2R_2$	CC(NCCCC[C@@H](C([R])=O)N[R])=O
113	Pip(NMe2)	 $C_8H_{15}N_2OR_2^+$	C[N+](C)(CC1)CCC1(C([R])=O)N[R]
114	K(Gly)	 $C_8H_{15}N_3O_2R_2$	NCC(NCCCC[C@@H](C([R])=O)N[R])=O
115	8Aoc、8Aoc(2)	 $C_8H_{15}NOR_2$	O=C(CCCCCCCN[R])[R]

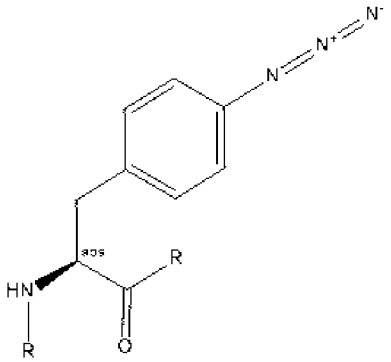
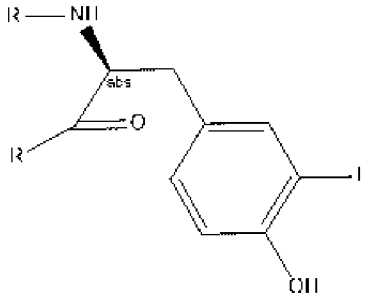
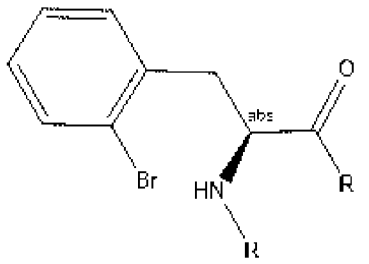
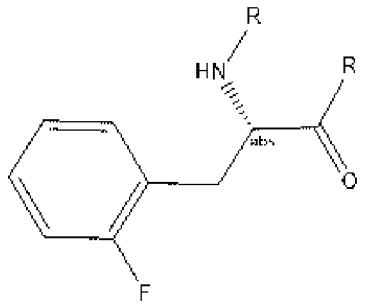
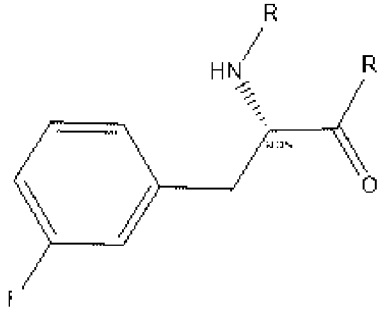
116	2Benzyl	 $C_8H_6OR_2$	O=C(c1c(C[R])ccccc1)[R]
117	6OH3Pya	 $C_8H_8N_2O_2R_2$	Oc1ncc(C[C@@H](C([R])=O)N[R])cc1
118	3Pya、3Pal、3-(2-吡啶基)-丙胺酸	 $C_8H_8N_2OR_2$	O=C([C@H](Cc1ccccc1)N[R])[R]
119	4Pya、4Pya、4Pal、(S)-2-胺基-3-(吡啶-4-基)丙酸 4PyridinAla	 $C_8H_8N_2OR_2$	O=C([C@H](Cc1ccncc1)N[R])[R]
120	dPal、dpal、d3Pya、3pya、3-吡啶基丙胺酸、(R)-2-胺基-3-(吡啶-3-基)丙酸	 $C_8H_8N_2OR_2$	O=C([C@@H](Cc1cnccc1)N[R])[R]

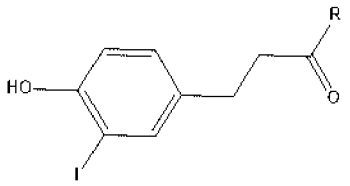
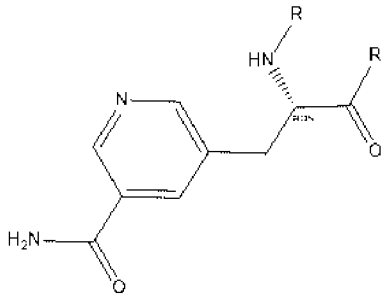
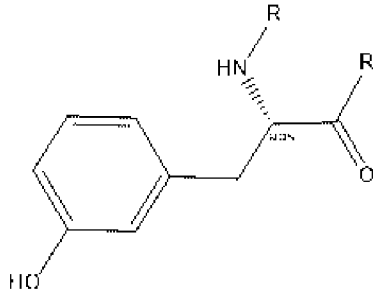
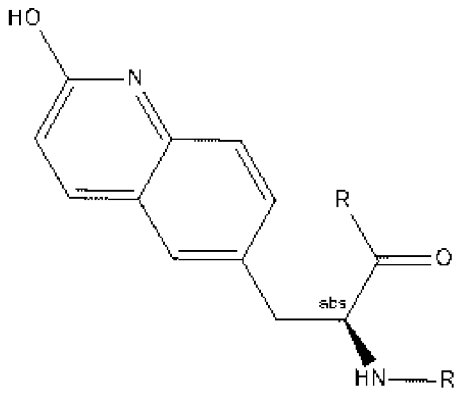
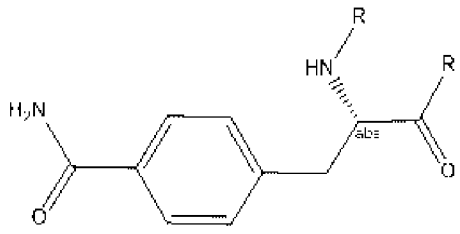
121	6MePyridazAla	 $C_8H_9N_3OR_2$	Cc1 cc(C[C@@H](C([R])=O)N[R])cnn 1
122	5MePyridinAla	 $C_9H_{10}N_2OR_2$	Cc1 cc(C[C@@H](C([R])=O)N[R])cnc 1
123	J、Aph、4-胺基苯基丙胺酸	 $C_9H_{10}N_2OR_2$	Nc1 ccc(C[C@@H](C([R])=O)N[R])cc1
124	NMe3Pya	 $C_9H_{10}N_2OR_2$	CN([C@@H](Cc1cnccc1)C([R])=O)[R] CN[C@@H](Cc1cnccc1)C=O
125	SMSBCO	 $C_9H_{10}NO_3SR$	CS(NCc(cc1)ccc1C([R])=O)(=O)=O
126	Me3Pya	 $C_9H_{11}N_2OR_2^+$	C[n+]1 cccc(C[C@@H](C([R])=O)N[R])c 1

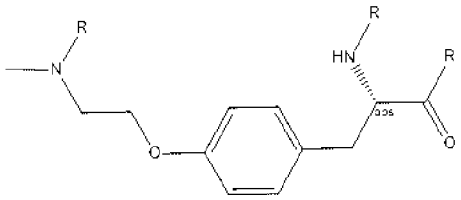
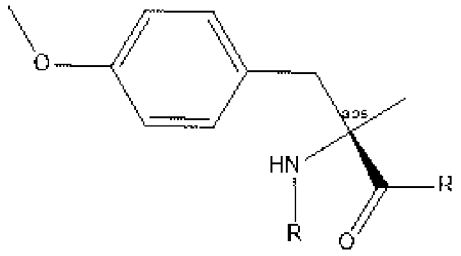
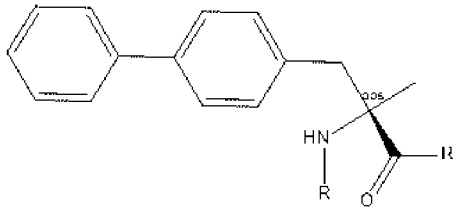
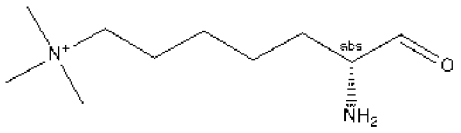
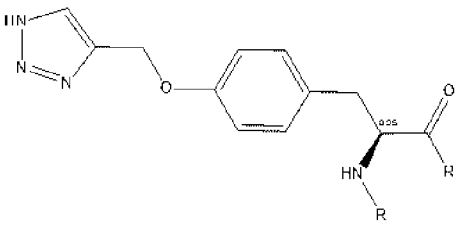
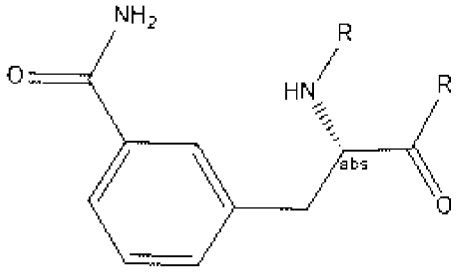
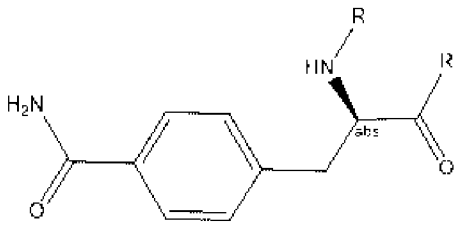
127	D(Pip)、(S)-2-胺基-4-側氧基-4-(哌啶-1-基)丁酸	 $C_9H_{14}N_2O_2R_2$	O=C(C[C@@H](C([R])=O)N[R])N1CCCCC1
128	D(NPip)	 $C_9H_{15}N_3O_2R_2$	O=C(C[C@@H](C([R])=O)N[R])NC1CCNCC1
129	N(環己基)Gly	 $C_9H_{15}NOR_2$	O=C(CN(CC1CCCCC1)[R])[R]
130	R7H、(R,E)-2-胺基-9-羥基壬-8-烯酸	 $C_9H_{15}NOR_2$	C=CCCCCC[C@H](C([R])=O)N[R] C=CCCCCC[C@H](C=O)N
131	K(COEt)	 $C_9H_{16}N_2O_2R_2$	CCC(NCCCC[C@@H](C([R])=O)N[R])=O

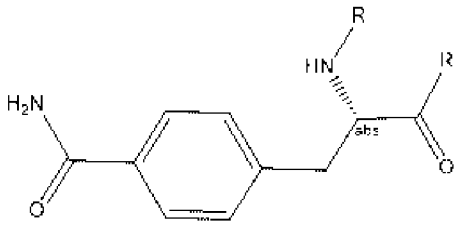
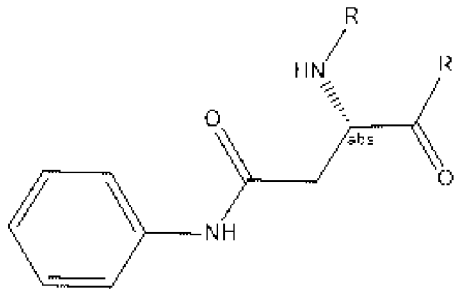
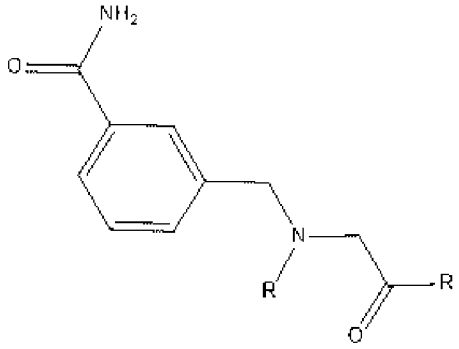
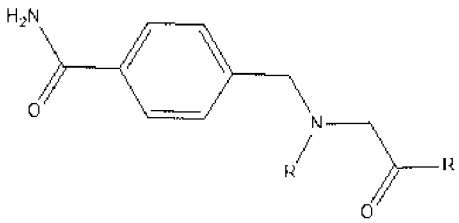
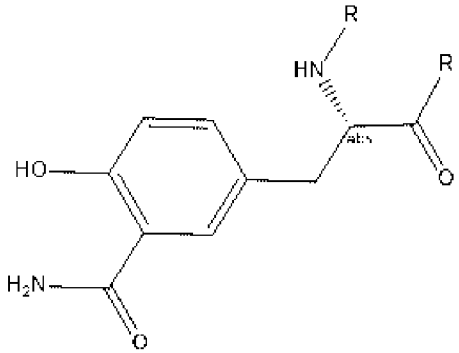
132	K(NMeAc)、KNMeAc	 $C_9H_{16}N_2O_2R_2$	CC(N(C)CCCC[C@@H](C([R])=O)N[R])=O
133	Q(NHtBu)	 $C_9H_{16}N_2O_2R_2$	CC(C)(C)NC(CC[C@@H](C([R])=O)N[R])=O
134	K(Me)3	 $C_9H_{19}N_2OR_2^+$	C[N+](C)(C)CCCC[C@@H](C([R])=O)N[R]
135	dK(Me)3、k(Me)3	 $C_9H_{19}N_2OR_2^+$	C[N+](C)(C)CCCC[C@H](C([R])=O)N[R]

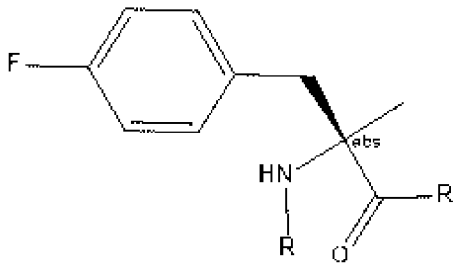
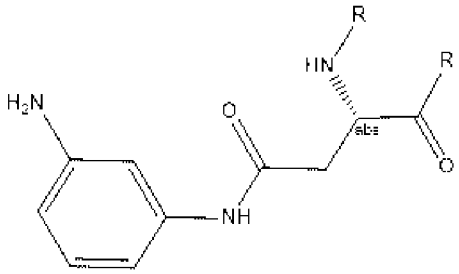
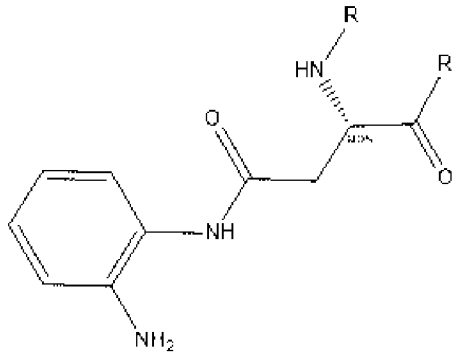
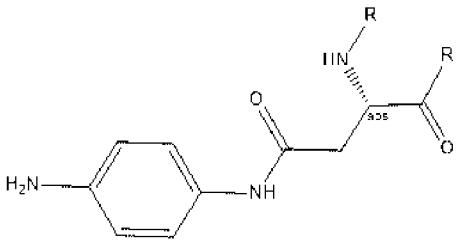
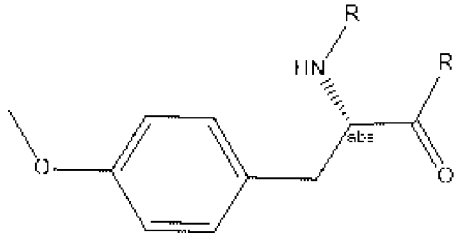
136	5cpaCO	 $C_9H_{19}NOR^+$	C[N+](C)(C)CCCCCC([R])=O
137	tetraFPhe	 $C_9H_5F_4NOR_2$	O=C([C@H](Cc(c(F)c(cc1F)F)c1F)N[R])[R]
138	5CF33Pya	 $C_9H_7F_3N_2OR_2$	O=C([C@H](Cc1cncc(C(F)(F)F)c1)N[R])[R] N[C@@H](Cc1cc(C(F)(F)F)cnc1)C=O
139	3,4diFPhe、4diFPhe	 $C_9H_7F_2NOR_2$	O=C([C@H](Cc(cc1)cc(F)c1F)N[R])[R]

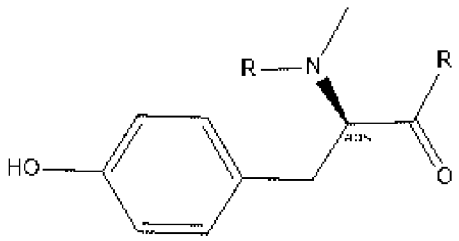
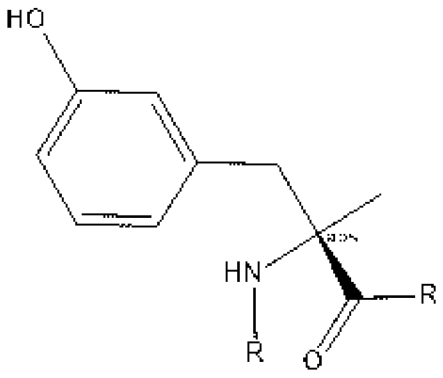
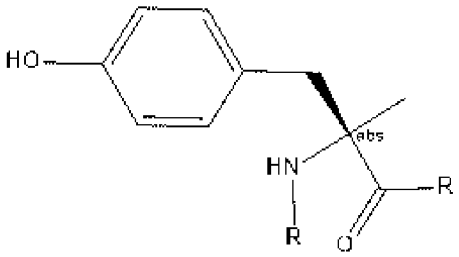
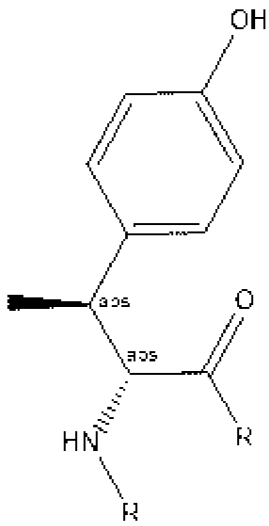
140	F(4N3)	 $C_9H_8N_4OR_2$	[N-]=[N+]=Nc1ccc(C[C@@H](C([R])=O)N[R])cc1
141	3FTyr	 $C_9H_8FNO_2R_2$	Oc(ccc(C[C@@H](C([R])=O)N[R])c1)c1F
142	2BrPhe、2BrF	 $C_9H_8BrNOR_2$	O=C([C@H](Cc(cccc1)c1Br)N[R])[R]
143	2FPHE、2FPhe	 $C_9H_8FNOR_2$	O=C([C@H](Cc(cccc1)c1F)N[R])[R]
144	3FPHE、3FPhe	 $C_9H_8FNOR_2$	O=C([C@H](Cc1cc(F)ccc1)N[R])[R]

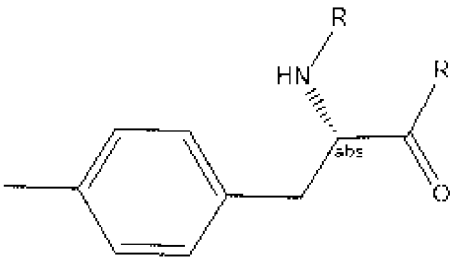
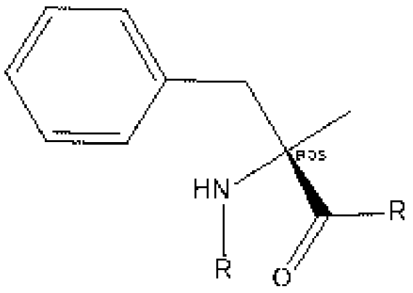
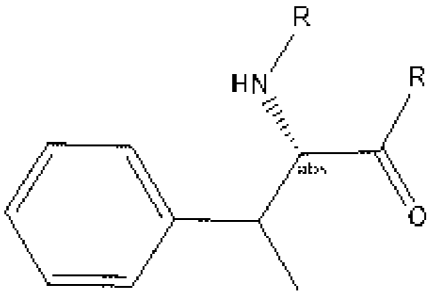
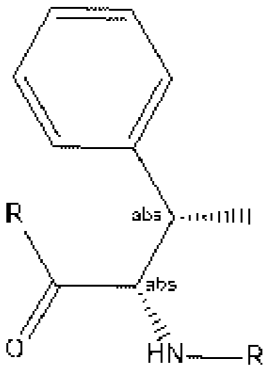
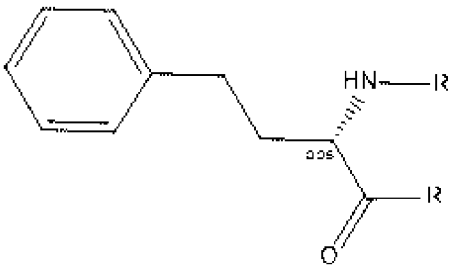
145	BHCO	 $C_9H_8IO_2R$	Oc(ccc(CCC([R])=O)c1)c1I
146	5AmPyridinAla	 $C_9H_9N_3O_2R_2$	NC(c1cc(C[C@@H](C([R])=O)N[R])cnc1)=O
147	mTYR、mY、mTyr	 $C_9H_9NO_2R$	Oc1cccc(C[C@@H](C([R])=O)N[R])c1
148	6OHQuin	 $C_{12}H_{10}N_2O_2R_2$	Oc1ccc(cc(C[C@@H](C([R])=O)N[R])cc2)c2n1
149	4AmF、4AmPhe	 $C_{10}H_{10}N_2O_2R_2$	NC(c1ccc(C[C@@H](C([R])=O)N[R])cc1)=O N[C@@H](Cc(cc1)ccc1C(N)=O)C=O

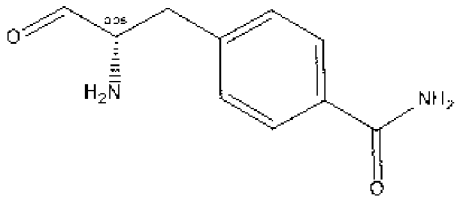
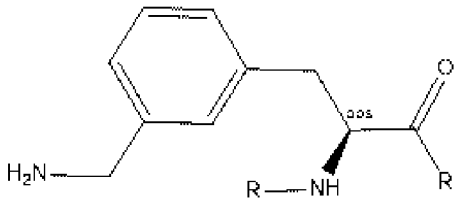
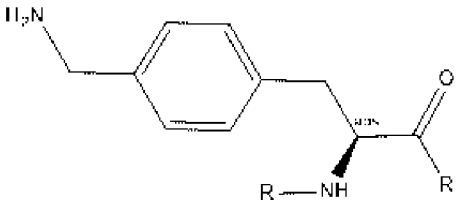
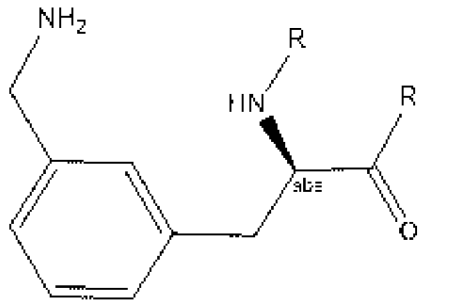
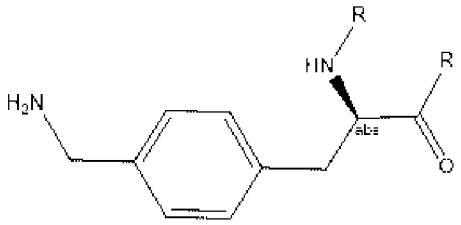
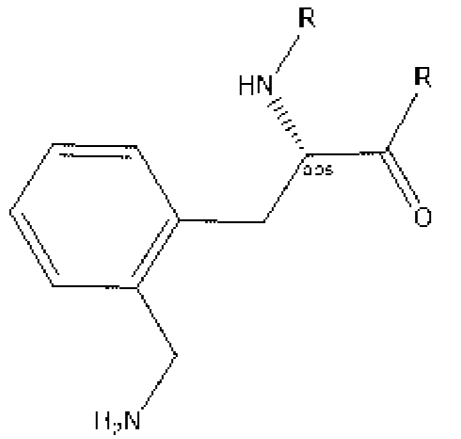
150	AEF(NMe(2))	 $C_{12}H_{15}N_2O_2R_3$	CN(CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)[R]
151	aMeY01	 $C_{11}H_{13}NO_2R_2$	C[C@](Cc(cc1)ccc1OC)(C([R])=O)N[R]
152	BiF	 $C_{16}H_{15}NOR_2$	C[C@](Cc(cc1)ccc1-c1ccccc1)(C([R])=O)N[R]
153	hdKMe3、hk(Me)3	 $C_{10}H_{23}N_2O^+$	C[N+](C)(C)CCCCC[C@H](C=O)N
154	Y(OTzl)	 $C_{12}H_{12}N_4O_2R_2$	O=C([C@H](Cc(cc1)ccc1OCc1c[nH]nn1)N[R])[R]
155	3CONH2F	 $C_{10}H_{10}N_2O_2R_2$	NC(c1cccc(C[C@@H](C([R])=O)N[R])c1)=O
156	4AmDF、4AmDPhe	 $C_{10}H_{10}N_2O_2R_2$	NC(c1ccc(C[C@H](C([R])=O)N[R])cc1)=O

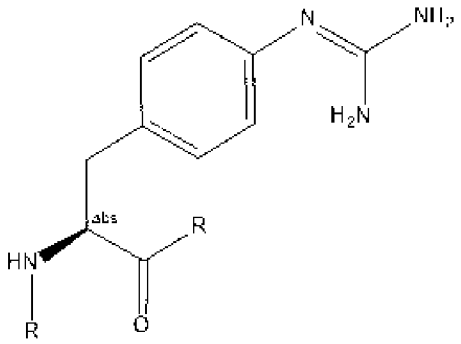
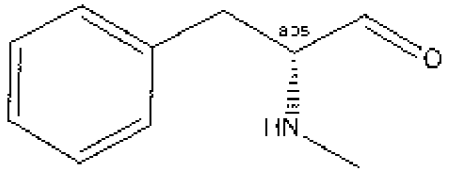
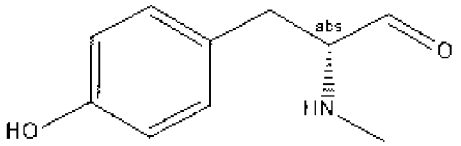
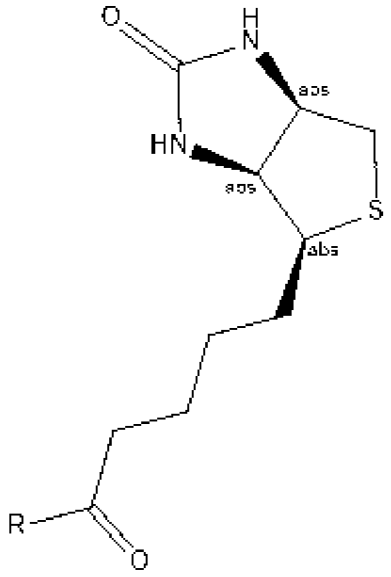
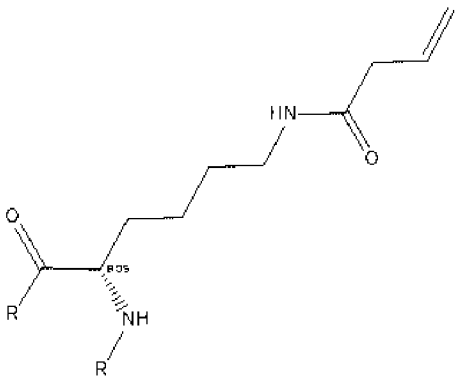
157	4AmF、4AmPhe	 $C_{10}H_{10}N_2O_2R_2$	NC(c1ccc(C[C@@H](C([R])=O)N[R])cc1)=O N[C@@H](Cc(cc1)ccc1C(N)=O)C=O
158	D(NPh)	 $C_{10}H_{10}N_2O_2R_2$	O=C(C[C@@H](C([R])=O)N[R])Nc1 ccccc1
159	N(3Am 苄基)Gly	 $C_{10}H_{10}N_2O_2R_2$	NC(c1cccc(CN(CC([R])=O)[R])c1)=O
160	N(4Am 苄基)Gly	 $C_{10}H_{10}N_2O_2R_2$	NC(c1ccc(CN(CC([R])=O)[R])cc1)=O
161	2AmTyr	 $C_{10}H_{10}N_2O_3R_2$	NC(c(cc(C[C@@H](C([R])=O)N[R])cc1)c1O)=O

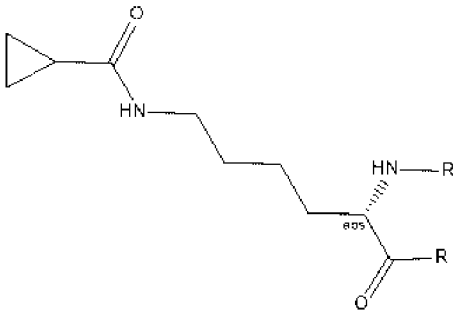
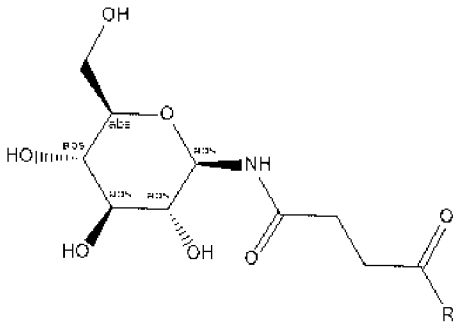
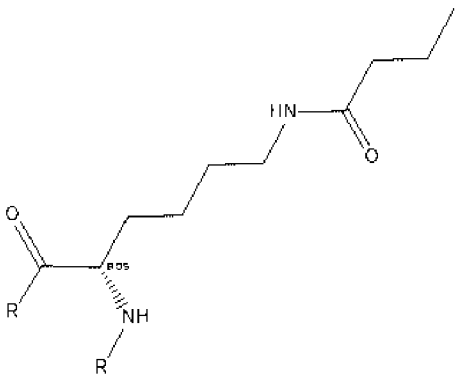
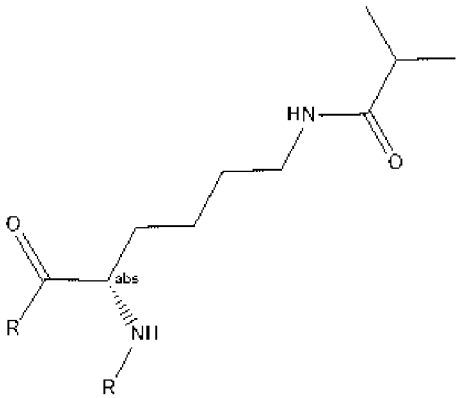
162	aMeFPhe	 $C_{10}H_{10}FNOR_2$	C[C@](Cc(cc1)ccc1F)(C([R])=O)N[R]
163	D(NmAn)	 $C_{10}H_{11}N_3O_2R_2$	Nc1cccc(NC(C[C@@H](C([R])=O)N[R])=O)c1
164	D(NoAn)	 $C_{10}H_{11}N_3O_2R_2$	Nc(cccc1)c1NC(C[C@@H](C([R])=O)N[R])=O
165	D(NpAn)	 $C_{10}H_{11}N_3O_2R_2$	Nc(cc1)ccc1NC(C[C@@H](C([R])=O)N[R])=O
166	4MeOF	 $C_{10}H_{11}NO_2R_2$	COc1ccc(C[C@@H](C([R])=O)N[R])cc1 COc1ccc(C[C@@H](C=O)N)cc1

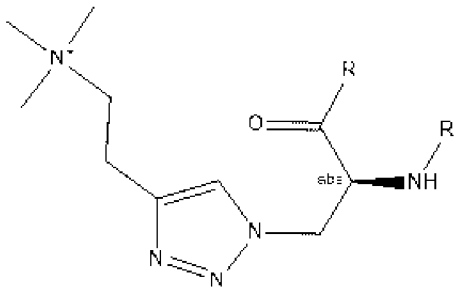
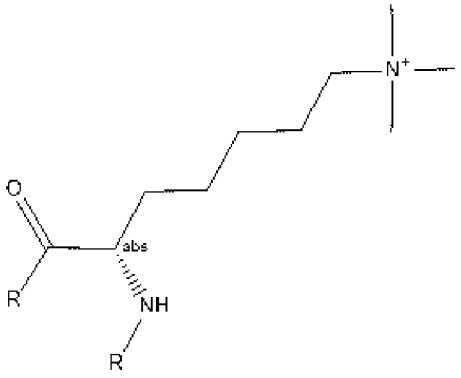
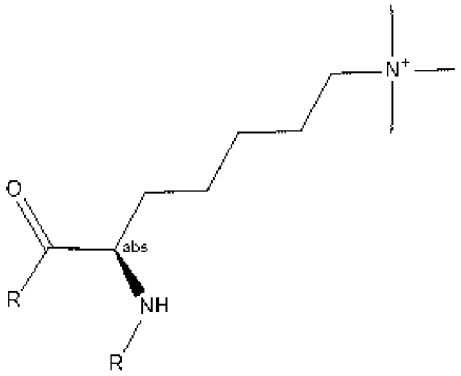
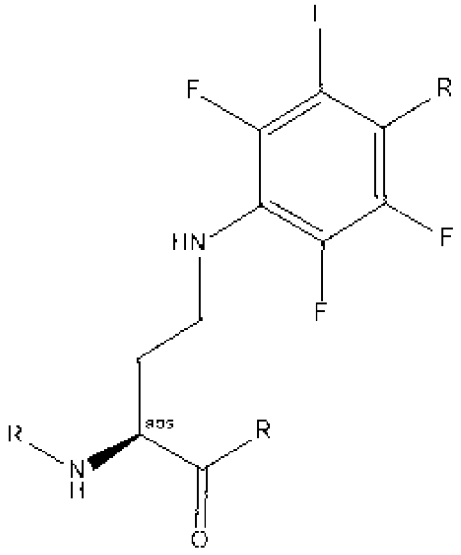
167	NMeDTyr、NMeDY、NMedTyr、NMedY、N-甲基-D-酪胺酸、dNMeTyr dNMeY	 $C_{10}H_{11}NO_2R_2$	CN([C@H](Cc(cc1)ccc1O)C([R])=O)[R]
168	aMe3OHPhe	 $C_{10}H_{11}NO_2R_2$	C[C@](Cc1cc(O)ccc1)(C([R])=O)N[R]
169	aMeY、aMeTyr	 $C_{10}H_{11}NO_2R_2$	C[C@](Cc(cc1)ccc1O)(C([R])=O)N[R]
170	bMeDTyr(2R3S) bMeDTyr(2R,3S)	 $C_{10}H_{11}NO_2R_2$	C[C@H]([C@H](C([R])=O)N[R])c(cc1)ccc1O

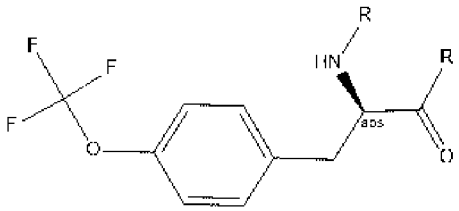
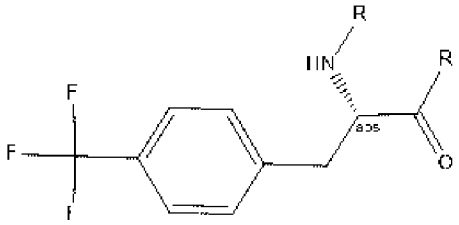
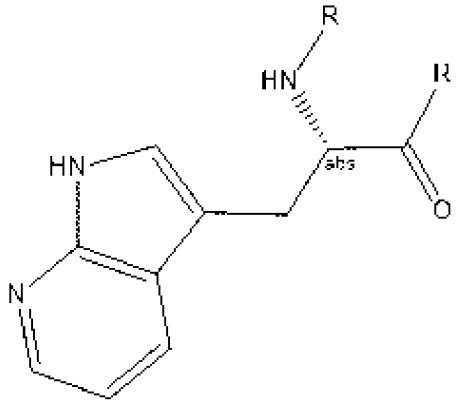
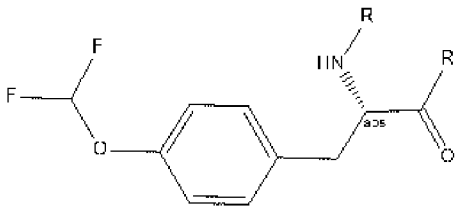
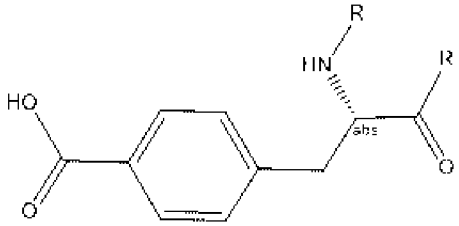
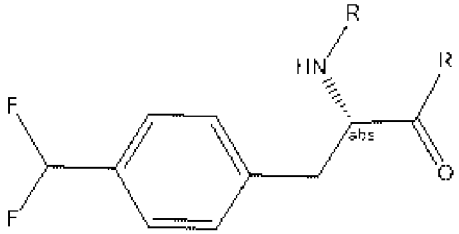
171	4MeF	 $C_{10}H_{11}NOR_2$	Cc1 ccc(C[C@@H](C([R])=O)N[R]) cc1
172	aMeF、aMeF α-甲基苯基丙胺酸	 $C_{10}H_{11}NOR_2$	C[C@](Cc1 ccccc1)(C([R])=O)N[R] C[C@](Cc1 ccccc1)(C=O)N
173	bMePhe	 $C_{10}H_{11}NOR_2$	CC([C@@H](C([R])=O)N[R])c1 ccccc1
174	bMePhe(2S3S) bMePhe(2S,3S)	 $C_{10}H_{11}NOR_2$	C[C@H]([C@@H](C([R])=O)N[R])c1 ccccc1
175	hF、hPhe、homoF、homoPhe	 $C_{10}H_{11}NOR_2$	O=C([C@H](CCc1 ccccc1)N[R])[R]

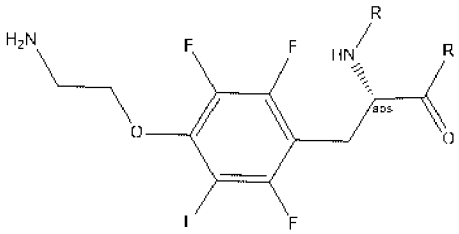
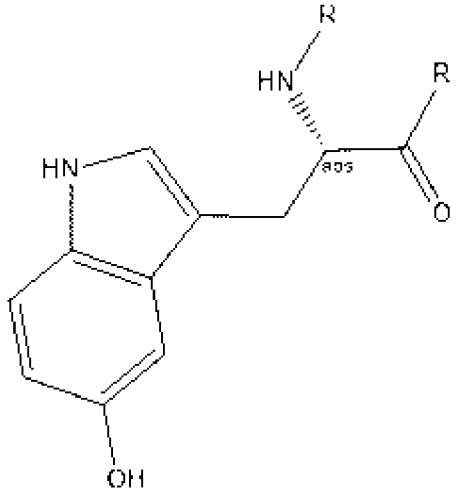
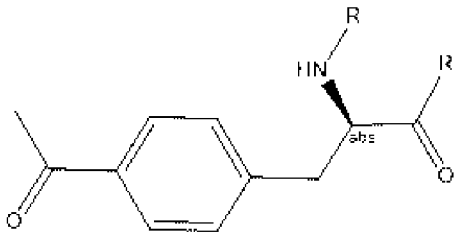
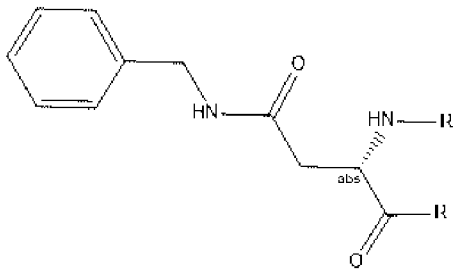
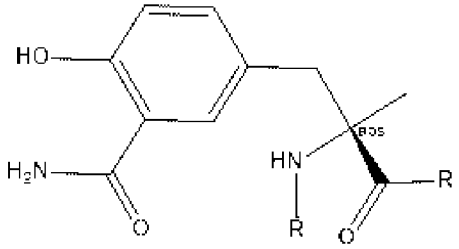
176	F4CONH2、4-胺甲醯基-L-苯基丙胺酸	 $C_{10}H_{12}N_2O_2$	N[C@@H](Cc(cc1)ccc1C(N)=O)C=O
177	Maf	 $C_{10}H_{12}N_2OR_2$	NCc1ccccc(C[C@@H](C([R])=O)N[R])c1
178	Paf	 $C_{10}H_{12}N_2OR_2$	NCc1ccc(C[C@@H](C([R])=O)N[R])cc1 NCc1ccc(C[C@@H](C=O)N)cc1
179	dMaf、maf	 $C_{10}H_{12}N_2OR_2$	NCc1ccccc(C[C@H](C([R])=O)N[R])c1
180	dPaf	 $C_{10}H_{12}N_2OR_2$	NCc1ccc(C[C@H](C([R])=O)N[R])cc1
181	oAMPhe	 $C_{10}H_{12}N_2OR_2$	NCc1c(C[C@@H](C([R])=O)N[R])cccc1

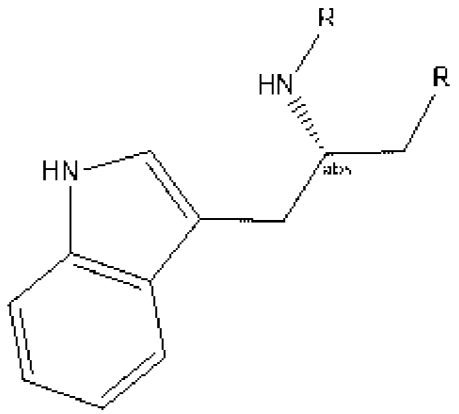
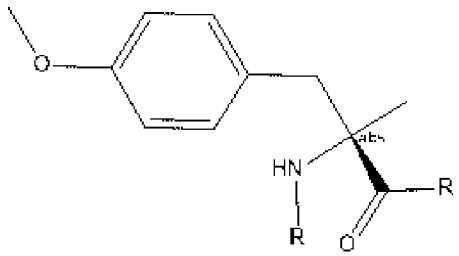
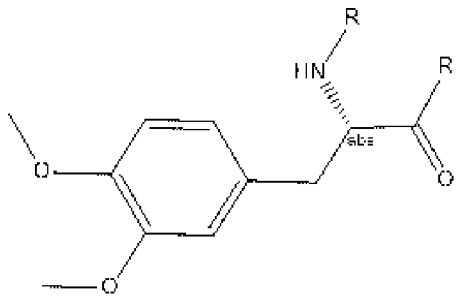
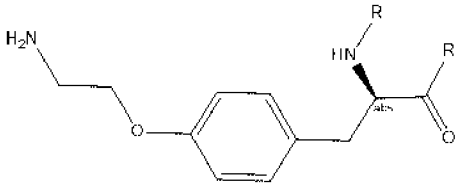
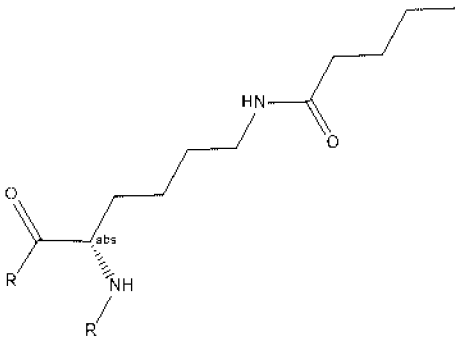
182	F(4G)	 $C_{10}H_{12}N_4OR_2$	NC(N)=Nc1ccc(C[C@@H](C([R])=O)N[R])cc1
183	NMeDTyr	 $C_{10}H_{13}NO$	CN[C@H](Cc1ccccc1)C=O
184	dNMeTyr dNMeY、D-N-甲基酪胺酸 N-甲基-D-酪胺酸	 $C_{10}H_{13}NO_2$	CN[C@H](Cc(cc1)ccc1O)C=O
185	生物素	 $C_{10}H_{15}N_2O_2SR$	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)[R]
186	K(CO2allyl)	 $C_{10}H_{16}N_2O_2R_2$	C=CCC(NCCCC[C@@H](C([R])=O)N[R])=OC=CCOC(NCCCC[C@@H](C([R])=O)N[R])=O

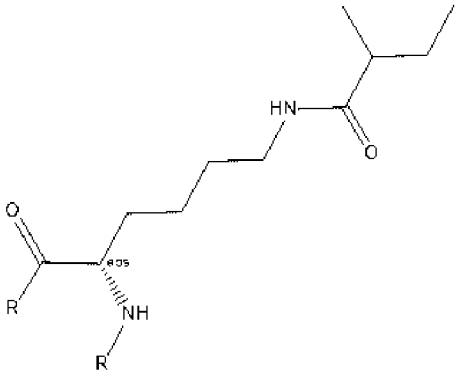
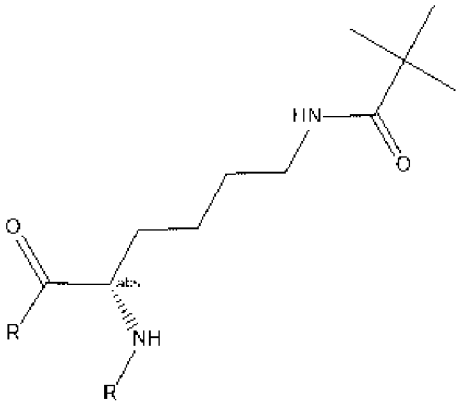
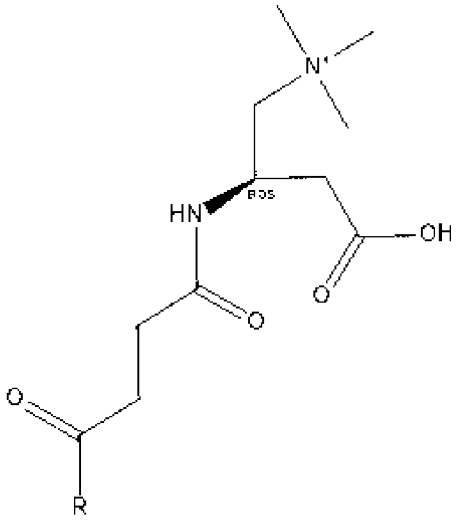
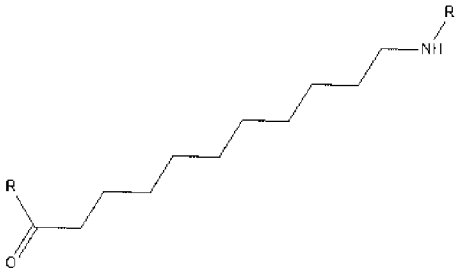
187	K(COcPr)	 $C_{10}H_{16}N_2O_2R_2$	O=C([C@H](CCCCNC(C1CC1)=O)N[R])[R]
188	DAGSuc	 $C_{10}H_{16}NO_7R$	OC[C@H]([C@H]([C@@H]([C@H]1O)O)O)O[C@H]1NC(CCC([R])=O)=O
189	K(COPr)	 $C_{10}H_{18}N_2O_2R_2$	CCCC(NCCCC[C@@H](C([R])=O)N[R])=O
190	K(COiPr)	 $C_{10}H_{18}N_2O_2R_2$	CC(C)C(NCCCC[C@@H](C([R])=O)N[R])=O

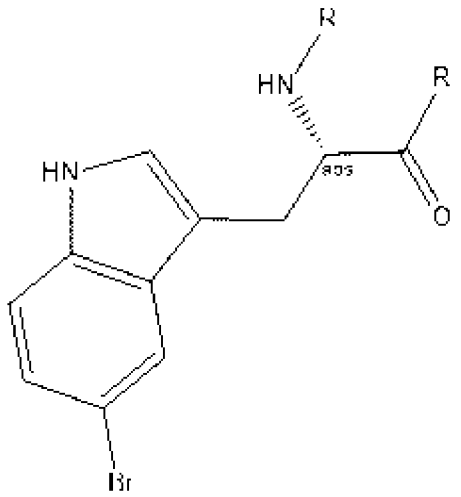
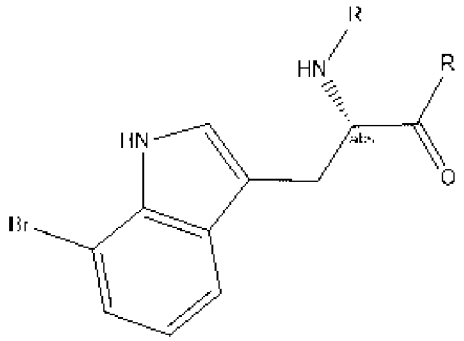
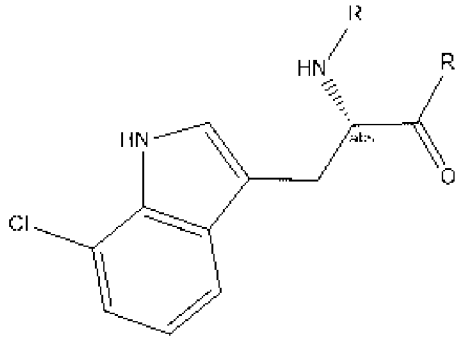
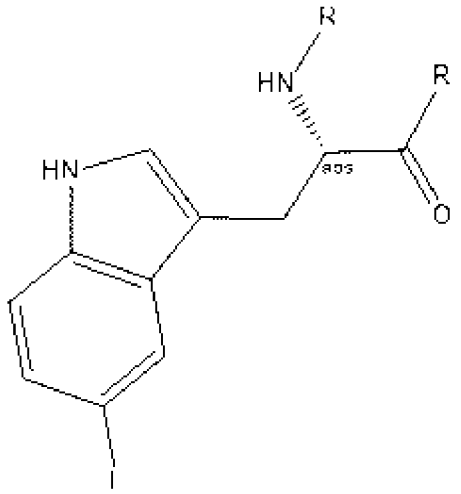
191	Tzl(Ch)	 $C_{10}H_{18}N_5OR_2^+$	C[N+](C)(C)CCc1cn(C[C@@H](C([R])=O)N[R])nn1
192	hK(Me)3、hKMe3	 $C_{10}H_{21}N_2OR_2^+$	C[N+](C)(C)CCCCC[C@@H](C([R])=O)N[R]
193	hdK(Me)3、hk(Me)3、hdKMe3	 $C_{10}H_{21}N_2OR_2^+$	C[N+](C)(C)CCCCC[C@H](C([R])=O)N[R]
194	Dap(pF(6))	 $C_{10}H_7F_4N_2OR_3$	O=C([C@H](CCNc(c(F)c(c([R])c1F)F)c1F)N[R])[R]

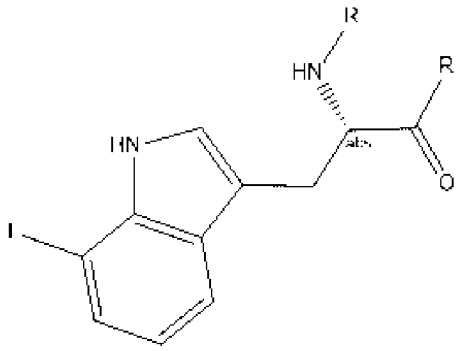
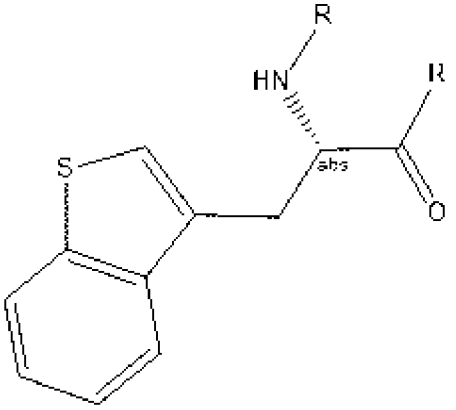
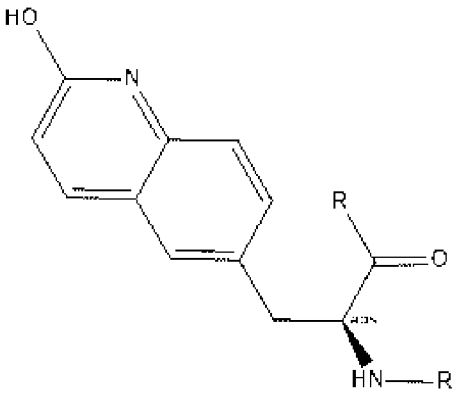
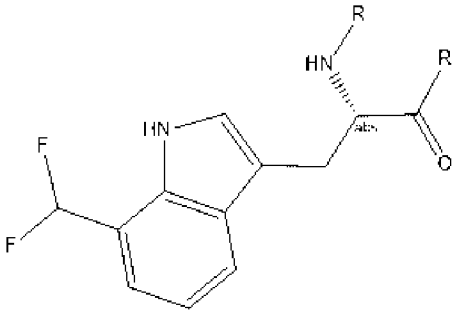
195	4OCF3DPhe	 $C_{10}H_8F_3NO_2R_2$	O=C([C@@H](Cc(cc1)ccc1OC(F)(F)F)N[R])[R]
196	CF3F	 $C_{10}H_8F_3NOR_2$	O=C([C@H](Cc1 ccc(C(F)(F)F)cc1)N[R])[R]
197	7AzaW	 $C_{10}H_9N_3OR_2$	O=C([C@H](Cc1c[nH]c2c1 cccn2)N[R])[R]
198	Y(CHF2)	 $C_{10}H_9F_2NO_2R_2$	O=C([C@H](Cc(cc1)ccc1OC(F)F)N[R])[R]
199	CXF	 $C_{10}H_9NO_3R_2$	OC(c1 ccc(C[C@@H](C([R])=O)N[R])cc1)=O
200	CHF2Phe	 $C_{10}H_9F_2NOR_2$	O=C([C@H](Cc1 ccc(C(F)F)cc1)N[R])[R]

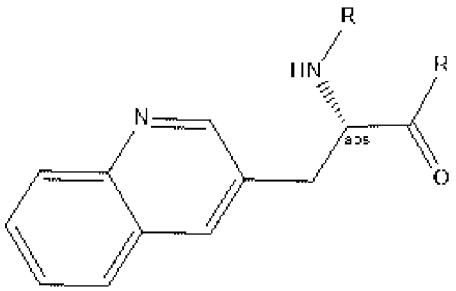
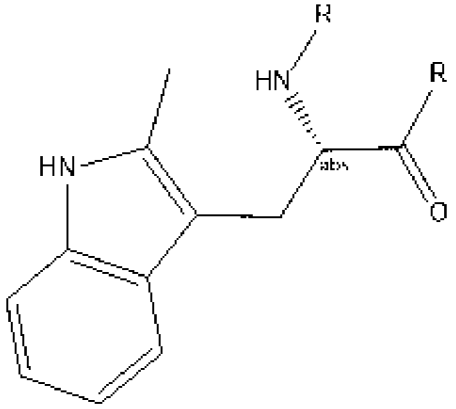
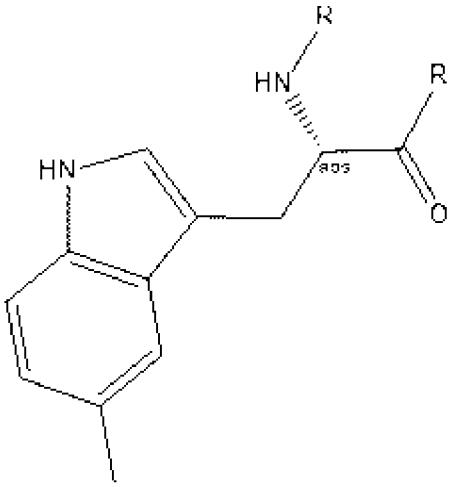
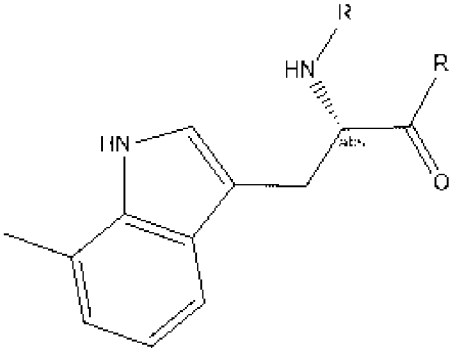
201	TetraFAEF	 $C_{11}H_{10}F_4N_2O_2R_2$	NCCOc(c(F)c(c(C[C@@H](C([R])=O)N[R])c1F)F)c1F
202	5OHW	 $C_{11}H_{10}N_2O_2R_2$	Oc(cc1)cc2c1[nH]cc2C[C@@H](C([R])=O)N[R]
203	4AcDPhe	 $C_{11}H_{11}NO_2R_2$	CC(c1ccc(C[C@H](C([R])=O)N[R])cc1)=O
204	D(NBzl)	 $C_{11}H_{12}N_2O_2R_2$	O=C(C[C@@H](C([R])=O)N[R])NCc1 ccccc1
205	aMe2AmTyr	 $C_{11}H_{12}N_2O_3R_2$	C[C@](Cc(cc1)cc(C(N)=O)c1O)(C([R])=O)N[R]

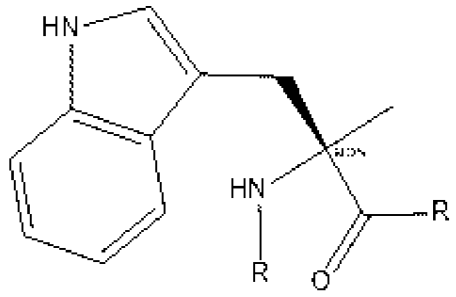
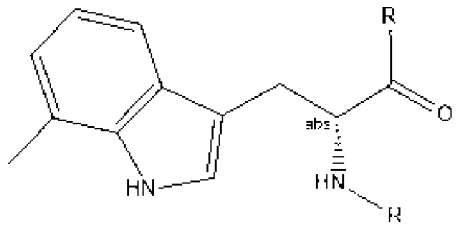
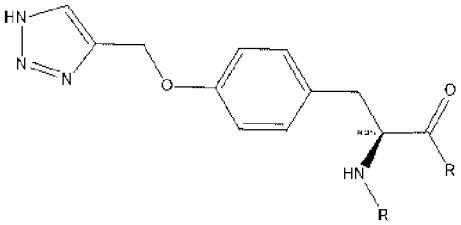
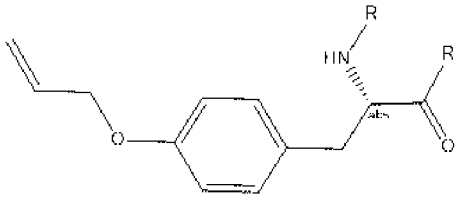
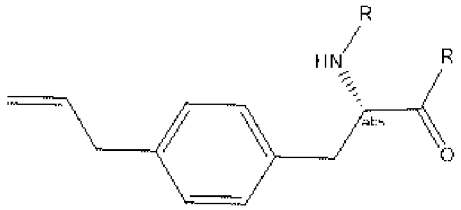
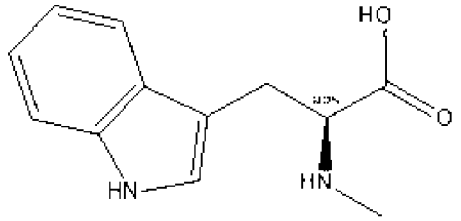
206	psiW	 $C_{11}H_{12}N_2R_2$	[R]C[C@H](Cc1c[nH]c2c1cccc2)N[R]
207	aMeY01	 $C_{11}H_{13}NO_2R_2$	C[C@](Cc(cc1)ccc1OC)(C([R])=O)N[R]
208	3OMeY01	 $C_{11}H_{13}NO_3R_2$	COc(ccc(C[C@@H](C([R])=O)N[R])c1)c1OC
209			
210	dAEF	 $C_{11}H_{14}N_2O_2R_2$	NCCOc1ccc(C[C@H](C([R])=O)N[R])cc1
211	K(COBu)	 $C_{11}H_{20}N_2O_2R_2$	CCCCC(NCCCC[C@@H](C([R])=O)N[R])=O

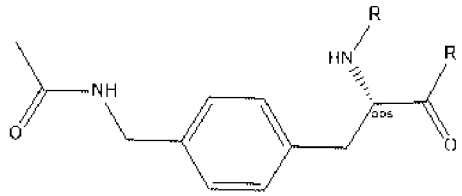
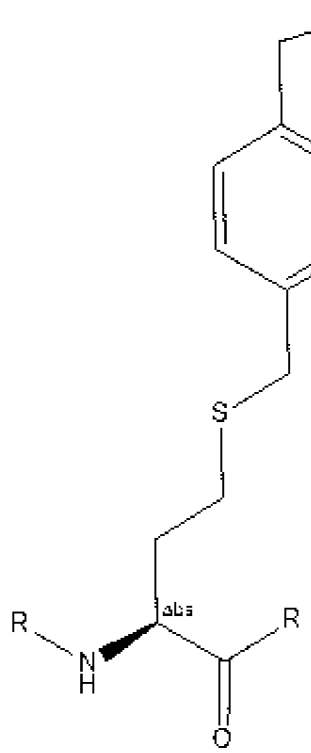
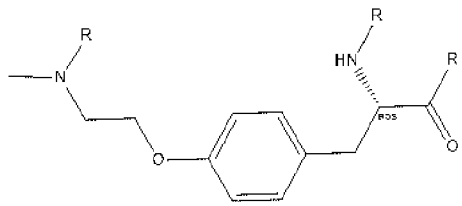
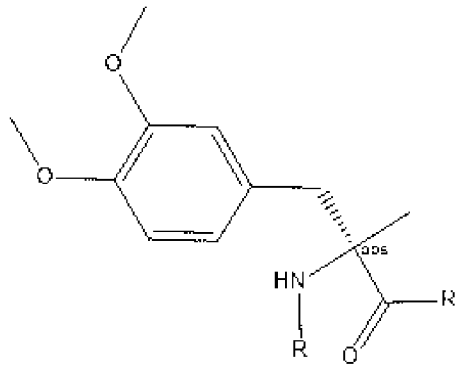
212	K(COiBu)	 $C_{11}H_{20}N_2O_2R_2$	CCC(C)C(NCCCC[C@@H](C([R])=O)N[R])=OCC(C)CC(NCCCC[C@@H](C([R])=O)N[R])=O
213	K(COtBu)	 $C_{11}H_{20}N_2O_2R_2$	CC(C)(C)C(NCCCC[C@@H](C([R])=O)N[R])=O
214	succiniccarn	 $C_{11}H_{20}N_2O_4R^+$	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CCC([R])=O)=O
215	Aun	 $C_{11}H_{21}NOR_2$	O=C(CCCCCCCCCCN[R])[R]

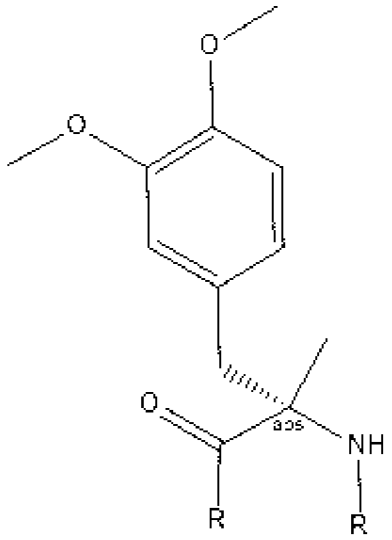
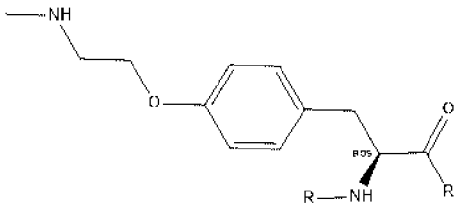
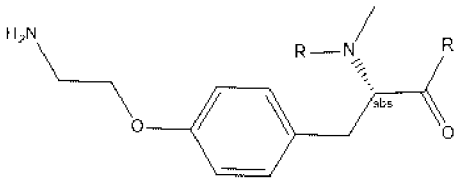
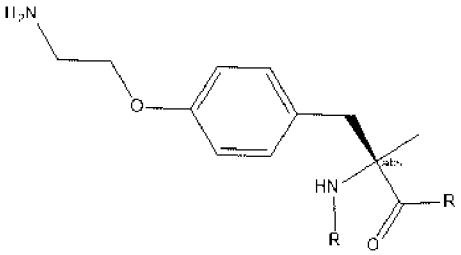
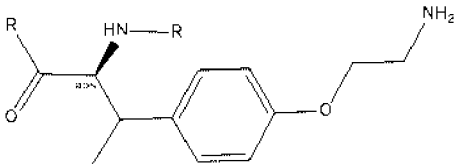
216	5BrW、5BrTrp	 $C_{11}H_9BrN_2OR_2$	O=C([C@H](Cc1c[nH]c(cc2)c1cc2Br)N[R])[R]
217	7BrTrp、7BrW	 $C_{11}H_9BrN_2OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2Br)N[R])[R]
218	7ClW、7ClTrp	 $C_{11}H_9ClN_2OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2Cl)N[R])[R]
219	5FW、5FTrp	 $C_{11}H_9FN_2OR_2$	O=C([C@H](Cc1c[nH]c(cc2)c1cc2F)N[R])[R]

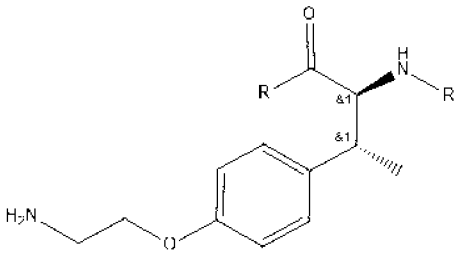
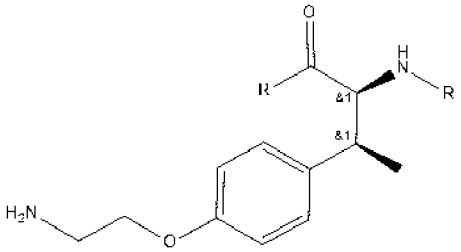
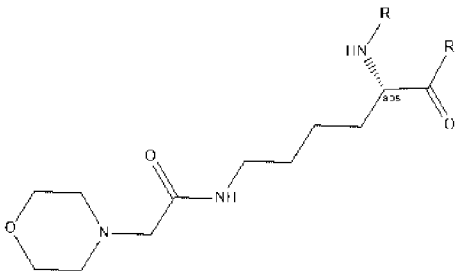
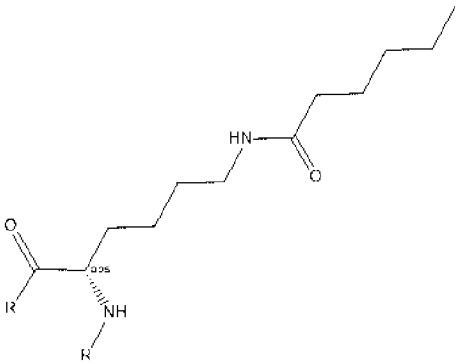
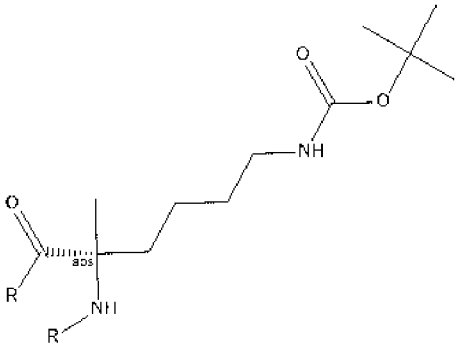
220	7FW、7FTrp	 $C_{11}H_9FN_2OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2F)N[R])[R]
221	BT、L-3-苯并噻吩基丙胺酸	 $C_{11}H_9NOSR_2$	O=C([C@H](Cc1csc2c1cccc2)N[R])[R]
222	2Quin 6OHQui	 $C_{12}H_{10}N_2O_2R_2$	Oc1ccc(cc(C[C@@H](C([R])=O)N[R])cc2)c2n1
223	7CF2H	 $C_{12}H_{10}F_2N_2OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2C(F)F)N[R])[R]

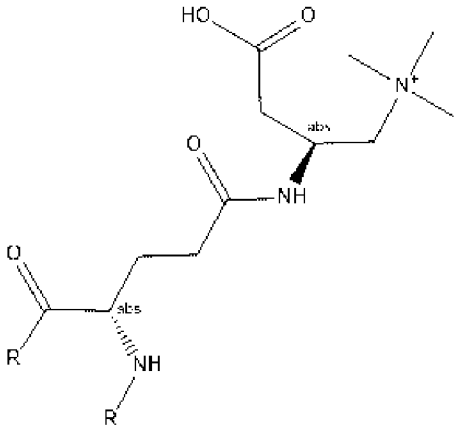
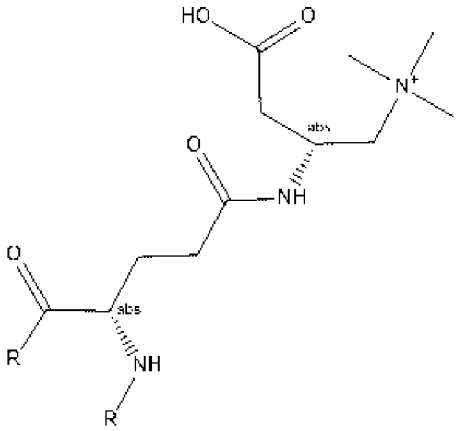
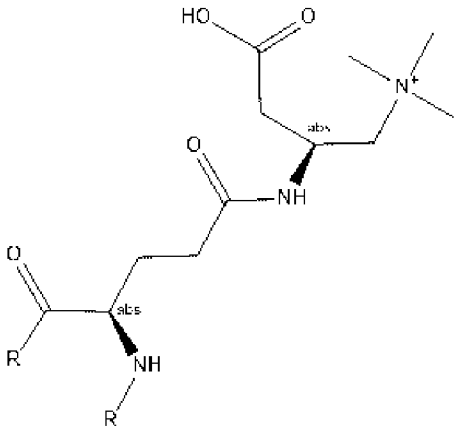
224	3QuinolAla	 $C_{12}H_{10}N_2OR_2$	O=C([C@H](Cc 1 cc2 ccccc2nc1)N[R]) [R]
225	2MeTrp、2MeW	 $C_{12}H_{12}N_2OR_2$	Cc1c(C[C@@H] (C([R])=O)N[R]) c(cccc2)c2[nH]1
226	5MeW、5MeTrp	 $C_{12}H_{12}N_2OR_2$	Cc(cc1)cc2c1[n H]cc2C[C@@H] (C([R])=O)N[R]
227	7MeW、 7(MeW)、7MeTrp	 $C_{12}H_{12}N_2OR_2$	Cc1 cccc2c1[nH]cc2 C[C@@H](C([R])=O)N[R] Cc1 cccc2c1[nH]cc2 C[C@@H](C=O)N

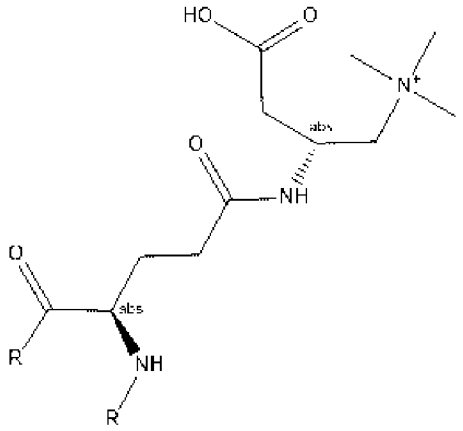
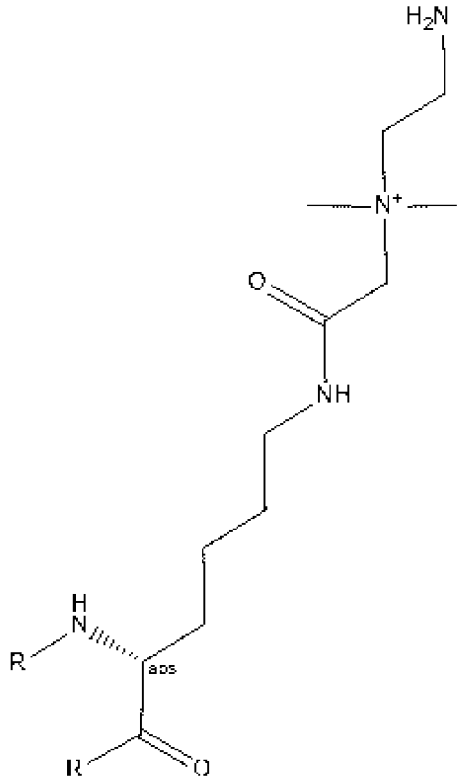
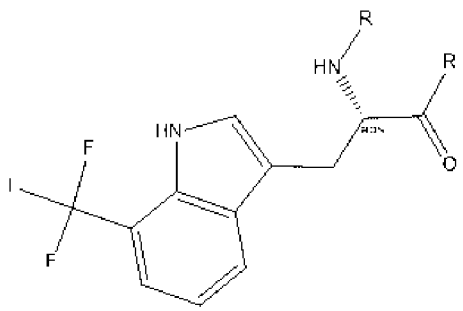
228	aMeW	 $C_{12}H_{12}N_2OR_2$	C[C@](Cc1c[nH]c2c1 cccc2)(C([R])=O)N[R]
229	dW7Me、7Mew、7MedW	 $C_{12}H_{12}N_2OR_2$	Cc1 cccc2c1[nH]cc2 C[C@H](C([R])=O)N[R]
230	Y(OTzl)	 $C_{12}H_{12}N_4O_2R_2$	O=C([C@H](Cc(cc1)ccc1OCc1c[nH]nn1)N[R])[R]
231	4AllylY	 $C_{12}H_{13}NO_2R_2$	C=CCOc1 ccc(C[C@@H](C([R])=O)N[R])cc1
232	4AllylF	 $C_{12}H_{13}NOR_2$	C=CCc1 ccc(C[C@@H](C([R])=O)N[R])cc1
233	meW、NMeW、NMeTrp、N-甲基-色胺酸	 $C_{12}H_{14}N_2O_2$	CN[C@@H](Cc1c[nH]c2c1 cccc2)C(O)=O

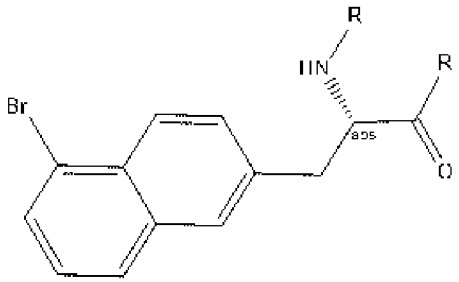
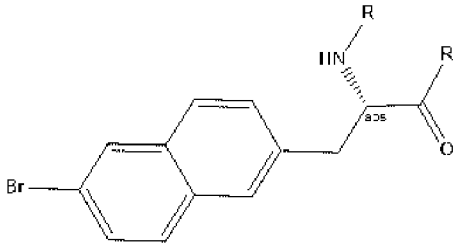
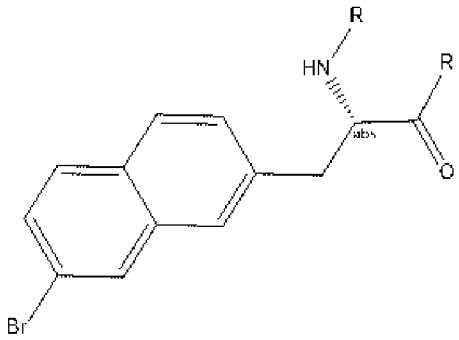
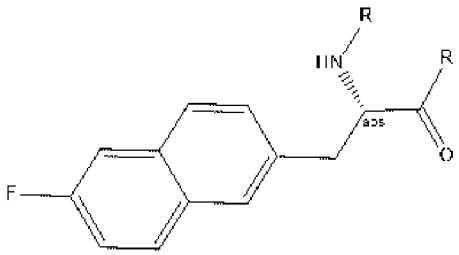
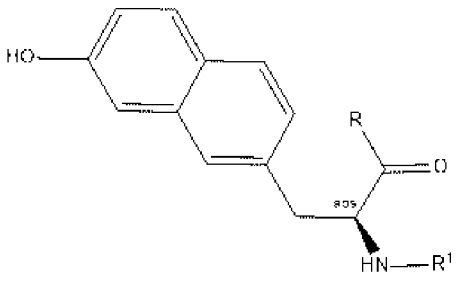
234	AAMPhe	 $C_{12}H_{14}N_2O_2R_2$	CC(NCc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O CC(NCc1ccc(C[C@@H](C=O)N)cc1)=O
235	hC(pXyl)	 $C_{12}H_{14}NOSR_3$	O=C([C@H](CCSCc1ccc(C[R])cc1)N[R])[R]
236	AEF(NMe(2))	 $C_{12}H_{15}N_2O_2R_3$	CN(CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)[R]
237	DY02	 $C_{12}H_{15}NO_3R_2$	C[C@@](Cc(cc1)cc(OC)c1OC)(C([R])=O)N[R]

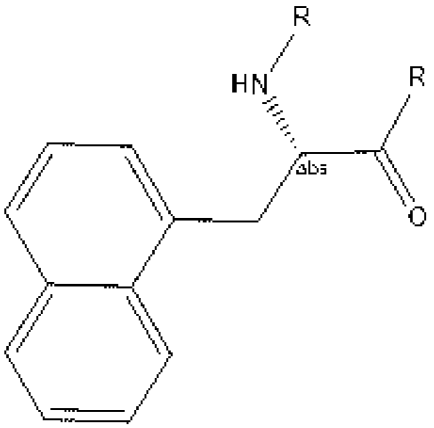
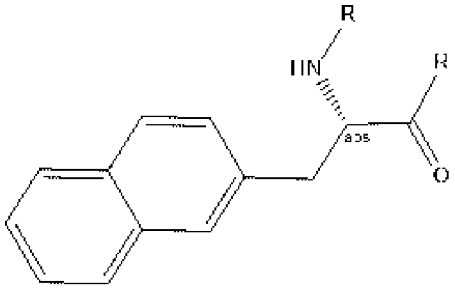
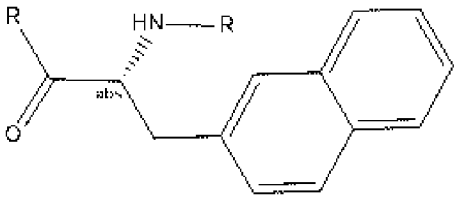
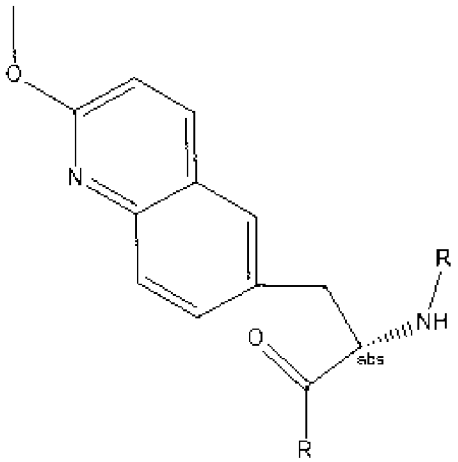
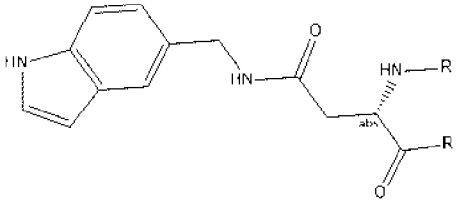
238	Y02	 $C_{12}H_{15}NO_3R_2$	C[C@](Cc(cc1)cc(OC)c1OC)(C([R])=O)N[R]
239	AEF(NMe)	 $C_{12}H_{16}N_2O_2R_2$	CNCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
240	NMeAEF	 $C_{12}H_{16}N_2O_2R_2$	CN([C@@H](Cc(cc1)ccc1OCCN)C([R])=O)[R] CN[C@@H](Cc(cc1)ccc1OCCN)C=O
241	aMeAEF	 $C_{12}H_{16}N_2O_2R_2$	C[C@](Cc(cc1)ccc1OCCN)(C([R])=O)N[R] CC(C)(C)OC(NCCOc1ccc(C[C@@](C)(C([R])=O)N[R])cc1)=O
242	bMeAEF	 $C_{12}H_{16}N_2O_2R_2$	CC([C@@H](C([R])=O)N[R])c(cc1)ccc1OCCN

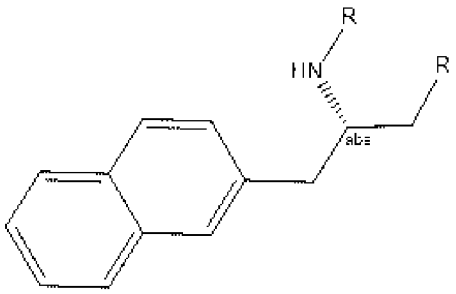
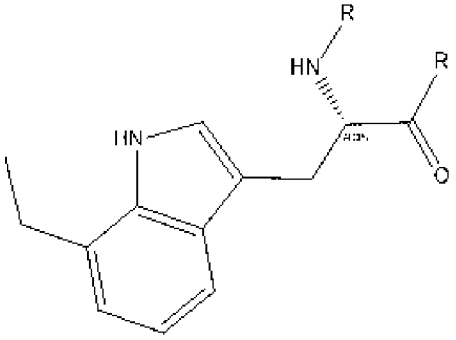
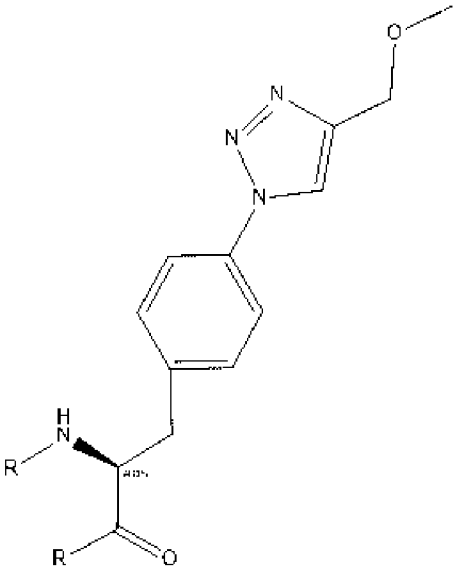
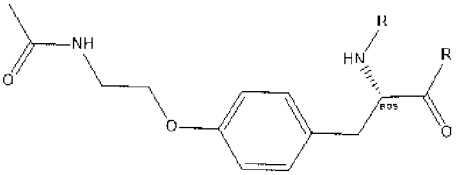
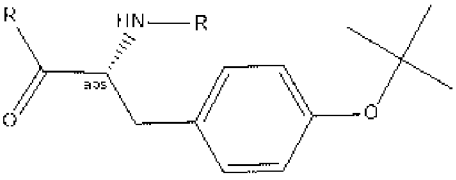
243	bMeAEF(2S,3R*)、bMeAEF(2S3R*)（*純的但組態未知）	 $C_{12}H_{16}N_2O_2R_2$	C[C@@H]([C@@H](C([R])=O)N[R])c(cc1)ccc1OCCN
244	bMeAEF(2S3S*)、bMeAEF(2S,3S*)（*純的但組態未知）	 $C_{12}H_{16}N_2O_2R_2$	C[C@H]([C@@H](C([R])=O)N[R])c(cc1)ccc1OCCN
245	K(Morph)	 $C_{12}H_{21}N_3O_3R_2$	O=C(CN1CCOCC1)NCCCC[C@@H](C([R])=O)N[R]
246	K(COPent)	 $C_{12}H_{22}N_2O_2R_2$	CCCCCC(NCCCC[C@@H](C([R])=O)N[R])=O
247	aMeK(Boc)	 $C_{12}H_{22}N_2O_3R_2$	CC(C)(C)OC(NCCCC[C@@](C)(C([R])=O)N[R])=O

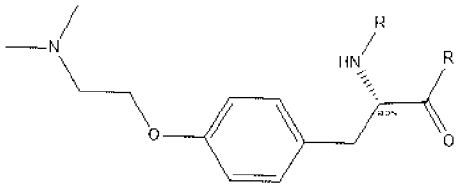
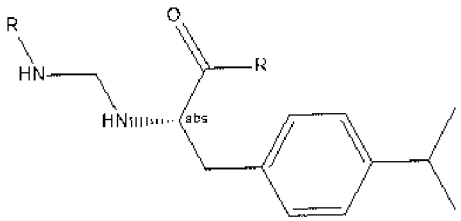
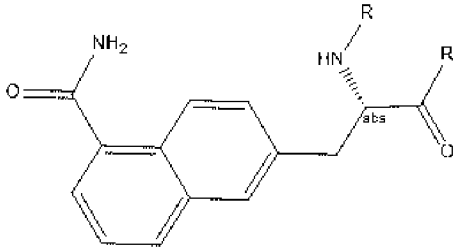
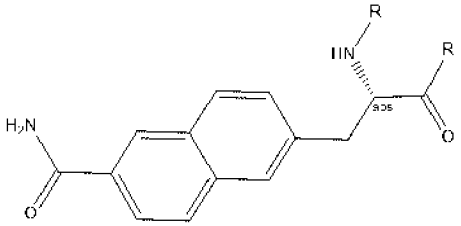
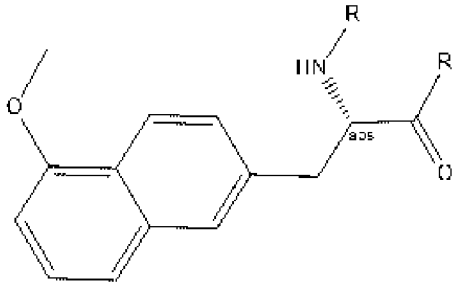
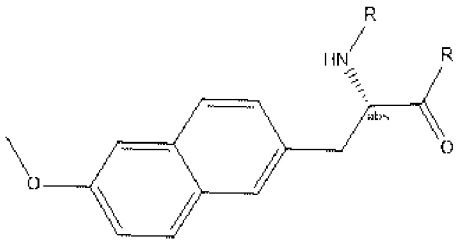
248	E(C)	 $C_{12}H_{22}N_3O_4R_2^+$	C[N+](C)(C)C[C@H](CC(O)=O)NC(CC[C@@H](C([R])=O)N[R])=O
249	E(c) (R)-2-((R)-4-胺基-4-羧基丁醯胺基)-3-羧基-N,N,N-三甲基丙-1-銨鹽、E(c)	 $C_{12}H_{22}N_3O_4R_2^+$	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CC[C@@H](C([R])=O)N[R])=O
250	e(C)、dE(C)	 $C_{12}H_{22}N_3O_4R_2^+$	C[N+](C)(C)C[C@H](CC(O)=O)NC(CC[C@H](C([R])=O)N[R])=O

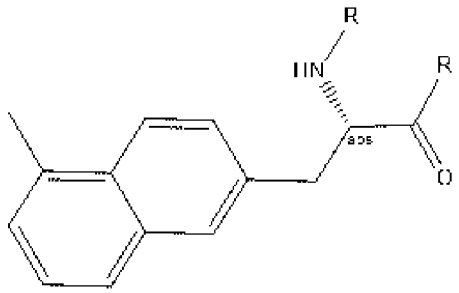
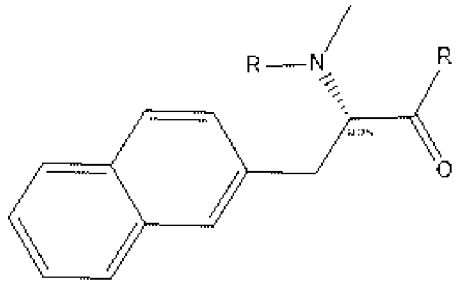
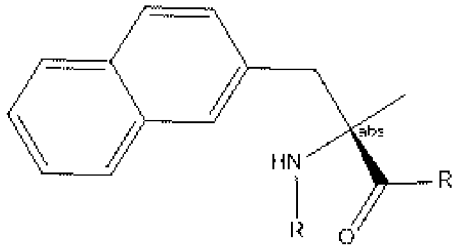
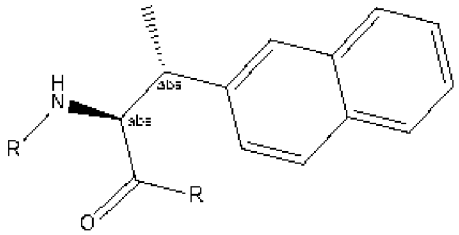
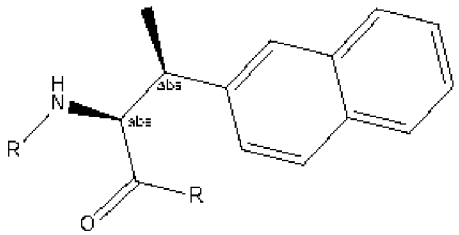
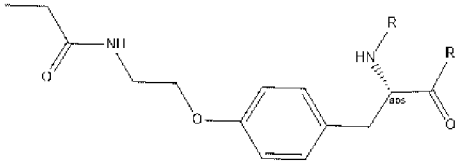
251	e(c)、dE(c)	 $C_{12}H_{22}N_3O_4R_2^+$	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CC[C@H](C([R])=O)N[R])=O
252	dK(SP6)、k(SP6)	 $C_{12}H_{25}N_4O_2R_2^+$	C[N+](C)(CCN)CC(NCCCC[C@H](C([R])=O)N[R])=O
253	7CF3W、(S)-2-胺基-3-(7-(三氟甲基)-1H-吲哚-3-基)丙酸	 $C_{12}H_9F_3N_2OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2C(F)(F)F)N[R])[R] N[C@@H](Cc1c[nH]c2c(C(F)(F)F)cccc12)C=O N[C@@H](Cc1c[nH]c2c(C(F)(F)F)cccc12)C=O

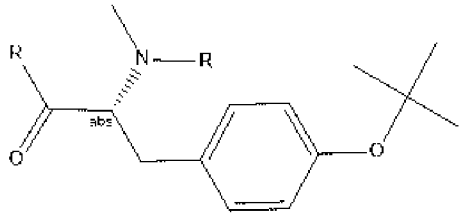
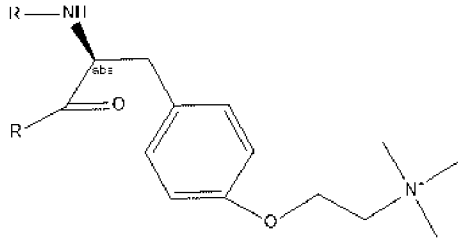
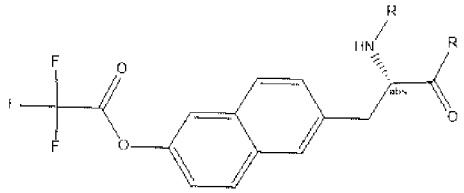
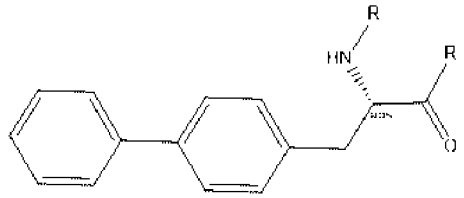
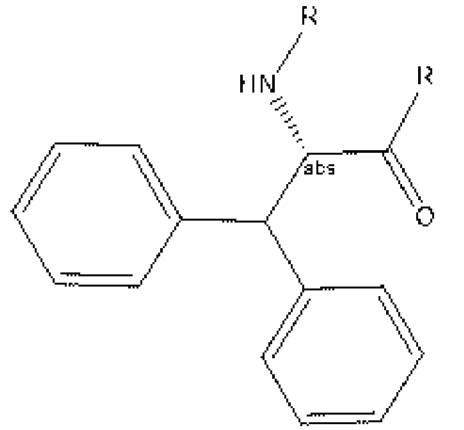
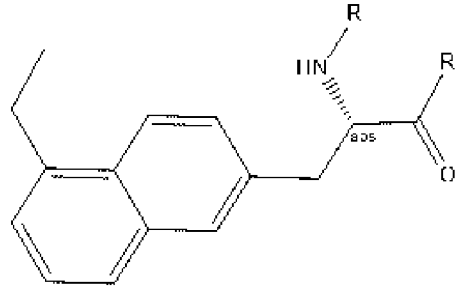
254	5Br2Nal	 $C_{13}H_{10}BrNOR_2$	O=C([C@H](Cc 1 cc2 cccc(Br)c2 cc1)N[R])[R]
255	6Br2Nal	 $C_{13}H_{10}BrNOR_2$	O=C([C@H](Cc (ccc1c2)cc1 ccc2Br)N[R])[R]
256	7Br2Nal	 $C_{13}H_{10}BrNOR_2$	O=C([C@H](Cc 1 cc2 cc(Br)ccc2 cc1)N[R])[R]
257	6F2Nal	 $C_{13}H_{10}FNOR_2$	O=C([C@H](Cc (ccc1c2)cc1 ccc2F)N[R])[R] N[C@@H](Cc1 ccc(cc(cc2)F)c2c 1)C=O
258	7OH2Nal	 $C_{13}H_{11}NO_2R_2$	Oc1 ccc(ccc(C[C@@ H](C([R])=O)N[R1])c2)c2c1

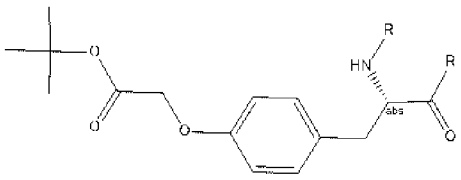
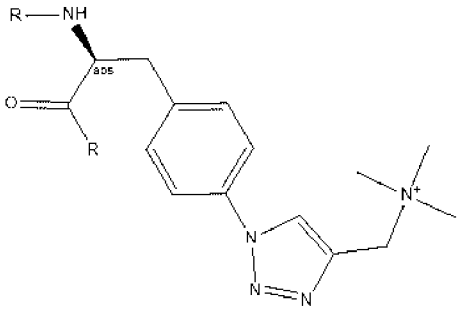
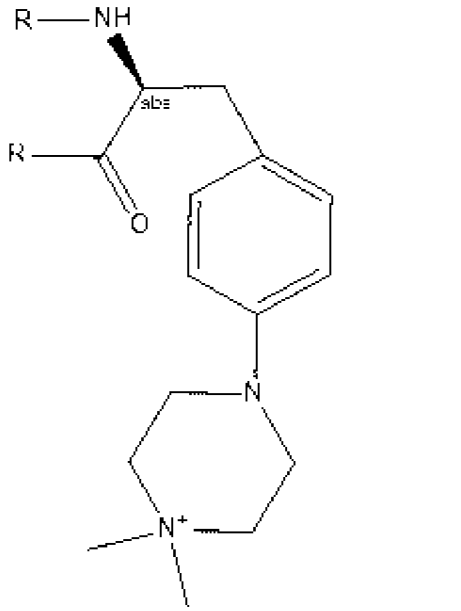
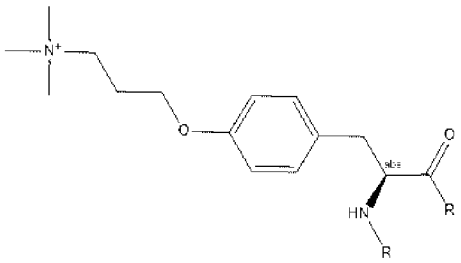
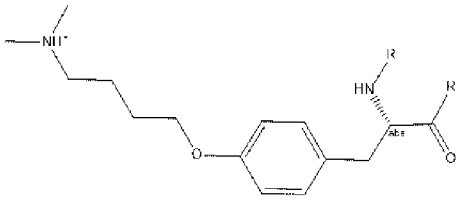
259	1Nal、Nal,	 $C_{13}H_{11}NOR_2$	O=C([C@H](Cc1 cccc2 ccccc12)N[R])[R]
260	2Nal	 $C_{13}H_{11}NOR_2$	O=C([C@H](Cc1 cc2 ccccc2 cc1)N[R])[R]
261	dNal、d2Nal	 $C_{13}H_{11}NOR_2$	O=C([C@@H](Cc1 cc2 ccccc2 cc1)N[R])[R]
262	6MeQui	 $C_{13}H_{12}N_2O_2R_2$	COc1 ccc(cc(C[C@@H](C([R])=O)N[R])cc2)c2n1
263	D(N5In)	 $C_{13}H_{13}N_3O_2R_2$	O=C(C[C@@H](C([R])=O)N[R])NCc(cc1)cc2c1[nH]cc2

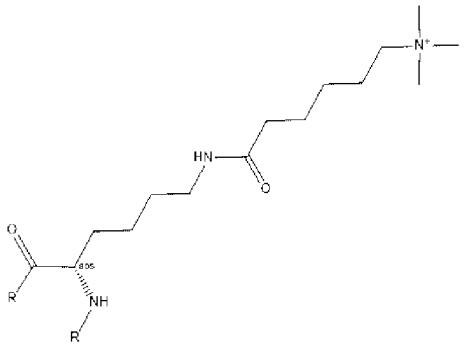
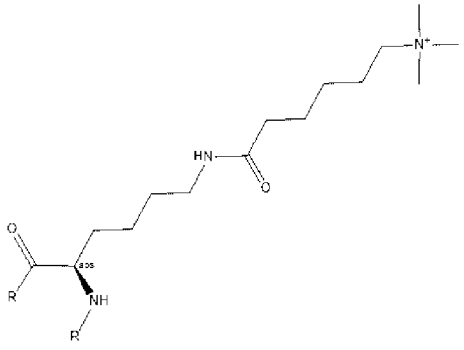
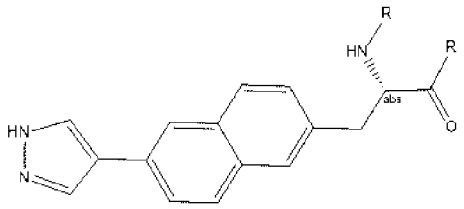
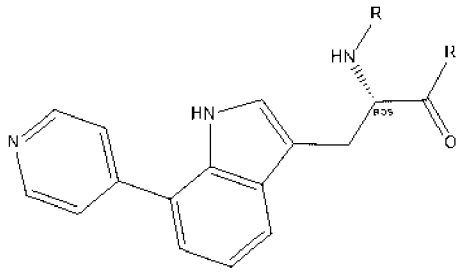
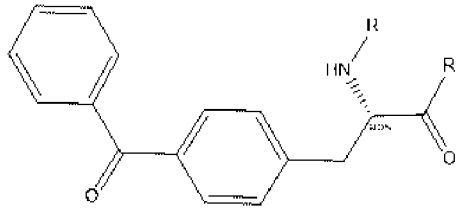
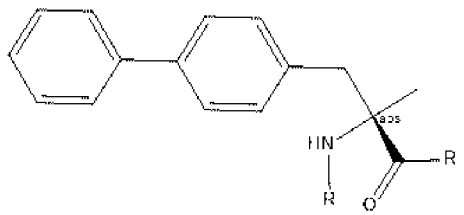
264	psi2Nal	 $C_{13}H_{13}NR_2$	[R]C[C@H](Cc1cc2 ccccc2 cc1)N[R]
265	7EtW	 $C_{13}H_{14}N_2OR_2$	CCc1 cccc2c1[nH]cc2 C[C@@H](C([R])=O)N[R]
266	F(4TzlMME)	 $C_{13}H_{14}N_4O_2R_2$	COCc1cn(-c2 ccc(C[C@@H](C([R])=O)N[R]) cc2)nn1
267	AcAEF	 $C_{13}H_{16}N_2O_3R_2$	CC(NCCOc1 ccc(C[C@@H](C([R])=O)N[R]) cc1)=O
268	tButY、Y(tBu)	 $C_{13}H_{17}NO_2R_2$	CC(C)(C)Oc1 ccc(C[C@H](C([R])=O)N[R])cc1

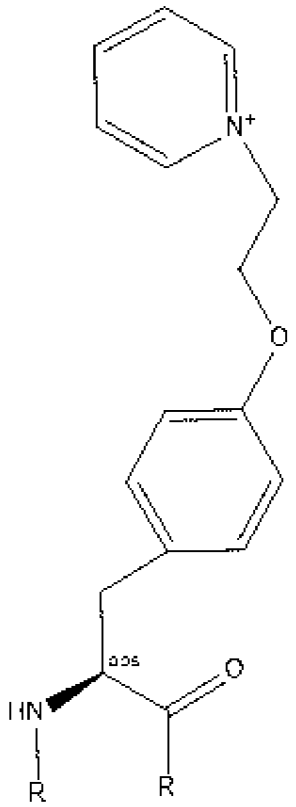
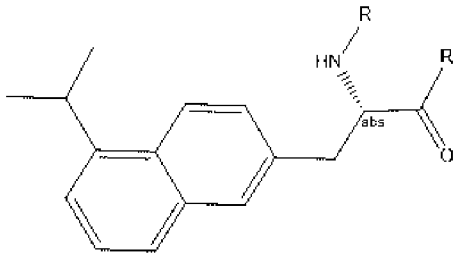
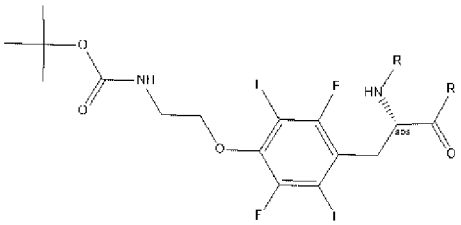
269	AEF(Me)2	 $C_{13}H_{18}N_2O_2R_2$	CN(C)CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
270	Z、Amp	 $C_{13}H_{18}N_2OR_2$	CC(C)c1ccc(C[C@@H](C([R])=O)NCN[R])cc1
271	5amido2Nal	 $C_{14}H_{12}N_2O_2R_2$	NC(c1c(ccc(C[C@@H](C([R])=O)N[R])c2)c2ccc1)=O
272	6amido2Nal	 $C_{14}H_{12}N_2O_2R_2$	NC(c1ccc(cc(C[C@@H](C([R])=O)N[R])cc2)c2c1)=O
273	5OMe2Nal	 $C_{14}H_{13}NO_2R_2$	COc1c(ccc(C[C@@H](C([R])=O)N[R])c2)c2ccc1
274	6OMe2Nal	 $C_{14}H_{13}NO_2R_2$	COc1ccc(cc(C[C@@H](C([R])=O)N[R])cc2)c2c1

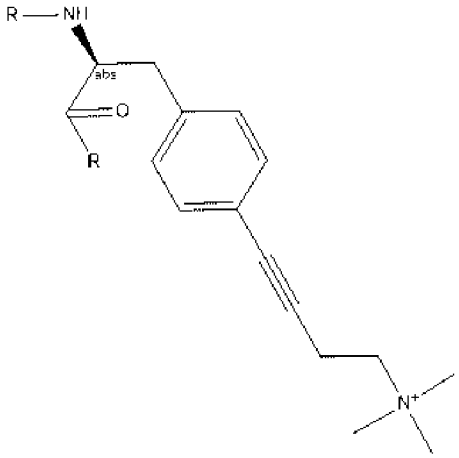
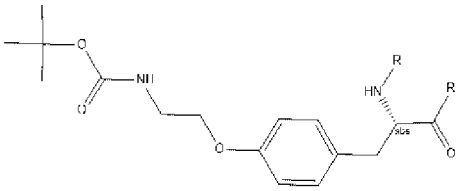
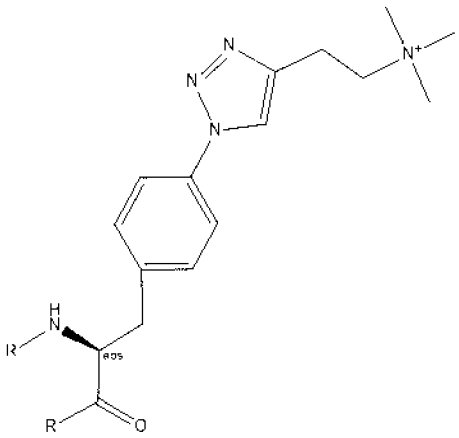
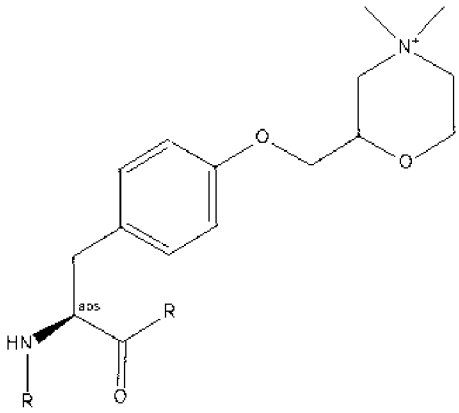
275	5Me2Nal	 $C_{14}H_{13}NOR_2$	Cc1c(ccc(C[C@@H](C([R])=O)N[R])c2)c2 ccc1
276	NMe2NAL	 $C_{14}H_{13}NOR_2$	CN([C@@H](Cc1 cc2 ccccc2 cc1)C([R])=O)[R] CN[C@@H](Cc1 cc2 ccccc2 cc1)C=O
277	aMe2Nal	 $C_{14}H_{13}NOR_2$	C[C@](Cc1 cc2 ccccc2 cc1)(C([R])=O)N[R]
278	bMe2Nal(2S,3R)、bMe2Nal(2S3R)	 $C_{14}H_{13}NOR_2$	C[C@@H]([C@@H](C([R])=O)N[R])c1 cc2 ccccc2 cc1
279	bMe2Nal(2S3S)、bMe2Nal(2S3R)	 $C_{14}H_{13}NOR_2$	C[C@H]([C@@H](C([R])=O)N[R])c1 cc2 ccccc2 cc1
280	AEF(EtCO)	 $C_{14}H_{18}N_2O_3R_2$	CCC(NCCOc1 ccc(C[C@@H](C([R])=O)N[R])cc1)=O

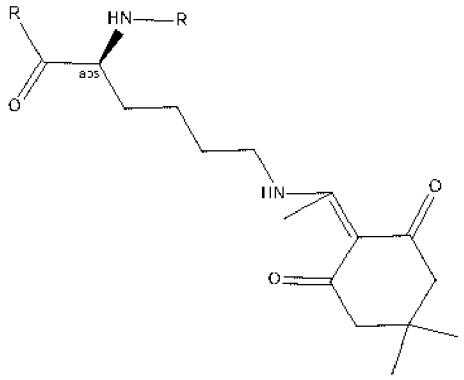
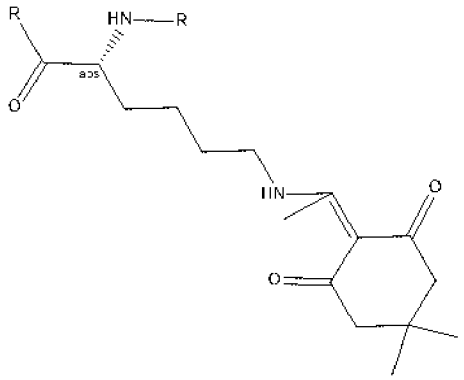
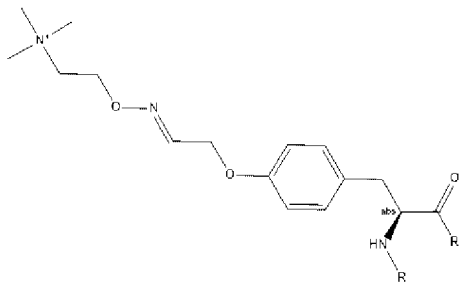
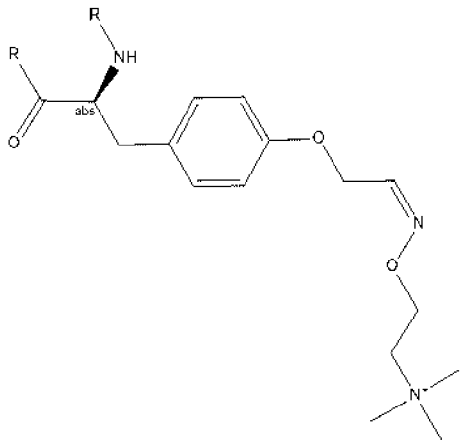
281	NMeY(tBu)	 $C_{14}H_{19}NO_2R_2$	CC(C)(C)Oc1ccc(C[C@H](C([R])=O)N(C)[R])cc1
282	AEF(NMe3)	 $C_{14}H_{21}N_2O_2R_2^+$	C[N+](C)(C)CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
283	6O(COCF3)2Nal	 $C_{15}H_{10}F_3NO_3R_2$	O=C([C@H](Cc(ccc1c2)cc1ccc2OC(C(F)(F)F)=O)N[R])[R]
284	BIF	 $C_{15}H_{13}NOR_2$	O=C([C@H](Cc(cc1)ccc1-c1ccccc1)N[R])[R]
285	DiPhAla	 $C_{15}H_{13}NOR_2$	O=C([C@H](C(c1ccccc1)c1ccccc1)N[R])[R]
286	5Et2Nal	 $C_{15}H_{15}NOR_2$	CCc1c(ccc(C[C@@H](C([R])=O)N[R])c2)c2ccc1

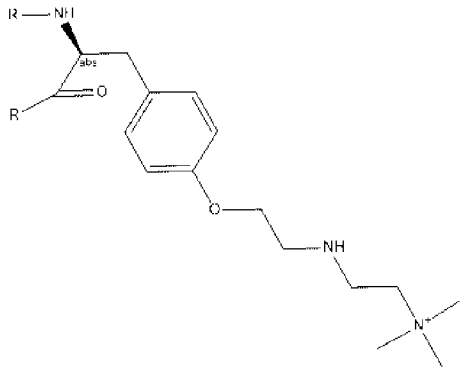
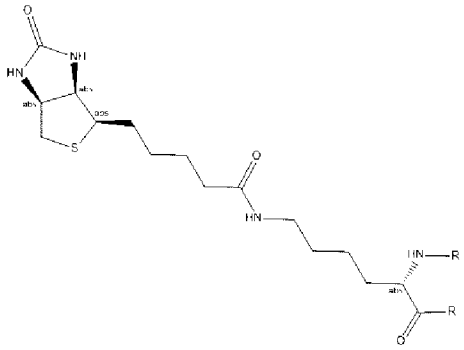
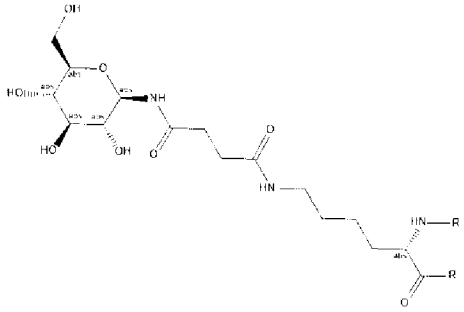
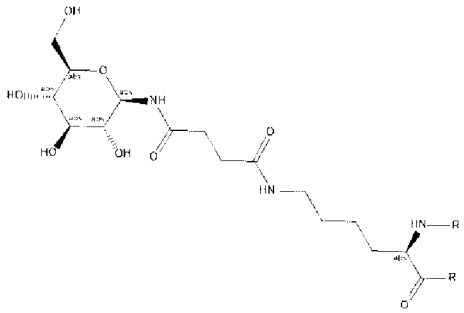
287	CMF	 $C_{15}H_{19}NO_4R_2$	CC(C)(C)OC(C Oc1 ccc(C[C@@H](C([R])=O)N[R]) cc1)=O
288	F(4TzlTMA1)	 $C_{15}H_{20}N_5OR_2^+$	C[N+](C)(C)Cc1 cn(-c2 ccc(C[C@@H](C([R])=O)N[R]) cc2)nn1
289	哌吡quatF	 $C_{15}H_{22}N_3OR_2^+$	C[N+](C)(CC1) CCN1c1 ccc(C[C@@H](C([R])=O)N[R]) cc1
290	TMA3F	 $C_{15}H_{23}N_2O_2R_2^+$	C[N+](C)(C)CC COc1 ccc(C[C@@H](C([R])=O)N[R]) cc1
291	TMA4F	 $C_{15}H_{23}N_2O_2R_2^+$	C[NH+](C)CCC COc1 ccc(C[C@@H](C([R])=O)N[R]) cc1

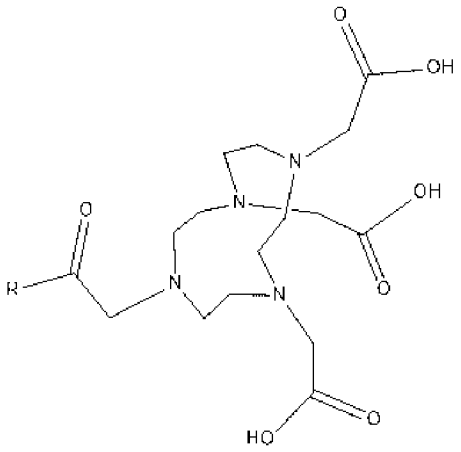
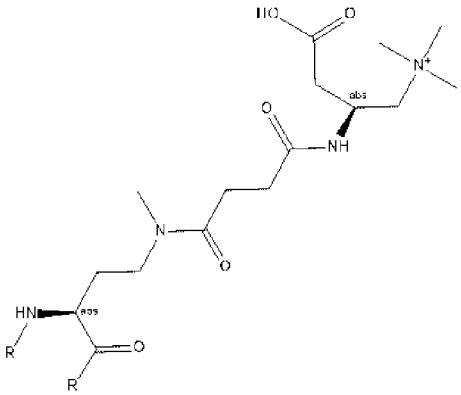
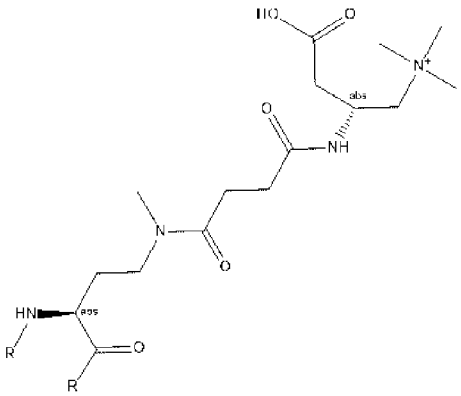
292	K5cpa、K(5cpa)、K(5cpaCO)	 $C_{15}H_{30}N_3O_2R_2^+$	C[N+](C)(C)CCCCCC(NCCCC[C@@H](C([R])=O)N[R])=O
293	dK(5cpa)、k(5cpa)、k(5cpaCO)	 $C_{15}H_{30}N_3O_2R_2^+$	C[N+](C)(C)CCCCCC(NCCCC[C@H](C([R])=O)N[R])=O
294	2Nal6(3 吡唑)	 $C_{16}H_{13}N_3OR_2$	O=C([C@H](Cc(ccc1c2)cc1ccc2-c1c[nH]nc1)N[R])[R]
295	7PyrTrp	 $C_{16}H_{13}N_3OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2-c1ccncc1)N[R])[R]
296	4BzF	 $C_{16}H_{13}NO_2R_2$	O=C([C@H](Cc(cc1)ccc1C(c1ccccc1)=O)N[R])[R]
297	aMeBiF	 $C_{16}H_{15}NOR_2$	C[C@](Cc(cc1)ccc1-c1ccccc1)(C([R])=O)N[R]

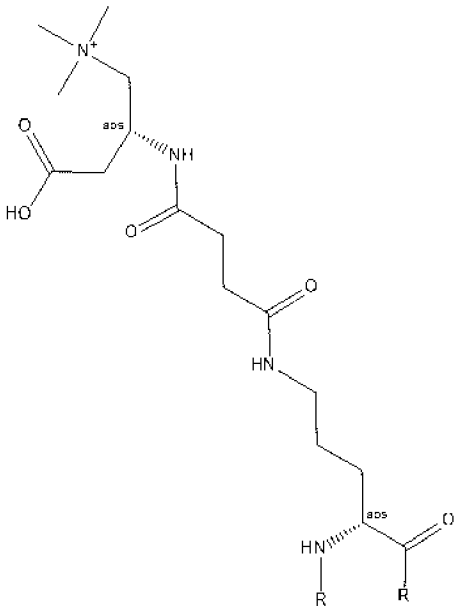
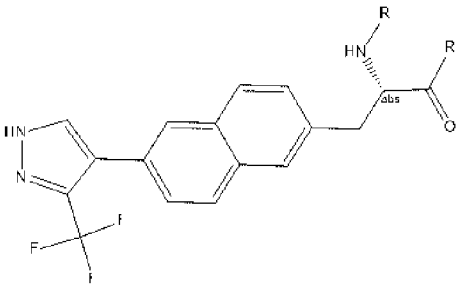
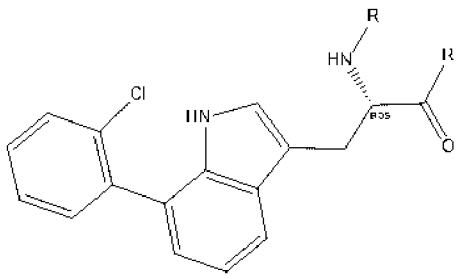
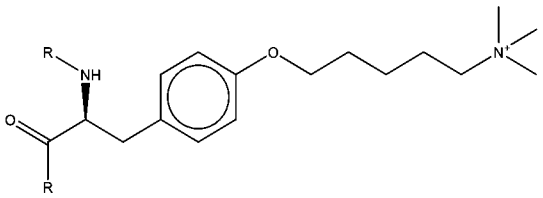
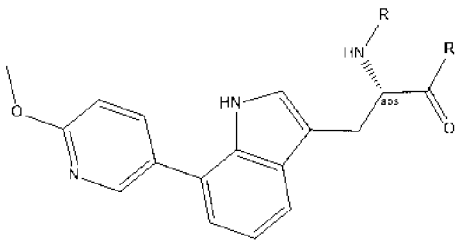
298	NPyEF	 $C_{16}H_{17}N_2O_2R_2^+$	O=C([C@H](Cc(cc1)ccc1OCC[n+]1ccccc1)N[R])[R]
299	5iPr2Nal	 $C_{16}H_{17}NOR_2$	CC(C)c1c(ccc(C[C@@H](C([R])=O)N[R])c2)c2ccc1
300	四 FAEF(Boc)	 $C_{16}H_{18}F_4N_2O_4R_2$	CC(C)(C)OC(NCCOc(c(F)c(c(C[C@@H](C([R])=O)N[R])c1F)F)c1F)=O

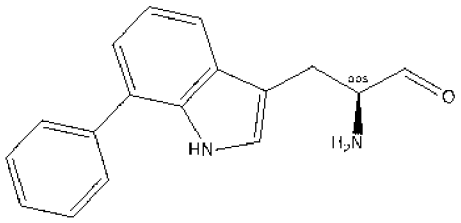
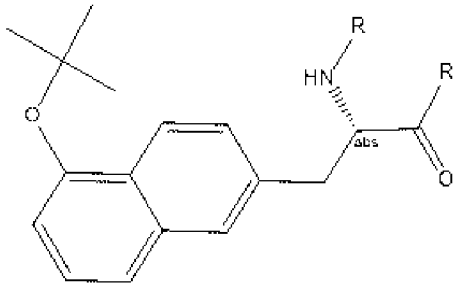
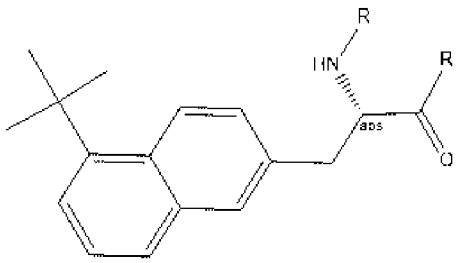
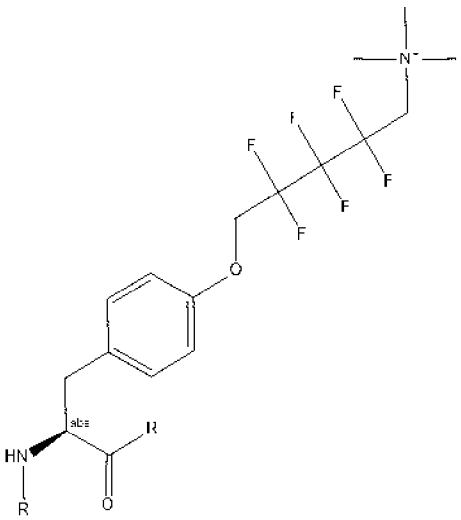
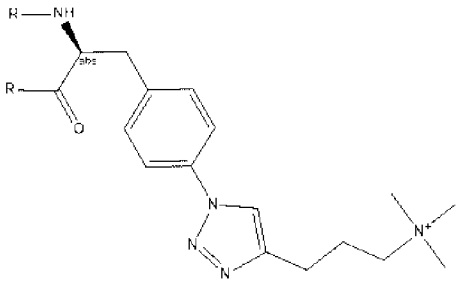
301	4TMABYF	 $C_{16}H_{21}N_2OR_2^+$	C[N+](C)(C)CC C#Cc1 ccc(C[C@@H](C([R])=O)N[R]) cc1
302	AEF(Boc)	 $C_{16}H_{22}N_2O_4R_2$	CC(C)(C)OC(N CCOc1 ccc(C[C@@H](C([R])=O)N[R]) cc1)=O
303	F(4TzlTMA2)	 $C_{16}H_{22}N_5OR_2^+$	C[N+](C)(C)CC c1cn(-c2 ccc(C[C@@H](C([R])=O)N[R]) cc2)nn1
304	DMPMF	 $C_{16}H_{23}N_2O_3R_2^+$	C[N+]1(C)CC(C Oc2 ccc(C[C@@H](C([R])=O)N[R]) cc2)OCC1

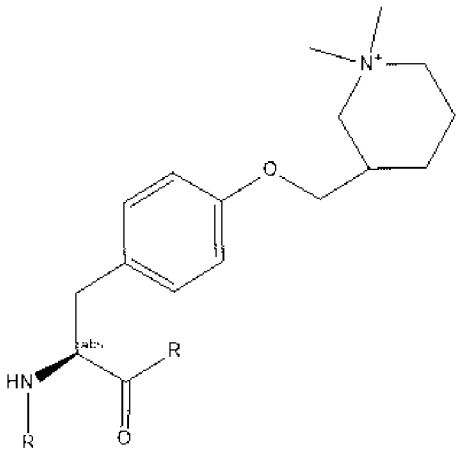
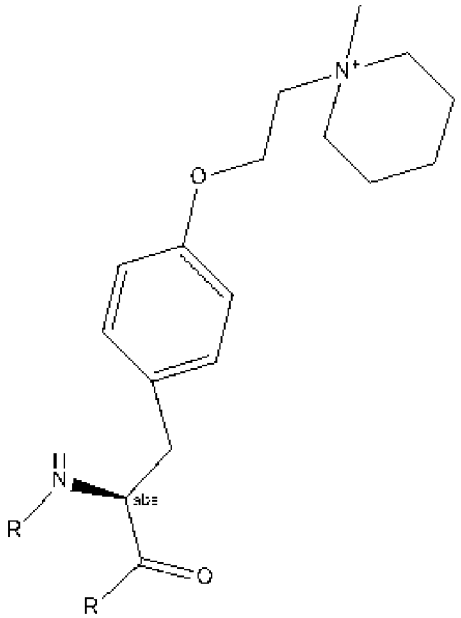
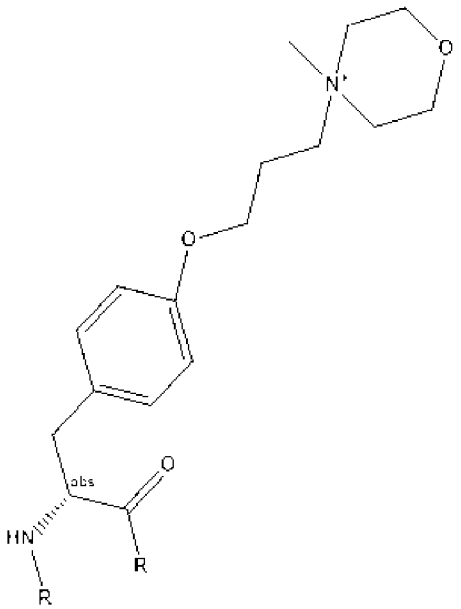
305	KDde、K(Dde)	 $C_{16}H_{24}N_2O_3R_2$	CC(C)(CC(C1=C(C)NCCCC[C@@H](C([R])=O)N[R])=O)CC1=O
306	dKDde、k(Dde)、dK(Dde)	 $C_{16}H_{24}N_2O_3R_2$	CC(C)(CC(C1=C(C)NCCCC[C@H](C([R])=O)N[R])=O)CC1=O
307	Y(OEOXIMECh)	 $C_{16}H_{24}N_3O_3R_2^+$	C[N+](C)(C)CCO/N=C/COc1ccc(C[C@@H](C([R])=O)N[R])cc1
308	Y(OZOXIMECh)	 $C_{16}H_{24}N_3O_3R_2^+$	C[N+](C)(C)CCO/N=C\COc1ccc(C[C@@H](C([R])=O)N[R])cc1

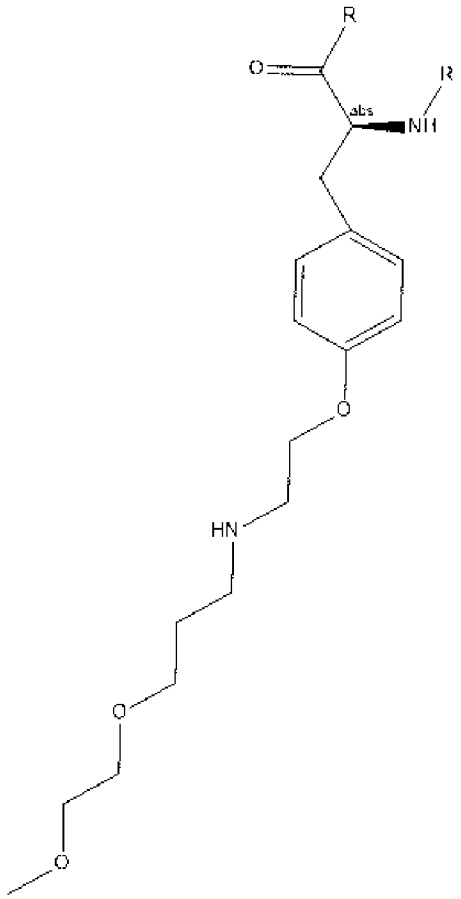
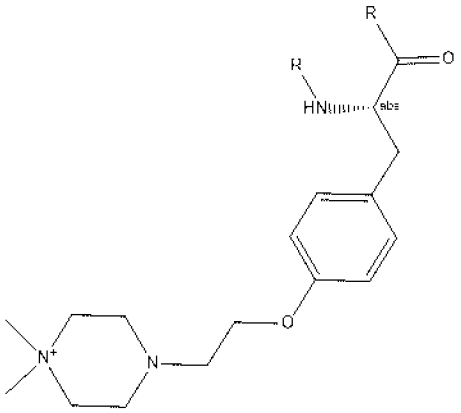
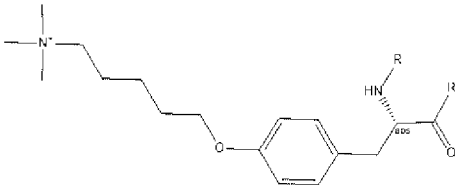
309	AEF(NHCh)	 $C_{16}H_{26}N_3O_2R_2^+$	C[N+](C)(C)CCNCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
310	K(Biotina)、K(生物素)	 $C_{16}H_{26}N_4O_3SR_2$	O=C(CCCC[C@H]([C@@H]1N2)SC[C@H]1NC2=O)NCCCC[C@@H](C([R])=O)N[R]
311	K(DAGSuc)	 $C_{16}H_{27}N_3O_8R_2$	OC[C@H]([C@H]([C@@H]([C@H]1O)O)O)O[C@H]1NC(CCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
312	k(DAGSuc)、dK(DAGSuc)	 $C_{16}H_{27}N_3O_8R_2$	OC[C@H]([C@H]([C@@H]([C@H]1O)O)O)O[C@H]1NC(CCC(NCCCC[C@H](C([R])=O)N[R])=O)=O

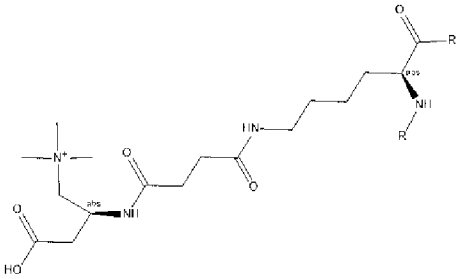
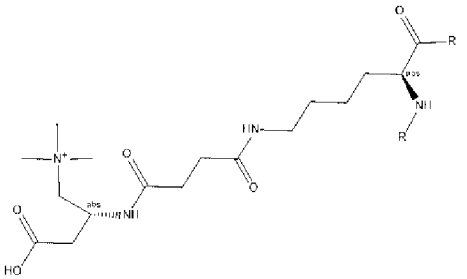
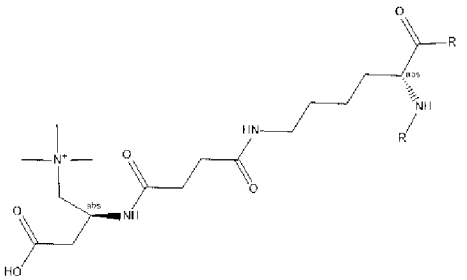
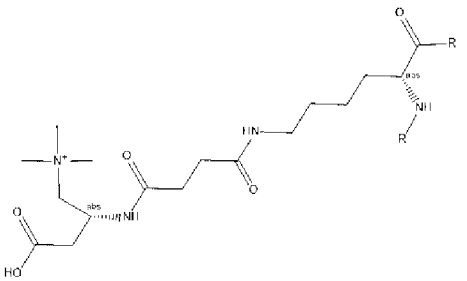
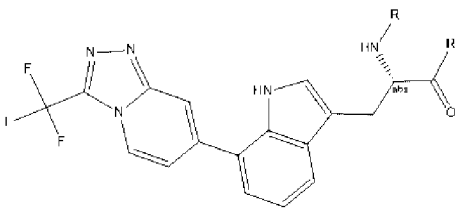
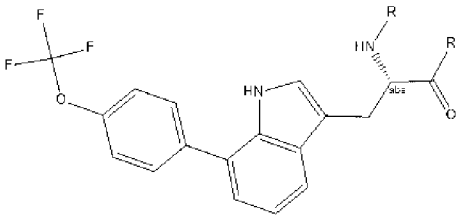
313	DOTA	 $C_{16}H_{27}N_4O_7R$	OC(CN1CCN(CC(O)=O)CCN(CC([R])=O)CCN(CC(O)=O)CC1)=O
314	Dab(NMeCarn)	 $C_{16}H_{29}N_4O_5R_2^+$	CN(CC[C@@H](C([R])=O)N[R])C(CCC(N[C@@H](CC(O)=O)C[N+](C)(C)C)=O)=O
315	Dab(NMecarn)	 $C_{16}H_{29}N_4O_5R_2^+$	CN(CC[C@@H](C([R])=O)N[R])C(CCC(N[C@H](CC(O)=O)C[N+](C)(C)C)=O)=O

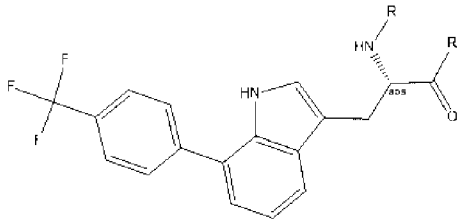
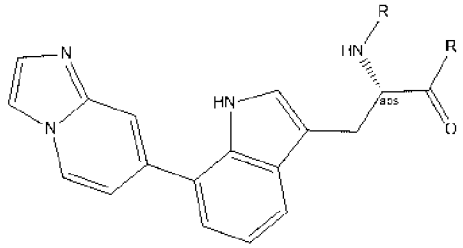
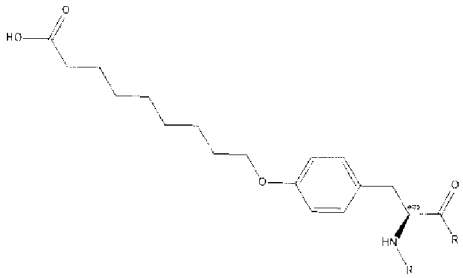
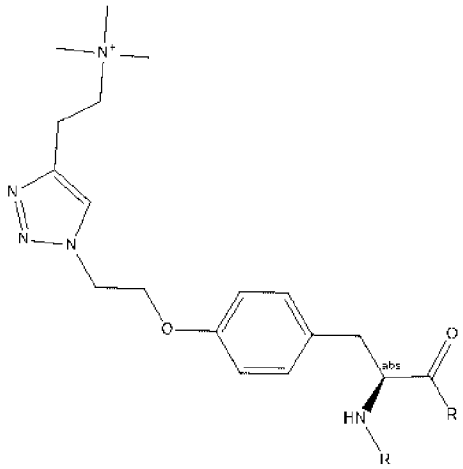
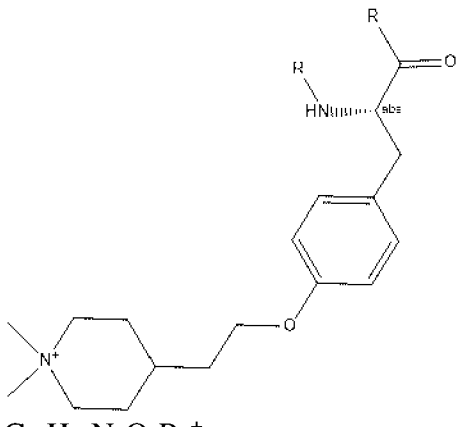
316	orn(d)	 $C_{16}H_{29}N_4O_5R_2^+$	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CCC(NCCC[C@H](C([R])=O)N[R])=O)=O
317	2Nal6((5CF3)3 吡唑)	 $C_{17}H_{12}F_3N_3OR_2$	O=C([C@H](Cc(ccc1c2)cc1ccc2-c1c[nH]nc1C(F)(F)F)N[R])[R]
318	7(2ClPh)W	 $C_{17}H_{13}ClN_2OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2-c(cccc1)c1Cl)N[R])[R]
319	TMAPF		C[N+](C)(CCCCCOc1ccc(C[C@H](N[R])C([R])=O)cc1)C
320	7(2OMe5Pyr)W	 $C_{17}H_{15}N_3O_2R_2$	COc(cc1)ncc1-c1cccc2c1[nH]cc2C[C@@H](C([R])=O)N[R]

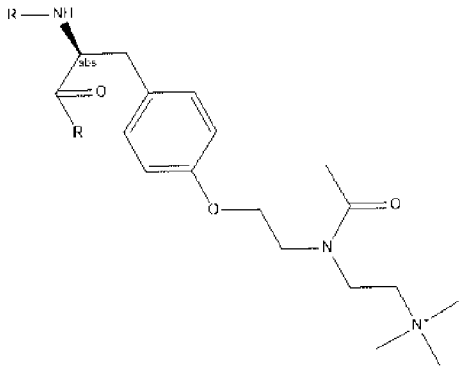
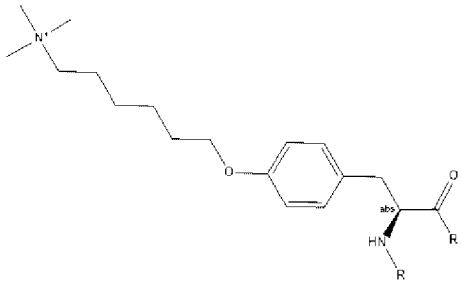
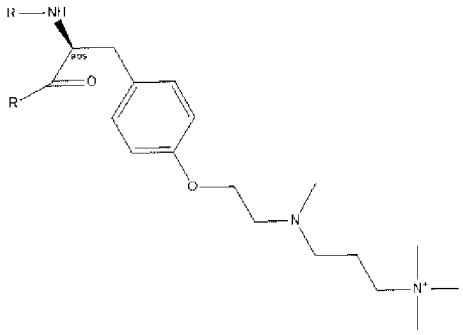
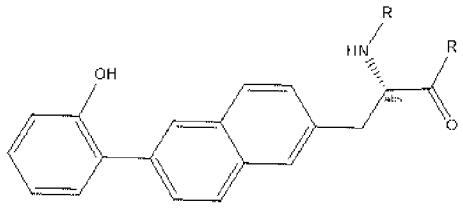
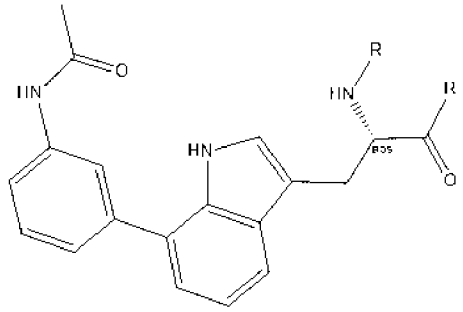
321	W-7Ph、7-苯基-L-色胺酸	 $C_{17}H_{16}N_2O$	N[C@@H](Cc1c[nH]c2c1 cccc2-c1 ccccc1)C=O
322	5OH2Nal	 (S)-2-胺基-3-(5-(三級丁氧基)萘-2-基)丙酸 $C_{17}H_{19}NO_2R_2$	CC(C)(C)Oc1c(ccc(C[C@@H](C([R])=O)N[R])c2)c2 ccc1
323	5tBu2Nal	 $C_{17}H_{19}NOR_2$	CC(C)(C)c1c(ccc(C[C@@H](C([R])=O)N[R])c2)c2 ccc1
324	hFTMAPF	 $C_{17}H_{21}F_6N_2O_2R_2^+$	C[N+](C)(C)CC(C(C(COc1ccc(C[C@@H](C([R])=O)N[R])cc1)(F)F)(F)F)(F)F
325	F(4TzlTMA3)	 $C_{17}H_{24}N_5OR_2^+$	C[N+](C)(C)CCCc1cn(-c2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1

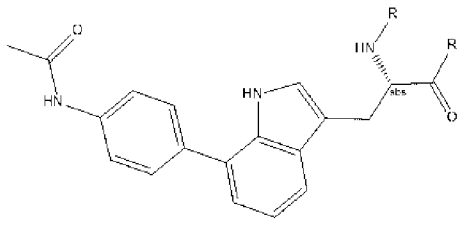
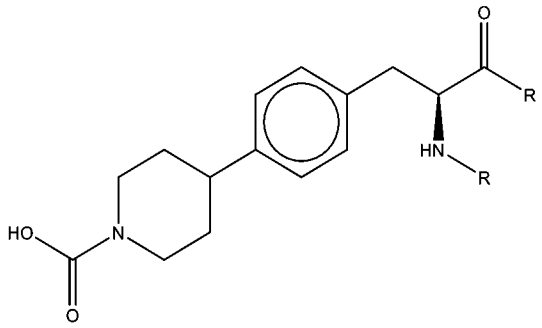
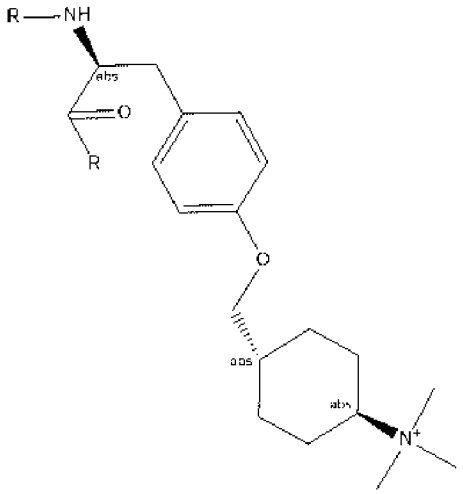
326	DMMMF	 $C_{17}H_{25}N_2O_2R_2^+$	C[N+]1(C)CC(COc2ccc(C[C@@H](C([R])=O)N[R])cc2)CCC1
327	MMoEF	 $C_{17}H_{25}N_2O_2R_2^+$	C[N+]1(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)CCCCC1
328	MMoPF	 $C_{17}H_{25}N_2O_3R_2^+$	C[N+]1(CCCOc2ccc(C[C@H](C([R])=O)N[R])cc2)CCOCC1

329	AEF(MEP)	 $C_{17}H_{26}N_2O_4R_2$	COCCOCCCNCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
330	4DMPzEF	 $C_{17}H_{26}N_3O_2R_2^+$	C[N+]1(C)CCN(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)CC1 C[N+]1(C)CCN(CCOc2ccc(C[C@@H](C=O)N)cc2)CC1
331	TMAPF	 $C_{17}H_{27}N_2O_2R_2^+$	C[N+](C)(C)CCCCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1 C[N+](C)(C)CCCCCOc1ccc(C[C@@H](C=O)N)cc1

332	K(D)、KCar	 $C_{17}H_{31}N_4O_5R_2^+$	C[N+](C)(C)C[C@H](CC(O)=O)NC(CCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
333	K(d)、KdCar	 $C_{17}H_{31}N_4O_5R_2^+$	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
334	k(D)、dKCar	 $C_{17}H_{31}N_4O_5R_2^+$	C[N+](C)(C)C[C@H](CC(O)=O)NC(CCC(NCCCC[C@H](C([R])=O)N[R])=O)=O
335	k(d)、dKdCar	 $C_{17}H_{31}N_4O_5R_2^+$	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CCC(NCCCC[C@H](C([R])=O)N[R])=O)=O
336	7(3CF3TAZP)W	 $C_{18}H_{12}F_3N_5OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2-c1cc2nnc(C(F)(F)F)n2cc1)N[R])[R]
337	7(4OCF3Ph)W	 $C_{18}H_{13}F_3N_2O_2R_2$	O=C([C@H](Cc1c[nH]c2c1cccc2-c(cc1)ccc1OC(F)(F)F)N[R])[R]

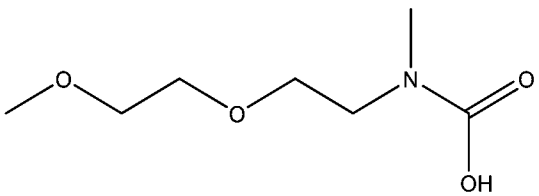
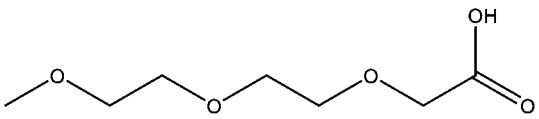
338	7(4CF3Ph)W	 $C_{18}H_{13}F_3N_2OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2-c1ccc(C(F)(F)F)cc1)N[R])[R]
339	7(7ImidPyr)W	 $C_{18}H_{14}N_4OR_2$	O=C([C@H](Cc1c[nH]c2c1cccc2-c1cc2nccn2cc1)N[R])[R]
340	Y(C9OH)	 $C_{18}H_{25}NO_4R_2$	OC(CCCCCCCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
341	Y(OTzlCh)	 $C_{18}H_{26}N_5O_2R_2^+$	C[N+](C)(C)CCc1cn(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1
342	4DMPEF	 $C_{18}H_{27}N_2O_2R_2^+$	C[N+]1(C)CCC(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)CC1 C[N+]1(C)CCC(CCOc2ccc(C[C@@H](C=O)N)cc2)CC1

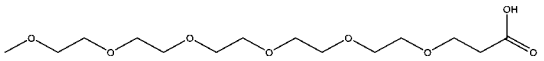
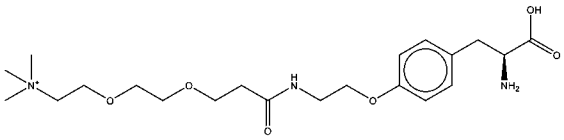
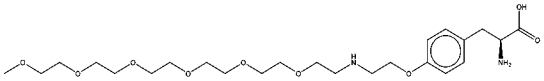
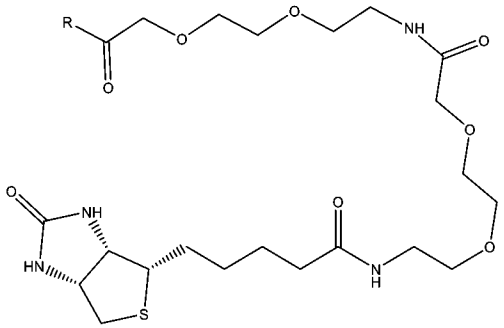
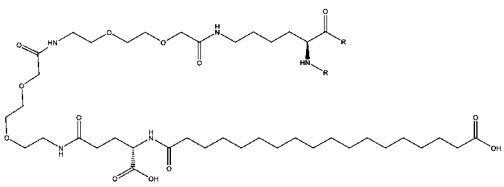
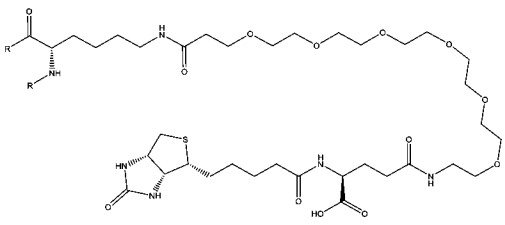
343	AEF(AcCh)	 $C_{18}H_{28}N_3O_3R_2^+$	CC(N(CC[N+](C)(C)C)CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
344	TMA6F	 $C_{18}H_{29}N_2O_2R_2^+$	C[N+](C)(C)CCCCCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
345	AEF(MePrpa)	 $C_{18}H_{30}N_3O_2R_2^+$	CN(CCC[N+](C)(C)C)CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
346	2Nal6(Ph2OH)	 $C_{19}H_{15}NO_2R_2$	Oc(cccc1)c1-c1ccc(cc(C[C@@H](C([R])=O)N[R])cc2)c2c1
347	7(3NAcPh)W	 $C_{19}H_{17}N_3O_2R_2$	CC(Nc1cccc(-c2cccc3c2[nH]cc3C[C@@H](C([R])=O)N[R])c1)=O

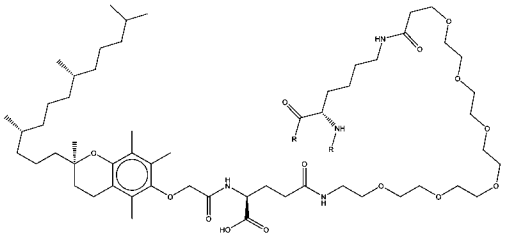
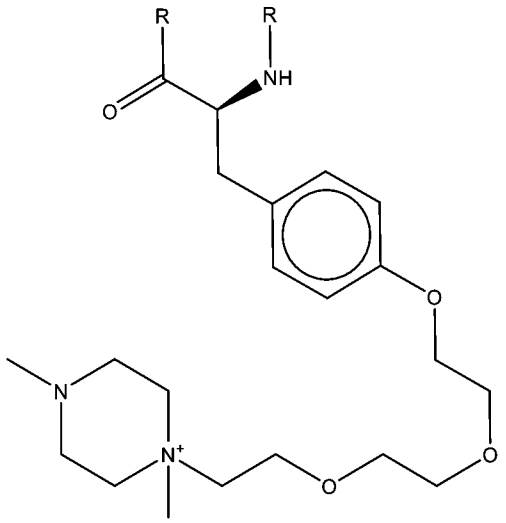
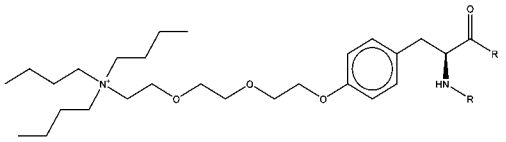
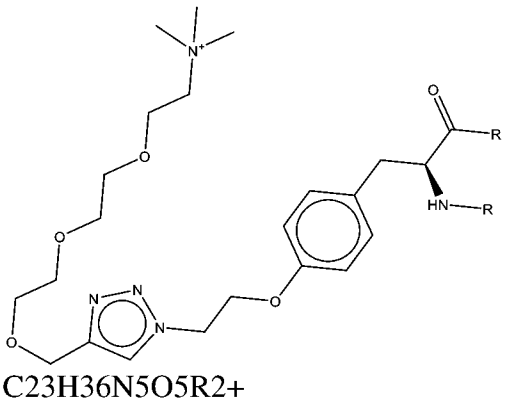
348	7(4NAcPh)W	 $C_{19}H_{17}N_3O_2R_2$	CC(Nc(cc1)ccc1-c1cccc2c1[nH]cc2C[C@@H](C([R])=O)N[R])=O
349	4PipF、4PipPhe	 $C_{19}H_{26}N_2O_3R_2$	CC(C)(C)OC(N(CC1)CCC1c1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
350	a	 $C_{19}H_{29}N_2O_2R_2^+$	C[N+](C)(C)[C@H]1CC[C@H](COc2ccc(C[C@@H](C([R])=O)N[R])cc2)CC1

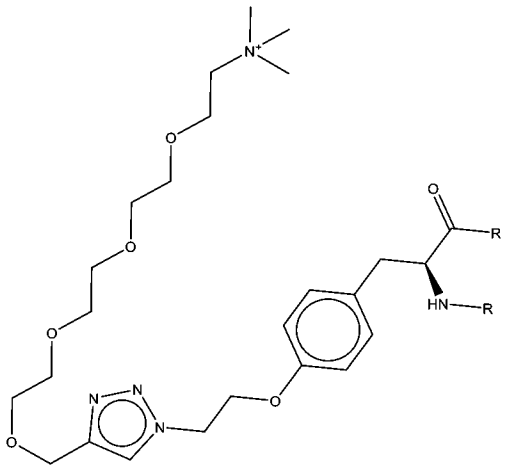
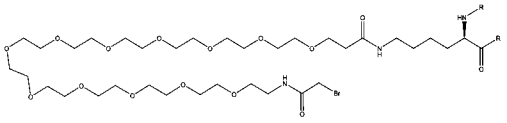
【0274】

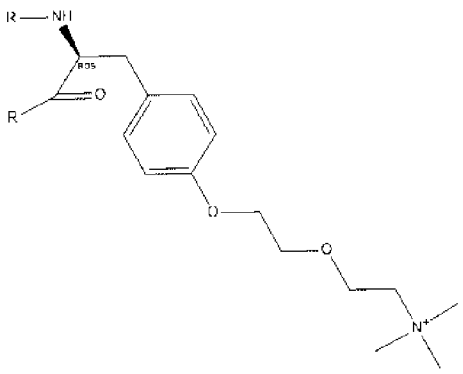
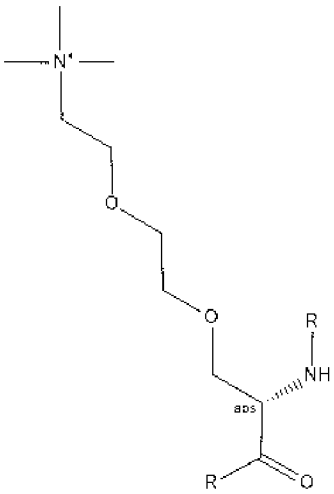
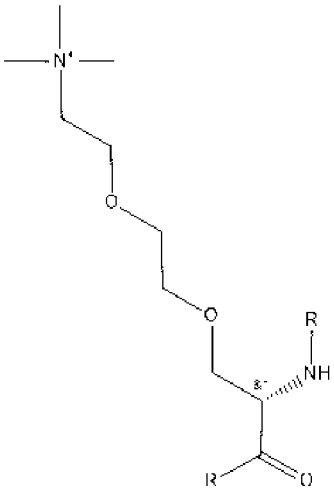
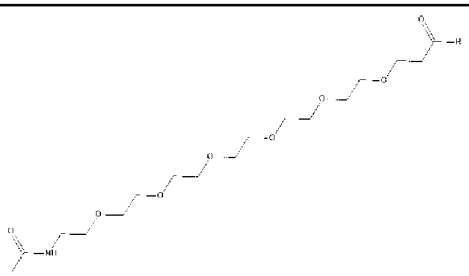
表2D：Peg單體及Peg共軛單體。

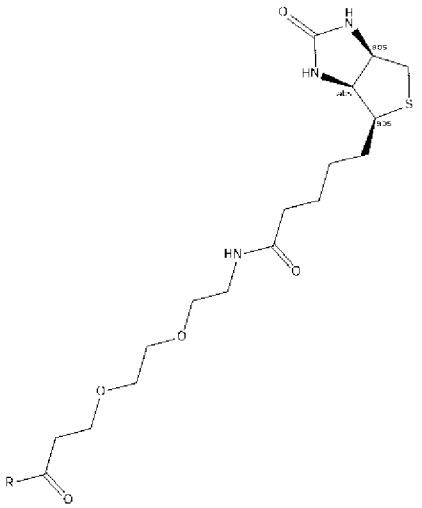
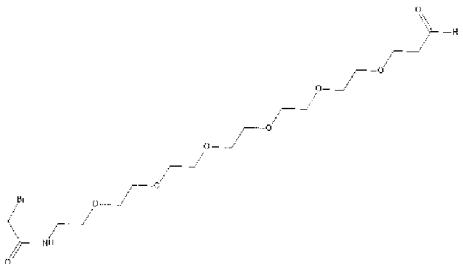
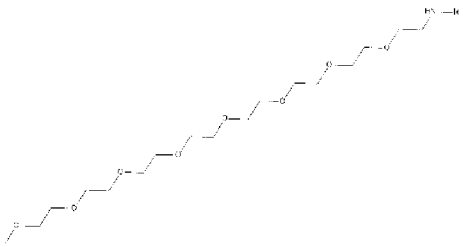
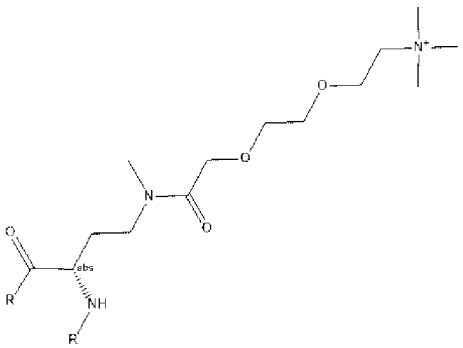
#	結構	名稱及同義詞	Smiles 結構
1	 C7H15NO3	CON(MePEG2)	CN(CCOCCOC)C=O
2	 C7H14O4	mPEG3CO	COCCOCCOCC=O

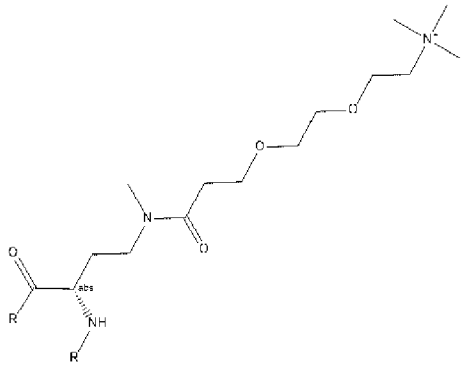
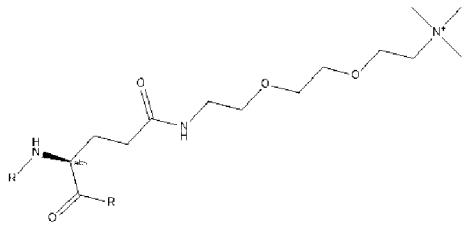
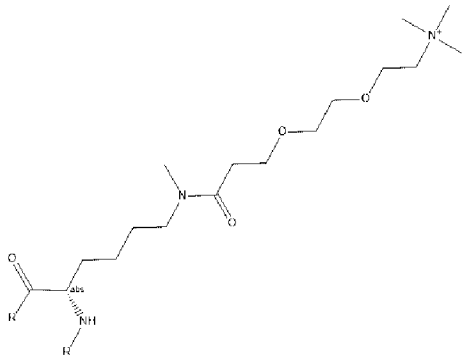
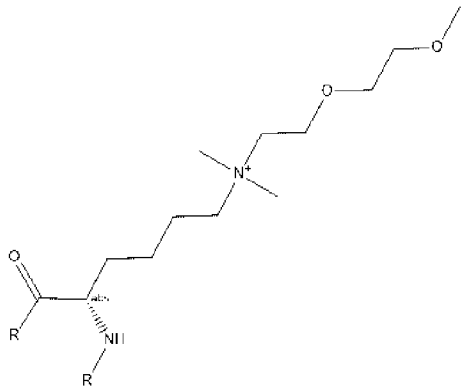
3	 C14H28O7	mPEG6CO	COCCOCCOCCOCCOCCOCCCO=O
4	 C21H36N3O5+	AEFNMePEG3a、AEF(NHcPEG3a)	C[N+](C)(C)CCOCCOCCC(NCCOc1ccc(C[C@@H](C=O)N)cc1)=O
5	 C24H42N2O8	AEFNmPEG6、AEF(NmPEG6)	COCCOCCOCCOCCOCCOCCNCCOc1ccc(C[C@@H](C=O)N)cc1
6	 C22H37N4O8SR	生物素 PEG2PEG2、生物素(PEG2PEG2)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCC(NCCOCCOCC([R])=O)=O
7	 C41H73N5O13R2	K(PEG2PEG2gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
8	 C36H62N6O13SR2	K(PEG6gE 生物素)	OC([C@H](CCC(NCCOCCOCCOCCOCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)NC(CCCC[C@H]([C@@H]1N2)SC[C@H]1NC2=O)=O)=O

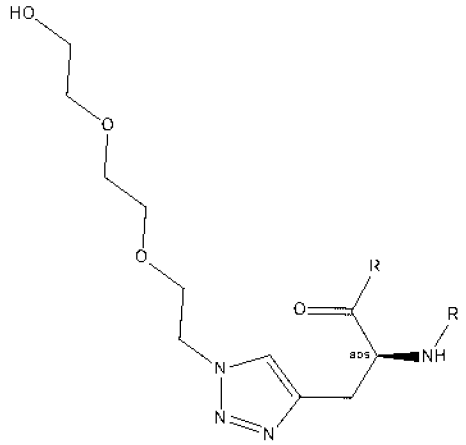
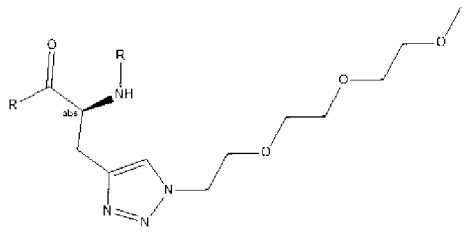
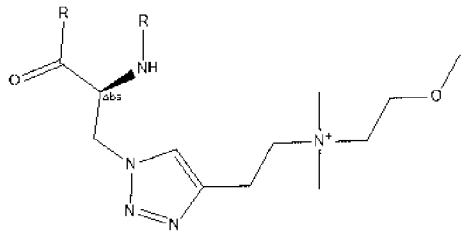
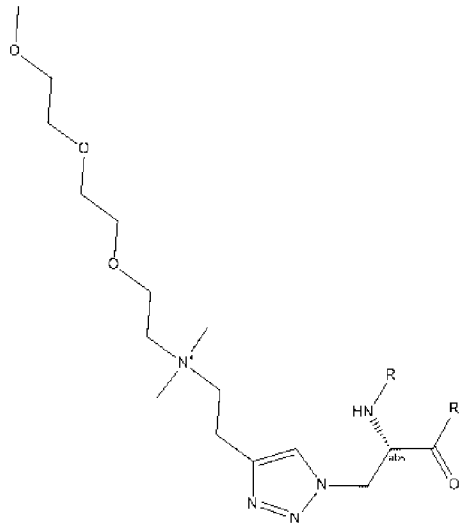
9	 C57H98N4O14R2	K(PEG6gEVitE)	CC(C)CCC[C@@H](C)CCC[C@@H](C)CCC[C@](C)(CC1)Oc(c(C)c2C)c1c(C)c2OCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)C(O)=O)=O
10	 C21H34N3O4R2+	MPzPEG3F	CN1CC[N+](C)(CCOCCOCCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)CC1
11	 C27H47N2O4R2+	TBAPEG3F	CCCC[N+](CCCC)(CCCC)CCOCCOCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
12	 C23H36N5O5R2+	Y(OTzlPEG3a)	C[N+](C)(C)CCOCCOCCOCc1cn(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1

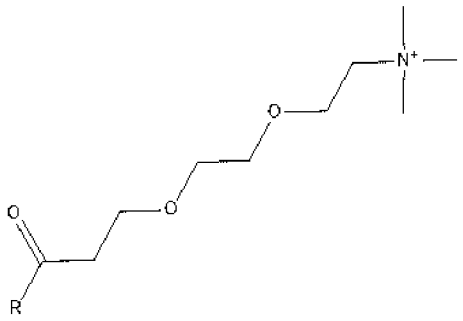
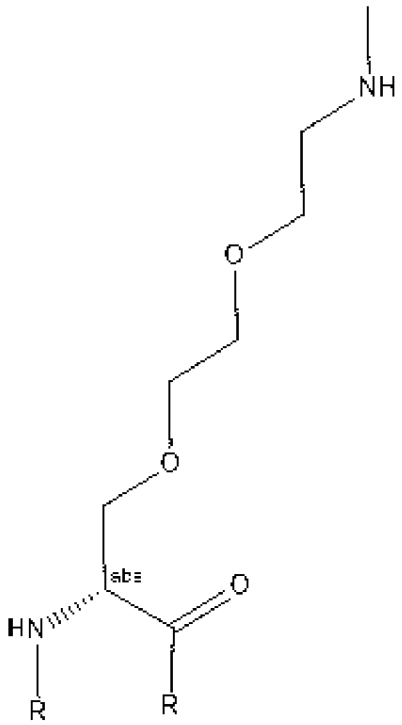
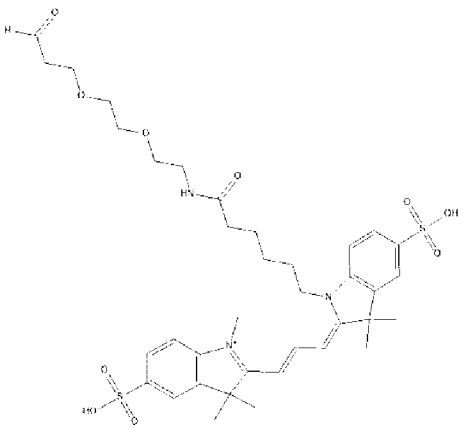
13	 C25H40N5O6R2+	Y(OTzlPEG4a)	C[N+](C)(C)CCOCCOCCOCCOCc1cn(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1
14	 C35H66BrN3O15R2	k(PEG6 生物素)、dK(PEG6 生物素)	O=C(CCOCCOCCOCCOC

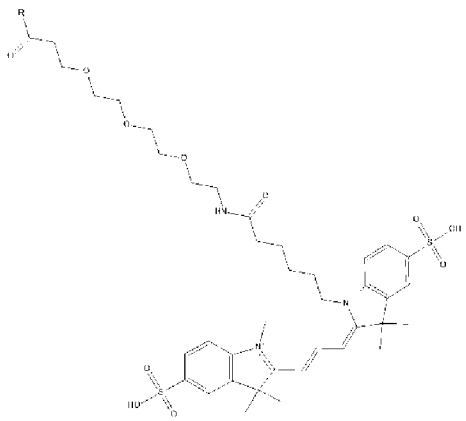
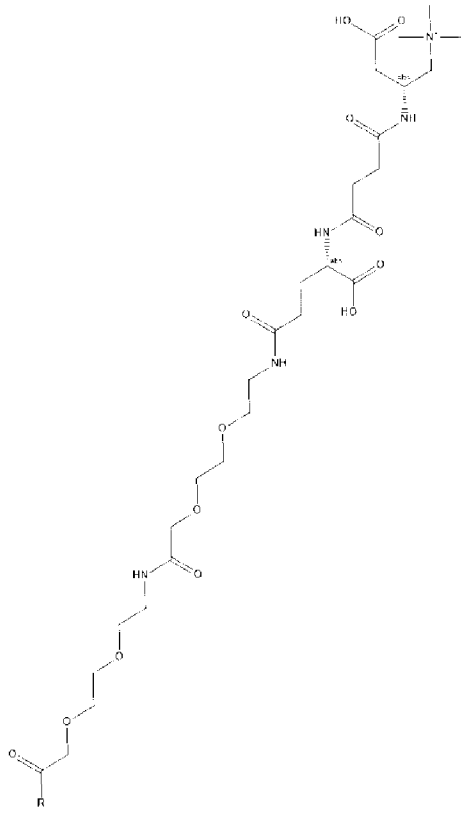
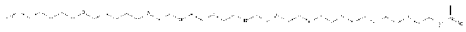
18	 C16H25N2O3R2+	C[N+](C)(C)CCOCCOc1 ccc(C[C@@H](C([R])=O)N[R])cc1
19	 C10H21N2O3R2+	C[N+](C)(C)CCOCCOC[C@@H](C([R])=O)N[R]
20	 C10H21N2O3R2+	C[N+](C)(C)CCOCCOCC(C([R])=O)N[R]
21	 C17H32NO8R	CC(NCCOCCOCCOCCOCCOCCOCCC([R])=O)=O

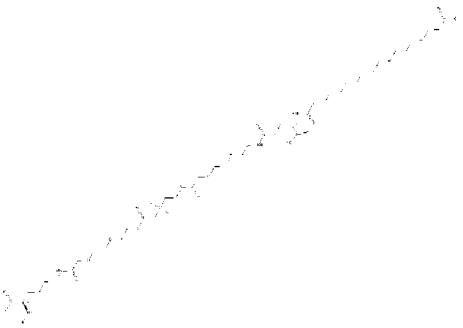
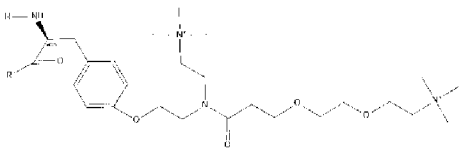
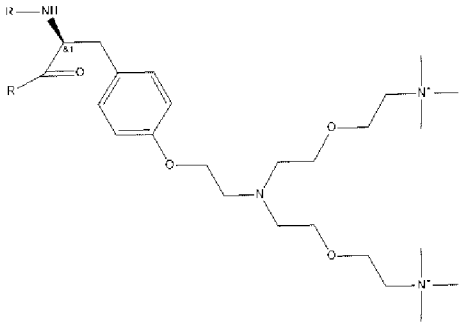
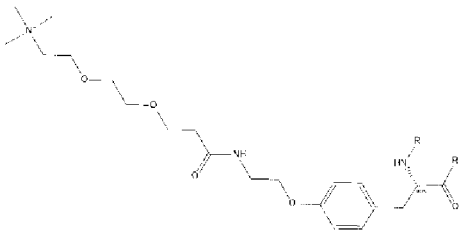
22	 C17H28N3O5SR	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCC([R])=O
23	 C17H31BrNO8R	O=C(CBr)NCCOCCOCCOCCOCCOCCOCCC([R])=O
24	 C17H36NO8R	COCCOCCOCCOCCOCCOCCOCCOCCN[R]
25	 C14H28N3O4R2+	CN(CC[C@@H](C([R])=O)N[R])C(COCCOCC[N+](C)(C)C)=O

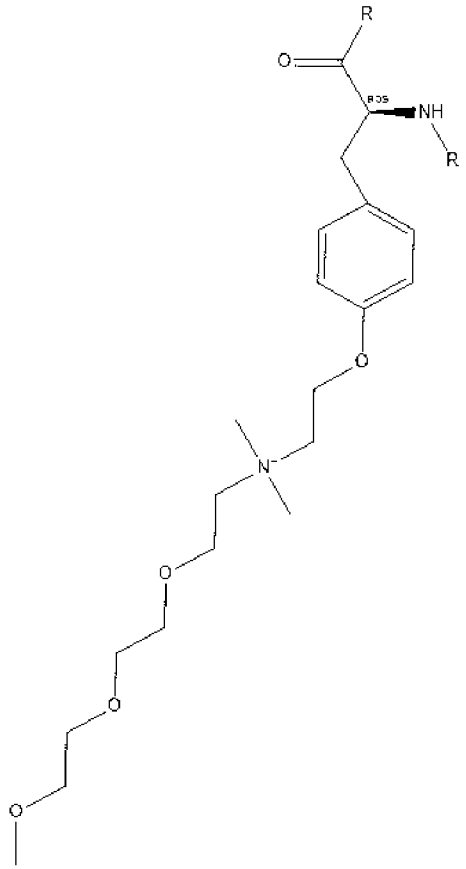
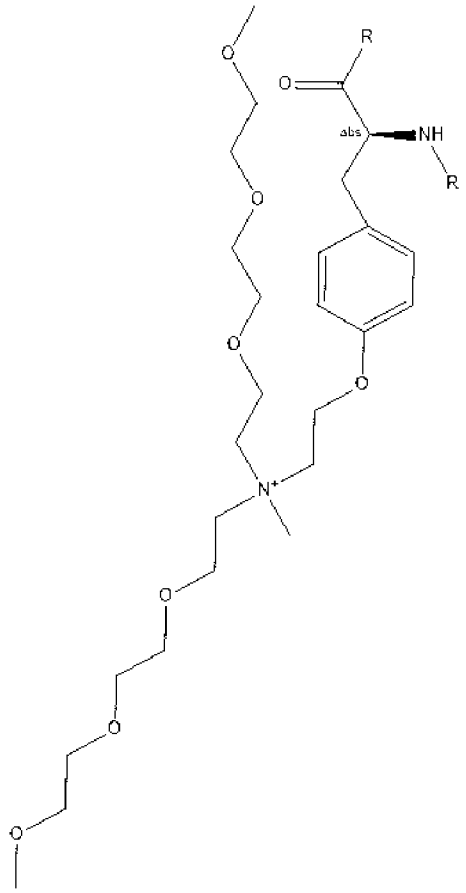
26	 C15H30N3O4R2+	CN(CC[C@@H](C([R])=O)N[R])C(CCOCCOCC[N+](C)(C)C)=O
27	 C14H28N3O4R2+	C[N+](C)(C)CCOCCOCCNC(CC[C@@H](C([R])=O)N[R])=O
28	 C17H34N3O4R2+	CN(CCCC[C@@H](C([R])=O)N[R])C(CCOCCOCC[N+](C)(C)C)=O
29	 C13H27N2O3R2+	C[N+](C)(CCCC[C@@H](C([R])=O)N[R])CCOCCOC

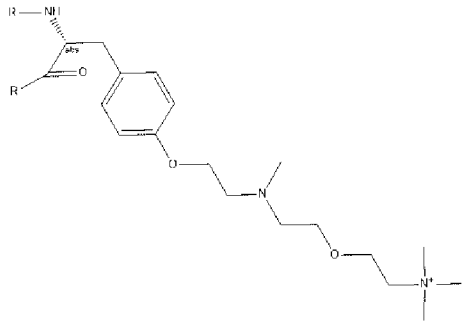
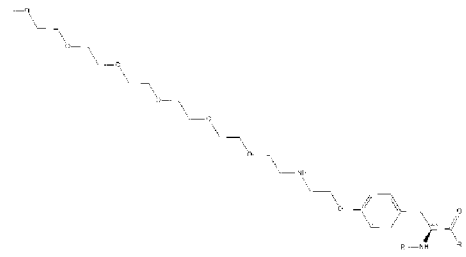
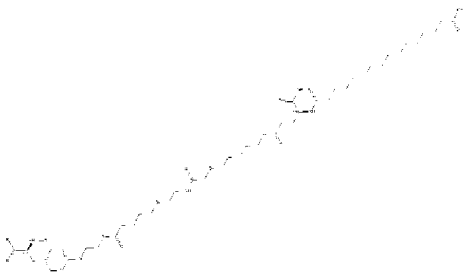
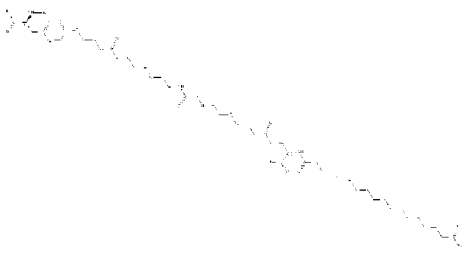
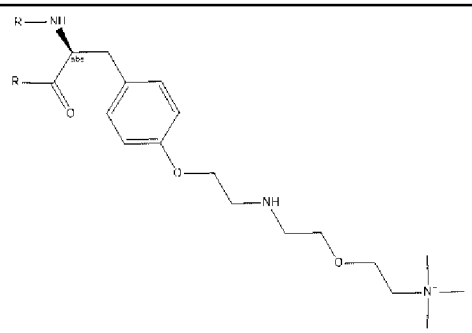
30	 C11H18N4O4R2	OCCOCCOCCn1nnc(C[C@@H](C([R])=O)N[R])c1
31	 C12H20N4O4R2	COCCOCCOCCn1nnc(C[C@@H](C([R])=O)N[R])c1
32	 C12H22N5O2R2+	C[N+](C)(CCc1cn(C[C@@H](C([R])=O)N[R])nn1)CCOC
33	 C16H30N5O4R2+	C[N+](C)(CCc1cn(C[C@@H](C([R])=O)N[R])nn1)CCOCCOCCOC

34	 C10H21NO3R+	C[N+](C)(C)CCOCCO CCC([R])=O	
35	 C8H16N2O3R2	CNCCOCCOC[C@H](C([R])=O)N[R]	
36	 C37H49N3O10S2R+	(SulfoCy3dPEG2)	CC1(C)c(cc(cc2) S(O)(=O)=O)c2[N+](C)=C1/C=C/ C=C(/C1(C)C)\N(CCCCCC(NCCO CCOCCC([R])=O)=O)c(cc2)c1 cc2S(O)(=O)=O

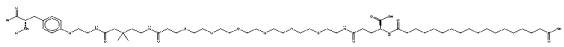
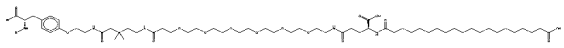
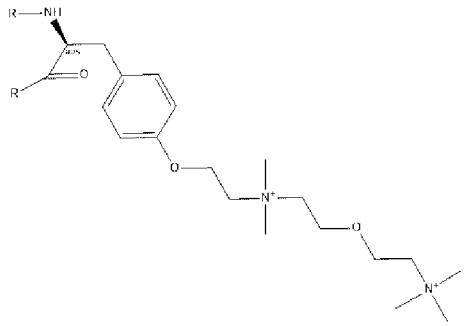
37	 C39H53N3O11S2R+	(SulfoCy3dPEG3)	CC1(C)c(cc(cc2)S(O)(=O)=O)c2[N+](C)=C1/C=C/C=C(/C1(C)C)\N(CCCCCC(NCCOCCOCCOCCC([R])=O)=O)c(cc2)c1cc2S(O)(=O)=O
38	 C28H49N5O13R+	(d)gEPEG2PEG2	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O)=O
39	 C29H57NO14	AcdPEG12CO	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC=O)=O
40	C23H45NO11	AcdPEG9CO	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC=O)=O

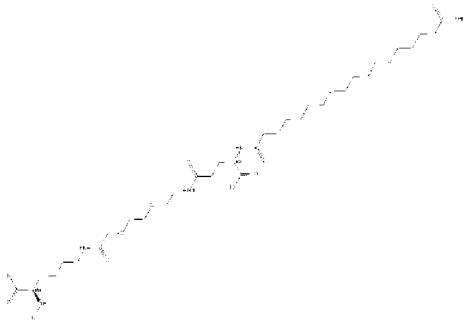
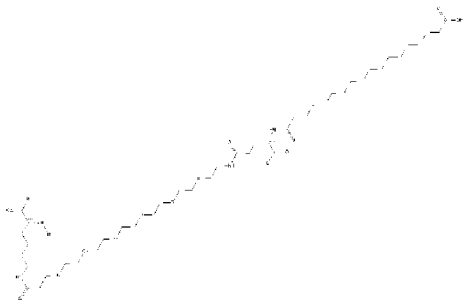
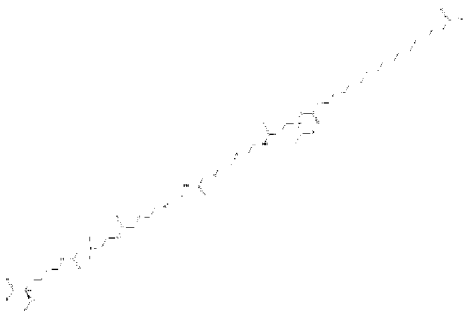
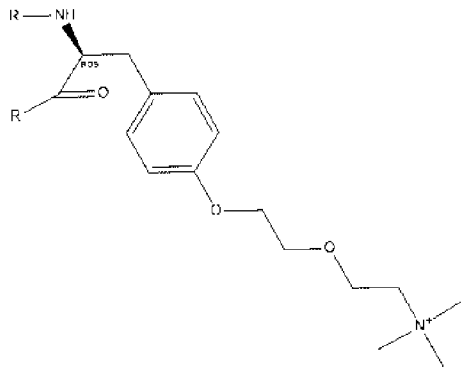
41	C42H75N4O15R	AEEP(PEG2PEG2gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCOCCOCCC([R])=O)=O)=O)=O)C(O)=O)=O)=O
42	 C47H86N7O14R2+	AEEPPEG2PEG2gEC18OH、k(PEG2Sp6PEG2gEC18OH)、dK(PEG2Sp6PEG2gEC18OH)	C[N+](C)(CCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)CC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O
43	 C26H46N4O5R2+2	AEF((Ch)cPEG3a)	C[N+](C)(C)CCN(CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)C(CCOCCOCC[N+](C)(C)C)=O
44	 C25H46N4O4R2+2	AEF(雙 PEG2a)(RS) AEF(雙 PEG2a)(S*) （RS 及 S*指示立體化學）	C[N+](C)(C)CCOCCN(CCOCC[N+](C)(C)C)CCOc1ccc(CC(C([R])=O)N[R])cc1
45	 C21H34N3O5R2+	AEF(NMePEG3a)、AEF(NMecPEG3aCO)	C[N+](C)(C)CCOCCOCCC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O

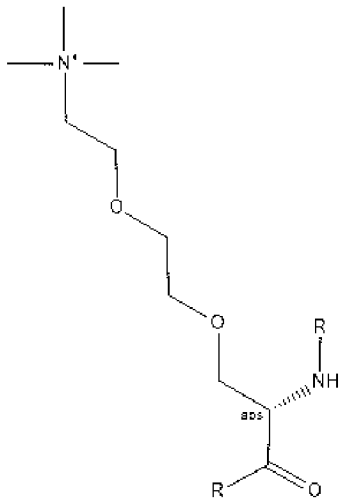
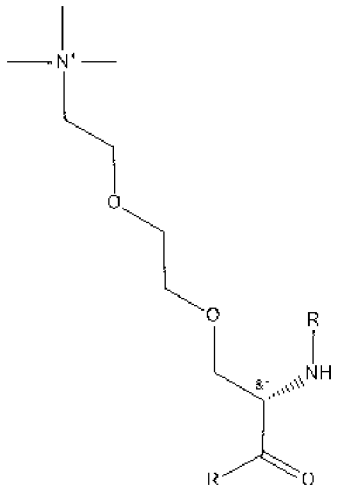
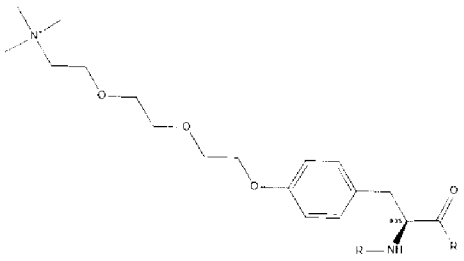
46	 C20H33N2O5R2+	AEF(NMe2mPEG3)	C[N+](C)(CCOCCOCCOC)CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
47	 C26H45N2O8R2+	AEF(NMe 雙 mPEG3)	C[N+](CCOCCOCCOC)(CCOCCOCCOC)CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1

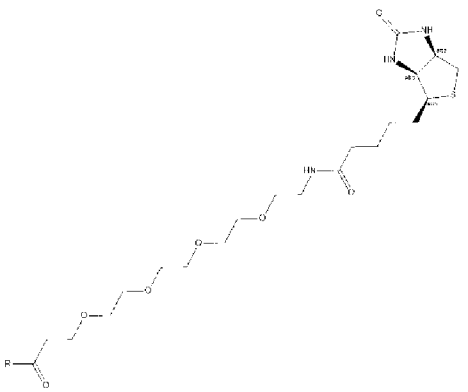
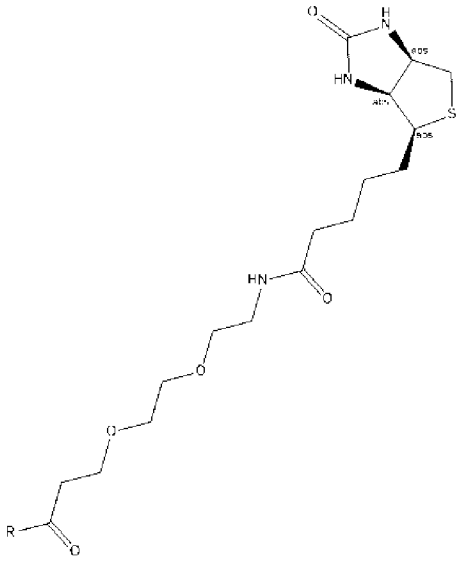
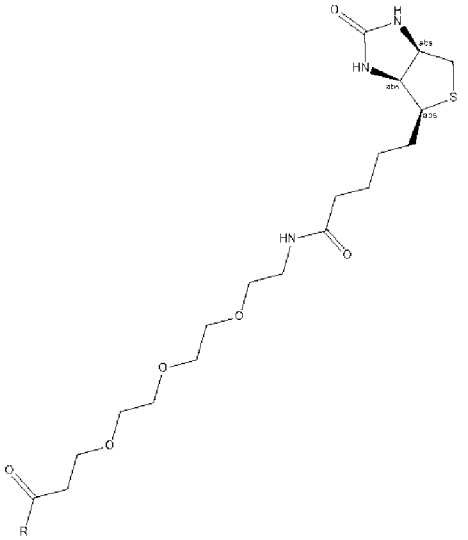
48	 C19H32N3O3R2+	AEF(NMePEG2a)	CN(CCOCC[N+](C)(C)C)CCOc1ccc(C[C@H](C([R])=O)N[R])cc1
49	 C24H40N2O8R2	AEF(NmPEG6)	COCCOCCOCCOCCOCCOCCNCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1
50	 C44H71N5O14R2	AEF(PEG2PEG2gEC16OH)	OC(CCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O)=O)=O)C(O)=O)=O)=O
51	 C46H75N5O14R2	AEF(PEG2PEG2gEC18OH)	OC(CCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O)=O)=O)C(O)=O)=O)=O
52	 C18H30N3O3R2+	AEF(Peg2a)、AEF(PEG2a)	C[N+](C)(C)CCOCCNCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1

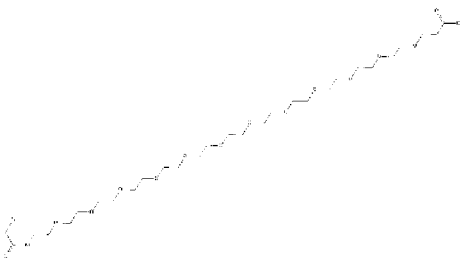
53	 C67H119N6O22R2+	AEF(SP6PEG12gEC18OH)	C[N+](C)(CCNC(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)CC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
54	 C69H123N6O22R2+	AEF(SP6PEG12gEC20OH)	C[N+](C)(CCNC(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)CC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
55	 C52H88N7O15R2+	AEF(SP6PEG2PEG2gEC18OH)	C[N+](C)(CCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)CC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O

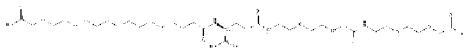
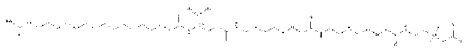
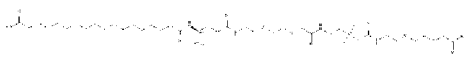
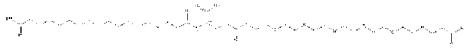
56	C54H92N7O15R2+	AEF(SP6PEG2PEG2gEC20OH)	C[N+](C)(CCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)CC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
57	 C55H95N6O16R2+	AEF(SP6PEG6gEC18OH)	C[N+](C)(CCNC(CCOCCOCCOCCOCCOCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)CC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
58	 C57H99N6O16R2+	AEF(SP6PEG6gEC20OH)	C[N+](C)(CCNC(CCOCCOCCOCCOCCOCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)CC(NCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
59	 C20H35N3O3R2+2	AEF(aPEG2a)	C[N+](C)(C)CCOCC[N+](C)(C)CCOc1ccc(C[C@@H](C([R])=O)N[R])cc1

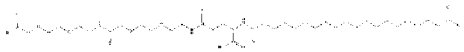
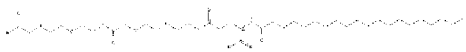
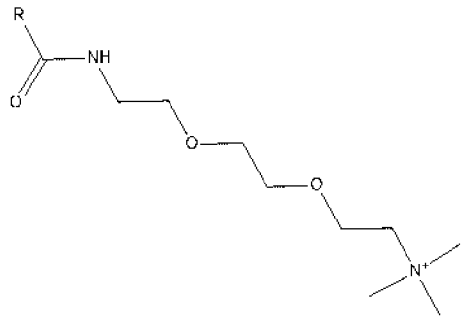
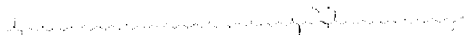
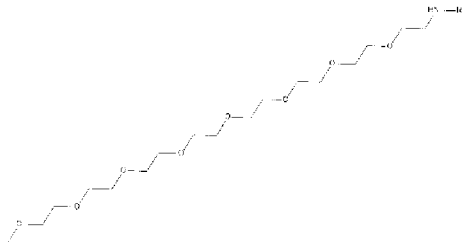
60	 C35H62N4O10R2	k(PEG2gEC18OH)、dK(PEG2gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
61	 C44H80N4O14R2	k(PEG6gEC18OH)、dK(PEG6gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
62	 C47H86N7O14R2+	、k(Sp6PEG2PEG2gEC18OH)、dK(Sp6PEG2PEG2gEC18OH)	C[N+](C)(CCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)CC(NCCCC[C@H](C([R])=O)N[R])=O
63	 C16H25N2O3R2+	APEG2F	C[N+](C)(C)CCOCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1

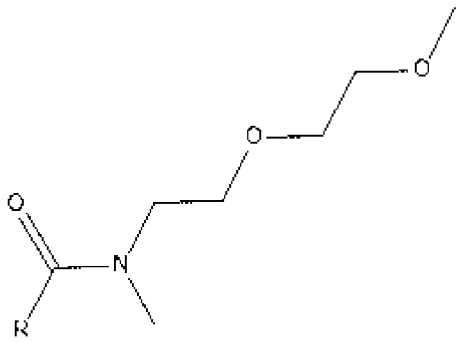
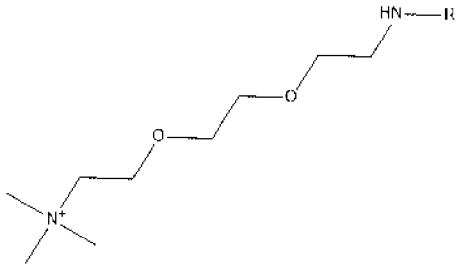
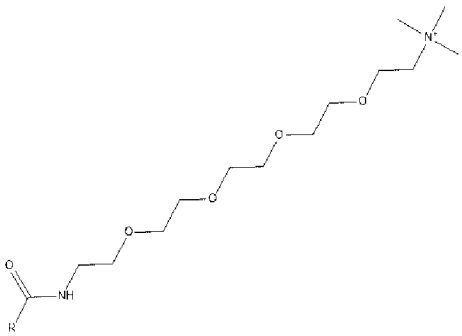
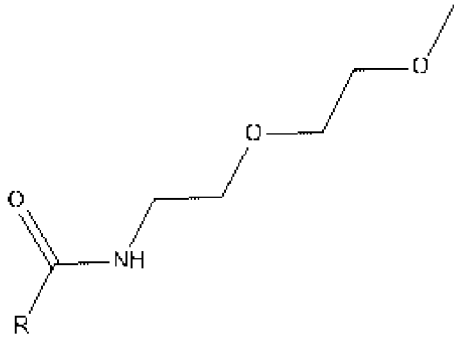
64	 C10H21N2O3R2+	APEG2ser	C[N+](C)(C)CCOCCOC[C@@H](C([R])=O)N[R]
65	 C10H21N2O3R2+	APEG2Ser(R*) APEG2Ser(S*)	C[N+](C)(C)CCOCCOCC(C([R])=O)N[R]
66	 C18H29N2O4R2+	APEG3F	C[N+](C)(C)CCOCCOCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1 C[N+](C)(C)CCOCCOCCOc1ccc(C[C@@H](C=O)N)cc1
67	C17H32NO8R	AcdPEG6CO	CC(NCCOCCOCCOCCOCCOCCOCCC([R])=O)=O

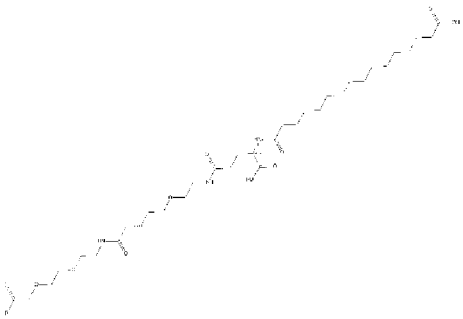
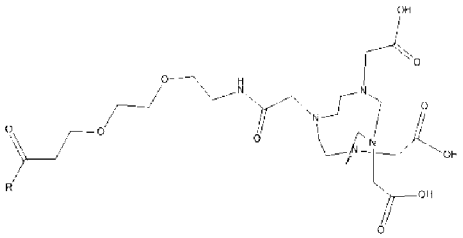
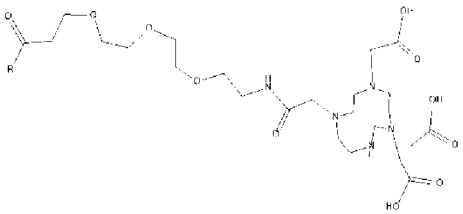
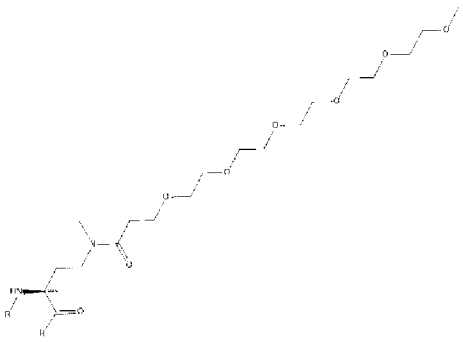
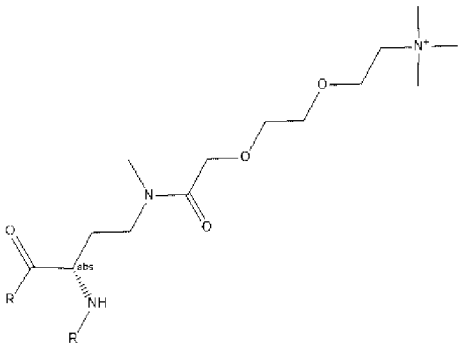
68	 C21H36N3O7SR	生物素 PEG4CO、生物素(PEG4CO)、生物素(PEG4)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCOCCOCCC([R])=O
69	 C17H28N3O5SR	生物素基(dPEG2)、生物素(dPEG2)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCC([R])=O
70	 C19H32N3O6SR	生物素基(dPEG3)、生物素(dPEG3)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCOCCC([R])=O

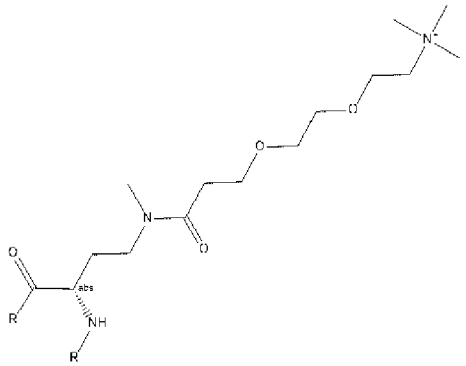
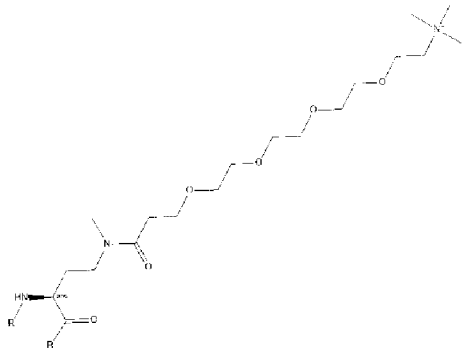
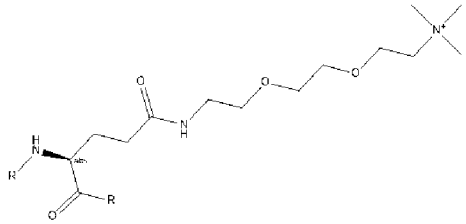
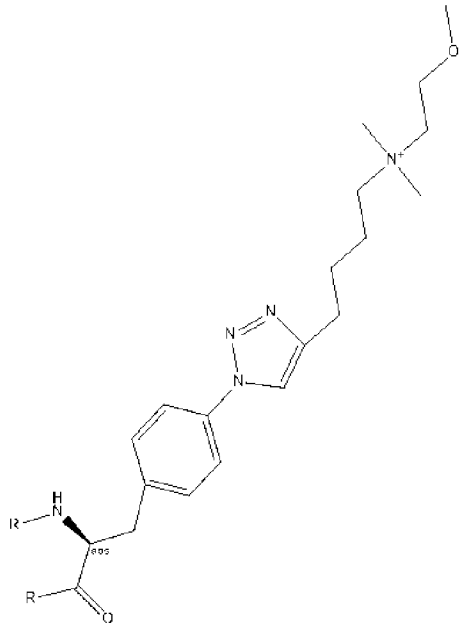
71	 C29H55BrNO14R	BrAcdPEG12CO	O=C(CBr)NCCOCCOCCOCCOCCOCOCCOCCOCCOC

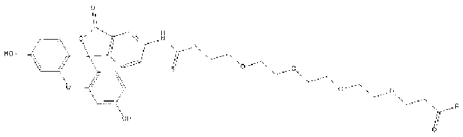
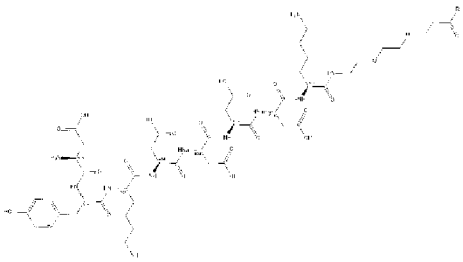
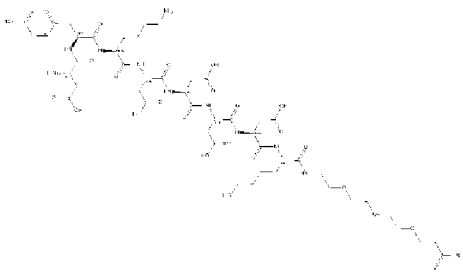
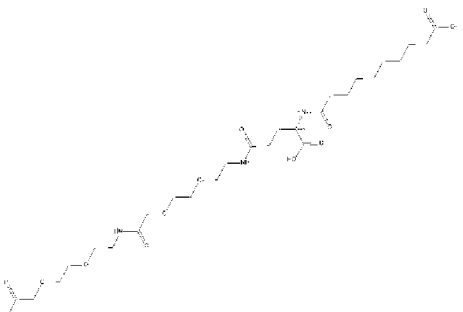
77	 C35H62N3O12R	C18OHgEPEG2PEG2、HOC18gEPEG2PEG2PEG2PEG2gEC18OH	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O)=O OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O)=O OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC=O)=O)=O)C(O)=O)=O)=O
78	 C41H75N5O13R+	C18OHgEPEG2PEG2SP6、HOC18gEPEG2PEG2SP6	C[N+](C)(CCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)CC([R])=O
79	 C41H75N5O13R+	C18OHgEPEG2SP6PEG2、HOC18gEPEG2SP6PEG2	C[N+](C)(CCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)CC(NCCOCCOCC([R])=O)=O
80	 C38H69N2O13R	C18OHgEPEG6、HOC18gEPEG6	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCOCC([R])=O)=O)C(O)=O)=O)=O

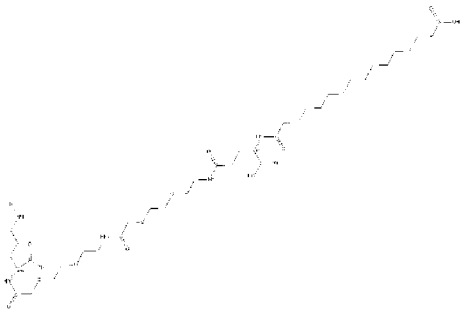
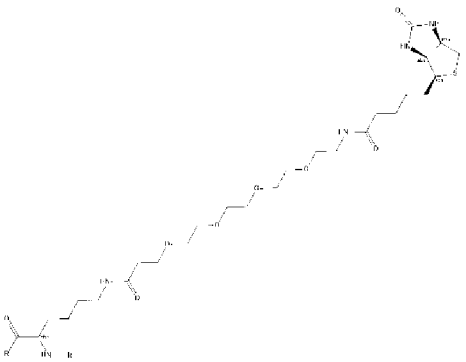
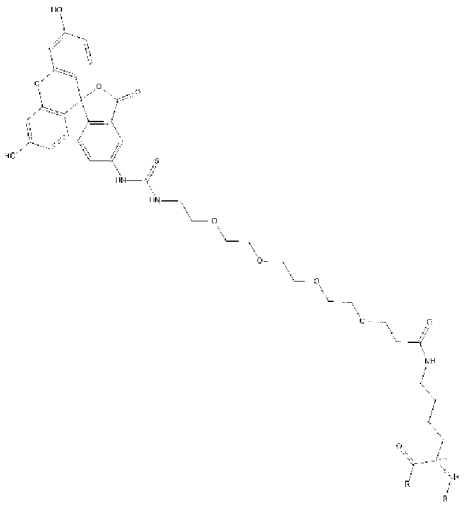
81	 C37H66N3O12R	C20OHgEPEG2PEG2、HOC20gEPEG2PEG2	OC(CCCCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O)=O
82	 C37H68N3O10R	C20gEPEG2PEG2	CCCCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O
83	 C10H22N2O3R+	CO(NHPEG3a) CON(PEG3a) CONHPEG3a	C[N+](C)(C)CCOCCOCCNC([R])=O
84	 C50H94N3O19R	CO(PEG12gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCNC([R])=O)=O)C(O)=O)=O)=O
85	C36H65N4O12R	CO(PEG2PEG2gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCCNC([R])=O)=O)=O)C(O)=O)=O)=O
86	 C17H36NO8R	CO(mPEG8)	COCCOCCOCCOCCOCCOCCOCCOCCN[R]

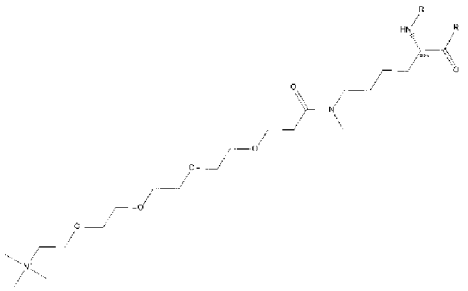
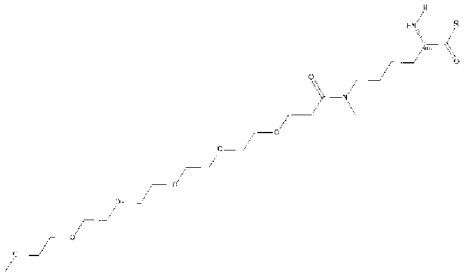
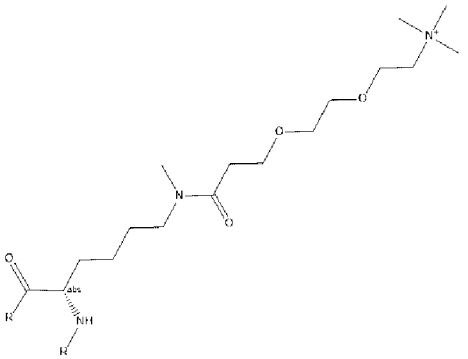
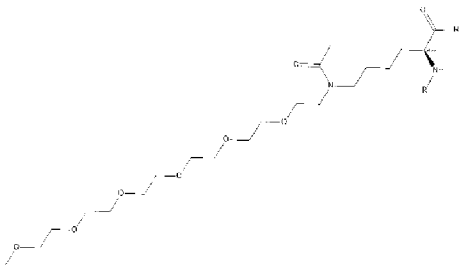
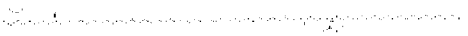
87	 C7H14NO3R	CON(MePEG2)	CN(CCOCCOC)C([R])=O
88	 C9H22N2O2R+	CONH(PEG3a)	C[N+](C)(C)CCOCCOCCN[R]
89	 C14H30N2O5R+	CONH(PEG5a)	C[N+](C)(C)CCOCCOCCOCCOCCNC([R])=O
90	 C6H12NO3R	CONH(mPEG2)	COCCOCCNC([R])=O

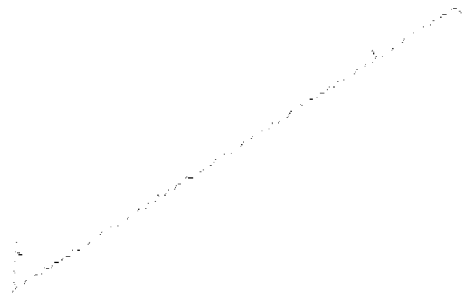
91	 C33H58N3O12R	PEG2PEG2gEC16OH	OC(CCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O)=O OC(CCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC=O)=O)=O)C(O)=O)=O)=O
92	 C23H40N5O10R	DOTA(dPEG2)	OC(CN1CCN(CC(O)=O)CCN(CC(O)=O)CCN(CC(NCCOCCOCCC([R])=O)=O)CC1)=O
93	 C25H44N5O11R	DOTA(dPEG3)	OC(CN1CCN(CC(O)=O)CCN(CC(O)=O)CCN(CC(NCCOCCOCCOCCC([R])=O)=O)CC1)=O
94	 C19H36N2O8R2	Dab(NMeCOmPEG6)	CN(CC[C@@H](C([R])=O)N[R])C(CCOCCOCCOCCOCCOCCOC)=O
95	 C14H28N3O4R2+	Dab(NMecPEG2aCO)、Dab(NMecPEG2a)	CN(CC[C@@H](C([R])=O)N[R])C(COCCOCC[N+](C)(C)C)=O

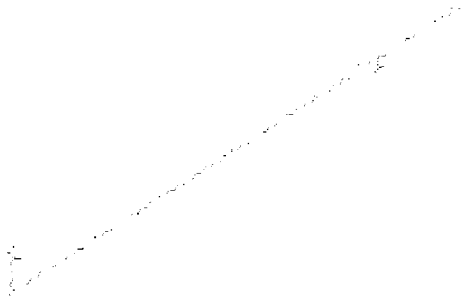
96	 C15H30N3O4R2+	Dab(NMecPEG3aCO)、Dab(NMecPEG3a)	CN(CC[C@@H](C([R])=O)N[R])C(CCOCCOCC[N+](C)(C)C)=O
97	 C19H38N3O6R2+	Dab(NMecPEG5aCO)、Dab(NMecPEG5a)	CN(CC[C@@H](C([R])=O)N[R])C(CCOCCOCCOCCOCC[N+](C)(C)C)=O
98	 C14H28N3O4R2+	E(COcPEG3a))	C[N+](C)(C)CCOCCOCCNC(CC[C@@H](C([R])=O)N[R])=O
99	 C20H30N5O2R2+	F(4TzlDMA4mPEG)	C[N+](C)(CCCCc1cn(-c2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1)CCOC

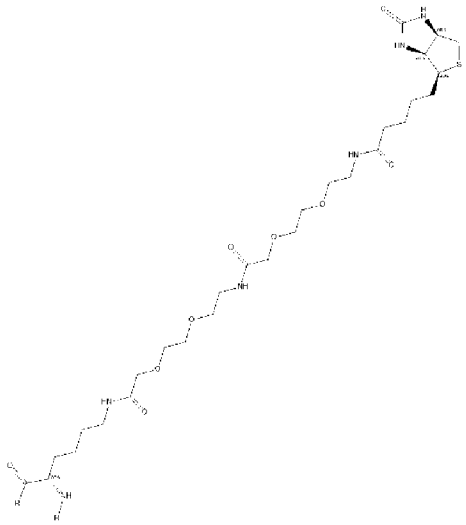
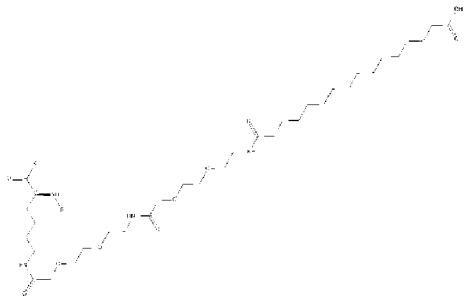
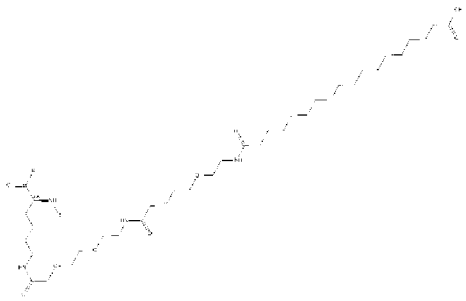
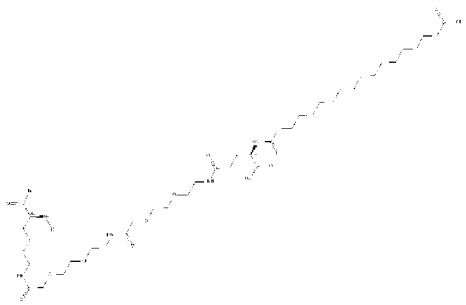
100	 C32H33N2O10SR	FITCPEG4CO	Oc1 cc(Oc2c(C3(c(cc4)c5 cc4NC(NCCOCC OCCOCCOCCC([R])=O)=S)OC5= O)ccc(O)c2)c3 cc1
101	 C48H72N11O22R	Flag 標籤(dPEG2)	NCCCC[C@@H] (C(NCCOCCOC CC([R])=O)=O)N C([C@H](CC(O) =O)NC([C@H](C C(O)=O)NC([C@ H](CC(O)=O)NC ([C@H](CC(O)= O)NC([C@H](C CCCN)NC([C@ H](Cc(cc1)ccc1O)NC([C@H](CC(O)=O)N)=O)=O) =O)=O)=O)=O)= O
102	 C50H76N11O23R	Flag 標籤(dPEG3)	NCCCC[C@@H] (C(NCCOCCOC COCCC([R])=O) =O)NC([C@H](C C(O)=O)NC([C@ H](CC(O)=O)NC ([C@H](CC(O)= O)NC([C@H](C C(O)=O)NC([C@ H](CCCCN)NC([C@H](Cc(cc1)cc c1O)NC([C@H](CC(O)=O)N)=O) =O)=O)=O)=O)= O)=O
103	 C27H46N3O12R	HOC10gEPEG2PEG2、HOC10gEPEG2PEG2CO	OC(CCCCCCCC C(N[C@@H](CC C(NCCOCCOCC (NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O)=O OC(CCCCCCCC C(N[C@@H](CC C(NCCOCCOCC (NCCOCCOCC= O)=O)=O)C(O)= O)=O)=O

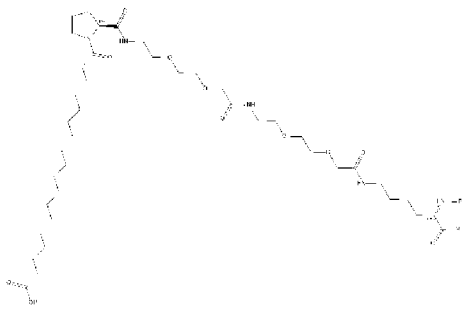
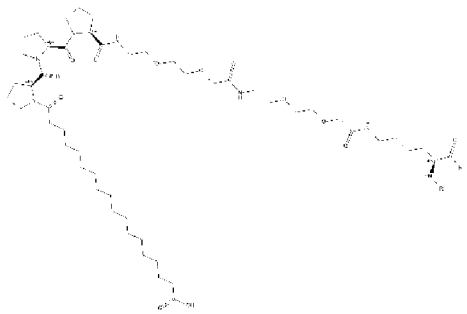
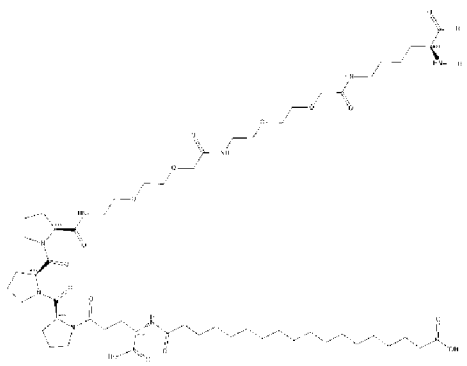
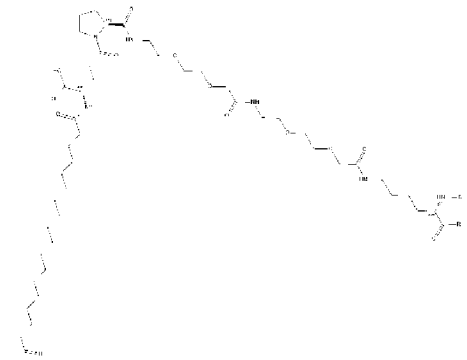
104	 C38H67N5O13R2	HOC16gEPEG2PEG2orn、HOC16OHgEPEG2PEG2orn(2)	OC(CCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(N[C@H](CCCN[R])C([R])=O)=O)=O)=O)C(O)=O)=O)=O NCCC[C@H](C=O)NC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O
105	 C27H47N5O8SR2	K(生物素 PEG4)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O
106	 C38H44N4O11SR2	K(FITCPEG4)	Oc1cc(Oc2c(C3(c(cc4)c5cc4NC(NCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=S)OC5=O)ccc(O)c2)c3 cc1

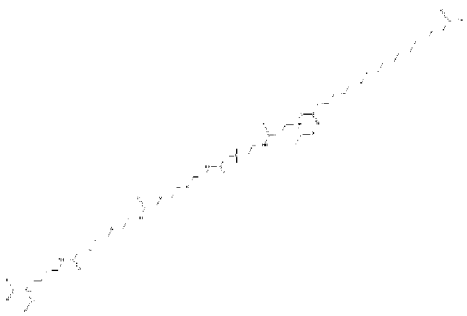
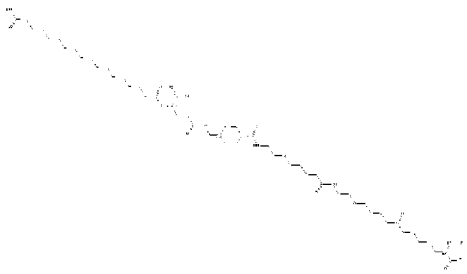
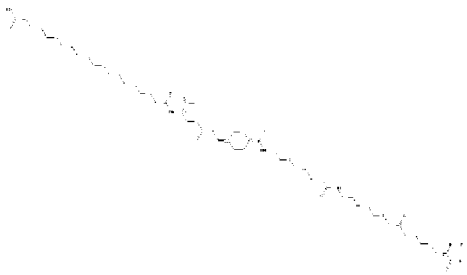
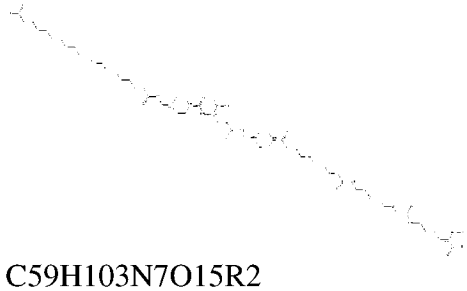
107	 C21H42N3O6R2+	K(NMeCOPEG4N+Me3)	CN(CCCC[C@@H](C([R])=O)N[R])C(CCOCCOCCOCCOCC[N+](C)(C)C)=O
108	 C21H40N2O8R2	K(NMeCOmPEG6)	CN(CCCC[C@@H](C([R])=O)N[R])C(CCOCCOCCOCCOCCOCCOC)=O
109	 C17H34N3O4R2+	K(NMePEG3a)、K(NMecPEG3a)、K(NMecPEG3aCO)	CN(CCCC[C@@H](C([R])=O)N[R])C(CCOCCOCC[N+](C)(C)C)=O
110	 C21H40N2O8R2	K(NmPEG6Ac)	CC(N(CCCC[C@@H](C([R])=O)N[R])CCOCCOCCOCCOCCOCCOC)=O
111	 C58H108N4O20R2	K(PEG12NMegENMeC18OH)	CN(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)C(CC[C@@H](C(O)=O)N(C)C(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O

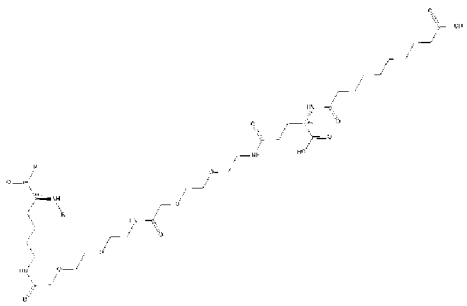
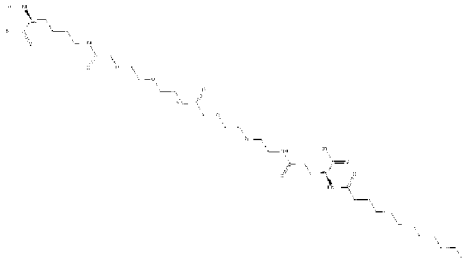
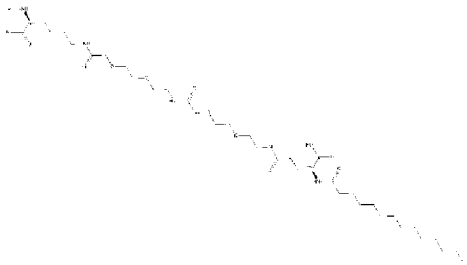
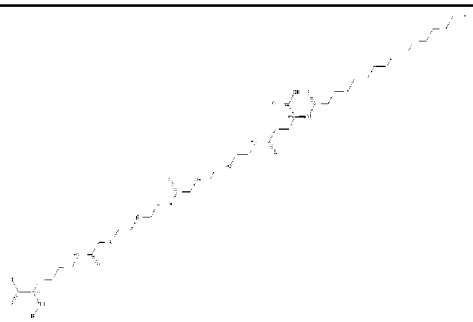
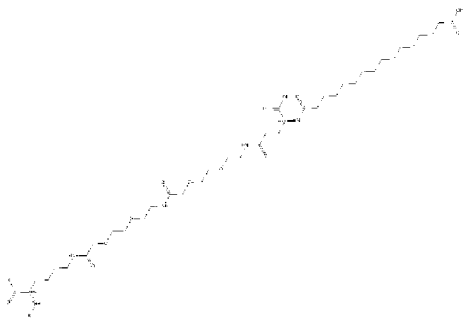
112	C59H110N8O18R2	K(PEG12NMegENMeC18 四唑)	CN(CCOCCOCCOCCOCCCOCCOCCOCCOCCCOCCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)C(CC[C@@H](C(O)=O)N(C)C(CCCCCCCCCCCCCCCCCCCCc1nnn[nH]1)=O)=O
113	C56H104N4O20R2	K(PEG12gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCCOCCOCCCOCCOCCCOCCOCCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
114	C58H108N4O20R2	K(PEG12gEC20OH)	OC(CCCCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCCOCCOCCCOCCOCCCOCCOCCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
115	 C75H145N3O29R2	K(PEG24C18OH)	OC(CCCCCCCCCCCCCCCCCC(NCCOCCOCCOCCOCCCOCCOCCCOCCOCCCOCCOCCCOCCOCCCOCCOCCCOCCOCCCOCCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O

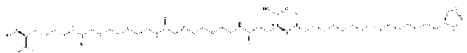
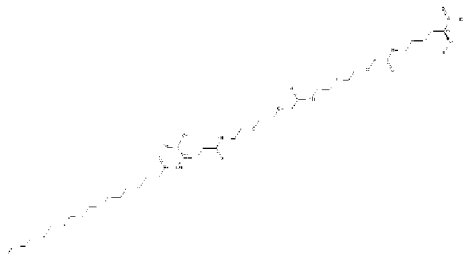
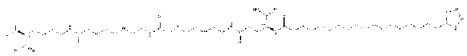
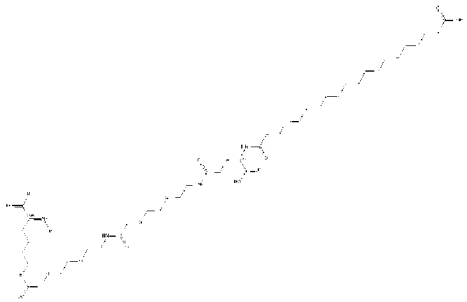
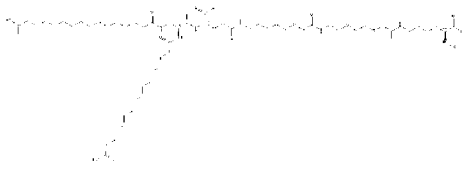
116	 C78H148N4O32R2	K(PEG24gEC16OH)	OC(CCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCO

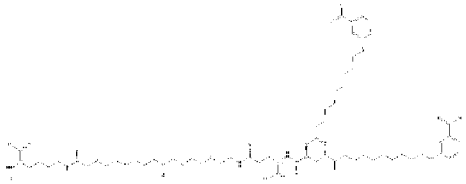
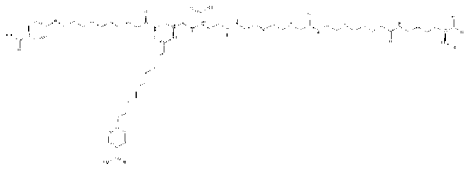
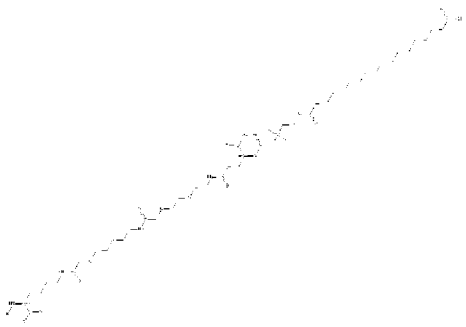
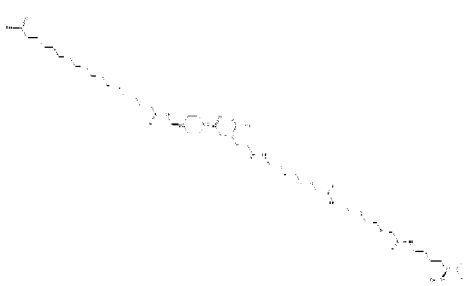
120	 C28H48N6O9SR2	K(PEG2PEG2 生物素)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
121	 C34H62N4O10R2	K(PEG2PEG2C16OH)	OC(CCCCCCCCCCCCCCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O
122	 C36H66N4O10R2	K(PEG2PEG2C18OH)	OC(CCCCCCCCCCCCCCCCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O
123	 C41H73N5O13R2	K(PEG2PEG2DgEC18OH)	OC(CCCCCCCCCCCCCCCCC(N[C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O

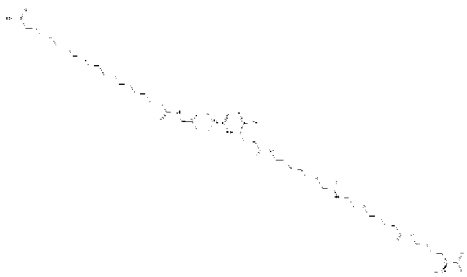
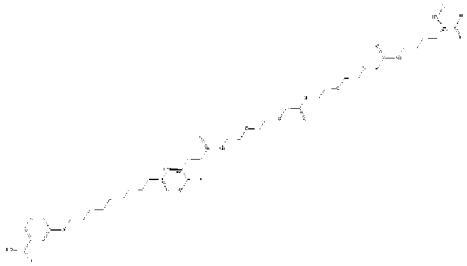
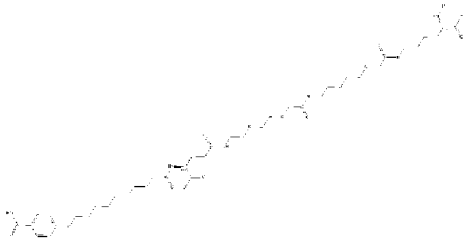
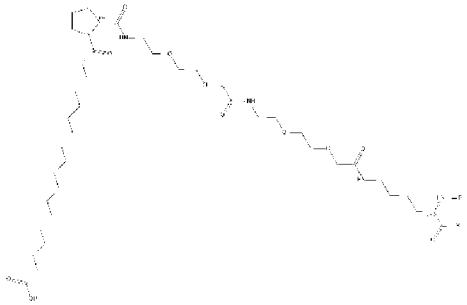
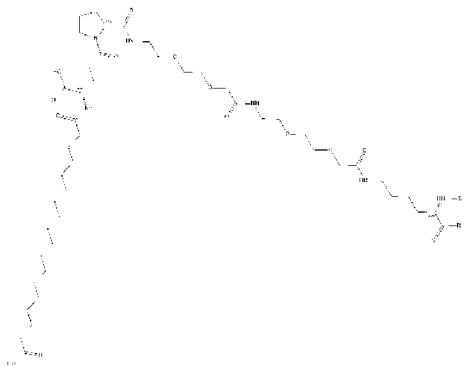
124	 C41H73N5O11R2	K(PEG2PEG2PC18OH)	OC(CCCCCCCCCCCCCCCCCC(N(CCC1)[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)=O
125	 C51H87N7O13R2	K(PEG2PEG2PPPC18OH)	OC(CCCCCCCCCCCCCCCCCC(N(CCC1)[C@@H]1C(N(CCC1)[C@@H]1C(N(CCC1)[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)=O)=O)=O
126	 C56H94N8O16R2	K(PEG2PEG2PPPgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@@H]1C(N(CCC1)[C@@H]1C(N(CCC1)[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)=O)=O)C(O)=O)=O)=O
127	 C46H80N6O14R2	K(PEG2PEG2PgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O)=O

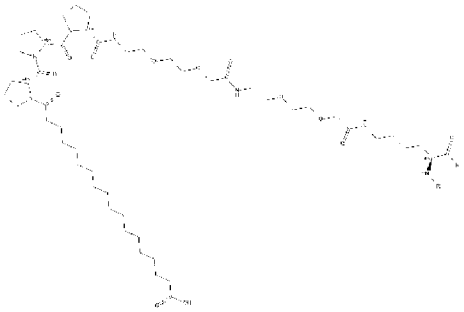
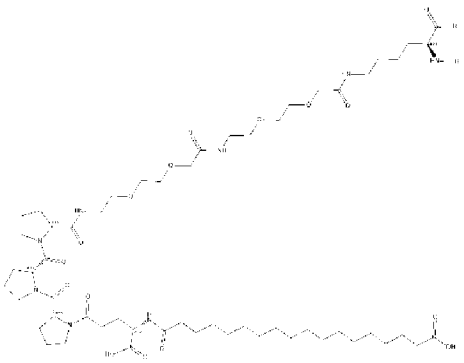
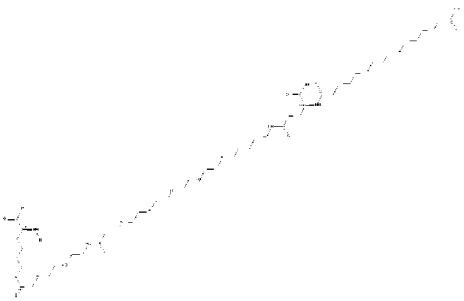
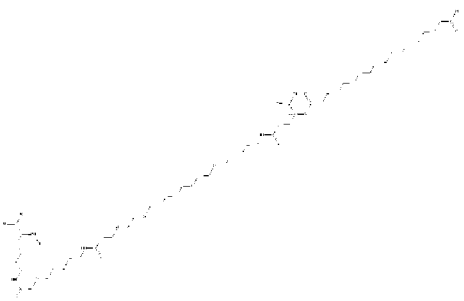
128	 C47H86N7O14R2+	K(PEG2PEG2Sp6gEC18OH)	C[N+](C)(CCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCC(O)=O)=O)=O)CC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O
129	 C49H86N6O14R2	K(PEG2PEG2TrxgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NC[C@H](CC1)CC[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O)=O
130	 C51H90N6O14R2	K(PEG2PEG2TrxgEC20OH)	OC(CCCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NC[C@H](CC1)CC[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O)=O
131	 C59H103N7O15R2	K(PEG2PEG2TrxgETrxC20OH)	OC(CCCCCCCCCCCCCCCCCC(NC[C@H](CC1)CC[C@@H]1C(N[C@@H](CCC(NC[C@H](CC1)CC[C@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O)=O

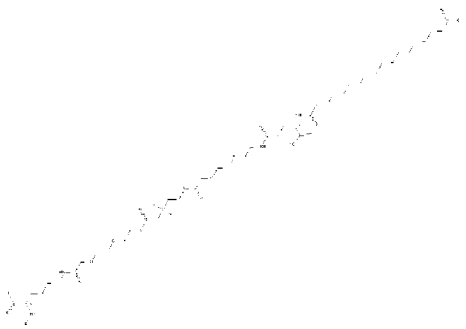
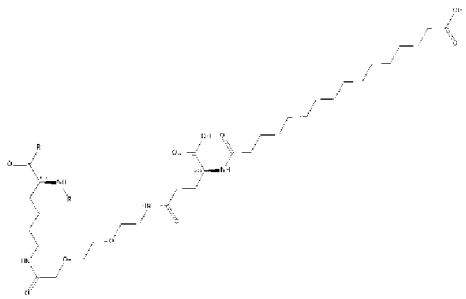
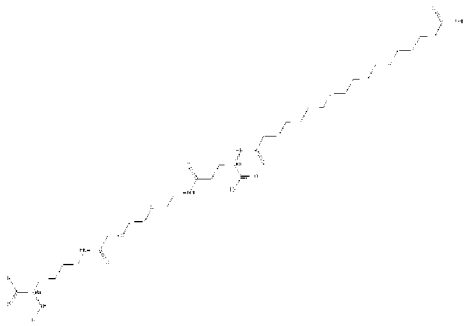
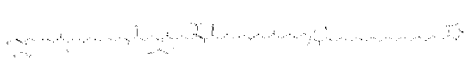
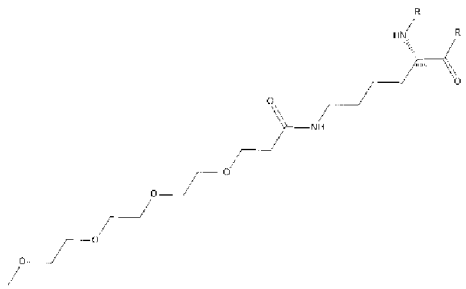
132	 C33H57N5O13R2	K(PEG2PEG2gEC10OH)	OC(CCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
133	 C35H63N5O11R2	K(PEG2PEG2gEC12)	CCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
134	 C37H67N5O11R2	K(PEG2PEG2gEC14) NMeK(PEG2PEG2gEC14)	CCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
135	 C39H71N5O11R2	K(PEG2PEG2gEC16)	CCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
136	 C39H69N5O13R2	K(PEG2PEG2gEC16OH)	OC(CCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O

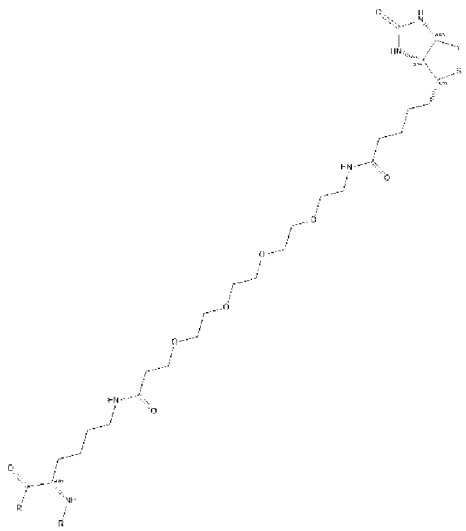
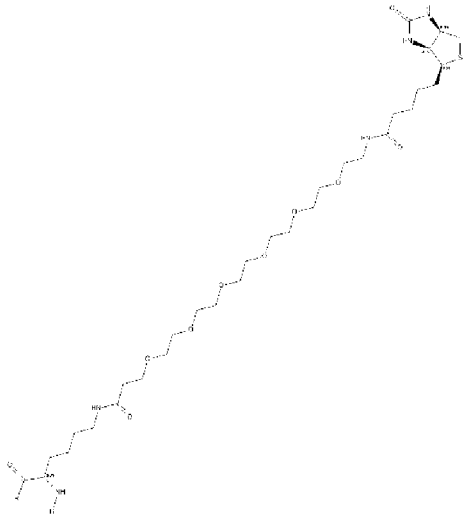
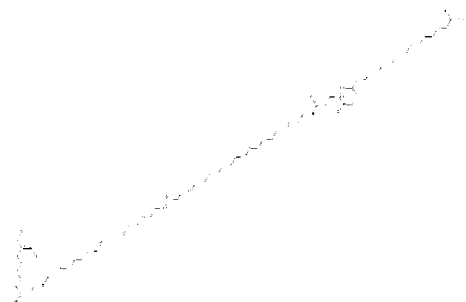
137	 C40H71N9O11R2	K(PEG2PEG2gEC16 四唑)	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCCCCCCCCc1nnn[nH]1)=O)=O
138	 C41H75N5O11R2	K(PEG2PEG2gEC18)	CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
139	 C42H75N9O11R2	K(PEG2PEG2gEC18 四唑)	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCC[C@@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCCCCCCCCCCc1nnn[nH]1)=O)=O
140	 C43H77N5O13R2	K(PEG2PEG2gEC20OH)	OC(CCCCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O
141	 C58H103N7O17R2	KPEG2PEG2gEDap(C16OH)2、K(PEG2PEG2gEDAP(C16OH)2)	OC(CCCCCCCCCCCCCCCC(NC[C@@H](C(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)NC(CCCCCCCCCCCCCCCC(O)=O)=O)=O

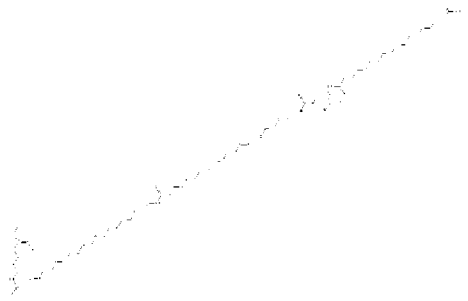
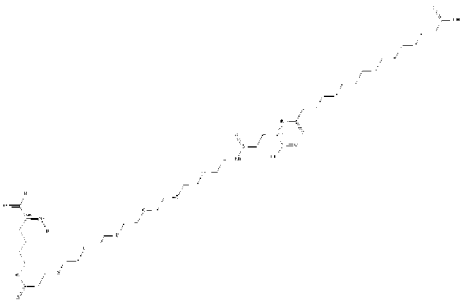
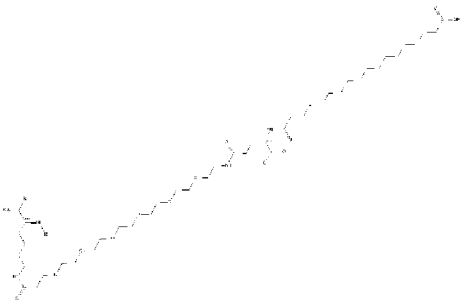
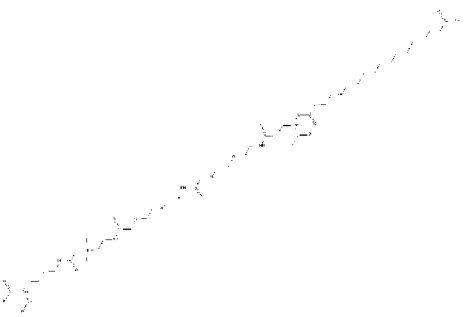
142	 C60H91N7O19R2	K(PEG2PEG2gEDAP(mXOH)2) KPEG2PEG2gEDAP(mXOH)2	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)NC([C@H](CNC(CCCCCCCCCCOc1cc(C(O)=O)ccc1)=O)NC(CCCCCCCCCCOc1cc(C(O)=O)ccc1)=O)=O)=O
143	 C60H91N7O19R2	K(PEG2PEG2gEDAP(pXOH)2) KPEG2PEG2gEDAP(pXOH)2	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)NC([C@H](CNC(CCCCCCCCCCOc(cc1)ccc1C(O)=O)=O)NC(CCCCCCCCCCOc(cc1)ccc1C(O)=O)=O)=O)=O
144	 C47H86N7O14R2+	K(PEG2PEG2gESp6C18OH)	C[N+](C)(CCNC(CCCCCCCCCCCCCCCCCC(O)=O)=O)CC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
145	 C49H86N6O14R2	K(PEG2PEG2gETrxC18OH)	OC(CCCCCCCCCCCCCCCCCC(NC[C@H](CC1)CC[C@@H]1C(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O)=O

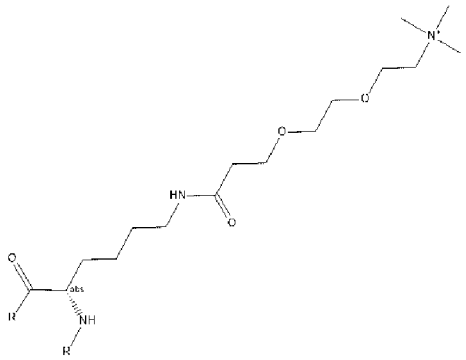
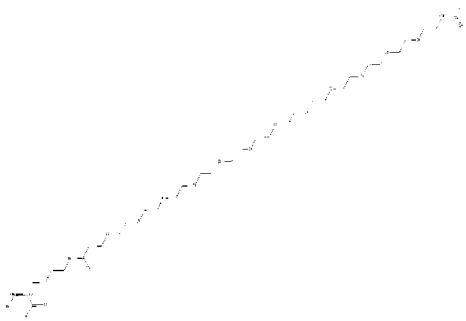
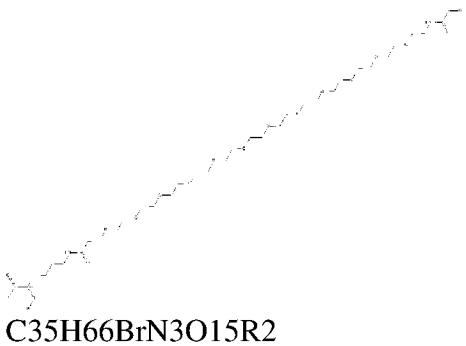
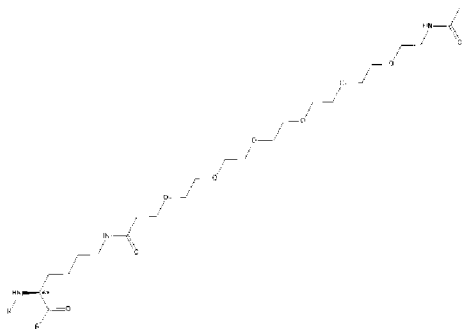
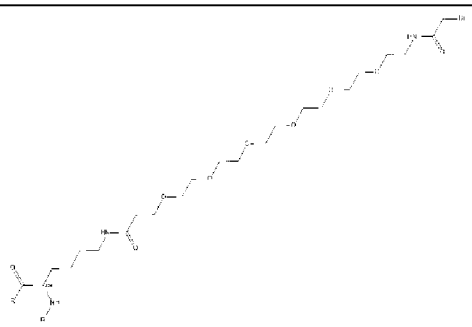
146	 C51H90N6O14R2	K(PEG2PEG2gETrxC20OH)	OC(CCCCCCCCCCCCCCCCCCCC(NC[C@H](CC1)CC[C@@H]1C(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O)=O
147	 C40H63N5O14R2	K(PEG2PEG2gEmXOH)	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCCOc1cc(C(O)=O)ccc1)=O)=O
148	 C40H63N5O14R2	K(PEG2PEG2gEpXOH)	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCOc(cc1)ccc1C(O)=O)=O)=O
149	 C41H73N5O11R2	K(PEG2PEG2pC18OH)	OC(CCCCCCCCCCCCCCCCCC(N(CCC1)[C@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)=O
150	 C46H80N6O14R2	K(PEG2PEG2pgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O

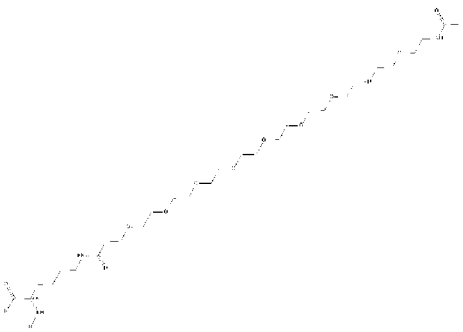
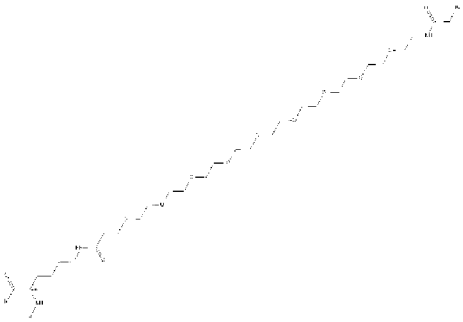
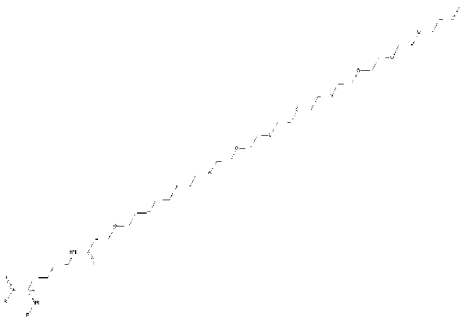
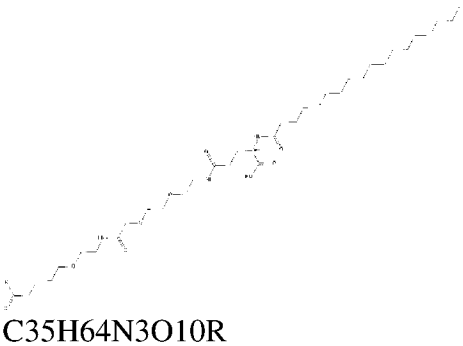
151	 C51H87N7O13R2	K(PEG2PEG2pppC18OH)	OC(CCCCCCCCCCCCCCCCCC(N(CCC1)[C@H]1C(N(CCC1)[C@H]1C(N(CCC1)[C@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)=O)=O)=O
152	 C56H94N8O16R2	K(PEG2PEG2pppgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@H]1C(N(CCC1)[C@H]1C(N(CCC1)[C@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)=O)=O)C(O)=O)=O)=O
153	 C48H87N5O17R2	K(PEG2PEG6gEC16OH)	OC(CCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
154	 C50H91N5O17R2	K(PEG2PEG6gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O

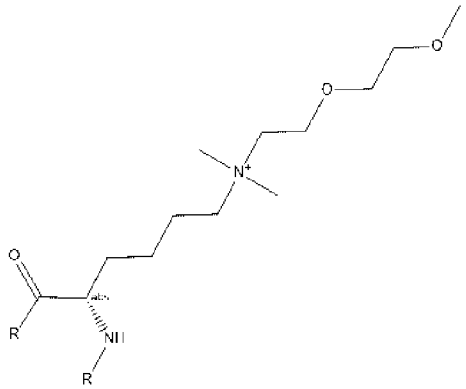
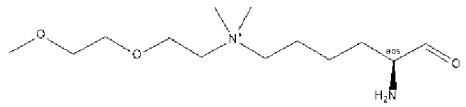
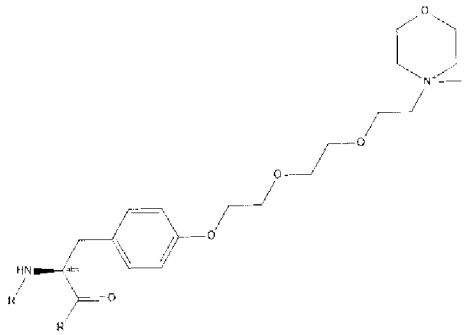
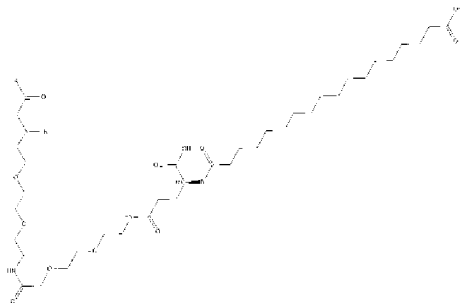
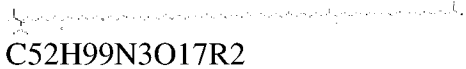
155	 C47H86N7O14R2+	K(PEG2Sp6PEG2gEC18OH)	C[N+](C)(CCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)CC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
156	 C33H58N4O10R2	K(PEG2gEC16OH)	OC(CCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
157	 C35H62N4O10R2	K(PEG2gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
158	 C49H85N11O17SR2	K(PEG2gEgEPEG24SBC16 四唑)	OC([C@H](CCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)NC(CC[C@@H](C(O)=O)NC(COCCOCCNC(CCCS(NC(CCCCCCCCCCCCCCCCCCCCc1nnn[nH]1)=O)(=O)=O)=O)=O)=O)=O
159	 C16H30N2O6R2	K(PEG3OMe)K(mPEG4)	COCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O

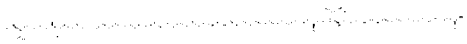
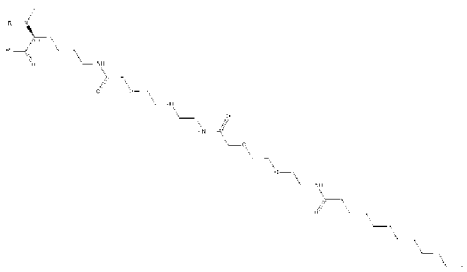
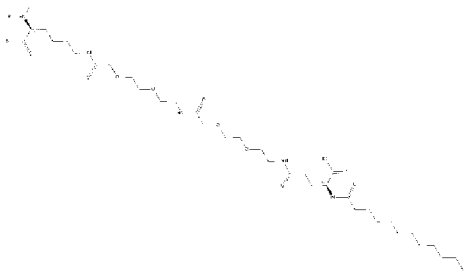
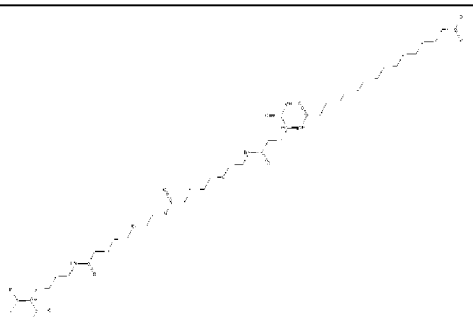
160	 C27H47N5O8SR2	K(PEG4Biotina)、K(PEG4 生物素)	O=C(CCCC[C@H]([C@@H]1N2)SC[C@H]1NC2=O)NCCOCCOCCOCCOCCC(NCCC[C@@H](C([R])=O)N[R])=O
161	 C31H55N5O10SR2	K(PEG6 生物素)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O
162	 C57H105N5O21R2	K(PEG6PEG6gEC16OH)	OC(CCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCC(NCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O

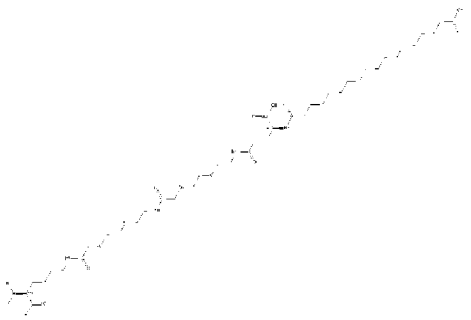
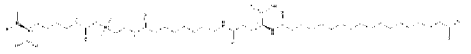
163	 C59H109N5O21R2	K(PEG6PEG6gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCC(NCCOCCOCCOCCOCCOCCOCCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
164	 C42H76N4O14R2	K(PEG6gEC16OH)	OC(CCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
165	 C44H80N4O14R2	K(PEG6gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O)C(O)=O)=O)=O
166	 C47H86N7O14R2+	K(Sp6PEG2PEG2gEC18OH)	C[N+](C)(CCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)CC(NCCCC[C@@H](C([R])=O)N[R])=O

167	 C16H32N3O4R2+	K(cPEG3a)、K(cPEG3aCO)	C[N+](C)(C)CCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O
168	 C35H67N3O15R2	K(dPEG12Ac)	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
169	 C35H66BrN3O15R2	K(dPEG12AcBr)	O=C(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCNC(CBr)=O)NCCCC[C@@H](C([R])=O)N[R]
170	 C23H43N3O9R2	K(dPEG6Ac)	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
171	 C23H42BrN3O9R2	K(dPEG6AcBr)	O=C(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCNC(CBr)=O)NCCCC[C@@H](C([R])=O)N[R]

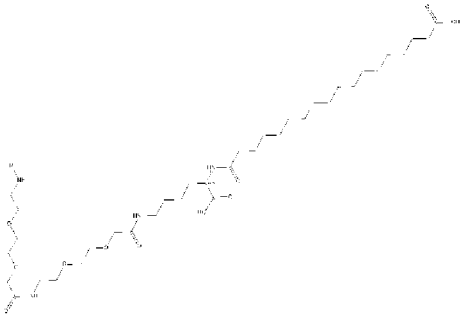
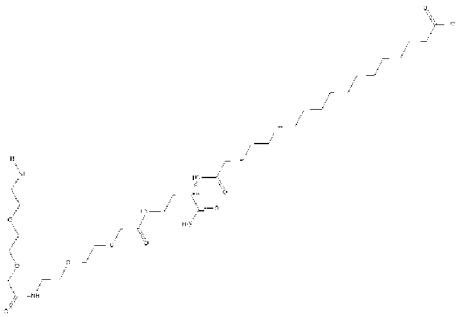
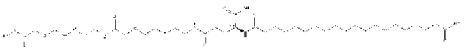
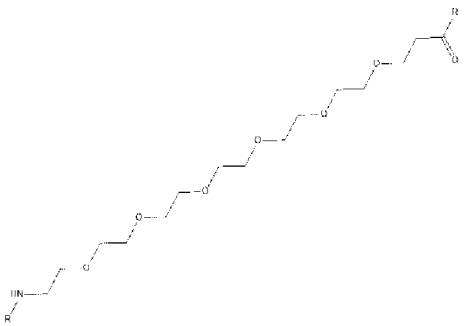
172	 C29H55N3O12R2	K(dPEG9Ac)	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@@H](C([R])=O)N[R])=O)=O
173	 C29H54BrN3O12R2	K(dPEG9AcBr)	O=C(CCOCCOCCOCCOCCOCCOCCOCCOCCNC(CBr)=O)NCCCC[C@@H](C([R])=O)N[R]
174	 C32H62N2O14R2	K(mPEG12)	COCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(NCCC[C@@H](C([R])=O)N[R])=O
175	 C35H64N3O10R	PEG2PEG2gEC18	CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC([R])=O)=O)=O)C(O)=O)=O CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC=O)=O)=O)C(O)=O)=O

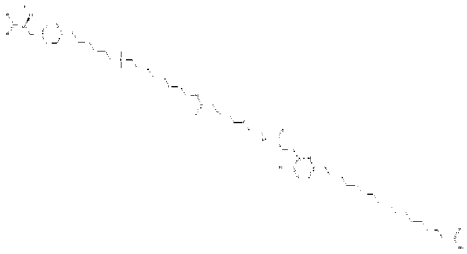
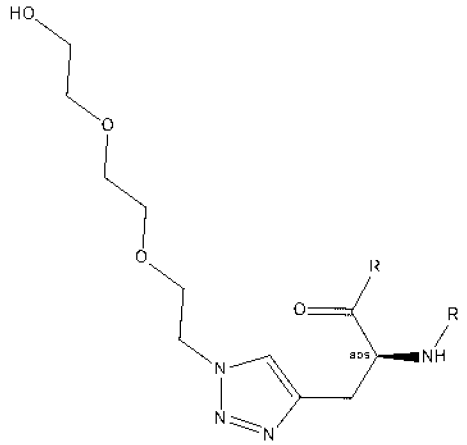
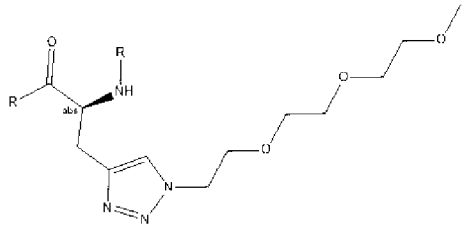
176	 C13H27N2O3R2+	Lys(N+Me2mPEG3)	C[N+](C)(CCCC[C@@H](C([R])=O)N[R])CCOCCOC
177	 C13H29N2O3+	LysQuatMe2mPEG3、Lys(N+(Me)2mPEG3)	C[N+](C)(CCCC[C@@H](C=O)N)CCOCCOC
178	 C20H31N2O5R2+	MMPEG3F	C[N+]1(CCOCCOCCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)CCOCC1
179	 C37H66N4O12R2	N(PEG2PEG2gEC18OH)Gly	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCCN(CC([R])=O)[R])=O)=O)C(O)=O)=O)=O
180	 C52H99N3O17R2	NMeK(PEG12C18OH)	CN([C@@H](CCCCNC(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCNC(CCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)C([R])=O)[R]

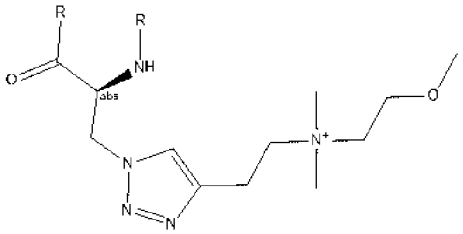
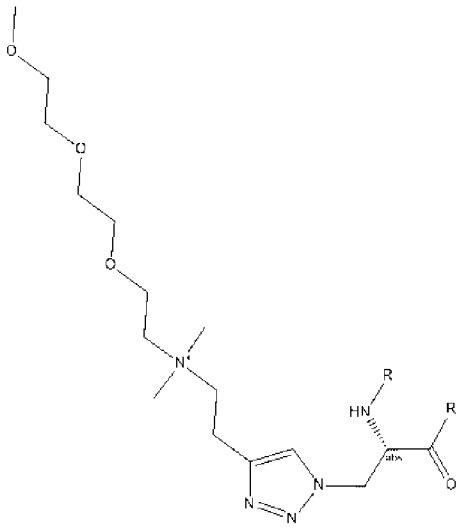
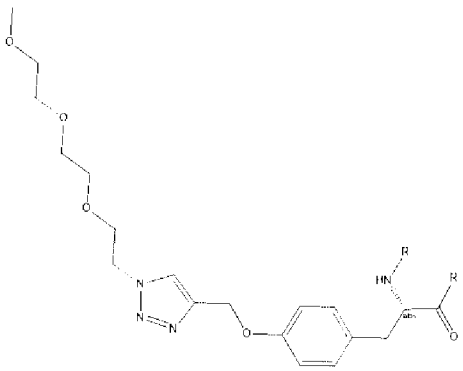
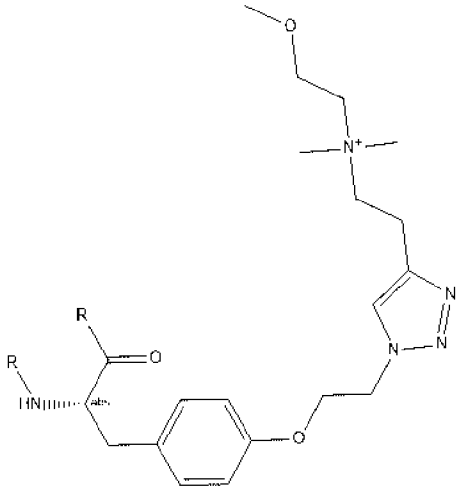
181	 C57H106N4O20R2	NMeK(PEG12gEC18OH)	CN([C@@H](CCCCNC(CCOCCOCCOCCOCCOCCOCCOCCCOCCOCCCOCCOCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)C([R])=O)[R]
182	C45H81N5O13R2	NMeK(PEG2NMePEG2NMegENMeC18OH)	CN(CCOCCOCC(N(C)CCOCCOCC(NCCCC[C@@H](C([R])=O)N(C)[R])=O)=O)C(CC[C@@H](C(O)=O)N(C)C(CCCCCCCCCCCCCCCCC(O)=O)=O)=O
183	 C31H58N4O8R2	NMeK(PEG2PEG2C12)	CCCCCCCCCCCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N(C)[R])=O)=O)=O
184	 C36H65N5O11R2	NMeK(PEG2PEG2gEC12)	CCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C([R])=O)N(C)[R])=O)=O)=O)C(O)=O)=O
185	 C40H71N5O13R2	NMeK(PEG2PEG2gEC16OH)	CN([C@@H](CCCCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)C([R])=O)[R]

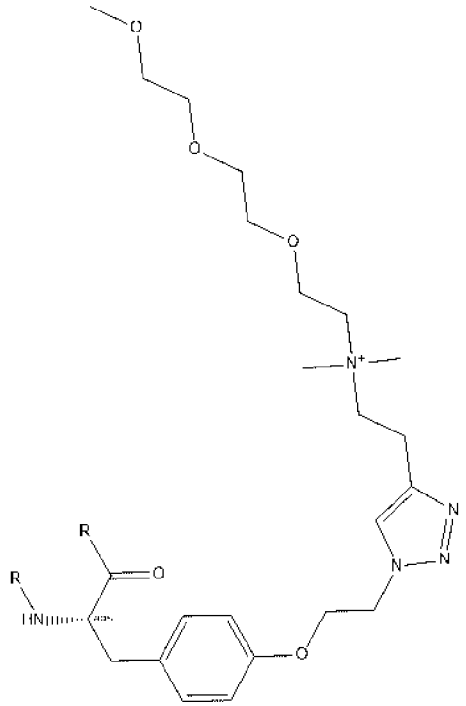
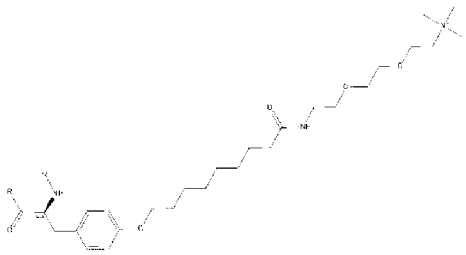
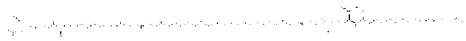
186	 C42H75N5O13R2	NMeK(PEG2PEG2gEC18OH)	CN([C@@H](CCCCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)=O)C([R])=O)[R]
187	C44H79N5O13R2	NMeK(PEG2PEG2gEC20OH)	CN([C@@H](CCCCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)=O)C([R])=O)[R]
188	C39H74N3O11R3	NMeK(PEG6C18OH)	CN([R])[R](CCCCNC(CCOCCOCCOCCOCCOCCOCCOCCNC(CCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)C([R])=O
189	C45H82N4O14R2	NMeK(PEG6gEC18OH)	CN([C@@H](CCCCNC(CCOCCOCCOCCOCCOCCOCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)=O)C([R])=O)[R]
190	 C42H77N6O11R2+	NMeK(SP6PEG2gEC18OH)	CN([C@@H](CCCCNC(C[N+](C)(C)CCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)=O)=O)C([R])=O)[R]

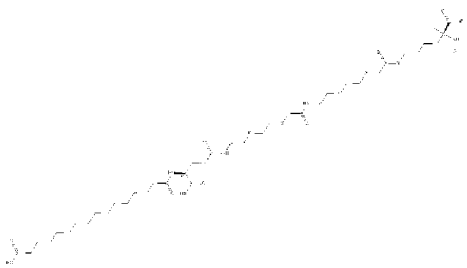
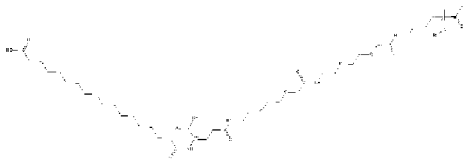
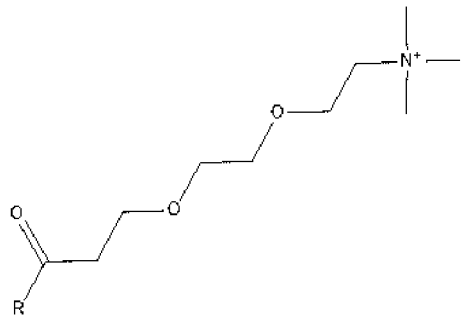
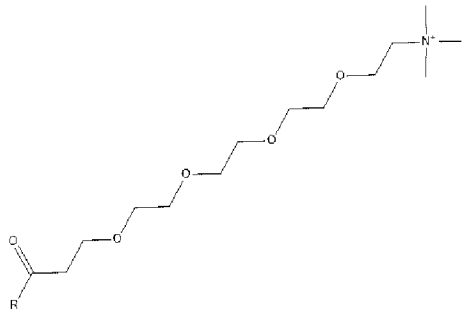
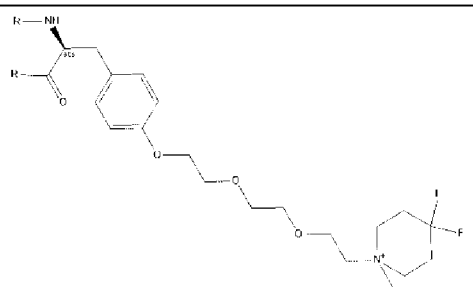
191	 C50H94N3O19R	PEG12gEC18OH	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCO

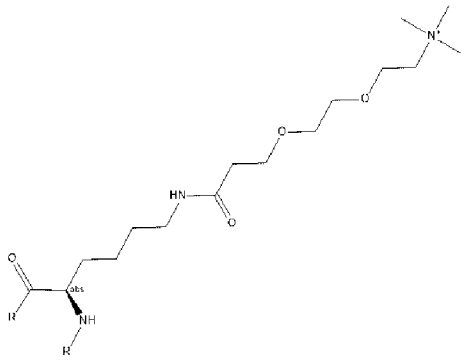
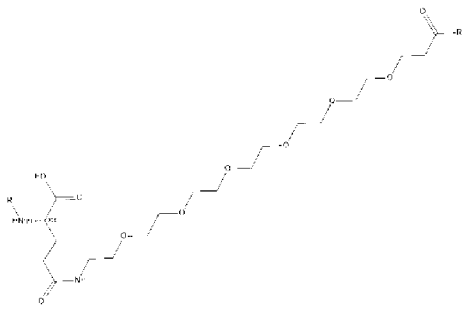
196	 C36H67N4O11R	PEG2PEG2eKC18OH	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCCCNC(COCCOCCNC(COCCOCCN[R])=O)=O)C(O)=O)=O)=O NCCOCCOCC(NCCOCCOCC(NCCCC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O
197	 C34H63N4O11R	PEG2PEG2gDabC18OH	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCNC(COCCOCCNC(COCCOCCN[R])=O)=O)C(O)=O)=O)=O NCCOCCOCC(NCCOCCOCC(NCC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O
198	 C37H67N4O12R	PEG2PEG2gEC20OH	OC(CCCCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(N[R])=O)=O)=O)C(O)=O)=O)=O
199	 C15H29NO7R2	PEG6	O=C(CCOCCOCCOCCOCCOCCOCCN[R])[R]
200	C26H52O13	Peg12-Ome Peg12OMe、Poly 乙基 ene12-O-甲基 Peg12-O 甲基	COCCOCCOCCOCCOCCO

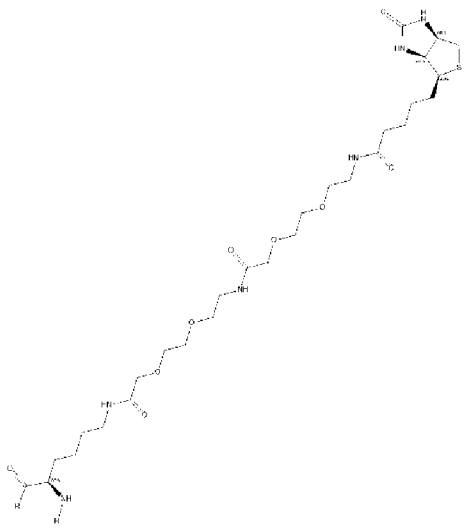
201	 C23H48O11	Peg12OMe、Peg12-O甲基	CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOC
202	 C54H100N4O18R2	Pip(PEG12gEC16)、Spiral_Pip_PEG12_IsoGlu_Palm	CCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(N(CC1)CCC1(C([R])=O)N[R])=O)=O)C(O)=O)=O
203	 C51H88N5O13R2+	TMAPF(PEG2PEG2gEC18OH)	C[N+](C)(CCCCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)CCOCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O
204	 C11H18N4O4R2	Tzl(PEG3OH)	OCCOCCOCCn1nnc(C[C@@H](C([R])=O)N[R])c1
205	 C12H20N4O4R2	Tzl(mPEG3)	COCCOCCOCCn1nnc(C[C@@H](C([R])=O)N[R])c1

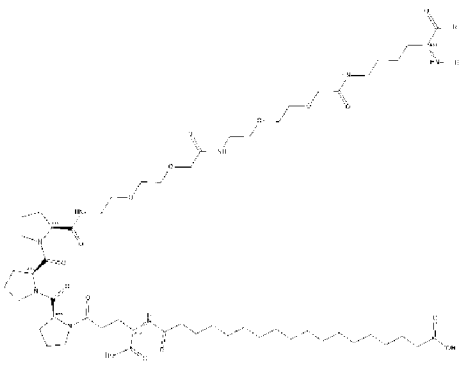
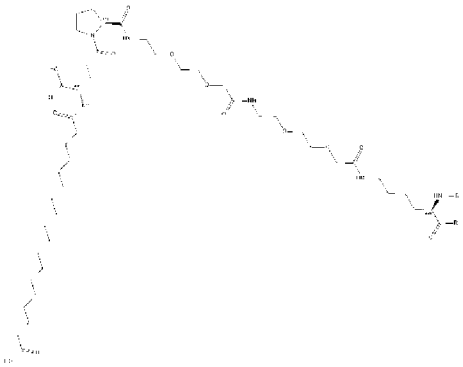
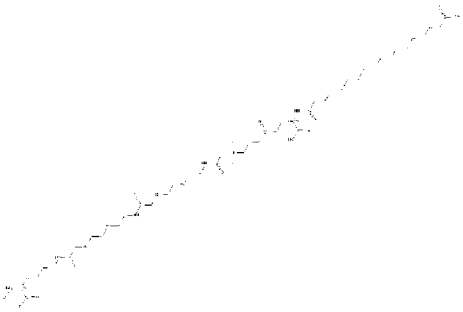
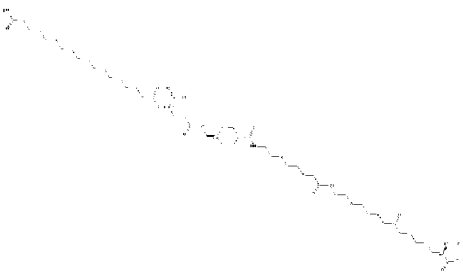
206	 C12H22N5O2R2+	TzlChmPEG	C[N+](C)(CCc1cn(C[C@@H](C([R])=O)N[R])nn1)CCOC
207	 C16H30N5O4R2+	TzlChmPEG3	C[N+](C)(CCc1cn(C[C@@H](C([R])=O)N[R])nn1)CCOCCOCCOC
208	 C19H26N4O5R2	Y(OTzl(mPEG3))	COCCOCCOCCn1nnc(COc2ccc(C[C@@H](C([R])=O)N[R])cc2)c1
209	 C20H30N5O3R2+	Y(OTzlChmPEG)	C[N+](C)(CCc1cn(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1)CCOC

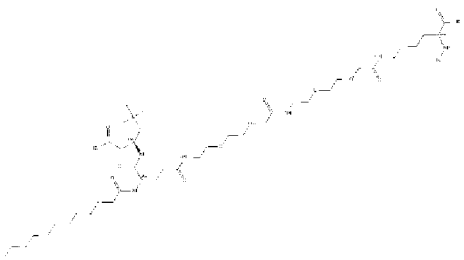
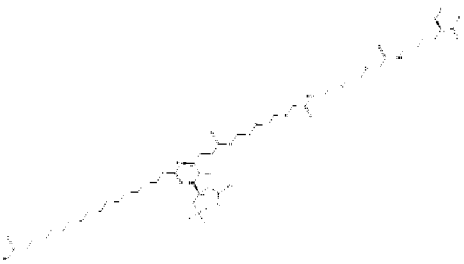
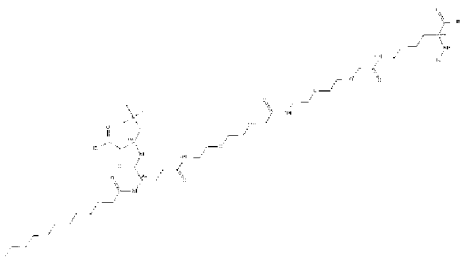
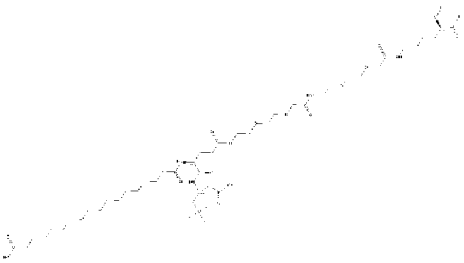
210	 C24H38N5O5R2+	Y(OTzlChmPEG3)	C[N+](C)(CCc1cn(CCOc2ccc(C[C@@H](C([R])=O)N[R])cc2)nn1)CCOCCOCCOC
211	 C27H46N3O5R2+	YC8CO(NHPEG3a)	C[N+](C)(C)CCOCCOCCNC(CCCCCCCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)=O
212	 C55H104N4O18R2	aMeK(PEG12gEC16)	CCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCO

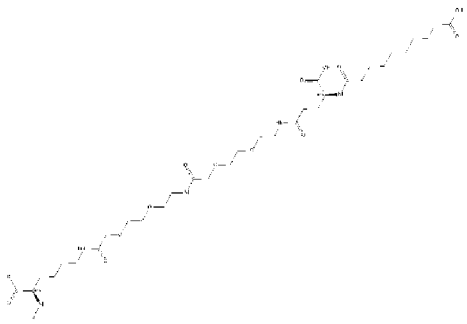
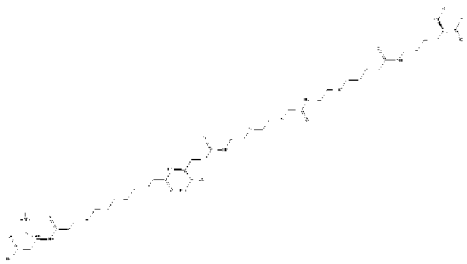
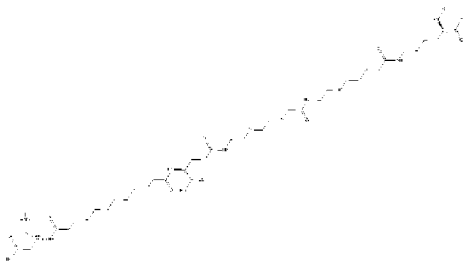
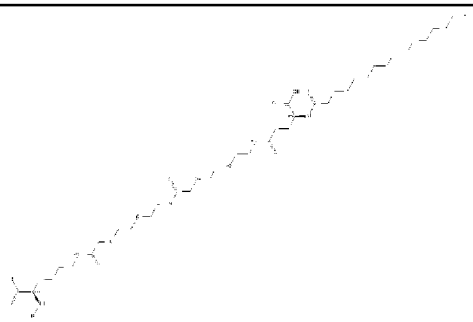
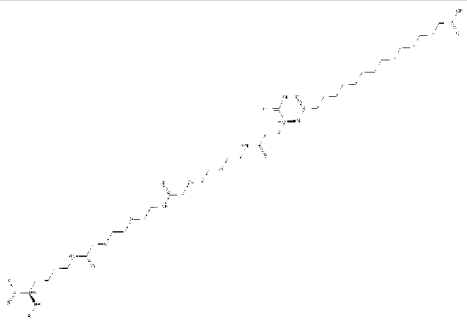
214	 C40H71N5O13R2	aMeK(PEG2PEG2gEC16OH)	C[C@](CCCCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)(C([R])=O)N[R]
215	 C42H75N5O13R2	aMeK(PEG2PEG2gEC18OH)	C[C@](CCCCNC(COCCOCCNC(COCCOCCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCC(O)=O)=O)=O)=O)=O)(C([R])=O)N[R]
216	 C10H21NO3R+	cPEG3aCO、cPEG3a	C[N+](C)(C)CCOCCOCCC([R])=O
217	 C14H29NO5R+	cPEG5aCO、cPEG5a	C[N+](C)(C)CCOCCOCCOCCOCCOCCC([R])=O
218	 C21H31F2N2O4R2+	dFPPEG3F	C[N+](CCOCCOCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)(CC1)CCC1(F)F

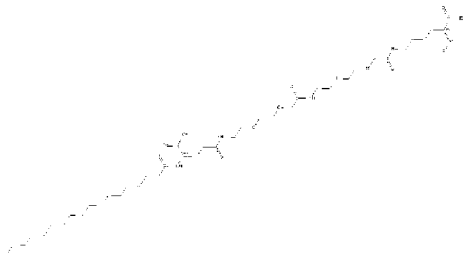
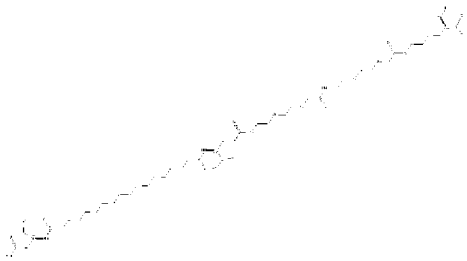
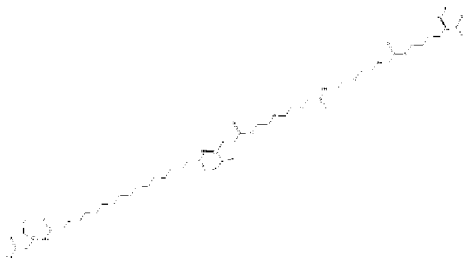
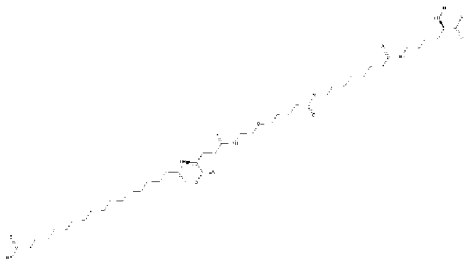
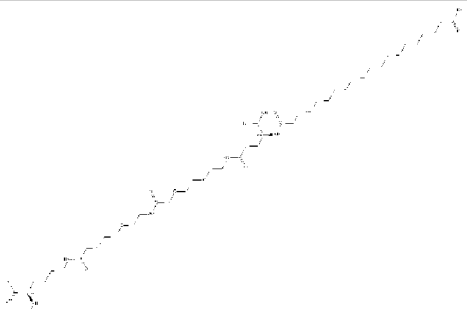
219	 C16H32N3O4R2+	dK(cPEG3a)、 k(cPEG3a)、 dK(cPEG3aCO)、 k(cPEG3aCO)	C[N+](C)(C)CCO CCOCCC(NCCC C[C@H](C([R])= O)N[R])=O
220	 C20H36N2O10R2	gEPEG6	OC([C@H](CCC(NCCOCCOCCO CCOCCOCCOC CC([R])=O)=O)N [R])=O
221	 C56H104N4O20R2	k(PEG12gEC18OH)、 dK(PEG12gEC18OH)	OC(CCCCCCCC CCCCCCCCC(N [C@@H](CCC(N CCOCCOCCOC COCCOCCOCC OCCOCCOCCO CCOCCOCCC(N CCCC[C@H](C([R])=O)N[R])=O) =O)C(O)=O)=O) =O
222	 C58H108N4O20R2	k(PEG12gEC20OH) dK(PEG12gEC20OH)	OC(CCCCCCCC CCCCCCCCCCC (N[C@@H](CCC (NCCOCCOCCO CCOCCOCCOC COCCOCCOCC OCCOCCOCCC(NCCCC[C@H](C ([R])=O)N[R])=O)=O)C(O)=O)=O) =O

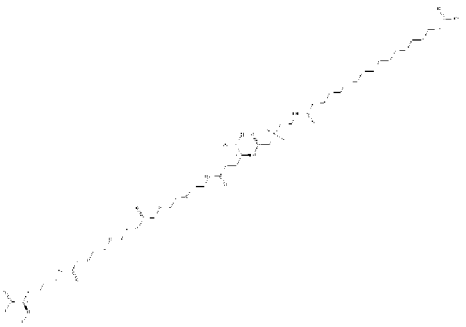
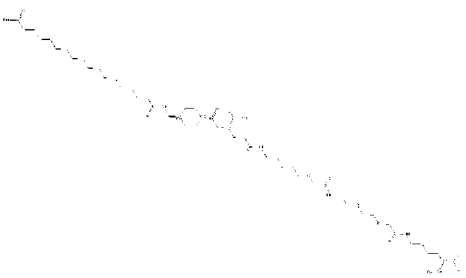
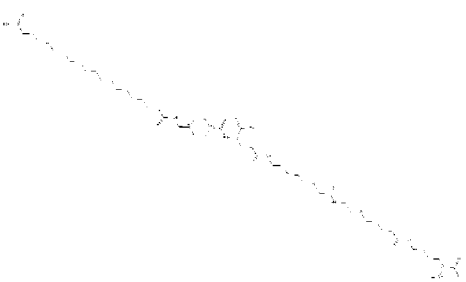
223	 C28H48N6O9SR2	dK(PEG2PEG2 生物素)、k(PEG2PEG2 生物素)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCO

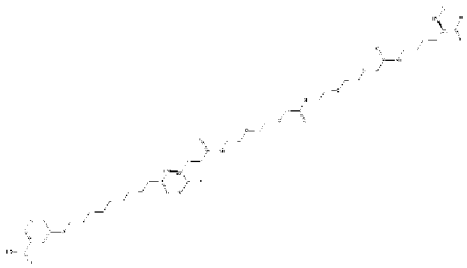
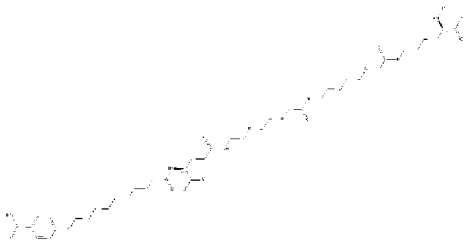
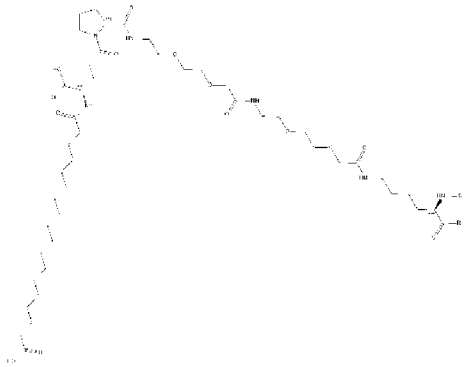
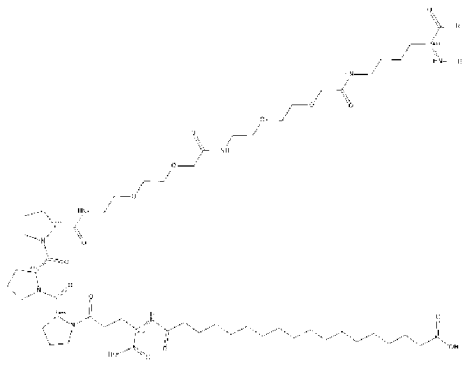
227	 C56H94N8O16R2	k(PEG2PEG2PPPgEC18OH) dK(PEG2PEG2PPPgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@@H]1C(N(CCC1)[C@@H]1C(N(CCC1)[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)=O)=O)C(O)=O)=O)=O
228	 C46H80N6O14R2	k(PEG2PEG2PgEC18OH)、 dK(PEG2PEG2PgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O
229	 C47H86N7O14R2+	k(PEG2PEG2Sp6gEC18OH)、 dK(PEG2PEG2Sp6gEC18OH)	C[N+](C)(CCNC(CC[C@@H](C(O)=O)NC(CCCCCCCCCCCCCCCCC(O)=O)=O)=O)CC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O
230	 C49H86N6O14R2	k(PEG2PEG2TrxgEC18OH)、 dK(PEG2PEG2TrxgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NC[C@H](CC1)CC[C@@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O)=O

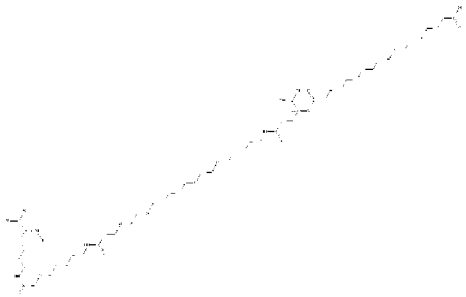
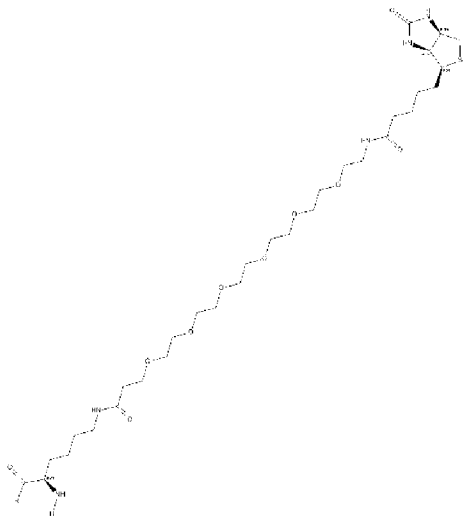
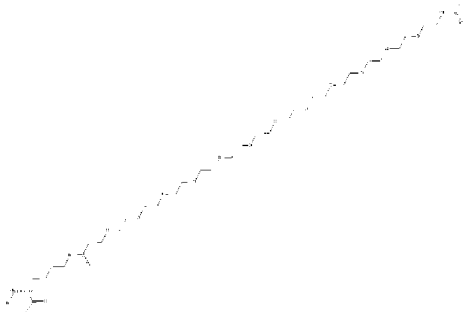
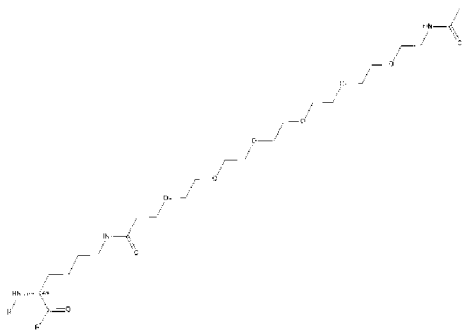
231	 C42H78N7O12R2+	k(PEG2PEG2gE(C)C12、dK(PEG2PEG2gE(C)C12	CCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(N[C@@H](CC(O)=O)C[N+](C)(C)C)=O)=O
232	 C48H88N7O14R2+	k(PEG2PEG2gE(C)C18OH、dK(PEG2PEG2gE(C)C18OH	C[N+](C)(C)C[C@H](CC(O)=O)NC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCCCCCCCCC(O)=O)=O)=O
233	 C42H78N7O12R2+	k(PEG2PEG2gE(c)C12、dK(PEG2PEG2gE(c)C12	CCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(N[C@H](CC(O)=O)C[N+](C)(C)C)=O)=O
234	 C48H88N7O14R2+	k(PEG2PEG2gE(c)C18OH、dK(PEG2PEG2gE(c)C18OH	C[N+](C)(C)C[C@@H](CC(O)=O)NC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCCCCCCCC(O)=O)=O)=O

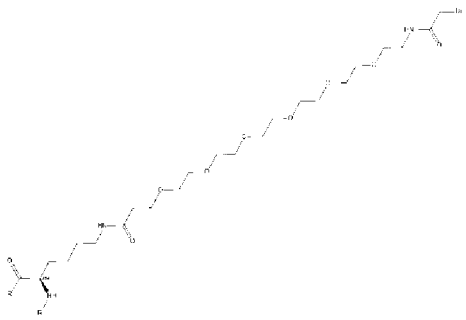
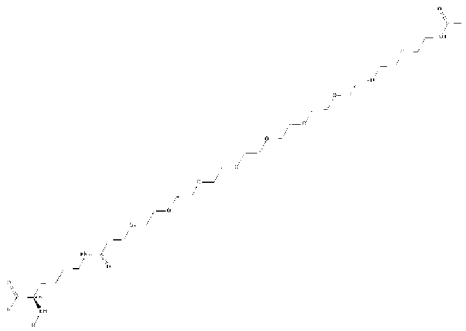
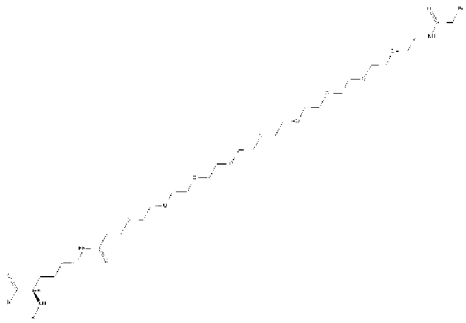
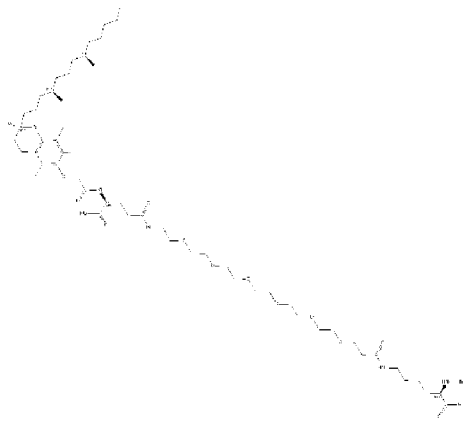
235	 C33H57N5O13R2	k(PEG2PEG2gEC10OH)、dK(PEG2PEG2gEC10OH)	OC(CCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
236	 C42H76N7O14R2+	k(PEG2PEG2gEC12OH(C)、dK(PEG2PEG2gEC12OH(C)	C[N+](C)(C)C[C@H](CC(O)=O)NC(CCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
237	 C42H76N7O14R2+	k(PEG2PEG2gEC12OH(c)、dK(PEG2PEG2gEC12OH(c)	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
238	 C39H71N5O11R2	k(PEG2PEG2gEC16)、dK(PEG2PEG2gEC16)	CCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
239	 C39H69N5O13R2	k(PEG2PEG2gEC16OH)、dK(PEG2PEG2gEC16OH)	OC(CCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O

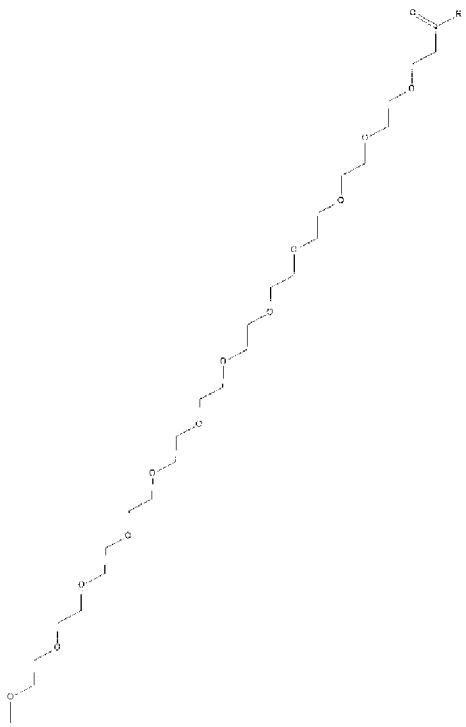
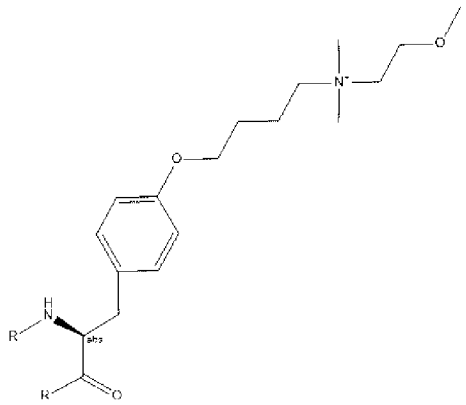
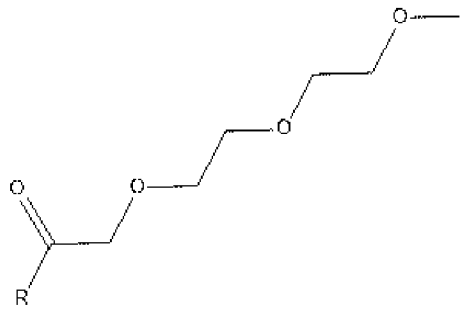
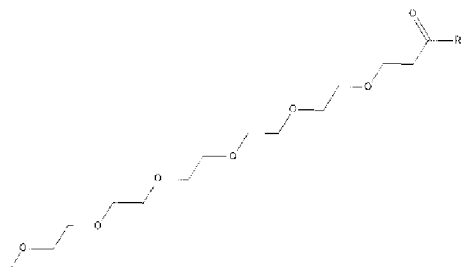
240	 C41H75N5O11R2	k(PEG2PEG2gEC18)、dK(PEG2PEG2gEC18)	CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
241	 C48H88N7O14R2+	k(PEG2PEG2gEC18OH(C)、dK(PEG2PEG2gEC18OH(C)	C[N+](C)(C)C[C@H](CC(O)=O)NC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
242	 C48H88N7O14R2+	k(PEG2PEG2gEC18OH(c)、dK(PEG2PEG2gEC18OH(c)	C[N+](C)(C)C[C@@H](CC(O)=O)NC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
243	 C41H73N5O13R2	k(PEG2PEG2gEC18OH)、dK(PEG2PEG2gEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
244	 C43H77N5O13R2	k(PEG2PEG2gEC20OH)、dK(PEG2PEG2gEC20OH)	OC(CCCCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O

245	C58H103N7O17R2	k(PEG2PEG2gEDAP(C16OH)2)、dK(PEG2PEG2gEDAP(C16OH)2)	OC(CCCCCCCCCCCCCCC(NC[C@@H](C(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)NC(CCCCCCCCCCCCCCC(O)=O)=O)=O)=O
246	 C47H86N7O14R2+	kPEG2PEG2gEDAP(C16OH)2；kPEG2PEG2gEDap(C16OH)2、k(PEG2PEG2gEDAP(C16OH)2)、dKPEG2PEG2gEDAP(C16OH)2；dKPEG2PEG2gEDap(C16OH)2、dK(PEG2PEG2gEDAP(C16OH)2)	C[N+](C)(CCNC(CCCCCCCCCCCCCCCC(O)=O)=O)CC(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O
247	 C49H86N6O14R2	kPEG2PEG2gEDAP(C16OH)2、dKPEG2PEG2gEDAP(C16OH)2	OC(CCCCCCCCCCCCCCCCC(NC[C@H](CC1)CC[C@@H]1C(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O)=O
248	 C51H90N6O14R2	k(PEG2PEG2gESp6C18OH)、dK(PEG2PEG2gESp6C18OH)	OC(CCCCCCCCCCCCCCCCCC(NC[C@H](CC1)CC[C@@H]1C(N[C@@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O)=O

249	 C40H63N5O14R2	k(PEG2PEG2gETrxC18OH)、dK(PEG2PEG2gETrxC18OH)	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCCOc1ccc(C(O)=O)ccc1)=O)=O
250	 C40H63N5O14R2	k(PEG2PEG2gETrxC20OH)、dK(PEG2PEG2gETrxC20OH)	OC([C@H](CCC(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)NC(CCCCCCCCCOc(cc1)ccc1C(O)=O)=O)=O
251	 C46H80N6O14R2	k(PEG2PEG2gEmXOH)、dK(PEG2PEG2gEmXOH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)=O)C(O)=O)=O)=O
252	 C56H94N8O16R2	k(PEG2PEG2gEpXOH)、dK(PEG2PEG2gEpXOH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(N(CCC1)[C@H]1C(N(CCC1)[C@H]1C(N(CCC1)[C@H]1C(NCCOCCOCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)=O)=O)=O)C(O)=O)=O

253	 C50H91N5O17R2	k(PEG2PEG2pgEC18OH)、dK(PEG2PEG2pgEC18OH)	OC(CCCCCCCCCCCCCCCCCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCCC(NCCOCCOCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)=O)C(O)=O)=O)=O
254	 C31H55N5O10SR2	k(PEG2PEG2pppgEC18OH)、dK(PEG2PEG2pppgEC18OH)	O=C(CCCC[C@@H]([C@H]1N2)SC[C@@H]1NC2=O)NCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@H](C([R])=O)N[R])=O
255	 C35H67N3O15R2	k(PEG2PEG6gEC18OH)、dK(PEG2PEG6gEC18OH)	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@H](C([R])=O)N[R])=O)=O
256	 C23H43N3O9R2	k(dPEG12AcBr)、dK(dPEG12AcBr)	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@H](C([R])=O)N[R])=O)=O

257	 C23H42BrN3O9R2	k(dPEG12AcVitE)、dK(dPEG12AcVitE)	O=C(CCOCCOCCOCCOCCOCCOCCNC(CBr)=O)NCCCC[C@H](C([R])=O)N[R]
258	 C29H55N3O12R2	k(dPEG6Ac)、dK(dPEG6Ac)	CC(NCCOCCOCCOCCOCCOCCOCCOCCOCCCC(NCCCC[C@H](C([R])=O)N[R])=O)=O
259	 C29H54BrN3O12R2	k(dPEG6AcBr)、dK(dPEG6AcBr)	O=C(CCOCCOCCOCCOCCOCCOCCOCCOCCNC(CBr)=O)NCCCC[C@H](C([R])=O)N[R]
260	 C57H98N4O14R2	k(dPEG9Ac)、dK(dPEG9Ac)	CC(C)CCC[C@@H](C)CCC[C@@H](C)CCC[C@](C)(CC1)Oc(c(C)c2C)c1c(C)c2OCC(N[C@@H](CCC(NCCOCCOCCOCCOCCOCCOCCOCCOCCC(NCCCC[C@H](C([R])=O)N[R])=O)=O)C(O)=O)=O

261	 C26H51O13R	mPEG12CO	COCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC([R])=O
262	 C18H29N2O3R2+	mPEG2TMA4F	C[N+](C)(CCCCOc1ccc(C[C@@H](C([R])=O)N[R])cc1)CCOC
263	 C7H13O4R	mPEG3CO	COCCOCCOCC([R])=O
264	 C14H27O7R	mPEG6CO	COCCOCCOCCOCCOCCOCCC([R])=O

1			

VIII. 實例

【0275】 下列實例說明本發明。這些實例不意欲限制本發明之範疇，而是對所屬技術領域中具有通常知識者提供指引以製備及使用本發明之化合物、組成物、及方法。雖然描述了本發明之特定態樣，所屬技術領域中具有通常知識者將認知到，可作出各種改變及修改而不偏離本發明之精神與範疇。

一般肽合成程序1

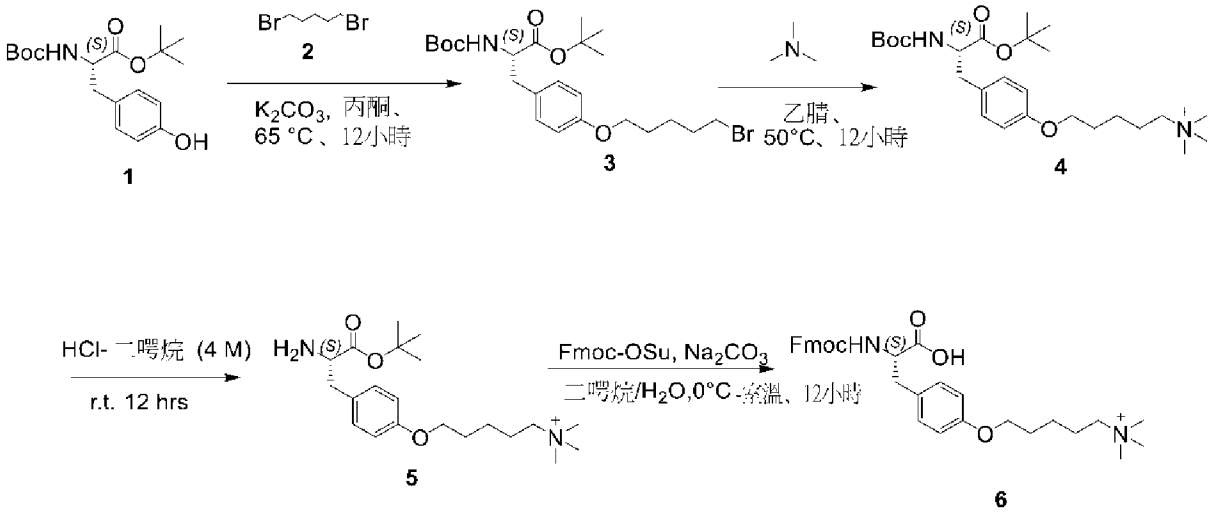
【0276】 本文中所述的IL-23R抑制劑化合物係以胺基酸單體使用標準基於Fmoc之固相合成在各種儀器（諸如Protein Technology的Symphony多通道合成儀及CEM微波肽合成儀）上合成。肽係使用各種偶合條件來組裝，諸如HBTU（O-苯并三唑-N,N,N',N'-四甲基-脲鎓-六氟-磷酸鹽）及二異丙基乙基胺(DIEA)、Oxyma/DIC、或PyAOP(7-吖苯并三唑-1-基氧基)三吡咯啶基鏻六氟磷酸鹽）、及DIEA。針對具有C-端醯胺之肽使用Rink Amide MBHA樹脂，而針對具有C-端酸之肽使用具有N-α-Fmoc受保護胺基酸之預載Wang Resin或2-氯三苯甲基樹脂。本發明之肽抑制劑係基於醫療化學最佳化及/或噬菌體顯示來進行識別及篩選以找出具有優異結合及/或抑制性質者。

某些經修飾胺基酸之製備

【0277】 某些經修飾胺基酸會出現在本文中所述的IL-23R抑制劑之序列中。適用於合成本文中所述的抑制劑之那些經修飾胺基酸、及其前驅物可自商

業來源獲得、如所屬技術領域中所述合成、或藉由任何合適途徑來獲得。例如，經取代色胺酸可藉由任何合適途徑來製備。某些經取代色胺酸之製備包括在七位置經取代者，諸如7-烷基-色胺酸（例如，7-乙基-L-色胺酸），其連同其他經取代色胺酸係描述於例如WO 2021/146441 Al中。某些額外經修飾胺基酸之合成係描述於下文中。

a. (S)-5-(4-(2-((((9H-芴-9-基)甲氧基)羰基)胺基)-2-羧基乙基)苯氧基)-N,N,N-三甲基戊-1-銨鹽(TMAPF)之合成



【0278】 向**1** (6.60 g, 19.7 mmol)、K_2CO_3 (4.09 g, 29.6 mmol)、及丙酮(50 mL)之混合物中加入**2** (4.99 g, 21.7 mmol)。將反應混合物加熱以回流並攪拌12小時。將反應混合物倒入水(500 mL)中然後用乙酸乙酯(500 mL × 3)萃取。將合併之有機萃取物用鹽水(500 mL)洗滌，以無水Na_2SO_4乾燥，過濾然後在減壓下濃縮而供給粗產物，將其藉由FCC純化（洗提液：石油醚：乙酸乙酯= 1：0至5：1）而供給呈淡無色油之粗產物**3** (5.26 g,產率：54.8%)。**MS (ESI)：**

$C_{23}H_{36}BrNO_5$質量計算為486.44，m/z測得為509.9 $[M+23]^+$。**^{1}H NMR** (400 MHz, $CDCl_3$): δ ppm 7.07 (d, *J*=8.4 Hz, 2 H), 6.81 (d, *J*=8.6 Hz, 2 H), 4.97 (br d, *J*=8.2 Hz, 1 H), 4.36 - 4.48 (m, 1 H), 3.95 (t, *J*=6.3 Hz, 2 H), 3.45 (t, *J*=6.8 Hz, 2 H), 3.00 (br d, *J*=3.7 Hz, 2 H), 1.87 - 2.01 (m, 2 H), 1.76 - 1.86 (m, 2 H), 1.62 - 1.69 (m, 2 H), 1.42 (d, *J*=2.8 Hz, 18 H).

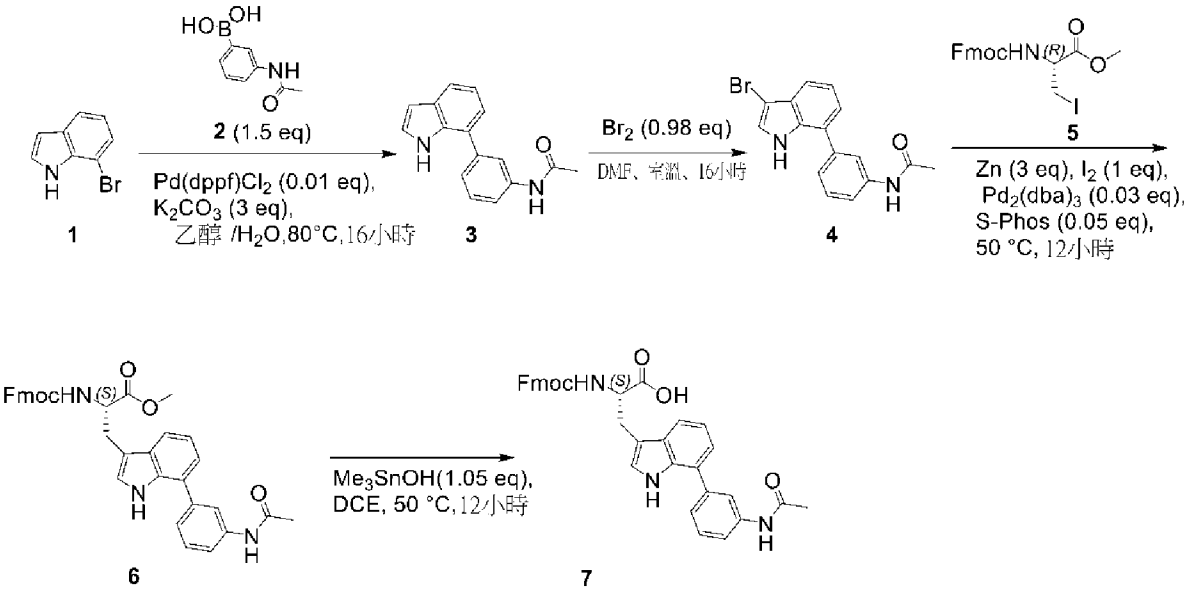
【0279】 向**3** (5.26 g, 10.8 mmol)於乙腈(50 mL)中之混合物中加入乙腈中之三甲胺(2 M, 8.11 mL)。將反應混合物在50℃下攪拌12小時。將反應混合物在減壓下濃縮而獲得呈淡黃色固體之產物**4** (5.0 g,產率：99.3%)。

【0280】 **MS (ESI)**：$C_{26}H_{45}N_2O_5$質量計算為465.646，m/z測得為465.2 $[M]^+$。將**4** (4.00 g, 8.59 mmol)於4M HCl-二噁烷(43.0 mL, 172 mmol)中之混合物在室溫下攪拌12小時。將溶劑在減壓下移除而獲得呈白色固體之產物**5** (3.00 g, 產率：粗製)，將其直接用於下一個步驟中。**MS (ESI)**：$C_{17}H_{29}N_2O_3$質量計算為309.424，m/z測得為309.1 $[M+H]^+$。

【0281】 將化合物**5** (3.00 g, 8.67 mmol)溶於圓底燒瓶中之二噁烷(20 mL)及水(20 mL)中。將Na_2CO_3 (1.38 g, 13.0 mol)加入，然後將溶液在冰浴中冷卻至0℃。接著將Fmoc-OSu (3.22 g, 9.54 mol)溶於二噁烷(20 mL)中然後在0℃下分批添加至溶液中。將反應在0℃下攪拌2小時。讓反應溫熱至室溫整夜。將反應用2N HCl (50 mL)酸化。將反應混合物藉由製備型HPLC純化並使用Xtimate C18 150*40 mm*5 um（洗提液：20%至50% (v/v) CH_3CN及H_2O含0.05% HCl）而供給產物。將產物懸浮於水(40 mL)中，使用乾冰/乙醇將混合物冷凍，接著凍縮至乾而供給呈淡黃色固體之標題化合物**6** (TMAPF, 3.57 g,產率：61.9%,純度：99.2%)。**MS (ESI)**：$C_{32}H_{39}N_2O_5$質量計算為531.662，m/z測得為531.4 $[M+H]^+$。

^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.89 (d, *J*=7.6 Hz, 2 H), 7.73 (d, *J*=8.2 Hz, 1 H), 7.65 (t, J=7.2 Hz, 2 H), 7.39 - 7.43 (m, 2 H), 7.27 -7.34 (m, 2 H), 7.19 (d, *J*=8.2 Hz, 2 H), 6.78 - 6.89 (m, 2 H), 4.06 - 4.25 (m, 4 H), 3.84 - 3.99 (m, 2 H), 3.25 - 3.37 (m, 2 H), 3.05 (s, 9 H), 3.00 (d, *J*=4.0 Hz, 1 H), 2.70 - 2.84 (m, 1 H), 1.63 - 1.82 (m, 4 H), 1.30 - 1.46 (m, 2 H)

b. (S)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)-3-(7-(3-乙醯胺基苯基)-1H-吲哚-3-基)丙酸(7-(3-N乙醯基-苯基)-色胺酸或7(3NAcPh)W)之合成



【0282】 向**1** (30.0 g, 153 mmol)、化合物**2** (41.1 g, 230 mmol)、及K_3PO_4 (97.4 g, 459 mmol)於H_2O/乙醇(500 mL)中之溶液中，在N_2氣氛下將Pd(dppf)Cl_2 (1.12 g, 1.53 mmol)加入。將混合物在80℃下攪拌16小時。將混合物過濾。將混合物濃縮，接著用乙酸乙酯(500 mL × 2)萃取，以無水Na_2SO_4乾燥。將有機層濃縮並藉由FCC純化（洗提液：石油醚/乙酸乙酯=1:0至55:45）而給出呈黃色油

之**3** (25.0 g,產率：62.5%) **MS (ESI)：**$C_{16}H_{14}N_2O$質量計算為250.295，m/z測得為251.0 [M+]。

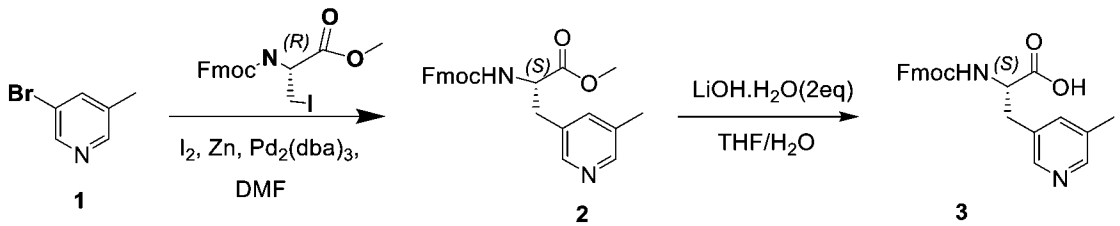
【0283】 向含有**3** (12.0 g, 47.9 mmol)於DMF (300 mL)中之溶液的1 L圓底燒瓶中，將溴(Br_2, 2.422 mL, 47.0 mmol)緩慢加入。將混合物在25℃下攪拌16小時。將溶液加入至亞硫酸鈉水溶液(500 mL)中，將混合物在25℃下攪拌2小時。將混合物過濾，將濾餅與H_2O (400 mL)混合然後在25℃下攪拌1小時。將混合物過濾，收集固體而給出呈粗產物之**4**，將其藉由製備型高效液相層析法純化（管柱：Phenomenex C18 250 × 50 mm × 10 um，條件：水(FA)-CAN (20%-60%)）。將混合物濃縮，用CH_2Cl_2 (1 L × 2)萃取，用鹽水洗滌，以無水Na_2SO_4乾燥。將有機層過濾然後濃縮而給出呈淡白色之**4** (9.70 g,產率：60.8%)。**MS (ESI)：**$C_{16}H_{13}BrN_2O$質量計算為329.191，m/z測得為328.8 [M]。

【0284】 向250 mL三頸圓底燒瓶中倒入活化Zn粉(5.84 g, 89.3 mmol)，將DMF (120 mL)及I_2 (382 mg, 1.50 mmol)在N_2氣氛下在室溫下加入。在攪拌20分鐘後，將**5** (13.6 g, 30.1 mmol)於DMF (30 mL)中之溶液加入至混合物中。將反應混合物在室溫下攪拌30分鐘，之後將**4** (9.70 g, 29.5 mmol)、參(二亞苄基丙酮)鈀(826 mg, 0.902 mmol)、2-二環己基膦基-2',6'-二甲氧基聯苯(617 mg, 1.50 mmol)在N_2氣氛下加入。將反應混合物在50℃下攪拌12小時，之後將溶劑在減壓下移除而給出粗產物**6**。將粗產物用乙酸乙酯(1500 mL)萃取。將萃取物用H_2O (500 mL × 2)、接著鹽水(500 mL)洗滌，之後將其以無水Na_2SO_4乾燥，過濾，然後在真空中濃縮至乾而給出粗中間物6，將其藉由矽膠層析法純化（0-

100%乙酸乙酯/石油醚(EtOAc/PE)）而供給呈棕黃色油之**6** (11.0 g,產率：63.8%)。**MS (ESI)：**$C_{35}H_{31}N_3O_5$質量計算為573.638，m/z測得為574.1 [M+1]。

【0285】 將中間物**6** (11.0 g, 19.2 mmol)、攪拌棒、Me_3SnOH (3.64 g, 20.1 mmol)、及DCE (150 mL)加入至250 mL圓底燒瓶中然後在50℃下攪拌12小時。向反應混合物中加入2 N HCl以將pH調整至6。製備用**1**之溶液起始的第二反應系列，然後將合併之反應混合物在減壓下濃縮而給出粗產物**7**，將其藉由製備型HPLC純化並使用Xtimate C18 150 × 40 mm × 5um（洗提液：38%至68% (v/v) CH_3CN及H_2O含0.05% HCl）而供給產物**7**。將產物懸浮於水(100 mL)中，使用乾冰/乙醇將混合物冷凍，接著凍縮至乾而供給呈白色固體之**7** (7(3NAcPh)W、11.8 g,產率：66.8%)。**MS (ESI)：**$C_{34}H_{29}N_3O_5$質量計算為559.611，m/z測得為560.0 [M+1]。**^{1}H NMR** DMSO-d_6 (400 MHz) δ 10.73 (s, 1 H), 10.10 (s, 1 H), 7.52 - 8.02 (m, 7 H), 6.96 - 7.52 (m, 9 H), 4.03 - 4.44 (m, 3 H), 3.25 (d, J = 13.2 Hz, 2 H), 3.01 - 3.15 (m, 1 H), 2.08 (s, 3 H).

c. (S)-2-((((9H-芴-9-基)甲氧基)羰基)胺基)-3-(6-(三級丁氧基)萘-2-基)丙酸(5-甲基-吡啶基-丙胺酸或5MePyridinAla之合成



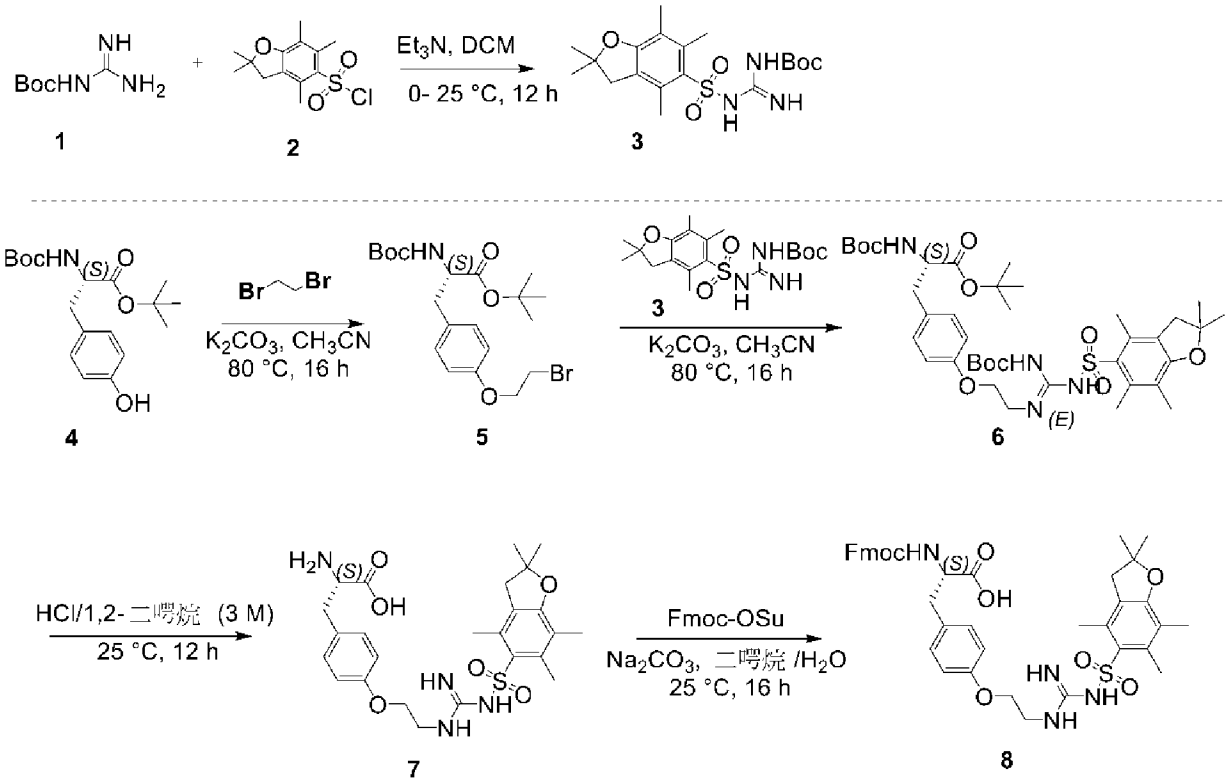
【0286】 將活化Zn粉(8.18 g, 125 mmol)、DMF (150 mL)、及I_2 (0.534 g, 2.11 mmol)在N_2氣氛下在室溫下攪拌20分鐘，之後將DMF (25 mL)中之2-((((9H-

茀-9-基)甲氧基)羰基)胺基)-3-碘丙酸(R)-甲酯(19.0 g, 42.1 mmol)加入。將反應混合物在室溫下攪拌30分鐘，之後將**1** (7.97 g, 46.3 mmol)、參(二亞苄基丙酮)鈀(1.16 g, 1.26 mmol)、及2-二環己基膦基-2',6'-二甲氧基聯苯(0.864 g, 2.11 mmol)於DMF (25 mL)中之混合物在N_2氣氛下加入。將所得反應混合物在50℃下攪拌12小時。將溶劑在減壓下移除而給出粗製物，將其藉由FCC純化（洗提液：石油醚：乙酸乙酯= 1：0至0：1及乙酸乙酯：甲醇= 1：0至2：1）而供給呈淡黃色液體之產物**2** (10.00 g, 57.0%產率)。**MS (ESI)：**$C_{25}H_{24}N_2O_4$質量計算為416.469，m/z測得為417.1 $[M+H]^+$。

【0287】　向**2** (9.50 g, 22.8 mmol)於THF (100 mL)中之混合物中加入H_2O (10 mL)中之$LiOH.H_2O$ (1.91 g, 45.6 mmol)。將混合物在0℃下攪拌1小時。TLC顯示大部分SM已耗盡。在冰浴中向反應混合物中逐滴加入HCl (1 N)至pH=5。將反應混合物在減壓下濃縮，接著倒入水(200 mL)中，將混合物用THF (200 mL x3)萃取。將有機層合併，用鹽水(100 mL)洗滌，以無水Na_2SO_4乾燥。在過濾後將有機層在減壓下濃縮而供給粗產物**3**，將其藉由FCC純化（洗提液：乙酸乙酯：甲醇=1:0至2:1）而獲得呈白色粉末之**3** (**5MePyridinAla**, 6.716 g,產率：72.3%)。**MS (ESI)：**$C_{24}H_{22}N_2O_4$質量計算為402.442，m/z測得為403.1 $[M+H]^+$。

^{1}H NMR DMSO-d_6 (Bruker_400 MHz): δ 8.18 (s, 2H), 7.88 (d, *J*=7.6 Hz, 2H), 7.63 (d, *J*=7.2 Hz, 2H), 7.45 - 7.26 (m, 5H), 6.81 (s, 1H), 4.33 - 4.21 (m, 1H), 4.20 - 4.09 (m, 2H), 3.95 (s, 1H), 3.06 -3.05 (m, 1H), 2.92 - 2.89 (m, 1H), 2.18 (s, 3H).

d. (S)-2-((((9H-茀-9-基)甲氧基)羰基)胺基)-3-(4-(2-(3-((2,2,4,6,7-五甲基-2,3-二氫苯并呋喃-5-基)磺醯基)胍基)乙氧基)苯基)丙酸(AEF(G))之合成



【0288】 將起始材料**1** (9.9 g, 62.2 mmol)、攪拌棒、Et_3N (14 mL, 101 mmol)、及二氯甲烷(DCM、250 mL)加入至500 mL圓底燒瓶中。在冰水浴下將所得混合物用**2** (10 g, 34.6 mmol)分批處理。接著將反應混合物在25℃下攪拌12小時。將反應混合物用H_2O (800 mL)稀釋，用DCM (400 mL × 2)萃取。將有機相萃取物合併，用鹽水(800 mL)洗滌，然後濃縮而給出呈黃色固體之粗中間物**3**。將粗中間物用乙酸乙酯(50 mL)研製然後將懸浮液經由過濾單離。將濾餅用乙酸乙酯(20 mL × 3)洗滌，之後在減壓下乾燥而給出呈白色固體之**3** (7.12 g, 49%)。**MS (ESI)**：$C_{19}H_{29}N_3O_5S_6$質量計算為411.5，m/z測得為412.1 $[M+H]^+$。

【0289】 將起始材料**4** (50.0 g, 148 mmol)、攪拌棒、DMF (300 mL)、及K_2CO_3 (102 g, 739 mmol)加入至氮吹掃1000 mL圓底燒瓶中。隨後將燒瓶排空並用氮再填充（3次），之後將1,2-二溴乙烷(154 mL, 1.78 mol)加入，然後將所得

混合物在80℃下在N_2氣氛下攪拌16小時。將反應混合物過濾然後在減壓下濃縮至乾而給出粗產物，使其經歷矽膠層析法（洗提液：EtOAc：石油醚= 0 - 60%）而給出呈淺黃色油之**5** (64 g, 96%)。**MS (ESI)**：$C_{20}H_{30}BrNO_5$質量計算為444.36，m/z測得為466.1 $[M+Na]^+$。

【0290】 將中間物**5** (6.1 g, 13.7 mmol)、**3** (6.2 g, 15.1 mmol)、K_2CO_3 (7.6 g, 55.0 mmol)、攪拌棒、及CH_3CN (100 mL)倒入250 mL圓底燒瓶中。將反應混合物在80℃下在N_2氣氛下攪拌16小時。將反應混合物冷卻至室溫，用H_2O (200 mL)稀釋，用乙酸乙酯(100 mL × 2)萃取。將有機相合併然後用鹽水(300 mL)洗滌並濃縮而給出粗中間物**6**。將粗中間物藉由快速管柱層析法純化（FCC，洗提液：乙酸乙酯/石油醚=0:1至2:1）而給出呈白色固體之**6** (6.62 g, 44.2%)。**MS (ESI)**：$C_{39}H_{58}N_4O_{10}S$質量計算為774.9，m/z測得為775.5 $[M+H]^+$。

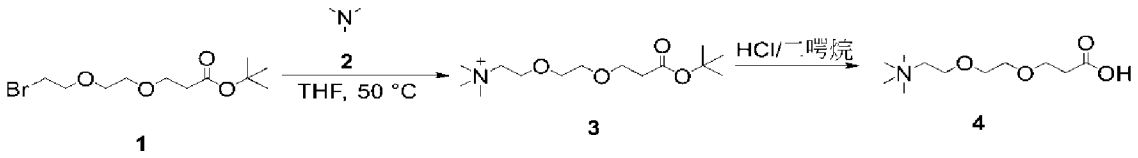
【0291】 將中間物**6** (6.6 g, 8.52 mmol)、HCl/1、4-二噁烷(90 mL, 4M)、攪拌棒、及1、4 -二噁烷(30 mL)倒入250 mL圓底燒瓶中。將所得混合物在25℃下攪拌12小時。將溶劑在減壓下移除而給出呈無色油之中間物**7** (7.8 g,粗產物)，將其直接用於下一個步驟中。**MS (ESI)**：$C_{25}H_{34}N_4O_6S$質量計算為518.6，m/z測得為519.2 $[M+H]^+$。

【0292】 將中間物**7** (7.80 g, 15.0 mmol)、攪拌棒、Na_2CO_3 (3.19 g, 30.1 mmol)、Fmoc-OSu (5.58 g, 16.5 mmol)、1,4-二噁烷(50 mL)、及H_2O (50 mL)在25℃下加入至250 mL圓底燒瓶中。將反應混合物在25℃下攪拌16小時，之後將其用HCl (2M)調整至pH = 5至6，然後將所得反應混合物用EtOAc (150 mL × 3)萃取。將來自萃取之有機相合併然後用鹽水(200 mL)洗滌並濃縮而給出粗中間

物**7**。將粗中間物藉由製備型HPLC純化並使用管柱：Phenomenex C18 150 × 40 mm × 5um（洗提液：42%至72% (v/v) CH_3CN及H_2O含0.1% HCl）而供給純產物。將產物懸浮於水(100 mL)中，使用乾冰/乙醇將混合物冷凍，接著凍縮至乾而供給呈白色固體之所欲產物**8** (**AEF(G)**、4 g, 36%)。**MS (ESI)**：$C_{40}H_{44}N_4O_8S$ 質量計算為740.9，m/z測得為741.3 $[M+H]^+$。**^{1}H NMR** (400 MHz, DMSO-d_6):

7.87 (d, J = 7.2 Hz, 2H), 7.71 - 7.62 (m, 2H), 7.39 (td, J = 4.0, 7.2 Hz, 2H), 7.29 (td, J = 7.6, 12.0 Hz, 2H), 7.14 (br d, J = 8.0 Hz, 2H), 6.99 - 6.85 (m, 1H), 6.77 (br d, J = 8.4 Hz, 2H), 6.59 - 6.50 (m, 1H), 4.21 - 4.06 (m, 4H), 3.88 (br s, 2H), 3.42 - 3.36 (m, 4H), 2.99 (br dd, J = 4.4, 14.0 Hz, 1H), 2.92 (s, 2H), 2.78 (br dd, J = 10.8, 13.6 Hz, 1H), 2.47 (br s, 3H), 2.41 (s, 3H), 1.97 (s, 3H), 1.38 (s, 6H).

e. 2-(2-(2-羧基乙氧基)乙氧基)-N,N,N-三甲基乙-1-銨鹽(cPEG3a)之合成

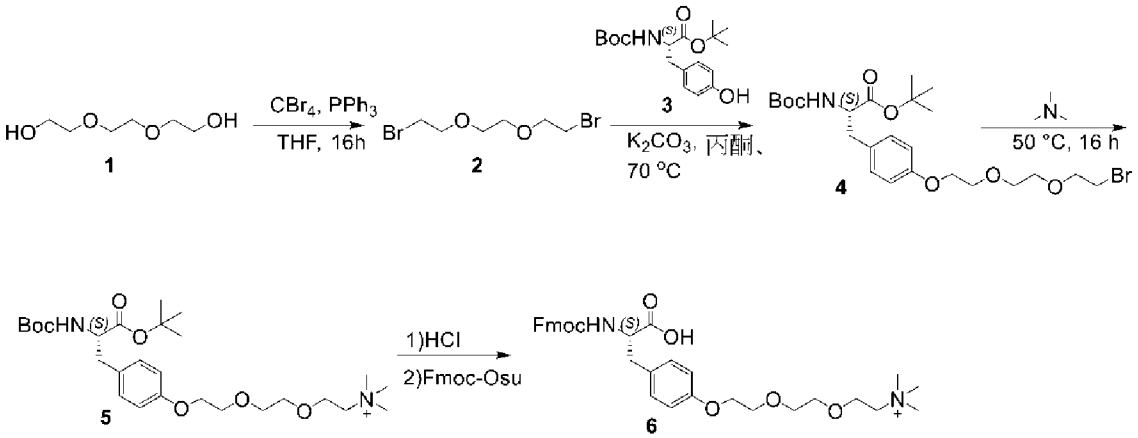


1　　3　　4

【0293】　將混合物1 (5.00 g, 16.8 mmol)及三甲胺2 (25 mL, 50 mmol,於THF中)於無水THF (10 mL)中在50℃下在N2下攪拌16小時。將混合物濃縮而給出呈黃色油之產物**3** (6.0 g,產率：99.8%)。**^{1}H NMR** (DMSO-d_6, 400 MHz): δ3.88 - 3.79 (m, 2H), 3.64 - 3.48 (m, 8H), 3.12 (s, 9H), 2.42 (t, *J* = 6.4 Hz, 2H), 1.39 (s, 9H). 將**3** (6.00 g, 16.8 mmol)及HCl/二噁烷(60 mL, 240 mmol)之混合物在25℃下在N2下攪拌16小時。將混合物濃縮而給出呈黃色油之產物**4** (**cPEG3a**、4.3 g,產率：

99.8%)。**^{1}H NMR** (D_2O, 400 MHz): δ3.96 - 3.87 (m, 2H), 3.74 (t, *J* = 5.6 Hz, 2H), 3.64 (s, 4H), 3.57 - 3.49 (m, 2H), 3.12 (s, 9H), 2.60 (t, *J* = 5.6 Hz, 2H).

f. (S)-2-(2-(2-(4-(2-((((9H-芴-9-基)甲氧基)羰基)胺基)-2-羧基乙基)苯氧基)乙氧基)乙氧基)-N,N,N-三甲基乙-1-銨鹽(APEG3F)之合成



【0294】 向1 (50.0 g, 333 mmol)於THF (1.3 L)中之混合物加入PPh3 (188 g, 716 mmol)，之後將CBr4 (243 g, 732 mmol)在0℃下極緩慢加入至混合物中。將混合物在室溫下攪拌整夜（16小時）接著在減壓下濃縮而給出粗中間物2。將石油醚(2.0 L)及乙酸乙酯(200 mL)加入至混合物中然後在25℃下攪拌0.5小時。將混合物過濾，在減壓下濃縮，然後藉由FCC純化（洗提液：石油醚：乙酸乙酯= 1：0至1：9）而給出呈無色油之中間物2 (52 g,產率：56.6%)。**^{1}H NMR** (400 MHz,氯仿-d): 3.91 - 3.81 (m, 4H), 3.75 - 3.68 (m, 4H), 3.55 - 3.46 (m, 4H).

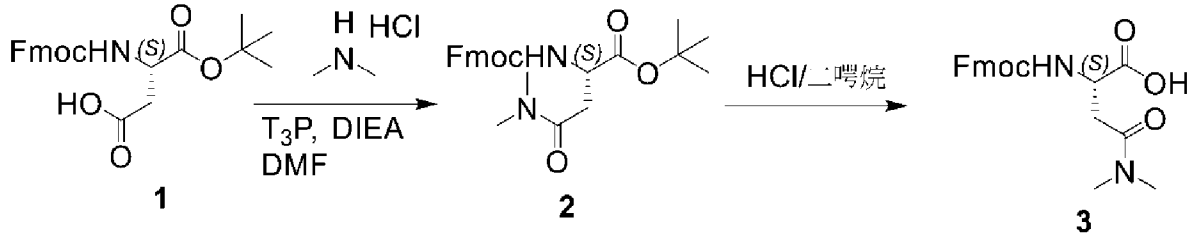
【0295】 向3 (45.9 g, 136 mmol)及K2CO3 (56.3 g, 408 mmol)於丙酮(1 L)中之溶液中在氮氣氛下加入2 (75.0 g, 272 mmol)。將混合物在70℃下攪拌16小

時。將混合物過濾並蒸發，然後將殘餘物藉由快速管柱層析法FCC純化（洗提液：石油醚：乙酸乙酯= 1:0至1:9）而給出呈淡黃色油之中間物**4** (45 g,產率：61.6%)。**MS (ESI)**：$C_{24}H_{38}BrNO_7$質量計算為532.47，m/z測得為433.8 [M-100]$^+$。

【0296】 將4 (51 g, 96 mmol)於三甲胺(239 mL, 2 M,於THF中)中之溶液在50℃下攪拌16小時。將混合物在減壓下濃縮而給出呈淡黃色油之粗中間物5 (56 g,粗製)，將其用於下一個步驟中而未經純化。**MS (ESI)**：C27H47N2O7+質量計算為511.67，m/z測得為511.4 [M]+

【0297】 將5 (56.0 g, 94.7 mmol)於HCl/二噁烷(592 mL, 4 M)中之混合物在25℃下攪拌16小時，之後將其在減壓下濃縮，溶於H_2O (200 mL)中，然後在0℃下用Na_2CO_3水溶液淬熄以調整pH = 7。接著將丙酮(150 mL)中之Na_2CO_3 (15.0 g, 142 mmol)及Fmoc-OSu (31.9 g, 94.4 mmol)在氮氣氛下加入然後在25℃下攪拌3小時。將混合物用2 M HCl酸化，調整至pH = 4然後在減壓下濃縮。將混合物用乙酸乙酯(300 mL x2)萃取。將水相在減壓下濃縮而給出粗產物**6**（H_2O溶液），將其藉由製備型HPLC純化並使用Phenomenex Gemini Xtimate C18 150*40 mm*5um，100A（洗提液：53%至83% (v/v)水(0.225%FA)-ACN）而供給呈灰白色固體之標題化合物**6** (**APEG3F,** 43 g,產率：78.8%)。**MS (ESI)**：$C_{18}H_{31}N_2O_5^+$質量計算為355.45，m/z測得為355.1 [M]+。**^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.40 (s, 1H), 7.88 (d, *J* = 7.6 Hz, 2H), 7.66 (d, *J* = 7.2 Hz, 2H), 7.44 - 7.36 (m, 2H), 7.31 (q, *J* = 7.2 Hz, 2H), 7.18 - 7.04 (m, 3H), 6.77 (d, *J* = 8.4 Hz,2H), 4.24 - 4.13 (m, 3H), 4.00 (d, *J* = 3.6 Hz, 3H), 3.81 (s, 2H), 3.73 - 3.67 (m, 2H), 3.58 (s,4H), 3.54 - 3.48 (m, 2H), 3.07 (s, 9H), 3.05 - 2.98 (m, 1H), 2.85 - 2.76 (m, 1H).

f. N2-(((9H-芴-9-基)甲氧基)羰基)-N4,N4-二甲基-L-天冬醯胺酸(N(N(Me)2)之合成

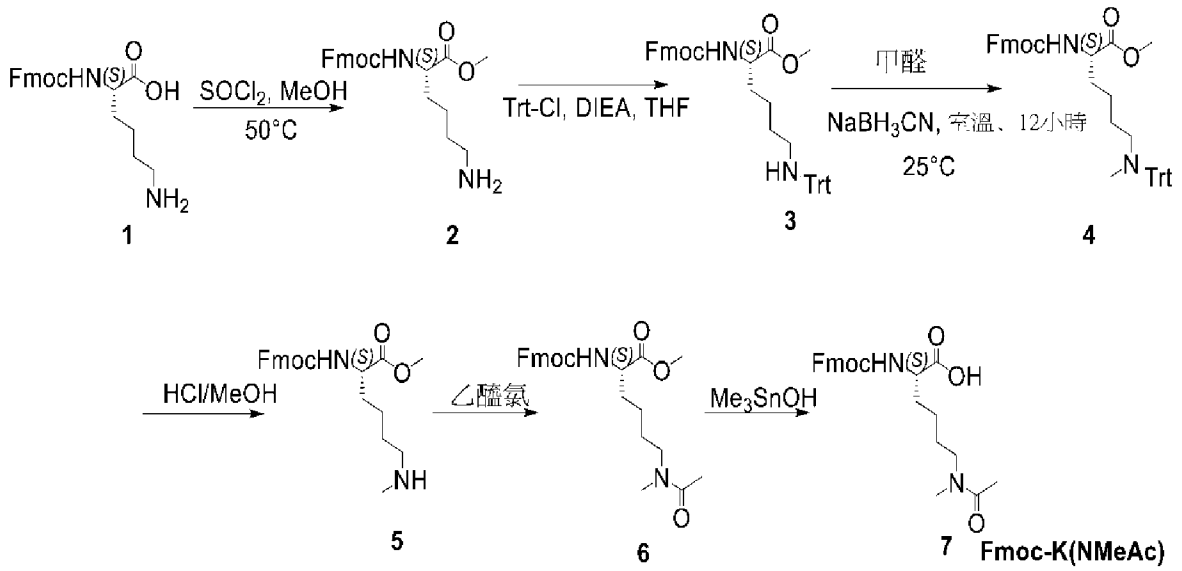


【0298】 向起始材料**1** (50 g, 122 mmol)、二甲基胺(10.9 mg, 134 mmol)、及二異丙基乙胺(DIEA, 62.0 g, 365 mmol)於DMF (200 mL)中之溶液中在0℃下用N_2除氣三次，然後將丙基膦酸酐(T_3P®, 109 g, 182 mmol)經由注射器加入。將混合物在20℃下攪拌12小時，之後將其倒入冰水(500 mL)中然後用乙酸乙酯(500 mLx3)萃取。將合併之有機萃取物用鹽水洗滌，以無水Na_2SO_4乾燥，過濾，然後在減壓下濃縮而供給粗中間物**2**，將其藉由快速管柱層析法純化（FCC，洗提液：石油醚：乙酸乙酯= 1：0至1：2）而供給呈淡黃色固體之**2** (45 g,產率：84.4%)。**MS (ESI)**：$C_{25}H_{30}N_2O_5$質量計算為438.52，m/z測得為439.2 $[M+H]^+$。

【0299】 將中間物**2** (45 g, 103 mmol)於HCl/二噁烷(1L, 4 M)中在20℃下攪拌16小時。將反應混合物過濾然後濃縮。將EtOAc (200 mL)加入至濃縮材料中，之後將石油醚(200 mL)逐滴加入。將混合物在20℃下攪拌3小時而產生固體，將其過濾而供給呈白色固體之**3** (**N(N(Me)2),** 25 g,產率：62.3%)。**MS (ESI)**：$C_{21}H_{22}N_2O_5$質量計算為382.41，m/z測得為383.1 $[M+H]^+$。**^{1}H NMR** (DMSO-d_6, 400 MHz): δ ppm 12.59 (s, 1H), 7.86 (d, *J*=7.6 Hz, 2H), 7.67 (d, *J*=7.2

Hz, 2H), 7.43 - 7.21 (m, 5H), 4.39 - 4.31 (m, 1H), 4.29 - 4.23 (m, 2H), 4.21 - 4.15 (m, 1H), 2.90 (s, 3H), 2.78 (s, 3H), 2.75 - 2.62 (m, 2H).

g. N2-(((9H-芴-9-基)甲氧基)羰基)-N6-乙醯基-N6-甲基-L-離胺酸(離胺酸N-(MeAc)或K(NMeAc))之合成



【0300】 將起始材料**1** (21 g, 57.0 mmol)及MeOH (300 mL)在燒瓶中在N_2氣氛下合併。將亞硫醯氯(8.14 g, 68.4 mmol)在15分鐘期間內在25℃之溫度下逐滴加入至燒瓶中而產生淡黃色混合物。將混合物在回流下加熱4小時。將所得黃色溶液在真空中濃縮。將乙酸乙酯(50 mL)加入至濃縮材料中然後將混合物在25℃下攪拌1小時。將固體過濾而供給呈白色固體之粗中間物**2** (23 g,粗製)。**MS (ESI)**：$C_{22}H_{26}N_2O_4$質量計算為382.45，m/z測得為383.5 $[M+H]^+$。

【0301】 向**2** (6.1 g, 14.6 mmol)及TEA (4.41、43.7 mmol)於100 mL的無水CH_2Cl_2/THF (100 mL)中之溶液中加入氯化三苯甲基(Trt-Cl, 4.47 g, 16.0 mmol)。將反應混合物在20℃下攪拌2小時。將反應混合物用水(80 mL)稀釋，用乙酸乙

酯(100 mLx2)萃取，用鹽水(20 mL)洗滌然後以Na_2SO_4乾燥。將合併之有機萃取物過濾然後在減壓下濃縮而供給粗中間物3，將其藉由FCC純化（洗提液：石油醚：乙酸乙酯= 1：0至1：2）而供給呈淡黃色固體之**3** (7 g,產率：76.7%)。**MS (ESI)**：$C_{41}H_{40}N_2O_4$質量計算為624.77，m/z測得為647.3 [M+Na]+。**^{1}H NMR** (DMSO-d_6, 400 MHz): δ ppm 7.84 (d, *J*=7.5 Hz, 2H), 7.71 (d, *J*=7.7 Hz, 1H), 7.66 (d, *J*=6.8 Hz, 2H), 7.36 (d, *J*=7.3 Hz, 9H), 7.29 - 7.20 (m, 8H), 7.17 - 7.08 (m, 3H), 4.29 - 4.22 (m, 2H), 4.21 - 4.11 (m, 1H), 3.97 - 3.91 (m, 1H), 3.56 (s, 3H), 2.56 - 2.50 (m, 1H), 1.91 (d, *J*=6.2 Hz, 2H), 1.55 (m, 2H), 1.46 - 1.31 (m, 2H), 1.26 (d, *J*=7.5 Hz, 2H).

【0302】　將**3** (5.20 g, 8.32 mmol)、甲醛(20.3 g, 250 mmol)、及$NaBH_3CN$ (2.62 g, 41.6 mmol)於甲醇(100 mL)中之溶液在25℃下攪拌16小時。將混合物用水(100 mL)淬熄，用二氯甲烷(200 mLx3)萃取，將有機層以無水Na_2SO_4乾燥，過濾，然後在減壓下濃縮。將殘餘物藉由快速層析法純化（FCC，洗提液：石油醚：乙酸乙酯= 1：0至1：9）而供給呈淡黃色固體之**4** (2.7 g,產率：41.2%)。**MS (ESI)**：$C_{42}H_{42}N_2O_4$質量計算為638.79，m/z測得為661.1$[M+Na]^+$。

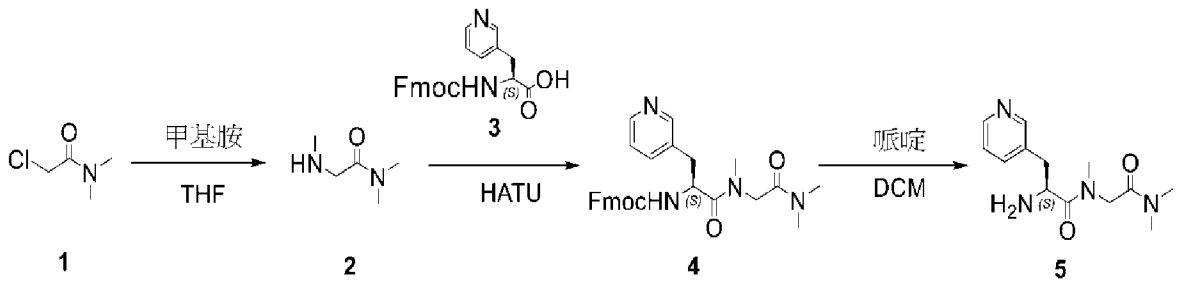
【0303】　將中間物**4** (80 g, 125 mmol)溶於HCl/MeOH (800 mL)中然後在20℃下攪拌1小時。將反應混合物在減壓下濃縮而供給粗產物。將乙酸乙酯(100 mL)及石油醚(200 mL)加入然後將反應混合物在20℃下攪拌4小時。將固體過濾而供給呈淡黃色固體之中間物**5** (60 g,粗製)。**MS (ESI)**：$C_{23}H_{28}N_2O_4$質量計算為396.48，m/z測得為397.1 $[M+H]^+$。

【0304】　向**5** (120 g, 277 mmol)於CH_2Cl_2 (1200 mL)中之溶液中在0℃下加入TEA (107 g, 832 mmol)。將乙醯氯(26.1 g, 333 mmol)加入然後將反應混合物

在20℃下攪拌2小時。將反應混合物用水(300 mL)稀釋，用CH_2Cl_2 (500 mLx2)萃取，用鹽水洗滌，然後以Na_2SO_4乾燥。將合併之有機萃取物過濾然後在減壓下濃縮而供給粗中間物**6**，將其藉由FCC純化（洗提液：石油醚：乙酸乙酯= 1：0至1：2）而供給呈淡黃色油之**6** (67 g,產率：38.0%)。**MS (ESI)**：$C_{25}H_{30}N_2O_5$質量計算為438.52，m/z測得為439.6 $[M+H]^+$。

【0305】 向6 (2.6 g, 5.93 mmol)於DCE (50 mL)中之溶液中加入Me3SnOH(1.61 g, 8.90 mmol)然後在20℃下攪拌16小時。將1 M HCl (5 mL)在0℃下逐滴加入。將混合物在室溫下攪拌0.5小時，以Na_2SO_4乾燥，然後過濾。將濾液濃縮然後將殘餘物藉由FCC純化（洗提液：CH_2Cl_2：MeOH=1:0至95:5）而供給呈淡黃色固體之**7** (**K(NMeAc)**, 2.02 g,產率：80.51%)。**MS (ESI)**：$C_{24}H_{28}N_2O_5$質量計算為424.49，m/z測得為425.1 $[M+H]+$。**^{1}H NMR** (DMSO-d_6, 400 MHz): δ 7.89 (d, *J*=7.6 Hz, 2H), 7.73 (d, *J*=7.2 Hz, 2H), 7.62 (m, 1H), 7.46 - 7.38 (m, 2H), 7.36 - 7.28 (m, 2H), 4.33 - 4.16 (m, 3H), 3.89 (s, 1H), 3.22 (m, 2H), 2.93 - 2.73 (m, 3H), 1.94 (d, *J*=7.2 Hz, 3H), 1.77 - 1.55 (m, 2H), 1.55 - 1.36 (m, 2H), 1.28 (m, 2H).

h. (S)-2-胺基-N-(2-(二甲基胺基)-2-側氧基乙基)-N-甲基-3-(吡啶-3-基)丙醯胺(NH2-3Pya-Sar-CON(Me)2)之合成



【0306】 向100-mL小瓶中倒入起始材料**1** (10 g, 82.3 mmol)然後將甲基胺溶液(51.1 g, 494 mmol, 30%於乙醇中)加入。將反應混合物在25℃下攪拌16小時，之後將混合物濃縮而給出粗中間物2。向粗中間物中，將石油醚(30 mL)加入然後將混合物在25℃下攪拌0.5小時而產出固體。將所得固體過濾而給出呈淺黃色固體之**2** (10 g,粗製)。**^{1}H NMR** (DMSO- d_6, 400 MHz): δ ppm 9.09 - 8.02 (m, 2H), 3.97 (s, 2H), 2.92 (s, 3H), 2.87 (s, 3H), 2.52 (s, 3H).

【0307】 向化合物**3** (9 g, 23.2 mmol)、中間物**2** (3.23 g, 27.81 mmol)、及DIEA (7.03 g, 69.5 mmol)之攪拌溶液中加入DMF (90 mL)中之HATU (10.6 g, 27.8 mmol)。將反應混合物在25℃下攪拌2小時接著倒入冰水(100 mL)中，然後用乙酸乙酯(200 mL x4)萃取。將合併之有機萃取物用鹽水(100 mL)洗滌，以無水Na_2SO_4乾燥，過濾，然後在減壓下濃縮而供給粗中間物**4**，將其藉由FCC純化（洗提液：CH_2Cl_2：MeOH = 1：0至95：5）而供給呈淡黃色固體之**4** (11 g,產率：96.5%)。**MS (ESI)：**$C_{28}H_{30}N_4O_4$質量計算為486.56，m/z測得為487.2 $[M+H]^+$。

【0308】 向**4** (10.5 g, 21.6 mmol)於DCM (400 mL)中之溶液中加入哌啶(5 mL, 50.5 mmol)。將反應混合物在室溫下在氮氣氛下攪拌16小時，接著將其在真空下濃縮。將殘餘物藉由FCC純化（洗提液：CH_2Cl_2：MeOH = 1：0至95：5）而供給呈淡黃色固體之粗產物**5** (5.5 g,不純)。接著將粗產物藉由製備型HPLC純化並使用Phenomenex Genimi NX C18 (150*40 mm*5um)（洗提液：1%至25% (v/v)水(0.04%NH_3H_2O+10 mM NH_4HCO_3)-MeCN）而供給純產物。收集純流份然後將其凍縮至乾而給出呈膠狀液體之**5** (**NH2-3Pya-Sar-CON(Me)$_2$**, 3.6

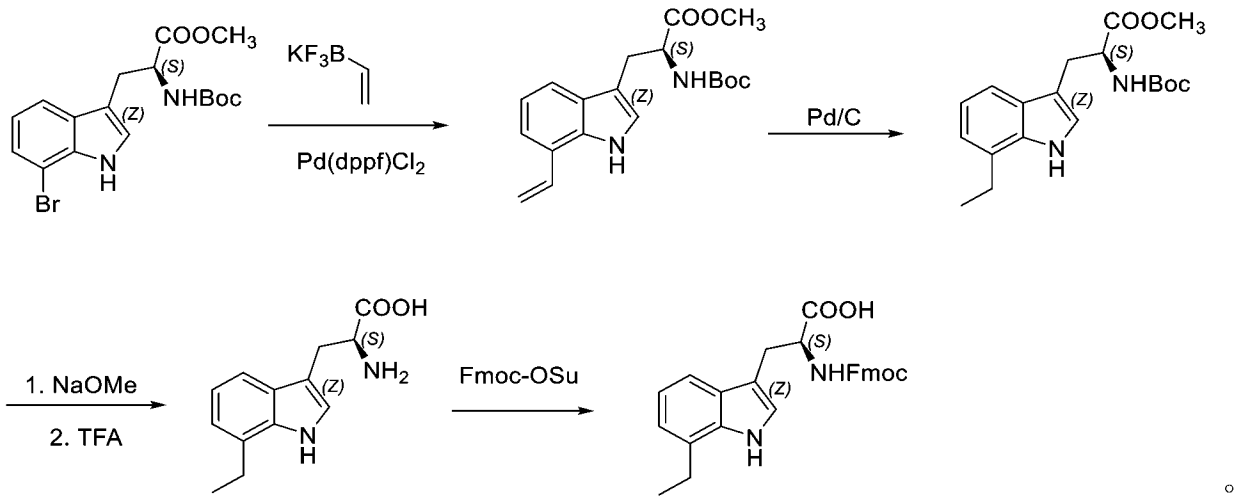
g,產率：62.7%)。**MS (ESI)**：$C_{13}H_{20}N_4O_2$質量計算為264.32，m/z測得為265.1 [M+H]+。**^{1}H NMR** (400 MHz, D_2O) δ ppm 8.44 - 8.22 (m, 2H), 7.76 - 7.54 (m, 1H), 7.34 (m, 1H), 4.31 - 4.19 (m, 1H), 4.18 - 3.96 (m, 2H), 2.95 (m, 3H), 2.92 - 2.85 (m, 6H), 2.77 (m, 2H).

i.經取代色胺酸之合成

【0309】 7-甲基色胺酸之合成。7-甲基色胺酸係購自商業來源。此外，該化合物可依照下述方式其中之一來合成。

【0310】 7-乙基色胺酸之合成。7-乙基色胺酸係依照方案1中所繪示之方法來合成：

方案1



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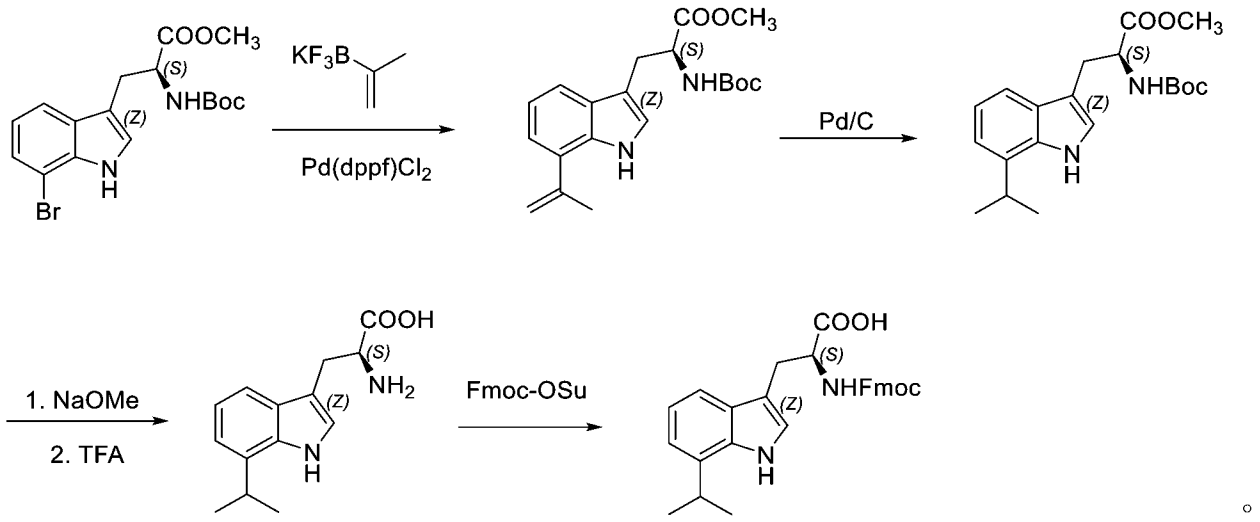
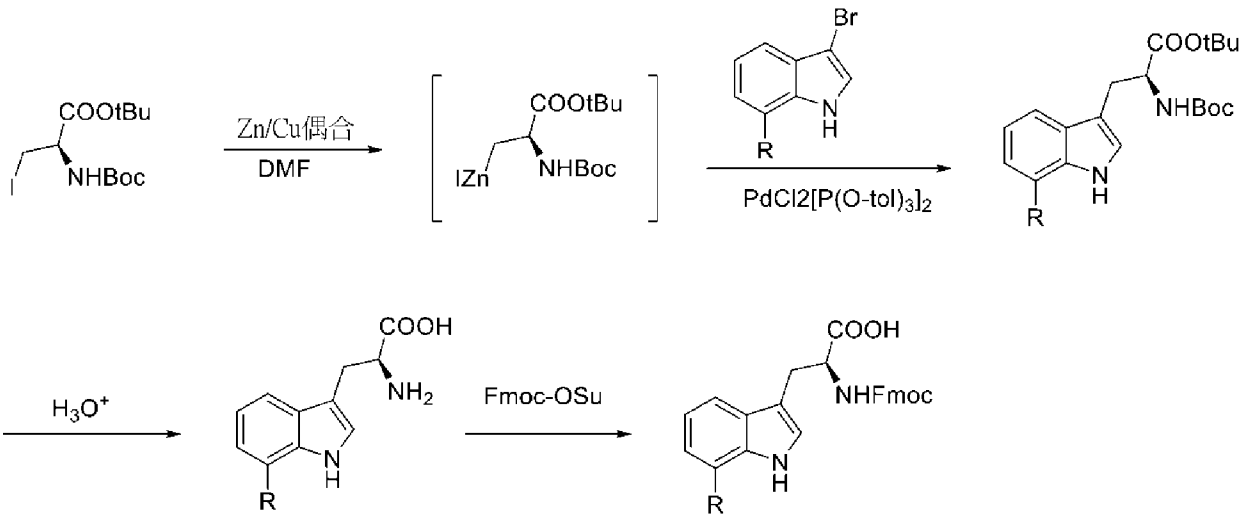
【0311】 7-異丙基色胺酸之合成。7-異丙基色胺酸係依照方案2中所繪示之方法來合成：

方案2



【0312】　額外7-經取代色胺酸之合成。額外7-經取代色胺酸係或可依照方案3A中所繪示之方法來合成：

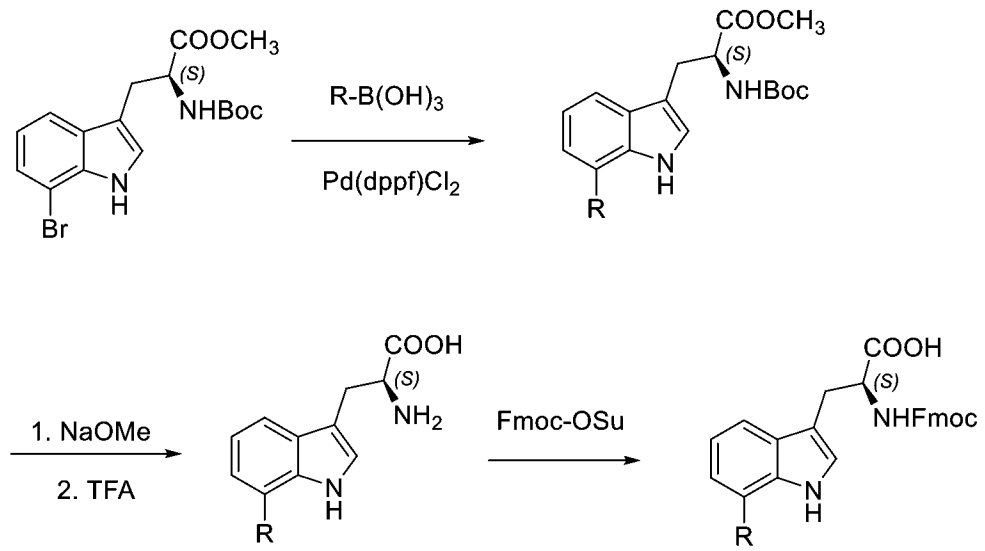
方案3A



其中R係氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基。

【0313】　7-芳基經取代色胺酸之合成。7-芳基經取代色胺酸係或可依照方案3B中所繪示之方法來合成：

方案3B

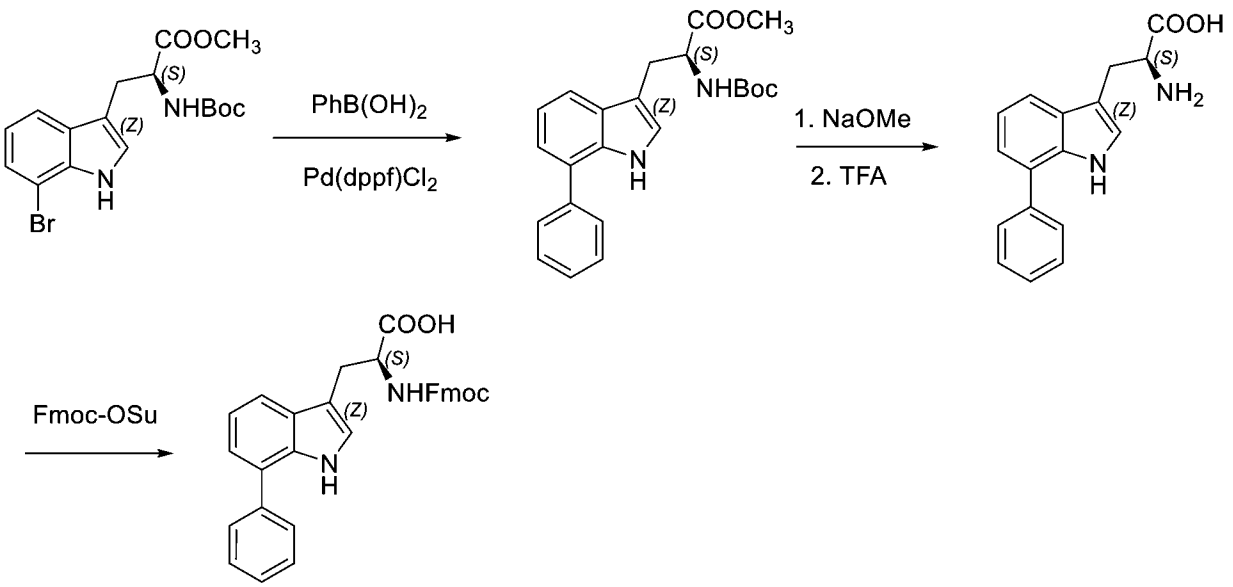


其中R係芳基、未經取代或經鹵基、烷基、氰基、鹵基烷基、羥基、或烷氧基所取代。

【0314】 特定代表性R基團係選自苯基、或3-Me-苯基。

【0315】 7-苯基經取代色胺酸之合成。7-苯基經取代色胺酸係或可依照方案4中所繪示之方法來合成：

方案4



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【0316】 使用芳基硼酸之Suzuki偶合。將無水甲苯(30 mL)中之3-(7-溴-1H-吲哚-3-基)-2-((三級丁氧基羰基)胺基)丙酸(S)-甲酯(4.0 g, 10.0 mmol)用氮吹掃10分鐘。將10 mL的水中之K_2CO_3 (2.0 g, 15.0 mmol)加入接著將苯基硼酸(1.47 g, 12.0 mmol)加入，然後將反應混合物用氮吹掃10分鐘。將Pd(dppf)Cl_2.DCM (0.58 g, 0.71 mmol)、乙醇(10 mL)、及THF (20 mL)加入，然後將反應混合物加熱至100 ºC伴隨攪拌8小時。將反應混合物在真空下濃縮然後將殘餘物溶於DCM (200 mL)中。將有機層用水及鹽水洗滌，以硫酸鈉乾燥然後濃縮。將粗產物藉由60-120-網目矽膠管柱層析法純化而產出呈帶泡沫固體之產物(3.6 g ,90%)。

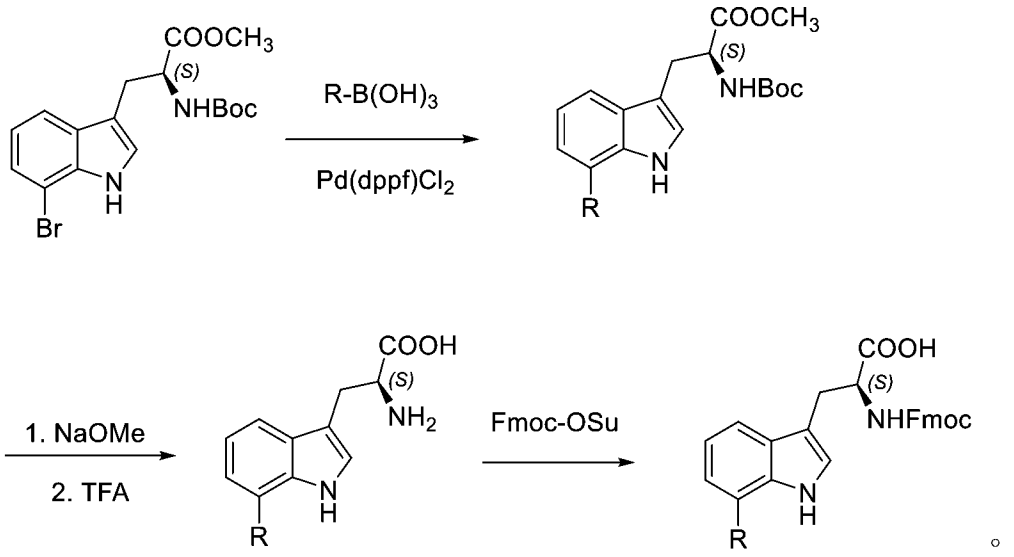
【0317】 水解。向2-((三級丁氧基羰基)胺基)-3-(7-苯基-1H-吲哚-3-基)丙酸(S)-甲酯(3.6 g, 9.1 mmol)於THF/MeOH/水(4:1:1)中之溶液中加入氫氧化鋰(1.15g、27.3 mmol)然後將溶液攪拌整夜。將溶液濃縮以移除溶劑，然後用足夠的水稀釋並用10%檸檬酸酸化。將含有產物之水層用乙酸乙酯(2 × 10 mL)萃取。將有機層用水及鹽水洗滌，以Na_2SO_4乾燥然後濃縮至所欲產物(3.3 g, 95%)。

【0318】 Boc去保護。向(S)-2-((三級丁氧基羰基)胺基)-3-(7-苯基-1H-吲哚-3-基)丙酸(3.3 g, 8.6 mmol)於二氯甲烷(13 mL)中之冰冷卻溶液中加入三氟乙酸(6.6 mL)然後將溶液在室溫下攪拌6小時。將溶液蒸發至乾再溶於二氯甲烷(10 mL)中用HCl/醚處理然後濃縮。將粗製鹽酸鹽懸浮於MTBE (25 mL)中，攪拌30分鐘然後過濾而得到(S)-2-胺基-3-(7-苯基-1H-吲哚-3-基)丙酸鹽酸鹽(1.8 g, 66%)。

【0319】 Fmoc保護。向(S)-2-胺基-3-(7-苯基-1H-吲哚-3-基)丙酸鹽酸鹽(1.8 g, 5.7 mmol)於THF/水(45 mL：13 mL)中之溶液中加入碳酸氫鈉(1.92 g, 22.8 mmol)接著分批加入N-(9-芴基甲氧基羰基氧基)琥珀醯亞胺(1.92 g, 5.7 mmol)。將所得混合物攪拌整夜然後濃縮以移除THF。將殘餘物用足夠的水稀釋並用2N HCl酸化，然後用乙酸乙酯(2 × 100 mL)萃取。將有機層用水及鹽水洗滌，以Na_2SO_4乾燥然後濃縮，將殘餘物懸浮於20% MTBE/己烷中而產出所欲產物(2.6 g, 92%)。

【0320】 7-雜芳基經取代色胺酸之合成。7-雜芳基經取代色胺酸係或可依照方案5中所繪示之方法來合成：

方案5



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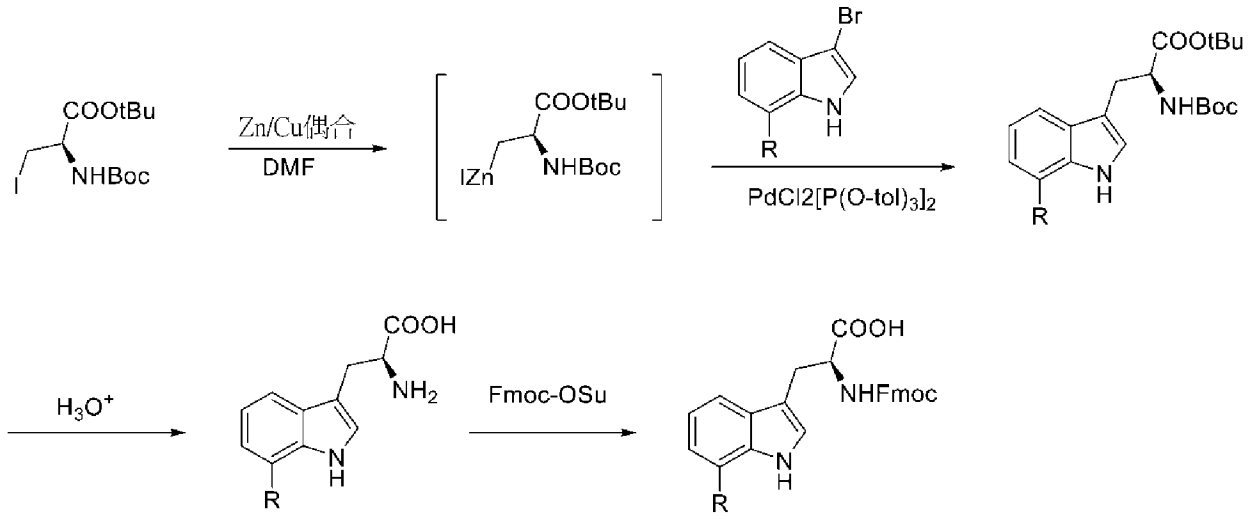
其中R係雜芳基、未經取代或經鹵基、鹵基、烷基、氰基、鹵基烷基、羥基、或烷氧基所取代。

【0321】 7-雜環烷基經取代色胺酸之合成。7-雜環烷基經取代色胺酸係或可依照方案6中所繪示之方法來合成：

方案6

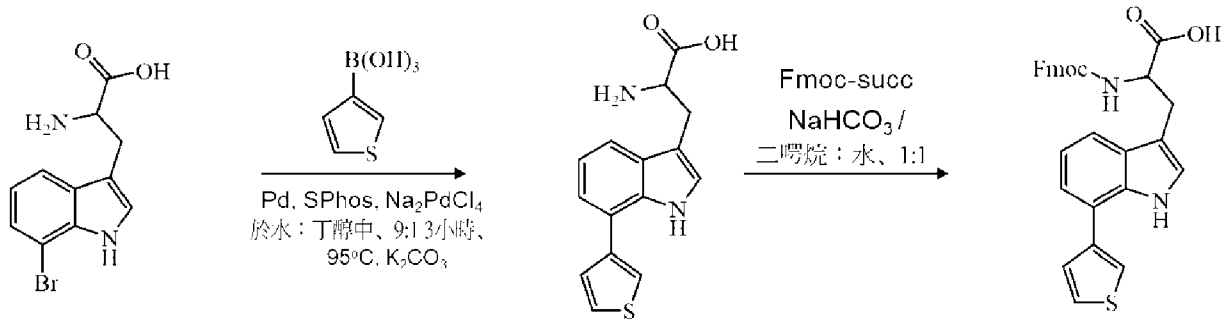


其中R係雜環烷基、未經取代或經烷基、或鹵基所取代。

【0322】 特定代表性R基團係選自噻吩基、吡啶基、哌啶基、及味啉基(morpholinyl)。

【0323】 7-噻吩基(硫苯基)經取代色胺酸之合成。7-噻吩基(硫苯基)經取代色胺酸係或可依照方案7中所繪示之方法來合成：

方案7



【0324】 Suzuki–Miyaura交叉偶合反應係使用Frese等人(ChemCatChem 2016, 8, 1799-1803)所述之修改方法來執行。使用Na_2PdCl_4作為Pd來源並結合

Buchwald配位基SPhos。此系統已知對於催化具挑戰性之受質組合即使在低溫下仍有優良結果。在我們的情況下，7溴Trp與硼酸之Suzuki–Miyaura交叉偶合反應供給了所要產物，隨後我們使用Fmoc-OSu將其保護起來。

【0325】 將L-7-(硫苯-3-基)-色胺酸：將7-溴-L-色胺酸(0.283 g, 1 mmol)、噻吩-3-硼酸(0.383 g, 3.00 mmol, 3 equiv.)、及K_2CO_3 (10 equiv.)置於燒瓶中然後用N_2吹掃。經除氣水：將1-丁醇(9:1、30 mL)經由注射器加入，然後將反應在95℃下攪拌。為了起始反應，在先前將Pd鹽及配位基在40℃下溫熱10分鐘後，將SPhos (6.2 mg, 15 mole %)及Na_2Cl_4Pd (15.2 mg, 5 mole %)轉移至混合物中。

【0326】 一旦完成，便將水性反應用H_2O (20 mL)稀釋然後藉由逐滴加入1 M HCl將溶液酸化至pH 1.0。將沉澱的鈀黑藉由過濾（Whatman，20 μm孔徑）移除然後將濾液凍乾。最後，將所得粗產物藉由製備型反相高效液相層析法(RP-HPLC)純化，並且使用C18管柱(5 μm, 250 × 50 mm)及50 mL/min之流率。分離係使用緩衝劑B於A中之線性梯度來達成（緩衝劑A：0.05% TFA水溶液；緩衝劑B：0.043% TFA，90%乙腈於水中）。分析係使用C18管柱(3 μm, 50 × 2 mm)及1 mL/min之流率來執行監測。接著將含有純產物之流份在凍乾器上凍乾。產出104 mg（36%產率）。MS (ESI) *m/z* 287.08 [M+H] +（C15H15O2NS計算為287.12）。

【0327】 Fmoc-L-7-(硫苯-3-基)-色胺酸：將胺基酸L-7-(硫苯-3-基)-色胺酸(31.5 mg, 0.11 mmol)溶於水及碳酸氫鈉(2 eq)中並伴隨攪拌。將所得溶液冷卻至5℃然後將Fmoc-OSu (44.53 mg, 1.05 eq)緩慢加入而為二噁烷中之溶液。將所得混合物在0°下攪拌1小時然後讓其溫熱整夜至室溫。接著將水加入然後將水層用

EtOAC萃取2次。將有機層用飽和碳酸氫鈉溶液回萃取兩次。將合併之水層用10% HCl酸化至1.0之pH，接著用EtOAC萃取3次。將合併之有機層乾燥（硫酸鈉）然後在真空中濃縮。將所得殘餘物藉由快速層析法純化(SiO2)並使用（甲苯，乙酸乙酯，(1:1)，1%乙酸）。產出50 mg（89%產率）。MS (ESI) *m/z* 509.10 [M+H] +（C15H15O2NS計算為508.59）。

組裝

【0328】 肽係使用標準基於Fmoc之固相合成在各種儀器上組裝。大致上，肽序列係組裝如下：將各反應小瓶中中之樹脂用DMF洗滌兩次，接著用20% 4-甲基哌啶或20%哌啶處理（Fmoc去保護）。接著將樹脂過濾並用DMF洗滌，然後用4-甲基哌啶或哌啶再處理。將樹脂再次用DMF洗滌，接著加入胺基酸及偶合試劑。在頻繁攪動一段指定時間後，將樹脂過濾然後用DMF洗滌。針對典型的本發明之肽，針對胺基酸執行雙重偶合。在完成偶合反應後，將樹脂用DMF洗滌，之後繼續進行下一個胺基酸偶合。

形成烯烴之環合岐化

【0329】 環合岐化之一個實例為將樹脂(100 μmol)用2 mL的DCM（3 × 1分鐘）接著2 mL的DCE（3 × 1分鐘）洗滌，之後用Grubb氏第一代催化劑在DCE中之6 mM溶液的2 mL溶液處理（4.94 mg ml−1；相對於樹脂取代為20 mol%）。將溶液在氮下回流整夜（12小時），之後進行排液。將樹脂用DMF（每次4 ml）洗滌三次；DCM (4 ml)，之後進行乾燥及切割。

切割

【0330】 在完成肽組裝後，藉由用切割試劑處理將肽自樹脂切割下來，諸如試劑K（82.5%三氟乙酸、5%水、5%苯基甲基硫醚、5%酚、2.5% 1,2-乙二硫醇）。切割試劑能夠成功地將肽自樹脂，以及所有其餘側鏈保護基切割下來。

【0331】 將切割下來的肽沉澱於冷二乙醚中，接著用乙醚洗滌兩次。將濾液倒出並將第二份等分試樣的冷乙醚加入，然後重複程序。將粗製肽溶於乙腈：水之溶液（7：3含1% TFA）中然後過濾。接著使用電灑游離質譜(ESI-MS) (Micromass/Waters ZQ)驗證線性肽之品質，之後將其純化。

經由氧化之雙硫鍵形成

【0332】 在一般Fmoc-SPPS程序後，將含有游離硫醇（例如diPen）之肽組裝在Rink Amide-MBHA樹脂上。藉由用切割試劑（90%三氟乙酸、5%水、2.5% 1,2-乙二硫醇、2.5%三-異丙基矽烷）處理將肽自樹脂切割下來。將切割下來的肽沉澱於冷二乙醚中，接著用乙醚洗滌兩次。將濾液倒出並將第二份等分試樣的冷乙醚加入，然後重複程序。將粗製肽溶於乙腈：水之溶液（7：3含1% TFA）中然後過濾而給出所要之未氧化肽粗製肽

【0333】 大致上，將切割下來之粗製肽（具有帶Cys、aMeCys、Pen、hCys、(D)Pen、(D)Cys、或(D)hCys之X4及X9）溶於20 mL的水：乙腈中。接著將乙酸中之飽和碘逐滴加入並伴隨攪拌，直到黃色持續出現。將溶液攪拌15分鐘，並且用分析型HPLC及LCMS監測反應。當反應完成時，將固體抗壞血酸加入，直到溶液變成透明。接著將溶劑混合物藉由先用水稀釋接著裝載至反相

HPLC機上來純化（條件之實例包括Luna C18擔體，10u，100A，動相A：含有0.1% TFA之水，動相B：含有0.1% TFA之乙腈(ACN)，梯度開始為5% B，然後在60分鐘期間內以15 ml/min之流率變化至50% B）。接著將含有純產物之流份在凍乾器上凍乾。

硫醚鍵形成

【0334】 在一般Fmoc-SPPS程序後，將含有游離硫醇（例如Cys）及hSer(OTBDMS)之肽組裝在Rink Amide-MBHA樹脂上。氯化係藉由將樹脂用DCM中之PPh_3 (10 equiv.)及Cl_3CCN (10 equiv.)處理2小時來進行。藉由用切割試劑（90%三氟乙酸、5%水、2.5% 1,2-乙二硫醇、2.5%三-異丙基矽烷）處理將肽自樹脂切割下來。將切割下來的肽沉澱於冷二乙醚中，接著用乙醚洗滌兩次。將濾液倒出並將第二份等分試樣的冷乙醚加入，然後重複程序。將粗製肽溶於乙腈：水之溶液（7：3含1% TFA）中然後過濾而給出所要之未環化粗製肽

【0335】 將在X4及X9位置或X9及X4位置具有游離硫醇（例如Cys、Pen、aMeCys、hCys、(D)Pen、(D)Cys或(D)hCys及鹼化烷基(hSer(Cl)）之粗製肽溶於0.1 M TRIS緩衝劑pH 8.5中。讓環化在室溫下進行整夜。接著將溶劑混合物藉由先用水稀釋兩倍接著裝載至反相HPLC機上來純化（Luna C18擔體，10u，100A，動相A：含有0.1% TFA之水，動相B：含有0.1% TFA之乙腈(ACN)，梯度開始為5% B，然後在60分鐘期間內以15 ml/min之流率變化至50% B）。接著將含有純產物之流份在凍乾器上凍乾。

純化

【0336】 分析及純化管柱及方法會有所變化且在所屬技術領域中係已知的。例如，分析型反相、高效液相層析法(HPLC)係在Gemini C18管柱(4.6 mm × 250 mm) (Phenomenex)上執行。半製備型反相HPLC係在Gemini 10 μm C18管柱(22 mm × 250 mm) (Phenomenex)或Jupiter® 10 μm，300 angstrom (Å) C18管柱(21.2 mm × 250 mm) (Phenomenex)上執行。分離係使用緩衝劑B於A中之線性梯度來達成（動相A：含有0.15% TFA之水，動相B：含有0.1% TFA)之乙腈(ACN)，流率為1 mL/min（分析型）及15 mL/min（製備型））。分離係使用緩衝劑B於A中之線性梯度來達成（動相A：含有0.15% TFA之水，動相B：含有0.1% TFA)之乙腈(ACN)，流率為1 mL/min（分析型）及15 mL/min（製備型））。

實例1B. ac-Pen(1:3)-E-T-Trp_7Me-Lys_Ac-Pen(1:3)-Phe_4_2ae-Nal-THP-Lys_Ac-N-H-Sar-am（中間物肽）

【0337】 中間物肽之TFA（三氟乙酸）鹽係以0.1 mmol規模合成。一旦完成，單離出60 mg的大約95%純中間物肽而呈白色粉末，代表大約30%之整體產率。

【0338】 中間物肽係使用Merrifield固相合成技術在Protein Technology多通道合成儀上合成，然後在Rink Amide MBHA (100-200網目, 0.8 mmol/g)樹脂上使用標準Fmoc保護合成條件來建構。藉由用強酸切割將所建構之肽與樹脂及

保護基分離，接著進行沉澱。接著將粗製較精簡之肽環化然後藉由反相、高效液相層析法(RP-HPLC)純化。凍乾純流份而給出中間物肽2之最終產物。

【0339】 澎潤樹脂：將125 mg的Rink Amide MBHA樹脂(0.1 mmol, 0.8 mmol/g裝載量)轉移至25 mL反應容器（用於Symphony肽合成儀）中。將樹脂用3.75 mL的DMF澎潤（3×10分鐘）。

【0340】 步驟1：Fmoc-Sar-OH（Fmoc-N-甲基甘胺酸）之偶合：Fmoc基團之去保護係藉由用2.5 mL的20%哌啶（在DMF中）對經澎潤Rink Amide樹脂處理兩次（分別為5及10分鐘）來達成。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-Sar-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0341】 步驟2：Fmoc-His(Trt)-OH之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-His(Trt)-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0342】 步驟3：Fmoc-Asn(Trt)-OH之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-His(Trt)-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0343】 步驟4：Fmoc-Lys(Ac)-OH之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc- Lys(Ac)-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0344】 步驟5：Fmoc-THP-OH（Fmoc-4-胺基-四氫哌喃-4-羧酸）之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-THP-OH（在DMF (100 mM)

中）及1.25 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0345】 步驟6：Fmoc-2Nal-OH（Fmoc-3-(2-萘基)-L-丙胺酸）之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-2Nal-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0346】 步驟7：Fmoc-Phe_4_2ae-OH（Fmoc-4-[2-(Boc-胺基)乙氧基]-L-苯丙胺酸）之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自2Nal-THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-Phe_4_2ae-OH（在DMF (100 mM)中）及1.25 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一

次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0347】 步驟8：Fmoc-L-Pen(Trt)-OH（Fmoc-S-三苯甲基-L-青黴胺）之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Phe_4_ae-2Nal-THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-L-Pen(Trt)-OH（在DMF (100 mM)中）及1.25 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0348】 步驟9：Fmoc-Lys(Ac)-OH之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Pen-Phe_4_ae-2Nal-THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc- Lys(Ac)-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0349】 步驟10：Fmoc-Trp_7Me-OH之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Lys(Ac)-Pen-Phe_4_ae-2Nal-THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-Trp_7Me-OH（在DMF (100 mM)中）及1.25 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0350】 步驟11：Fmoc-Thr(tBu)-OH之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Trp_7Me-Lys(Ac)-Pen-Phe_4_ae-2Nal-THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-Thr(tBu)-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0351】 步驟12：Fmoc-Glu(OtBu)-OH之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Thr-Trp_7Me-Lys(Ac)-Pen-Phe_4_ae-2Nal-THP-

Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-Glu(OtBu)-OH（在DMF (200 mM)中）及2.5 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0352】 步驟13：Fmoc-L-Pen(Trt)-OH（Fmoc-S-三苯甲基-L-青黴胺）之偶合：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Glu-Thr-Trp_7Me-Lys(Ac)-Pen-Phe_4_ae-2Nal-THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的胺基酸Fmoc-L-Pen(Trt)-OH（在DMF (100 mM)中）及1.25 mL的偶合試劑HBTU-DIEA混合物（在DMF（200及220 mM）中）。將偶合反應混合1小時，過濾然後重複一次（雙重偶合）。在完成偶合反應後，先將樹脂用6.25 mL的DMF洗滌（3×0.1分鐘），之後再開始下一個去保護/偶合循環。

【0353】 步驟14：乙醯基加蓋：將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌，然後藉由用2.5 mL的20%哌啶（在DMF中）處理兩次（分別為5及10分鐘）將Fmoc基團自Pen-Glu-Thr-Trp_7Me-Lys(Ac)-Pen-Phe_4_ae-2Nal-THP-Lys(Ac)-Asn-His-Sar-Rink Amide樹脂之N-端移除。在去保護後，將樹脂用3.75 mL的DMF（3×0.1分鐘）洗滌接著加入2.5 mL的20%酸性酐（在DMF中）及2.5 mL的10% DIEA（在DMF中）。將乙醯基反應混合1小時，過濾然後重複一次

（雙重偶合）。在完成乙醯基化後，將樹脂用6.25 mL的DMF（6×0.1分鐘）及6.25 mL的DCM（6×0.1分鐘）洗滌，接著在氮下乾燥20分鐘，之後用TFA進行切割。

【0354】 步驟15：TFA切割及醚沉澱：在完成肽組裝後，將乾燥之樹脂轉移至20 mL玻璃小瓶中。向其中加入10 mL的TFA切割雞尾酒組合試劑（90/5/2.5/2.5的TFA/水/Tips/DODT）然後在室溫下攪拌2小時。切割試劑能夠將肽自樹脂，以及所有其餘側鏈保護基切割下來。之後，將大部分的TFA在氮下吹除，接著將20 mL的冷加入至肽切割混合物之剩餘部分而形成白色沉澱物。將醚混合在4℃下以3000 rpm離心3分鐘，然後將醚層（含有側鏈保護基）傾析至廢料中並多執行2次沉澱物之醚洗滌（每次20 mL）。將粗製線性肽（丸粒）溶於40 mL的乙腈：水(1:1)中然後通過0.45 μm RC膜過濾以移除樹脂。

【0355】 步驟16：經由氧化之雙硫鍵形成：將粗製線性肽氧化而未經純化。在切割步驟後，將40 mL的50%乙腈（於水中）中之粗製線性肽用水稀釋至100 mL以成為20%乙腈（於水中）之最終有機溶劑含量。向其中逐滴加入碘於甲醇中之飽和溶液同時攪拌，直到黃色持續而不會退去。將稍微有色之溶液攪拌額外5分鐘，之後藉由加入一撮固體抗壞血酸將多餘的碘淬熄，直到溶液變成透明。

【0356】 步驟17：單環肽（雙硫鍵）之RP-HPLC純化：此純化係使用RP-HPLC來進行。將半製備型管柱Gemini 5 μm C18管柱(21.2 mm×250 mm) (Phenomenex®)以20 mL/min之流率使用100%動相A（MPA = 0.1% TFA於水中）來平衡。將100 mL的經淬熄氧化肽以20 mL/min直接裝載至平衡後之管柱中，

然後用20%動相B（MPB = 0.1% TFA於乙腈中）洗滌5分鐘。分離係使用20至50% MPB之線性梯度在30分鐘期間內以20 mL/min來達成。將所欲之氧化肽以大約30% MPB洗提。將純流份合併及凍乾而給出60 mg的經純化氧化肽，其呈TFA鹽之形式，產率為30%。

【0357】 步驟18：特性分析：在凍乾後給出白色粉末，藉由分析型HPLC得出純度>95%。低解析度液相層析法–質譜法(LC-MS)給出648.7之三價離子$[M+3H]^{3+}$及972.4之二價離子$[M+2H]^{2+}$。實驗質量符合1943.27 Da之理論分子量。

實例1C下. ac-Pen(1:3)-E(2:3)-T-Trp_7Me-Lys_Ac-Pen(1:3)-Phe_4_2ae(2:3)-Nal-THP-Lys_Ac-N-H-Sar-am

【0358】 雙環標題化合物之TFA（三氟乙酸）鹽係以0.01 mmol規模使用如先前所述之經純化單環肽前驅物（步驟1至17）來合成，接著進行內醯胺鍵形成（在殘基Glu與Phe_4_2ae之間）然後藉由RP-HPLC純化。一旦完成，單離出10 mg的大約95%純標題化合物而呈白色粉末，代表內醯胺鍵形成步驟之產率為50%而總產率為15%。

【0359】 步驟18：內醯胺鍵形成：將20 mg的經純化氧化中間物肽(大約0.01 mmol)溶於10 mL的N N-二甲基甲醯胺(DMF)中。向其中加入(苯羊三唑-1-基-氧基三吡咯啶基鏻六氟磷酸酯(PyBOP) (0.04 mmol, 4當量)，接著加入N,N-二異丙基乙基胺(DIEA) (0.05 mmol, 5當量)。將混合物在室溫下攪拌並藉由分析型HPLC監測反應。反應在30分鐘內完成，然後將混合物用水中之20%乙腈稀釋至100 mL，DMF之最終含量<10%，之後將其裝載至HPLC以進行純化。

【0360】 步驟19：雙環肽（雙硫鍵及內醯胺鍵）之RP-HPLC純化：第2次純化係使用與先前於步驟17中所述相同之程序進行。所欲之雙環肽比單環肽晚洗提出來（大約35% MPB）。將純流份合併及凍乾而給出10 mg的經純化雙環肽，其呈TFA鹽之形式，內醯胺鍵形成步驟之產率為50%而總產率為15%。

【0361】 步驟20：特性分析：在凍乾後，標題化合物給出白色粉末，藉由分析型HPLC得出純度>95%。低解析度液相層析法–質譜法(LC-MS)給出642.5之三價離子$[M+3H]^{3+}$及963.5之二價離子$[M+2H]^{2+}$。實驗質量符合1925.26 Da之理論分子量。

實例1D. ac-Pen(1:3)-Dap(2:3)-T-Trp_7Me-Lys_Ac-Pen(1:3)-Phe_4_2ae(3:3)-Nal-THP-Lys_Ac-N-H-Sar-am-PEG4DA(x,2:1,3:2)

【0362】 雙環標題化合物之TFA（三氟乙酸）鹽係以0.01 mmol規模使用其對應之經純化單環（雙硫鍵）肽前驅物來合成，而第2環化係使用預活化之二酸鍵聯物來進行，該鍵聯物在殘基Dap(2:3)及Phe_4_2ae Glu之側鏈上偶聯至一級胺，接著使用RP-HPLC進行純化。一旦完成，單離出10 mg的大約95%純標題化合物而呈白色粉末，代表第2環化步驟之產率為50%而總產率為15%。

【0363】 單環前驅物之製備：經純化單環前驅物（雙硫鍵）之製備方式類似於如先前所述之中間物（步驟1至17），除了步驟12，使用Fmoc-L-Dap(Boc)-OH（Nα-Fmoc-Nβ-Boc-L-2,3-二胺基丙酸）之胺基酸代替Fmoc-Glu(OtBu)-OH。

【0364】 步驟18：將二酸鍵聯物活化：雙-PEG4-酸(PEG4DA) (294 mg, 1 mmol)、N-羥基琥珀醯亞胺(NHS) (2.2 mmol, 2.2當量)、及N,N'-二環己基碳二亞

胺(DCC) (2.2 mmol, 2.2當量)溶於10 mL N-甲基-2-吡咯啶酮(NMP)。將混合物在室溫下攪拌以完全溶解固體起始材料。沉澱在10分鐘內出現，然後將反應混合物進一步在室溫下攪拌整夜，接著進行過濾以移除沉澱之二環己基脲(DCU)。將活化之鍵聯物放在4℃之密閉玻璃小瓶中，之後用於第2環化。預活化鍵聯物之額定濃度為大約0.1 M。

【0365】 步驟19：經由預活化二酸鍵聯物(PEG4DA-NHS)之雙環形成：將20 mg的經純化單環前驅物(大約0.01 mmol)溶於10 mL的N N-二甲基甲醯胺(DMF)中。向其中在10分鐘期間內分次加入預活化二酸鍵聯物(PEG4DA-NHS) (0.1 M於NMP中, 0.01 mmol, 1當量)及N,N-二異丙基乙基胺(DIEA) (0.1 mmol, 10當量)。將混合物在室溫下攪拌並藉由分析型HPLC監測反應。可能需要多餘當量的PEG4DA-NHS以驅使反應完成。反應在1小時後完成，然後將混合物用水中之20%乙腈稀釋至100 mL，DMF之最終含量<10%，之後將其裝載至HPLC以進行純化。

【0366】 步驟20：雙環肽之RP-HPLC純化：第2次純化係使用與先前於步驟17中所述相同之程序進行。所欲之雙環肽比單環肽晚洗提出來（大約35% MPB）。將純流份合併及凍乾而給出10 mg的經純化雙環肽，其呈TFA鹽之形式，內醯胺鍵形成步驟之產率為50%而總產率為15%。

【0367】 步驟21：特性分析：在凍乾後，標題化合物給出白色粉末，藉由分析型HPLC得出純度>95%。低解析度液相層析法–質譜法(LC-MS)給出720.1之三價離子$[M+3H]^{3+}$及1080.1之二價離子$[M+2H]^{2+}$。實驗質量符合2158.52 Da之理論分子量。

實例1E.Ac-[Pen]*-E-T-[W(7-Me)]-[Lys(Ac)]-[Pen]*-Phe[4-(2-胺基乙氧基)]**-[2-Nal]-[THP]-E-N-[3-Pal]-Sarc-NH_2（*Pen-Pen形成雙硫鍵）（**Glu及Phe[4-(2-胺基乙氧基)之側鏈形成內醯胺鍵）**

【0368】 標題化合物之合成係使用FMOC固相肽合成技術來製備。

【0369】 標題化合物係在Rink Amide MBHA樹脂上使用文獻中所記述之標準FMOC保護合成條件來建構。藉由用強酸切割將所建構之肽與樹脂及保護基分離，接著進行沉澱。執行用以形成雙硫鍵之氧化，接著藉由RPHPLC進行純化然後進行相對離子交換。凍乾純流份而給出最終產物。

【0370】 澎潤樹脂：將10 g的Rink Amide MBHA固相樹脂(0.66 mmol/g裝載量)轉移至具有過濾器玻料、磨砂玻璃接頭、及真空側臂之250 ml肽容器中。將樹脂用DMF洗滌3次。

【0371】 步驟1：FMOC-Sarc-OH之偶合：樹脂結合FMOC基團之去保護係藉由加入2樹脂床體積的DMF中之20% 4-甲基-哌啶至經澎潤樹脂並搖動3至5分鐘來實行，之後排液並加入第二份2-樹脂-床體積的4-甲基哌啶溶液並搖動額外20至30分鐘。在去保護後，將樹脂用DMF洗滌3次並伴隨搖動。將FMOC-Sarc-OH (3 eq, 6.2 g)連同Oxyma (4.5 eq, 4.22g)溶於100 ml DMF中。酸之預活化係藉由加入DIC (3.9 eq, 4 ml)並伴隨搖動15分鐘，之後加入至去保護之樹脂。接著在大約15分鐘的偶合後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入。偶合反應之進度係比色Kaiser測試來監測。一旦判斷反應完成，便將樹脂用DMF洗滌3次並伴隨搖動，之後開始下一個去保護/偶合循環。

【0372】 步驟2：FMOC-3Pal-OH之偶合：FMOC去保護再次係藉由依序加入兩次2-樹脂-床體積的DMF中之20% 4-甲基-哌啶來達成，一次3至5分鐘而一次20至30分鐘，在處理之間進行排液。接著將樹脂洗滌3次，之後用受保護之3-吡啶基丙胺酸(3Pal)進行偶合。將FMOC-3Pal-OH (3 eq, 7.8g)連同Oxyma (4.5eq, 4.22g)溶於DMF中。用DIC (3.9 eq, 4 ml)進行預活化15分鐘，之後加入至Sarc-Amide樹脂。在15分鐘後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0373】 步驟3：FMOC-Asn(Trt)-OH之偶合：將FMOC自樹脂結合3Pal之N-端移除，然後如先前所述洗滌。將FMOC-Asn(Trt)-OH (2eq, 8g)連同Oxyma (3eq, 2.81g)溶於100 mL的DMF中。將DIC (2.6 eq, 2.65 ml)加入以進行酸之預活化大約15分鐘，之後加入至3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (1.4 eq, 1.43 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0374】 步驟4：FMOC-Lys(Ac)-OH之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。將FMOC-Lys(Ac)-OH (2 eq, 5.4 g)連同Oxyma (3 eq, 2.81 g)溶於100 mL的DMF中。將DIC (2.6 eq, 2.65 ml)加入以進行酸之預活化大約15分鐘，之後加入至Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (1.4 eq, 1.43 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0375】 步驟5：FMOC-THP-OH之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。將FMOC-THP-OH (3 eq, 7.36 g)連同Oxyma (4.5 eq, 4.22g)溶於100 mL的DMF中。將DIC (3.9 eq, 4 ml)加入以進行酸之預活化大約15分鐘，之後加入至Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0376】 步驟6：FMOC-L-Ala(2-萘基)-OH (Nal)之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。FMOC-L-Ala(2-萘基)-OH (3 eq, 8.66 g)連同Oxyma (4.5 eq, 4.22g)溶於100 mL的DMF中。將DIC (3.9 eq, 4 ml)加入以進行酸之預活化大約15分鐘，之後加入至THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0377】 步驟7：FMOC-4-[2-(Boc-胺基-乙氧基)]-L-苯基丙胺酸(FMOC-AEF)之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。將FMOC-4-[2-(Boc-胺基-乙氧基)]-L-苯基丙胺酸(3 eq, 10.8 g)連同Oxyma (4.5 eq, 4.22g)溶於100 mL的DMF中。將DIC (3.9 eq, 4 ml)加入以進行酸之預活化大約15分鐘，之後加入至Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入至反應中。一旦

反應完成（如藉由Kaiser測試所判定），便將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0378】 步驟8：FMOC-Pen(Trt)-OH之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。將FMOC-Pen(Trt)-OH (3 eq, 12.14 g)連同Oxyma (4.5 eq, 4.22g)溶於100 mL的DMF中。將DIC (3.9 eq, 4 ml)加入以進行酸之預活化大約15分鐘，之後加入至AEF-Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0379】 步驟9：FMOC-Lys(Ac)-OH之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。將FMOC-Lys(Ac)-OH (2 eq, 5.4 g)連同Oxyma (3 eq, 2.81 g)溶於100 mL的DMF中。將DIC (2.6 eq, 2.65 ml)加入以進行酸之預活化大約15分鐘，之後加入至Pen(Trt)-AEF-Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (1.4 eq, 1.43 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0380】 步驟10：FMOC-7-Me-Trp-OH之偶合：將FMOC自樹脂結合肽之N-7-端移除，然後將樹脂如先前所述洗滌。將FMOC-7-Me-Trp-OH (2 eq, 5.81 g)連同Oxyma (3 eq, 2.81 g)溶於100 mL的DMF中。將DIC (2.6 eq, 2.65 ml)加入以進行酸之預活化大約15分鐘，之後加入至Lys(Ac)-Pen(Trt)-AEF-Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的

DIC (1.4 eq, 1.43 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0381】 步驟11：FMOC-Thr(tBu)-OH之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。將FMOC-Thr(tBu)-OH (4 eq, 10.5g)連同Oxyma (6 eq, 5.62 g)溶於100 mL的DMF中。將DIC (5.2 eq, 5.3 ml)加入以進行酸之預活化大約15分鐘，之後加入至7MeTrp-Lys(Ac)-Pen(Trt)-AEF-Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0382】 步驟12：FMOC-Glu(OtBu)-OH之偶合：將FMOC自樹脂結合天冬醯胺酸之N-端移除，然後將樹脂如先前所述用DMF洗滌。將FMOC-Glu(OtBu)-OH (2 eq, 5.91 g)連同Oxyma (3eq, 2.81g)溶於100 mL的DMF中。將DIC (2.6 eq, 2.65 ml)加入以進行酸之預活化大約15分鐘，之後加入至Thr(tBu)-7MeTrp-Lys(Ac)-Pen(Trt)-AEF-Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (1.4 eq, 1.43 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便將樹脂用DMF洗滌3次，之後開始下一個去保護/偶合循環。

【0383】 步驟13：FMOC-Pen(Trt)-OH之偶合：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。FMOC- Pen(Trt)-OH (2 eq, 8.1 g)連同Oxyma (3 eq, 2.81 g)溶於100 mL的DMF中。將DIC (2.6 eq, 2.65 ml)加入以進行酸之預活化大約15分鐘，之後加入至Glu(OtBu)-Thr(tBu)-7MeTrp-Lys(Ac)-

Pen(Trt)-AEF-Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂。在大約15分鐘後，將額外等分試樣的DIC (2.6 eq, 2.65 ml)加入至反應中。一旦反應完成（如藉由Kaiser測試所判定），便再次將樹脂用DMF洗滌3次，之後進行所構築肽之最終去保護及乙酸加蓋。

【0384】 步驟14：乙醯基加蓋：將FMOC自樹脂結合肽之N-端移除，然後將樹脂如先前所述洗滌。將150 mL的加蓋試劑A（THF/乙酐/吡啶，80:10:10）加入所建構之Pen(Trt)- Glu(OtBu)-Thr(tBu)-7MeTrp-Lys(Ac)-Pen(Trt)-AEF-Nal-THP-Lys(Ac)-Asn(Trt)-3Pal-Sarc-Amide樹脂中然後搖動30分鐘。將樹脂用DMF洗滌3次接著用DCM洗滌5次。將樹脂分配至5至50 ml離心管中然後置於真空下1.5小時，之後用TFA進行切割。

【0385】 步驟15：TFA切割及醚沉澱：製備200 mL的TFA切割雞尾酒組合試劑(90/5/2.5/2.5 TFA/水/Tips/DODT)。將40 mL的切割雞尾酒組合試劑加入至這5個含有受保護樹脂結合肽之管的各者中，然後搖動兩小時。將用完的樹脂濾除然後將濾液均勻分配至18至50 ml離心管中以進行沉澱。將冷的二乙醚加入至各管中而形成白色沉澱物，接著將其離心。將醚傾析至廢料中並多執行2次沉澱物之醚洗滌。將所得白色沉澱物餅在櫃中乾燥整夜而給出粗製還原肽。

【0386】 步驟16：雙硫鍵氧化：將粗製肽氧化然後以四個1L批次純化。將大約2.5 g的粗製肽溶於1L 20% ACN/水中。在攪拌下，將碘於乙酸/甲醇中之飽和溶液逐滴加入至1L肽溶液中，直到I_2之黃色/棕色持續而不會退去。讓淺黃色溶液靜置5分鐘，之後用一撮抗壞血酸將多餘的碘淬熄。

【0387】 步驟17：RP-HPLC純化：RP-HPLC純化係在各I2氧化後立即執行。將製備型純化管柱(Phenomenex, Luna, C18(2), 100A, 250×50 mm)以70 ml/min用MPA中之20% MPB（MPA = 0.1% TFA/水，MPB = 0.1% TFA於ACN中）平衡。將1 L的經淬熄氧化肽以70 ml/min裝載至經平衡管柱中。在溶劑前部洗提出來後，在60分鐘期間內以70 ml/min執行25至45% MPB之梯度。所欲材料係單離於流份中並各自藉由分析型RPHPLC來進行分析。將純流份自全部四次純化合併然後凍乾而給出經純化TFA鹽，其可立即用於進行經由內醯胺形成之雙環化。

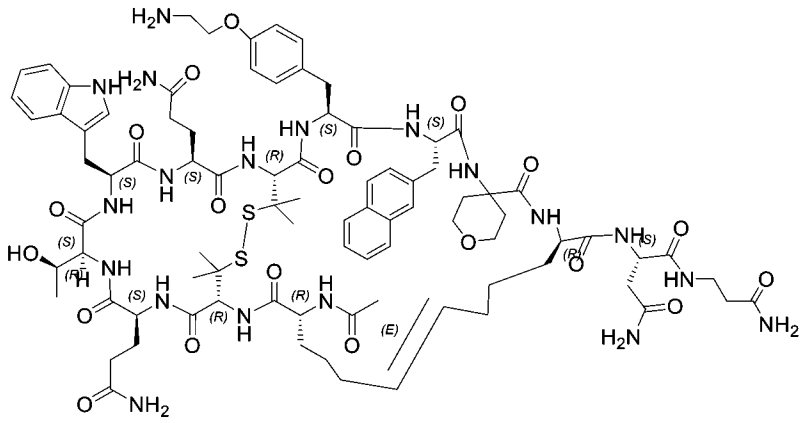
【0388】 步驟18：內醯胺形成而給出雙環：將經純化Pen-Pen雙硫鍵單環肽(800 mg)溶於150 mL的50/50 DMF/DCM (大約5 mg/mL)中。向攪拌中之肽中加入二異丙基乙胺(大約5 eq, 360 ul)，接著加入PyBop (大約4eq, 864 mg)。藉由RP-HPLC監測反應。一旦所有單環起始材料皆轉化為雙環形式，便將溶液用水中之10%乙腈中和並稀釋至1L。稀釋溶液可立即用於RP-HPLC純化。

【0389】 步驟19：RP-HPLC純化：RP-HPLC純化係在內醯胺形成及稀釋後立即執行。將製備型純化管柱(Phenomenex, Luna, C18(2), 100A, 250×50 mm)用MPA中之20% MPB以70 ml/min平衡（MPA = 0.1% TFA/水，MPB = 0.1% TFA於ACN中）。將1 L的經中和雙環肽以70 ml/min裝載至經平衡管柱中。在溶劑前部洗提出來後，在60分鐘期間內以70 ml/min執行25至45% MPB之梯度。所欲材料係單離於流份中並各自藉由分析型RPHPLC來進行分析。將來自所有四次純化之純流份合併然後凍乾而給出經純化TFA鹽，其可立即用於進行相對離子交換。

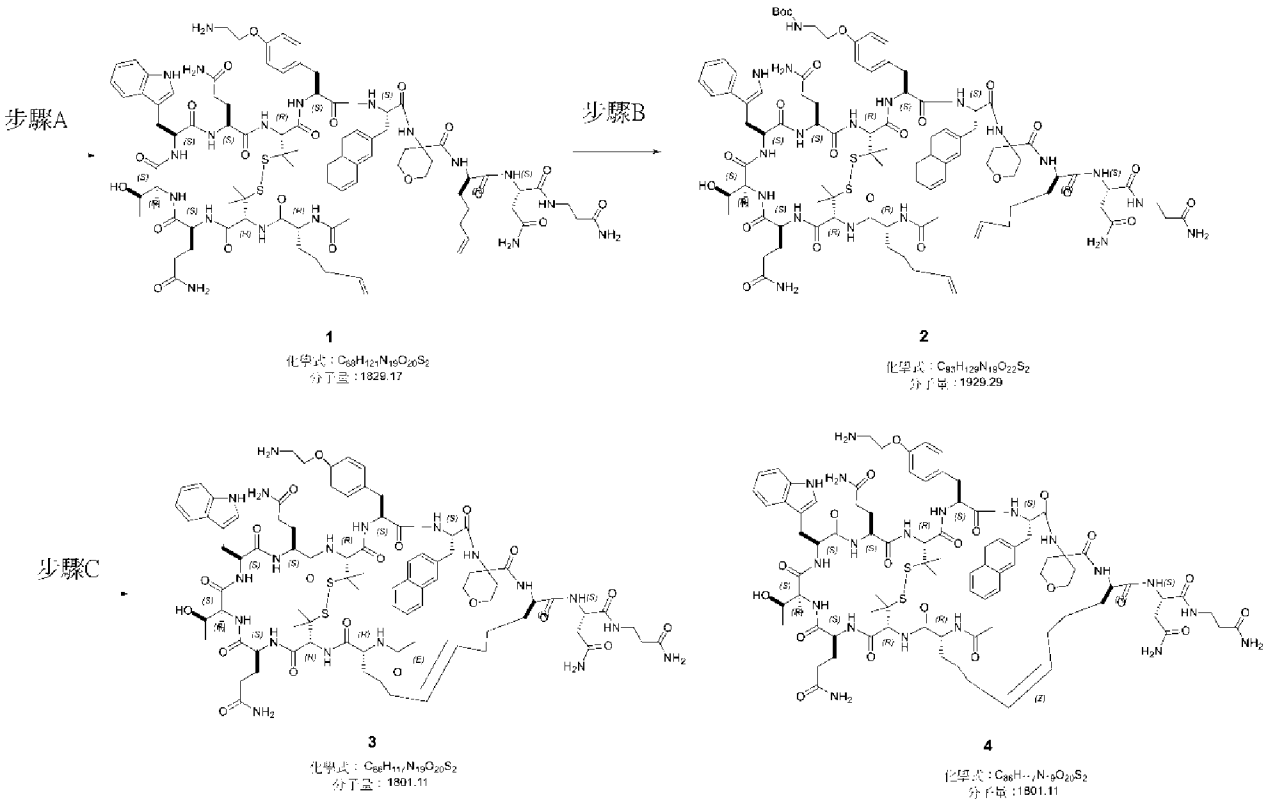
【0390】 步驟20：相對離子交換為乙酸根：將相同之製備型RP-HPLC管柱用MPA中之5% MPB以70 ml/min平衡（MPA = 0.3% AcOH於水中，MPB = 0.3% AcOH於ACN中，MPC = 0.5M NH4OAc於水中）。將經純化肽TFA鹽溶於50/50 ACN/水中然後稀釋至15% ACN。將溶液以70 ml/min裝載至經平衡管柱中然後將溶劑前部洗提出來。將所捕捉之肽用MPA中之5% MPB洗滌5分鐘。接著將所捕捉之肽用MPC中之5% MPB以70 ml/min洗滌40分鐘以將相對離子交換為乙酸根。將所捕捉之肽用MPA中之5% MPB以70 ml/min洗滌10分鐘以將所有NH4OAc自系統中清除。最終，將肽用MPA中之5至70% MPB在60分鐘期間內洗提然後收集於流份中。

【0391】 步驟21：最終凍乾及分析：將所收集之流份藉由分析型RP-HPLC分析，然後將所有>95%純度之流份合併。將合併之流份凍乾而給出呈白色粉末且純度>95%之標題化合物，如藉由RPHPLC所判定。肽身份係使用經純化標題化合物之LC/MS來確認，給出肽之2價狀態M+2/2為969原子質量單位而分子離子為1936原子質量單位。

實例1F.Ac-O2R-Pen-Q-T-W-Q-Pen-Phe[4-(2-胺基乙氧基)]-[2-Nal]-[THP]-O2R-N-[bA]-NH2



（烯烴顯示為E，但未指定）



【0392】　化合物**1**之合成係使用Fmoc受保護胺基酸在固相Rink Amide MBHA（NovaBiochem，0.33 meq/g，100-200網目）上使用CEM Liberty Blue自動化微波肽合成儀來合成。肽係以0.22 mmol規模合成。第一個殘基(bAla)係使用NMP中之3 eq的胺基酸、3 eq的HOAt、及3 eq的DIC在室溫下手動結合整夜。典型反應條件如下：去保護條件：DMF中之20%哌啶(v/v)（2分鐘在90℃

下）；殘基偶合條件：將受保護胺基酸（2.5 mL的0.4 M胺基酸儲備溶液於DMF中）遞送至樹脂中，接著遞送DIC活化劑（2 mL的0.5 M溶液於DMF中）、及Oxyma Pure（1 mL的1 M溶液於DMF中）然後讓其在90℃下反應2分鐘。針對2Nal執行雙重偶合。游離胺基之加蓋係使用DMF中之10eq的乙酐來執行。

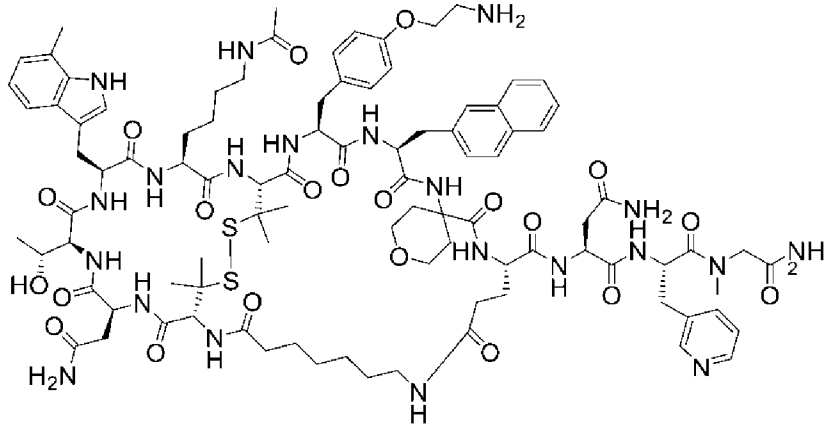
【0393】　在組裝結束時，將肽樹脂用DMF、MeOH、DCM、Et_2O洗滌。使用87.5% TFA、5%酚、2.5%三異丙基矽烷、及5%水在室溫下將肽自固體擔體中切割下來1.5小時。將樹脂過濾接著加入至冷的甲基三級丁醚中以將肽沉澱。在離心後，將肽丸粒用新鮮的冷二乙醚洗滌以移除有機清除劑。重複程序兩次。將最終丸粒乾燥，再懸浮於H2O及乙腈1:1 + 0.1% TFA中然後攪拌整夜。接著凍乾而供給所欲之受保護中間物化合物**1**（產率：80.4%）。LCMS分析C88H121N19O20S2計算為：1829.17；測得為：916.4 $(M+2)^{2+}$。

【0394】　將沉澱之固體粗中間物13-1溶於水：乙腈(1 mg/mL)中。接著將乙酸中之飽和碘逐滴加入並伴隨攪拌，直到黃色持續出現。將溶液攪拌30分鐘，並且用UPLC-MS監測反應。當反應完成時，將固體抗壞血酸加入，直到溶液變成透明。將DIPEA加入直到溶液變成鹼性。將1.5eq.的Boc酐加入。將溶液攪拌60分鐘，並且用UPLC-MS監測反應。將反應混合物用CH_3COOH淬熄。接著將溶劑混合物凍乾並將所得材料溶於2.5 mL的DMSO中，然後藉由C4反相HPLC純化（Waters Deltapak C4 (40 × 200 mm, 15 μm, 300Å)，使用作為洗提液(A) 0.1% TFA於水中及(B) 0.1% TFA，梯度開始為30% B，然後在20分鐘期間內以80 ml/min之流率變化至45% B）。收集含有純產物之流份接著凍乾而供給中

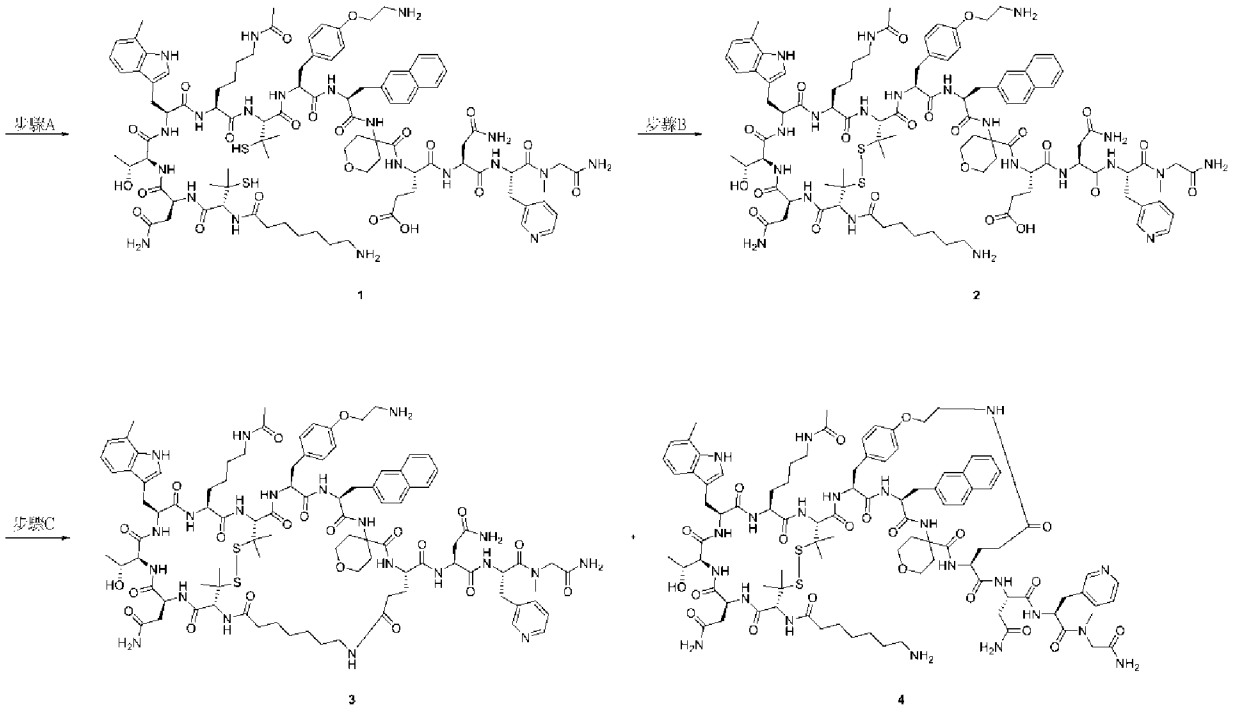
間物化合物**2**。（產率：40%）。LCMS分析C93H129N19O22S2計算為：1929.29；測得為：965.5 $(M+2)^{2+}$。

【0395】 將中間物**2**溶於含5% AcOH之無水DCE (1 mg/mL)中。將Grubbs 2催化劑(0.25 eq) (CAS：246047-72-3)加入，在60℃下在N_2氣氛下攪拌，並且藉由UPLC-MS監測。反應在30分鐘後幾乎完成，在此時將額外0.2 eq的催化劑加入。在2小時後，讓反應混合物冷卻至室溫然後將SilaMet DMT清除劑樹脂加入（裝載量：0.57 mmol/g，相對於催化劑為8 eq）。攪拌整夜。接著，將反應混合物在減壓下濃縮至乾而獲得異構物**3及4**之混合物。將混合物用10 mL的溶液(v/v) (95%TFA, 5%H_2O)處理以移除Boc保護基歷時10分鐘，接著濃縮至乾。將反應粗製物再溶於2 mL的DMSO中然後藉由反相HPLC純化(Phenomenex Luna C18, 30×250 mm, 5 μm, 100Å)。動相A：+ 0.1% TFA，動相B：乙腈(ACN) + 0.1% TFA，梯度開始為20% B，然後在25分鐘期間內以45 mL/min之流率變化至30% B。接著將含有第一洗提異構物之所收集流份凍乾而供給標題化合物之第一異構物。LCMS分析C86H117N19O20S2計算為：1801.12；測得為：1801.6 $(M+1)^{+}$。接著將含有第二洗提異構物之所收集流份凍乾而供給標題**4**之第二異構物。LCMS分析C86H117N19O20S2計算為：1801.12；測得為：901.1 $(M+2)^{2+}$。

實例1G. 7Ahp(2)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-E(2)-N-3Pya-Sar-CONH2



化學式：$C_{95}H_{129}N_{21}O_{21}S_2$
精確質量：1963.91



【0396】　線性肽係使用CEM Liberty Blue自動微波肽合成儀使用標準Fmoc肽合成使用Rink Amide MBHA樹脂（NovaBiochem，0.34 mmol/g，100-200網目）來合成。將Fmoc-受保護胺基酸(5 mL, 0.2 M, 1 mmol)使用DIC (2 mL, 0.5 M, 1 mmol)及Oxyma Pure (1 mL, 1 M, 1 mmol)在90℃下偶合3.5分鐘。雙重偶合係用於Sar、THP、及Thr以及用於在Sar、THP、及Thr之後結合的殘基。Fmoc去保護係使用DMF中之20%哌啶(v/v)在90℃下進行1分鐘。在CEM Razor

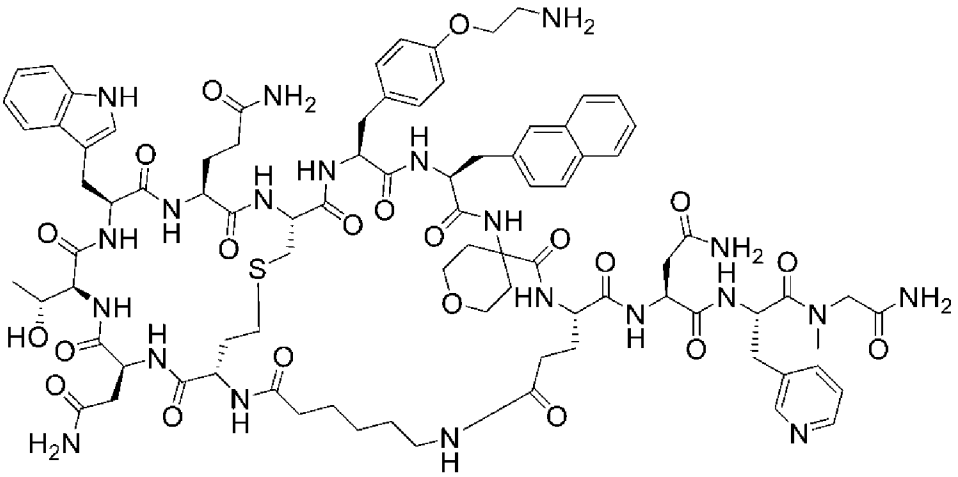
切割系統上藉由用92.5% TFA、2.5%三異丙基矽烷、2.5% 2,2'-(乙二氧基)二乙烷硫醇(DODT)、及2.5%水在42℃下處理30分鐘，將肽去保護及自固體擔體切割下來。將樹脂過濾然後用TFA洗滌。將濾液濃縮然後用冷的甲基三級丁醚(MTBE)沉澱。將混合物離心，然後將丸粒用新鮮的冷MTBE洗滌。重複此兩次。將肽丸粒乾燥，再溶於水中/乙腈+ 0.1% TFA中，然後凍乾整夜而供給所欲中間物**1**（產率：97%）。LCMS分析$C_{95}H_{133}N_{21}O_{22}S_2$計算為：1983.94；測得為：1984.9 $(M+H)^+$、993.0 $(M+2H)^{2+}$。

【0397】 將粗中間物**1**溶於30%乙腈/H_2O (2 mg/mL)中。將甲醇中之碘(0.1 M)逐滴加入並伴隨攪拌，直到黃色持續出現。在攪拌大約2小時後，藉由HPLC判定反應完成。將反應藉由加入水中之1M抗壞血酸淬熄直到溶液變成透明。將溶液濃縮然後凍乾。將所得丸粒溶於DMSO中然後藉由反相在Biotage Selekt (Biotage Sfar Bio C18 D – Duo 300 Å, 20 um, 25g管柱)上使用洗提液(A) 0.1% TFA於水中及(B) 0.1% TFA於乙腈中及20% B至55% B之梯度在10 CV期間內純化。收集含有純產物之流份然後凍乾而供給中間物**2**。（產率：30.3%）LCMS分析$C_{95}H_{131}N_{21}O_{22}S_2$計算為：1983.35；測得為：992.0 $(M+2H)^{2+}$及1983.8 $(M+H)^+$。

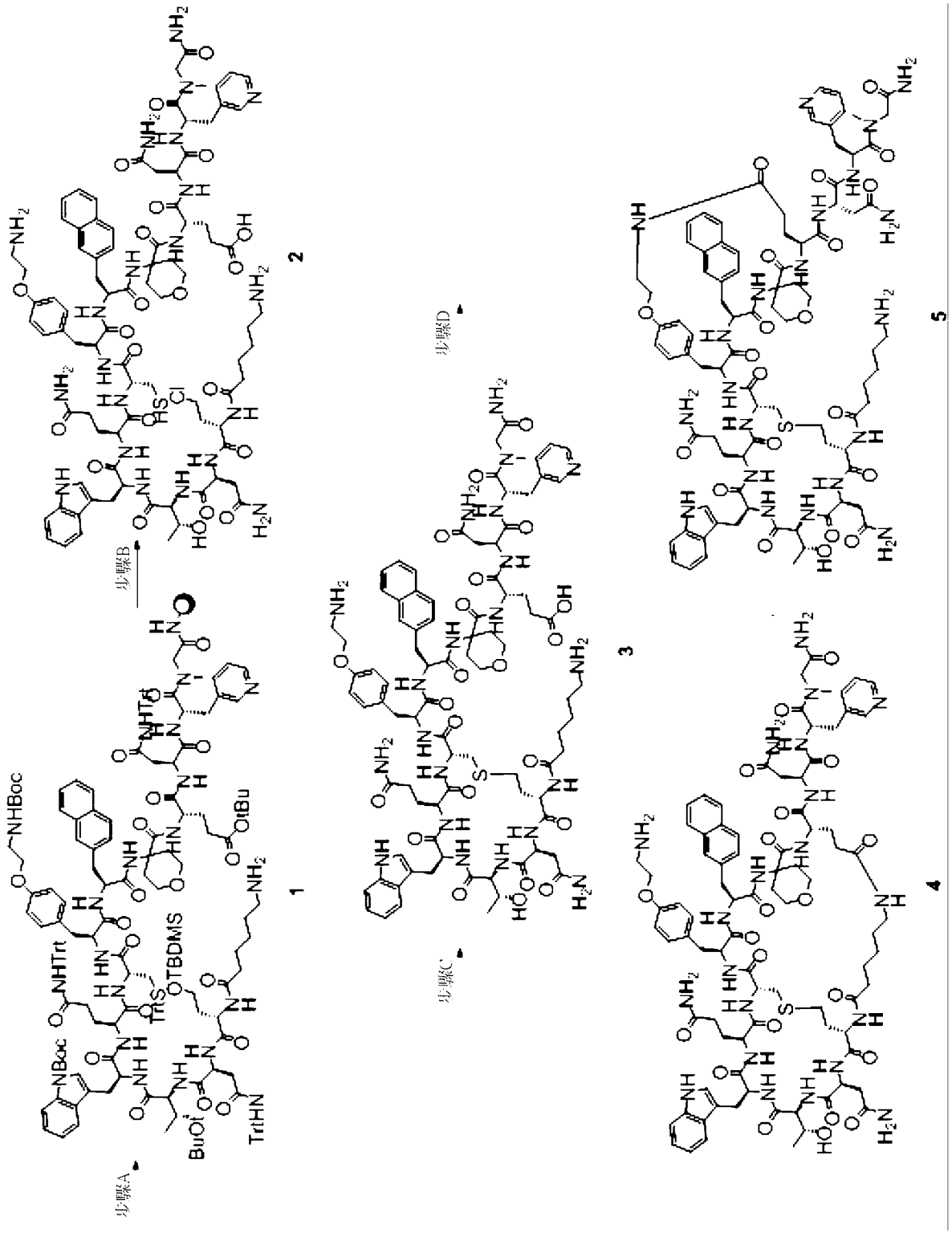
【0398】 將經純化中間物**2**溶於DMF (0.005 M)中。向此溶液中加入PyBOP (2 eq)及DIEA (4 eq)然後將反應在室溫下攪拌。一旦反應完成（如藉由LCMS判定），將反應濃縮然後藉由反相HPLC (Waters XSelect CSH Prep C18, 5 um OBD管柱, 19×150 mm, 25 mL/min)使用洗提液(A) 0.1% TFA於水中及(B) 0.1% TFA於乙腈中及26% B至33% B之梯度在10分鐘期間內純化。收集含有純

產物之流份然後凍乾而供給標題化合物**3**。（產率：13%）LCMS分析 $C_{95}H_{129}N_{21}O_{21}S_2$計算為：1965.3；測得為：1964.8 $(M+H)^+$、1986.8 $(M+Na)^+$、及983.0 $(M+2H)^{2+}$。

實例1H. 6Ahx(2)-Abu(1)-N-T-W-Q-C(1)-AEF-2Nal-THP-E(2)-N-3Pya-Sar-CONH2



化學式：$C_{87}H_{113}N_{21}O_{21}S$
精確質量：1819.81



【0399】 **1**之線性肽合成係使用CEM Liberty Blue自動微波肽合成儀使用標準Fmoc肽合成使用Rink Amide MBHA樹脂（NovaBiochem，0.34 mmol/g，100-200網目）來進行。將Fmoc-受保護胺基酸(5 mL, 0.2 M, 1 mmol)使用DIC (2

mL, 0.5 M, 1 mmol)及Oxyma Pure (1 mL, 1 M, 1 mmol)在90℃下偶合3.5分鐘。雙重偶合係用於Sar、THP、及Thr以及用於在Sar、THP、及Thr之後結合的殘基。Fmoc去保護係使用DMF中之20%哌啶(v/v)在90℃下進行1分鐘。

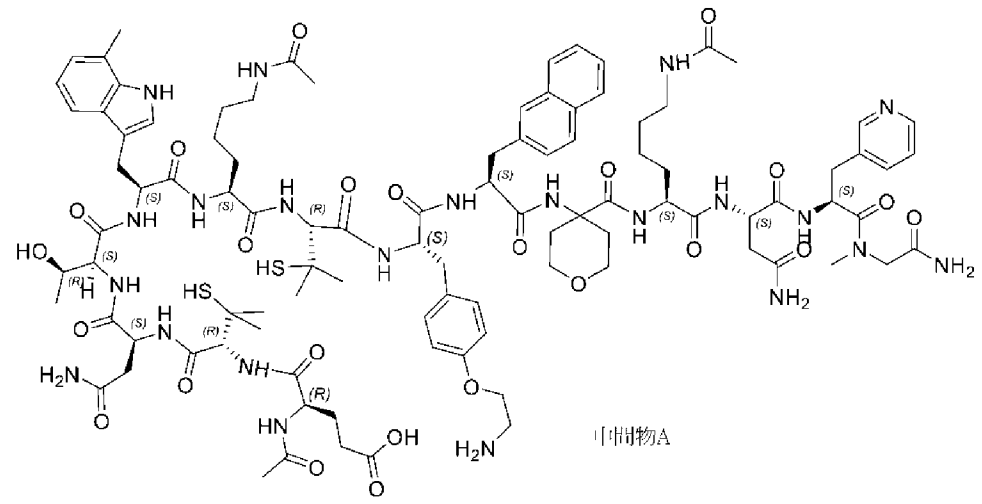
【0400】 將樹脂結合肽中間物**1**用二氯三苯基磷烷(10 eq)、α-蒎烯(15 eq)、及苯基甲基硫醚(15 eq)於無水DCM中之溶液處理15分鐘。將樹脂排液然後用DCM洗滌。將二氯三苯基磷烷(10 eq)、α-蒎烯(15 eq)、及苯基甲基硫醚(15 eq)於無水DCM中之新鮮溶液加入然後將混合物在旋轉搖動器上培養3小時。將樹脂用DMF及DCM洗滌。藉由使用92.5% TFA、2.5%三異丙基矽烷、2.5% 2,2'-(乙二氧基)二乙硫醇(DODT)、及2.5%水在室溫下處理2小時，將肽去保護及自固體擔體切割下來。將樹脂過濾然後用TFA洗滌。將濾液濃縮然後用冷的甲基三級丁醚(MTBE)沉澱。將混合物離心，然後將丸粒用新鮮的冷MTBE洗滌。重複此兩次。將肽丸粒乾燥，再溶於水中/乙腈+ 0.1% TFA中，然後凍乾整夜而供給中間物**2**（產率：76%）。LCMS分析$C_{87}H_{116}ClN_{21}O_{22}S$計算為：1873.80；測得為：938.5 $(M+2H)^{2+}$。

【0401】 將粗製肽溶於DMF (2 mg/mL)中。將NaI (1.5 eq)及EDTA (1.5 eq)加入至肽溶液中而為10 mg/mL溶液，接著加入0.1 M Na_2CO_3 (10 eq)。將反應在室溫下攪拌整夜，用TFA淬熄，濃縮，然後藉由反相在ISCO (Biotage Sfar Bio C18 D – Duo 300 Å, 20 um, 25g管柱)上使用洗提液(A) 0.1% TFA於水中及(B) 0.1% TFA於乙腈中及20% B至55% B之梯度在10 CV期間內純化。收集含有純產物之流份然後凍乾而供給中間物**3**。（產率：21%）LCMS分析$C_{87}H_{115}N_{21}O_{22}S$計算為：1837.82；測得為：1838.8 $(M+H)^+$、1860.7 $(M+Na)^+$、920.0 $(M+2H)^{2+}$。

【0402】 將經純化肽溶於DMF (0.005 M)中。向此溶液中加入PyBOP (2 eq)及DIEA (4 eq)然後將反應在室溫下攪拌。一旦反應完成（如藉由LCMS判定），將反應濃縮然後藉由反相HPLC (Waters XSelect CSH Prep C18, 5 um OBD管柱, 19×150 mm, 25 mL/min)使用洗提液(A) 0.1% TFA於水中及(B) 0.1% TFA於乙腈中及20% B至28% B之梯度在10分鐘期間內純化。收集含有純產物之流份然後凍乾而供給標題化合物。（產率：5%）LCMS分析$C_{87}H_{113}N_{21}O_{21}S$計算為：1819.81；測得為：1820.8 $(M+H)^+$、1842.7 $(M+Na)^+$、911 $(M+2H)^{2+}$。

實例1 I. MeCO-Glu-Pen-N-T-7MeW-K(Ac)-Pen-AEF-2Nal-THP-K(Ac)-N-3Pya-Sar-CONH2

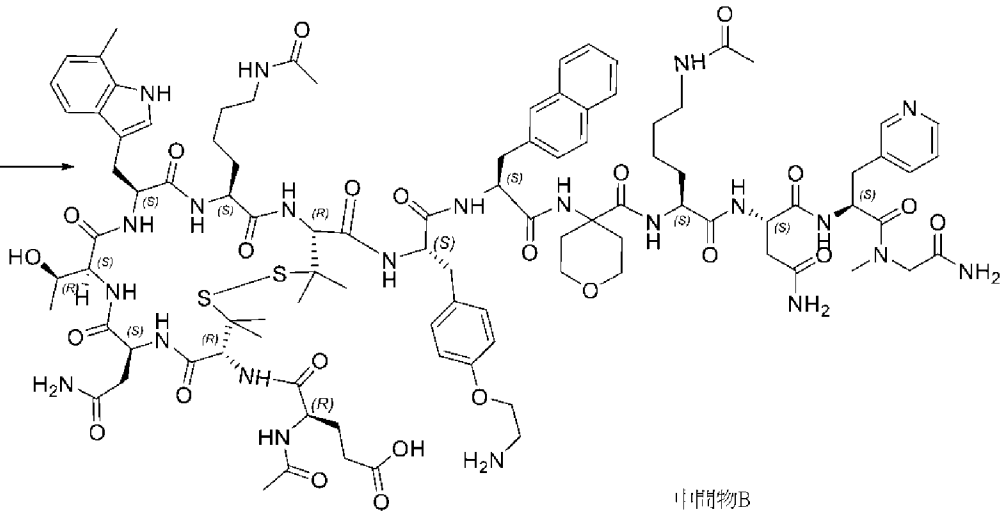
步驟A



中間物A

化學式：$C_{98}H_{136}N_{22}O_{24}S_2$
分子量：2070.42

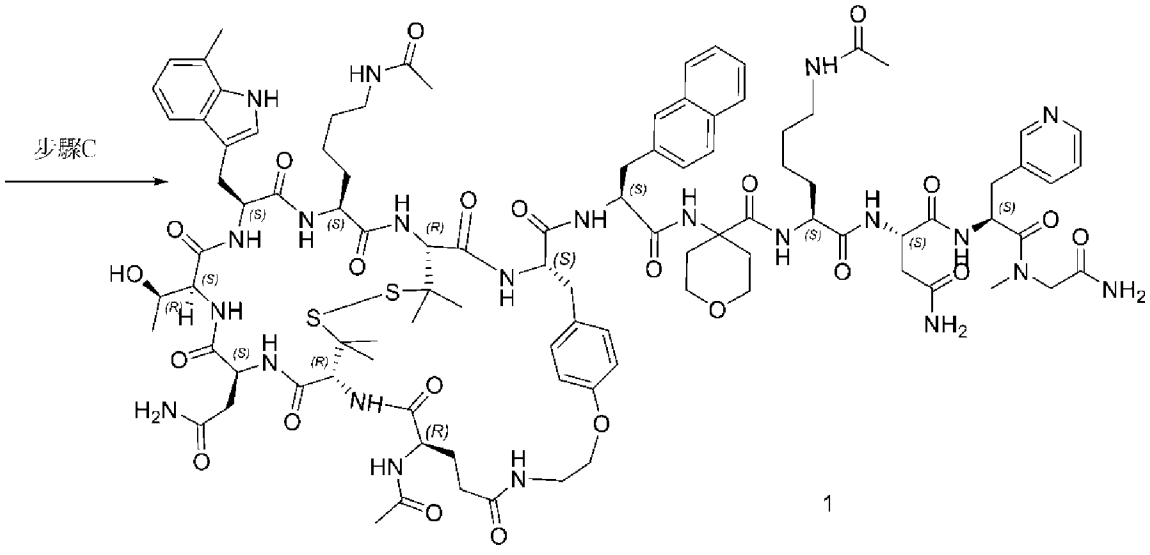
步驟B



中間物B

化學式：$C_{98}H_{134}N_{22}O_{24}S_2$
分子量：2068.40

步驟C



1

化學式：$C_{98}H_{132}N_{22}O_{23}S_2$
分子量：2050.39

【0403】 肽係藉由標準固相肽合成(SPPS)使用Fmoc/t-Bu化學來合成。組裝係在Rink-amide AM樹脂(220 μmol, 100至200網目；裝載量0.35 mmol/g)上在Cem Liberty Blue微波肽合成儀(CEM Inc.)上執行。在肽於固相上組裝期間，側鏈保護基：針對Thr及Glu為三級丁基；針對Pen及Asn為三苯甲基；針對AEF為三級丁氧基-羰基。將所有胺基酸以0.4 M濃度溶於DMF中。醯化反應係在90℃下在MW照射下執行3分鐘並使用相對於樹脂游離胺基5倍過量的活化胺基酸。將胺基酸用等莫耳量的DMF中之0.5M DIC溶液及DMF中之1M Oxyma溶液活化。針對3Pya15及2Nal10執行雙重醯化反應。Fmoc去保護係使用DMF中之20%(V/V)哌啶來執行。游離胺基之加蓋係使用DMF中之10eq的乙酐來手動執行。

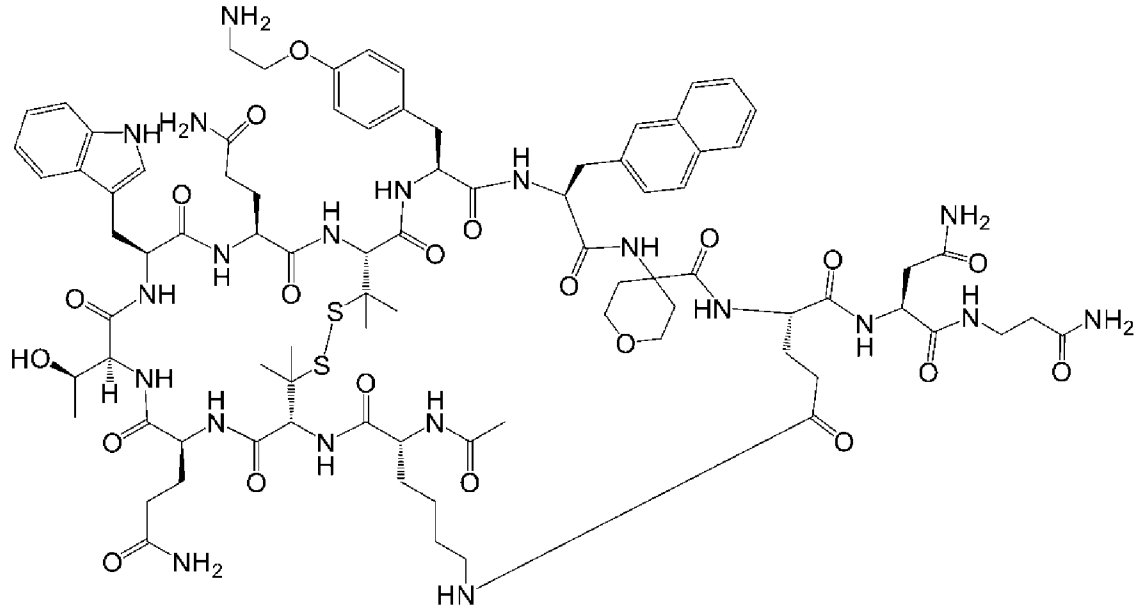
【0404】 在組裝結束時，將樹脂用DMF、MeOH、DCM、Et_2O洗滌。在室溫下使用30 mL的TFA溶液(v/v)（87.5% TFA、5% H2O、2.5% TIPS、5%酚），將肽自固體擔體切割下來大約1.5小時。接著將樹脂過濾然後沉澱於冷的MTBE (135 mL)中。在離心後，將肽丸粒用新鮮的冷二乙醚洗滌以移除有機清除劑。重複程序兩次。將最終丸粒乾燥，再懸浮於H2O及乙腈1:1 + 0.1% TFA中然後攪拌整夜，接著凍乾而供給所欲線性中間物166-1（產率83.4%）。LCMS分析C98H136N22O24S2計算為：2070.42Da；測得為：1036.6 $(M+2)^{2+}$。

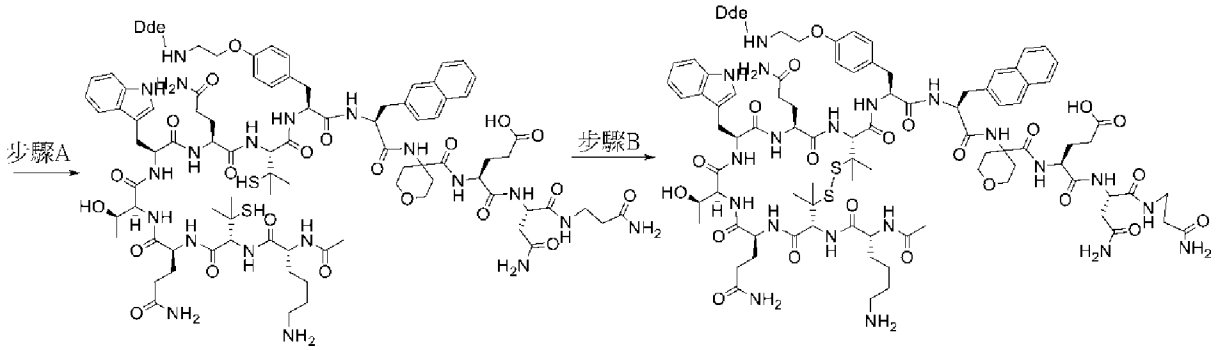
【0405】 將粗製肽溶於CAN/H_2O (5 mg/mL)中。接著將乙酸中之飽和碘在攪拌下逐滴加入，直到黃色持續出現。反應在20分鐘內完成（藉由UPLC-MS監測）。將固體抗壞血酸加入直到溶液變成透明。在凍乾後，將粗中間物166-2

原樣用於下一個步驟中。LCMS分析C98H134N22O24S2計算為：2068.40Da；測得為：1035.4 $(M+2)^{2+}$。

【0406】 將中間物166-2溶於DMF (0.5 mg/mL)中。將HATU (2Eq)及Dipea (4 Eq)加入。讓反應在室溫下攪拌60分鐘（藉由UPLC-MS監測）。將溶劑在真空中蒸發。藉由反相HPLC使用製備型Waters DeltaPak C18 (200×40 mm, 100 Å, 15 µm)純化。動相A：+ 0.1% TFA，動相B：乙腈(ACN) + 0.1% TFA。使用下列之洗提液B梯度：在5min期間內20%B至20%B，在25min期間內至35%B，流率80 mL/min，波長214 nm。將所收集之流份凍乾而供給標題化合物**1（產率**10%）。LCMS分析C98H132N22O23S2計算為：2050.39Da；測得為：1025.84 $(M+2)^{2+}$。

實例1 J. MeCO-k(2)-Pen(3)-Q-T-W-Q-Pen(3)-AEF-2Nal-THP-E(2)-N-bAla-CONH2



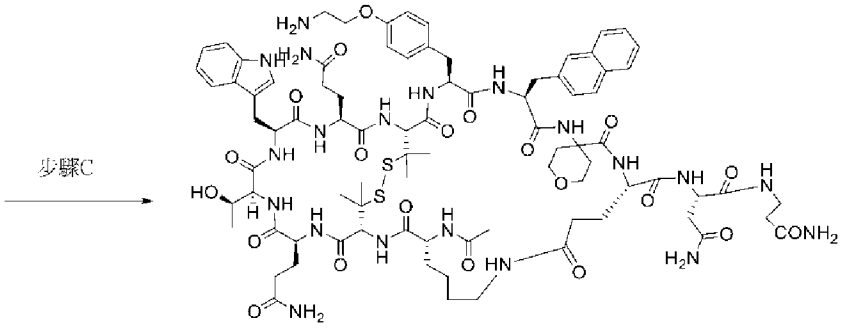


化學式：$C_{95}H_{132}N_{20}O_{24}S_2$
分子量：2002.34

1

化學式：$C_{95}H_{130}N_{20}O_{24}S_2$
分子量：2000.32

2



化學式：$C_{85}H_{116}N_{20}O_{21}S_2$
分子量：1818.10

3

【0407】　步驟A –中間物化合物**1**之合成合成係使用Fmoc受保護胺基酸在固相Rink Amide MBHA（NovaBiochem，0.33 meq/g，100-200網目）上使用

CEM Liberty Blue自動化微波肽合成儀來合成。肽係以0.22 mmol規模合成。第一個殘基(bAla)係使用NMP中之3 eq的胺基酸、3 eq的HOAt、及3 eq的DIC在室溫下手動結合整夜。典型反應條件如下：去保護條件：DMF中之20%哌啶(v/v)（2分鐘在90℃下）；殘基偶合條件：將受保護胺基酸（2.5 mL的0.4 M胺基酸儲備溶液於DMF中）遞送至樹脂中，接著遞送DIC活化劑（2 mL的0.5 M溶液於DMF中）、及Oxyma Pure（1 mL的1 M溶液於DMF中）然後讓其在90℃下反應2分鐘。針對2Nal執行雙重偶合。游離胺基之加蓋係使用DMF中之10eq的乙酐來執行。

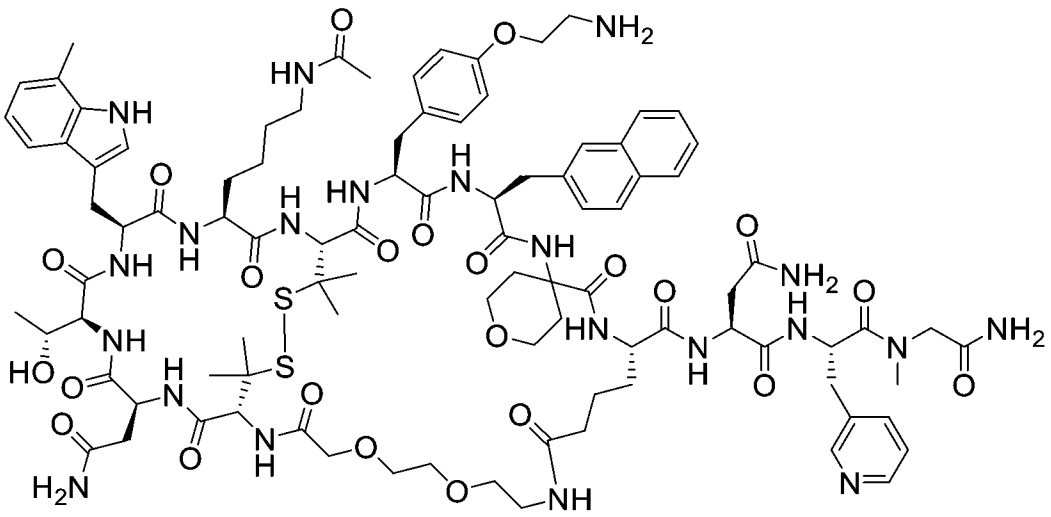
【0408】 在組裝結束時，將肽樹脂用DMF、MeOH、DCM、Et2O洗滌。使用87.58% TFA、5%酚、2.5%三異丙基矽烷、及5%水在室溫下將肽自固體擔體中切割下來1.5小時。將樹脂過濾接著加入至冷的甲基三級丁醚中以將肽沉澱。在離心後，將肽丸粒用新鮮的冷二乙醚洗滌以移除有機清除劑。重複程序兩次。將最終丸粒乾燥，再懸浮於H2O及乙腈1:1 + 0.1% TFA中然後攪拌整夜。接著凍乾而供給所欲之受保護中間物化合物**1**（產率：86%）。LCMS分析C95H132N20O24S2計算為：2002.34；測得為：1001.9 (M+2)2+

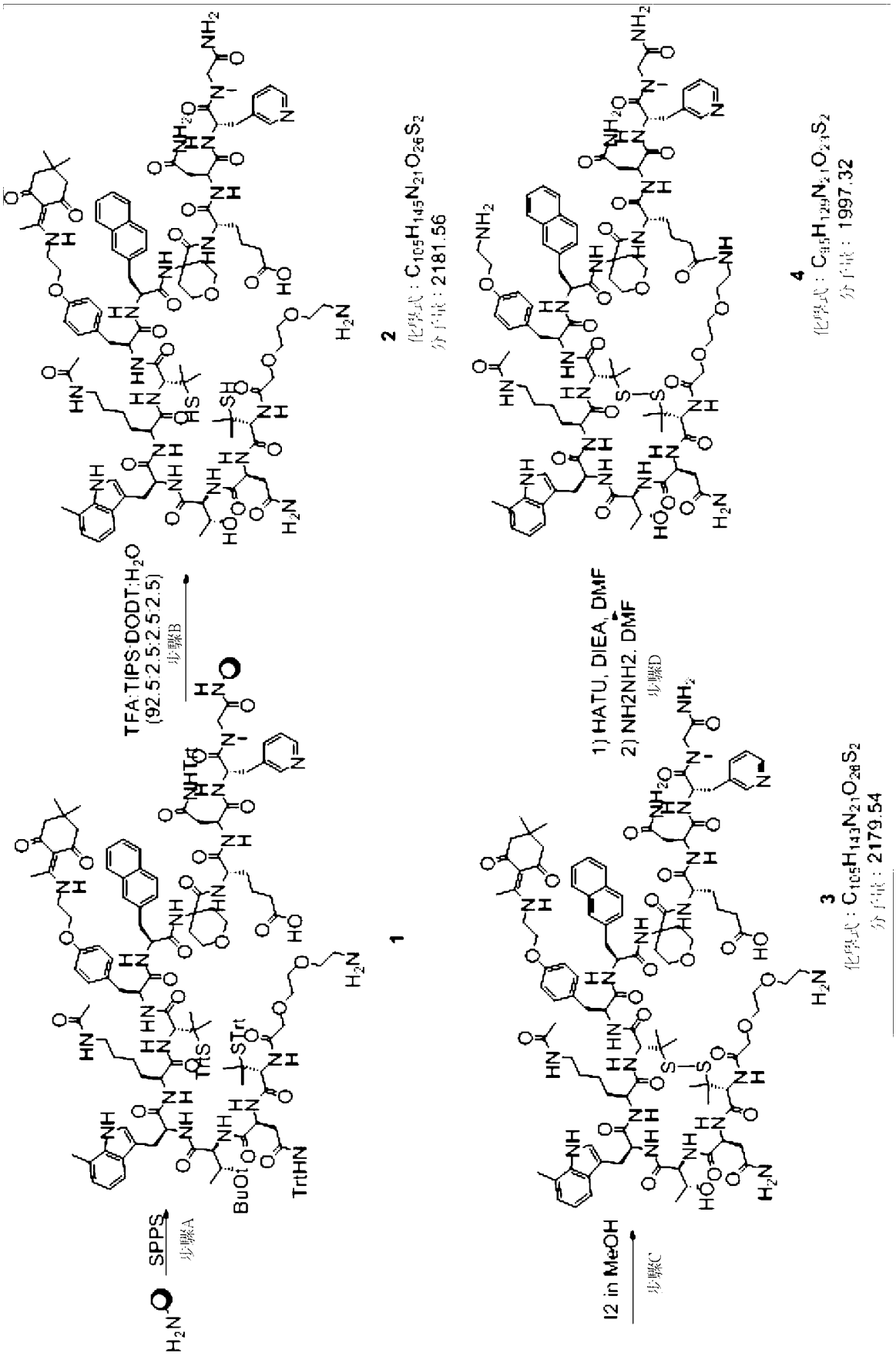
【0409】 步驟B –中間物化合物**2**之合成將來自步驟A之沉澱固體粗製肽溶於水/乙腈1:1 (1 mg/mL)中。接著將乙酸中之飽和碘逐滴加入並伴隨攪拌，直到黃色持續出現。將溶液攪拌15分鐘，並且用UPLC-MS監測反應。當反應完成時，將固體抗壞血酸加入，直到溶液變成透明。接著將溶劑混合物凍乾並將所得材料溶於DMSO中，然後藉由反相HPLC (Deltapak C4, 40×200 mm, 15 µm, 300Å)純化。動相A：+ 0.1% TFA，動相B：乙腈(ACN) + 0.1% TFA，梯度開始

為20% B，然後在25分鐘期間內在80 mL/min之流率變化至35% B。接著將含有純產物之所收集流份凍乾而供給化合物**2**（產率：48%）。LCMS分析C95H130N20O24S2計算為：2000.32；測得為：1001.1(M+2)2+

【0410】　步驟C –中間物化合物**3**之合成將化合物**2**溶於DMF (0.5 mg/mL)中。將DMF (5 mL)中之HATU (1.1 eq)及DIPEA (3 eq)逐滴加入。將所得溶液在室溫下攪拌5分鐘（藉由UPLC-MS監測）。在完成環化後，將肼單水合物(20 eq)加入以移除Dde保護基。去保護在30分鐘後完成（藉由UPLC-MS監測）。將反應混合物用TFA淬熄然後濃縮至乾。將反應粗製物再溶於4 mL的DMSO中然後藉由反相HPLC以兩次運行純化(Deltapak C18, 40×200 mm, 15 µm, 100Å)。動相A：+ 0.1% TFA，動相B：乙腈(ACN) + 0.1% TFA，梯度開始為20% B，然後在25分鐘期間內在80 mL/min之流率變化至35% B。接著將含有純產物之所收集流份凍乾而供給化合物**3**（產率：49%）。LCMS分析C85H116N20O21S2計算為：1818.10；測得為：909.9 (M+2)2+

實例1 K. PEG2(2)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-hE(2)-N-3Pya-Sar-CONH2




SPPS
步驟A
TFA:TIPS:DODT:H2O
(92.5:2.5:2.5:2.5)
步驟B
1
2
化學式：C105H145N21O26S2
分子量：2181.56
1) HATU, DIEA, DMF
2) NH2NH2, DMF
步驟D
I2 in MeOH
步驟C
3
化學式：C105H143N21O26S2
分子量：2179.54
4
化學式：C85H120N21O23S2
分子量：1997.32

【0411】 步驟A –中間物化合物**1**之合成合成係使用標準Fmoc固相肽合成在Rink Amide MBHALL樹脂(NovaBiochem, 0.34 mmol/g, 100至200網目)上執行。樹脂結合肽係CEM Liberty Blue自動微波肽合成儀上以1 mmol規模合成。典型反應條件如下：去保護條件：DMF中之20%哌啶(v/v)（10 mL, 1.5分鐘在90℃下）；殘基偶合條件：將受保護胺基酸（5 mL的0.4 M胺基酸儲備溶液於DMF中）遞送至樹脂中，接著DIC活化劑（2 mL的0.5 M溶液於DMF中）、及Oxyma Pure（1 mL的1 M溶液於DMF中）然後讓其在90℃下反應3.5分鐘。針對Sar、3Pya、THP、及2Nal執行雙重偶合。針對AEF(Dde)執行手動偶合。將Fmoc-AEF(Dde)-OH (1.5 eq)用DMF中HOAt (1.5 eq)及DIC (1.5 eq)活化20分鐘，接著加入至樹脂中然後在室溫下混合16小時。

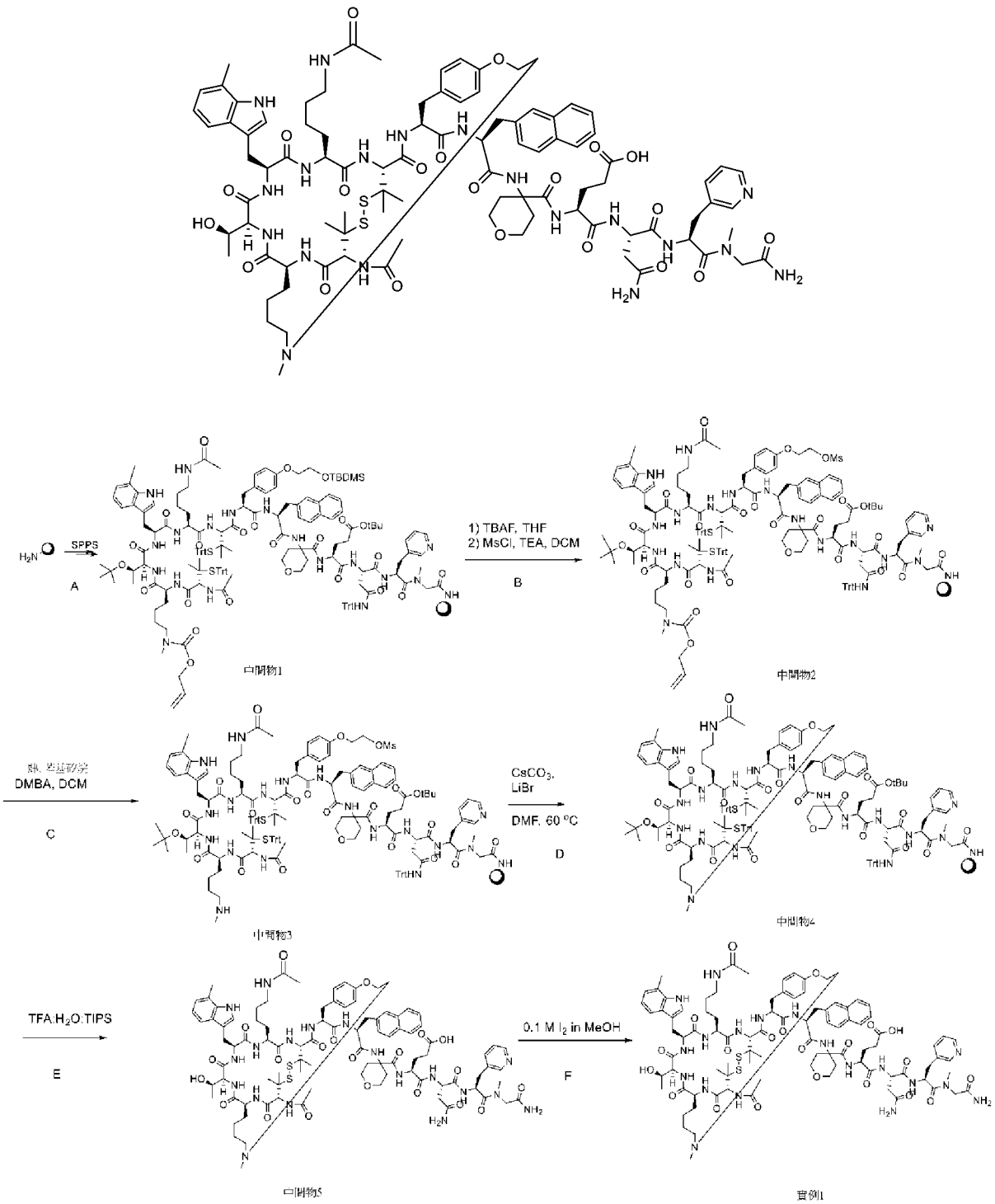
【0412】 步驟B –中間物化合物**2**之合成在完成組裝後，將肽樹脂用DMF、MeOH、DCM洗滌。在CEM Razor切割站上藉由將樹脂用92.5% TFA、2.5%水、2.5%三異丙基矽烷(TIPS)、及2.5% 3,6-二噁-1,8-辛二硫醇(DODT)在42℃下處理30分鐘將肽去保護及自固體擔體切割下來。將樹脂過濾然後用TFA洗滌。將混合物濃縮接著加入至冷的甲基三級丁醚中以將肽沉澱。在離心後，將肽丸粒用新鮮的冷甲基三級丁醚洗滌。再重複此一次。將最終丸粒乾燥、再懸浮於水及乙腈(1:1) + 0.1% TFA中然後凍乾而供給所欲中間物**2**（產率：89.7%）LCMS分析$C_{105}H_{145}N_{21}O_{26}S_2$計算為：2181.56；測得為：1091.3 $(M+2H)^{2+}$及727.8 $(M+3H)^{3+}$。

【0413】 步驟C –中間物化合物3之合成將中間物2溶於水:乙腈(1:1) (1 mg/mL)中。將甲醇中之碘(0.1 M)逐滴加入並伴隨攪拌，直到黃色持續出現。藉

由HPLC-MS監測反應。當反應完成時，將水中之抗壞血酸(1 M)加入，直到溶液變成透明。將反應濃縮然後凍乾。將粗製材料溶於DMSO中然後藉由反相在ISCO (Biotage Sfar Bio C18 D – Duo 300 Å, 20 uM, 50g管柱, 40 mL/min)上使用洗提液(A) 0.1% TFA於水中及(B) 0.1% TFA於乙腈中及20% B至55% B之梯度在10 CV期間內純化。收集含有純產物之流份然後凍乾而供給中間物**3**。（產率：32%）LCMS分析$C_{105}H_{143}N_{21}O_{26}S_2$計算為：2119.55；測得為：1090.4 $(M+2H)^{2+}$及727.1 $(M+3H)^{3+}$。

【0414】　步驟D –化合物**4**之合成將中間物**3** (292.1 mg, 0.121 mmol)溶於DMF (25 mL, 0.005 M)中。向此溶液中加入HATU (69.2 mg,0.182 mmol)及*N*,*N*-二異丙基乙基胺(84.5 uL、0.485 mmol)然後在室溫下攪拌。藉由HPLC-MS監測反應。一旦反應完成，便將肼(38.9 uL, 1.21 mmol)加入然後在室溫下攪拌1小時。將混合物濃縮，溶於DMSO中然後藉由反相HPLC (Waters XSelect CSH Prep C18, 5 um OBD管柱, 19×150 mm, 25 mL/min)使用洗提液(A) 0.1% TFA於水中及(B) 0.1% TFA於乙腈中及22% B至27% B之梯度在10分鐘期間內純化。收集含有純產物之流份然後凍乾而供給化合物**3**。（產率：14%）LCMS分析$C_{95}H_{129}N_{21}O_{23}S_2$計算為：1997.33；測得為：1996.6 $(M+H)^+$及998.9 $(M+2H)^{2+}$。

實例1 L. MeCO-Pen(3)-K(NMe)(5)-T-7MeW-K(Ac)-Pen(3)-AEF(5)-2Nal-THP-E-N-3Pya-Sar-CONH2



【0415】 步驟A –中間物化合物**1**之合成-合成係使用Fmoc受保護胺基酸在固相Rink amide MBHA樹脂（Novabiochem，0.42 mmol/g，100-200網目）上使用Biotage Syro II平行肽合成儀來合成。肽係以0.05 mmol規模合成。典型反應條件如下：去保護條件：Fmoc去保護係以2階段使用DMF (1 mL)中之40%哌

啶在室溫下執行3分鐘，接著使用DMF (1 mL)中之20%哌啶執行9分鐘。殘基偶合條件：將Fmoc-受保護胺基酸（0.5 mL的0.5 M胺基酸儲備溶液於DMF中，0.25 mmol）遞送至樹脂中，接著將HATU（0.52 mL的0.48 M儲備溶液於DMF中，0.25 mmol）、及4-甲基味啉(0.25 mL, 2M, 0.5 mmol)然後讓其在室溫下反應1小時。殘基[Y(OEtOTBDMS)]係使用手動偶合條件來偶合：將Fmoc-受保護胺基酸(0.125 mmol)、HATU (0.125 mmol)、及4-甲基味啉(0.35 mmol)於DMF (8 mL)中之混合物加入至樹脂(0.05 mmol)中，接著在室溫下混合2小時。將肽 Ac_2O/NMM/DMF (1:1:3) (1 mL)加蓋。

【0416】 步驟B –中間物化合物**2**之合成-將中間物**1** (0.15 mmol)於THF中(8 mL)澎潤15分鐘，接著將TBAF (1.5 mL, 1 M於THF中, 1.5 mmol)加入。將反應在室溫下混合1小時。接著將樹脂排液，用DMF (8 mL, 3次)及DCM (8 mL, 3次)洗滌。向DCM (10 mL)中之所得樹脂中加入DCM (5 ml)中之TEA (0.834 mL, 0.728 g/mL, 6 mmol)，接著緩慢加入甲磺醯氯(0.233 mL, 1.48 g/mL, 3 mmol)於DCM (5 mL)中之溶液。將反應在室溫下混合1小時，接著排液，用DMF（3次）及DCM（3次）洗滌。將樹脂用TFA微切割便顯示所欲產物。LCMS分析 $C_{97}H_{133}N_{19}O_{24}S_2$計算為：2013.368；測得為：1007.0 $(M+2)^{2+}$。

【0417】 步驟C –中間物化合物**3**之合成-在N_2下向DCM (5 mL)中之中間物**2** (0.15 mmol)加入DCM (2 mL)中之苯基矽烷(0.286 mL, 0.877 g/mL, 2.25 mmol)及DCM (2 mL)中之1,3-二甲基巴比妥酸(354.9 mg, 2.25 mmol)歷時1至2分鐘。肆(三苯基膦)鈀(0) (87.5 mg, 0.075 mmol)於DCM (2 mL)加入然後將反應在室溫下混合40分鐘。將樹脂排液然後用DCM (8 x)洗滌。將樹脂用TFA微切割便

顯示所欲產物。LCMS分析$C_{93}H_{129}N_{19}O_{22}S_2$計算為：1929.293；測得為：965.0 $(M+2)^{2+}$

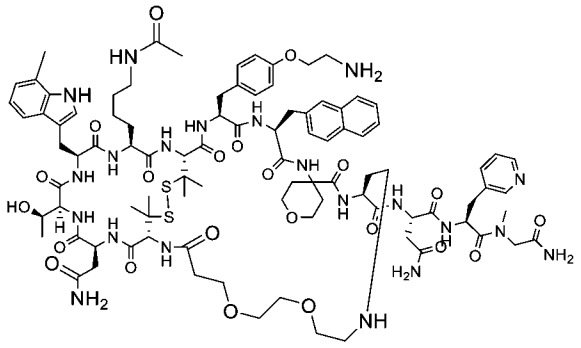
【0418】 步驟D –中間物化合物**4**之合成-將中間物**3** (0.15 mmol)於DMF (10 mL)中澎潤15分鐘，接著加入至Cs_2CO_3之飽和DMF (400 mL)溶液中。接著將溴化鋰(1302.6 mg, 15 mmol)加入然後將反應混合物在60 ºC下加熱1小時。接著將樹脂冷卻至室溫，排液，用水（3次）、DMF（3次）、及DCM（3次）洗滌。將樹脂用TFA微切割便顯示所欲產物。LCMS分析$C_{93}H_{127}N_{19}O_{21}S_2$計算為：1911.278，測得為：956.3 $(M+2)^{2+}$

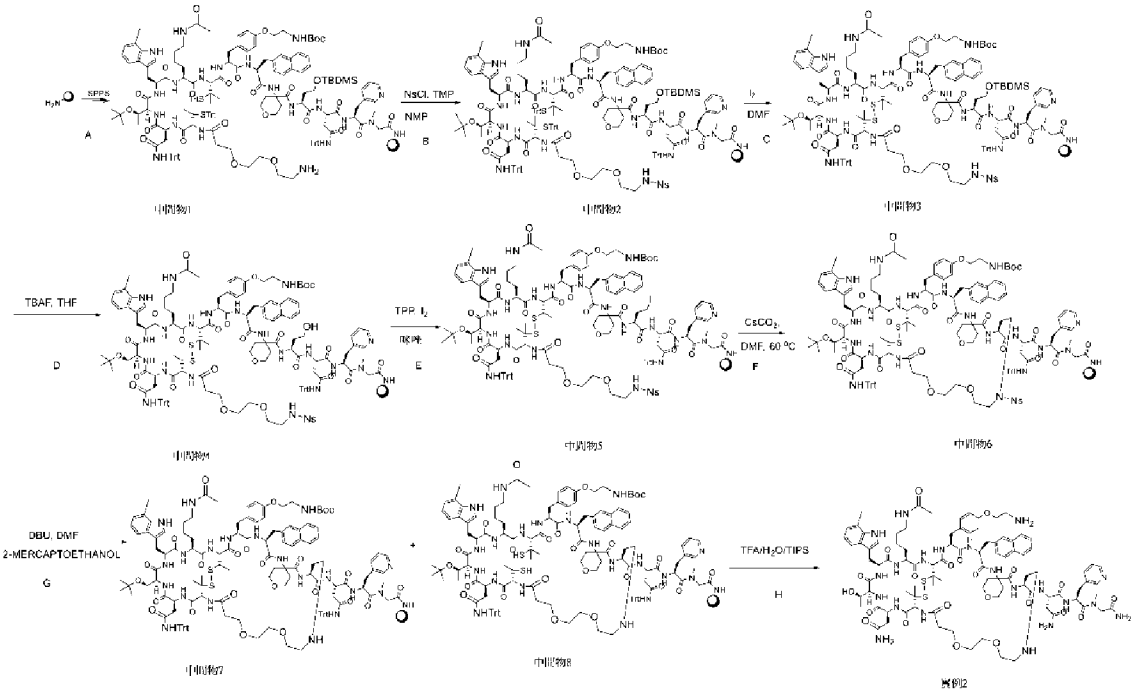
【0419】 步驟E –化合物**5**之合成-在CEM Razor切割站上將中間物化合物**4** (0.15 mmol)用TFA/H_2O/TIPS 92.5/5/2.5之雞尾酒組合試劑溶液在42 ºC下處理30分鐘。接著將混合物濃縮然後加入至冷的甲基三級丁醚中以將肽沉澱。在離心後，將肽丸粒用新鮮的冷甲基三級丁醚洗滌以移除有機清除劑。重複程序兩次。將最終丸粒乾燥，再懸浮於H_2O及乙腈中，接著凍乾而供給呈淺黃色固體之所欲受保護中間物化合物**5**。LCMS分析$C_{93}H_{127}N_{19}O_{21}S_2$計算為：1911.278測得為：956.3 $(M+2)^{2+}$

【0420】 步驟F –化合物**1**之合成-將來自步驟E之中間物粗製肽**5**溶於40% ACN/水(50 mL)中。接著將甲醇中之碘(0.1 M)逐滴加入並伴隨攪拌，直到黃色持續出現。用UPLC-MS監測反應。當反應完成時，將固體抗壞血酸加入，直到溶液變成透明。接著將溶劑混合物凍乾並將所得材料溶於DMSO中，然後藉由製備型HPLC純化。收集含有純產物之流份接著凍乾而供給呈白色粉末之所欲產物。LCMS分析$C_{93}H_{125}N_{19}O_{21}S_2$計算為：1909.26；測得為：955.0 $(M+2)^{2+}$

【0421】

實例1 M. AEEP(5)-Pen(3)-N-T-7MeW-K(Ac)-Pen(3)-AEF-2Nal-THP-hSer(5)-N-3Pya-Sar-CONH2





【0422】 步驟A–中間物**1**之合成-合成係使用Fmoc受保護胺基酸在固相Rink amide MBHA（Novabiochem，0.42 mmol/g，100-200網目）上使用CEM Liberty Blue自動化微波肽合成儀來執行。肽係以0.25 mmol規模合成。典型反應條件如下：去保護條件：Fmoc去保護係使用DMF (10 mL)中之20%哌啶在微波條件（90℃，1分鐘）下執行。殘基偶合條件：將Fmoc-受保護胺基酸（0.5 mL

的0.2 M胺基酸儲備溶液於DMF中，1 mmol）遞送至樹脂中，接著在90℃下遞送N,N'-二異丙基碳二亞胺(2.041 mL, 0.5 M, 1 mmol)及(氫亞胺基)氰基乙酸乙酯(1 mL, 1 M, 1 mmol)歷時3.5分鐘。針對3Pya、THP、及Thr以及在THP及Thr（2Nal及N）之後結合的殘基使用雙重偶合。Fmoc去保護係使用DMF (10 mL)中之20%哌啶在微波條件下在90℃下進行1分鐘。將樹脂用TFA微切割便顯示所欲產物。LCMS分析$C_{94}H_{133}N_{21}O_{23}S_2$計算為：1989.349；測得為：995.5 $(M+2)^{2+}$

【0423】　步驟B –中間物**2**之合成-向樹脂中間物**1** (0.25 mmol)中加入2-硝基苯磺醯氯(221.6 mg, 1 mmol)及2,4,6-三甲基吡啶(330.4 µL, 0.917 g/mL, 2.5 mmol)於NMP (20 mL)中之溶液。將樹脂在室溫下混合50分鐘。將樹脂排液，用DMF（3次）及DCM（3次）洗滌。將樹脂微切割便顯示所欲產物之形成。LCMS分析$C_{100}H_{136}N_{22}O_{27}S_3$計算為：2174.509；測得為：1087.8 $(M+2)^{2+}$

【0424】　步驟C –中間物**3**之合成-將樹脂中間物**2** (0.5 mmol)於DMF (50 mL)中澎潤10分鐘。向此混合物中緩慢加入DMF (10 mL)中之碘(636 mg, 2.5 mmol)，使用另一份2 mL的DMF沖洗小瓶然後加入至反應容器中。將樹脂在室溫下混合0.5小時。將樹脂排液。接著將樹脂用DMF、DMF中之飽和抗壞血酸鈉溶液、DMF、及DCM洗滌。將樹脂乾燥以用於下一個步驟中。將樹脂微切割便顯示所欲產物之形成。LCMS分析$C_{100}H_{134}N_{22}O_{27}S_3$計算為：2172.493；測得為：1086.8 $(M+2)^{2+}$

【0425】　步驟D–中間物**4**之合成-將樹脂中間物**3** (0.5 mmol)於THF (40 mL)中澎潤15分鐘，接著將TBAF（1M於THF中）(2.5 mL, 1 M, 2.5 mmol)加

入。將反應在室溫下混合1小時。將樹脂排液，用DMF（3次）及DCM（3次）洗滌。

【0426】 步驟E–中間物**5**之合成-將樹脂中間物**4** (0.32 mmol)於DMF (30 mL)中澎潤15分鐘，接著加熱至50 ºC。將碘(812 mg, 3.2 mmol)、TPP (1678 mg, 6.4 mmol)、及咪唑(217.85 mg, 3.2 mmol)於DMF (13 mL)中之預混溶液加入。將反應在50 ºC下混合30分鐘，接著排液，用DMF（3次）及DCM（3次）洗滌。將樹脂微切割便顯示所欲產物之形成。LCMS分析$C_{100}H_{133}IN_{22}O_{26}S_3$計算為：2282.39；測得為：1141.4 $(M+2)^{2+}$

【0427】 步驟F –中間物**6**之合成-將樹脂中間物**5** (0.32 mmol)於DMF (10 mL)中澎潤15分鐘，接著加入至DMF (80 mL)中之飽和$CsCO_3$溶液然後將反應混合物在60 ºC下加熱1小時。將樹脂冷卻至室溫，排液，用水（3次）、DMF（3次）、及DCM（3次）洗滌。將樹脂微切割便顯示所欲產物之形成。LCMS分析$C_{100}H_{132}N_{22}O_{26}S_3$計算為：2154.478；測得為：1077.8 $(M+2)^{2+}$

【0428】 步驟G –**中間物7及中間物8**之合成-將中間物**6** (0.3 mmol)於DMF (12 mL)中澎潤15分鐘，接著將1,8-二吖雙環[5.4.0]十一-7-烯(224.1 µL, 1.019 g/mL, 1.5 mmol)於DMF (3 mL)中之溶液加入，接著將2-巰基乙醇(210.4 µL, 1.114 g/mL, 3 mmol)於DMF (3 mL)中之溶液加入。將反應混合物混合20分鐘。將樹脂用DCM及DMF洗滌。將新鮮之溶液B及C加入至樹脂中然後混合另外20分鐘。將樹脂用DMF、MeOH、及DCM洗滌然後用於下一個步驟。將樹脂微切割便顯示所欲產物中間物7與副產物中間物8之混合物之形成。LCMS分析

$C_{94}H_{129}N_{21}O_{22}S_2$及$C_{94}H_{131}N_{21}O_{22}S_2$計算為1969.318、1971.334測得為：985.0及986.0 $(M+2)^{2+}$

【0429】 步驟H –實例**02**之合成-在CEM Razor切割站上將中間物化合物**7**及**8**用TFA/H_2O/TIPS 92.5/5/2.5之雞尾酒組合試劑溶液在42 ℃下處理30分鐘。接著將混合物濃縮然後加入至冷的甲基三級丁醚中以將肽沉澱。在離心後，將肽丸粒用新鮮的冷甲基三級丁醚洗滌以移除有機清除劑。重複程序兩次。接著將粗製物溶於50% ACN/水(0.005 M)中。向此攪拌溶液中逐滴加入MeOH中之碘(0.1 M)直到其保持黃色。將反應攪拌10分鐘接著用水中之1M抗壞血酸淬熄。將反應凍乾然後送交藉由製備型HPLC純化。將含有產物之流份合併然後乾燥而給出呈白色固體之標題化合物。LCMS分析$C_{94}H_{129}N_{21}O_{22}S_2$計算為：1969.318；測得為：985.0 $(M+2)^{2+}$

實例2.對介白素-23與介白素-23受體之結合的抑制

【0430】 執行肽最佳化以識別出在低濃度（例如，IC50 <10 nM）下具有活性的IL-23傳訊之肽抑制劑。如下所述對肽進行測試，以識別出抑制IL-23與人類IL-23R之結合及抑制IL-23/IL-23R功能性活性的肽。

【0431】 如下所述執行檢定以判定肽活性，並且這些檢定之結果係提供於表3A至表3H中。人類ELISA指的是下述的IL23-IL23R競爭性結合檢定，大鼠ELISA指的是下述的大鼠IL-23R競爭性結合ELISA檢定，而pStat3HTRF指的是下述的DB細胞IL-23RpSTAT3細胞檢定。表3A至表3H中所繪示的肽係經由這些肽中的兩個Pen殘基之間所形成的雙硫鍵橋而環化。表3A至表3H中所繪示的肽係經由所標示胺基酸殘基之間的硫醚鍵而環化。針對某些肽，殘基Abu係存在

於所標示之處，而在其他實施例（例如，關於非環化形式者）中，Abu可指為hSer(Cl)或homoSer殘基。

IL23-IL23R競爭性結合ELISA

【0432】 將Immulon® 4HBX盤用50 ng/孔的IL23R_huFC塗佈然後在4℃下培養整夜。將孔用PBST洗滌四次，用含有3%脫脂乳之PBS在室溫下阻斷1小時，然後再次用PBST洗滌四次。將稀釋於檢定緩衝劑（含有1%脫脂乳之PBS）中的測試肽及IL-23之連續稀釋液（最終濃度為2 nM）加入至各孔中，然後在室溫下培養2小時。在將孔洗滌後，將結合IL-23藉由用50 ng/孔的稀釋於檢定緩衝劑中之山羊抗-p40多株抗體(R&D Systems #AF309)在室溫下培養1小時來偵測。再次將孔用PBST洗滌四次。接著將1:5000稀釋於檢定緩衝劑中之二次抗體HRP接合驢抗山羊IgG (Jackson ImmunoResearch Laboratories #705-035-147)加入，然後在室溫下培養30分鐘。最後將盤如上洗滌。使用TMB One Component HRP Membrane Substrate將信號視覺化，用2 M硫酸淬熄，然後以分光光度方式在450 nm讀取。

大鼠IL-23R競爭性結合ELISA

【0433】 將檢定盤用300 ng/孔的大鼠IL-23R_huFC塗佈然後在4℃下培養整夜。將孔洗滌，阻斷，然後再次洗滌。將測試肽及IL-23之連續稀釋液（最終濃度為7 nM）加入至各孔中，然後在室溫下培養2小時。在將孔洗滌後，將結合IL-23用山羊抗-p40多株抗體接著HRP接合驢抗山羊IgG來偵測。使用TMB

One Component HRP Membrane Substrate將信號視覺化，然後用2 M硫酸淬熄。針對各種測試肽，由這些數據所判定之IC50值係示於表3A至表3H中。

【0434】

DB細胞IL23R pSTAT3細胞檢定

【0435】 IL-23在支持及維持體內Th17分化上扮演主要角色。據認為此程序主要透過信號轉導物及轉錄活化物3 (Signal Transducer and Activator of Transcription 3, STAT3)來介導，而STAT3之磷酸化（產出pSTAT3）導致了RORC及促發炎性IL-17之向上調控。此細胞檢定檢驗了當用IL-23於測試化合物存在下進行刺激時，pSTAT3於IL-23R表現DB細胞中之水準。將培養於RPMI-1640培養基(ATCC #30-2001)中之DB細胞(ATCC #CRL-2289)以5 X 10E5細胞/孔接種於96孔組織培養盤中，該培養基補充有10% FBS及1%麩醯胺酸。將測試肽及IL-23之連續稀釋液（最終濃度為0.5 nM）加入至各孔中，然後在37℃下於5% CO_2加濕培養器中培養30分鐘。細胞溶胞產物中之phospho-STAT3水準變化係使用Cisbio HTRF pSTAT3 Cellular Assay Kit（細胞檢定套組），根據製造商之Two Plate Assay（兩盤檢定）規程來偵測。由這些數據所判定之IC50值係示於表3A至表3H中。若未顯示，則是數據尚未判定。

實例3.基於NK細胞之檢定

【0436】 將藉由去除性選汰而純化自健康捐贈人之人類周邊血液(Miltenyi Biotech, Cat # 130-092-657)的自然殺手(NK)細胞在完全培養基（RPMI 1640，含有10% FBS、L-麩醯胺酸、及青黴素-鏈黴素）中於25 ng/mL之IL-2 (RnD, Cat # 202-IL-010/CF)存在下培養。在7天後，將細胞離心，然後以1E6細

胞/mL再懸浮於完全培養基中。將在預定EC_{50}至EC_{75}下之重組IL-23及在10 ng/mL下之IL-18 (RnD, Cat # B003-5)與不同濃度的肽混合，然後加入至以每孔1E5細胞接種之NK細胞中。在20至24小時後，使用Quantikine ELISA (RnD, Cat # DIF50)定量上清液中之IFNγ。顯示由這些數據所判定之IC_{50}值。若未顯示，則是數據尚未判定。

實例4.IL-23R受體檢定

【0437】 將化合物連續稀釋於100% (v/v) DMSO中然後使用Echo聲波施配器(Labcyte)施覆至1536孔未處理黑色檢定盤(Corning # 9146)中。將3 μL的HEK293細胞（含有IL-23R、IL-12Rβ1、及由STAT誘導性啟動子(Promega)所驅動之螢火蟲螢光素酶報導子基因）加入至盤中（4000細胞/孔），接著加入3 μL的20 ng/mL IL-23（等同於EC_{90}濃度）。在5小時後，在37℃、5% CO_2、95%相對濕度下，將細胞置於20℃下然後用BioGlo試劑(Promega)根據製造商之指示處理。發光係在Pherastar FSX (BMG LabTech)上測量。將數據對IL-23處理（0%抑制）及30 μM的對照抑制劑（100%抑制）進行標準化，並使用4參數Hill方程式判定IC_{50}值。數據係示於下表中。假使曾進行多次測量，則重複次數會伴隨平均值顯示，標示在IC_{50}值後面的括號中。

【0438】

表3

化合物編號	IC_{50} (1×10^{-6} M (μM))		化合物編號	IC_{50} (μM)
201			210	0.0022
202	7.15		211	0.0015

化合物編號	IC_{50} (1×10^{-6} M (μM))		化合物編號	IC_{50} (μM)
203	0.0088		212	
204	0.015		213	.0096
205	0.0076		214	0.12
206	0.2		215	.019
207	0.0029		216	0.25
208	0.003		217	.031
209	.0027			

【0439】

表4

化合物編號	**IC_{50} (μM)**
201	0.0034
209	0.0037
213	0.009
4	0.33
25	0.83
137	0.43
139	>16.61
218	>16.61
219	>16.61
220	>16.61
221	~9.41
222	>16.61
223	~7.27
224	8.32
225	>16.61
226	2.66
227	3.52
228	>16.61
229	0.29
230	2.32
231	0.17
232	>16.61
233	>16.61
234	0.25
235	>16.61
236	>16.61
237	0.29
238	>16.61
239	>16.61
240	7.72
241	>16.61
242	>16.61
243	0.0021
244	0.0026
245	1.35
246	0.0054
247	3.56
248	>16.61
249	>16.61
250	0.0032
251	0.034
252	0.0028
253	0.27
254	0.29
255	0.006
256	
257	7.15
258	0.0088
259	0.015
260	0.0076
261	0.2
262	0.0029
263	0.003
264	0.0027
265	0.0022
266	0.0015
267	
268	0.0096
269	0.12
270	0.19
271	0.25
272	0.031
273	0.3
274	0.07
275	0.069
276	0.031
277	0.0029
278	0.0042
279	0.0024
280	0.0039
281	0.0038
282	0.0047
283	0.0049
284	0.0067
285	0.0049
286	0.0071
287	0.02
288	0.0066
289	0.0059
290	0.0046
291	0.009
292	0.0029
293	
294	0.0041
295	0.0044
296	0.0037
297	0.0028
298	0.001
299	0.0045
300	0.0045
301	0.0018
302	0.0028
303	0.0031
304	0.011

305	0.0018
306	0.0095
307	0.0018
308	
309	
310	
311	
312	0.036
313	0.016

314	0.021
315	0.029
316	0.039
317	0.017
318	0.0025
319	0.0028
320	0.0021
321	5.23
322	0.0013

323	0.0018
324	0.35
325	0.0016
326	0.0038
327	0.077
328	0.14

PBMC pSTAT3檢定

【0440】 將來自健康捐贈人之冷凍保存周邊血液單核細胞(PBMC)解凍，然後在ImmunoCult-XF T細胞擴增培養基(XF-TCEM)中洗滌兩次，該培養基補充有CTL抗凝聚洗劑。計數細胞，以每mL XF-TCEM（補充有青黴素/鏈黴素及100 ng/mL IL-1β (BioLegend, 579404)）2×105細胞再懸浮，然後在塗佈有抗-CD3 (eBioscience, 16-0037-85 or BD Pharmingen, 555329)之組織培養瓶中在37℃下在5% CO2中培養。在培養第4天，收集PBMC，在補充有0.1% BSA (RPMI-BSA)之RPMI-1640中洗滌兩次，然後在直立組織培養瓶中之RPMI-BSA中在37℃下在5% CO2中培養4小時。在此「飢餓處理(starvation)」後，將30 μL RPMI-BSA中之總共6×10^4細胞轉移至384孔盤之各孔中，該盤用肽或DMSO預點染。將細胞培養30分鐘，之後以5 ng/mL之最終濃度加入IL-23。將細胞用細胞介素在37 ℃下在5% CO2中刺激30分鐘，轉移至冰上歷時10分鐘，然後將細胞溶解。將細胞溶胞產物儲存於-80℃下，直到使用phospho-STAT組合試劑套組(Meso Scale Discovery, K15202D)測量磷酸化STAT3。針對來自實例之數者，使用PBMC所產生之結果係提供於下**表5**中，連同來自採用上述HEK293細胞之IL23R報導子檢定的數據。結果係針對單次檢定或作為多次重複檢定（如由IC50值後面的括號中所標示）之平均值而記述。

【0441】

表5.

Compd	PBMC pSTAT3 IC50 (nM)	SEQ ID NO:
221	1100	166

226	96	171
288	0.004	233
202	0.0155	2
250	0.0277	195
289	0.0056	234
265	0.0020	210
327	0.40	272
320	0.0036	265
319	0.0079	264

【0442】 雖然前述發明已藉由說明和實例之方式某種程度詳細地描述以達清晰及理解之目的，所屬技術領域中具有通常知識者將認知到，可實施某些改變及修改而不偏離隨附申請專利範圍之範疇。本發明之完整範疇應參照申請專利範圍（連同其等效者之完整範疇）及說明書（連同此類變化）來決定。此外，本文中所提供之各參考文獻係以引用方式全文併入，如同各參考文獻係以引用方式個別併入。假使本申請案與本文中所提供之參考文獻之間存在衝突，則以本申請案為準。

【符號說明】

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【發明申請專利範圍】

【請求項1】一種式(I')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X4-X5-T-X7-X8-X9-AEF-2Nal-X12-X13-N-X15-meG-R2 (I')

其中：

R1係7Ahp、6Ahx、5Ava、Peg2、AEEP、或AEEP(Ns)；

X4係Pen、Abu、aMeC、hC、或C；

X5係N或K(PEG2PEG2gEC18OH)；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係KAc、Q、K(NMeAc)、K(PEG2PEG2gEC18OH)、dKAc、dQ、dK(NMeAc)、或dK(PEG2PEG2gEC18OH)；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP或aMeK；

X13係E、dE、hE、D、dD、或hSer；

X15係不存在或3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵，及
- R1 與 X13 之間的第二醯胺鍵或硫醚鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項2】一種式(II')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1- X3-X4-X5-T-7MeW-K(Ac)-X9-AEF-X11-THP-X13-N-X15-X16-R2　(II')

其中：

R1係Gaba、pFS、bAla、或HOC16gEPEG2PEG2orn；

X3係dR、G、k(PEG2PEG2gEC18OH)、R、dG、或dK(PEG2PEG2gEC18OH)；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、或Q；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、dD、或Dap(pF(6))；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bA`la、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；

X16係不存在、meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、B、或dD；及

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4與X9之間的第一雙硫鍵或硫醚鍵，及
- R1與X13之間的第二鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項3】一種式(III')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-X12-X13-N-3Pya-meG-R2　(III')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、5Cpa、或cPEG3aCO；

X3係R5H、R6H、R7H、S5H、S6H、S7H、K、dK、Orn、d-Orn、Dap、Dab(COCH2)、dHe、或hK；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、Q或N(N(Me)2)、dN、dQ、或dN(N(Me)2)；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、

7PyrW、A、BT、或D7MeW；X8係K(Ac)、Q、K(NMeAc)、或dK(Ac)、dQ、或dK(NMeAc)；

X8係KAc、Q、K(NMeAc)、dK、dQ、dKAc、或dK(NMeAc)；

X9係Pen、Abu、aMeC、hC、或C；

X10係AEF或TMAPF；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP或aMeK；

X13係R5H、R6H、R7H、S5H、S6H、S7H、C、E、hE、KNMe、dC、dE、dhE、或dKNMe；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- X3 與 X13 之間的第二醯胺、硫醚、或脂族鍵。

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項4】一種式(IV')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X3-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-X16- R2　(IV')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、7Ahp、6Ahx、或5Ava；

X3係不存在、dR、R、d-Orn、或Orn；

X4係Pen、Abu、aMeC、hC、或C；

X5係Q、dQ、dN、或N；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；X8係Q、KAc、dQ、或dKAc；

X8係KAc、Q、dKAc、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、aMeE、Aad、hE、K、dE、dAad、dhE、或dK；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、

5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；

X16係不存在、meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、B、或dD；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；
- AEF 與 X13 之間的第二醯胺鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項5】一種式V'之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X4-N-T-X7-X8-X9-F4CONH2-X11-THP-X13-N-3Pya-meG-R2 (V')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X4係Pen、Abu、aMeC、hC、或C；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、

7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係K或dK；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、或dD；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由下列而環化：

- 形成 X4 與 X9 之間的第一雙硫鍵或硫醚鍵
- X8 與 X13 之間的第二醯胺鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項6】一種式(VI')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X3-A-X5-T-X7-X8-A-AEF-X11-THP-X13-N-X15-R2 (VI')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係E、dE、D、或dD；

X5係E、dE、D、或dD；

X7係W或7MeW；

X8係KAc或dK(Ac)；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係KAc或dK(Ac)；

X15係不存在3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、L、或不存在；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X5 與 X10 之間的第一醯胺鍵；及
- X3 與 X15 之間的第二醯胺鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項7】一種式(VII')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X3-X4-N-T-X7-K(Ac)-X9-X10-X11-THP-X13-N-3Pya-X16-R2 (VII')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係D、dK、E、dDap、dD、K、dE、或Dap；

X4係Pen、Abu、aMeC、hC、或C；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X9係Pen、Abu、aMeC、hC、或C；

X10係AEF、F4CONH2、或F4Ome；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係KAc或dKAc；

X16係不存在、meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、B、或dD；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- X3 與 X16 之間的第二醯胺鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項8】一種式(VIII')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X4-X5-X6-X7-X8-X9-X10-X11-X12-X13-X14-3Pya-meG-R2　(VIII')

其中：

R1係CF3CO、5cpaCO、cPeg3aCO、C_1至C_4烷基C(O)-、或經氰基、Cl、F所取代之C_1至C_4烷基C(O)-、或MeCo；

X4係Pen、Abu、aMeC、hC、或C；

X5係E、Dap、或K(NMe)、dE、D、dD、或dK(NMe)；

X6係T、L、dT、dL、I、或dI；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、

7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係KAc、KPeg12、KAcMor、Q(N(Me)2)、K(Me)3、hK(Me)3；K(NMeAc)、K(mPEG12)、A、或Q、dKAc、dKPeg12、dKacMor、dQ(N(Me)2)、KAc；kPeg12、KPeg12、KacMor、Q(N(Me)2)、K(Me)3、hK(Me)3、K(NMeAc)；K(mPEG12)、dA、dQ、dhK(Me)3、dK(NMeAc)、dK(mPEG12)、dA、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X10係AEF或AEF(NMe)；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP、aMeLeu、或A；

X13係KAc、A、L、K(NMeAc)、Q(N(Me)2))、K(Me)3、E、dKAc、dA；dL、dK(NMeAc)、dQ(N(Me)2))、dK(Me)3、或dE；

X14係L、N、或S；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- X5 與 X10 之間的第二醯胺或脂族(RCM)鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項9】一種式(IX')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-THP-X13-X14-3Pya-meG-R2 (IX')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、或HOC18gEPEG2PEG2CO；

X3係R、dR、K、dK、dK(Me)3、K(Me)3、dK(PEG2PEG2gEC18OH)、或K(PEG2PEG2gEC18OH)；

X4係Pen、Abu、aMeC、hC、或C；

X5係E、或dE；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、

7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係KAc或dK(Ac)；

X9係Pen、Abu、aMeC、hC、或C；

X10係AEF或AEF(NMe)；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係KAc、E、dK(Ac)、或dE；

X14係L、N、或S；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- X5 與 X10 之間的第二醯胺或脂族(RCM)鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項10】一種式(X')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

X5-T-X7-X8-A-AEF-X11-THP-X13-3Pya (X')

其中：

X5係E、dE、D、或dD；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係KAc或dK(Ac)；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；且

X13係不存在、KAc、或dK(Ac)；且

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X5 與 AEF 之間的第一雙硫鍵或硫醚鍵；及
- X5 之胺基端與 3Pya 之羧基端之間的第二環化。

【請求項11】一種式(XI')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-R2　　(XI')

其中：

R1係7Ahp、6Ahx、5Ava AEEP、或dK(PEG2PEG2gEC18OH)；；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、Q、dN、或dQ，

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係KAc、Q、dKAc、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、或dD；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、

3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- R1 與 X13 之間的第二醯胺或脂族(RCM)鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項12】一種式(XII')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X4-N-T-X7-X8-X9-AEF-2Nal-X12-X13-N-3Pya-X16-R2 (XII')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X4係Pen、Abu、aMeC、hC、或C；

X6係3Hyp、T、3OHPro、或dT；

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、

7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；

X8係、R5H、R6H、R7H、S5H、S6H、或S7H；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係、R5H、R6H、R7H、S5H、S6H、或S7H；

X16係不存在、meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、B、或dD；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- X3 與 X10、X13、或 X16 中之一者之間的第二醯胺或脂族(RCM)鍵。

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項13】一種式(XIII')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X4-X5-T-X7-X8-X9-AEF-2Nal-THP-X13-N-X15-X16-X17-R2 (XIII')

其中：

R1係7Ahp、6Ahx、5Ava、AEEP、或dK(PEG2PEG2gEC18OH)；

X4係Pen、Abu、aMeC、hC、或C；，

X5係N、Q、dN、或dQ，

X7係W、7MeW、3Pya、7(2ClPh)W、7(3(1NMepip)pyraz)W、7(3(6AzaInd1Me))W、7(3CF3TAZP)W、7(3NAcPh)W、7(3NPyrazPh)W、7(3NpyrlonePh)W、7(3UrPh)W、7(4(CpCNPh))W、7(4CF3Ph)W、7(4NAcPh)W、7(4OCF3Ph)W、7(4OMePh)W、7(4Paz)W、7(5(2(4OMePh)Pyr))W、7(5(Ina7Pyr))W、7(6(1)7dMeNDAZ))W、7(6(2MeNDAZ))W、7(7(124TAZP))W、7(7Imzpy)W、7BrW、7EtW、7PhW、7PyrW、A、BT、或D7MeW；X8係KAc、Q、dKAc、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dE、D、或dD；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、

3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；

X16係不存在、meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、D、dD、或NMeK(PEG2PEG2gEC18OH)；

X17係不存在、K(PEG2PEG2gEC18OH)、或dK(PEG2PEG2gEC18OH)，且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- R1 與 X13 之間的第二醯胺鍵；

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項14】一種式(XIV')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

其中：

R1-X3-X4-X5-X6-X7-X8-X9-AEF-X11-X12-X13-N-X15-X16-X17-R2-R3 (XIV')

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-;

X3係DK或不存在；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、Q、Dap、dN、或dQ，

X6係N、T、或K；

X7係W、7meW、dW、或d7MeW；

X8係KAc、Q、dKAc、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X12係THP、aMeL、或aMedL；

X13係E、KAc、dE、D、dD、或dKAc；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；

X16係不存在、meG、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、B、或dD；

R2係-NH_2或–NH-R_3；且

R3係PEG4、PEG4DA、或C6-C20飽和或不飽和二羧酸（例如，1,10-癸二酸、1,12-十二烷二酸、1,14-十四烷二酸、或1,16-十六烷二酸）。

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- AEF 與 R3 之間的第二醯胺鍵。

【請求項15】一種介白素-23受體之雙環肽抑制劑，其包含式(XV')之胺基酸序列

R1-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-R2　　(XV')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-；

X4係Pen、Abu、aMeC、hC、或C；

X5係E、dE、D、或dD；

X7係W、7meW、dW、或d7MeW；

X8係KAc、Q、dKAc、或dQ；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、KAc、dE、D、dD、或dKAc；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、

3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- AEF 與 X5 之間的第二醯胺鍵；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項16】一種式(XVI')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-X15-R2　　(式XVI')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-；

X4係Pen、Abu、aMeC、hC、或C；

X5係N、L、dN、或dL；

X7係W、7meW、dW、或d7MeW；

X8係KAc、或dKAc；

X9係Pen、Abu、aMeC、hC、或C；

X10係F4CONH_2、4AmF、或dF4CONH_2；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、dK、dDap、K、Dap、或dE；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- X13 與 X15、或 X13 與 X16 之間的第二醯胺鍵。

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項17】一種式(XVII')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-THP-X13-X14-X15-X16-R2 (XVII')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-；

X3係Orn、E、dOrn、或dE；

X4係Pen、Abu、aMeC、hC、或C；

X5係N或dN；

X7係W、7meW、dW、或d7MeW；

X8係KAc、或dKAc；

X9係Pen、Abu、aMeC、hC、或C；

X10係F4CONH2或AEF；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係E、KAc、dKAc、或dE；，

X14係不存在或N；

X15係不存在、3Pya、3MeH、H、F、hF、Y、dY、Y(CHF2)、PAF、oAMPhe、F(CF3)、dPaf、D3Pya、ACIPA(SR)、6OH3Pya、5PyrimidAla、5MePyridinAla、5MeH、5AmPyridinAla、4TriazolAla、4PyridinAla、4Pya、3QuinolAla、3OHPhe、3AmPyrazolAla、2AmTyr、1MeH、THP、bAla、NMedY、K、dK、NMeY、NmedY、N、dH、dN、dL、Aib、或L；

X16係不存在、4(R)OHPro、4(S)胺基Pro、4diFPro、5(R)diMePro、aMeP、N(3Am苄基)Gly、N(環己基)Gly、N(異丁基)Gly、P、dP、K、dK、E、dE、R、dR、D、dD、dDap、meG、Dap、或dMeG；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4與X9之間的第一雙硫鍵或硫醚鍵；及
- X3與X10、X13、或X16中之一者之間的第二醯胺鍵。

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項18】一種式(XVIII')之介白素-23受體之三環肽抑制劑，其包含胺基酸序列：

R1-X3-X4-X5-T-X7-X8-X9-AEF-X11-THP-X13-N-3Pya-meG-X17-R2　(XVIII')

其中：

R1係C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-，

X3係K、dK、E、或dE；

X4係Pen、Abu、aMeC、hC、或C；

X5係E、dE、D、或dD；

X7係W或7MeW；

X8係KAc或dK(Ac)；

X9係Pen、Abu、aMeC、hC、或C；

X11係2-Nal、Phe(2-Me)、Phe(3-Me)、Phe(4-Me)、Phe(3,4-二甲氧基)、2Quin、3Quin、1-Nal、未經取代Trp、或經氰基、鹵基、烷基、鹵基烷基、羥基、或烷氧基所取代之Trp；

X13係KAc或dK(Ac)；

X17係E、dE、K、dK、D、或dD；且

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；

其中：

該介白素-23受體之三環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵及
- X3 與 X17 之間的第二鍵，及
- X5 與 AEF 之間的第三鍵；

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項19】一種式(XIX')之介白素-23受體之雙環肽抑制劑其包含胺基酸序列：

R1-X3-X4-X5-T-X7-X8-X9-X10-X11-X12-X13-X14-X15-X16-X17-R2　(XIX')

其中：

R1係7Ahp、6Ahx、5Ava、Peg2、PEGNMe、AEEP、AEEP(Ns)、Gaba、pFS、bAla、C_1至C_4烷基C(O)-、或經Cl、F、或氰基所取代之C_1至C_4烷基C(O)-、5cpaCO、或cPEG3aCO；

X3係不存在、dR、R、G、R5H、R6H、R7H、S5H、S6H、S7H,、K、dK、Orn、dOrn、Dap、dDap、Dab、dDab、Dab(COCH2)、dDab(COCH2)、hE、dhE、hK、dhK、dSer(MePEG2)、Ser(MePEG2)；

X4係Pen、Abu、或C；

X5係N、dN、Q、dQ、N(N(Me)2)、或dN(N(Me)2)；

X7係W、dW、7MeW、或d7MeW；

X8係K(Ac)、dK(Ac)、Q、dQ、K(NMeAc)、或dK(NMeAc)；

X9係Pen、Abu、或C；

X10係AEF、TMAPF、或AEF(NHPEG3a)；

X11係2Nal；

X12係THP、Acpx、或aMeK；

X13係E、dE、hE、dhE、aMeE、d-aMeE、D、dD、Aad、dAad、K、dK、hSer、dhSer、Dap(pF)、R5H、R6H、R7H、S5H、S6H、S7H、C、dC、K(NMe)、或dK(NMe)；

X15係3Pal、H、dH、3MeH、3MedH、F、dF、aMeF、aMedF、THP、bAla、NMeTyr、NMedY、K、或dK；

X16係不存在或meG、NMedY；

R2係-NH_2、N(H)(C_1-C_4烷基)、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$，及

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4與X9之間的第一雙硫鍵或硫醚鍵；及
- R1與X13之間或X3與X13之間第二醯胺、脂族(RCM)、烷基胺、或硫醚鍵聯；且

R2之各烷基可選地係經Cl、F、或氰基所取代；

【請求項20】一種式(XX')之介白素-23受體之雙環肽抑制劑，其包含胺基酸序列：

R1-X3-X4-X5-X6-X7-X8-X9-X10-X11-X12-X13-X14-X15-X16-R2 (XX')

其中：

R1係CF3CO、5cpaCO、cPEG3aCO、C1至C4烷基C(O)-、或經氰基、Cl、或F所取代之C1至C4烷基C(O)-；

X3係不存在、R、dR、K、dK、K(Me)3、dK(Me)3、hK(Me)3、dhK(Me)3、K(d、或dK(d)；

X4係Pen、Abu、或C；

X5係E、dE、D、dD、K、dK、K(a)、K(Ac)、K(cPEG3aCO)、K(d)、K(G)、Dap、或K(NMe)、dK(NMe)、K(NNs)、或dK(NNs)；

X6係選自T、L、dT、dL、I、或dI；

X7係W、7MeW、7PhW、dW、d7MeW、d7PhW、或7(3NAcPh)W；

X8係K(Ac)、dK(Ac)、hK(Me)3、dhK(Me)3、K(Me)3、dK(Me)3、K(NMeAc)、dK(NMeAc)、K(NMecPEG3a)、Q(N(Me)2)、KPeg12、dKPeg12、KAcMor、A、Q、dKacMor、dQ(N(Me)2)、K(mPEG12)、dA、dQ、或dK(mPEG12)；

X9係Pen、Abu、或C；

X10係AEF或AEF(NMe)；

X11係2Nal；

X12係THP、aMeLeu、或A；

X13係E、dE、K(Ac)、dK(Ac)、K(Me)3、dK(Me)3、K(NMeAc)、dK(NMeAc)、K(NMecPEG3a)、Q(N(Me)2)、dQ(N(Me)2)、A、dA、L、或dL；

X14係L、N、或S；

X15係3Pal、L、dL、或Aib

X16係meG；且

R2係-NH_2、N(H)(C_1-C_4 alklyl、-HN(C_1-C_4烷基)、-N(C_1-C_4烷基)$_2$；且

其中：

該介白素-23受體之雙環肽抑制劑係藉由形成下列而環化：

- X4 與 X9 之間的第一雙硫鍵或硫醚鍵；及
- X5 與 X10 之間的第二醯胺或烷基胺鍵聯；且

R2之各烷基可選地係經Cl、F、或氰基所取代。

【請求項21】一種化合物或其醫藥上可接受之鹽，其各別係選自表1A、表1B、表1C、表1D、表1E、表1F、表1G或表1H之化合物。

【請求項22】一種醫藥組成物，其包含：

- 如請求項 1 至 21 中任一項所述之化合物或其醫藥上可接受之鹽；及
- 醫藥上可接受之載劑、賦形劑、或稀釋劑。

【請求項23】如請求項22所述之醫藥組成物，其進一步包含腸溶衣。

【請求項24】如請求項23所述之醫藥組成物，其中該腸溶衣保護該醫藥組成物且在患者或對象之下胃腸系統內釋放該醫藥組成物。

【請求項25】一種用於治療自體免疫、發炎性疾病、或相關病症之方法，其包含投予治療有效量的：

- 如請求項 1 至 21 中任一項所述之化合物或其醫藥上可接受之鹽；或
- 如請求項 22 至 24 中任一項所述之醫藥組成物

至有需要之對象或患者中。

【請求項26】一種治療有效量的：

[a] 如請求項 1 至 21 中任一項所述之化合物或其醫藥上可接受之鹽；或

[b] 如請求項 22 至 24 中任一項所述之醫藥組成物，於製造用於治療自體免疫、發炎性疾病、或相關病症的藥劑之用途。

【請求項27】如請求項25所述之用於治療自體免疫、發炎性疾病、或相關病症之方法或如請求項26所述之用途，其中該自體免疫、發炎性疾病、或相關病症係選自多發性硬化症、氣喘、類風濕性關節炎、腸道發炎、發炎性腸疾(inflammatory bowel disease, IBD)、幼年型IBD、青年期IBD、Crohn氏症、潰瘍性結腸炎、肉瘤病、全身性紅斑性狼瘡、關節黏連性脊椎炎（中軸性脊椎關節炎）、牛皮癬性關節炎、或牛皮癬。特定而言，疾病或病症可係牛皮癬（例如，斑塊型牛皮癬、滴狀牛皮癬、反轉型牛皮癬、膿疱性牛皮癬、掌蹠膿疱症、尋常牛皮癬、或紅皮性牛皮癬）、異位性皮膚炎、痤瘡異位、潰瘍性結腸炎、Crohn氏症、乳糜瀉（非熱帶性口瘡）、與血清反應陰性關節病變相關聯之腸病變、顯微鏡性結腸炎、膠原性結腸炎、嗜伊紅性胃腸炎/食道炎、與放射或化學療法相關聯之結腸炎、與如在白血球黏附分子缺乏症-1中的先天免疫性病症相關聯之結腸炎、慢性肉芽腫疾病、肝糖貯積病第1b型、Hermansky-Pudlak氏症候群、Chediak-Higashi氏症候群、Wiskott-Aldrich氏症候群、囊炎、直腸結腸切除術及回腸肛管吻合術後產生之囊炎、胃腸癌、胰臟炎、胰島素依

賴性糖尿病、乳腺炎、膽囊炎、膽管炎、原發性膽汁性肝硬化、病毒相關腸病變、膽管週圍炎、慢性支氣管炎、慢性竇炎、氣喘、眼色素層炎、或移植物抗宿主疾病。

【請求項28】如請求項27所述之用於治療自體免疫、發炎性疾病、或相關病症之方法或用途，其中該自體免疫、發炎性疾病、或相關病症係選自發炎性腸疾(IBD)、潰瘍性結腸炎(Ulcerative colitis, UC)、Crohn氏症(CD)、牛皮癬(psoriasis, PsO)、或牛皮癬性關節炎(psoriatic arthritis, PsA)。

【請求項29】一種用於治療係發炎性腸疾(IBD)、Crohn氏症、潰瘍性結腸炎、牛皮癬、或牛皮癬性關節炎之發炎性疾病之方法，其包含投予治療有效量的：

- 如請求項 1 至 21 中任一項所述之化合物或其醫藥上可接受之鹽；或
- 如請求項 22 至 24 中任一項所述之醫藥組成物

至有需要之對象或患者中。

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