Supporting information for:
Selective inhibitors of human neuraminidase 1 (NEU1)

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Protein expression

Optimized Neu3 and Neu4 genes were synthesized and subcloned into vector pMAL-c2x in DNA2.0. The plasmids of MBP-Neu3 and MBP-Neu4 were transformed into expression cells, *E. coli* TB1. Protein was isolated by culturing *E. coli* TB1 cells containing plasmid pMBP-*Neu3* or *Neu4* in LB medium containing 0.2% glucose and ampicillin (100 μg/mL). The culture was grown at 30 °C with shaking until the OD_{600} reached 0.3. The temperature was decreased to 20 °C, and fusion protein was induced by adding IPTG to a final concentration of 0.3 mM when OD_{600} reached 0.5-0.6. Cells were harvested by centrifugation after 20 h of induction. The pellet was resuspended (50 mL per liter of medium) in resuspension buffer (20 mM MOPS, pH 7.2, 300 mM NaCl, 1mM EDTA, 10% glycerol and 0.05% triton X-100) and supplemented with a protease inhibitor tablet (Roche). The lysate was passed through a cell disruptor once at 20,000 psi and then immediately pelleted by centrifugation at 105,000 x g for 60 min at 4 °C. The supernatant was loaded onto an amylose column (New England Biolabs) equilibrated with 20 mM MOPS (10% glycerol and 300 mM NaCl, pH 7.2). MBP-fusion protein was eluted with running buffer containing 10% glycerol (v/v) and 10 mM maltose.

Table S1: HPLC Gradient elution used to check purity of inhibitors

Purity of compounds for enzymatic assay was tested by HPLC using a C18 reverse phase column (XTerra RP C18, analytical, particle size: 3.5 μm, column dimensions: 4.8 × 150 mm). The gradient elution program was summarized below where solvent A was 0.1% trifluoroacetic acid in milliQ water and solvent B was 0.1% trifluoroacetic acid in acetonitrile. See Figure S4 for HPLC traces.

Time	Flow rate (mL/min)	A%	B%
0	1	100	0
3	1	100	0
13	1	0	100
18	1	0	100

Table S2: Summary of HPLC and HRMS data for tested compounds

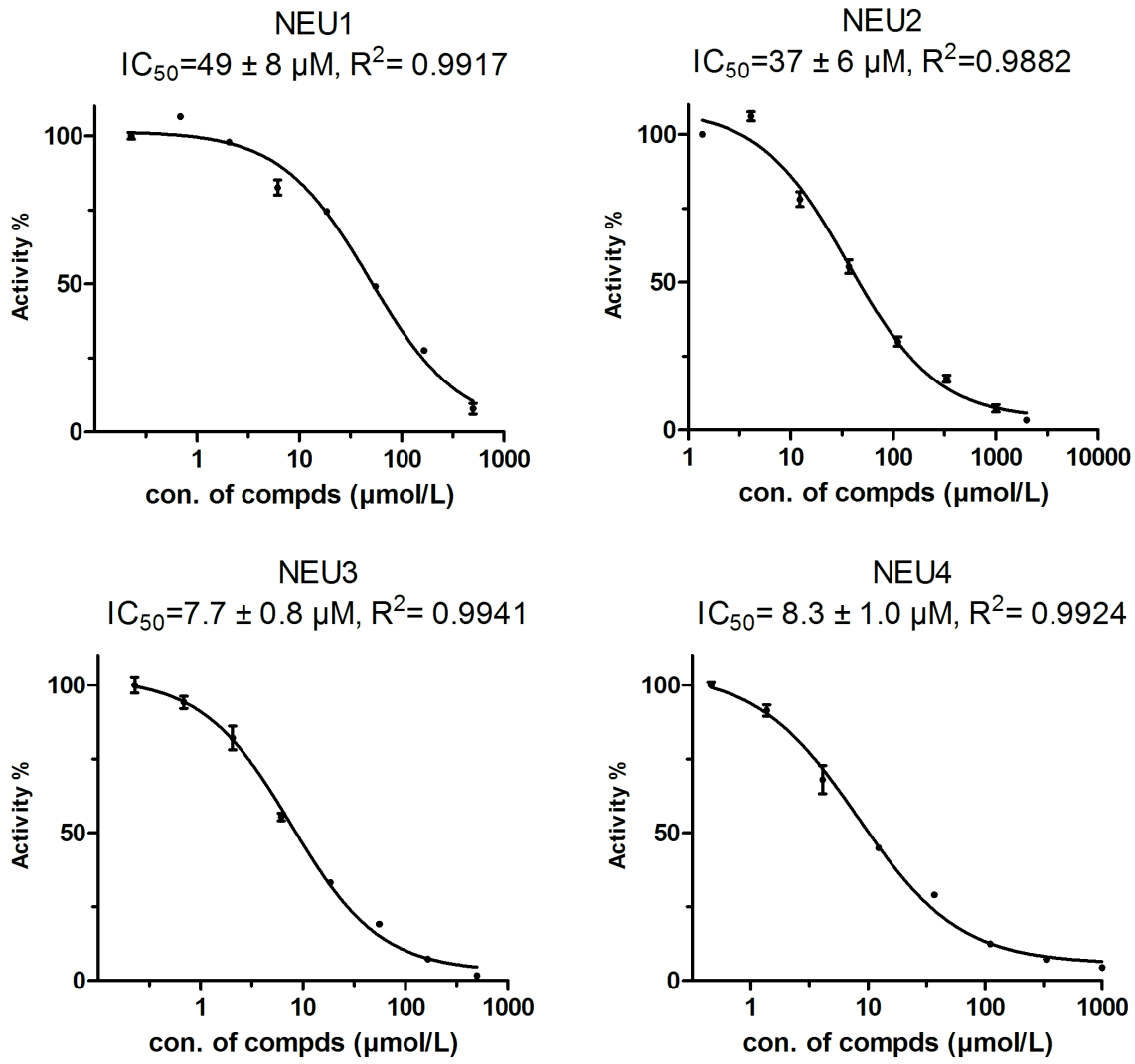
Compound	HPLC Trace		HRMS	
	Retention Time min	Area %	Calculated m/z	Found m/z
DANA (1)	1.657	98.70	290.0876	290.0879
Neu5AcN$_3$2en (6)	2.208	97.67	331.0890	331.0894
C9-BA-DANA (8)	1.864	99.97	373.1616	373.1614
11a	2.115	99.71	304.1032	304.1039
11b	3.562	96.09	318.1189	318.1196
11c	8.546	97.15	332.1345	332.1348
11d	9.866	98.07	346.1507	346.1506
11e	10.696	99.05	360.1664	360.1665
11f	3.586	99.13	318.1194	318.1193
11g	7.692	97.26	333.1351	333.1348
11h	9.950	97.93	346.1507	346.1496
11i	3.188	96.35	316.1032	316.1030
11j	4.858	95.21	330.1189	330.1195
11k	9.295	99.36	352.1038	352.1035
11l	1.667	98.98	347.1460	347.1458
13a	8.342	96.24	448.1468	448.1481
13b	11.757	96.96	490.1574	490.1584
13c	5.140	99.78	448.1468	448.1481
13d	10.781	99.32	447.1516	447.1520
13e	13.667	97.20	463.1465	463.1471
13f	13.872	95.09	451.1265	451.1271
13g	13.403	95.96	501.1233	501.1243

13h	12.199	97.12	477.1258	477.1268
13i	11.645	96.35	427.1834	427.1837
15a	8.088	97.62	359.1460	359.1453
15b	11.240	96.84	387.1773	387.1766
15c	12.120	96.14	401.1929	401.1931
15d	6.950	95.86	359.1460	359.1458
15e	10.131	95.32	373.1616	373.1617
15f	10.456	96.86	387.1773	387.1765
15g	10.141	97.23	393.1303	393.1302
15h	11.757	96.96	450.1518	450.1525
15i	4.455	99.32	408.1412	408.1415
15j	9.600	95.50	450.1518	450.1515
15k	5.202	97.68	408.1412	408.1411
15l	9.447	96.58	549.2202	549.2207
15m	11.753	99.59	411.1885	411.1889
17a	12.937	98.19	443.2399	443.2396
17b	10.757	96.19	415.2086	415.2081
17c	11.769	99.89	387.1773	387.1770
17d	12.273	99.58	401.1929	401.1926
17e	11.351	98.88	373.1616	373.1615
17f	12.030	97.16	387.1773	387.1774
17g	12.084	96.27	401.1929	401.1929
17h	12.363	97.55	415.2086	415.2088
22	9.353	97.76	387.1885	387.1879

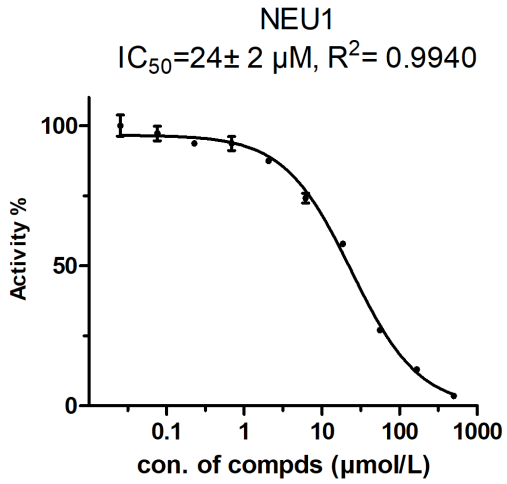
Figure S1: Inhibition of human neuraminidase isoforms

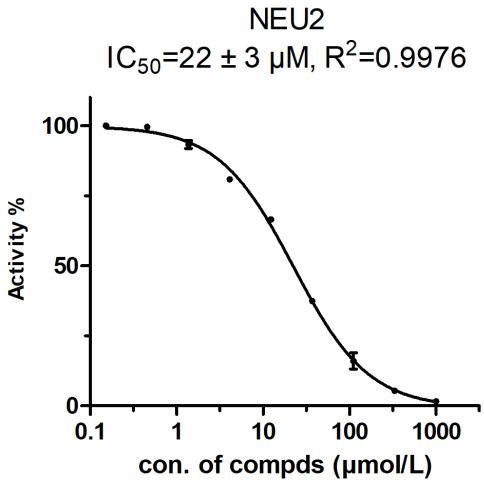
IC_{50} curves using 4MU-NANA as substrate

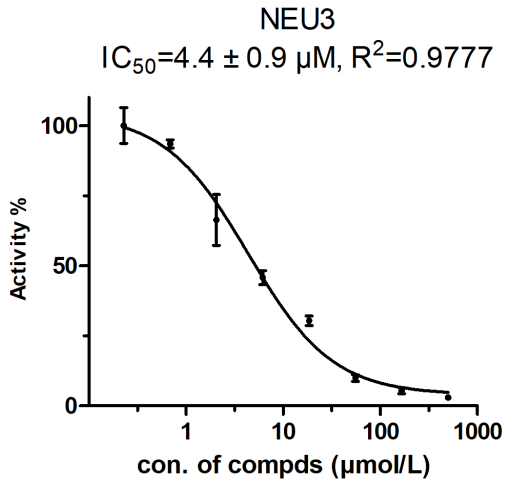
1(DANA)

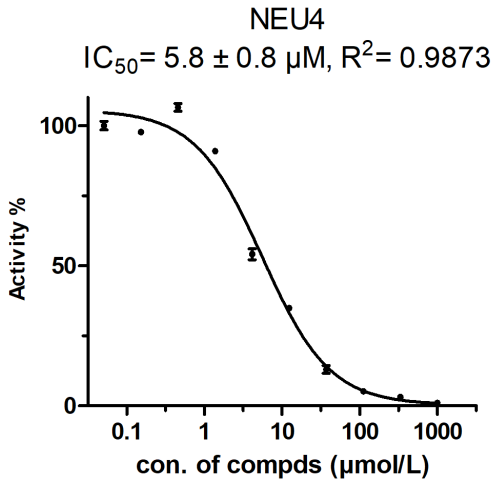


6(Neu5AcN$_3$2en)

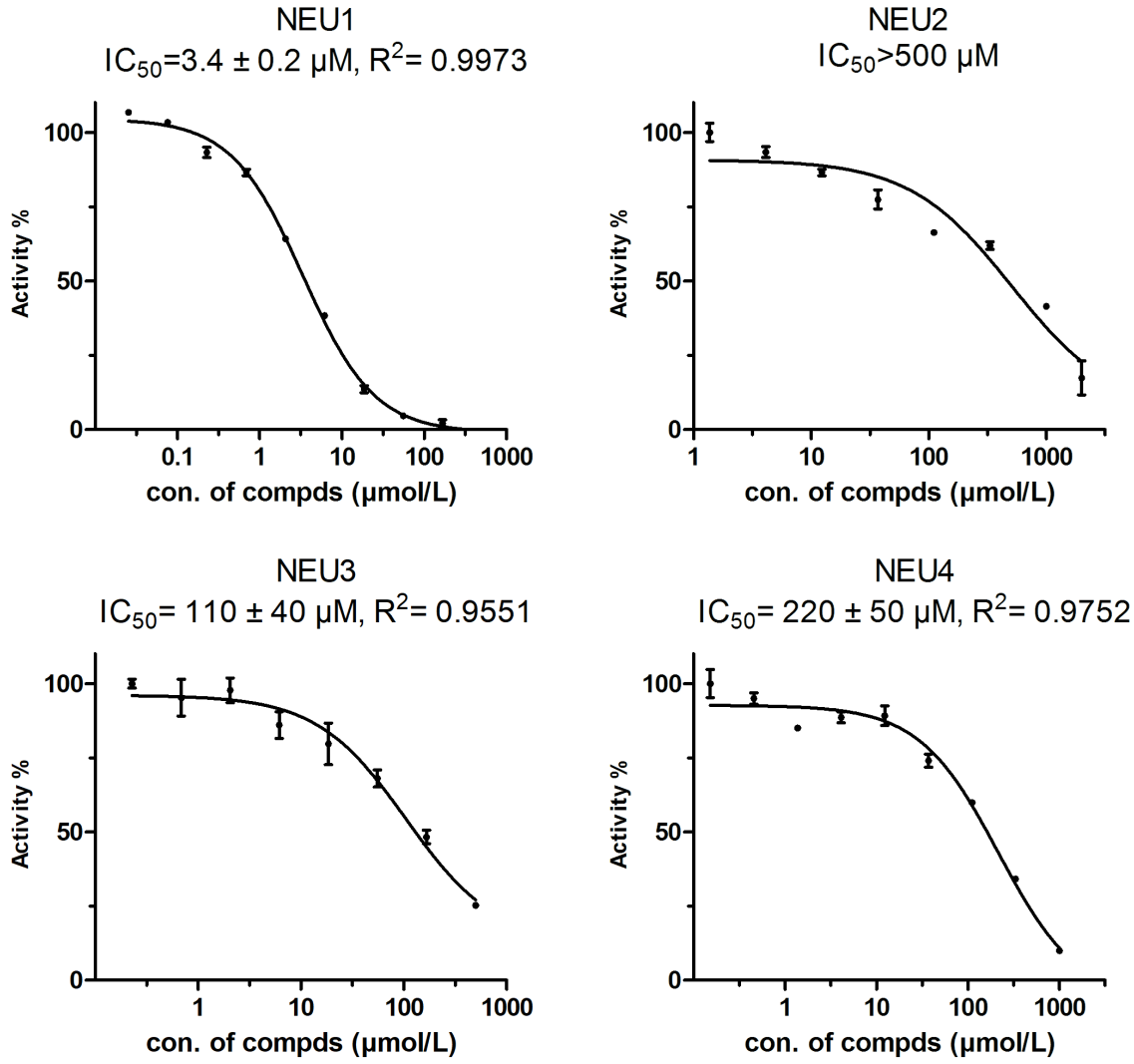




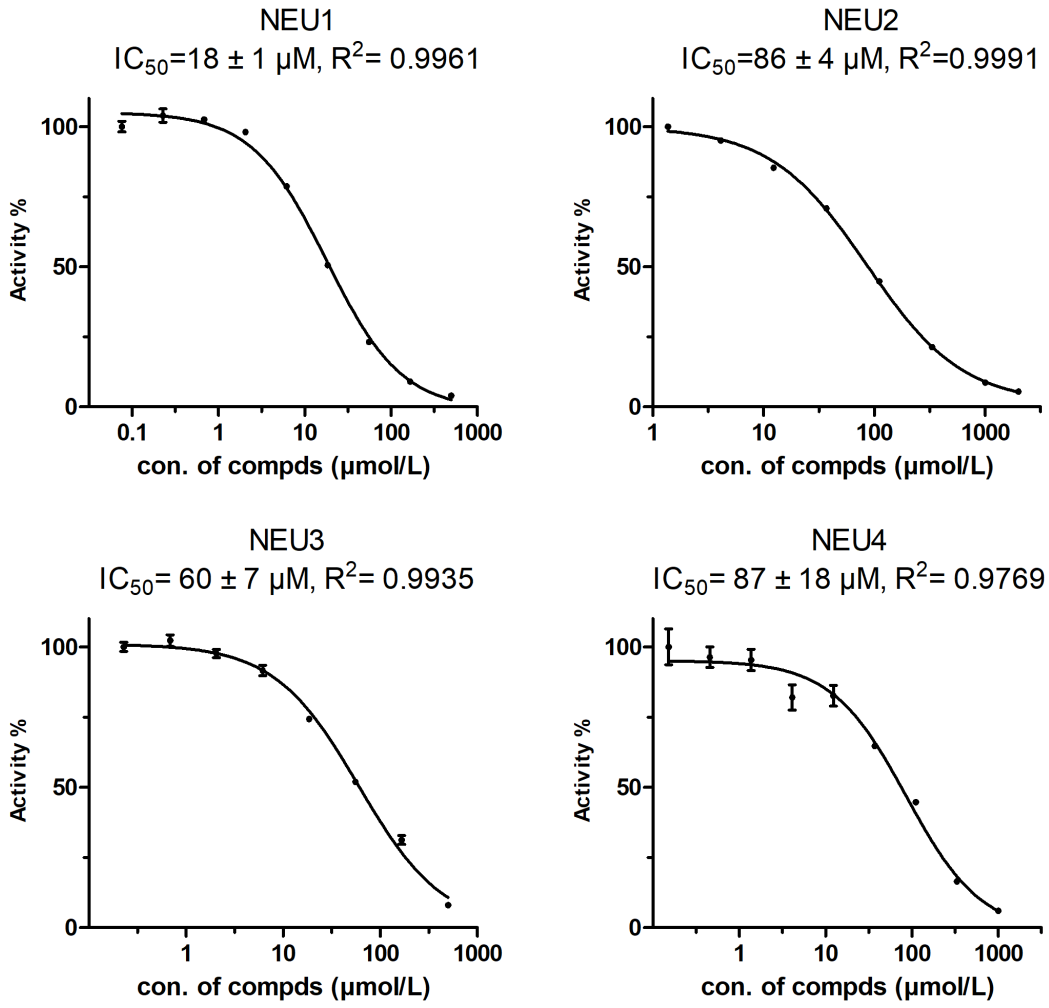




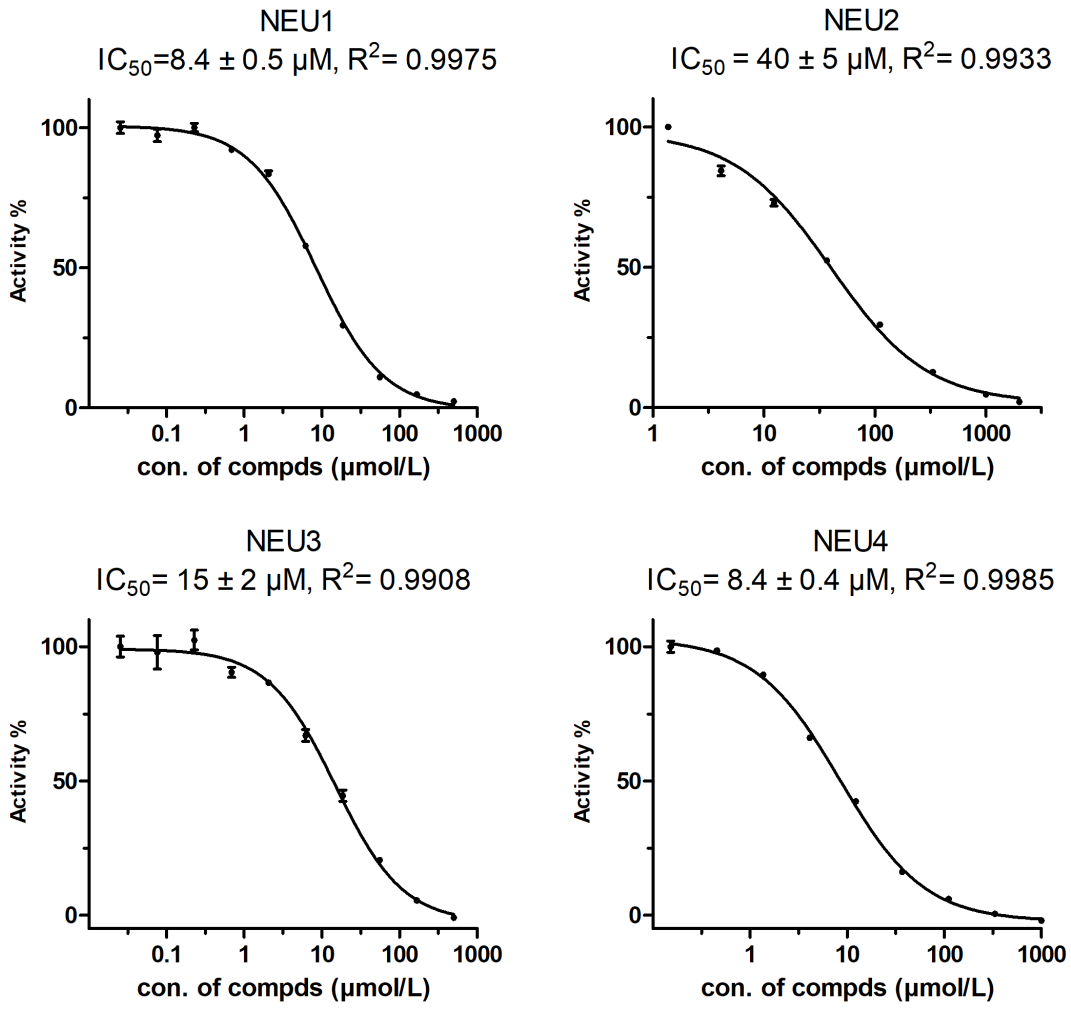
8(C9-BA-DANA)


NEU1
IC50=3.4 ± 0.2 μM, R2= 0.9973
Activity %
con. of compds (μmol/L)
NEU2
IC50>500 μM
Activity %
con. of compds (μmol/L)
NEU3
IC50= 110 ± 40 μM, R2= 0.9551
Activity %
con. of compds (μmol/L)
NEU4
IC50= 220 ± 50 μM, R2= 0.9752
Activity %
con. of compds (μmol/L)

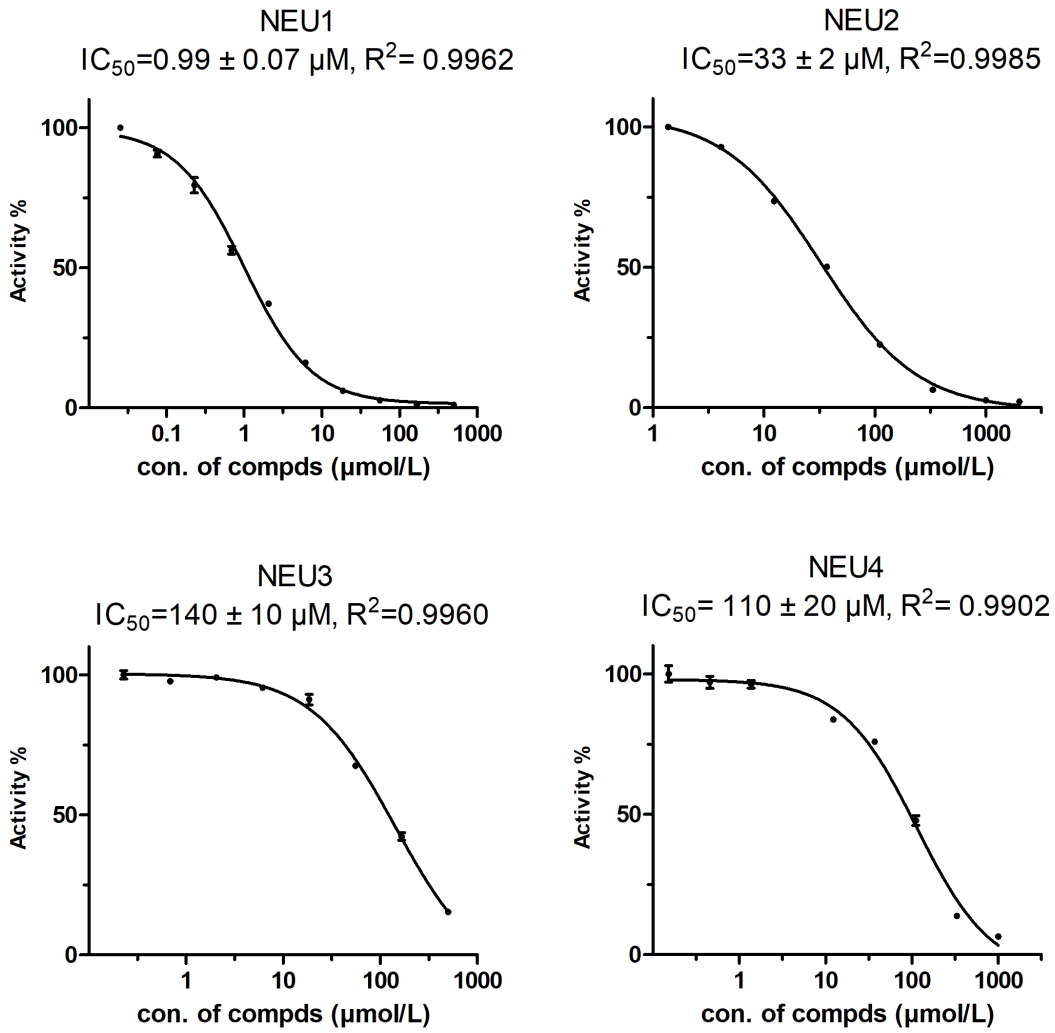
11a


NEU1
IC50=18 ± 1 μM, R2= 0.9961
NEU2
IC50=86 ± 4 μM, R2=0.9991
NEU3
IC50= 60 ± 7 μM, R2= 0.9935
NEU4
IC50= 87 ± 18 μM, R2= 0.9769
Activity %
con. of compds (μmol/L)

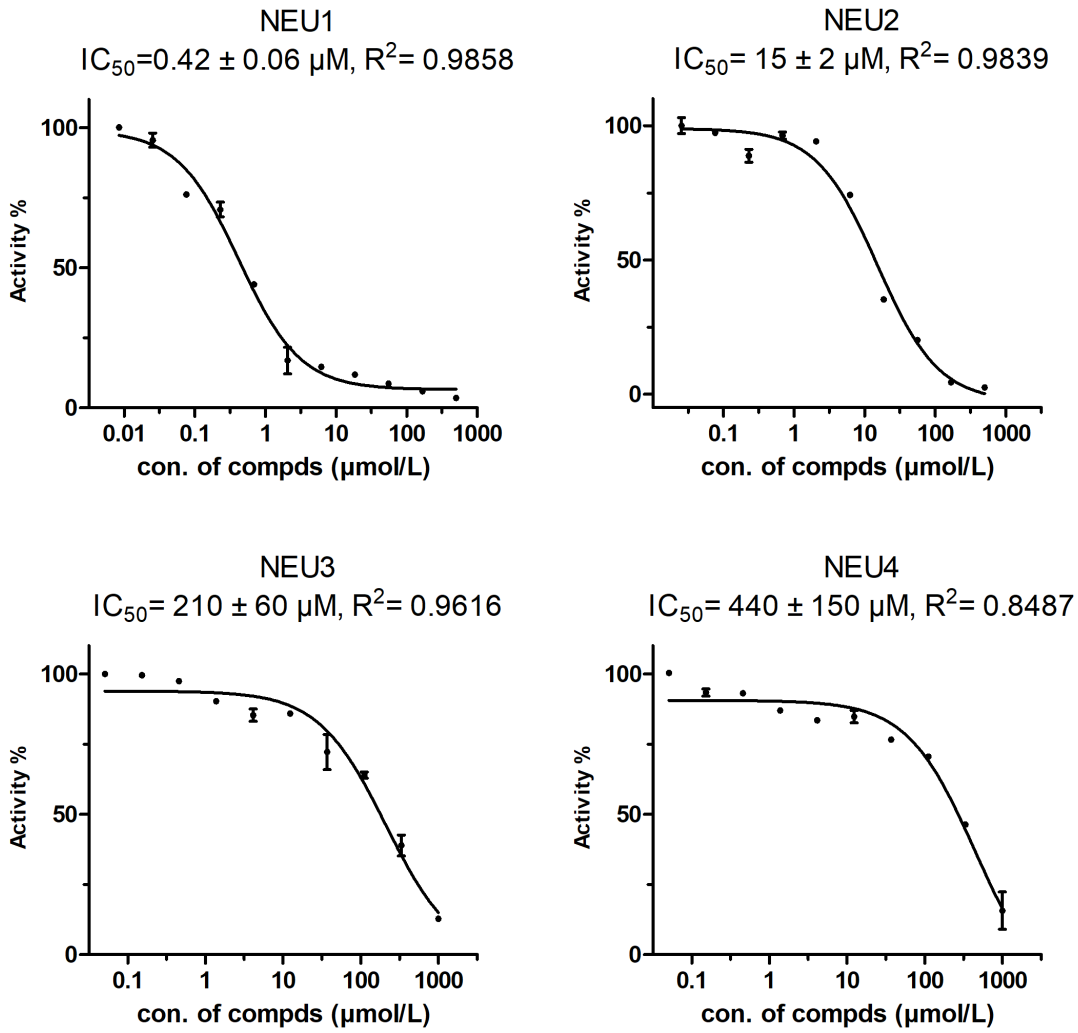
11b


NEU1
IC50=8.4 ± 0.5 μM, R2= 0.9975
NEU2
IC50 = 40 ± 5 μM, R2= 0.9933
NEU3
IC50= 15 ± 2 μM, R2= 0.9908
NEU4
IC50= 8.4 ± 0.4 μM, R2= 0.9985
Activity %
con. of compds (μmol/L)

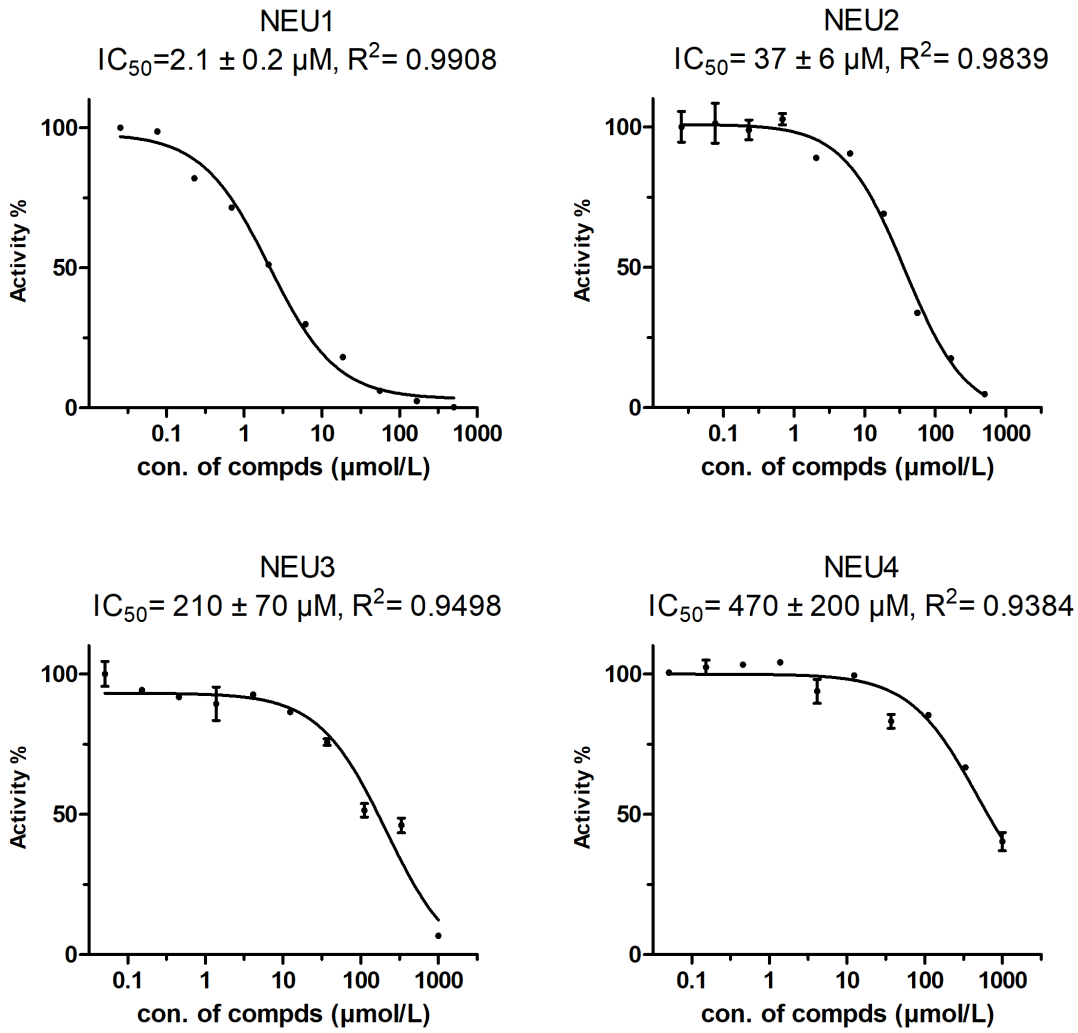
11c


NEU1
IC50=0.99 ± 0.07 μM, R2= 0.9962
NEU2
IC50=33 ± 2 μM, R2=0.9985
NEU3
IC50=140 ± 10 μM, R2=0.9960
NEU4
IC50= 110 ± 20 μM, R2= 0.9902
Activity %
con. of compds (μmol/L)

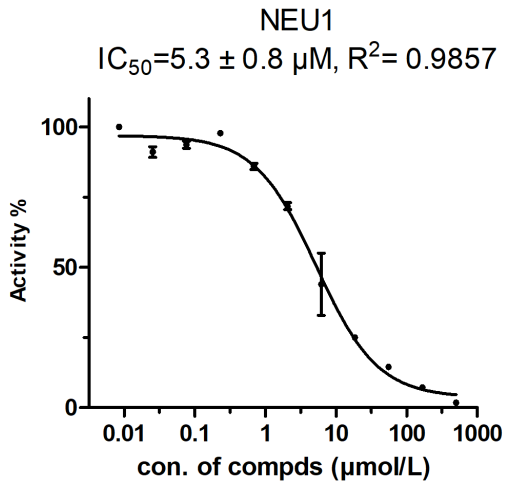
11d

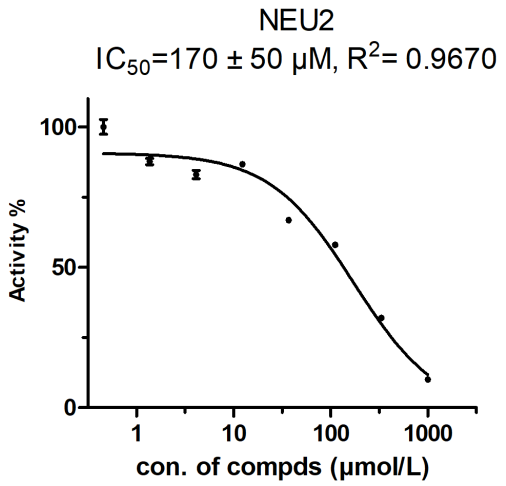

NEU1
IC50=0.42 ± 0.06 μM, R2= 0.9858
NEU2
IC50= 15 ± 2 μM, R2= 0.9839
NEU3
IC50= 210 ± 60 μM, R2= 0.9616
NEU4
IC50= 440 ± 150 μM, R2= 0.8487
Activity %
con. of compds (μmol/L)

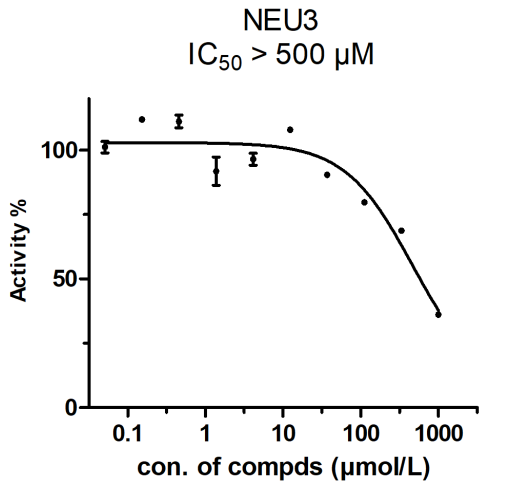
11e

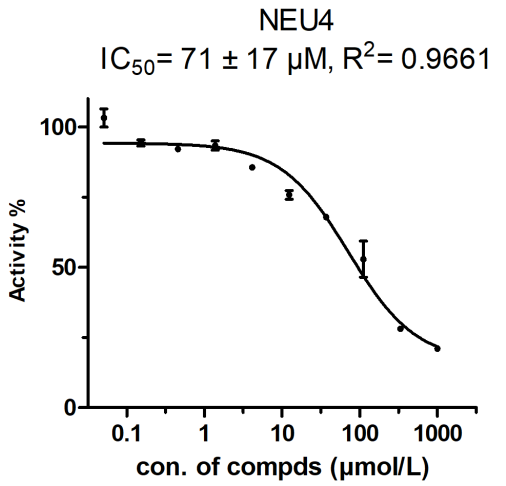

NEU1
IC50=2.1 ± 0.2 μM, R2= 0.9908
NEU2
IC50= 37 ± 6 μM, R2= 0.9839
NEU3
IC50= 210 ± 70 μM, R2= 0.9498
NEU4
IC50= 470 ± 200 μM, R2= 0.9384
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

11f

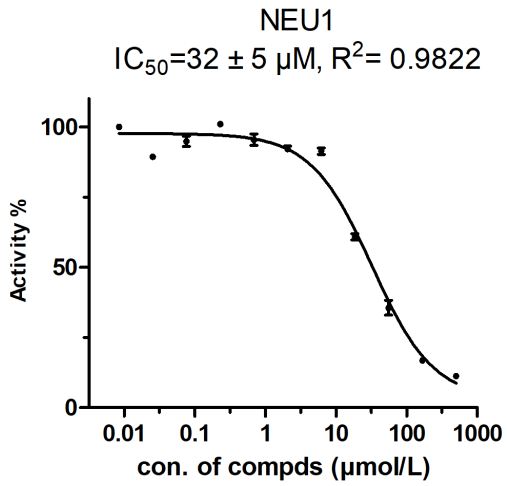

NEU1
IC50=5.3 ± 0.8 μM, R2= 0.9857
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)

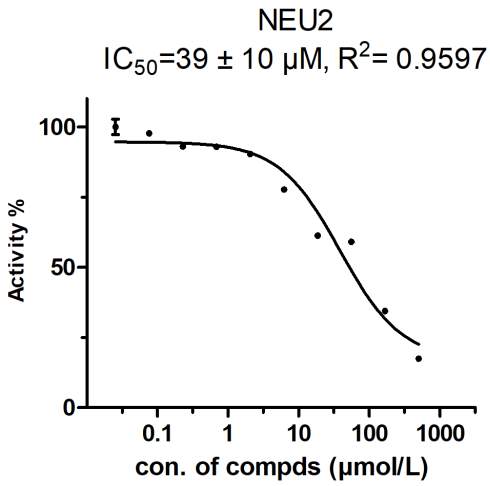

NEU2
IC50=170 ± 50 μM, R2= 0.9670
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

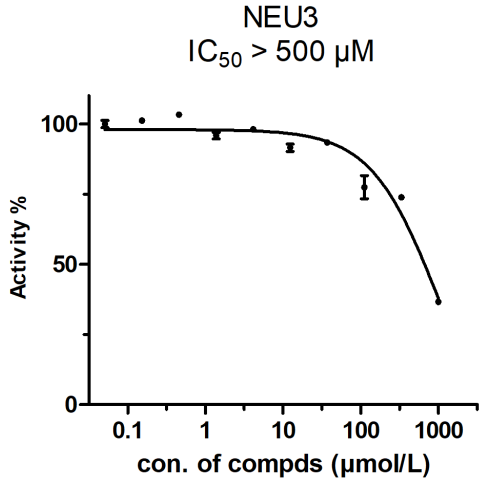

NEU3
IC50 > 500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

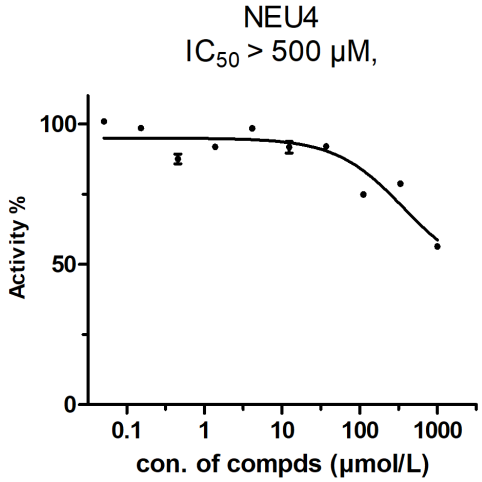

NEU4
IC50= 71 ± 17 μM, R2= 0.9661
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

11g

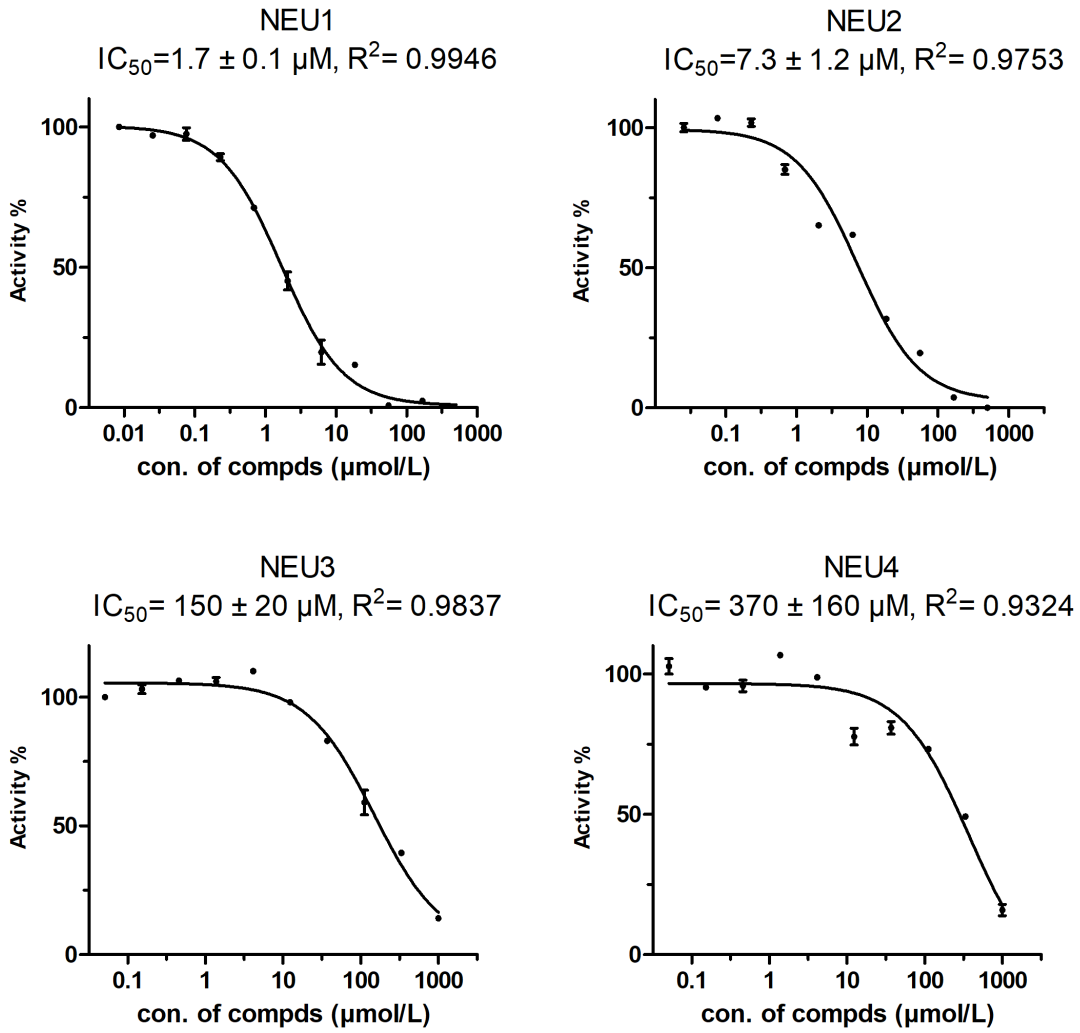

NEU1
IC50=32 ± 5 μM, R2= 0.9822
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50=39 ± 10 μM, R2= 0.9597
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

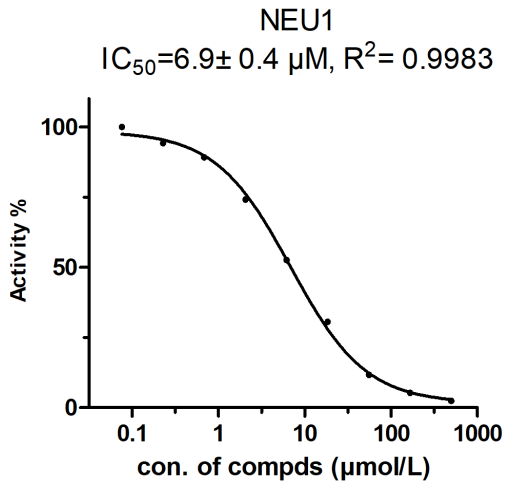

NEU3
IC50 > 500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

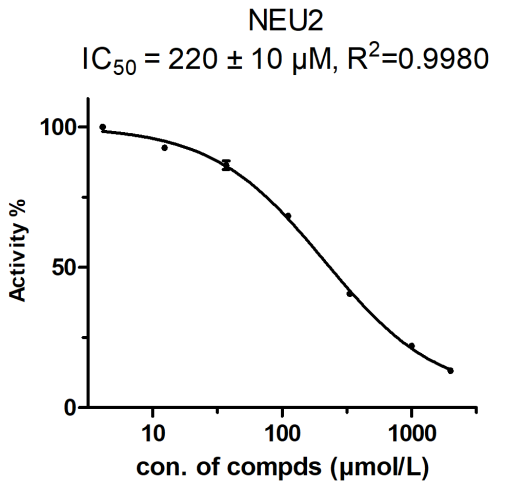

NEU4
IC50 > 500 μM,
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

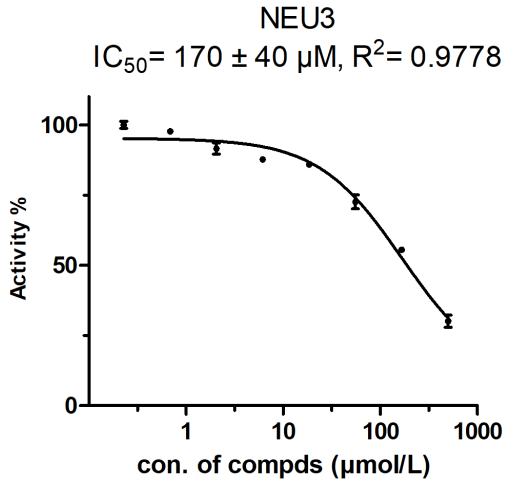
11h

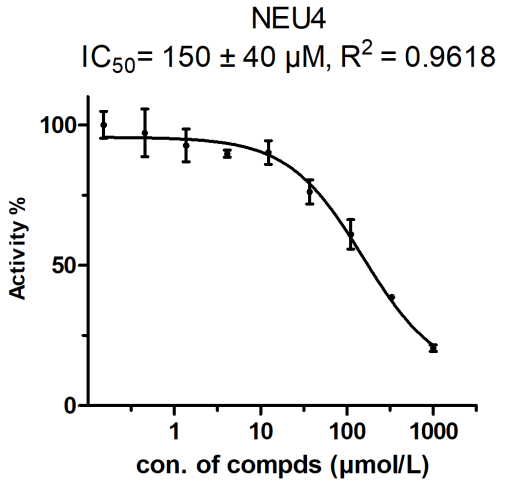

NEU1
IC50=1.7 ± 0.1 μM, R2= 0.9946
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50=7.3 ± 1.2 μM, R2= 0.9753
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 150 ± 20 μM, R2= 0.9837
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50= 370 ± 160 μM, R2= 0.9324
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

11i

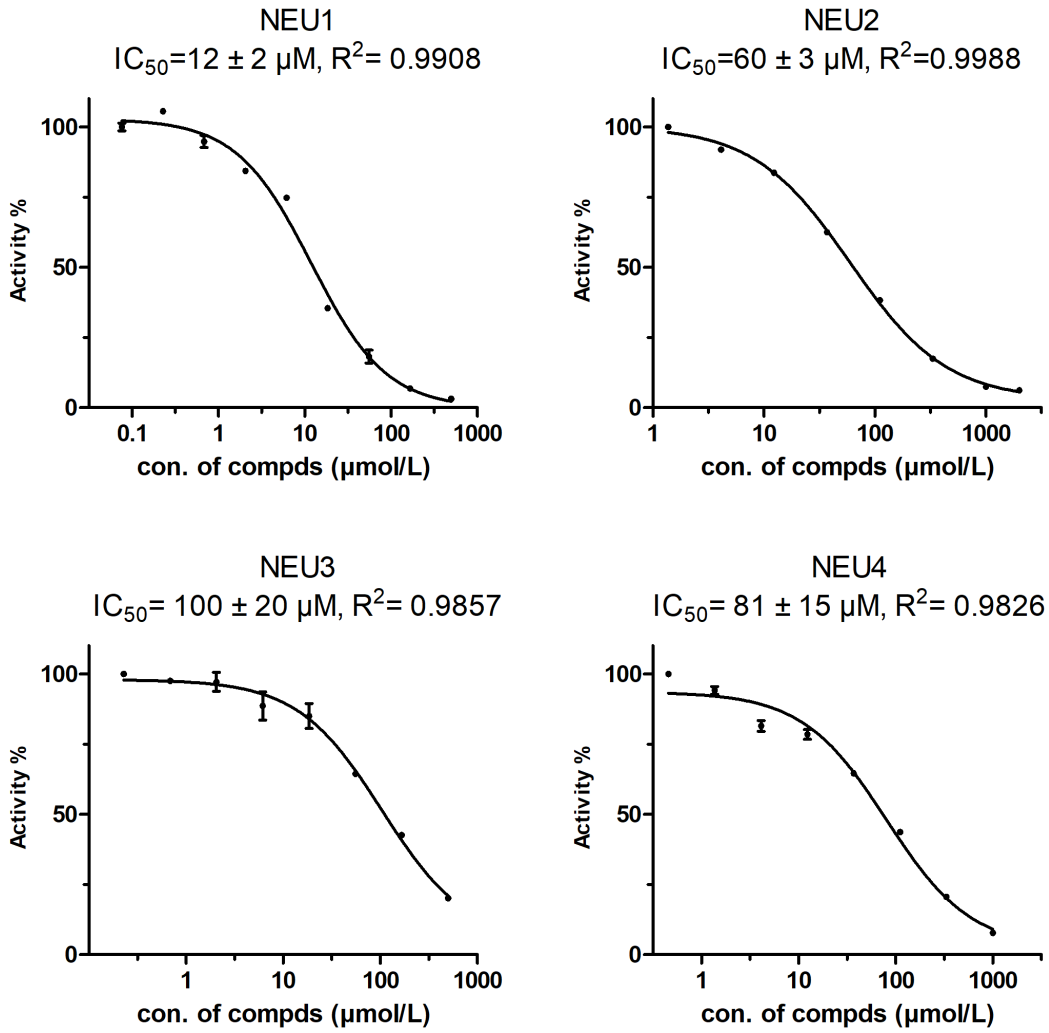

NEU1
IC50=6.9± 0.4 μM, R2= 0.9983
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50 = 220 ± 10 μM, R2=0.9980
Activity %
100
50
0
10
100
1000
con. of compds (μmol/L)

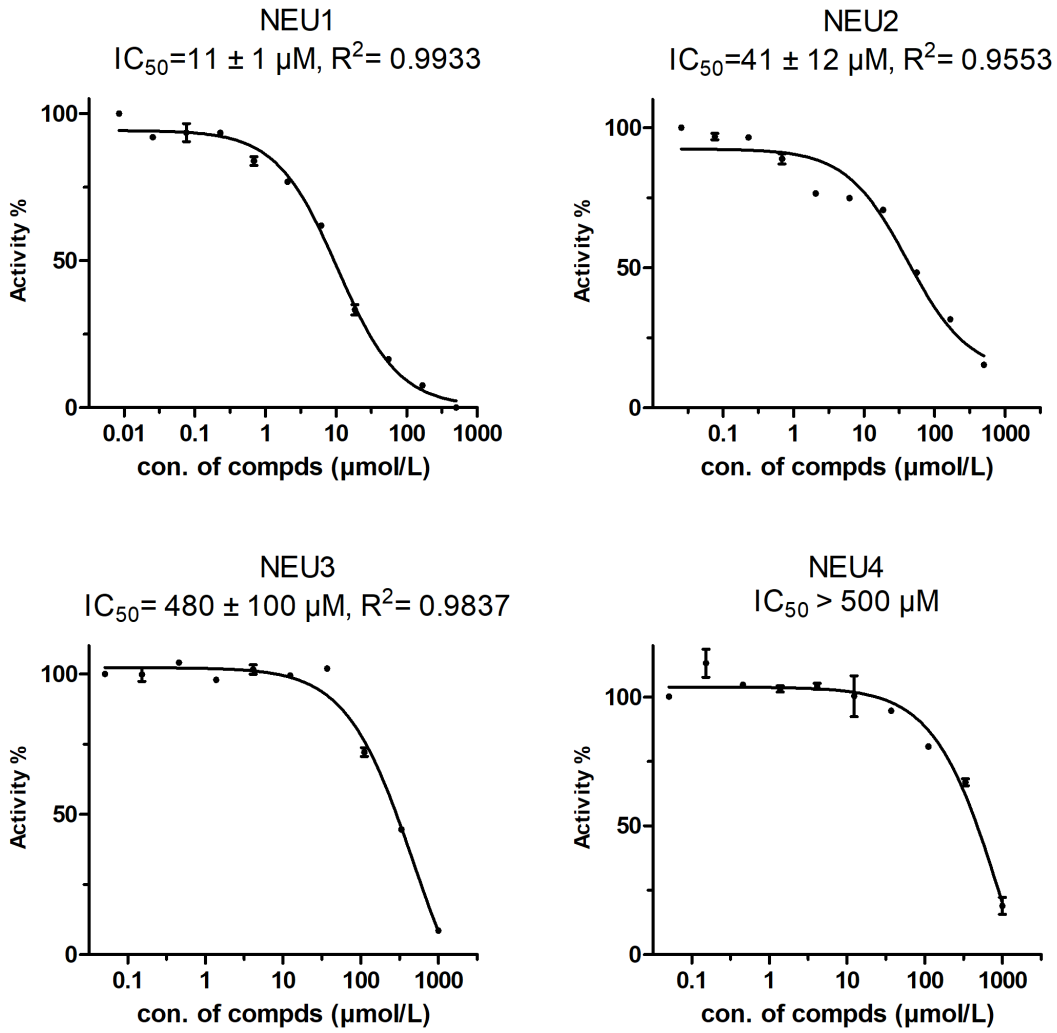

NEU3
IC50= 170 ± 40 μM, R2= 0.9778
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)


NEU4
IC50= 150 ± 40 μM, R2 = 0.9618
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

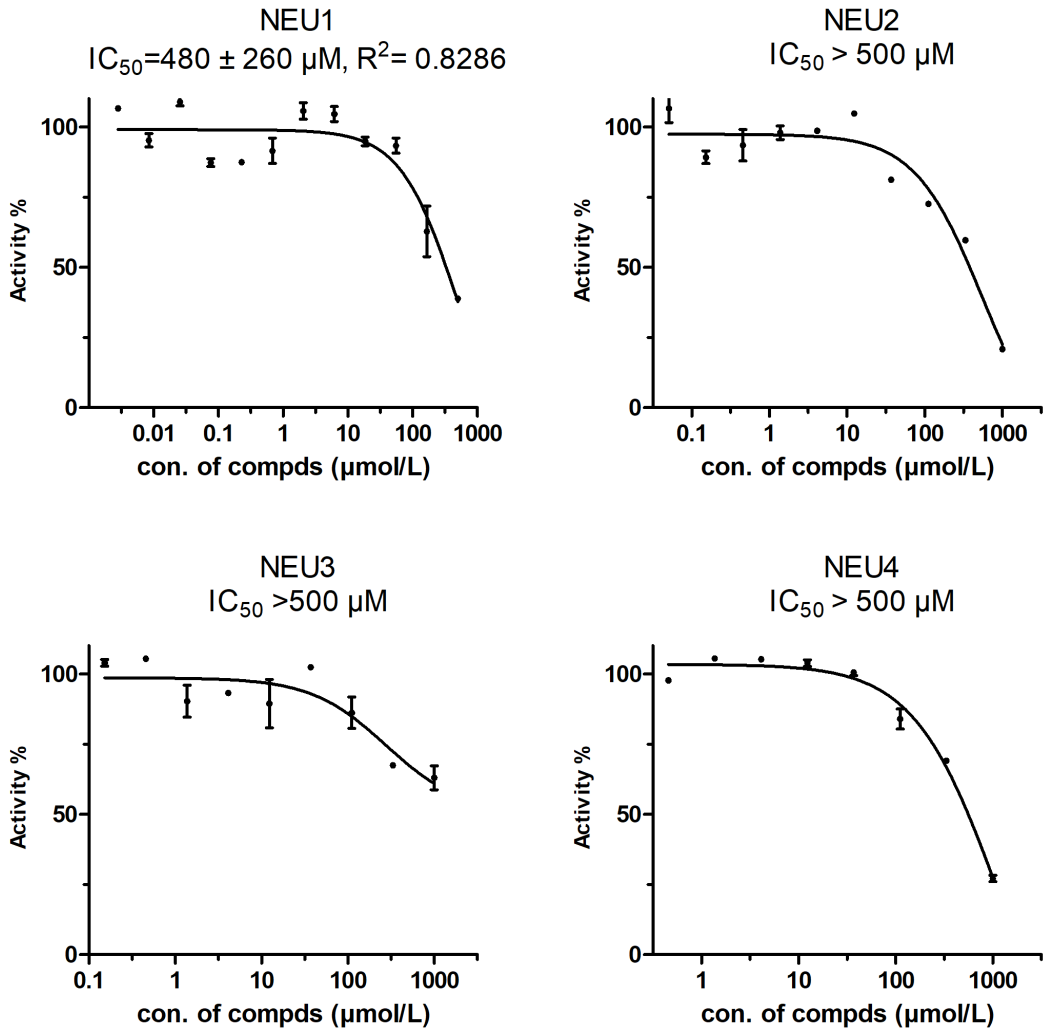
11j


NEU1
IC50=12 ± 2 μM, R2= 0.9908
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50=60 ± 3 μM, R2=0.9988
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 100 ± 20 μM, R2= 0.9857
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50= 81 ± 15 μM, R2= 0.9826
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

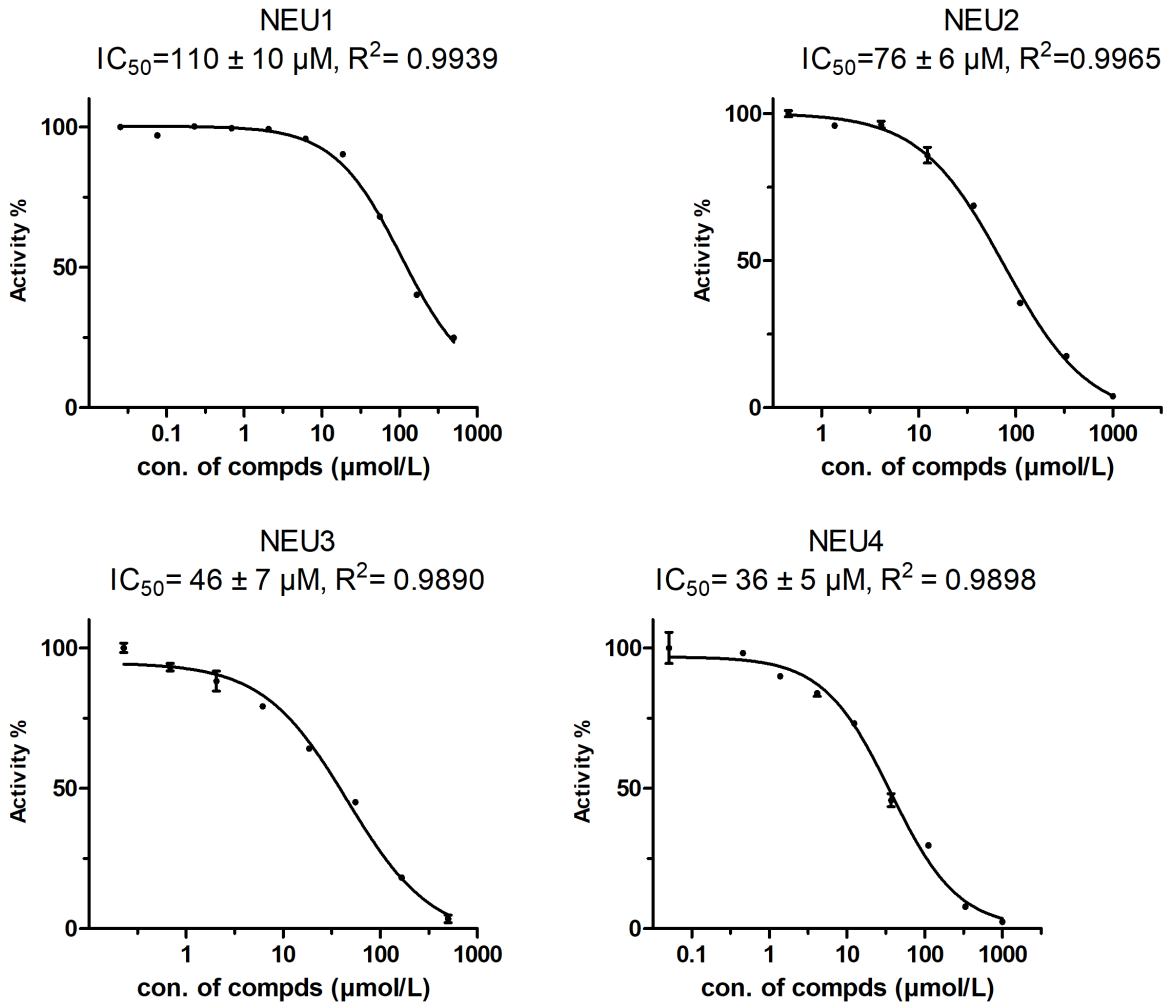
11k


NEU1
IC50=11 ± 1 μM, R2= 0.9933
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50=41 ± 12 μM, R2= 0.9553
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 480 ± 100 μM, R2= 0.9837
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50 > 500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

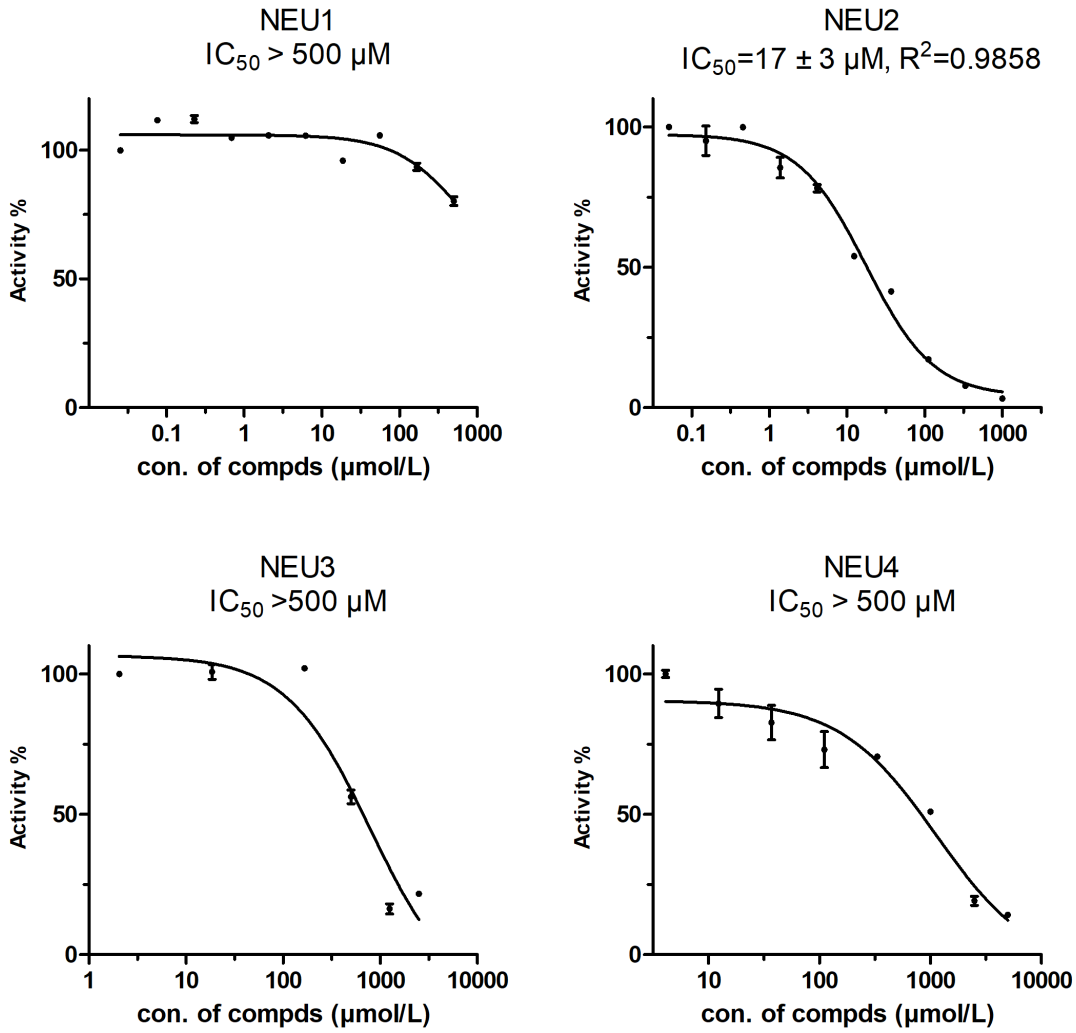
11l


NEU1
IC50=480 ± 260 μM, R2= 0.8286
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50 > 500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50 >500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50 > 500 μM
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

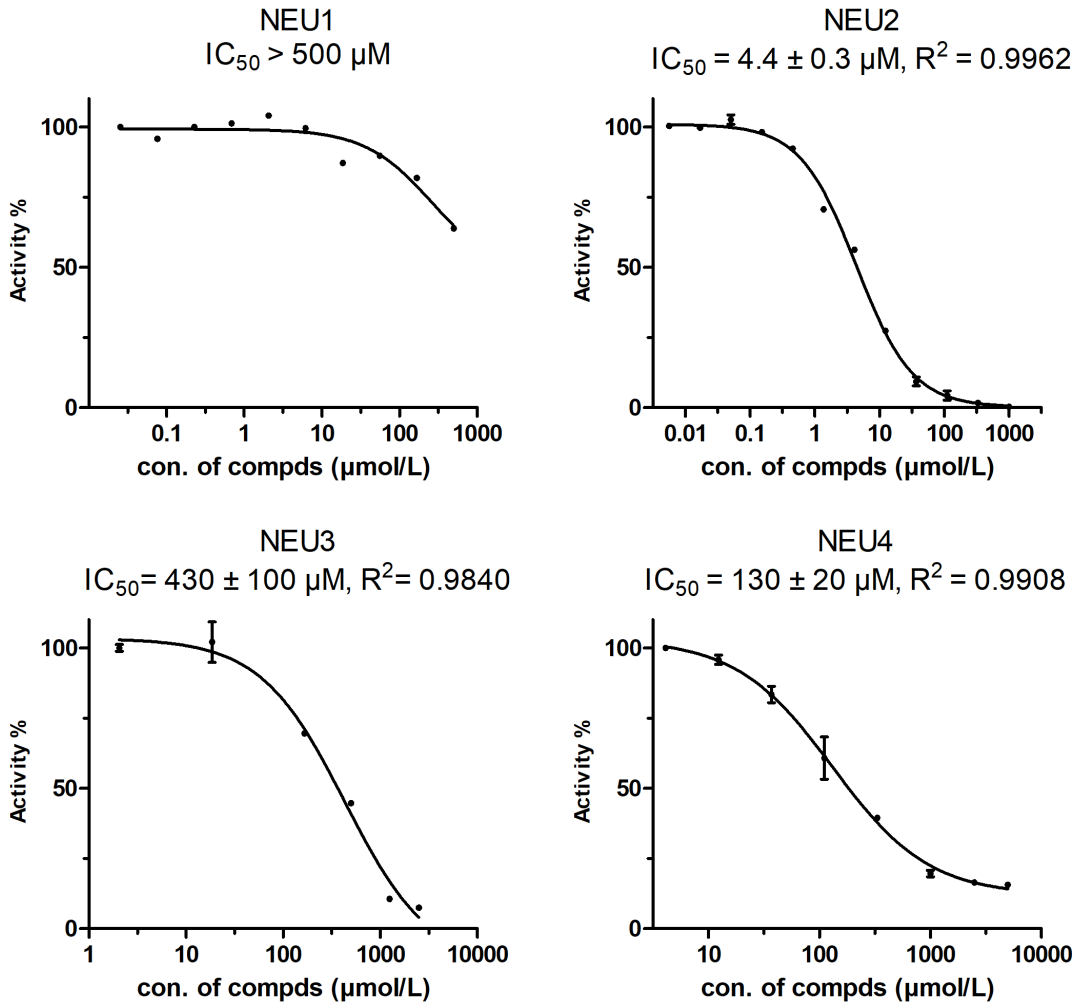
13a


NEU1
IC50=110 ± 10 μM, R2= 0.9939
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50=76 ± 6 μM, R2=0.9965
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 46 ± 7 μM, R2= 0.9890
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50= 36 ± 5 μM, R2 = 0.9898
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

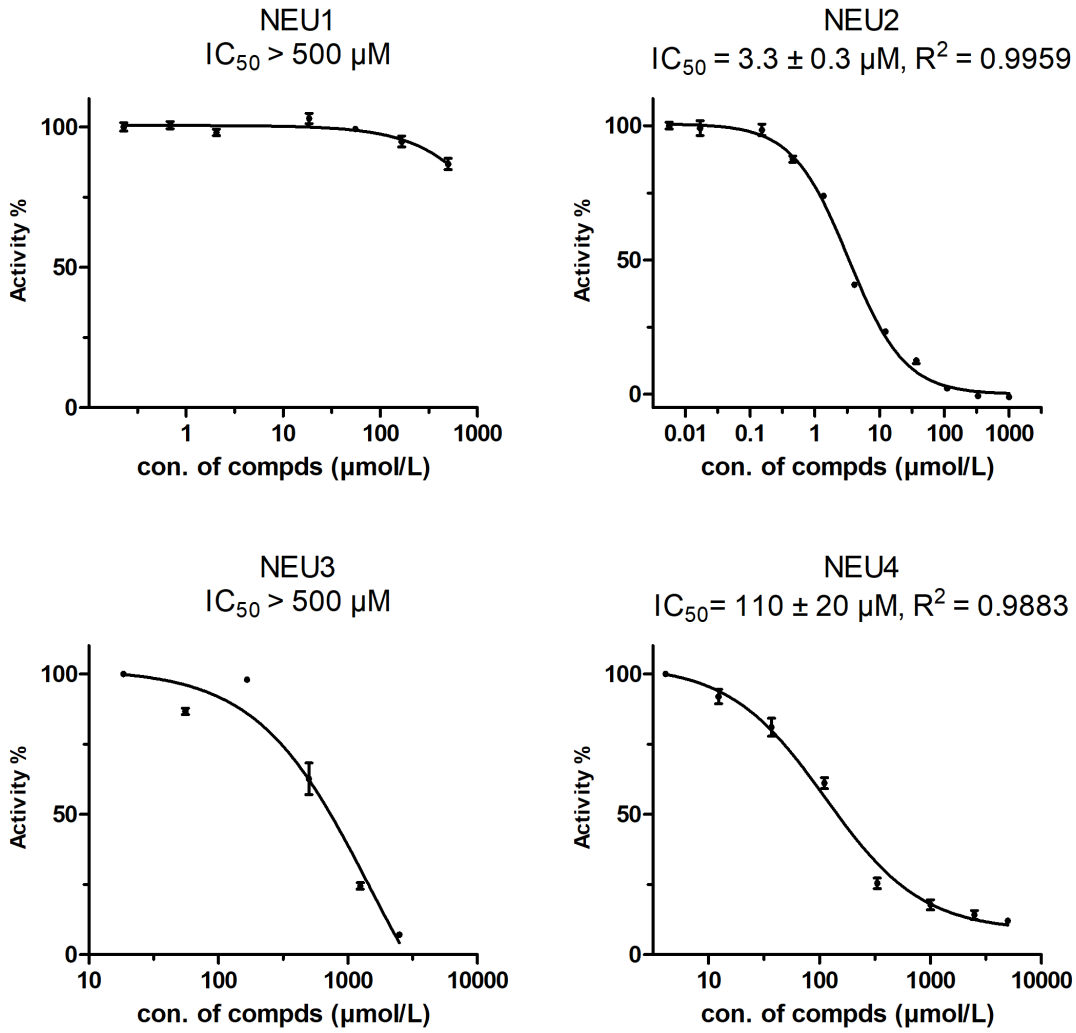
13b


NEU1
IC50 > 500 μM
NEU2
IC50=17 ± 3 μM, R2=0.9858
NEU3
IC50 >500 μM
NEU4
IC50 > 500 μM
Activity %
con. of compds (μmol/L)

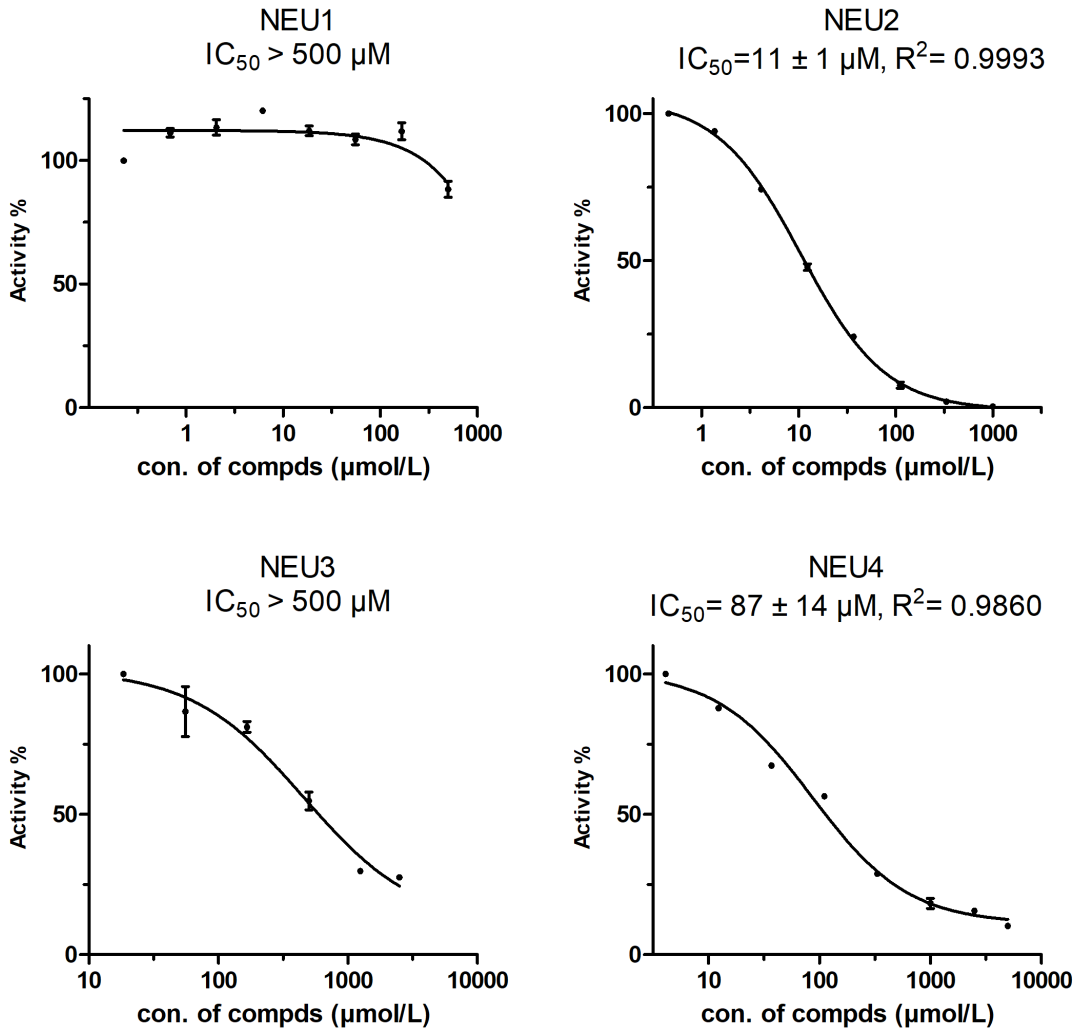
13c


NEU1
IC50 > 500 μM
NEU2
IC50 = 4.4 ± 0.3 μM, R2 = 0.9962
NEU3
IC50= 430 ± 100 μM, R2= 0.9840
NEU4
IC50 = 130 ± 20 μM, R2 = 0.9908
Activity %
con. of compds (μmol/L)

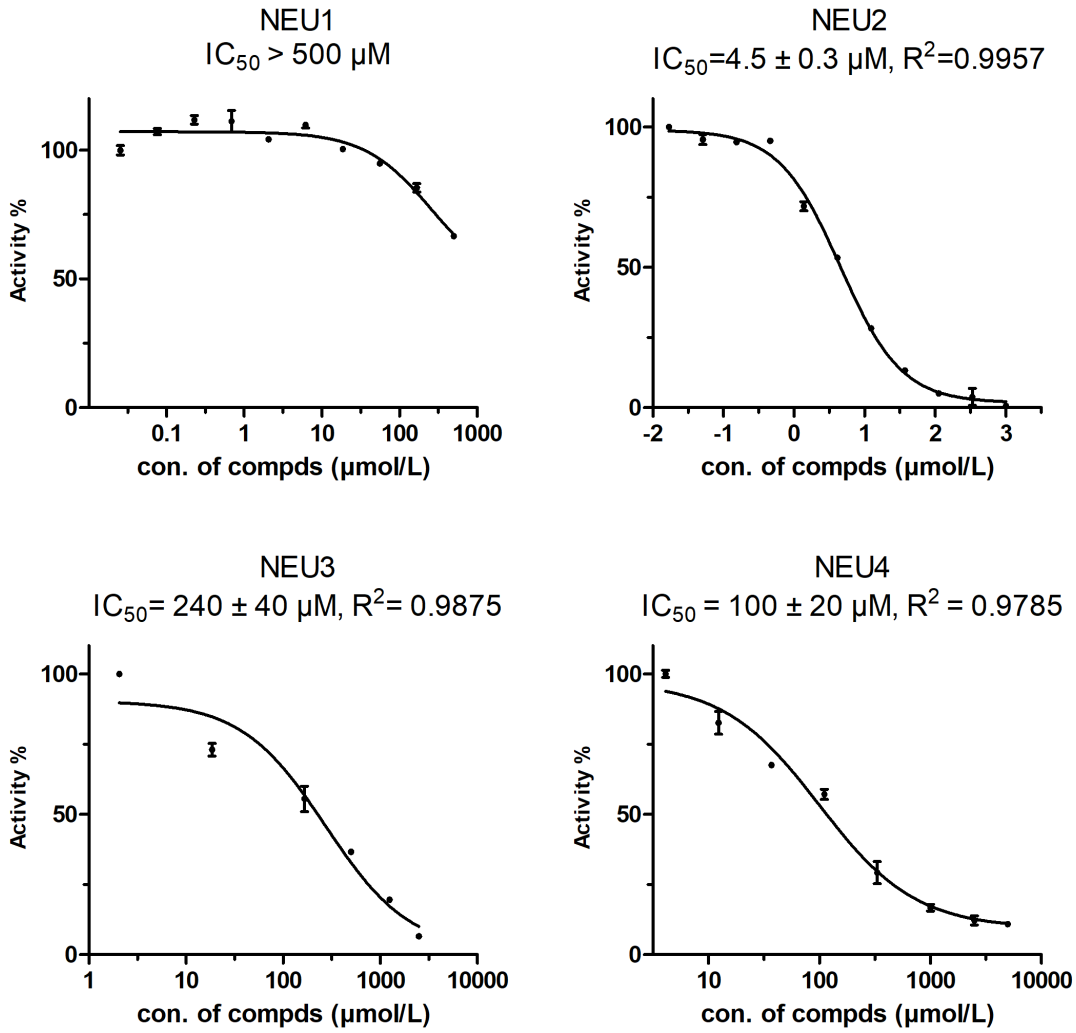
13d


NEU1
IC50 > 500 μM
NEU2
IC50 = 3.3 ± 0.3 μM, R2 = 0.9959
NEU3
IC50 > 500 μM
NEU4
IC50= 110 ± 20 μM, R2 = 0.9883
Activity %
con. of compds (μmol/L)

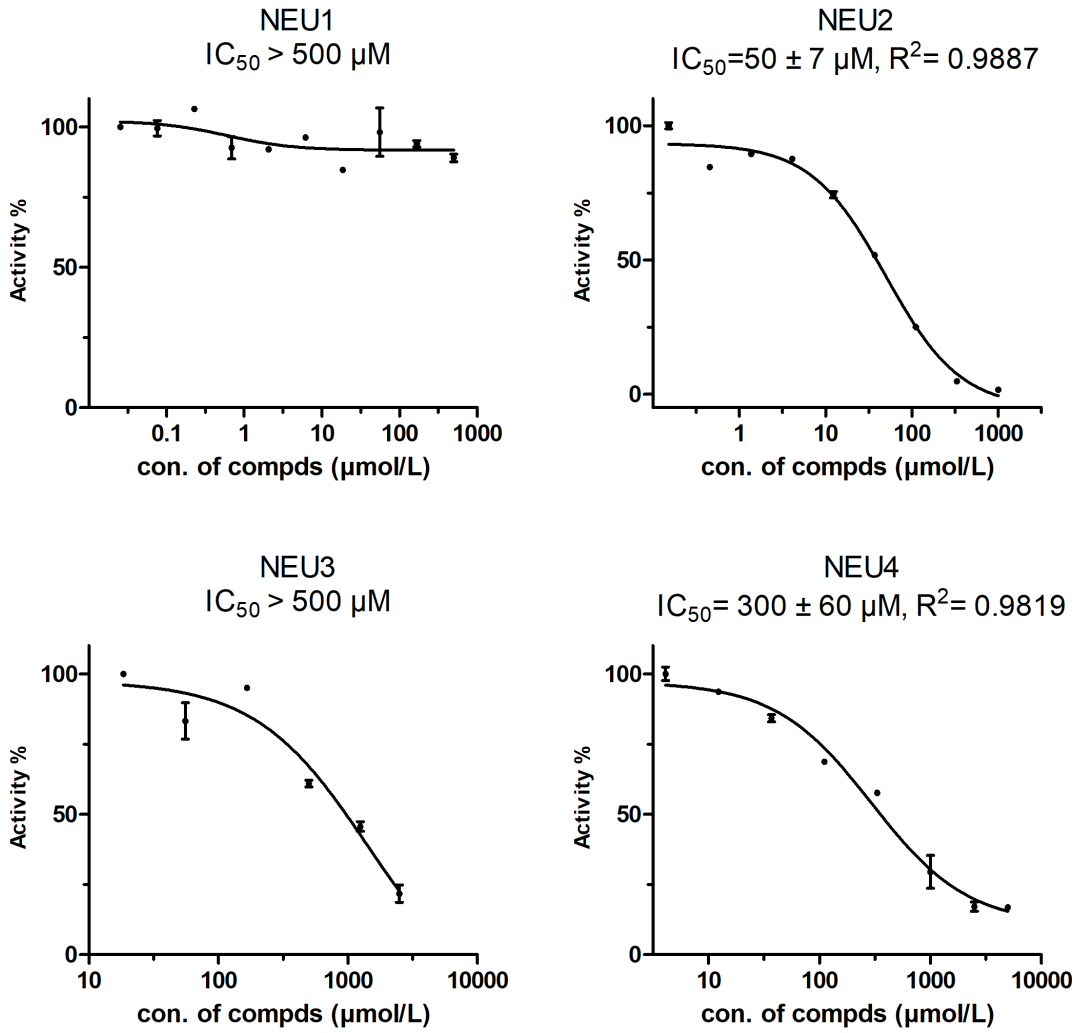
13e


NEU1
IC50 > 500 μM
NEU2
IC50=11 ± 1 μM, R2= 0.9993
NEU3
IC50 > 500 μM
NEU4
IC50= 87 ± 14 μM, R2= 0.9860
Activity %
con. of compds (μmol/L)

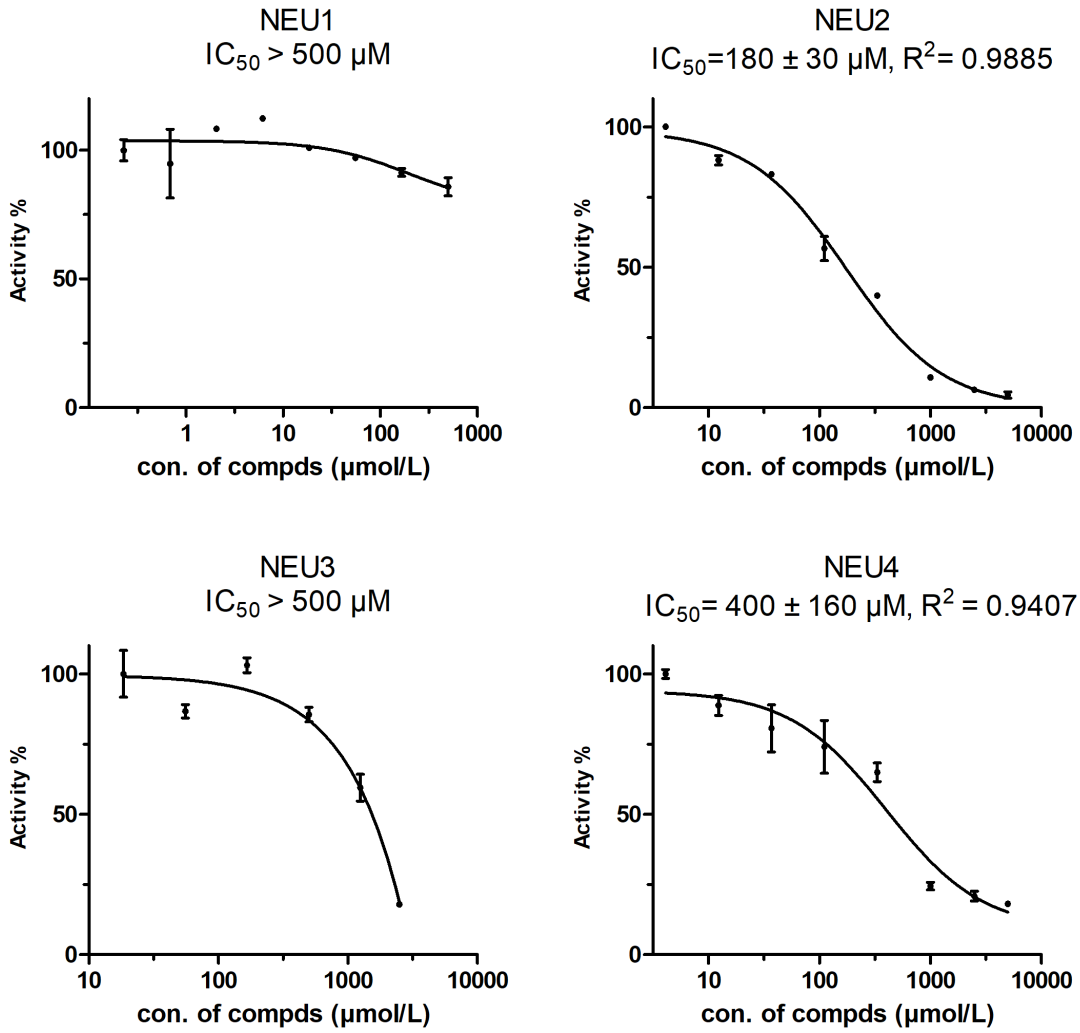
13f


NEU1
IC50 > 500 μM
Activity %
con. of compds (μmol/L)
NEU2
IC50=4.5 ± 0.3 μM, R2=0.9957
Activity %
con. of compds (μmol/L)
NEU3
IC50= 240 ± 40 μM, R2= 0.9875
Activity %
con. of compds (μmol/L)
NEU4
IC50 = 100 ± 20 μM, R2 = 0.9785
Activity %
con. of compds (μmol/L)

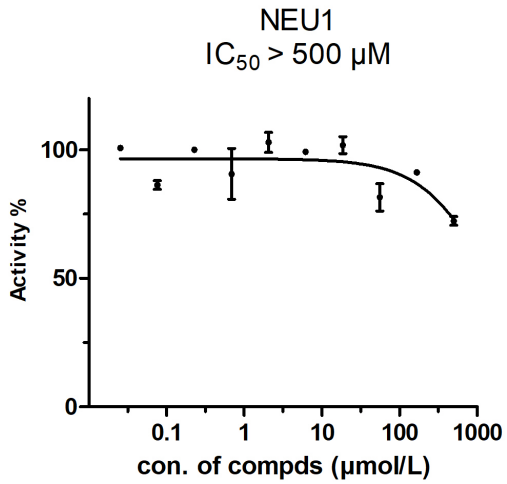
13g

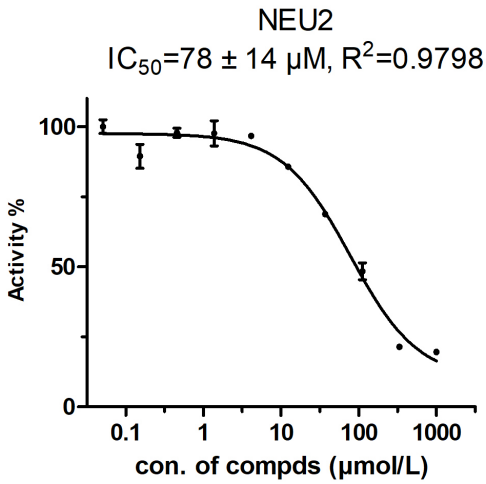

NEU1
IC50 > 500 μM
NEU2
IC50=50 ± 7 μM, R2= 0.9887
NEU3
IC50 > 500 μM
NEU4
IC50= 300 ± 60 μM, R2= 0.9819
Activity %
con. of compds (μmol/L)

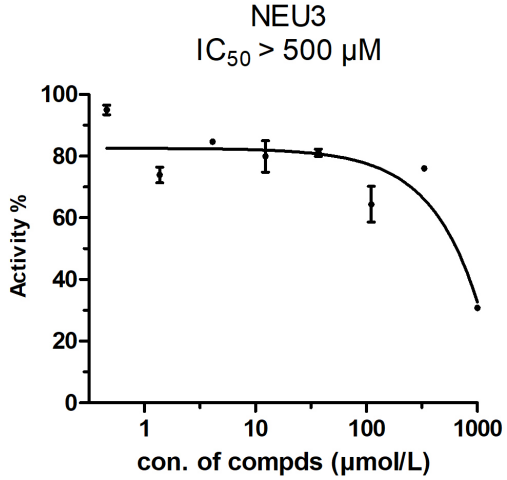
13h

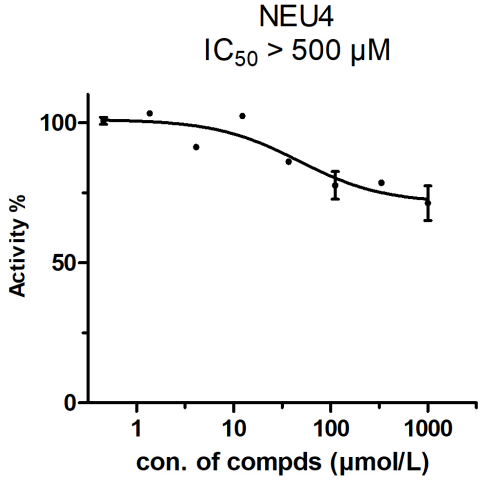

NEU1
IC50 > 500 μM
NEU2
IC50=180 ± 30 μM, R2= 0.9885
NEU3
IC50 > 500 μM
NEU4
IC50= 400 ± 160 μM, R2 = 0.9407
Activity %
con. of compds (μmol/L)

13i

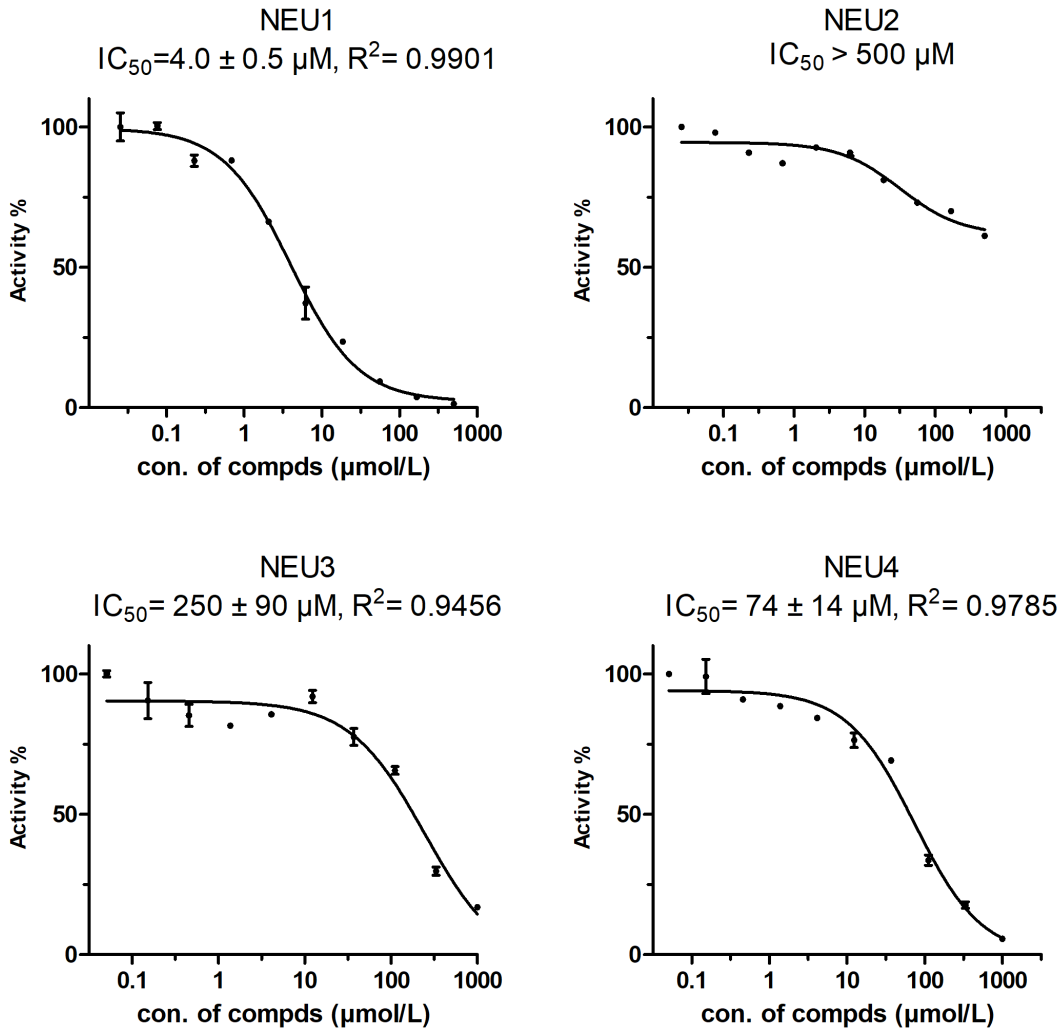

NEU1
IC50 > 500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50=78 ± 14 μM, R2=0.9798
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

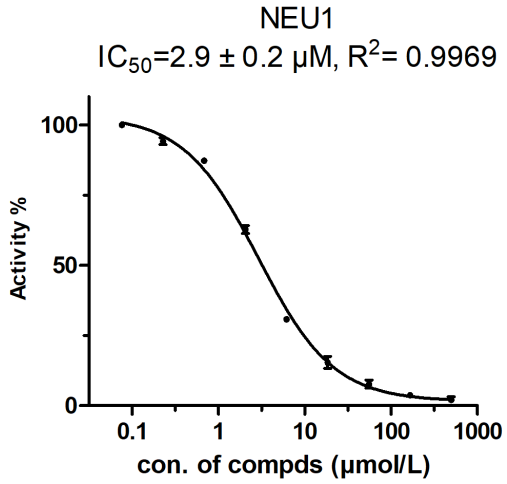

NEU3
IC50 > 500 μM
Activity %
100
80
60
40
20
0
1
10
100
1000
con. of compds (μmol/L)

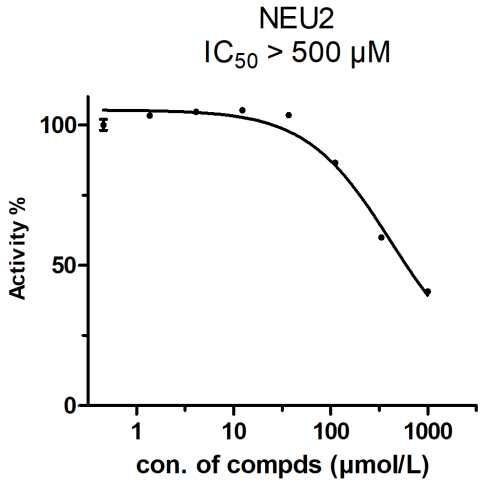

NEU4
IC50 > 500 μM
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

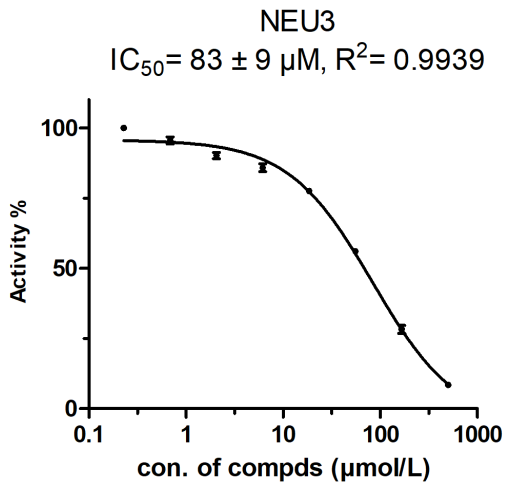
15a

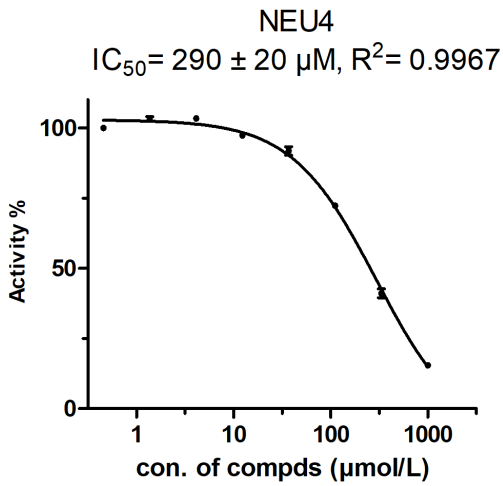

NEU1
IC50=4.0 ± 0.5 μM, R2= 0.9901
NEU2
IC50 > 500 μM
NEU3
IC50= 250 ± 90 μM, R2= 0.9456
NEU4
IC50= 74 ± 14 μM, R2= 0.9785
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

15b

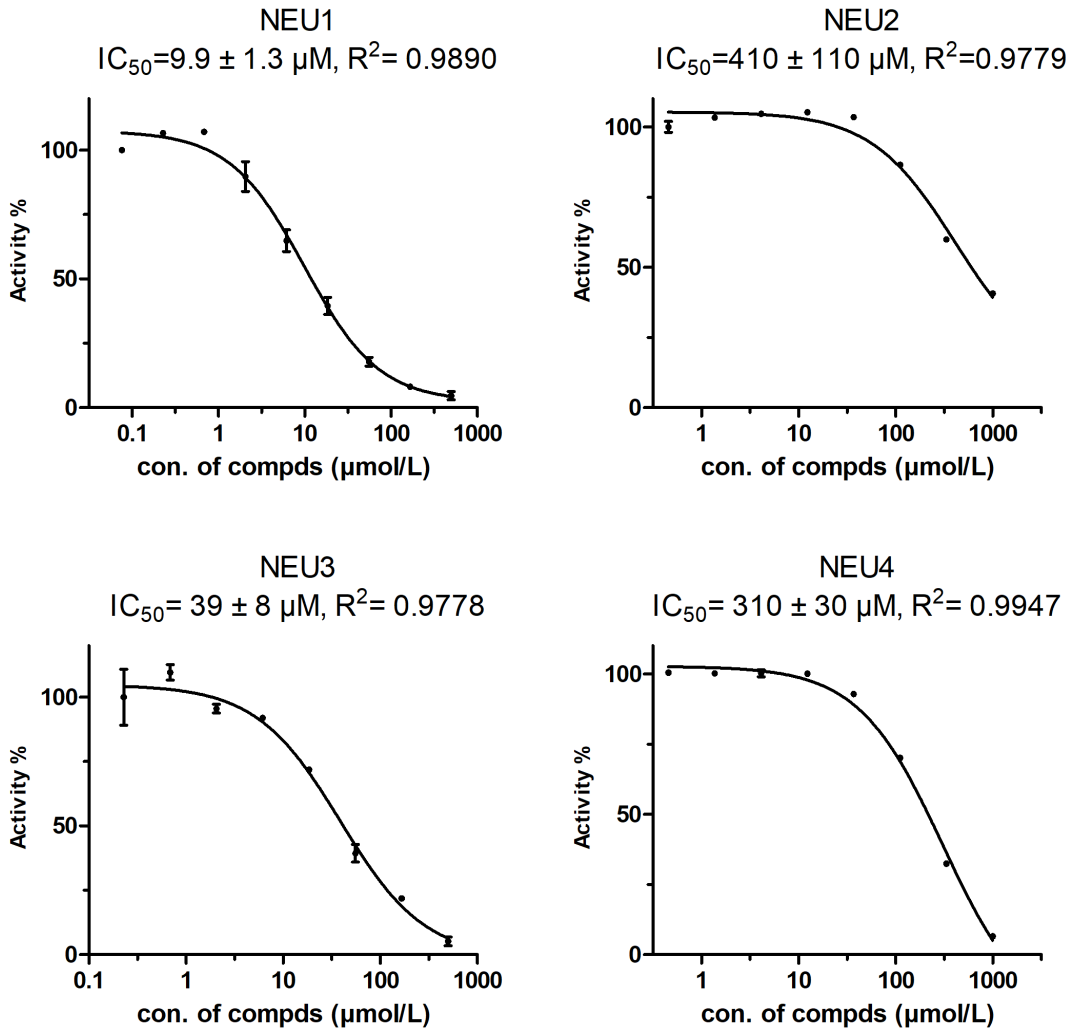

NEU1
IC50=2.9 ± 0.2 μM, R2= 0.9969
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50 > 500 μM
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

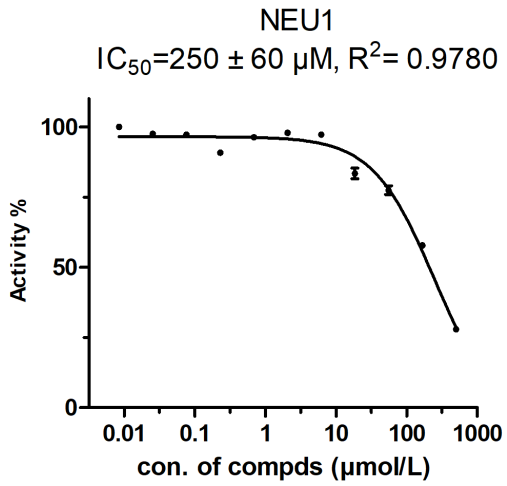

NEU3
IC50= 83 ± 9 μM, R2= 0.9939
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

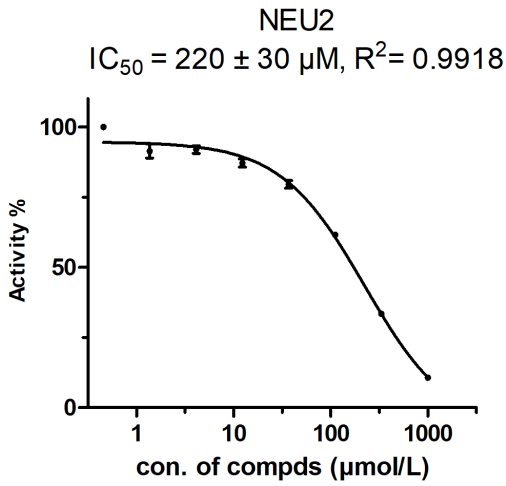

NEU4
IC50= 290 ± 20 μM, R2= 0.9967
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

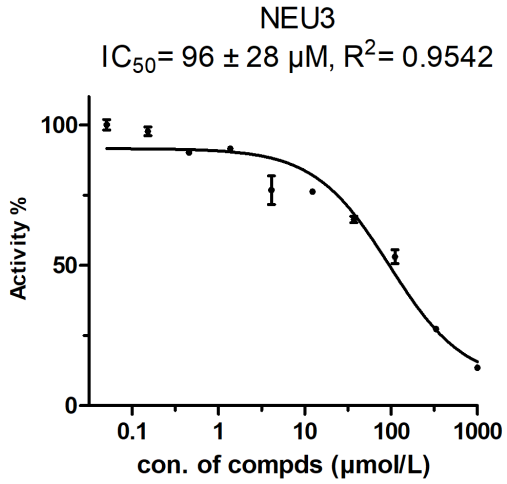
15c

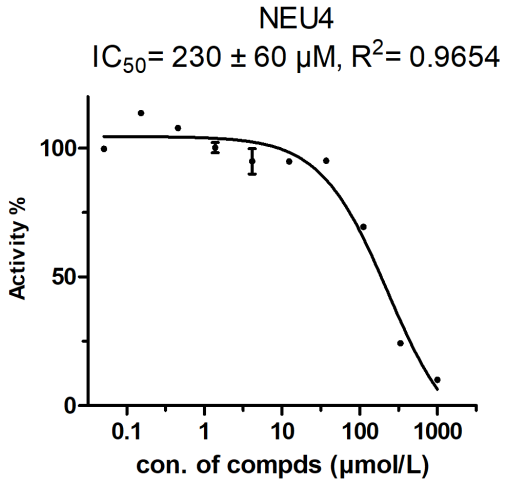

NEU1
IC50=9.9 ± 1.3 μM, R2= 0.9890
Activity %
con. of compds (μmol/L)
NEU2
IC50=410 ± 110 μM, R2=0.9779
Activity %
con. of compds (μmol/L)
NEU3
IC50= 39 ± 8 μM, R2= 0.9778
Activity %
con. of compds (μmol/L)
NEU4
IC50= 310 ± 30 μM, R2= 0.9947
Activity %
con. of compds (μmol/L)

15d

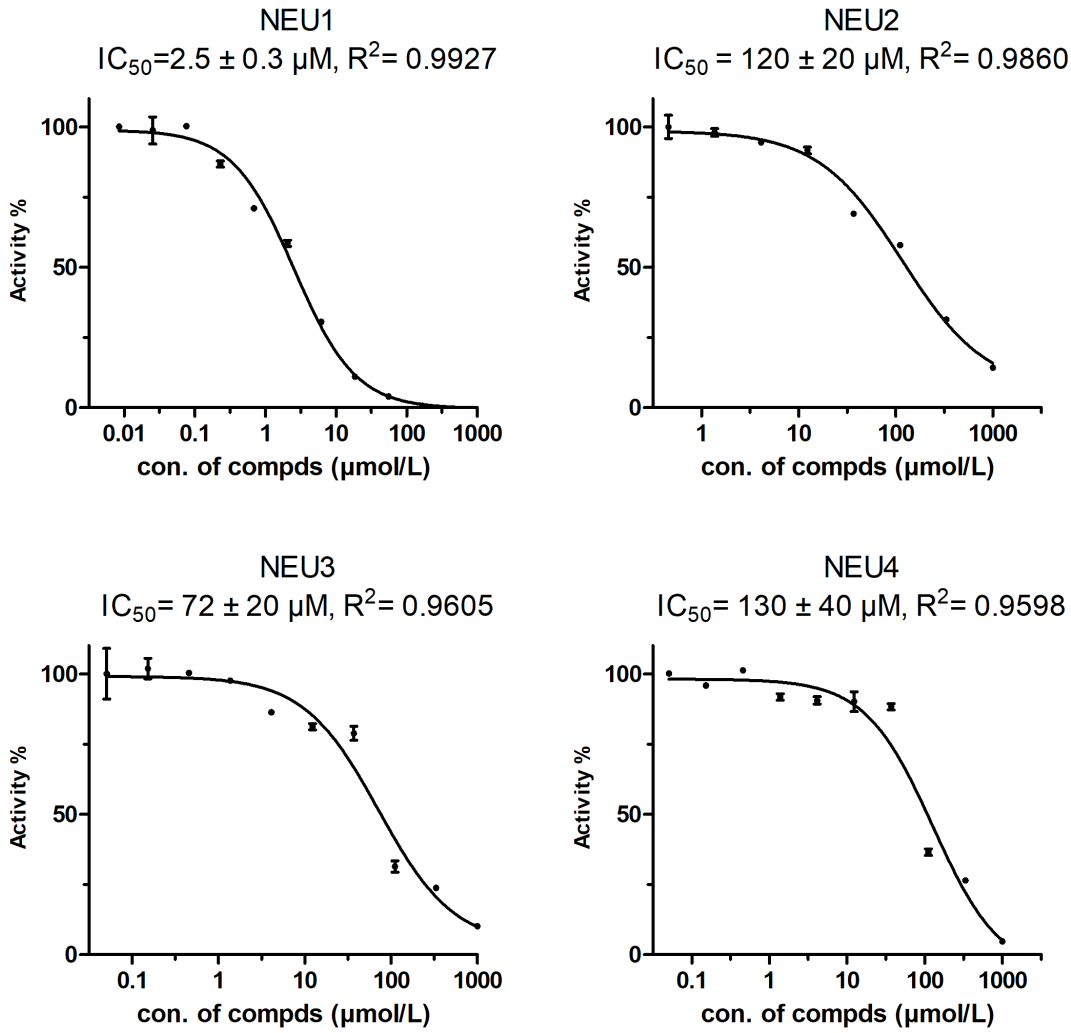

NEU1
IC50=250 ± 60 μM, R2= 0.9780
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50 = 220 ± 30 μM, R2= 0.9918
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

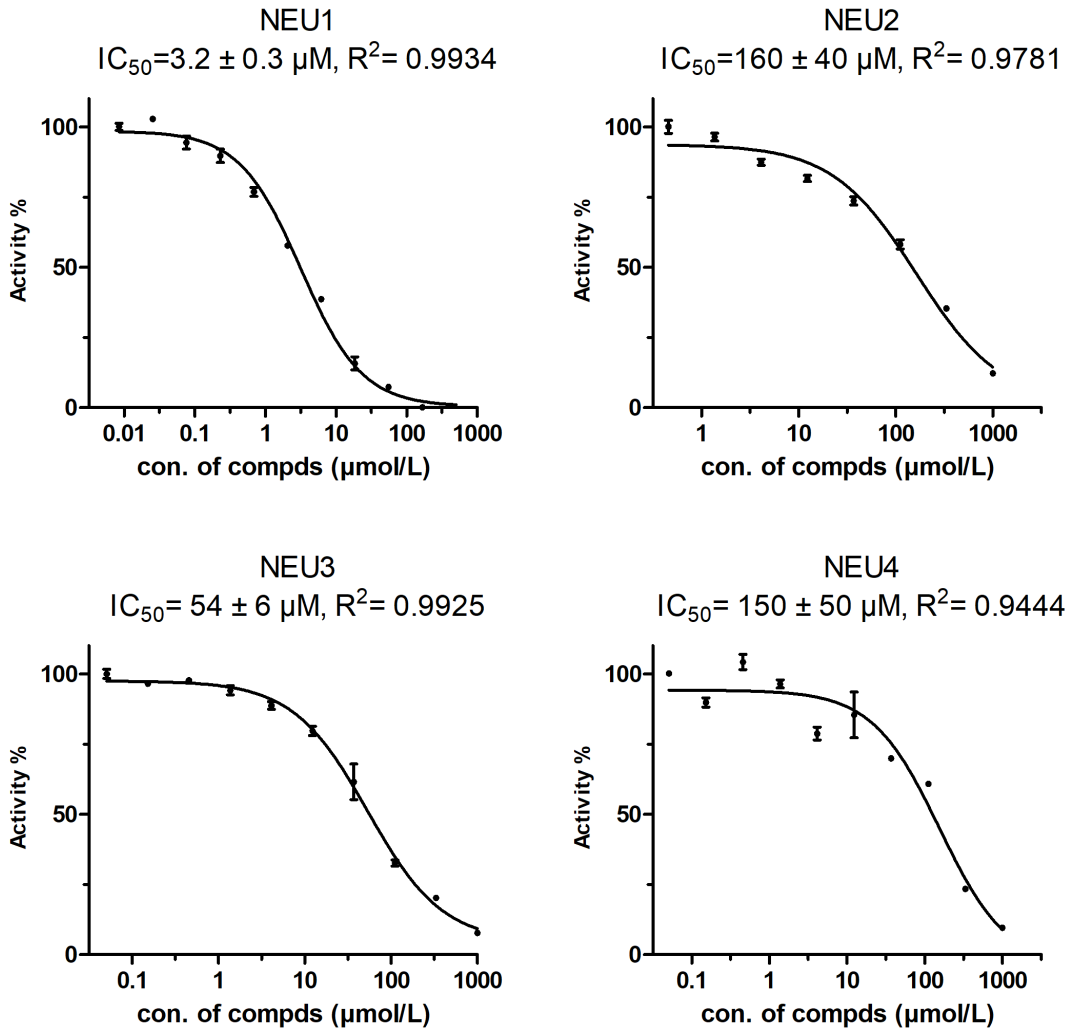

NEU3
IC50= 96 ± 28 μM, R2= 0.9542
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU4
IC50= 230 ± 60 μM, R2= 0.9654
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

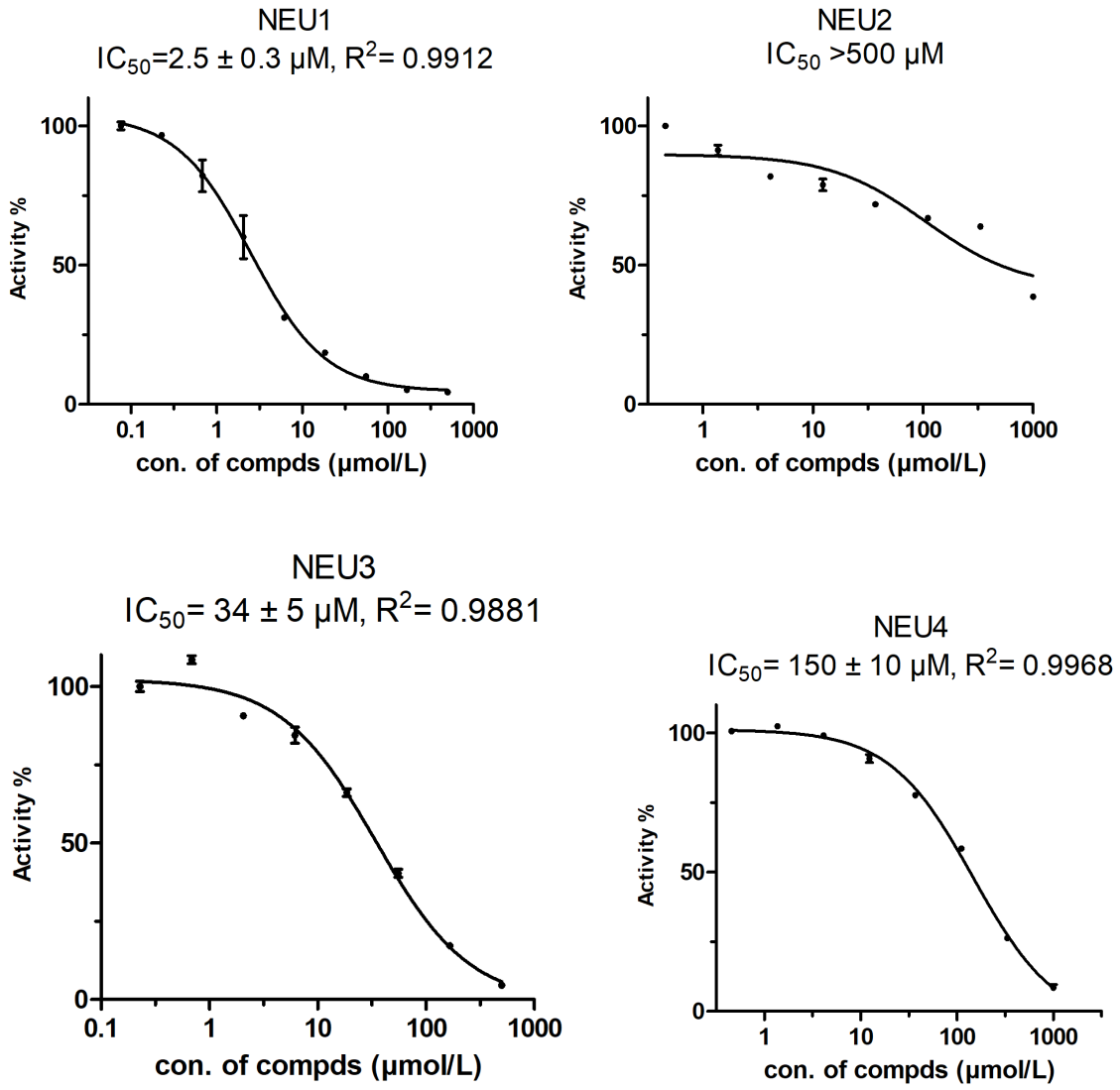
15e


NEU1
IC50=2.5 ± 0.3 μM, R2= 0.9927
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50 = 120 ± 20 μM, R2= 0.9860
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 72 ± 20 μM, R2= 0.9605
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50= 130 ± 40 μM, R2= 0.9598
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

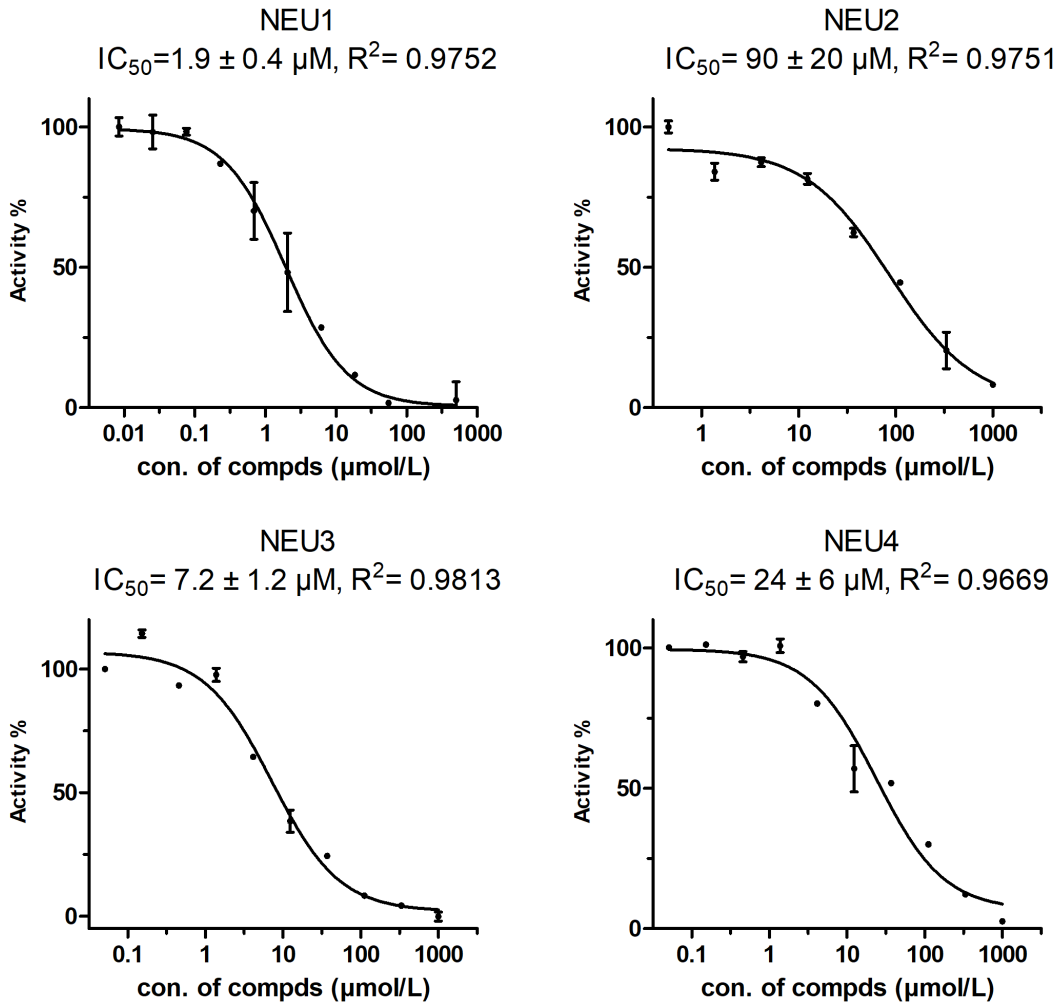
15f


NEU1
IC50=3.2 ± 0.3 μM, R2= 0.9934
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50=160 ± 40 μM, R2= 0.9781
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 54 ± 6 μM, R2= 0.9925
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50= 150 ± 50 μM, R2= 0.9444
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

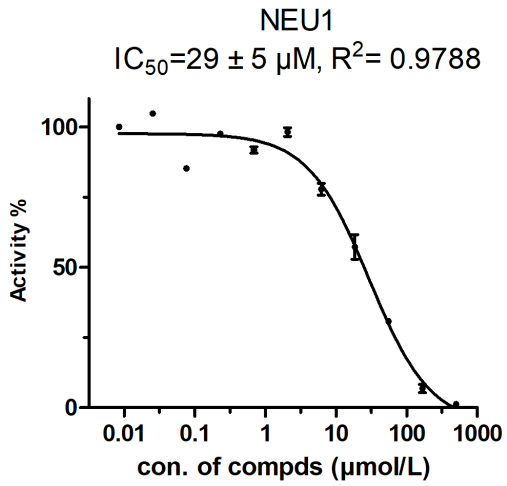
15g

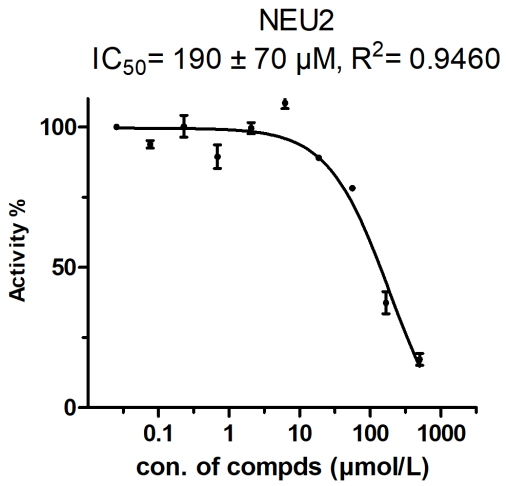

NEU1
IC50=2.5 ± 0.3 μM, R2= 0.9912
Activity %
con. of compds (μmol/L)
NEU2
IC50 >500 μM
Activity %
con. of compds (μmol/L)
NEU3
IC50= 34 ± 5 μM, R2= 0.9881
Activity %
con. of compds (μmol/L)
NEU4
IC50= 150 ± 10 μM, R2= 0.9968
Activity %
con. of compds (μmol/L)

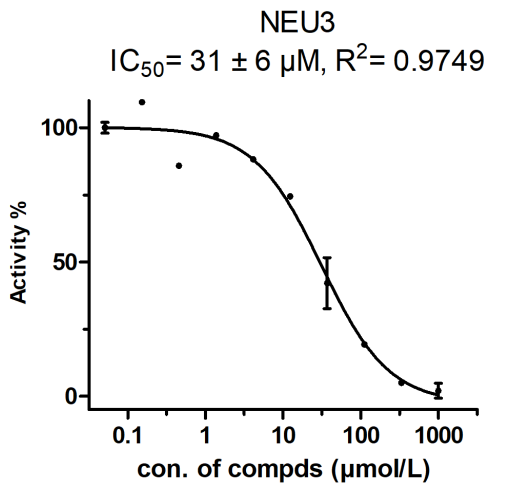
15h

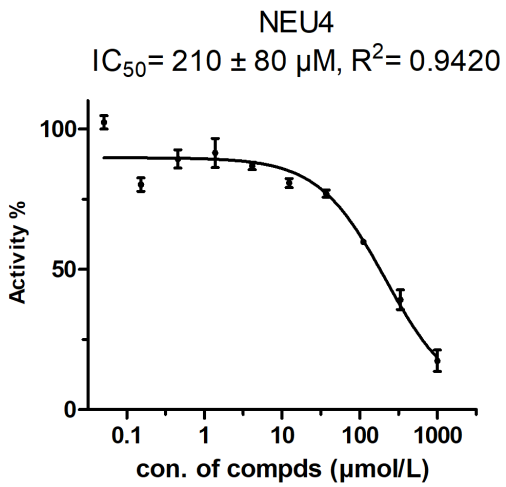

NEU1
IC50=1.9 ± 0.4 μM, R2= 0.9752
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50= 90 ± 20 μM, R2= 0.9751
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 7.2 ± 1.2 μM, R2= 0.9813
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50= 24 ± 6 μM, R2= 0.9669
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

15i

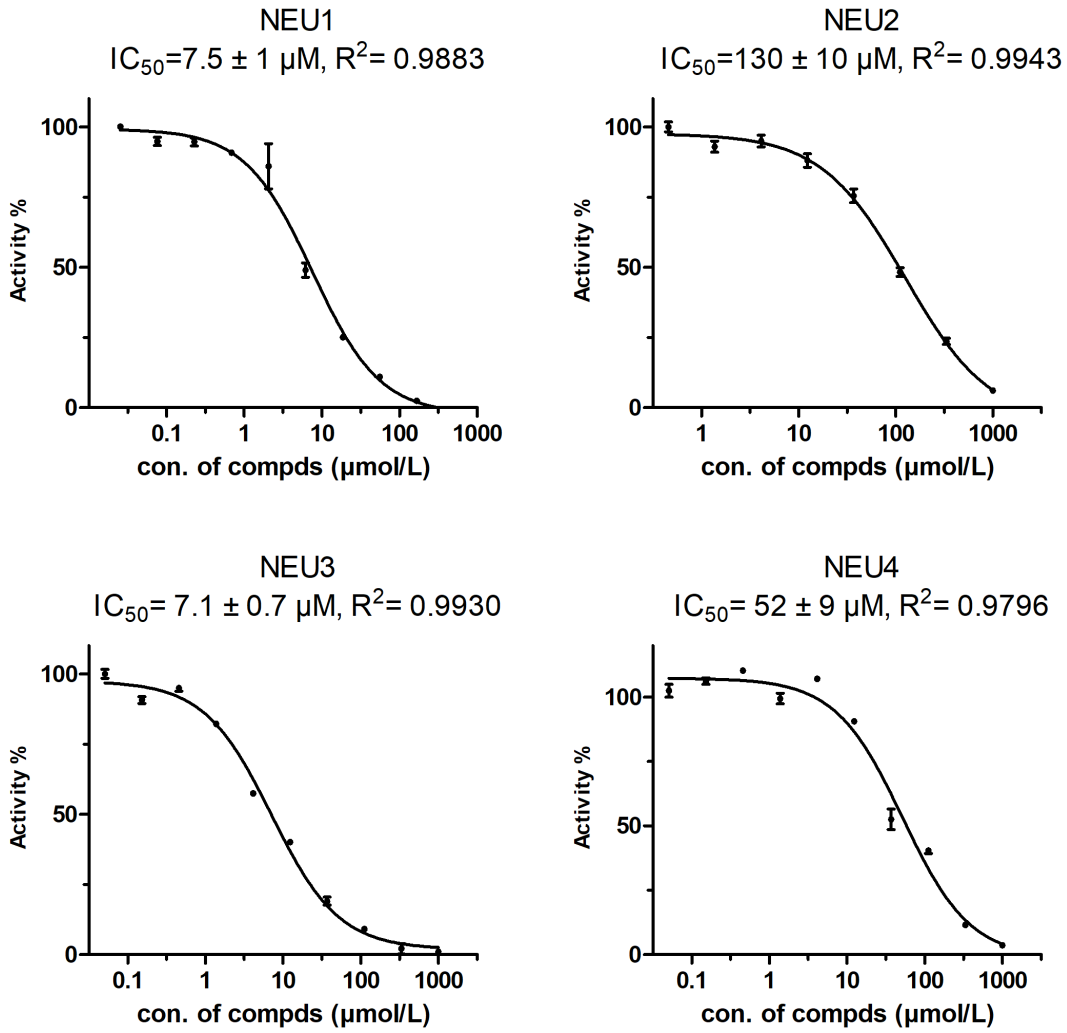

NEU1
IC50=29 ± 5 μM, R2= 0.9788
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50= 190 ± 70 μM, R2= 0.9460
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

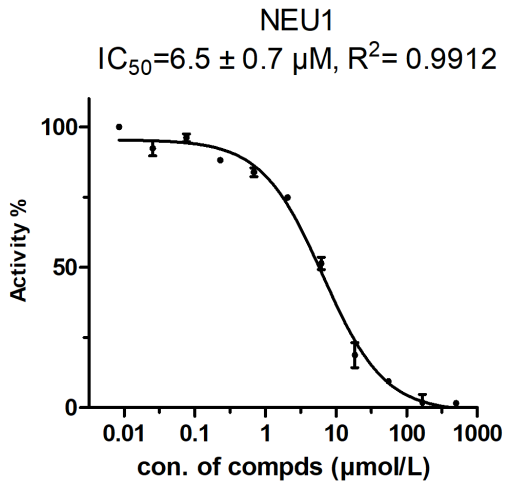

NEU3
IC50= 31 ± 6 μM, R2= 0.9749
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

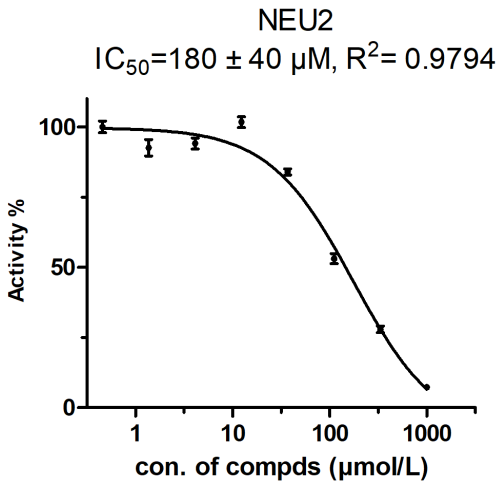

NEU4
IC50= 210 ± 80 μM, R2= 0.9420
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

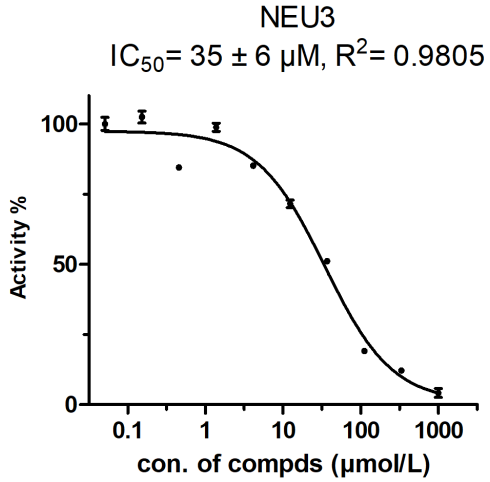
15j

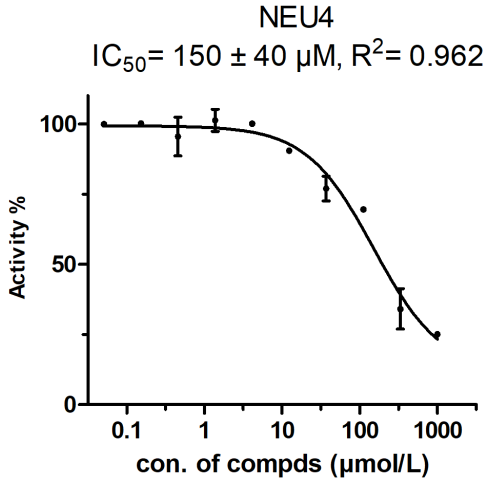

NEU1
IC50=7.5 ± 1 μM, R2= 0.9883
NEU2
IC50=130 ± 10 μM, R2= 0.9943
NEU3
IC50= 7.1 ± 0.7 μM, R2= 0.9930
NEU4
IC50= 52 ± 9 μM, R2= 0.9796
Activity %
con. of compds (μmol/L)

15k

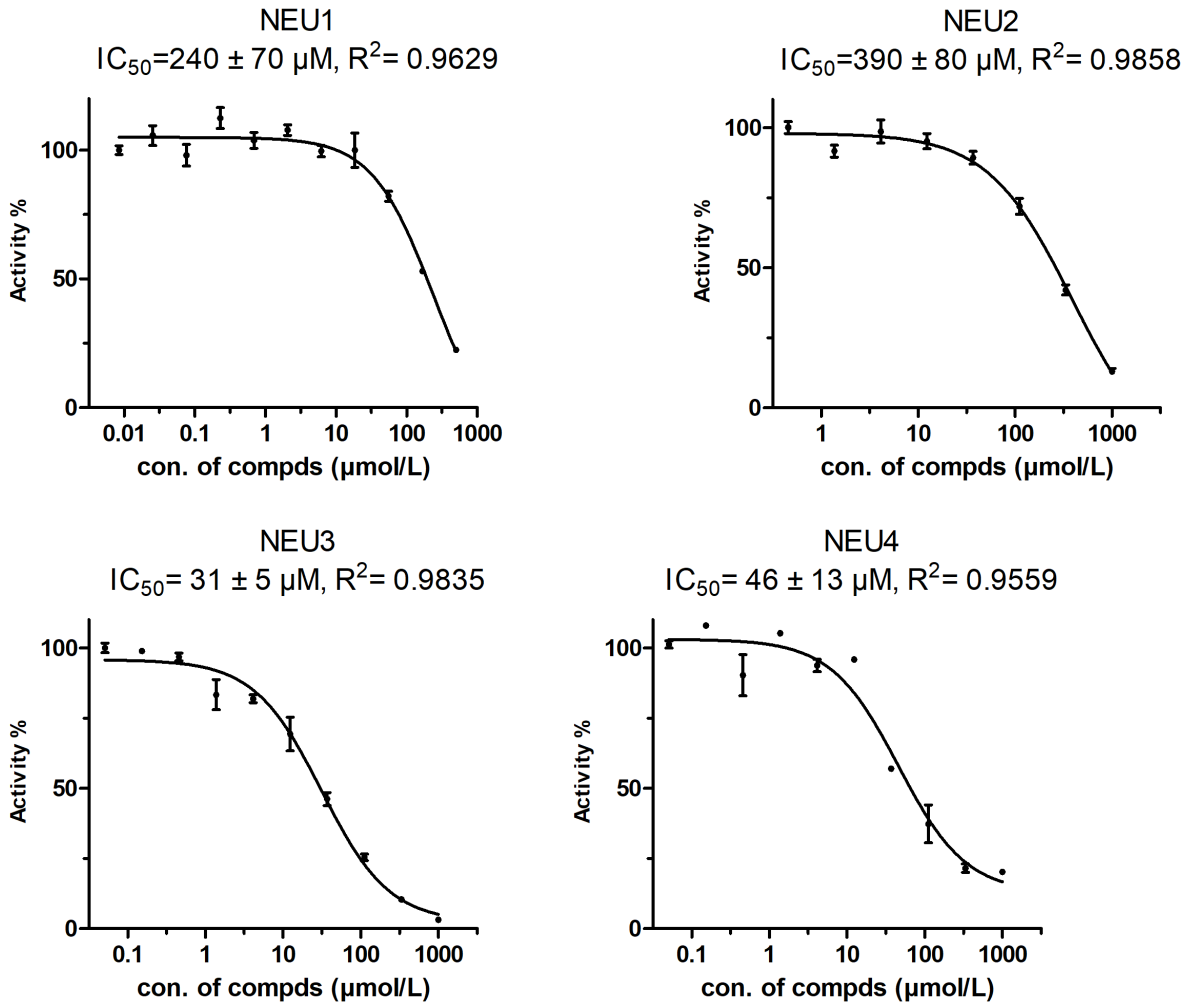

NEU1
IC50=6.5 ± 0.7 μM, R2= 0.9912
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50=180 ± 40 μM, R2= 0.9794
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

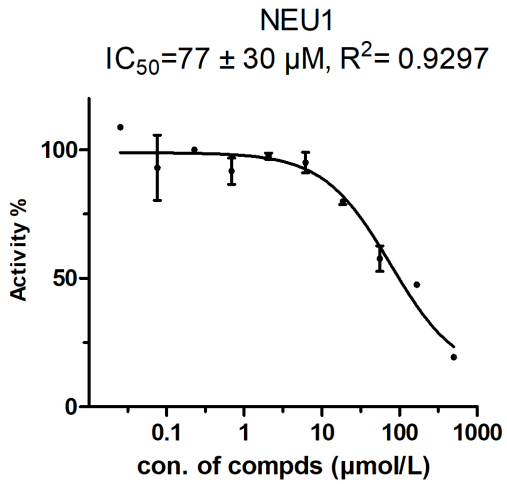

NEU3
IC50= 35 ± 6 μM, R2= 0.9805
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

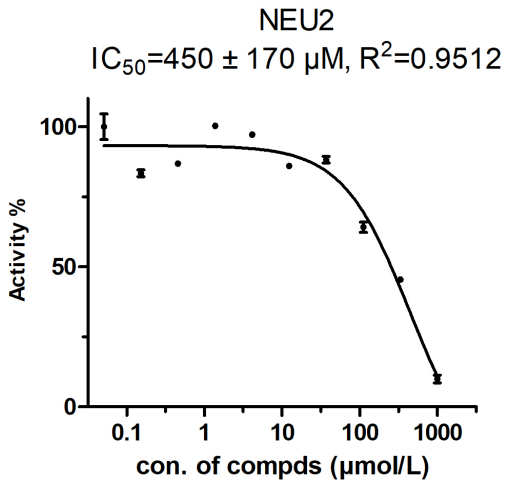

NEU4
IC50= 150 ± 40 μM, R2= 0.9621
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

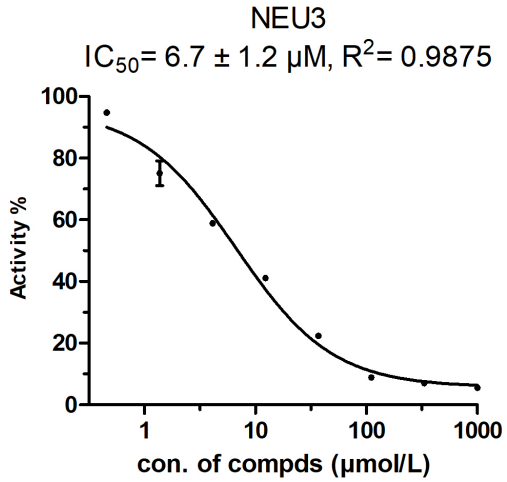
15l

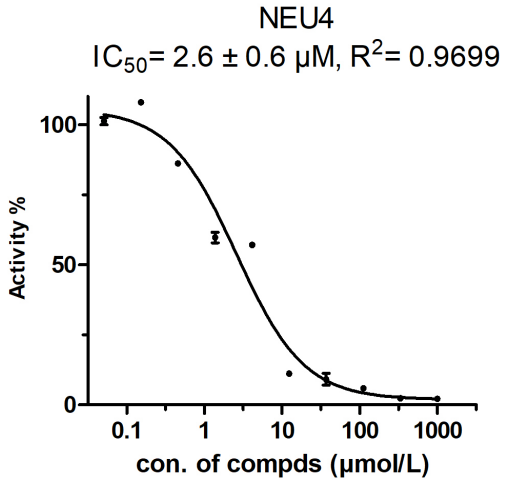

NEU1
IC50=240 ± 70 μM, R2= 0.9629
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50=390 ± 80 μM, R2= 0.9858
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50= 31 ± 5 μM, R2= 0.9835
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50= 46 ± 13 μM, R2= 0.9559
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

15m

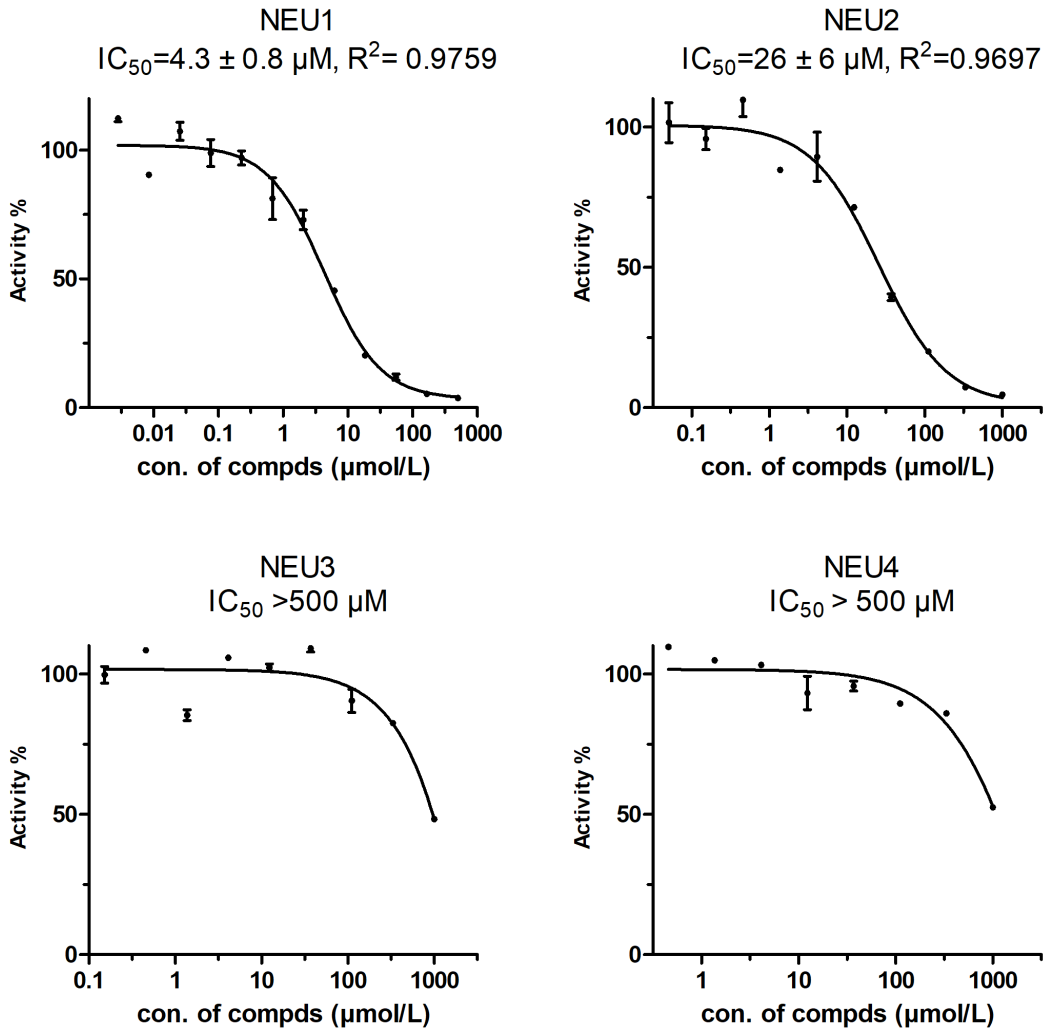

NEU1
IC50=77 ± 30 μM, R2= 0.9297
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)


NEU2
IC50=450 ± 170 μM, R2=0.9512
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

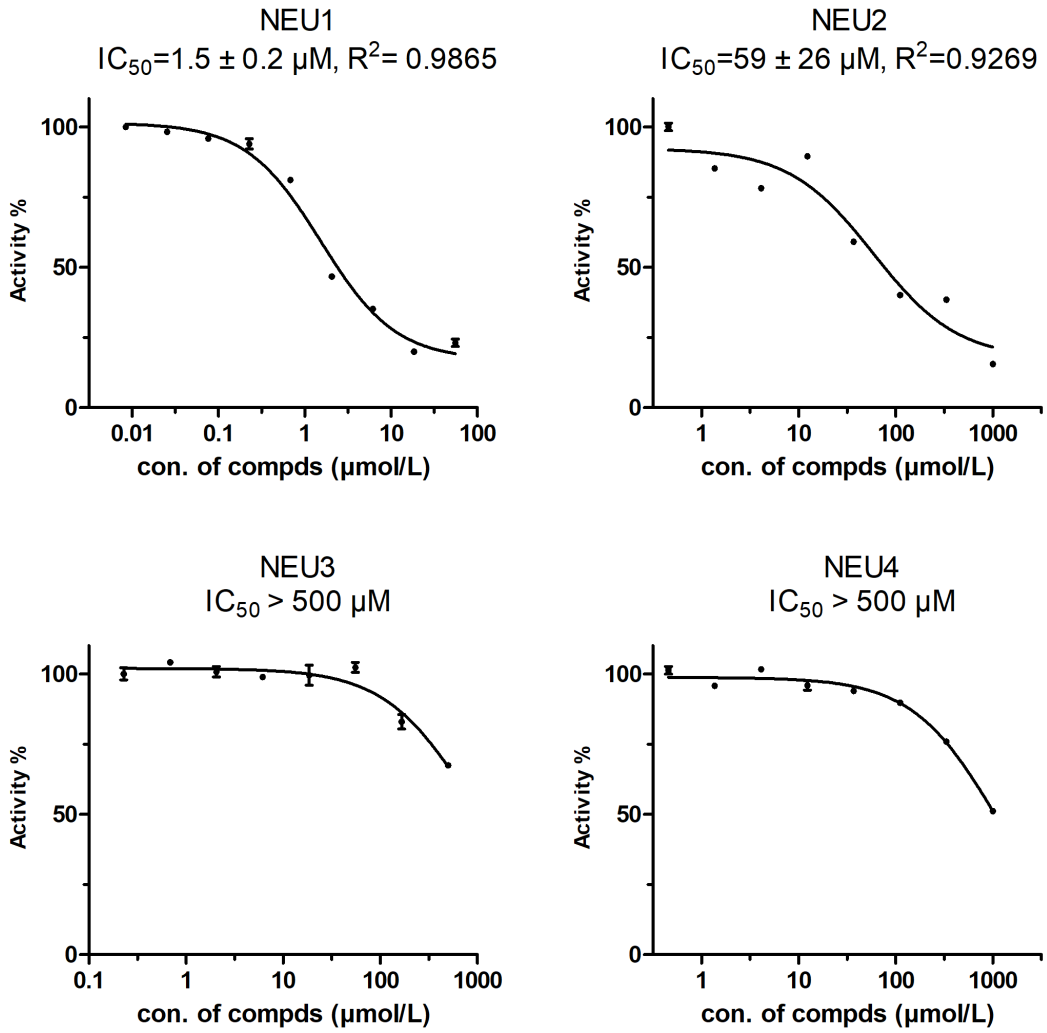

NEU3
IC50= 6.7 ± 1.2 μM, R2= 0.9875
Activity %
100
80
60
40
20
0
1
10
100
1000
con. of compds (μmol/L)


NEU4
IC50= 2.6 ± 0.6 μM, R2= 0.9699
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)

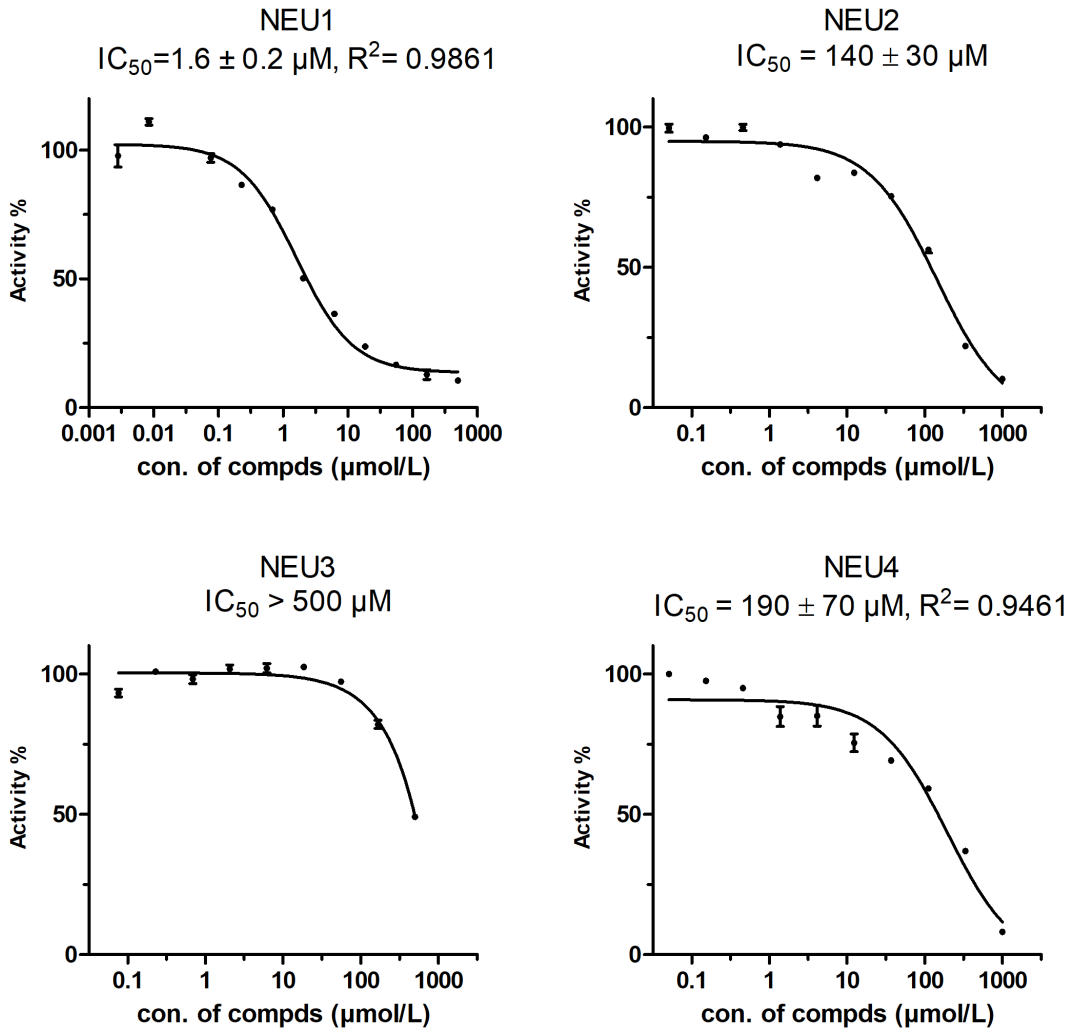
17a


NEU1
IC50=4.3 ± 0.8 μM, R2= 0.9759
Activity %
100
50
0
0.01
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU2
IC50=26 ± 6 μM, R2=0.9697
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50 >500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50 > 500 μM
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

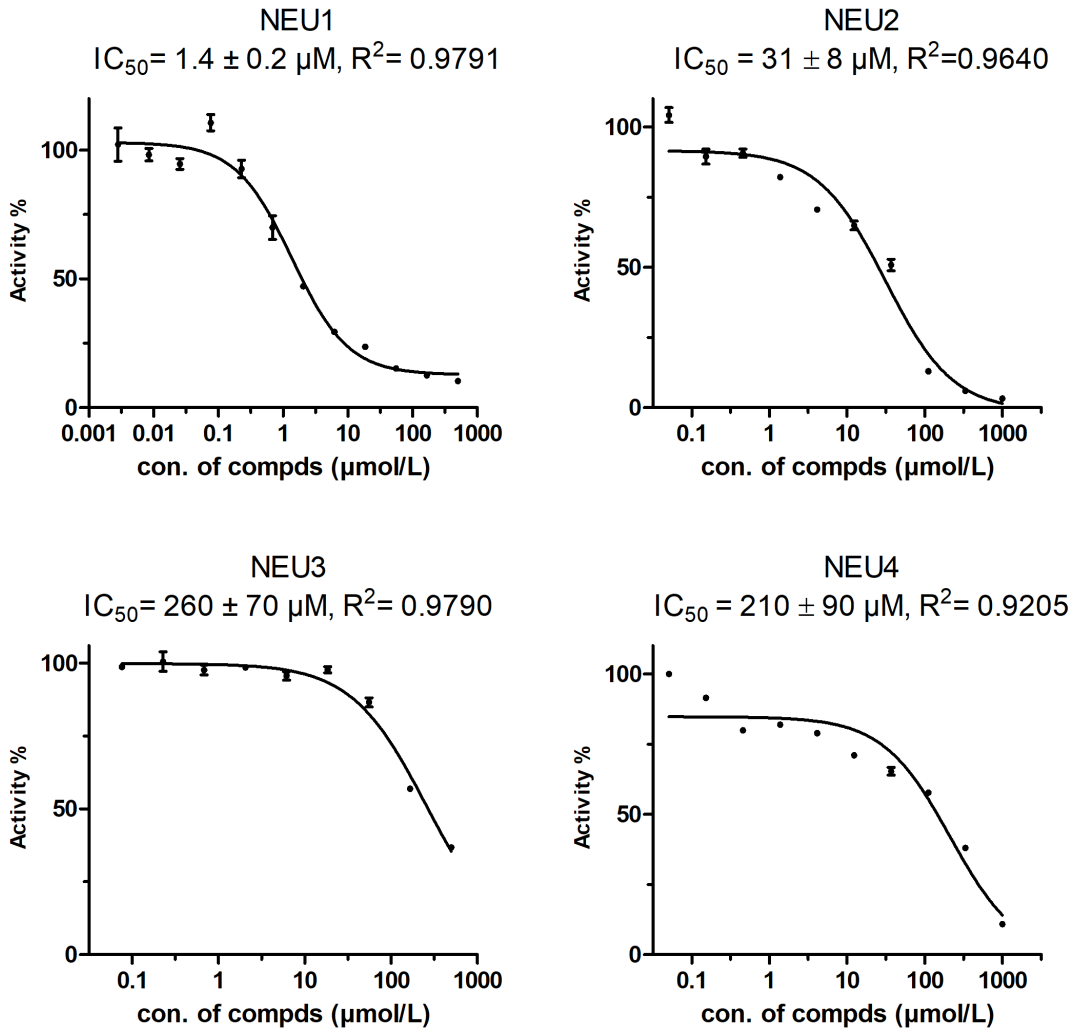
17b


NEU1
IC50=1.5 ± 0.2 μM, R2= 0.9865
Activity %
100
50
0
0.01
0.1
1
10
100
con. of compds (μmol/L)
NEU2
IC50=59 ± 26 μM, R2=0.9269
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)
NEU3
IC50 > 500 μM
Activity %
100
50
0
0.1
1
10
100
1000
con. of compds (μmol/L)
NEU4
IC50 > 500 μM
Activity %
100
50
0
1
10
100
1000
con. of compds (μmol/L)

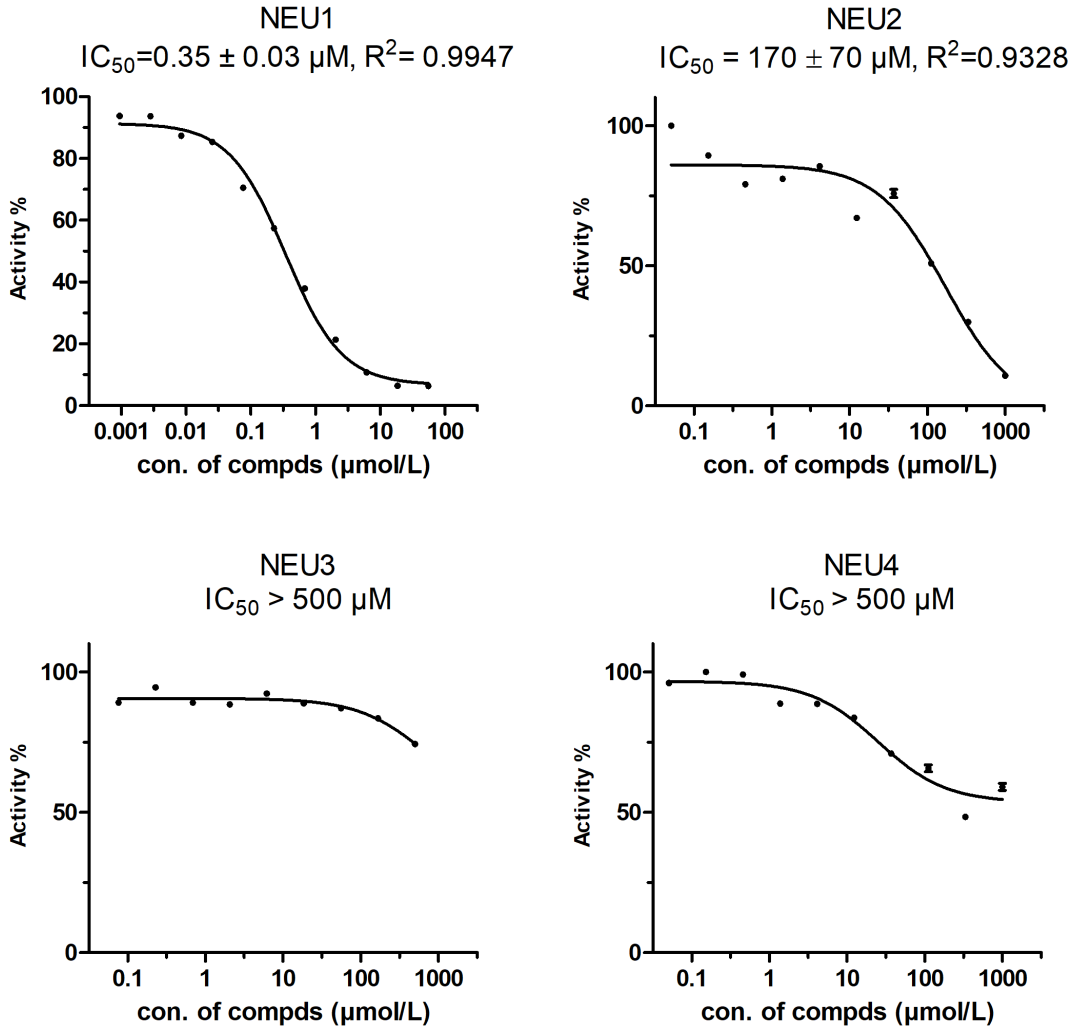
17c


NEU1
IC50=1.6 ± 0.2 μM, R2= 0.9861
Activity %
con. of compds (μmol/L)
NEU2
IC50 = 140 ± 30 μM
Activity %
con. of compds (μmol/L)
NEU3
IC50 > 500 μM
Activity %
con. of compds (μmol/L)
NEU4
IC50 = 190 ± 70 μM, R2= 0.9461
Activity %
con. of compds (μmol/L)

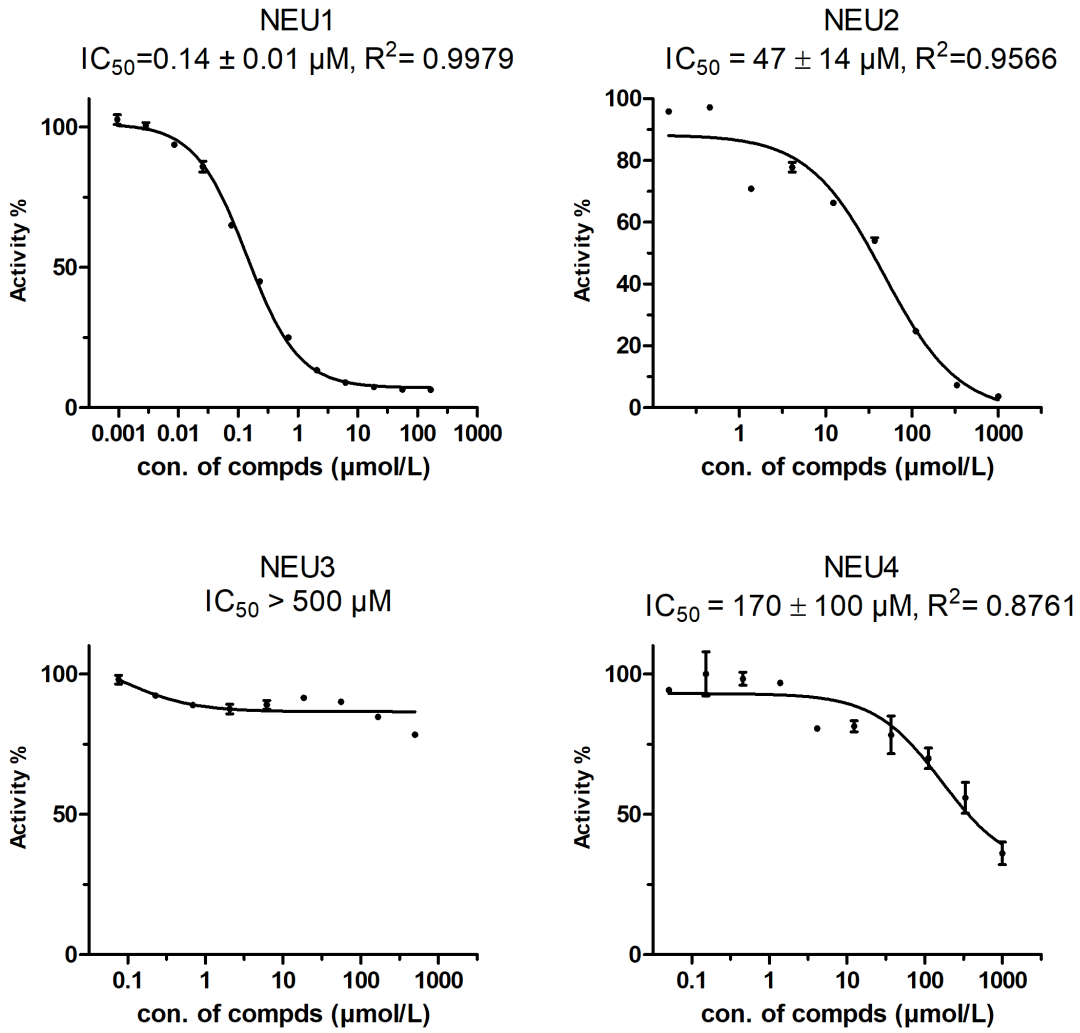
17d


NEU1
IC50= 1.4 ± 0.2 μM, R2= 0.9791
NEU2
IC50 = 31 ± 8 μM, R2=0.9640
NEU3
IC50= 260 ± 70 μM, R2= 0.9790
NEU4
IC50 = 210 ± 90 μM, R2= 0.9205
Activity %
con. of compds (μmol/L)
0
50
100
0.001
0.01
0.1
1
10
100
1000

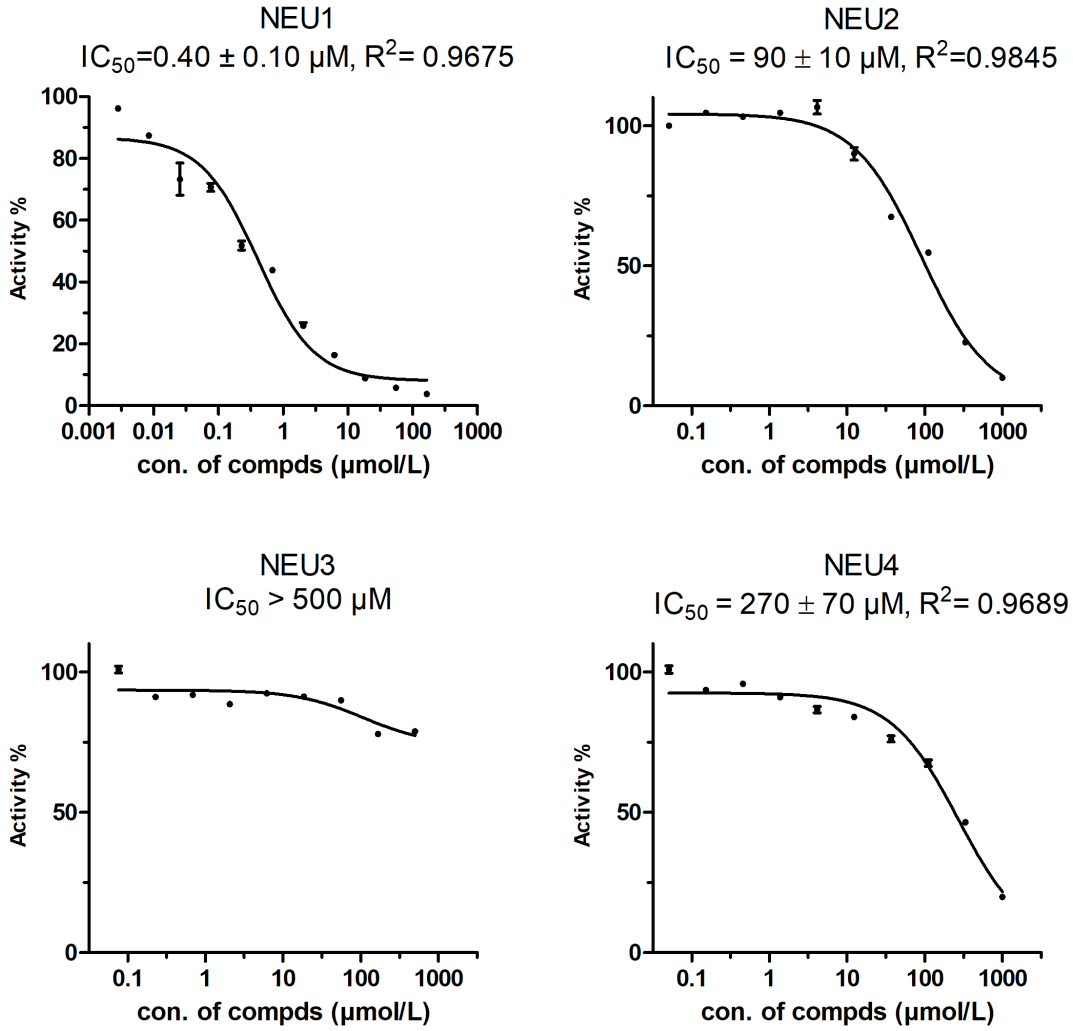
17e


NEU1
IC50=0.35 ± 0.03 μM, R2= 0.9947
Activity %
con. of compds (μmol/L)
NEU2
IC50 = 170 ± 70 μM, R2=0.9328
Activity %
con. of compds (μmol/L)
NEU3
IC50 > 500 μM
Activity %
con. of compds (μmol/L)
NEU4
IC50 > 500 μM
Activity %
con. of compds (μmol/L)

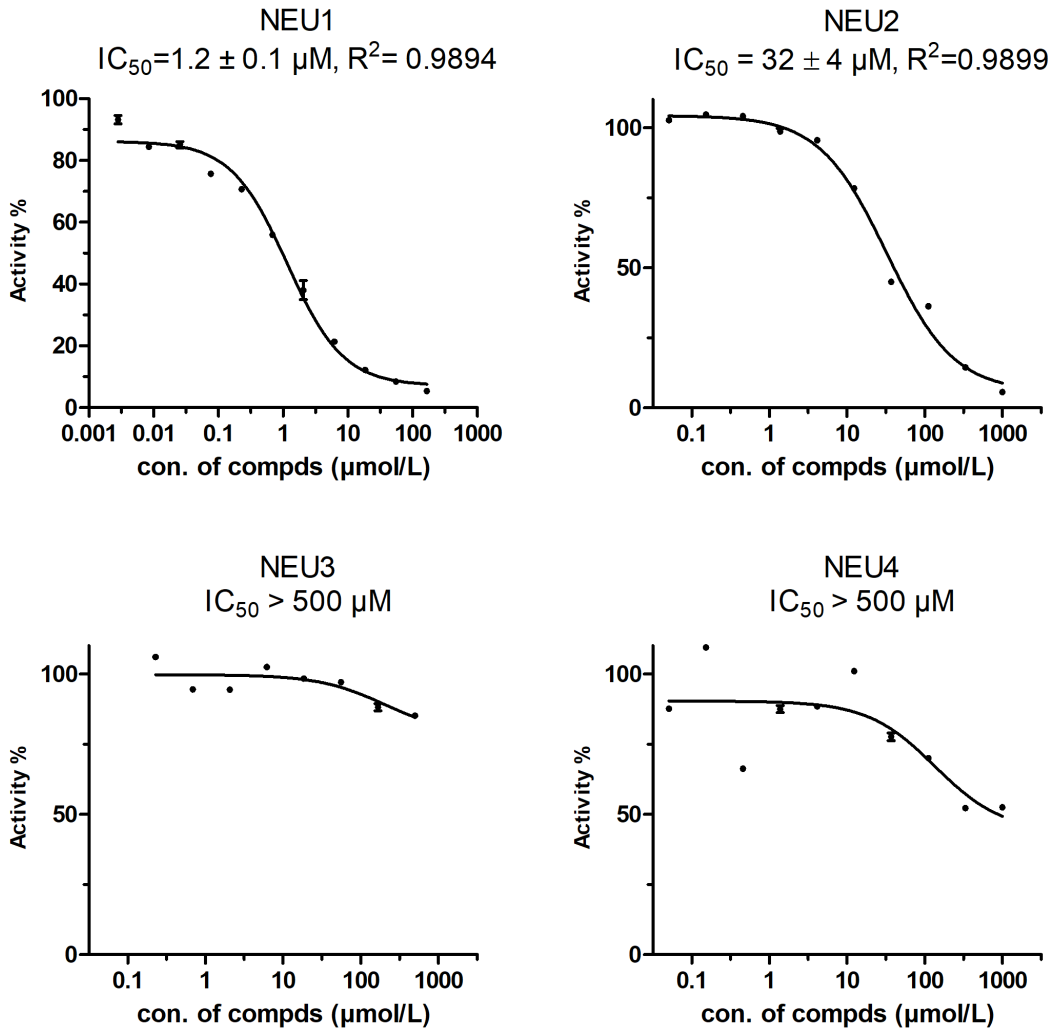
17f


NEU1
IC50=0.14 ± 0.01 μM, R2= 0.9979
Activity %
100
50
0
0.001 0.01 0.1 1 10 100 1000
con. of compds (μmol/L)
NEU2
IC50 = 47 ± 14 μM, R2=0.9566
Activity %
100
80
60
40
20
0
1 10 100 1000
con. of compds (μmol/L)
NEU3
IC50 > 500 μM
Activity %
100
50
0
0.1 1 10 100 1000
con. of compds (μmol/L)
NEU4
IC50 = 170 ± 100 μM, R2= 0.8761
Activity %
100
50
0
0.1 1 10 100 1000
con. of compds (μmol/L)

17g


NEU1
IC50=0.40 ± 0.10 μM, R2= 0.9675
Activity %
con. of compds (μmol/L)
NEU2
IC50 = 90 ± 10 μM, R2=0.9845
Activity %
con. of compds (μmol/L)
NEU3
IC50 > 500 μM
Activity %
con. of compds (μmol/L)
NEU4
IC50 = 270 ± 70 μM, R2= 0.9689
Activity %
con. of compds (μmol/L)

17h


NEU1
IC50=1.2 ± 0.1 μM, R2= 0.9894
Activity %
con. of compds (μmol/L)
NEU2
IC50 = 32 ± 4 μM, R2=0.9899
Activity %
con. of compds (μmol/L)
NEU3
IC50 > 500 μM
Activity %
con. of compds (μmol/L)
NEU4
IC50 > 500 μM
Activity %
con. of compds (μmol/L)

22

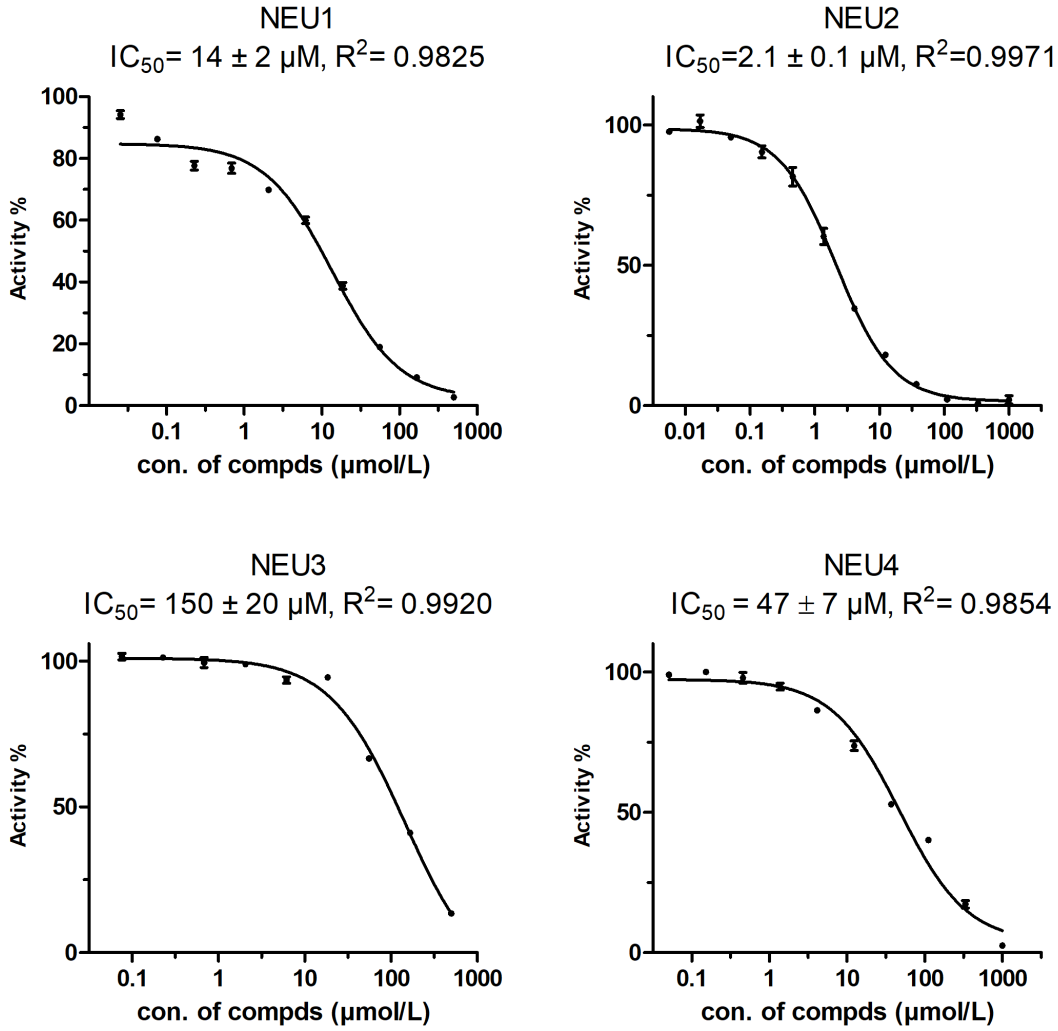

NEU1
IC50= 14 ± 2 μM, R2= 0.9825
Activity %
con. of compds (μmol/L)
NEU2
IC50=2.1 ± 0.1 μM, R2=0.9971
Activity %
con. of compds (μmol/L)
NEU3
IC50= 150 ± 20 μM, R2= 0.9920
Activity %
con. of compds (μmol/L)
NEU4
IC50 = 47 ± 7 μM, R2= 0.9854
Activity %
con. of compds (μmol/L)

Table S3: K_i determinations using a noncompetitive inhibition model[a]

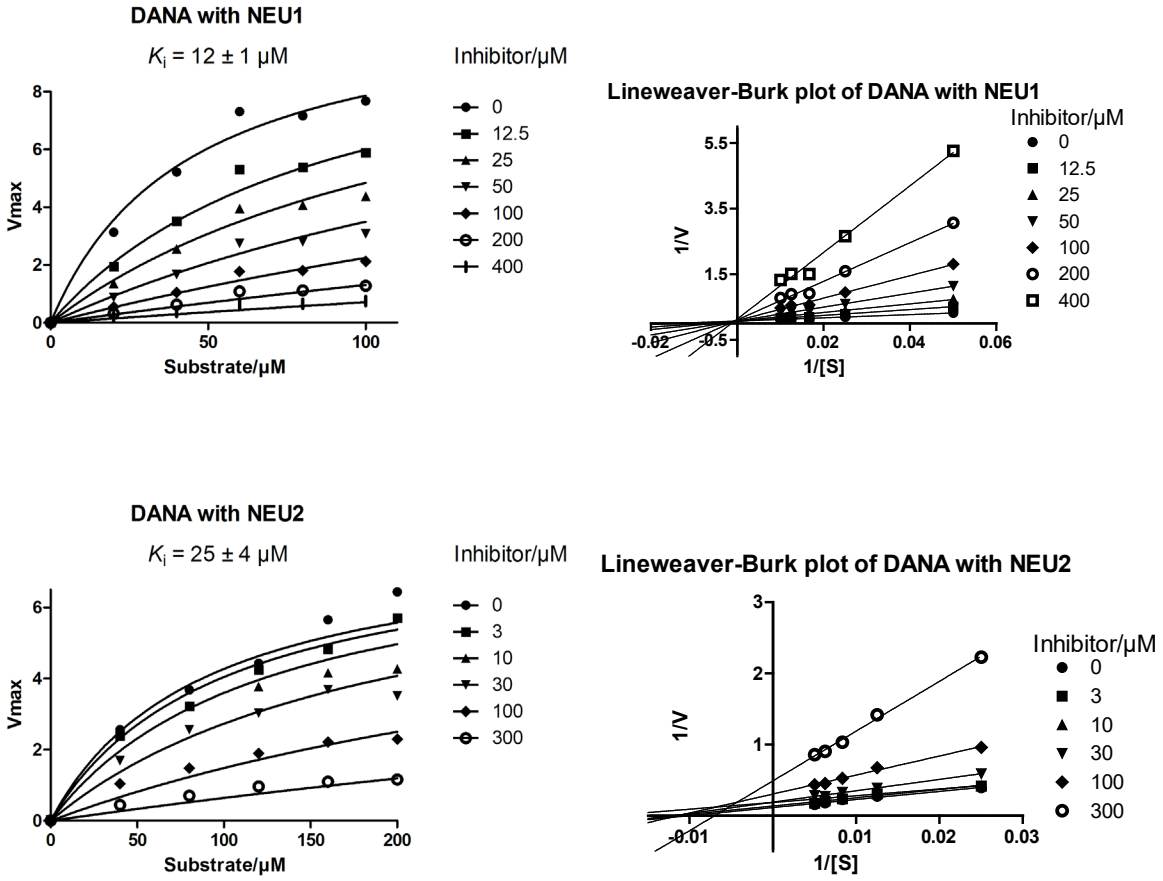
Compd.	NEU1		NEU2	
	α	K_i[μM]	α	K_i[μM]
DANA	4.4	17 ± 4	0.32	130 ± 99
8	1.2	1.6 ± 0.9	ND	
11c	infinite	0.24 ± 0.03	ND	
11d	4.7	0.25 ± 0.06	ND	
17f	7.2	0.066 ± 0.13	ND	
13c	ND		0.024	67 ± 476
13d	ND		0.69	11 ± 6
22	ND		12	1.7 ± 0.5

[a] Data were fit to a noncompetitive inhibition model, also called a mixed inhibition model, using the kinetic data shown in Fig S2 with the following equation[1]:

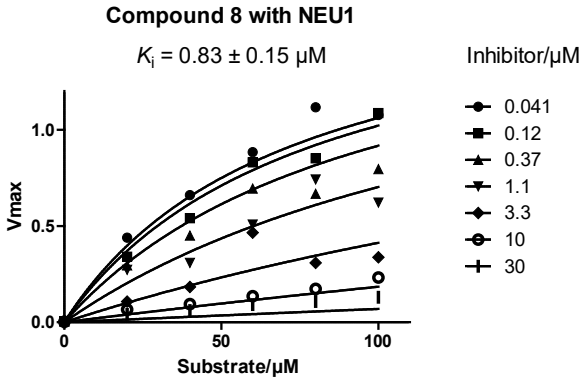
$$\mathbf{V} = \frac{\mathbf{V_{max}[S]}}{[\boldsymbol{S}]\left(\mathbf{1} + \frac{[\boldsymbol{I}]}{\boldsymbol{\alpha K_i}}\right) + \boldsymbol{K_m}(\mathbf{1} + \frac{[\boldsymbol{I}]}{\boldsymbol{K_i}})}$$

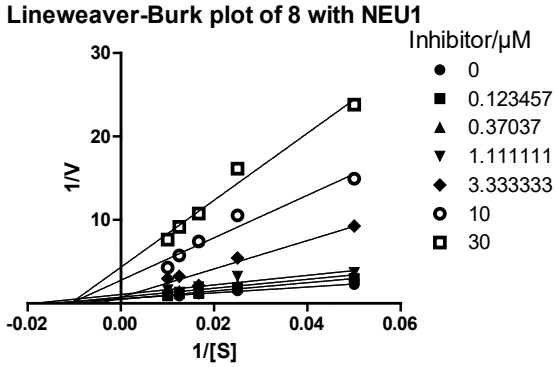
Figure S2: Curves for K_i determinations using a competitive inhibition model and Lineweaver-Burke plots.

DANA

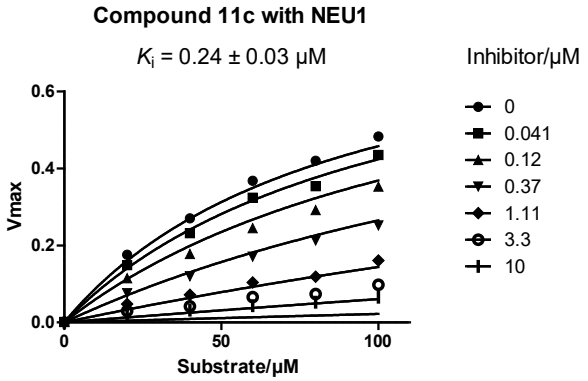


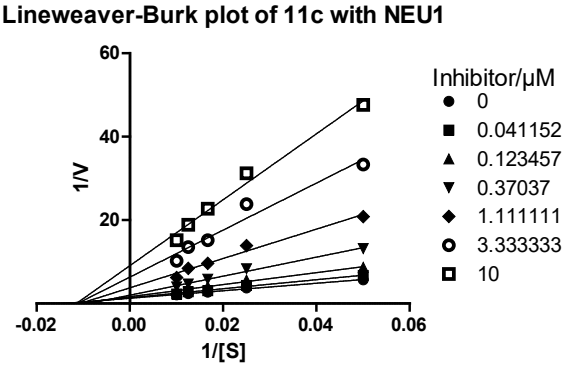
8


Compound 8 with NEU1
K_i = 0.83 ± 0.15 μM
Vmax
Substrate/μM
Inhibitor/μM
0.041
0.12
0.37
1.1
3.3
10
30

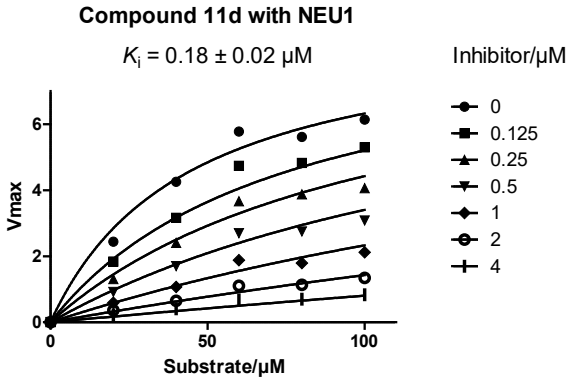

Lineweaver-Burk plot of 8 with NEU1
1/V
1/[S]
Inhibitor/μM
0
0.123457
0.37037
1.111111
3.333333
10
30

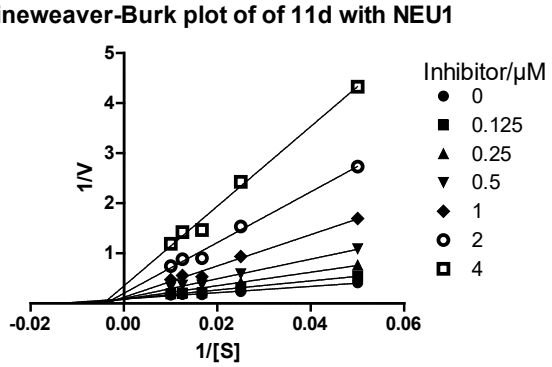
11c


Compound 11c with NEU1
K_i = 0.24 ± 0.03 μM
Vmax
Substrate/μM
Inhibitor/μM
0
0.041
0.12
0.37
1.11
3.3
10

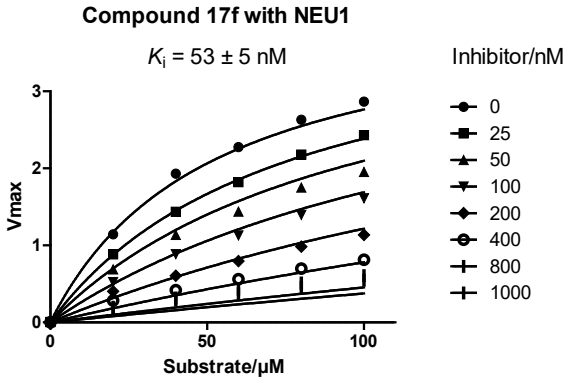

Lineweaver-Burk plot of 11c with NEU1
1/V
1/[S]
Inhibitor/μM
0
0.041152
0.123457
0.37037
1.111111
3.333333
10

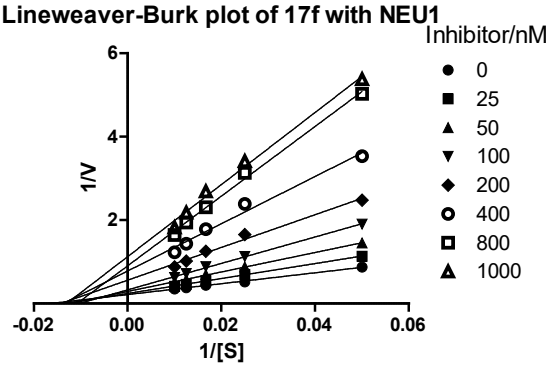
11d


Compound 11d with NEU1
K_i = 0.18 ± 0.02 μM
Vmax
Substrate/μM
Inhibitor/μM
0
0.125
0.25
0.5
1
2
4

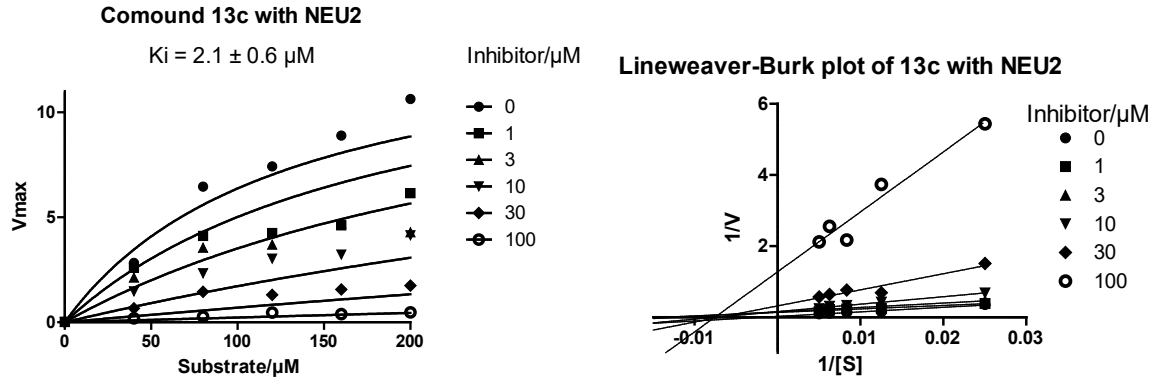

Lineweaver-Burk plot of of 11d with NEU1
1/V
1/[S]
Inhibitor/μM
0
0.125
0.25
0.5
1
2
4

17f

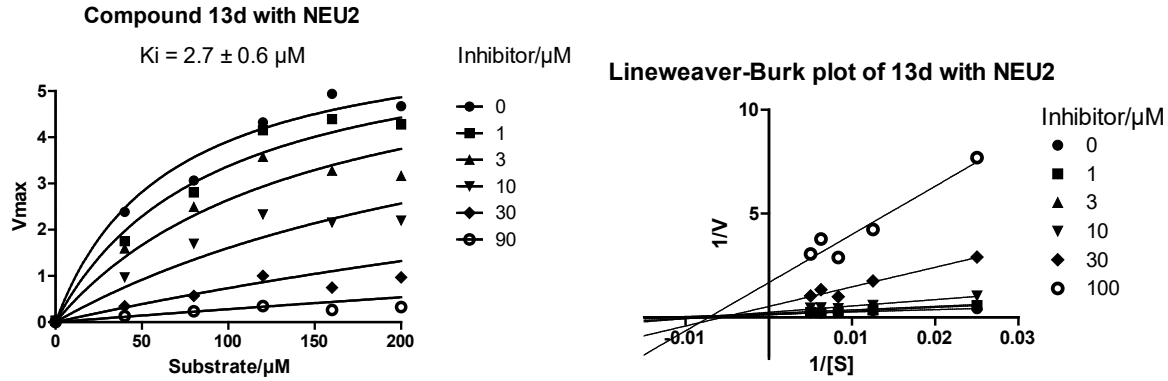

Compound 17f with NEU1
K_i = 53 ± 5 nM
Vmax
Substrate/μM
Inhibitor/nM
0
25
50
100
200
400
800
1000


Lineweaver-Burk plot of 17f with NEU1
1/V
1/[S]
Inhibitor/nM
0
25
50
100
200
400
800
1000

13c


Comound 13c with NEU2
Ki = 2.1 ± 0.6 μM
Inhibitor/μM
0
1
3
10
30
100
Vmax
Substrate/μM
Lineweaver-Burk plot of 13c with NEU2
1/V
1/[S]

13d


Compound 13d with NEU2
Ki = 2.7 ± 0.6 μM
Inhibitor/μM
0
1
3
10
30
90
Vmax
Substrate/μM
Lineweaver-Burk plot of 13d with NEU2
1/V
1/[S]

22

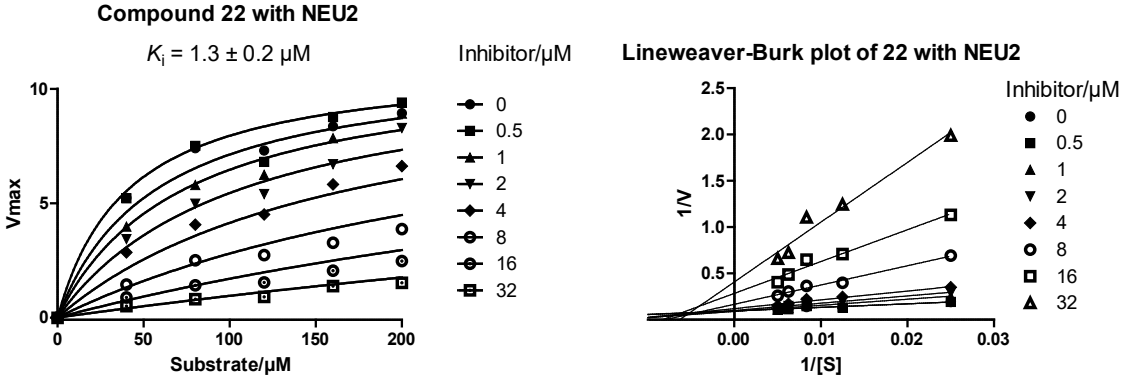
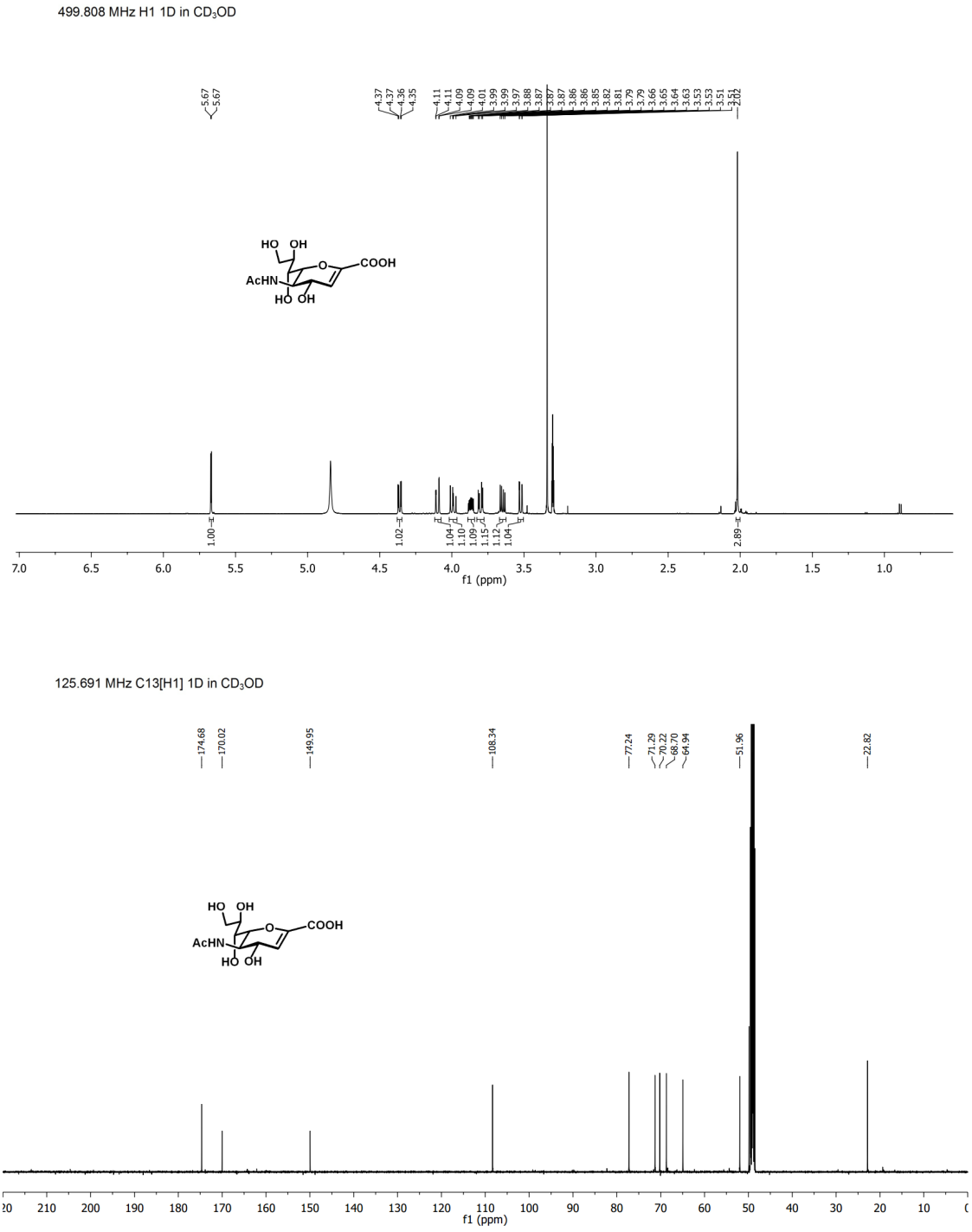
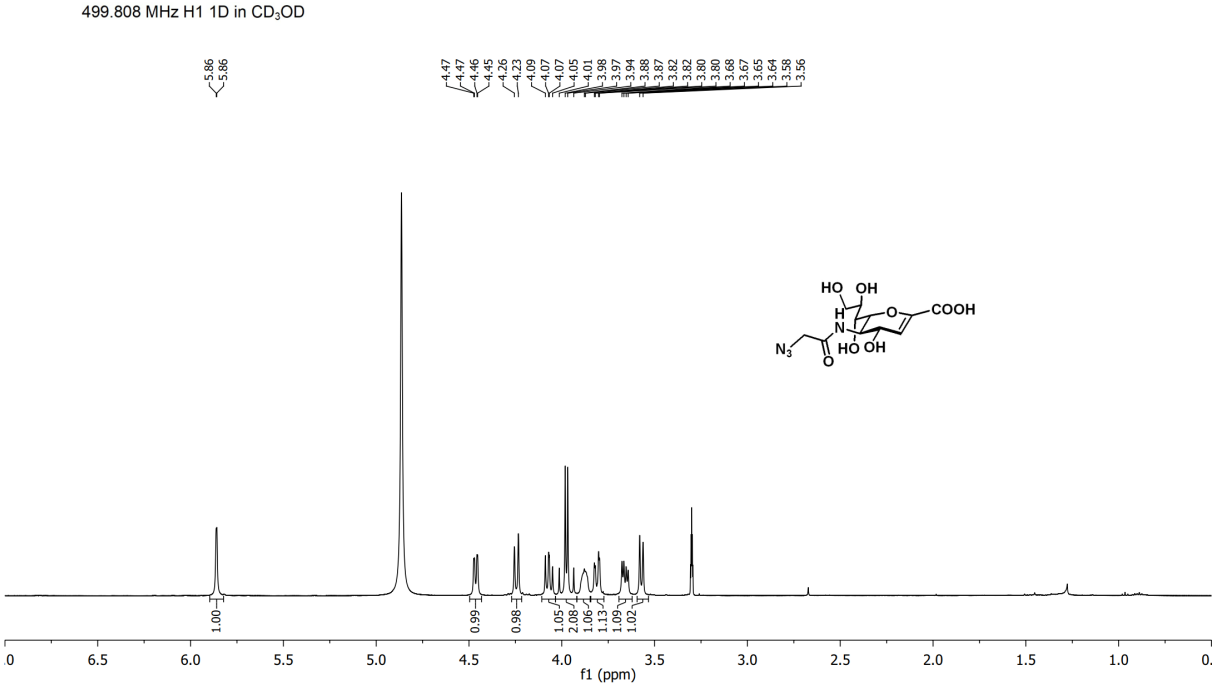

Compound 22 with NEU2
K_i = 1.3 ± 0.2 μM
Inhibitor/μM
0
0.5
1
2
4
8
16
32
Vmax
Substrate/μM
Lineweaver-Burk plot of 22 with NEU2
1/V
1/[S]

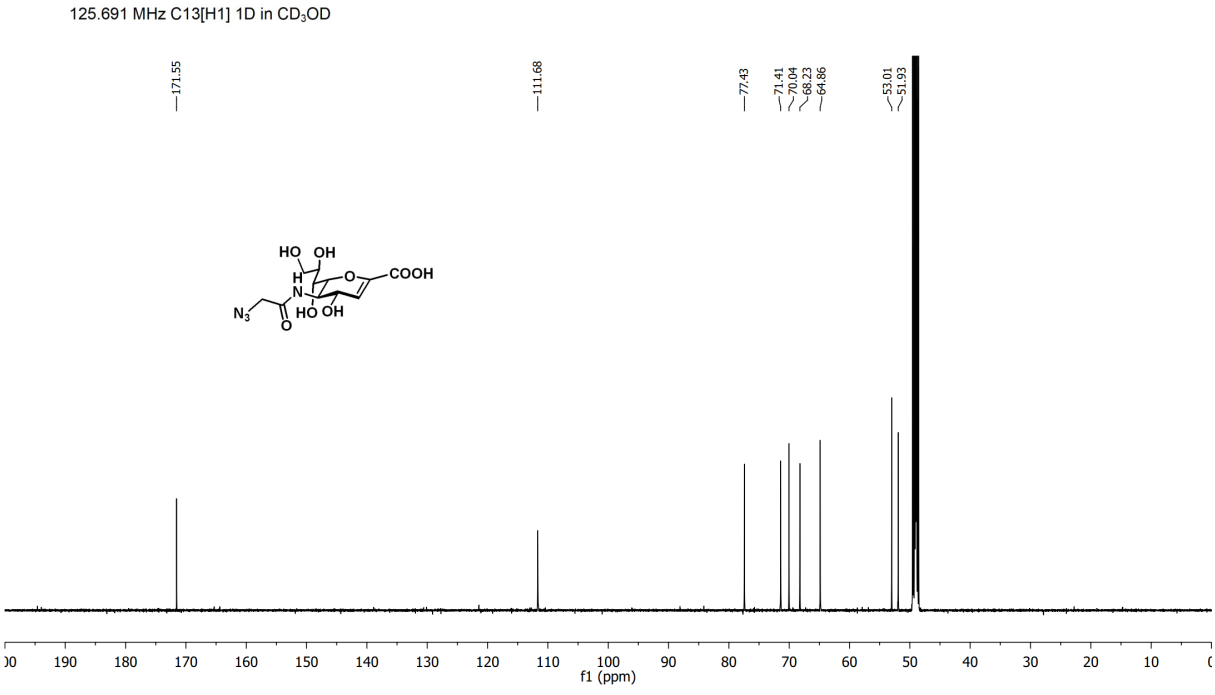
Figure S3: NMR (^{1}H and ^{13}C) spectra

1(DANA)



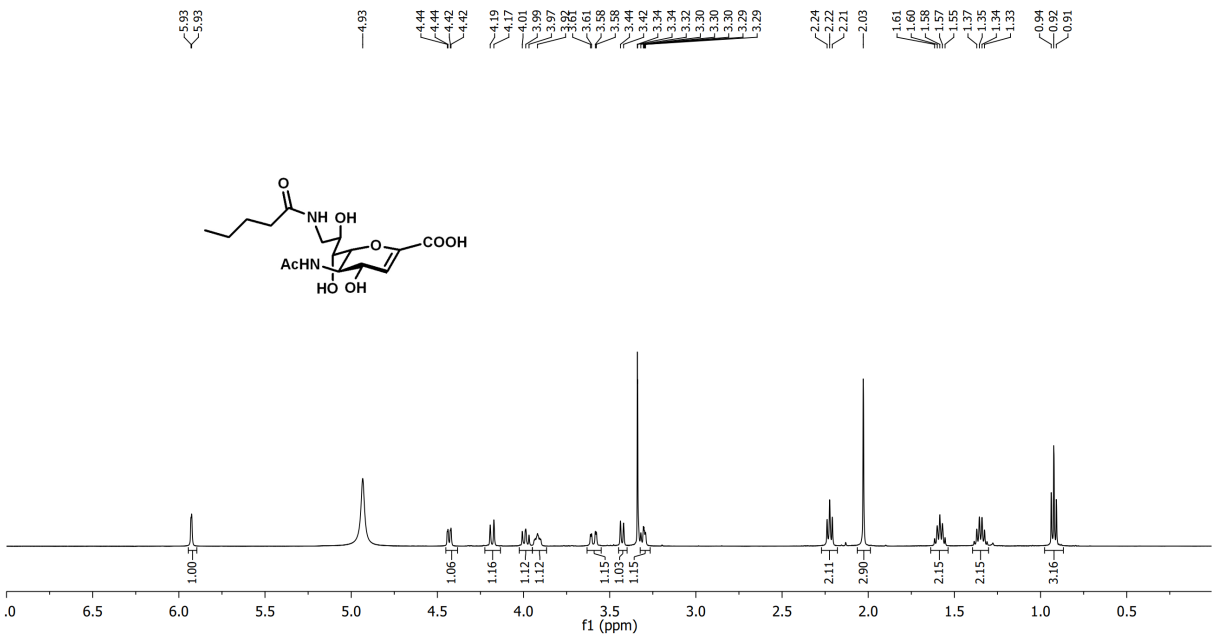
6(Neu5AcN$_3$2en)



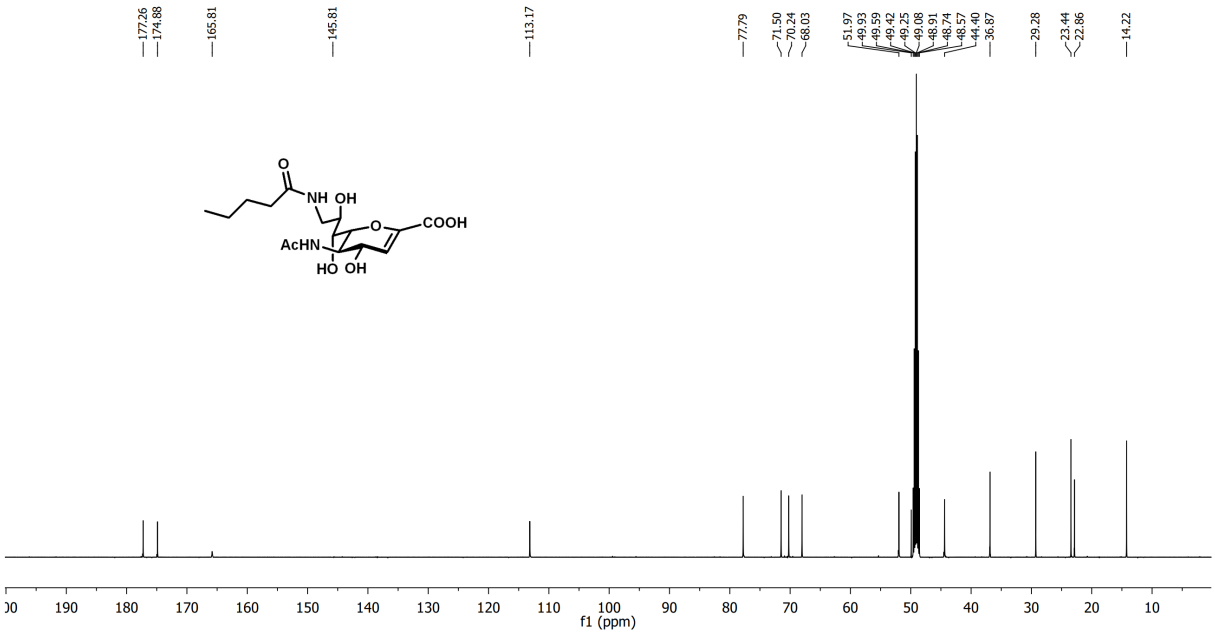


8(C9-BA-DANA)

499.808 MHz H1 1D in CD_3OD

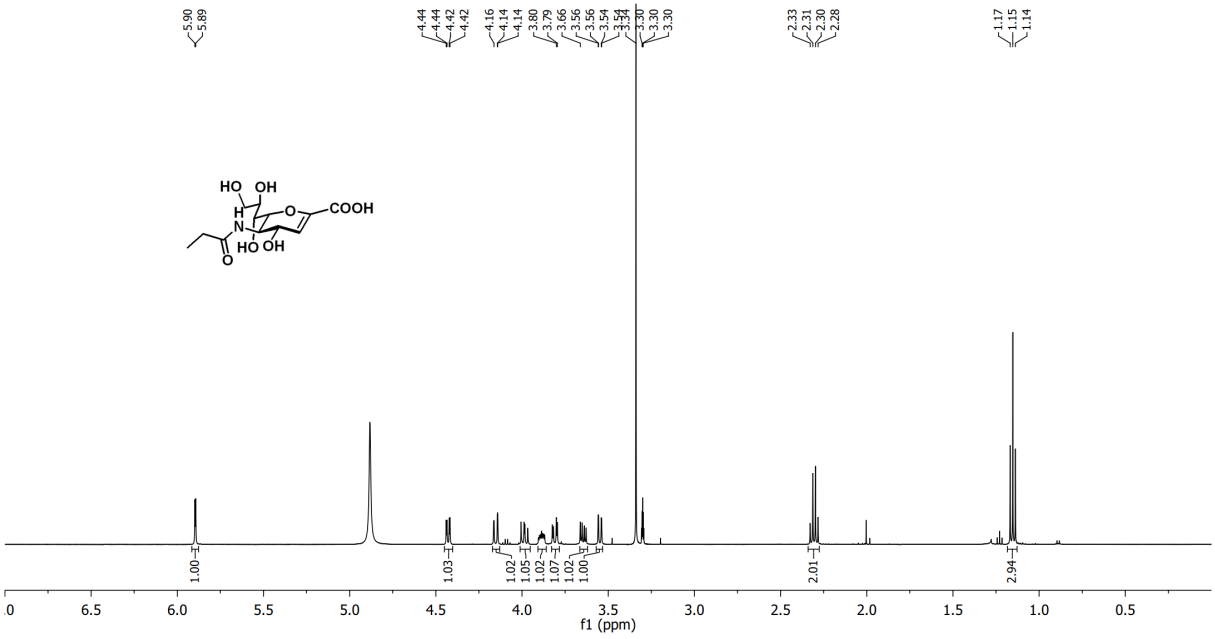


125.691 MHz C13[H1] 1D in CD_3OD

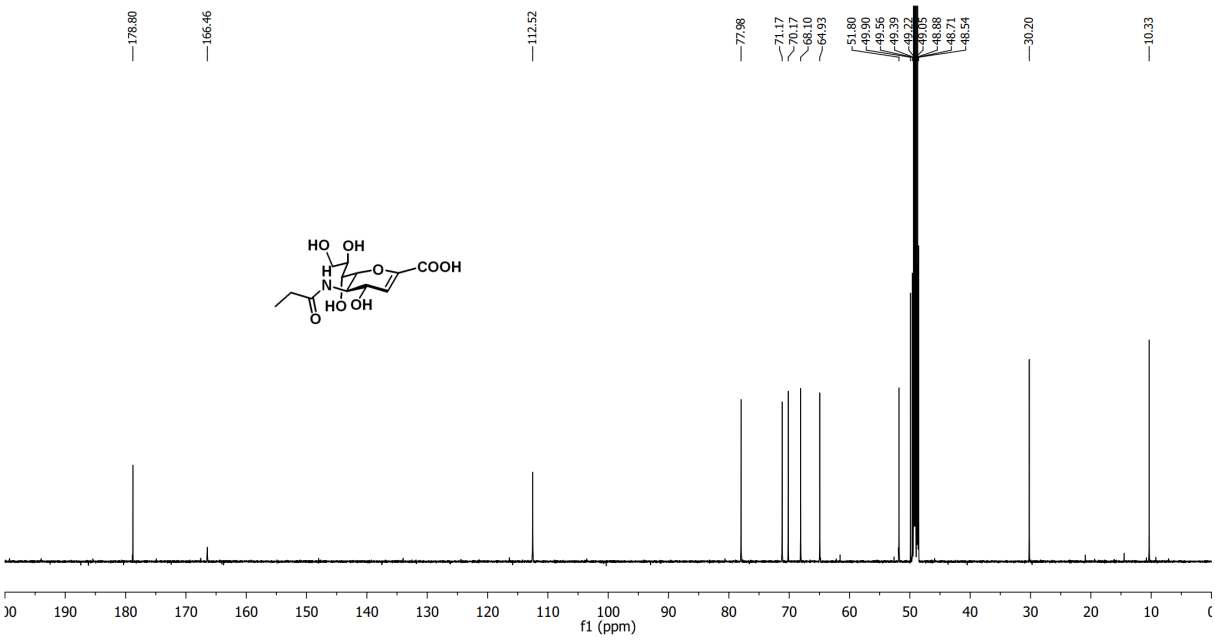


11a

499.808 MHz H1 1D in CD_3OD

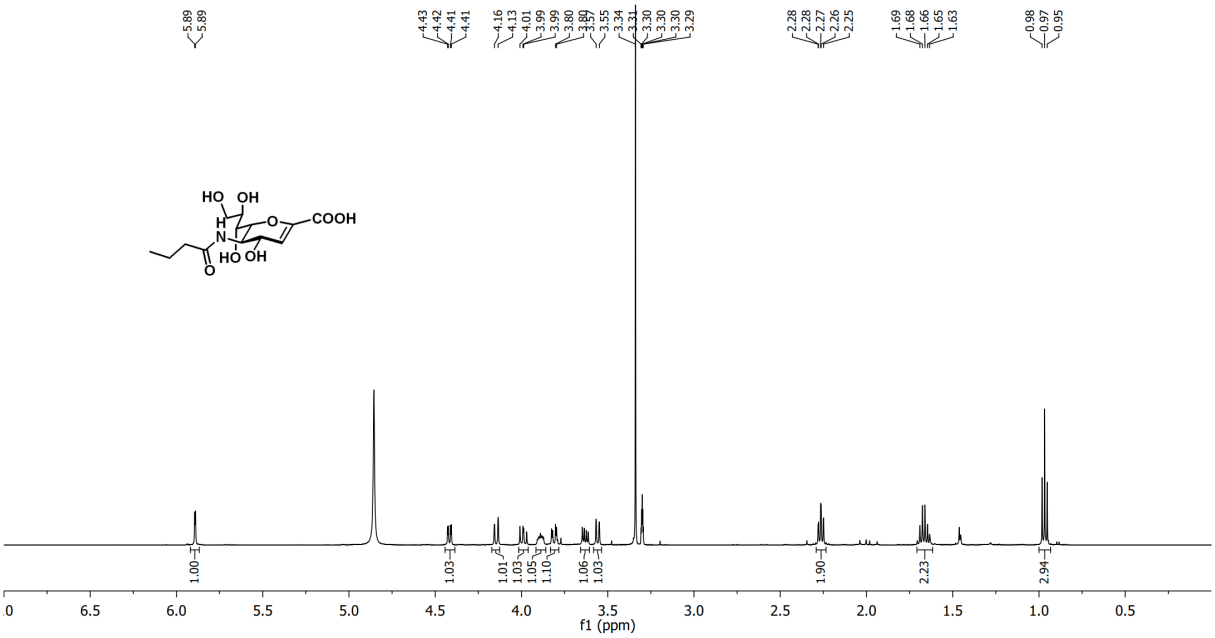


125.691 MHz C13[H1] 1D in CD_3OD

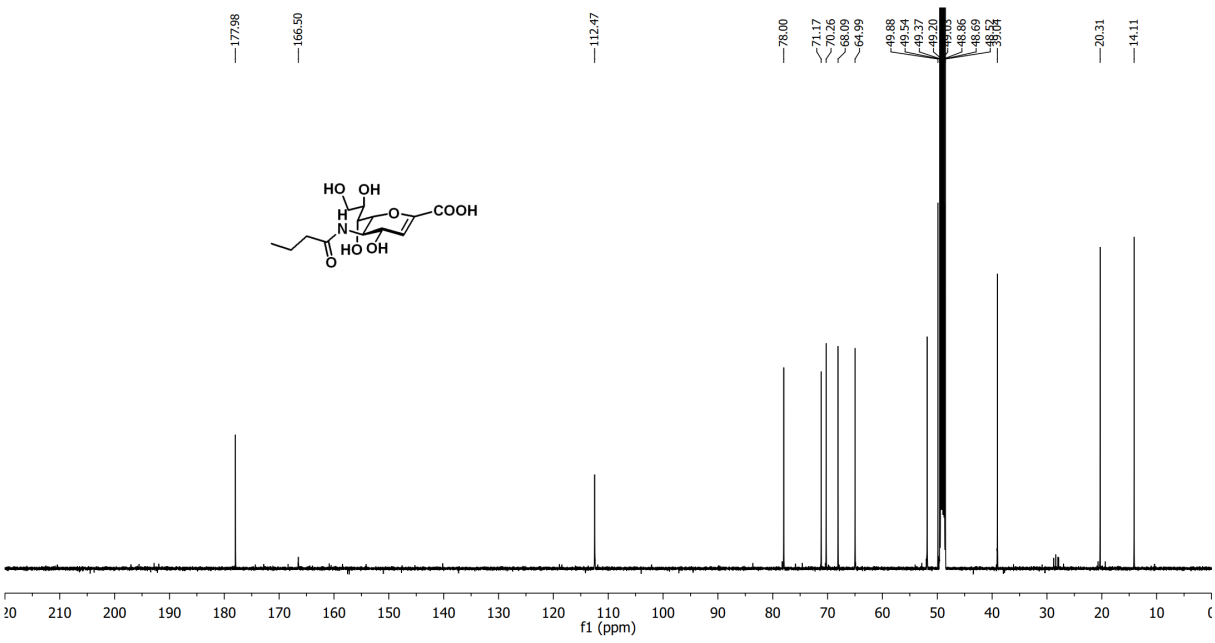


11b

499.808 MHz H1 1D in CD_3OD

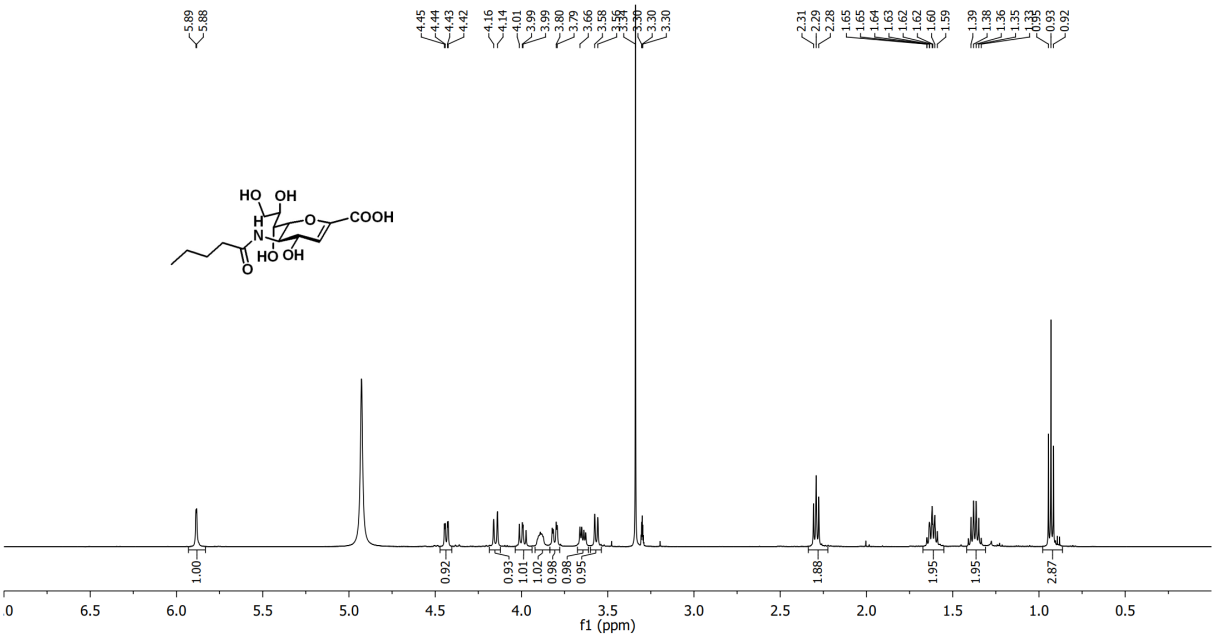


125.691 MHz C13[H1] 1D in CD_3OD

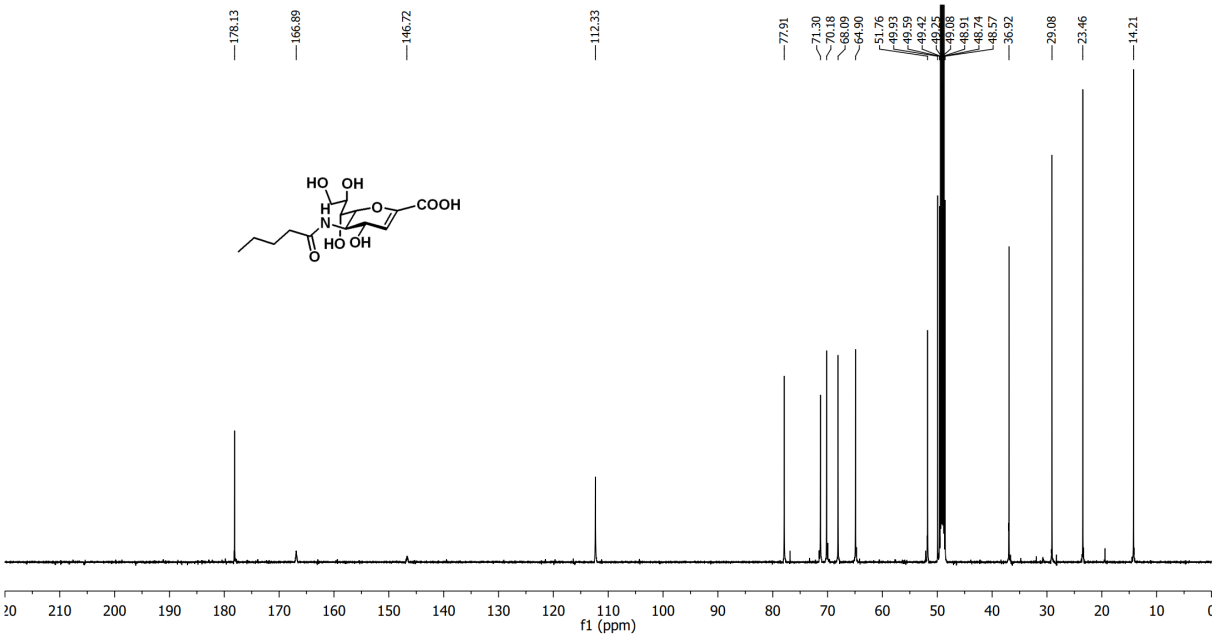


11c

499.808 MHz H1 1D in CD_3OD

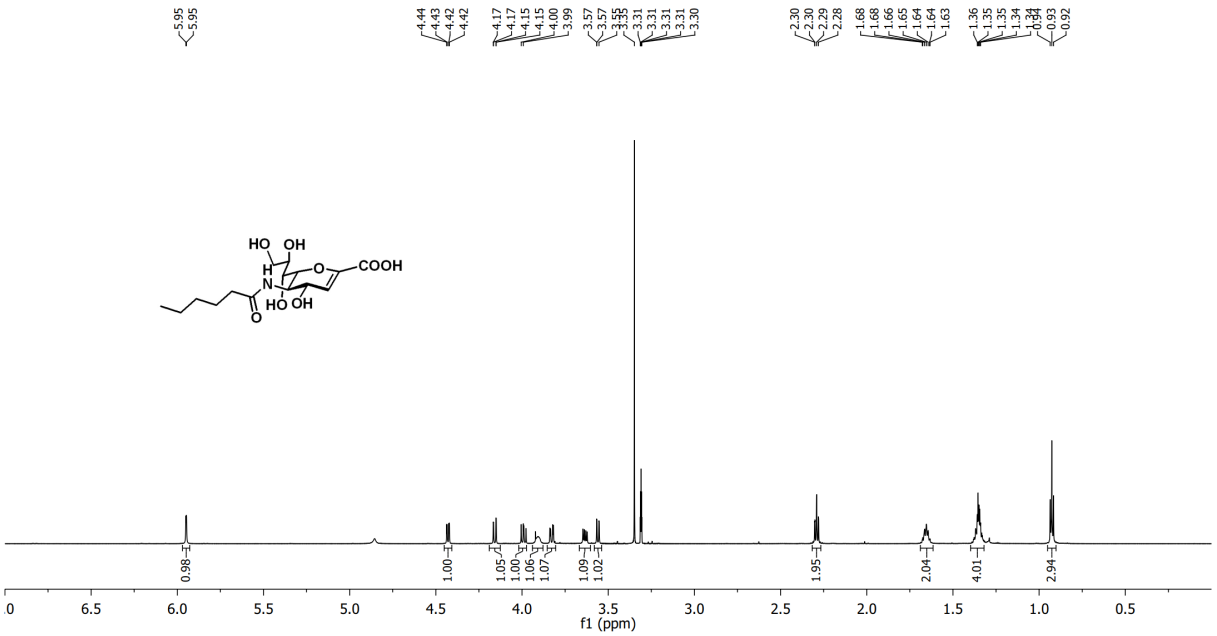


125.691 MHz C13[H1] 1D in CD_3OD

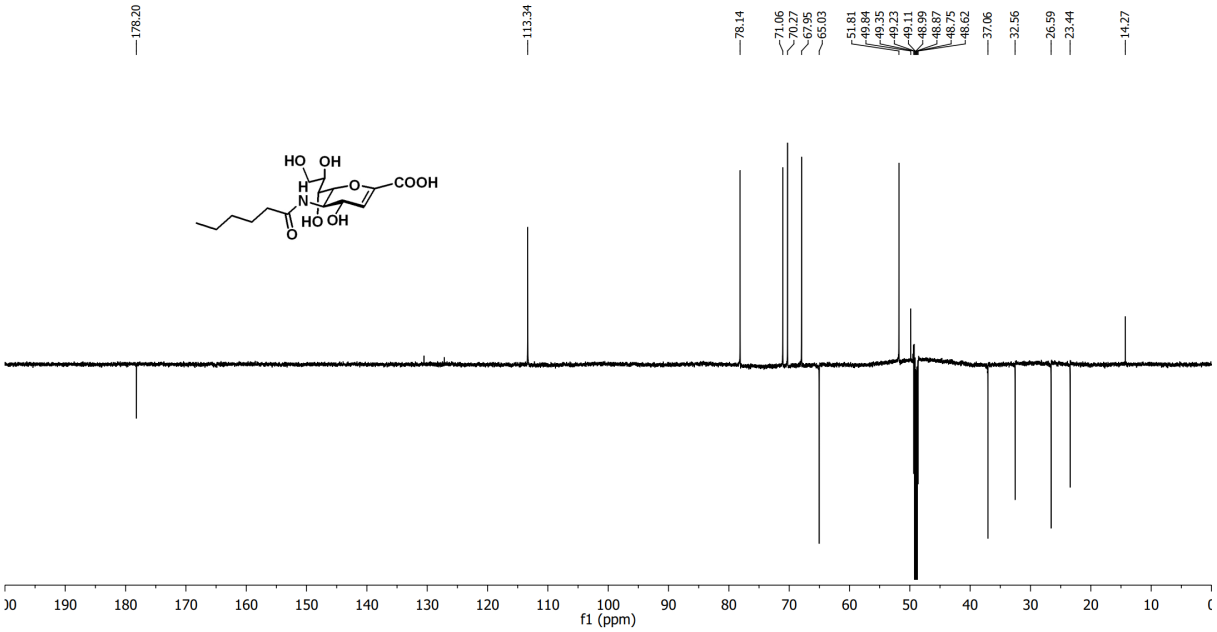


11d

699.765 MHz H1 1D in CD_3OD

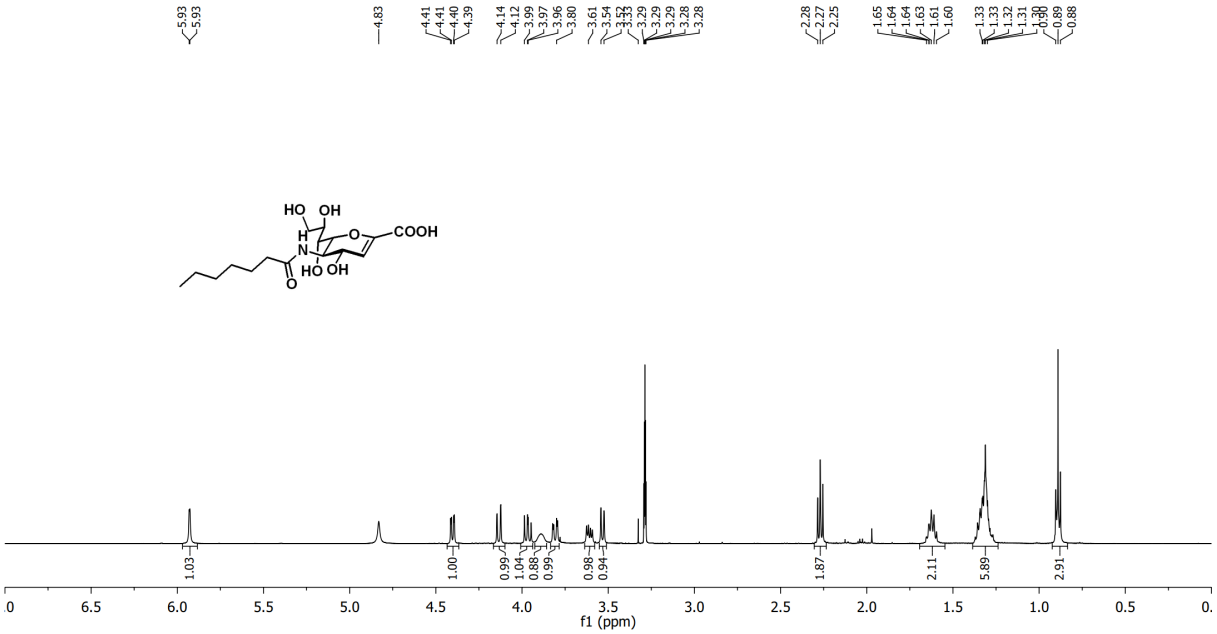


175.975 MHz C13 1D DEPTq in CD_3OD

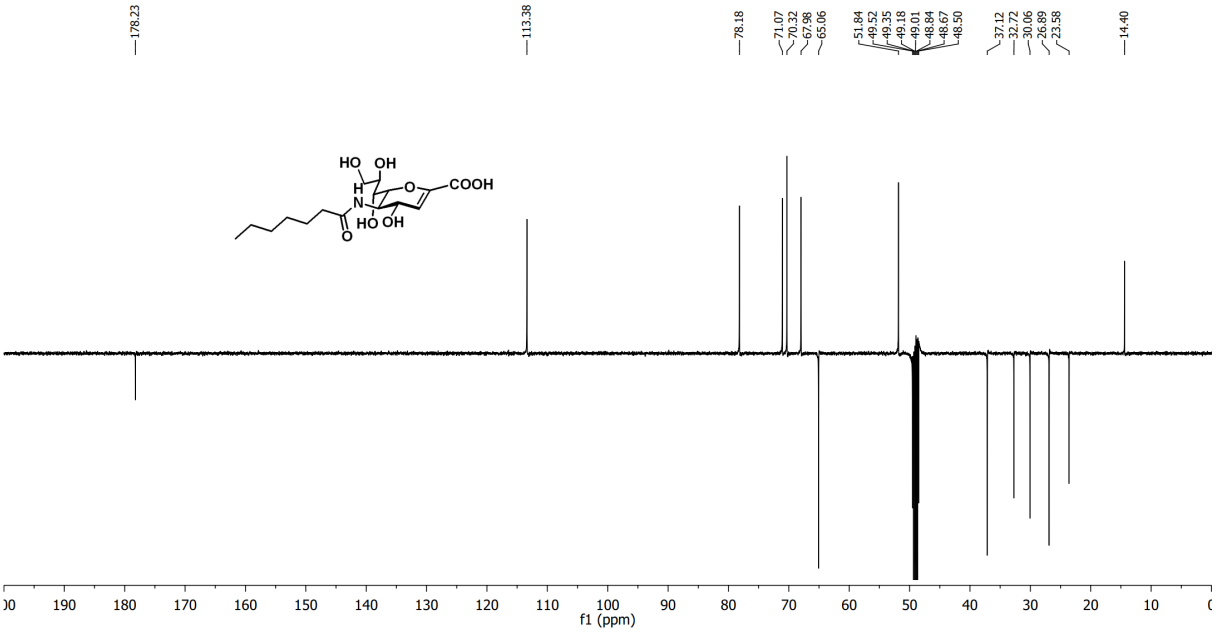


11e

499.799 MHz H1 1D in CD_3OD

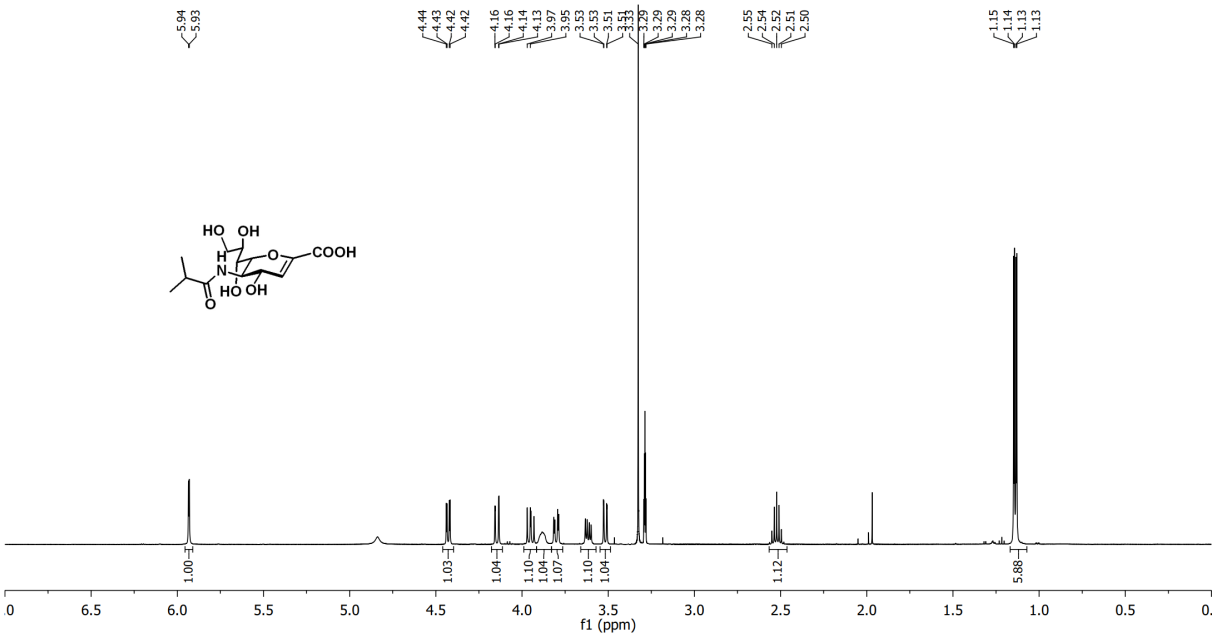


125.688 MHz C13[H1] DEPTq in CD_3OD

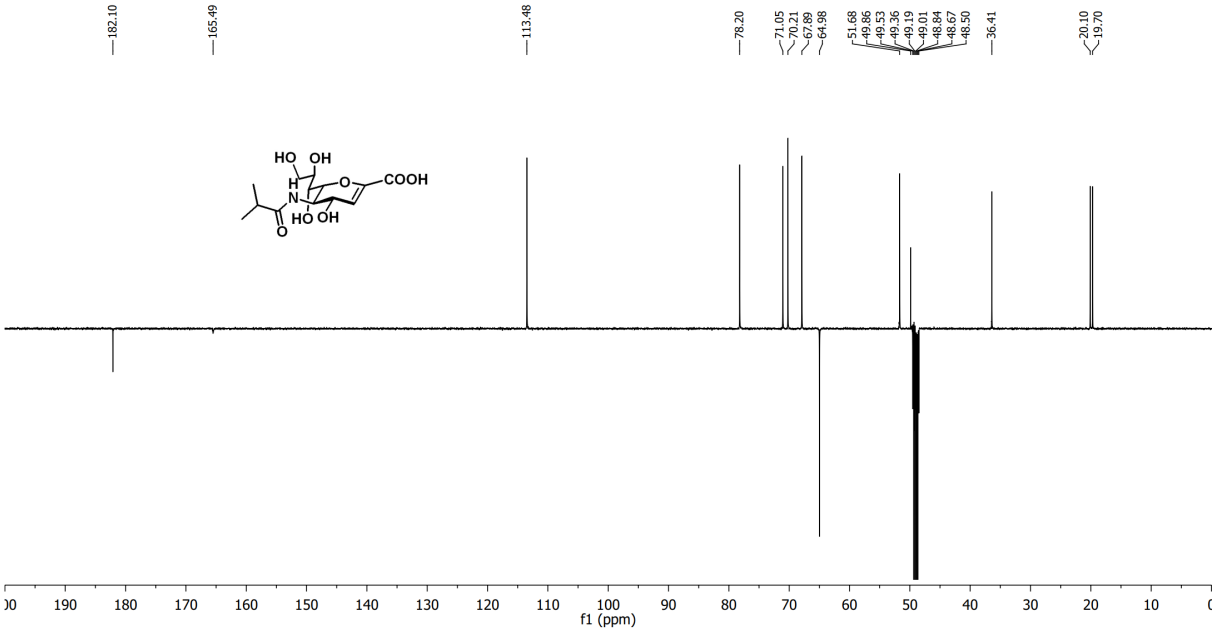


11f

499.799 MHz H1 1D in CD_3OD

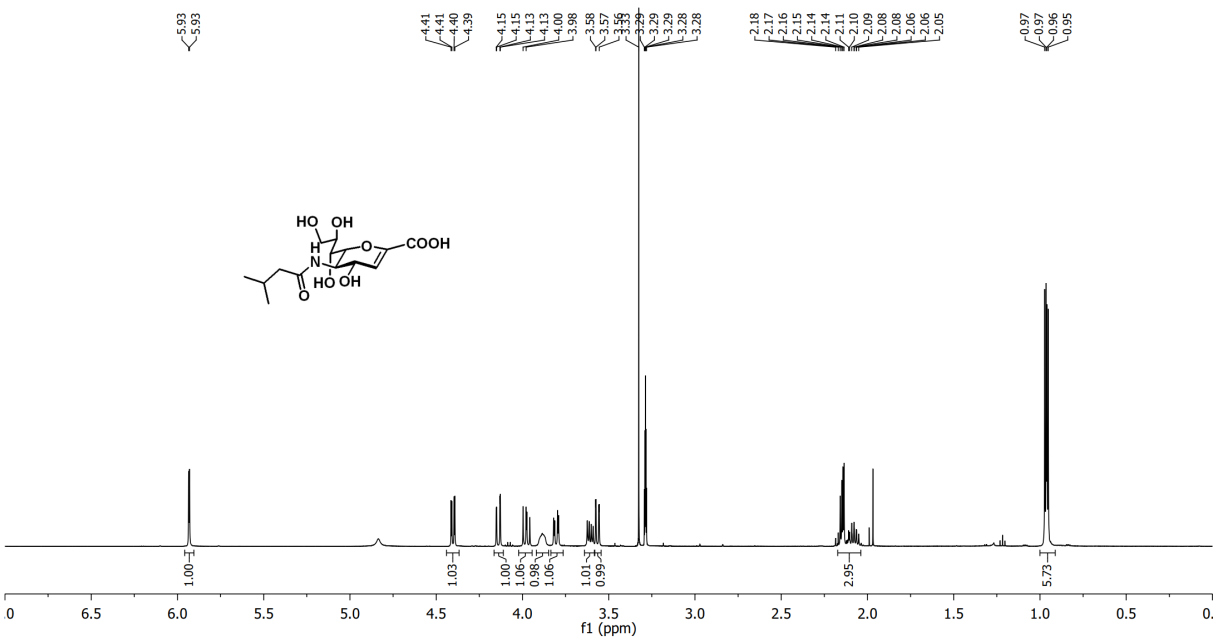


125.688 MHz C13[H1] DEPTq in CD_3OD

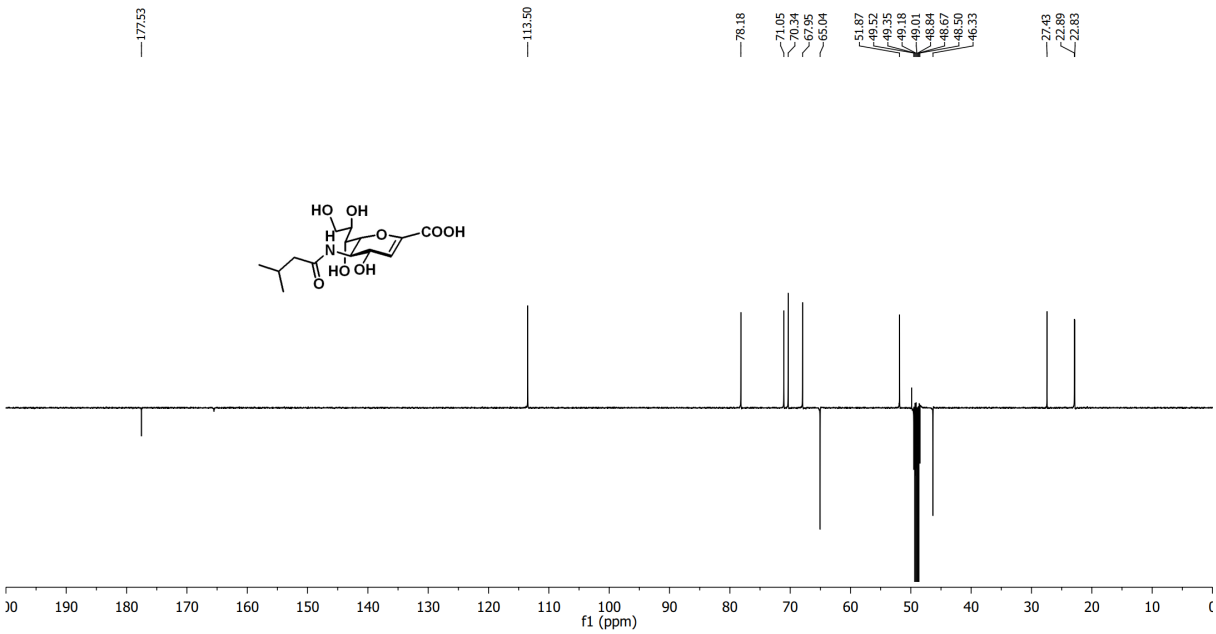


11g

499.808 MHz H1 1D in CD_3OD

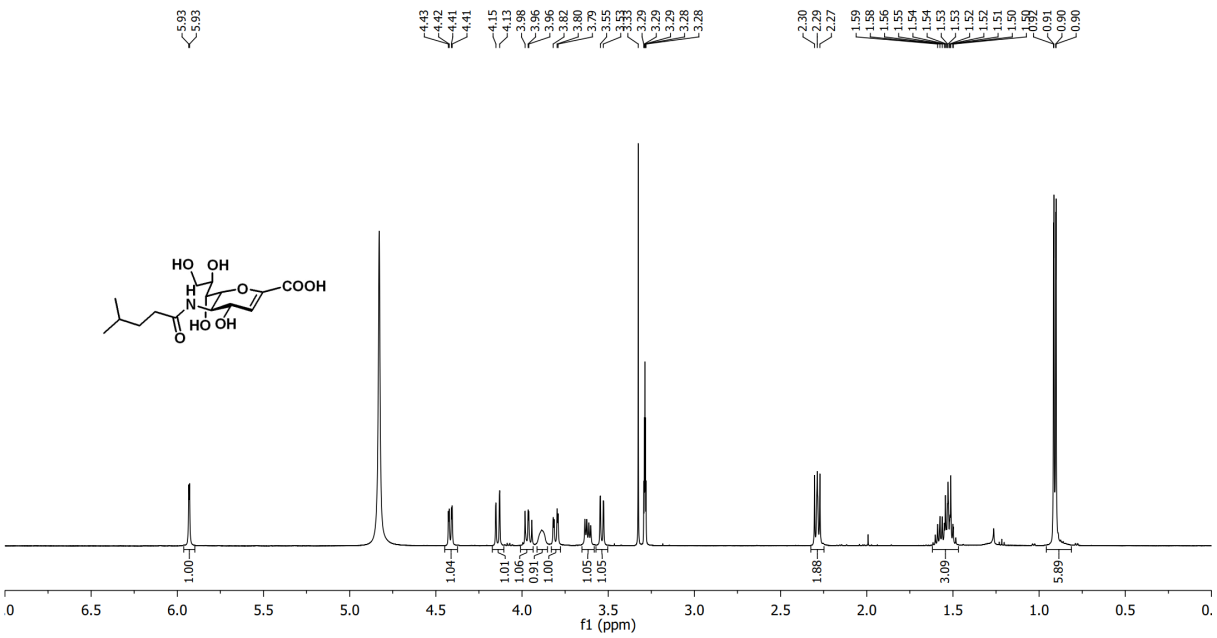


125.688 MHz C13[H1] DEPTq in CD_3OD

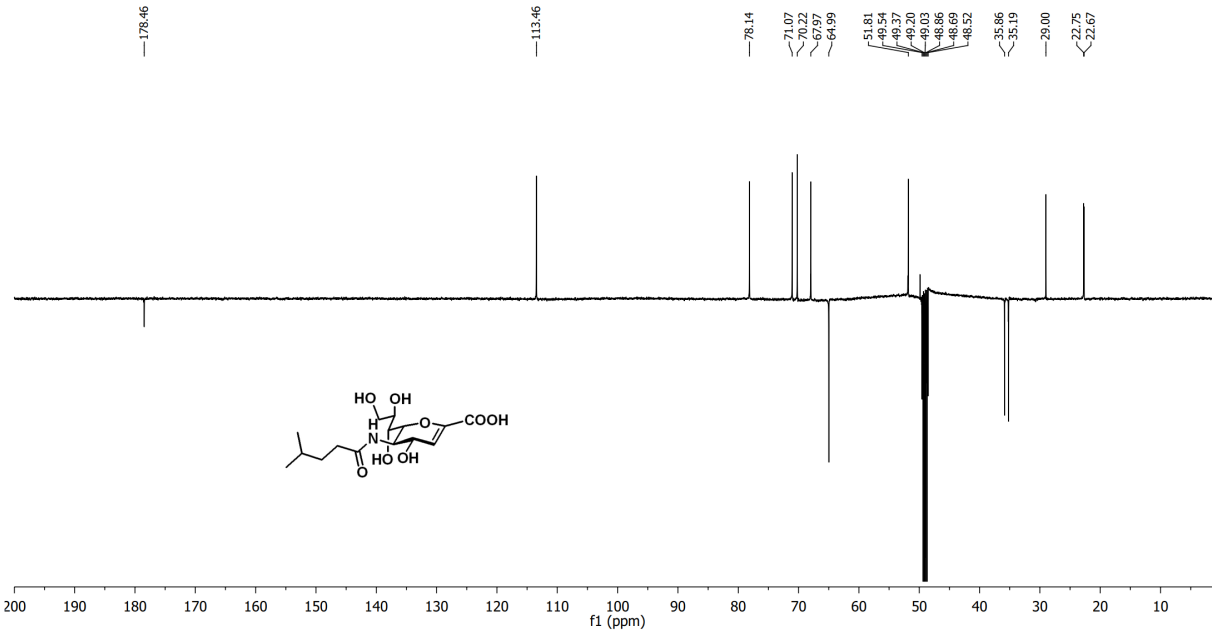


11h

499.799 MHz H1 1D in CD_3OD

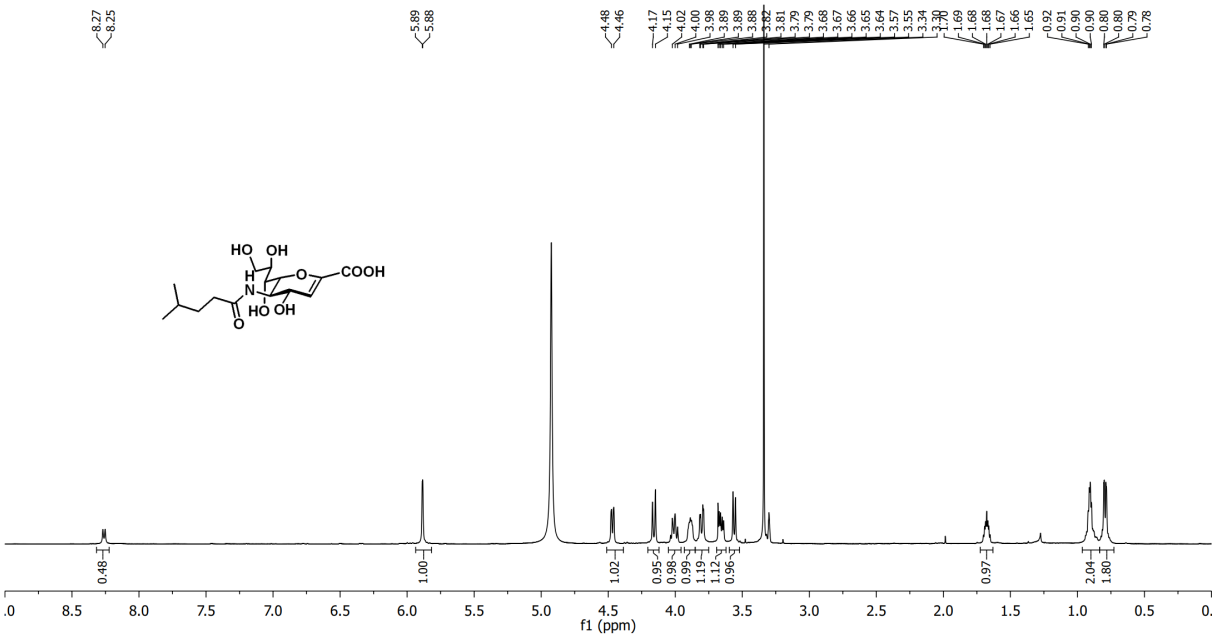


125.688 MHz C13[H1] DEPTq in CD_3OD

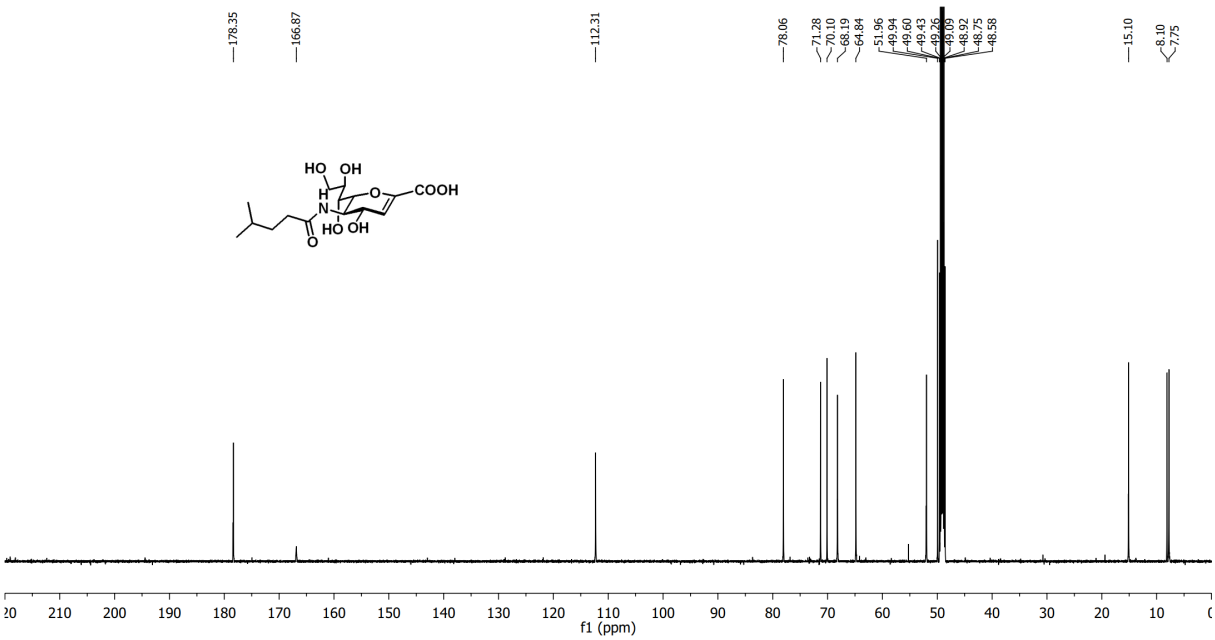


11i

499.808 MHz H1 1D in CD_3OD

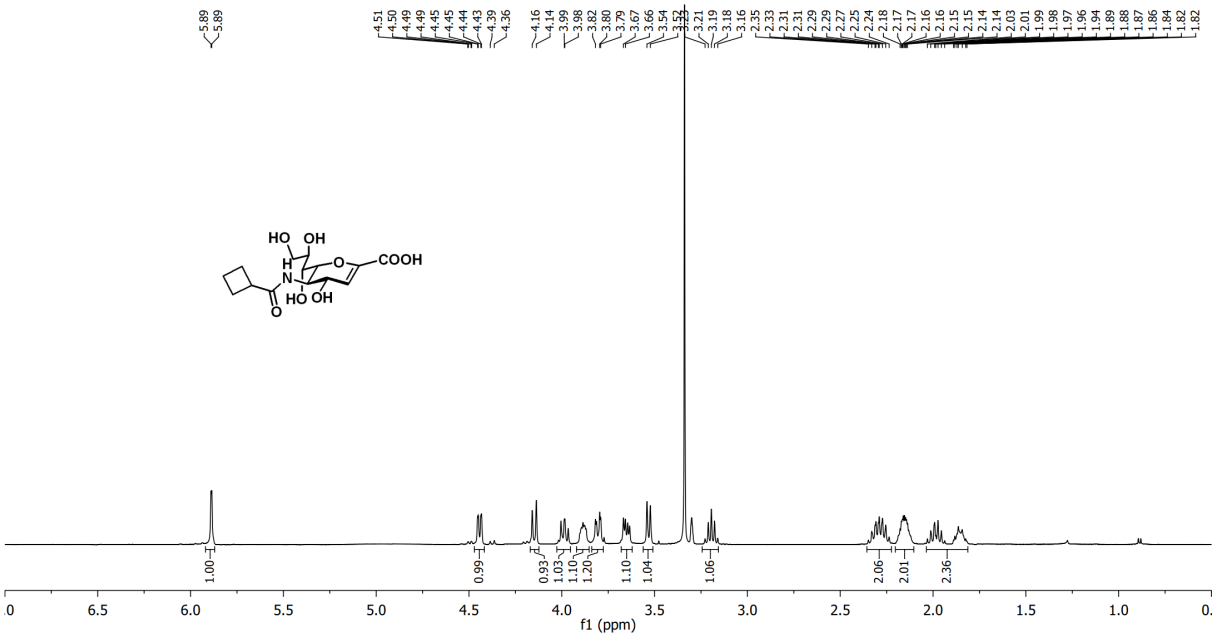


125.691 MHz C13[H1] 1D in CD_3OD

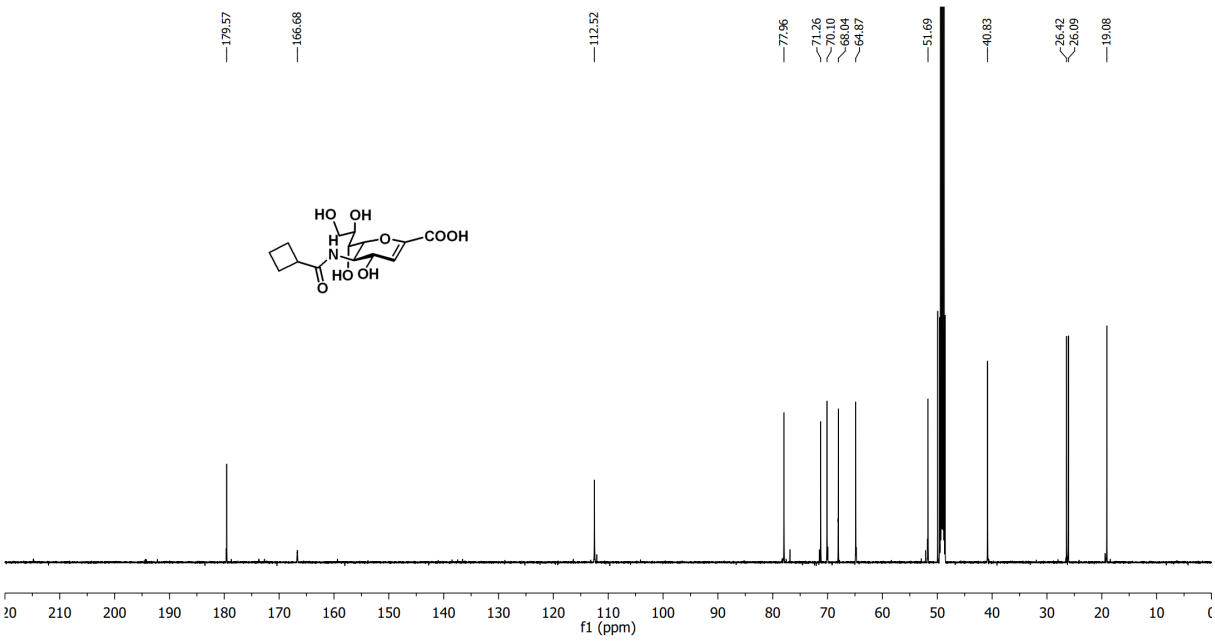


11j

499.808 MHz H1 1D in CD_3OD

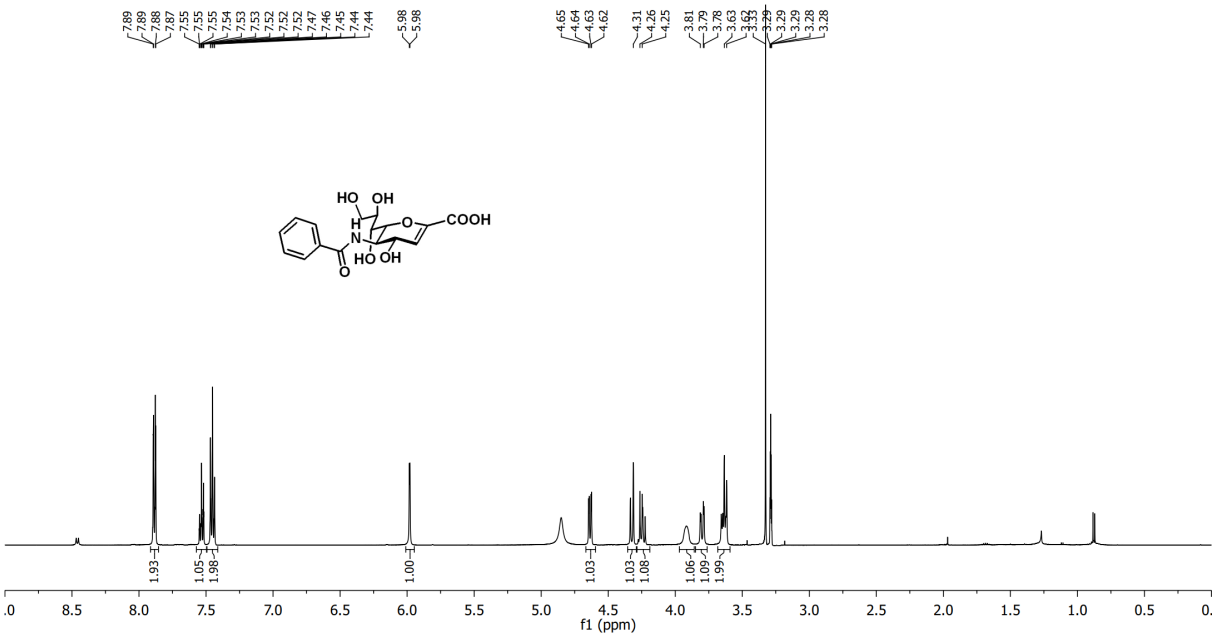


125.691 MHz C13[H1] 1D in CD_3OD

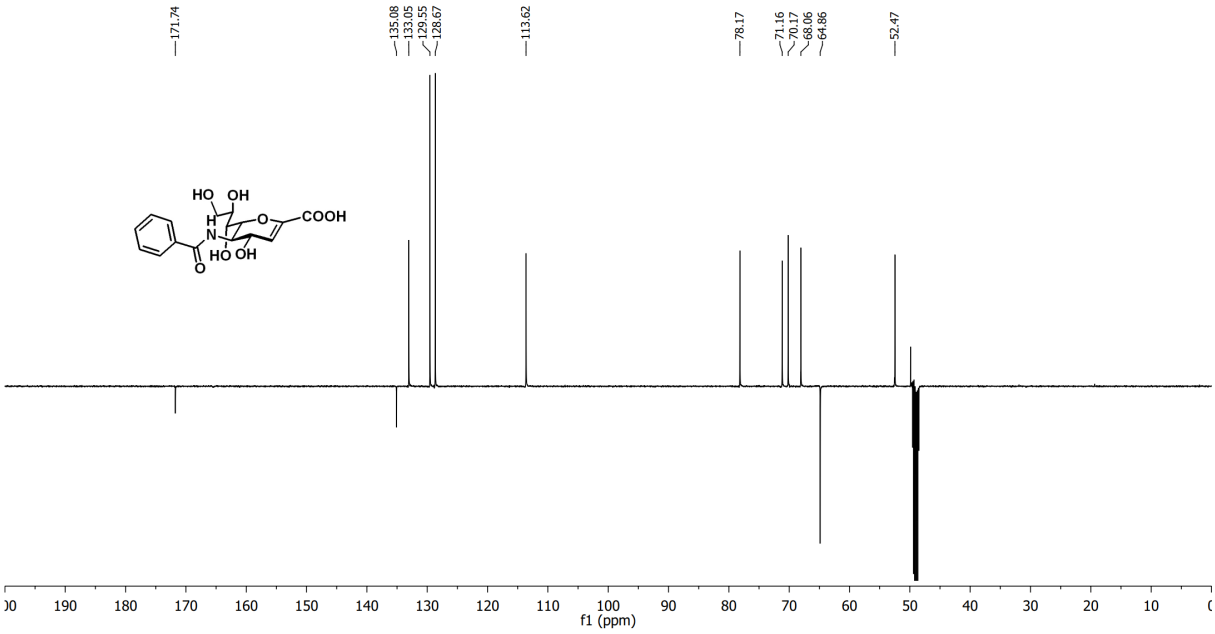


11k

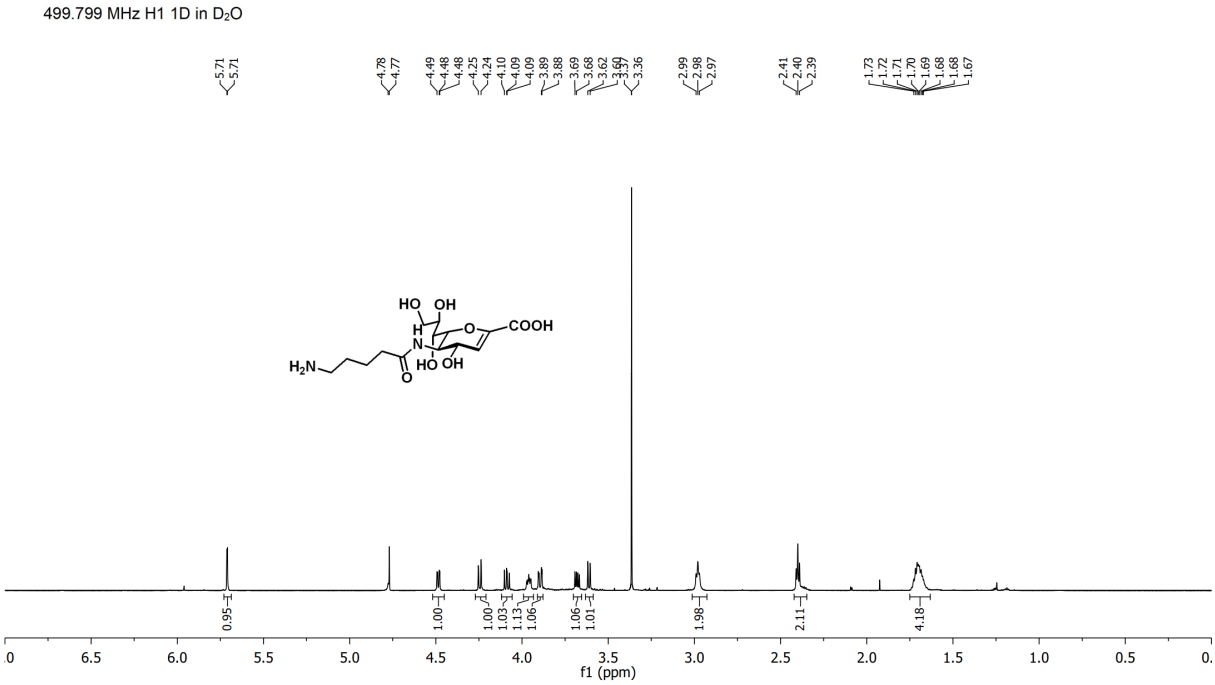
499.799 MHz H1 1D in CD_3OD

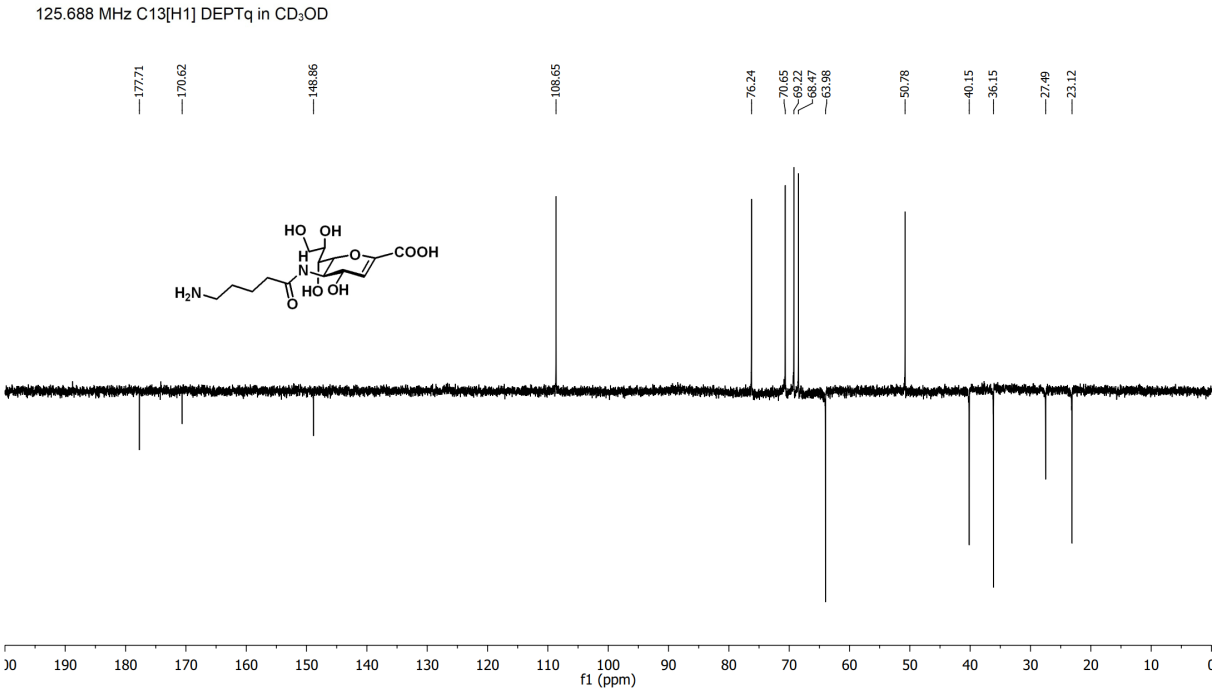


125.688 MHz C13[H1] DEPTq in CD_3OD

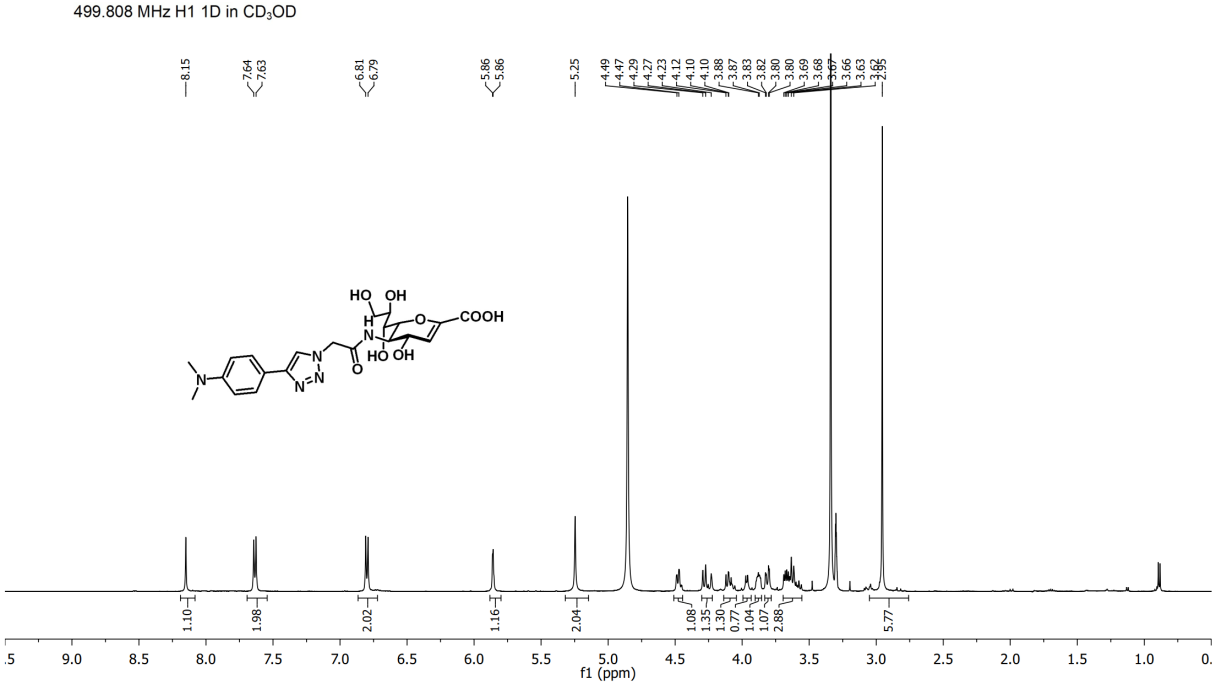


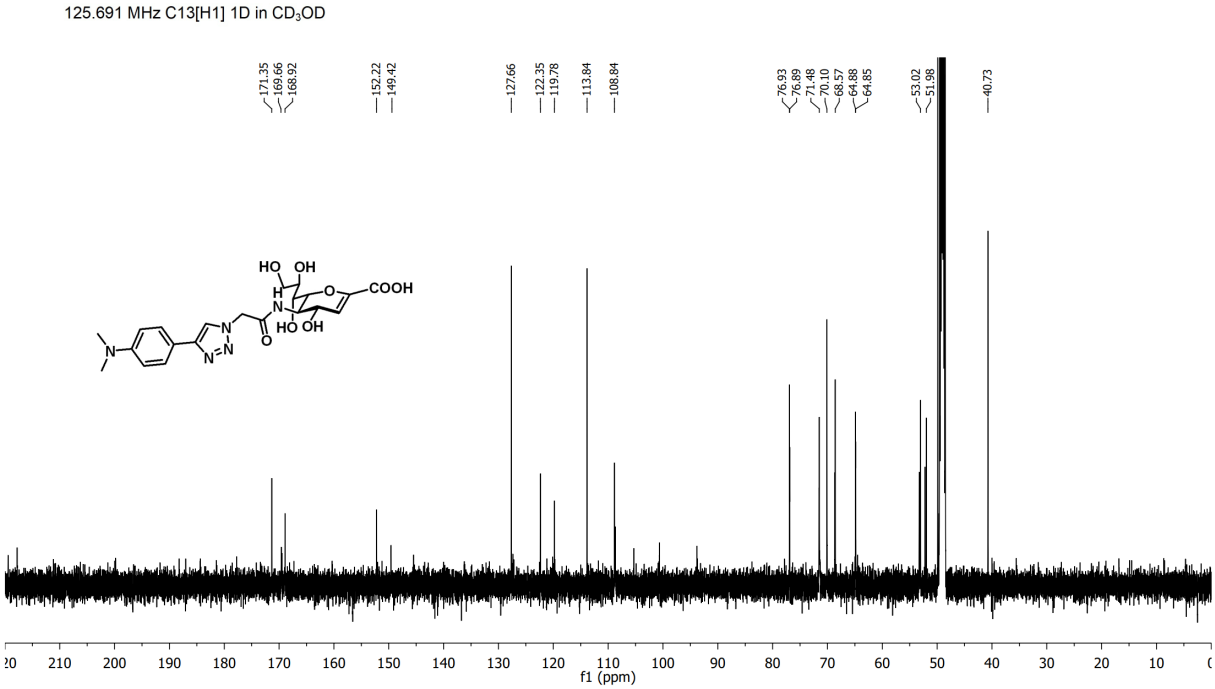
11l


499.799 MHz H1 1D in D2O
5.71
5.71
4.78
4.77
4.49
4.48
4.48
4.25
4.24
4.10
4.09
4.09
3.89
3.88
3.69
3.68
3.62
3.60
3.37
3.36
2.99
2.98
2.97
2.41
2.40
2.39
1.73
1.72
1.71
1.70
1.69
1.68
1.68
1.67
HO OH
H
O
COOH
N
H2N
HO OH
O
0.95
1.00
1.00
1.03
1.13
1.06
1.06
1.01
1.98
2.11
4.18
f1 (ppm)

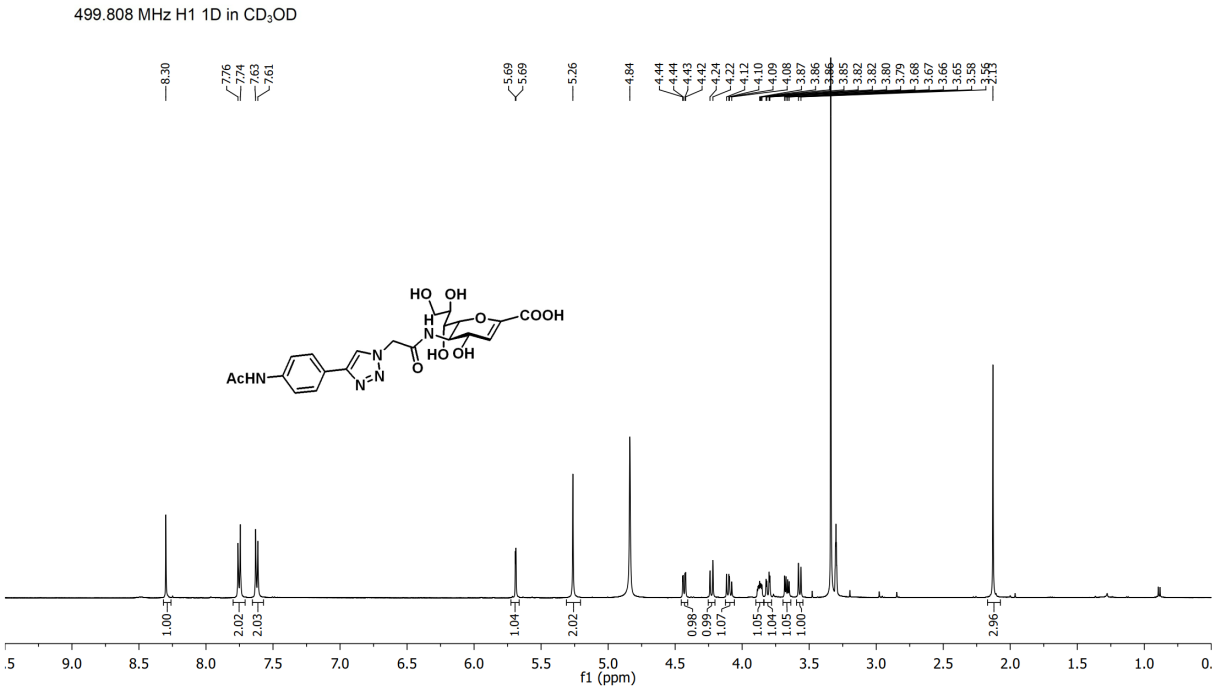

125.688 MHz C13[H1] DEPTq in CD3OD
177.71
170.62
148.86
108.65
76.24
70.65
69.22
68.47
63.98
50.78
40.15
36.15
27.49
23.12
HO OH
H
O
COOH
N
H2N
HO OH
O
f1 (ppm)

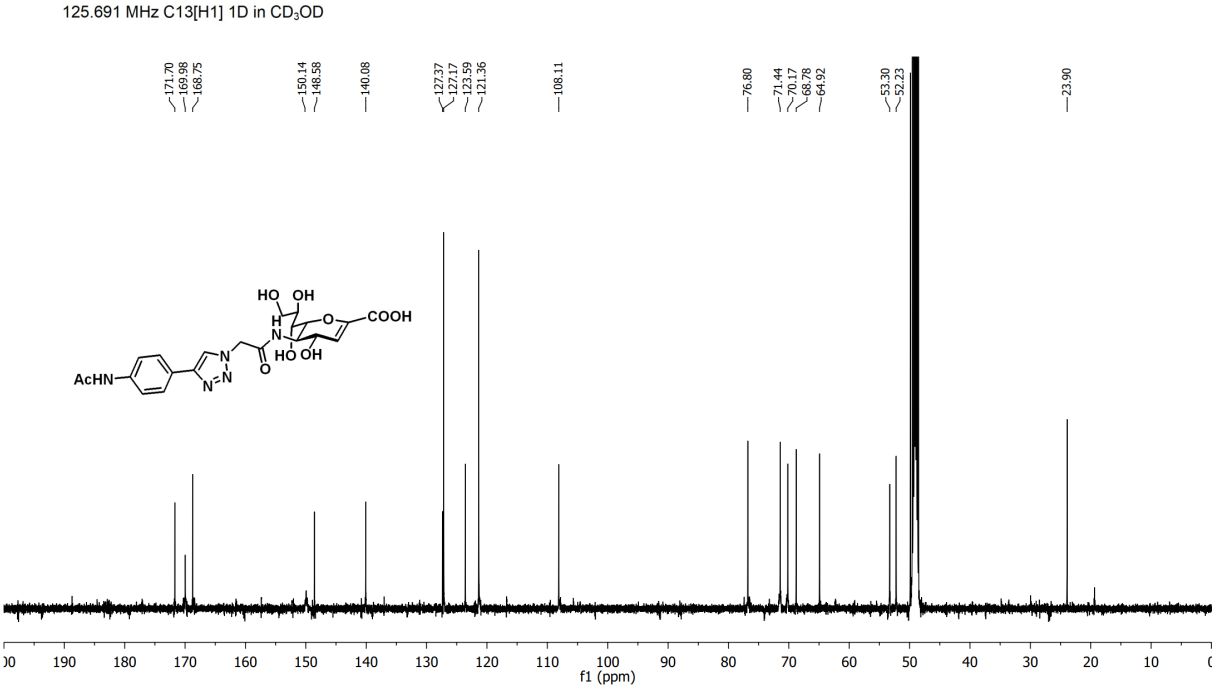
13a


499.808 MHz H1 1D in CD3OD
8.15
7.64
7.63
6.81
6.79
5.86
5.86
5.25
4.49
4.47
4.29
4.27
4.23
4.12
4.10
4.10
3.88
3.87
3.83
3.82
3.80
3.80
3.69
3.68
3.67
3.66
3.63
2.95
HO OH
COOH
HO OH
1.10
1.98
2.02
1.16
2.04
1.08
1.35
1.30
0.77
1.04
1.07
2.88
5.77
f1 (ppm)

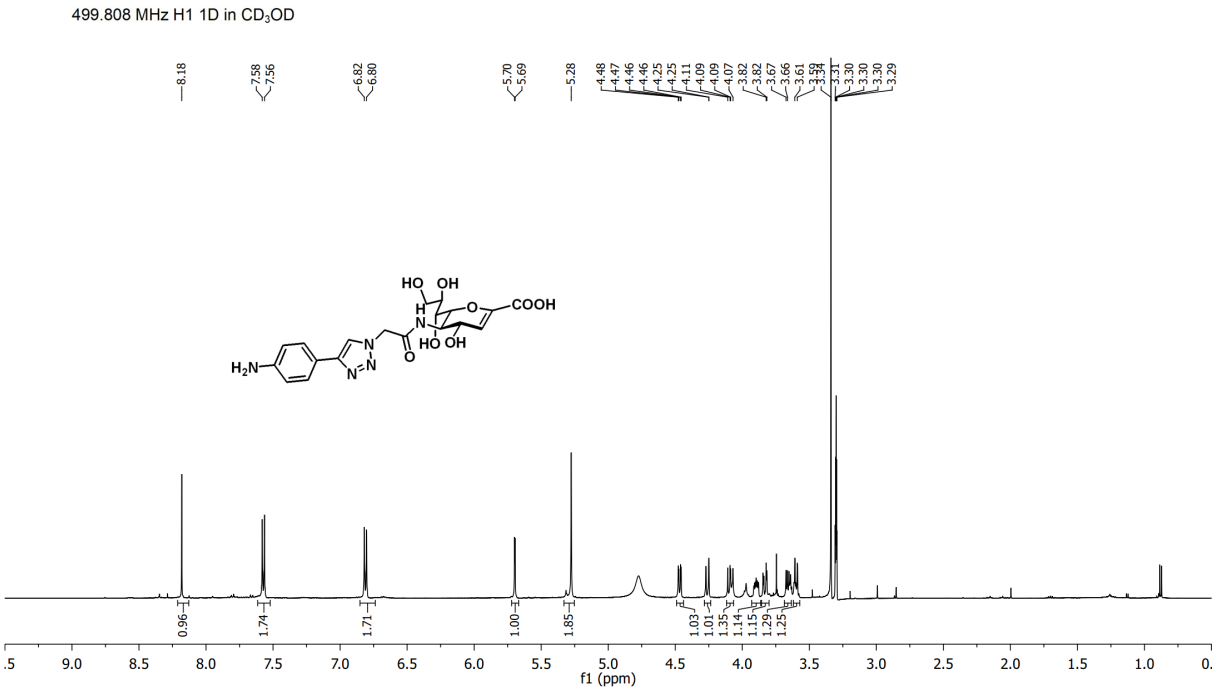

125.691 MHz C13[H1] 1D in CD3OD
171.35
169.66
168.92
152.22
149.42
127.66
122.35
119.78
113.84
108.84
76.93
76.89
71.48
70.10
68.57
64.88
64.85
53.02
51.98
40.73
HO OH
COOH
HO OH
f1 (ppm)

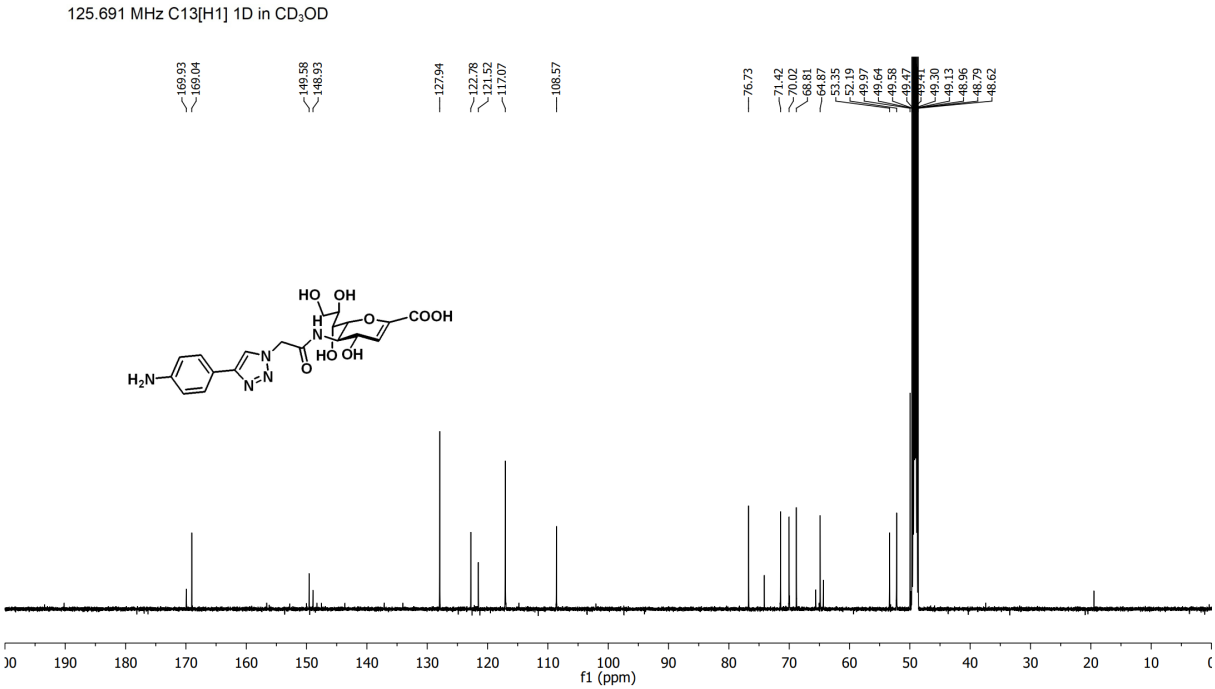
13b


499.808 MHz H1 1D in CD3OD
8.30
7.76
7.74
7.63
7.61
5.69
5.69
5.26
4.84
4.44
4.44
4.43
4.42
4.24
4.22
4.12
4.10
4.09
4.08
3.87
3.86
3.86
3.85
3.82
3.82
3.80
3.79
3.68
3.67
3.66
3.65
3.58
2.15
HO OH
COOH
AcHN
HO OH
1.00
2.02
2.03
1.04
2.02
0.98
0.99
1.07
1.05
1.04
1.05
1.00
2.96
f1 (ppm)


125.691 MHz C13[H1] 1D in CD3OD
171.70
169.98
168.75
150.14
148.58
140.08
127.37
127.17
123.59
121.36
108.11
76.80
71.44
70.17
68.78
64.92
53.30
52.23
23.90
HO OH
COOH
AcHN
HO OH
f1 (ppm)

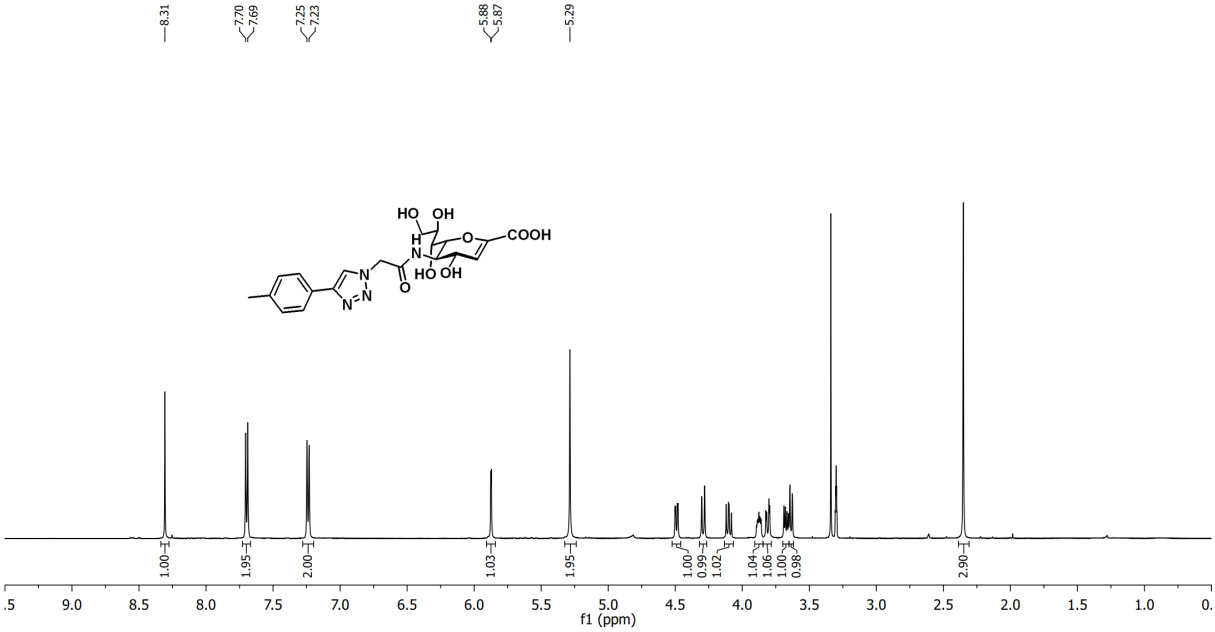
13c


499.808 MHz H1 1D in CD3OD
8.18
7.58
7.56
6.82
6.80
5.70
5.69
5.28
4.48
4.47
4.46
4.46
4.25
4.25
4.11
4.09
4.09
4.07
3.82
3.82
3.67
3.66
3.61
3.59
3.34
3.31
3.30
3.30
3.30
3.29
HO OH
H
N
O
COOH
HO OH
O
N
N
N
H2N
0.96
1.74
1.71
1.00
1.85
1.03
1.01
1.35
1.14
1.15
1.29
1.25
f1 (ppm)

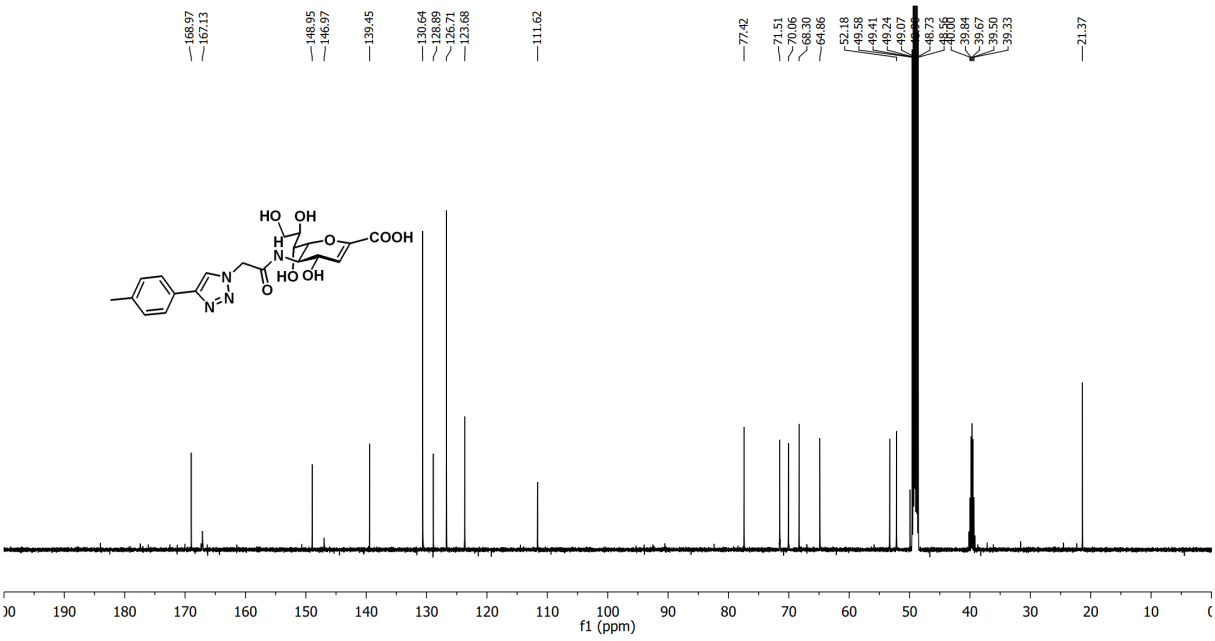

125.691 MHz C13[H1] 1D in CD3OD
169.93
169.04
149.58
148.93
127.94
122.78
121.52
117.07
108.57
76.73
71.42
70.02
68.81
64.87
53.35
52.19
49.97
49.64
49.58
49.47
49.41
49.30
49.13
48.96
48.79
48.62
HO OH
H
N
O
COOH
HO OH
O
N
N
N
H2N
f1 (ppm)

13d

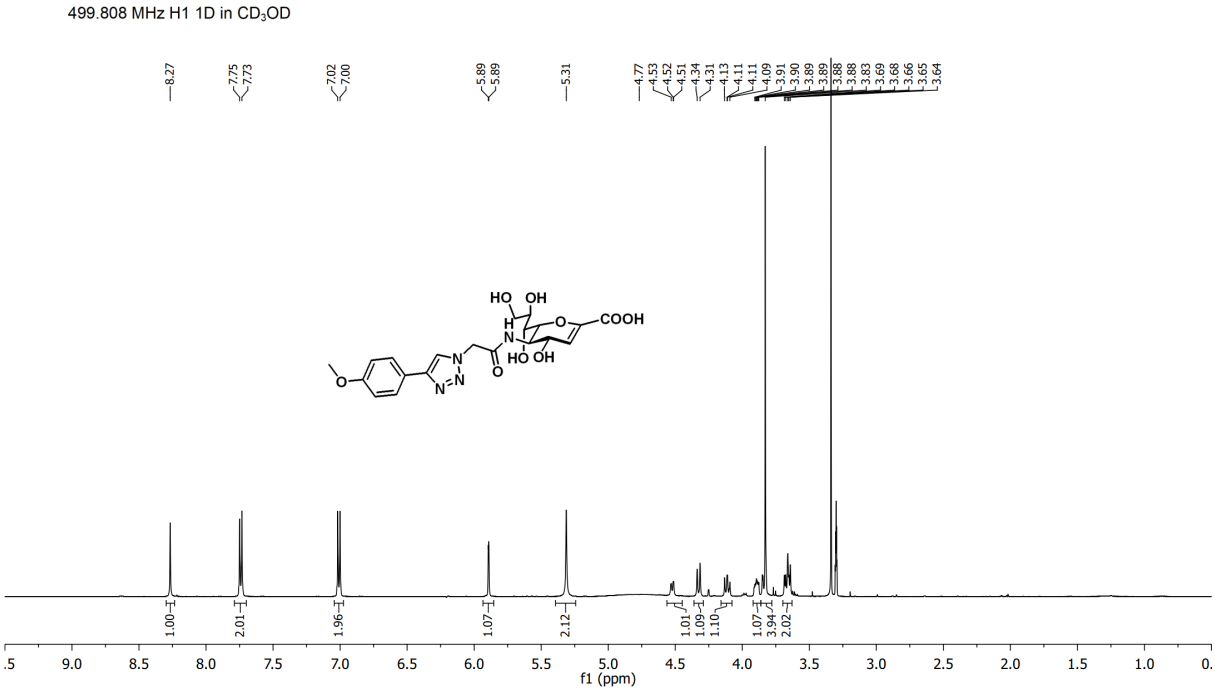
499.808 MHz H1 1D in CD_3OD

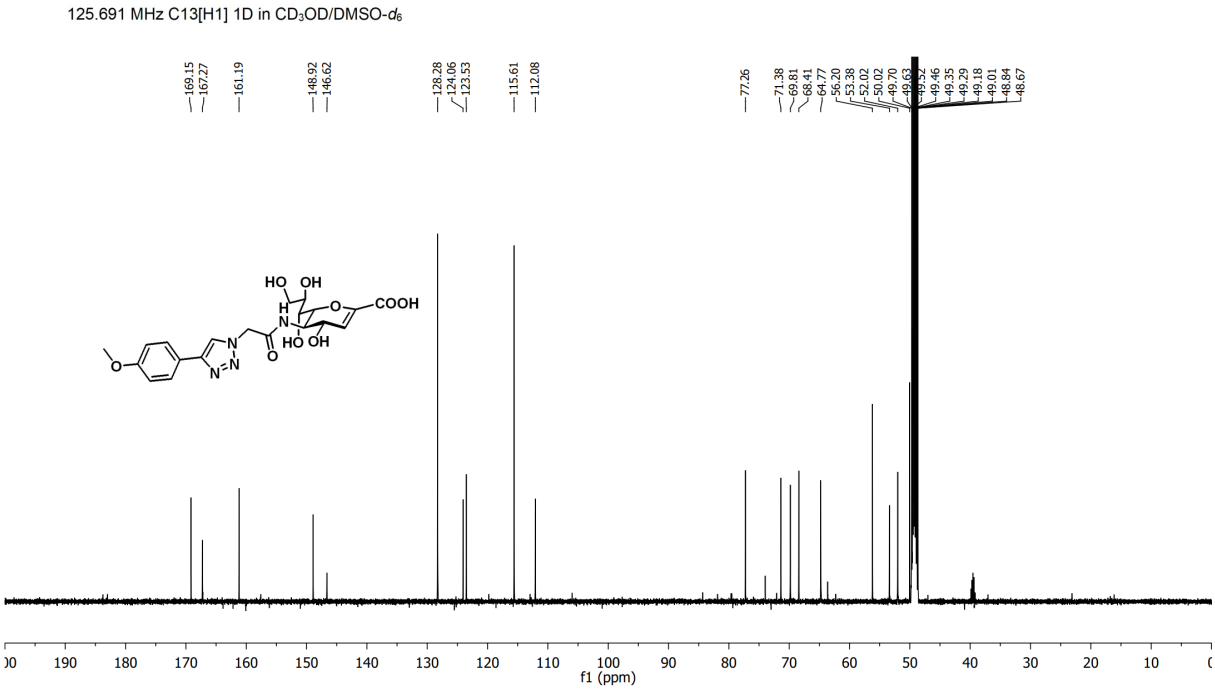


125.691 MHz C13[H1] 1D in $CD_3OD/DMSO\text{-}d_6$

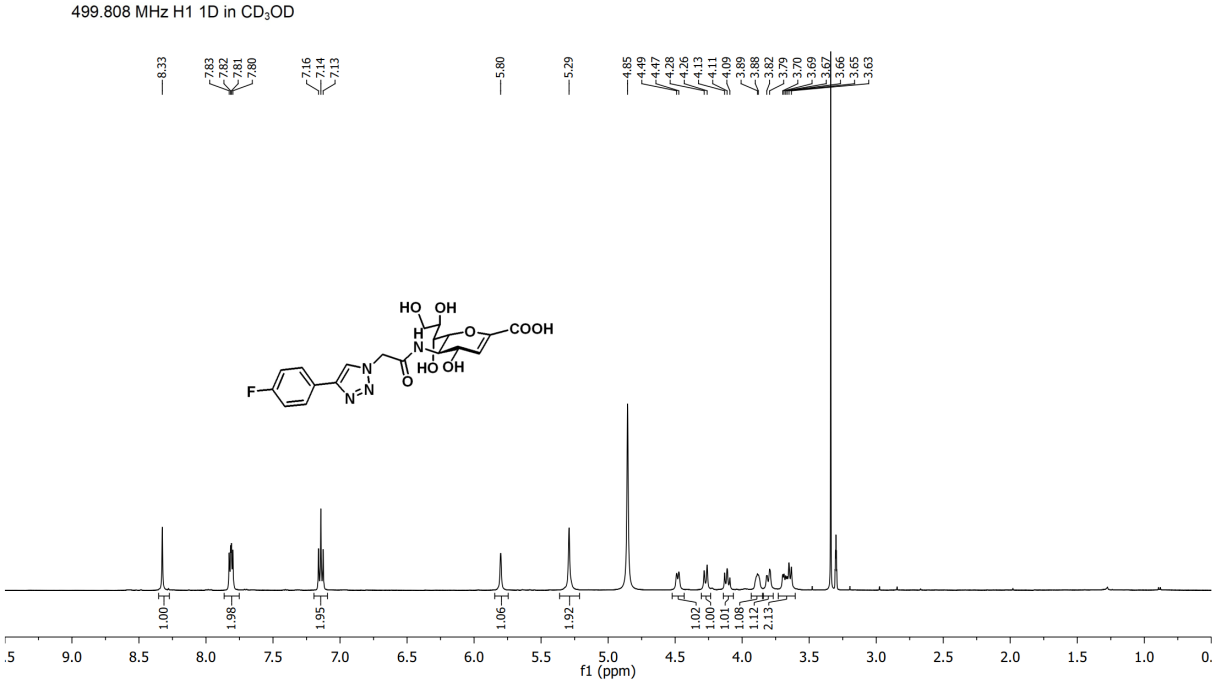


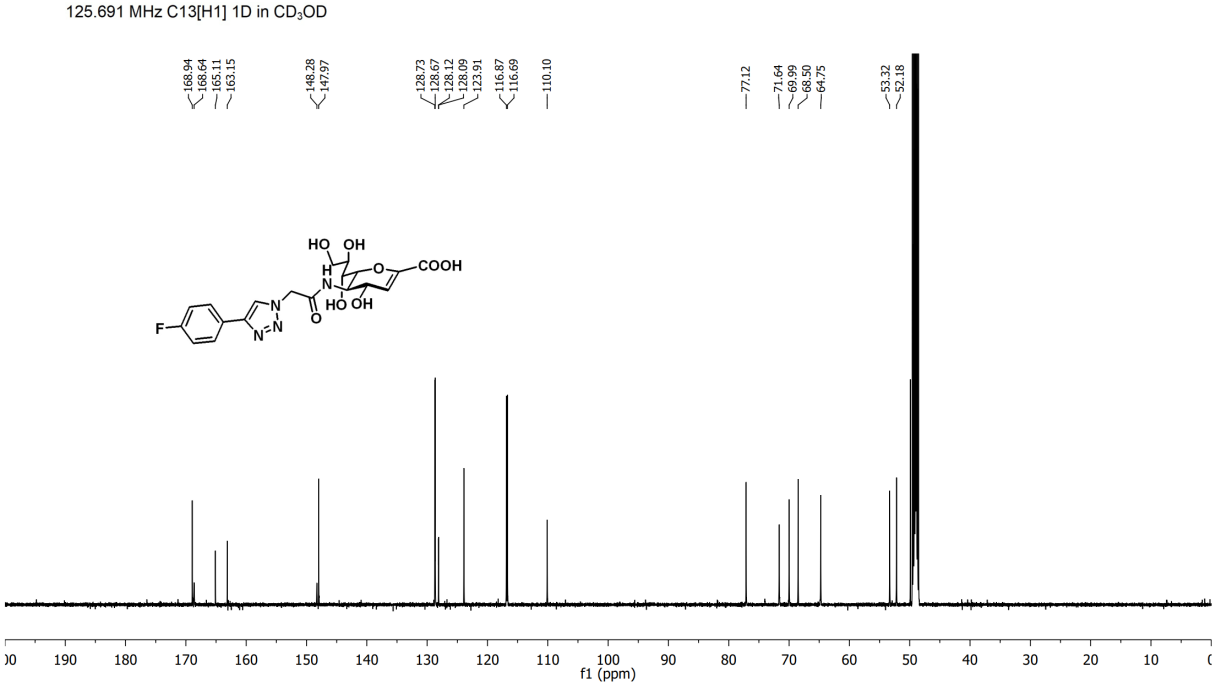
13e


499.808 MHz H1 1D in CD3OD
8.27
7.75
7.73
7.02
7.00
5.89
5.89
5.31
4.77
4.53
4.52
4.51
4.34
4.31
4.13
4.11
4.11
4.09
3.91
3.90
3.89
3.89
3.88
3.88
3.83
3.69
3.68
3.66
3.65
3.64
HO OH
COOH
HO OH
1.00
2.01
1.96
1.07
2.12
1.01
1.09
1.10
1.07
3.94
2.02
f1 (ppm)

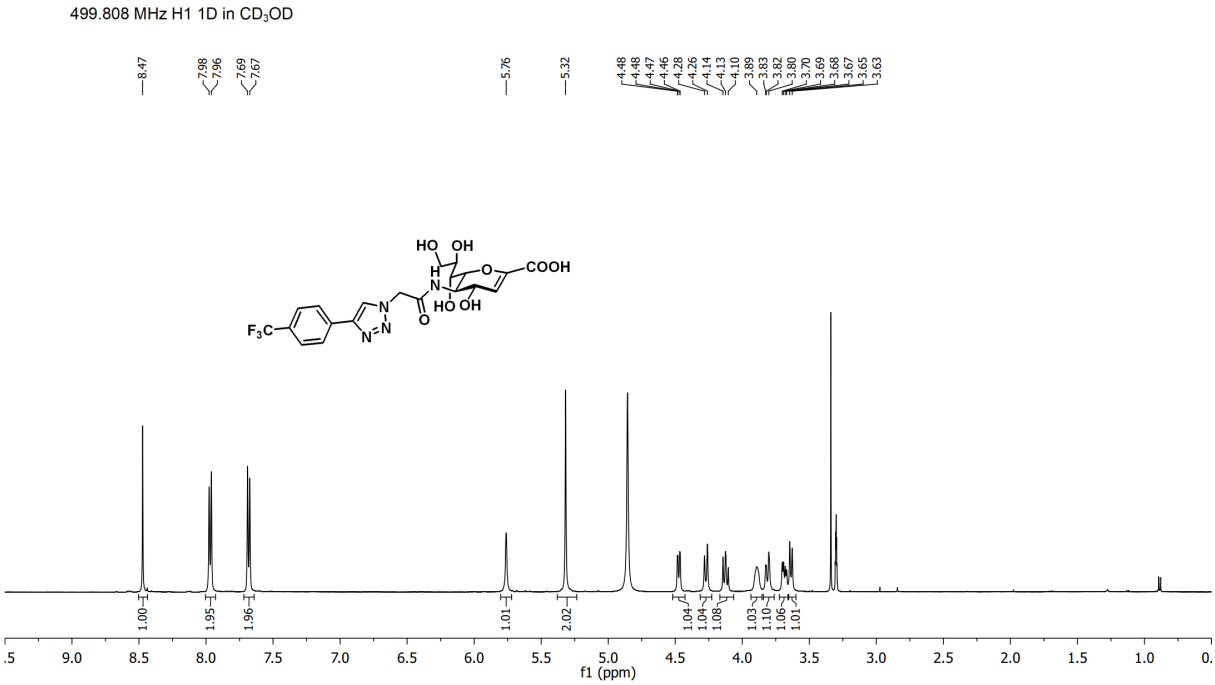

125.691 MHz C13[H1] 1D in CD3OD/DMSO-d6
169.15
167.27
161.19
148.92
146.62
128.28
124.06
123.53
115.61
112.08
77.26
71.38
69.81
68.41
64.77
56.20
53.38
52.02
50.02
49.70
49.63
49.46
49.35
49.29
49.18
49.01
48.84
48.67
HO OH
COOH
HO OH
f1 (ppm)

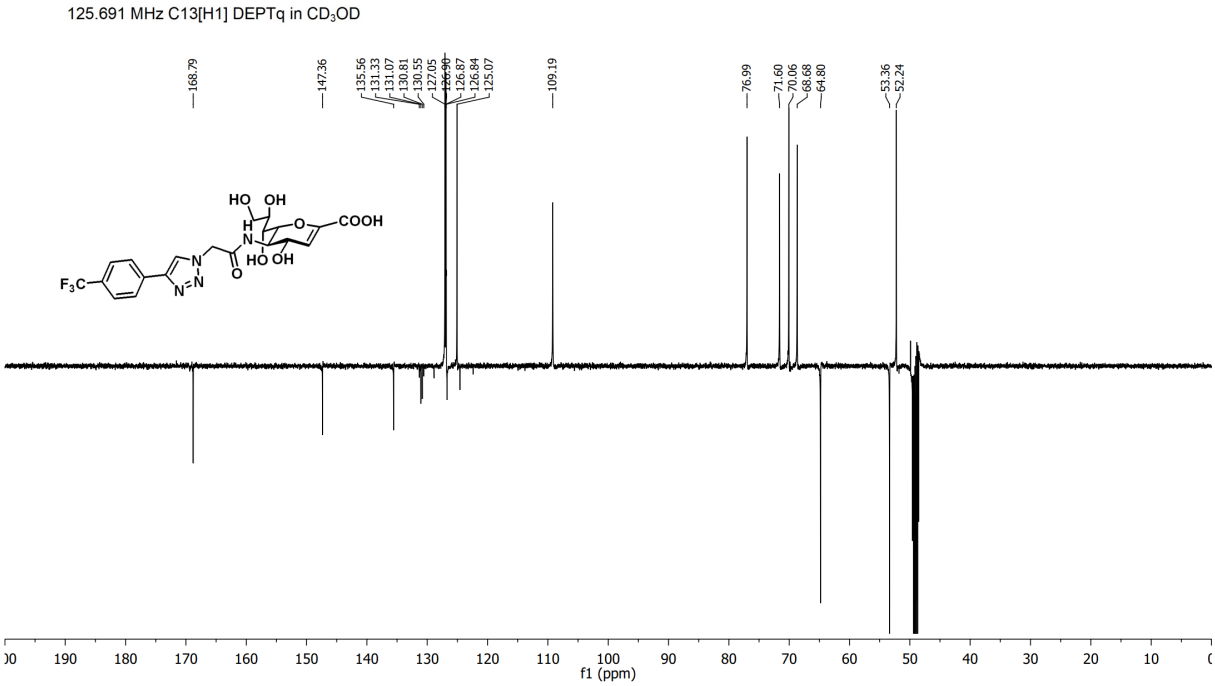
13f


499.808 MHz H1 1D in CD3OD
8.33
7.83
7.82
7.81
7.80
7.16
7.14
7.13
5.80
5.29
4.85
4.49
4.47
4.28
4.26
4.13
4.11
4.09
3.89
3.88
3.82
3.79
3.70
3.69
3.67
3.66
3.65
3.63
HO OH
COOH
HO OH
F
1.00
1.98
1.95
1.06
1.92
1.02
1.00
1.01
1.08
1.12
2.13
f1 (ppm)


125.691 MHz C13[H1] 1D in CD3OD
168.94
168.64
165.11
163.15
148.28
147.97
128.73
128.67
128.12
128.09
123.91
116.87
116.69
110.10
77.12
71.64
69.99
68.50
64.75
53.32
52.18
HO OH
COOH
HO OH
F
f1 (ppm)

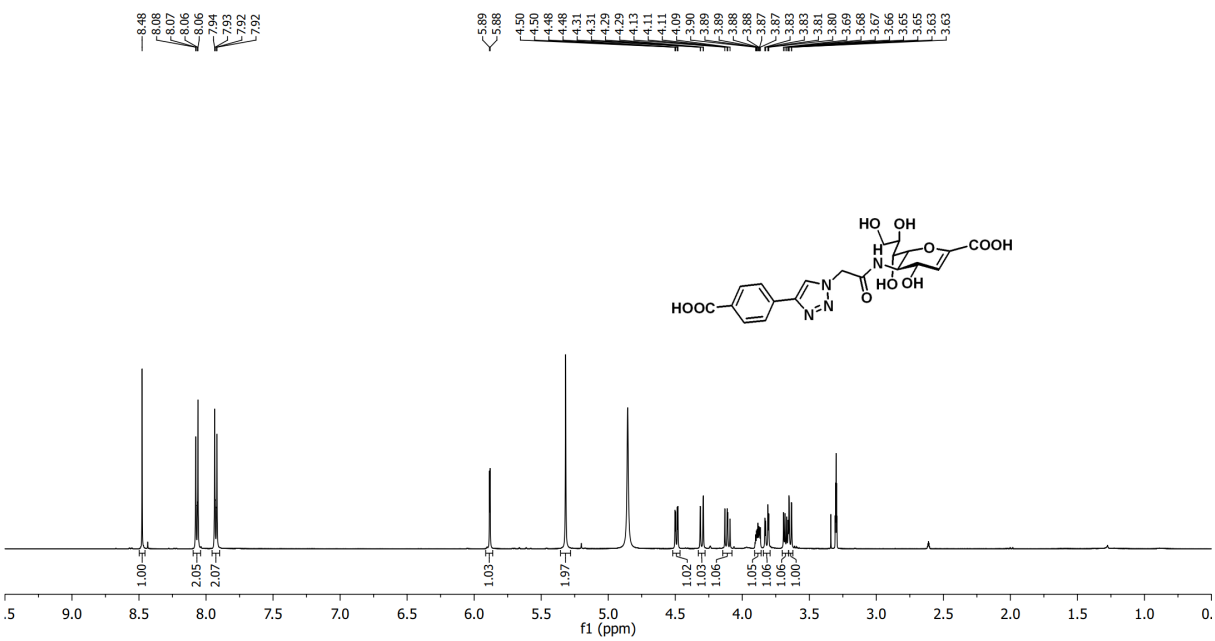
13g


499.808 MHz H1 1D in CD3OD
8.47
7.98
7.96
7.69
7.67
5.76
5.32
4.48
4.48
4.47
4.46
4.28
4.26
4.14
4.13
4.10
3.89
3.83
3.82
3.80
3.70
3.69
3.68
3.67
3.65
3.63
HO OH
H
O
COOH
N
HO OH
O
F3C
N
N
1.00
1.95
1.96
1.01
2.02
1.04
1.04
1.08
1.03
1.10
1.06
1.01
f1 (ppm)

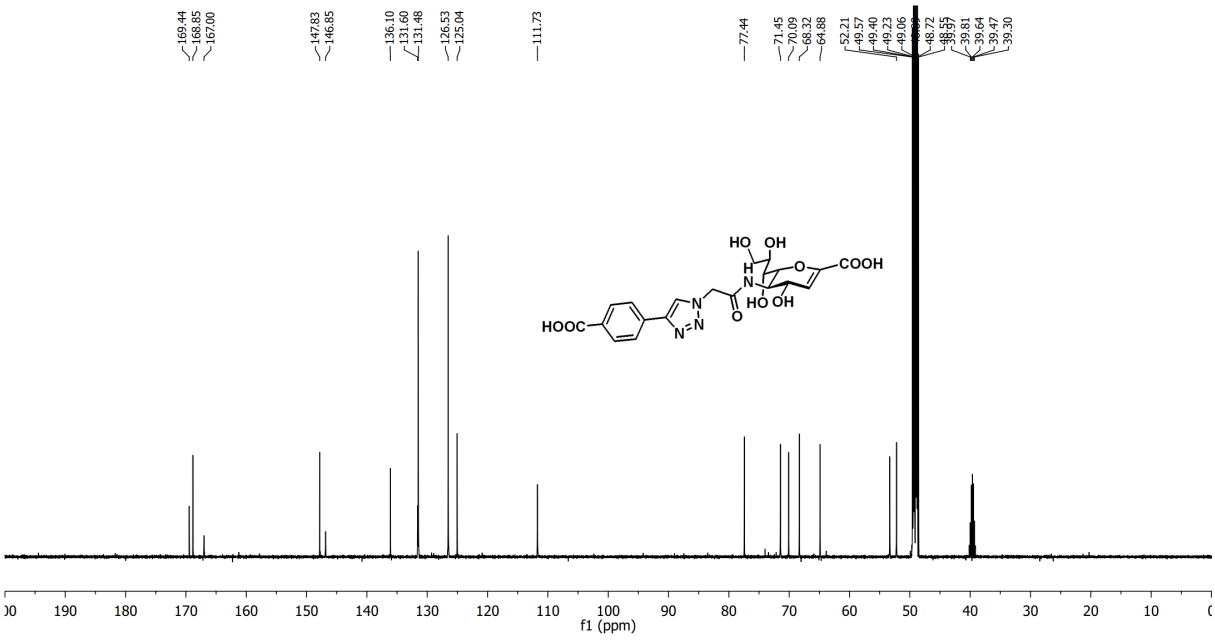

125.691 MHz C13[H1] DEPTq in CD3OD
168.79
147.36
135.56
131.33
131.07
130.81
130.55
127.05
126.90
126.87
126.84
125.07
109.19
76.99
71.60
70.06
68.68
64.80
53.36
52.24
HO OH
H
O
COOH
N
HO OH
O
F3C
N
N
f1 (ppm)

13h

499.808 MHz H1 1D in CD_3OD

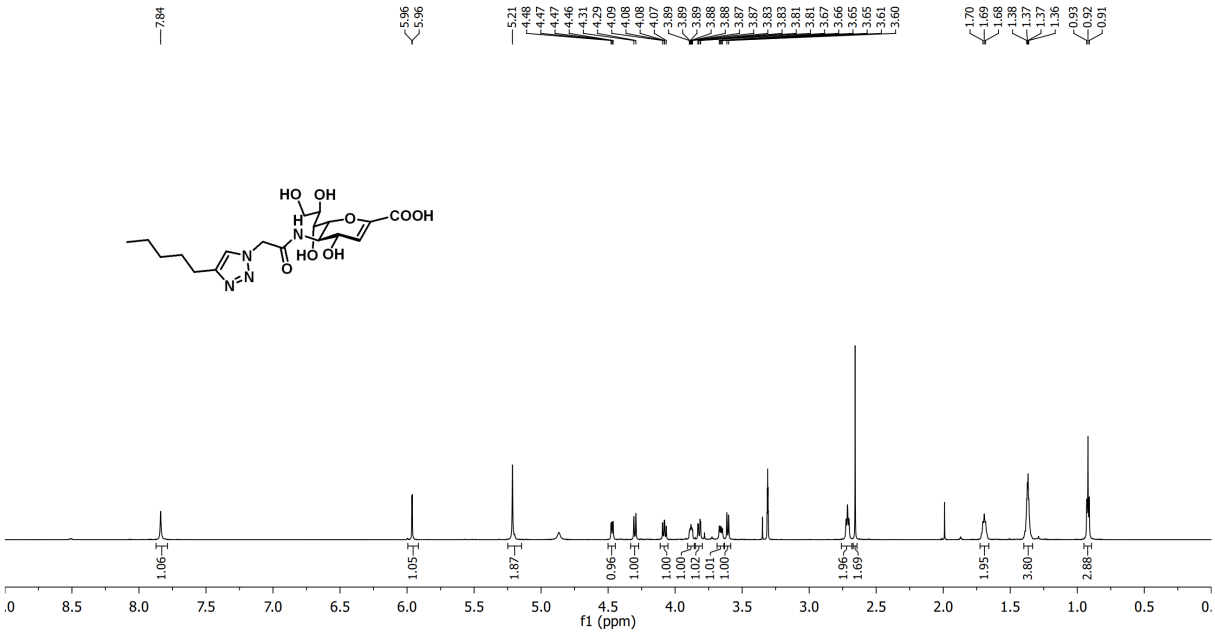


125.691 MHz C13[H1] 1D in CD_3OD

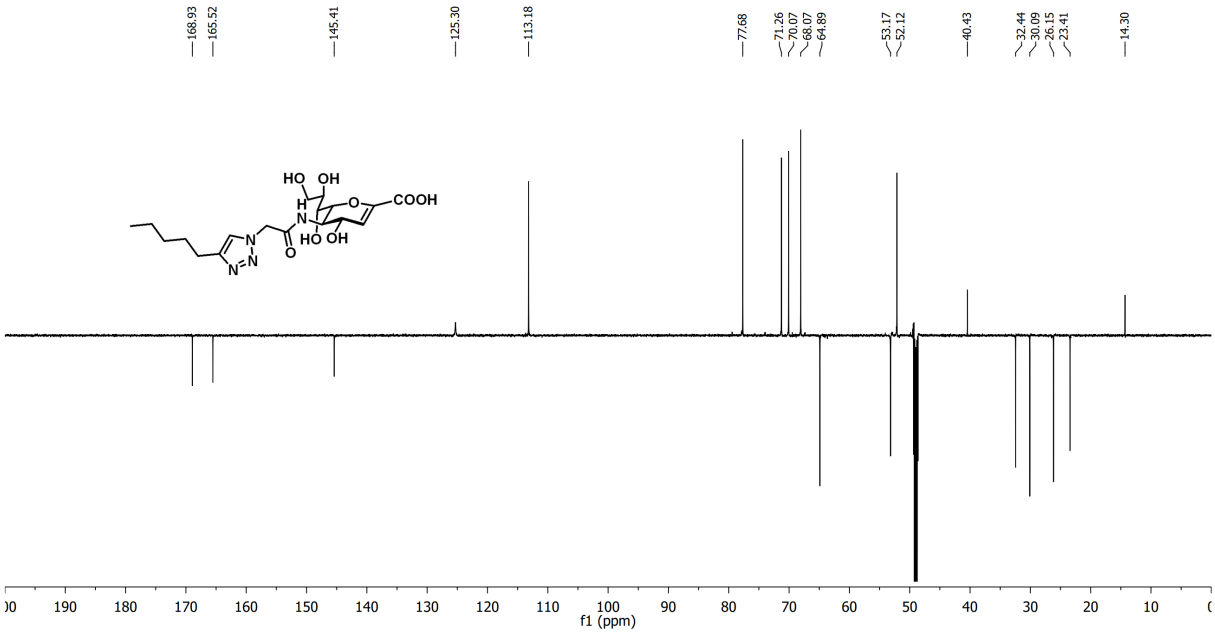


13i

499.799 MHz H1 1D in CD_3OD

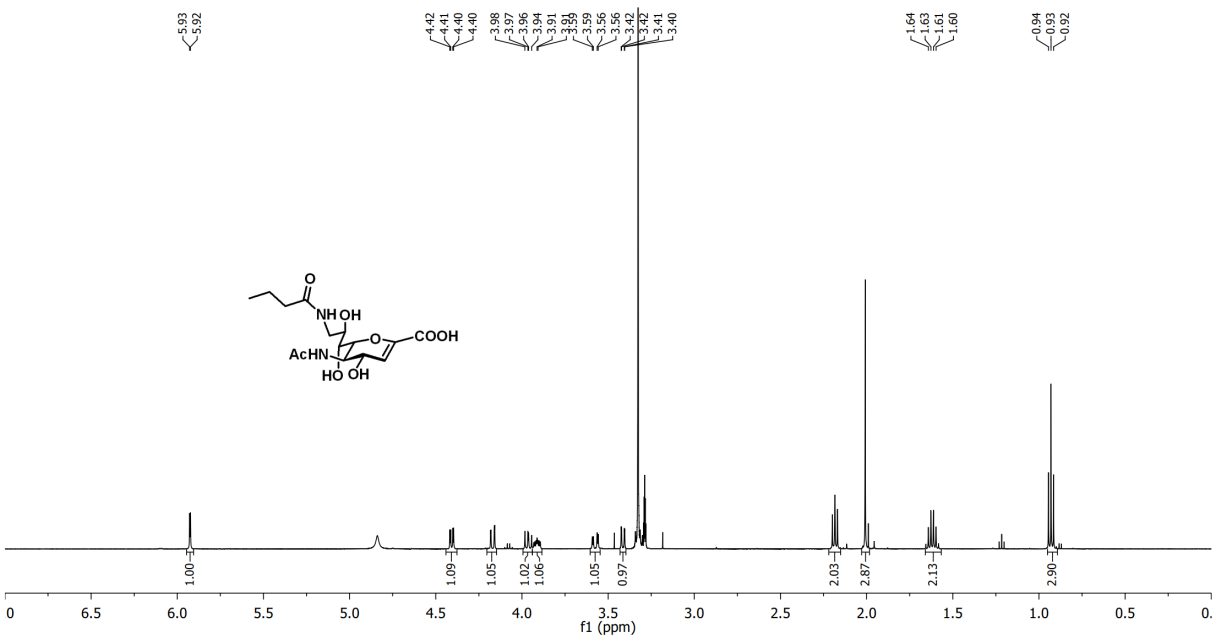


125.688 MHz C13[H1] DEPTq in CD_3OD

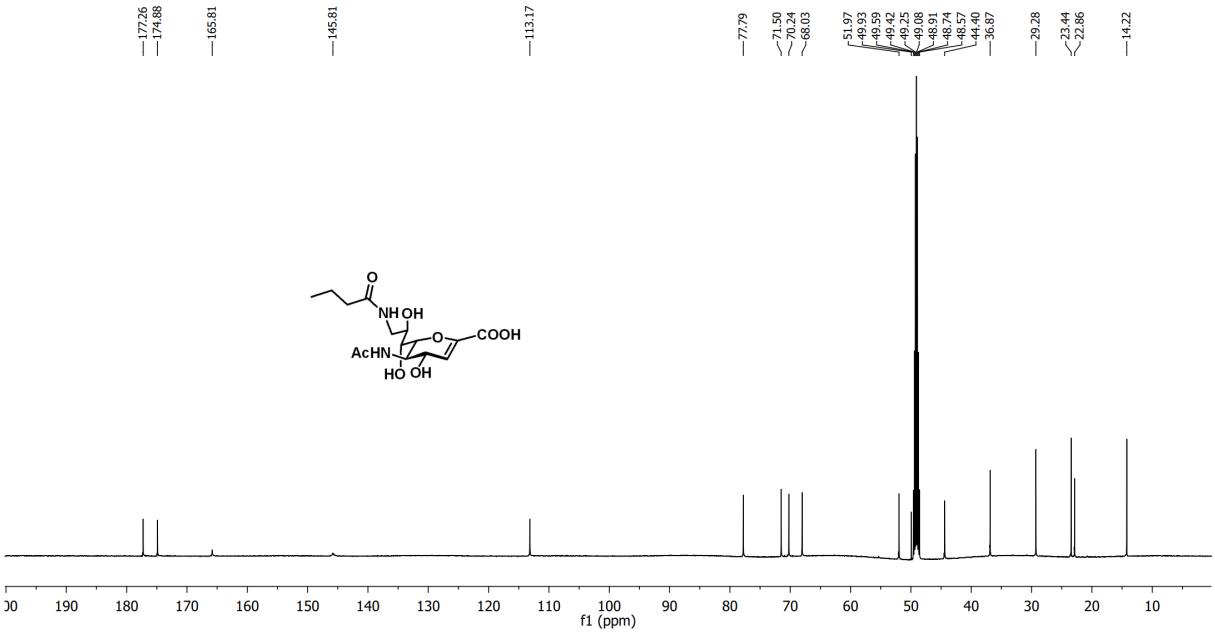


15a

499.808 MHz H1 1D in CD_3OD

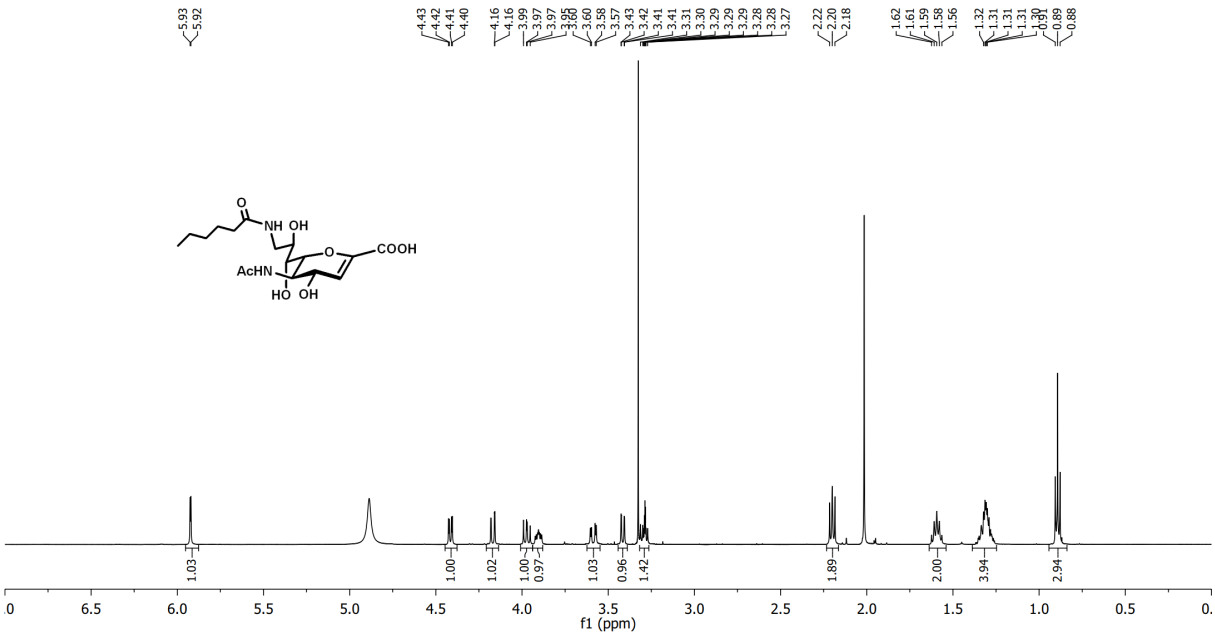


125.691 MHz C13[H1] 1D in CD_3OD

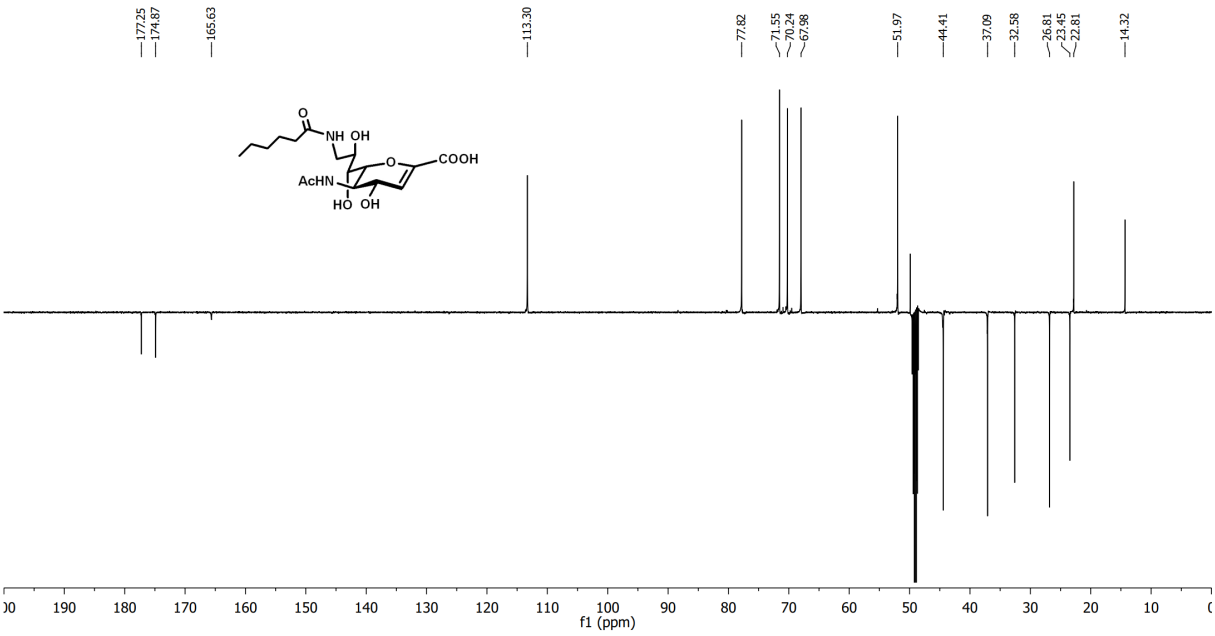


15b

499.808 MHz H1 1D in CD_3OD

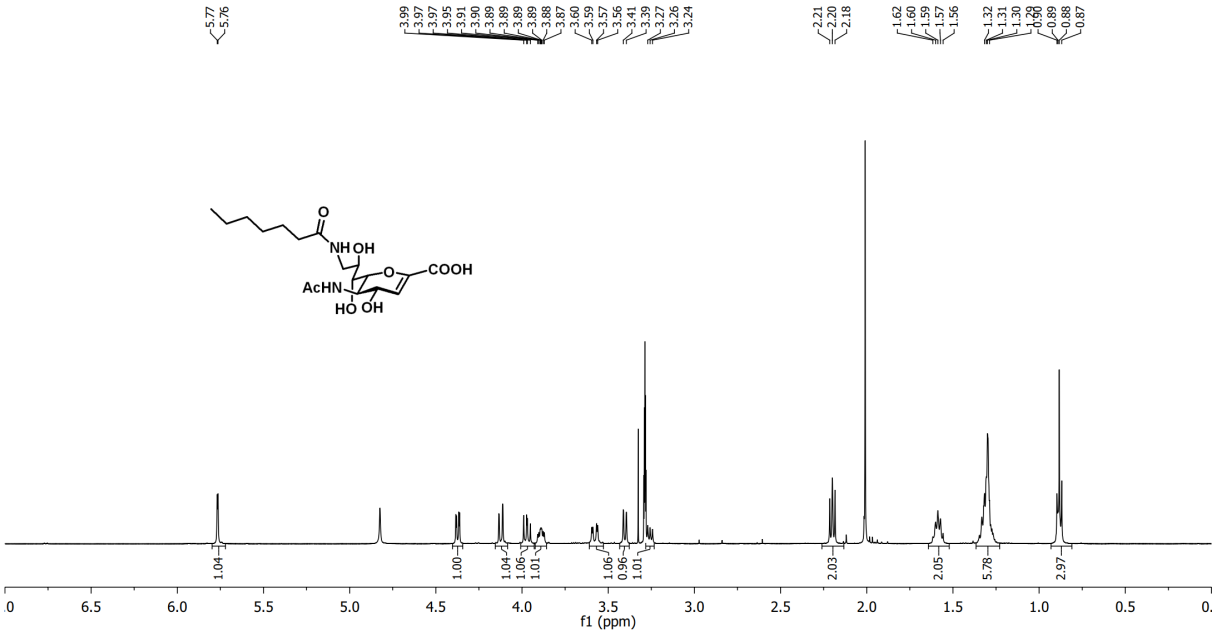


125.691 MHz C13[H1] 1D in CD_3OD

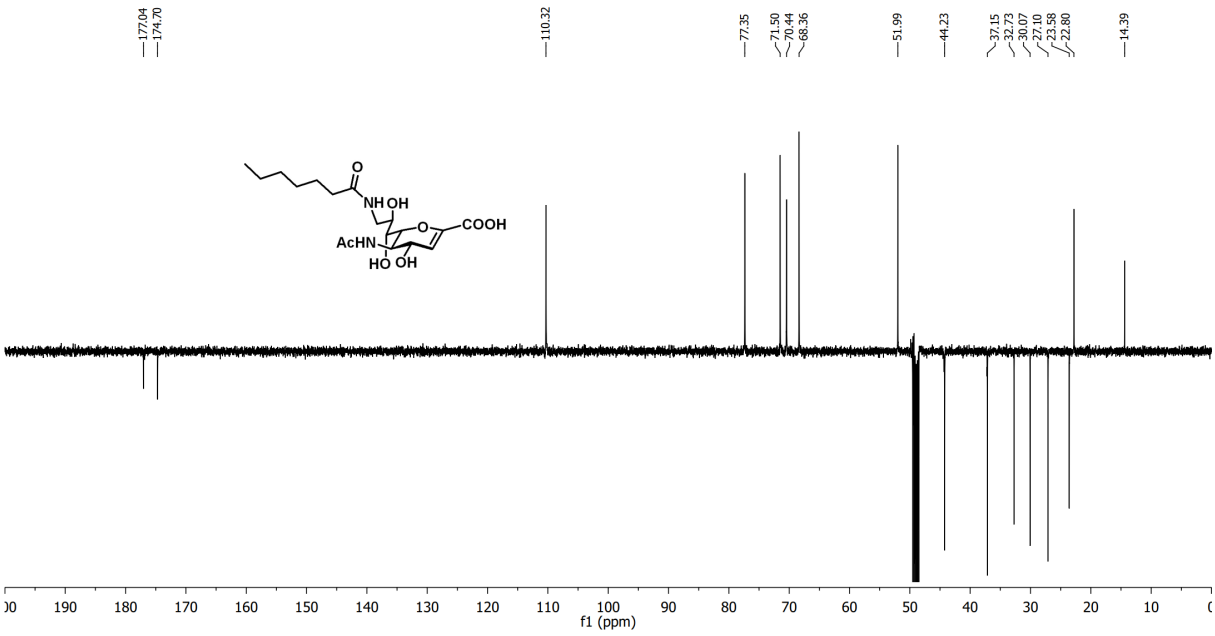


15c

499.799 MHz H1 1D in CD_3OD

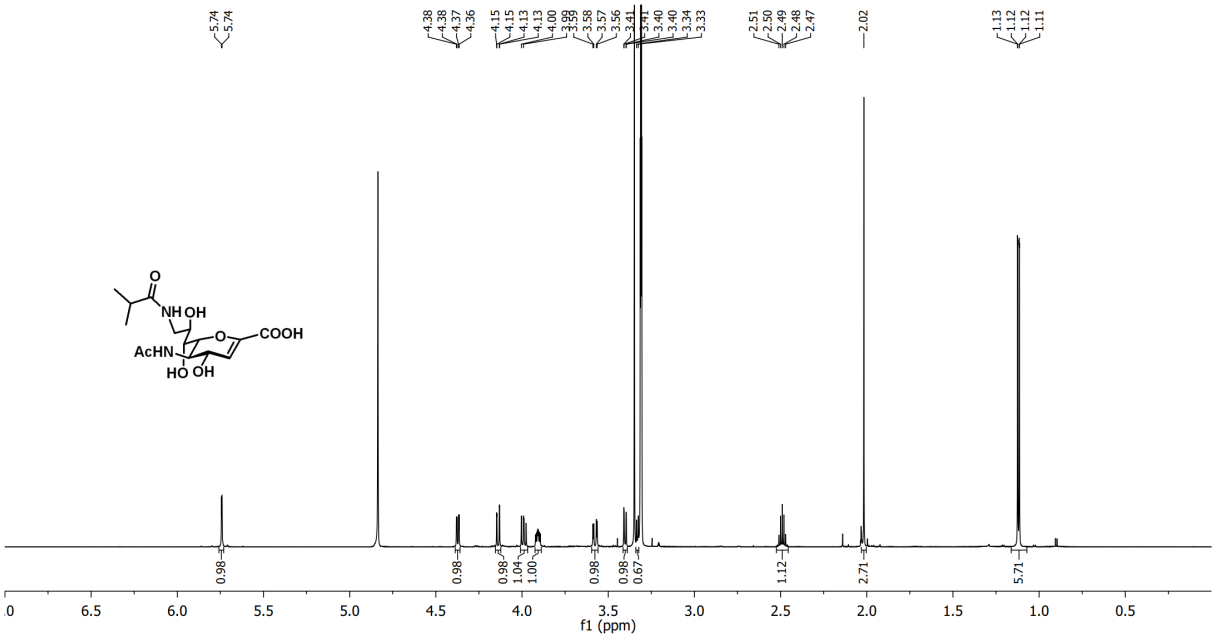


125.688 MHz C13[H1] 1D in CD_3OD

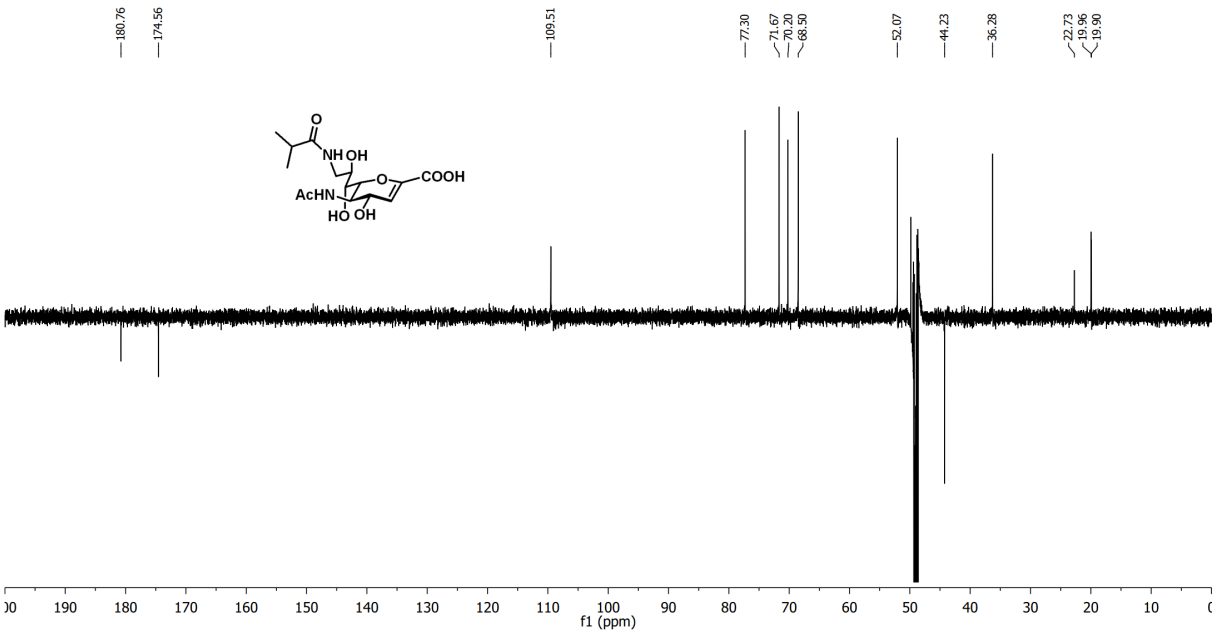


15d

699.765 MHz H1 1D in CD_3OD

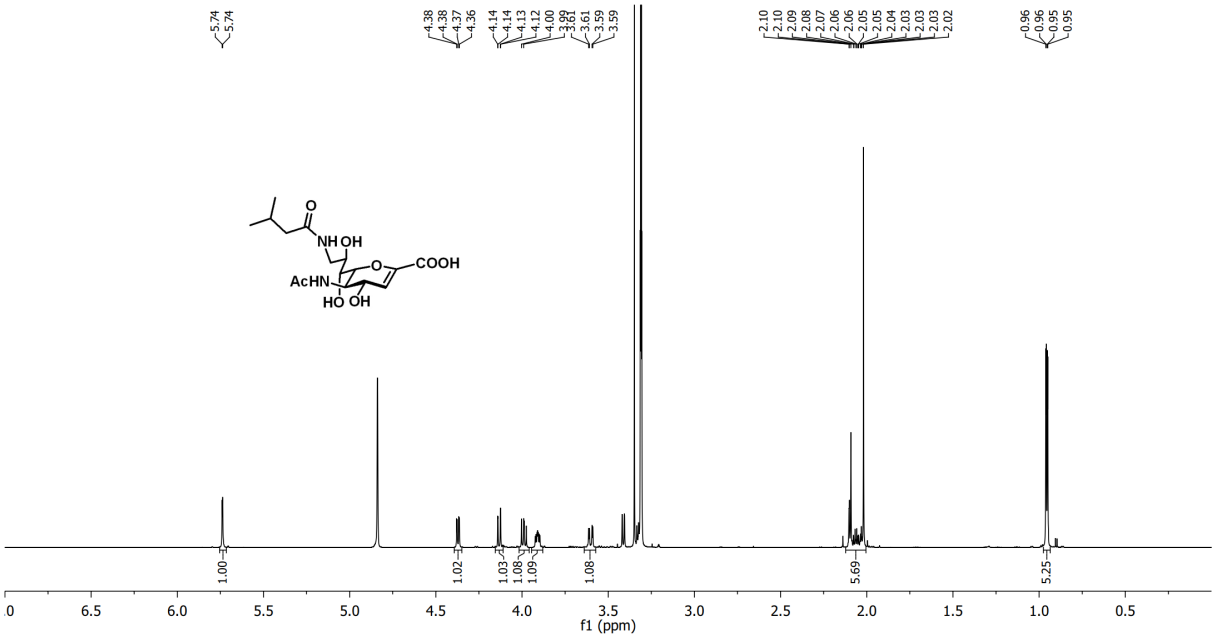


175.975 MHz C13[H1] DEPTq in CD_3OD

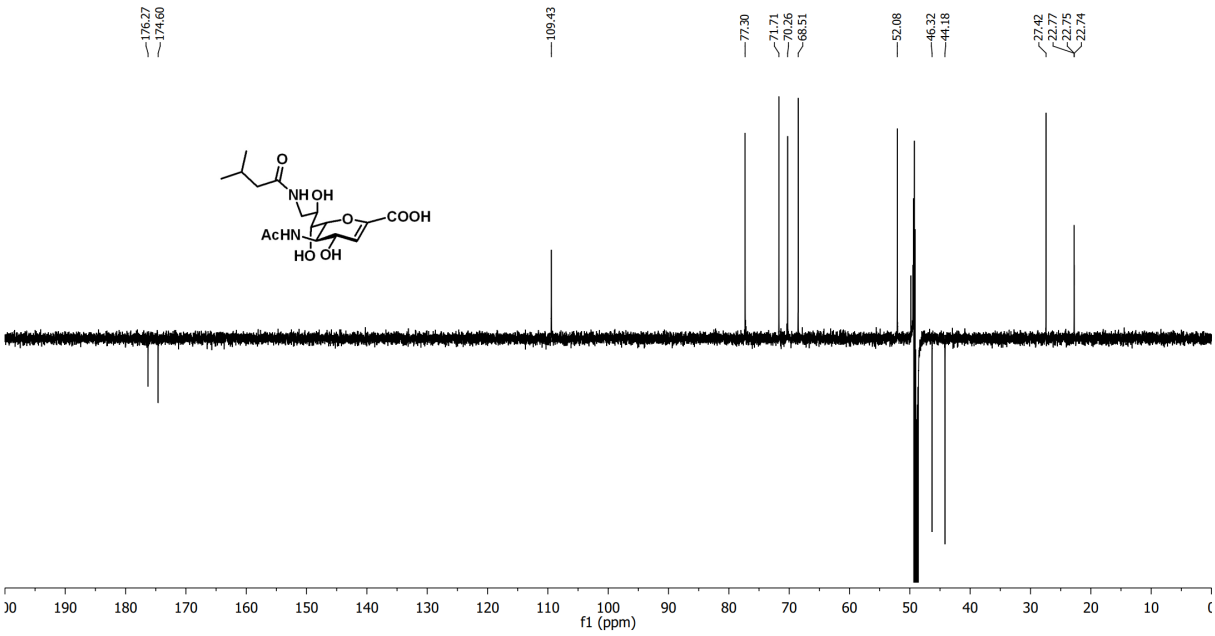


15e

699.765 MHz H1 1D in CD_3OD

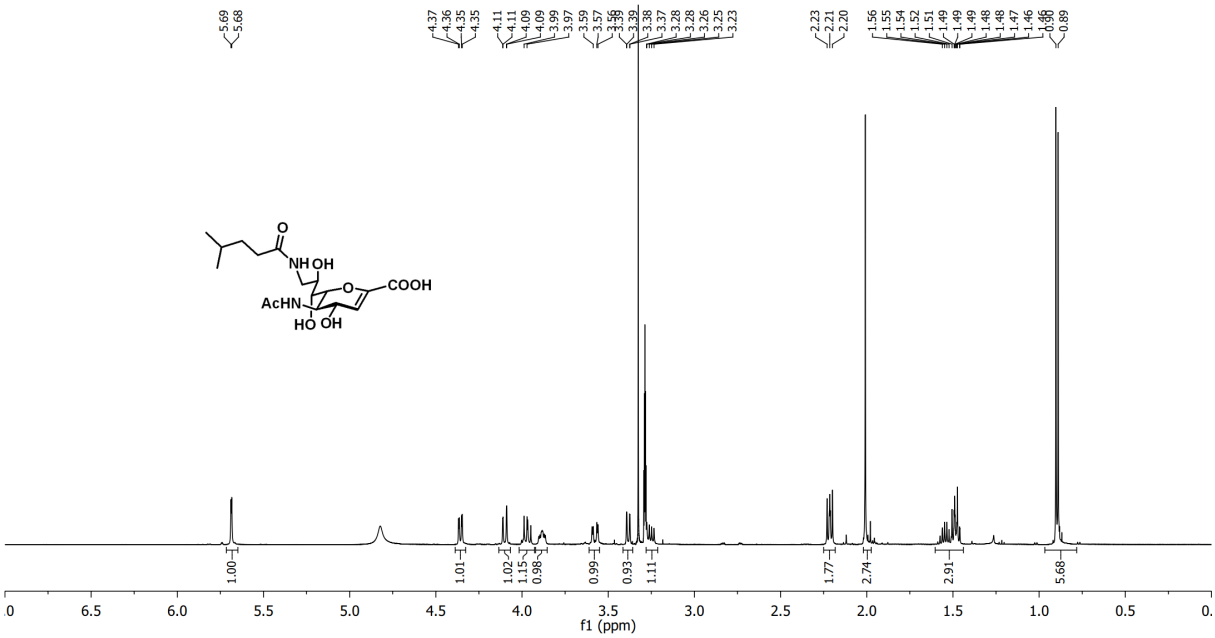


175.975 MHz C13[H1] DEPTq in CD_3OD

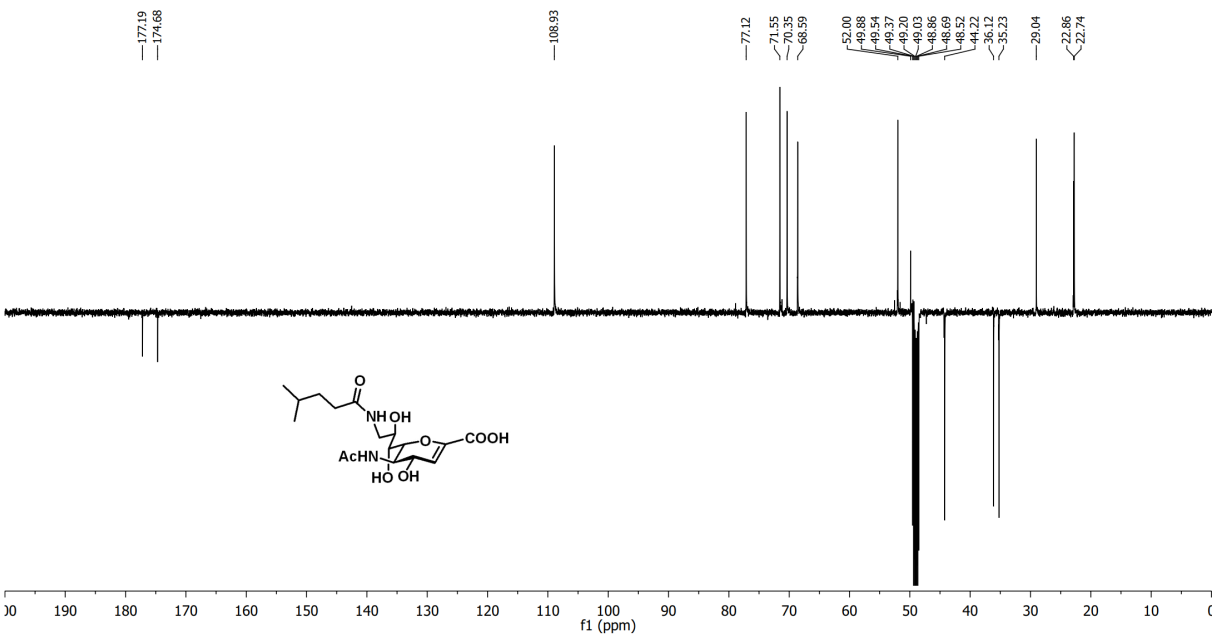


15f

499.799 MHz H1 1D in CD_3OD

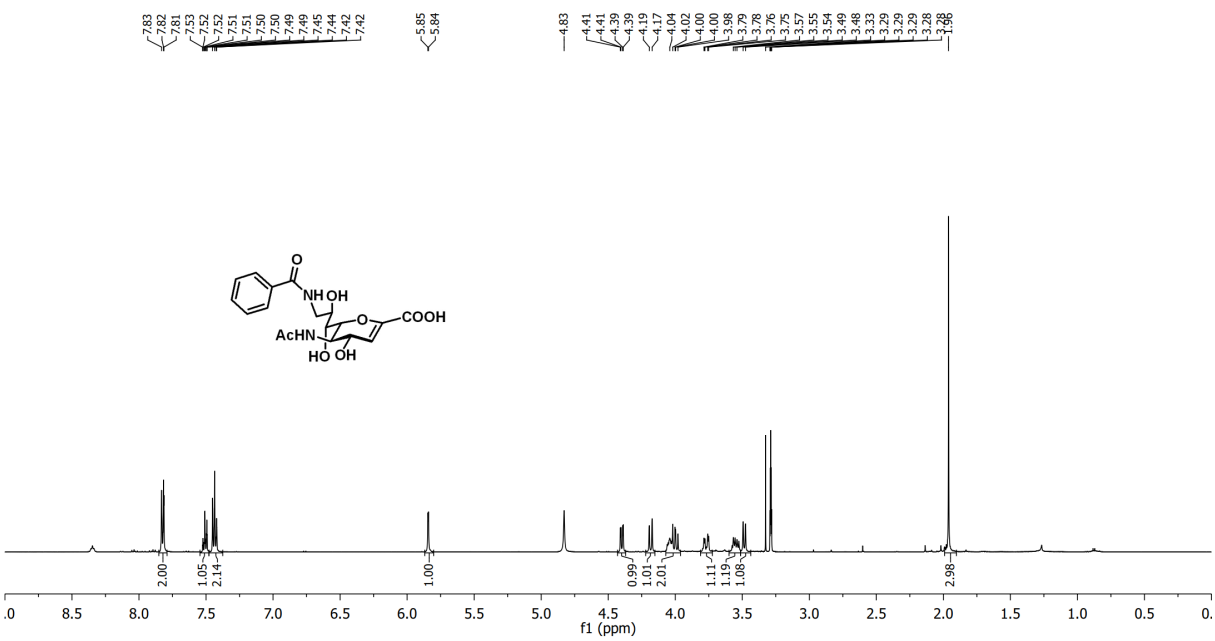


125.688 MHz C13[H1] DEPTq in CD_3OD

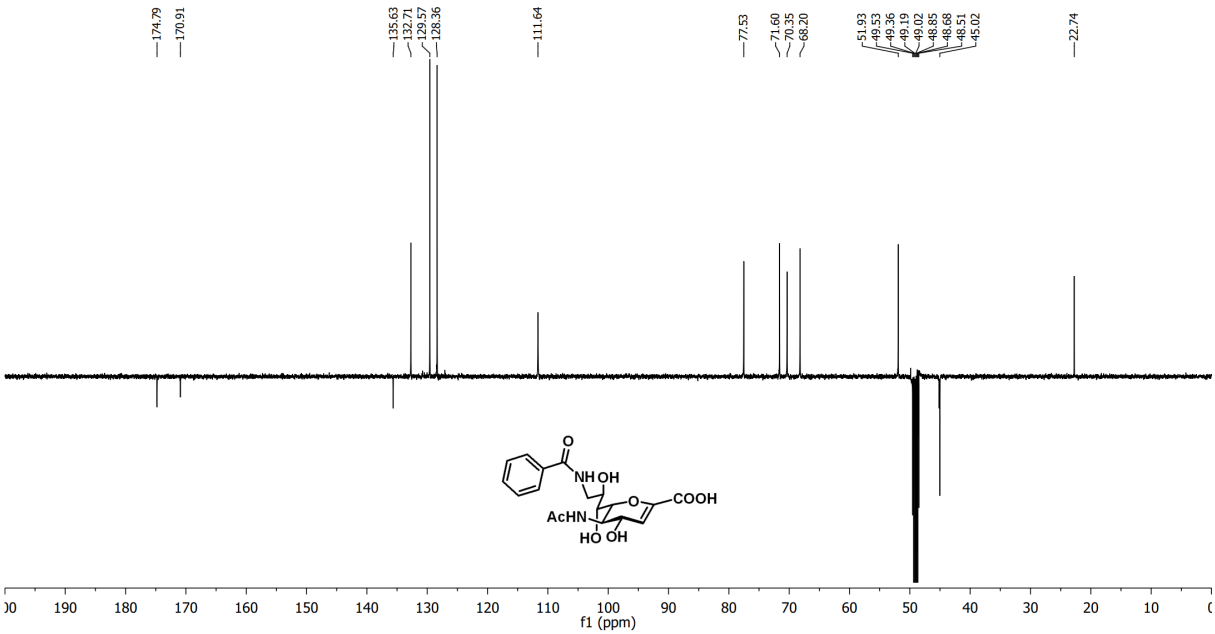


15g

499.799 MHz H1 1D in CD_3OD

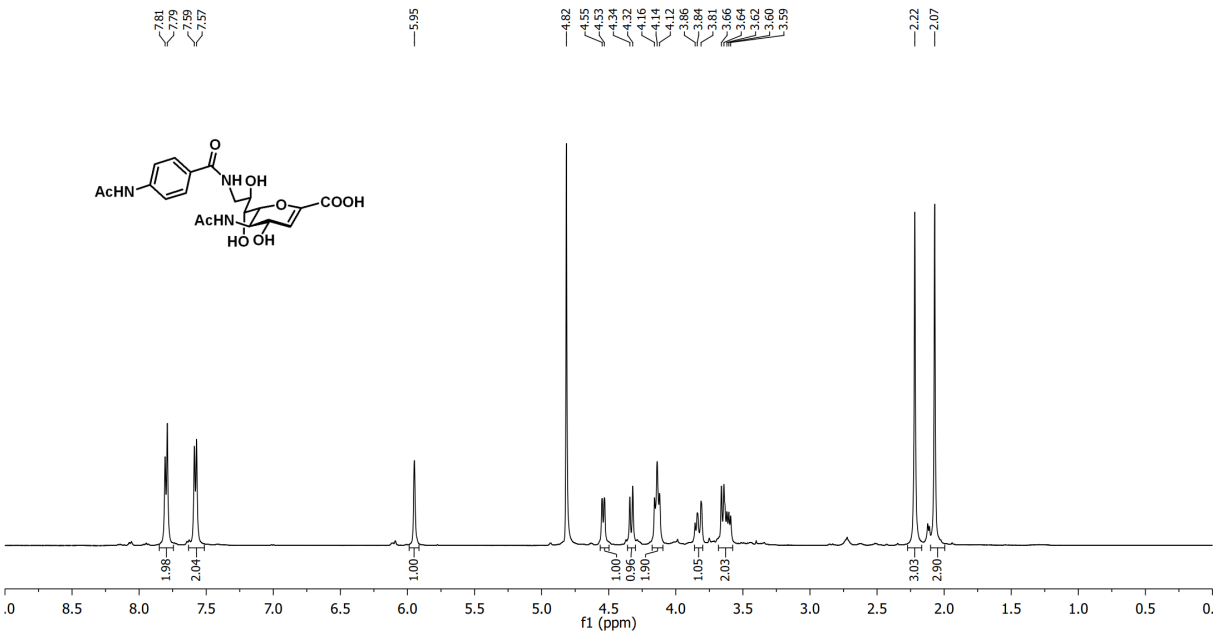


125.688 MHz C13[H1] 1D in CD_3OD

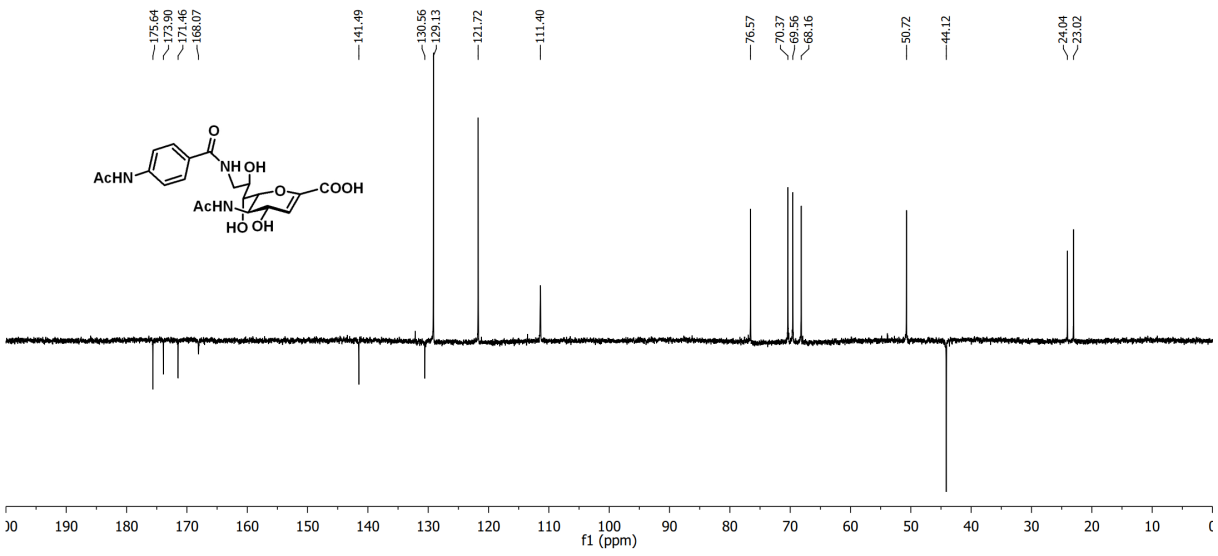


15h

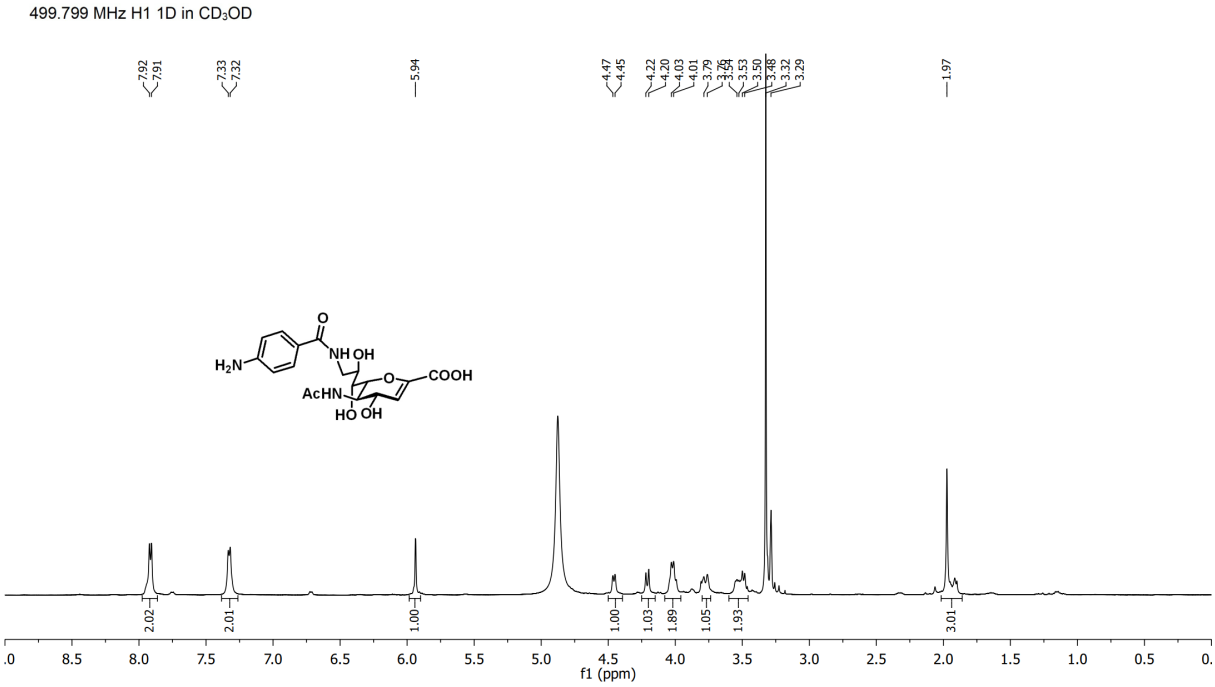
499.808 MHz H1 1D in D_2O

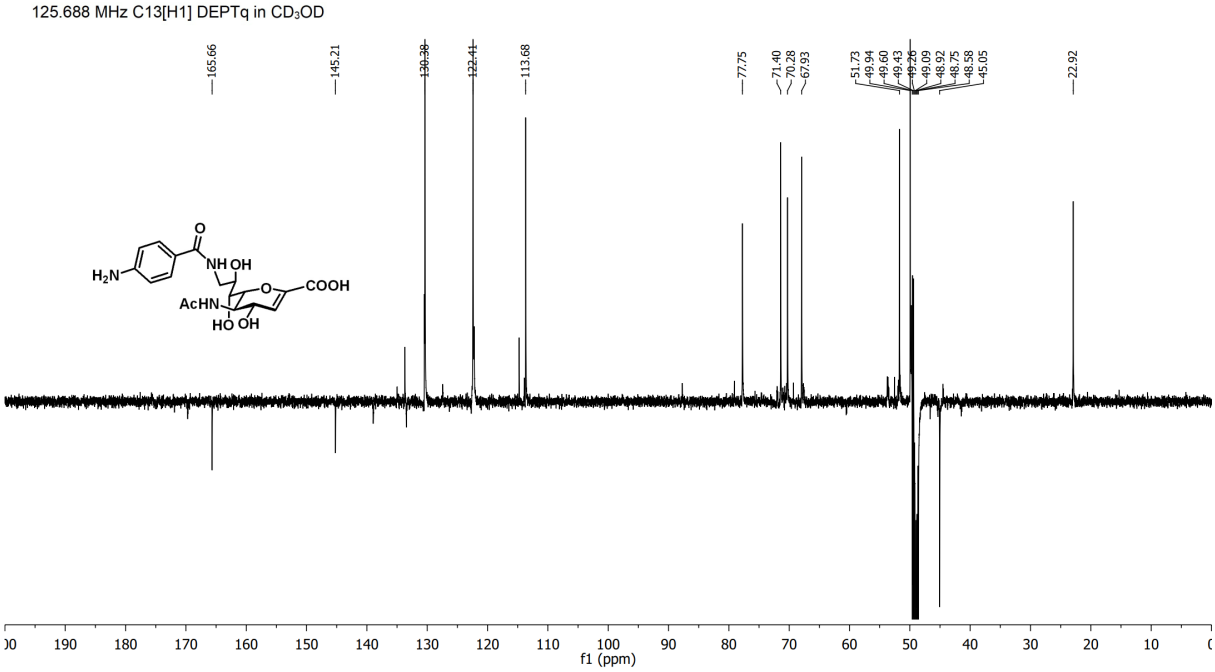


125.688 MHz C13[H1] DEPTq in D_2O



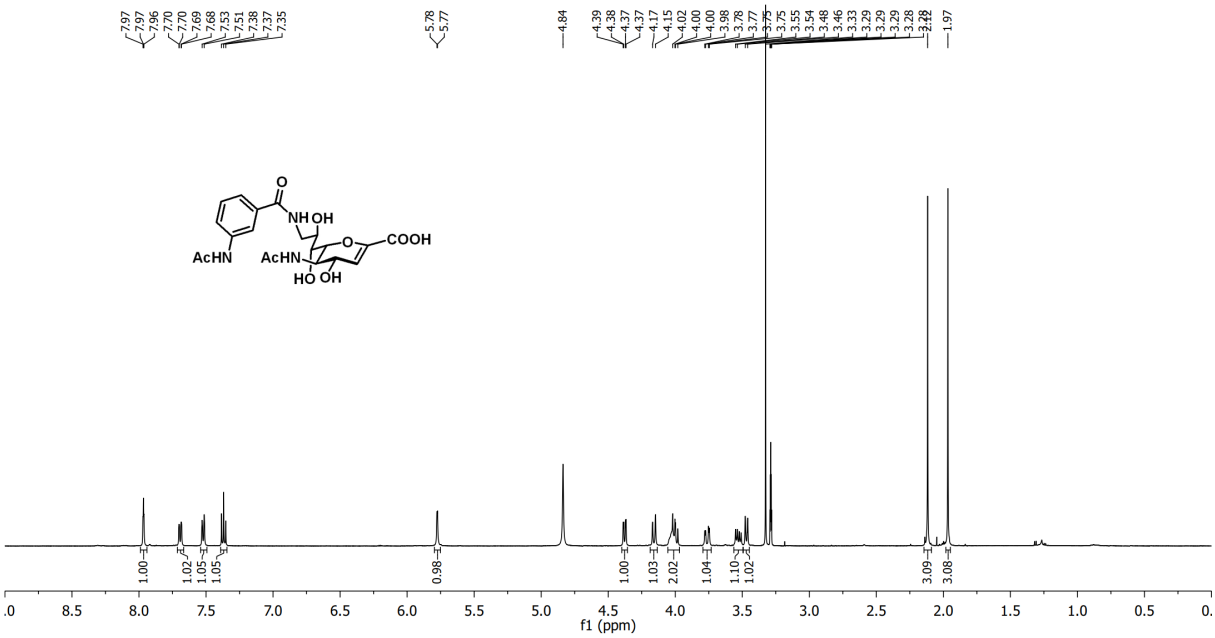
15i


499.799 MHz H1 1D in CD3OD
7.92
7.91
7.33
7.32
5.94
4.47
4.45
4.22
4.20
4.03
4.01
3.79
3.76
3.54
3.53
3.50
3.48
3.32
3.29
1.97
2.02
2.01
1.00
1.00
1.03
1.89
1.05
1.93
3.01
f1 (ppm)

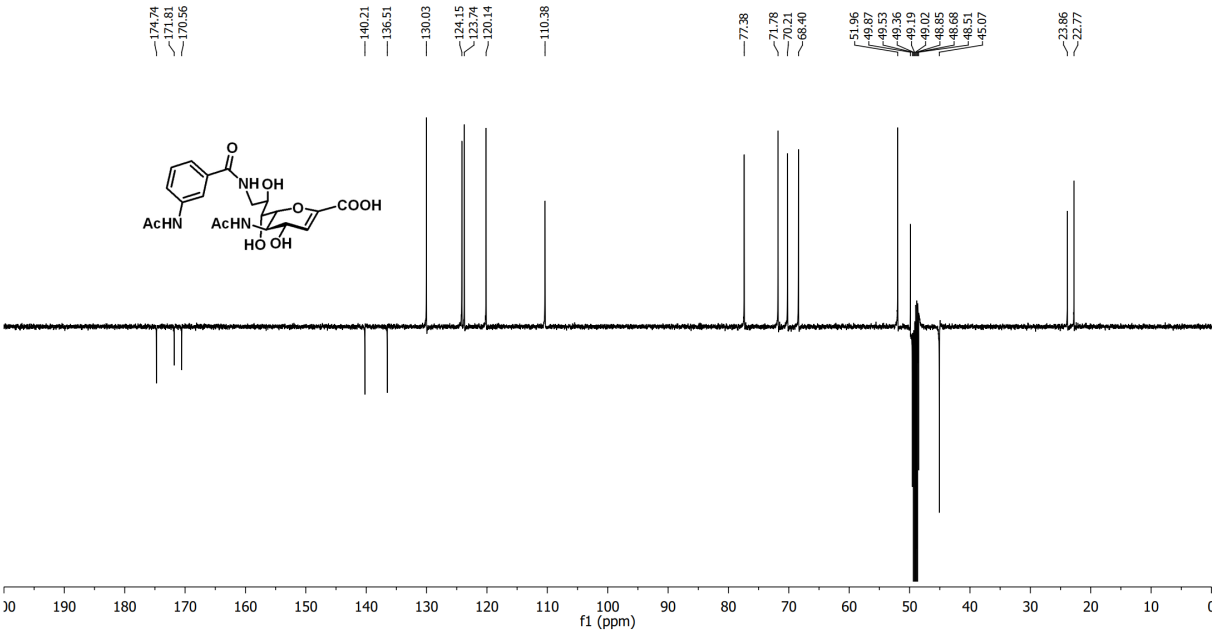

125.688 MHz C13[H1] DEPTq in CD3OD
165.66
145.21
130.38
122.41
113.68
77.75
71.40
70.28
67.93
51.73
49.94
49.60
49.43
49.26
49.09
48.92
48.75
48.58
45.05
22.92
f1 (ppm)

15j

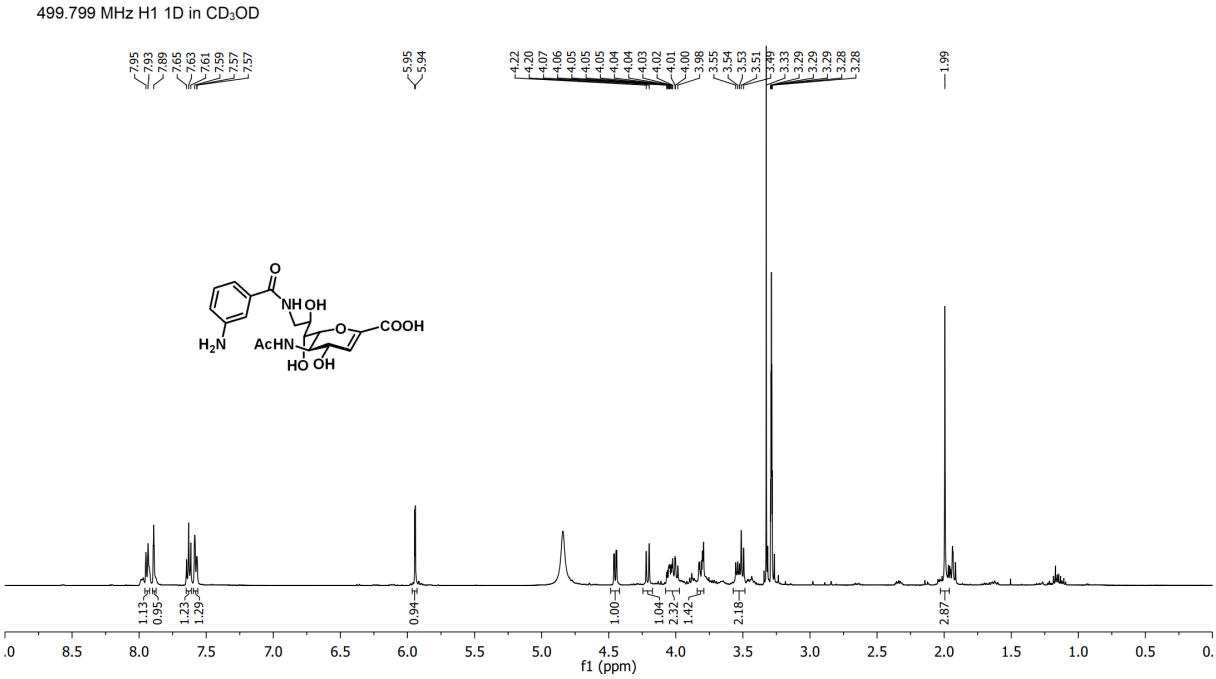
499.799 MHz H1 1D in CD_3OD

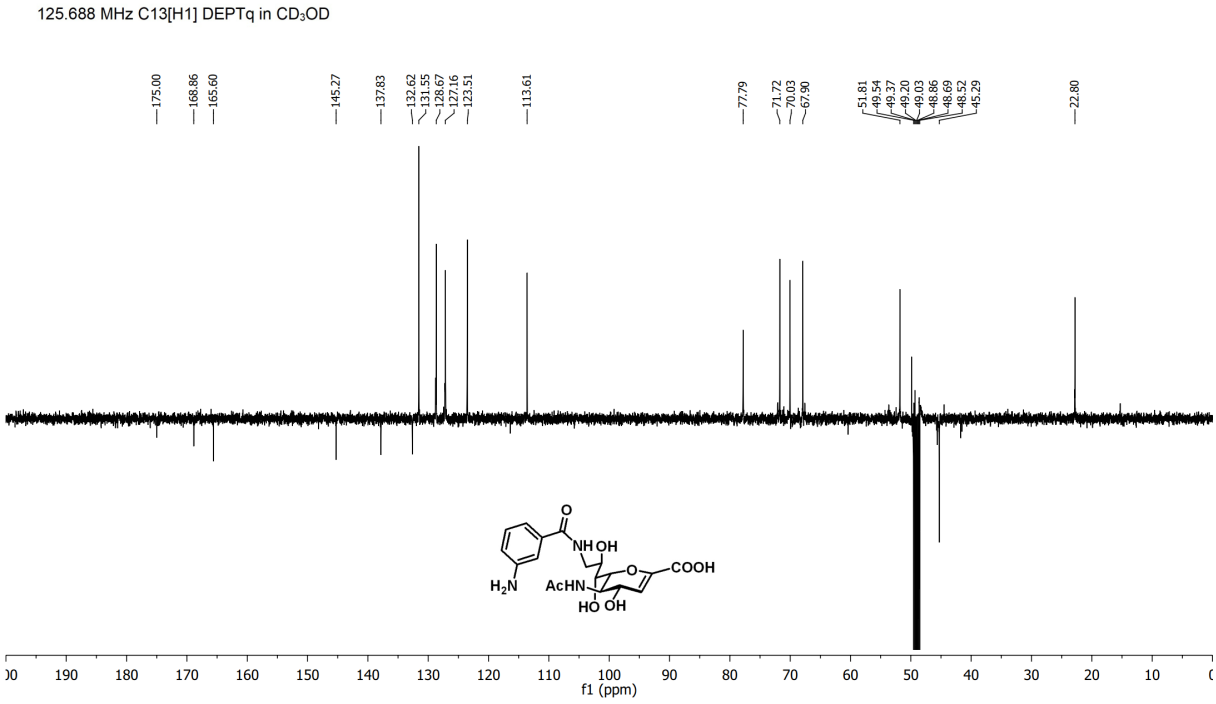


125.688 MHz C13[H1] DEPTq in CD_3OD



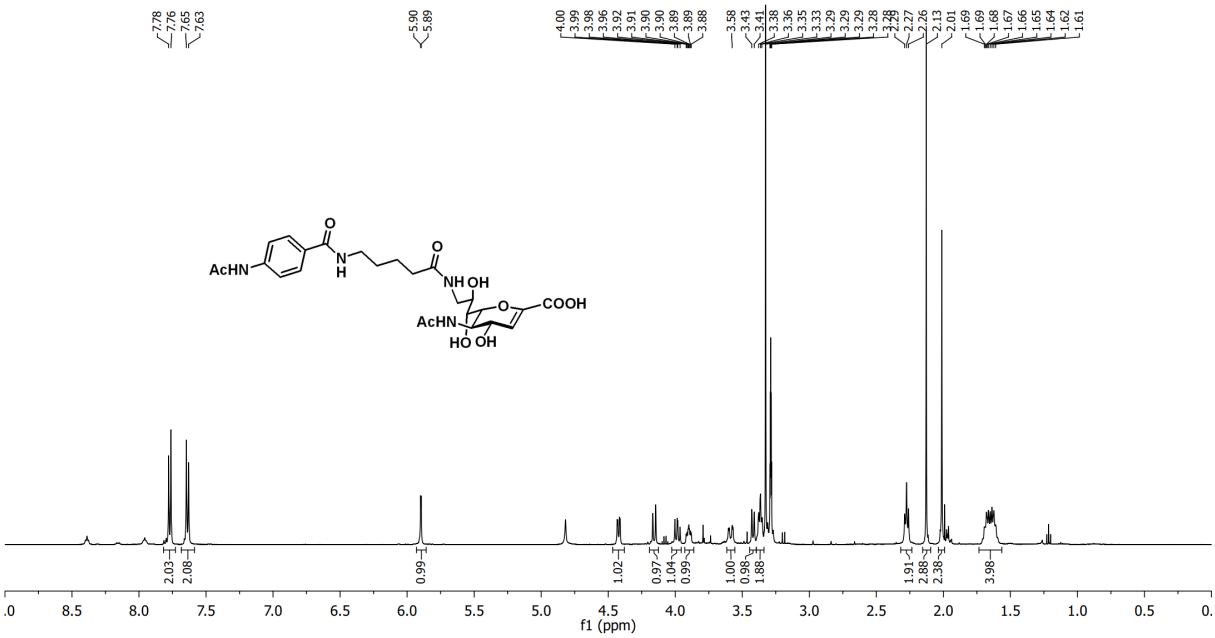
15k


499.799 MHz H1 1D in CD3OD
7.95
7.93
7.89
7.65
7.63
7.61
7.59
7.57
7.57
5.95
5.94
4.22
4.20
4.07
4.06
4.05
4.05
4.05
4.04
4.04
4.03
4.02
4.01
4.00
3.98
3.55
3.54
3.53
3.51
3.49
3.33
3.29
3.29
3.29
3.28
3.28
1.99
1.13
0.95
1.23
1.29
0.94
1.00
1.04
2.32
1.42
2.18
2.87
f1 (ppm)

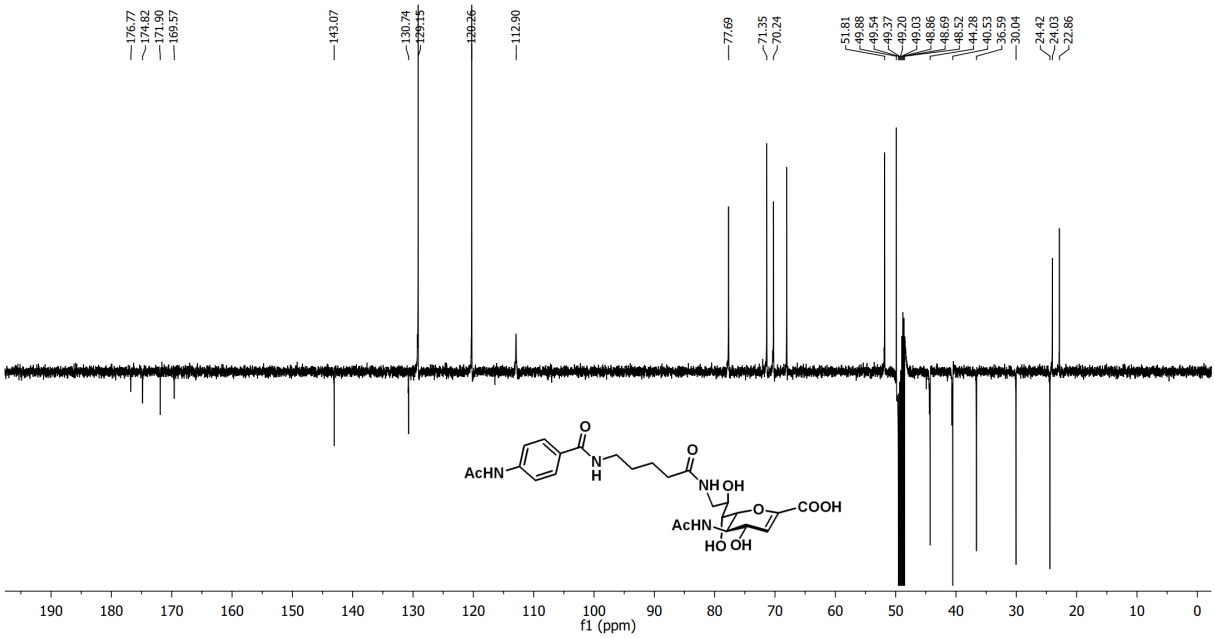

125.688 MHz C13[H1] DEPTq in CD3OD
175.00
168.86
165.60
145.27
137.83
132.62
131.55
128.67
127.16
123.51
113.61
77.79
71.72
70.03
67.90
51.81
49.54
49.37
49.20
49.03
48.86
48.69
48.52
45.29
22.80
f1 (ppm)

15l

499.799 MHz H1 1D in CD_3OD

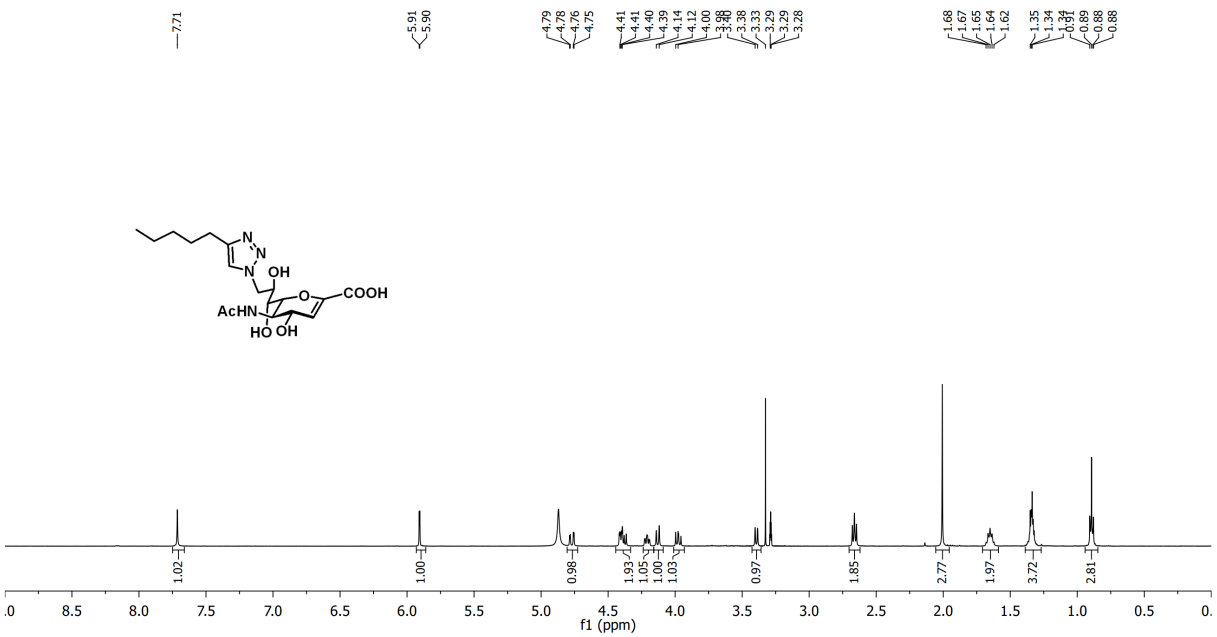


125.688 MHz C13[H1] DEPTq in CD_3OD

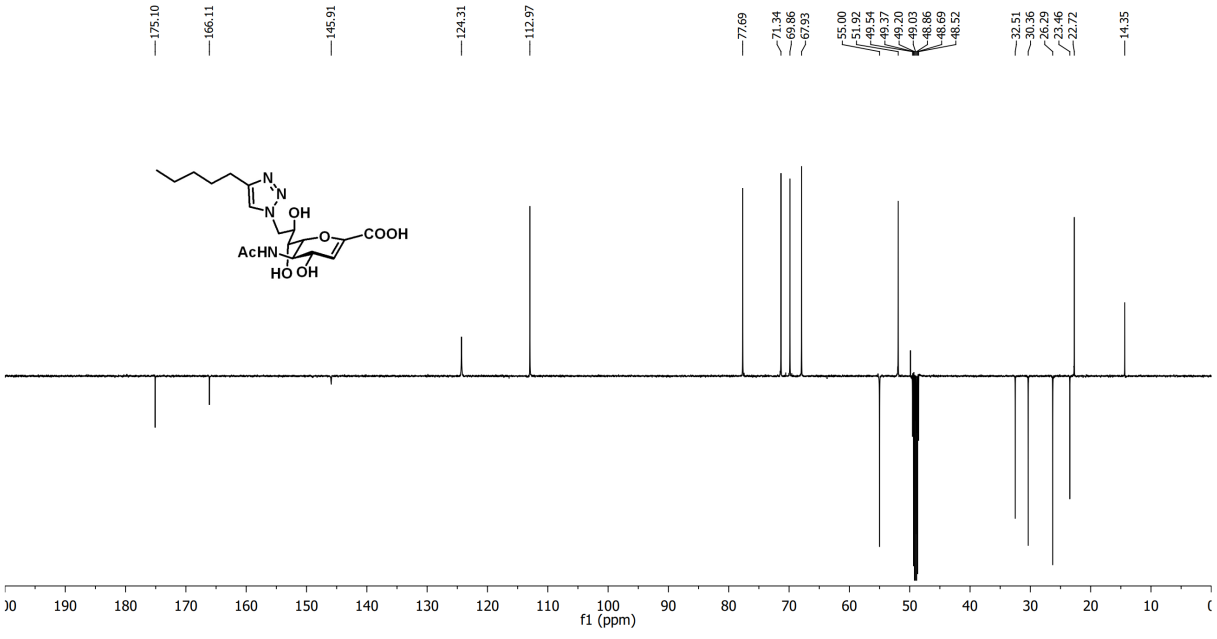


15m

499.799 MHz H1 1D in CD_3OD

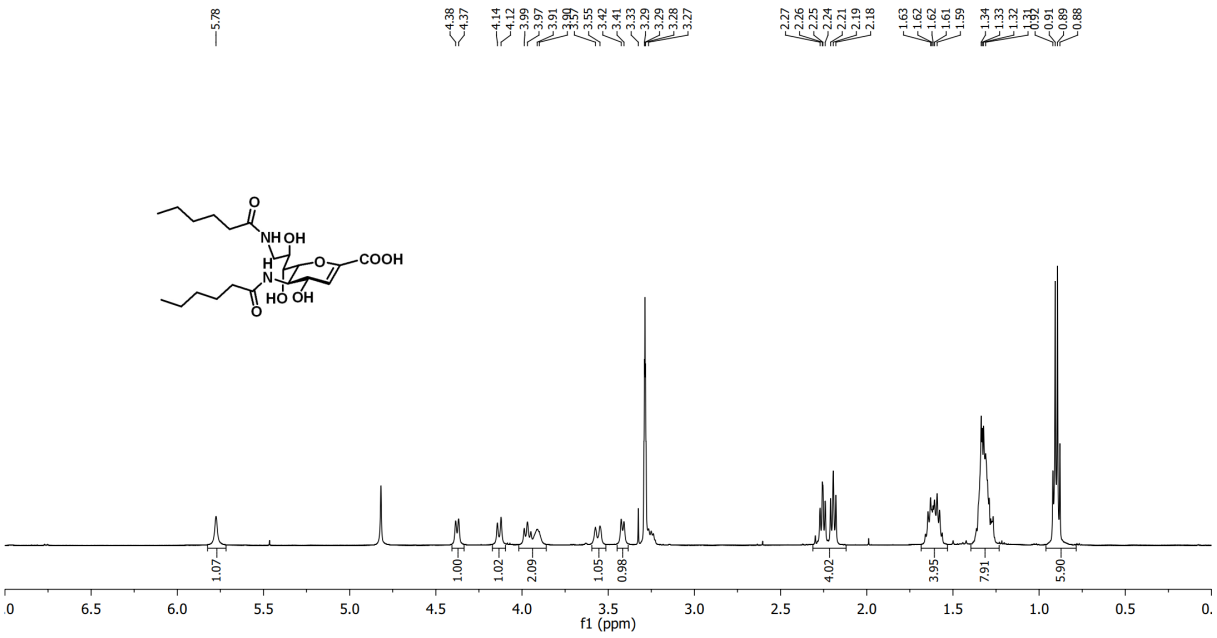


125.688 MHz C13[H1] DEPTq in CD_3OD

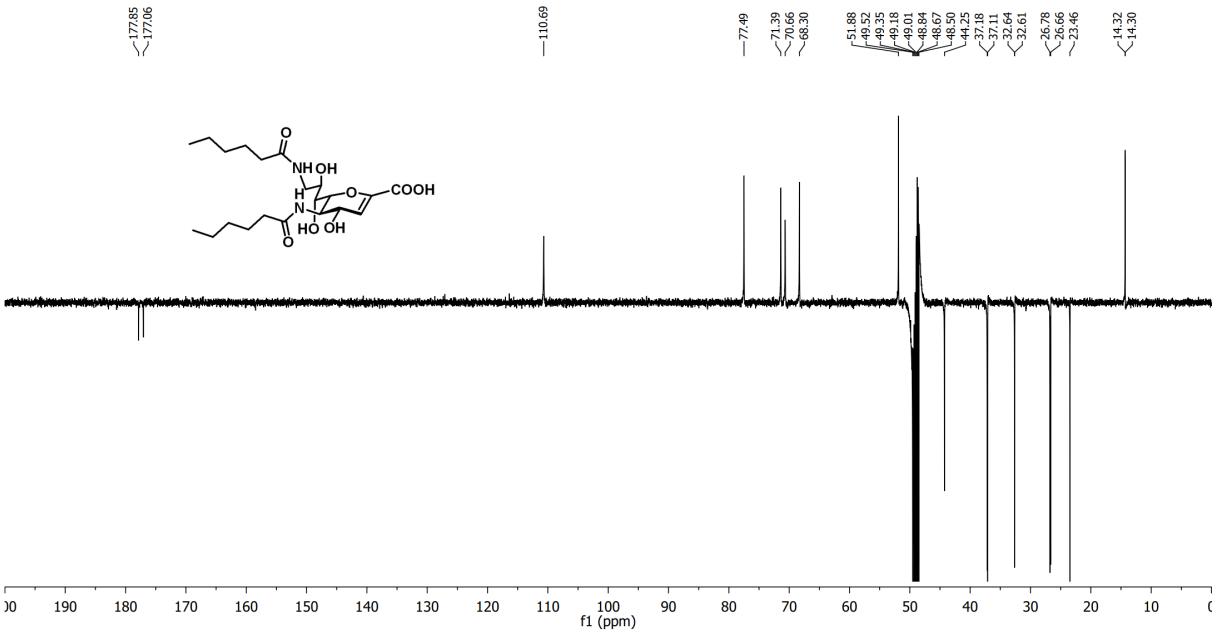


17a

499.799 MHz H1 1D in CD_3OD

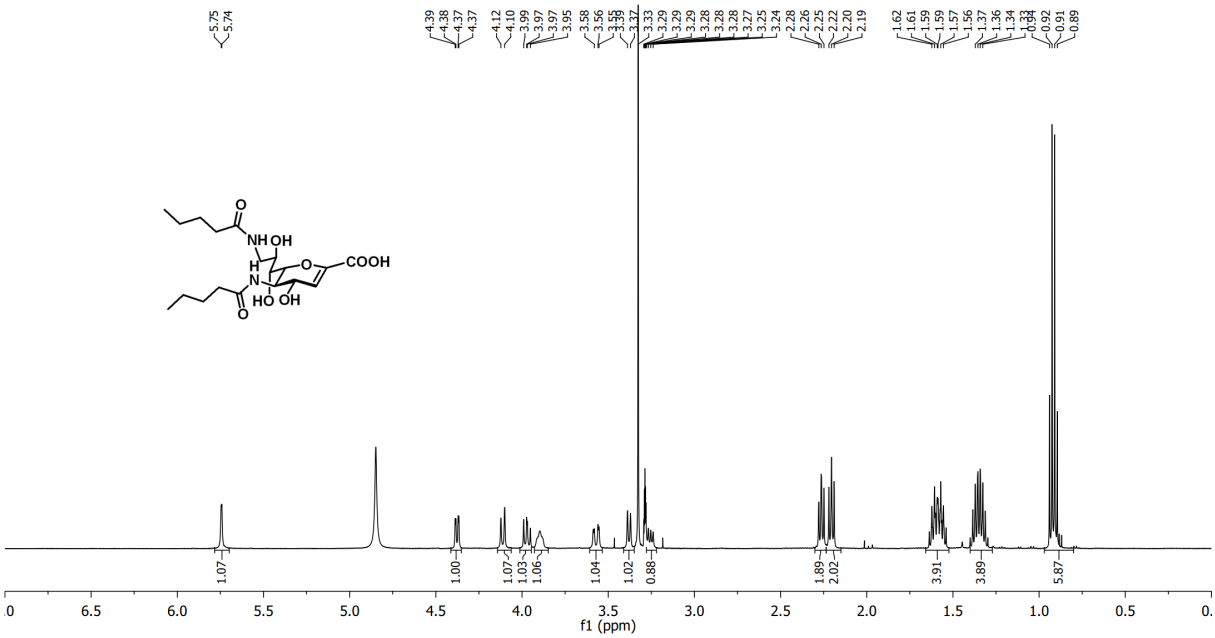


125.688 MHz C13[H1] DEPTq in CD_3OD

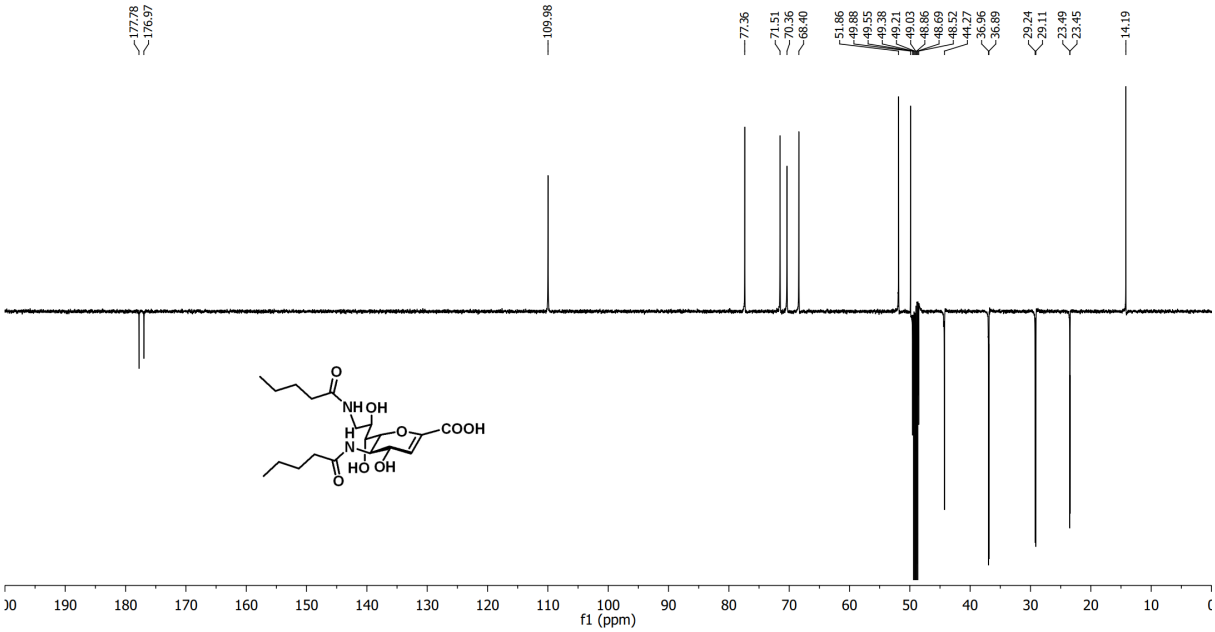


17b

499.799 MHz H1 1D in CD_3OD

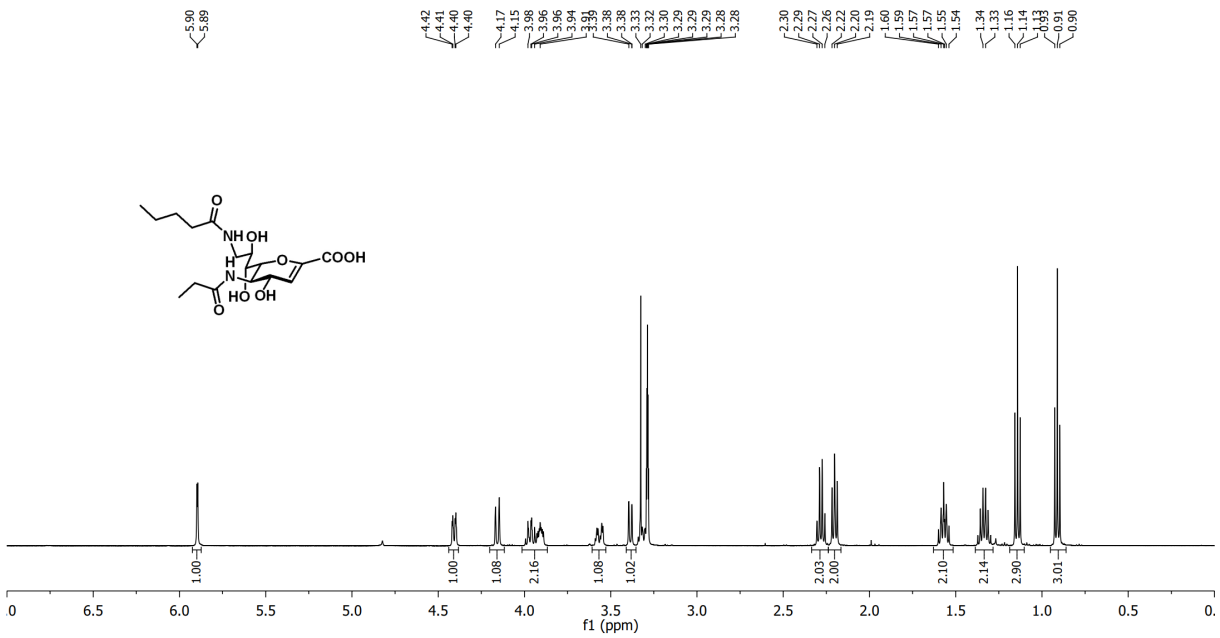


125.688 MHz C13[H1] 1D in CD_3OD

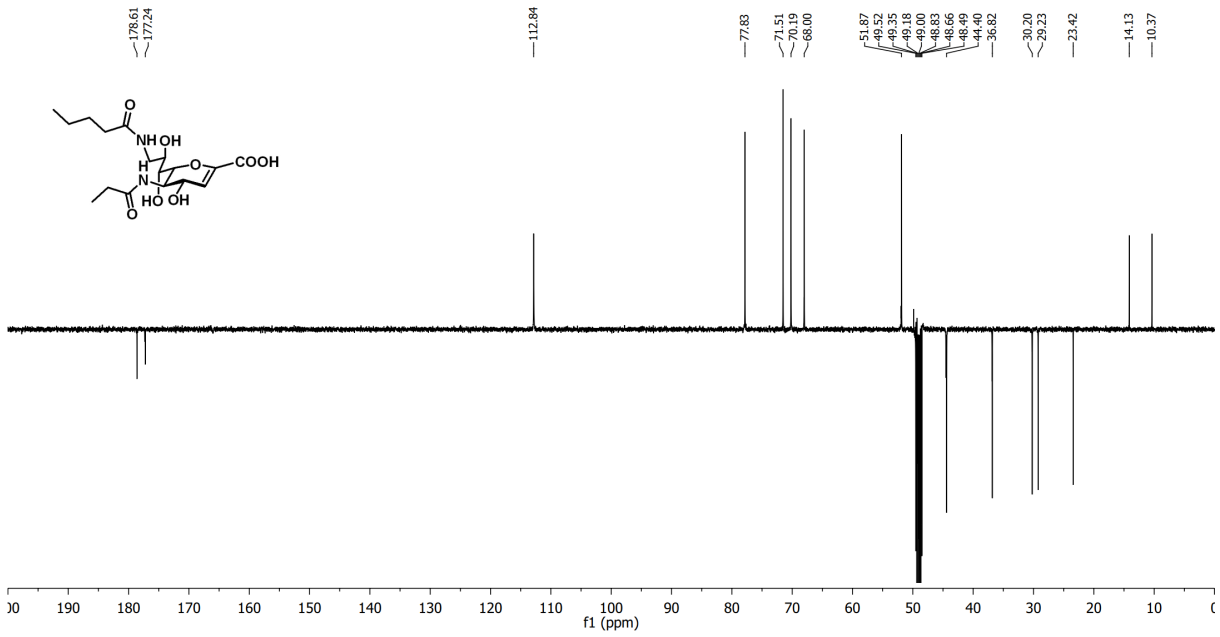


17c

499.799 MHz H1 1D in CD_3OD

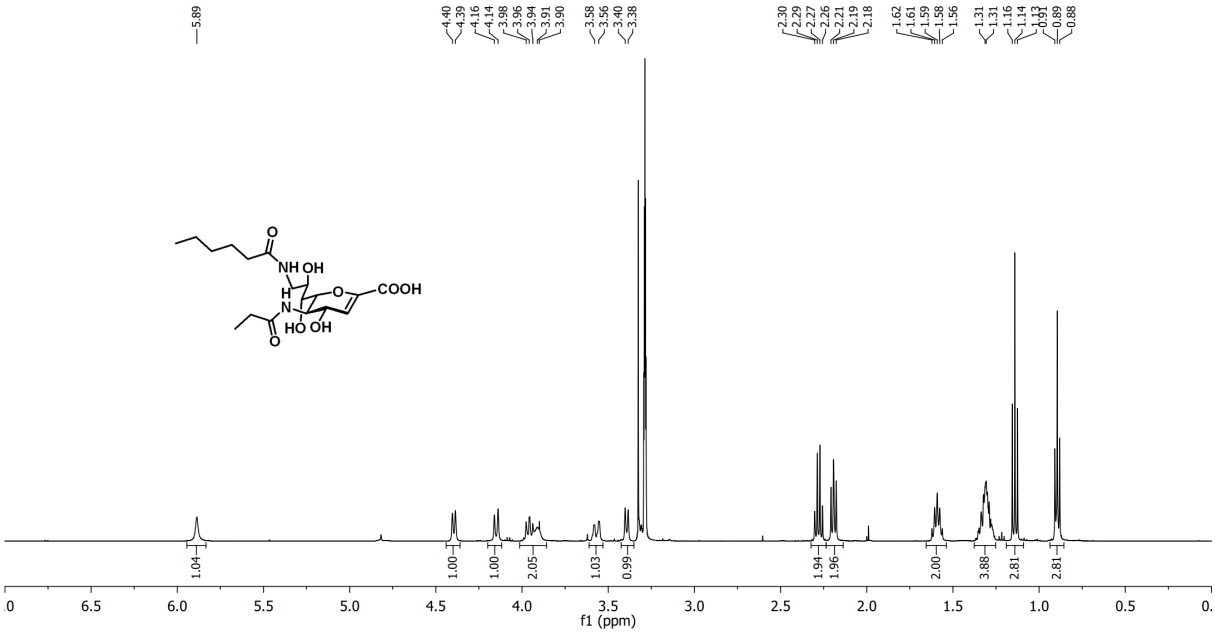


125.688 MHz C13[H1] DEPTq in CD_3OD

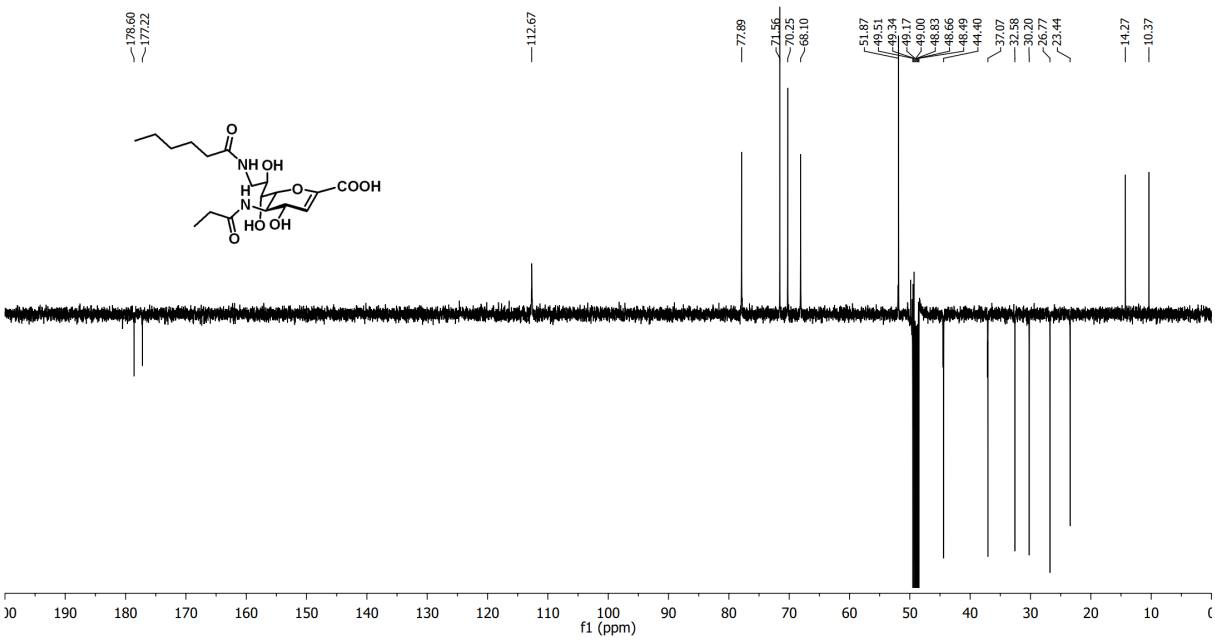


17d

499.799 MHz H1 1D in CD_3OD

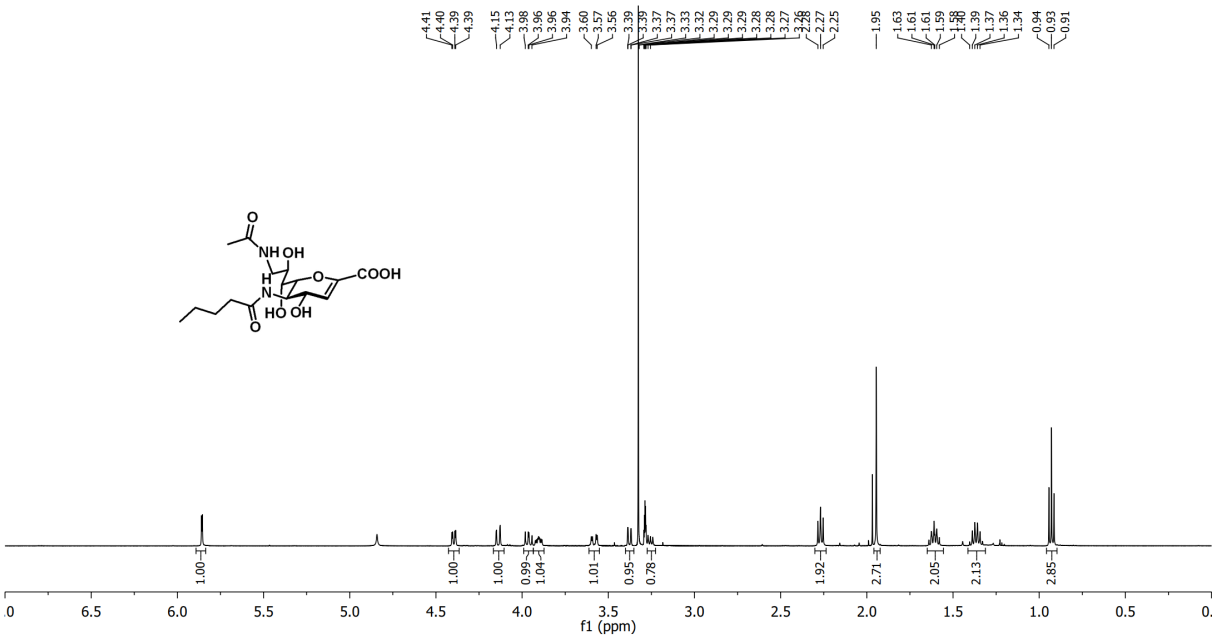


125.688 MHz C13[H1] DEPTq in CD_3OD

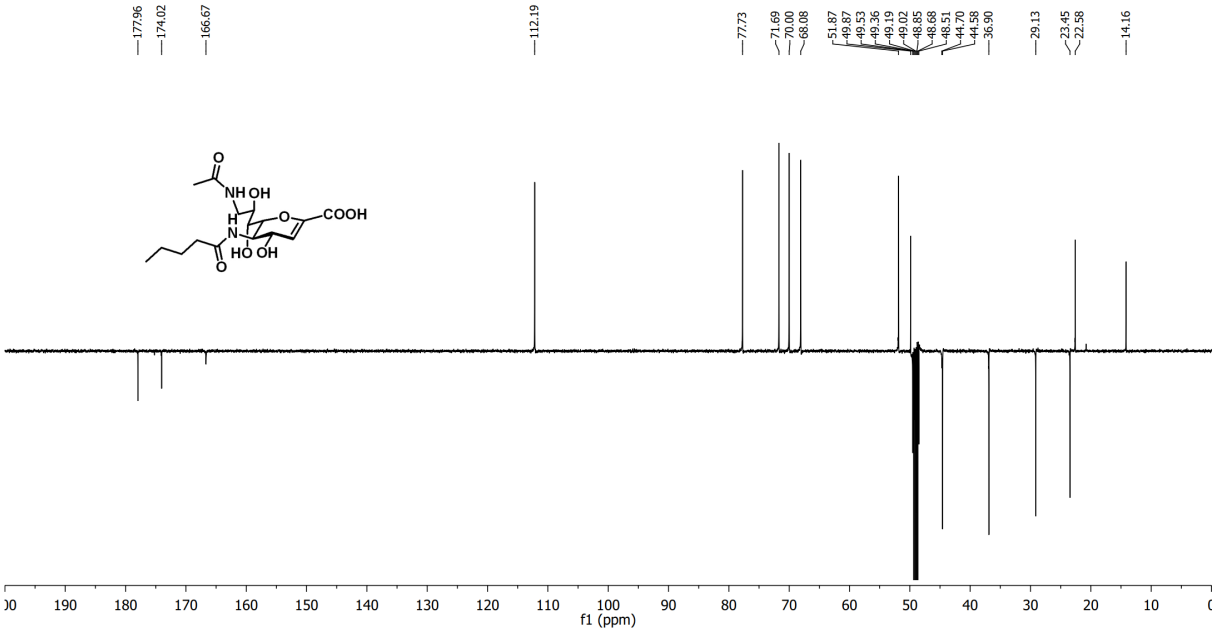


17e

499.799 MHz H1 1D in CD_3OD

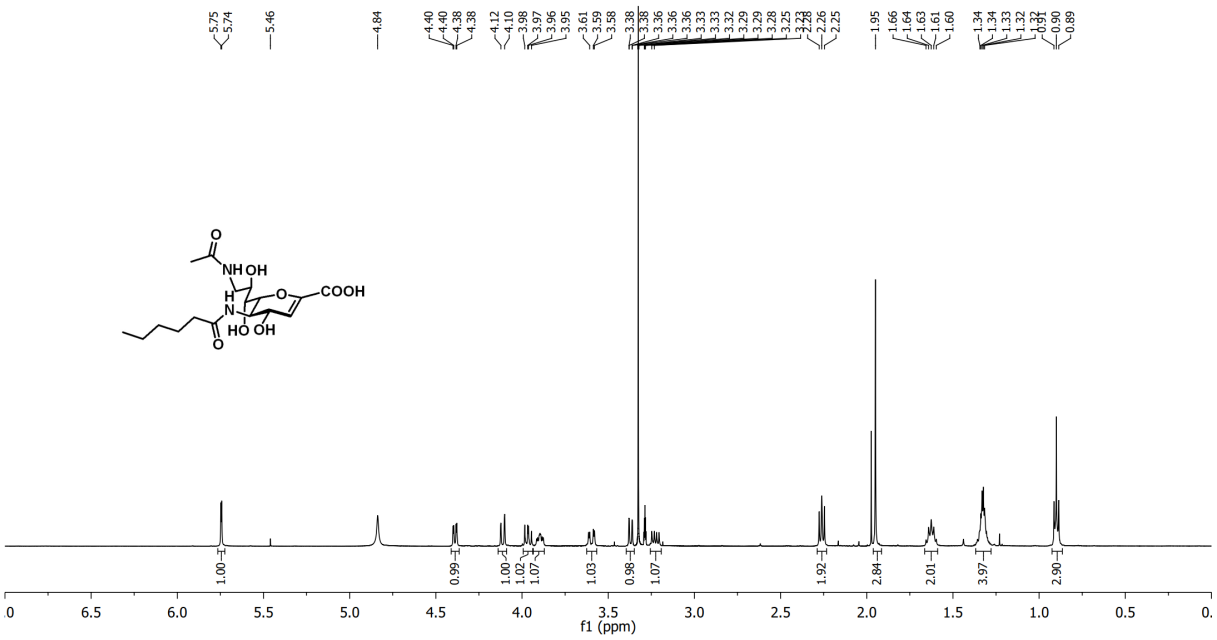


125.688 MHz C13[H1] DEPTq in CD_3OD

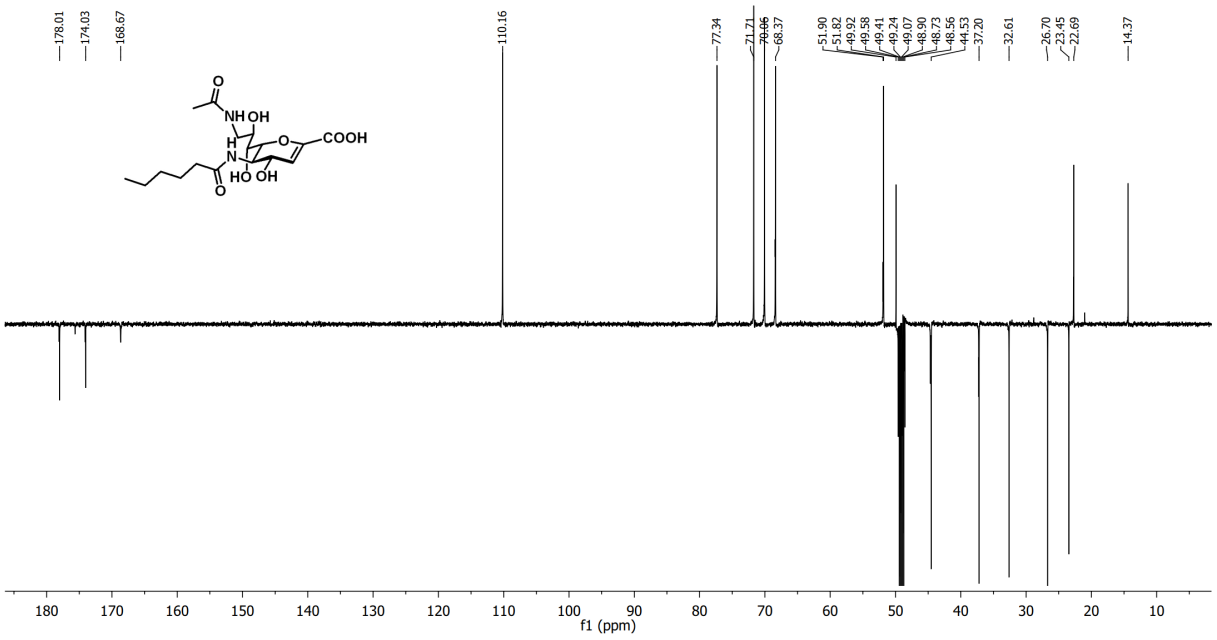


17f

499.799 MHz H1 1D in CD_3OD

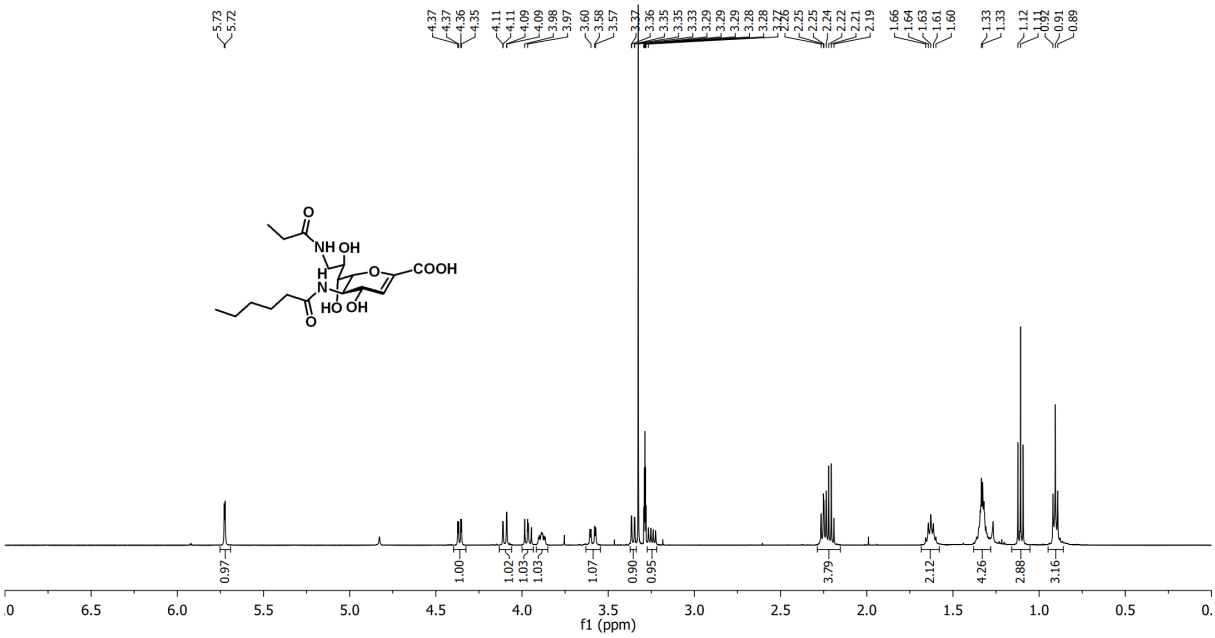


125.688 MHz C13[H1] DEPTq in CD_3OD

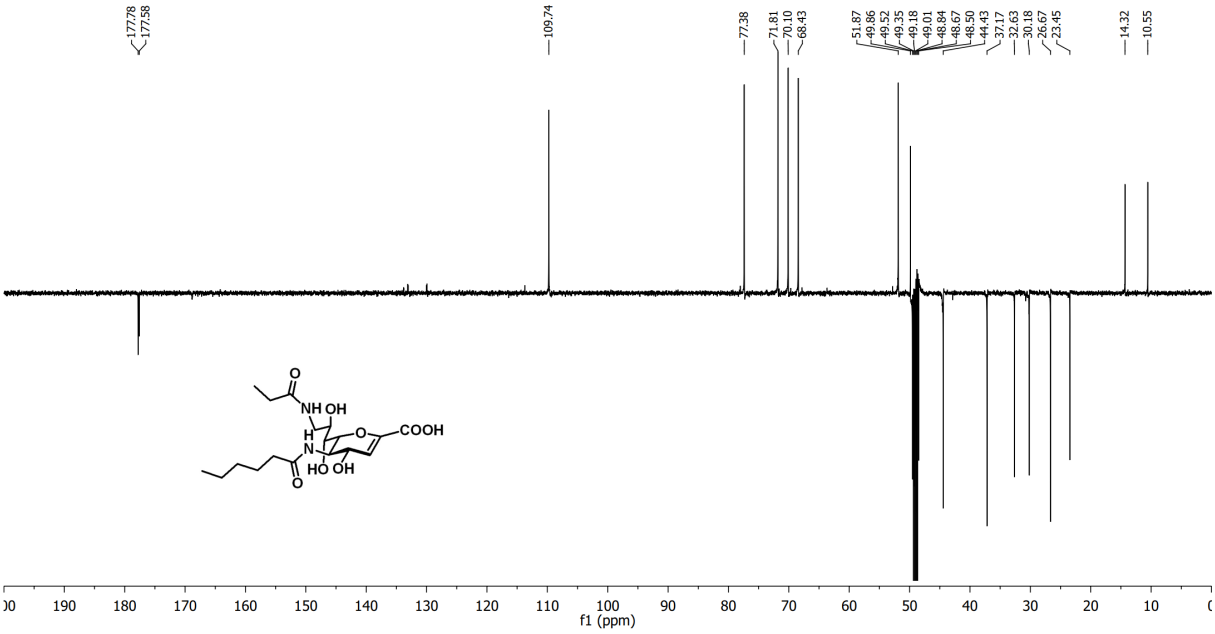


17g

499.799 MHz H1 1D in CD_3OD

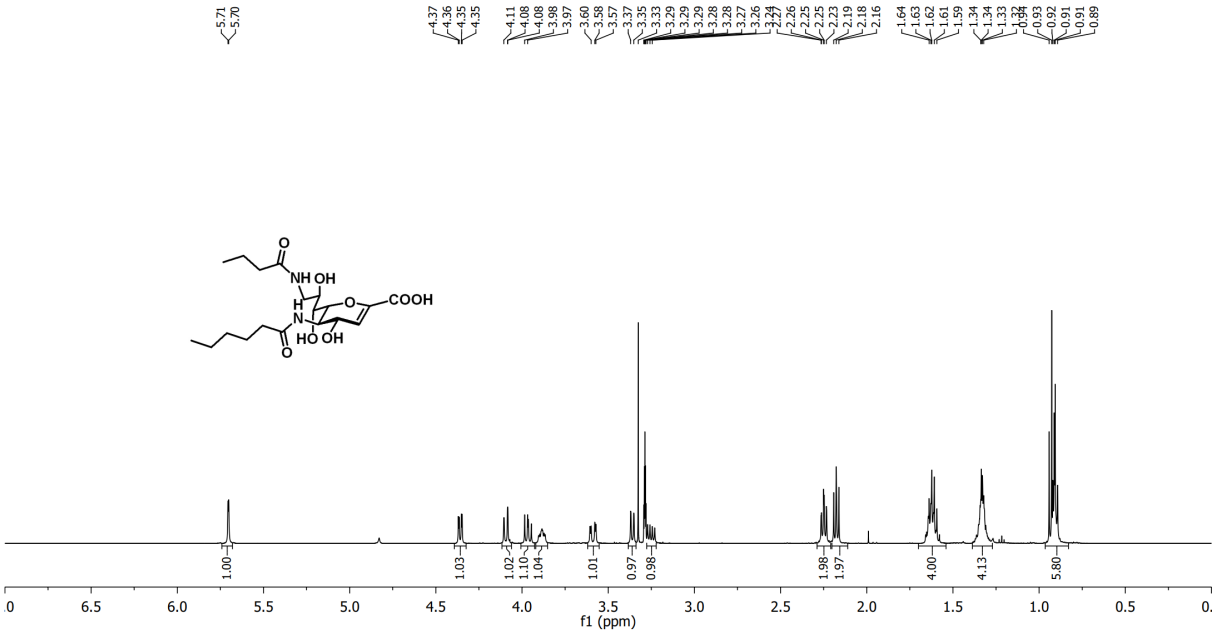


125.688 MHz C13[H1] DEPTq in CD_3OD

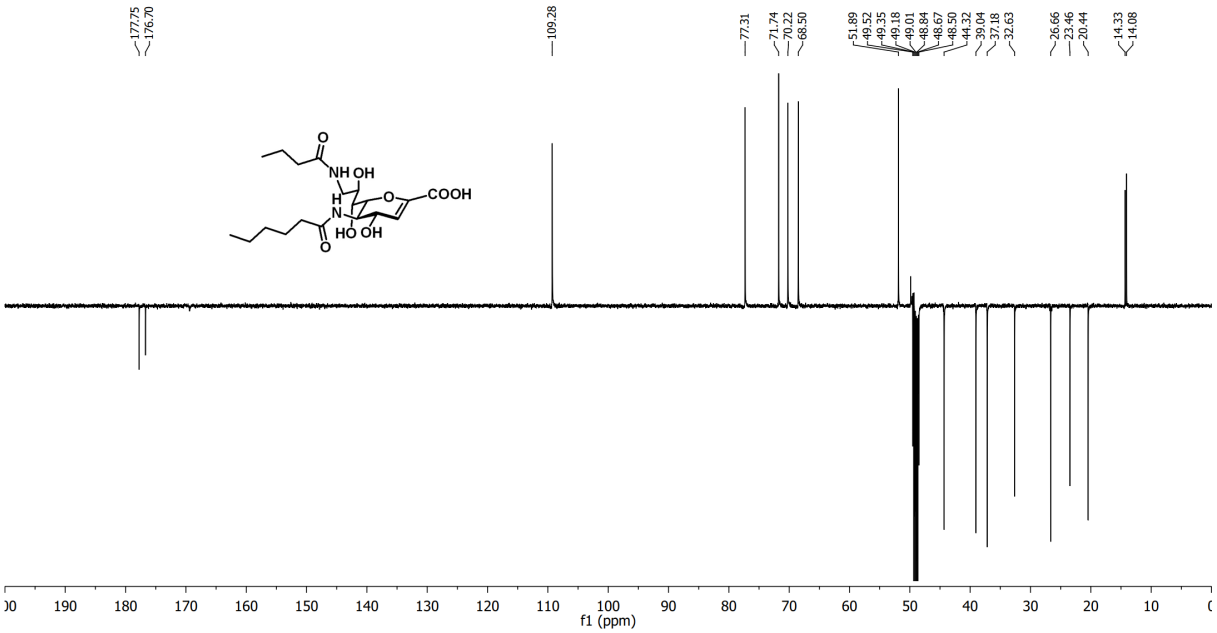


17h

499.799 MHz H1 1D in CD_3OD

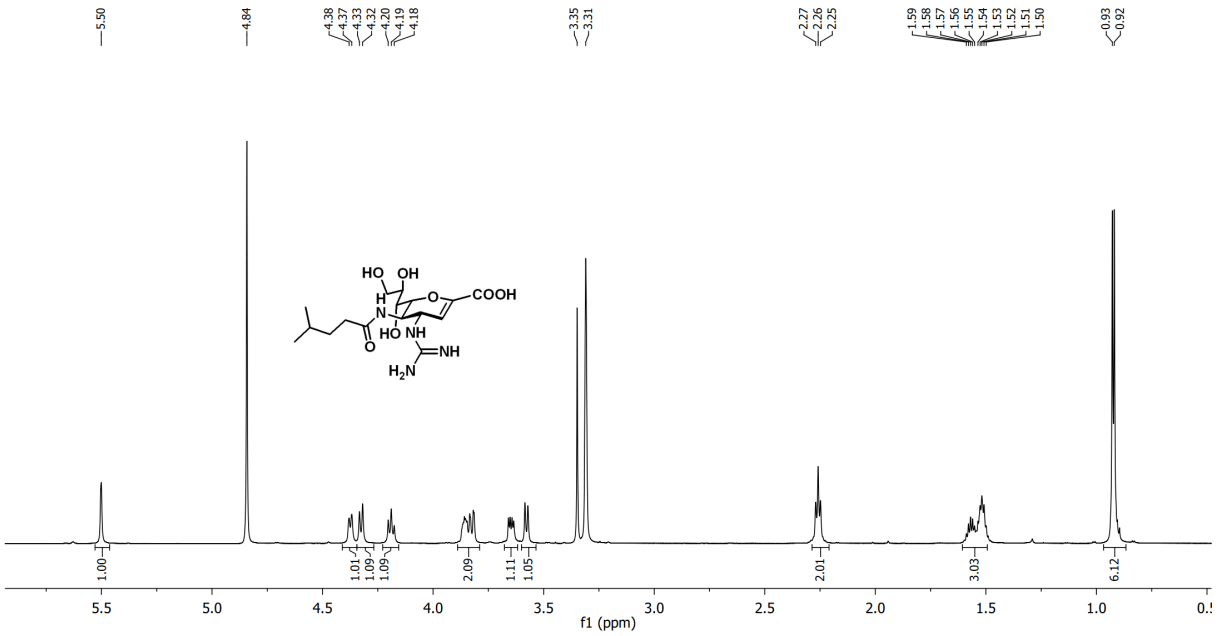


125.688 MHz C13[H1] DEPTq in CD_3OD



22

699.765 MHz H1 1D in CD_3OD



175.975 MHz C13[H1] DEPTq in CD_3OD

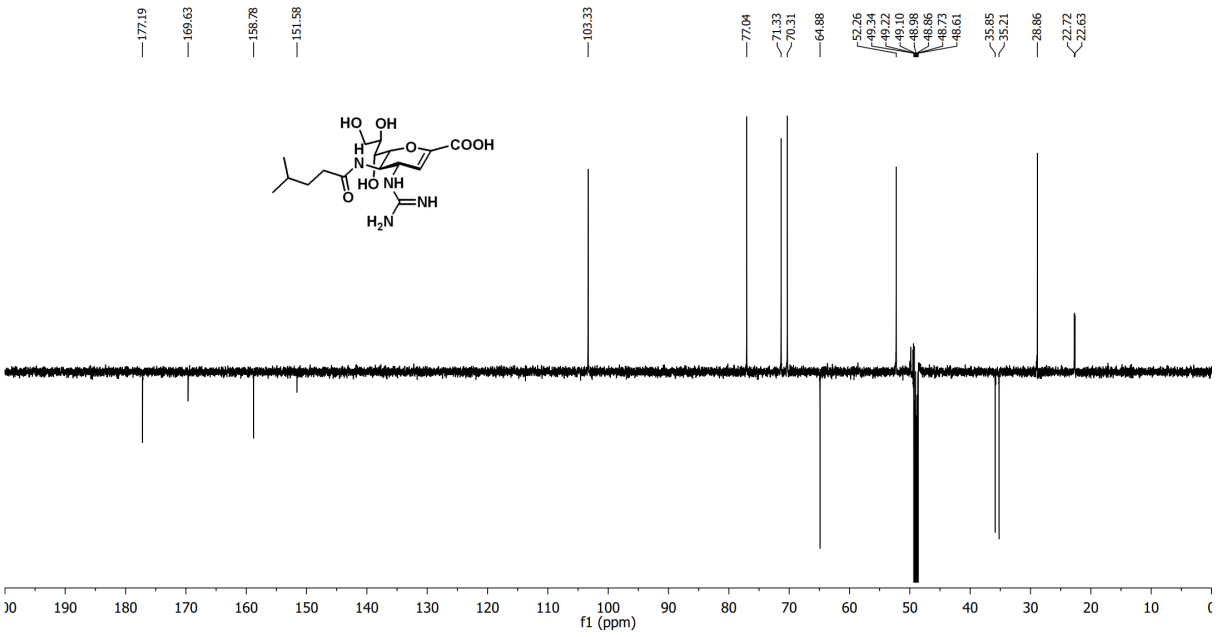
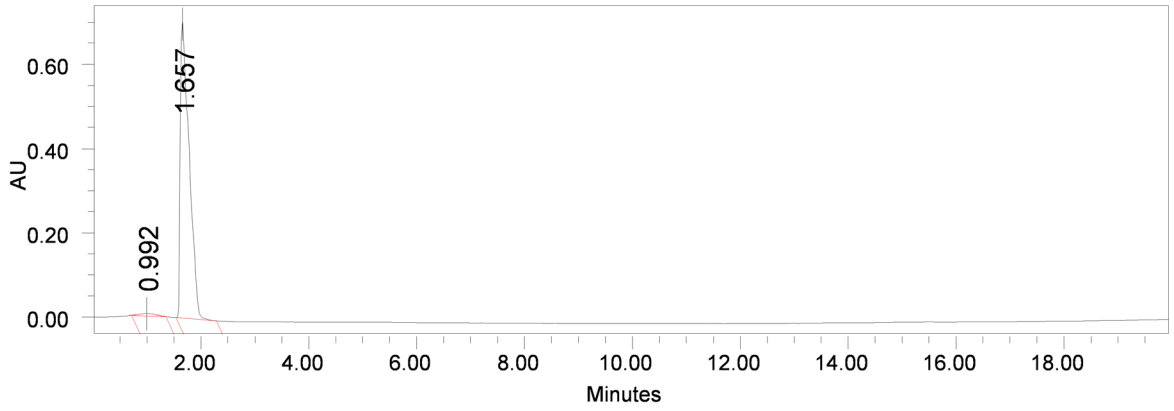


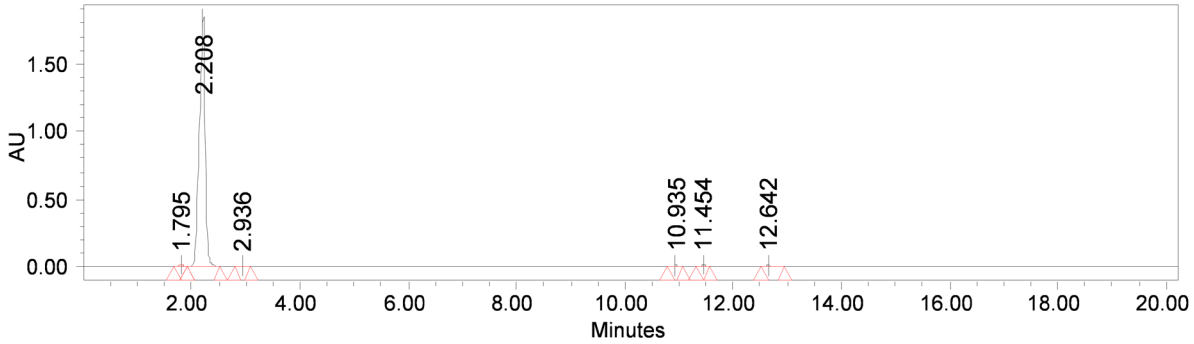
Figure S4: HPLC traces

1(DANA)



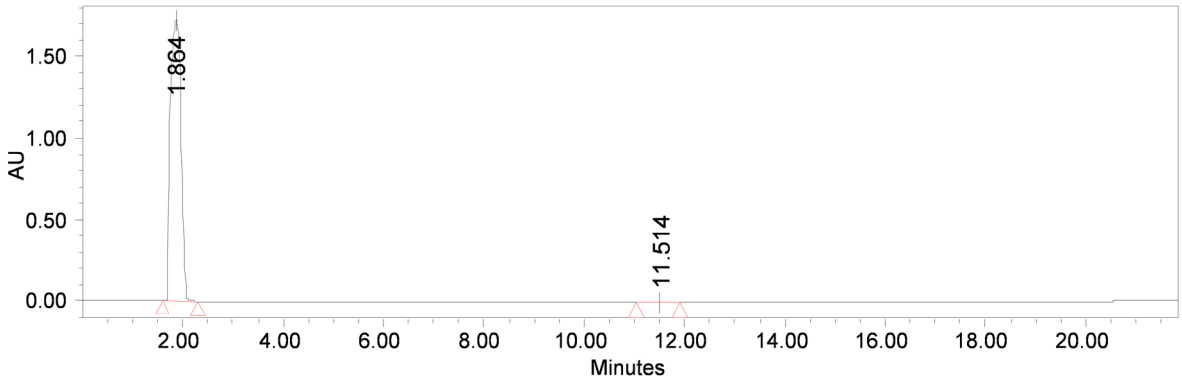
	Retention Time	Area	% Area
1	0.992	206327	2.49
2	1.657	8083296	97.51

6(Neu5AcN$_3$2en)



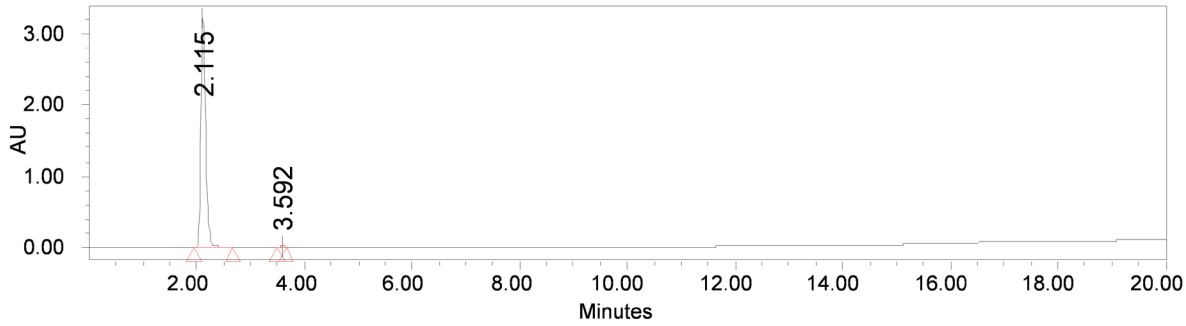
	Retention Time	Area	% Area
1	1.795	102641	0.69
2	2.208	14609215	97.67
3	2.936	58635	0.39
4	10.935	61798	0.41
5	11.454	66473	0.44
6	12.642	58879	0.39

8(C9-BA-DANA)



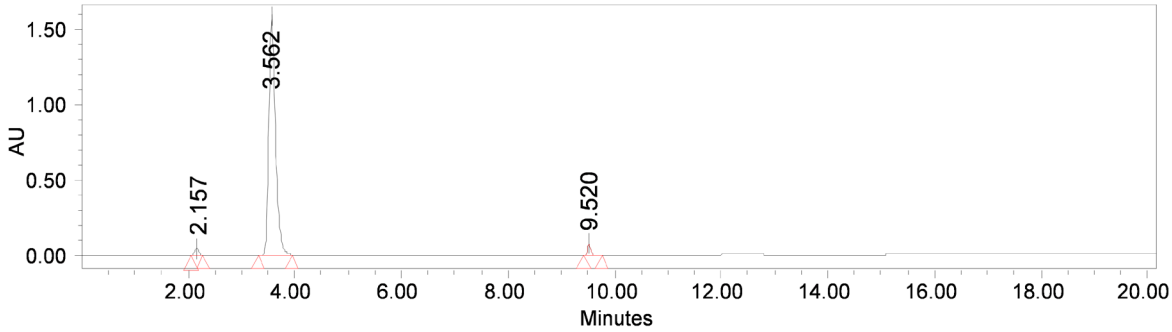
	Retention Time	Area	% Area
1	1.864	25156549	99.97
2	11.514	7667	0.03

11a



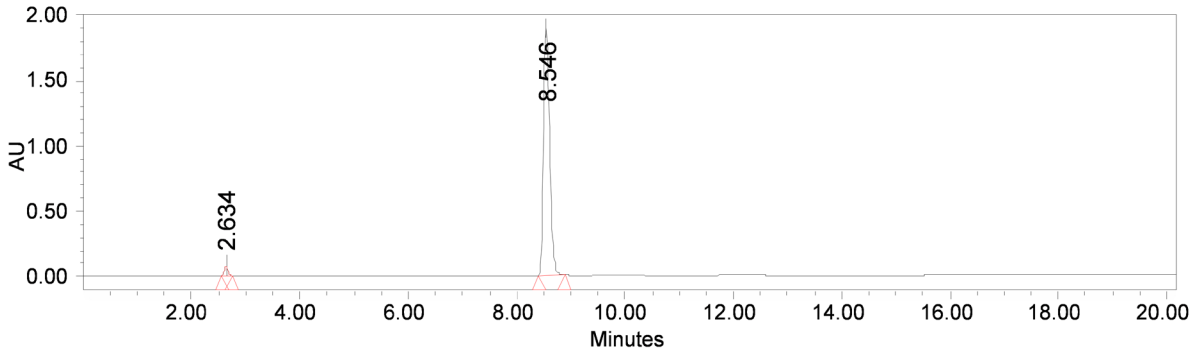
	Retention Time	Area	% Area
1	2.115	21117740	99.71
2	3.592	60690	0.29

11b



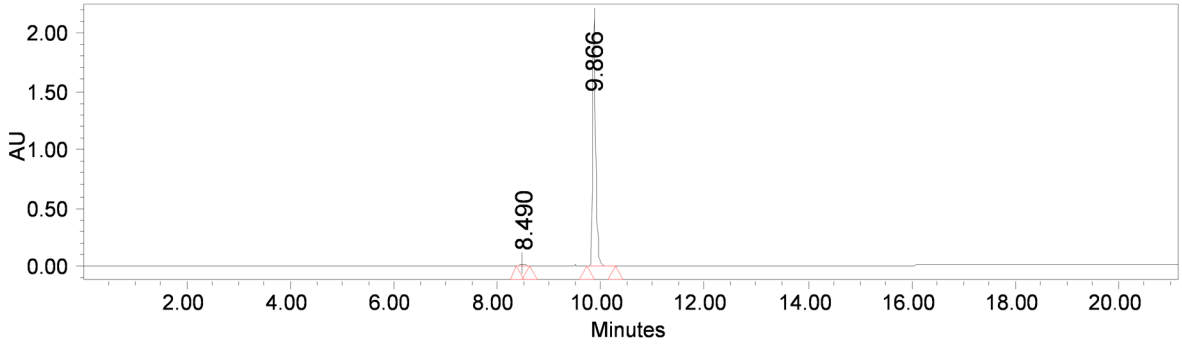
	Retention Time	Area	% Area
1	2.157	257098	1.71
2	3.562	14450419	96.09
3	9.520	331511	2.20

11c



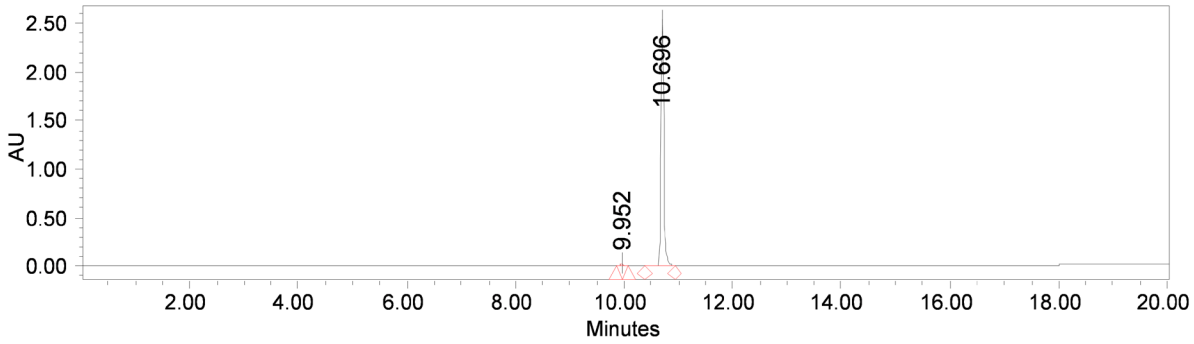
	Retention Time	Area	% Area
1	2.634	418103	2.85
2	8.546	14249347	97.15

11d



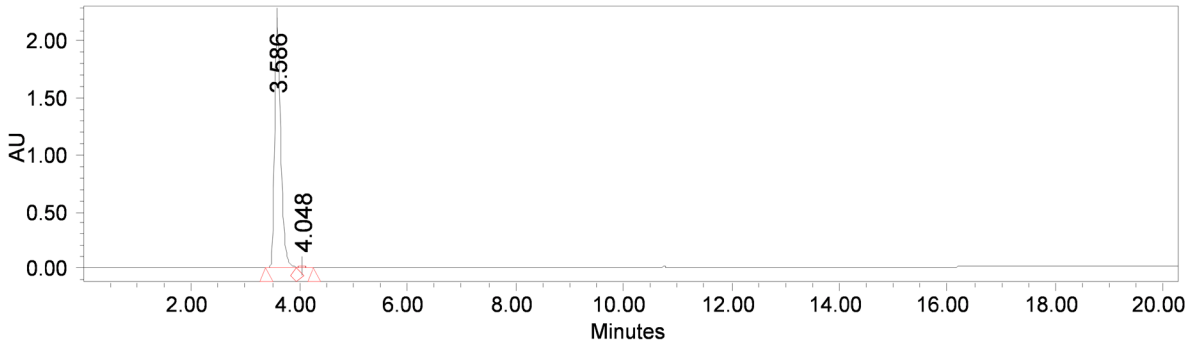
	Retention Time	Area	% Area
1	8.490	152736	1.93
2	9.866	7765075	98.07

11e



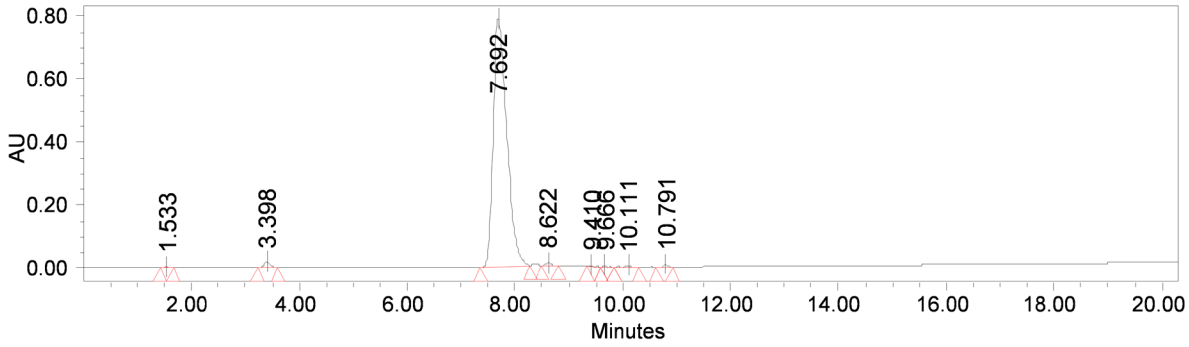
	Retention Time	Area	% Area
1	9.952	92676	0.95
2	10.696	9692986	99.05

11f



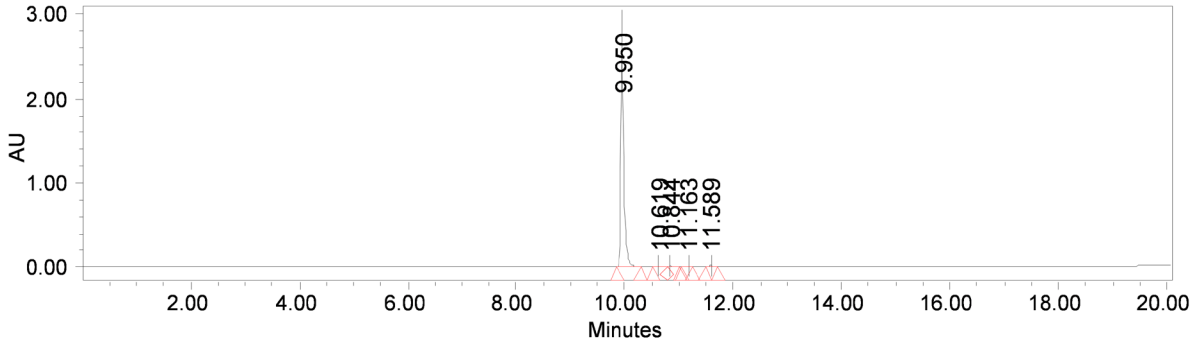
	Retention Time	Area	% Area
1	3.586	18463333	99.13
2	4.048	161496	0.87

11g



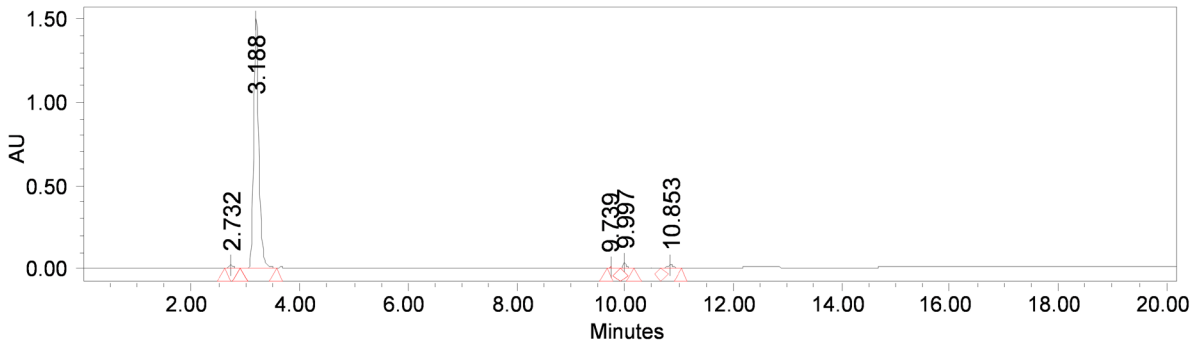
	Retention Time	Area	% Area
1	1.533	24281	0.17
2	3.398	155851	1.09
3	7.692	13864145	97.26
4	8.622	59974	0.42
5	9.410	32166	0.23
6	9.666	30659	0.22
7	10.111	47474	0.33
8	10.791	40680	0.29

11h



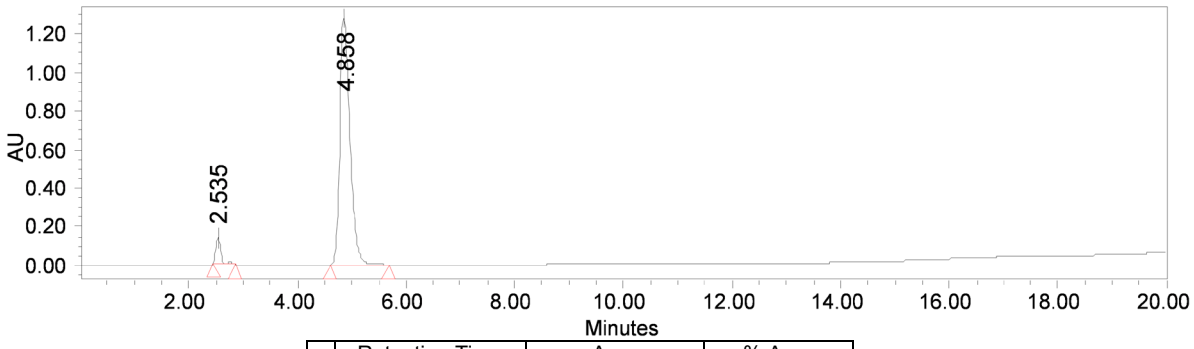
	Retention Time	Area	% Area
1	9.950	12524844	97.93
2	10.619	63271	0.49
3	10.844	94979	0.74
4	11.163	40353	0.32
5	11.589	65812	0.51

11i



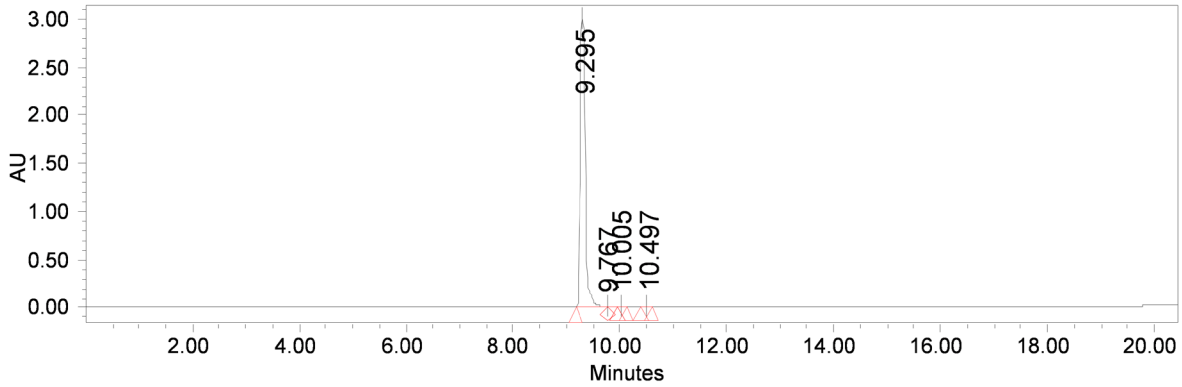
	Retention Time	Area	% Area
1	2.732	126624	1.14
2	3.188	10659916	96.35
3	9.739	30487	0.28
4	9.997	128279	1.16
5	10.853	117976	1.07

11j



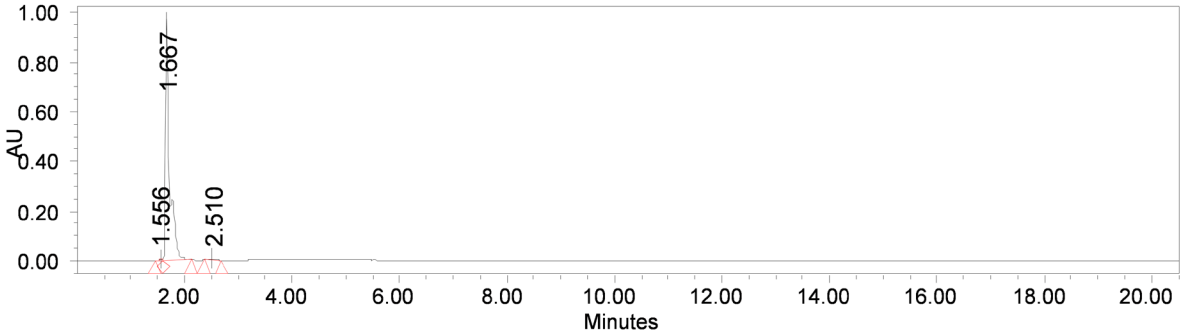
	Retention Time	Area	% Area
1	2.535	839355	4.79
2	4.858	16685134	95.21

11k



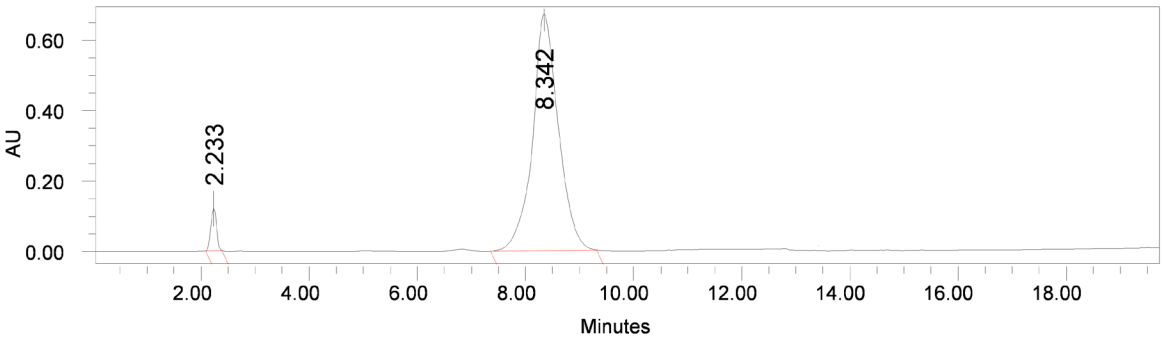
	Retention Time	Area	% Area
1	9.295	19652995	99.36
2	9.767	31767	0.16
3	10.005	37271	0.19
4	10.497	57686	0.29

11l



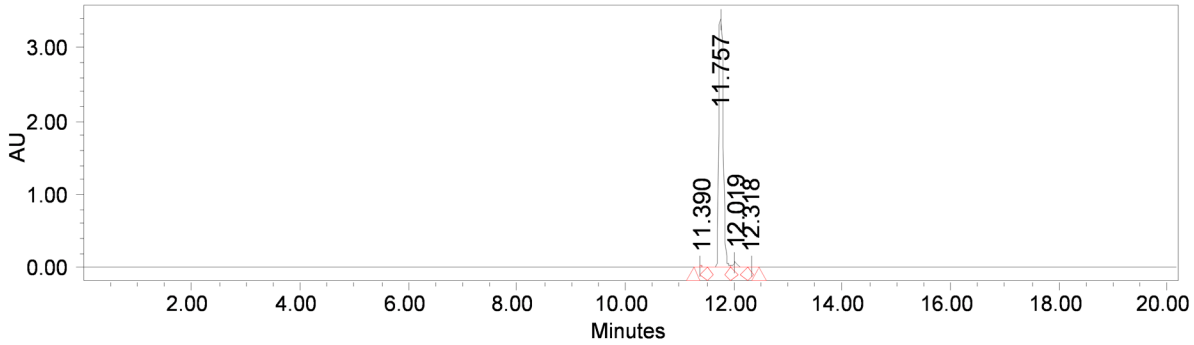
	Retention Time	Area	% Area
1	1.556	16378	0.32
2	1.667	5123519	98.98
3	2.510	36463	0.70

13a



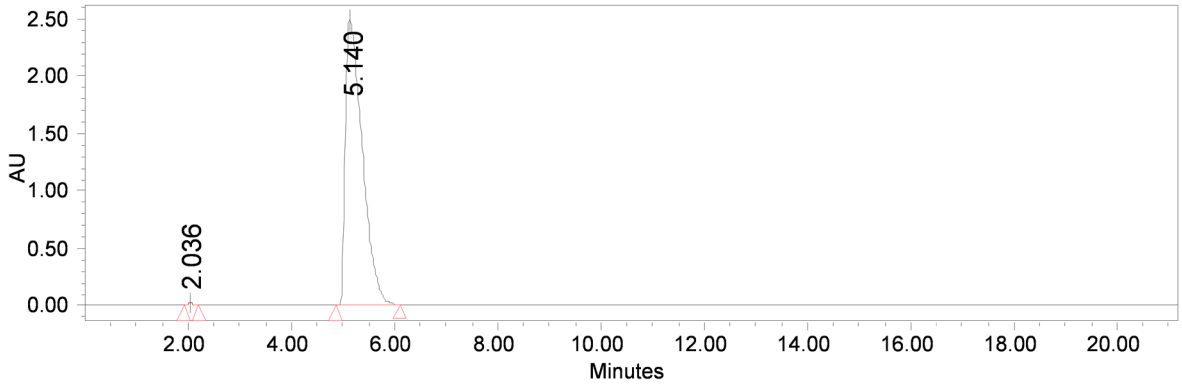
	Retention Time	Area	% Area
1	2.233	869431	3.76
2	8.342	22276794	96.24

13b



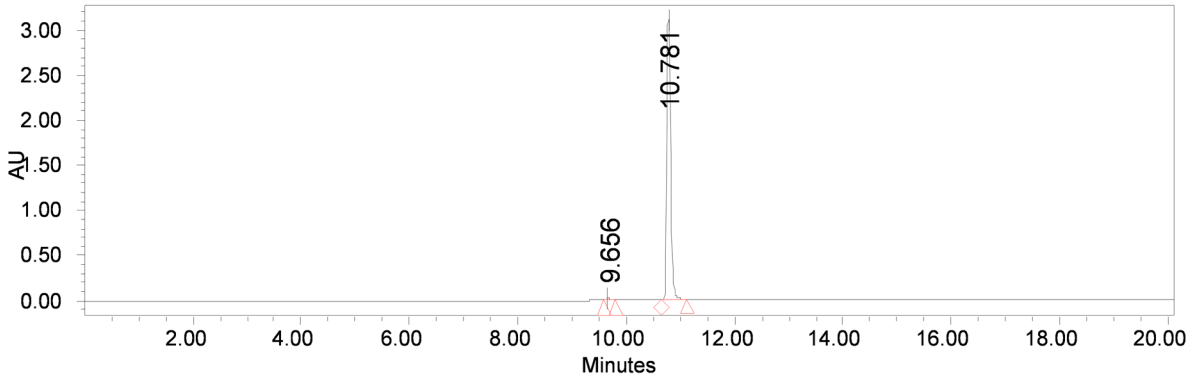
	Retention Time	Area	% Area
1	11.390	112187	0.58
2	11.757	18722426	96.96
3	12.019	416036	2.15
4	12.318	59118	0.31

13c



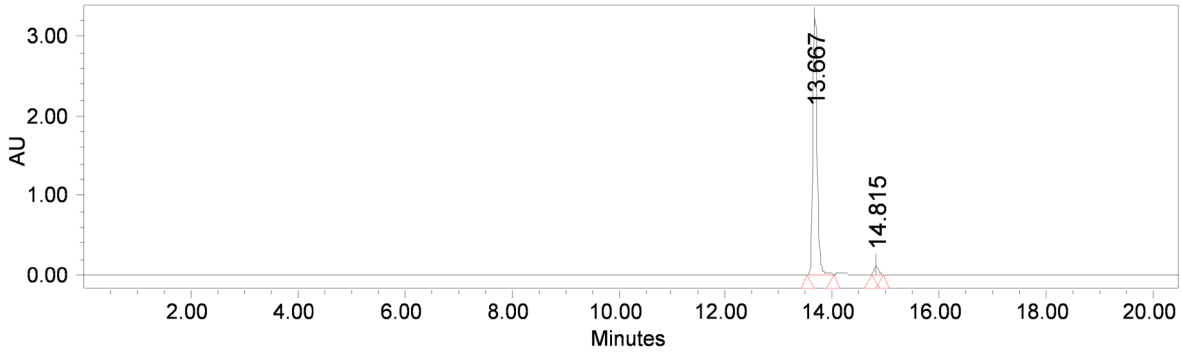
	Retention Time	Area	% Area
1	2.036	127653	0.22
2	5.140	57051847	99.78

13d



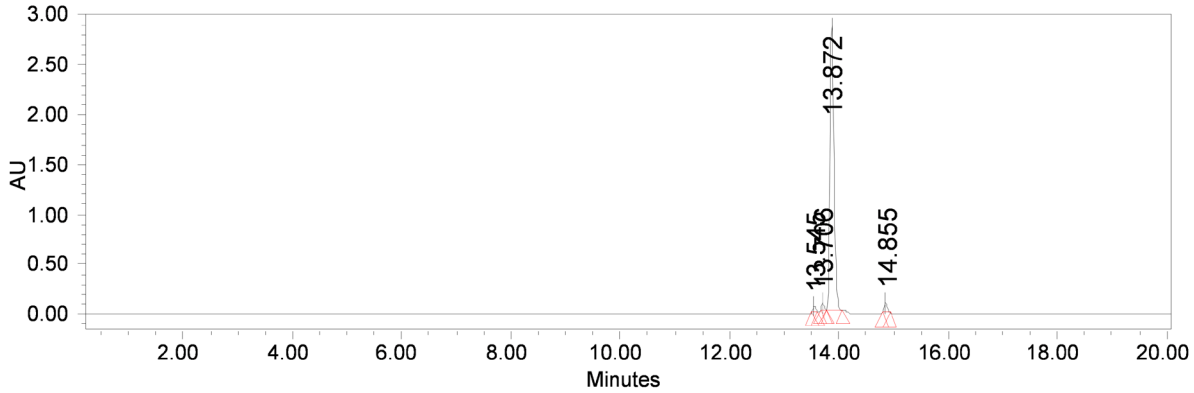
	Retention Time	Area	% Area
1	9.656	101508	0.68
2	10.781	14916758	99.32

13e



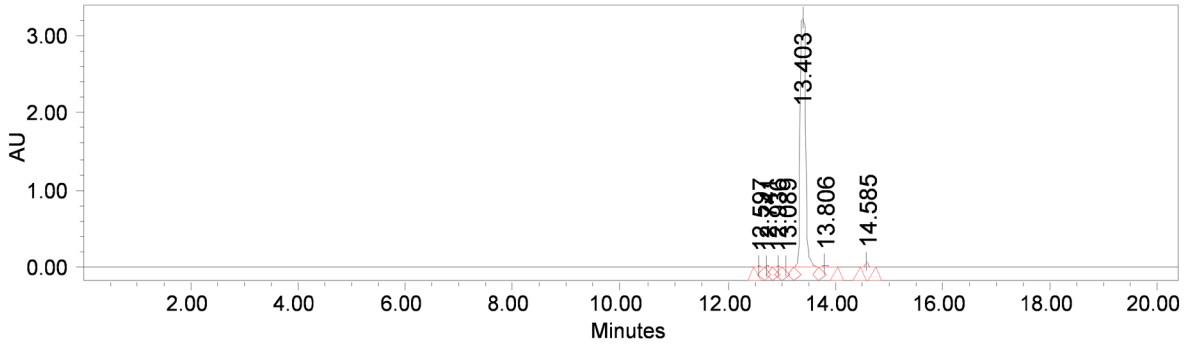
	Retention Time	Area	% Area
1	13.667	19963692	97.20
2	14.815	574610	2.80

13f



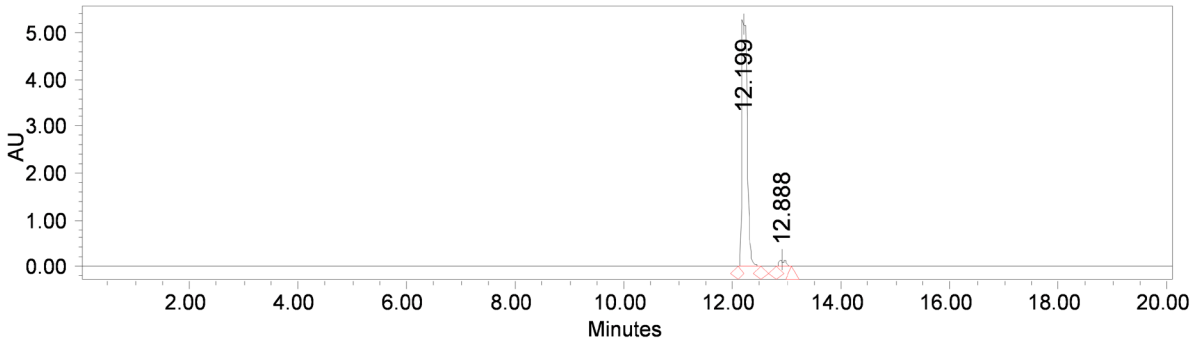
	Retention Time	Area	% Area
1	13.545	214494	1.24
2	13.706	218927	1.27
3	13.872	16440809	95.09
4	14.855	415979	2.41

13g



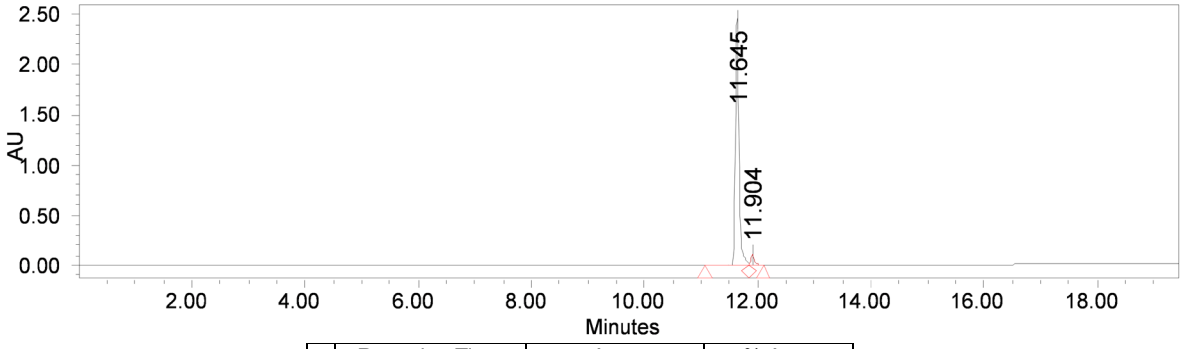
	Retention Time	Area	% Area
1	12.597	94077	0.42
2	12.741	98389	0.44
3	12.936	89595	0.40
4	13.089	73873	0.33
5	13.403	21376798	95.96
6	13.806	248740	1.12
7	14.585	295061	1.32

13h



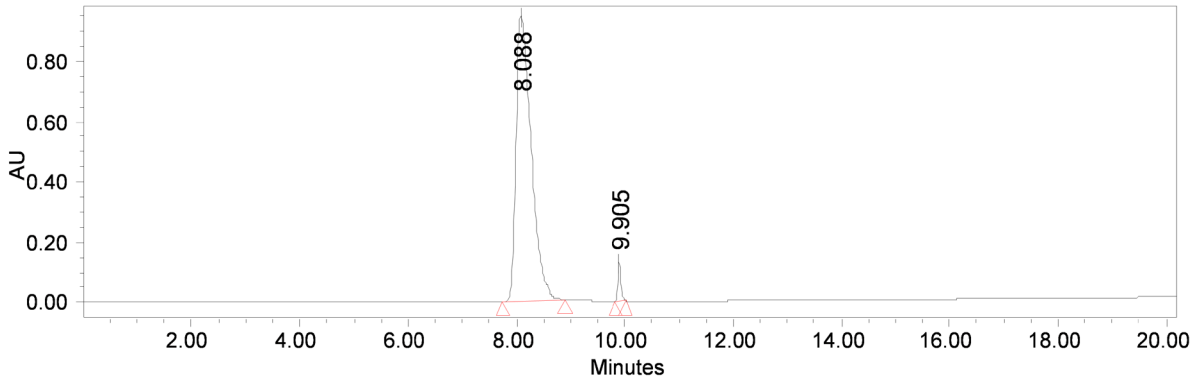
	Retention Time	Area	% Area
1	12.199	38968281	97.12
2	12.888	1154296	2.88

13i



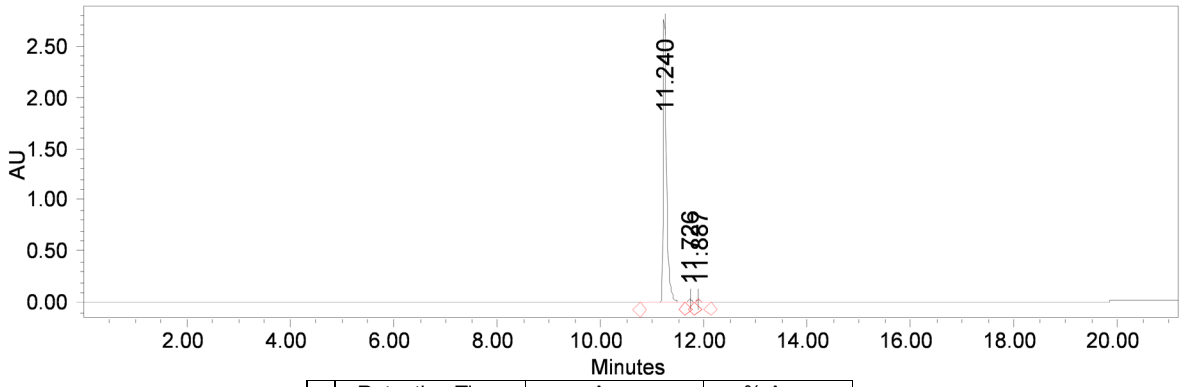
	Retention Time	Area	% Area
1	11.645	11220601	96.35
2	11.904	424542	3.65

15a



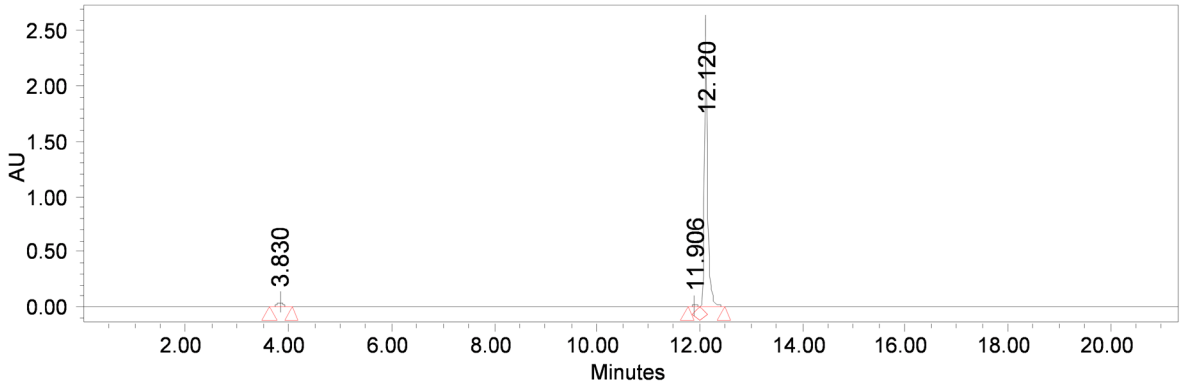
	Retention Time	Area	% Area
1	8.088	18511320	97.62
2	9.905	451821	2.38

15b



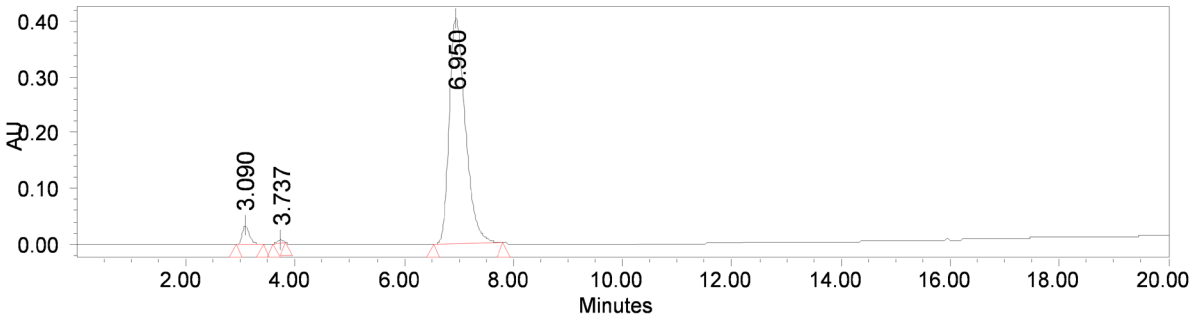
	Retention Time	Area	% Area
1	11.240	12634056	96.84
2	11.726	214509	1.64
3	11.887	197865	1.52

15c



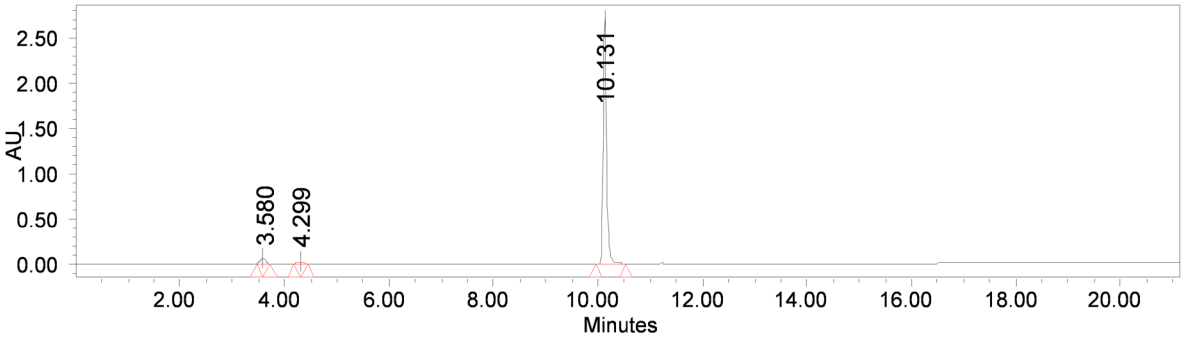
	Retention Time	Area	% Area	Height
1	3.830	375477	3.03	43104
2	11.906	102377	0.83	15456
3	12.120	11912150	96.14	2554777

15d



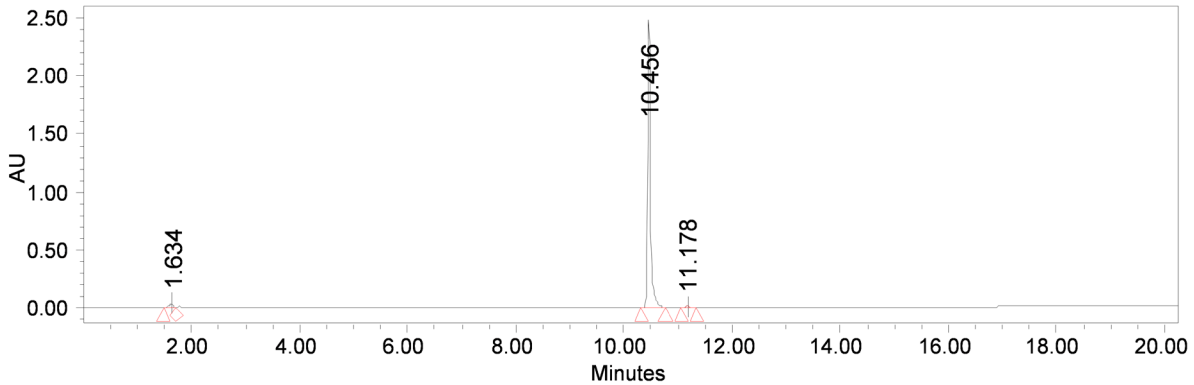
	Retention Time	Area	% Area
1	3.090	313111	3.58
2	3.737	48462	0.55
3	6.950	8372437	95.86

15e



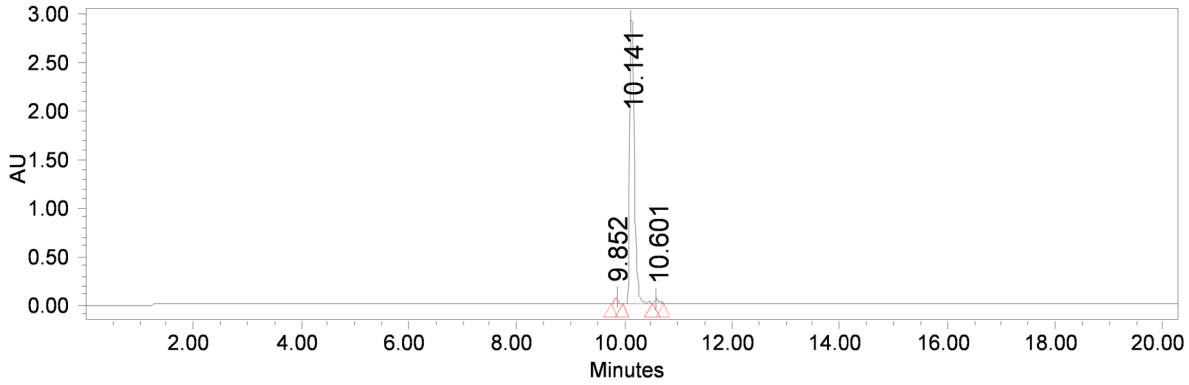
	Retention Time	Area	% Area
1	3.580	417805	3.26
2	4.299	181580	1.42
3	10.131	12203930	95.32

15f



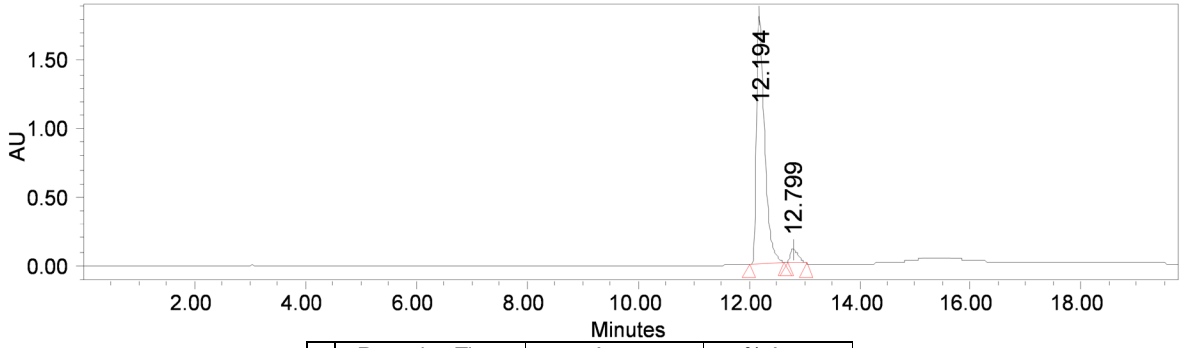
	Retention Time	Area	% Area
1	1.634	243816	2.42
2	10.456	9779345	96.86
3	11.178	72697	0.72

15g



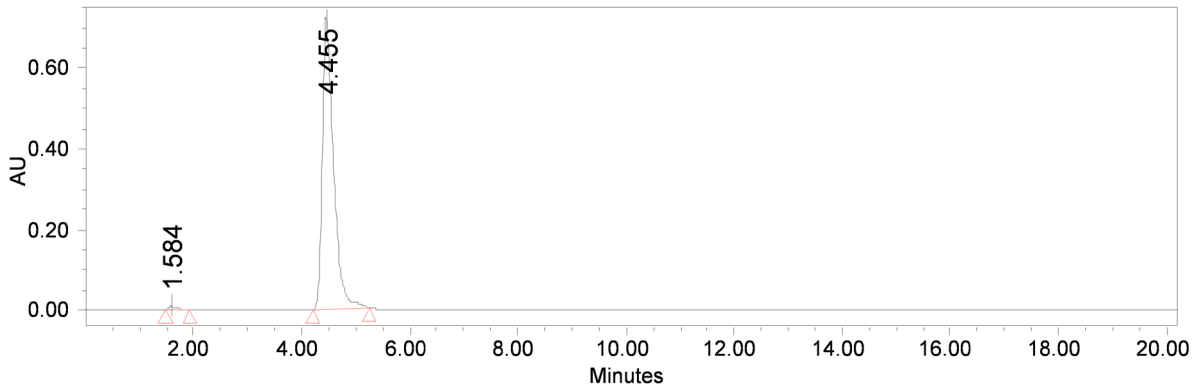
	Retention Time	Area	% Area
1	9.852	270258	1.62
2	10.141	16244973	97.23
3	10.601	192267	1.15

15h



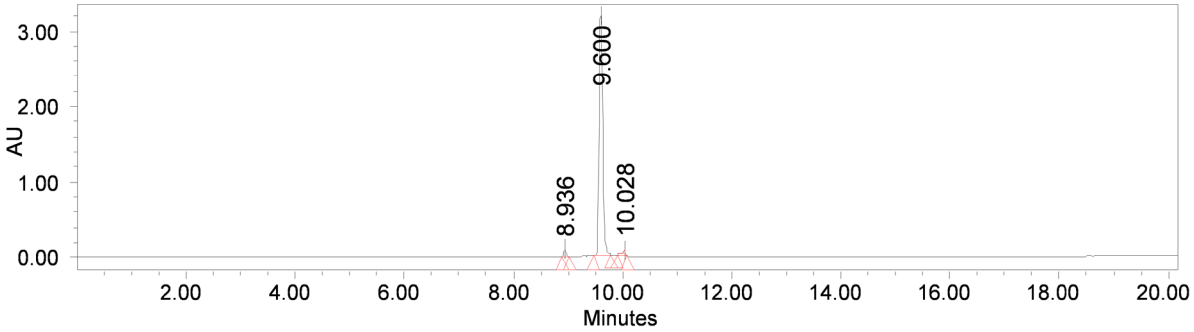
	Retention Time	Area	% Area
1	11.390	112187	0.58
2	11.757	18722426	96.96
3	12.019	416036	2.15
4	12.318	59118	0.31

15i



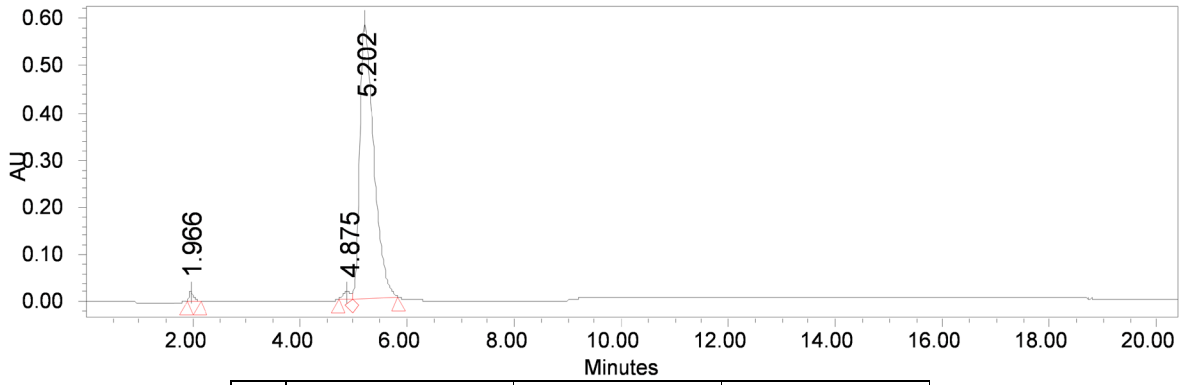
	Retention Time	Area	% Area
1	1.584	71417	0.68
2	4.455	10367309	99.32

15j



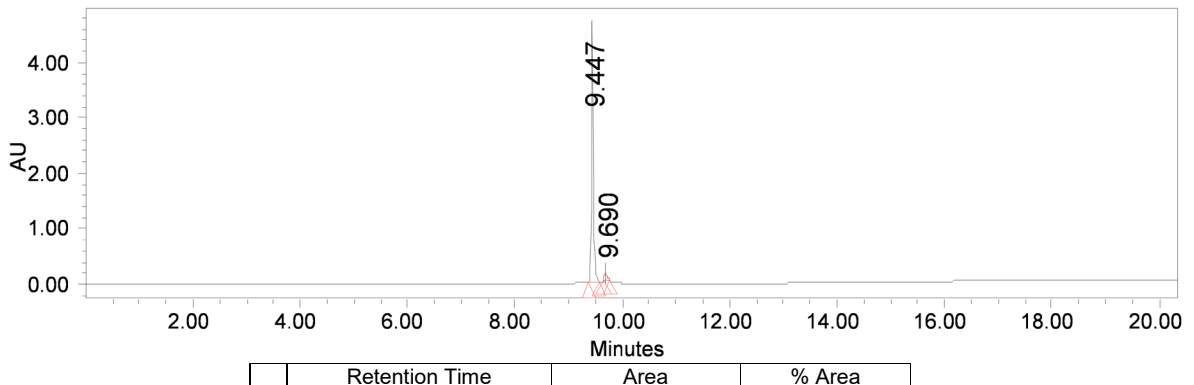
	Retention Time	Area	% Area
1	8.936	326138	2.11
2	9.600	14789970	95.50
3	10.028	370792	2.39

15k



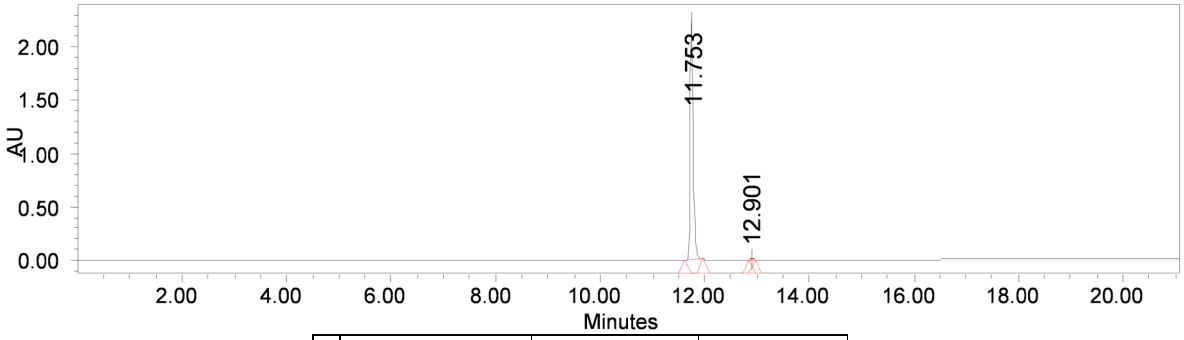
	Retention Time	Area	% Area
1	1.966	111379	1.02
2	4.875	143322	1.31
3	5.202	10717974	97.68

15l



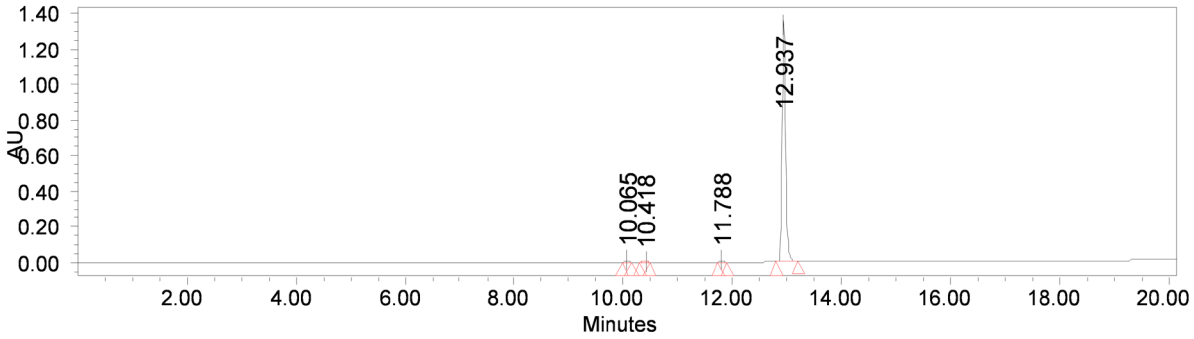
	Retention Time	Area	% Area
1	9.447	13258947	96.58
2	9.690	469080	3.42

15m



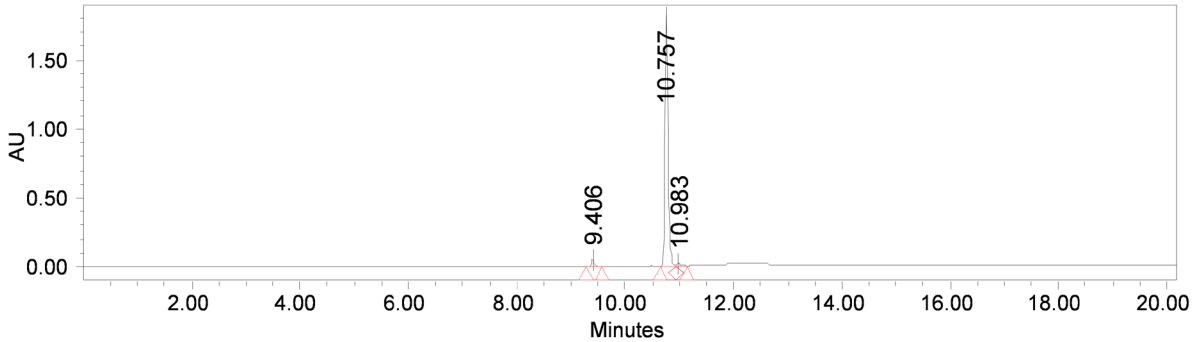
	Retention Time	Area	% Area
1	11.753	9597354	99.59
2	12.901	39144	0.41

17a



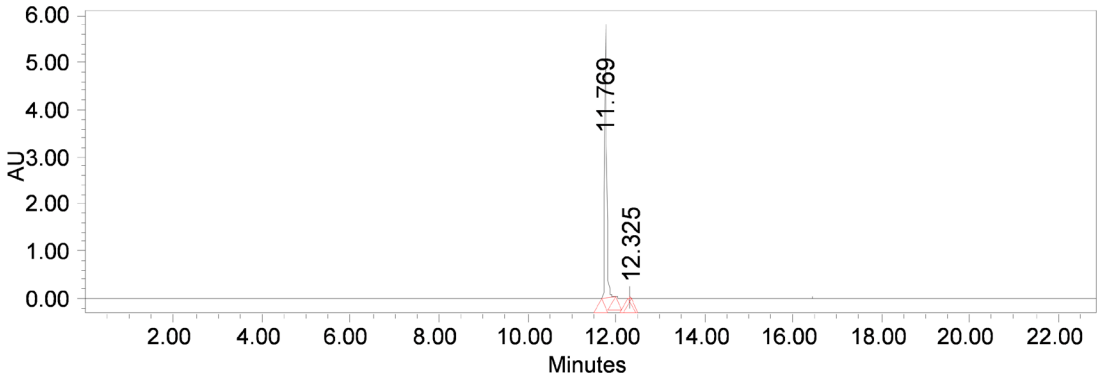
	Retention Time	Area	% Area
1	10.065	49465	0.79
2	10.418	25352	0.41
3	11.788	38115	0.61
4	12.937	6114601	98.19

17b



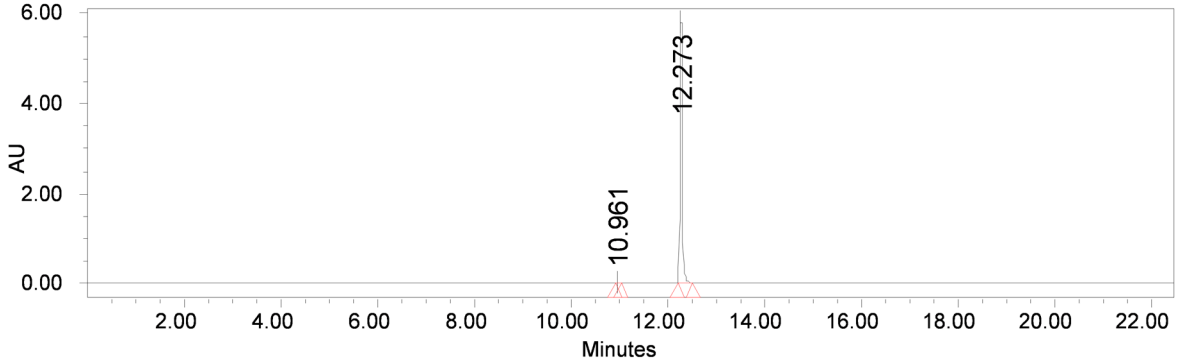
	Retention Time	Area	% Area
1	9.406	181285	2.58
2	10.757	6754467	96.19
3	10.983	86195	1.23

17c



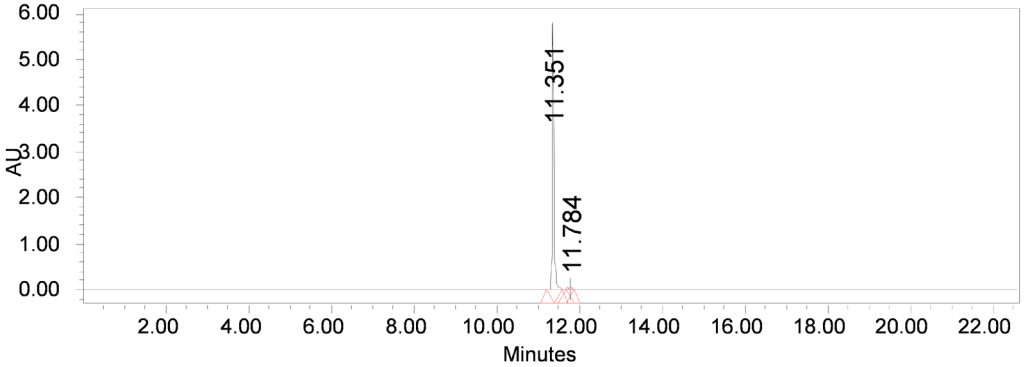
	Retention Time	Area	% Area
1	11.769	15572120	99.89
2	12.325	16859	0.11

17d



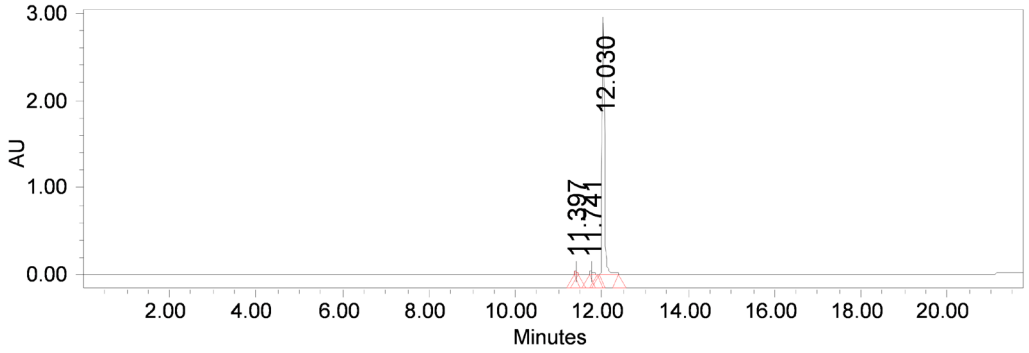
	Retention Time	Area	% Area
1	10.961	73329	0.42
2	12.273	17334002	99.58

17e



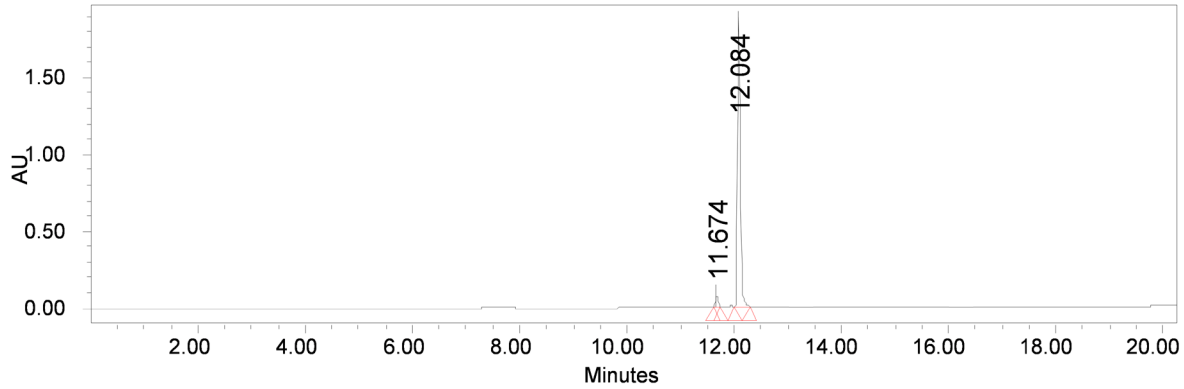
	Retention Time	Area	% Area
1	11.351	14272533	98.88
2	11.784	162317	1.12

17f



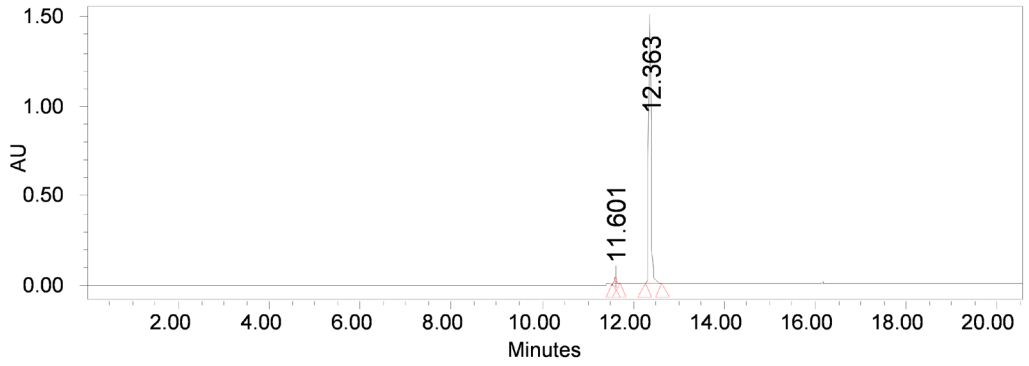
	Retention Time	Area	% Area
1	11.397	112987	1.08
2	11.741	184288	1.76
3	12.030	10155499	97.16

17g



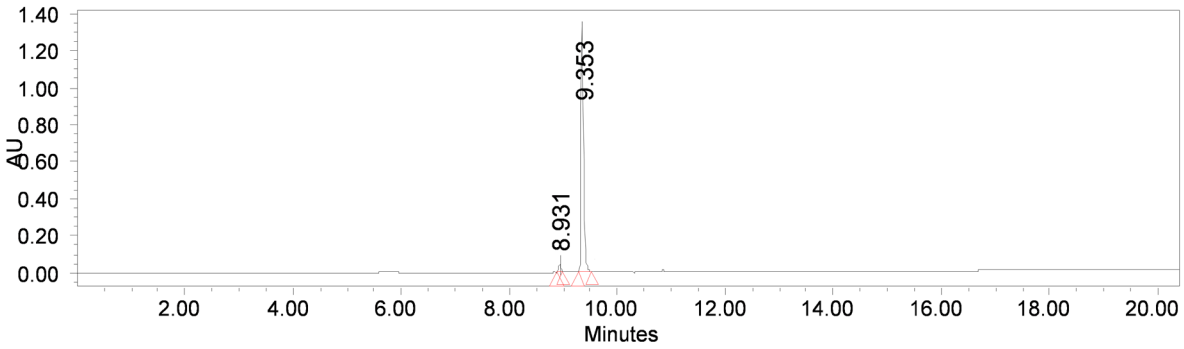
	Retention Time	Area	% Area
1	11.674	246370	3.73
2	12.084	6362942	96.27

17h



	Retention Time	Area	% Area
1	11.601	135485	2.45
2	12.363	5398484	97.55

22



	Retention Time	Area	% Area
1	8.931	109273	2.24
2	9.353	4758872	97.76

References

1. Kenakin, T. P. Chapter 6 - Enzymes as Drug Targets. In *Pharmacology in Drug Discovery*, Kenakin, T. P., Ed. Academic Press: Boston, 2012; pp 105-124.