



ENAMINE

Glycomimetics Library

2,700 in-stock compounds

Library design outline

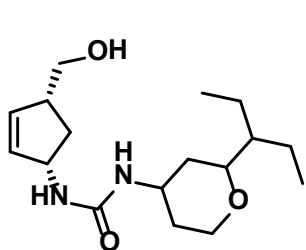
- **Privileged core fragments and side chain functionalities**
 - cyclic amino alcohols, cyclic glycols
 - O,N-containing aliphatic rings
 - polyalcohols
- **Nature-likeness scoring algorithm**
 - Taverna 2.5 workbench, similarity to available NP databases
- **MedChem structural filters, removal of common and trivial chemotypes**
 - PAINS, REOS, Elli Lilly rules and strict Enamine filters

Molecular filters

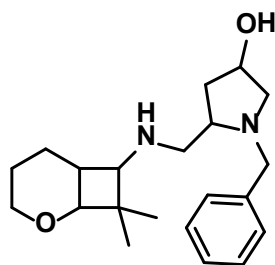
MW	140 – 450
ClogP	-3 – 4
HbAcc	2 – 10
HbD	1 – 6
TPSA	32 – 160
Ring count	1 – 5
Fsp ³	0.3 – 1
S +Cl	≤ 2
Sulfo and cyano group count	≤ 1

Training set of known glycosides was collected from the public available e-databases, scientific literature and evaluated to define the optimal range of Molecular parameters

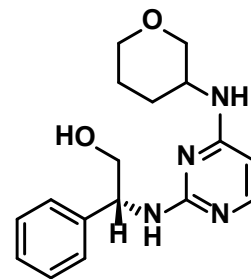
Examples of compounds in Glycomimetics library



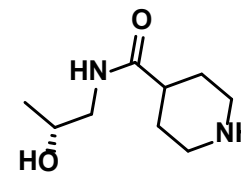
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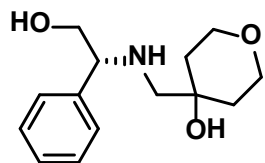
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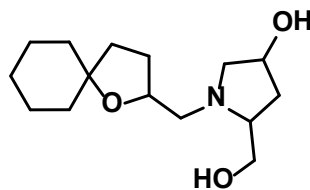
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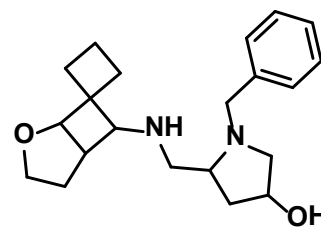
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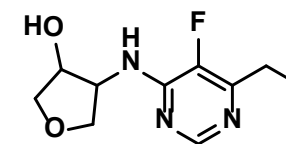
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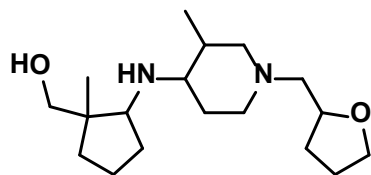
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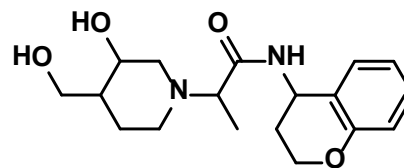
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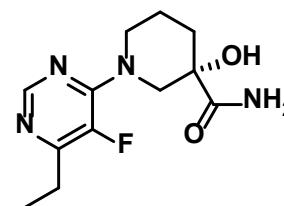
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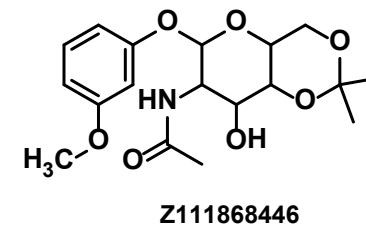
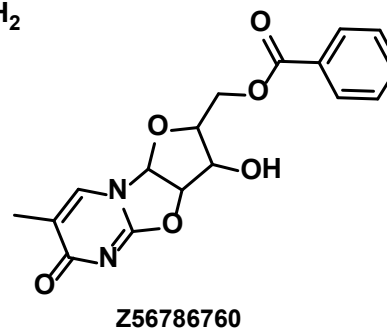
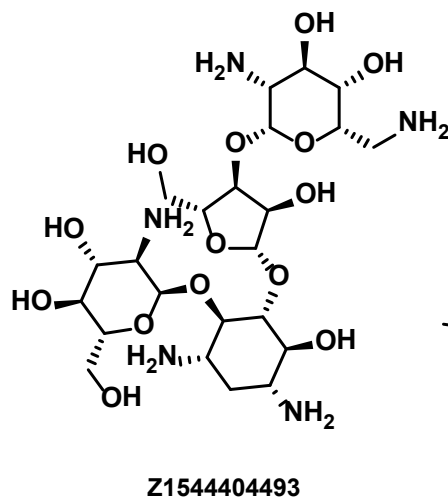
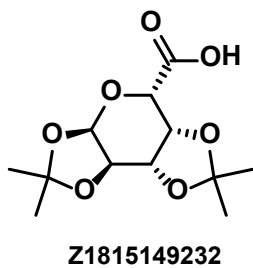
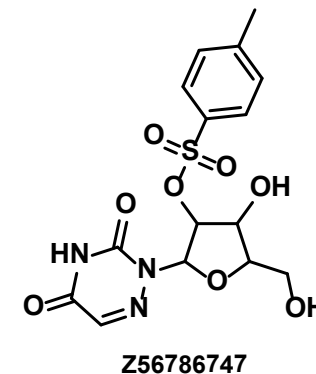
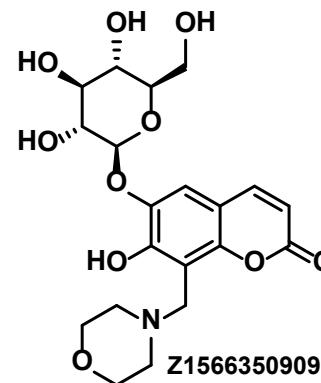
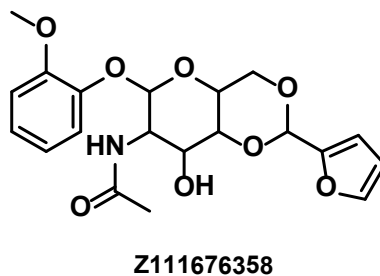
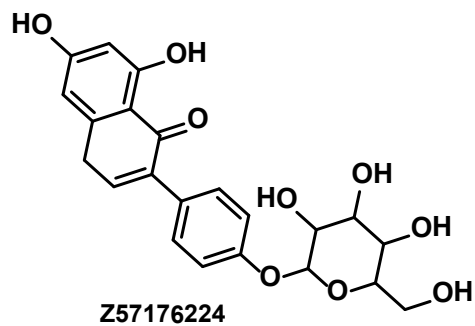


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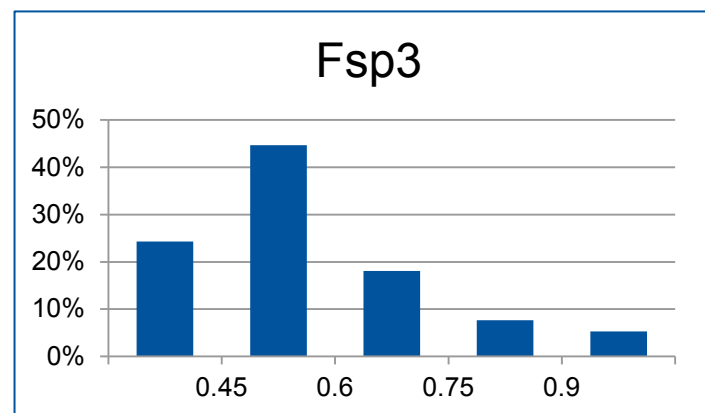
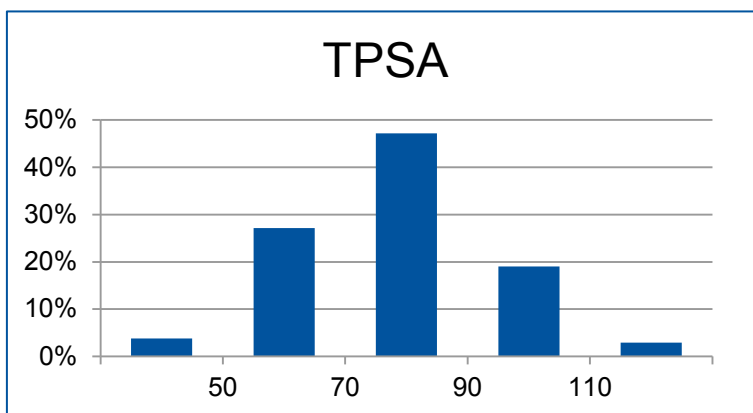
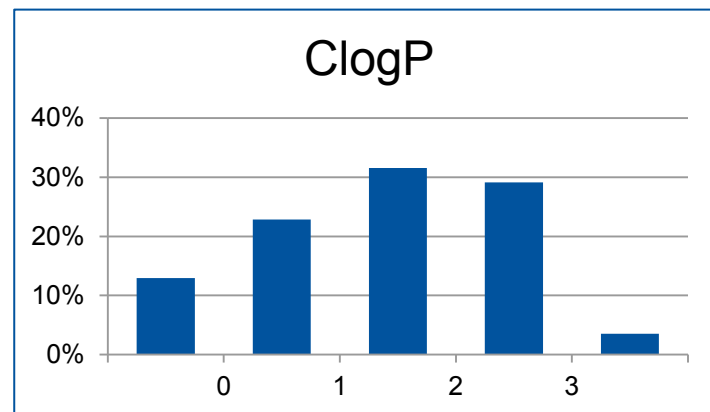
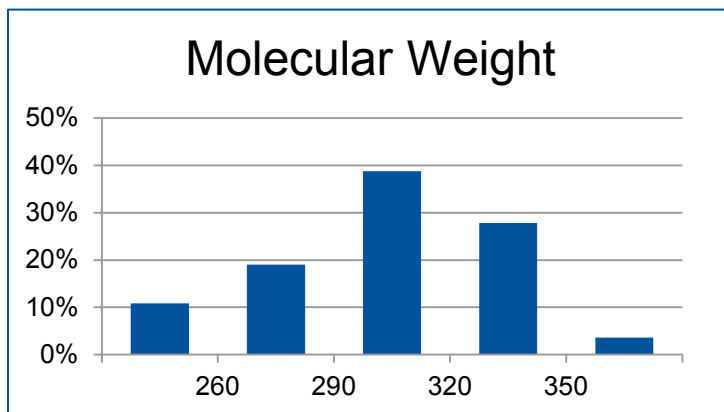


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Examples of Glycomimetics included in the library

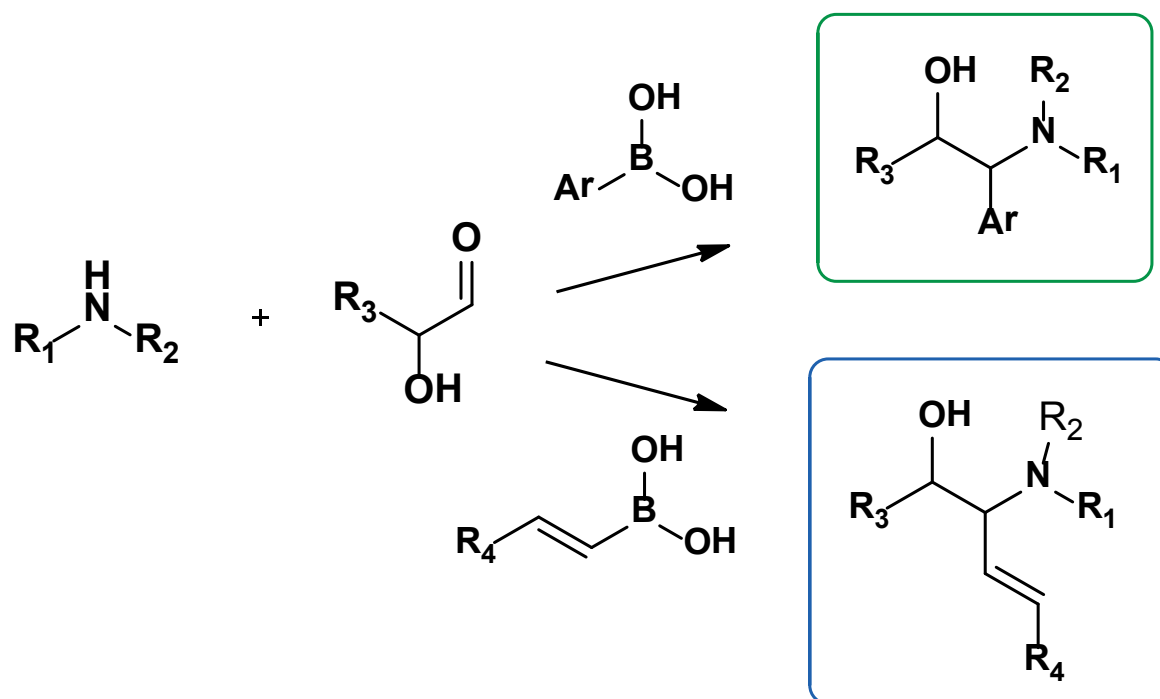


Molecular profile of the library



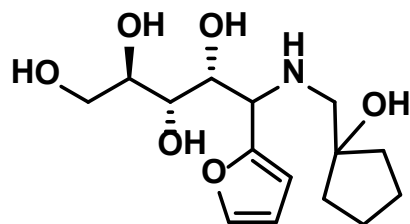
Synthesis of amino sugars *via* Petasis reaction

Validated synthetic approach, safe chemistry

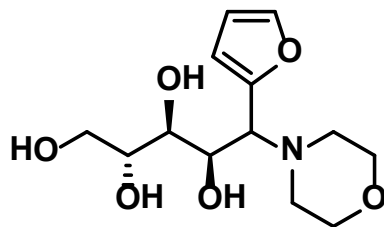


- Room temperature reaction without any additional reagents
- Solvents: water / acetonitrile

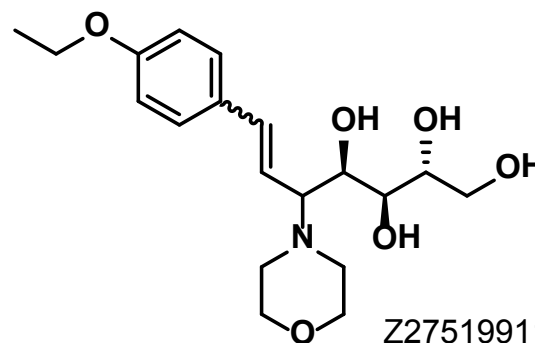
Examples of synthesized molecules



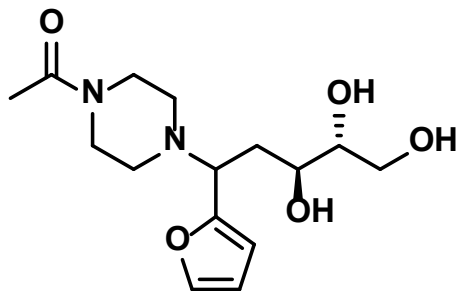
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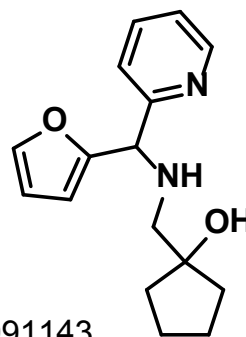
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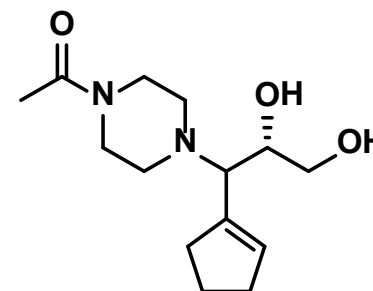
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Z2754391669



Z2751991143



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