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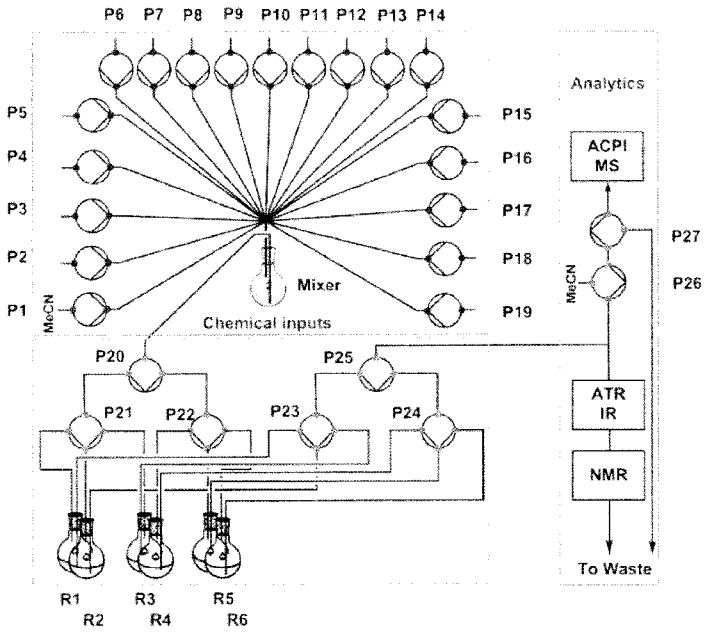
(54) Title: PREDICTING CHEMICAL REACTIONS USING MACHINE LEARNING

Fig. 1



(57) Abstract: The present invention provides a method to generate a predictive model for a reaction set, which reaction set is the sum of the reaction outcomes for a plurality of chemical inputs. Also provided is a system for generating a predictive model for a reaction set, which system may be used in the method. The system comprises a synthesiser for conducting reactions, which synthesiser is an automated synthesiser, an analytical unit for monitoring reactions performed by the synthesiser, and a control unit suitably programmed with a machine learning algorithm, for analysing analytical data from the analytical unit, and for controlling the synthesiser.

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[Continued on next page]

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A. CLASSIFICATION OF SUBJECT MATTER
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B. FIELDS SEARCHED

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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, BIOSIS, EMBASE, INSPEC, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

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X	COLEY C. W. ET AL: "Machine Learning in Computer-Aided Synthesis Planning", ACCOUNTS OF CHEMICAL RESEARCH, vol. 51, no. 5, 1 May 2018 (2018-05-01), pages 1281-1289, XP055660945, US ISSN: 0001-4842, DOI: 10.1021/acs.accounts.8b00087 the whole document	1-14

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[X] Further documents are listed in the continuation of Box C.

[X] See patent family annex.

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