Subject: chemical complexity calculation
Posted by yunforce on Fri, 23 Aug 2024 03:30:37 GMT
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Dear Datawarror team,
In our recent analysis of chemical synthesis routes, we have frequently incorporated a chemical complexity metric known as Cm (T. Böttcher, J. Chem. Inf. Model. 56, 462–470 (2016)). Although there are numerous methods for calculating molecular complexity, the Cm index appears to be particularly favored by organic synthetic chemists. When analyzing the "direction of travel" of a synthetic route in chemical space, we typically need to quantitatively analyze molecules across three dimensions: Cm, Fsp3, and Mw.(similar to Science 375, 1270–1274 (2022); Nat. Prod. Rep. 2024,doi:10.1039/D4NP00015C)

While exploring this domain, I have noticed that DataWarrior offers an option for calculating molecular complexity, but I remain uncertain about the specific methodology and reliability of this feature. To enhance our research efficiency and accuracy, I propose the possibility of adding a Cm calculation option within DataWarrior's "Chemistry" menu, under the "From Chemical Structure" submenu, specifically in a new "Calculate Descriptor" feature.

By implementing this feature, we would be able to directly utilize DataWarrior's built-in three-dimensional data analysis software for our analyses, eliminating the need to switch to Python for calculations followed by the use of Matplotlib for plotting. This would greatly streamline our workflow and improve research efficiency.

File Attachments

1) Snipaste_2024-08-23_11-22-52.png, downloaded 987 times

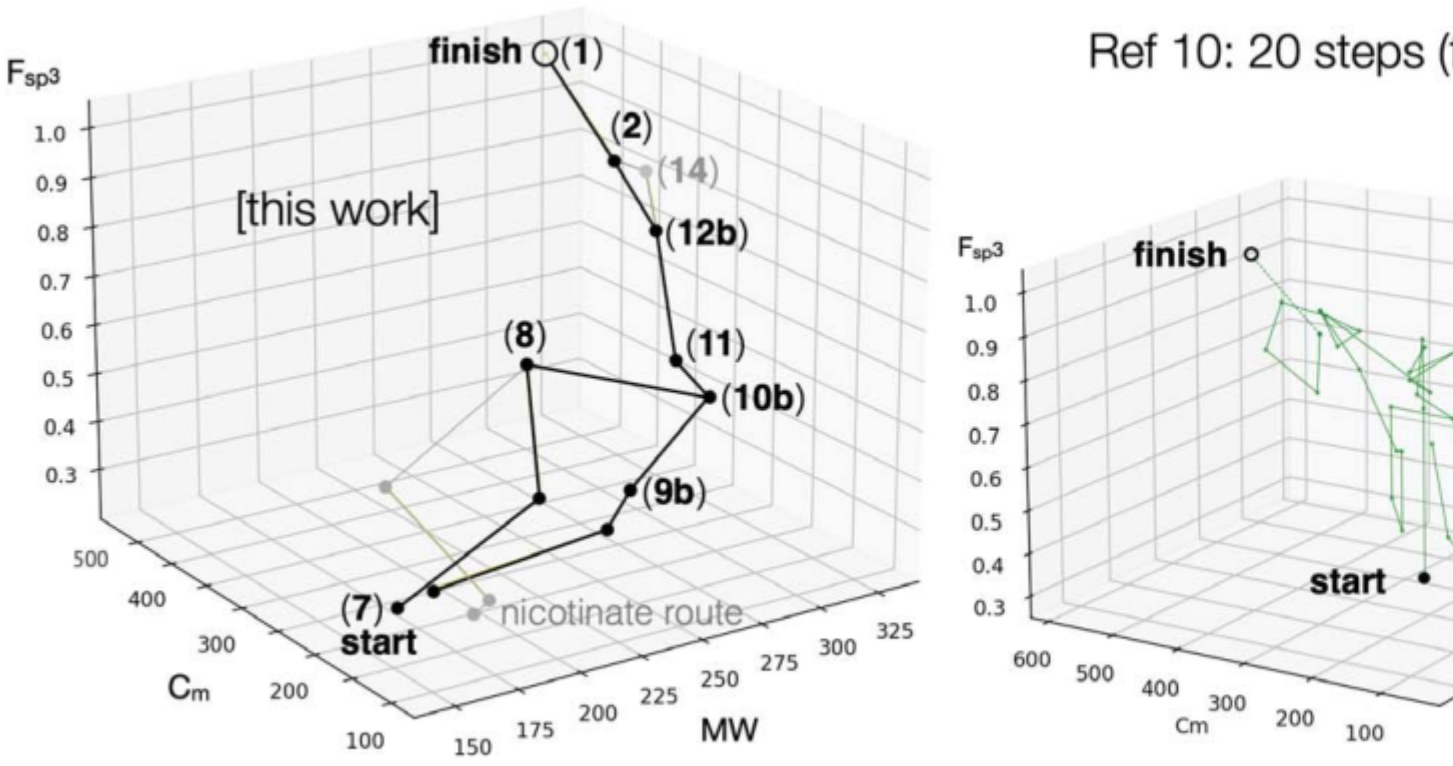
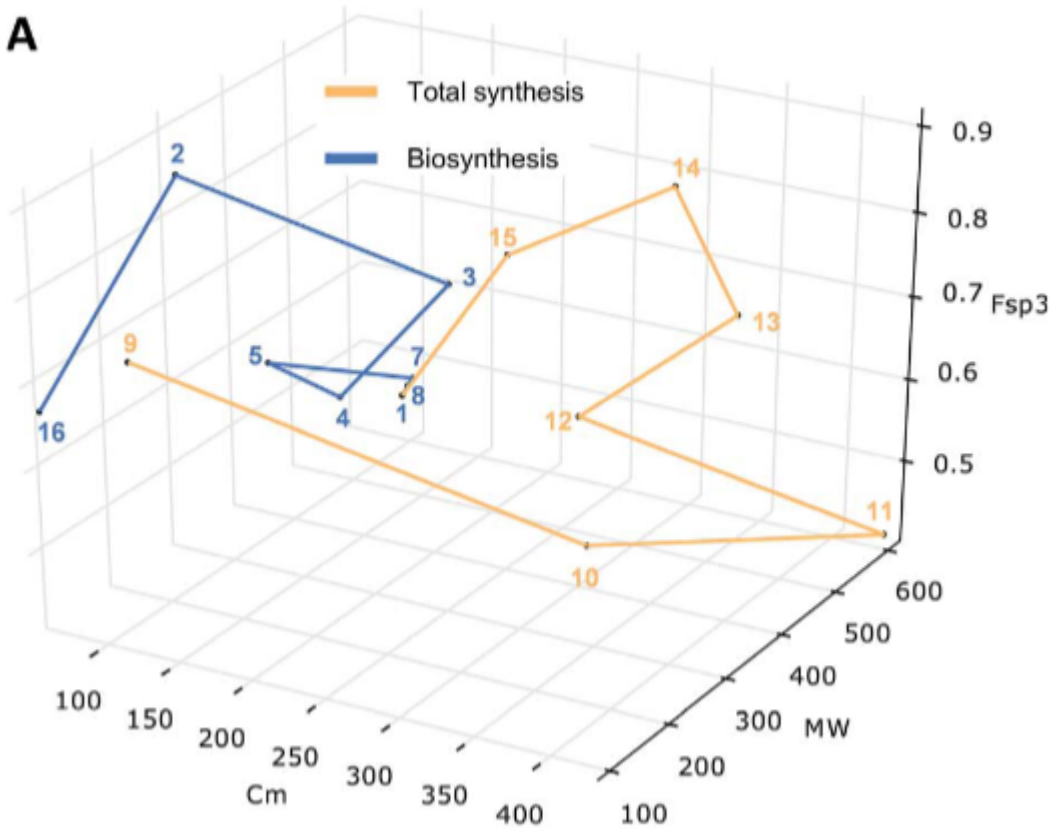


Fig. 4. Himgaline syntheses as walks through a chemical space. Plots ar

2) Snipaste_2024-08-23_11-29-08.png, downloaded 957 times


A
Total synthesis
Biosynthesis
Fsp3
MW
Cm
0.9
0.8
0.7
0.6
0.5
600
500
400
300
200
100
100
150
200
250
300
350
400
1
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