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REAXYS: An excellent tool for cracking chemistry problems

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Abstract

Medicinal Chemistry is the basis of successful drug discovery and its principal component is effective synthetic organic chemistry. It takes numerous years to become an experienced medicinal chemist who can predict the outcome of various chemical reactions correctly and provide the most efficient synthetic scheme to a pharmaceutically active and safe compound or compound library. Even then, Merck quote, more than half of the cornerstone reactions we attempt are failing (Science 02, 2015), and non-yielding synthesis steps are part of the reasons why the amount of investment into pharmaceutical research and development (R&D) is high (2016, $157 billion). The design of an effective synthesis route to a correctly substituted molecule can become a rate-limiting process and occasionally, molecules are not synthesized, because it simply takes too long to find suitable chemistries. If we want to prepare any molecule of interest quickly and with lower failure rate than today, a disruptive synthesis prediction technology will be required. In line with such a paradigm shift we will need chemists that combine excellent synthesis knowledge as well as competence in machine learning methods and artificial intelligence (AI).

For the first time computer-aided retro synthesis tools, which can predict reactions correctly, are available and do not rest on the input of rules from researchers. Waller and Segler et al. (Nature, March 2018) in collaboration with Elsevier have developed a 'deep learning' computer program that produces blueprints for the sequences of reactions needed to create small organic molecules, such as pharmaceutical active molecules. This novel artificial-intelligence tool has processed nearly every reaction ever published (> 15 million) and has the potential to transform the way synthetic & medicinal chemists work in the future. Segler & Waller et al. tested the synthetic routes that the program generated in a double-blind trial with 45 organic chemists from two institutes in China and Germany and the routes have proven scientifically sound and robust. Increasing the success rate in synthetic chemistry would have a huge benefit in terms of treating diseases more resourcefully, discovering more sustainable chemical solutions and minimizing expenditure in R&D. Reaxys-PAI Predictive Retrosynthetic solution, developed in collaboration between Elsevier and Waller and Segler et al., deploys next generation AI technologies to augment chemical synthesis knowledge, drives innovation and helps to save time and cost.

Biography

Friedrich Kroll obtained his PhD in Chemistry at the University of Marburg and his MBA from the University of Potsdam. He is a successful drug and technology developer. Currently, he is Head of Scientific Affairs promoting information technologies in academia and in drug discovery.

Publications

1. Solid phase supports
2. 3, 4-dihydro-1H-isoquinolin-2-yl-derivatives
3. Capture Compound Mass Spectrometry: An exceptional and fast method for the identification of the mechanism of toxicity in drugs
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7. G. Ö rlygsson, BT Golding, and W. Buckel. 1995. Evidence for a mechanism involving transient fragmentation in coenzyme-B12-dependent carbon skeleton rearrangements
8. Vinyl sulphone modified polymer

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