

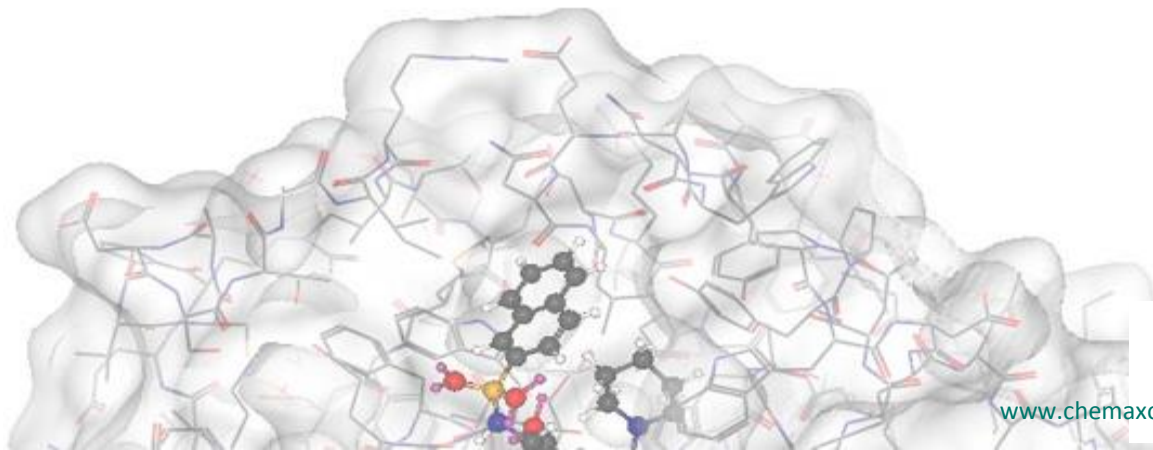


ChemAxon
discovery informatics



Design of synthetically accessible virtual libraries with Plexus

Ágnes Peragovics

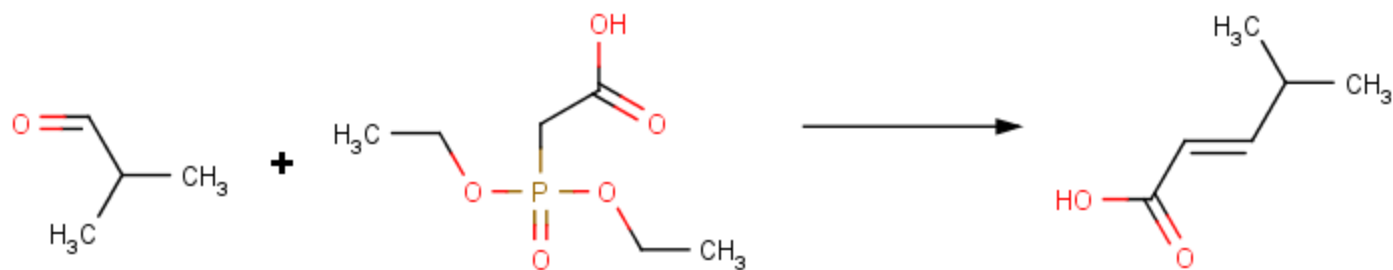
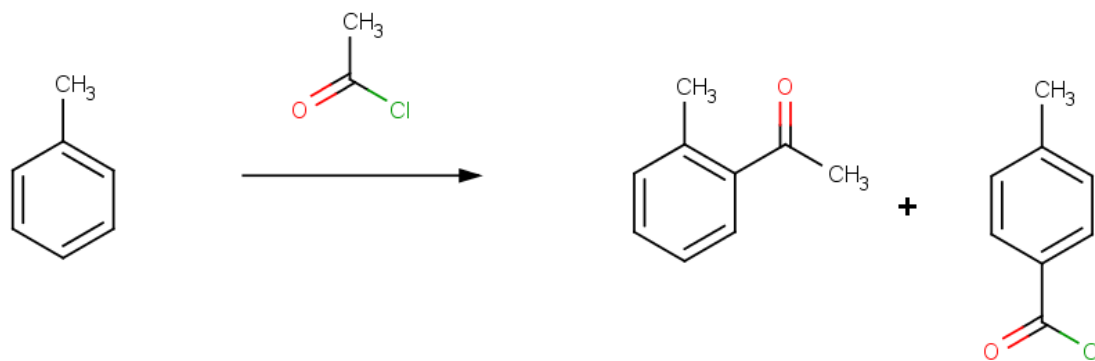


Plexus

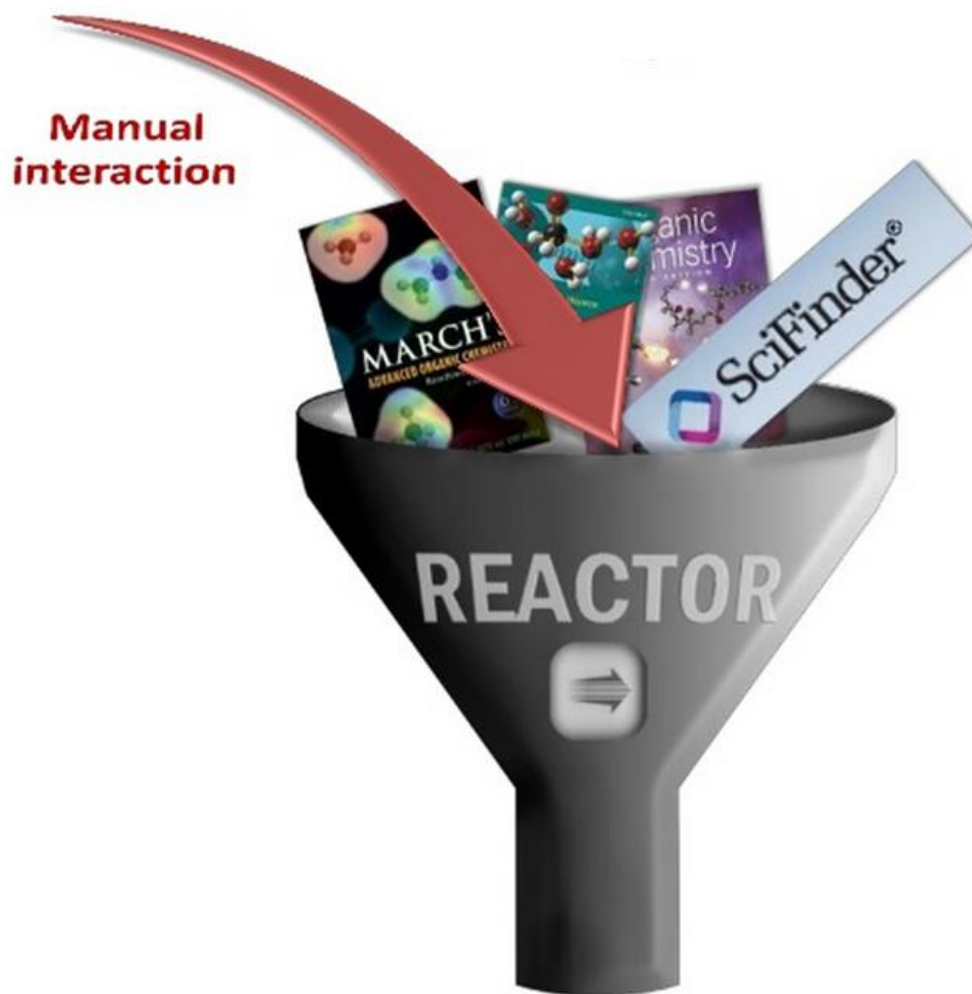
Plexus Suite: web-based application which gathers and connects key research processes using our cheminformatics toolkits.

Plexus Discovery: first available module supporting library design workflows.

Reaction based enumeration



Knowledge-based library

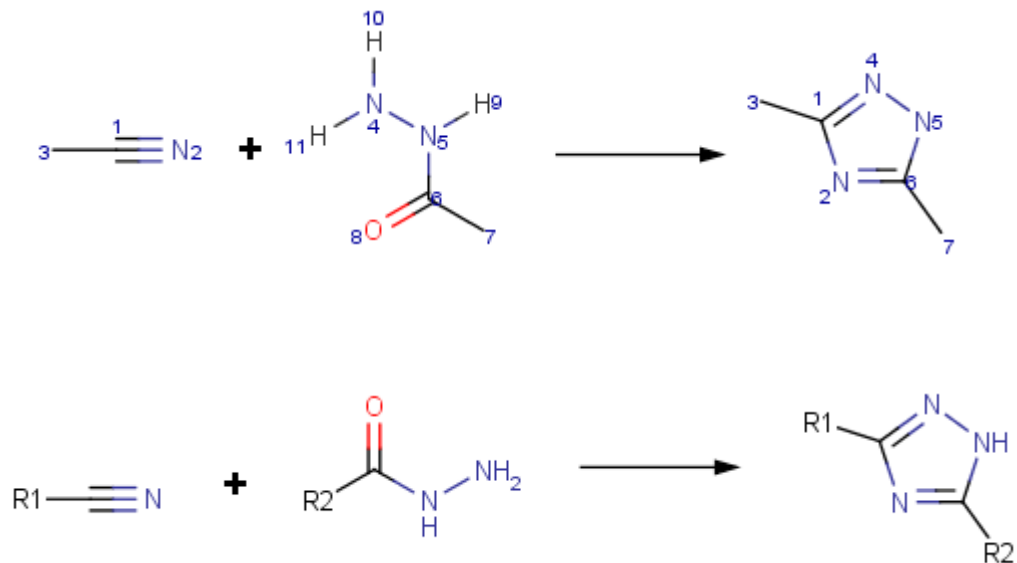


Reactions

Over **200**
organic chemical
reactions
from literature

1. 1,2,4-Oxadiazole formation
2. 1,2,4-Triazole formation from nitrile and hydrazide
3. 2,3-Dihydro benzimidazole formation from diamine and carbonyls
4. Acylation of alcohols with phosgene
5. Acylation of nucleophiles with carboxylic acid anhydrides
6. Acylation of amine
7. Acylation of nucleophiles with acid chlorides
8. Acylation of nucleophiles with carboxylic acids
9. Addition of alcohols to alkynes
10. Addition of hydrogen cyanide to alkynes
11. Aldol reaction revised
12. Alkylation of amines with alkyl halides
13. Alkyl Lithium formation from alkyl halides
14. Alkylation of phenols with benzyl chloride
15. Allylic halogenation of alkenes
16. Alpha-Alkylation of beta-keto esters
17. Alpha-alkylation of esters
18. Alpha halogenation of carboxylic acids
19. Amide synthesis from carboxylic acid
20. Amine sulfonation
21. Arylation of amines
22. Baylis-Hillman vinyl alkylation
23. Benzidine rearrangement
24. Benzilic type rearrangement
25. Benzimidazole formation from 1,2-phenyldiamine and carbonyls
26. Benzothiazole formation from 2-aminothiophenol and aldehyde
27. Benzoxazole formation from 2-aminophenol carbonyls
28. Beta HX elimination (Zaitsev elimination)
29. Birch reduction

1,2,4-triazole formation from nitrile and hydrazide



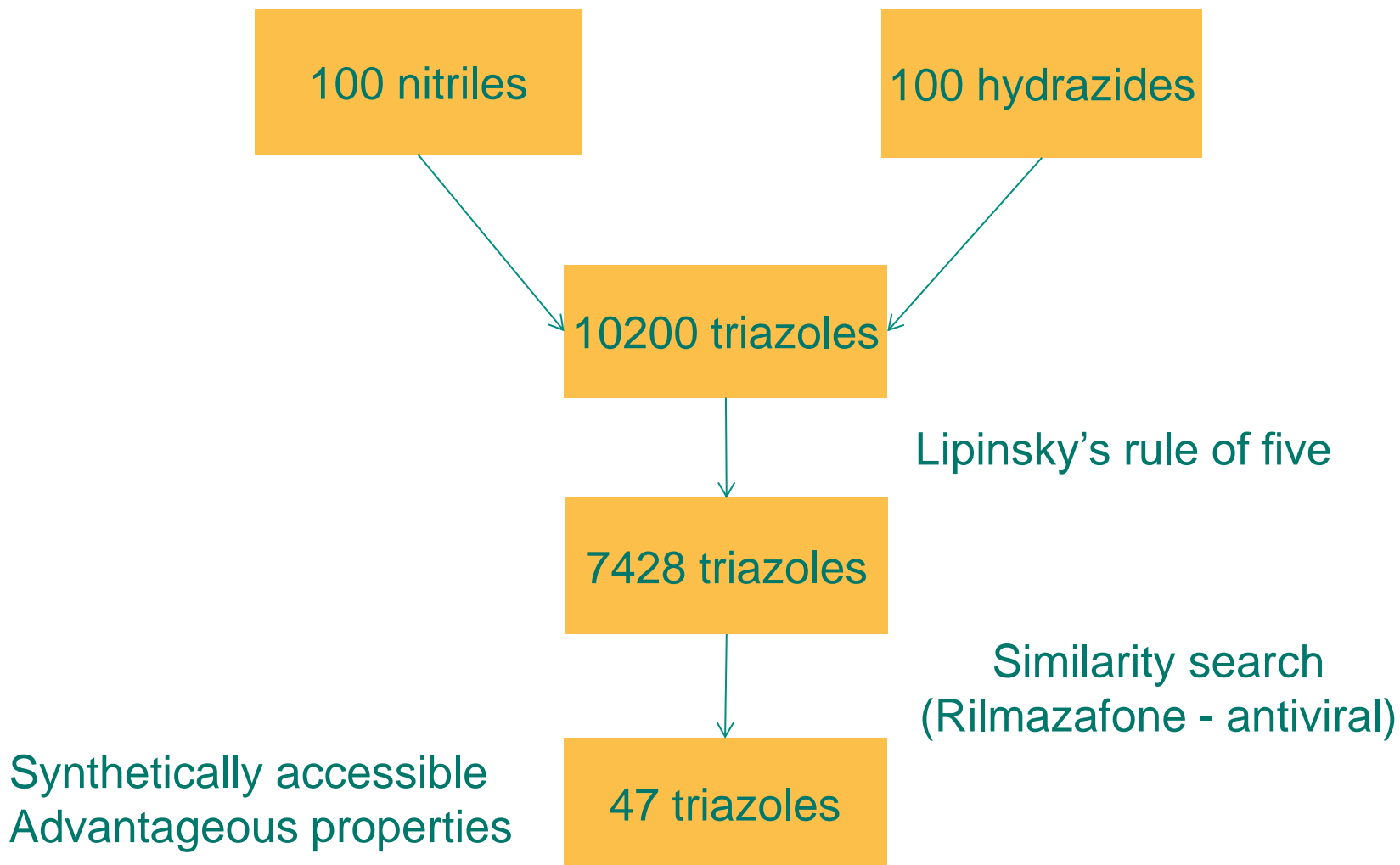
100 nitriles and 100 hydrazides from



Demonstration

[For the video click here](#)

Summary



Try Plexus Discovery online!

plexus.chemaxon.com

Provide us some feedback!

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ChemAxon Developers



Thank you for your attention!

Questions?