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Environmental sustainability assessment of pharmaceutical synthesis steps: case studies and resource consumption modeling

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The pharmaceutical and fine chemical industries are eager more and more to strive for innovative products and technologies. To accomplish this, resources should be used more efficiently within a life cycle perspective as being a major driver of both production and consumption. This study unravels resource consumption patterns in the production of Active Pharmaceutical Ingredients (APIs) through Exergy Analysis (EA) and Exergetic Life Cycle Analysis (ELCA) of five selected APIs. A multilevel approach (process, plant and cradle-togate level) enables identifying and locating resource losses throughout the complete manufacturing supply chain. Results showed that 58% of cumulative resource extraction was due to industrial processes in the supply chain, while only 42% proved to be related to the on-site manufacturing processes. Of all chemicals considered (accounting for about 80% of cumulative resource consumption), solvents and primary building blocks proved to be most significant. Second, multiple linear regression models are proposed in order to estimate resource consumption of API synthesis steps. An optimal set of predictor variables is postulated to balance model complexity and embedded information on the one hand and usability, readily availability of data and capability of merging models with existing Enterprise Resource Planning (ERP) data systems on the other hand. The use of organic solvents, the molar efficiency and duration of an API synthesis step showed to be the most significant predictor variables. The authors want to address that including additional predictor variables might in some cases be an unnecessary, time consuming task which might not benefit to the predictive character and can eventually deteriorate the model interpretation. In future, ideally, an organization should be able to derive the environmental impact of its portfolio from ERP data, linking supply chains back to the cradle of resource extraction.