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(54) Title: ACTIVE LEARNING MODEL VALIDATION

(57) Abstract: Method(s), apparatus, and computer-implemented method(s) are provided for training a machine learning (ML) technique to generate a property model for predicting whether a compound has a particular property. An iterative procedure/feedback loop may be performed for generating the property model, the procedure including: generating a prediction result list for a plurality of compounds and their association with the particular property based on the property model; validating the property model based on compounds from the prediction result list having an association with the particular property; and updating the property model based on the property model validation. The procedure/loop may be repeated using the updated property model until it is determined the property model has been validly trained. The property model validation may include selecting a shortlist of compounds, performing simulation analysis and/or laboratory analysis on the shortlist of compounds in relation to the particular property and using the simulation and/or laboratory results in updating the property model.



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INTERNATIONAL SEARCH REPORT

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A. CLASSIFICATION OF SUBJECT MATTER
INV. G16C20/30 G16C20/70
ADD.
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED
Minimum documentation searched (classification system followed by classification symbols)
G16C
Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
EPO-Internal, WPI Data, BIOSIS, EMBASE, INSPEC

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	POPOVA M. ET AL: "Deep Reinforcement Learning for De-Novo Drug Design", ARXIV.ORG, CORNELL UNIVERSITY LIBRARY, 201 OLIN LIBRARY CORNELL UNIVERSITY ITHACA, NY 14853, 29 November 2017 (2017-11-29), XP081150300, DOI: 10.1126/SCIADV.AAP7885 the whole document ----- -/--	1-30,33, 35-37

Further documents are listed in the continuation of Box C.

See patent family annex.

* Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier application or patent but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art

"&" document member of the same patent family

Date of the actual completion of the international search 30 October 2019	Date of mailing of the international search report 11/11/2019
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Name and mailing address of the ISA/ European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Fax: (+31-70) 340-3016	Authorized officer Godzina, Przemysław
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INTERNATIONAL SEARCH REPORT

International application No.
PCT/GB2019/050921

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. Claims Nos.: 31, 32, 34
because they relate to subject matter not required to be searched by this Authority, namely:
A meaningful search is not possible on the basis of claims 31, 32 and 34 because claims 31, 32 and 34 are directed to presentation of information (R. 39.1(v) PCT).
2. Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:
3. Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
2. As all searchable claims could be searched without effort justifying an additional fees, this Authority did not invite payment of additional fees.
3. As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:
4. No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.
- The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.
- No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International application No

PCT/GB2019/050921

C(Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT		
Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	EL-TELBANY M. E. ET AL: "Drug design: The machine learning roles", 2014 INTERNATIONAL CONFERENCE ON ENGINEERING AND TECHNOLOGY (ICET), IEEE, 19 April 2014 (2014-04-19), pages 1-6, XP032725760, DOI: 10.1109/ICENGTECHNOL.2014.7016794 [retrieved on 2015-01-20] the whole document	1-30,33, 35-37
X	----- OLIVECRONA M. ET AL: "Molecular de-novo design through deep reinforcement learning", JOURNAL OF CHEMINFORMATICS, vol. 9, no. 48, 4 September 2017 (2017-09-04), XP055637190, DOI: 10.1186/s13321-017-0235-x the whole document	1-30,33, 35-37
X	----- SEGLER M. H. S. ET AL: "Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks", ACS CENTRAL SCIENCE, vol. 4, no. 1, 28 December 2017 (2017-12-28), pages 120-131, XP055637179, ISSN: 2374-7943, DOI: 10.1021/acscentsci.7b00512 the whole document	1-30,33, 35-37
X	----- MITCHELL J. B. O.: "Machine learning methods in chemoinformatics : Machine learning methods in chemoinformatics", WILEY INTERDISCIPLINARY REVIEWS: COMPUTATIONAL MOLECULAR SCIENCE, vol. 4, no. 5, 24 February 2014 (2014-02-24), pages 468-481, XP055585883, ISSN: 1759-0876, DOI: 10.1002/wcms.1183 the whole document	1-30,33, 35-37
X	----- US 2005/278124 A1 (DUFFY NIGEL P [US] ET AL) 15 December 2005 (2005-12-15) the whole document	1-30,33, 35-37

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No

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Patent document cited in search report	Publication date	Patent family member(s)	Publication date
US 2005278124	A1	NONE	