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Abstract Title: Retrosynthetic software for practicing chemists: Novel and efficient in silico pathway design validated at the bench

Lindsey Rickershauser, Ph.D., Sarah L. Trice, Ph.D.

[1] *First Author Affiliation (MilliporeSigma)*
[2] *Second Author Affiliation (MilliporeSigma)*

Abstract

In a continuously evolving landscape of in silico chemical intelligence and machine learning, computer assisted synthetic planning has come to the forefront of discussion in the cheminformatics space. Herein, we describe an experiment in which Chematica, a retrosynthetic design software, was used to plan synthetic pathways of eight structurally diverse bioactive and natural products. In each instance, the computer-planned routes were not only executed successfully in the laboratory, but also offered significant improvements over previous routes, circumvented patented routes and/or produced targets not synthesized previously. Chematica's unique approach to building their expert database of known reactions by hand coding each transformation has allowed this tool to become a bench chemist's ally by 'learning' chemistry much like a chemist would themselves, and suggesting diverse pathways towards their targets, thus generating ideas and providing cost effective routes based on each user's unique needs. As a product of over 15 years of research, this unique tool is poised to not only get better with time, but also revolutionize the way chemists approach designing pathways to their complex targets.

Keywords—*Computer-aided Retrosynthetic Design; Cheminformatics; Retrosynthesis; AI*

Professional Biography (100-150 words)

Lindsey Hess Rickershauser, Ph.D., is currently a Technical Application Scientist in the Cheminformatics Technologies division of MilliporeSigma, a business of Merck KGaA, Darmstadt, Germany. She got her Ph.D. in organic chemistry in 2010, working under Professor Gary Posner at Johns Hopkins University. During her Ph.D. work, her concentrations were on synthesizing analogs of vitamin D and artemisinin dimers for biological activity, and synthetic methodologies of enantioselective sigmatropic rearrangements. From there, she had a short venture at Chemical Abstracts Services in the cheminformatics space, after which, she joined Cerilliant Corporation (then a subsidiary of Sigma-Aldrich) as a senior scientist specializing in certified reference materials in the clinical, diagnostic & forensic industries. During her six-year tenure as a senior scientist, she specialized in stable label isotope incorporation to both pharmaceutical and illicit drugs and their metabolites (concentrating on D and 13C incorporation). From there, she then joined the Cheminformatics Technologies division where she has been actively part of launching the retrosynthetic design software acquired in 2017.



Email Id: Lindsey.rickershauser@sial.com

Any Comments: