Bringing retrosynthesis in-house: customized, interpretable planning on your own chemistry with SynPlanner

Tagir Akhmetshin[1], Almaz Gilmullin[1], Guillaume Schmitz[1], Olga Klimchuk[1], Dragos Horvath[1], Timur Madzhidov[2], Alexandre Varnek[1,3*]

[1]*Laboratory of Chemoinformatics, UMR 7140 CNRS, University of Strasbourg, 4, rue B. Pascal, 67000 Strasbourg, France*
[2] *Chemistry Solutions, Life Science Solutions, Elsevier, Nielsen House, John Smith Drive, Oxford OX4 2WB, United Kingdom*
[3] *Institute of Chemical Reaction Design and Development, Hokkaido University, Japan*

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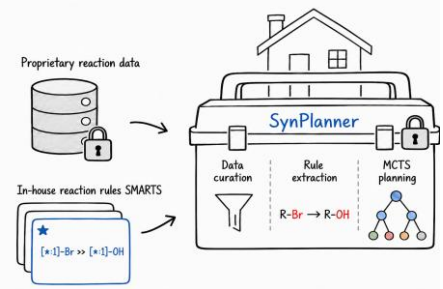
For discovery groups, a retrosynthesis planner is most useful when it reflects their own reaction chemistry, not only a generic model trained on public reactions such as USPTO dataset.[1,2] Their data are proprietary, a planner is trusted only when its reasoning can be inspected, and most groups have no practical path from raw reaction data to a customized planner they can run locally on sensitive data.

SynPlanner[3] is an open-source, end-to-end tool that closes this gap. It builds a customized, interpretable planner from a group's own reaction data, covering the full path from data curation and reaction-rule extraction to Monte Carlo Tree Search planning, and runs locally.

Even within such a planner, a transformation seen in only a handful of reactions can be missed. Priority-rule injection lets a chemist supply a small curated rule set that is tried ahead of the learned policy during the search, so routes are built around the chosen chemistry. We demonstrate this on the Ugi four-component reaction and show that injected rules recover chemist-intended routes that the default planner misses. The same mechanism extends to other rare or proprietary transformations the group trusts, so it can plan on its own chemistry from a handful of examples, without retraining the validated model or exposing the data behind it.



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