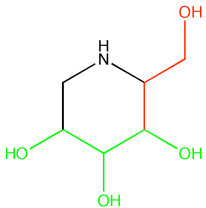
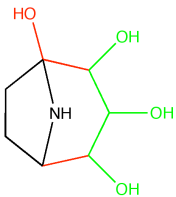
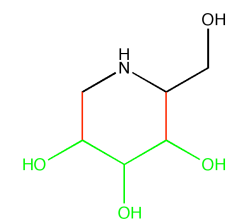


Table S3. Multiple common anchor substructures (blue) identified from weakly homologous threading templates for D-xylose isomerase from *Arthrobacter sp.* (PDB-ID: 1die) compared to the conserved substrate substructure reported by Chiang *et al.* (red). The overlap between both substructures is colored in green. The anchor substructures are presented for selected ligand clusters obtained for top-ranked binding pockets.

	Ligands	PDB-ID	SID [*]	TM-score/RMSD [†]	SCOP superfamily/family	EC [‡]
Target protein	 1-Deoxynojirmycin	1die	-	-	Xylose isomerase-like/ Xylose isomerase	5.3.1.5
Cluster: 1 Templates: 12 RMSD [§] : 3.49 Å	 Calystegine B2	2cbv	19.5%	0.53/4.65 Å	(Trans)glycosidases/ Family 1 of glycosyl hydrolase	3.2.1.21



1-Deoxynojirimycin

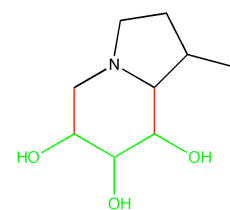
1oim

19.5%

0.53/4.64 Å

(Trans)glycosidases/
Family 1 of glycosyl hydrolase

3.2.1.21



Castanospermine

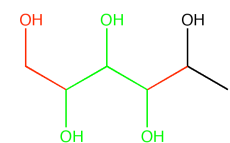
2cbu

19.7%

0.54/4.67 Å

(Trans)glycosidases/
Family 1 of glycosyl hydrolase

3.2.1.21



L-rhamnitol

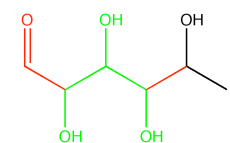
1de5

19.3%

0.68/3.45 Å

Xylose isomerase-like/
L-rhamnose isomerase

5.3.1.14



L-rhamnose

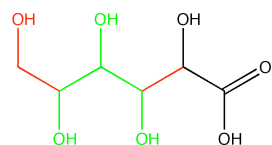
1de6

19.3%

0.68/3.50 Å

Xylose isomerase-like/
L-rhamnose isomerase

5.3.1.14



Gluconic acid

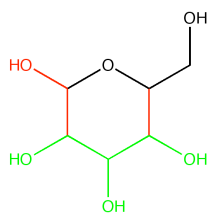
1bgg

18.8%

0.53/4.66 Å

(Trans)glycosidases/
Family 1 of glycosyl hydrolase

3.2.1.21



α-D-glucose

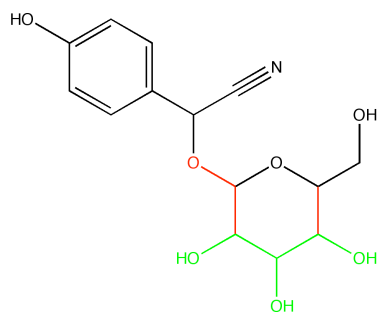
1hiz

16.4%

0.55/5.05 Å

(Trans)glycosidases/
Beta-glycanases

3.2.1.8



Dhurrin

1e55

20.1%

0.49/4.69 Å

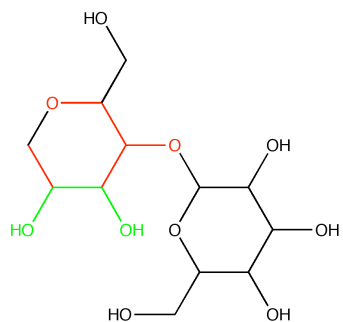
(Trans)glycosidases/
Family 1 of glycosyl hydrolase

3.2.1.21

Cluster: 2

Templates: 12

RMSD^S: 5.61 Å



β -D-mannose- α -D-mannose

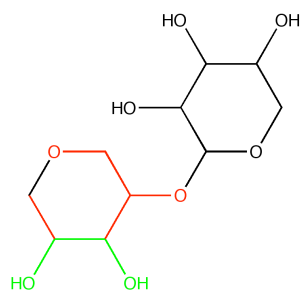
2man

15.3%

0.63/4.38 Å

(Trans)glycosidases/
Beta-glycanases

3.2.1.78



Xylobiose

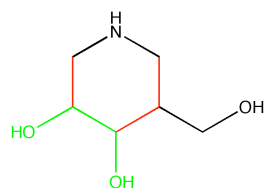
1vbr

17.9%

0.62/4.89 Å

(Trans)glycosidases/
Beta-glycanases

3.2.1.8



5-Hydroxymethyl-3,4-
dihydropiperidine

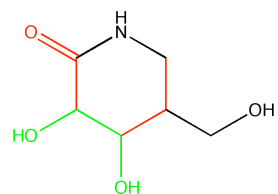
1oif

19.8%

0.53/4.61 Å

(Trans)glycosidases/
Family 1 of glycosyl hydrolase

3.2.1.21



(3S,4R,5R)-3,4-dihydroxy-5-(hydroxymethyl)piperidin-2-one

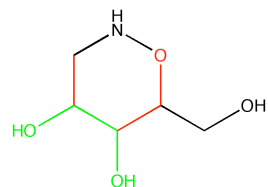
1uz4

19.2%

0.54/4.75 Å

(Trans)glycosidases/
Beta-glycanases

-



Tetrahydrooxazine

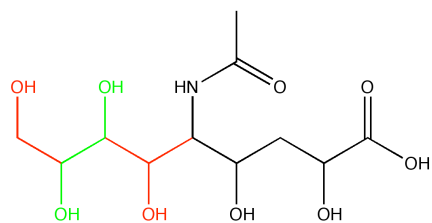
1w3j

19.3%

0.53/4.62 Å

(Trans)glycosidases/
Beta-glycanases

3.2.1.21



2,4,6,7,8,9-Hexahydroxy-5-methylcarboxamido nonanoic acid

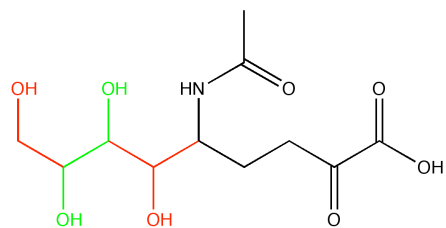
1f73

17.5%

0.59/3.92 Å

Aldolase/Class I aldolase

4.1.3.3



6,7,8,9-Tetrahydroxy-5-methylcarboxamido-2-oxononanoic acid

1f74

17.5%

0.58/4.11 Å

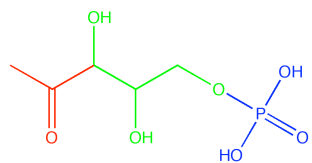
Aldolase/Class I aldolase

4.1.3.3

Cluster: 3

Templates: 12

RMSD^S: 3.86 Å



1-Deoxy-D-xylulose-5-phosphate

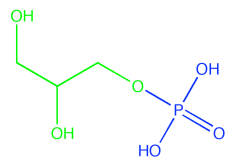
1ixn

19.6%

0.69/3.76 Å

Pyridoxine 5'-phosphate
synthase/
Pyridoxine 5'-phosphate
synthase

-



Glycerol-3-phosphate

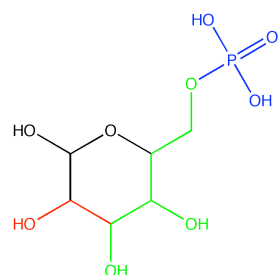
1ixo

19.3%

0.71/3.78 Å

Pyridoxine 5'-phosphate
synthase/
Pyridoxine 5'-phosphate
synthase

-



β -Galactose-6-phosphate

4pbg

21.2%

0.51/4.49 Å

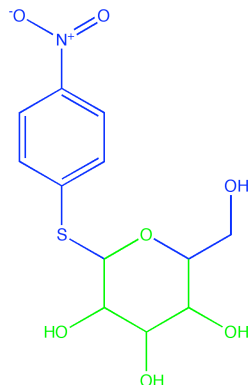
(Trans)glycosidases/
Family 1 of glycosyl hydrolase

3.2.1.85

Cluster: 4

Templates: 2

RMSD[§]: 0.71 Å



Para-nitrophenyl-1-thio- β -D-glucopyranoside

1e1f

19.5%

0.49/4.67 Å

(Trans)glycosidases/
Family 1 of glycosyl hydrolase

3.2.1.21

*Sequence identity. [†]TM-score and C α RMSD of the aligned region reported by TM-align. [‡]Enzyme Commission nomenclature. [§]Average pairwise RMSD of the anchor heavy atoms calculated for all ligands that belong to a particular cluster.