Subject: Re: retrosyntheis tools
Posted by nbehrnd on Thu, 27 Jan 2022 06:54:38 GMT
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Your question does not clarify if your interest is about the classical rules, or about contemporary implementation of retrosynthethic algorithms into computer programs. For the former (humanoid recognition of pattern, disconnection into known precursors) E. J. Corey was one prominent author who formalized the approaches.[1, 2] But there are plenty publications about the later as well[3,4,5] and a listing here is opinionated and incomplete. You may use the references below to expand the bibliographic search further.

Norwid

[1] Corey, Nobel lecture in Angewandte 1991, 30, 455-465; https://doi.org/10.1002/anie.199104553.
[2] E. J. Corey, X-M. Cheng (1995). The Logic of Chemical Synthesis. New York: Wiley. ISBN 978-0-471-11594-6.

Angewandte 2016, 55, 5904-5937; https://doi.org/10.1002/anie.201506101
[4] Badowski, T. et al. Synergy Between Expert and Machine-Learning Approaches Allows for Improved Retrosynthetic Planning. Angewandte 2019, 55, 725-730; https://doi.org/10.1002/anie.201912083
[5] Thakkar, A. et al. Retrosynthetic accessibility score (RAscore) – rapid machine learned synthesizability classification from AI driven retrosynthetic planning. Chem. Sci. 2021, 12, 3339-3349; https://doi.org/10.1039/D0SC05401A.