Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Glycal mediated synthesis of piperidine alkaloids: fagomine, 4-*epi*-fagomine, 2-deoxynojirimycin and an advanced intermediate, iminoglycal

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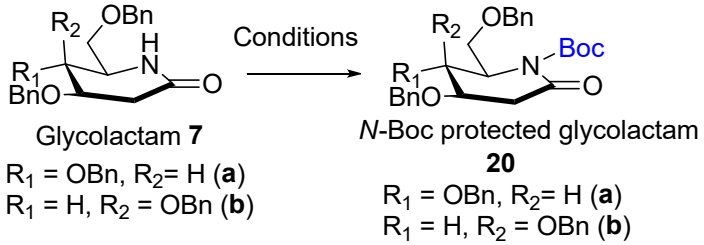
Table 1. Attempt for *N*-protection of 2-deoxyglycolactam.

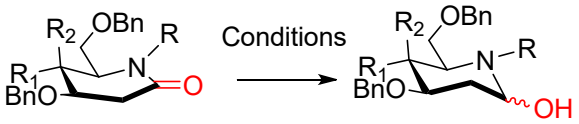


Glycolactam **7**
R_1 = OBn, R_2= H (**a**)
R_1 = H, R_2 = OBn (**b**)

N-Boc protected glycolactam **20**
R_1 = OBn, R_2= H (**a**)
R_1 = H, R_2 = OBn (**b**)

Entry	Reagents and condition	Remark
1	Boc_2O, Py, DMAP, rt	Sm recovered
2	Boc_2O, $NaHCO_3$, H_2O -THF, rt	Sm recovered
3	Boc_2O, CH_3CN, NEt_3, DMAP (cat)	Sm recovered
4	Boc_2O, DCM, NEt_3, DMAP (cat), 0 ºC then rt	**2-deoxygluconolactam-*N*-Boc (20a) 95%** **2-deoxygalactonolactam-*N*-Boc (20b) 79%**

Table 2. Conditions for partial reduction of 2-deoxyglycolactams **7a/b** and 2-deoxyglycolactam-*N*-Boc **20a/b**.

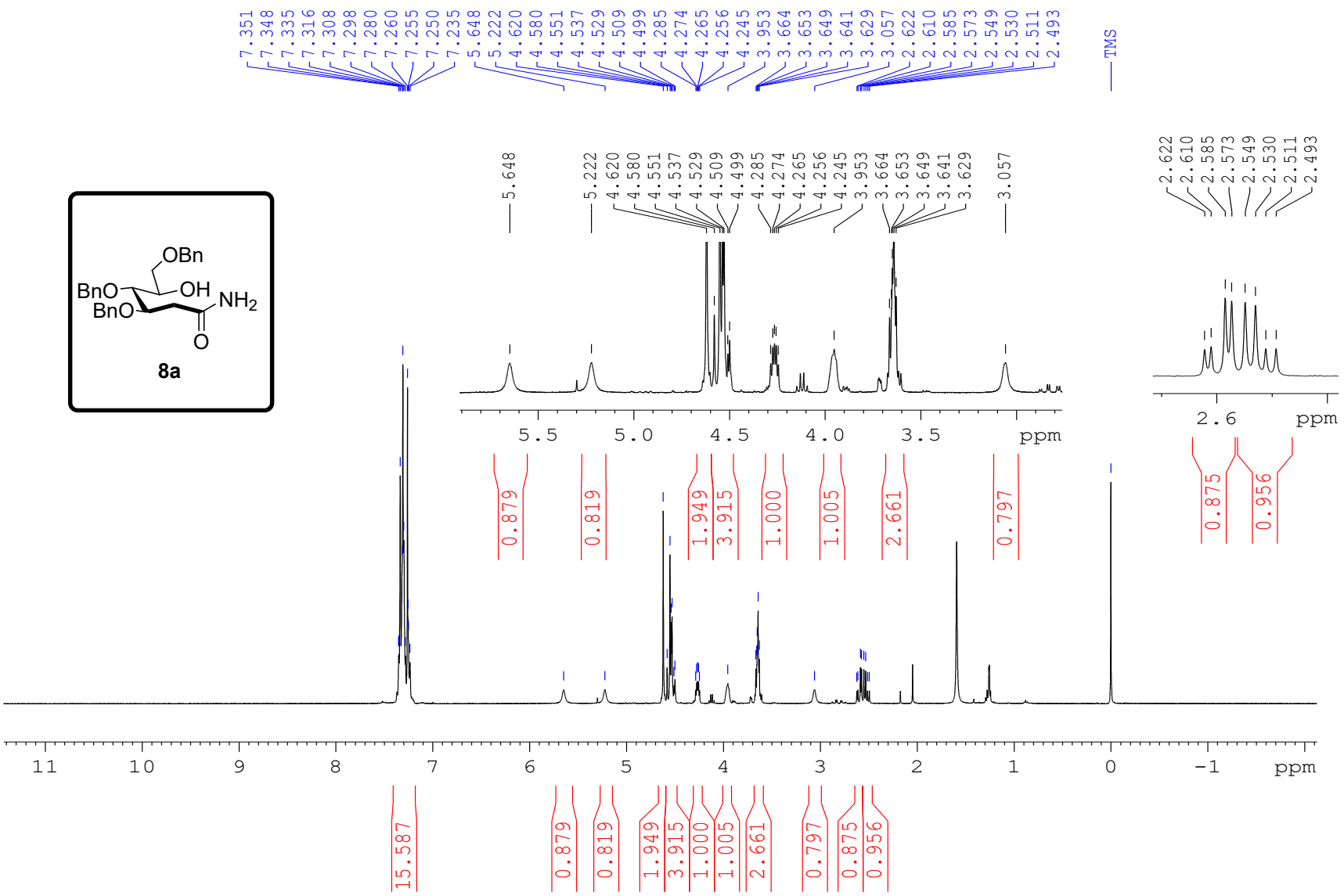


R=H
2-deoxyglycolactam **7a/b**
R=Boc
2-deoxyglycolactam-*N*-Boc **20a/b**

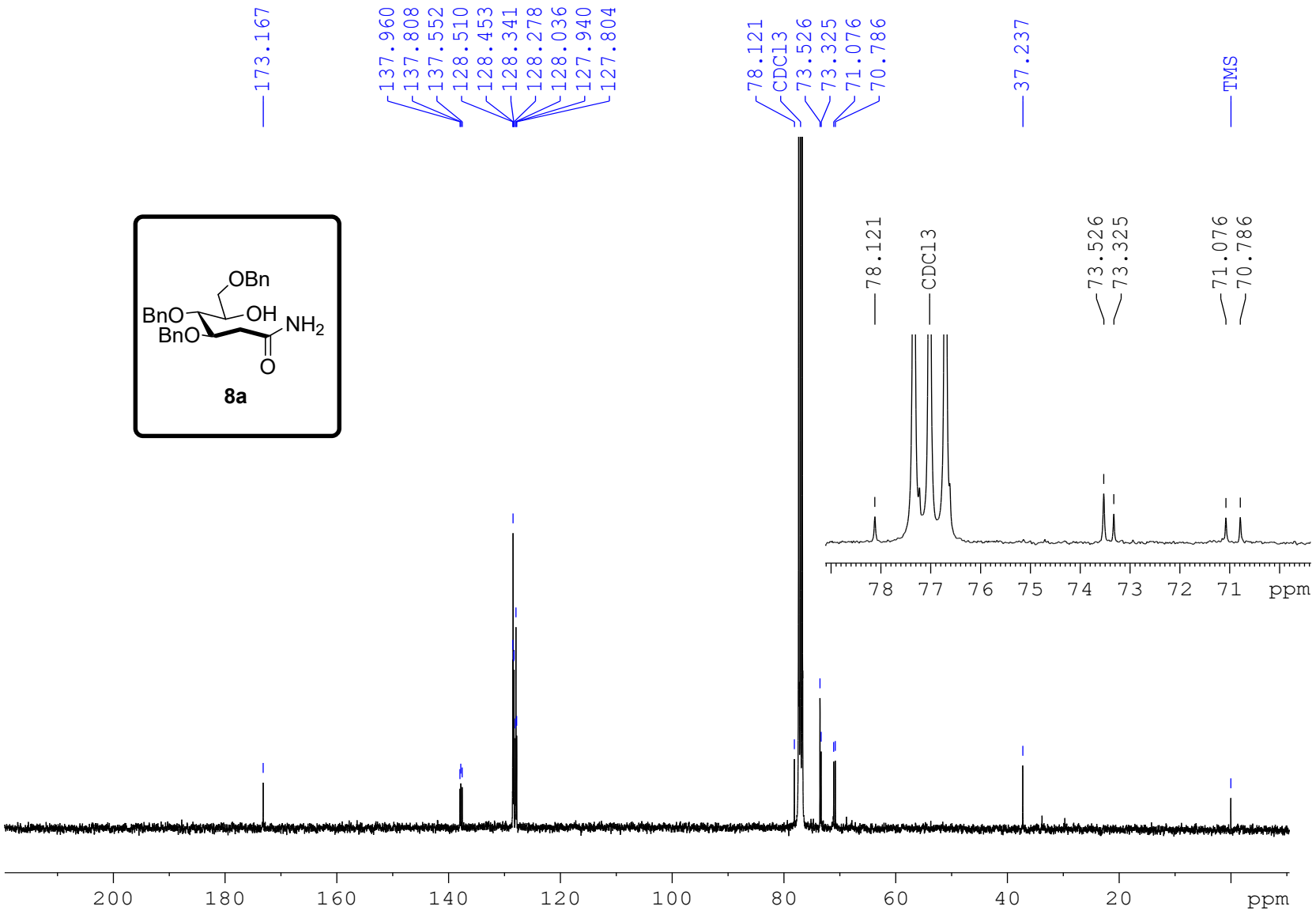
R_1 = OBn, R_2 = H (**a**)
R_1 = H, R_2 = OBn (**b**)

Entry	Reagents and condition	Remark
1	$NaBH_4$, MeOH, 0 ºC	Sm recovered
2	$NaBH_4$, MeOH, 0 ºC, then rt	Sm recovered
3	$NaBH_4$, THF-MeOH, 0 ºC, then rt	Sm recovered
4	$NaBH_4$, THF-MeOH, rt	Sm recovered

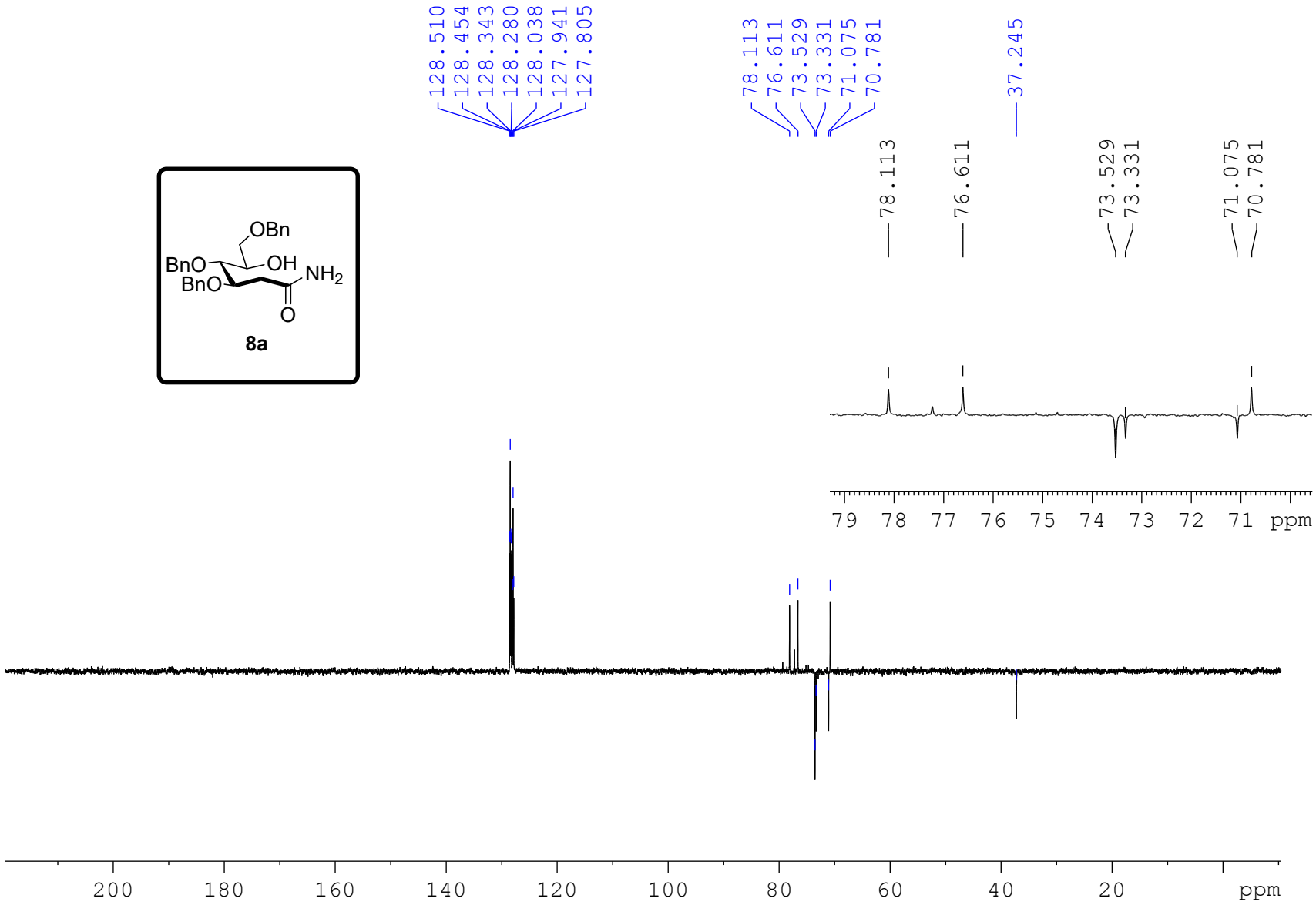
^{1}H NMR of **8a** (400 MHz, $CDCl_3$)



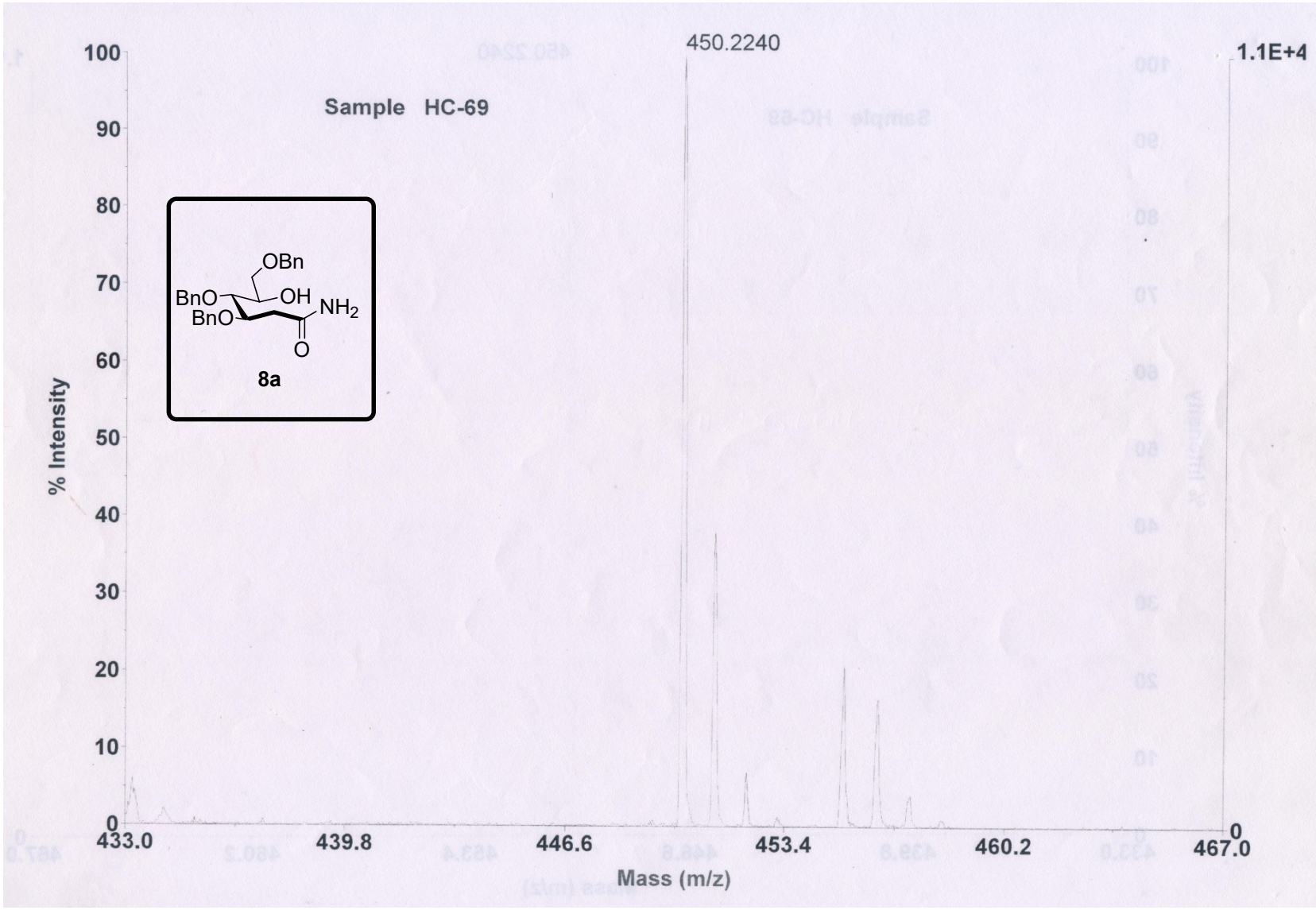
^{13}C NMR of **8a** (100 MHz, $CDCl_3$)



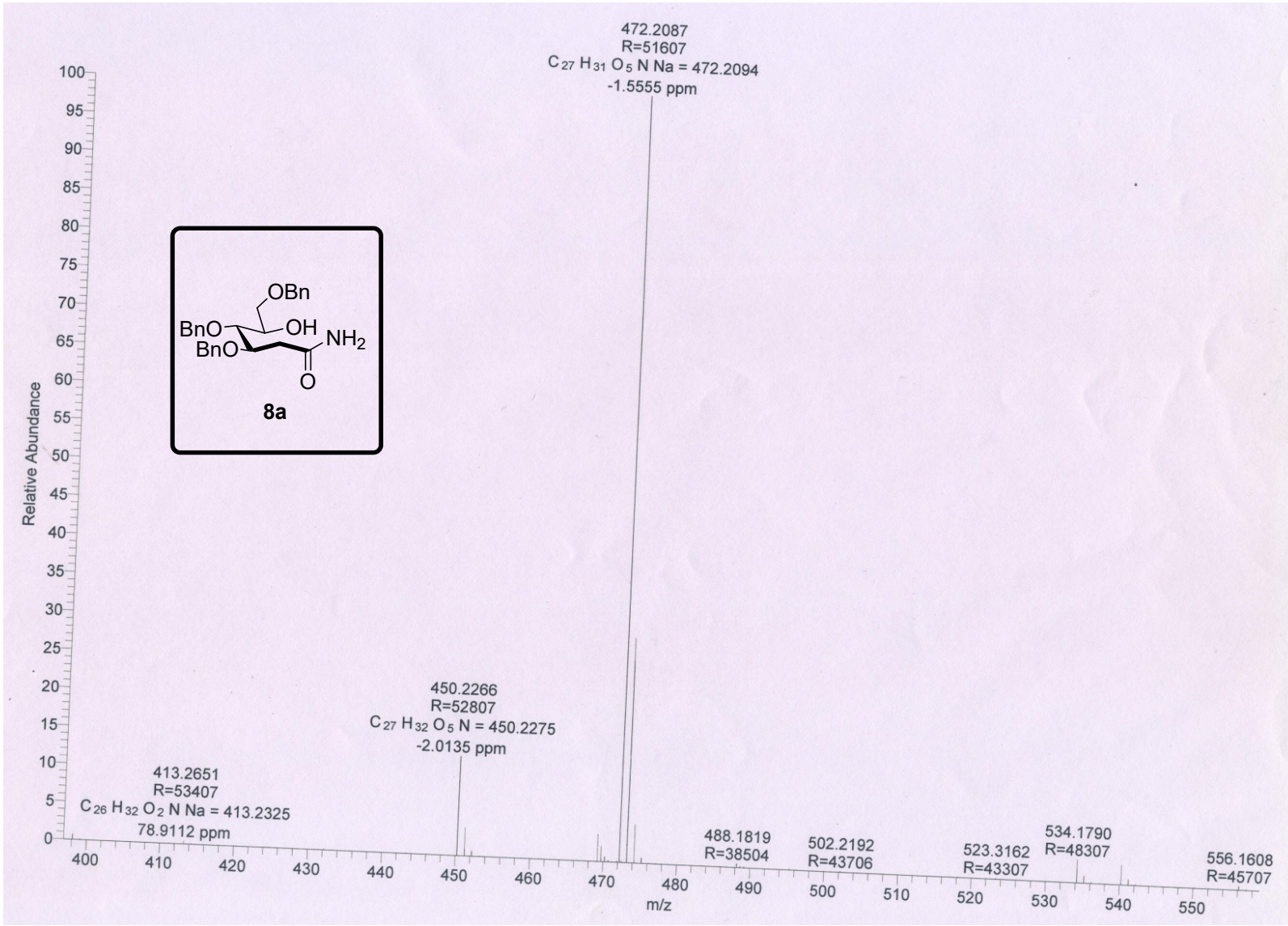
DEPT of **8a** (100 MHz, $CDCl_3$)



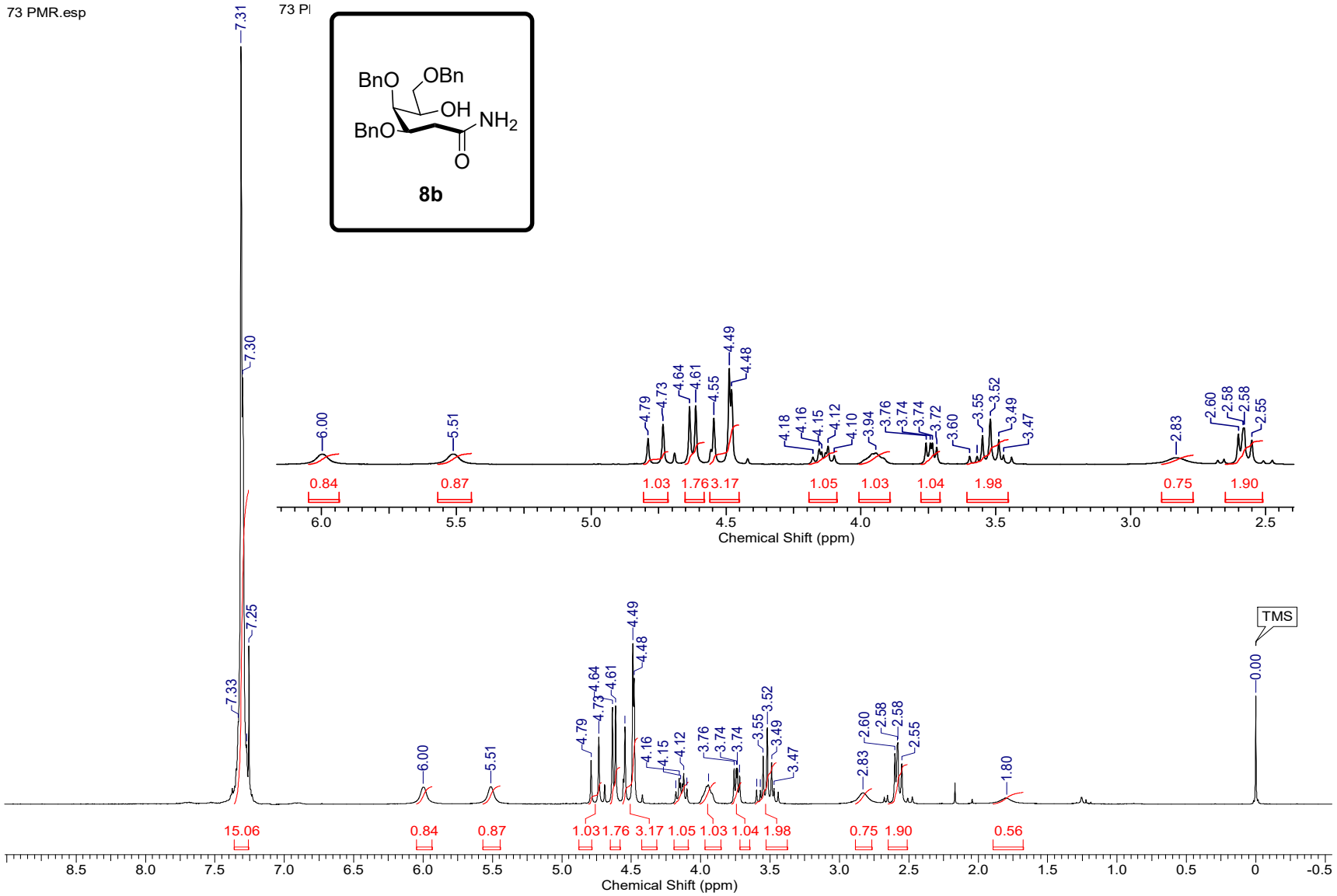
ESI-MS of **8a**


Sample HC-69
450.2240
1.1E+4
% Intensity
Mass (m/z)
100
90
80
70
60
50
40
30
20
10
0
433.0
439.8
446.6
453.4
460.2
467.0
OBn
BnO
OH
NH2
BnO
O
8a

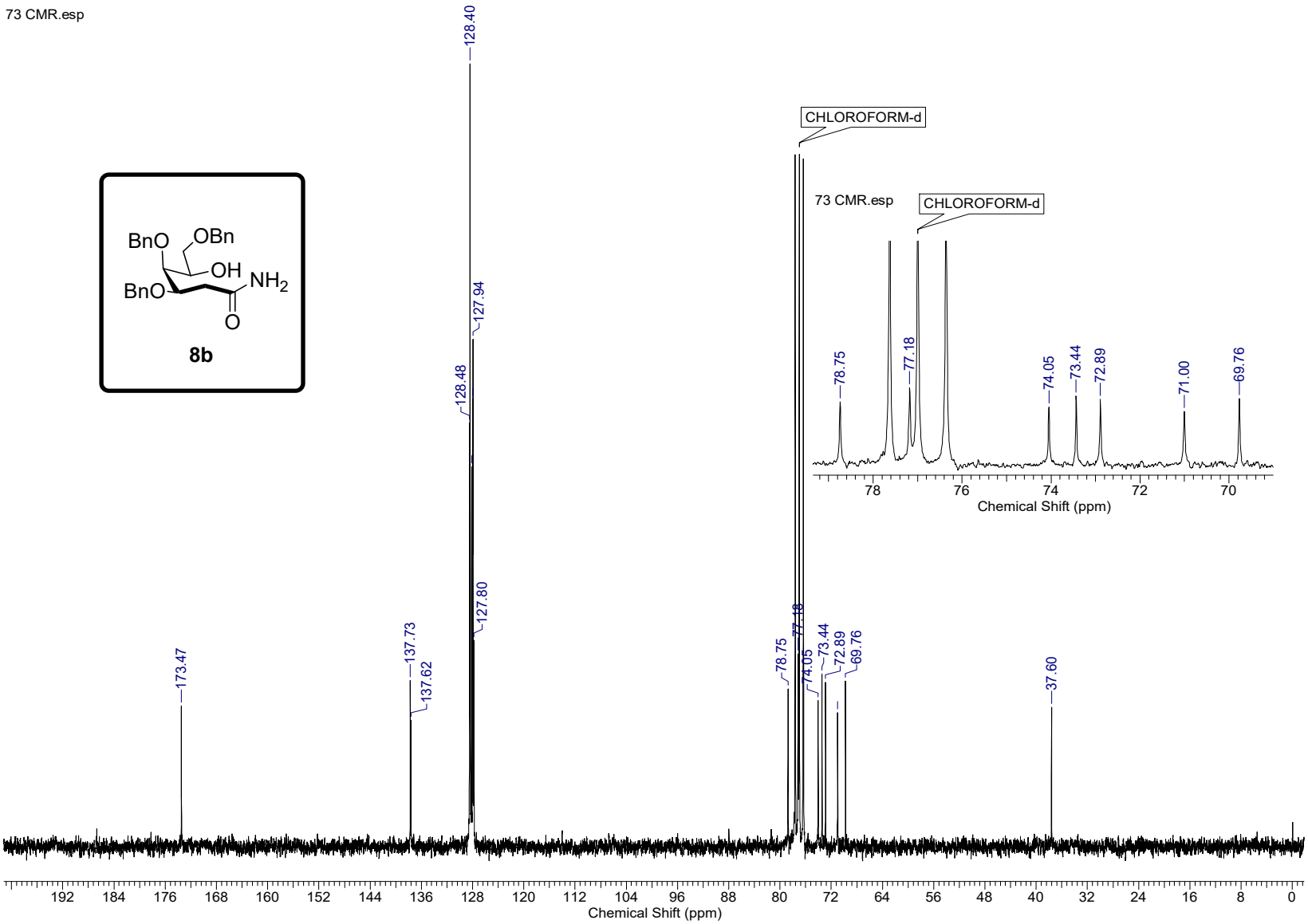
HRMS (ESI) of **8a**



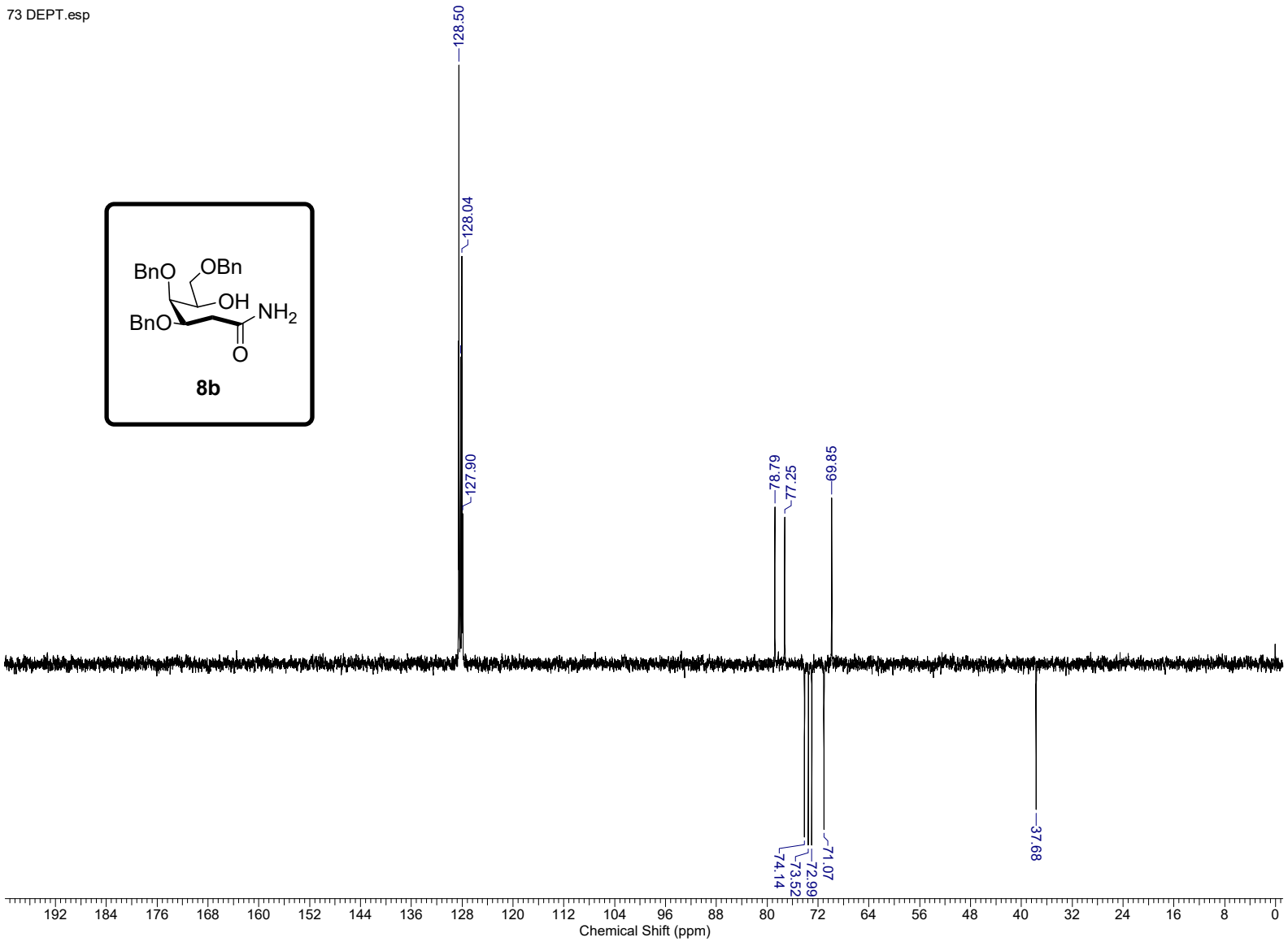
^{1}H NMR of **8b** (400 MHz, $CDCl_3$)



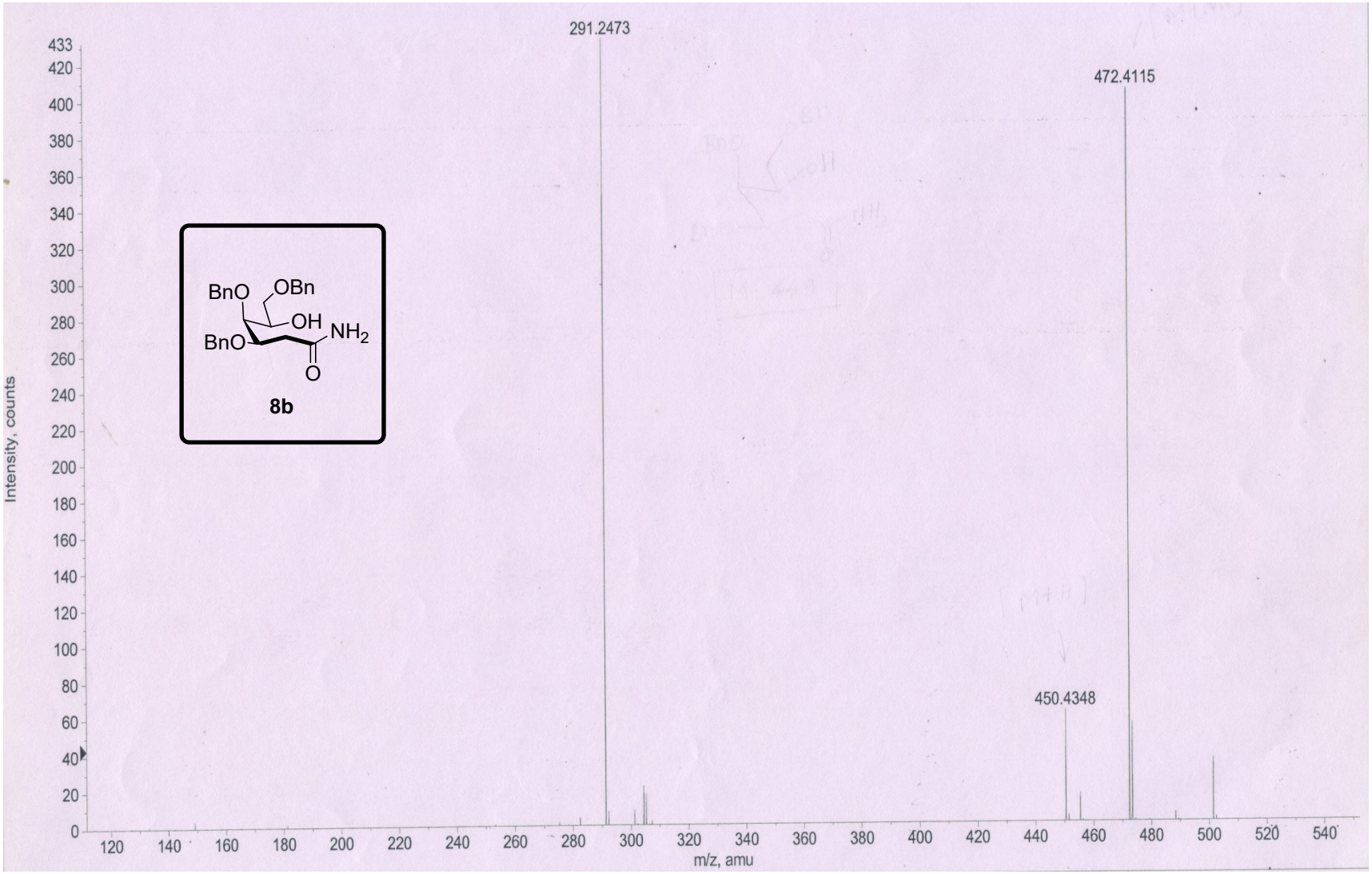
^{13}C NMR of **8b** (50 MHz, $CDCl_3$)



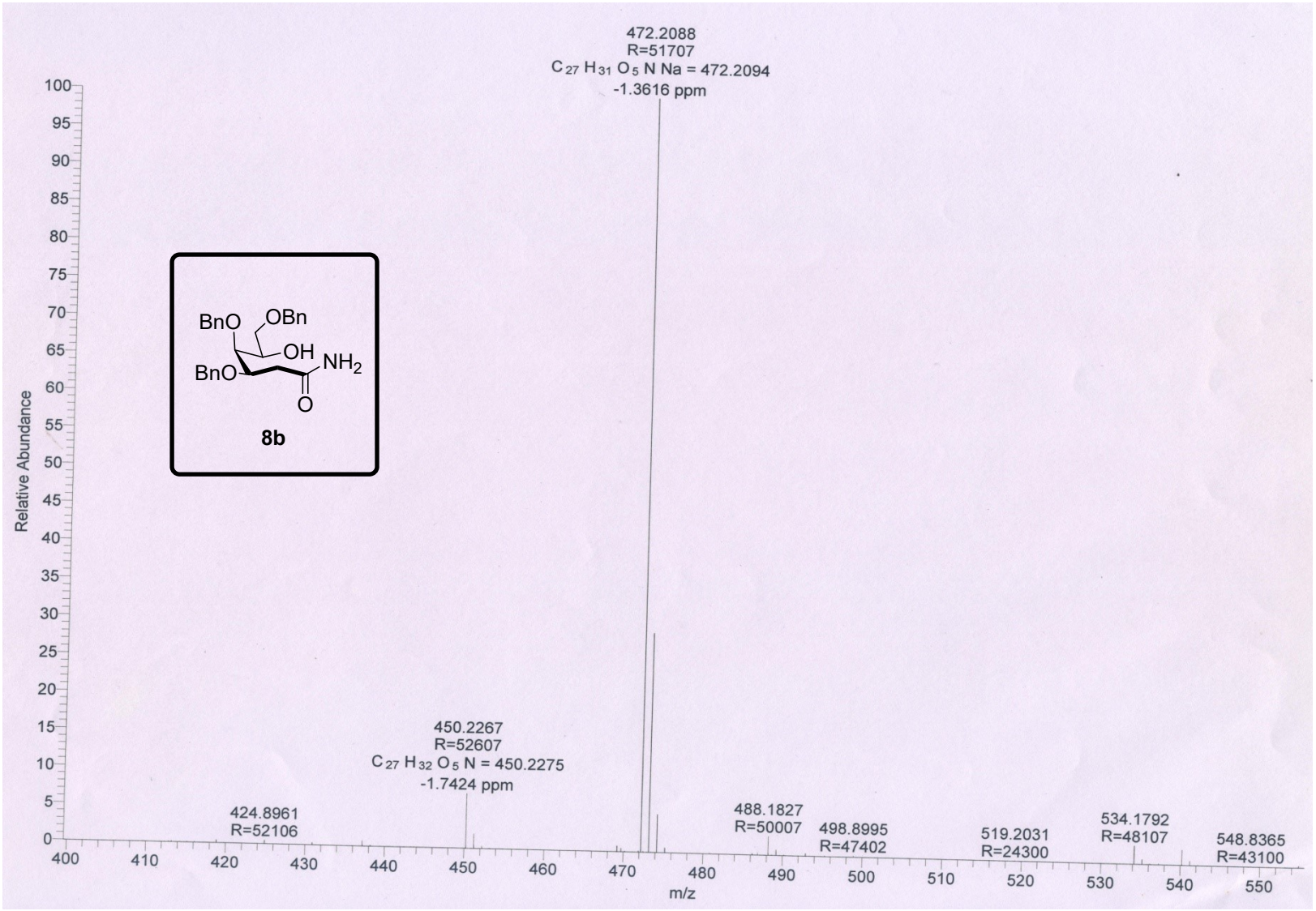
DEPT of **8b** (50 MHz, $CDCl_3$)



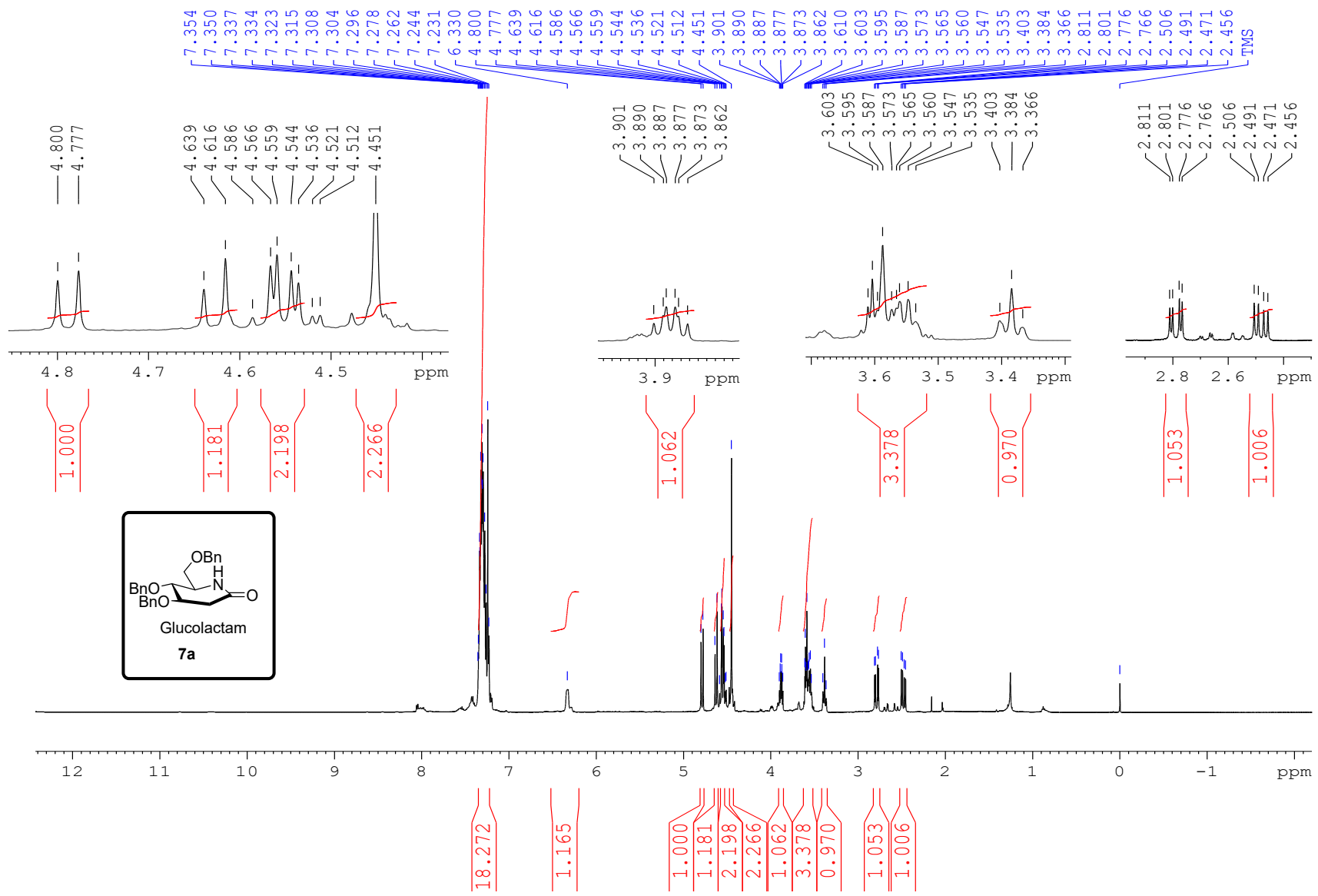
ESI-MS of **8b**


291.2473
472.4115
450.4348
BnO
OBn
OH
NH2
BnO
O
8b
Intensity, counts
m/z, amu

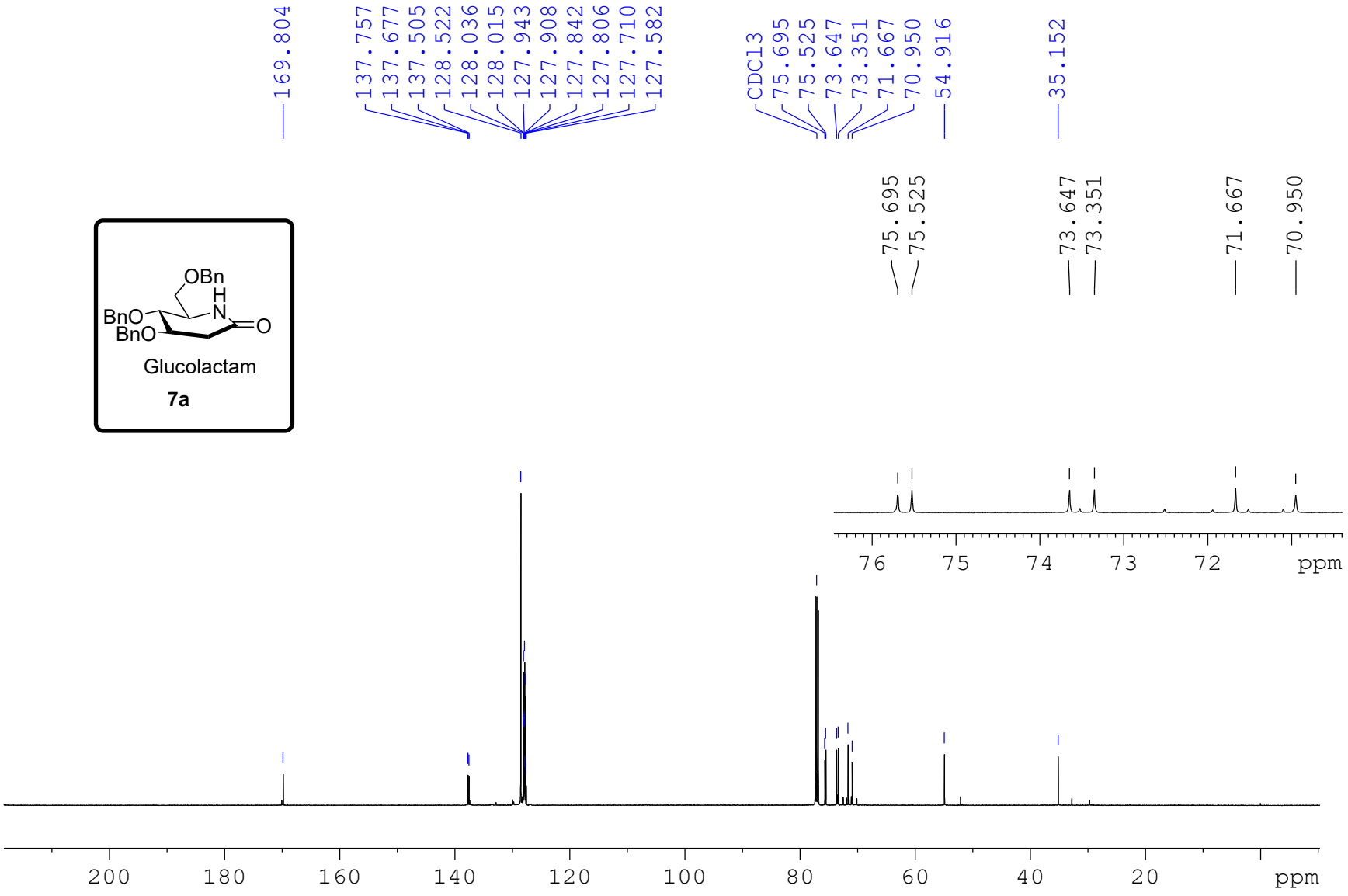
HRMS (ESI) of **8b**



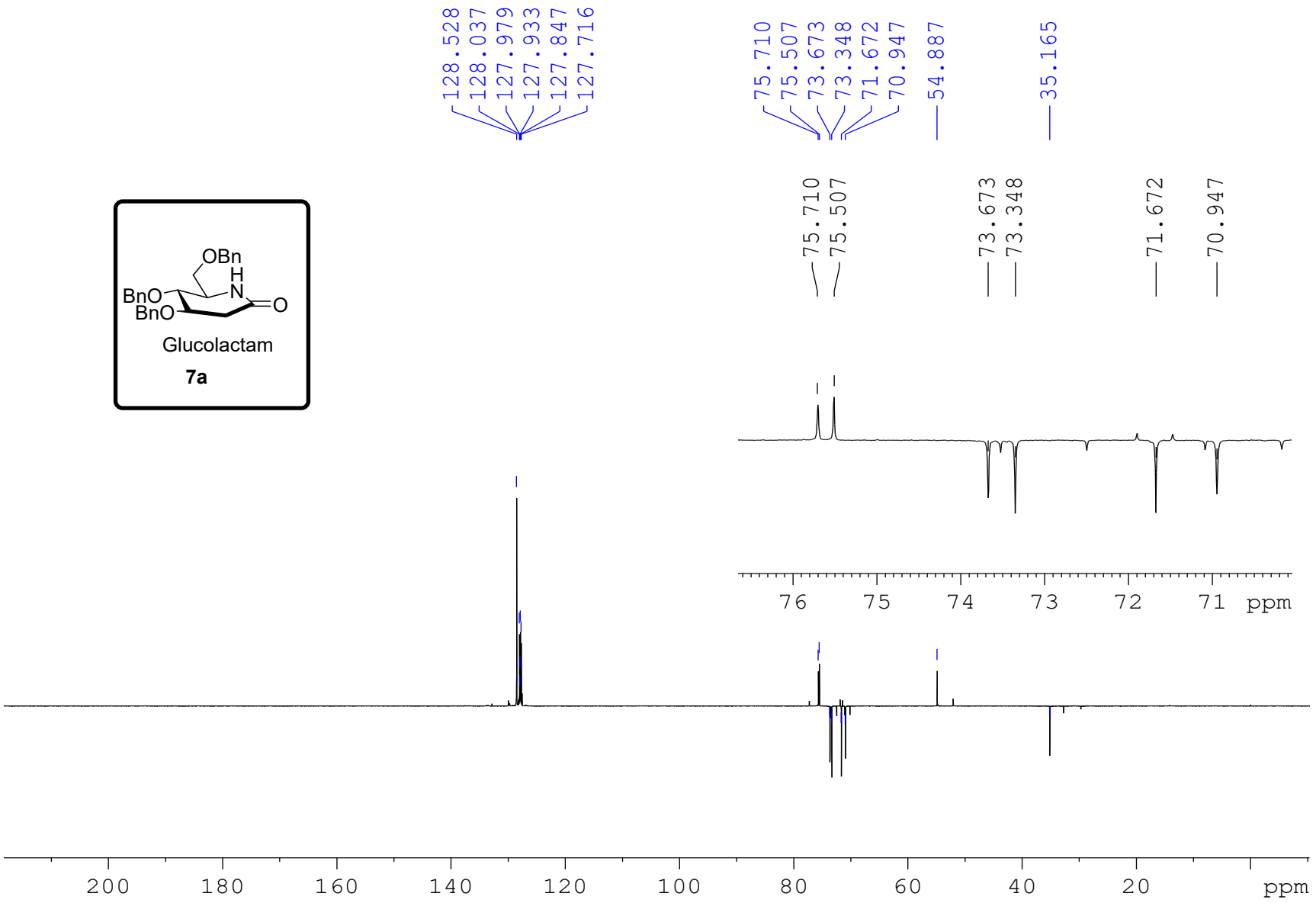
^{1}H NMR of **7a** (500MHz, $CDCl_3$)



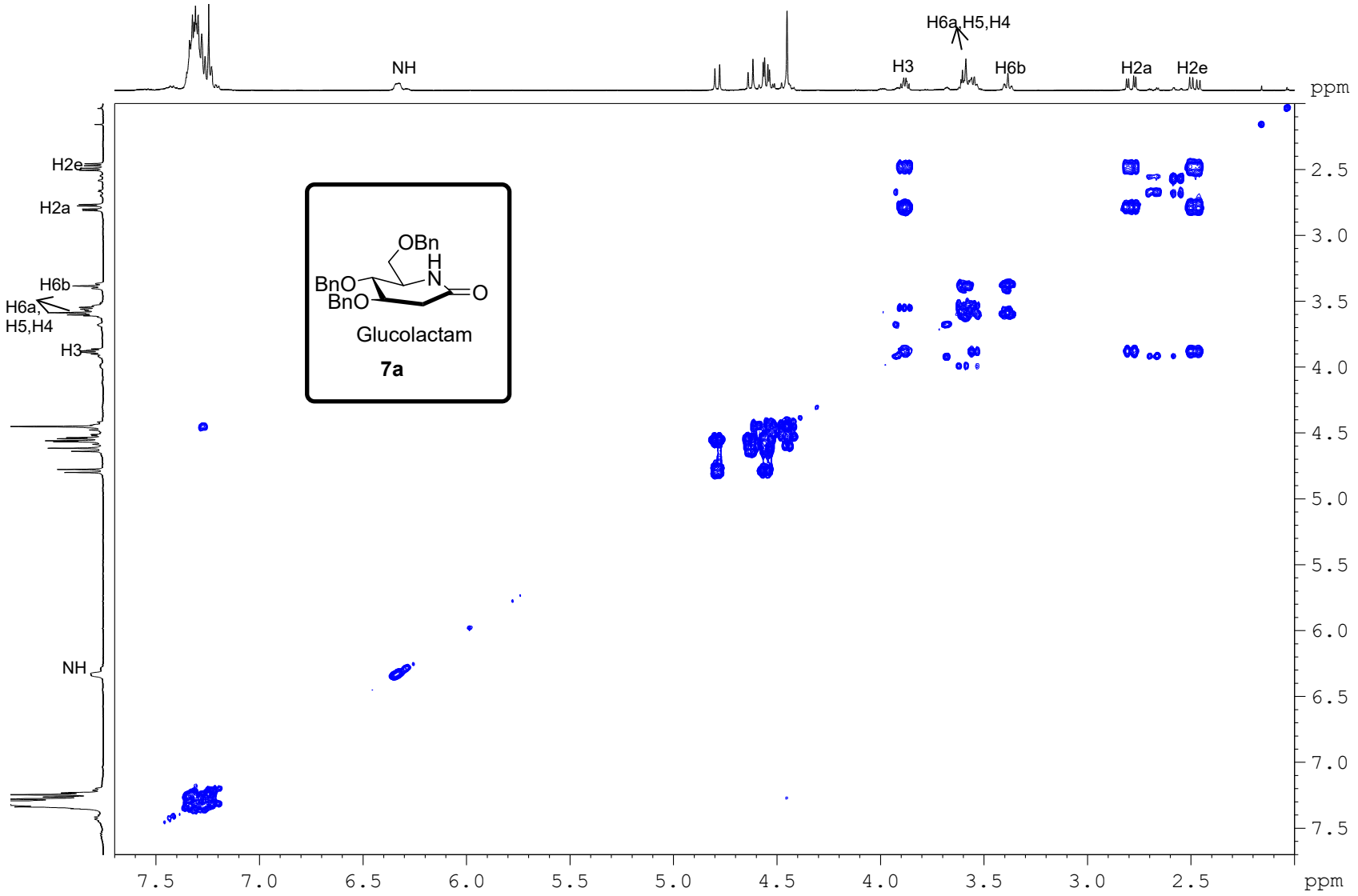
^{13}C NMR of **7a** (125MHz, $CDCl_3$)



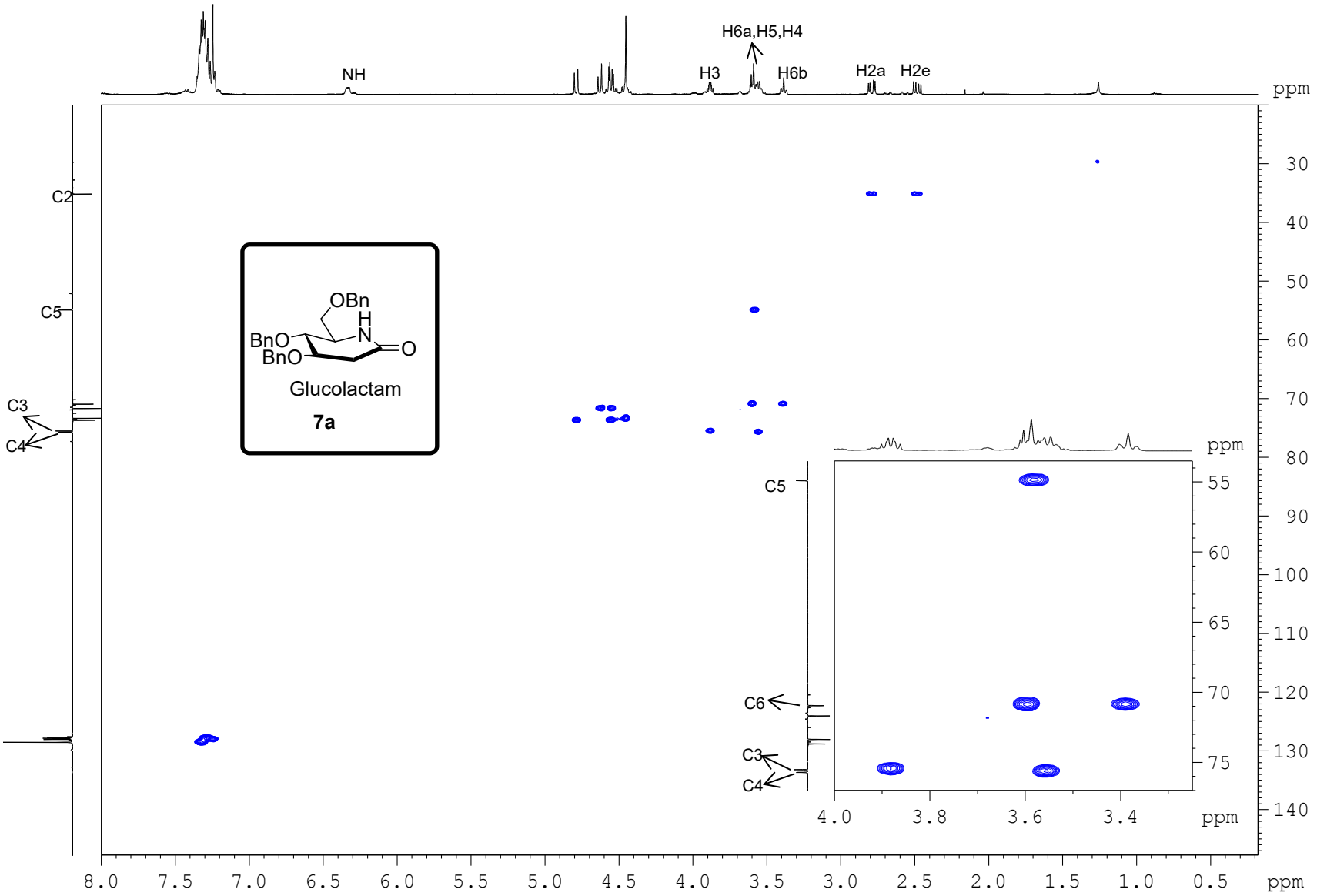
DEPT of **7a** (100MHz, $CDCl_3$)



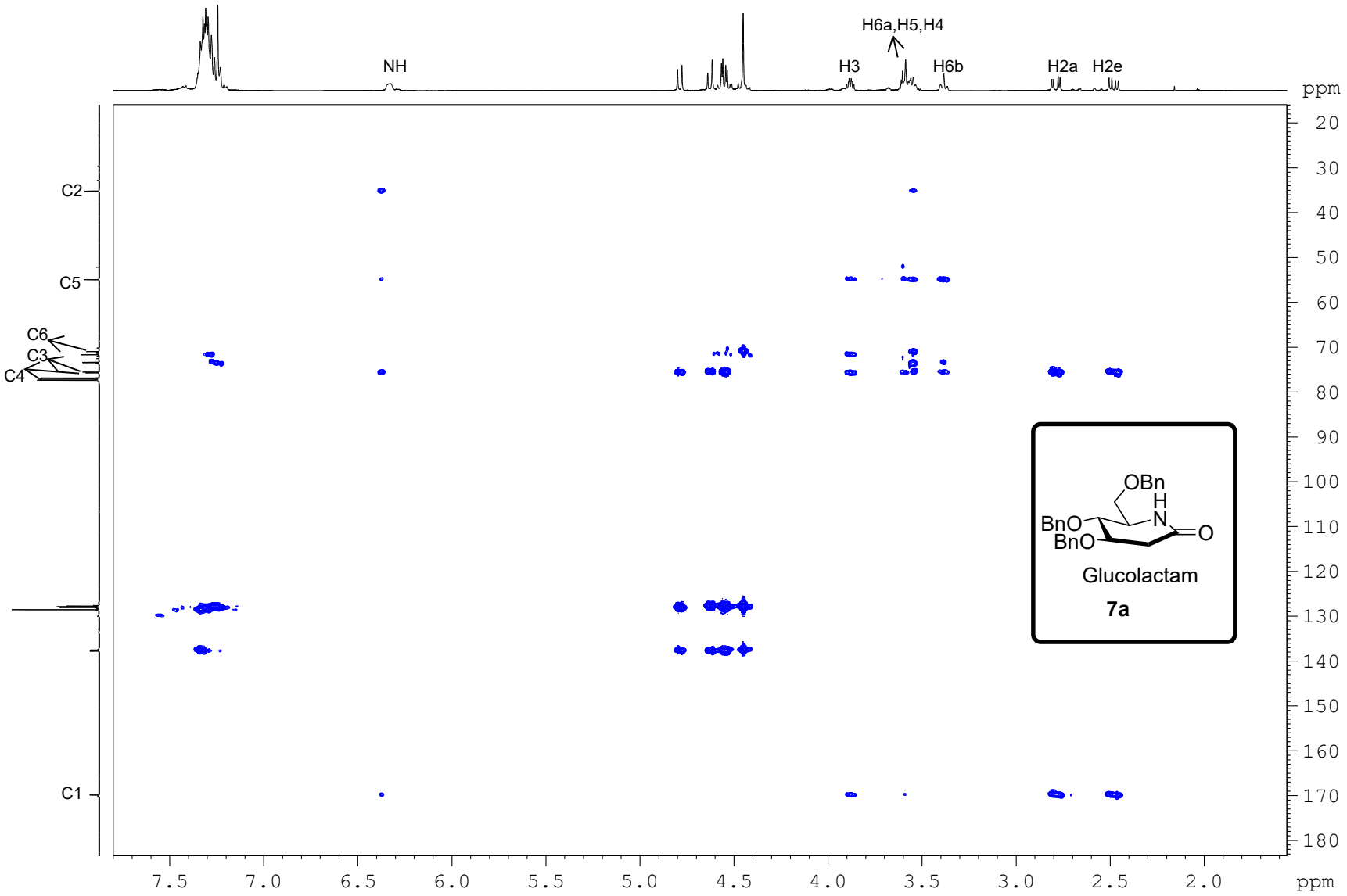
^{1}H-^{1}H COSY of **7a** (400MHz, $CDCl_3$, 298 K)

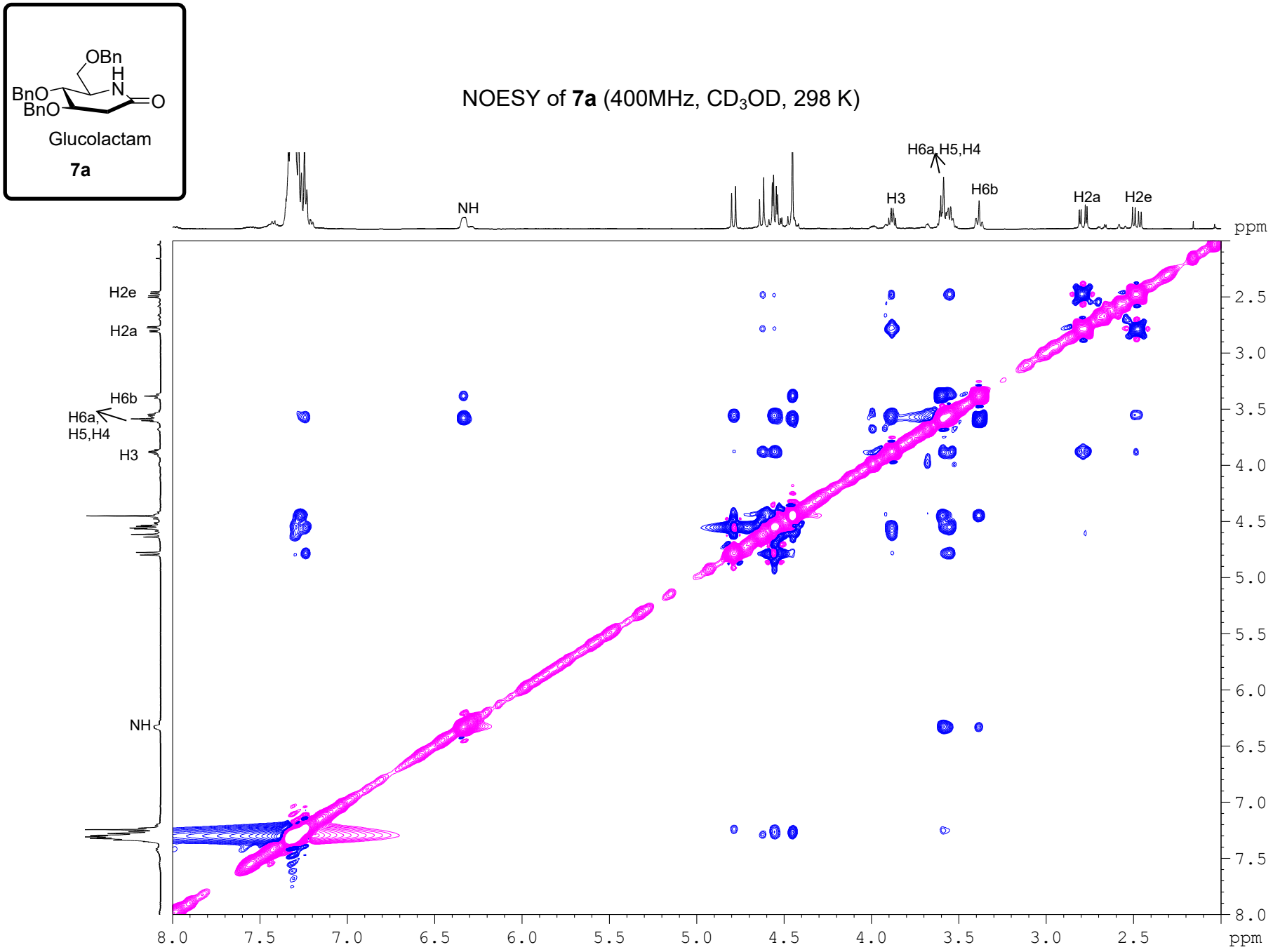


HSQC of **7a** (400MHz, $CDCl_3$, 298 K)

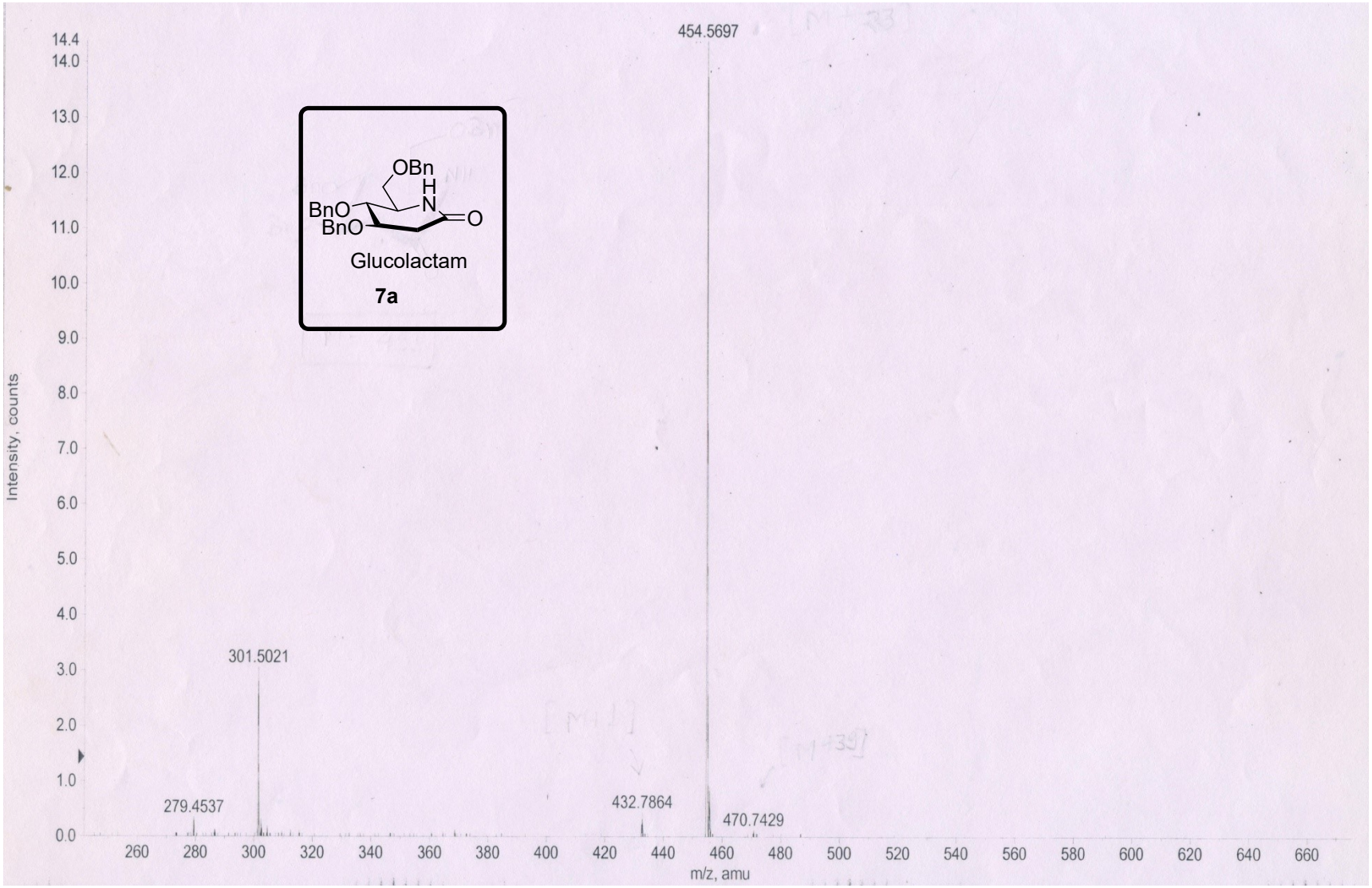


HMBC of **7a** (400MHz, $CDCl_3$, 298 K)

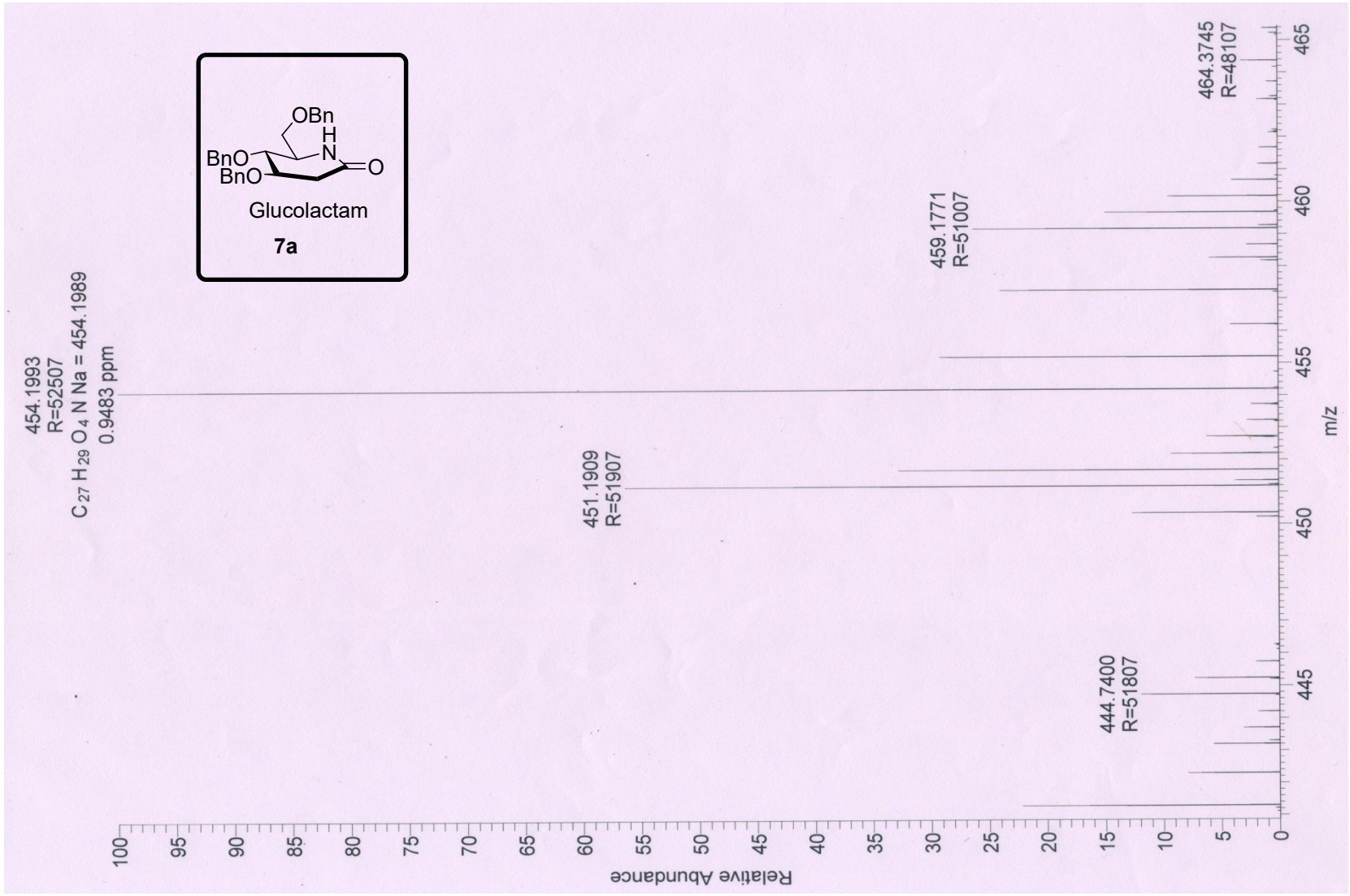



OBn
H
N
BnO
BnO
O
Glucolactam
7a
NOESY of 7a (400MHz, CD3OD, 298 K)
H6a,H5,H4
H3
H6b
H2a
H2e
NH
ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5

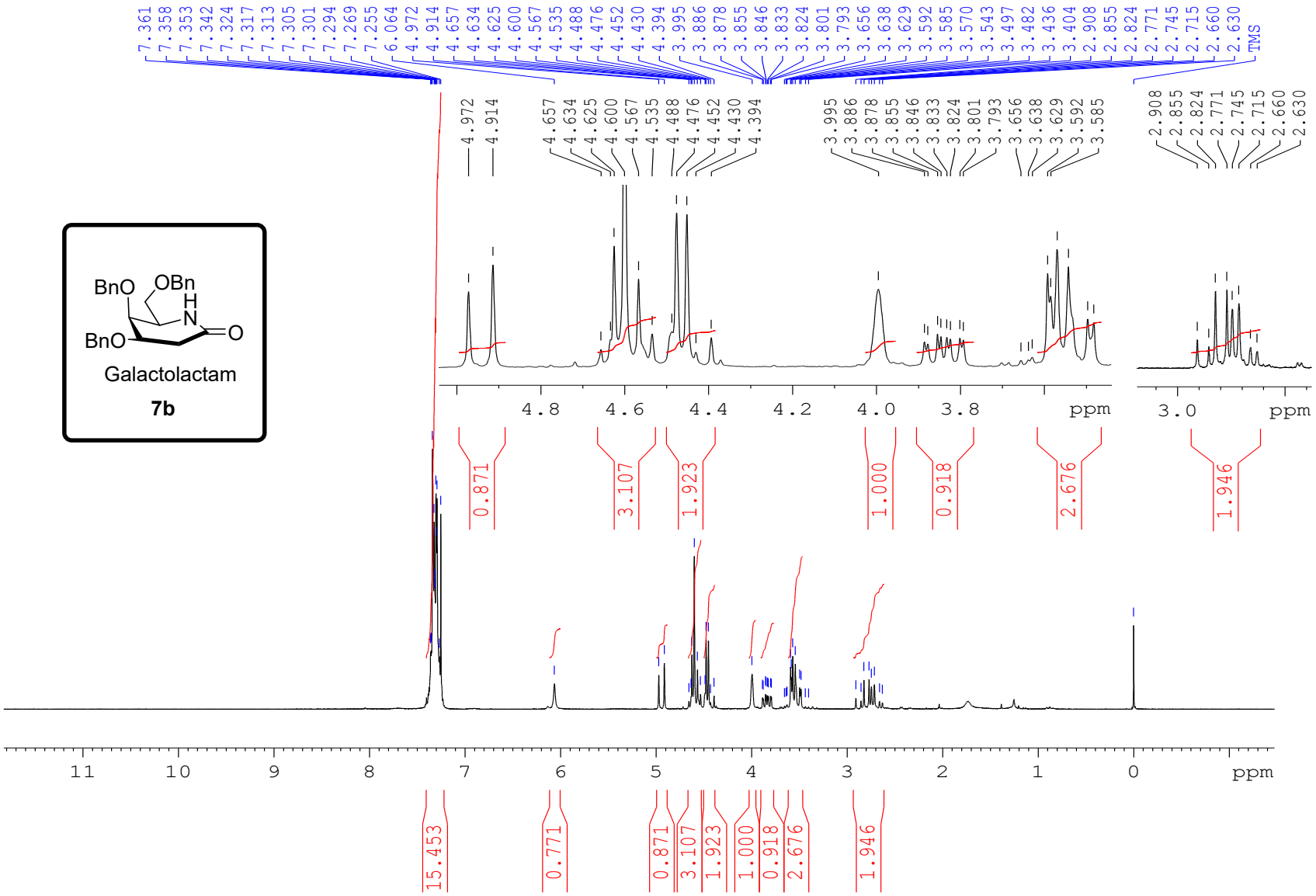
ES-MS of **7a**


454.5697
OBn
H
N
BnO
BnO
O
Glucolactam
7a
301.5021
279.4537
432.7864
470.7429
Intensity, counts
m/z, amu

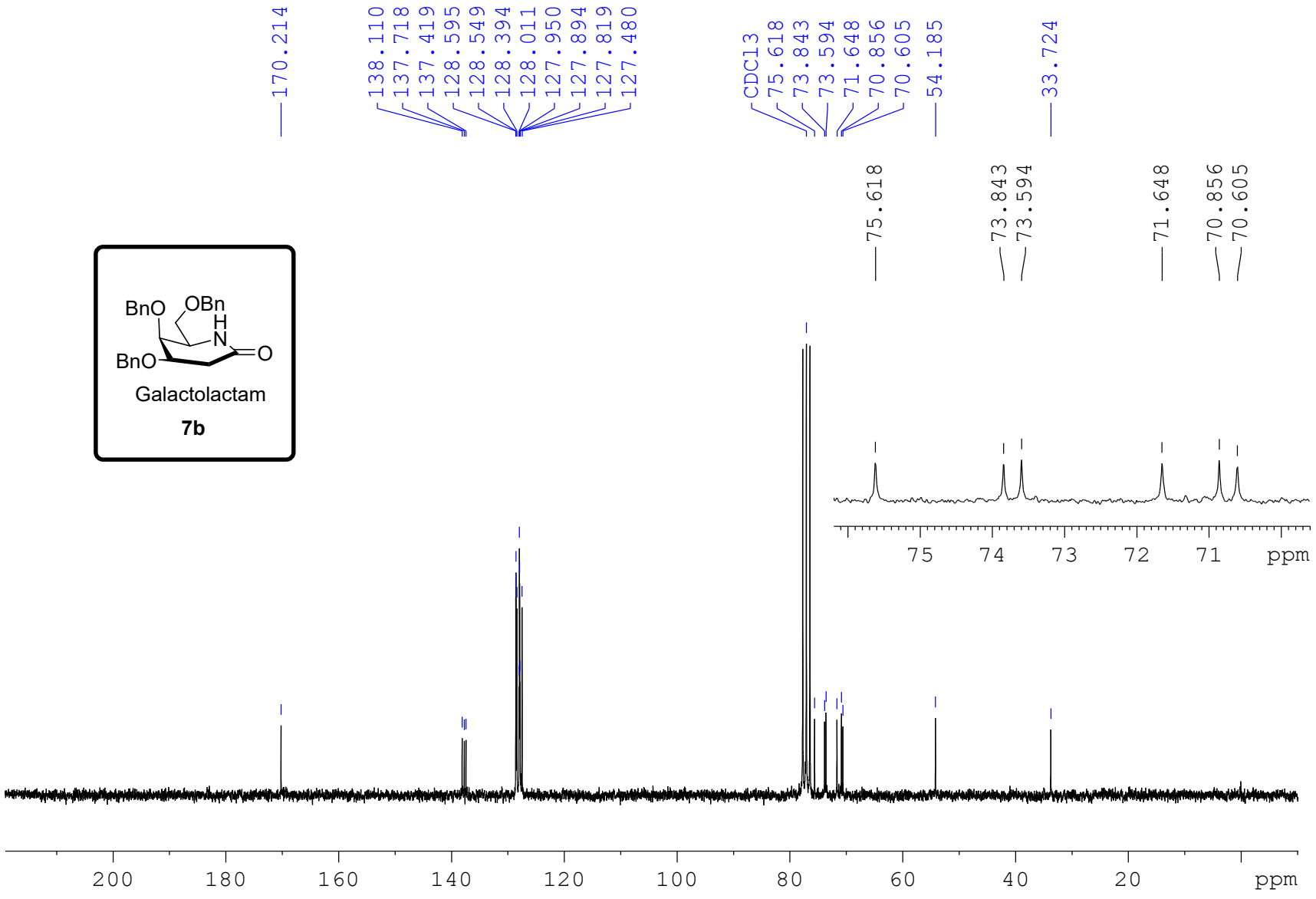
HRMS (ESI) of **7a**



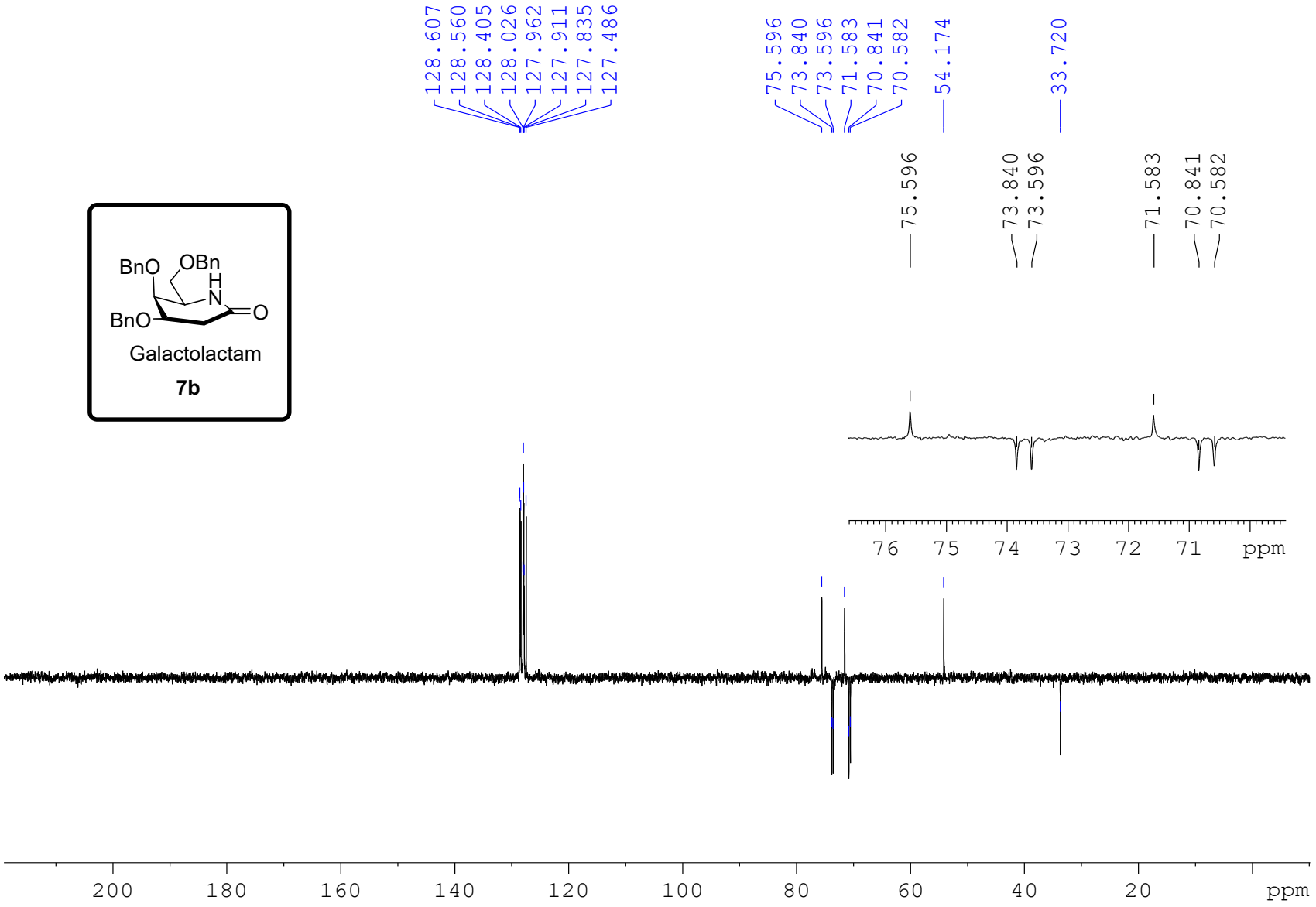
^{1}H NMR of **7b** (200MHz, $CDCl_3$)



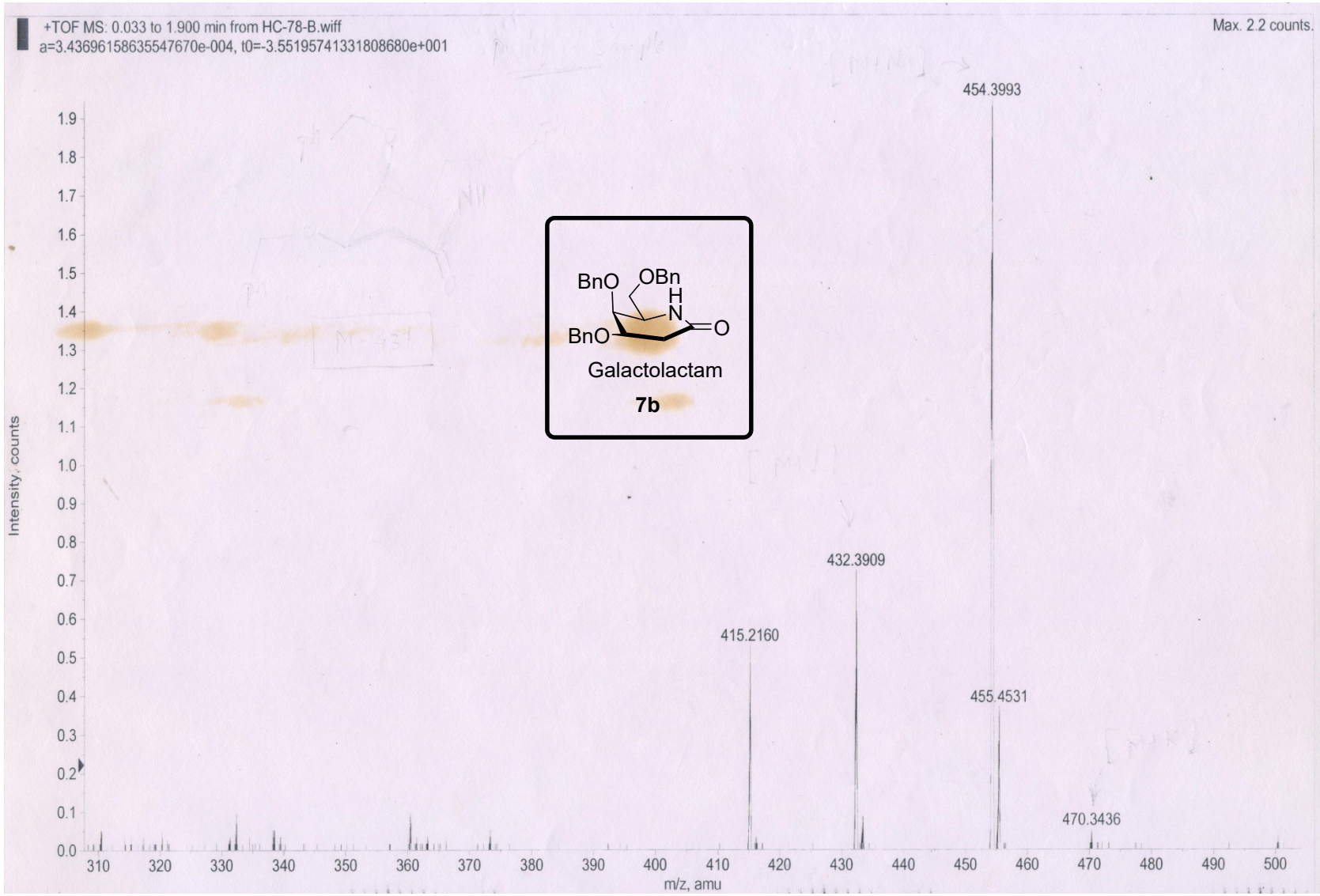
^{13}C NMR of **7b** (50MHz, $CDCl_3$)



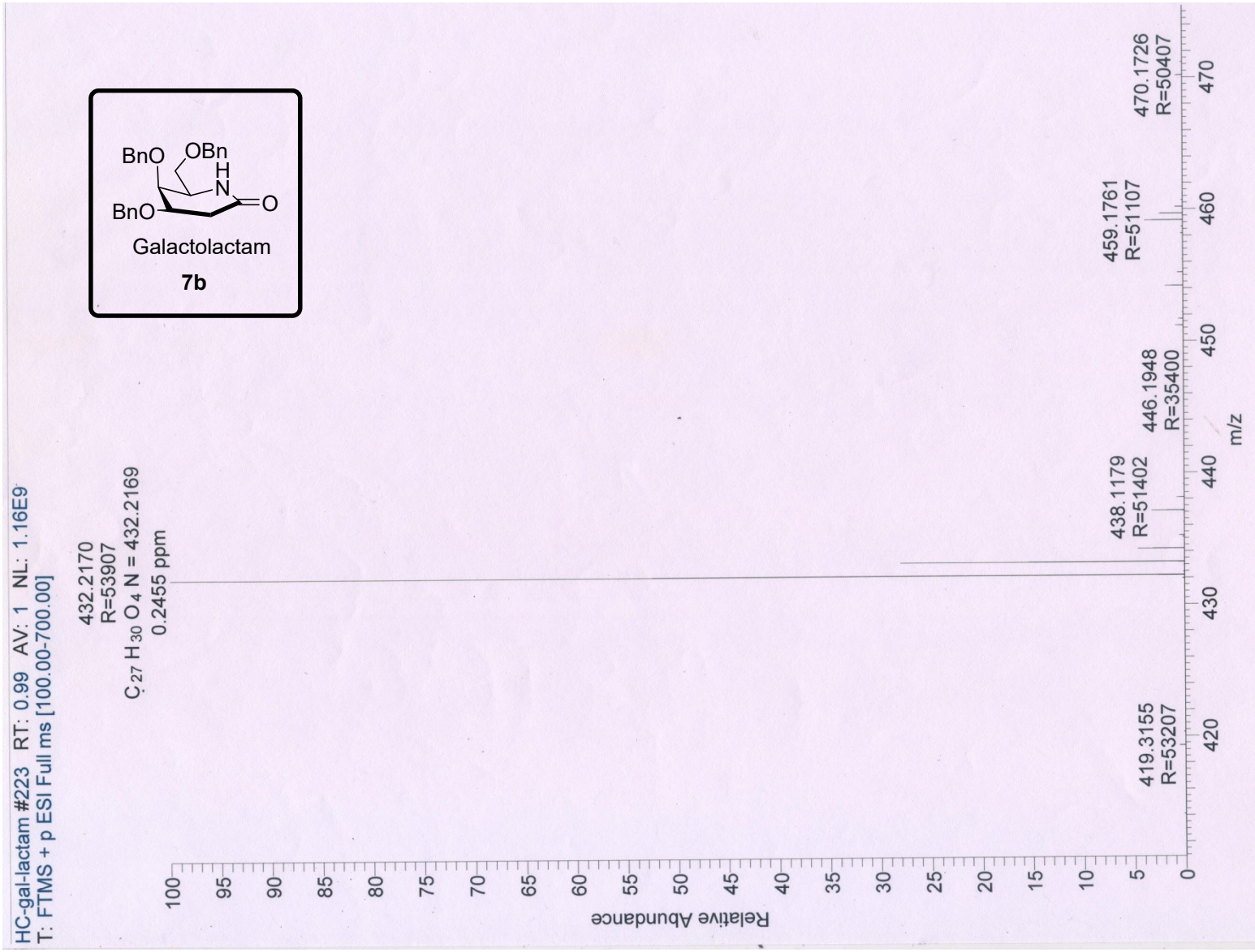
DEPT of **7b** (100MHz, $CDCl_3$)



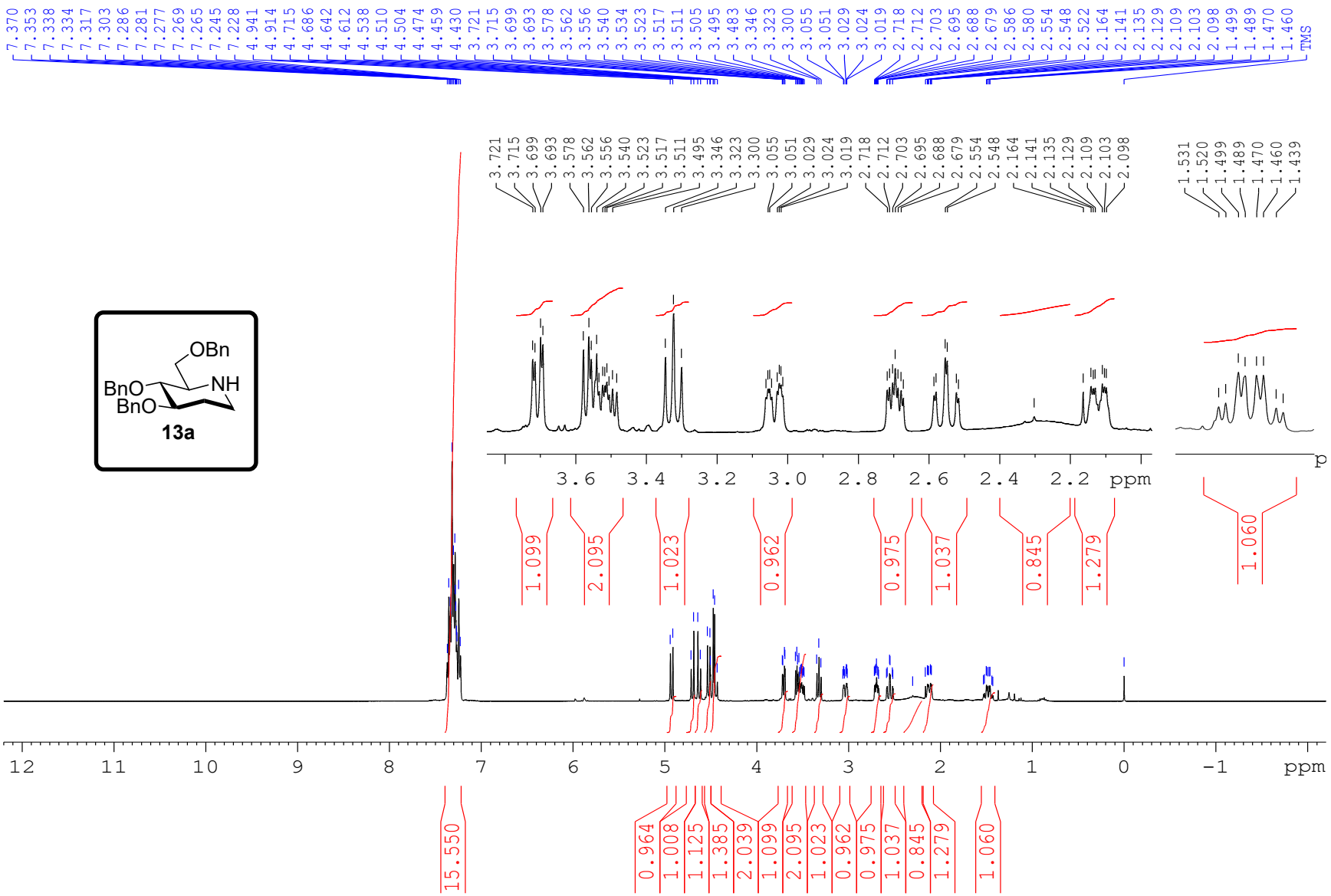
ESI-MS of **7b**


+TOF MS: 0.033 to 1.900 min from HC-78-B.wiff
a=3.43696158635547670e-004, t0=-3.55195741331808680e+001
Max. 2.2 counts.
454.3993
432.3909
415.2160
455.4531
470.3436
BnO
OBn
H
N
O
BnO
Galactolactam
7b
Intensity, counts
m/z, amu

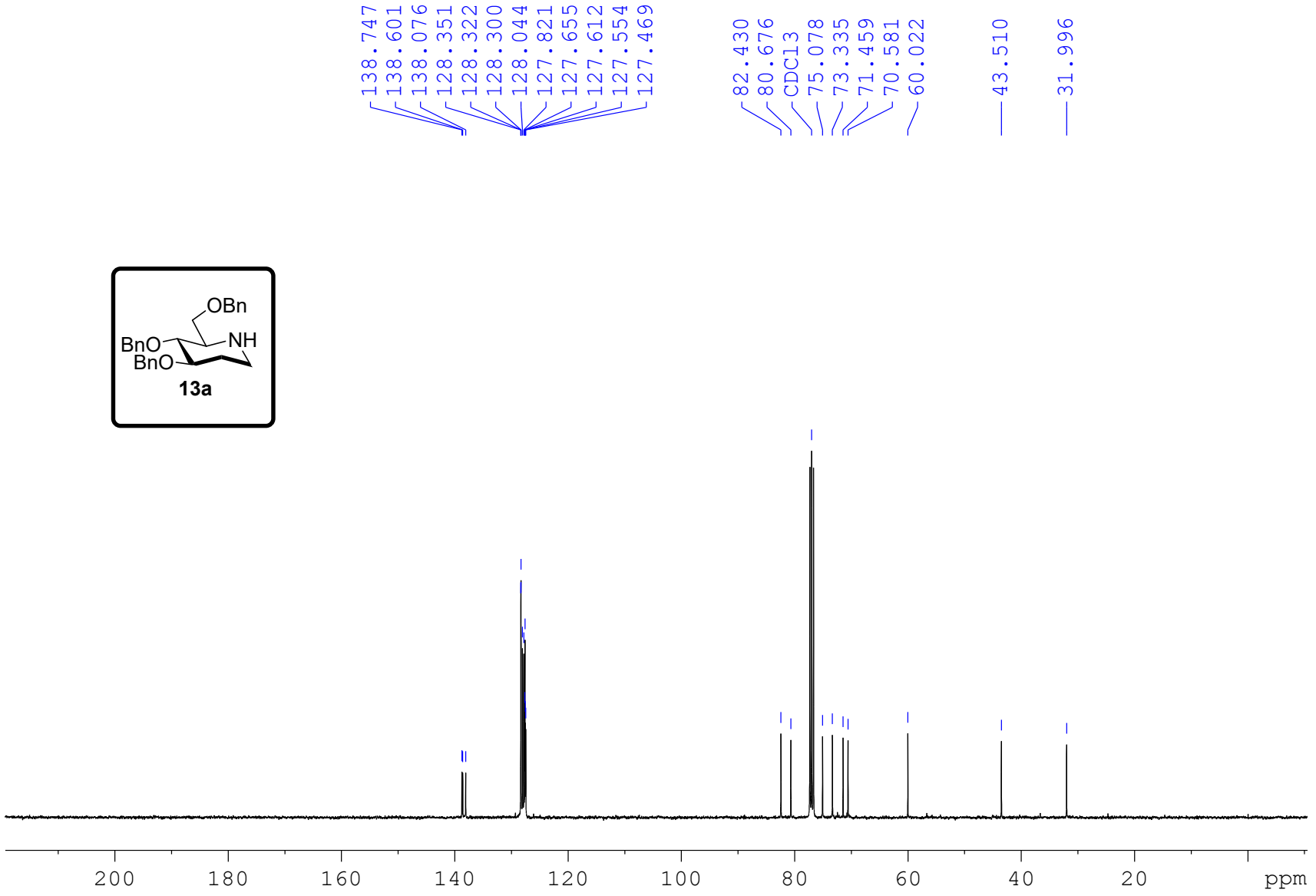
HRMS (ESI) of **7b**



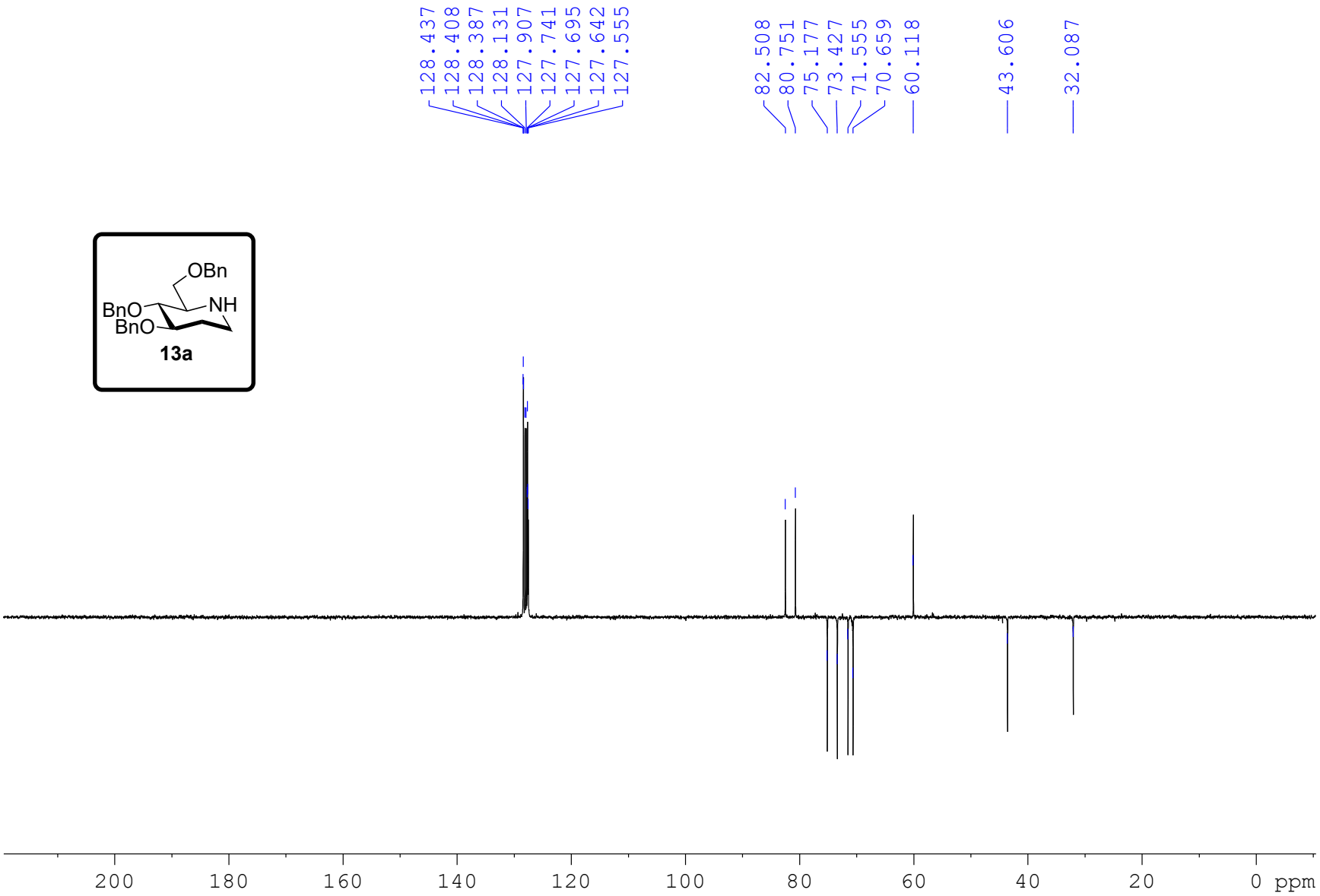
^{1}H NMR of **13a** (400MHz, $CDCl_3$)

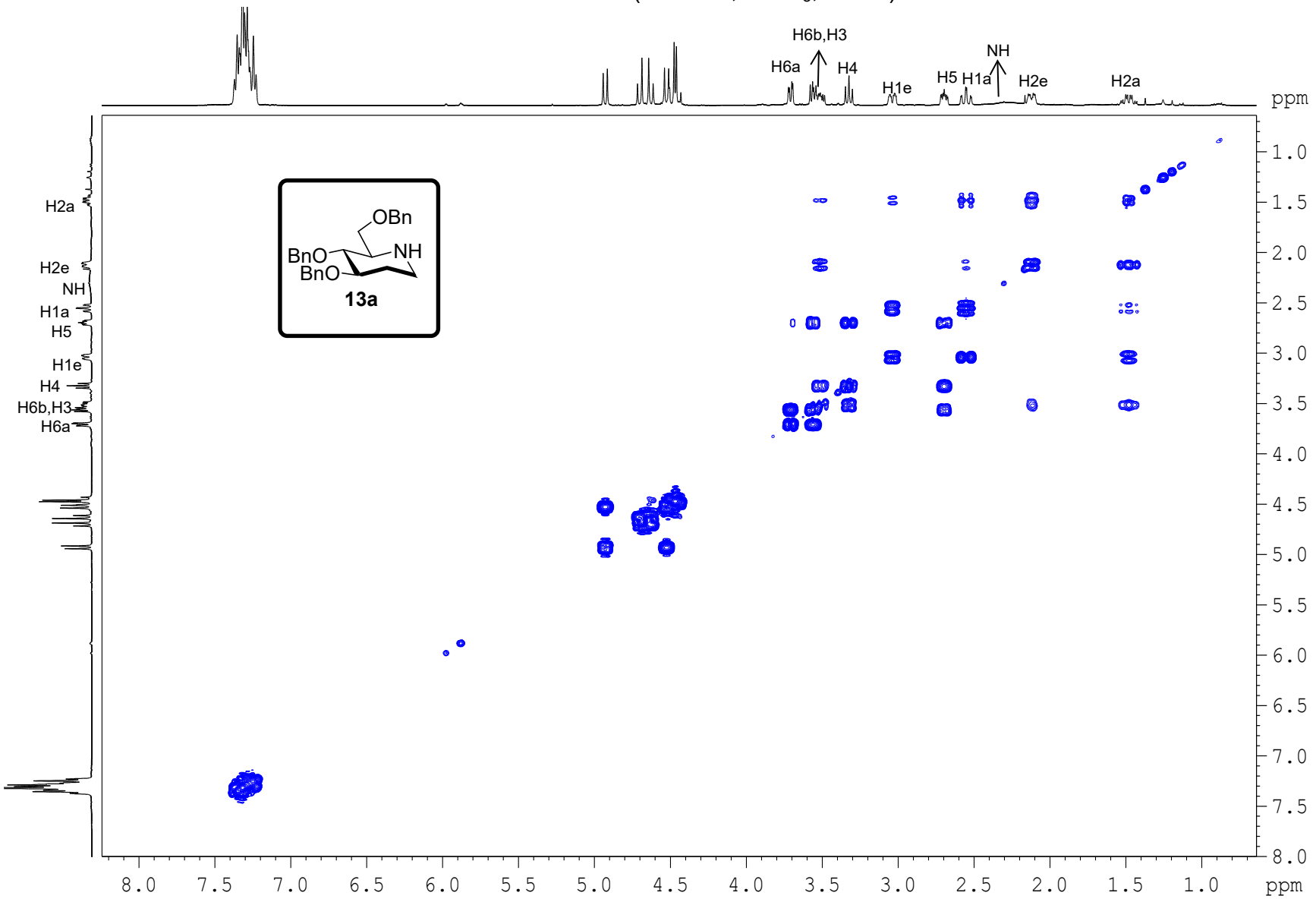


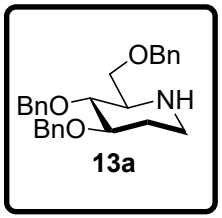
^{13}C NMR of **13a** in (100 MHz $CDCl_3$)



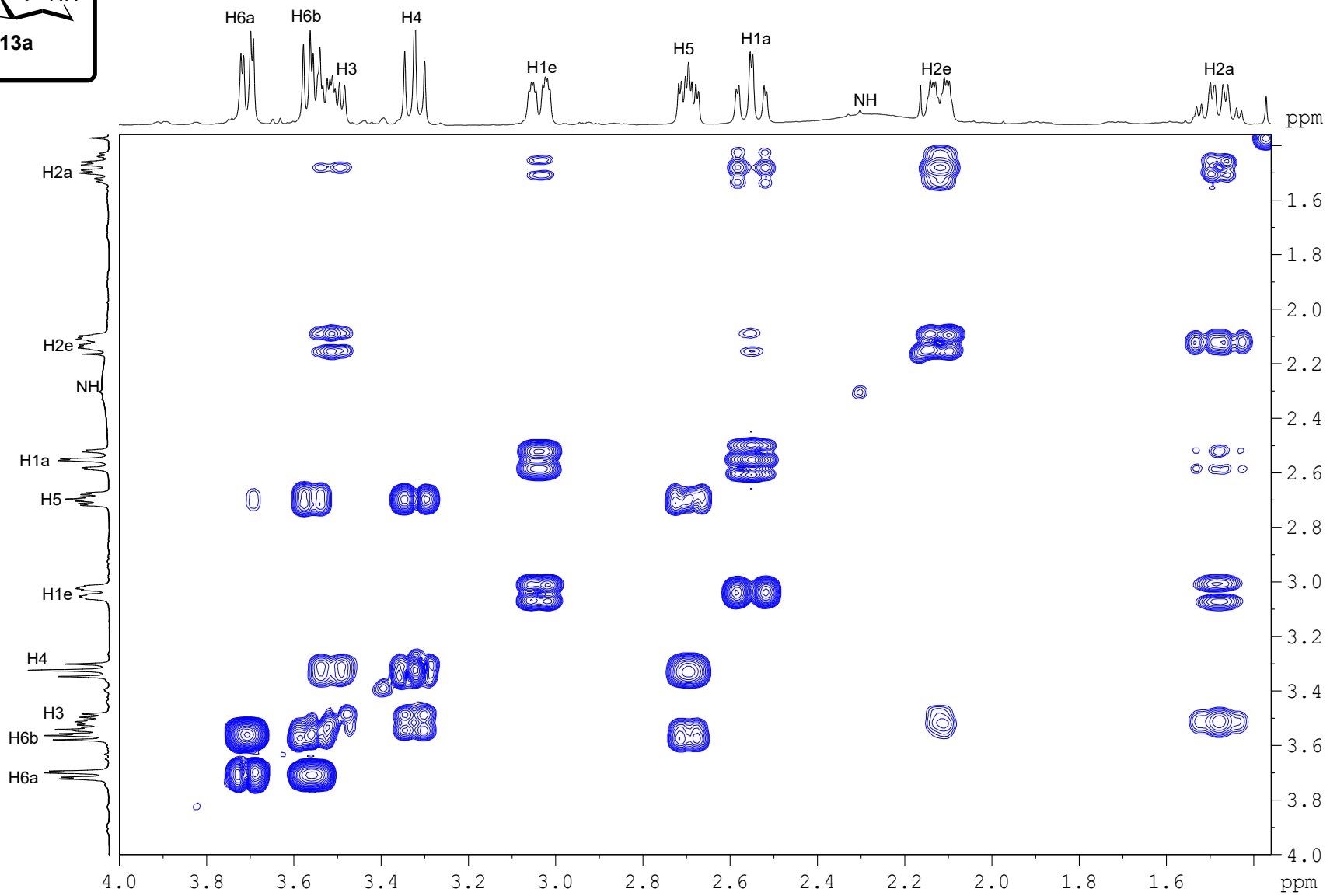
DEPT of **11'a** in (100 MHz $CDCl_3$)

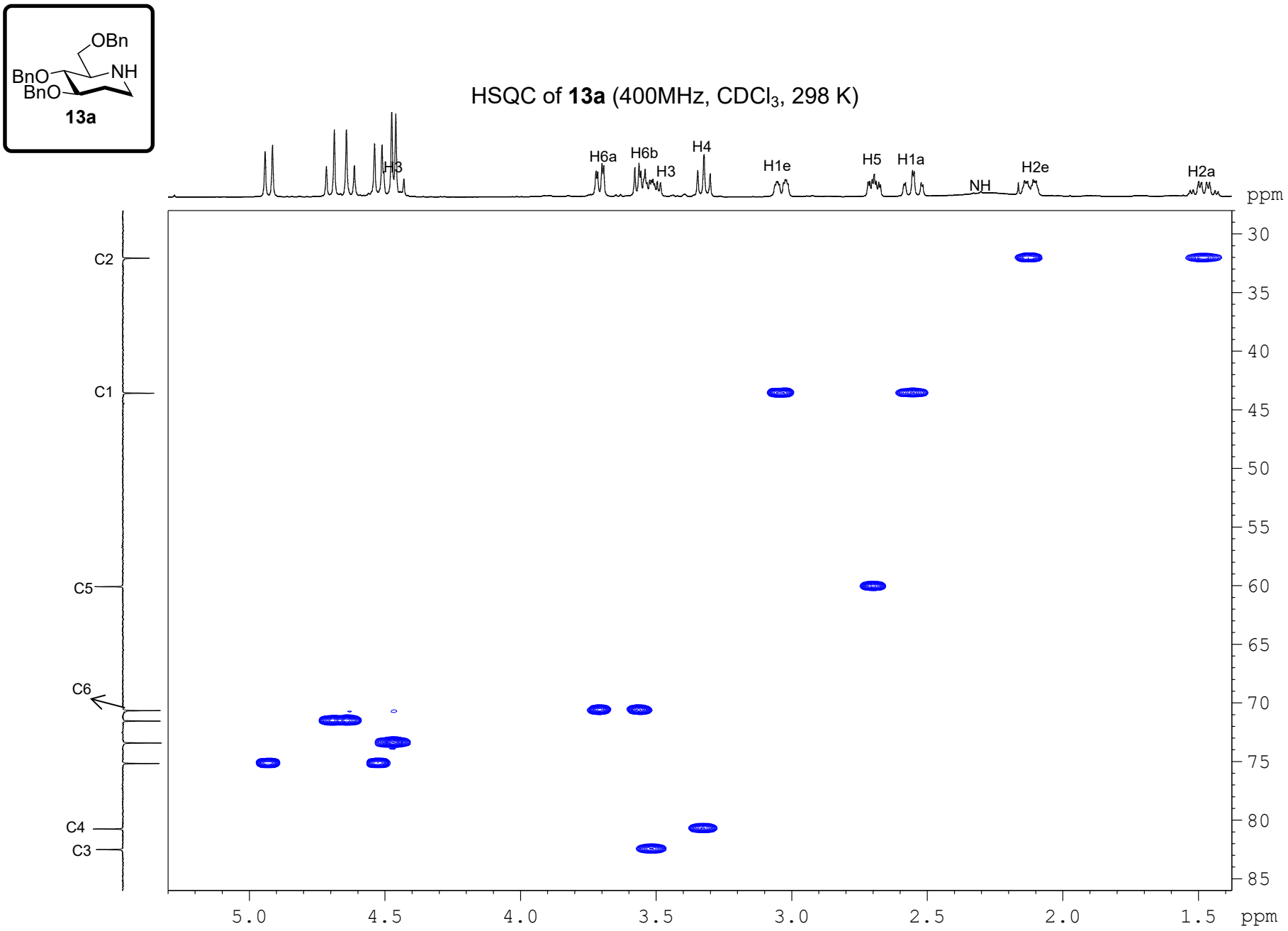


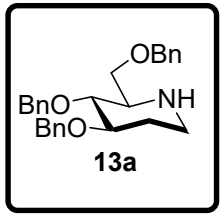

^{1}H-^{1}H COSY of **13a** (400MHz, $CDCl_3$, 298 K)
H6b,H3
H6a
H4
H1e
H5
H1a
NH
H2e
H2a
ppm
OBn
BnO
BnO
NH
13a
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0



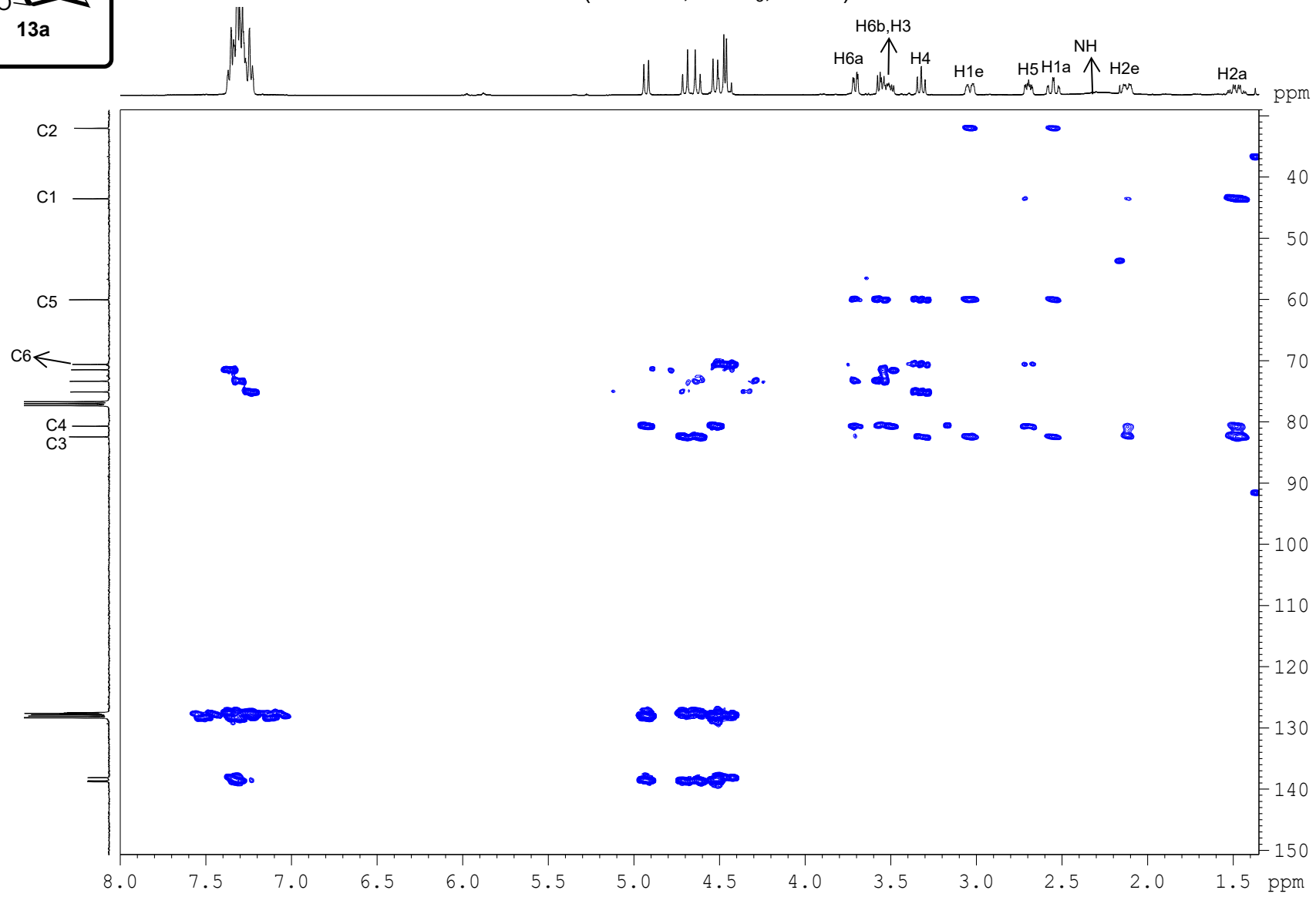
^{1}H-^{1}H COSY offset of **13a** (400MHz, $CDCl_3$, 298 K)

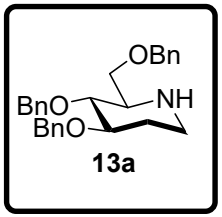



OBn
BnO
NH
BnO
13a
HSQC of 13a (400MHz, CDCl3, 298 K)
H3
H6a
H6b
H3
H4
H1e
H5
H1a
NH
H2e
H2a
ppm
C2
C1
C5
C6
C4
C3
30
35
40
45
50
55
60
65
70
75
80
85
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm



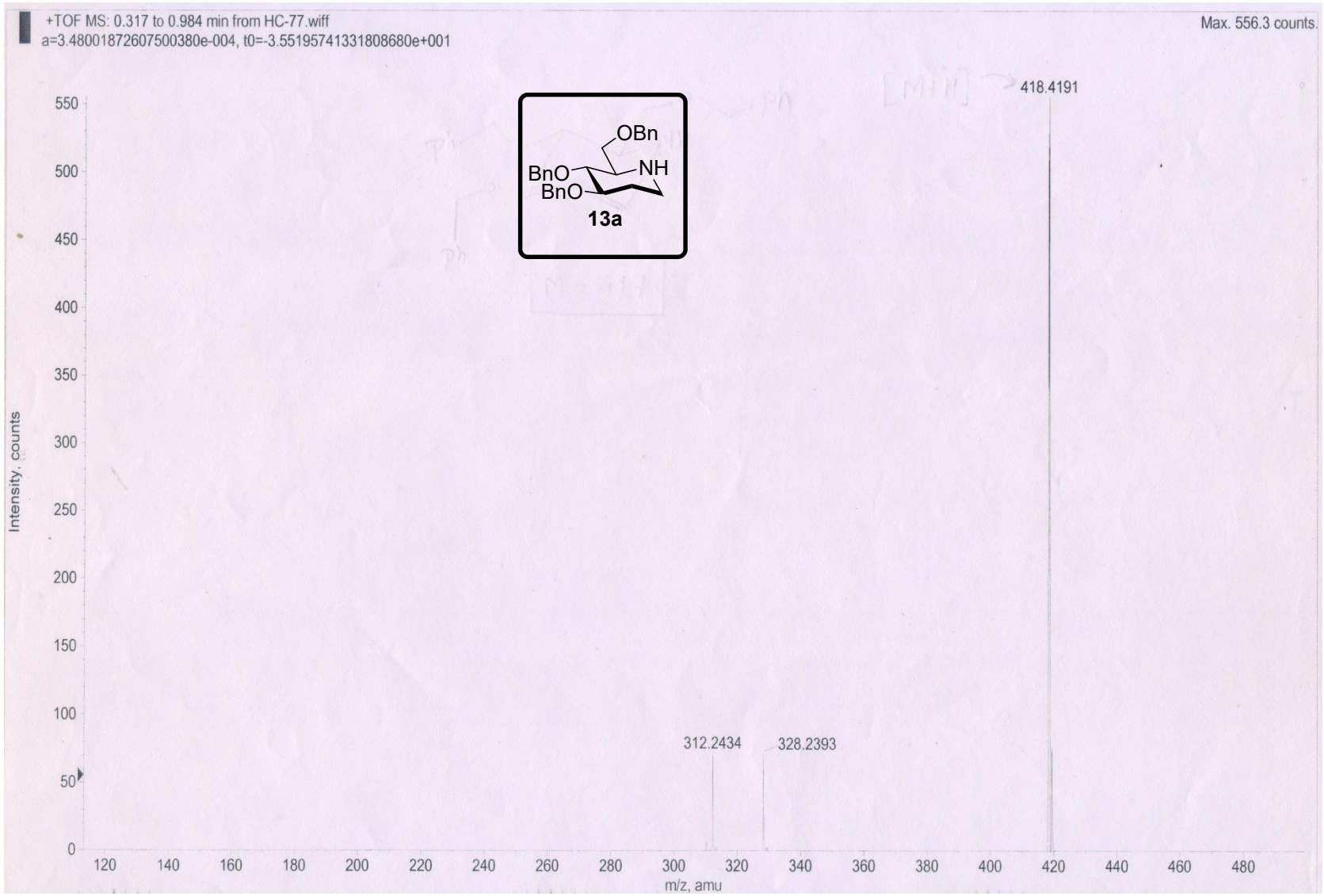
HMBC **13a** (400MHz, $CDCl_3$, 298 K)



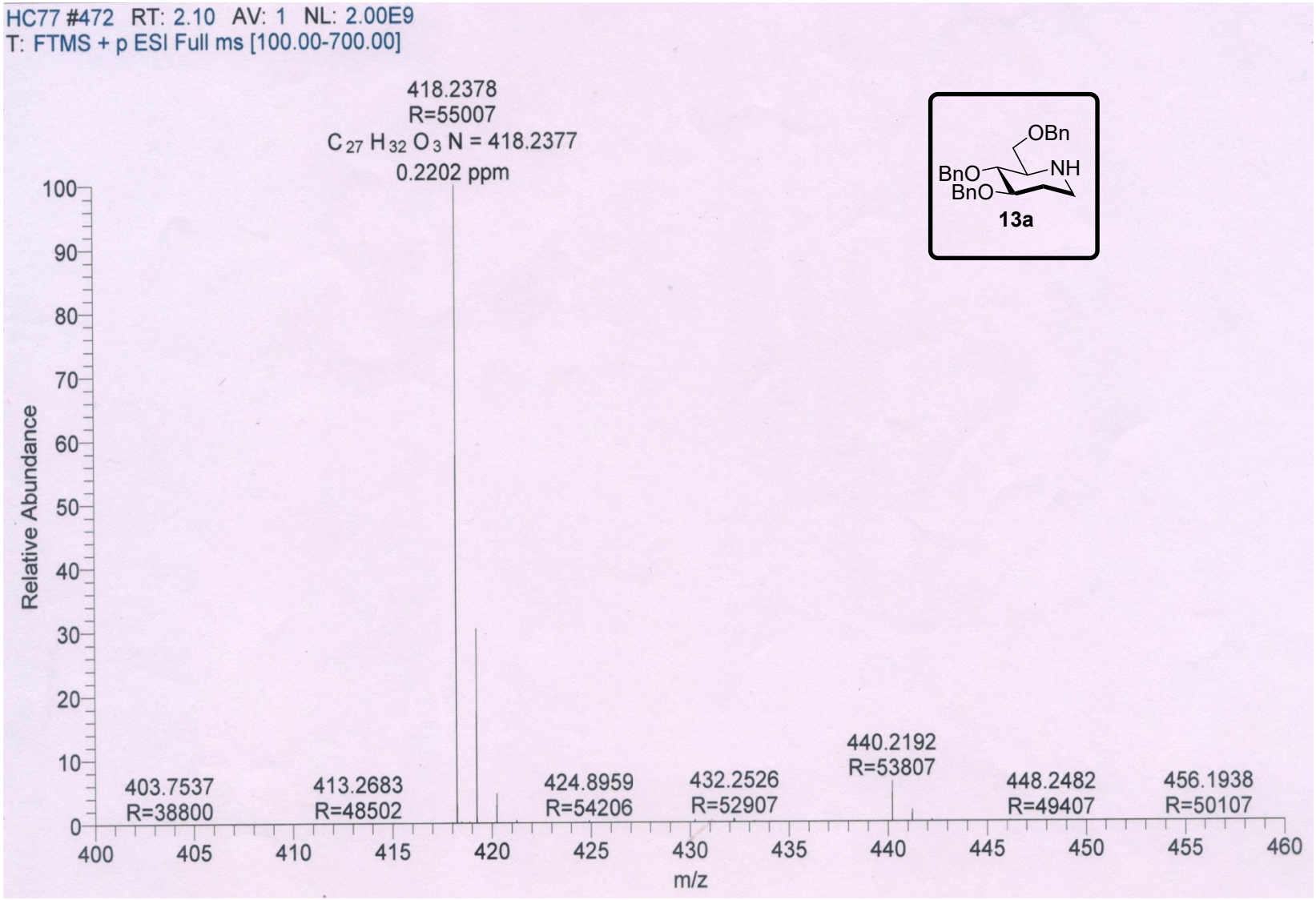


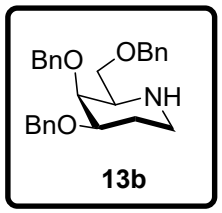
NOESY of **13a** (400MHz, $CDCl_3$, 298 K)

ESI-MS of **13a**

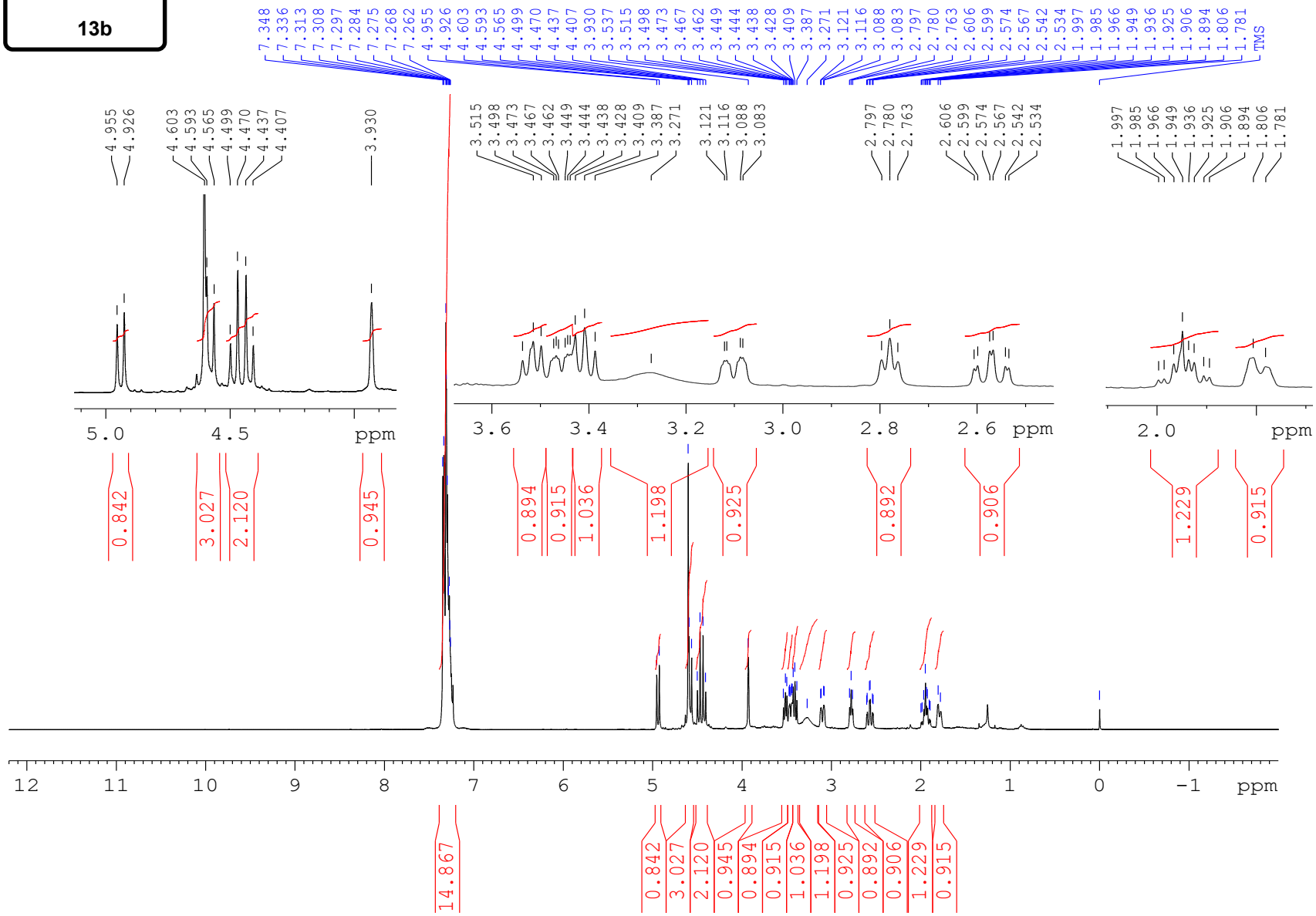

+TOF MS: 0.317 to 0.984 min from HC-77.wiff
a=3.48001872607500380e-004, t0=-3.55195741331808680e+001
Max. 556.3 counts.
418.4191
312.2434
328.2393
OBn
BnO
BnO
NH
13a
Intensity, counts
m/z, amu

HRMS (ESI) of **13a**

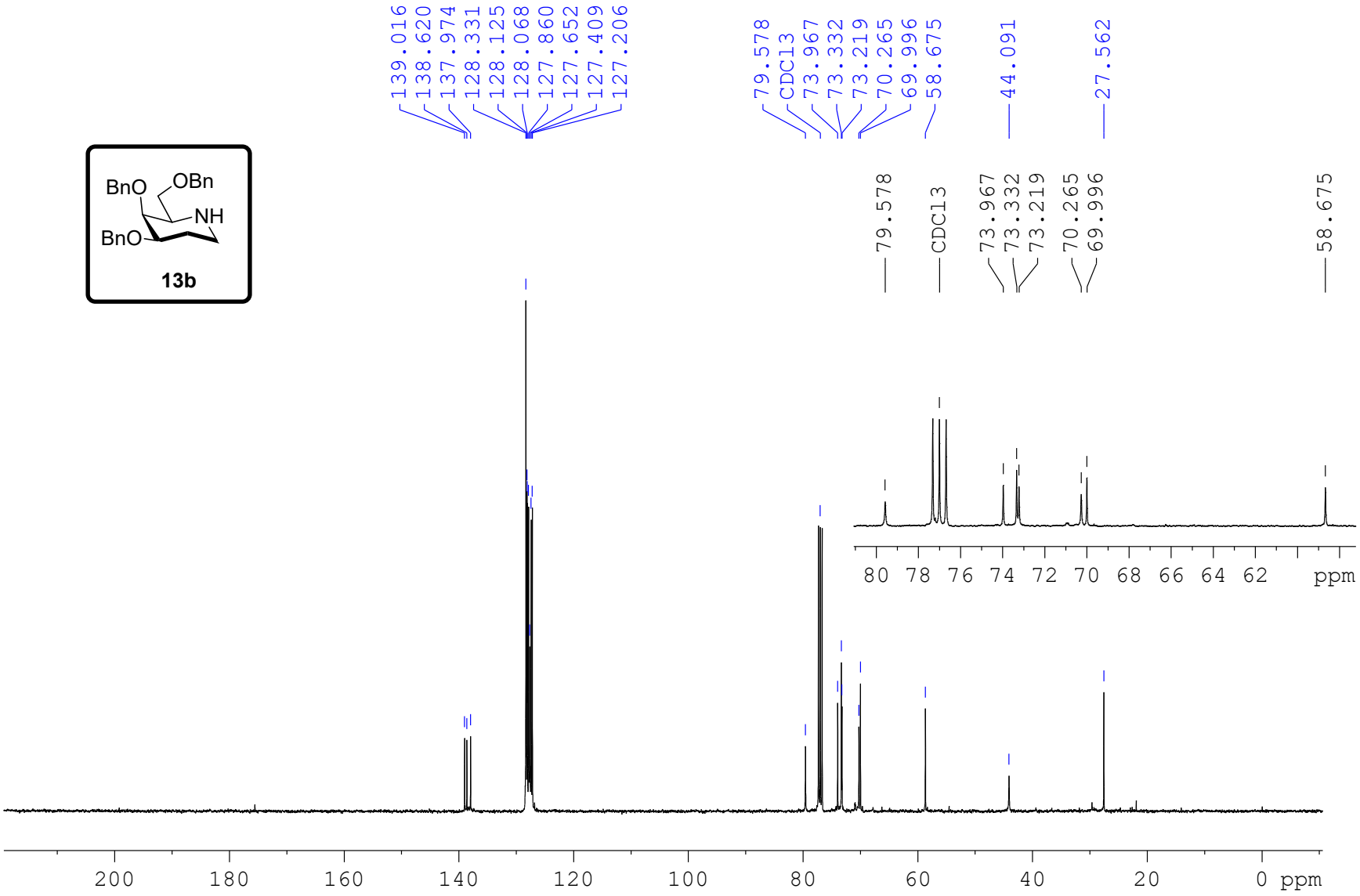




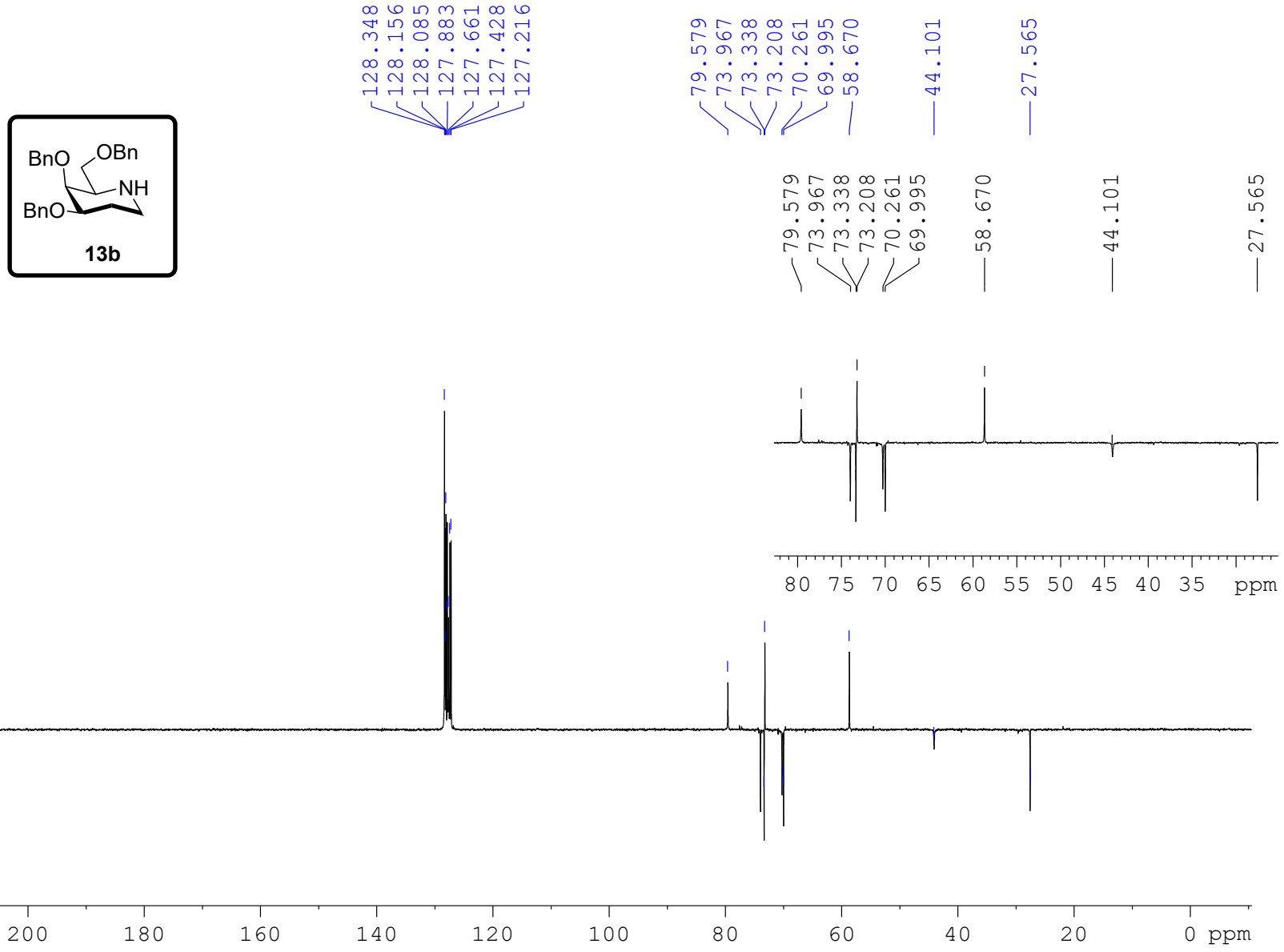
^{1}H NMR of **13b** (400 MHz $CDCl_3$)

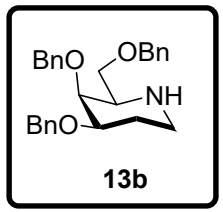


^{13}C NMR of **13b** (100 MHz $CDCl_3$)

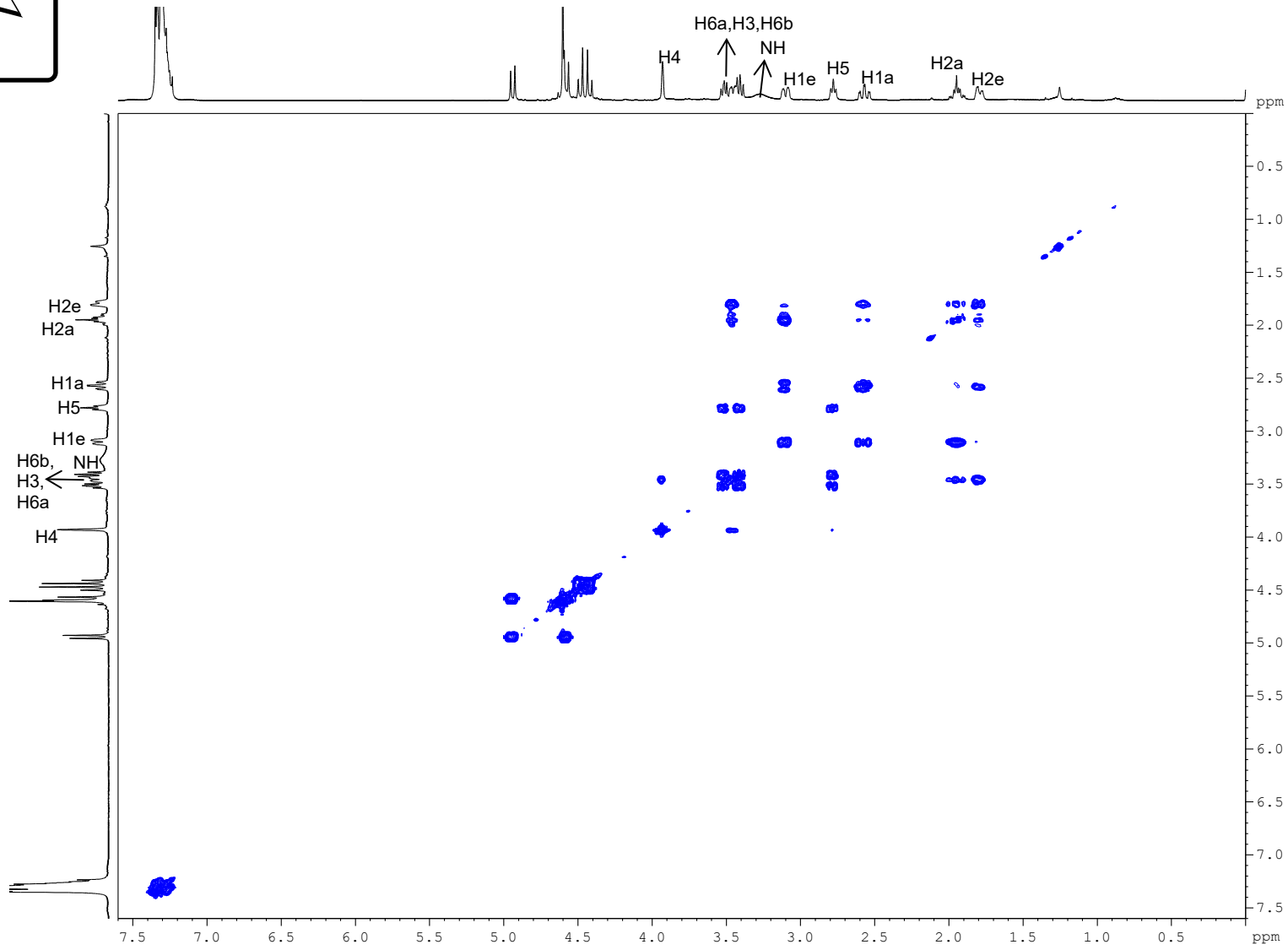


DEPT of **13b** (100 MHz $CDCl_3$)

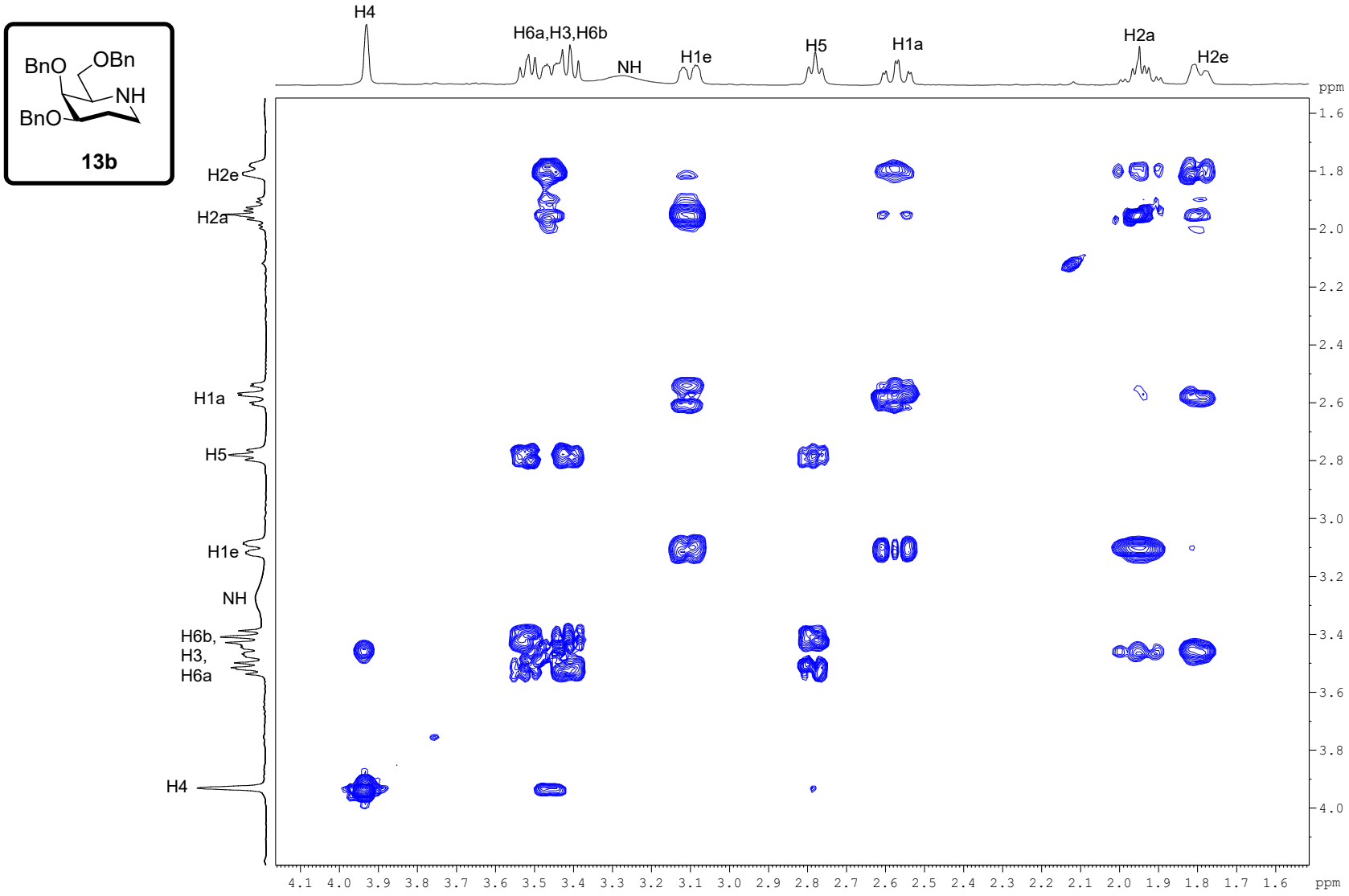


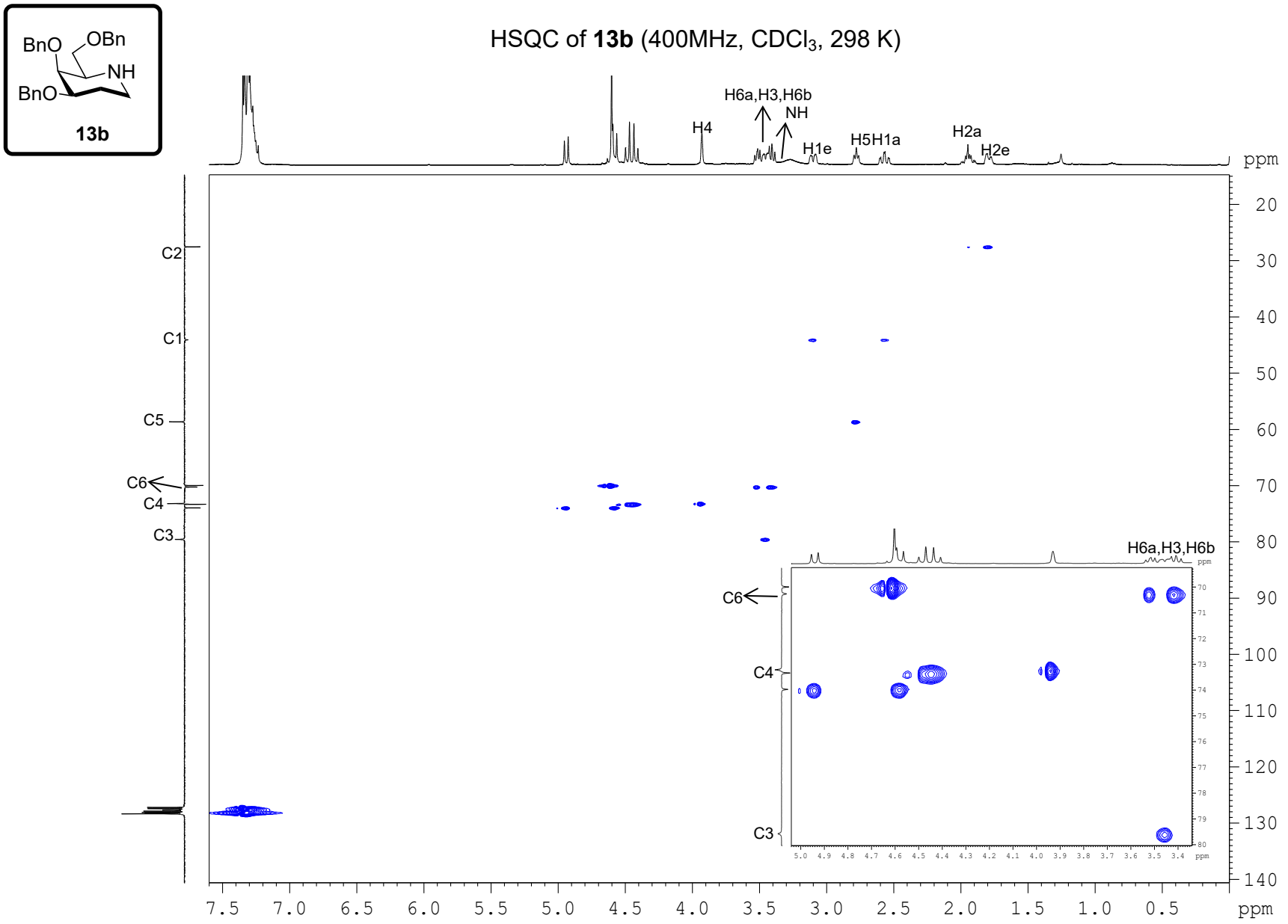


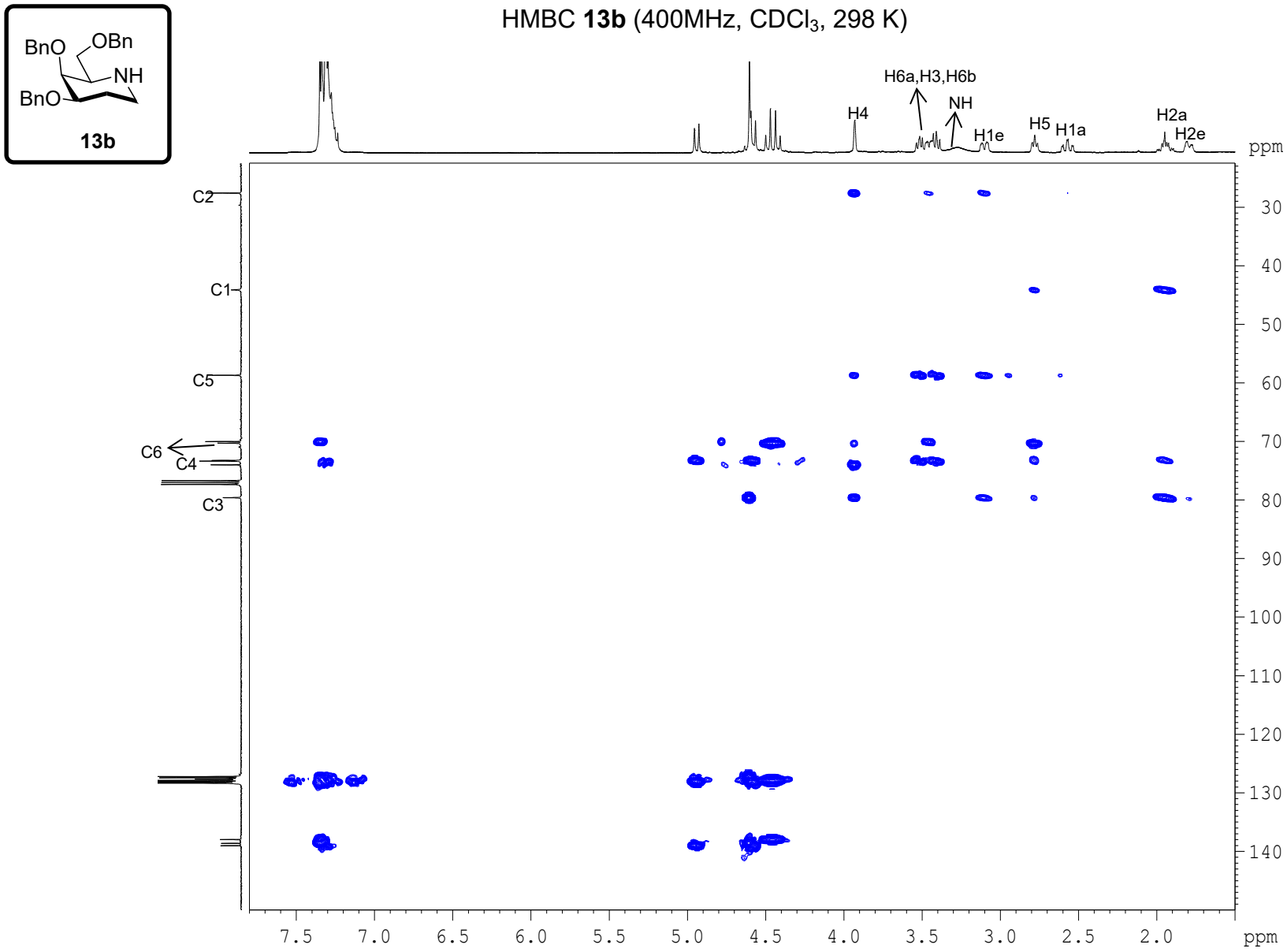
^{1}H-^{1}H COSY of **13b** (400MHz, $CDCl_3$, 298 K)

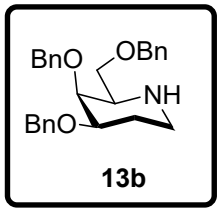


^{1}H-^{1}H COSY offset of **13b** (400MHz, $CDCl_3$, 298 K)

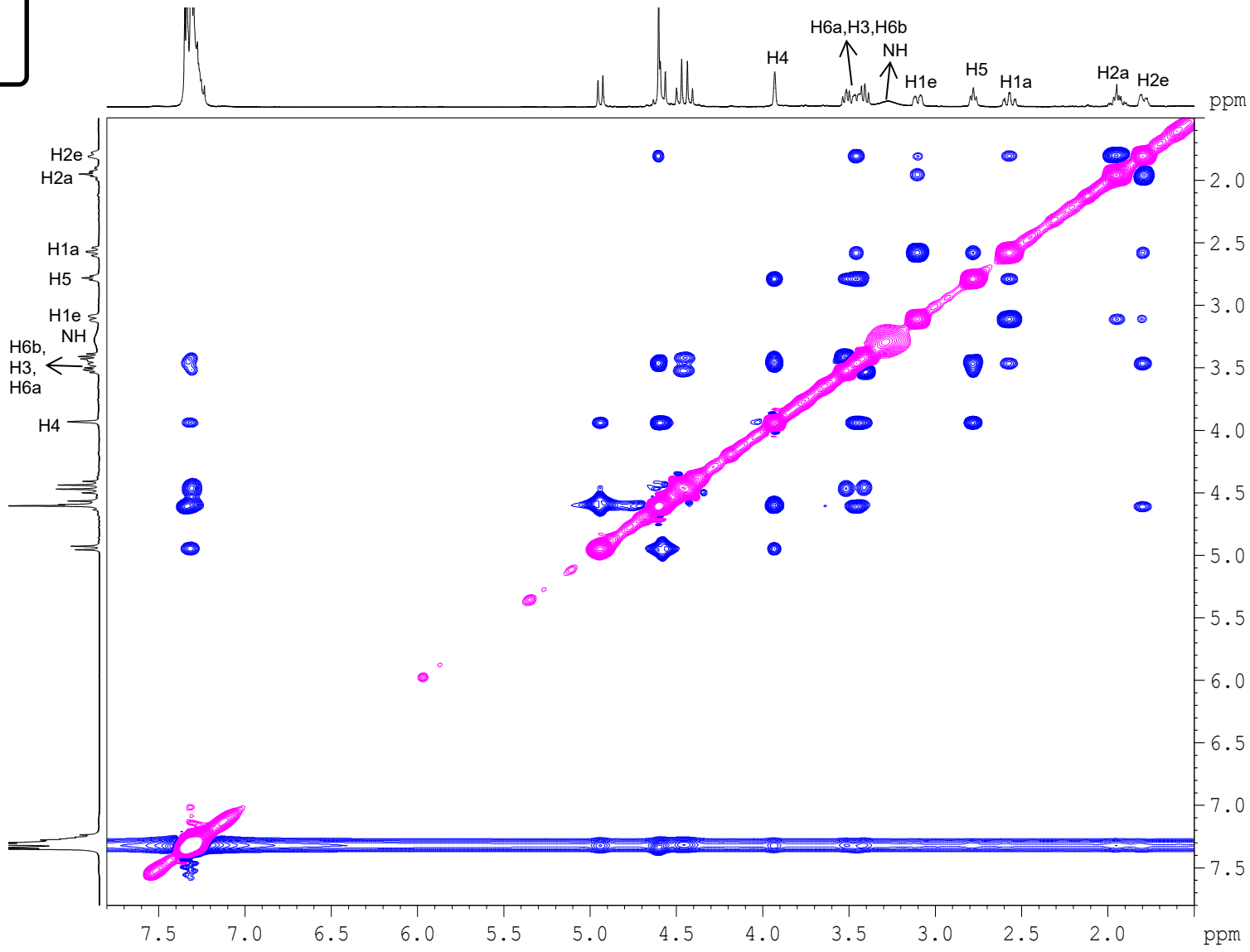



BnO
OBn
NH
BnO
13b
HSQC of 13b (400MHz, CDCl3, 298 K)
H6a,H3,H6b
NH
H4
H1e
H5H1a
H2a
H2e
ppm
C2
C1
C5
C6
C4
C3
H6a,H3,H6b
C6
C4
C3
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
20 30 40 50 60 70 80 90 100 110 120 130 140

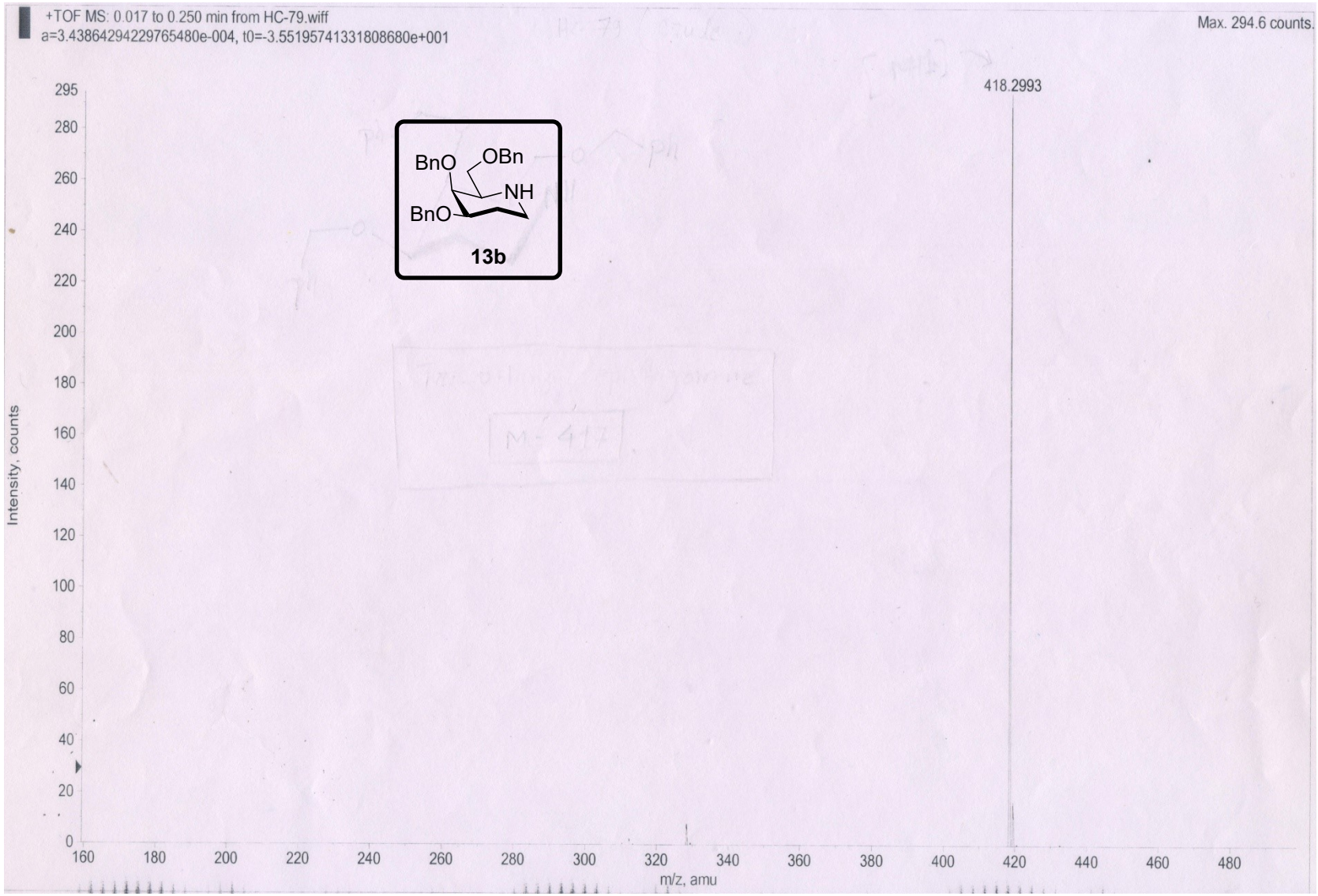

BnO
OBn
NH
BnO
13b
HMBC 13b (400MHz, CDCl3, 298 K)
H6a,H3,H6b
H4
NH
H1e
H5
H1a
H2a
H2e
ppm
C2
C1
C5
C6
C4
C3
30
40
50
60
70
80
90
100
110
120
130
140
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm



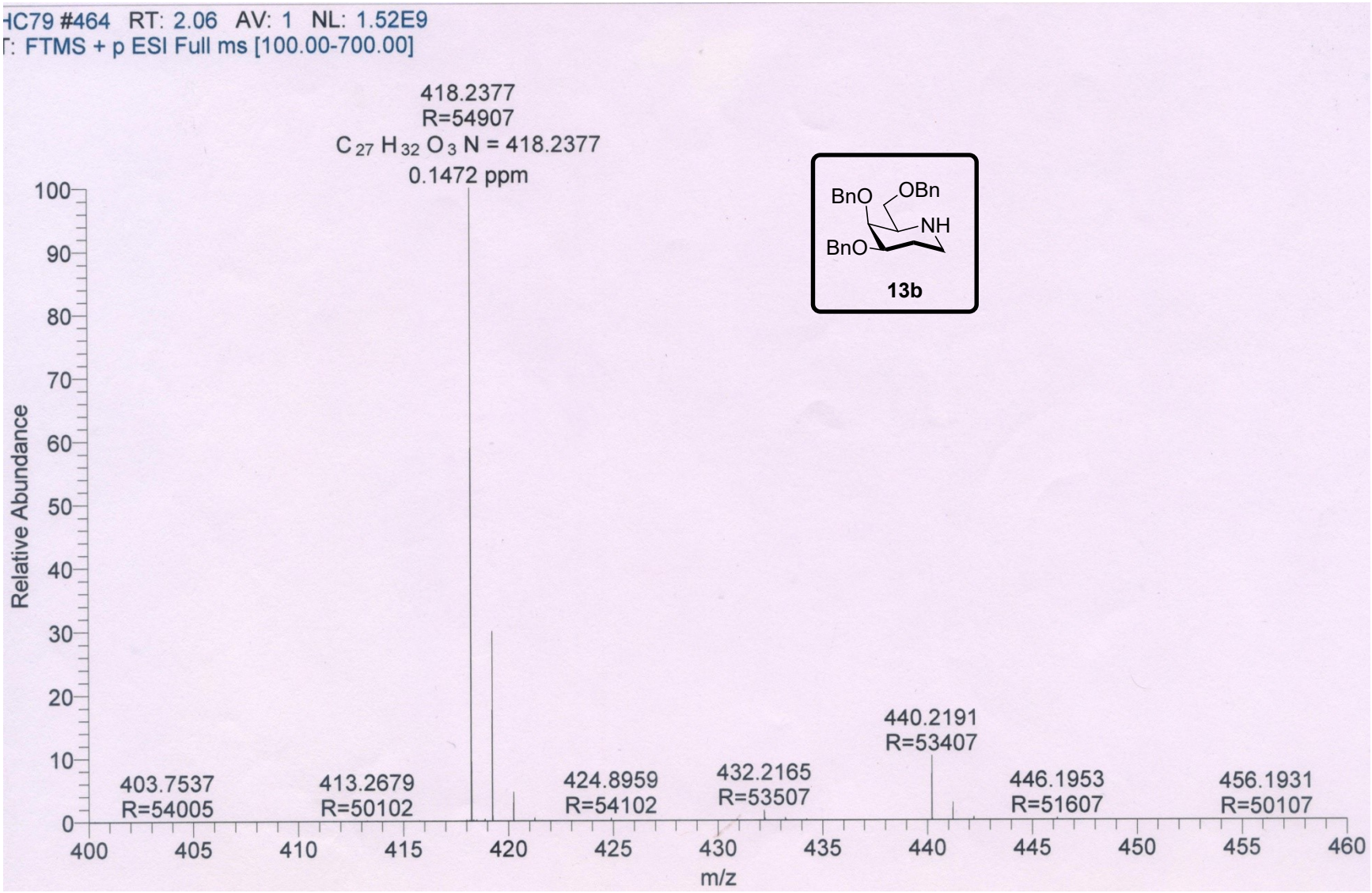
NOESY **13b** (400MHz, $CDCl_3$, 298 K)



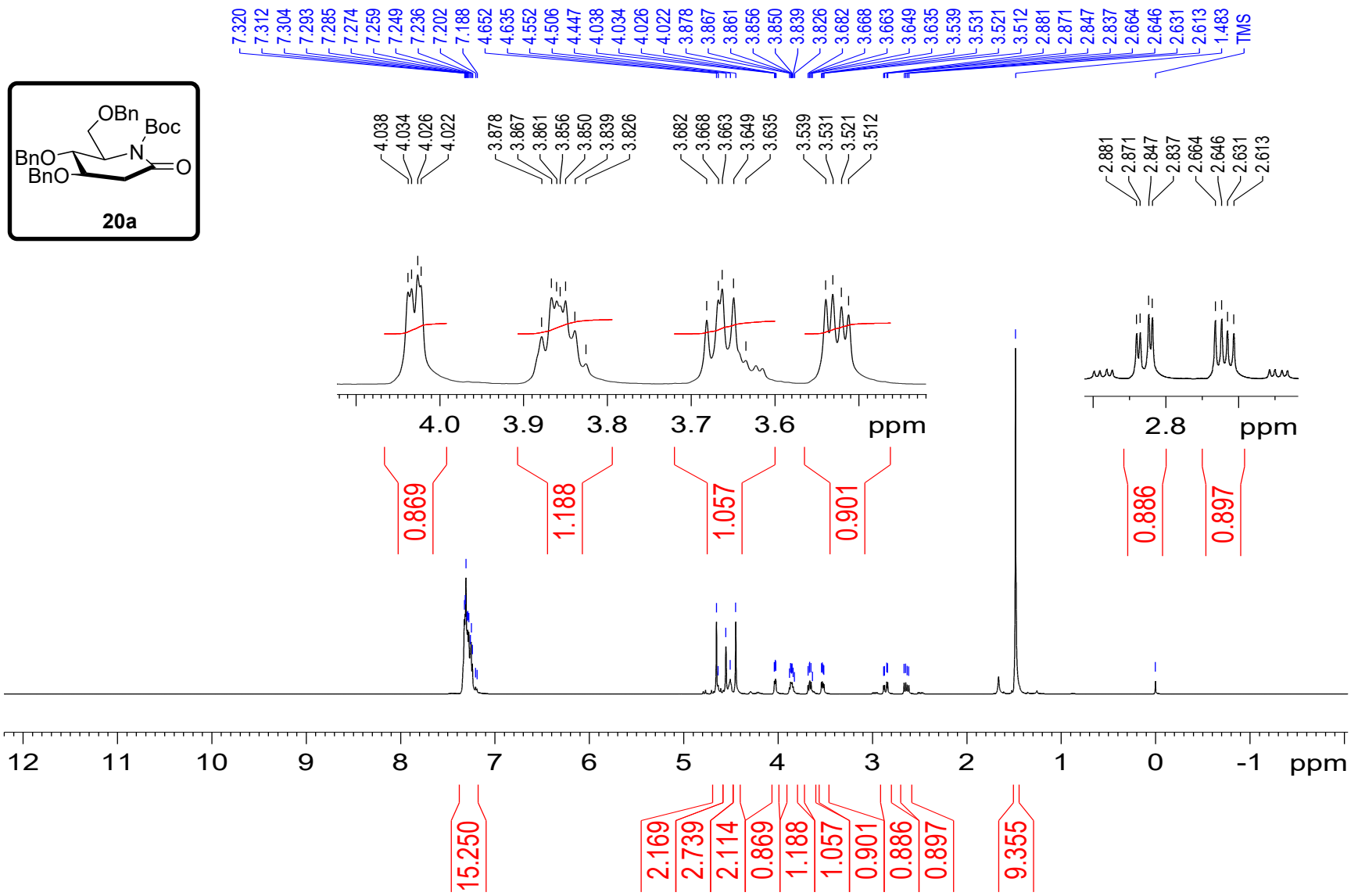
ESI-MS of **13b**


+TOF MS: 0.017 to 0.250 min from HC-79.wiff
a=3.43864294229765480e-004, t0=-3.55195741331808680e+001
Max. 294.6 counts.
418.2993
BnO
OBn
NH
BnO
13b
Intensity, counts
m/z, amu

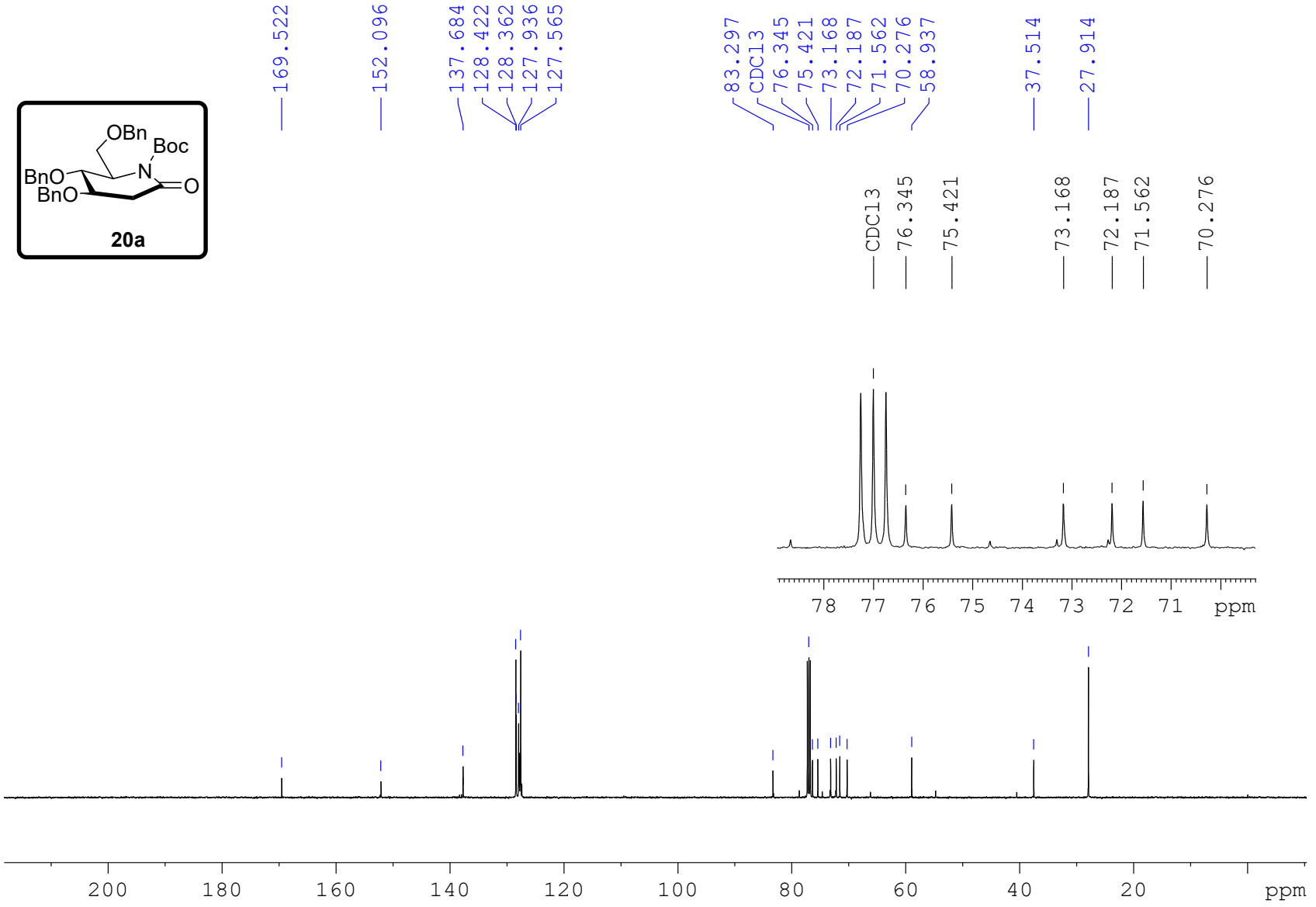
HRMS of **13b**


HC79 #464 RT: 2.06 AV: 1 NL: 1.52E9
T: FTMS + p ESI Full ms [100.00-700.00]
418.2377
R=54907
C 27 H 32 O 3 N = 418.2377
0.1472 ppm
BnO
OBn
NH
BnO
13b
Relative Abundance
m/z
403.7537
R=54005
413.2679
R=50102
424.8959
R=54102
432.2165
R=53507
440.2191
R=53407
446.1953
R=51607
456.1931
R=50107

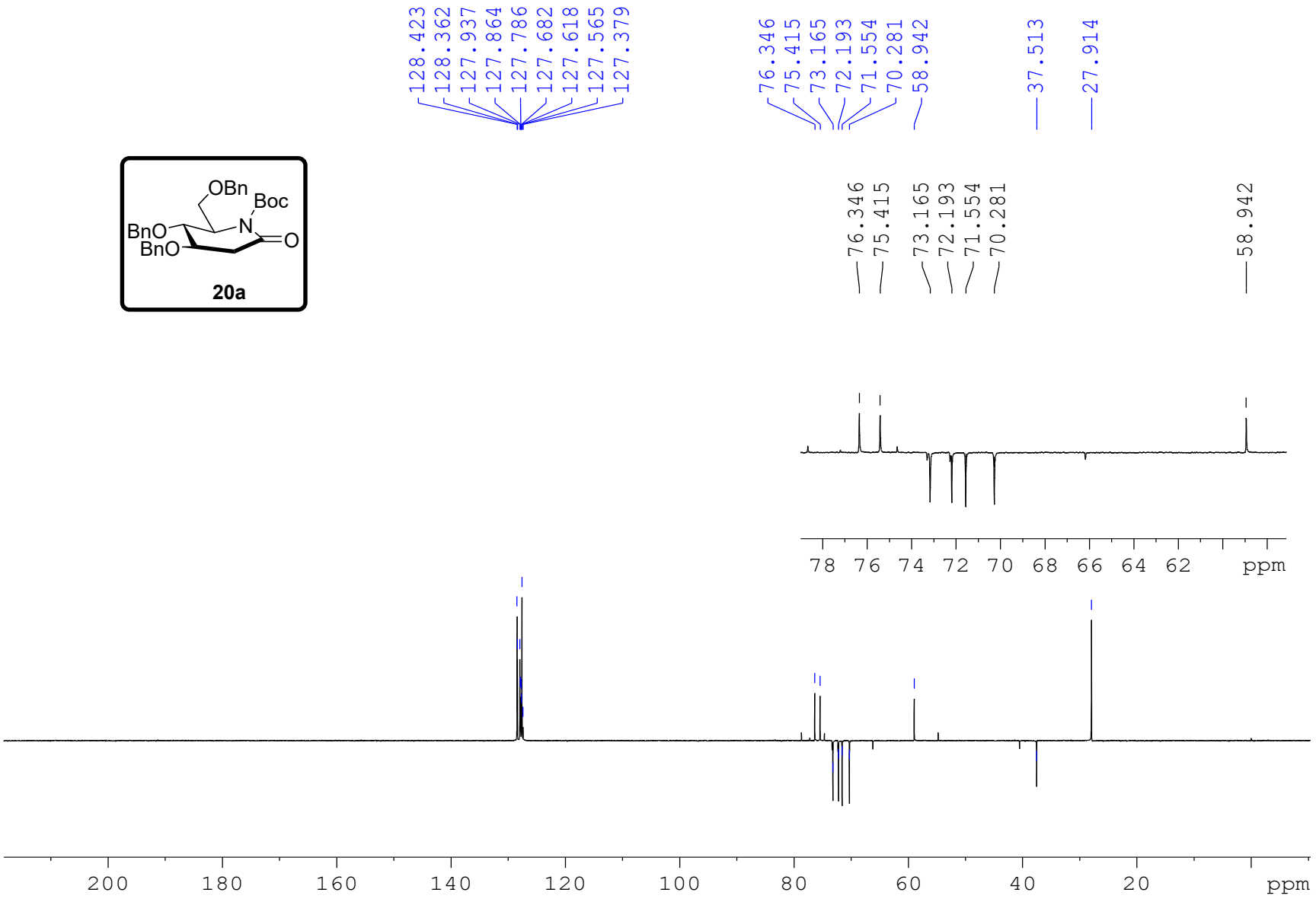
^{1}H NMR of **20a** (500 MHz, $CDCl_3$)



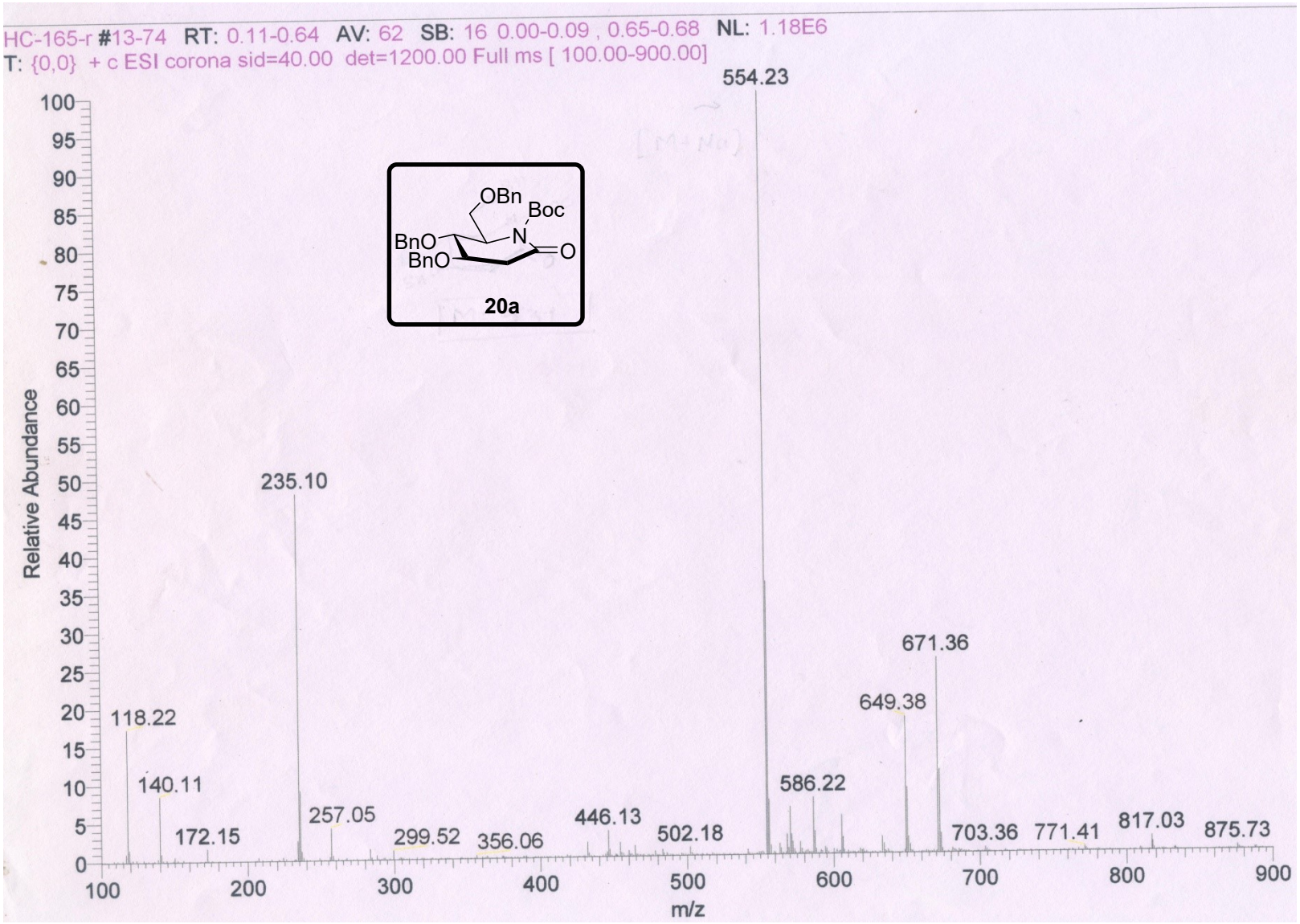
^{13}C NMR of **20a** (125 MHz, $CDCl_3$)



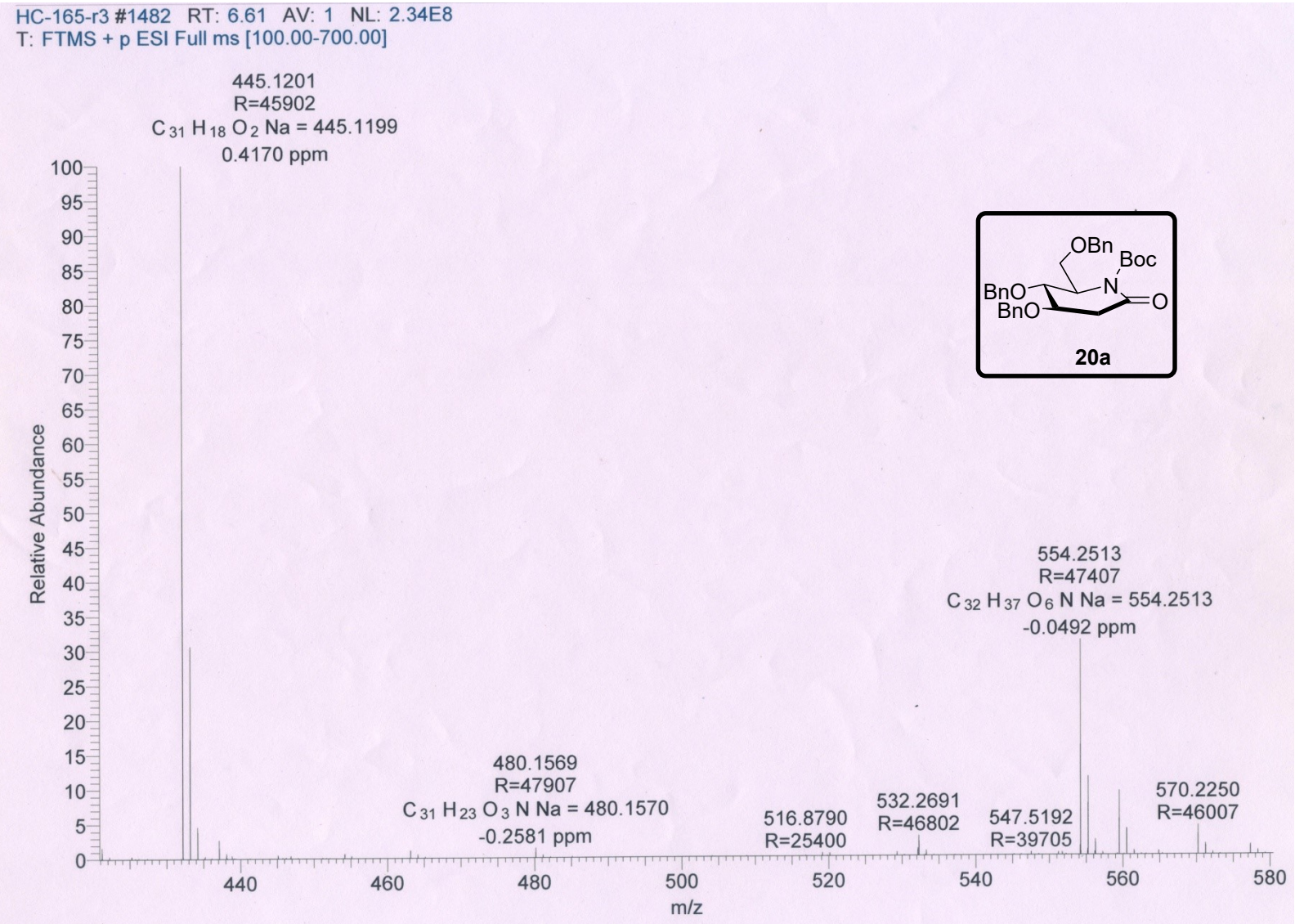
DEPT of **20a** (125 MHz, $CDCl_3$)



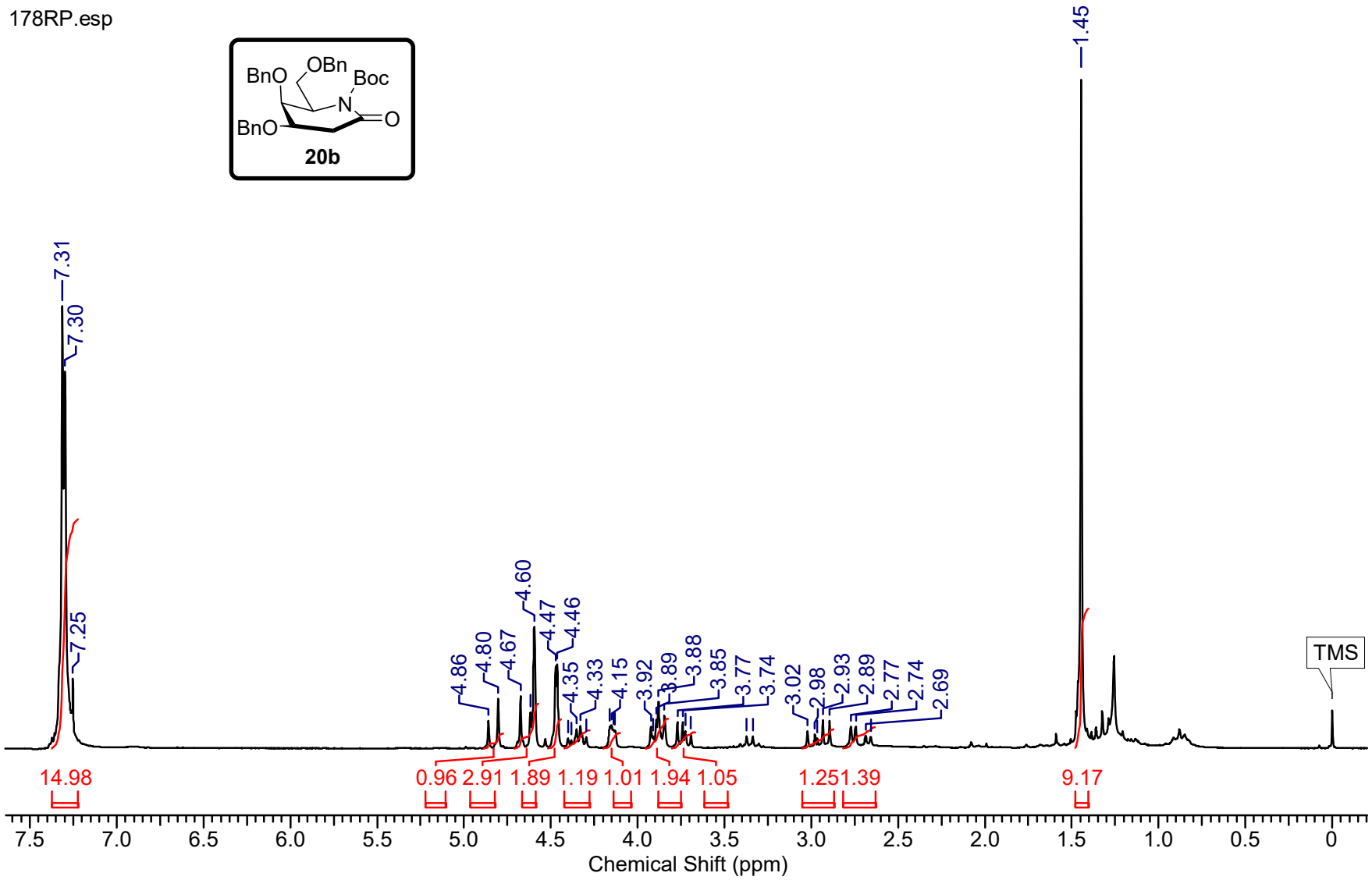
ESI-MS of **20a**


HC-165-r #13-74 RT: 0.11-0.64 AV: 62 SB: 16 0.00-0.09 , 0.65-0.68 NL: 1.18E6
T: {0,0} + c ESI corona sid=40.00 det=1200.00 Full ms [100.00-900.00]
OBn
Boc
N
BnO
BnO
O
20a
Relative Abundance
m/z
554.23
235.10
671.36
649.38
118.22
140.11
586.22
257.05
446.13
172.15
299.52
356.06
502.18
703.36
771.41
817.03
875.73

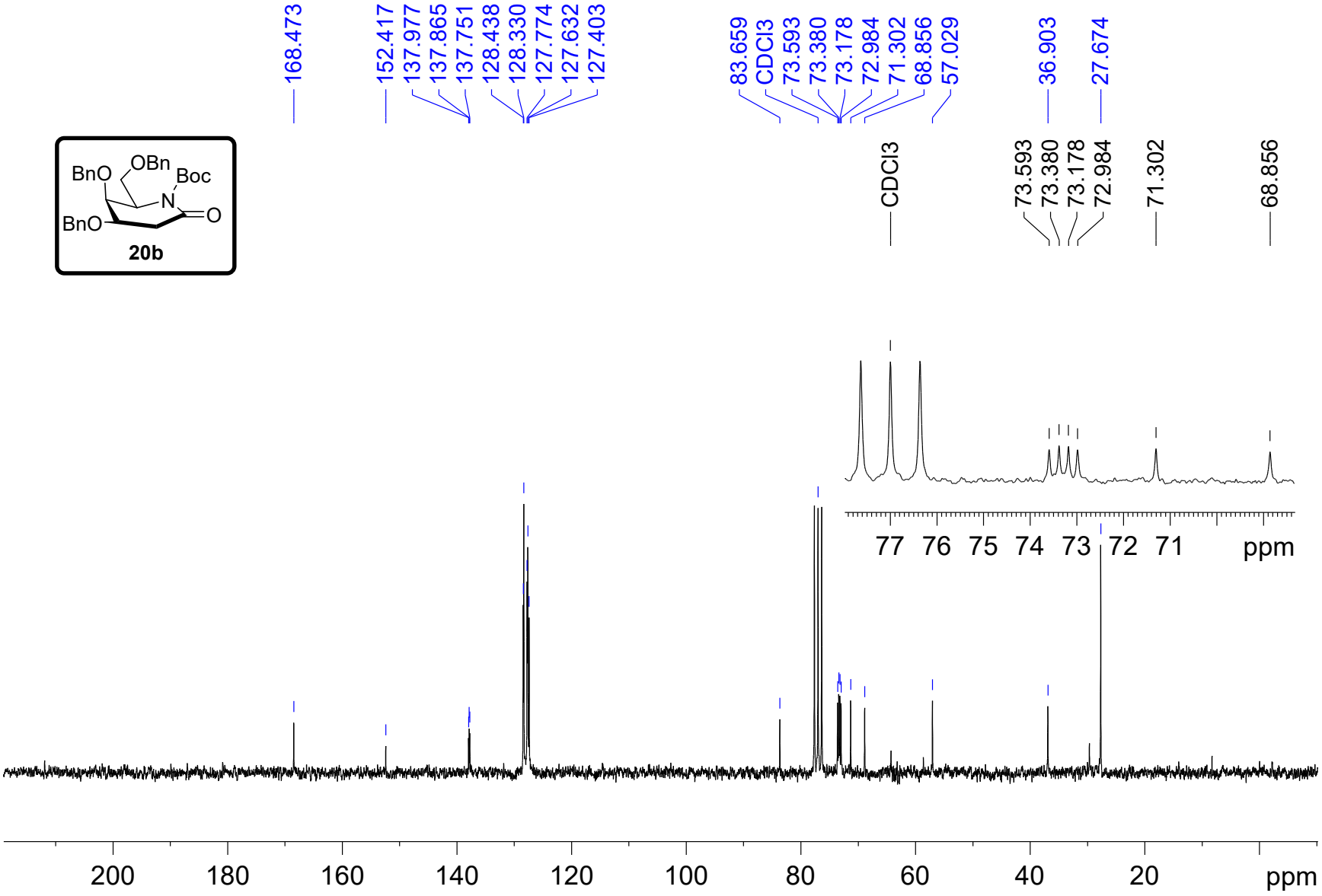
HRMS (ESI) of **20a**



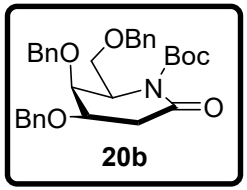
^{1}H NMR of **20b** (200 MHz, $CDCl_3$)



^{13}C NMR of **20b** (50 MHz, $CDCl_3$)

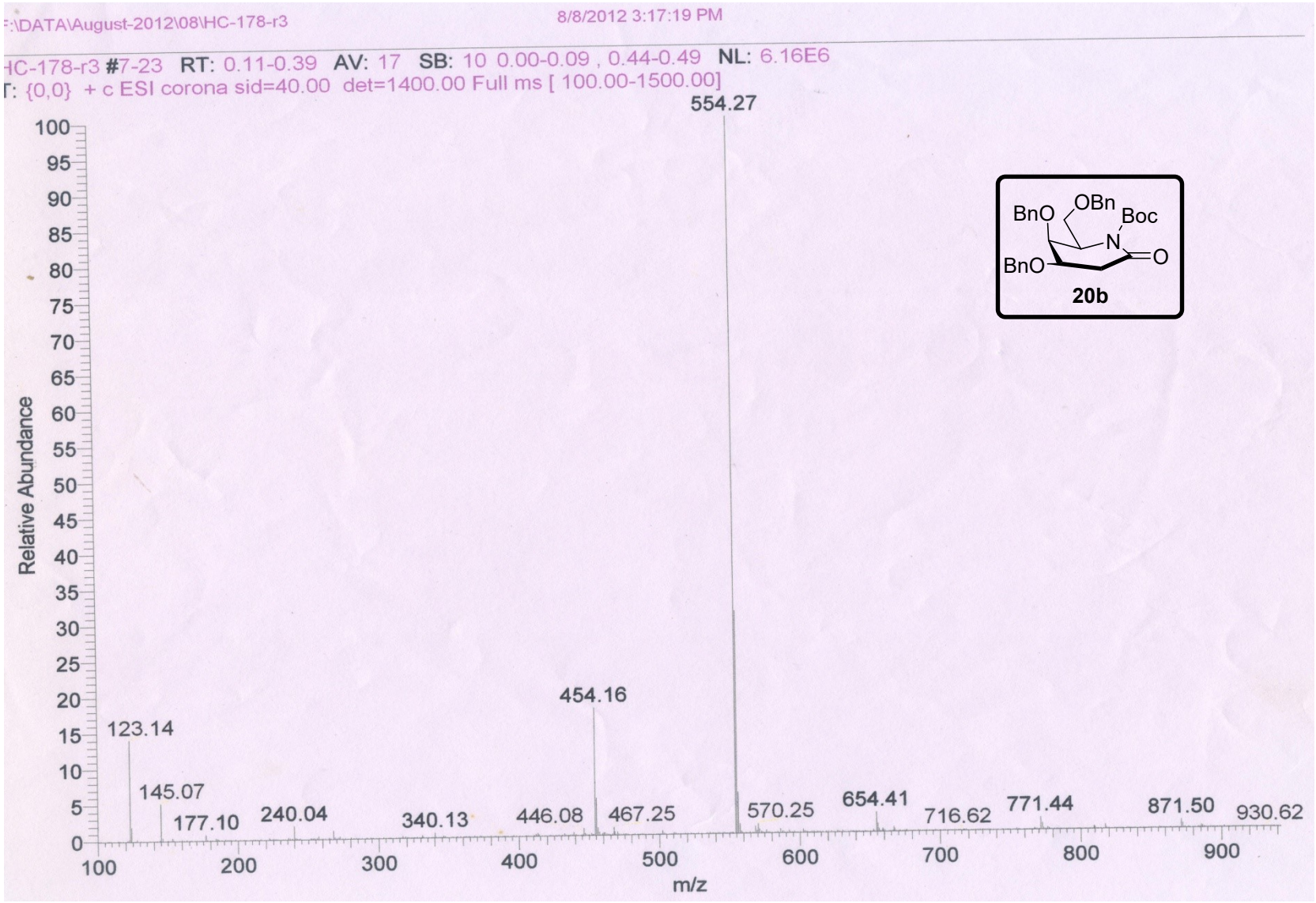


DEPT of **20b** (50 MHz, $CDCl_3$)

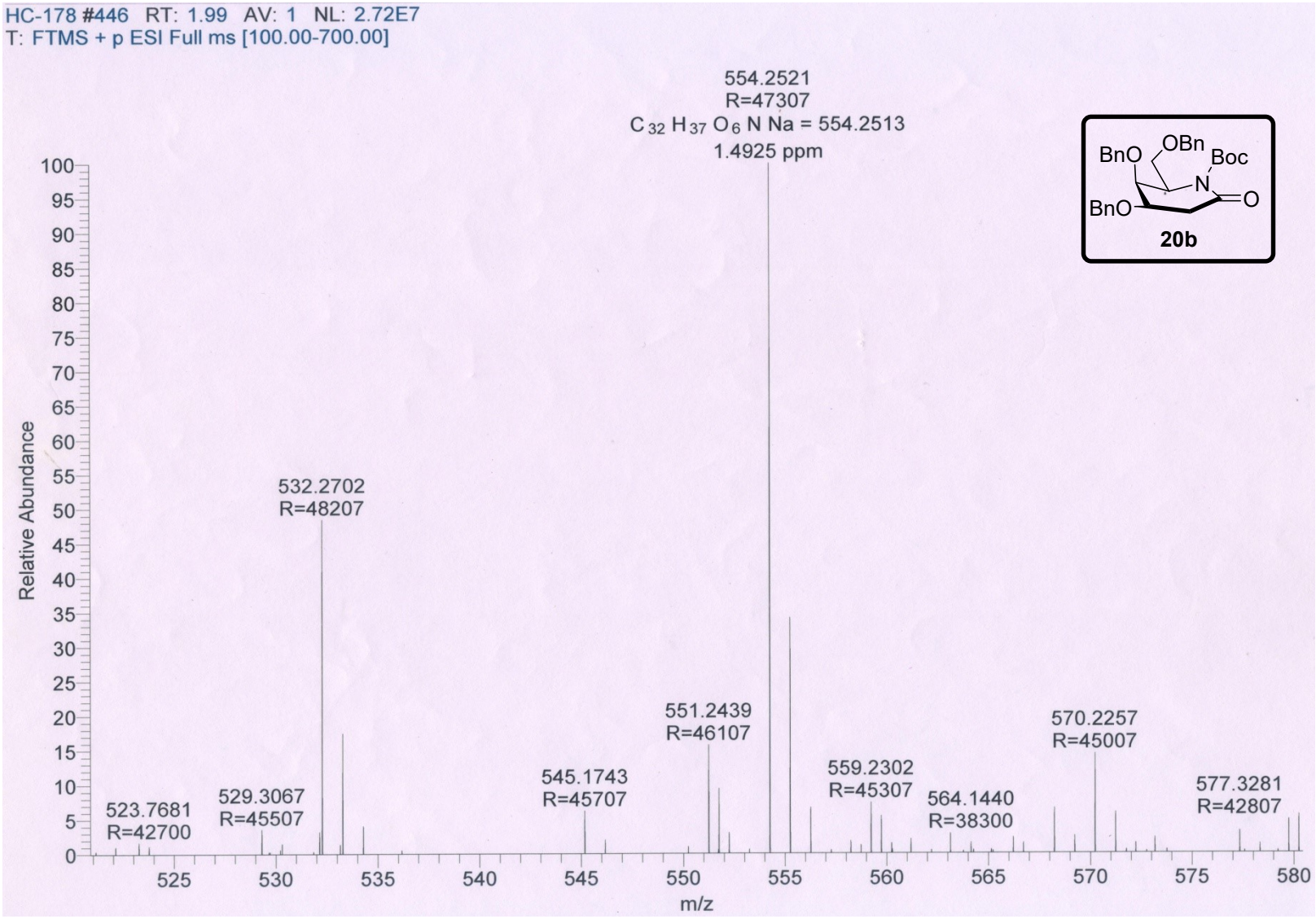


20b

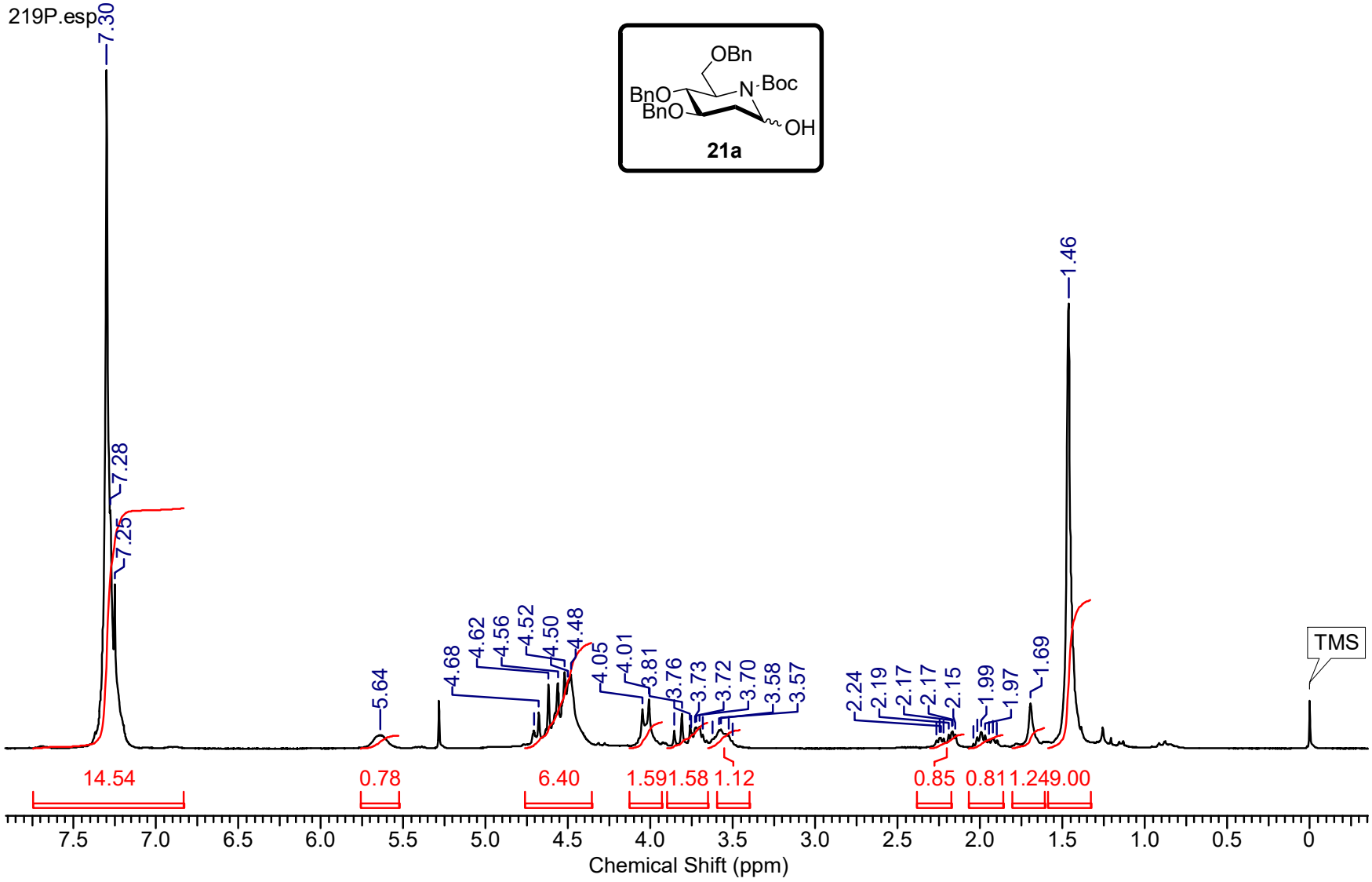
ESI-MS of **20b**


F:\DATA\August-2012\08\HC-178-r3
8/8/2012 3:17:19 PM
HC-178-r3 #7-23 RT: 0.11-0.39 AV: 17 SB: 10 0.00-0.09 , 0.44-0.49 NL: 6.16E6
Γ: {0,0} + c ESI corona sid=40.00 det=1400.00 Full ms [100.00-1500.00]
554.27
454.16
123.14
145.07
177.10
240.04
340.13
446.08
467.25
570.25
654.41
716.62
771.44
871.50
930.62
Relative Abundance
m/z
BnO
OBn
Boc
N
O
BnO
20b

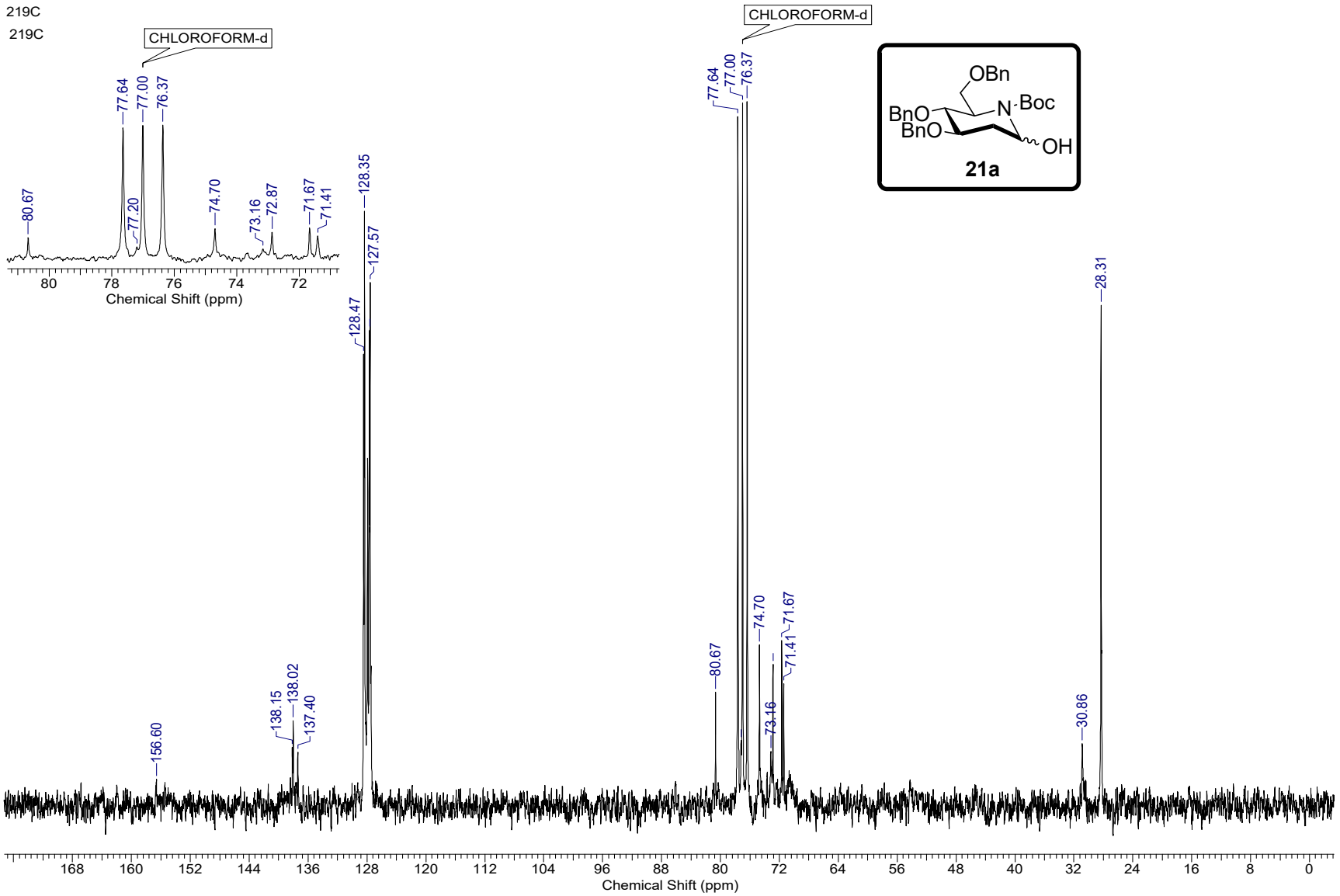
HRMS of **20b**


HC-178 #446 RT: 1.99 AV: 1 NL: 2.72E7
T: FTMS + p ESI Full ms [100.00-700.00]
554.2521
R=47307
C 32 H 37 O 6 N Na = 554.2513
1.4925 ppm
BnO
OBn
Boc
N
O
BnO
20b
532.2702
R=48207
523.7681
R=42700
529.3067
R=45507
545.1743
R=45707
551.2439
R=46107
559.2302
R=45307
564.1440
R=38300
570.2257
R=45007
577.3281
R=42807
Relative Abundance
m/z

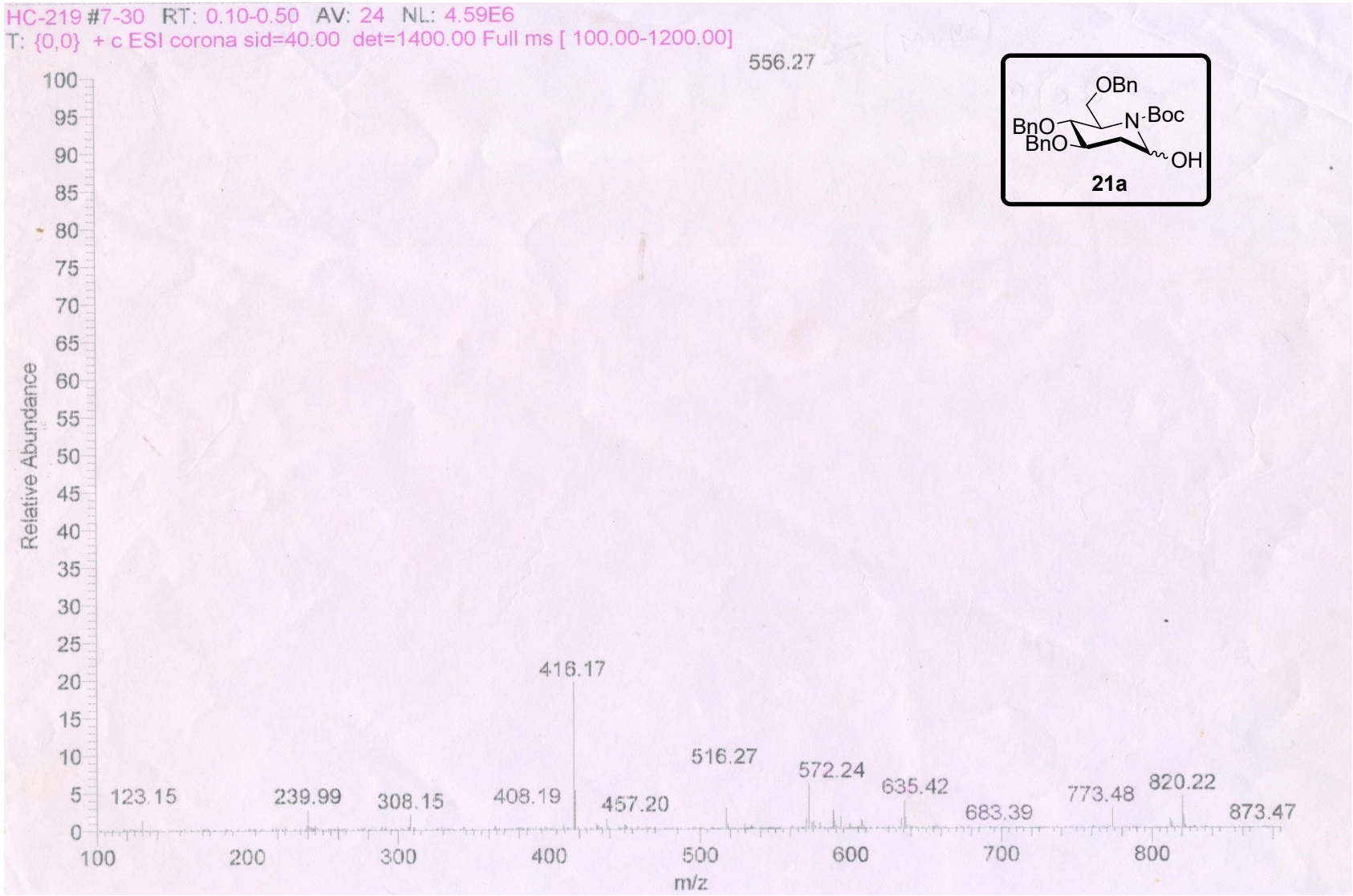
^{1}H NMR of **21a** (200 MHz, $CDCl_3$)



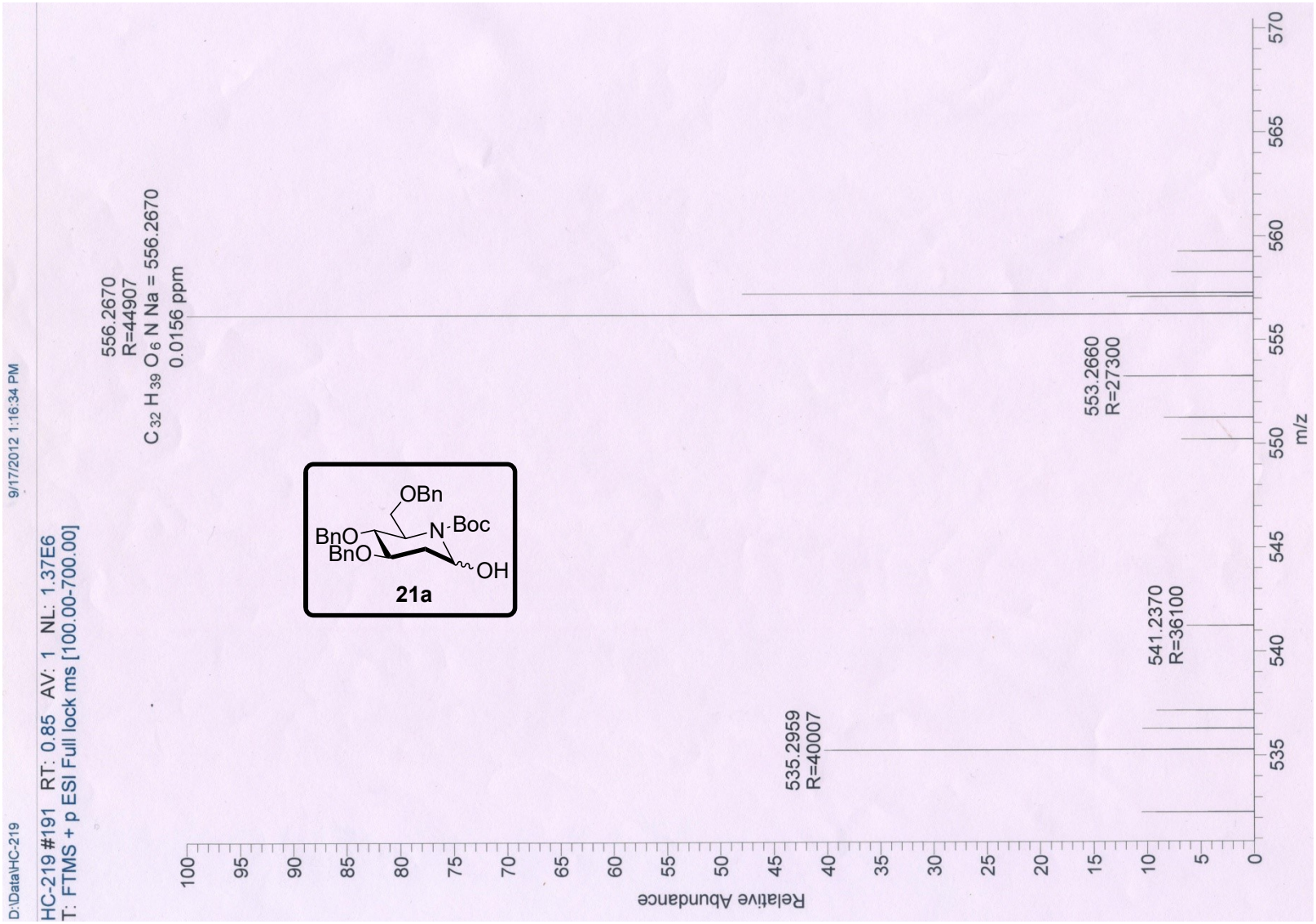
^{13}C NMR of **21a** (50 MHz, $CDCl_3$)



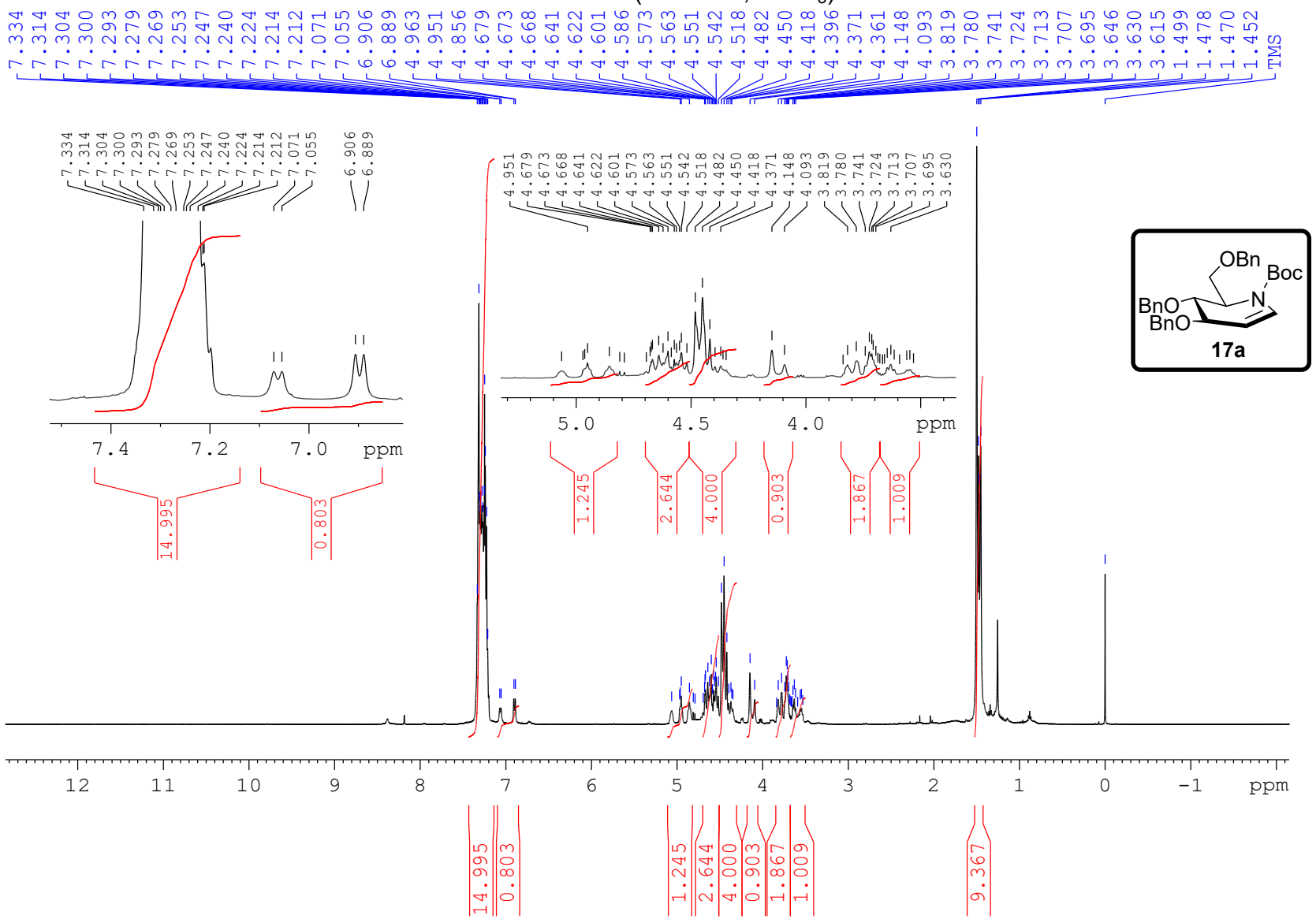
ESI-MS of **21a**

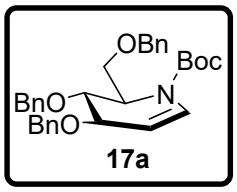

HC-219 #7-30 RT: 0.10-0.50 AV: 24 NL: 4.59E6
T: {0,0} + c ESI corona sid=40.00 det=1400.00 Full ms [100.00-1200.00]
556.27
OBn
BnO
BnO
N·Boc
OH
21a
Relative Abundance
m/z
416.17
516.27
572.24
635.42
123.15
239.99
308.15
408.19
457.20
683.39
773.48
820.22
873.47

HRMS (ESI) of **21a**



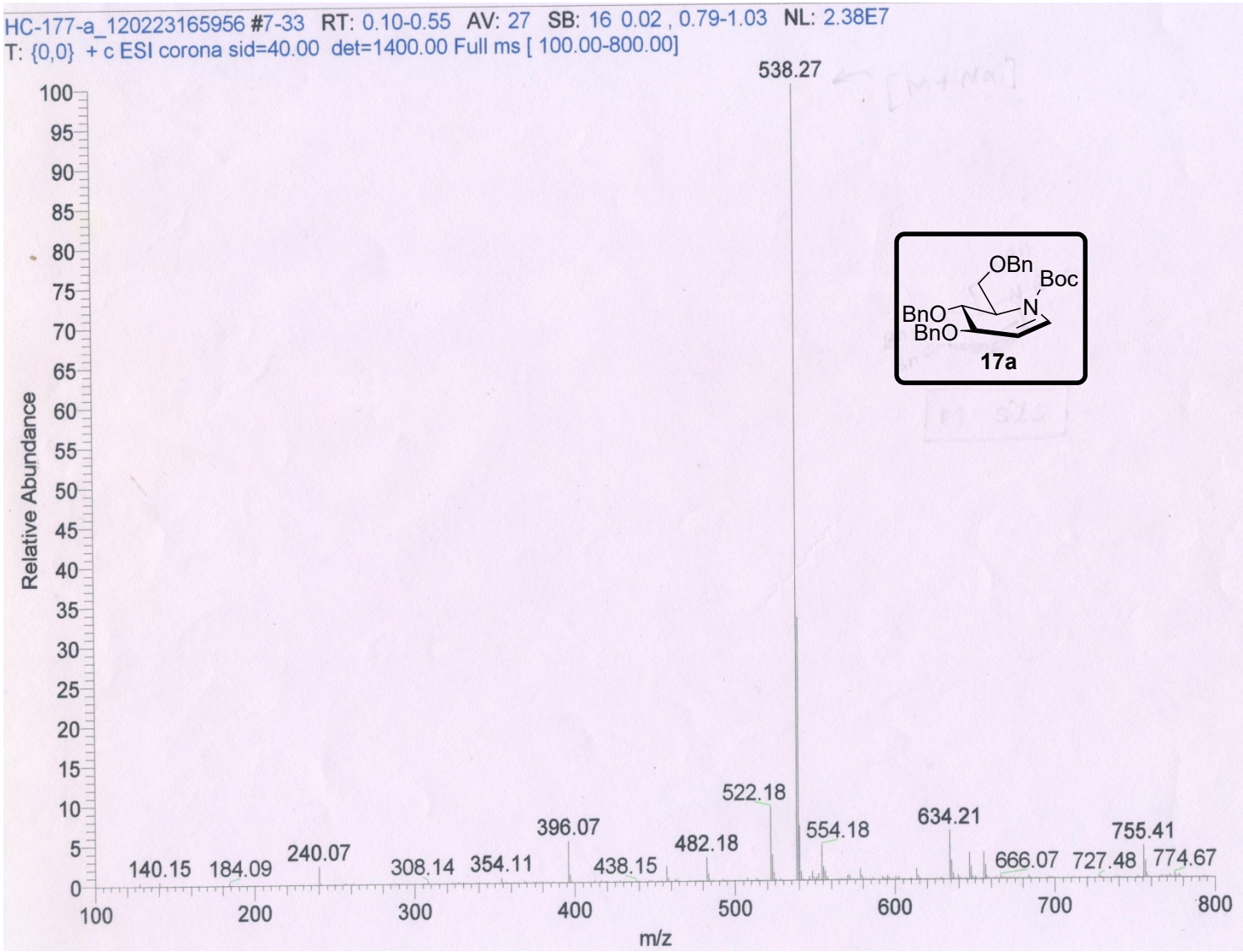
^{1}H NMR of **17a** (500 MHz, $CDCl_3$)



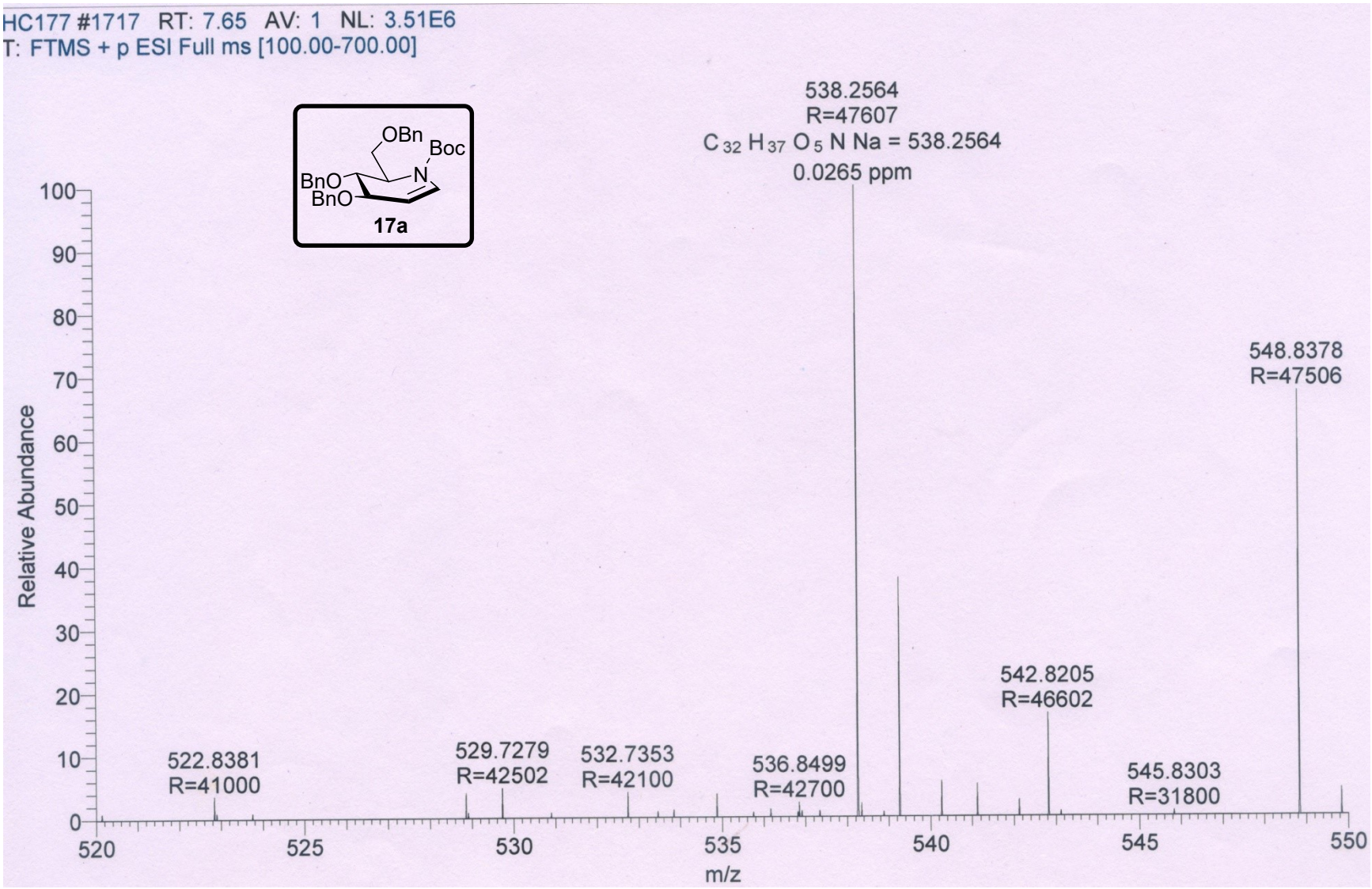


^{13}C NMR of **17a** (125 MHz, $CDCl_3$)

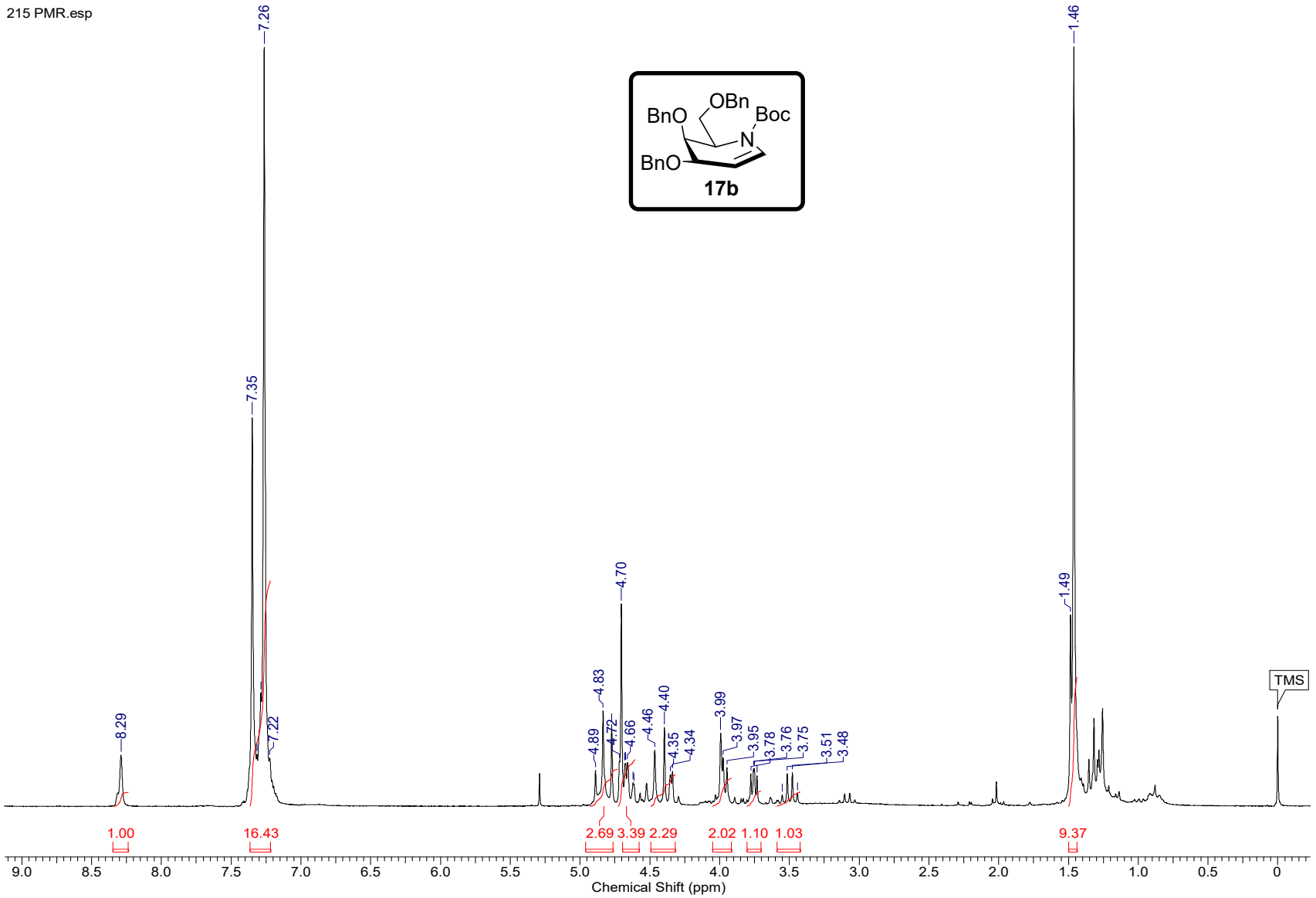
ESI-MS of **17a**


HC-177-a_120223165956 #7-33 RT: 0.10-0.55 AV: 27 SB: 16 0.02 , 0.79-1.03 NL: 2.38E7
T: {0,0} + c ESI corona sid=40.00 det=1400.00 Full ms [100.00-800.00]
538.27
522.18
396.07
634.21
554.18
482.18
755.41
240.07
140.15
184.09
308.14
354.11
438.15
666.07
727.48
774.67
Relative Abundance
m/z
OBn
Boc
N
BnO
BnO
17a

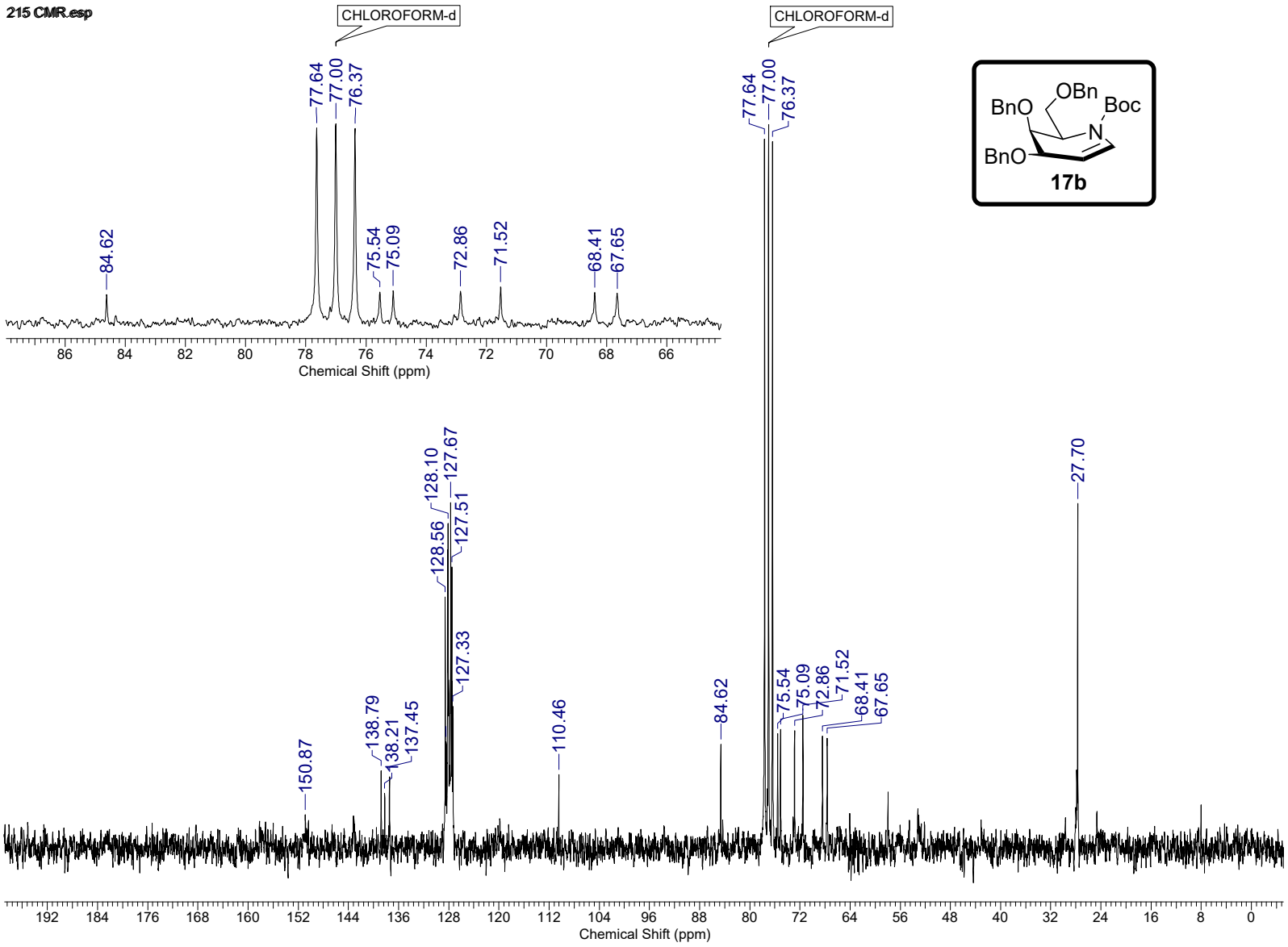
HRMS (ESI) of **17a**



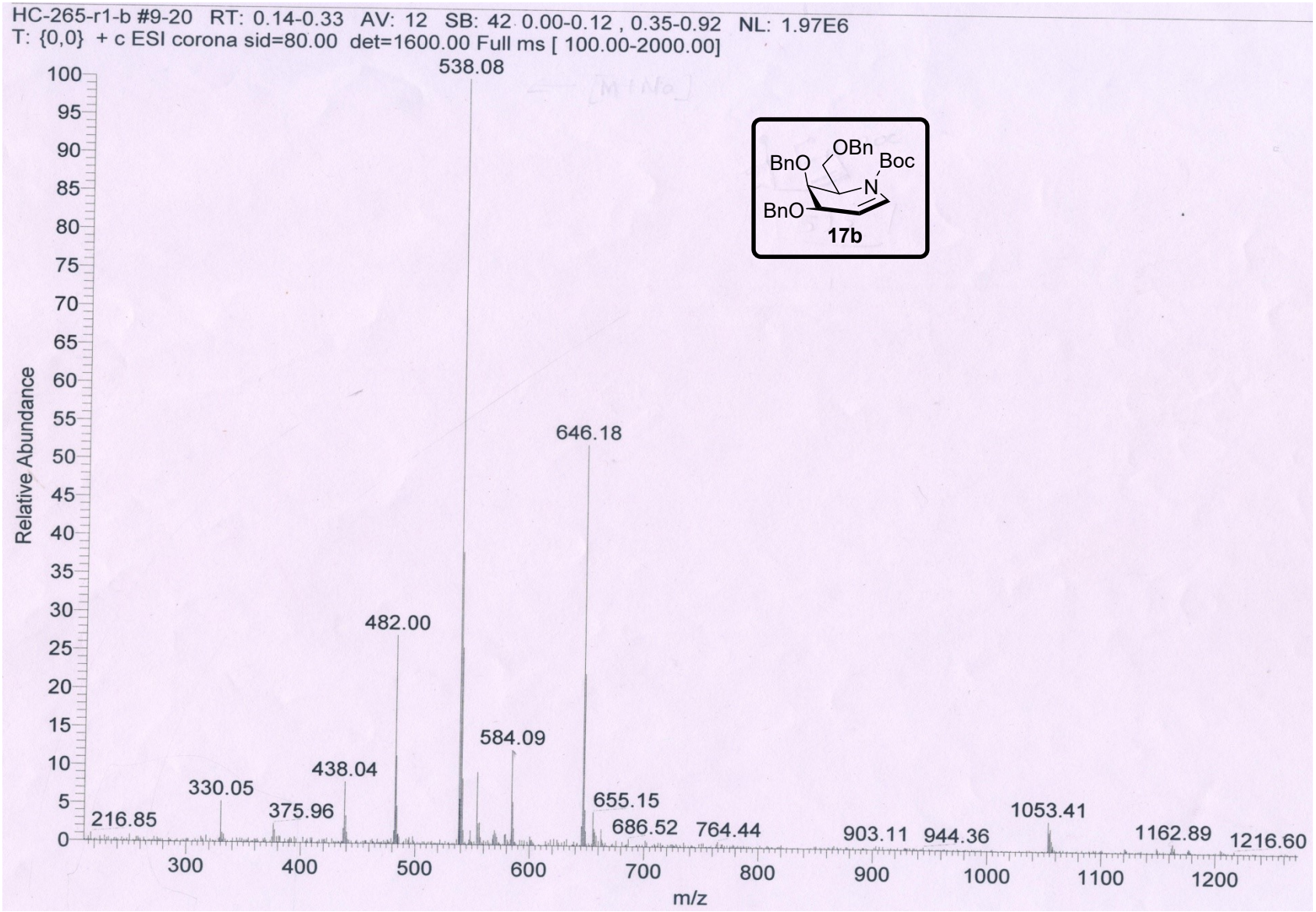
^{1}H NMR of **17b** (200 MHz, $CDCl_3$)



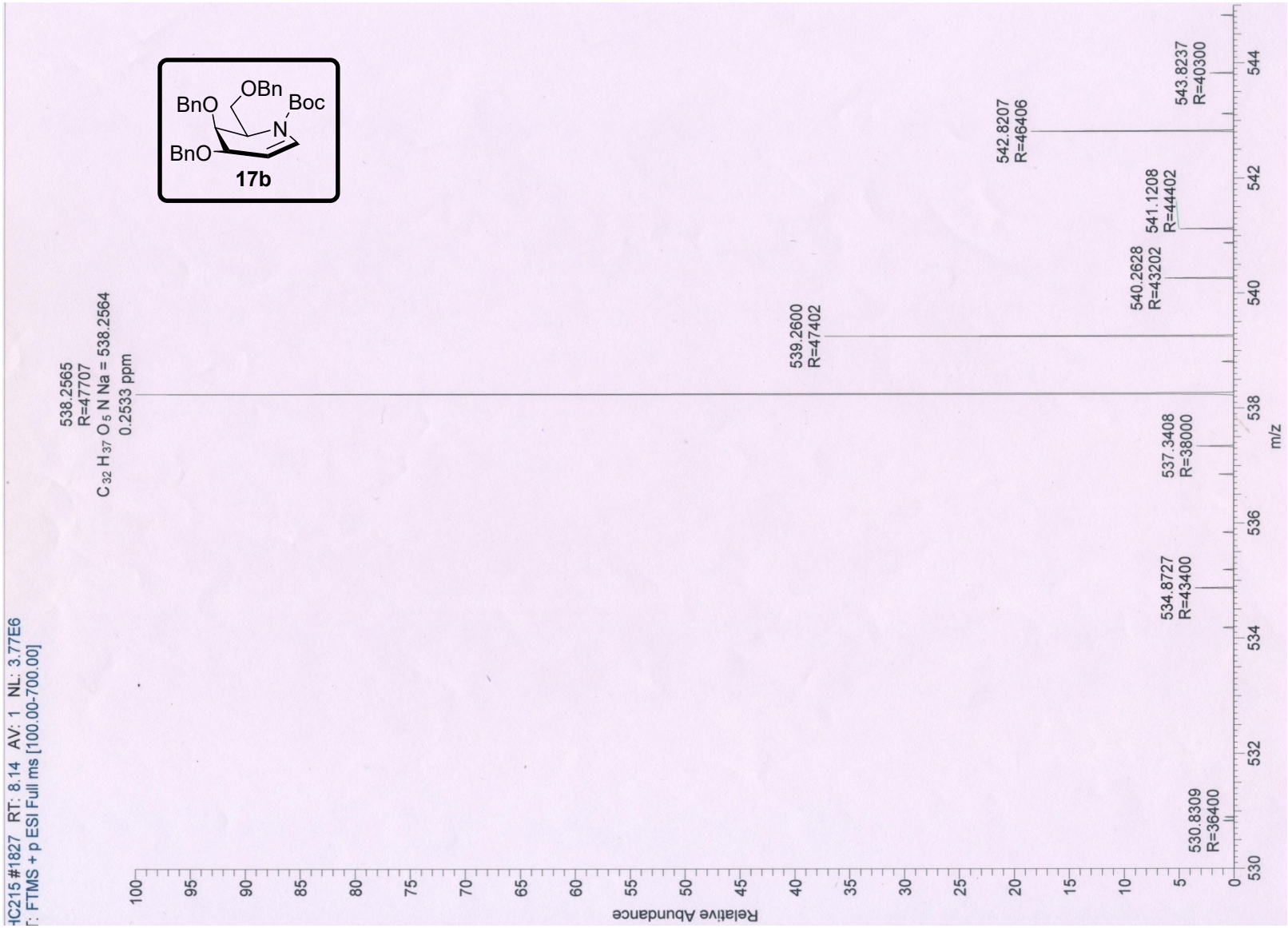
^{13}C NMR of **17b** (50 MHz, $CDCl_3$)



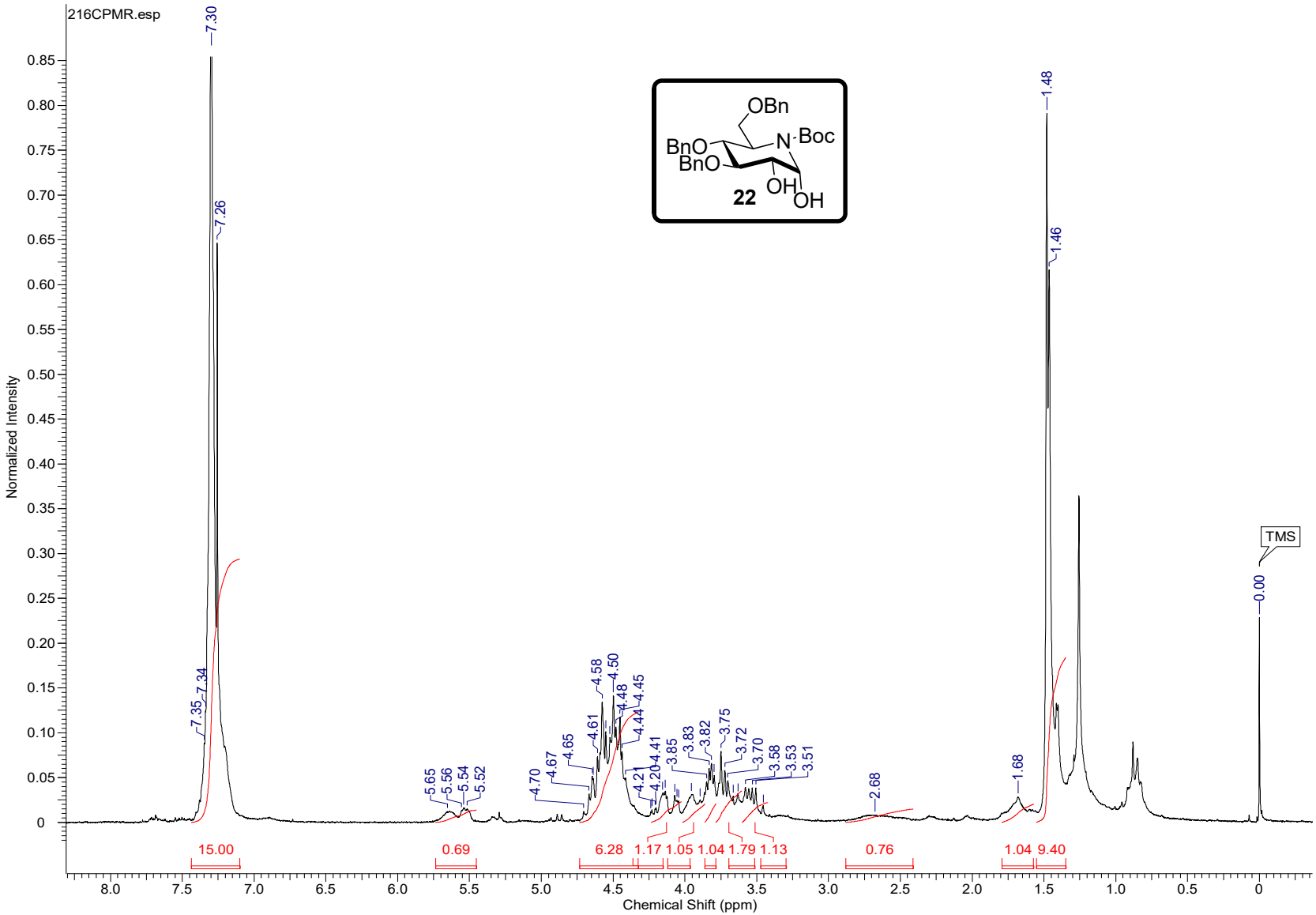
ESI-MS of **17b**


HC-265-r1-b #9-20 RT: 0.14-0.33 AV: 12 SB: 42 0.00-0.12 , 0.35-0.92 NL: 1.97E6
T: {0,0} + c ESI corona sid=80.00 det=1600.00 Full ms [100.00-2000.00]
Relative Abundance
m/z
538.08
646.18
482.00
584.09
438.04
330.05
375.96
216.85
655.15
686.52
764.44
903.11
944.36
1053.41
1162.89
1216.60
OBn
BnO
Boc
N
BnO
17b

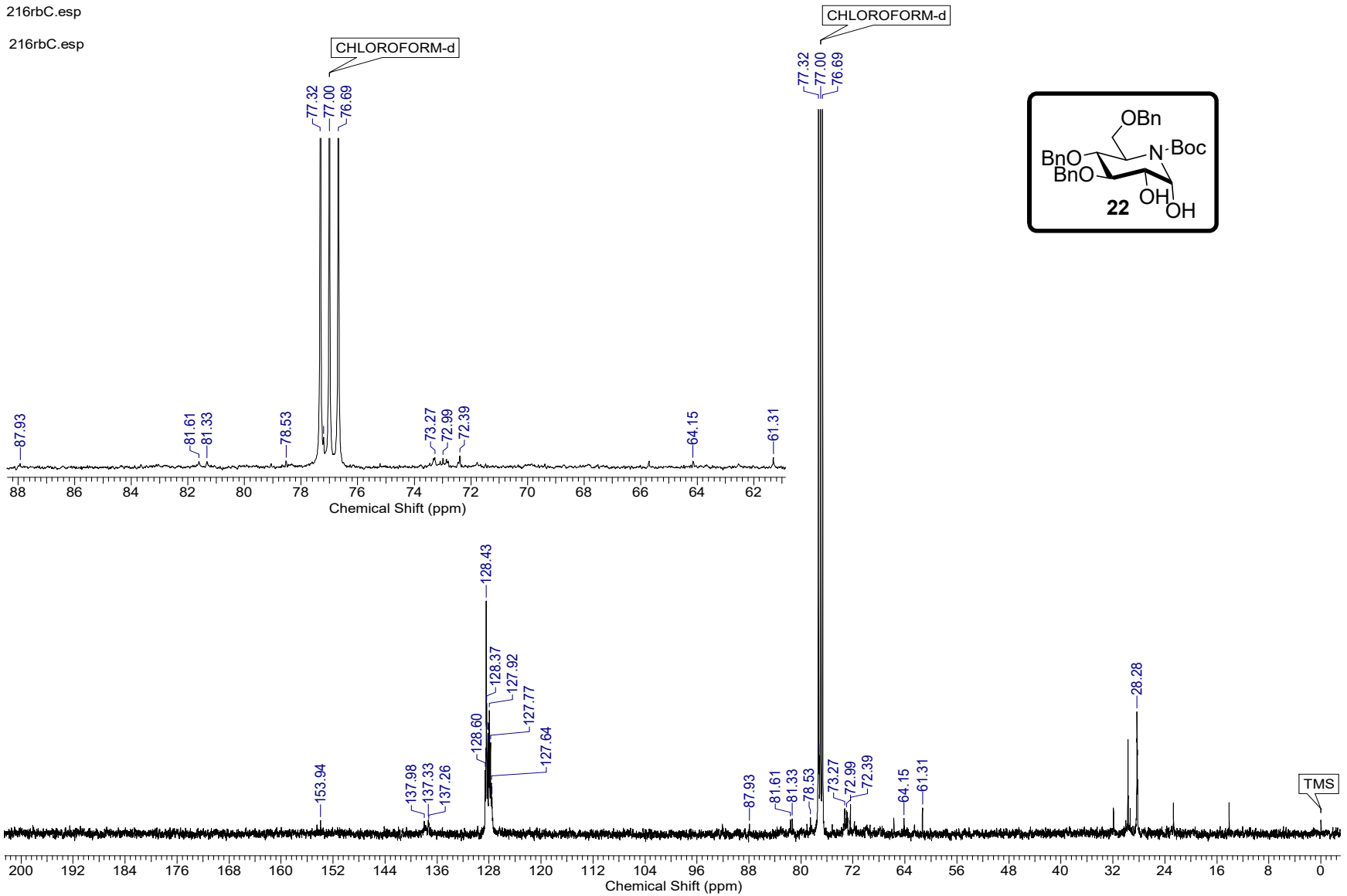
HRMS (ESI) of **17b**



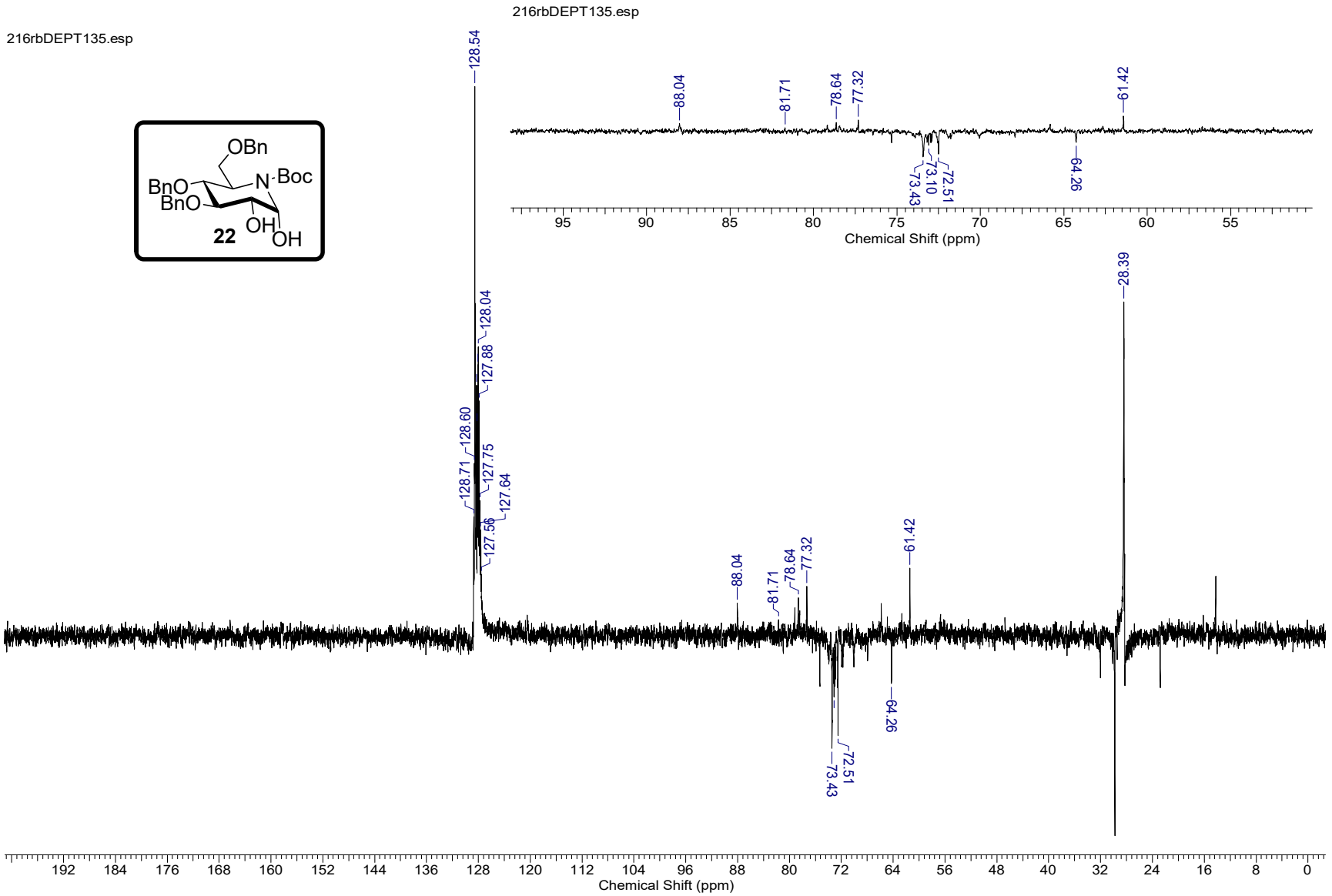
^{1}H NMR of **22** (200MHz, $CDCl_3$)



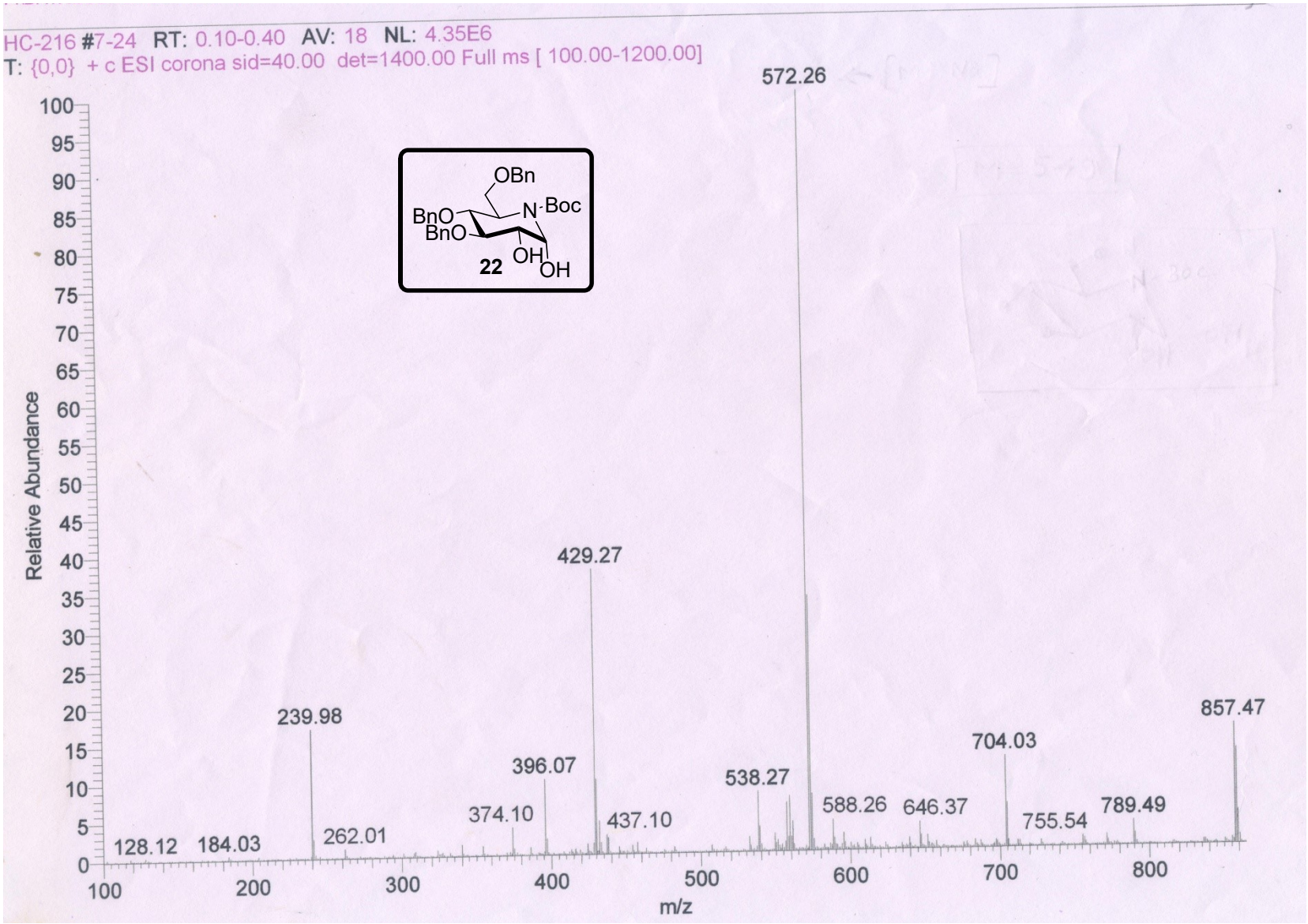
^{13}C NMR of **22** (50MHz, $CDCl_3$)


216rbC.esp
216rbC.esp
CHLOROFORM-d
77.32
77.00
76.69
87.93
81.61
81.33
78.53
73.27
72.99
72.39
64.15
61.31
Chemical Shift (ppm)
CHLOROFORM-d
77.32
77.00
76.69
OBn
BnO
BnO
N·Boc
OH
OH
22
128.43
128.37
127.92
127.77
128.60
127.64
153.94
137.98
137.33
137.26
87.93
81.61
81.33
78.53
73.27
72.99
72.39
64.15
61.31
28.28
TMS
Chemical Shift (ppm)

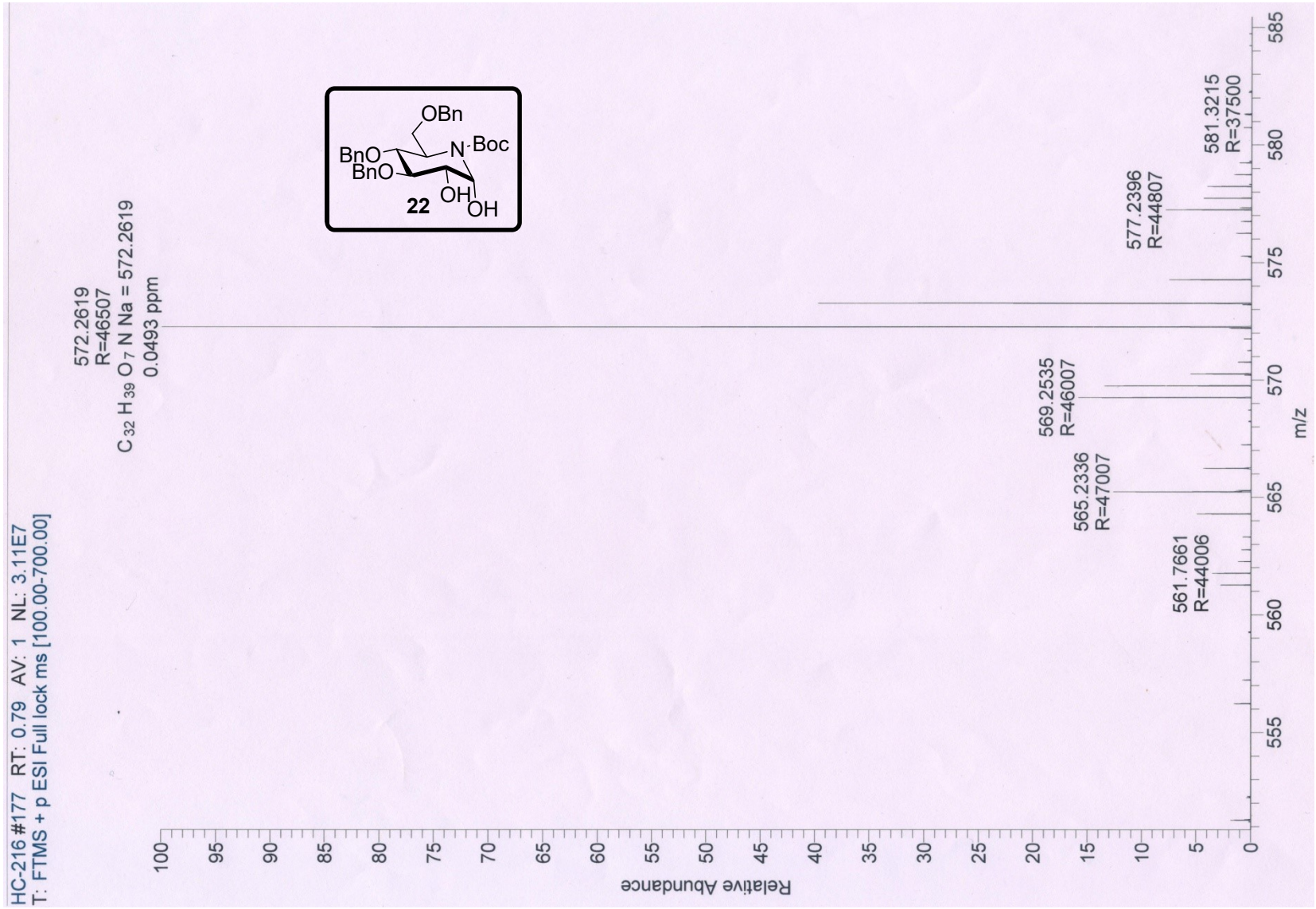
DEPT of **22** (100MHz, $CDCl_3$)



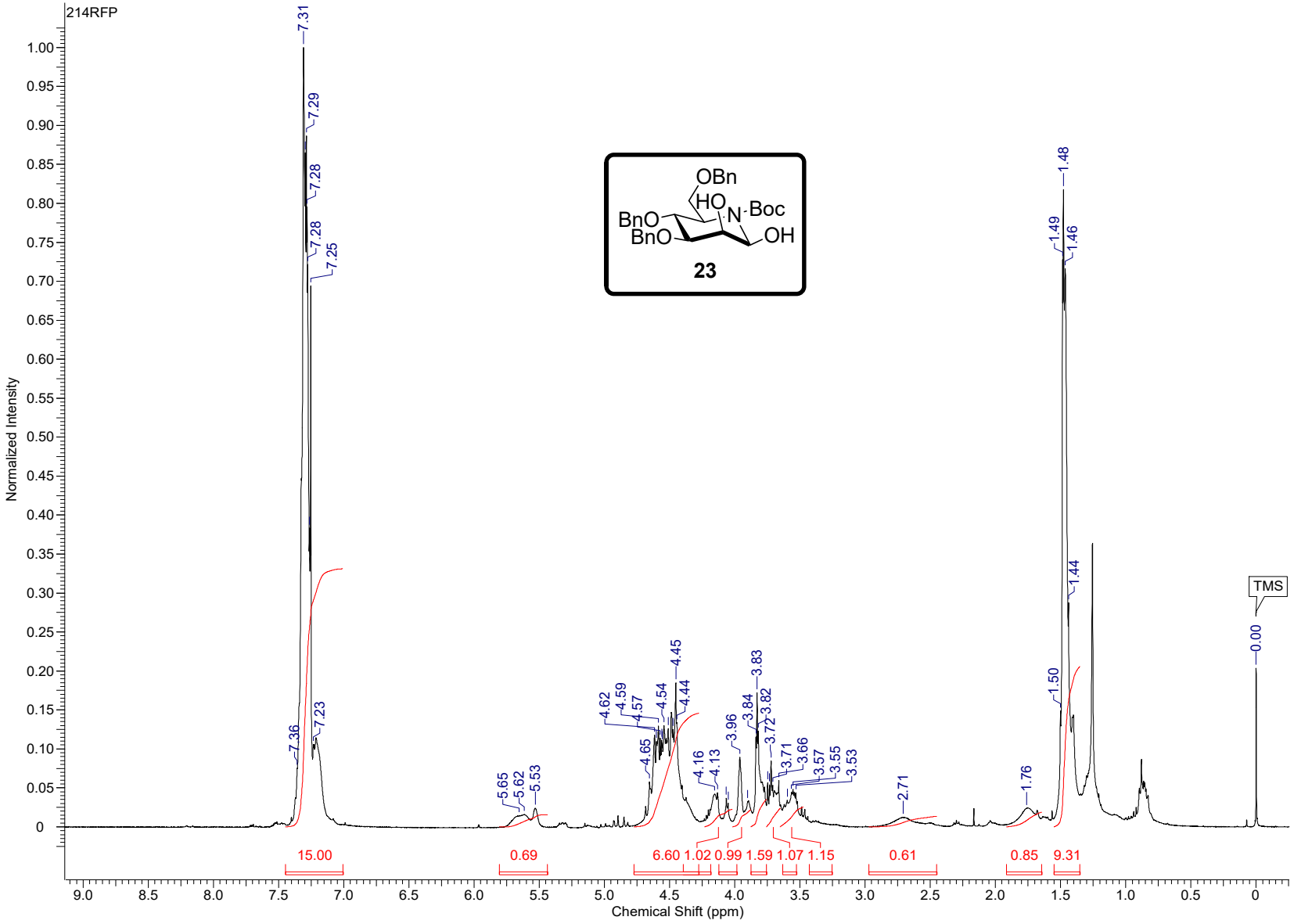
ESI-MS of **22**


HC-216 #7-24 RT: 0.10-0.40 AV: 18 NL: 4.35E6
T: {0,0} + c ESI corona sid=40.00 det=1400.00 Full ms [100.00-1200.00]
OBn
BnO
BnO
N·Boc
OH
OH
22
Relative Abundance
m/z
572.26
429.27
239.98
396.07
538.27
704.03
857.47
374.10
437.10
588.26
646.37
755.54
789.49
128.12
184.03
262.01

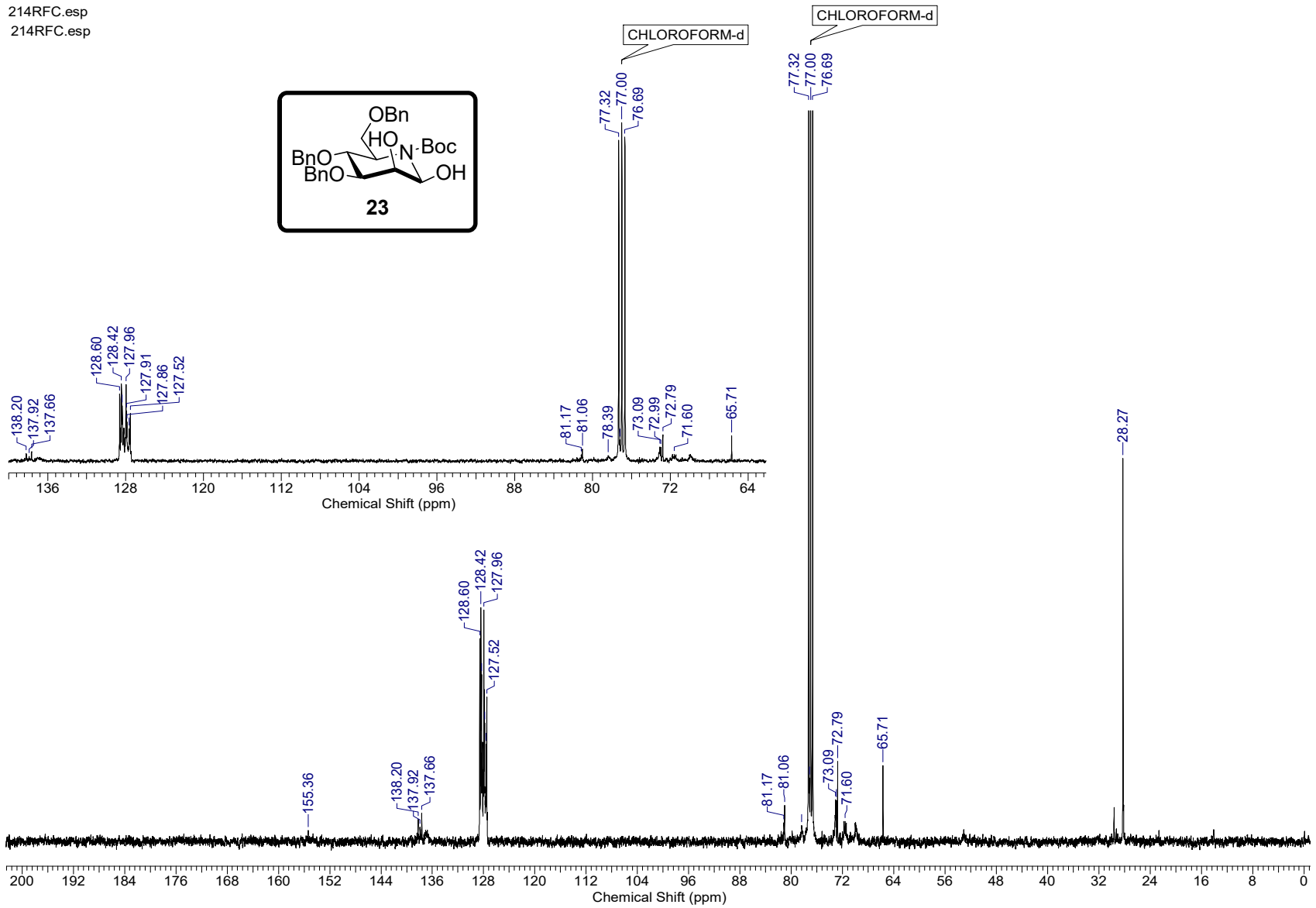
HRMS (ESI) of **22**



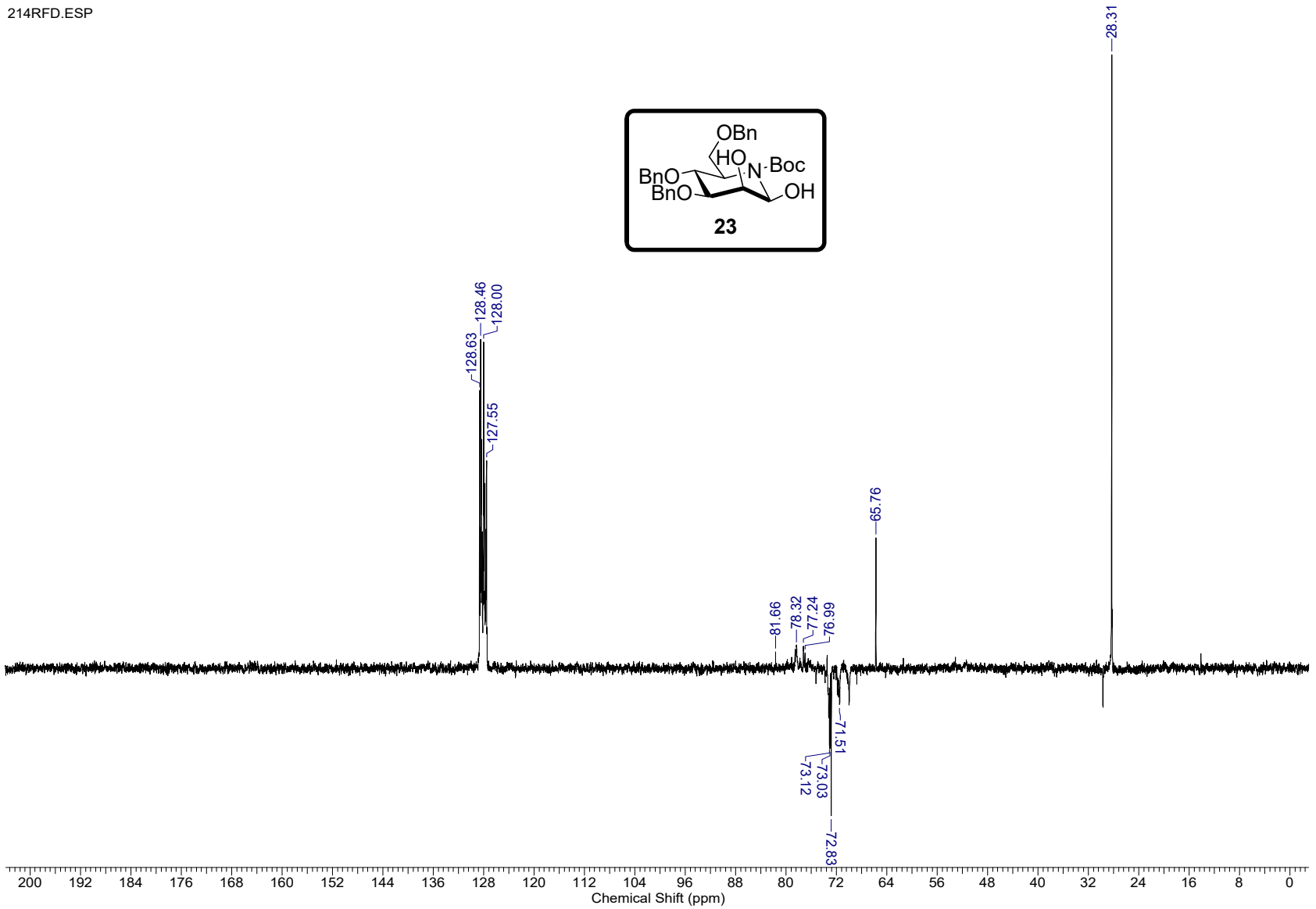
^{1}H NMR of **23** (400MHz, $CDCl_3$)



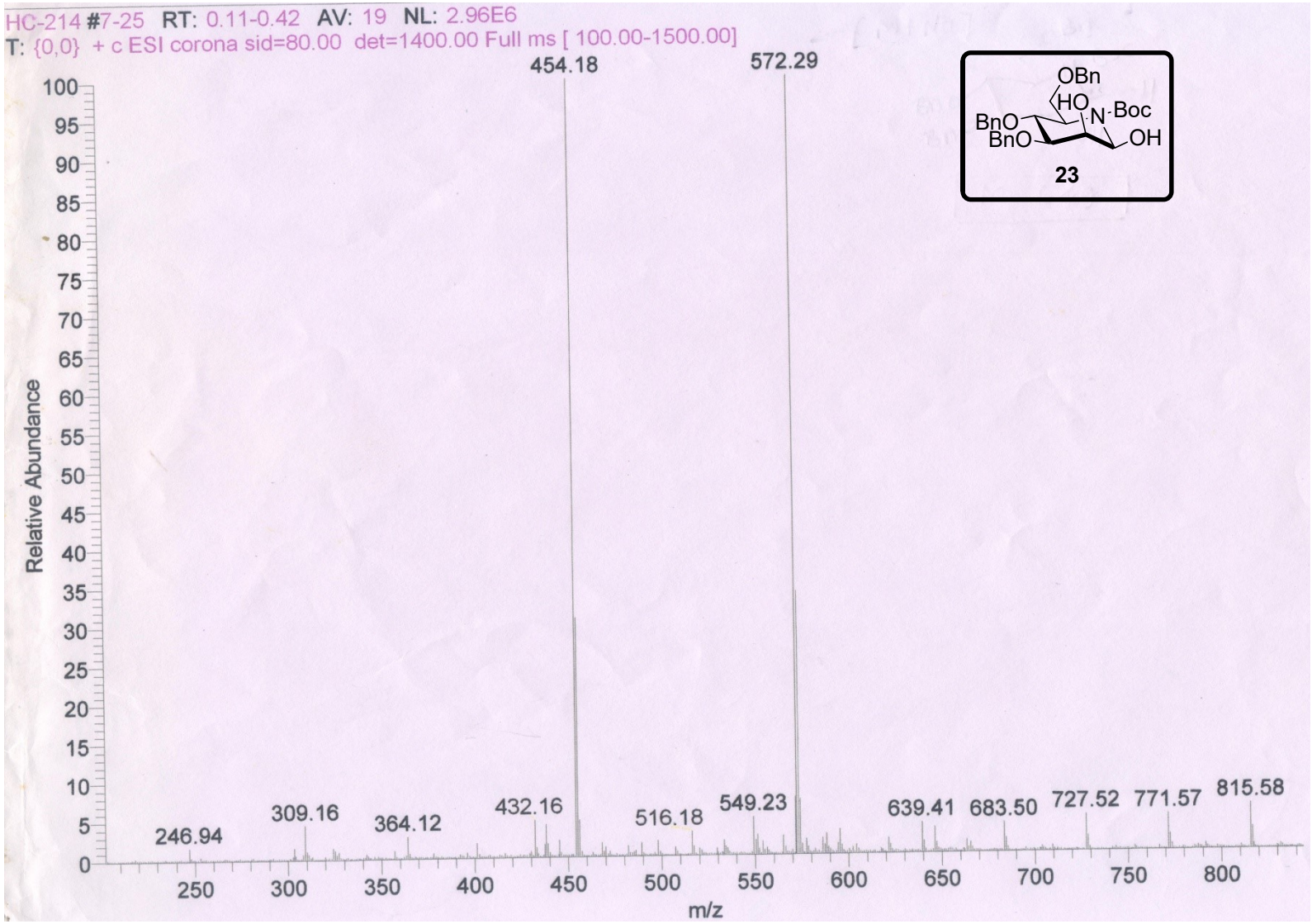
^{13}C NMR of **23** (100MHz, $CDCl_3$)



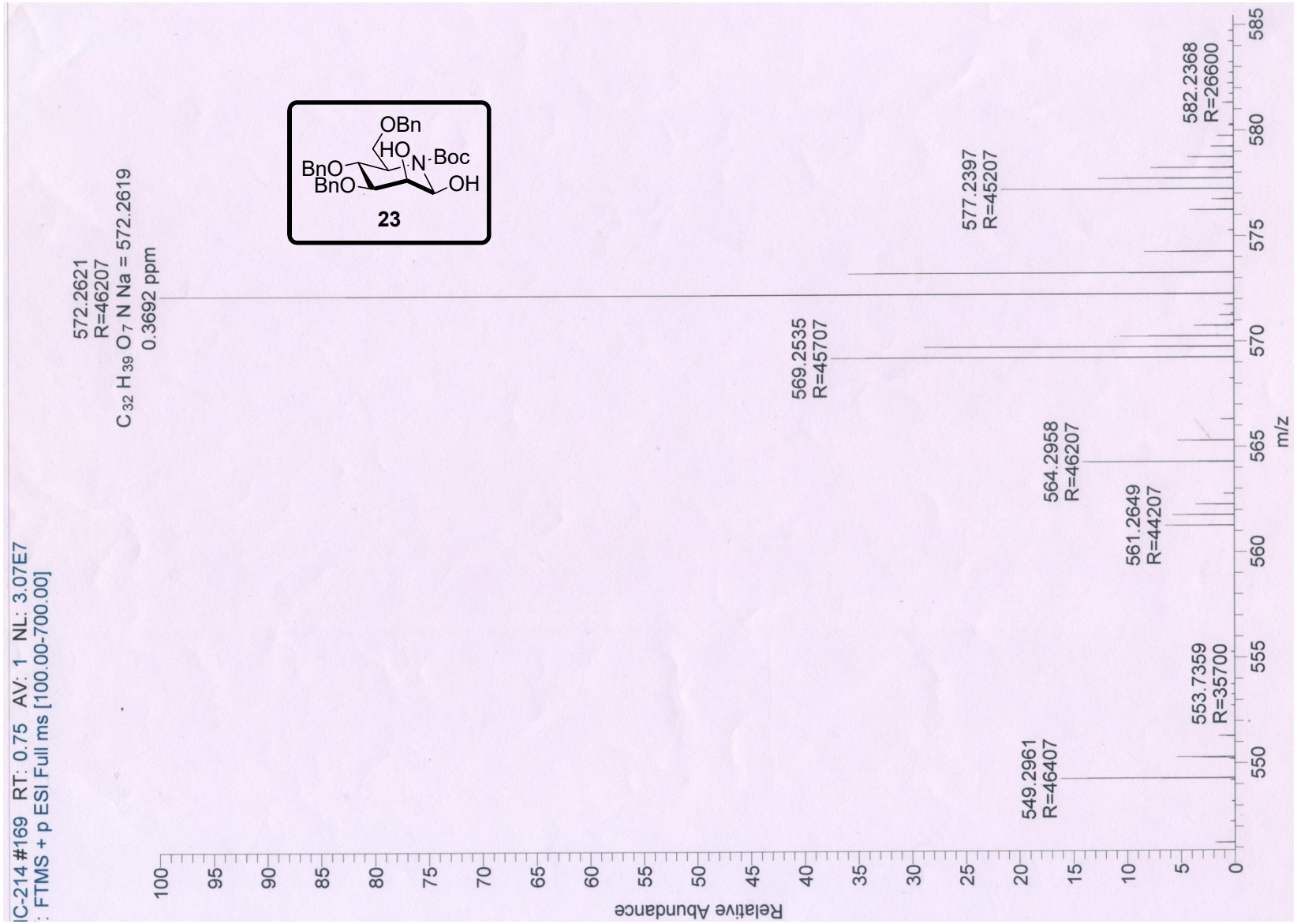
DEPT of **23** (100MHz, $CDCl_3$)



ESI-MS of **23**


HC-214 #7-25 RT: 0.11-0.42 AV: 19 NL: 2.96E6
T: {0,0} + c ESI corona sid=80.00 det=1400.00 Full ms [100.00-1500.00]
454.18
572.29
OBn
HO
N·Boc
BnO
BnO
OH
23
Relative Abundance
m/z
246.94
309.16
364.12
432.16
516.18
549.23
639.41
683.50
727.52
771.57
815.58

HRMS (ESI) of **23**



Computational details

All the minima and transition states, reported in this study, were fully optimized at the M06-2X/6-31G** level of theory[1] using the Gaussian 09 suite of quantum-chemical programs.[2] The stationary points on the potential-energy surface were characterized by evaluating the vibrational frequencies. The transition states were characterized by a single imaginary frequency. The zero-point vibrational energy corrections and thermal corrections were applied to the "bottom-of-the-well" values to obtain values for the Gibbs free energy at the room temperature. The effect of the solvent dielectric on the stability of chemical species was determined by full geometry optimizations in the dielectric continuum of toluene (ε = 2.3741) using the Conductor like Polarization Continuum Model (CPCM),[3] the CPCM (toluene)/M06-2X/6-31G** level of theory. All the energies were calculated with respect to the infinitely separated reactants. However, to investigate the influence of noncovalent interactions on the energetics of this reaction step, the reactant complexes (corresponding to the reactants **20a** and **20b**, see manuscript for the structures) were optimized by keeping the reactive species (**20a/b** with the Super-Hydride) together in a single structure. The same strategy was employed for obtaining the optimized geometries of the final products for the above-specified reaction steps. A direct comparison of the energies of the reactant and the product complexes is expected to minimize the errors in the computation of the translational entropy in determining the relative free energy values. This approach has been applied in several previous studies.[4]

The complete structures of the substrates (**20a/b**) (along with protecting groups, -Bn and -Boc) had been considered, as the benzyl protecting groups are capable of making noncovalent interactions with the cation.[5] Also, considering the presence of the lone pairs (on carbonyl, alkoxy, and ester groups, which may have a differential binding with the cation) and phenyl groups at the substrate, which may interact with a cation and thus alter the energetics, the counter cation of Super-Hydride, Li^+, was included into the calculations. Thus, the cation-π interactions involving Li^+ cation and the benzyl protecting group of the reactants and lone pair – cation interactions involving Li^+ and lone pairs on nearby oxygen atoms of the substrate had been considered to obtain the energetically favourable pathways.

Since the substrates (**20a/b**) are prochiral, the approach of Super-Hydride to both, *re* and *si*, faces of the substrates had been considered, revealing two different modes of the approach of the

Super-Hydride to the substrate. Each mode of approach is associated with two different conformations of reactant and product complexes and the transition state geometry depending upon the relative orientation of the carbamate ester group on the lactam (*N*-Boc protecting group), which coordinates with the Li^+ through one of its oxygen. The conformation in which the Li^+ cation is associated with the alkoxy oxygen of the *N*-Boc group is referred to as conformation C_1 (conformation 1) and the conformation in which the Li^+ cation is linked to the carbonyl moiety of the *N*-Boc group is referred to as conformation C_2 (conformation 2). Please refer to Figures S1 and S2 for the structural details of the conformations C_1 and C_2. A weak cation – π interaction has been seen to be present in all the geometries (mostly the transition state geometries and the product complexes) belonging to conformation 2 of the *re* face approach. Therefore, two different pathways (each with two different conformations of reactant and product complexes and transition state geometries) have been investigated for both the substrates, **20a** and **20b.**

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Table 3. The gas-phase relative energy values in kcal/mol for the reduction of the 2-deoxygluconolactam-*N*-Boc **20a** to 2-deoxygluconolactamol-*N*-Boc **21a**.

Molecular Description			ΔE	Δ(E+ZPE)	ΔH	ΔG
2-deoxygluconolactam-*N*-Boc **20a**	R_S		0.0	0.0	0.0	0.0
	C_1^r	R_C	-39.8	-37.4	-37.8	-21.2
		T_1	-26.8	-24.8	-26.0	-6.1
		I_1	-35.9	-32.6	-33.0	-15.7
	C_2^r	R_C	-44.0	-41.5	-41.9	**-25.5**
		T_1	-29.3	-27.4	-28.4	**-10.4**
		I_1	-47.0	-43.3	-43.6	**-26.7**
	C_1^s	R_C	-36.7	-34.3	-34.7	-16.9
		T_1	-25.1	-23.2	-24.3	-4.8
		I_1	-44.2	-40.7	-41.2	-23.5
	C_2^s	R_C	-43.4	-40.7	-41.3	**-23.0**
		T_1	-31.9	-30.3	-31.5	**-10.5**
		I_1	-52.4	-48.0	-48.8	**-29.7**

Rs, Rc, T_1, I_1 represent infinitely separated reactants, the reactant complex, the transition state and product respectively for this particular step of the reaction.

r and s represent the *re* and *si* faces of the substrate on which the attack of the Super-Hydride occurs. C_1 and C_2 represent two different conformations of the reactant and product complexes and the transition state geometries. The conformation in which the Li^+ cation is associated with the alkoxy oxygen of the *N*-Boc group is referred to as C_1 and the conformation in which the Li^+ cation is linked to the carbonyl moiety of the *N*-Boc group is referred to as C_2.

Table 4. The gas-phase relative energy values in kcal/mol for the reduction of 2-deoxygalactonolactam-*N*-Boc **20b** to 2-deoxygalactonolactamol-*N*-Boc **21b**.

Molecular Description			ΔE	Δ(E+ZPE)	ΔH	ΔG
2-deoxygalactonolactam-*N*-Boc **20b**	R_S		0.0	0.0	0.0	0.0
	C_1^r	R_C	-36.9	-35.2	-35.5	-17.2
		T_1	-18.6	-17.1	-17.9	1.1
		I_1	-27.1	-24.2	-24.3	-9.1
	C_2^r	R_C	-43.1	-41.3	-41.3	**-25.6**
		T_1	-25.6	-24.2	-25.1	**-6.0**
		I_1	-37.9	-34.7	-34.8	**-17.8**
	C_1^s	R_C	-32.3	-31.0	-31.6	-13.2
		T_1	-19.8	-18.7	-19.7	0.7
		I_1	-49.0	-45.1	-45.6	-27.6
	C_2^s	R_C	-36.1	-34.3	-34.5	**-17.8**
		T_1	-27.4	-26.5	-27.4	**-9.3**
		I_1	-49.0	-45.1	-45.6	**-26.6**

R_s, R_c, T_1, I_1 represent infinitely separated reactants, the reactant complex, the transition state and product respectively for this particular step of the reaction.

r and s represent the *re* and *si* faces of the substrate on which the attack of the Super-Hydride occurs. C_1 and C_2 represent two different conformations of the reactant and product complexes and the transition state geometries. The conformation in which the Li^+ cation is associated with

the alkoxy oxygen of the *N*-Boc group is referred to as C_1 and the conformation in which the Li^+ cation is linked to the carbonyl moiety of the *N*-Boc group is referred to as C_2.

Table 5. The solvent-phase relative energy values in kcal/mol for the reduction of 2-deoxyglycolactam-*N*-Boc **20a**/**b** to 2-deoxyglycolactamol-*N*-Boc **21a**/**b**.

Molecular Description			ΔE	Δ(E+ZPE)	ΔH	ΔG
2-deoxygluconolactam-*N*-Boc **20a**	R_S		0.0	0.0	0.0	0.0
	C_2^r	R_C	-34.5	-31.8	-32.2	-15.3
		T_1	-23.9	-22.3	-23.4	-2.5
		I_1	-38.6	-34.8	-35.3	-17.2
	C_2^s	R_C	-33.8	-31.9	-32.3	-15.0
		T_1	-21.4	-19.7	-21.0	0.3
		I_1	-41.7	-38.0	-38.5	-20.9
2-deoxygalactonolactam-*N*-Boc **20b**	R_S		0.0	0.0	0.0	0.0
	C_2^r	R_C	-33.2	-31.6	-31.6	-17.5
		T_1	-16.4	-15.5	-16.2	0.1
		I_1	-32.1	-29.2	-29.3	-13.7
	C_2^s	R_C	-27.7	-26.6	-26.6	-12.7
		T_1	-16.0	-15.2	-16.0	1.6
		I_1	-37.8	-33.9	-34.5	-16.3

R_s, R_c, T_1, I_1 represent infinitely separated reactants, the reactant complex, the transition state and product respectively for this particular step of the reaction.

r and s represent the *re* and *si* faces of the substrate on which the attack of the Super-Hydride occurs. C_2 represents the most favourable gas-phase pathway in the given mode of attack of Super-Hydride to the prochiral substrate.

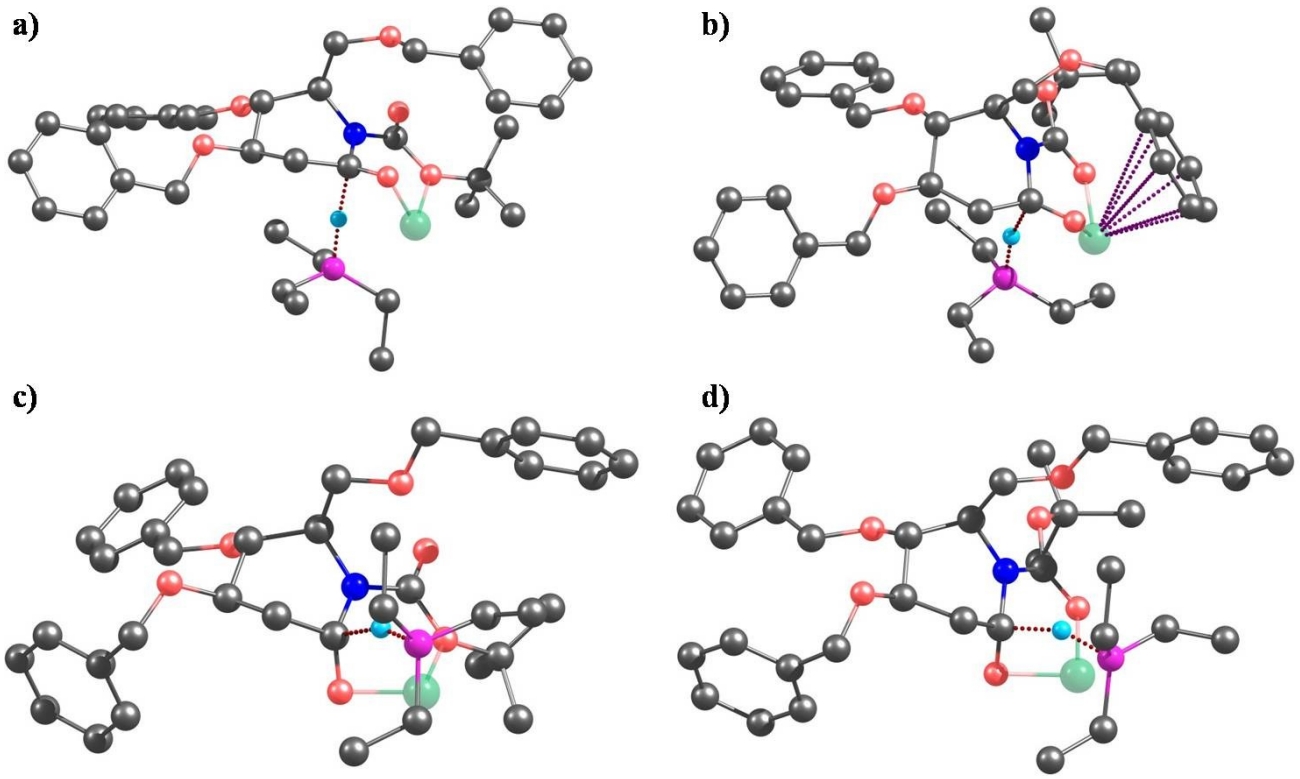


Figure S1. The optimized gas-phase transition state geometries at the M06-2X/6-31G** level of theory depicting different modes of approaches of the Super-Hydride to the different faces of 2-deoxygluconolactam-*N*-Boc **20a**. a) and b) represent conformations 1 and 2, respectively, for the *re* face attack whereas c) and d) represent conformations 1 and 2, respectively, for the *si* face attack of the Super-Hydride to the 2-deoxygluconolactam-*N*-Boc **20a**. The two conformations for each face of the attack were obtained with respect to the relative orientation of the *N*-Boc group that is linked to the Li+ through one of its oxygen through a covalent linkage. Hydrogen atoms that are not part of the reaction coordinate have been removed for clarity. Color codes: black - carbon, coral - oxygen, cyan - hydrogen, light green - lithium, fuchsia - boron, blue - nitrogen. The dotted pink lines represented cation–π interaction and dotted maroon lines represented bond breaking/bond forming.

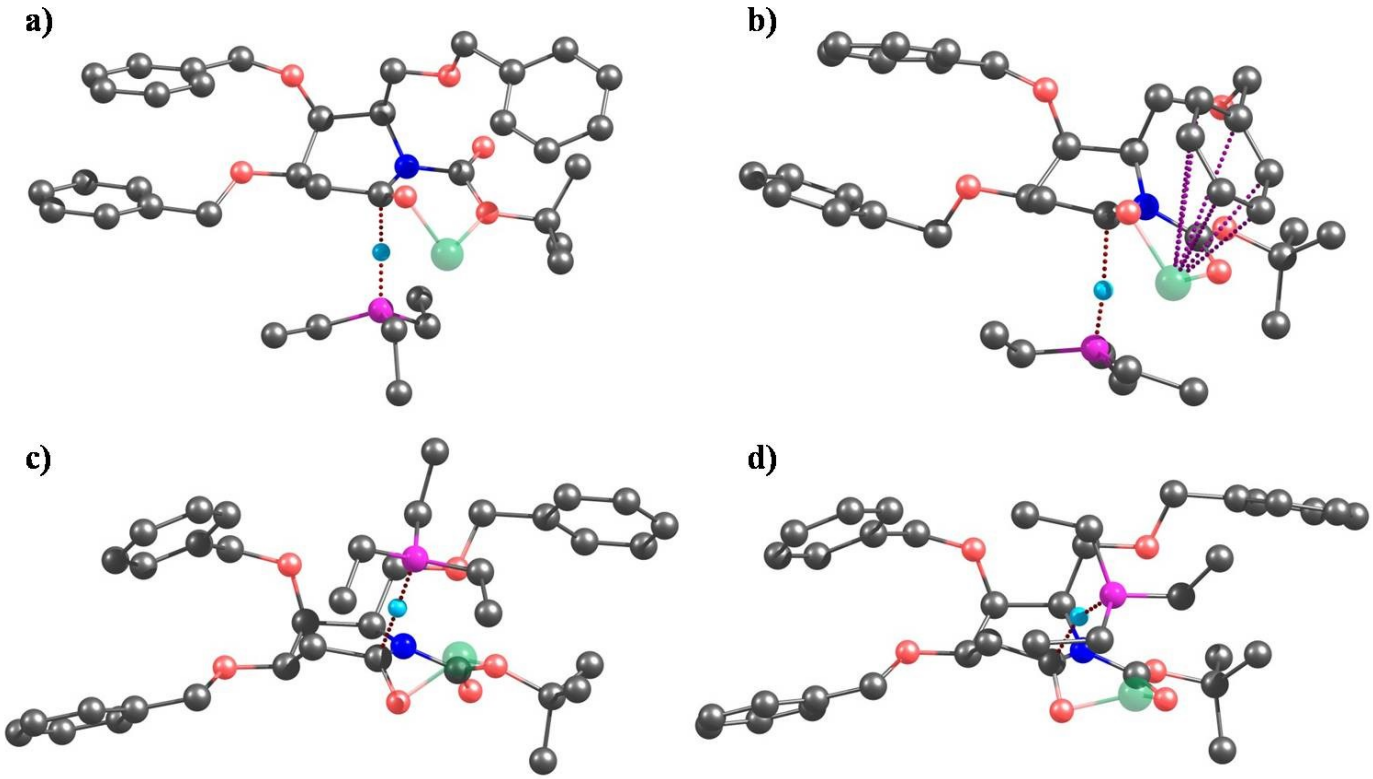


Figure S2. The optimized gas-phase transition state geometries at the M06-2X/6-31G** level of theory depicting different modes of approaches of the Super-Hydride to the different faces of 2-deoxygalactonolactam-*N*-Boc **20b**. a) and b) represent conformations 1 and 2, respectively, for the *re* face attack whereas c) and d) represent conformations 1 and 2, respectively, for the *si* face attack of the Super-Hydride to 2-deoxygalactonolactam-*N*-Boc **20b**. The two conformations for each face of the attack were obtained with respect to the relative orientation of the *N*-Boc group that is linked to the Li+ through one of its oxygen through a covalent linkage. Hydrogen atoms that are not part of the reaction coordinate have been removed for clarity. Color codes: black - carbon, coral - oxygen, cyan - hydrogen, light green - lithium, fuchsia - boron, blue - nitrogen. The dotted pink lines represented cation–π interaction and dotted maroon lines represent bond breaking/bond forming.

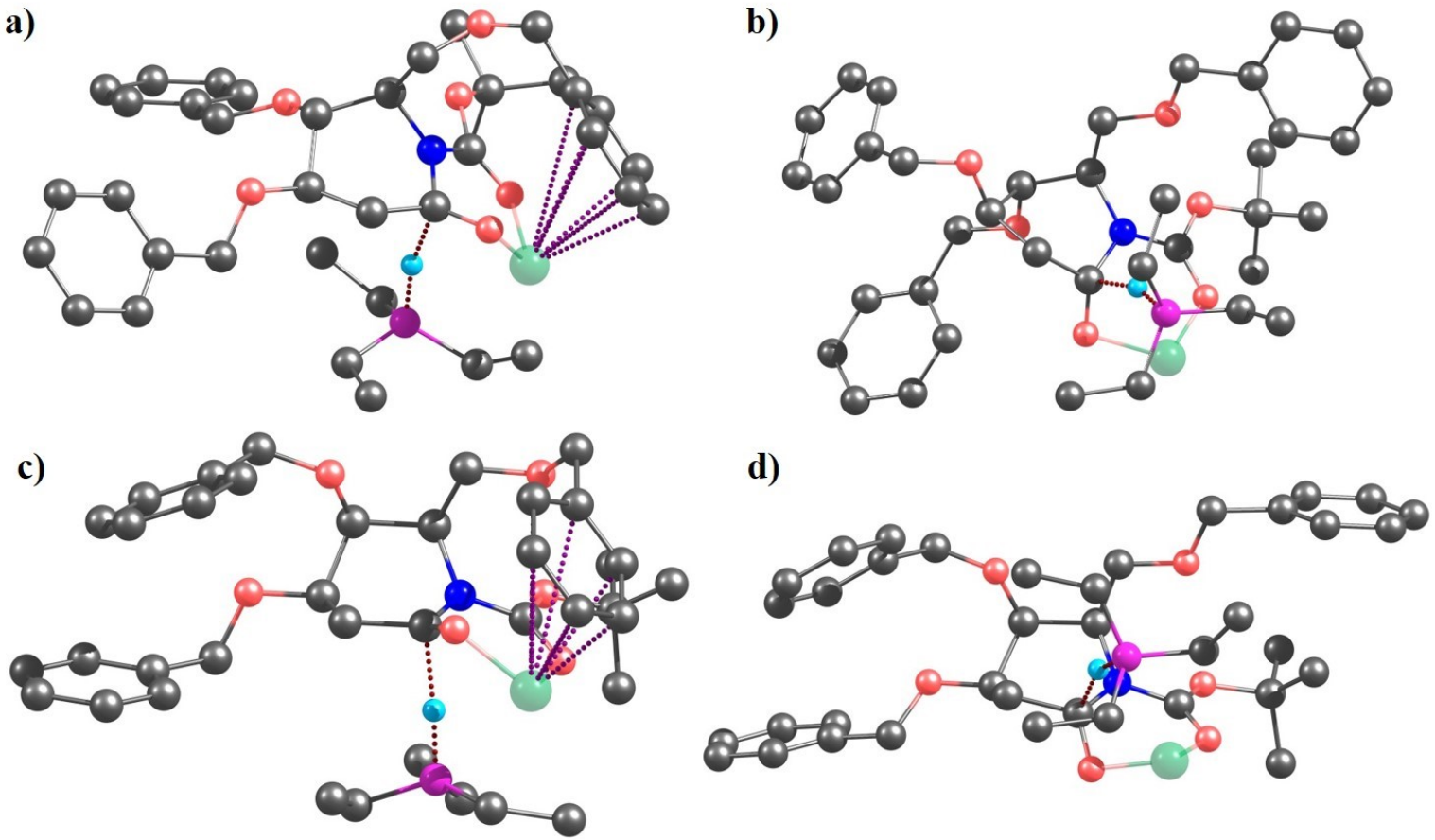


Figure S3. The solvent-phase optimized transition state geometries at the CPCM (toluene)/M06-2X/6-31G** level of theory depicting different modes of approaches of Super-Hydride to the 2-deoxyglycolactam-*N*-Boc **20a**/**b** : a) *re* face attack to the **20a**, (b) *si* face attack to the **20a**, c) *re* face attack to the 2-deoxygalactonolactam-*N*-Boc **20b** and d) *si* face attack to the 2-deoxygalactonolactam-**20b**. Only the lowest energy conformations (conformation 2) from the gas phase optimized geometries for each mode of approach have been considered for the solvent-phase calculations. Hydrogen atoms that are not part of the reaction coordinate have been removed for clarity. Color codes: black - carbon, coral - oxygen, cyan - hydrogen, light green - lithium, fuchsia - boron, blue - nitrogen. The dotted pink lines represented cation–π interaction and dotted maroon lines represent bond breaking/bond forming.

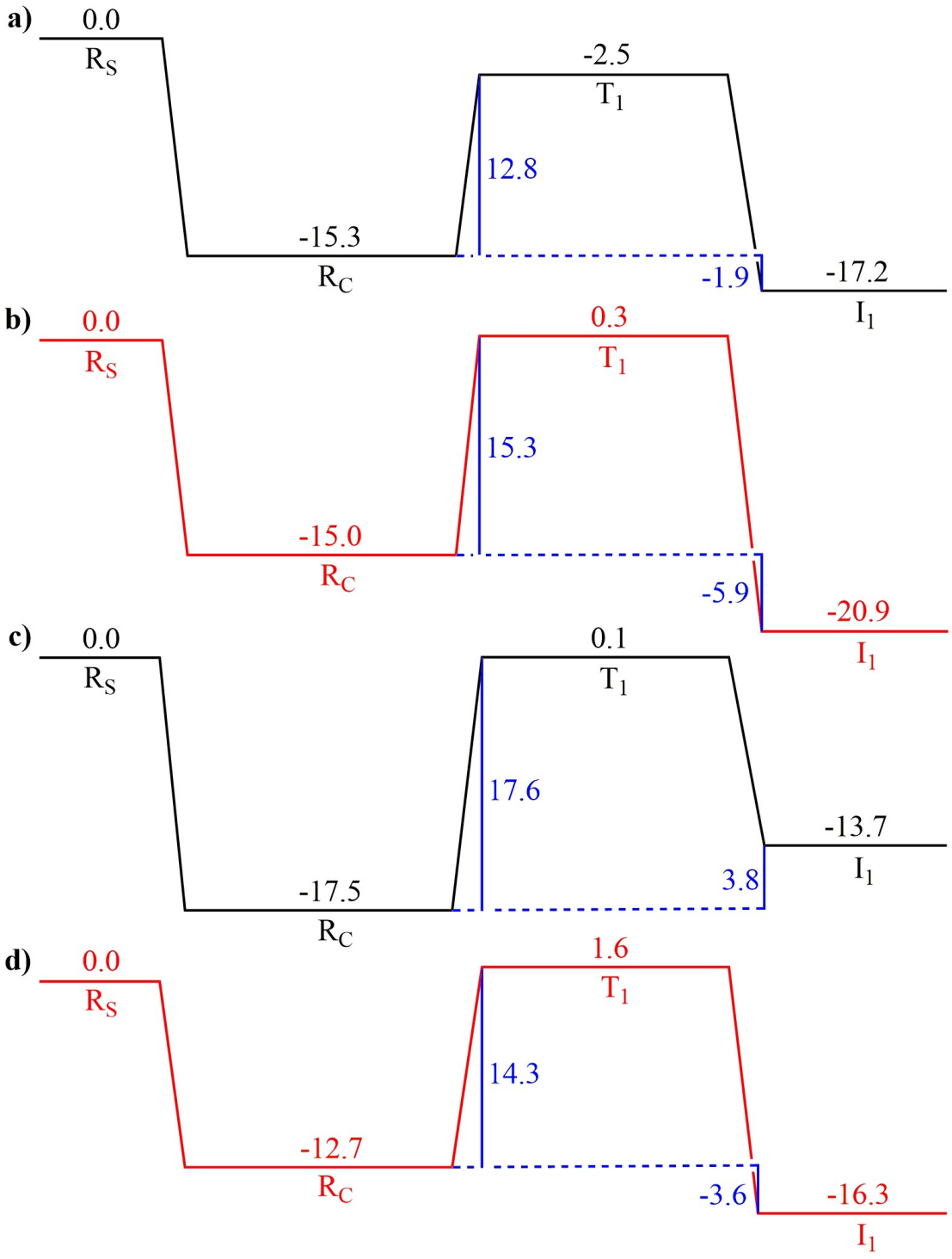
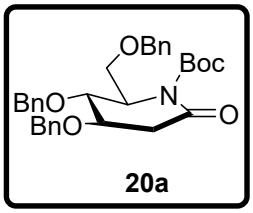


Figure S4. The solvent-phase free energy profile for reduction of the 2-deoxyglycolactam-*N*-Boc **20a**/**b** to 2-deoxyglycolactamol-*N*-Boc **21a**/**b** representing approach of the Super-Hydride to a) *re* face of **20a**, b) *si* face of **20a**, c) *re* face of **20b**, and d) *si* face of **20b**. R_s, R_c, T_1, I_1 represent infinitely separated reactants, the reactant complex, the transition state geometry and the product complex, respectively. All the values are in kcal/mol.

XYZ coordinates of the DFT optimized geometries

2-deoxygluconolactam-*N*-Boc (20a)



20a

glu_re_reactant_gas_conformation1

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C	3.243150	4.101881	-2.892129
C	4.619302	4.236643	-3.043575
C	5.457384	3.173278	-2.713193
C	2.995259	0.552291	-1.533017
O	1.591554	0.509336	-1.693706
C	1.009063	-0.743190	-1.435682
C	1.292089	-1.241461	-0.017206
C	0.139048	-2.135753	0.455157
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N	-1.293208	-0.418567	-0.475193
C	-0.493622	-0.589378	-1.709216
O	2.512877	-1.938861	-0.032296
C	3.201170	-1.923477	1.203560
C	4.620826	-2.391074	1.006019
C	5.410286	-2.644787	2.129267
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H	-0.750109	-1.570830	-3.603672
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H	-5.634923	2.069456	2.061197
H	-5.172532	0.362062	1.883438
H	-4.121696	1.507393	2.767180
H	-0.016283	-2.949540	-0.261327
H	-0.380536	1.063554	1.594690
H	1.887799	1.766848	3.819910
H	2.137522	1.082833	2.240430
H	2.246334	-0.749368	3.951889
H	0.671224	-0.275719	4.583950
H	0.785520	-0.980093	2.978325
H	-0.693898	3.854271	1.911599
H	0.928416	3.841917	2.555951
H	1.047663	4.194877	0.086984
H	1.714939	2.605352	0.459587
H	0.084706	2.732741	-0.183827
H	-2.085268	2.245135	3.431796
H	-1.409521	0.777912	4.163323
H	-1.425884	2.683106	5.767720
H	0.221675	2.137208	5.430226
H	-0.385074	3.606994	4.672468

glu_re_TS_gas_conformation1

C	5.624898	-2.703182	-1.849632
C	4.837582	-1.552633	-1.789444
C	5.315655	-0.368590	-2.349203
C	6.566741	-0.337182	-2.959141
C	7.352004	-1.485285	-3.010617
C	6.877502	-2.670179	-2.453013
C	3.507951	-1.593323	-1.079678
O	2.698705	-0.529127	-1.531358
C	1.496449	-0.359849	-0.802834
C	1.127448	1.123409	-0.871661
C	-0.385128	1.364071	-0.814698
N	-1.146568	0.261833	-0.201205
C	-0.931668	-1.088585	-0.647280
C	0.393900	-1.241641	-1.366106
C	-0.952784	1.702955	-2.205953
O	-2.357390	1.736099	-2.174296
C	-2.966043	0.661859	-2.875547
C	-4.405001	0.542946	-2.455059
C	-5.226567	1.672235	-2.414296
C	-6.565538	1.552812	-2.056915
C	-7.098132	0.302745	-1.742946
C	-6.282506	-0.824762	-1.778451
C	-4.936546	-0.703427	-2.123808
O	1.693790	1.870017	0.182795
C	3.099359	1.798149	0.274402
C	3.584435	2.715811	1.367753
C	2.711907	3.259808	2.308289
C	3.203891	4.076110	3.324778
C	4.564593	4.352189	3.410706
C	5.439018	3.807879	2.471914
C	4.949331	2.995486	1.456194
O	-1.899268	-1.827375	-0.987157
C	-2.144991	0.652735	0.677638
O	-2.940848	-0.381150	1.062185
C	-4.150255	-0.109701	1.869542
C	-4.990643	1.000839	1.248129
O	-2.278408	1.778175	1.087569
C	-4.912284	-1.428744	1.775650
C	-3.728793	0.196290	3.298553
B	-0.182686	-2.393895	1.865868
C	1.101938	-3.267380	1.405670
C	0.796060	-4.417909	0.436683
C	0.041661	-1.261203	2.999992
C	1.200302	-0.278745	2.805310
C	-1.481333	-3.350657	2.225934
C	-1.143111	-4.335985	3.354943
H	1.513659	1.500574	-1.836335
H	1.649001	-0.614547	0.254880
H	0.671251	-2.295772	-1.322551
H	-0.546440	2.222393	-0.163823
H	-0.572748	2.690709	-2.494326
H	-0.594802	0.986371	-2.958944
H	-2.901599	0.853583	-3.958713
H	-2.453591	-0.284228	-2.665318
H	-4.286004	-1.574599	-2.133820
H	-6.692547	-1.800584	-1.534024
H	-8.144544	0.210303	-1.469828
H	-7.196599	2.435348	-2.024496
H	-4.801955	2.643413	-2.650355
H	3.422712	0.769291	0.497685

H	3.555815	2.073218	-0.690057
H	5.632152	2.572323	0.722448
H	6.502013	4.019991	2.529397
H	4.943648	4.989835	4.202934
H	2.517245	4.497540	4.052359
H	1.651791	3.043035	2.235723
H	3.665968	-1.497733	0.008669
H	3.019051	-2.566029	-1.245507
H	5.252283	-3.631427	-1.422899
H	7.480521	-3.571709	-2.493782
H	8.326875	-1.458707	-3.486824
H	6.928726	0.587889	-3.397102
H	4.691988	0.518266	-2.317440
H	-5.986185	0.966995	1.700809
H	-4.555167	1.983307	1.415567
H	-5.100602	0.834018	0.174013
H	-4.622382	0.361881	3.907669
H	-3.167617	-0.640059	3.726425
H	-3.111618	1.095513	3.327988
H	-5.849328	-1.352314	2.332119
H	-5.154462	-1.646981	0.729814
H	-4.347087	-2.258751	2.214279
H	0.218811	-1.000930	-2.422889
H	-0.485085	-1.677704	0.739654
H	1.578843	-3.682181	2.307872
H	1.875304	-2.623275	0.967170
H	1.700618	-4.879536	0.024725
H	0.229540	-5.215056	0.930509
H	0.178800	-4.087670	-0.408520
H	-0.884315	-0.682347	3.145359
H	0.194965	-1.790006	3.954504
H	1.389129	0.327708	3.697634
H	2.136062	-0.803922	2.572213
H	0.999319	0.420505	1.986656
H	-2.335628	-2.752085	2.595486
H	-1.842505	-3.964658	1.375068
H	-1.996505	-4.963916	3.629078
H	-0.321866	-4.996082	3.063897
H	-0.824396	-3.795452	4.250092
Li	-2.427851	-2.194966	0.700712

glu_re_product_gas_conformation1

C	3.349769	3.792802	-1.429864
C	2.257471	2.989865	-1.759587
C	1.031960	3.585724	-2.057423
C	0.904680	4.972016	-2.015568
C	1.995970	5.771150	-1.685736
C	3.222491	5.177550	-1.395646
C	2.410779	1.489016	-1.776741
O	1.131802	0.904132	-1.761726
C	1.131260	-0.506839	-1.655118
C	1.598134	-0.936224	-0.250441
C	0.554965	-1.738538	0.513375
C	-0.803502	-1.030199	0.594537
N	-1.185385	-0.642270	-0.851246
C	-0.299778	-0.932261	-1.977167
O	2.829286	-1.621801	-0.406002
C	3.544452	-1.788596	0.796789
C	4.983614	-2.125723	0.494831
C	5.752143	-2.798459	1.444966
C	7.096836	-3.064378	1.207084
C	7.683987	-2.667176	0.008439
C	6.918601	-2.003509	-0.946374
C	5.574959	-1.730972	-0.704498
C	-0.392647	-2.381177	-2.487855
O	-1.734063	-2.798312	-2.619653
C	-2.253968	-3.478085	-1.498960
C	-3.615941	-2.955844	-1.114804
C	-4.263562	-1.960172	-1.844940
C	-5.488876	-1.452064	-1.405259
C	-6.065202	-1.915324	-0.225337
C	-5.422610	-2.919473	0.508249
C	-4.212240	-3.443029	0.057376
C	-2.121411	0.313644	-1.079455
O	-2.274654	0.972681	-2.088226
O	-1.729682	-1.768086	1.216277
O	-2.978453	0.426609	-0.001789
C	-3.609155	1.710469	0.292074
C	-2.500040	2.733860	0.499408
C	-4.594518	2.126794	-0.794488
C	-4.357437	1.419572	1.588704
Li	-3.365893	-1.316911	0.770518
C	-1.367099	1.138611	3.979984
C	-2.253103	2.356455	4.247676
B	0.079213	1.367978	3.394980
C	0.519635	2.746748	2.751418
C	1.358365	2.656956	1.467115
C	1.130132	0.186198	3.459230
C	0.649449	-1.151275	4.028463
H	1.825271	-0.944736	-2.392108
H	1.776143	-0.003509	0.311699
H	0.874365	-1.895366	1.546447

H	-0.637459	-0.290256	-2.792402
H	0.051582	-2.407422	-3.488846
H	0.174517	-3.085452	-1.868213
H	-2.324173	-4.553086	-1.723921
H	-1.616725	-3.348980	-0.614525
H	-3.697092	-4.203047	0.639193
H	-5.865213	-3.294777	1.425703
H	-7.010082	-1.508743	0.120976
H	-5.985709	-0.681236	-1.985680
H	-3.786074	-1.571057	-2.738203
H	3.007874	1.172186	-0.906105
H	2.959687	1.162163	-2.676470
H	4.303008	3.329002	-1.186072
H	4.077674	5.792287	-1.132884
H	1.891817	6.850996	-1.651812
H	-0.054037	5.429658	-2.240207
H	0.183096	2.954802	-2.301735
H	3.501497	-0.852397	1.382004
H	3.098484	-2.576841	1.421435
H	5.292917	-3.118159	2.377521
H	7.683671	-3.589233	1.954347
H	8.731268	-2.878753	-0.182195
H	7.369306	-1.696435	-1.885191
H	4.968248	-1.221222	-1.445415
H	-5.148697	3.004528	-0.447395
H	-4.085523	2.361376	-1.726859
H	-5.309916	1.319242	-0.972312
H	-2.918881	3.677020	0.862494
H	-1.787282	2.358004	1.240793
H	-1.968612	2.923811	-0.436394
H	-4.828322	2.329433	1.969766
H	-5.148166	0.680295	1.407660
H	-3.672815	1.040407	2.352597
H	0.425599	-2.734739	0.081683
H	-0.634235	-0.038551	1.081586
H	2.002071	0.556576	4.023102
H	1.527007	0.040324	2.444500
H	1.423635	-1.923893	3.963640
H	0.373769	-1.058730	5.083773
H	-0.231463	-1.513408	3.485404
H	-0.330221	3.420449	2.592756
H	1.122349	3.239350	3.534366
H	1.637078	3.644693	1.086936
H	2.285327	2.095635	1.635033
H	0.811356	2.150623	0.660441
H	-1.823910	0.465476	3.225207
H	-1.315984	0.504204	4.874004
H	-3.240848	2.072677	4.625582
H	-1.794767	3.014412	4.992839
H	-2.408370	2.956681	3.345903

glu_re_reactant_gas_conformation2

C	2.027544	3.594561	-1.629938
C	2.910008	2.620456	-1.169599
C	4.207449	2.989619	-0.808671
C	4.619006	4.312849	-0.911702
C	3.733419	5.285222	-1.372540
C	2.439008	4.921860	-1.728516
C	2.508640	1.171238	-1.051491
O	1.126695	1.040406	-1.316895
C	0.659477	-0.278849	-1.466193
C	1.030356	-1.177802	-0.283947
C	-0.065751	-2.231945	-0.077349
C	-1.284836	-1.477614	0.388216
N	-1.599222	-0.366959	-0.397015
C	-0.859832	-0.152499	-1.662647
O	2.278287	-1.762412	-0.563035
C	3.033651	-2.090506	0.586825
C	4.438926	-2.461057	0.183881
C	4.895268	-2.284933	-1.120155
C	6.208954	-2.611467	-1.452377
C	7.074094	-3.111842	-0.485434
C	6.620521	-3.288527	0.820609
C	5.309596	-2.966892	1.151703
C	-1.430845	-1.022194	-2.781181
O	-2.793427	-0.705789	-2.945308
C	-3.638219	-1.840186	-3.079501
C	-3.823479	-2.562263	-1.766572
C	-3.231494	-3.802093	-1.525721
C	-3.386631	-4.434809	-0.291870
C	-4.137166	-3.828292	0.708889
C	-4.722511	-2.582656	0.481107
C	-4.562493	-1.954240	-0.747196
C	-2.564031	0.560762	0.020009
O	-3.149069	0.497528	1.089597
Li	-2.051503	-0.167596	2.536745
O	-1.834683	-1.752574	1.442387
O	-2.743278	1.506119	-0.875965
C	-3.526440	2.711704	-0.564089
C	-3.328008	3.548893	-1.820755
C	-4.991296	2.333544	-0.385485
C	-2.934079	3.409960	0.654522

C	0.059837	2.589932	2.901424
C	0.923256	2.965121	1.692380
B	-0.110642	0.977925	3.080245
C	1.319917	0.217000	3.313526
C	1.226038	-1.298690	3.511321
C	-1.165731	0.605689	4.325323
C	-2.459901	1.437997	4.422520
H	1.106402	-0.740835	-2.365192
H	1.082289	-0.547660	0.619848
H	0.190292	-2.937375	0.713607
H	-1.034597	0.881968	-1.945420
H	-0.878779	-0.804652	-3.706356
H	-1.302980	-2.089063	-2.560528
H	-4.593086	-1.446949	-3.438370
H	-3.245265	-2.526085	-3.843489
H	-2.659190	-4.284860	-2.315469
H	-2.924042	-5.400941	-0.117276
H	-4.257370	-4.316051	1.670565
H	-5.293742	-2.097250	1.265901
H	-5.010060	-0.978354	-0.924202
H	2.741510	0.812684	-0.036776
H	3.087424	0.552418	-1.755474
H	4.897172	2.233552	-0.439968
H	5.629640	4.587378	-0.626434
H	4.051609	6.320014	-1.448471
H	1.742151	5.674851	-2.083697
H	1.017055	3.307209	-1.897807
H	3.054182	-1.228753	1.272993
H	2.566829	-2.922428	1.136095
H	4.955351	-3.105218	2.170872
H	7.289280	-3.679582	1.580780
H	8.096978	-3.364736	-0.745427
H	6.555758	-2.473397	-2.471774
H	4.214208	-1.899226	-1.870189
H	-0.237078	-2.790650	-1.001425
H	-0.551490	0.575952	1.968041
H	1.824722	0.653098	4.190020
H	1.998756	0.427470	2.469356
H	2.201461	-1.795786	3.602077
H	0.660159	-1.543533	4.417075
H	0.690852	-1.776987	2.677319
H	-0.921064	3.077040	2.783998
H	0.495645	3.037338	3.809468
H	0.956024	4.042719	1.487397
H	1.962468	2.638966	1.822969
H	0.554962	2.467271	0.783372
H	-1.422916	-0.473692	4.403651
H	-0.595323	0.772674	5.247787
H	-3.097295	1.144479	5.263674
H	-2.210923	2.495503	4.541024
H	-3.090094	1.392938	3.517874
H	-3.900112	4.476388	-1.740581
H	-2.271427	3.799965	-1.946803
H	-3.666747	2.997504	-2.701590
H	-3.378674	4.405460	0.740590
H	-3.129101	2.860586	1.576330
H	-1.851477	3.523598	0.538752
H	-5.582832	3.246529	-0.273713
H	-5.350938	1.798538	-1.269518
H	-5.133845	1.713343	0.499944

glu_re_TS_gas_conformation2

C	1.407613	3.945066	-0.724205
C	2.561870	3.183949	-0.902933
C	3.808045	3.808224	-0.841907
C	3.901524	5.174194	-0.599448
C	2.746377	5.931579	-0.417245
C	1.501510	5.313348	-0.481006
C	2.487922	1.692515	-1.123167
O	1.147861	1.342290	-1.377620
C	0.868818	-0.038191	-1.491316
C	1.307604	-0.810073	-0.242043
C	0.311276	-1.900226	0.127170
C	-1.080646	-1.347772	0.379253
N	-1.342836	-0.163231	-0.423018
C	-0.645358	-0.091323	-1.713516
O	2.592184	-1.336201	-0.509033
C	3.384060	-1.554915	0.639718
C	4.781888	-1.931215	0.218673
C	5.291419	-1.517367	-1.011636
C	6.598693	-1.833142	-1.371031
C	7.409244	-2.559151	-0.502775
C	6.904311	-2.973637	0.726946
C	5.595367	-2.664062	1.083017
C	-1.177278	-1.183840	-2.641530
O	-2.464225	-0.780283	-3.063117
C	-3.419747	-1.824521	-3.126440
C	-4.021311	-2.140634	-1.774490
C	-4.061434	-3.441419	-1.275734
C	-4.643960	-3.707993	-0.039318
C	-5.195240	-2.671389	0.709012
C	-5.154716	-1.365934	0.218687

C	-4.566041	-1.105007	-1.014018
C	-2.250021	0.771283	-0.020050
O	-2.907159	0.670135	1.015097
Li	-2.722975	-0.910896	2.009479
O	-2.009506	-2.078347	0.758344
O	-2.320037	1.807977	-0.844769
C	-3.092872	3.004308	-0.503131
C	-2.778920	3.935881	-1.667674
C	-4.580033	2.670643	-0.467157
C	-2.592164	3.594948	0.810642
C	-0.394113	1.380707	3.109283
C	0.613825	1.979401	2.123457
B	-0.523872	-0.235680	3.068346
C	0.837679	-1.051161	3.436877
C	0.670948	-2.558803	3.678070
C	-1.797863	-0.816630	3.964145
C	-3.024330	0.085699	4.218705
H	1.400133	-0.468101	-2.357095
H	1.347461	-0.093577	0.591332
H	0.619536	-2.428855	1.029521
H	-0.914244	0.856911	-2.176395
H	-0.514718	-1.290665	-3.512317
H	-1.231655	-2.153251	-2.128838
H	-4.197573	-1.463478	-3.807002
H	-2.984023	-2.729702	-3.573027
H	-3.629357	-4.252394	-1.857248
H	-4.663832	-4.723853	0.341658
H	-5.664703	-2.880556	1.665947
H	-5.585871	-0.550321	0.793854
H	-4.515525	-0.087289	-1.394608
H	2.868247	1.177593	-0.227773
H	3.129669	1.389542	-1.966284
H	4.711848	3.219487	-0.982727
H	4.876671	5.648641	-0.552021
H	2.818372	6.997565	-0.226779
H	0.595776	5.896142	-0.339279
H	0.442585	3.451020	-0.775520
H	3.410854	-0.633355	1.246635
H	2.954347	-2.342257	1.277628
H	5.199526	-2.997646	2.039218
H	7.527315	-3.546848	1.406234
H	8.428181	-2.805334	-0.783941
H	6.985079	-1.510754	-2.332981
H	4.649795	-0.960407	-1.686330
H	0.246076	-2.644794	-0.675949
H	-0.707349	-0.505125	1.774928
H	1.266998	-0.603990	4.347787
H	1.607596	-0.893385	2.668430
H	1.628545	-3.087477	3.757607
H	0.125703	-2.750381	4.607953
H	0.088892	-3.043572	2.883851
H	-1.371174	1.849706	2.925709
H	-0.112841	1.681804	4.131826
H	0.728586	3.065362	2.225829
H	1.612261	1.540060	2.253794
H	0.314038	1.787178	1.082991
H	-2.120556	-1.836305	3.666881
H	-1.352381	-1.007281	4.948764
H	-3.759053	-0.390451	4.876330
H	-2.699548	1.013823	4.696164
H	-3.560568	0.415366	3.316056
H	-3.339329	4.867602	-1.556539
H	-1.711340	4.170361	-1.696002
H	-3.058680	3.467114	-2.614511
H	-3.010943	4.598325	0.930250
H	-2.887571	2.985818	1.664724
H	-1.499868	3.675771	0.797003
H	-5.147588	3.586719	-0.280326
H	-4.900170	2.262977	-1.430548
H	-4.802684	1.954125	0.324632

glu_re_product_gas_conformation2

C	-4.520727	-2.901207	-0.849727
C	-4.020421	-1.961853	-1.764374
C	-4.663210	-0.732547	-1.892064
C	-5.793840	-0.445909	-1.123939
C	-6.277368	-1.370195	-0.204087
C	-5.634949	-2.604750	-0.066302
C	-2.790482	-2.313381	-2.563937
O	-2.225848	-1.169646	-3.178069
C	-0.824263	-1.066985	-3.062463
C	-0.434576	-0.095141	-1.934911
C	1.074190	-0.009530	-1.680338
C	1.541326	-0.965501	-0.573145
C	0.566548	-2.105941	-0.320149
C	-0.770593	-1.566164	0.206304
N	-1.145569	-0.370089	-0.692808
O	1.287274	1.339740	-1.310075
C	2.611835	1.718640	-1.026924
C	2.591297	3.113306	-0.446730
C	3.790323	3.778360	-0.187689
C	3.783580	5.048737	0.378054

C	2.575541	5.669282	0.690394
C	1.377420	5.010731	0.430429
C	1.384271	3.738830	-0.137230
O	2.848684	-1.395652	-0.910766
C	3.601205	-1.844247	0.192010
C	5.047979	-2.004301	-0.203598
C	5.896983	-2.772050	0.594969
C	7.245759	-2.893140	0.279733
C	7.758464	-2.252506	-0.846024
C	6.913866	-1.491911	-1.649023
C	5.564340	-1.364285	-1.328868
O	-1.731916	-2.480122	0.333543
Li	-3.237956	-1.610991	0.745810
C	-2.031127	0.499087	-0.172325
O	-2.746924	0.216892	0.807041
O	-2.072762	1.688842	-0.781074
C	0.691540	1.379077	2.367289
C	-0.342638	0.759968	3.314386
B	-0.447376	-0.817164	3.386464
C	0.858516	-1.711971	3.260524
C	0.639891	-3.223777	3.136643
C	-1.820929	-1.531673	3.700551
C	-3.047189	-0.663642	3.991781
H	1.635551	-0.249065	-2.599905
H	1.586129	-0.364625	0.351148
H	0.955962	-2.773908	0.453422
H	-0.741161	0.896658	-2.265208
H	-0.441086	-0.654659	-4.003085
H	-0.373204	-2.056939	-2.935660
H	-3.059395	-3.042732	-3.343087
H	-2.088605	-2.780240	-1.863089
H	-4.005023	-3.850784	-0.730481
H	-6.007700	-3.337590	0.643083
H	-7.149143	-1.138459	0.398796
H	-6.291835	0.511658	-1.237895
H	-4.259407	-0.003666	-2.587964
H	3.080505	1.032283	-0.305312
H	3.225109	1.684923	-1.942479
H	4.735346	3.296052	-0.427485
H	4.722710	5.555801	0.576027
H	2.570507	6.660438	1.132572
H	0.430051	5.486325	0.669949
H	0.458341	3.211707	-0.343222
H	3.524469	-1.108209	1.012978
H	3.211735	-2.796634	0.582240
H	5.496197	-3.279439	1.469509
H	7.895201	-3.494194	0.908344
H	8.809688	-2.350337	-1.097427
H	7.306547	-0.995867	-2.531346
H	4.898001	-0.778954	-1.953224
H	0.412913	-2.719421	-1.212574
H	-0.540600	-1.041081	1.162093
H	1.474558	-1.491467	4.148464
H	1.472629	-1.353890	2.421591
H	1.576605	-3.760567	2.951344
H	0.204424	-3.638569	4.050844
H	-0.052101	-3.453307	2.317958
H	-1.326227	1.202822	3.125342
H	-0.098574	1.051436	4.352330
H	0.791267	2.459859	2.512017
H	1.687677	0.942464	2.505359
H	0.411789	1.226532	1.315401
H	-1.991386	-2.178496	2.819009
H	-1.666065	-2.255110	4.514458
H	-3.936386	-1.267048	4.205406
H	-2.878740	-0.019802	4.861433
H	-3.276797	-0.006752	3.146777
C	-2.845387	2.805175	-0.246548
C	-2.469982	3.946145	-1.186300
C	-4.337266	2.512121	-0.337057
C	-2.410847	3.121554	1.181099
H	-4.896887	3.397022	-0.019597
H	-4.611178	2.285471	-1.371993
H	-4.608931	1.670784	0.300853
H	-3.028229	4.846177	-0.915977
H	-1.400615	4.165172	-1.124653
H	-2.710306	3.681502	-2.219243
H	-2.811935	4.098131	1.468285
H	-2.776829	2.370747	1.881513
H	-1.318367	3.166392	1.244973

glu_si_reactant_gas_conformation1

C	4.910456	-2.354895	2.064433
C	4.881156	-2.119704	0.691481
C	5.616085	-1.055515	0.166805
C	6.361624	-0.228859	0.997111
C	6.390653	-0.473660	2.369884
C	5.670446	-1.538933	2.901588
C	4.033919	-2.949260	-0.243188
O	3.137337	-2.139094	-0.996029
C	2.070802	-1.617334	-0.234313
C	1.685995	-0.268463	-0.810912

C	0.434437	0.317296	-0.134458
N	-0.384005	-0.646306	0.636570
C	-0.310556	-2.016238	0.484749
C	0.852461	-2.528016	-0.321138
C	-0.441488	0.979382	-1.192130
O	-1.532745	1.590690	-0.560313
C	-2.336338	2.339172	-1.458396
C	-3.479669	2.931657	-0.680688
C	-3.205908	3.740252	0.424720
C	-4.243472	4.275219	1.179526
C	-5.567583	4.005183	0.835427
C	-5.846700	3.205385	-0.268930
C	-4.805010	2.670866	-1.025228
O	2.710229	0.684099	-0.646989
C	3.541389	0.865300	-1.778586
C	4.719400	1.725022	-1.393374
C	4.666382	2.567431	-0.283589
C	5.764813	3.355594	0.050366
C	6.924424	3.310124	-0.719308
C	6.982403	2.468080	-1.828153
C	5.884743	1.679609	-2.160633
O	-1.124072	-2.791260	0.979349
C	-1.231595	-0.025060	1.608880
O	-2.403025	-0.652205	1.715054
C	-3.365878	-0.288326	2.779838
C	-3.901560	1.108955	2.510978
O	-0.881693	0.939488	2.229493
C	-4.450126	-1.348638	2.622540
C	-2.686184	-0.416783	4.137887
Li	-2.787739	-2.020536	0.286003
B	-3.388459	-2.083601	-1.718837
C	-4.245214	-0.777753	-1.174793
C	-5.762710	-0.911741	-1.329795
C	-3.475282	-2.238410	-3.336472
C	-3.152782	-0.957412	-4.111875
C	-3.859563	-3.496131	-0.969514
C	-2.949488	-4.694680	-1.257152
H	1.483689	-0.423781	-1.883949
H	2.381455	-1.469821	0.811272
H	1.057682	-3.541109	0.030224
H	0.778319	1.065405	0.582027
H	0.175253	1.718363	-1.731687
H	-0.790504	0.216859	-1.908527
H	-1.720699	3.135150	-1.907903
H	-2.702822	1.696725	-2.271690
H	-5.024628	2.034476	-1.878449
H	-6.875180	2.990303	-0.541624
H	-6.378475	4.419620	1.426194
H	-4.020611	4.898393	2.040145
H	-2.171216	3.923478	0.702247
H	3.887415	-0.104308	-2.156463
H	2.964484	1.351830	-2.582855
H	5.936140	1.015052	-3.020400
H	7.883886	2.421353	-2.430804
H	7.780324	3.922859	-0.455188
H	5.716394	4.003691	0.919817
H	3.769649	2.583311	0.325384
H	3.484690	-3.720551	0.316380
H	4.652897	-3.455282	-0.989414
H	4.333402	-3.176648	2.482485
H	5.688484	-1.729340	3.969959
H	6.972218	0.168432	3.023712
H	6.906347	0.609187	0.569916
H	5.596511	-0.871738	-0.903354
H	-4.675706	1.338983	3.249412
H	-3.107864	1.852083	2.589119
H	-4.346434	1.172334	1.512325
H	-3.444418	-0.307777	4.917892
H	-2.229163	-1.405653	4.239209
H	-1.925752	0.350438	4.279544
H	-5.210094	-1.208481	3.394943
H	-4.943867	-1.270740	1.648469
H	-4.025799	-2.352010	2.738022
H	0.518973	-2.606693	-1.365419
H	-2.173596	-1.861249	-1.440396
H	-4.045076	-0.461972	-0.133966
H	-3.902424	0.091230	-1.747896
H	-4.476883	-2.585861	-3.634920
H	-2.788012	-3.026431	-3.674183
H	-4.871365	-3.710860	-1.340118
H	-4.026556	-3.462799	0.133975
H	-3.099131	-1.111962	-5.195517
H	-3.907291	-0.180742	-3.935440
H	-2.186910	-0.542272	-3.792292
H	-6.305183	-0.003112	-1.037656
H	-6.027411	-1.138263	-2.368678
H	-6.153612	-1.735154	-0.719411
H	-3.309715	-5.627416	-0.809445
H	-2.865760	-4.857093	-2.335570
H	-1.937653	-4.512731	-0.875302

glu_si_TS_gas_conformation1

C	4.385949	-2.335927	-0.804189
C	4.276062	-1.637139	-2.008964
C	5.418076	-1.097564	-2.596453
C	6.665057	-1.263429	-1.996418
C	6.772692	-1.964628	-0.799866
C	5.629874	-2.497439	-0.203696
C	2.920175	-1.469332	-2.642509
O	2.003901	-1.138851	-1.620694
C	0.690090	-0.949445	-2.065027
C	-0.220479	-0.919447	-0.829956
C	-1.613201	-0.362399	-1.157873
C	-1.783165	1.124097	-0.798234
C	-0.423291	1.815228	-0.672855
C	0.292614	1.176729	0.501710
N	0.405282	-0.252656	0.320285
O	-2.535362	-1.188653	-0.484576
C	-3.895094	-0.901015	-0.751665
C	-4.737549	-2.099185	-0.390867
C	-6.073265	-1.922494	-0.029100
C	-6.879706	-3.021006	0.252497
C	-6.353225	-4.308475	0.186547
C	-5.017534	-4.488419	-0.162342
C	-4.213509	-3.389963	-0.452307
O	-2.575198	1.718611	-1.810002
C	-3.228461	2.920038	-1.418696
C	-4.445051	2.639754	-0.571635
C	-5.627135	2.211211	-1.180781
C	-6.731544	1.862060	-0.411723
C	-6.660136	1.928378	0.980193
C	-5.487956	2.356783	1.595549
C	-4.386929	2.717346	0.820318
O	0.105172	1.633225	1.666243
C	1.129040	-1.074589	1.159189
O	1.159421	-2.280645	1.082025
O	1.825941	-0.370749	2.088135
C	2.458561	-1.063959	3.217898
C	2.940450	0.095767	4.087265
C	1.421406	-1.886479	3.974688
C	3.629766	-1.898801	2.718220
B	2.859275	2.376100	0.102606
C	2.819873	2.997796	-1.385399
C	2.991786	1.967561	-2.502151
C	2.728140	3.527612	1.270795
C	1.582114	4.538171	1.148931
C	4.023410	1.275047	0.379618
C	5.427828	1.809359	0.061007
H	-1.772481	-0.438640	-2.248317
H	-2.293360	1.167403	0.175866
H	-0.527116	2.876517	-0.440334
H	-0.368282	-1.949848	-0.506807
H	0.361259	-1.781452	-2.708494
H	0.610534	-0.028807	-2.664740
H	2.600618	-2.404547	-3.131440
H	2.949012	-0.682791	-3.411609
H	5.330853	-0.536335	-3.523574
H	7.548496	-0.834479	-2.458455
H	7.742378	-2.091299	-0.328806
H	5.709378	-3.040267	0.733877
H	3.483256	-2.720700	-0.335157
H	-4.231217	-0.022210	-0.183323
H	-4.018676	-0.654595	-1.819210
H	-3.169405	-3.522394	-0.714033
H	-4.598368	-5.488890	-0.207933
H	-6.978634	-5.166023	0.413677
H	-7.917458	-2.871014	0.534120
H	-6.476256	-0.914610	0.039432
H	-2.536696	3.585736	-0.885384
H	-3.515717	3.410339	-2.352803
H	-3.470618	3.054599	1.300400
H	-5.428761	2.411470	2.677637
H	-7.519589	1.649669	1.581656
H	-7.647560	1.534525	-0.894038
H	-5.671813	2.143049	-2.264853
H	4.202425	-2.263399	3.576515
H	3.272336	-2.750594	2.138229
H	4.285524	-1.289802	2.088832
H	1.869572	-2.248523	4.904323
H	0.557796	-1.264127	4.227079
H	1.087967	-2.740753	3.387389
H	3.405825	-0.288772	4.997592
H	3.691069	0.699867	3.564911
H	2.094847	0.726982	4.386240
H	0.139931	1.721465	-1.604373
H	1.700926	1.614750	0.126667
H	4.039889	0.926074	1.427059
H	3.839842	0.369265	-0.214232
H	3.618026	3.753368	-1.462030
H	1.887383	3.554889	-1.554144
H	3.685447	4.060996	1.170193
H	2.786023	3.193742	2.331601
H	2.925603	2.406710	-3.503592
H	3.954906	1.449770	-2.423185

H	2.224655	1.191791	-2.417139
H	6.200601	1.052689	0.232413
H	5.502013	2.120121	-0.986347
H	5.672371	2.684744	0.673721
H	1.662553	5.347757	1.881524
H	1.581888	4.994690	0.154941
H	0.615103	4.048117	1.297196
Li	1.914322	1.559173	1.988960

glu_si_product_gas_conformation1

C	4.381206	-2.278953	-0.483776
C	4.366855	-1.762911	-1.782092
C	5.572495	-1.475697	-2.420158
C	6.785716	-1.727054	-1.782582
C	6.798776	-2.253330	-0.494374
C	5.593739	-2.518401	0.156182
C	3.051781	-1.568313	-2.493144
O	2.071866	-1.229037	-1.542018
C	0.774331	-1.134317	-2.071275
C	-0.212859	-1.014406	-0.898149
C	-1.597360	-0.534635	-1.355029
C	-1.793855	0.968608	-1.128922
C	-0.457365	1.697323	-1.152971
C	0.318346	1.316504	0.113884
N	0.316141	-0.201411	0.198310
O	-2.529684	-1.323147	-0.645169
C	-3.886868	-1.036088	-0.917456
C	-4.744482	-2.154100	-0.380967
C	-6.040848	-1.883644	0.056930
C	-6.861973	-2.911646	0.511087
C	-6.388448	-4.220687	0.541421
C	-5.090799	-4.493756	0.116142
C	-4.272955	-3.466425	-0.344635
O	-2.686389	1.436350	-2.130961
C	-3.303082	2.679518	-1.831617
C	-4.379763	2.550596	-0.780407
C	-5.674576	2.179727	-1.150054
C	-6.657136	1.980800	-0.185134
C	-6.347491	2.141056	1.164885
C	-5.059787	2.511650	1.542180
C	-4.080752	2.721846	0.573229
O	-0.212341	1.915650	1.196486
C	0.983343	-0.894991	1.147998
O	1.106183	-2.102701	1.207966
O	1.537049	-0.079041	2.127561
C	2.164852	-0.706460	3.295665
C	2.613670	0.499037	4.123068
C	1.131123	-1.515892	4.073188
C	3.376676	-1.543082	2.894669
B	3.294216	2.610613	0.063579
C	3.055918	3.036718	-1.441679
C	3.098133	1.901974	-2.468842
C	2.886702	3.588759	1.243997
C	1.809210	4.640765	0.974150
C	4.076534	1.279321	0.398076
C	5.559579	1.345478	-0.013944
H	-1.707834	-0.716091	-2.440177
H	-2.222935	1.089799	-0.125138
H	-0.599917	2.778532	-1.085467
H	-0.350024	-2.014620	-0.487812
H	0.517856	-2.038623	-2.645875
H	0.710667	-0.282901	-2.766633
H	2.762319	-2.500909	-3.006097
H	3.139943	-0.784939	-3.262854
H	5.562676	-1.057191	-3.424003
H	7.719012	-1.503837	-2.289818
H	7.742895	-2.447582	0.004790
H	5.598175	-2.920507	1.165490
H	3.433594	-2.476297	0.012206
H	-4.190097	-0.084969	-0.459405
H	-4.033486	-0.925861	-2.004437
H	-3.255731	-3.666748	-0.664094
H	-4.712850	-5.511179	0.146344
H	-7.025242	-5.022919	0.900992
H	-7.868719	-2.689129	0.851495
H	-6.399761	-0.856775	0.050131
H	-2.555884	3.418111	-1.512078
H	-3.735107	3.023684	-2.775582
H	-3.069371	2.996991	0.867511
H	-4.815636	2.636407	2.592266
H	-7.110451	1.980338	1.920028
H	-7.662241	1.698134	-0.483418
H	-5.906616	2.038892	-2.202924
H	3.962710	-1.770223	3.790634
H	3.064647	-2.475898	2.426963
H	4.008922	-0.990188	2.194166
H	1.571572	-1.846760	5.018355
H	0.254576	-0.899732	4.300074
H	0.812159	-2.386840	3.503176
H	3.119014	0.162519	5.030861
H	3.308739	1.129744	3.559885
H	1.755155	1.099722	4.460908

H	0.082836	1.493224	-2.082596
H	1.392643	1.568868	-0.048186
H	4.022980	1.044526	1.468196
H	3.600277	0.437051	-0.127492
H	3.824604	3.791876	-1.679365
H	2.104901	3.579346	-1.528008
H	3.836525	4.079474	1.523889
H	2.648393	3.008093	2.153452
H	2.866551	2.250133	-3.480203
H	4.078766	1.414727	-2.497752
H	2.376163	1.123121	-2.199771
H	6.056137	0.386418	0.160717
H	5.678538	1.584204	-1.075064
H	6.095177	2.113518	0.554781
H	1.657554	5.304118	1.831586
H	2.083904	5.266884	0.120320
H	0.854973	4.151185	0.752082
Li	0.882427	1.654645	2.492898

glu_si_reactant_gas_conformation2

C	4.827832	-2.873855	1.167223
C	4.828504	-2.888867	-0.227244
C	5.957167	-2.431438	-0.913031
C	7.064277	-1.962391	-0.216430
C	7.051453	-1.941669	1.179092
C	5.933377	-2.397390	1.870271
C	3.607531	-3.306916	-1.007408
O	2.898226	-2.178765	-1.510717
C	2.033167	-1.558529	-0.581050
C	1.786373	-0.123992	-1.064313
C	0.387447	0.415037	-0.723549
N	-0.267914	-0.281306	0.406205
C	-0.235633	-1.661688	0.479010
C	0.713139	-2.320227	-0.489520
C	-0.593344	0.435354	-1.892604
O	-1.723355	1.127510	-1.433183
C	-2.869112	0.947964	-2.261582
C	-3.978818	1.777193	-1.683064
C	-4.806231	1.229117	-0.703691
C	-5.789121	2.008330	-0.100419
C	-5.938177	3.344848	-0.463543
C	-5.109581	3.899040	-1.438003
C	-4.134481	3.114974	-2.047544
O	2.687355	0.804564	-0.508384
C	4.057766	0.557131	-0.781031
C	4.839079	1.820487	-0.527089
C	6.108493	1.756997	0.045217
C	6.854729	2.917131	0.236030
C	6.331299	4.151861	-0.135012
C	5.058417	4.221249	-0.697549
C	4.316993	3.061426	-0.894146
O	-0.874732	-2.316784	1.288322
C	-1.138245	0.458753	1.242727
O	-2.110272	-0.022939	1.792488
O	-0.716966	1.694411	1.367434
Li	-2.752566	-1.809921	1.398659
C	-3.441008	-3.919415	0.611820
C	-2.483287	-4.503655	-0.431204
B	-4.252492	-2.568437	0.095100
C	-5.109032	-1.895821	1.355123
C	-6.250243	-2.803681	1.831512
C	-5.201103	-2.952006	-1.172671
C	-6.095626	-1.839921	-1.727450
H	1.898668	-0.150318	-2.162592
H	2.501404	-1.499495	0.414633
H	0.838504	-3.349719	-0.151226
H	0.539243	1.444466	-0.403712
H	-0.135419	0.941972	-2.756971
H	-0.864424	-0.588175	-2.199724
H	-2.632431	1.267991	-3.287500
H	-3.144916	-0.116370	-2.274444
H	-3.484637	3.542422	-2.807255
H	-5.227348	4.939307	-1.724814
H	-6.703515	3.954348	0.007030
H	-6.434566	1.569672	0.654870
H	-4.668460	0.190011	-0.417167
H	4.440932	-0.255617	-0.149852
H	4.171654	0.232744	-1.827879
H	3.320260	3.109240	-1.321127
H	4.642959	5.182672	-0.983190
H	6.908889	5.057801	0.018907
H	7.841495	2.856378	0.684439
H	6.507462	0.791996	0.348895
H	2.953498	-3.936314	-0.389771
H	3.894143	-3.884976	-1.889672
H	3.957061	-3.239059	1.707227
H	5.921565	-2.386332	2.955167
H	7.915465	-1.575386	1.724673
H	7.937638	-1.611778	-0.757436
H	5.955820	-2.435929	-2.000079
H	0.250676	-2.356477	-1.483470
H	-3.386999	-1.724788	-0.305779

H	-4.513360	-1.654268	2.263870
H	-5.541795	-0.925430	1.071626
H	-5.840018	-3.802700	-0.887157
H	-4.581796	-3.332011	-1.997884
H	-4.199699	-4.677590	0.852390
H	-2.884028	-3.817125	1.565117
H	-6.770142	-2.194025	-2.515920
H	-6.720973	-1.391021	-0.944793
H	-5.500406	-1.025932	-2.158066
H	-6.815414	-2.375298	2.666756
H	-6.956422	-2.987875	1.015529
H	-5.871404	-3.778737	2.154708
H	-1.871164	-5.328410	-0.048181
H	-3.038879	-4.879520	-1.295721
H	-1.801546	-3.729710	-0.807830
C	-1.471545	2.695185	2.143989
C	-0.666446	3.962943	1.892991
C	-2.884550	2.830199	1.596309
C	-1.439981	2.304701	3.616067
H	-1.108093	4.792835	2.449936
H	0.369269	3.832331	2.216662
H	-0.676227	4.211454	0.828638
H	-1.897141	3.105928	4.203267
H	-1.996911	1.383983	3.793281
H	-0.408099	2.176563	3.954758
H	-3.350982	3.711804	2.045674
H	-2.860802	2.963754	0.510977
H	-3.493949	1.957083	1.828194

glu_si_TS_gas_conformation2

C	3.609772	3.485158	-6.371578
C	3.775725	3.772106	-5.016403
C	4.415211	4.953941	-4.643532
C	4.895365	5.831952	-5.611480
C	4.730216	5.539681	-6.962355
C	4.082778	4.365376	-7.339448
C	3.306471	2.801363	-3.962481
O	2.127485	2.160377	-4.417133
C	1.819183	0.953628	-3.755142
C	1.639947	1.142184	-2.238388
C	0.470048	0.308426	-1.710962
C	-0.775613	0.869321	-2.363263
N	-0.678910	0.787362	-3.815851
C	0.578050	0.389857	-4.465389
O	2.863363	0.786520	-1.621662
C	3.048680	1.333625	-0.321351
C	3.403220	2.799014	-0.379338
C	2.429422	3.783163	-0.202413
C	2.749389	5.130343	-0.360934
C	4.050417	5.502413	-0.686423
C	5.032890	4.525321	-0.853055
C	4.707128	3.182143	-0.703456
C	0.686486	-1.125452	-4.671453
O	-0.555975	-1.588961	-5.117323
C	-0.562828	-2.956546	-5.463596
C	-1.990270	-3.395769	-5.667868
C	-2.974455	-2.454920	-5.964444
C	-4.296773	-2.851496	-6.141148
C	-4.643538	-4.195231	-6.031365
C	-3.661610	-5.139628	-5.740183
C	-2.341350	-4.740842	-5.555683
C	-1.789587	1.106947	-4.548286
O	-1.557389	1.187234	-5.854544
C	-2.514548	1.840628	-6.751917
C	-2.797402	3.256494	-6.259463
O	-1.346027	1.874964	-1.860394
O	-2.895841	1.294782	-4.042446
C	-1.750138	1.873077	-8.069610
C	-3.786493	1.010393	-6.891408
Li	-3.011694	1.098230	-2.165114
C	-3.217171	-0.095543	-0.176298
B	-2.680850	-1.024419	-1.414941
C	-1.789156	-2.287168	-0.952062
C	-1.282903	-3.125001	-2.127668
C	-2.203994	0.328778	0.891215
C	-3.798896	-1.340759	-2.554386
C	-4.769239	-2.446653	-2.113580
H	2.649483	0.236355	-3.882171
H	1.409480	2.204286	-2.068699
H	0.344295	0.423980	-0.633319
H	0.561510	0.853444	-5.450843
H	1.476196	-1.309448	-5.418295
H	0.982732	-1.651119	-3.749652
H	0.030671	-3.109368	-6.380354
H	-0.099324	-3.557120	-4.665692
H	-1.580968	-5.477569	-5.307000
H	-3.926725	-6.187639	-5.642967
H	-5.675035	-4.506011	-6.162664
H	-5.057728	-2.105370	-6.351734
H	-2.693778	-1.408628	-6.019638
H	3.127852	3.332546	-3.017117
H	4.082481	2.044861	-3.761068

H	3.093300	2.574170	-6.655746
H	3.944561	4.135936	-8.391589
H	5.099024	6.226572	-7.717498
H	5.389933	6.750269	-5.310228
H	4.527395	5.186590	-3.587086
H	2.154714	1.181352	0.298176
H	3.866477	0.757484	0.119608
H	1.411958	3.491868	0.050565
H	1.982813	5.886931	-0.229715
H	4.301283	6.551618	-0.807377
H	6.049638	4.812994	-1.102331
H	5.465108	2.416411	-0.848178
H	0.613888	-0.752378	-1.929143
H	-1.719214	-0.304742	-2.105045
H	-4.408881	-0.464229	-2.839680
H	-3.306212	-1.652601	-3.484157
H	-2.384018	-2.919389	-0.274604
H	-0.930896	-1.956669	-0.350263
H	-3.972349	-0.749887	0.286675
H	-3.828890	0.793915	-0.438876
H	-0.573349	-3.905047	-1.828277
H	-2.107225	-3.609578	-2.663165
H	-0.793576	-2.473114	-2.860993
H	-5.503087	-2.680513	-2.892205
H	-4.231781	-3.372238	-1.883636
H	-5.321153	-2.160576	-1.211182
H	-2.685144	0.772243	1.768994
H	-1.624632	-0.533577	1.234984
H	-1.508687	1.068983	0.484450
H	-2.377432	2.309339	-8.851109
H	-0.841469	2.472786	-7.971583
H	-1.472956	0.858645	-8.367368
H	-3.344419	3.799476	-7.035000
H	-3.393345	3.252100	-5.346921
H	-1.856467	3.781509	-6.071501
H	-4.481546	1.541558	-7.548527
H	-3.565294	0.042274	-7.348673
H	-4.264702	0.854977	-5.923781

glu_si_product_gas_conformation2

C	-5.715643	1.301490	-2.581949
C	-4.451951	1.489576	-2.020413
C	-4.345172	1.855920	-0.679204
C	-5.495338	2.015209	0.091560
C	-6.754158	1.815796	-0.467650
C	-6.862013	1.463697	-1.811701
C	-3.221120	1.235759	-2.858027
O	-2.088655	1.265136	-2.029106
C	-0.904232	0.796866	-2.625420
C	0.084039	0.636028	-1.470017
C	1.558869	0.399435	-1.825257
C	1.930795	-1.081676	-1.745745
C	0.724716	-1.929589	-2.114930
C	-0.278799	-1.885682	-0.946561
N	-0.391195	-0.388219	-0.538588
O	2.264081	1.194168	-0.887104
C	3.674388	1.102093	-0.935788
C	4.252305	2.155566	-0.024969
C	3.603730	3.377031	0.162315
C	4.161274	4.350010	0.986614
C	5.376094	4.114704	1.626055
C	6.026824	2.897577	1.442503
C	5.463584	1.921130	0.626048
O	3.045352	-1.292940	-2.599171
C	3.749352	-2.501267	-2.347420
C	4.560836	-2.443992	-1.074440
C	4.006756	-2.844600	0.144274
C	4.731433	-2.702464	1.325883
C	6.018051	-2.171773	1.298229
C	6.583362	-1.784776	0.084138
C	5.853725	-1.916450	-1.093548
O	0.131834	-2.665460	0.059175
Li	-0.803852	-2.552971	1.514379
C	-0.991579	-0.039708	0.600927
O	-1.439279	-0.842298	1.449400
O	-1.102239	1.285443	0.801000
C	-0.714085	1.844554	2.093737
C	-1.803941	1.597774	3.129332
C	0.635143	1.260661	2.501434
C	-0.582135	3.331065	1.786769
C	-2.938394	-3.034114	2.841282
C	-2.411321	-4.427136	2.457487
B	-3.563963	-2.101905	1.703737
C	-4.359238	-0.811223	2.144878
C	-5.878120	-1.061496	2.095461
C	-3.644020	-2.625709	0.214747
C	-3.935297	-1.578964	-0.862804
H	1.772899	0.746537	-2.851301
H	2.187555	-1.295830	-0.699132
H	0.991307	-2.983350	-2.211327
H	0.066159	1.590255	-0.945972
H	-0.512161	1.520160	-3.357723

H	-1.098135	-0.150262	-3.148451
H	-3.133376	1.987182	-3.660289
H	-3.311424	0.249195	-3.342900
H	-5.801712	1.006751	-3.625599
H	-7.839145	1.305287	-2.257198
H	-7.646748	1.930772	0.139280
H	-5.404547	2.283921	1.140593
H	-3.359612	1.975926	-0.238140
H	4.018156	0.109385	-0.619030
H	4.021519	1.245821	-1.971892
H	2.656155	3.550042	-0.337492
H	3.647289	5.295689	1.129682
H	5.810407	4.873886	2.268891
H	6.969251	2.703698	1.945391
H	5.957389	0.960353	0.498344
H	3.056697	-3.352268	-2.309715
H	4.407345	-2.637899	-3.210141
H	2.993725	-3.244047	0.166317
H	4.289824	-3.007917	2.269305
H	6.582011	-2.064640	2.219519
H	7.590512	-1.379622	0.056466
H	6.284918	-1.600237	-2.040398
H	0.315595	-1.602911	-3.077224
H	-1.292447	-2.128702	-1.323560
H	-4.080101	-0.487255	3.155415
H	-4.114378	0.014326	1.464182
H	-4.457891	-3.373979	0.232711
H	-2.753905	-3.213617	-0.054344
H	-3.734125	-3.164117	3.589600
H	-2.184952	-2.451049	3.397771
H	-4.006670	-2.027319	-1.860188
H	-4.873658	-1.048416	-0.670550
H	-3.148427	-0.815684	-0.896190
H	-6.441409	-0.169592	2.386156
H	-6.205251	-1.337070	1.087953
H	-6.175002	-1.871486	2.771428
H	-2.024763	-4.973953	3.322072
H	-3.213896	-5.025680	2.017279
H	-1.618075	-4.429292	1.694937
H	-0.317607	3.879157	2.694703
H	0.199411	3.493262	1.039373
H	-1.527092	3.723121	1.400815
H	1.011593	1.784548	3.384125
H	0.544665	0.198821	2.747035
H	1.358044	1.378677	1.686716
H	-1.573977	2.156820	4.041481
H	-2.768544	1.941464	2.742930
H	-1.884752	0.536778	3.366057

glu_re_reactant_solvent

C	2.050832	3.584806	-1.725159
C	2.912301	2.618582	-1.209064
C	4.185326	2.998584	-0.778006
C	4.593895	4.324804	-0.866031
C	3.728595	5.289241	-1.380486
C	2.457847	4.915155	-1.807300
C	2.514753	1.166602	-1.113715
O	1.122392	1.043779	-1.321063
C	0.652187	-0.275585	-1.482273
C	1.032566	-1.180702	-0.307885
C	-0.062481	-2.234203	-0.094464
C	-1.274998	-1.478516	0.385790
N	-1.594405	-0.364091	-0.388019
C	-0.869224	-0.148725	-1.663518
O	2.281492	-1.763394	-0.590424
C	3.015035	-2.128689	0.563909
C	4.424040	-2.498763	0.175293
C	4.958174	-2.129381	-1.058011
C	6.278931	-2.444542	-1.373012
C	7.075866	-3.125654	-0.457875
C	6.544691	-3.497061	0.776157
C	5.224895	-3.188036	1.088370
C	-1.447733	-1.019689	-2.777318
O	-2.814141	-0.708340	-2.926914
C	-3.653949	-1.848879	-3.056948
C	-3.830126	-2.570240	-1.741985
C	-3.231652	-3.807879	-1.503170
C	-3.389184	-4.446420	-0.272220
C	-4.149035	-3.848516	0.727460
C	-4.738852	-2.603967	0.502309
C	-4.575214	-1.968789	-0.722582
C	-2.565614	0.555923	0.036544
O	-3.126393	0.499166	1.119031
Li	-2.071614	-0.211118	2.592627
O	-1.816715	-1.760024	1.443505
O	-2.772799	1.486603	-0.868059
C	-3.571667	2.686182	-0.565490
C	-3.424009	3.494706	-1.847446
C	-5.024304	2.290254	-0.336016
C	-2.956183	3.423708	0.617799
C	0.170828	2.627265	2.879675
C	1.086461	2.941291	1.692467

B	-0.083714	1.027088	3.095395
C	1.315369	0.204235	3.320690
C	1.161854	-1.307780	3.511589
C	-1.125071	0.760460	4.369907
C	-2.389057	1.638905	4.419816
H	1.091123	-0.725815	-2.389742
H	1.092164	-0.552579	0.597253
H	0.200029	-2.943790	0.690572
H	-1.048223	0.885780	-1.943922
H	-0.905324	-0.798790	-3.706702
H	-1.314033	-2.086067	-2.561136
H	-4.613001	-1.462134	-3.411295
H	-3.258999	-2.532577	-3.820766
H	-2.653358	-4.284760	-2.291795
H	-2.923109	-5.411367	-0.100237
H	-4.276761	-4.344007	1.684445
H	-5.321796	-2.127992	1.284597
H	-5.030718	-0.996547	-0.899169
H	2.796788	0.776993	-0.123326
H	3.057158	0.569800	-1.864179
H	4.857930	2.249668	-0.365983
H	5.584795	4.608304	-0.525733
H	4.043385	6.325968	-1.443242
H	1.776555	5.661252	-2.204525
H	1.058289	3.290309	-2.047655
H	3.031957	-1.282334	1.269589
H	2.533893	-2.969357	1.085440
H	4.810919	-3.482586	2.050017
H	7.157585	-4.032763	1.494099
H	8.104421	-3.369247	-0.703931
H	6.684627	-2.154822	-2.337383
H	4.331592	-1.604804	-1.770994
H	-0.243850	-2.790316	-1.017791
H	-0.574593	0.619296	2.008597
H	1.843355	0.615681	4.196974
H	1.998205	0.386065	2.473539
H	2.116427	-1.842932	3.606576
H	0.577487	-1.535900	4.410647
H	0.618679	-1.758663	2.668350
H	-0.783095	3.155385	2.723306
H	0.599278	3.073134	3.793608
H	1.195257	4.014124	1.485769
H	2.097879	2.544686	1.846519
H	0.707940	2.469103	0.775724
H	-1.416339	-0.300386	4.518390
H	-0.539750	0.966173	5.276998
H	-3.037138	1.415743	5.274674
H	-2.108584	2.693980	4.477544
H	-3.013428	1.554504	3.515574
H	-3.999457	4.419890	-1.767015
H	-2.374557	3.748382	-2.019146
H	-3.792842	2.921502	-2.701974
H	-3.432685	4.403652	0.708128
H	-3.094563	2.881451	1.554104
H	-1.884729	3.574736	0.452902
H	-5.626123	3.197991	-0.238911
H	-5.397964	1.722286	-1.193090
H	-5.135701	1.696819	0.571571

glu_re_TS_solvent

C	1.702668	3.969200	-0.156928
C	2.809173	3.190945	-0.497869
C	4.081341	3.764837	-0.470962
C	4.247318	5.096638	-0.104217
C	3.139448	5.871055	0.236237
C	1.868763	5.303440	0.208130
C	2.653821	1.734143	-0.861966
O	1.297076	1.488185	-1.156194
C	0.968120	0.157124	-1.499077
C	1.374164	-0.833864	-0.404036
C	0.354355	-1.953310	-0.251883
C	-1.031727	-1.433463	0.076578
N	-1.278501	-0.133048	-0.501414
C	-0.545737	0.185252	-1.736388
O	2.651688	-1.335952	-0.748566
C	3.403089	-1.805802	0.353595
C	4.759174	-2.257688	-0.123935
C	5.376453	-1.634087	-1.209313
C	6.645020	-2.034136	-1.619972
C	7.311120	-3.055828	-0.946082
C	6.699918	-3.679106	0.139081
C	5.427766	-3.283954	0.544132
C	-1.064682	-0.692117	-2.875555
O	-2.363045	-0.237074	-3.200977
C	-3.286706	-1.269376	-3.506416
C	-3.904336	-1.869381	-2.262435
C	-3.909875	-3.244190	-2.031490
C	-4.522663	-3.768714	-0.895423
C	-5.138941	-2.918875	0.020055
C	-5.130123	-1.540463	-0.200276
C	-4.510257	-1.022655	-1.332815
C	-2.222285	0.698779	0.033618

O	-2.921730	0.392290	0.996395
Li	-2.905856	-1.360886	1.700959
O	-1.960458	-2.207724	0.347594
O	-2.271350	1.874773	-0.575024
C	-3.101551	2.968247	-0.058280
C	-2.734242	4.119556	-0.986408
C	-4.575760	2.609816	-0.202257
C	-2.712670	3.291719	1.380252
C	-0.326017	0.843938	3.219258
C	0.695738	1.584854	2.351160
B	-0.457474	-0.749700	2.920272
C	0.912635	-1.595378	3.200702
C	0.769753	-3.124188	3.209684
C	-1.736718	-1.455338	3.702756
C	-2.933379	-0.573980	4.113494
H	1.489716	-0.135841	-2.425299
H	1.416320	-0.282025	0.546361
H	0.637914	-2.638316	0.547187
H	-0.789446	1.212992	-1.999805
H	-0.404350	-0.597560	-3.748658
H	-1.093264	-1.749831	-2.582874
H	-4.063752	-0.796053	-4.114994
H	-2.815008	-2.050186	-4.118301
H	-3.434182	-3.910495	-2.747099
H	-4.520362	-4.840648	-0.725599
H	-5.630933	-3.328785	0.897285
H	-5.611029	-0.869302	0.507148
H	-4.488121	0.050879	-1.504975
H	2.992765	1.111957	-0.019307
H	3.286186	1.479120	-1.726755
H	4.947167	3.164912	-0.741075
H	5.241586	5.531890	-0.088307
H	3.267925	6.910738	0.519743
H	1.000283	5.899636	0.471729
H	0.715624	3.519489	-0.181919
H	3.513681	-0.994046	1.092775
H	2.888608	-2.633477	0.863545
H	4.946954	-3.779348	1.383959
H	7.209195	-4.480456	0.664892
H	8.299490	-3.367638	-1.267950
H	7.115319	-1.547393	-2.468674
H	4.849923	-0.843753	-1.734712
H	0.294752	-2.540148	-1.176978
H	-0.634213	-0.822203	1.623725
H	1.310632	-1.285752	4.181461
H	1.700080	-1.314096	2.486741
H	1.733486	-3.647032	3.250308
H	0.189025	-3.459408	4.075772
H	0.232045	-3.493356	2.326963
H	-1.300595	1.337262	3.094050
H	-0.061669	0.987392	4.281003
H	0.797199	2.647589	2.606510
H	1.696603	1.139190	2.437134
H	0.417688	1.536222	1.289040
H	-2.082822	-2.390175	3.214744
H	-1.317336	-1.848642	4.639316
H	-3.711859	-1.137333	4.640293
H	-2.586532	0.216315	4.785057
H	-3.413538	-0.038168	3.283047
H	-3.326359	5.001380	-0.730395
H	-1.674227	4.368761	-0.887651
H	-2.936209	3.849549	-2.026007
H	-3.148926	4.256342	1.654346
H	-3.069702	2.531903	2.075292
H	-1.623612	3.367256	1.467999
H	-5.182390	3.462165	0.115909
H	-4.811549	2.395739	-1.248845
H	-4.834180	1.747409	0.414190

glu_re_product_solvent

C	1.502919	3.814638	-0.419624
C	2.657636	3.098962	-0.737336
C	3.896108	3.740038	-0.678790
C	3.982277	5.076839	-0.303195
C	2.826799	5.788498	0.016624
C	1.589229	5.153932	-0.043218
C	2.588892	1.637891	-1.112966
O	1.240604	1.294611	-1.319369
C	0.974200	-0.072686	-1.577924
C	1.460750	-0.961138	-0.427078
C	0.463470	-2.065004	-0.112710
C	-0.854777	-1.473628	0.421756
N	-1.172012	-0.249489	-0.439379
C	-0.548357	-0.126124	-1.749969
O	2.748261	-1.446057	-0.771737
C	3.536859	-1.790543	0.345740
C	4.924686	-2.163159	-0.111094
C	5.452611	-1.636119	-1.290324
C	6.748190	-1.959871	-1.685135
C	7.530045	-2.806139	-0.902270
C	7.007820	-3.331805	0.277530
C	5.709956	-3.014344	0.667558

C	-1.096532	-1.207445	-2.685929
O	-2.280611	-0.688905	-3.273906
C	-3.273102	-1.666840	-3.498362
C	-4.081479	-1.950392	-2.249928
C	-4.467747	-3.244163	-1.905203
C	-5.257099	-3.473884	-0.779990
C	-5.682541	-2.403029	0.004473
C	-5.297189	-1.101938	-0.334456
C	-4.486269	-0.881952	-1.446633
C	-2.057162	0.624672	0.056565
O	-2.713656	0.399891	1.091117
Li	-3.285899	-1.453594	1.103901
O	-1.861300	-2.345564	0.517079
O	-2.176516	1.752504	-0.656818
C	-2.934850	2.895384	-0.158143
C	-2.686143	3.949258	-1.231287
C	-4.420809	2.563627	-0.068943
C	-2.373966	3.353044	1.184608
C	-0.200254	1.083725	3.374004
C	0.771166	1.611828	2.312698
B	-0.321569	-0.480040	3.573940
C	0.958715	-1.408192	3.432628
C	0.712387	-2.920420	3.434105
C	-1.680553	-1.137120	4.044581
C	-2.868443	-0.219665	4.340807
H	1.482476	-0.391059	-2.502480
H	1.542512	-0.312224	0.459785
H	0.853136	-2.726279	0.666822
H	-0.835453	0.832284	-2.184143
H	-0.371069	-1.453096	-3.475082
H	-1.330012	-2.114560	-2.117826
H	-3.930634	-1.258060	-4.273273
H	-2.837870	-2.596078	-3.891379
H	-4.143324	-4.081780	-2.517150
H	-5.544983	-4.486910	-0.518413
H	-6.318772	-2.576663	0.867110
H	-5.635244	-0.259118	0.262788
H	-4.162086	0.122879	-1.705863
H	3.034964	1.036717	-0.305341
H	3.180887	1.440105	-2.021160
H	4.798597	3.187565	-0.929821
H	4.951066	5.564719	-0.261335
H	2.892522	6.831615	0.309024
H	0.683921	5.701556	0.202933
H	0.543341	3.309639	-0.472404
H	3.589583	-0.929516	1.036353
H	3.090011	-2.623724	0.908980
H	5.300312	-3.434553	1.582801
H	7.608539	-3.996363	0.890426
H	8.539242	-3.058860	-1.211294
H	7.147746	-1.551277	-2.608127
H	4.834326	-0.985046	-1.899607
H	0.284017	-2.688984	-0.994607
H	-0.600047	-0.986237	1.391519
H	1.626688	-1.137382	4.267659
H	1.529471	-1.125092	2.537090
H	1.629901	-3.487257	3.243290
H	0.313573	-3.259043	4.395208
H	-0.019973	-3.198532	2.667265
H	-1.188958	1.527186	3.218939
H	0.118544	1.446032	4.368572
H	0.879786	2.700720	2.359206
H	1.773635	1.181746	2.423516
H	0.421759	1.370034	1.299927
H	-1.933616	-1.855819	3.243414
H	-1.475298	-1.785914	4.909226
H	-3.752200	-0.783121	4.658996
H	-2.629330	0.489032	5.140767
H	-3.138161	0.366475	3.457095
H	-3.228806	4.865106	-0.984415
H	-1.619618	4.180958	-1.301225
H	-3.029664	3.587742	-2.203965
H	-2.802689	4.326425	1.439560
H	-2.616689	2.642058	1.975203
H	-1.285593	3.460807	1.123571
H	-4.972154	3.466468	0.208752
H	-4.797613	2.222597	-1.037898
H	-4.599989	1.797237	0.685302

glu_si_reactant_solvent

C	4.746008	-2.985191	1.005644
C	4.804146	-2.929858	-0.387411
C	5.975329	-2.478915	-1.003234
C	7.067597	-2.084179	-0.238712
C	6.995989	-2.129032	1.154752
C	5.835584	-2.580710	1.776340
C	3.602689	-3.268352	-1.233602
O	2.927759	-2.091436	-1.677112
C	2.060398	-1.511607	-0.724246
C	1.861101	-0.040800	-1.110089
C	0.462177	0.504970	-0.784901
N	-0.241562	-0.240360	0.285984

C	-0.230383	-1.623509	0.285948
C	0.721548	-2.246623	-0.701531
C	-0.468429	0.605827	-1.990714
O	-1.638116	1.236235	-1.533698
C	-2.716846	1.154484	-2.458835
C	-3.896008	1.857301	-1.848348
C	-4.683776	1.188436	-0.910284
C	-5.734475	1.849063	-0.279862
C	-5.993805	3.186911	-0.573231
C	-5.207875	3.860051	-1.506281
C	-4.162753	3.194680	-2.143403
O	2.764252	0.817666	-0.450256
C	4.133499	0.576355	-0.731321
C	4.935784	1.796078	-0.352822
C	6.248498	1.650035	0.097086
C	7.019131	2.769244	0.401142
C	6.478099	4.045848	0.269376
C	5.164244	4.196136	-0.169615
C	4.397450	3.077104	-0.482338
O	-0.895405	-2.313278	1.045639
C	-1.111654	0.473644	1.142102
O	-2.082127	-0.024199	1.682270
O	-0.704178	1.709952	1.294651
Li	-2.733708	-1.819547	1.413891
C	-3.658915	-3.942449	0.938666
C	-2.823386	-4.747573	-0.062272
B	-4.393361	-2.600796	0.293410
C	-5.126727	-1.696304	1.481220
C	-6.360606	-2.387503	2.075990
C	-5.446275	-3.048792	-0.868325
C	-6.216167	-1.914322	-1.550582
H	2.015201	0.017759	-2.201097
H	2.510529	-1.532077	0.280657
H	0.825748	-3.294352	-0.417507
H	0.619056	1.511997	-0.404367
H	0.019526	1.192098	-2.783946
H	-0.701106	-0.390101	-2.400138
H	-2.427038	1.624375	-3.409735
H	-2.950742	0.096835	-2.650622
H	-3.547200	3.716661	-2.871648
H	-5.410641	4.900560	-1.739476
H	-6.811306	3.702804	-0.079463
H	-6.347656	1.319265	0.443500
H	-4.466464	0.149420	-0.671166
H	4.499056	-0.298887	-0.177707
H	4.254942	0.351484	-1.802867
H	3.372030	3.188156	-0.819346
H	4.735076	5.188257	-0.269485
H	7.074701	4.918840	0.513864
H	8.038518	2.643676	0.752391
H	6.663518	0.651847	0.215393
H	2.917497	-3.926409	-0.684280
H	3.908447	-3.785687	-2.146382
H	3.843696	-3.350106	1.490983
H	5.778388	-2.623433	2.859074
H	7.847194	-1.818481	1.752215
H	7.974904	-1.739631	-0.725198
H	6.021986	-2.431675	-2.088275
H	0.276855	-2.216759	-1.703330
H	-3.500577	-1.888208	-0.255711
H	-4.479237	-1.432101	2.343636
H	-5.437900	-0.718480	1.085009
H	-6.172853	-3.756757	-0.437799
H	-4.925470	-3.621138	-1.649365
H	-4.456837	-4.589468	1.332075
H	-3.024706	-3.767112	1.832439
H	-6.968225	-2.276240	-2.262313
H	-6.738225	-1.280858	-0.821428
H	-5.537279	-1.257032	-2.106911
H	-6.830918	-1.808418	2.879010
H	-7.118150	-2.551793	1.302720
H	-6.104655	-3.370408	2.486960
H	-2.319800	-5.609970	0.390121
H	-3.449981	-5.126123	-0.875805
H	-2.051023	-4.114604	-0.515954
C	-1.477420	2.691991	2.080674
C	-0.683168	3.971369	1.856455
C	-2.886022	2.820988	1.518999
C	-1.457213	2.281074	3.546966
H	-1.142519	4.788789	2.417124
H	0.348550	3.848113	2.195502
H	-0.679363	4.233121	0.795105
H	-1.924000	3.072448	4.139628
H	-2.010424	1.355068	3.707180
H	-0.427688	2.154291	3.892792
H	-3.365457	3.689068	1.980391
H	-2.851679	2.974312	0.436519
H	-3.489160	1.937455	1.728066

glu_si_TS_solvent

C	-3.787966	1.916979	0.785003
C	-4.347749	0.736672	1.269689

C	-5.728901	0.668268	1.476162
C	-6.543946	1.754293	1.179181
C	-5.983583	2.929153	0.675827
C	-4.608194	3.006502	0.485469
C	-3.511991	-0.485179	1.587550
O	-2.120129	-0.287892	1.398033
C	-1.550353	-1.001604	0.319156
C	-1.860771	-0.320569	-1.025989
C	-0.810237	0.750729	-1.383041
C	-0.118043	1.338877	-0.166622
N	0.490907	0.306621	0.652390
C	-0.049911	-1.065763	0.595933
O	-1.854434	-1.290842	-2.064723
C	-3.111620	-1.465969	-2.701927
C	-4.154771	-2.050096	-1.776863
C	-5.320645	-1.350908	-1.471579
C	-6.261603	-1.892822	-0.594997
C	-6.029583	-3.129720	-0.002486
C	-4.858321	-3.832263	-0.295410
C	-3.930314	-3.296285	-1.180498
C	0.685053	-1.966371	-0.394406
O	2.050135	-1.937920	-0.063723
C	2.845928	-2.697597	-0.946357
C	4.294104	-2.319155	-0.766162
C	4.634920	-1.078546	-0.228921
C	5.970898	-0.702283	-0.113452
C	6.979088	-1.565667	-0.535774
C	6.643193	-2.808898	-1.068544
C	5.307185	-3.184514	-1.179906
C	1.369331	0.694286	1.627437
O	1.689074	-0.286668	2.457030
C	2.606206	-0.072647	3.580717
C	2.038844	0.980608	4.525988
O	-0.521166	2.396141	0.376058
O	1.824541	1.835566	1.703229
C	2.621170	-1.443557	4.245297
C	3.994815	0.285463	3.064944
Li	1.202872	3.177105	0.505254
C	1.301604	4.036401	-1.812623
B	2.009193	2.566382	-1.658237
C	2.070956	1.702830	-3.024647
C	2.685855	0.313252	-2.821692
C	-0.084959	4.108055	-2.460496
C	3.428395	2.631216	-0.846301
C	4.566846	3.162576	-1.730509
H	-1.945245	-2.026293	0.279915
H	-2.854555	0.135022	-0.941593
H	-1.254401	1.573013	-1.945022
H	0.083183	-1.487457	1.592356
H	0.274578	-2.985115	-0.305034
H	0.536303	-1.645953	-1.434710
H	2.701004	-3.774342	-0.767945
H	2.542763	-2.494288	-1.986713
H	5.049864	-4.157668	-1.591362
H	7.423370	-3.489831	-1.394040
H	8.020775	-1.274131	-0.448103
H	6.219112	0.268869	0.306097
H	3.840627	-0.415544	0.098978
H	-3.868475	-1.332038	0.981531
H	-3.659891	-0.757420	2.639982
H	-2.712387	1.990892	0.652297
H	-4.162739	3.920523	0.104164
H	-6.617171	3.778310	0.440247
H	-7.615548	1.686710	1.340352
H	-6.165212	-0.249047	1.865785
H	-3.466687	-0.509404	-3.109811
H	-2.917571	-2.142686	-3.538944
H	-5.491546	-0.371233	-1.911788
H	-7.164955	-1.336878	-0.365352
H	-6.756526	-3.548790	0.685910
H	-4.675230	-4.798021	0.164872
H	-3.014864	-3.836392	-1.410279
H	-0.062109	0.274561	-2.019894
H	1.192076	1.794621	-0.909987
H	3.391653	3.265329	0.057261
H	3.711637	1.637455	-0.474867
H	2.654519	2.251476	-3.780723
H	1.070586	1.594595	-3.466941
H	2.012369	4.596557	-2.440397
H	1.278755	4.652583	-0.891122
H	2.584340	-0.339107	-3.697344
H	3.753480	0.378555	-2.582541
H	2.219883	-0.194423	-1.964556
H	5.518462	3.229972	-1.191646
H	4.724722	2.509604	-2.595128
H	4.339268	4.161380	-2.119411
H	-0.372885	5.132908	-2.718952
H	-0.115008	3.517442	-3.381925
H	-0.848457	3.712885	-1.783637
H	3.309320	-1.436394	5.093959
H	1.622593	-1.705971	4.604692
H	2.949678	-2.202112	3.530057

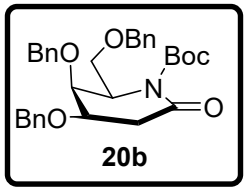
H	2.630005	0.984742	5.445844
H	2.071796	1.975022	4.081631
H	1.004664	0.734868	4.783291
H	4.672413	0.384397	3.917804
H	4.372209	-0.509382	2.416565
H	3.984758	1.226501	2.512739

glu_si_product_solvent

C	-5.657576	1.517784	-2.714395
C	-4.423469	1.501018	-2.061069
C	-4.364832	1.804933	-0.701444
C	-5.532555	2.113292	-0.004285
C	-6.762022	2.124299	-0.656219
C	-6.821261	1.827121	-2.017518
C	-3.178920	1.120788	-2.827075
O	-2.075544	1.154780	-1.957791
C	-0.881117	0.662641	-2.515762
C	0.098053	0.542360	-1.346681
C	1.580187	0.380050	-1.710031
C	2.034289	-1.080471	-1.675433
C	0.862011	-1.997667	-1.982680
C	-0.087086	-1.992163	-0.769489
N	-0.330636	-0.505329	-0.417055
O	2.264570	1.180303	-0.759386
C	3.672583	1.201125	-0.892605
C	4.229714	2.251943	0.034013
C	3.522100	3.426827	0.294988
C	4.061298	4.402009	1.129589
C	5.316017	4.215310	1.706856
C	6.025456	3.044586	1.450393
C	5.481298	2.065941	0.622527
O	3.112387	-1.215415	-2.591418
C	3.901438	-2.383140	-2.399691
C	4.758836	-2.308512	-1.157903
C	4.282617	-2.781515	0.068097
C	5.046264	-2.637280	1.224724
C	6.297047	-2.027754	1.164388
C	6.785307	-1.564866	-0.057249
C	6.016508	-1.702282	-1.209604
O	0.443542	-2.680348	0.252678
Li	-0.402227	-2.570979	1.785235
C	-1.016546	-0.203008	0.690825
O	-1.429966	-1.043036	1.517686
O	-1.250134	1.109704	0.867311
C	-0.999480	1.716663	2.173311
C	-2.129202	1.392281	3.140873
C	0.362741	1.255129	2.682434
C	-0.974697	3.205460	1.849893
C	-3.285706	-3.108873	2.823796
C	-2.661405	-4.477879	2.537904
B	-3.721252	-2.206637	1.591877
C	-4.526984	-0.879305	1.887260
C	-6.032227	-1.105580	1.648673
C	-3.615341	-2.760975	0.115213
C	-3.743576	-1.739434	-1.018051
H	1.765487	0.767043	-2.726538
H	2.363915	-1.291746	-0.649356
H	1.186600	-3.035155	-2.083274
H	0.035149	1.494389	-0.820569
H	-0.483221	1.358315	-3.270733
H	-1.068393	-0.304157	-3.003981
H	-3.024936	1.807636	-3.675296
H	-3.301380	0.108105	-3.245798
H	-5.707963	1.278906	-3.774389
H	-7.775249	1.832071	-2.535449
H	-7.669309	2.360720	-0.109435
H	-5.478602	2.335605	1.058162
H	-3.405297	1.774959	-0.192650
H	4.109314	0.223246	-0.651791
H	3.941556	1.422821	-1.938184
H	2.543549	3.563097	-0.154419
H	3.501592	5.310388	1.330443
H	5.735509	4.975579	2.358063
H	6.999303	2.888353	1.904013
H	6.024724	1.142258	0.435824
H	3.265710	-3.277087	-2.361534
H	4.531915	-2.454292	-3.290022
H	3.297151	-3.242002	0.117145
H	4.664580	-3.002705	2.172907
H	6.893061	-1.918414	2.064950
H	7.763934	-1.097415	-0.110928
H	6.390589	-1.331781	-2.160902
H	0.387812	-1.708332	-2.926432
H	-1.085126	-2.352868	-1.084329
H	-4.378437	-0.532146	2.917338
H	-4.180037	-0.077877	1.222641
H	-4.424625	-3.508531	0.031837
H	-2.694925	-3.349602	-0.002745
H	-4.186658	-3.246044	3.442258
H	-2.627469	-2.498213	3.461062
H	-3.639273	-2.206821	-2.004148
H	-4.711695	-1.227926	-0.993343

H	-2.979941	-0.956279	-0.939012
H	-6.610163	-0.194767	1.833852
H	-6.233461	-1.413720	0.617620
H	-6.427917	-1.886995	2.307279
H	-2.384609	-5.011168	3.452188
H	-3.356239	-5.114052	1.980825
H	-1.761445	-4.415353	1.911771
H	-0.821105	3.783865	2.764524
H	-0.163410	3.429569	1.151547
H	-1.922930	3.509166	1.397392
H	0.635583	1.828223	3.572359
H	0.343680	0.195564	2.952139
H	1.125764	1.415285	1.913127
H	-1.986257	1.955671	4.067998
H	-3.089445	1.679460	2.701401
H	-2.156981	0.325543	3.364788

2-deoxygalactonolactam-*N*-Boc (20b)



20b

gal_re_reactant_gas_conformation1

C	-3.959991	-5.515810	-0.796710
C	-2.806106	-6.196408	-0.401012
C	-2.828714	-6.953171	0.766728
C	-3.990783	-7.037351	1.531210
C	-5.135242	-6.352807	1.135996
C	-5.117527	-5.589298	-0.031318
C	-1.553526	-6.082325	-1.228223
O	-1.295764	-4.702372	-1.419971
C	-0.266082	-4.390654	-2.314197
C	-0.282569	-2.868107	-2.459085
C	0.957954	-2.390645	-3.258036
N	1.749919	-3.517131	-3.806513
C	2.132981	-4.530559	-2.929868
C	1.129100	-4.798761	-1.832615
O	-0.230951	-2.234241	-1.196026
C	-1.449370	-2.110929	-0.474151
C	-1.462865	-2.930378	0.795434
C	-0.279363	-3.339549	1.404825
C	-0.314601	-4.086122	2.580077
C	-1.534449	-4.419495	3.161942
C	-2.720197	-3.999511	2.563883
C	-2.682059	-3.261144	1.385739
C	1.909920	-1.520279	-2.421418
O	3.066092	-1.332527	-3.198295
C	4.187132	-0.817334	-2.503264
C	5.424791	-1.495077	-3.033811
C	5.564314	-2.874737	-2.857620
C	6.677224	-3.540179	-3.358361
C	7.661066	-2.830488	-4.048784
C	7.525315	-1.457859	-4.231455
C	6.408531	-0.793082	-3.725056
C	2.300899	-3.279410	-5.084942
O	3.142132	-4.247635	-5.478442
C	4.012069	-4.016365	-6.660419
C	3.173223	-4.066543	-7.929150
O	3.141844	-5.209173	-3.063978
O	1.978750	-2.335188	-5.755529

C	4.763343	-2.699594	-6.502875
C	4.987234	-5.184923	-6.574530
Li	2.813267	-6.111766	-4.783725
C	2.611178	-8.325794	-4.352051
B	1.243871	-7.516345	-4.848175
C	-0.108028	-8.361687	-4.525494
C	-0.155194	-8.925276	-3.101421
C	2.756487	-9.673917	-5.069987
C	1.350791	-7.077724	-6.438234
C	0.329366	-6.016573	-6.855302
H	-1.201159	-2.568390	-2.980013
H	-0.447452	-4.862063	-3.295044
H	1.214318	-5.866342	-1.619162
H	0.646069	-1.816278	-4.127632
H	1.418436	-0.574467	-2.162601
H	2.159263	-2.032048	-1.479520
H	4.248526	0.271760	-2.629870
H	4.084601	-1.024610	-1.427725
H	4.791245	-3.431836	-2.335263
H	6.777431	-4.611018	-3.207641
H	8.530695	-3.347794	-4.441687
H	8.286250	-0.903219	-4.771089
H	6.296950	0.277360	-3.876219
H	-1.670937	-6.574219	-2.207092
H	-0.718052	-6.570103	-0.708304
H	-1.928235	-7.469512	1.088145
H	-3.996198	-7.628753	2.441437
H	-6.040076	-6.412230	1.732856
H	-6.009289	-5.054761	-0.344193
H	-3.935635	-4.915706	-1.702190
H	5.534763	-2.653461	-7.277066
H	4.103425	-1.840268	-6.613705
H	5.254849	-2.655785	-5.527929
H	3.839238	-3.971071	-8.791833
H	2.641089	-5.017718	-8.007197
H	2.452883	-3.248265	-7.948157
H	5.706133	-5.120182	-7.394820
H	5.535069	-5.147983	-5.627685
H	4.473295	-6.148514	-6.666643
H	1.377178	-4.241249	-0.922126
H	1.134236	-6.452336	-4.184300
H	-0.229107	-9.192219	-5.237733
H	-0.989700	-7.721841	-4.682720
H	-1.139506	-9.319005	-2.820887
H	0.568565	-9.737530	-2.971514
H	0.115009	-8.153797	-2.367847
H	2.359737	-6.732151	-6.748832
H	1.205067	-7.979638	-7.049075
H	0.347042	-5.777606	-7.925256
H	-0.684077	-6.349859	-6.610024
H	0.491871	-5.076035	-6.309048
H	3.591116	-7.811992	-4.496978
H	2.575334	-8.494946	-3.266768
H	3.624231	-10.249840	-4.730766
H	1.865854	-10.289691	-4.907983
H	2.854529	-9.533796	-6.152231
H	-1.558499	-1.046637	-0.226287
H	-2.300068	-2.402871	-1.099952
H	-3.611483	-2.961705	0.907512
H	-3.677547	-4.268942	2.998646
H	-1.561458	-5.006621	4.074418
H	0.613851	-4.406464	3.043207
H	0.669016	-3.068654	0.950822

gal_re_TS_gas_conformation1

C	-0.431212	-3.745002	1.228621
C	-1.545169	-3.087429	0.713942
C	-2.769637	-3.208843	1.373176
C	-2.882956	-3.984085	2.521227
C	-1.767832	-4.650189	3.025017
C	-0.543132	-4.528155	2.375864
C	-1.456368	-2.228283	-0.527525
C	-0.327062	-2.957505	-2.543278
C	0.952017	-2.524653	-3.301286
N	1.578151	-3.660386	-4.003932
C	1.970722	-4.790983	-3.163784
C	0.932657	-5.036557	-2.073230
C	-0.425996	-4.488003	-2.494672
C	1.998400	-1.868294	-2.384923
O	3.167806	-1.707309	-3.151203
C	4.279559	-1.252773	-2.405390
C	5.535586	-1.753104	-3.069466
C	5.810041	-3.124261	-3.038605
C	6.944114	-3.623833	-3.669974
C	7.805872	-2.761643	-4.349976
C	7.532314	-1.398232	-4.387502
C	6.400104	-0.896495	-3.745439
O	-1.490898	-4.754082	-1.615243
C	-1.625513	-6.072990	-1.131746
C	-2.909555	-6.160793	-0.347724
C	-2.977667	-6.946863	0.799683
C	-4.165688	-7.046669	1.519581

C	-5.294295	-6.349671	1.100266
C	-5.231490	-5.559702	-0.046651
C	-4.047485	-5.470612	-0.770246
O	3.190715	-5.019414	-2.931152
C	2.196857	-3.318408	-5.191264
O	1.923433	-2.338302	-5.840847
O	3.105850	-4.246025	-5.592746
C	3.962419	-3.969961	-6.761504
C	4.691612	-2.642428	-6.585119
C	4.966993	-5.118211	-6.705088
C	3.124784	-4.018442	-8.032195
Li	3.371053	-5.827305	-4.555522
C	2.818100	-7.993040	-4.105486
C	2.857331	-9.369510	-4.798165
B	1.476802	-7.199635	-4.622561
C	1.411791	-6.901723	-6.215806
C	0.294761	-5.942293	-6.634339
C	0.101053	-7.845172	-4.042136
C	0.162686	-8.650589	-2.737424
H	-1.218580	-2.560828	-3.047183
H	-0.656573	-4.866347	-3.504599
H	0.923221	-6.107537	-1.875106
H	0.698072	-1.811711	-4.084503
H	1.613381	-0.909700	-2.014141
H	2.205800	-2.501833	-1.510320
H	4.277315	-0.155030	-2.338530
H	4.223769	-1.651638	-1.381164
H	5.114748	-3.792391	-2.536585
H	7.163326	-4.687299	-3.626106
H	8.690425	-3.152899	-4.842912
H	8.198324	-0.723553	-4.916069
H	6.182482	0.167781	-3.778649
H	-1.633618	-6.784404	-1.972162
H	-0.783625	-6.335949	-0.474923
H	-2.088337	-7.468277	1.144683
H	-4.203137	-7.657605	2.416241
H	-6.219448	-6.418906	1.664000
H	-6.109468	-5.013042	-0.377389
H	-3.987362	-4.848828	-1.658240
H	5.488292	-2.583061	-7.332877
H	4.018610	-1.796370	-6.711935
H	5.146911	-2.592675	-5.592756
H	3.781742	-3.872621	-8.894869
H	2.628020	-4.986963	-8.134768
H	2.374358	-3.227542	-8.022087
H	5.666767	-5.041193	-7.540455
H	5.549351	-5.062893	-5.777131
H	4.470906	-6.093225	-6.784459
H	1.275150	-4.531207	-1.163357
H	1.517615	-5.903218	-4.071322
H	-0.280689	-8.516105	-4.828290
H	-0.677007	-7.074185	-3.957499
H	-0.821760	-9.032871	-2.445322
H	0.827469	-9.514574	-2.833874
H	0.542738	-8.065388	-1.892768
H	2.367002	-6.544171	-6.630796
H	1.246595	-7.873345	-6.706118
H	0.238323	-5.798741	-7.718632
H	-0.678759	-6.319566	-6.303688
H	0.425675	-4.953889	-6.178256
H	3.828250	-7.572455	-4.292711
H	2.792927	-8.125691	-3.016846
H	3.625189	-10.023153	-4.373679
H	1.895668	-9.883813	-4.712284
H	3.065537	-9.259107	-5.866896
H	-1.500905	-1.168879	-0.239953
H	-2.318928	-2.442129	-1.168879
H	-3.649608	-2.714115	0.967926
H	-3.848435	-4.091966	3.005529
H	-1.855947	-5.267294	3.913870
H	0.331917	-5.040802	2.764389
H	0.523292	-3.636469	0.724341
O	-0.244836	-2.411931	-1.240500

gal_re_product_gas_conformation1

C	3.511389	-2.099190	0.019046
C	4.006838	-1.625525	-1.193394
C	5.386533	-1.608833	-1.404070
C	6.260024	-2.043979	-0.414077
C	5.760490	-2.501258	0.803662
C	4.385325	-2.528535	1.016387
C	3.087283	-1.153011	-2.297011
O	1.749799	-0.971192	-1.863679
C	1.227950	0.344191	-1.863808
C	1.671128	1.125381	-0.615970
C	0.929243	0.568209	0.592940
C	-0.569413	0.907965	0.504958
N	-0.929376	1.099742	-0.911331
C	-0.320474	0.216425	-1.900514
O	3.074561	1.000730	-0.587272
C	3.722334	1.313083	0.625913
C	5.211428	1.280822	0.393729

C	5.751538	1.688465	-0.827146
C	7.126357	1.652709	-1.033507
C	7.976548	1.219529	-0.017601
C	7.443223	0.821030	1.204205
C	6.065505	0.846850	1.404780
C	-0.776521	-1.239004	-1.696682
O	-2.192516	-1.224554	-1.510379
C	-2.814754	-2.489615	-1.701719
C	-4.231858	-2.355241	-1.200176
C	-4.798621	-3.321734	-0.367843
C	-6.103607	-3.172184	0.094400
C	-6.846136	-2.049188	-0.262618
C	-6.279346	-1.070872	-1.076432
C	-4.976013	-1.219439	-1.545145
C	-2.089333	1.739175	-1.277152
O	-2.725889	2.235442	-0.196140
O	-1.359666	-0.101012	1.030056
O	-2.495020	1.831495	-2.420991
Li	-2.859581	-0.657794	0.243294
C	-3.069244	-1.169950	2.481205
B	-1.639438	-0.335029	2.554939
C	-1.846178	1.090025	3.328007
C	-0.589244	1.799016	3.845711
C	-4.311065	-0.323481	2.137496
C	-0.436876	-1.251708	3.163389
C	-0.248309	-2.598855	2.458943
H	1.584048	0.874104	-2.758194
H	1.396606	2.186025	-0.745796
H	1.313763	0.965659	1.534317
H	-0.700685	0.549833	-2.866179
H	-0.525405	-1.828172	-2.584605
H	-0.305677	-1.700376	-0.822972
H	-2.784376	-2.750991	-2.768216
H	-2.277816	-3.266620	-1.138856
H	-4.213986	-4.190420	-0.077055
H	-6.535151	-3.927008	0.743363
H	-7.860984	-1.931416	0.102878
H	-6.851535	-0.190068	-1.350505
H	-4.524746	-0.456374	-2.176966
H	3.404602	2.309211	0.978056
H	3.466010	0.581196	1.404109
H	5.648006	0.502156	2.347467
H	8.097915	0.473794	1.997575
H	9.049613	1.192146	-0.179431
H	7.537153	1.965171	-1.988890
H	5.080951	2.011410	-1.617265
H	1.046360	-0.519095	0.630388
H	-0.768468	1.860802	1.007708
H	-0.618061	-1.430019	4.234539
H	0.516169	-0.701260	3.125918
H	0.637798	-3.148889	2.797128
H	-1.112737	-3.255394	2.615129
H	-0.150003	-2.457295	1.373042
H	-2.408218	1.782119	2.678668
H	-2.505010	0.915341	4.193244
H	-0.817393	2.734325	4.369968
H	-0.038485	1.159561	4.543226
H	0.108234	2.052520	3.037480
H	-2.994651	-2.027493	1.777685
H	-3.253712	-1.661602	3.444455
H	-5.203634	-0.914924	1.902256
H	-4.552539	0.336645	2.975882
H	-4.151242	0.379840	1.298628
H	3.061798	-1.907475	-3.095496
H	3.485084	-0.224380	-2.722186
H	5.782425	-1.225571	-2.342047
H	7.331373	-2.000575	-0.583345
H	6.441077	-2.828415	1.583644
H	3.985798	-2.888007	1.960155
H	2.438289	-2.128295	0.178814
C	-3.829085	3.175965	-0.362661
C	-4.150439	3.579069	1.071420
C	-3.368091	4.386046	-1.169595
C	-5.024695	2.477892	-1.003890
H	-4.962990	4.310537	1.076470
H	-4.455994	2.708150	1.657795
H	-3.272333	4.022337	1.548222
H	-4.159618	5.140732	-1.167778
H	-2.477867	4.824255	-0.708930
H	-3.142840	4.111929	-2.200203
H	-5.888318	3.149278	-0.982883
H	-4.809975	2.203534	-2.037159
H	-5.280205	1.579127	-0.432339

gal_re_reactant_gas_conformation2

C	4.305803	1.680273	0.424495
C	4.243918	1.516540	-0.959910
C	5.423173	1.290404	-1.671564
C	6.647841	1.227340	-1.013037
C	6.701534	1.399772	0.369019
C	5.528928	1.623762	1.086544
C	2.922009	1.564130	-1.680735

O	2.382044	0.247189	-1.833121
C	1.042668	0.126905	-1.422418
C	0.403586	-1.101107	-2.059167
C	-1.114543	-1.058515	-1.771645
N	-1.455941	-0.279052	-0.553680
C	-0.536164	-0.135148	0.501283
C	0.907681	-0.024257	0.087361
C	-1.681084	-2.471976	-1.614645
O	-3.062999	-2.414304	-1.334194
C	-3.473610	-3.403062	-0.394338
C	-3.033532	-3.065125	1.010293
C	-3.693158	-2.050854	1.708031
C	-3.279321	-1.682035	2.982227
C	-2.192361	-2.321313	3.574169
C	-1.526408	-3.332606	2.888444
C	-1.948964	-3.704281	1.613839
O	-0.881326	0.006178	1.661211
C	-2.717167	0.316354	-0.463025
O	-3.169020	0.822232	0.553204
O	-3.316493	0.335064	-1.635585
C	-4.664639	0.886635	-1.797830
C	-5.638468	0.155506	-0.880681
C	-4.629693	2.390959	-1.558904
C	-4.962996	0.562860	-3.256294
Li	-1.896386	1.651807	1.751668
C	-1.641195	3.662488	2.448709
B	-0.667744	3.485933	1.101200
C	-0.982490	4.652785	0.006882
C	-0.071926	4.582013	-1.222498
C	-3.143697	3.888378	2.204694
C	0.909326	3.470369	1.552126
C	1.262015	2.604877	2.769042
H	0.555466	-1.074065	-3.147604
O	0.904317	-2.314404	-1.540745
H	0.466673	1.008701	-1.749814
H	1.273476	0.864246	0.613851
H	-1.599181	-0.552395	-2.604533
H	-1.494408	-3.043418	-2.534759
H	-1.137205	-2.957709	-0.800219
H	-4.565546	-3.425187	-0.457101
H	-3.095561	-4.391133	-0.692781
H	-1.437107	-4.505446	1.084900
H	-0.679166	-3.833611	3.345801
H	-1.863768	-2.029165	4.566216
H	-3.803330	-0.892821	3.513042
H	-4.537125	-1.547329	1.243745
H	3.049827	1.995747	-2.681284
H	2.217487	2.199378	-1.129388
H	3.393816	1.872986	0.984722
H	5.565504	1.762882	2.162365
H	7.656422	1.363360	0.884442
H	7.559829	1.056204	-1.576428
H	5.377935	1.169246	-2.751444
H	1.475348	-0.890325	0.440289
H	-0.909712	2.409125	0.480540
H	1.226432	4.504390	1.764338
H	1.539639	3.164228	0.700691
H	2.340087	2.558863	2.973894
H	0.790895	2.999221	3.676337
H	0.905392	1.571537	2.658128
H	-2.027330	4.601567	-0.336710
H	-0.873074	5.647300	0.469518
H	-0.316762	5.323633	-1.992278
H	0.977875	4.734388	-0.946480
H	-0.139015	3.589633	-1.692184
H	-1.517981	2.879960	3.230962
H	-1.242159	4.548793	2.959199
H	-3.707382	4.057285	3.128870
H	-3.289394	4.757807	1.558062
H	-3.628912	3.047163	1.685247
H	-5.960547	0.921540	-3.520861
H	-4.233138	1.046102	-3.910949
H	-4.917902	-0.518038	-3.413692
H	-5.610977	2.813008	-1.793964
H	-4.384183	2.625244	-0.522445
H	-3.887003	2.859307	-2.210661
H	-6.661017	0.416695	-1.166413
H	-5.507993	-0.924663	-1.000881
H	-5.486121	0.427880	0.163797
C	2.240523	-2.668835	-1.897856
H	2.189968	-3.690587	-2.294006
H	2.619458	-2.007404	-2.682668
C	3.146831	-2.625896	-0.692323
C	4.357920	-1.940943	-0.725850
C	5.179412	-1.903842	0.398605
C	4.786100	-2.544933	1.568847
C	3.571943	-3.229315	1.611529
C	2.759252	-3.273558	0.484210
H	4.648017	-1.409206	-1.626897
H	6.112128	-1.350649	0.360661
H	5.419132	-2.507962	2.449756
H	3.259879	-3.727660	2.524167

H	1.805329	-3.794504	0.515702

gal_re_TS_gas_conformation2

C	1.525469	3.393088	-0.538915
C	2.585085	3.212912	-1.429817
C	3.388515	4.300838	-1.763872
C	3.133104	5.559937	-1.223446
C	2.068818	5.734240	-0.344406
C	1.264562	4.647294	-0.001813
C	2.877443	1.837114	-1.962731
O	3.373959	1.063752	-0.883790
C	3.665546	-0.278523	-1.200823
C	5.127355	-0.554116	-0.839426
C	5.443822	-2.064965	-0.993812
N	4.279423	-2.827473	-1.486075
C	3.027681	-2.660321	-0.757396
C	2.789485	-1.212631	-0.387269
C	5.924856	-2.740889	0.293572
O	6.313154	-4.054988	-0.060042
C	6.182557	-4.997890	0.993816
C	4.767007	-5.511132	1.131767
C	4.236627	-6.328483	0.131783
C	2.926221	-6.790391	0.211556
C	2.128791	-6.436555	1.301493
C	2.651433	-5.627699	2.305697
C	3.964167	-5.169965	2.219273
O	2.529572	-3.586753	-0.101952
C	4.457489	-3.901193	-2.314146
O	3.622764	-4.790323	-2.468689
O	5.595155	-3.831702	-2.992157
C	5.992425	-4.881974	-3.925734
C	6.126684	-6.209797	-3.188168
C	5.007280	-4.951765	-5.087064
C	7.356533	-4.391954	-4.397509
Li	2.006789	-4.658730	-1.511060
C	0.193024	-4.169329	-2.615672
B	1.080762	-2.810623	-2.973980
C	1.757958	-2.853499	-4.449634
C	2.774314	-1.739140	-4.716715
C	0.549343	-5.507475	-3.296764
C	0.215147	-1.464538	-2.664290
C	-0.670274	-1.518166	-1.410689
H	5.780347	0.026563	-1.505872
O	5.391937	-0.186815	0.501072
H	3.514232	-0.475568	-2.271786
H	1.732795	-0.980939	-0.517664
H	6.223437	-2.188928	-1.742658
H	6.767642	-2.191988	0.728633
H	5.106958	-2.754087	1.028601
H	6.856539	-5.820336	0.733829
H	6.529865	-4.564522	1.942470
H	4.369986	-4.537998	3.006030
H	2.036300	-5.349543	3.155071
H	1.108780	-6.801980	1.372086
H	2.534840	-7.446577	-0.562756
H	4.857555	-6.601975	-0.716128
H	3.617687	1.887007	-2.776127
H	1.965172	1.373269	-2.366524
H	0.917124	2.536881	-0.259646
H	0.441779	4.777613	0.694065
H	1.865765	6.714792	0.075329
H	3.761363	6.403321	-1.492323
H	4.218605	4.161836	-2.452179
H	3.029643	-1.095086	0.676345
H	2.108369	-2.702085	-2.153975
H	-0.430387	-1.256826	-3.532723
H	0.878383	-0.587199	-2.600809
H	-1.106931	-0.546223	-1.153421
H	-1.503038	-2.215359	-1.549843
H	-0.119573	-1.877135	-0.531652
H	2.253464	-3.818517	-4.627363
H	0.956852	-2.791212	-5.204146
H	3.133125	-1.721481	-5.752946
H	2.348960	-0.749963	-4.504377
H	3.656758	-1.857511	-4.072440
H	0.033302	-4.319264	-1.527218
H	-0.820415	-3.916740	-2.952654
H	-0.139681	-6.311896	-3.018050
H	0.500789	-5.386721	-4.382259
H	1.570141	-5.872482	-3.106633
H	7.773048	-5.093927	-5.123828
H	7.263423	-3.411210	-4.870822
H	8.042740	-4.311189	-3.550316
H	5.415325	-5.606776	-5.862492
H	4.042307	-5.343415	-4.764687
H	4.858395	-3.956399	-5.516184
H	6.661880	-6.922580	-3.821823
H	6.699866	-6.059635	-2.267744
H	5.147769	-6.624321	-2.944341
C	5.664425	1.186329	0.744253
H	6.642604	1.230358	1.243003
H	5.739793	1.737830	-0.199825

C	4.624288	1.842487	1.620316
C	4.423558	3.219842	1.539796
C	3.505878	3.849134	2.374218
C	2.766941	3.101848	3.287990
C	2.959472	1.725153	3.367113
C	3.889676	1.098901	2.542176
H	4.971761	3.804346	0.804457
H	3.351120	4.920206	2.290310
H	2.041649	3.588848	3.932328
H	2.384740	1.136232	4.075493
H	4.048904	0.026436	2.603168

gal_re_product_gas_conformation2

C	-5.332584	0.950048	1.711100
C	-4.891136	1.347179	0.447846
C	-5.819182	1.811586	-0.481273
C	-7.171302	1.882306	-0.156922
C	-7.607796	1.478225	1.101164
C	-6.684007	1.010295	2.034077
C	-3.427491	1.291615	0.089974
O	-2.845584	0.195620	0.754361
C	-1.441293	0.068524	0.675570
C	-1.150363	-1.396052	1.045909
C	0.345253	-1.732694	0.803403
N	1.108366	-0.503602	0.630644
C	0.735960	0.443906	-0.508986
C	-0.795226	0.373007	-0.668931
C	0.561762	-2.637537	-0.427877
O	1.953155	-2.734455	-0.658802
C	2.351750	-2.604198	-2.008870
C	3.653803	-1.844401	-2.068342
C	3.894312	-0.934245	-3.105547
C	5.064753	-0.175587	-3.125261
C	6.014231	-0.328451	-2.112430
C	5.784459	-1.239750	-1.084934
C	4.608281	-1.989176	-1.059633
H	-1.403744	-1.546928	2.104992
O	1.424618	0.224925	-1.634959
C	2.350038	-0.365602	1.120971
O	2.640412	-1.189085	2.137976
C	3.728941	-0.885069	3.057584
C	3.530225	0.507124	3.650363
O	3.158961	0.477297	0.688812
C	3.560879	-1.954383	4.131641
C	5.085368	-1.026255	2.375365
Li	3.148488	0.427156	-1.227186
C	3.283306	3.204769	-1.464736
C	4.720480	2.904002	-1.027594
B	2.201045	3.495420	-0.342916
C	0.734711	3.887016	-0.797670
C	0.347912	3.531608	-2.237646
C	2.617507	3.562261	1.180115
C	1.540537	3.216913	2.212093
O	-1.914773	-2.288674	0.256491
H	-0.976022	0.723520	1.433531
H	-1.113837	1.337571	-1.073406
H	0.750794	-2.249501	1.673214
H	0.130256	-3.625739	-0.237912
H	0.059154	-2.209031	-1.299719
H	2.472582	-3.600646	-2.461135
H	1.605215	-2.038150	-2.574273
H	3.134298	-0.784827	-3.867265
H	5.227709	0.544536	-3.921194
H	6.919148	0.270407	-2.120248
H	6.514906	-1.356675	-0.290535
H	4.398806	-2.669258	-0.239591
H	-2.922353	2.227813	0.385595
H	-3.327160	1.184949	-0.999265
H	-5.483906	2.098609	-1.474791
H	-7.884955	2.240674	-0.892530
H	-8.662596	1.524864	1.353679
H	-7.019199	0.691365	3.016379
H	-4.607350	0.573908	2.425754
H	-1.054780	-0.390976	-1.408112
H	0.952274	1.426816	-0.037129
H	0.662080	4.978508	-0.647159
H	-0.003151	3.474521	-0.095616
H	-0.693388	3.788633	-2.456633
H	0.973237	4.067687	-2.959480
H	0.485542	2.459816	-2.421546
H	3.513336	2.956626	1.356002
H	2.943695	4.607323	1.331280
H	1.901634	3.340064	3.238181
H	0.652142	3.845127	2.095746
H	1.222897	2.172506	2.099227
H	2.871739	2.416642	-2.120486
H	3.278675	4.081323	-2.132196
H	5.388318	2.745415	-1.880493
H	5.127422	3.734251	-0.441511
H	4.779995	2.018155	-0.383205
H	5.874539	-0.918617	3.125775
H	5.176679	-2.018933	1.924273

H	5.216794	-0.266636	1.605174
H	4.332515	-1.839905	4.897177
H	2.579880	-1.865996	4.605276
H	3.647690	-2.950607	3.690351
H	4.259138	0.668261	4.449619
H	3.661053	1.281280	2.892455
H	2.526172	0.593070	4.076794
C	-3.251831	-2.529968	0.654855
H	-3.363436	-3.618222	0.760366
H	-3.452590	-2.074777	1.631826
C	-4.269540	-2.022672	-0.342350
C	-5.615186	-1.967376	0.024445
C	-6.577851	-1.521549	-0.873631
C	-6.202906	-1.124650	-2.155463
C	-4.863261	-1.180980	-2.528356
C	-3.900524	-1.632719	-1.627159
H	-5.908860	-2.251965	1.032534
H	-7.616841	-1.460188	-0.565200
H	-6.950402	-0.763265	-2.854997
H	-4.563120	-0.873725	-3.525867
H	-2.854097	-1.680486	-1.910299

gal_si_reactant_gas_conformation1

C	6.517855	0.433729	-1.252929
C	5.407493	-0.363657	-1.530310
C	5.590354	-1.719773	-1.800690
C	6.868915	-2.269890	-1.794145
C	7.975268	-1.468723	-1.524058
C	7.797323	-0.114048	-1.254693
C	4.027650	0.243296	-1.548073
O	3.099290	-0.728485	-1.107629
C	1.739924	-0.422971	-1.306425
C	0.944297	-1.418658	-0.467315
C	-0.545589	-1.302935	-0.794430
N	-0.987301	0.107669	-0.878181
C	-0.146035	1.202979	-0.949849
C	1.339699	0.981976	-0.873252
C	-1.370825	-2.017486	0.272603
O	-2.737545	-1.777435	0.035961
C	-3.532379	-2.191416	1.138275
C	-4.931610	-1.666644	0.973959
C	-5.848358	-2.330940	0.157902
C	-7.141657	-1.839651	0.003772
C	-7.529653	-0.678953	0.670687
C	-6.619209	-0.008831	1.484010
C	-5.322402	-0.498032	1.629984
O	1.088922	-1.187967	0.913332
C	2.330640	-1.540839	1.521724
C	3.134830	-0.316911	1.888874
C	2.486598	0.783338	2.456416
C	3.207314	1.921217	2.805532
C	4.586043	1.963739	2.597634
C	5.236689	0.867233	2.038092
C	4.511669	-0.269358	1.681961
O	-0.609472	2.335932	-1.062861
C	-2.278835	0.273847	-1.497645
O	-3.024151	1.172511	-0.852636
C	-4.191788	1.767525	-1.559642
C	-5.215596	0.692109	-1.897079
O	-2.567280	-0.320679	-2.496377
C	-4.758669	2.737534	-0.535366
C	-3.673368	2.507393	-2.786143
Li	-1.834286	2.172065	0.547014
C	-2.430298	3.305489	2.273736
C	-2.129423	4.527327	1.384540
B	-1.149851	2.261948	2.585860
C	-1.704924	0.708558	2.692224
C	-2.601159	0.483136	3.915577
C	-0.323490	2.710954	3.913968
C	0.278816	4.118497	3.854935
H	1.272633	-2.438547	-0.721182
H	1.478399	-0.564733	-2.371017
H	1.639771	1.159535	0.166576
H	-0.732193	-1.754210	-1.775076
H	-1.140566	-3.095028	0.233112
H	-1.085633	-1.632538	1.256313
H	-3.094401	-1.804498	2.069239
H	-3.535524	-3.290942	1.191977
H	-4.607635	0.023215	2.262693
H	-6.917443	0.893327	2.009598
H	-8.540269	-0.299448	0.558210
H	-7.848206	-2.363924	-0.631729
H	-5.542991	-3.237377	-0.358191
H	2.067583	-2.097023	2.429335
H	2.911262	-2.196433	0.864554
H	5.017798	-1.111228	1.215201
H	6.308051	0.894872	1.862485
H	5.149913	2.850433	2.869891
H	2.686045	2.769086	3.240547
H	1.407857	0.761269	2.597387
H	3.768504	0.570103	-2.569285
H	4.006302	1.122630	-0.888654

H	6.375692	1.486117	-1.019586
H	8.654212	0.514512	-1.033735
H	8.971608	-1.898848	-1.517172
H	7.002235	-3.327401	-1.999642
H	4.722113	-2.339214	-2.000058
H	-6.136127	1.187657	-2.220423
H	-4.867643	0.035018	-2.692081
H	-5.441877	0.097077	-1.010794
H	-4.504716	3.044647	-3.250593
H	-2.904463	3.229455	-2.496763
H	-3.259747	1.814980	-3.521036
H	-5.635087	3.232612	-0.961022
H	-5.066765	2.202087	0.366673
H	-4.029802	3.509909	-0.270406
H	1.785074	1.764861	-1.490183
H	-0.351529	2.318143	1.616762
H	-2.786205	3.670928	3.244814
H	-3.322686	2.782886	1.869266
H	-2.271988	0.390102	1.789752
H	-0.853129	0.011513	2.741228
H	-3.033748	-0.525061	3.974055
H	-2.034074	0.641327	4.837427
H	-3.435268	1.196918	3.933896
H	-0.982087	2.662506	4.794918
H	0.480784	1.989043	4.126321
H	0.934758	4.341561	4.705592
H	0.861855	4.261486	2.935678
H	-0.507426	4.882492	3.853144
H	-2.986276	5.203106	1.275283
H	-1.295665	5.100144	1.797206
H	-1.808012	4.261631	0.362652

gal_si_TS_gas_conformation1

C	-5.869067	-1.830278	0.553498
C	-4.935700	-1.257197	1.418567
C	-5.278920	-0.103073	2.123875
C	-6.543155	0.464909	1.976001
C	-7.471190	-0.116938	1.115950
C	-7.131415	-1.264739	0.401556
C	-3.564026	-1.859119	1.565964
O	-2.788010	-1.495607	0.441078
C	-1.419161	-1.767472	0.628215
C	-0.613957	-1.093673	-0.487741
C	0.896481	-1.237281	-0.230122
C	1.638665	-0.074172	-0.880334
C	1.187048	1.198513	-0.165231
C	-0.251622	1.487938	-0.578608
N	-1.062787	0.300274	-0.706038
O	1.118384	-1.294285	1.166085
C	2.384926	-1.772414	1.607902
C	3.260467	-0.663445	2.144862
C	2.712140	0.312739	2.978870
C	3.501580	1.349471	3.467142
C	4.856136	1.407487	3.143201
C	5.413195	0.425998	2.327698
C	4.616033	-0.601688	1.828136
O	3.013333	-0.367817	-0.775758
C	3.894974	0.687457	-1.097616
C	5.275865	0.122909	-1.319415
C	5.449068	-1.153192	-1.855967
C	6.729194	-1.658619	-2.065631
C	7.847232	-0.891484	-1.747942
C	7.679283	0.384196	-1.214729
C	6.399057	0.884766	-0.996876
O	-0.460434	2.421529	-1.425510
C	-2.251426	0.378622	-1.435355
O	-2.635867	-0.469278	-2.198474
O	-2.947502	1.513572	-1.158567
C	-4.129842	1.841302	-1.972858
C	-4.490129	3.249430	-1.507989
C	-3.766926	1.863972	-3.455239
C	-5.244810	0.863763	-1.634013
H	1.237554	-2.179747	-0.683066
H	1.354519	-0.012123	-1.945852
H	1.290681	1.066046	0.913873
H	-0.831739	-1.606415	-1.428998
H	-1.218408	-2.851324	0.598357
H	-1.092440	-1.390375	1.600423
H	-3.088338	-1.486021	2.486047
H	-3.626822	-2.956352	1.638672
H	-4.551319	0.345544	2.796365
H	-6.803738	1.357391	2.536330
H	-8.457493	0.321890	1.001982
H	-7.851409	-1.718425	-0.272305
H	-5.597711	-2.722102	-0.005154
H	2.169916	-2.491110	2.408570
H	2.902982	-2.299326	0.799171
H	5.045981	-1.340722	1.156461
H	6.464062	0.466710	2.056959
H	5.472851	2.215902	3.523139
H	3.056349	2.113138	4.098120
H	1.653368	0.268392	3.224971

H	3.544701	1.202058	-2.007806
H	3.928803	1.423891	-0.281612
H	6.267018	1.870094	-0.556389
H	8.545672	0.985242	-0.956911
H	8.844464	-1.287952	-1.909754
H	6.854509	-2.654677	-2.478771
H	4.572437	-1.748246	-2.089880
H	-6.159568	1.161976	-2.155693
H	-4.976570	-0.149266	-1.933197
H	-5.436437	0.874810	-0.557325
H	-4.581888	2.340931	-4.007307
H	-2.854464	2.449104	-3.608437
H	-3.613985	0.860342	-3.847361
H	-5.375186	3.596080	-2.046630
H	-4.714311	3.267804	-0.437901
H	-3.681927	3.960298	-1.728640
H	1.756448	2.073391	-0.478966
H	-0.726251	2.038895	0.680824
B	-1.171108	2.507364	1.898089
C	0.149129	3.210555	2.506300
C	-2.486652	3.452869	1.626389
C	-1.578195	1.091243	2.554089
H	-2.912091	3.599020	2.628032
C	-2.345599	4.861295	1.009697
H	-3.273158	2.874615	1.111156
C	-2.104254	1.194694	3.991676
H	-2.329149	0.593076	1.919869
H	-0.695258	0.433264	2.552945
H	-2.359696	0.217204	4.419467
H	-1.358919	1.652345	4.651418
H	-3.005790	1.816596	4.048449
H	-0.121625	3.680252	3.466233
H	0.863810	2.419686	2.774379
C	0.881930	4.244352	1.637925
H	1.887872	4.458528	2.015376
H	0.988275	3.894746	0.604257
H	0.350030	5.199020	1.593086
H	-3.315548	5.324170	0.797935
H	-1.809420	5.515196	1.700571
H	-1.754217	4.918618	0.078179
Li	-1.883570	3.002421	-0.459633

gal_si_product_gas_conformation1

C	6.386568	1.109775	0.795270
C	5.395575	1.162710	-0.185374
C	5.762551	1.401578	-1.509479
C	7.101372	1.583214	-1.846531
C	8.085771	1.534273	-0.862983
C	7.724036	1.298345	0.461308
C	3.946899	0.978597	0.195518
O	3.248977	0.431098	-0.897417
C	1.844551	0.594038	-0.889505
C	1.294815	-0.355249	-1.952709
C	-0.256924	-0.321454	-1.921728
N	-0.739948	0.835232	-1.152043
C	-0.308282	0.906089	0.317509
C	1.114397	0.292363	0.407871
C	-0.860223	-1.624010	-1.356775
O	-2.256045	-1.454563	-1.225797
C	-2.866358	-2.640026	-0.758870
C	-4.356351	-2.435292	-0.686872
C	-5.055491	-2.082065	-1.843193
C	-6.428583	-1.871082	-1.798723
C	-7.118452	-2.009012	-0.594593
C	-6.429282	-2.362402	0.560795
C	-5.051851	-2.574118	0.512802
O	1.661832	-1.702649	-1.721545
C	3.013894	-2.065701	-1.935474
C	3.747942	-2.292063	-0.632813
C	3.068246	-2.797420	0.476311
C	3.735714	-3.003345	1.680202
C	5.095342	-2.716281	1.784540
C	5.781052	-2.223438	0.677474
C	5.108893	-2.012017	-0.523650
O	-0.309597	2.152585	0.806183
C	-1.865163	1.406192	-1.658717
O	-2.552137	2.209707	-0.756026
C	-3.869588	2.733640	-1.135106
C	-4.830060	1.579716	-1.376131
O	-2.270591	1.279912	-2.797089
C	-4.293488	3.519867	0.105285
C	-3.760969	3.682865	-2.325691
Li	-1.802556	2.981814	0.782701
C	-2.709982	1.495767	2.830943
C	-2.384270	2.935546	3.244968
B	-1.687665	0.303366	3.070722
C	-2.254327	-1.129747	2.669833
C	-3.063847	-1.741715	3.829247
C	-0.262900	0.343337	3.743429
C	0.470517	1.660326	4.003329
H	1.667441	-0.045118	-2.939701
H	1.600375	1.628484	-1.177589

H	1.116787	-0.787699	0.589348
H	-0.644360	-0.201387	-2.932348
H	-0.639146	-2.452672	-2.041682
H	-0.424836	-1.875469	-0.378793
H	-2.467216	-2.911029	0.231572
H	-2.635027	-3.469264	-1.447732
H	-4.511615	-2.848183	1.415835
H	-6.959992	-2.472530	1.501266
H	-8.190670	-1.843324	-0.560007
H	-6.962867	-1.593658	-2.702307
H	-4.506205	-1.952207	-2.771895
H	2.991517	-3.000653	-2.510850
H	3.537399	-1.309431	-2.530126
H	5.639688	-1.583651	-1.370418
H	6.835585	-1.975929	0.751567
H	5.615706	-2.873029	2.724206
H	3.194374	-3.388964	2.538963
H	2.006998	-3.013022	0.389287
H	3.508084	1.949725	0.477940
H	3.878189	0.311191	1.068528
H	6.107457	0.898134	1.824718
H	8.485791	1.248703	1.233314
H	9.129289	1.674495	-1.126676
H	7.376635	1.763454	-2.881278
H	4.989370	1.426153	-2.270206
H	-5.843317	1.969695	-1.513554
H	-4.539744	1.019314	-2.262695
H	-4.832420	0.898207	-0.518625
H	-4.710535	4.213912	-2.443067
H	-2.975401	4.424144	-2.145795
H	-3.533374	3.143091	-3.241627
H	-5.273607	3.972742	-0.059462
H	-4.370165	2.869183	0.982239
H	-3.599363	4.348001	0.312129
H	1.572149	0.784856	1.267517
H	-1.022542	0.219219	0.829436
H	-3.670430	1.196908	3.279137
H	-2.922736	1.415682	1.750046
H	-2.903238	-1.048355	1.786441
H	-1.438821	-1.816226	2.404968
H	-3.449092	-2.734229	3.574742
H	-2.451217	-1.855027	4.729436
H	-3.922833	-1.115544	4.092436
H	-0.390152	-0.213252	4.689657
H	0.379518	-0.322412	3.147928
H	1.457169	1.483149	4.442582
H	0.602654	2.200548	3.060981
H	-0.080639	2.303287	4.695958
H	-3.151672	3.648238	2.912995
H	-2.330804	3.028988	4.332451
H	-1.402509	3.254328	2.874624

gal_si_reactant_gas_conformation2

C	-7.015946	-0.959761	0.854334
C	-5.873667	-1.604158	0.379715
C	-5.993270	-2.536846	-0.651269
C	-7.241256	-2.820408	-1.197985
C	-8.380018	-2.179704	-0.715761
C	-8.265480	-1.249263	0.313590
C	-4.528087	-1.294473	0.983740
O	-3.545686	-1.351166	-0.032126
C	-2.213845	-1.277040	0.418339
C	-1.326530	-1.140892	-0.812946
C	0.145777	-1.316217	-0.412166
N	0.421527	-0.745633	0.931199
C	-0.456962	0.133323	1.565829
C	-1.931486	-0.076768	1.313960
C	1.033375	-0.617464	-1.440589
O	2.386457	-0.911171	-1.190254
C	3.236321	0.006721	-1.873369
C	4.638775	-0.538370	-1.879349
C	4.859703	-1.872841	-2.228730
C	6.144110	-2.403538	-2.206262
C	7.224111	-1.598189	-1.845354
C	7.012115	-0.264120	-1.512249
C	5.722191	0.264408	-1.526388
O	-1.440395	0.131702	-1.407110
C	-2.637542	0.434762	-2.124691
C	-3.465528	1.450160	-1.375451
C	-2.847984	2.609976	-0.897504
C	-3.572636	3.537984	-0.157093
C	-4.927588	3.322591	0.096126
C	-5.550489	2.177301	-0.392007
C	-4.819154	1.241505	-1.122089
O	-0.091679	0.976849	2.368185
C	1.651455	-1.046718	1.553949
O	2.204354	-0.306137	2.346050
O	2.050236	-2.256788	1.237316
Li	1.735209	1.564514	2.124271
B	2.366104	2.829637	0.553890
C	3.796359	2.348556	1.249500
C	4.813435	3.490490	1.367409

C	2.623141	3.573053	-0.882697
C	1.525313	3.404549	-1.940193
C	1.515375	3.791797	1.610583
C	0.104577	4.183773	1.158664
H	-1.586421	-1.924562	-1.539790
H	-1.946787	-2.207654	0.950770
H	-2.333317	0.837816	0.866992
H	0.382949	-2.381316	-0.366537
H	0.741868	-0.952228	-2.449516
H	0.852244	0.459736	-1.368948
H	3.191504	0.988008	-1.383046
H	2.876433	0.126046	-2.908549
H	5.550590	1.301022	-1.246201
H	7.849408	0.365859	-1.229672
H	8.227721	-2.011197	-1.824992
H	6.306494	-3.443874	-2.471384
H	4.009458	-2.492166	-2.500648
H	-2.311443	0.850701	-3.085009
H	-3.218781	-0.473717	-2.312067
H	-5.298741	0.332012	-1.475606
H	-6.604060	1.999081	-0.197757
H	-5.493754	4.046459	0.673700
H	-3.076872	4.425438	0.224393
H	-1.787527	2.766385	-1.083168
H	-4.283016	-2.023489	1.774937
H	-4.556649	-0.294011	1.437988
H	-6.922933	-0.218159	1.643971
H	-9.147816	-0.740446	0.688584
H	-9.352194	-2.399653	-1.144897
H	-7.325809	-3.543189	-2.003328
H	-5.099793	-3.022887	-1.029595
H	-2.375116	-0.182417	2.308298
H	1.682330	1.794883	0.323639
H	2.106659	4.706965	1.756322
H	1.426773	3.403548	2.650568
H	3.708410	1.911175	2.266894
H	4.242240	1.532795	0.657662
H	5.772689	3.168078	1.788120
H	5.013785	3.931183	0.385092
H	4.430168	4.294900	2.004446
H	2.783573	4.649368	-0.713165
H	3.570757	3.225390	-1.328796
H	1.442320	2.358399	-2.259311
H	0.541885	3.688493	-1.551727
H	1.705941	4.001134	-2.842508
H	-0.442885	4.762503	1.911944
H	0.147133	4.791118	0.248644
H	-0.492195	3.290944	0.930144
C	3.366630	-2.756085	1.679983
C	3.564407	-3.959524	0.769275
C	4.469678	-1.727279	1.452669
C	3.239845	-3.160878	3.141929
H	5.430129	-2.250704	1.432120
H	4.332189	-1.242355	0.485117
H	4.494595	-0.966151	2.231449
H	4.490711	-4.475551	1.033285
H	2.730609	-4.659784	0.869280
H	3.630052	-3.623502	-0.268947
H	4.185407	-3.595064	3.478682
H	3.019917	-2.289551	3.762429
H	2.450693	-3.906887	3.269838

gal_si_TS_gas_conformation2

C	-5.813132	-1.606342	0.340438
C	-4.684094	-1.147861	1.018603
C	-4.610758	0.194725	1.390191
C	-5.653322	1.065654	1.086434
C	-6.775683	0.604158	0.403333
C	-6.852791	-0.734910	0.028887
C	-3.550733	-2.094224	1.327845
O	-2.955457	-1.718528	2.552426
C	-1.631211	-2.149264	2.751697
C	-1.308627	-1.893551	4.221105
C	0.161726	-2.304941	4.519348
N	0.848777	-2.869402	3.337620
C	0.160394	-3.789146	2.421797
C	-1.359209	-3.636613	2.516669
C	0.277884	-3.255503	5.710126
O	1.643289	-3.339405	6.057934
C	1.854207	-4.249562	7.124078
C	3.310431	-4.196902	7.492355
C	3.837410	-3.029229	8.049147
C	5.200696	-2.919486	8.296798
C	6.050244	-3.984211	7.995995
C	5.529269	-5.155859	7.455610
C	4.162380	-5.260473	7.204304
O	-2.153287	-2.648410	5.071473
C	-3.487802	-2.182169	5.251019
C	-4.506921	-3.055214	4.555027
C	-4.388109	-4.444551	4.605931
C	-5.316147	-5.258725	3.963753
C	-6.388443	-4.690035	3.279067

C	-6.523816	-3.304643	3.241306
C	-5.584505	-2.492928	3.873005
O	0.642485	-3.944297	1.266147
C	2.207744	-2.694490	3.203845
O	2.930178	-3.410186	2.512877
O	2.662674	-1.653568	3.882924
Li	2.108582	-4.909424	1.763113
B	0.923281	-6.322650	3.345493
C	2.461630	-6.133862	3.884057
C	2.988815	-7.449609	4.481805
C	-0.042937	-6.987459	4.473373
C	-1.510346	-6.551739	4.536127
C	0.831577	-7.021504	1.873320
C	-0.568469	-7.170145	1.275123
H	-1.444649	-0.825709	4.442329
H	-0.955036	-1.554107	2.116067
H	-1.817155	-4.216452	3.317796
H	0.719138	-1.405468	4.776327
H	-0.311105	-2.868818	6.551820
H	-0.112323	-4.249155	5.447919
H	1.566471	-5.266680	6.816628
H	1.222626	-3.962409	7.979932
H	3.753822	-6.167390	6.766963
H	6.185981	-5.987967	7.222215
H	7.115420	-3.899762	8.186818
H	5.602970	-2.006006	8.723704
H	3.170077	-2.200520	8.272697
H	-3.668093	-2.199959	6.333380
H	-3.585394	-1.148561	4.901422
H	-5.671178	-1.411451	3.800230
H	-7.347221	-2.847428	2.700876
H	-7.113651	-5.323491	2.777932
H	-5.200866	-6.337783	4.001200
H	-3.557425	-4.889084	5.144392
H	-2.800867	-2.056722	0.521058
H	-3.933851	-3.123342	1.391436
H	-5.883961	-2.657604	0.071937
H	-7.728075	-1.103607	-0.496925
H	-7.588844	1.283414	0.168220
H	-5.590092	2.107652	1.384626
H	-3.738358	0.542088	1.934267
H	-1.736142	-3.989874	1.556464
H	0.394752	-5.053433	3.151501
H	1.266288	-8.023343	2.017311
H	1.478819	-6.594915	1.080464
H	3.209254	-5.838928	3.124996
H	2.522401	-5.337536	4.642128
H	4.038828	-7.372358	4.785588
H	2.408176	-7.749686	5.360032
H	2.919986	-8.269973	3.759137
H	-0.002178	-8.078867	4.328678
H	0.387298	-6.825343	5.473466
H	-1.588408	-5.528579	4.919027
H	-1.997432	-6.559363	3.555624
H	-2.102949	-7.187155	5.204854
H	-0.553261	-7.634826	0.284029
H	-1.197729	-7.791181	1.919124
H	-1.050561	-6.192174	1.174601
C	4.103021	-1.459124	4.082925
C	4.125159	-0.430380	5.206340
C	4.783088	-2.748883	4.536773
C	4.701438	-0.902276	2.798086
H	5.722234	-2.495299	5.037632
H	4.145742	-3.266720	5.257388
H	4.993184	-3.417007	3.702477
H	5.156797	-0.155975	5.440894
H	3.577903	0.469696	4.913260
H	3.659678	-0.857370	6.098965
H	5.760325	-0.679692	2.958899
H	4.614697	-1.630150	1.989620
H	4.192366	0.021082	2.508481

gal_si_product_gas_conformation2

C	-6.700757	-0.092816	1.160116
C	-5.552486	-0.869488	1.002205
C	-5.683672	-2.245568	0.816886
C	-6.945243	-2.834531	0.790248
C	-8.087219	-2.055432	0.954601
C	-7.961545	-0.680957	1.142290
C	-4.191415	-0.218791	1.039859
O	-3.299226	-0.976394	0.255961
C	-1.926074	-0.772142	0.517582
C	-1.164946	-1.448417	-0.620074
C	0.368837	-1.261976	-0.413742
N	0.691552	-0.592770	0.856286
C	-0.100041	0.634915	1.357943
C	-1.425953	0.662546	0.578022
C	1.027960	-0.510776	-1.575255
O	2.424207	-0.557797	-1.370971
C	3.140862	0.114115	-2.389084
C	4.597114	-0.224815	-2.219842
C	5.007997	-1.548039	-2.399248

C	6.324673	-1.919055	-2.154927
C	7.249600	-0.963715	-1.733845
C	6.852001	0.358797	-1.568107
C	5.528681	0.725946	-1.811481
O	-1.471580	-0.884705	-1.886035
C	-2.759001	-1.114096	-2.437096
C	-3.647314	0.106341	-2.336479
C	-3.099934	1.383873	-2.464420
C	-3.907277	2.512585	-2.358048
C	-5.276104	2.375123	-2.136072
C	-5.830355	1.102540	-2.023004
C	-5.018229	-0.024426	-2.122598
O	-0.322308	0.580159	2.676296
C	1.823497	-0.911987	1.510379
O	2.326733	-0.228427	2.426213
O	2.369031	-2.064206	1.121661
Li	1.183710	0.648182	3.530532
B	2.093624	3.424129	0.964945
C	3.239525	2.494932	0.391383
C	4.420946	2.226839	1.332108
C	1.289206	4.379640	-0.012773
C	0.024459	3.689206	-0.562257
C	1.804646	3.469450	2.519801
C	0.385581	3.827324	2.975854
H	-1.417810	-2.518482	-0.640063
H	-1.665595	-1.256627	1.471787
H	-1.334821	1.069140	-0.433055
H	0.835339	-2.245537	-0.376675
H	0.765552	-0.985778	-2.528149
H	0.674396	0.532063	-1.610566
H	2.977357	1.200748	-2.322929
H	2.780703	-0.221490	-3.374781
H	5.213424	1.755386	-1.665330
H	7.567784	1.106559	-1.241264
H	8.277930	-1.250882	-1.538323
H	6.631594	-2.951499	-2.290825
H	4.279159	-2.288897	-2.718832
H	-2.592235	-1.358189	-3.494403
H	-3.245878	-1.969939	-1.957868
H	-5.450025	-1.013271	-1.987561
H	-6.892324	0.981169	-1.831924
H	-5.905833	3.255137	-2.050076
H	-3.466672	3.501027	-2.447781
H	-2.030181	1.486195	-2.627618
H	-3.824774	-0.160748	2.077695
H	-4.268823	0.807681	0.649698
H	-6.603585	0.983721	1.279836
H	-8.847431	-0.064959	1.263131
H	-9.070215	-2.515094	0.930938
H	-7.036925	-3.905910	0.639408
H	-4.787711	-2.841576	0.677811
H	-2.080669	1.315746	1.157765
H	0.522969	1.504701	1.045201
H	2.510267	4.243591	2.875338
H	2.170074	2.554617	3.011847
H	2.768986	1.524782	0.140111
H	3.599022	2.898888	-0.565049
H	5.184456	1.604044	0.854850
H	4.901072	3.159248	1.648559
H	4.088276	1.696198	2.228550
H	0.983717	5.301750	0.497620
H	1.917151	4.677387	-0.861006
H	0.279337	2.765464	-1.094721
H	-0.668168	3.420691	0.241535
H	-0.511087	4.337292	-1.262396
H	0.342630	4.032846	4.050637
H	0.022969	4.721581	2.460049
H	-0.305505	3.003405	2.770904
C	3.711522	-2.457115	1.532059
C	3.992178	-3.635208	0.606325
C	4.716584	-1.335751	1.279989
C	3.685699	-2.898768	2.990748
H	5.722837	-1.761025	1.215202
H	4.490211	-0.848635	0.326750
H	4.694856	-0.589891	2.073547
H	4.972940	-4.063341	0.829850
H	3.230577	-4.409532	0.732541
H	3.983677	-3.292873	-0.431758
H	4.669885	-3.285155	3.272039
H	3.440913	-2.056068	3.638766
H	2.947227	-3.692342	3.135383

gal_re_reactant_solvent

C	4.578266	1.119596	0.427244
C	4.549402	0.940165	-0.956998
C	5.711114	0.524281	-1.610367
C	6.883564	0.293463	-0.895069
C	6.903984	0.480862	0.486078
C	5.747812	0.891201	1.146694
C	3.283535	1.186028	-1.739761
O	2.501512	-0.006865	-1.858170
C	1.176803	0.124396	-1.403509

C	0.304279	-0.980208	-1.985689
C	-1.165572	-0.621106	-1.703603
N	-1.328880	0.132945	-0.431038
C	-0.357643	0.069325	0.583144
C	1.072673	0.030987	0.112538
C	-2.026725	-1.881066	-1.646524
O	-3.379900	-1.514821	-1.477667
C	-4.191059	-2.609838	-1.094039
C	-3.945597	-3.060073	0.331133
C	-3.600373	-2.129885	1.314226
C	-3.401986	-2.538258	2.629760
C	-3.554954	-3.878910	2.978154
C	-3.900677	-4.810121	2.002490
C	-4.086766	-4.402109	0.683605
O	-0.638900	0.156930	1.767327
C	-2.458144	0.939254	-0.254577
O	-2.815384	1.388873	0.825784
O	-3.033150	1.201051	-1.404787
C	-4.331441	1.886677	-1.477309
C	-5.346388	1.193404	-0.574395
C	-4.130294	3.355977	-1.134506
C	-4.705537	1.698284	-2.941249
Li	-1.431804	1.953007	2.082817
C	-0.848672	4.046881	2.643582
B	0.003465	3.673511	1.262588
C	-0.223338	4.813658	0.115104
C	0.555160	4.542635	-1.175702
C	-2.318686	4.461040	2.464900
C	1.590894	3.462195	1.618294
C	1.893642	2.543455	2.808864
H	0.444897	-1.032476	-3.074162
O	0.558029	-2.242043	-1.406063
H	0.757928	1.087207	-1.739705
H	1.530742	0.901737	0.596197
H	-1.513207	0.031378	-2.504211
H	-1.890670	-2.451076	-2.577783
H	-1.687981	-2.504288	-0.811746
H	-5.223501	-2.261434	-1.206758
H	-4.050264	-3.454048	-1.785090
H	-4.340914	-5.133784	-0.079578
H	-4.014363	-5.857270	2.264614
H	-3.400512	-4.196749	4.004256
H	-3.126917	-1.807175	3.383905
H	-3.482233	-1.082907	1.049927
H	3.529138	1.525632	-2.752865
H	2.693175	1.974673	-1.255276
H	3.685037	1.460148	0.945738
H	5.757563	1.042921	2.221508
H	7.819179	0.309638	1.044175
H	7.782455	-0.022076	-1.415507
H	5.697444	0.390595	-2.689491
H	1.571400	-0.870575	0.480024
H	-0.413702	2.608494	0.731707
H	2.047686	4.445813	1.818158
H	2.130926	3.086189	0.732538
H	2.966625	2.375942	2.973140
H	1.496699	2.966388	3.738501
H	1.424884	1.556162	2.690217
H	-1.290712	4.902207	-0.141112
H	0.066548	5.805697	0.500737
H	0.354029	5.269918	-1.971878
H	1.636796	4.548799	-0.997018
H	0.303921	3.548029	-1.572118
H	-0.788384	3.283213	3.447472
H	-0.309670	4.891399	3.096365
H	-2.807660	4.729928	3.407898
H	-2.389821	5.321892	1.794082
H	-2.929848	3.670957	2.002845
H	-5.661900	2.186123	-3.143504
H	-3.943511	2.137805	-3.589941
H	-4.791823	0.632045	-3.166938
H	-5.075905	3.888444	-1.269659
H	-3.803274	3.477583	-0.100476
H	-3.383017	3.800078	-1.797888
H	-6.347582	1.539167	-0.844671
H	-5.296543	0.111976	-0.732417
H	-5.172031	1.411060	0.478860
C	1.779198	-2.880918	-1.783983
H	1.507481	-3.891223	-2.111996
H	2.244279	-2.354834	-2.623333
C	2.734706	-2.956697	-0.618870
C	4.036719	-2.473499	-0.721252
C	4.902980	-2.541150	0.368276
C	4.464607	-3.082151	1.573409
C	3.160134	-3.564164	1.685019
C	2.301878	-3.506413	0.591899
H	4.365498	-2.015559	-1.649559
H	5.909855	-2.146757	0.277023
H	5.133844	-3.123916	2.426987
H	2.813203	-3.984485	2.623810
H	1.282314	-3.873973	0.676422

gal_re_TS_solvent

C	4.335155	1.427913	0.713027
C	4.367911	1.624014	-0.669663
C	5.602227	1.718205	-1.311052
C	6.788294	1.627629	-0.583916
C	6.745643	1.437713	0.794683
C	5.515137	1.333845	1.442197
C	3.081469	1.718491	-1.450981
O	2.518998	0.424103	-1.646590
C	1.146461	0.321605	-1.341379
C	0.574975	-0.894024	-2.065311
C	-0.949156	-0.966544	-1.794696
N	-1.381644	-0.032048	-0.732395
C	-0.574859	0.030403	0.472685
C	0.904019	0.130478	0.151553
C	-1.407744	-2.371010	-1.394046
O	-2.816185	-2.344469	-1.258243
C	-3.309859	-3.314855	-0.343030
C	-3.178873	-2.862510	1.093948
C	-4.041282	-1.874658	1.577109
C	-3.929855	-1.410573	2.885664
C	-2.942200	-1.930027	3.726755
C	-2.084976	-2.920216	3.256104
C	-2.206858	-3.384183	1.947161
O	-0.984252	-0.427023	1.550266
C	-2.669357	0.433665	-0.729990
O	-3.257175	0.814586	0.279657
O	-3.176792	0.505453	-1.951329
C	-4.561188	0.918442	-2.179530
C	-5.514535	-0.001881	-1.424357
C	-4.729263	2.383766	-1.797249
C	-4.710913	0.724815	-3.683646
Li	-2.461111	0.622829	1.969469
C	-1.772302	2.748038	2.688511
B	-0.900474	2.859845	1.284125
C	-1.593556	3.813161	0.162521
C	-0.966722	3.699420	-1.230593
C	-3.292284	2.995383	2.640829
C	0.650233	3.253015	1.624568
C	1.282102	2.532797	2.824650
H	0.749976	-0.791863	-3.144436
O	1.150822	-2.105182	-1.613008
H	0.607313	1.214814	-1.692372
H	1.313901	0.960666	0.724855
H	-1.479571	-0.663319	-2.696002
H	-1.105831	-3.105005	-2.151661
H	-0.926535	-2.640702	-0.445267
H	-4.365712	-3.448134	-0.597776
H	-2.799759	-4.275922	-0.494510
H	-1.539251	-4.162738	1.585298
H	-1.321782	-3.332283	3.908095
H	-2.855703	-1.573707	4.748568
H	-4.625294	-0.661371	3.257340
H	-4.806778	-1.471784	0.920300
H	3.265371	2.174830	-2.431875
H	2.368136	2.356992	-0.914615
H	3.378346	1.355285	1.224373
H	5.475241	1.184329	2.516660
H	7.667801	1.371704	1.363751
H	7.743471	1.710212	-1.093259
H	5.634230	1.871553	-2.386923
H	1.390363	-0.793177	0.483198
H	-0.842153	1.695998	0.693494
H	0.682900	4.336535	1.826190
H	1.303848	3.123691	0.746785
H	2.337196	2.793669	2.974584
H	0.756460	2.783445	3.751948
H	1.224315	1.440383	2.728876
H	-2.665254	3.584391	0.071662
H	-1.544271	4.864082	0.494079
H	-1.377239	4.414723	-1.954002
H	0.118842	3.857915	-1.197350
H	-1.131982	2.693799	-1.641152
H	-1.540732	1.834759	3.275760
H	-1.357816	3.526669	3.345047
H	-3.765768	2.904721	3.625380
H	-3.483588	4.008855	2.276080
H	-3.832907	2.340198	1.945557
H	-5.715497	1.018382	-3.997079
H	-3.982490	1.338177	-4.220185
H	-4.551442	-0.324163	-3.947720
H	-5.715183	2.728546	-2.122108
H	-4.642279	2.520767	-0.718665
H	-3.966703	2.990984	-2.294165
H	-6.524563	0.122022	-1.824125
H	-5.204170	-1.041986	-1.565983
H	-5.527922	0.231863	-0.359330
C	2.473281	-2.388744	-2.059740
H	2.444679	-3.399309	-2.487155
H	2.774245	-1.690003	-2.846185
C	3.468184	-2.348642	-0.924542
C	4.727532	-1.776293	-1.097028
C	5.654875	-1.783014	-0.059208

C	5.322883	-2.349044	1.169126
C	4.061576	-2.912634	1.352929
C	3.141583	-2.917458	0.307861
H	4.973635	-1.299543	-2.042374
H	6.625217	-1.318294	-0.201682
H	6.040349	-2.341211	1.983906
H	3.794830	-3.350170	2.310111
H	2.154859	-3.352317	0.446215

gal_re_product_solvent

C	-5.239915	1.111624	1.386962
C	-4.832838	1.177450	0.052991
C	-5.795501	1.313288	-0.945309
C	-7.148072	1.385052	-0.619436
C	-7.549027	1.311395	0.711382
C	-6.590392	1.173936	1.714330
C	-3.368395	1.114273	-0.303345
O	-2.729678	0.265455	0.620811
C	-1.321331	0.194780	0.576025
C	-0.961530	-1.075294	1.365135
C	0.550231	-1.396863	1.218184
N	1.258100	-0.240742	0.679765
C	0.844911	0.317323	-0.676511
C	-0.677615	0.114342	-0.801124
C	0.811899	-2.617157	0.312083
O	2.204800	-2.707859	0.089871
C	2.569722	-2.994191	-1.242721
C	3.896133	-2.349736	-1.562223
C	4.273553	-2.172651	-2.899024
C	5.484271	-1.565146	-3.219166
C	6.336660	-1.123845	-2.204740
C	5.966291	-1.293626	-0.873274
C	4.749972	-1.901746	-0.552009
H	-1.211646	-0.916148	2.423053
O	1.557633	-0.166954	-1.702168
C	2.493684	0.089246	1.094199
O	2.829408	-0.421627	2.287870
C	3.900949	0.166720	3.086156
C	3.620853	1.650253	3.302724
O	3.256187	0.818555	0.434956
C	3.791689	-0.595904	4.401599
C	5.264157	-0.072201	2.446372
Li	3.293181	0.154597	-1.387276
C	2.184609	3.228094	-2.293800
C	3.708852	3.275570	-2.157988
B	1.316879	3.618857	-1.035429
C	-0.257836	3.750830	-1.172076
C	-0.873392	3.496288	-2.549712
C	1.989800	3.914348	0.364992
C	1.142439	3.633798	1.608788
O	-1.678921	-2.198089	0.883115
H	-0.897752	1.068971	1.102021
H	-1.049365	0.889038	-1.476828
H	0.973918	-1.609105	2.199289
H	0.436079	-3.524125	0.796998
H	0.284404	-2.498256	-0.638707
H	2.636270	-4.082695	-1.395743
H	1.823870	-2.581365	-1.930435
H	3.604976	-2.502398	-3.690218
H	5.761090	-1.429255	-4.259764
H	7.280150	-0.648894	-2.453019
H	6.621566	-0.950196	-0.078584
H	4.439983	-2.017006	0.481745
H	-2.917757	2.121808	-0.270801
H	-3.260511	0.730979	-1.327745
H	-5.485636	1.343857	-1.986991
H	-7.888770	1.484868	-1.406954
H	-8.603115	1.358734	0.966814
H	-6.897615	1.114743	2.754174
H	-4.488279	0.988658	2.160107
H	-0.884930	-0.852582	-1.269512
H	1.001409	1.405485	-0.505711
H	-0.543481	4.750577	-0.808677
H	-0.703766	3.071132	-0.428149
H	-1.968063	3.495919	-2.520101
H	-0.565069	4.262091	-3.268491
H	-0.551107	2.531651	-2.957029
H	2.951730	3.396175	0.446496
H	2.243027	4.989106	0.327593
H	1.644479	3.947023	2.529787
H	0.175867	4.146157	1.567233
H	0.940634	2.558104	1.697270
H	1.863367	2.196058	-2.530066
H	1.859738	3.811521	-3.166953
H	4.214040	2.923131	-3.063497
H	4.061705	4.293623	-1.962002
H	4.051770	2.661762	-1.316908
H	6.041123	0.306870	3.116782
H	5.434546	-1.143922	2.304532
H	5.339199	0.438664	1.486682
H	4.554385	-0.242299	5.099971
H	2.806723	-0.443587	4.850362

H	3.938988	-1.666042	4.233727
H	4.352015	2.058008	4.006146
H	3.684686	2.205823	2.365285
H	2.621866	1.783380	3.728240
C	-3.004306	-2.374779	1.350287
H	-3.062632	-3.383492	1.782300
H	-3.232963	-1.655944	2.145563
C	-4.041856	-2.242606	0.257333
C	-5.392631	-2.184856	0.605811
C	-6.374115	-2.070371	-0.372556
C	-6.014740	-2.014860	-1.717886
C	-4.669888	-2.076388	-2.071794
C	-3.688142	-2.193318	-1.088599
H	-5.677335	-2.206569	1.655623
H	-7.418567	-2.003133	-0.083895
H	-6.778097	-1.912720	-2.483050
H	-4.380193	-2.033004	-3.117715
H	-2.637946	-2.238329	-1.357641

gal_si_reactant_solvent

C	-7.005726	-1.013837	0.859433
C	-5.857959	-1.640924	0.373897
C	-5.970460	-2.556288	-0.674174
C	-7.216186	-2.840186	-1.226794
C	-8.360627	-2.216794	-0.733363
C	-8.253383	-1.303616	0.312705
C	-4.513969	-1.333872	0.983267
O	-3.536927	-1.335775	-0.040827
C	-2.204237	-1.268496	0.408320
C	-1.318043	-1.115170	-0.820891
C	0.150670	-1.303251	-0.419550
N	0.432425	-0.724620	0.919737
C	-0.449895	0.141984	1.561575
C	-1.923996	-0.077468	1.317672
C	1.046768	-0.617513	-1.448111
O	2.398580	-0.910497	-1.182143
C	3.258202	-0.008514	-1.871631
C	4.653583	-0.572432	-1.879405
C	4.853565	-1.915742	-2.208844
C	6.131802	-2.462335	-2.192561
C	7.226832	-1.665201	-1.857612
C	7.035711	-0.322692	-1.544222
C	5.751751	0.221616	-1.552362
O	-1.428951	0.170203	-1.393711
C	-2.622070	0.474063	-2.119146
C	-3.465108	1.475821	-1.367521
C	-2.871177	2.653130	-0.902519
C	-3.609966	3.570598	-0.162120
C	-4.957378	3.326166	0.106085
C	-5.557934	2.162660	-0.368200
C	-4.811815	1.239322	-1.099396
O	-0.084459	0.987743	2.364915
C	1.660406	-1.032931	1.542338
O	2.228892	-0.285119	2.318041
O	2.040928	-2.252527	1.243475
Li	1.747380	1.588223	2.159818
B	2.364505	2.878711	0.554567
C	3.805013	2.444511	1.257318
C	4.781065	3.620080	1.391947
C	2.620181	3.601910	-0.895266
C	1.537844	3.395480	-1.962228
C	1.487649	3.846194	1.583126
C	0.072124	4.198112	1.112297
H	-1.576769	-1.885188	-1.561231
H	-1.936556	-2.204205	0.929224
H	-2.337456	0.838882	0.885052
H	0.373651	-2.370819	-0.368616
H	0.764565	-0.961737	-2.455670
H	0.869285	0.460716	-1.387168
H	3.229177	0.976699	-1.385996
H	2.897966	0.111762	-2.906190
H	5.598058	1.266007	-1.291165
H	7.884264	0.300979	-1.281906
H	8.225146	-2.090851	-1.841497
H	6.277364	-3.509076	-2.441244
H	3.993395	-2.529623	-2.460495
H	-2.292119	0.902012	-3.072710
H	-3.194819	-0.436023	-2.321585
H	-5.272533	0.316312	-1.442191
H	-6.604658	1.961232	-0.160031
H	-5.534656	4.040408	0.684562
H	-3.133341	4.473938	0.206584
H	-1.817666	2.834757	-1.102836
H	-4.252023	-2.089010	1.742904
H	-4.555032	-0.354123	1.479172
H	-6.919583	-0.286396	1.662766
H	-9.139601	-0.808355	0.696531
H	-9.330991	-2.436818	-1.166630
H	-7.294422	-3.549237	-2.044905
H	-5.073874	-3.029867	-1.061203
H	-2.359403	-0.201802	2.313475
H	1.706020	1.827221	0.338512

H	2.057037	4.778247	1.713617
H	1.399330	3.475243	2.627370
H	3.726209	1.991241	2.267167
H	4.281542	1.654717	0.654204
H	5.751056	3.328726	1.811314
H	4.968372	4.078317	0.414992
H	4.368014	4.402982	2.037662
H	2.759328	4.684620	-0.743974
H	3.578717	3.261333	-1.323671
H	1.485556	2.344435	-2.270020
H	0.543467	3.658830	-1.587037
H	1.711941	3.986257	-2.870185
H	-0.493569	4.785204	1.845902
H	0.104733	4.781836	0.186323
H	-0.504903	3.287819	0.903309
C	3.336124	-2.781584	1.714132
C	3.508626	-4.014225	0.838107
C	4.471631	-1.792605	1.471510
C	3.183096	-3.146814	3.183830
H	5.416131	-2.344362	1.485000
H	4.360524	-1.335273	0.486648
H	4.507836	-1.010139	2.228628
H	4.409938	-4.555092	1.136171
H	2.648590	-4.681580	0.938557
H	3.608252	-3.711171	-0.207772
H	4.112906	-3.599238	3.539436
H	2.981004	-2.256377	3.782869
H	2.372181	-3.867417	3.319680

gal_si_TS_solvent

C	-6.641053	-0.964775	1.018886
C	-5.431658	-1.572620	0.683839
C	-5.446211	-2.784179	-0.010307
C	-6.654361	-3.379234	-0.360439
C	-7.860542	-2.770797	-0.016800
C	-7.851713	-1.562053	0.674418
C	-4.121842	-0.937245	1.077045
O	-3.205719	-1.074213	0.008000
C	-1.847851	-0.981507	0.362412
C	-1.047555	-1.006378	-0.935948
C	0.472144	-0.964330	-0.618151
N	0.760860	-0.787444	0.825520
C	-0.044641	0.088611	1.655932
C	-1.445510	0.305227	1.084429
C	1.215865	0.082257	-1.445540
O	2.598649	-0.176151	-1.318835
C	3.373719	0.783936	-2.018708
C	4.814001	0.362031	-1.934045
C	5.221805	-0.816936	-2.563251
C	6.526388	-1.276443	-2.421622
C	7.438983	-0.554162	-1.651877
C	7.042370	0.627510	-1.032439
C	5.731722	1.082619	-1.172747
O	-1.364396	0.108579	-1.748919
C	-2.566906	0.032465	-2.515926
C	-3.579161	1.060838	-2.068790
C	-3.218296	2.408525	-2.011827
C	-4.131609	3.368857	-1.586093
C	-5.425621	2.991319	-1.230167
C	-5.798944	1.651412	-1.303852
C	-4.877536	0.691932	-1.718216
O	0.063970	0.015723	2.904501
C	1.932133	-1.313830	1.337530
O	2.484896	-0.905252	2.354912
O	2.380383	-2.335197	0.628652
Li	1.782059	0.609233	3.224833
B	1.379915	2.528398	1.483919
C	2.958036	2.060921	1.467258
C	3.896393	3.265651	1.288410
C	1.035468	3.522773	0.233928
C	-0.368227	3.449342	-0.376559
C	0.896282	3.089008	2.939792
C	-0.561934	3.543241	3.035594
H	-1.275081	-1.928177	-1.487410
H	-1.571050	-1.852214	0.979965
H	-1.507831	1.139740	0.384954
H	0.890828	-1.935243	-0.877862
H	0.906050	0.007034	-2.495973
H	0.980800	1.093879	-1.086622
H	3.232694	1.781384	-1.575817
H	3.040281	0.826783	-3.067481
H	5.412414	1.996401	-0.678150
H	7.749732	1.193677	-0.434775
H	8.457398	-0.912366	-1.539601
H	6.834265	-2.195511	-2.910636
H	4.503516	-1.377935	-3.156000
H	-2.280807	0.224264	-3.557681
H	-2.999951	-0.970412	-2.452609
H	-5.161459	-0.356836	-1.744335
H	-6.803272	1.345428	-1.025888
H	-6.139170	3.738799	-0.897677
H	-3.833397	4.411661	-1.535548

H	-2.212635	2.703731	-2.295878
H	-3.717182	-1.429734	1.975985
H	-4.281350	0.123323	1.315139
H	-6.633746	-0.011971	1.542325
H	-8.786820	-1.078023	0.937979
H	-8.802369	-3.234414	-0.292264
H	-6.655965	-4.318508	-0.904591
H	-4.502919	-3.244874	-0.287291
H	-2.071966	0.516396	1.952218
H	0.635364	1.439459	1.263521
H	1.549711	3.945893	3.171580
H	1.071385	2.403351	3.790688
H	3.313452	1.550576	2.381434
H	3.145429	1.330883	0.663956
H	4.954110	2.989444	1.370851
H	3.752616	3.738891	0.311400
H	3.702896	4.034259	2.045265
H	1.227547	4.557327	0.563144
H	1.753771	3.356583	-0.584354
H	-0.524591	2.488603	-0.879915
H	-1.159953	3.538738	0.374444
H	-0.539960	4.233005	-1.125787
H	-0.837114	3.879474	4.041338
H	-0.754211	4.373003	2.348613
H	-1.240511	2.726554	2.762154
C	3.705377	-2.915924	0.881331
C	3.913721	-3.776889	-0.357835
C	4.781881	-1.837026	0.957824
C	3.632226	-3.761999	2.145278
H	5.756147	-2.303647	0.785051
H	4.615811	-1.094663	0.173610
H	4.795381	-1.339412	1.926963
H	4.860031	-4.317599	-0.278049
H	3.101835	-4.501319	-0.464008
H	3.944484	-3.140151	-1.246415
H	4.593886	-4.258632	2.302261
H	3.415507	-3.137402	3.013530
H	2.857848	-4.527883	2.048420

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C	-6.680813	-0.164307	1.111461
C	-5.538266	-0.943619	0.925298
C	-5.680731	-2.306307	0.661520
C	-6.947826	-2.880109	0.587543
C	-8.084478	-2.098819	0.781670
C	-7.947660	-0.737482	1.045897
C	-4.170637	-0.312919	1.022492
O	-3.282471	-1.004404	0.175592
C	-1.908052	-0.844554	0.464605
C	-1.142702	-1.413832	-0.728265
C	0.390942	-1.225258	-0.512579
N	0.710829	-0.716560	0.830057
C	-0.075794	0.447555	1.464075
C	-1.393038	0.569813	0.676223
C	1.025746	-0.324810	-1.578505
O	2.423109	-0.365178	-1.384319
C	3.128151	0.373877	-2.364997
C	4.587017	0.032036	-2.225648
C	5.010269	-1.267123	-2.519913
C	6.330705	-1.646300	-2.307440
C	7.247361	-0.722754	-1.803483
C	6.837616	0.577354	-1.523787
C	5.510433	0.952091	-1.734637
O	-1.459371	-0.746430	-1.940477
C	-2.745425	-0.940298	-2.508049
C	-3.630257	0.272957	-2.323359
C	-3.072583	1.552759	-2.344178
C	-3.874947	2.677350	-2.171803
C	-5.249062	2.534314	-1.986672
C	-5.812652	1.260443	-1.976087
C	-5.005779	0.137050	-2.142885
O	-0.312876	0.237734	2.765640
C	1.855558	-1.085508	1.438083
O	2.336943	-0.509941	2.431810
O	2.427102	-2.170563	0.908182
Li	1.148322	0.069467	3.738112
B	2.025857	3.407791	1.213909
C	3.193193	2.560987	0.563758
C	4.335790	2.139481	1.494926
C	1.196500	4.414416	0.312775
C	-0.040461	3.708955	-0.279608
C	1.713305	3.270934	2.756243
C	0.289596	3.571989	3.233023
H	-1.381890	-2.481084	-0.839217
H	-1.661084	-1.428149	1.365065
H	-1.283896	1.072445	-0.289063
H	0.875393	-2.196451	-0.605445
H	0.770343	-0.693310	-2.578836
H	0.651392	0.707513	-1.492154
H	2.960024	1.453147	-2.230302
H	2.762930	0.096599	-3.366257
H	5.186173	1.962298	-1.500263

H	7.547083	1.300522	-1.134031
H	8.278238	-1.016760	-1.633274
H	6.646594	-2.660139	-2.533237
H	4.289620	-1.983862	-2.905981
H	-2.579667	-1.110318	-3.579948
H	-3.231970	-1.827780	-2.091002
H	-5.445087	-0.856447	-2.090011
H	-6.879057	1.135124	-1.813930
H	-5.875322	3.410020	-1.847479
H	-3.427223	3.666690	-2.180499
H	-1.999240	1.659061	-2.478750
H	-3.808622	-0.354437	2.062821
H	-4.236022	0.746166	0.730357
H	-6.575063	0.902738	1.291991
H	-8.828669	-0.119494	1.189636
H	-9.071480	-2.546197	0.720503
H	-7.048080	-3.940372	0.376246
H	-4.790225	-2.904733	0.498643
H	-2.049322	1.173884	1.305997
H	0.551747	1.344640	1.265592
H	2.419338	3.987903	3.215924
H	2.045245	2.291492	3.127180
H	2.714116	1.644405	0.166713
H	3.586939	3.083855	-0.318828
H	5.109823	1.581675	0.957578
H	4.813452	3.007957	1.961345
H	3.962073	1.488912	2.290184
H	0.855470	5.281576	0.892304
H	1.807657	4.798148	-0.512852
H	0.252113	2.839018	-0.879170
H	-0.712801	3.351044	0.506580
H	-0.612429	4.378996	-0.928558
H	0.234815	3.656086	4.323514
H	-0.085969	4.510823	2.813757
H	-0.386672	2.764062	2.936176
C	3.752922	-2.618206	1.317080
C	4.051098	-3.711537	0.296897
C	4.776156	-1.492090	1.197362
C	3.688104	-3.199381	2.725573
H	5.782276	-1.922524	1.209784
H	4.639076	-0.967159	0.247049
H	4.684550	-0.777383	2.014538
H	5.022869	-4.165130	0.508360
H	3.283426	-4.489243	0.336077
H	4.073993	-3.284171	-0.709034
H	4.653360	-3.648762	2.976986
H	3.462690	-2.420872	3.455107
H	2.921649	-3.978095	2.778738