

(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]

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ResidueID:[110042] Sugar:[D-Gal-b] ParentID:[110041] ChildID:[Pos4=ID110043]

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ResidueID:[110043] Sugar:[D-Gal-a] ParentID:[110042] ChildID:[Pos3=ID110044]

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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]