

a) **tab1**

Query Structure Parameter Settings About Auto-CHO

Edit Glycan by GlycanBuilder Search Building Block Library Globo-H SSEA-4 OligoLacNAc

btn1

GlycanBuilder

File Edit Structure View Help

Linkage ? ? ? ? ? Chirality ? Ring ? 2nd bond ? ? ? ?

m/z: 1491.7302 [MONO,perMe,Na,0,freeEnd]

b) **tab7**

Result Visualization Result Text

Save Result Text

btn4

Building Blocks for Searching: ALL
Block(s) for Searching:
GalNAc[NPhth,OH,OCIAc,OTIPS] PredictedRRV=11.971
Index9941 GalNAc[NPhth,OH,NO2Bz,OTBDPS] PredictedRRV=25.804
Index10735 GalNAc[NPhth,OH,NO2Bz,OTBS] PredictedRRV=29.159
Index15044 GalNAc[NPhth,OH,OTBDPS,OCIAc] PredictedRRV=55.4

RESULT:
ResidueID:[110041] Sugar:[D-Glc-b] ParentID:[Root] ChildID:[Pos4=ID110042]
--
ResidueID:[110042] Sugar:[D-Gal-b] ParentID:[110041] ChildID:[Pos4=ID110043]
--
ResidueID:[110043] Sugar:[D-Gal-a] ParentID:[110042] ChildID:[Pos3=ID110044]
--
ResidueID:[110044] Sugar:[D-GalNAc-b] ParentID:[110043] ChildID:[Pos3=ID110045]

Solution 1:
Fragment 1[Fragment Yield=94%][Deprotect=N/A][HasSatbleProductAnomer=Yes][LeavingGroup=STol]
BBL RRV=1462.00 Type=Exp. Index=117 ProtectingGroup=[2:OBz,3:2,4:OPh,5:-,6:OPh]
BBL RRV=32.00 Type=Exp. Index=45 ProtectingGroup=[2:NHTroc,3:OH,4:OBz,5:-,6:OBz]

Solution 2:
Fragment 1[Fragment Yield=94%][Deprotect=N/A][HasSatbleProductAnomer=Yes][LeavingGroup=STol]
BBL RRV=1306.00 Type=Exp. Index=114 ProtectingGroup=[2:OLev,3:2,4:OPh,5:-,6:OPh]
BBL RRV=32.00 Type=Exp. Index=45 ProtectingGroup=[2:NHTroc,3:OH,4:OBz,5:-,6:OBz]

Done

c) **tab5**

Experimental Building Block Library Virtual Building Block Library

Library for Searching

Use Experimental Library Only
Use Experimental and Virtual Libraries

Filtering **Filtering Options**

Sugar Type Gal Glc Man GalNAc GlcNAc GlcN GlcA

Product Anomer Alpha Beta

R2 ALL OH OAc OBn OBz OCIAc OLev NO2Bz OPMB OTBDPS >>

R3 ALL OH OAc OBn OBz OCIAc OLev NO2Bz OPMB OTBDPS >>

R4 ALL OH OAc OBn OBz OCIAc OLev NO2Bz OPMB OTBDPS >>

R6 ALL OH OAc OBn OBz OCIAc OLev NO2Bz OPMB OTBDPS >>

btn5 **btn6** **btn7**

Show Selected Virtual BBL(s) Show Filtered Virtual BBL(s) Show All Virtual BBLs

Selection	Sugar Type	Product Anomer	R2	R3	R4	R6	Predicted RRV	Feedback [BBL ID]
☐	GalNAc	Beta	NPhth	OH	OCIAc	OTBS	6.774	To rate [3666]
☐	GalNAc	Beta	NPhth	OH	OCIAc	OCIAc	8.366	To rate [4393]
☐	GalNAc	Beta	NPhth	OH	NO2Bz	NO2Bz	9.42	To rate [4849]
☐	GalNAc	Beta	NPhth	OH	OCIAc	OTBDPS	9.516	To rate [4891]
☒	GalNAc	Beta	NPhth	OH	OCIAc	OTIPS	11.971	To rate [5885]
☐	GalNAc	Beta	NPhth	OH	OBz	OBz	14.324	To rate [6715]
☐	GalNAc	Beta	NPhth	OH	NO2Bz	OCIAc	15.354	To rate [7068]
☐	GalNAc	Beta	NPhth	OH	OBz	OCIAc	15.775	To rate [7216]
☐	GalNAc	Beta	NPhth	OH	OCIAc	OBz	16.861	To rate [7588]
☐	GalNAc	Beta	NPhth	OH	NO2Bz	OBz	16.942	To rate [7611]
☐	GalNAc	Beta	NPhth	OH	OCIAc	NO2Bz	17.748	To rate [7851]
☐	GalNAc	Beta	NPhth	OH	OBz	NO2Bz	20.016	To rate [8492]
☐	GalNAc	Beta	NPhth	OH	OBz	OTBS	21.088	To rate [8769]
☐	GalNAc	Beta	NPhth	OH	OBz	OTBDPS	22.91	To rate [9253]
☒	GalNAc	Beta	NPhth	OH	NO2Bz	OTBDPS	25.804	To rate [9942]
☒	GalNAc	Beta	NPhth	OH	NO2Bz	OTBS	29.159	To rate [10736]
☐	GalNAc	Beta	NPhth	OH	OTBS	OCIAc	44.817	To rate [13596]
☐	GalNAc	Beta	NPhth	OH	OBz	OTIPS	48.94	To rate [14190]