Improving Retrosynthetic Planning With New Algorithms

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SynPlanner is a new multi-step retrosynthesis software with SOTA performances. The multi-step retrosynthetic search is powered by tree search algorithms. We apply a range of search algorithms, including variants Monte Carlo Tree Search to SynPlanner in order to elicit the best combination. In addition, we compare different evaluation heuristics that can guide the search. All on 860 molecules selected for their Synthetic Accessibility Score, or being used as multi-step retrosynthesis benchmark.

We show that the right algorithm, Nested Monte Carlo Tree Search, paired with a powerful evaluation heuristic, the mass of the molecules absent from the stock in the super node, can increase the search efficiency. This new tree search method allowed SynPlanner to solve up to twice as many complex molecules, and divide the search times by more than 10 times compared to SOTA. Outperforming all past open softwares for multi-step retrosynthesis.

We then combine this algorithmic and heuristic efficiency with parallelization and search space pruning techniques, which leads to an even faster search and new molecules being solved.