

Title (en)

METHOD FOR CREATING A DATABASE ENABLING THE SELECTION OF AT LEAST ONE REACTION-CAPABLE CATALYST

Title (de)

VERFAHREN ZUR ERSTELLUNG EINER DATENBANK, DIE DIE AUSWAHL WENIGSTENS EINES REAKTIONSFÄHIGEN KATALYSATORS ERMÖGLICHT

Title (fr)

PROCEDE POUR CONSTITUER UNE BASE DE DONNEES PERMETTANT DE SELECTIONNER AU MOINS UN CATALYSEUR ADAPTE A UNE REACTION

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Application

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Abstract (en)

[origin: WO2005077864A1] The invention relates to a method for creating a database enabling, in particular, the selection of at least one reaction-capable catalyst, comprising the following steps: a) preparing a number of different reaction media containing the same reactivity probe and each having at least one catalyst; b) analyzing, by means of an analytic method, each reaction medium after reaction, and; c) assigning, in the database, an analysis result according to step b) to the reactivity probe, this result characterizing different reaction products obtained from said reactivity probe. The database is a relational database containing: a first entity in which items of information relative to the reaction patterns listed in the data base are recorded; a second entity containing items of information relative to the state of bindings of at least one reaction pattern listed in the first entity; a third entity in which items of information associated with different reaction media are stored, and; at least one fourth entity in which items of information are stored that are linked to the analysis results of the reaction media at the end of a reaction.

IPC 8 full level

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