A Reaction Database for Small Molecule Pharmaceutical Processes Integrated with Process Information

This article describes the development of a reaction database with the objective to collect data for multiphase reactions involved in small molecule pharmaceutical processes with a search engine to retrieve necessary data in investigations of reaction-separation schemes, such as the role of organic solvents in reaction performance improvement. The focus of this reaction database is to provide a data rich environment with process information available to assist during the early stage synthesis of pharmaceutical products. The database is structured in terms of reaction classification of reaction types; compounds participating in the reaction; use of organic solvents and their function; information for single step and multistep reactions; target products; reaction conditions and reaction data. Information for reactor scale-up together with information for the separation and other relevant information for each reaction and reference are also available in the database. Additionally, the retrieved information obtained from the database can be evaluated in terms of sustainability using well-known “green” metrics published in the scientific literature. The application of the database is illustrated through the synthesis of ibuprofen, for which data on different reaction pathways have been retrieved from the database and compared using “green” chemistry metrics.

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