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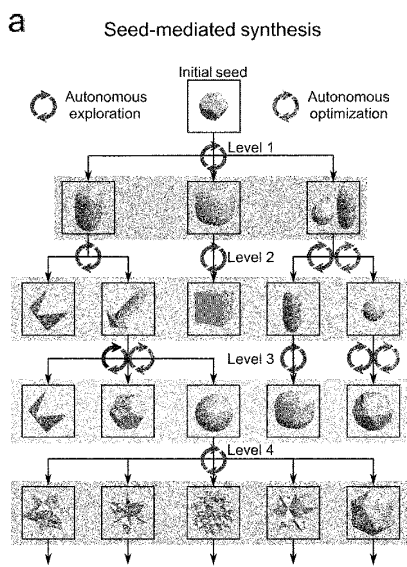
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(54) Title: AUTONOMOUS EXPLORATION FOR THE SYNTHESIS OF CHEMICAL LIBRARIES

Fig. 1a



(57) Abstract: The invention provides a method for the exploration of chemical space through a multigenerational series of synthetic stages. In a first stage, a series of reactions is performed. The products of the first series are analysed, and a first product from the series of reactions is selected. The first product is used as a chemical input for each of the reactions in a second series of reactions. The products of the second series are analysed. The first and second stages are performed autonomously. The selection of a product in the first stage comprises the comparison of the products from the first series of reactions against a fitness function, where the selected product has a superior fitness compared with one or more other products in the first series. Each reaction in the first series differs in one or more chemical and/or physical inputs. Each reaction in the second series differs in one or more chemical and/or physical inputs. The invention also provides an automated exploration apparatus for performing the method, and the apparatus comprises a controller, and a chemical synthesiser and an analytical unit which are operable by the controller, as described herein.

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