Electronic Supplementary Material (ESI) for RSC Advances.

“Armed and Disarmed” Theory in the Addition of Azide Radical to Glucals

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Supporting Information

1. General azidonitration procedure

Under Ar condition, CAN (3mmol, 3 equiv) was added in portion-wise to the mixture of NaN_3 (1.5mmol, 1.5equiv.) and glycan derivative (1mmol, 1equiv.) in 10 ml anhydrous MeCN at -30°C. The reaction was monitored by TLC. After the complete conversion of starting materials, EtOAc (30ml, 300% v/v) and water (20ml, 200% v/v) were added to the reaction suspension and the mixture was kept stirring until the solution turned into pale yellow. The separated organic layer was washed with brine, dried over Na_2SO_4 and evaporated to dryness. The crude product was purified by silica gel chromatography immediately to afford the corresponding compound.

2. Characterization of compounds in Table 1

6a, 7a

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 – 7.27 (m, 40H), 7.18 – 7.11 (m, 5H), 6.28 (d, *J* = 4.0 Hz, 1H), 6.17 (s, 2H), 4.88 (d, *J* = 2.6 Hz, 2H), 4.83 – 4.77 (m, 3H), 4.76 – 4.72 (m, 3H), 4.65 (d, *J* = 12.1 Hz, 2H), 4.60 (d, *J* = 12.0 Hz, 1H), 4.54 (d, *J* = 10.9 Hz, 1H), 4.51 – 4.45 (m, 5H), 4.03 (dd, *J* = 9.1 Hz, 2H), 3.96 – 3.90 (m, *J* = 6.7 Hz, 5H), 3.89 – 3.83 (m, *J* = 8.1 Hz, 4H), 3.81 – 3.72 (m, 5H), 3.67 – 3.61 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 137.92, 137.86, 137.68, 137.60, 137.44, 137.34, 128.71, 128.60, 128.54, 128.51, 128.47, 128.27, 128.17, 128.15, 128.03, 127.97, 127.93, 127.80, 127.72, 98.32, 97.57, 80.33, 79.15, 77.29, 75.80, 75.25, 75.20, 74.57, 73.82, 73.64, 73.60, 73.50, 73.20, 67.98, 67.59, 61.71, 58.85.

HRMS $C_{27}H_{28}N_4NaO_7$ [M+Na^+] =543.1858 (543.1856)

6b, 7b

^{1}H NMR (400 MHz, $CDCl_3$) (mannose configuration): δ 7.67 – 7.59 (m, 4H), 7.47 – 7.34 (m, 6H), 6.22 (d, J = 2.0 Hz, 1H), 5.47 (dd, J = 9.7 Hz, 1H), 5.24 (dd, J = 9.4, 3.8 Hz, 1H), 4.17 (dd, J = 3.7, 2.1 Hz, 1H), 3.91 (ddd, J = 10.1, 4.4, 2.6 Hz, 1H), 3.76 – 3.65 (m, 2H), 2.11 (s, 3H), 1.93 (s, 3H), 1.05 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 169.93, 169.14, 135.70, 135.63, 133.02, 132.91, 129.88, 129.80, 127.73, 127.71, 97.92, 97.51, 73.93, 73.38, 70.70, 65.24, 62.07, 60.61, 58.80, 26.65, 26.61, 20.55, 20.50, 19.19.

HRMS $C_{26}H_{32}N_4NaO_9Si$ [M+Na^+] =595.1835 (595.1836)

6c, 7c

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 – 7.64 (m, 4H), 7.43 – 7.27 (m, 14H), 7.20 – 7.14 (m, 2H), 6.17 (d, *J* = 1.1 Hz, 1H), 4.87 (d, *J* = 10.8 Hz, 1H), 4.80 – 4.70 (m, 2H), 4.62 (d, *J* = 10.8 Hz, 1H), 4.13 (dd, *J* = 9.6, 8.4 Hz, 1H), 3.98 – 3.91 (m, 3H), 3.83 (dd, *J* = 11.5, 1.6 Hz, 1H), 3.79 – 3.74 (m, 1H), 1.06 (s, 10H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 137.88, 137.33, 135.89, 135.62, 133.51, 132.94, 129.72, 128.69, 128.48, 128.25, 128.05, 127.89, 127.75, 127.64, 98.51, 79.09, 75.53, 75.28, 73.36, 73.22, 62.13, 58.87, 26.75.

HRMS $C_{36}H_{40}N_4NaO_7Si$ [M+Na^+]= 691.2564(691.2564)

6d

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 – 7.73 (m, 4H), 7.64 (d, J = 6.2 Hz, 4H), 7.52 – 7.37 (m,

12H), 6.27 (d, J = 2.6 Hz, 1H), 5.39 (dd, J = 8.1, 3.8 Hz, 1H), 5.12 (dd, J = 9.4 Hz, 1H), 5.01 – 4.90 (m, 2H), 4.83 (d, J = 8.1 Hz, 1H), 4.44 (t, J = 8.9 Hz, 1H), 4.13 – 4.09 (m, 1H), 3.97 (dd, J = 11.9, 2.2 Hz, 1H), 3.88 – 3.82 (m, 1H), 3.80 – 3.68 (m, 3H), 3.53 (ddd, J = 9.6, 5.2, 2.5 Hz, 1H), 2.09 (s, 3H), 2.00 (s, 3H), 1.79 (s, 3H), 1.78 (s, 3H), 1.11 (s, 9H), 1.10 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 170.26, 169.88, 169.32, 168.86, 135.97, 135.59, 135.55, 135.46, 133.21, 132.96, 132.93, 132.03, 130.05, 129.99, 129.88, 128.05, 127.80, 127.77, 127.74, 100.80, 98.26, 75.29, 74.46, 73.43, 72.76, 71.64, 70.10, 68.66, 63.09, 60.94, 58.92, 20.61, 20.58, 20.46, 20.39, 19.34, 19.10.

HRMS $C_{52}H_{64}N_4O_{16}Si_2$ [M+NH_4^+] =1074.4188(1074.4200)

6e

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.22 (d, *J* = 1.5 Hz, 1H), 5.40 (dd, *J* = 9.8 Hz, 1H), 5.31 (dd, *J* = 9.8, 3.8 Hz, 1H), 4.22 (dd, *J* = 3.7, 1.9 Hz, 1H), 3.92 – 3.87 (m, 1H), 3.73 (dd, *J* = 13.1, 2.1 Hz, 1H), 3.61 (dd, *J* = 13.0, 3.7 Hz, 1H), 2.14 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 170.34, 169.86, 97.22, 73.39, 70.20, 65.18, 60.67, 58.83, 20.63, 20.43.

HRMS $C_{10}H_{15}N_4O_9$ [M+H^+] = 335.0840 (335.0839)

6f, 7f

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.16 (d, *J* = 3.4 Hz, 1H), 5.61 (d, *J* = 8.8 Hz, 2H), 5.42 (dd, *J* = 7.1, 3.5 Hz, 1H), 5.27 (dd, *J* = 9.5 Hz, 4H), 5.15 (dd, *J* = 9.7 Hz, 2H), 5.00 (dd, *J* = 9.7, 3.4 Hz, 2H), 4.91 (dd, *J* = 9.3, 8.1 Hz, 2H), 4.73 (dd, *J* = 4.0 Hz, 2H), 4.33 (dd, *J* = 6.7 Hz, 1H), 4.27 – 4.19 (m, 2H), 4.16 – 4.12 (m, 3H), 4.03 (dd, *J* = 9.6 Hz, 3H), 3.97 (dd, *J* = 12.5, 1.4 Hz, 2H), 3.87 (dd, *J* = 12.4, 1.9 Hz, 1H), 3.81 (dd, *J* = 12.8, 2.4 Hz, 3H), 3.77 (dd, *J* = 4.6, 2.1 Hz, 2H), 3.75 – 3.73 (m, 1H), 3.69 – 3.65 (m, 2H), 3.62 – 3.60 (m, 2H), 3.59 – 3.57 (m, 2H), 3.55 – 3.51 (m, 2H), 2.27 – 2.21 (m, 9H), 2.11 – 2.08 (m, 9H), 2.08 – 2.06 (m, *J* = 4.2 Hz, 9H), 2.03 – 2.02 (m, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 170.52, 170.42, 170.25, 170.23, 170.17, 170.13, 169.32, 169.19, 100.89, 100.07, 97.89, 76.10, 74.47, 74.31, 74.02, 73.59, 72.79, 72.75, 72.62, 72.50, 71.89, 71.72, 68.62, 68.59, 61.18, 60.69, 60.44, 59.49, 20.74, 20.59, 20.55.

HRMS $C_{20}H_{28}N_4$ Na O_{16} [M+Na^+] =603.1400 (603.1398)

3. Synthesis of S8

6e **S8**

A solution of the **6e** (334 mg, 1 mmol, 1eq) and Et_3N (0.5 mL, 5 mmol, 5eq) in 5 mL glacial acid was heated to 100°C for 25 min. The reaction was monitored by TLC. After the complete conversion of starting materials, the solution was diluted with dichloromethane and washed with water. After dryness over anhydrous sodium sulfate, evaporation of solvent gave syrup. Ac_2O (0.1 mL, 1 mmol, 1eq), Et_3N (0.1 mL, 1 mmol, 1eq) and the syrup was dissolved in EtOAc (5 mL). Pd/C (10%, 30 mg) was added to this solution under N_2. The suspension was degassed under vacuum and purged with H_2 three times. The mixture was stirred under H_2 (1 atm) at 25℃ for 1.5 h. The mixture was filtered through a pad of Celite and the pad was washed with EtOAc. After purification by column chromatograph, the title compound was obtained as white foam **S8** (250

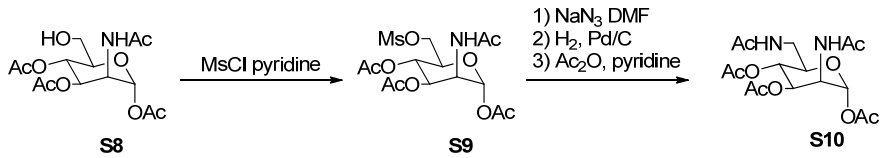
mg, 75%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.32 (d, *J* = 9.2 Hz, 1H), 6.03 (d, *J* = 1.5 Hz, 1H), 5.38 (dd, *J* = 10.3, 4.5 Hz, 1H), 5.20 (dd, *J* = 10.2 Hz, 1H), 4.66 (ddd, *J* = 9.3, 4.5, 1.7 Hz, 1H), 3.86 – 3.79 (m, 1H), 3.73 (dd, *J* = 12.9, 2.0 Hz, 1H), 3.59 (dd, *J* = 12.9, 3.3 Hz, 1H), 2.17 (s, 3H), 2.10 (s, 3H), 2.04 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 170.71, 170.57, 170.15, 168.57, 92.02, 72.39, 68.78, 65.60, 60.61, 49.23, 22.93, 20.86, 20.73, 20.69.

In accord with the literature U. Aich, C. T. Campbell, N. Elmouelhi, C. A. Weier, S. G. Sampathkumar, S. S. Choi and K. J. Yarema, *ACS Chem Bio*, 2008, 3, 230.

4. Synthesis of S10



S8 **S9** **S10**

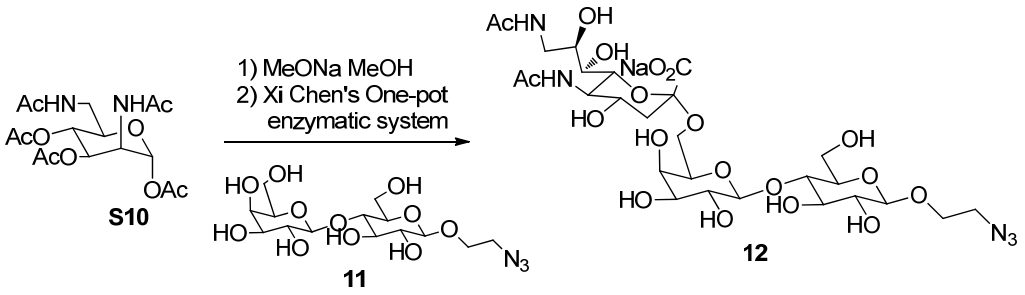
Flasks were heated before use under vacuum for 30 minutes and purged with N_2 for 10 minutes. To a solution of compound **S8** (347 mg, 1 mmol) and pyridine (155 μL, 2equiv) in DCM (anhydrous, 5 mL) was added drop-wise methanesulfonyl chloride (155 μL, 2equiv) with stirring under ice-bath. After stirring for 8 h, the solution was poured into ice water. The aqueous layer was extracted with DCM (40 mL×2). The combined organic layer was washed with brine and dried over Na_2SO_4. The crude product **S9** was dissolved in DMF (5 mL) and treated by sodium azide (650 mg 10equiv). The reaction mixture was stirring for 10h at 60ºC. After removal of solvent by evaporation, extraction and purification by column chromatograph, the product was dissolved in EtOH (10 mL) and Pd/C (10%, 50 mg) was added to this solution under N_2. The suspension was degassed under vacuum and purged with H_2 three times. The mixture was stirred under H_2 (1 atm) at 25℃ for 1.5 h. The suspension was filtered through a pad of Celite and the pad was washed with EtOH. The combined filtrates were concentrated to dryness, followed by acetylation using Ac_2O and pyridine. After purification by column chromatograph, the title compound **S10** was obtained as a white powder (55% yield, 213 mg).

^{1}H NMR (400 MHz, MeOD): δ 5.96 (d, *J* = 1.1 Hz, 1H), 5.27 (dd, *J* = 10.2, 4.4 Hz, 1H), 5.19 (dd, *J* = 10.0 Hz, 1H), 4.60 (dd, *J* = 4.2, 1.3 Hz, 1H), 4.01 (ddd, *J* = 9.6, 6.9, 2.7 Hz, 1H), 3.46 (dd, *J* = 14.2, 6.8 Hz, 1H), 3.37 (dd, *J* = 14.5, 2.7 Hz, 1H), 2.18 (s, 3H), 2.09 (s, 3H), 2.07 (s, 3H), 1.99 (s, 3H), 1.97 (s, 3H).

^{13}C NMR (100 MHz, MeOD): δ 173.74, 173.54, 171.65, 171.53, 170.15, 93.39, 72.31, 70.69, 67.79, 50.69, 40.86, 22.50, 22.38, 20.66.

HRMS $C_{16}H_{24}N_2$ Na O_9 [M+Na^+]=411.1380 (411.1380)

5. Synthesis of trisaccharide 12



Compound **S10** (0.74mmol, 287mmol, 1 eq) was treated with MeONa/MeOH (pH=9.0, 5 ml). After 30min, the reaction was quenched by H^+ resin and filtered. The solution was concentrated under vacuum. According to the protocol reported in the literature[2] , the crude product was added to a solution of 25 ml Tris-HCl buffer solution (10 mM, pH=8.0), pyruvate sodium (244 mg, 3 eq.), cytidine-5'-triphosphate (29 mg, 1.5 eq.), $MgCl_2$ (10 mM), compound **11** (334 mg, 0.81 mmol, 1.1 eq), E. coli K-12 sialic acid aldolase (1 UN), N. meningitides CMP-sialic acid synthetase (NmCSS, 1 UN) and Photobacterium damsela α-2,6-sialyltransferase (Pd2,6ST, 1 UN). The reaction mixture was incubated at 25 ℃ for 8 h with shaking (120 rpm). Then the reaction was allowed to boil for 5 min and cooled to room temperature. The precipitation was removed by centrifugation (6000 rpm, 10 min). The residual aqueous solution was purified by Bio-Gel P2 gel. The corresponding product **10** was converted to the trisaccharide **12** in 80% yield

^{13}C NMR (100 MHz, $CDCl_3$): δ 177.35, 176.92, 175.97, 105.71, 104.55, 102.83, 82.08, 77.18, 77.08, 76.19, 75.19, 74.85, 73.27, 72.46, 72.40, 71.03, 70.84, 66.14, 62.73, 54.27, 53.02, 44.68, 42.58, 24.57, 24.37.

^1H NMR (400 MHz, D_2O): δ 4.42 (d, *J* = 8.0 Hz, 1H), 4.31 (d, *J* = 7.8 Hz, 1H), 3.94 (ddd, *J* = 9.8, 4.6 Hz, 1H), 3.89 – 3.78 (m, 4H), 3.77 – 3.65 (m, 4H), 3.62 (dd, *J* = 10.4, 1.7 Hz, 1H), 3.57 – 3.38 (m, 10H), 3.33 (dd, *J* = 9.0, 1.6 Hz, 1H), 3.24 (dd, *J* = 8.5 Hz, 1H), 3.16 (dd, *J* = 14.0, 7.9 Hz, 1H), 2.58 (dd, *J* = 12.4, 4.6 Hz, 1H), 1.90 (s, 3H), 1.90 (s, 3H), 1.61 (dd, *J* = 12.2 Hz, 1H).

HRMS $C_{27}H_{44}N_5O_{19}$ $[M-H^+]$=742.2640(742.2630)

6. The conformational screen of compounds **5e, 3b, 5c,**

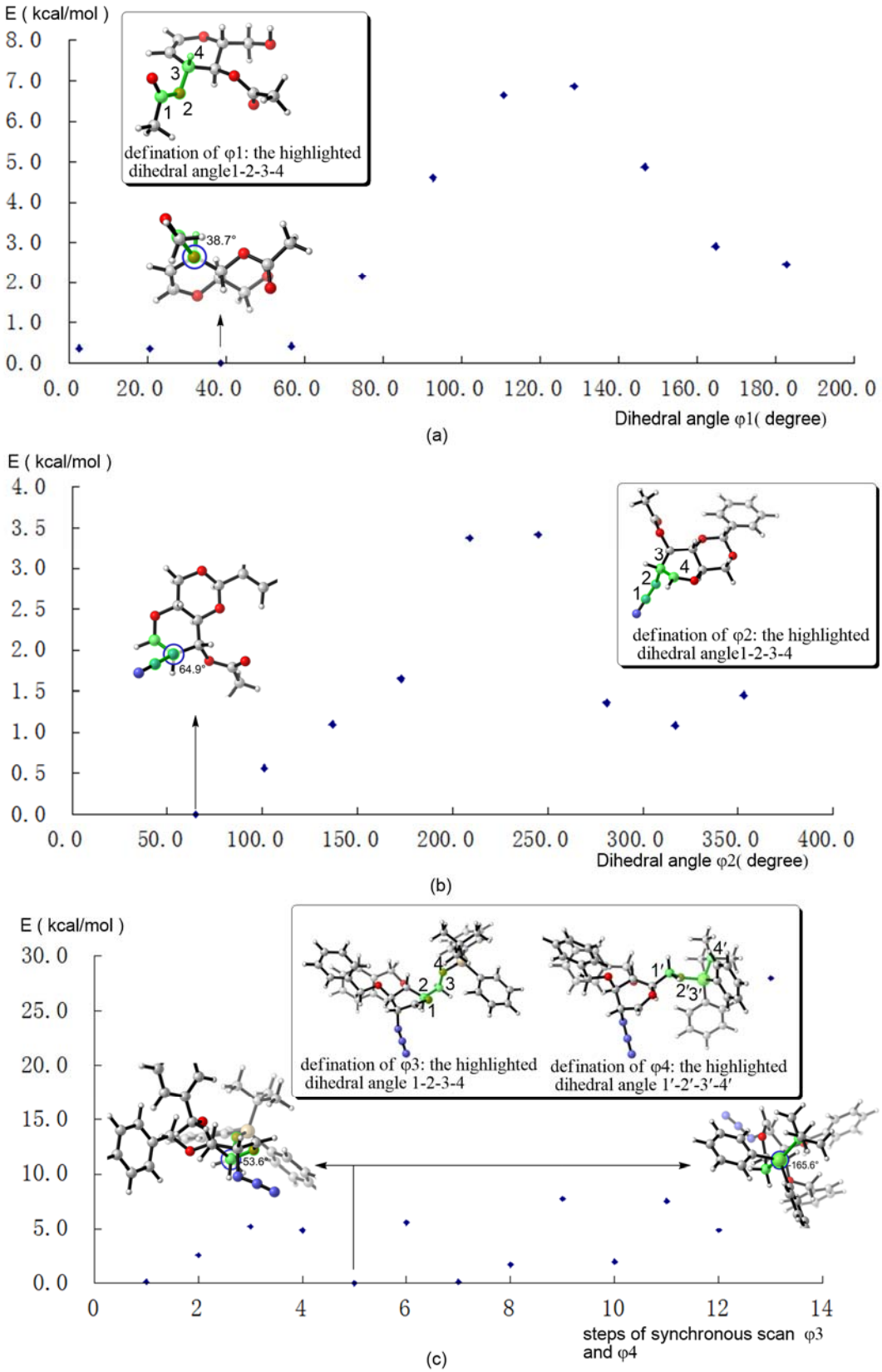


Figure S1. Scan of the torsion angles to determine (a) the compound **5e** orientation (b) the compound **3b** orientation (c) the compound **5c** orientation

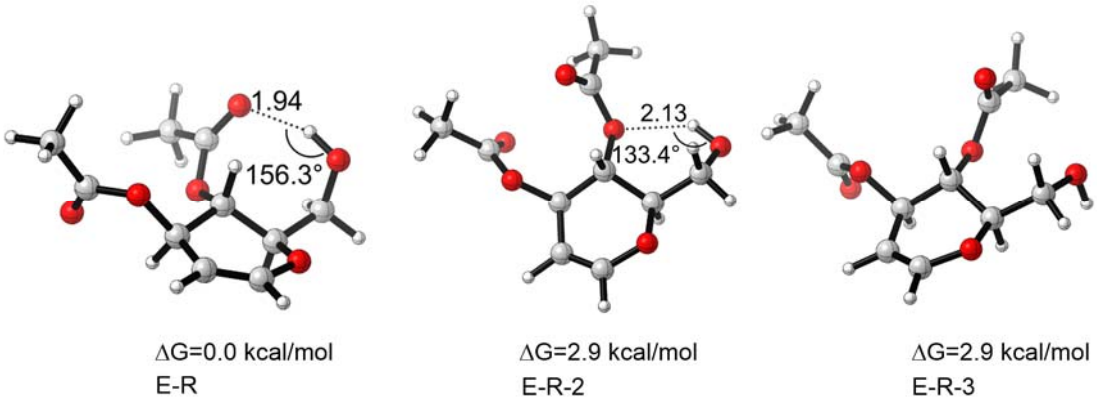


Figure S2. Geometries and relative Gibbs free energies of isomers of E-R. All energies are relative to E-R in Figure 1(b).

In order to locate the most stable geometries of ManNAc derivatives C, E and P, we performed conformational search by using tortional angle scan method. As illustrated in Figure S1, we investigated the potential energy versus group orientations, and presented the geometry and torsion angle of each energy minima.

Based on the most stable geometries as shown in Figure S1 (a), we further confirmed hydrogen bond structure which was implied by experiment. As shown in Figure S2, we compared the free energies of three possible isomers with and without hydrogen bond, including E-R, E-R-2 and E-R-3.

The most stable isomer (E-R) involves O---H-O hydrogen bonding which lies in an eight-membered ring. Though E-R-2 also involves O---H-O hydrogen bonding, it is 2.9 kcal/mol less stable than E-R due to the more strained six-membered ring with hydrogen bonding. The isomer E-R-3 does not involve hydrogen bonding, and it is 2.9 kcal/mol less stable than E-R. The stability of E-R comes from a stronger hygrogen bond interaction, which can be indicated in shorter hydrogen bond length(O---H) and larger hydrogen bond angle(O---H-O). As shown in Figure S1, the hydrogen bond length of E-R is 1.94 Å, shorter than that of E-R-2 and the hydrogen bond angle is 156.3° , larger than that of E-R-2. Thus, the free energy of E-R is lower than that of E-R-2.

Based on the most stable geometries as shown in Figure S1 and S2, we computed the reaction pathways as discussed in Figure 1 and Figure 3 in the text.

7. Electron density study of intermediates

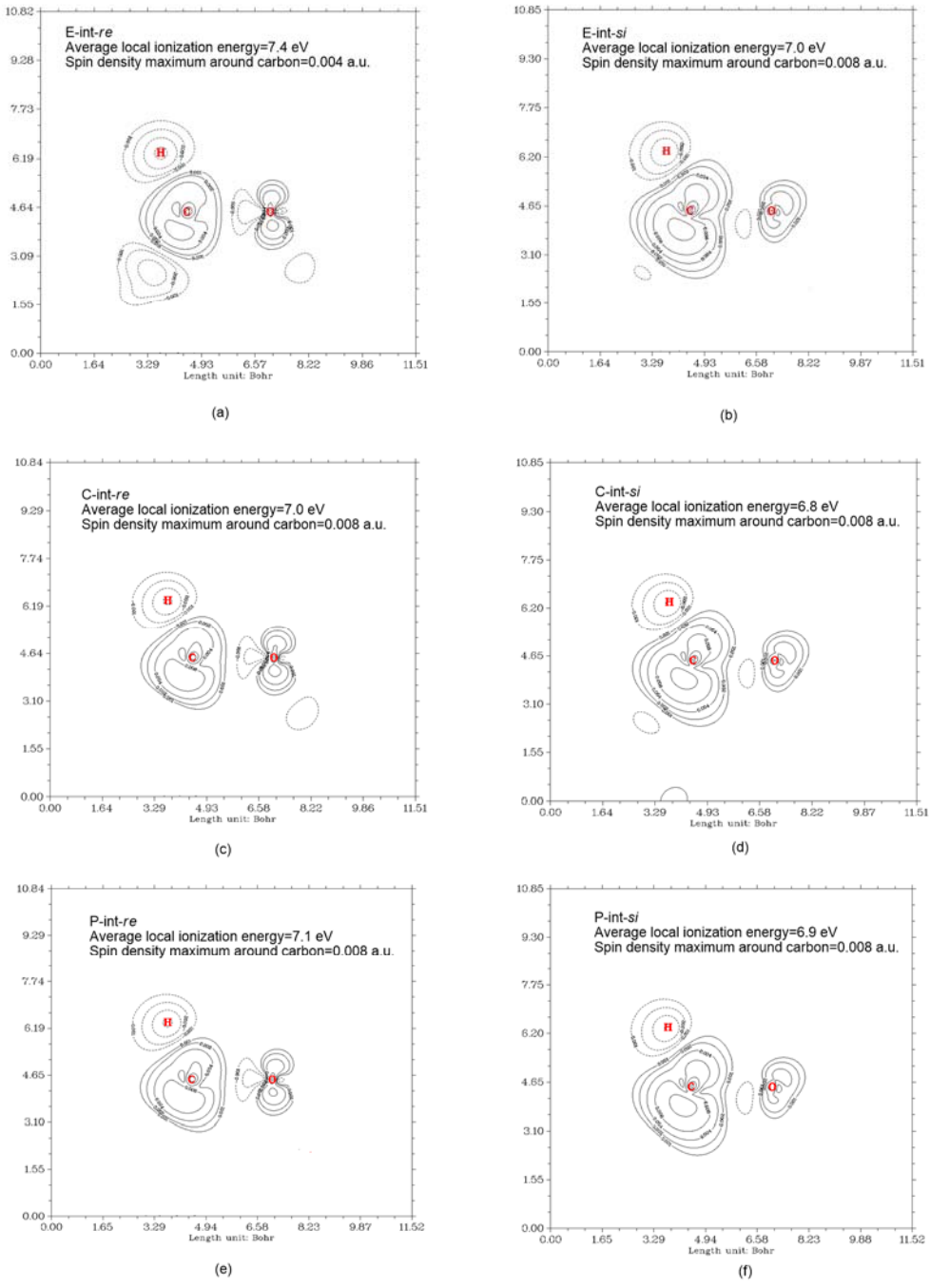


Figure S3. Spin electron density contour maps and average local ionization energy of intermediates: (a),(b) intermediates of compound **5e**, (c),(d) intermediates of compound **5c**, (e),(f) intermediates of compound **3b**,

In order to measure the oxidizability of intermediates of compound **5e**, **5c**, **3b**, we calculated average local ionization energies and spin electron density contour maps. As shown in Figure S3, the average local ionization energy of intermediate of compound **5e** in the axial addition is 7.4 eV, which is obviously larger than that of

intermediate of compound **5e** in the equatorial addition (7.0 eV). And the Spin density maximum around carbon of intermediate of compound **5e** in the equatorial addition is 0.004 a.u., which is lower than that in the axial addition (0.008 a.u.). Both evidences indicate that the oxidizability of intermediate of compound **5e** in the equatorial addition is obviously worse than that in the axial addition, making it likely to transform to intermediate of compound **5e** in the axial addition via thermodynamic equilibrium as shown in Figure 1(b) of the text, thus confirming the thermodynamic-control mechanism. In comparison, the oxidizability differences between intermediates of compound **5c** and **3b** are relatively small (**5c** equatorial addition: 7.0 eV, 0.008 a.u. versus **5c** axial addition: 6.8 eV, 0.008 a.u.,**3b** equatorial addition: 7.1 eV, 0.008 a.u. versus **3b** axial addition: 6.9 eV, 0.008 a.u.), thus confirming the kinetic-control mechanism.

8. The Cartesian coordinates (Å), SCF energies and Gibbs free energies at 298K for the optimized structures.

N_3, UB3LYP/6-31G(d)
Total SCF energy in solvent acetonitrile: -164.1385430 a.u.
Thermal free energy correction in gas phase: -0.009946 a.u.
Gibbs free energy in solvent acetonitrile at 298K: -164.1484890 a.u.
Gibbs free energy in gas phase at 298K: -164.1484880 a.u.
UX3LYP/6-311+G(d,p)
Total SCF energy in solvent acetonitrile: -164.118764 a.u.
Gibbs free energy in solvent acetonitrile at 298K: -164.131207 a.u.
Charge and Multiplicity: 0 2
Cartesian coordinates:

ATOM	X	Y	Z
N	1.16272700	0.22410700	0.00000000
N	0.00000000	0.00073300	0.00000000
N	-1.16272700	-0.22484000	0.00000000

E-Reactant, B3LYP/6-31G(d)
Total SCF energy in solvent acetonitrile: -840.8464030 a.u.
Thermal free energy correction in gas phase: 0.1959300 a.u.
Gibbs free energy in solvent acetonitrile at 298K: -840.6504730 a.u.
Gibbs free energy in gas phase at 298K: -840.6316510 a.u.
UX3LYP/6-311+G(d,p)
Total SCF energy in solvent acetonitrile: -840.7618986 a.u.
Gibbs free energy in solvent acetonitrile at 298K: -1004.697176 a.u.
Charge and Multiplicity: 0 1
Cartesian coordinates:

ATOM	X	Y	Z
C	0.46056700	-0.17449300	-0.05808900
C	1.83462700	-0.59263000	-0.60279200

O	2.20992100	-1.88259300	-0.09155600
C	1.23059200	-2.82064600	-0.02940200
C	-0.07805800	-2.59200800	-0.18154400
C	-0.61554900	-1.20905900	-0.38861100
O	0.04734500	1.06470200	-0.67960800
C	0.17120800	2.22426500	-0.00038900
O	-1.73677700	-1.01753500	0.51938000
C	-2.84559600	-0.39251400	0.04260200
C	2.96372100	0.37531800	-0.22751800
O	0.75316700	2.33779400	1.06233300
H	0.52273000	-0.03995600	1.02375500
H	1.77287400	-0.66684900	-1.69990900
H	1.64670500	-3.80491100	0.16175600
H	-0.78115600	-3.41550900	-0.12905500
H	-0.98954700	-1.03925500	-1.40285500
H	2.84657100	1.29526400	-0.82139500
C	-3.89355700	-0.29765700	1.12728800
H	-3.49828900	0.25556900	1.98552100
H	-4.77820600	0.20488500	0.73493000
H	-4.15920000	-1.29903800	1.48130900
O	-2.96935400	0.02090900	-1.08855800
C	-0.50603700	3.34762400	-0.74263300
H	-0.45316400	4.26216800	-0.15155300
H	-0.01374500	3.50250000	-1.70881200
H	-1.54687100	3.07992700	-0.94933100
H	3.90640400	-0.09243800	-0.53006600
O	3.05117600	0.63551300	1.15319200
H	2.34957400	1.27812600	1.37076800

E-Ts-*re*, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1004.982526 a.u.

Thermal free energy correction in gas phase: 0.200893 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.781633 a.u.

Gibbs free energy in gas phase at 298K: -1004.762593 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1004.880118 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.679225 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	-0.39740400	-0.46219700	-0.10618400
C	0.40841600	-1.76060100	0.03240500
O	1.43065300	-1.80134300	-0.99554100

C	2.14006100	-0.68599000	-1.19346400
C	1.89450000	0.51210400	-0.52412000
C	0.48615400	0.79164200	-0.03541700
O	-1.34388200	-0.37589800	0.97786300
C	-2.65285800	-0.60968900	0.72974700
O	-0.04022200	1.81604600	-0.91685200
C	-0.94154800	2.69802900	-0.39924300
C	-0.43827500	-3.02499200	-0.14670000
O	-3.07044000	-1.09902400	-0.30328500
H	-0.92799400	-0.48349700	-1.06101300
H	0.91978400	-1.77733100	1.00317800
H	2.99456300	-0.84843700	-1.84140900
H	2.42840300	1.38197600	-0.89213300
H	0.49685800	1.17527900	0.98559600
H	-1.05578700	-3.15593100	0.75479500
N	2.75864100	0.39759100	1.22747900
N	3.96604300	0.32666800	1.08300500
N	5.11509600	0.25777200	0.95280600
C	-1.32850600	3.71846600	-1.44208400
H	-1.76281600	3.21840000	-2.31392200
H	-2.04962500	4.41636400	-1.01586900
H	-0.44152400	4.26082900	-1.78509900
O	-1.36089900	2.65126900	0.73427900
C	-3.49948500	-0.16479700	1.89056100
H	-4.53605500	-0.45995400	1.72675100
H	-3.12279500	-0.59511200	2.82345500
H	-3.42285500	0.92439900	1.97996900
H	0.24746900	-3.87676100	-0.20106800
O	-1.20142500	-3.02435500	-1.32965700
H	-1.98271300	-2.45983900	-1.17371500

E-Int-*re*, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1004.987374 a.u.

Thermal free energy correction in gas phase: 0.203018 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.784356 a.u.

Gibbs free energy in gas phase at 298K: -1004.768550 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1004.881873 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.678855 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	-0.33730500	-0.39208900	-0.06561700
C	0.56287800	-1.61997000	-0.27297000

O	1.50694700	-1.34892400	-1.32672800
C	2.16647600	-0.16498000	-1.27276700
C	1.94630300	0.76692800	-0.15384100
C	0.44793000	0.91743600	0.16347100
O	-1.16460900	-0.60804000	1.09666700
C	-2.47399700	-0.89198800	0.91458000
O	-0.02338200	1.95977700	-0.72053300
C	-1.18763100	2.57659500	-0.38532800
C	-0.21760900	-2.87409100	-0.68623200
O	-2.95815100	-1.21102300	-0.15496500
H	-0.96728300	-0.28185700	-0.95035900
H	1.12002300	-1.82278000	0.65126300
H	2.99893700	-0.10564100	-1.96234400
H	2.35587400	1.75136100	-0.40035300
H	0.31346800	1.23604900	1.19878900
H	-0.74291200	-3.26008500	0.20060100
N	2.56896400	0.32079300	1.18523900
N	3.79620100	0.19539300	1.16470700
N	4.92892700	0.05192700	1.23118100
C	-1.51698100	3.66203100	-1.38028500
H	-1.63152300	3.22924300	-2.37959700
H	-2.44151900	4.15752500	-1.08305600
H	-0.70063400	4.38959100	-1.43096500
O	-1.85236200	2.27645400	0.58141800
C	-3.23983100	-0.73854300	2.19991000
H	-4.22110600	-1.20427800	2.10397200
H	-2.68582600	-1.17229500	3.03682200
H	-3.35793000	0.33280100	2.39827400
H	0.51443500	-3.62945700	-0.99012100
O	-1.08669200	-2.66957900	-1.77572700
H	-1.88805800	-2.23425100	-1.42740400

E-Ts-*si*, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1004.984087 a.u.

Thermal free energy correction in gas phase: 0.202635 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.781452 a.u.

Gibbs free energy in gas phase at 298K: -1004.759373 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1004.885222 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.682587 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	0.83015300	-0.03825500	-0.21903300

C	1.71430200	-1.08493600	-0.91980300
O	1.10997800	-2.40353900	-0.89555000
C	-0.22097300	-2.52511500	-0.94001700
C	-1.11209600	-1.49295400	-0.66303400
C	-0.58649200	-0.07792900	-0.77503600
O	1.35573200	1.27694200	-0.50145600
C	2.12160600	1.88118200	0.43775300
O	-1.37905900	0.86506900	-0.04092700
C	-2.48753300	1.34736200	-0.67576400
C	3.11182800	-1.23526000	-0.30454300
O	2.52524500	1.33287300	1.44388500
H	0.81043500	-0.21241300	0.85753200
H	1.81725900	-0.80558300	-1.97786600
H	-0.53304500	-3.55718900	-1.05243900
H	-0.59219200	0.22442900	-1.82825800
H	3.70753600	-0.35407800	-0.58820600
N	-1.37350000	-1.63697400	1.30969900
N	-2.53869200	-1.36321000	1.51402100
N	-3.65288900	-1.10142700	1.71599200
C	-3.26173800	2.26355000	0.23482100
H	-2.59402000	2.96083500	0.74833500
H	-4.01052600	2.80441900	-0.34488800
H	-3.75981900	1.65439300	0.99789500
O	-2.79307800	1.03336000	-1.80397100
C	2.39701000	3.31466800	0.06464200
H	3.11836900	3.74065800	0.76217500
H	2.77626500	3.37584400	-0.95985700
H	1.46413200	3.88747700	0.10256000
H	3.57929200	-2.10968300	-0.76931000
O	3.09719000	-1.45179400	1.08304500
H	2.95415000	-0.58382500	1.50507400
H	-2.14673700	-1.65118800	-0.95085100

E-Int-*si*, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1004.993075 a.u.

Thermal free energy correction in gas phase: 0.204432 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.788643 a.u.

Gibbs free energy in gas phase at 298K: -1004.770387 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1004.890987 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1004.686555 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM X Y Z

C	0.81431800	-0.06014600	-0.18241000
C	1.67557400	-1.12937300	-0.88002600
O	1.06183000	-2.42667800	-0.78491100
C	-0.26361600	-2.52575200	-1.06876800
C	-1.20393000	-1.50634300	-0.52719200
C	-0.61340700	-0.09650400	-0.70746500
O	1.33540900	1.25197100	-0.49934900
C	2.12054900	1.87498300	0.40789800
O	-1.37548700	0.87809700	0.02332700
C	-2.44231200	1.43378200	-0.62200000
C	3.08677200	-1.26347400	-0.29267500
O	2.53027000	1.35747800	1.42854000
H	0.82818800	-0.21265200	0.89793400
H	1.75491600	-0.86763100	-1.94631700
H	-0.58122300	-3.55940600	-1.15741700
H	-0.63682300	0.15985700	-1.77026800
H	3.68252800	-0.39670800	-0.61848900
N	-1.43431700	-1.77337100	0.94806900
N	-2.53825000	-1.41796200	1.37002300
N	-3.53758500	-1.14418100	1.85531600
C	-3.16381100	2.39605100	0.28619000
H	-2.45888500	3.08605100	0.75883400
H	-3.91100900	2.94618100	-0.28657100
H	-3.65763600	1.83129200	1.08532800
O	-2.75642800	1.15022800	-1.75534300
C	2.41352200	3.29100700	-0.01781300
H	3.12890100	3.73822000	0.67256100
H	2.81036600	3.30616000	-1.03752900
H	1.48638200	3.87402900	-0.01998500
H	3.53726900	-2.15713100	-0.73664600
O	3.10817700	-1.43212400	1.10380000
H	2.97688600	-0.55003900	1.49886900
H	-2.16090600	-1.56678500	-1.05711100

C-Reactant, B3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile: -1986.360252 a.u.

Thermal free energy correction in gas phase: 0.6005280 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1985.759724 a.u.

Gibbs free energy in gas phase at 298K: -1985.722157 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1985.996614 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -2149.527293 a.u.

Charge and Multiplicity: 0 1

Cartesian coordinates:

ATOM X Y Z

C	-1.55267500	-0.66485500	-0.40742900
C	-0.16247100	-0.98894800	-0.98189400
O	0.11770200	-2.39869500	-0.88919400
C	-0.90048100	-3.23065400	-1.23609500
C	-2.17225400	-2.86207400	-1.41687200
C	-2.63538100	-1.44950500	-1.16343100
O	-1.73632600	0.73792900	-0.53017100
C	-2.54204800	1.33837400	0.48555900
C	-2.71047400	2.81108000	0.19246400
C	-2.89244800	3.71406900	1.24641600
C	-3.10873600	5.06924900	0.99442100
C	-3.13440700	5.54101000	-0.31913400
C	-2.94438500	4.64779700	-1.37523100
C	-2.73765100	3.29118600	-1.12211600
O	-3.82266500	-1.41101000	-0.36005800
C	-5.02589900	-1.63686700	-1.08160800
C	-6.19689600	-1.62428200	-0.12650200
C	-6.08425300	-2.19372100	1.14802500
C	-7.18095600	-2.21830800	2.00917300
C	-8.40565400	-1.68133400	1.60538300
C	-8.52472800	-1.11210900	0.33697200
C	-7.42378600	-1.08014600	-0.52077300
C	3.07716500	2.58995300	-0.03247500
C	0.95808200	-0.25876000	-0.25767300
O	2.16869200	-0.43536600	-0.97809400
Si	3.71008000	-0.17748200	-0.36615300
C	3.70090100	1.47344800	0.56253600
C	4.25945200	1.65393300	1.84116500
C	3.02815700	3.82793400	0.60886000
C	3.60548800	3.98303800	1.87060400
C	4.21888200	2.89184200	2.48656400
C	4.15941400	-1.61590200	0.77772100
C	5.35030000	-1.65894000	1.53021600
C	5.66473900	-2.75403400	2.33663200
C	4.79160700	-3.84079300	2.40958400
C	3.61083200	-3.82636800	1.66648000
C	3.30100800	-2.72973400	0.85888000
C	4.82894000	-0.16007800	-1.92382900
C	4.70340200	-1.52482300	-2.63651200
C	4.38131100	0.95351300	-2.89406100
C	6.30087300	0.07813200	-1.52739800
H	-1.58447700	-0.97088900	0.64905900
H	-0.13865300	-0.70940600	-2.04477800
H	-0.54663300	-4.25088000	-1.35129200

H	-2.89773500	-3.61278700	-1.71221800
H	-2.83667800	-0.91372400	-2.10581500
H	-2.06552600	1.20255800	1.46959400
H	-3.51702800	0.83633900	0.52441900
H	-2.86268000	3.35480400	2.27312200
H	-3.24761700	5.75702800	1.82458400
H	-3.29633800	6.59719900	-0.51779700
H	-2.95704800	5.00781800	-2.40097100
H	-2.58194700	2.59667800	-1.94107300
H	-4.98026500	-2.60776300	-1.60277400
H	-5.15647600	-0.86502400	-1.85731900
H	-5.12867400	-2.60227500	1.46127200
H	-7.07962200	-2.65810700	2.99809100
H	-9.25957900	-1.70193700	2.27733500
H	-9.47096800	-0.68367200	0.01706200
H	-7.51912200	-0.62436300	-1.50411900
H	2.61200700	2.48989000	-1.00994000
H	1.03672400	-0.65663900	0.76412900
H	0.69886000	0.80285700	-0.19711600
H	4.72131400	0.81495200	2.35333000
H	2.53614300	4.66875300	0.12654500
H	3.56996100	4.94629800	2.37320200
H	4.66050600	3.00088300	3.47410100
H	6.05333100	-0.83027800	1.48759700
H	6.59109900	-2.75903800	2.90577800
H	5.03317700	-4.69438100	3.03798500
H	2.92886100	-4.67203900	1.71255800
H	2.38341300	-2.74470000	0.27729400
H	3.66924300	-1.72833000	-2.93550900
H	5.03668900	-2.35085900	-1.99784500
H	5.32435700	-1.53606600	-3.54430400
H	3.33463000	0.83092200	-3.19425500
H	4.99548000	0.92638300	-3.80604500
H	4.49595600	1.95066600	-2.45370700
H	6.93503200	0.10437800	-2.42528200
H	6.68494100	-0.72050300	-0.88209900
H	6.43517000	1.03321100	-1.00424200

C-Ts-*re*, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-2150.498413 a.u.

Thermal free energy correction in gas phase: 0.607097 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -2149.891316 a.u.

Gibbs free energy in gas phase at 298K: -2149.853340 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -2150.117057 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -2149.50996 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	1.19066300	-0.02278900	-0.07073700
C	-0.13686100	-0.45546100	0.57230900
O	-0.29377000	-1.89071300	0.42078200
C	0.77618500	-2.64225900	0.70600300
C	2.00585900	-2.11528700	1.09351500
C	2.37623100	-0.70303100	0.63885400
O	1.22451200	1.39091800	-0.00241600
C	2.19164100	2.05888800	-0.81708700
C	3.40103500	2.54444500	-0.04085700
C	4.62710900	2.71835500	-0.69326700
C	5.73213000	3.22492100	-0.00695800
C	5.62567700	3.55567600	1.34564400
C	4.40684300	3.37998400	2.00420600
C	3.29997600	2.88262300	1.31397400
O	3.44659200	-0.75294800	-0.30005800
C	4.74302300	-0.84492900	0.29298800
C	5.77535400	-1.06235900	-0.78803600
C	5.50728700	-1.89719900	-1.88003000
C	6.48405000	-2.13028500	-2.84790500
C	7.74406700	-1.53852300	-2.73284600
C	8.01800400	-0.70491600	-1.64774200
C	7.03609200	-0.46423700	-0.68503000
C	-3.70919800	2.90220100	0.26992900
C	-1.35850100	0.19101100	-0.05957900
O	-2.50466400	-0.17072100	0.69111400
Si	-4.09588400	0.06628400	0.20160400
C	-4.23406200	1.82823100	-0.47938800
C	-4.80398800	2.13346200	-1.72904900
C	-3.76608200	4.21552300	-0.19738700
C	-4.35195900	4.49167000	-1.43436600
C	-4.86803600	3.44649100	-2.20067900
C	-4.51146200	-1.22176000	-1.11943100
C	-5.72212200	-1.22663600	-1.84080300
C	-6.00791800	-2.21992400	-2.77912100
C	-5.08622800	-3.24055800	-3.01872200
C	-3.88441700	-3.26379500	-2.31025200
C	-3.60367300	-2.26884700	-1.37134600
C	-5.12145200	-0.23582200	1.79153600
C	-4.84755300	-1.67458300	2.28362800

C	-4.71499300	0.75635700	2.90168200
C	-6.62801900	-0.07400300	1.49774700
H	1.19679500	-0.35533100	-1.12124400
H	-0.12102000	-0.24342100	1.64767000
H	0.54604600	-3.70248000	0.70700500
H	2.82436000	-2.82781100	1.12273700
H	2.65752100	-0.10008400	1.50972400
H	1.66359400	2.92051000	-1.24750500
H	2.50804000	1.41267600	-1.64385900
H	4.72314200	2.44626600	-1.74203500
H	6.67766000	3.35145100	-0.52779100
H	6.48631700	3.94546700	1.88268600
H	4.31556800	3.63217300	3.05751000
H	2.35167100	2.74487000	1.82426300
H	4.76868200	-1.68251200	1.00886200
H	4.96085600	0.07156500	0.85795000
H	4.52476500	-2.34957200	-1.97262800
H	6.26187600	-2.77654300	-3.69326400
H	8.50518500	-1.72293800	-3.48637900
H	8.99312000	-0.23404400	-1.55371100
H	7.24746400	0.19890100	0.15049600
H	-3.23954100	2.71147400	1.23174000
H	-1.43904300	-0.14308200	-1.10431200
H	-1.21454100	1.27585600	-0.05766800
H	-5.19311300	1.33581800	-2.35493700
H	-3.35188200	5.02221100	0.40224300
H	-4.39926100	5.51401600	-1.80072000
H	-5.31591400	3.65104900	-3.16998900
H	-6.46253300	-0.44862300	-1.66954000
H	-6.95037700	-2.19790200	-3.32059700
H	-5.30633900	-4.01481300	-3.74928700
H	-3.16513000	-4.06013500	-2.48553000
H	-2.66991500	-2.31317400	-0.81744200
H	-3.78734800	-1.82589800	2.51395700
H	-5.14084000	-2.42374200	1.53927800
H	-5.42182500	-1.87487300	3.19977600
H	-3.64606000	0.68945900	3.13361800
H	-5.26975600	0.53378000	3.82464000
H	-4.94266500	1.79286900	2.62793000
H	-7.21044400	-0.23965600	2.41538900
H	-6.98103200	-0.79866400	0.75481400
H	-6.87104400	0.93240500	1.13431000
N	1.92542400	-1.78676200	3.03113000
N	1.79494000	-2.84251500	3.62202000

N	1.67102900	-3.84552800	4.19051100

C-Int-*re*, UB3LYP/6-31G(d)
Total SCF energy in solvent acetonitrile:-2150.502556 a.u.
Thermal free energy correction in gas phase: 0.608249 a.u.
Gibbs free energy in solvent acetonitrile at 298K: -2149.894307 a.u.
Gibbs free energy in gas phase at 298K: -2149.859937 a.u.
UX3LYP/6-311+G(d,p)
Total SCF energy in solvent acetonitrile: -2150.119883 a.u.
Gibbs free energy in solvent acetonitrile at 298K: -2149.511634 a.u.
Charge and Multiplicity: 0 2
Cartesian coordinates:

ATOM	X	Y	Z
C	1.20732300	0.04030600	0.04538500
C	-0.12972100	-0.38688900	0.67500700
O	-0.28889900	-1.81127900	0.50436700
C	0.81024600	-2.57746300	0.72546900
C	2.00335900	-2.00369600	1.37445700
C	2.39657900	-0.62771200	0.76595900
O	1.25221900	1.45667300	0.08497200
C	2.21012700	2.09661700	-0.76040800
C	3.44755500	2.57231300	-0.02217900
C	4.66455800	2.69865300	-0.70189200
C	5.79521700	3.19441600	-0.04991700
C	5.72345200	3.56232300	1.29535100
C	4.51368300	3.43428000	1.98122800
C	3.38176900	2.94742300	1.32524400
O	3.42639400	-0.76656600	-0.20255900
C	4.74298000	-0.86094400	0.33939700
C	5.72470300	-1.13992900	-0.77444900
C	5.39223600	-2.00545000	-1.82407300
C	6.32108000	-2.29261100	-2.82405900
C	7.59670900	-1.72491100	-2.78367600
C	7.93451700	-0.86117200	-1.74094900
C	7.00061800	-0.56645300	-0.74601500
C	-3.74552200	2.93292400	0.05926500
C	-1.33414200	0.27839800	0.02706100
O	-2.50060700	-0.06114600	0.76061600
Si	-4.07267800	0.09163100	0.18942800
C	-4.22659200	1.79644100	-0.62435600
C	-4.76633700	1.99855300	-1.90784100
C	-3.81664800	4.20792500	-0.50257500
C	-4.37300900	4.38168800	-1.77139600
C	-4.84476900	3.27287100	-2.47424200

C	-4.41035700	-1.29748500	-1.04925700
C	-5.60205200	-1.38543000	-1.79651200
C	-5.83610400	-2.44503400	-2.67441400
C	-4.87918700	-3.45016000	-2.82566700
C	-3.69489000	-3.39025400	-2.09035500
C	-3.46536300	-2.32915400	-1.21160100
C	-5.15922100	-0.11110200	1.75457900
C	-4.86991300	-1.49416600	2.38044900
C	-4.82848100	0.98389200	2.79083200
C	-6.65582700	-0.02161100	1.38830800
H	1.21941400	-0.31185700	-0.99800300
H	-0.12982900	-0.16658300	1.74995300
H	0.58680600	-3.63817100	0.71763700
H	2.84039000	-2.70143100	1.26466000
H	2.72138900	0.02677000	1.58425300
H	1.68756100	2.96193500	-1.19026600
H	2.49518500	1.43451400	-1.58648400
H	4.73283800	2.39812800	-1.74506500
H	6.73310000	3.28435500	-0.59182600
H	6.60377900	3.94417500	1.80555500
H	4.44933600	3.71643000	3.02897400
H	2.44003500	2.84673300	1.85620800
H	4.78509500	-1.67191100	1.08547800
H	5.00175000	0.07241600	0.85807600
H	4.39709300	-2.43793500	-1.85868300
H	6.04890400	-2.96183400	-3.63625400
H	8.32035800	-1.95095000	-3.56237100
H	8.92210200	-0.40853300	-1.70556700
H	7.26171400	0.12043800	0.05568800
H	-3.29840900	2.82151400	1.04403400
H	-1.40271100	-0.05628300	-1.01800500
H	-1.17775800	1.36138600	0.03025800
H	-5.11871400	1.14912200	-2.48556700
H	-3.43642100	5.06471100	0.04818600
H	-4.43133000	5.37399700	-2.21147400
H	-5.26867500	3.39739500	-3.46765200
H	-6.36829900	-0.62064400	-1.69306800
H	-6.76513700	-2.48665200	-3.23761000
H	-5.05829400	-4.27642900	-3.50904100
H	-2.94785600	-4.17298900	-2.19798100
H	-2.54262400	-2.30738300	-0.63850100
H	-3.81971100	-1.59074900	2.67647400
H	-5.10066500	-2.31227500	1.68836000
H	-5.48712000	-1.63591700	3.27954300

H	-3.76716500	0.97600900	3.06365800
H	-5.40953200	0.81894200	3.70981000
H	-5.08009400	1.98461000	2.42161100
H	-7.27153800	-0.12275000	2.29367800
H	-6.95757300	-0.82016500	0.70079700
H	-6.91046800	0.94041300	0.92599500
N	1.82391300	-1.73187400	2.88384900
N	1.56827900	-2.72905800	3.56314000
N	1.32727100	-3.60067000	4.26450400

C-Ts-*si*, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-2150.500601 a.u.

Thermal free energy correction in gas phase: 0.605053 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -2149.895548 a.u.

Gibbs free energy in gas phase at 298K: -2149.854328 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -2150.120832 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -2149.515779 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	1.37158600	-0.48645600	0.38626100
C	0.01279800	-0.79106600	1.04240100
O	-0.22585200	-2.21354300	1.22575100
C	0.81027300	-3.03000500	1.44645200
C	2.14180100	-2.70478900	1.20922300
C	2.49669700	-1.22819500	1.11959500
O	1.54094400	0.91737700	0.48323600
C	2.17029300	1.52593300	-0.66086100
C	2.39279700	2.98518100	-0.36006600
C	3.63454200	3.42734100	0.11067300
C	3.84293000	4.77468700	0.40854600
C	2.80660200	5.69489900	0.24106400
C	1.56291700	5.26245500	-0.22498500
C	1.35861300	3.91527100	-0.52336900
O	3.70589500	-0.94437000	0.45195000
C	4.89162100	-1.25901200	1.17571000
C	6.08376000	-0.93768900	0.30789800
C	6.14538200	-1.43253200	-1.00227200
C	7.25290300	-1.16168100	-1.80371500
C	8.31327500	-0.39913000	-1.30523400
C	8.25721000	0.09643800	-0.00275400
C	7.14332400	-0.16864600	0.79780400
C	-3.08700400	2.74079100	0.01827300

C	-1.15244900	-0.24761900	0.23282600
O	-2.33687000	-0.32370700	1.00743800
Si	-3.87608200	0.02129100	0.42090700
C	-3.75963500	1.64086300	-0.55475000
C	-4.27362100	1.80649200	-1.85390100
C	-2.95101100	3.95040700	-0.66445200
C	-3.48524700	4.09200200	-1.94710200
C	-4.14417200	3.01558400	-2.54126200
C	-4.43060500	-1.41843800	-0.67095900
C	-5.61343500	-1.39952900	-1.43654700
C	-6.00434900	-2.50064000	-2.20024600
C	-5.21920800	-3.65482800	-2.21522100
C	-4.04861600	-3.70252600	-1.45736200
C	-3.66279400	-2.59914400	-0.69345000
C	-4.96296900	0.14493200	1.99409200
C	-4.89474500	-1.20453100	2.74323600
C	-4.44996200	1.26078600	2.92877900
C	-6.42706900	0.44396000	1.60827200
H	1.36802000	-0.81919300	-0.66023700
H	-0.00695300	-0.33697900	2.04037900
H	0.48532500	-4.03704300	1.68734800
H	2.54828200	-0.82664000	2.14742300
H	1.51429300	1.40696800	-1.53682200
H	3.11843000	1.02176400	-0.86794500
H	4.44094800	2.70915000	0.23976700
H	4.81368100	5.10627400	0.76768000
H	2.96799100	6.74534100	0.46889100
H	0.75452900	5.97640500	-0.36085000
H	0.38900300	3.58205100	-0.88720700
H	4.89919000	-2.32793900	1.44103400
H	4.92686200	-0.68587800	2.11594500
H	5.31514300	-2.01906600	-1.38548500
H	7.29089700	-1.54738000	-2.81913200
H	9.17694500	-0.19115300	-1.93132800
H	9.07513600	0.69466300	0.39012100
H	7.09926900	0.22544600	1.81090700
H	-2.65338600	2.65138400	1.01109800
H	-1.24275800	-0.82996400	-0.69514200
H	-0.92451200	0.79136300	-0.02913700
H	-4.77059100	0.97727500	-2.34874200
H	-2.43023500	4.78114800	-0.19452200
H	-3.38290900	5.03311600	-2.48134100
H	-4.55287800	3.11334300	-3.54387100
H	-6.24870600	-0.51667700	-1.43805100

H	-6.92197500	-2.45773700	-2.78164800
H	-5.52072600	-4.51265800	-2.81080000
H	-3.43517200	-4.60003100	-1.45879400
H	-2.75595600	-2.66032200	-0.09757700
H	-3.86861100	-1.44720800	3.04077500
H	-5.27163900	-2.03156900	2.13076800
H	-5.50753300	-1.16110400	3.65539500
H	-3.40498000	1.09935400	3.21679600
H	-5.04956500	1.28283700	3.85032400
H	-4.52849000	2.25131100	2.46635100
H	-7.04708000	0.52346300	2.51271400
H	-6.85796100	-0.35065100	0.98815200
H	-6.52278900	1.39136400	1.06302200
N	2.46872500	-3.23799300	-0.68672900
N	2.47142700	-4.45201400	-0.73670900
N	2.47459200	-5.61210300	-0.79136700
H	2.87586700	-3.38359800	1.63210300

C-Int-*si*, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-2150.508408 a.u.

Thermal free energy correction in gas phase: 0.610986 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -2149.897422 a.u.

Gibbs free energy in gas phase at 298K: -2149.861186 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -2150.12625 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -2149.515264a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	-1.29992400	-0.77093900	-0.26219800
C	0.07458600	-1.01313700	-0.91452400
O	0.41282500	-2.41631400	-0.91605200
C	-0.53858000	-3.29900300	-1.32303400
C	-1.94678900	-3.12129300	-0.86982300
C	-2.35345700	-1.64025300	-0.95853700
O	-1.62127000	0.60698900	-0.40862300
C	-2.17043600	1.21400300	0.77421600
C	-2.47665000	2.66056800	0.48064400
C	-1.43630800	3.57995300	0.28842700
C	-1.71481100	4.91688800	0.01033700
C	-3.03952700	5.35445600	-0.07408000
C	-4.08139800	4.44748000	0.11956400
C	-3.79973600	3.10686800	0.39284100
O	-3.63398200	-1.45137500	-0.37599000

C	-4.56303300	-0.75393400	-1.20725000
C	-5.86742500	-0.55449500	-0.47096900
C	-6.33034900	-1.48959200	0.46259400
C	-7.56110600	-1.30308000	1.09348500
C	-8.34709400	-0.18824300	0.79513200
C	-7.89219900	0.74669400	-0.13596400
C	-6.65703900	0.56564900	-0.76045100
C	3.07274800	2.78061700	-0.14563300
C	1.19954700	-0.28270800	-0.20152700
O	2.37271300	-0.33747900	-0.99740300
Si	3.91034400	0.06195700	-0.45161400
C	3.77619100	1.71818900	0.46058000
C	4.30834000	1.94778100	1.74221200
C	2.92562300	4.01528200	0.48811000
C	3.47782600	4.22028500	1.75451300
C	4.16660600	3.18193700	2.38126000
C	4.52165400	-1.31520100	0.69030000
C	5.72122600	-1.23216500	1.42549800
C	6.15804800	-2.28696100	2.22858800
C	5.40284500	-3.45789000	2.31484100
C	4.21620600	-3.56829900	1.58919500
C	3.78363800	-2.51156100	0.78507400
C	4.97030000	0.14955600	-2.04635400
C	4.91975900	-1.22885400	-2.74228200
C	4.41776300	1.21691100	-3.01446900
C	6.43285300	0.49520600	-1.69612600
H	-1.25744700	-1.05184000	0.79850400
H	0.03684400	-0.66971900	-1.95729800
H	-0.13202400	-4.29703100	-1.45191900
H	-2.61431700	-3.72931200	-1.49268800
H	-2.37539800	-1.36191500	-2.02182200
H	-1.43559700	1.13483500	1.59061700
H	-3.07584300	0.67857500	1.08140100
H	-0.40376200	3.24632400	0.36112300
H	-0.89935700	5.62083400	-0.13480800
H	-3.25634000	6.39821000	-0.28590400
H	-5.11398200	4.78140600	0.05961500
H	-4.61456100	2.40215500	0.54205900
H	-4.73414100	-1.33683800	-2.12871900
H	-4.14458700	0.21563800	-1.50731700
H	-5.72242000	-2.35557800	0.70282200
H	-7.90611700	-2.03367300	1.82044000
H	-9.30549000	-0.04704600	1.28768800
H	-8.49362900	1.62083400	-0.37165300

H	-6.30308700	1.30122500	-1.48003700
H	2.62597800	2.64120500	-1.12694000
H	1.35961600	-0.74884800	0.78098200
H	0.89034400	0.75692700	-0.04620100
H	4.83036500	1.14942100	2.26138700
H	2.38280400	4.81708000	-0.00673500
H	3.36605200	5.18086100	2.25087900
H	4.58982800	3.32907900	3.37179500
H	6.33352500	-0.33480400	1.37156400
H	7.08759900	-2.19509000	2.78490200
H	5.74003300	-4.28004800	2.94099600
H	3.62556300	-4.47921300	1.64684000
H	2.86366500	-2.62274500	0.21743500
H	3.89409100	-1.50565300	-3.00987700
H	5.32677800	-2.02309700	-2.10618100
H	5.51459400	-1.20684400	-3.66709800
H	3.37268000	1.02081400	-3.27981900
H	5.00292200	1.21728700	-3.94560300
H	4.48047000	2.22586800	-2.59107300
H	7.03713300	0.55542900	-2.61264500
H	6.89122400	-0.26616100	-1.05442900
H	6.51468500	1.46367900	-1.18678700
N	-2.07211500	-3.58861200	0.56929100
N	-3.17681600	-4.04797900	0.86908000
N	-4.14895400	-4.52033500	1.24398600

P-Reactant, B3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile: -1075.03455888 a.u.

Thermal free energy correction in gas phase: 0.301528 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1074.733031 a.u.

Gibbs free energy in gas phase at 298K: -1074.697487 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1074.847466 a.u.

Gibbs free energy in solvent acetonitrile -1074.667199 a.u

Charge and Multiplicity: 0 1

Cartesian coordinates:

ATOM	X	Y	Z
C	-0.5357820	1.42911300	0.10992500
C	-1.4612820	2.62043800	-0.15818000
O	-0.8553720	3.85932300	0.22051300
C	0.4463320	3.97823100	-0.17932900
C	1.2044450	2.98609300	-0.66015800
C	0.7349320	1.54726200	-0.71951800
O	-1.2347340	0.23329200	-0.21455700

C	-2.4195810	0.10452900	0.55268700
C	-3.0854560	-1.21094500	0.21885400
C	-4.4772190	-1.33795500	0.27272000
C	-5.0788520	-2.56976800	0.01147200
C	-4.2960580	-3.68234100	-0.30067000
C	-2.9063290	-3.55773500	-0.35198600
C	-2.3016890	-2.32789400	-0.09213500
O	1.6990580	0.65291600	-0.16560400
C	-2.7524520	2.43193400	0.63498600
O	-3.3193990	1.16924900	0.30171400
H	-0.2505690	1.42483800	1.17465300
H	-1.6918710	2.65107000	-1.23235100
H	0.7957630	4.99920100	-0.06102400
H	2.2228540	3.21158100	-0.95893400
H	0.5085910	1.23448200	-1.75159000
H	-2.1366710	0.14233400	1.62280900
H	-5.0825730	-0.46973400	0.50903400
H	-6.1614490	-2.65843300	0.05013400
H	-4.7661310	-4.64116300	-0.50335300
H	-2.2902530	-4.41902900	-0.59676600
H	-1.2227460	-2.22435200	-0.13845300
H	-3.4951000	3.19346100	0.38499400
H	-2.5317890	2.49327300	1.71288000
C	2.7060440	0.24709900	-1.07906300
H	3.1975270	1.12960700	-1.52419300
H	2.2590240	-0.31999600	-1.91183700
C	3.7352290	-0.59826600	-0.36362700
C	4.0527040	-0.36053600	0.97864500
C	4.4193340	-1.60385800	-1.05552900
C	5.0383880	-1.11550300	1.61478900
H	3.5114580	0.40838000	1.52002900
C	5.4117360	-2.35362800	-0.42265200
H	4.1720970	-1.80530400	-2.09594300
C	5.7237240	-2.11156300	0.91609000
H	5.2714970	-0.92540700	2.65940100
H	5.9333220	-3.13254100	-0.97281100
H	6.4915820	-2.69875000	1.41285900

P-Ts-re, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1239.174722 a.u.

Thermal free energy correction in gas phase: 0.314867 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.859855 a.u.

Gibbs free energy in gas phase at 298K: -1238.831055 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1238.970956 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.656089 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	0.49895800	0.84013300	-0.66849500
C	1.15171800	2.22020300	-0.78688900
O	0.28411300	3.12601200	-1.49823200
C	-1.00639000	3.08276400	-1.12329100
C	-1.49914600	2.23473900	-0.13150100
C	-0.77572100	0.91526200	0.16366200
O	1.42329700	-0.05365000	-0.06620400
C	2.62777900	-0.15322400	-0.81647900
C	3.55155100	-1.11545900	-0.11958700
C	3.95347000	-2.29359000	-0.75139000
C	4.80932600	-3.18495900	-0.10083600
C	5.26502100	-2.89801600	1.18581500
C	4.86381800	-1.71904600	1.82121900
C	4.01006500	-0.83019500	1.17192800
O	-1.59154200	-0.18885600	-0.19504300
C	-2.46774600	-0.62500000	0.84141300
C	-3.37856100	-1.70890100	0.31434000
C	-3.85371700	-1.67333200	-1.00199800
C	-4.73259700	-2.65388900	-1.46198400
C	-5.15370000	-3.67743400	-0.61030400
C	-4.68366600	-3.71894600	0.70304100
C	-3.79690000	-2.74258900	1.15930700
C	2.46299900	2.08489400	-1.55566800
O	3.27158800	1.10895600	-0.91010000
H	0.23144700	0.48852100	-1.67933500
H	1.33230800	2.63031600	0.21309100
H	-1.59572700	3.86094400	-1.59604300
H	-2.58155700	2.19272500	-0.05891500
H	-0.50721000	0.87137600	1.22587300
H	2.37887900	-0.50199900	-1.83463500
H	3.59680300	-2.51700400	-1.75415300
H	5.11792100	-4.09999800	-0.59892200
H	5.93128800	-3.58997700	1.69416100
H	5.21790700	-1.49381000	2.82360400
H	3.69463400	0.08790200	1.65719700
H	-3.06687200	0.22408300	1.21116900
H	-1.88117200	-0.99644700	1.69522200
H	-3.51730000	-0.88297500	-1.66539800
H	-5.08946200	-2.61871300	-2.48813500

H	-5.83911300	-4.44038200	-0.96966600
H	-4.99851200	-4.51636200	1.37098700
H	-3.42442100	-2.78668500	2.18056200
H	3.02969100	3.01904500	-1.56194200
H	2.24823200	1.79488600	-2.59711700
N	-1.19226100	3.13277600	1.59900600
N	-1.84258700	4.16012800	1.65087900
N	-2.45897700	5.14057800	1.70657400

P-Int-re, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1239.182521 a.u.

Thermal free energy correction in gas phase: 0.316846 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.865675 a.u.

Gibbs free energy in gas phase at 298K: -1238.837688 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1238.967587 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.650741 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	0.49384600	0.80416400	-0.60290500
C	1.14603500	2.17860300	-0.78234600
O	0.25976700	3.06003000	-1.48519300
C	-1.04946600	2.97041300	-1.11501200
C	-1.43321700	2.27469500	0.13488000
C	-0.74580300	0.88242900	0.28457600
O	1.43833500	-0.08971700	-0.02775200
C	2.60756700	-0.21077800	-0.82924700
C	3.55155500	-1.17153400	-0.15627100
C	3.83094500	-2.41093500	-0.73488400
C	4.69676600	-3.30519500	-0.10171300
C	5.28654100	-2.95959800	1.11414500
C	5.00869400	-1.71915700	1.69610700
C	4.14372200	-0.82813200	1.06467300
O	-1.61257200	-0.16660100	-0.10761600
C	-2.48618700	-0.61853300	0.92169300
C	-3.45909800	-1.62828500	0.35856900
C	-3.94947800	-1.50477100	-0.94675800
C	-4.88429900	-2.41591800	-1.43840500
C	-5.34592100	-3.45662600	-0.62966100
C	-4.86059400	-3.58560700	0.67246100
C	-3.91853800	-2.67879600	1.16025600
C	2.42472800	2.01222600	-1.60059400
O	3.25596000	1.04195000	-0.97337500

H	0.17928700	0.44017200	-1.59524900
H	1.38111200	2.60658100	0.19993400
H	-1.66373200	3.73251500	-1.58060700
H	-2.51958900	2.13566600	0.14333700
H	-0.43447300	0.76225500	1.33029500
H	2.30983500	-0.57583300	-1.82865500
H	3.37083900	-2.67959700	-1.68296000
H	4.90980200	-4.26769400	-0.55881800
H	5.96191900	-3.65312900	1.60821300
H	5.46787900	-1.44761700	2.64291700
H	3.92504400	0.13844400	1.50699000
H	-3.03943500	0.23481300	1.35035000
H	-1.90120200	-1.06314400	1.74130200
H	-3.58066800	-0.70186000	-1.57700100
H	-5.25265200	-2.31323200	-2.45590900
H	-6.07462100	-4.16551800	-1.01374400
H	-5.20694800	-4.39750600	1.30654800
H	-3.53460700	-2.79123400	2.17202100
H	2.99814300	2.94093300	-1.65191000
H	2.16243600	1.70305700	-2.62530700
N	-1.05055400	3.04828400	1.41064300
N	-1.57788100	4.15807100	1.52396200
N	-2.01971700	5.19716800	1.70858800

P-Ts-si, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1239.173461 a.u.

Thermal free energy correction in gas phase: 0.318355 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.855106 a.u.

Gibbs free energy in gas phase at 298K: -1238.825544 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1238.975708 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.657353 a.u.

Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	0.53842600	-1.44921500	-0.01296100
C	1.34403800	-2.64451800	-0.53781000
O	0.62577800	-3.88974300	-0.45394900
C	-0.68638300	-3.83973000	-0.75108200
C	-1.45397300	-2.67747000	-0.71202700
C	-0.76642900	-1.32437100	-0.79858300
O	1.35883300	-0.29509900	-0.16938900
C	2.55880100	-0.40783300	0.59639500
C	3.35512000	0.85760900	0.41845900

C	4.05119600	1.09150800	-0.77290900
C	4.75619100	2.28085300	-0.94733800
C	4.76769100	3.24523600	0.06427000
C	4.07363000	3.01528600	1.25251200
C	3.36952800	1.82256200	1.42814900
O	-1.64014700	-0.32607100	-0.32947600
C	-1.42454300	0.97493200	-0.87632600
C	-2.56258100	1.89208100	-0.48804900
C	-3.80996000	1.39771000	-0.09305400
C	-4.84859600	2.27865000	0.21577000
C	-4.65721200	3.65781000	0.12540400
C	-3.41305700	4.15626300	-0.26727600
C	-2.37217100	3.27761700	-0.56540900
C	2.63819300	-2.75007900	0.26501200
O	3.33414900	-1.51142200	0.16149600
H	0.28619900	-1.59806700	1.04686000
H	1.58923100	-2.46637700	-1.59237800
H	-1.12320200	-4.82756100	-0.84153500
H	-2.44549100	-2.73681800	-1.15183100
H	-0.51831000	-1.12707600	-1.85692700
H	4.04295100	0.33445600	-1.55028800
H	5.29829100	2.45684000	-1.87261300
H	5.31856400	4.17181400	-0.07378500
H	4.08114100	3.76044800	2.04320500
H	2.82782400	1.64282100	2.35382500
H	-1.36304000	0.89717600	-1.97645100
H	-0.46676500	1.38099700	-0.52986400
H	-3.96253500	0.32732300	-0.00853200
H	-5.81011100	1.88092800	0.52989200
H	-5.46840300	4.34034300	0.36507500
H	-3.24975900	5.22896800	-0.33269600
H	-1.40113700	3.67182800	-0.85967200
H	3.30129600	-3.52255200	-0.13184500
H	2.40519900	-2.98749700	1.31481200
N	-2.05239400	-2.65864800	1.19440700
N	-3.24511700	-2.43251500	1.16588600
N	-4.38762400	-2.22581600	1.14591800
H	2.27763600	-0.55985500	1.65294000

P-Int-si, UB3LYP/6-31G(d)

Total SCF energy in solvent acetonitrile:-1239.182521 a.u.

Thermal free energy correction in gas phase: 0.319859 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.862662 a.u.

Gibbs free energy in gas phase at 298K: -1238.838049 a.u.

UX3LYP/6-311+G(d,p)

Total SCF energy in solvent acetonitrile: -1238.976771 a.u.

Gibbs free energy in solvent acetonitrile at 298K: -1238.656912 a.u.

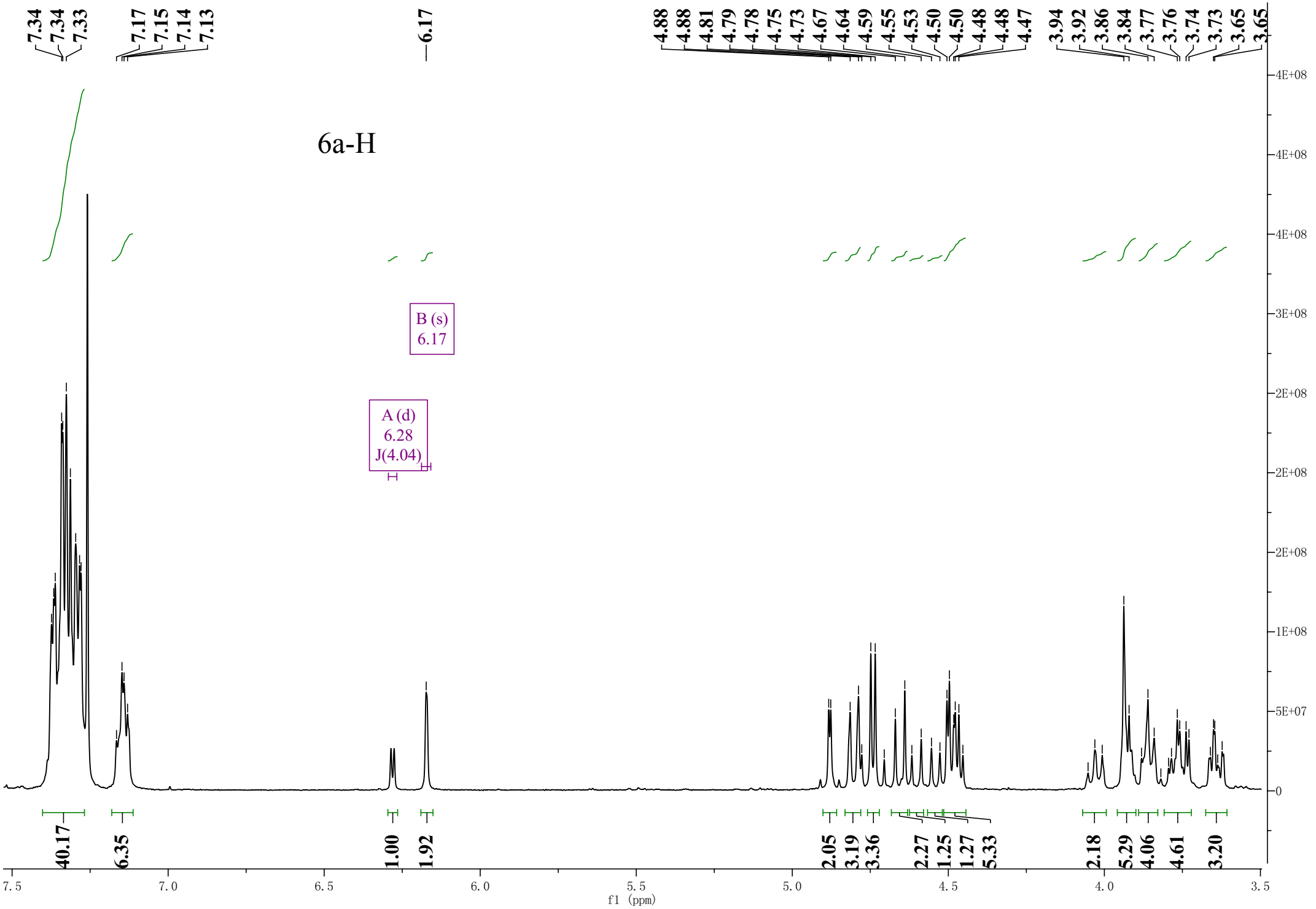
Charge and Multiplicity: 0 2

Cartesian coordinates:

ATOM	X	Y	Z
C	0.51762300	-1.47912200	0.03926200
C	1.32504300	-2.67821700	-0.47425700
O	0.61344200	-3.90996000	-0.32890300
C	-0.66017400	-3.89506000	-0.82195600
C	-1.54369700	-2.71691000	-0.56234900
C	-0.79474700	-1.37451700	-0.73354300
O	1.32027000	-0.31329200	-0.13362800
C	2.53422700	-0.40830200	0.61139700
C	3.31286400	0.86517700	0.40902000
C	3.99300900	1.09198500	-0.79288600
C	4.68186100	2.28719500	-0.99055100
C	4.69311600	3.26486900	0.00823500
C	4.01483700	3.04219600	1.20695300
C	3.32694100	1.84358000	1.40565900
O	-1.64624600	-0.34310600	-0.28653200
C	-1.42069400	0.93513800	-0.88427900
C	-2.51834300	1.89511100	-0.48540800
C	-3.78570000	1.44869000	-0.09687400
C	-4.78919700	2.36604100	0.22007700
C	-4.54241000	3.73741100	0.14325700
C	-3.27898600	4.18915600	-0.24357200
C	-2.27317400	3.27251100	-0.54891000
C	2.63540700	-2.75195900	0.30475700
O	3.31476700	-1.50507100	0.17520600
H	0.28370800	-1.61942000	1.10597600
H	1.54822100	-2.51660700	-1.53769100
H	-1.09331800	-4.88981400	-0.84436700
H	-2.39377400	-2.74260400	-1.25429500
H	-0.56558000	-1.24525500	-1.80400500
H	3.98528800	0.32431300	-1.55974000
H	5.21178000	2.45732500	-1.92398800
H	5.23160400	4.19591100	-0.14779700
H	4.02238200	3.79756200	1.98798200
H	2.79794500	1.66929300	2.33974100
H	-1.40418000	0.81801600	-1.98227100
H	-0.44098500	1.32548700	-0.58734600
H	-3.97954500	0.38424800	-0.02468600
H	-5.76657600	2.00468400	0.52928200

H	-5.32594100	4.44940300	0.38896300
H	-3.07278900	5.25500500	-0.29815500
H	-1.28663900	3.63015500	-0.83755300
H	3.30202700	-3.52024300	-0.09408700
H	2.42677800	-2.97900400	1.36216700
N	-2.06947500	-2.81717300	0.85487900
N	-3.22545500	-2.41299200	1.00804400
N	-4.29610600	-2.09614600	1.25337100
H	2.27214900	-0.55266800	1.67448200

9. Spectrum of the compounds


6a-H
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7.34
7.33
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7.13
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4.88
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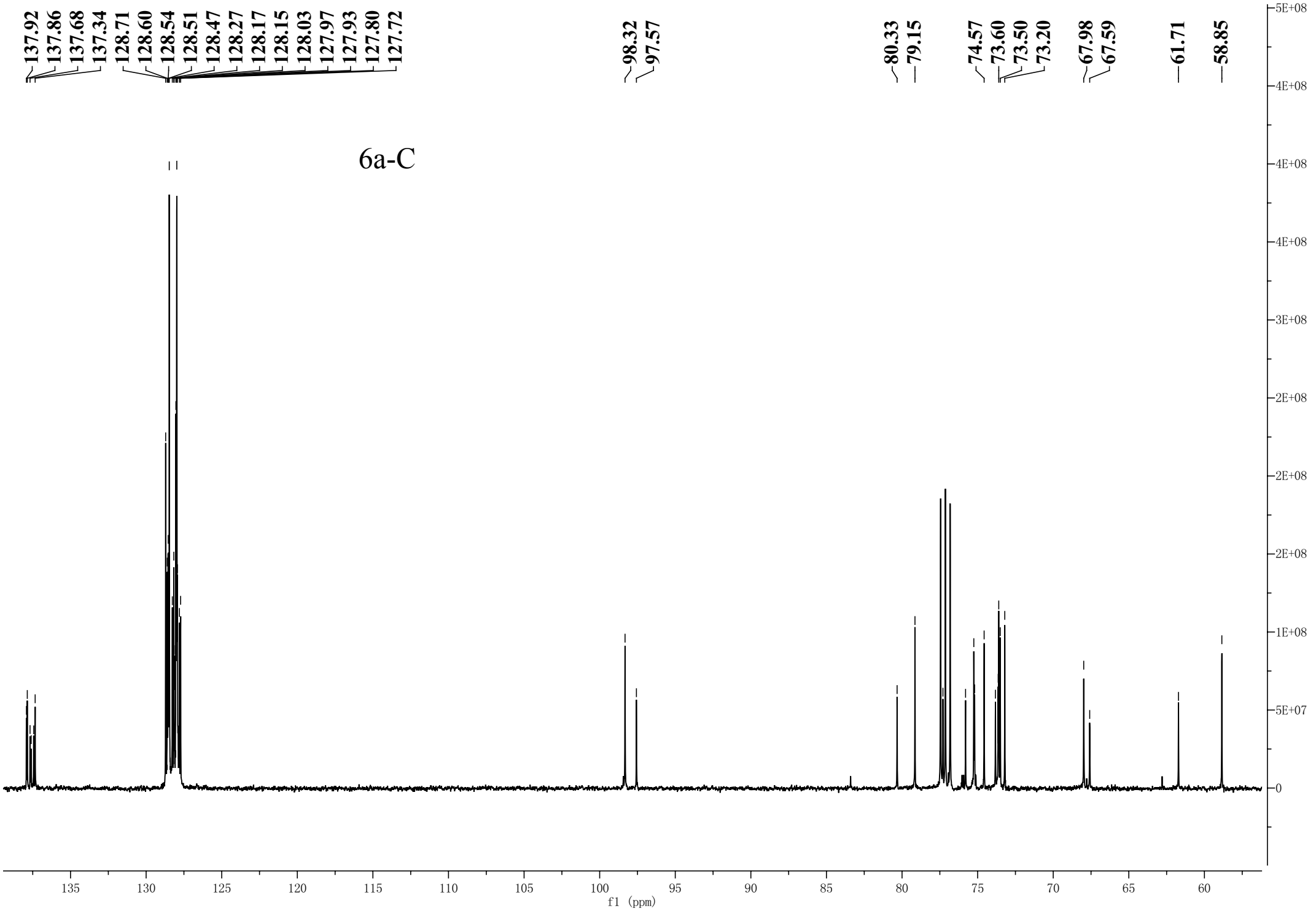
4.79
4.78
4.75
4.73
4.67
4.64
4.59
4.55
4.53
4.50
4.50
4.48
4.48
4.47
3.94
3.92
3.86
3.84
3.77
3.76
3.74
3.73
3.65
3.65
B (s)
6.17
A (d)
6.28
J(4.04)
40.17
6.35
1.00
1.92
2.05
3.19
3.36
2.27
1.25
1.27
5.33
2.18
5.29
4.06
4.61
3.20
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
f1 (ppm)
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0


137.92
137.86
137.68
137.34
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128.60
128.54
128.51
128.47
128.27
128.17
128.15
128.03
127.97
127.93
127.80
127.72
98.32
97.57
80.33
79.15
74.57
73.60
73.50
73.20
67.98
67.59
61.71
58.85
6a-C
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
135
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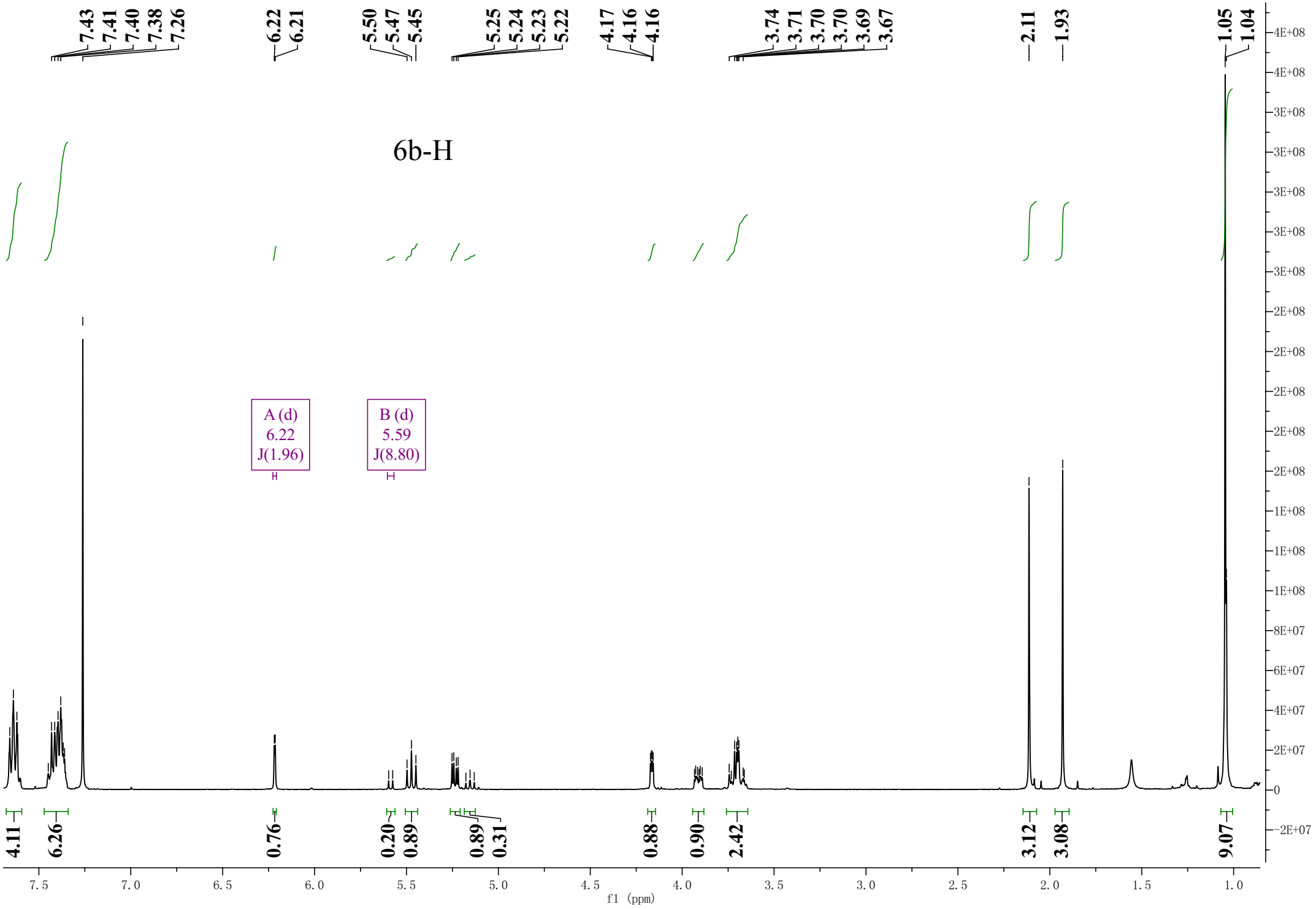
125
120
115
110
105
100
95
90
85
80
75
70
65
60
f1 (ppm)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6.22
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5.50
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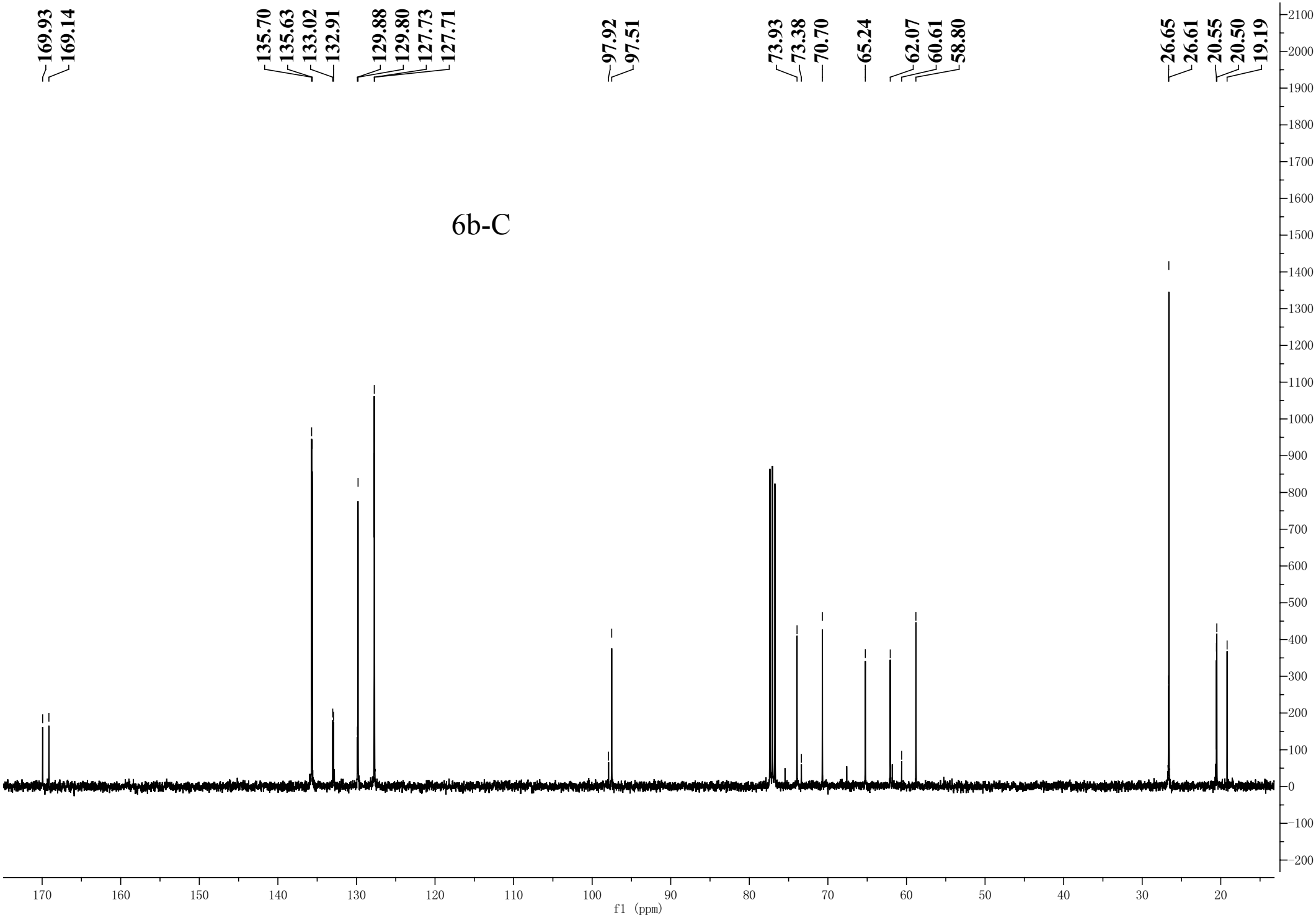
5.45
5.25
5.24
5.23
5.22
4.17
4.16
4.16
3.74
3.71
3.70
3.70
3.69
3.67
2.11
1.93
1.05
1.04
6b-H
A (d)
6.22
J(1.96)
B (d)
5.59
J(8.80)
4.11
6.26
0.76
0.20
0.89
0.89
0.31
0.88
0.90
2.42
3.12
3.08
9.07
f1 (ppm)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169.14
135.70
135.63
133.02
132.91
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129.80
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127.71
97.92
97.51
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73.38
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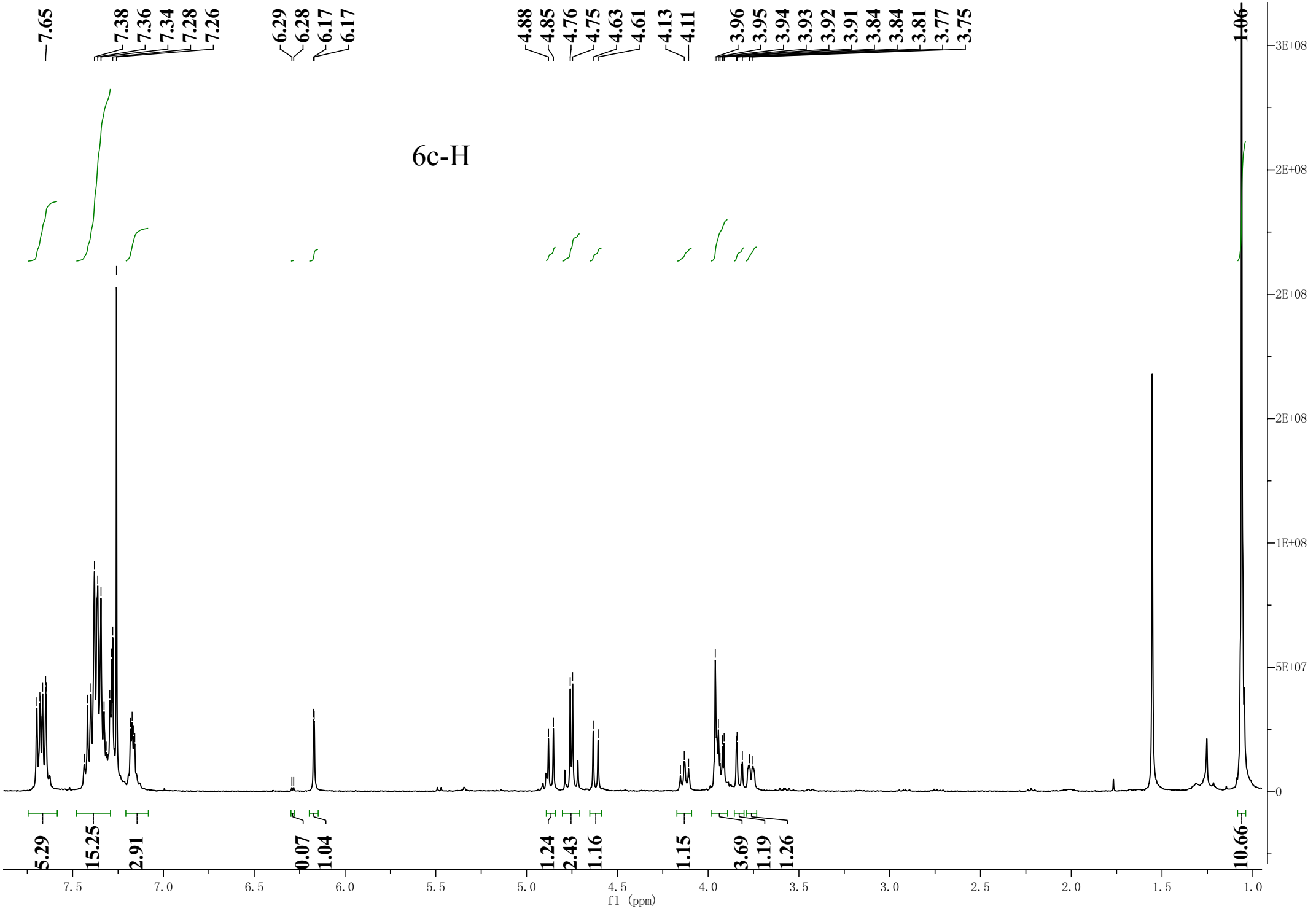
20.55
20.50
19.19
6b-C
f1 (ppm)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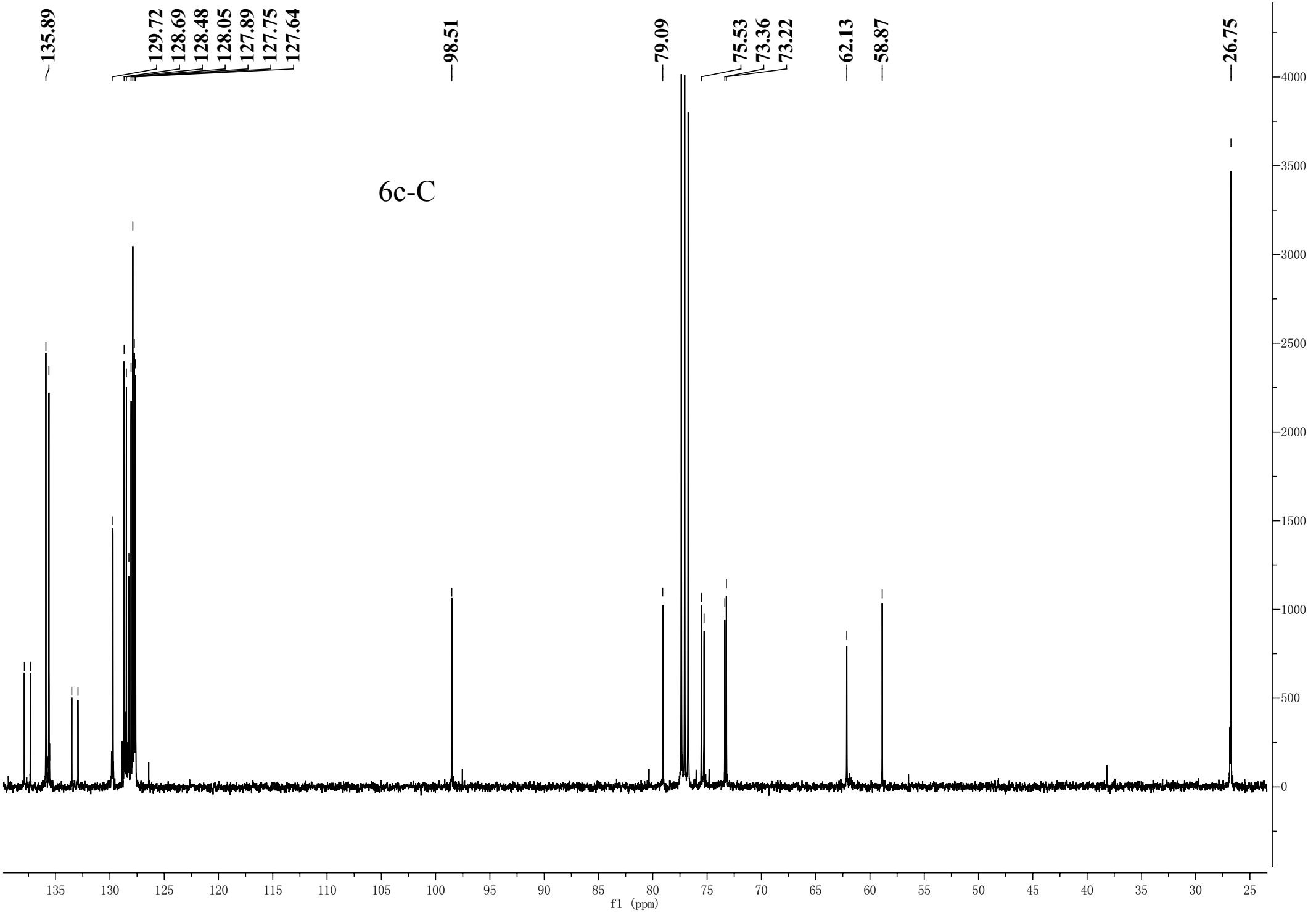
7.36
7.34
7.28
7.26
6.29
6.28
6.17
6.17
4.88
4.85
4.76
4.75
4.63
4.61
4.13
4.11
3.96
3.95
3.94
3.93
3.92
3.91
3.84
3.84
3.81
3.77
3.75
1.06
6c-H
5.29
15.25
2.91
0.07
1.04
1.24
2.43
1.16
1.15
3.69
1.19
1.26
10.66
f1 (ppm)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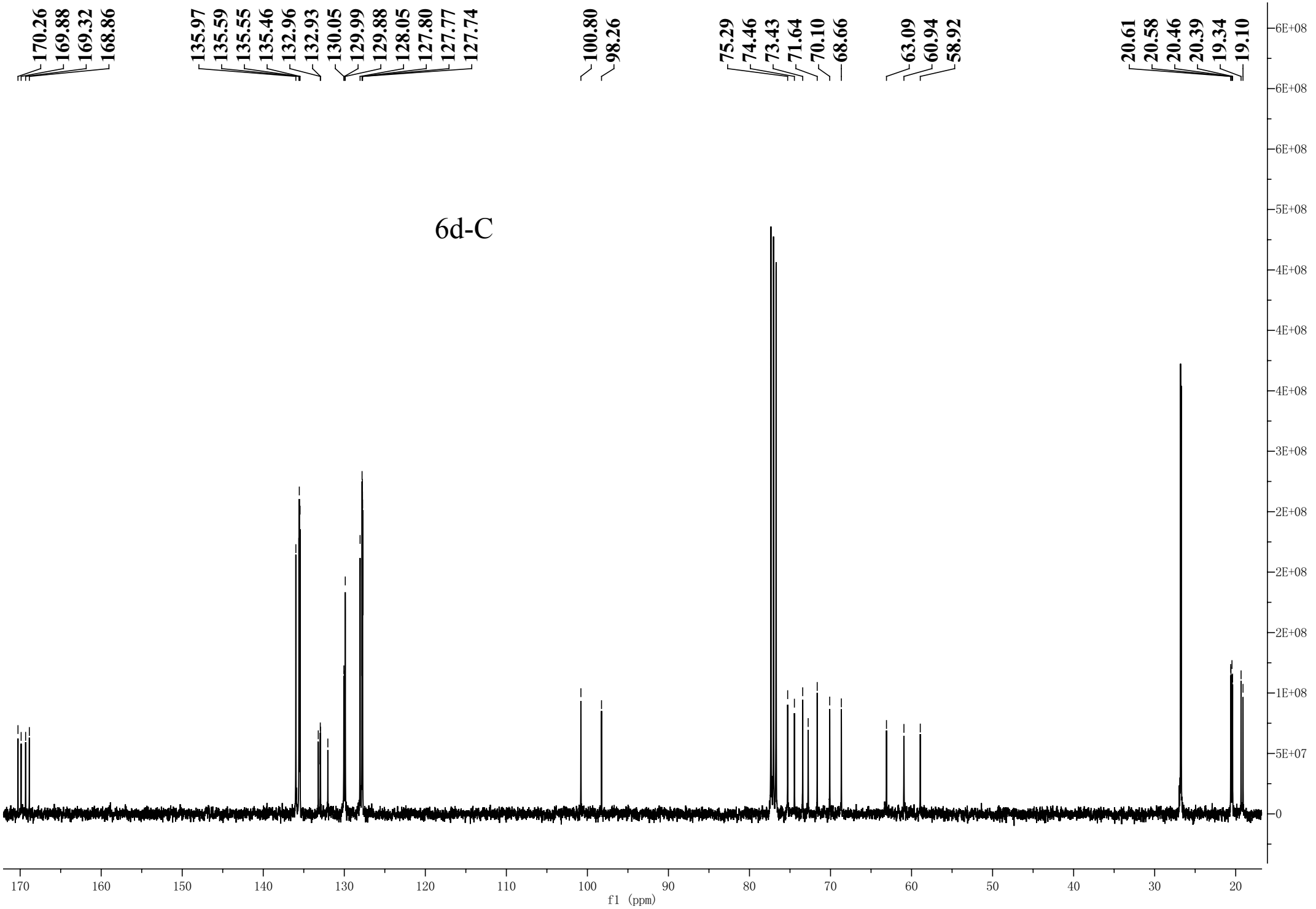
128.69
128.48
128.05
127.89
127.75
127.64
98.51
79.09
75.53
73.36
73.22
62.13
58.87
26.75
6c-C
4000
3500
3000
2500
2000
1500
1000
500
0
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
f1 (ppm)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169.32
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135.59
135.55
135.46
132.96
132.93
130.05
129.99
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128.05
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127.77
127.74
100.80
98.26
75.29
74.46
73.43
71.64
70.10
68.66
63.09
60.94
58.92
20.61
20.58
20.46
20.39
19.34
19.10
6d-C
6E+08
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
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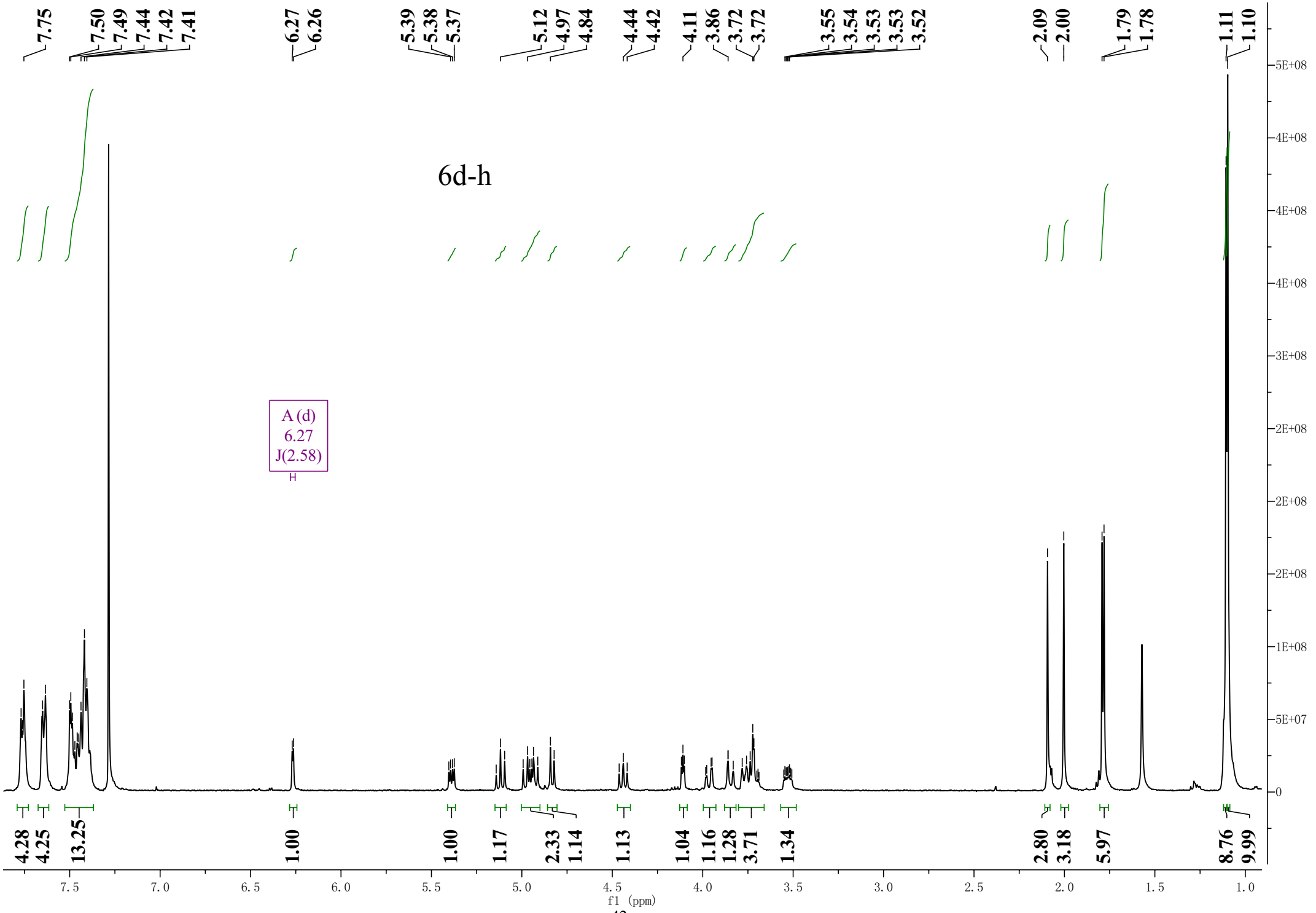
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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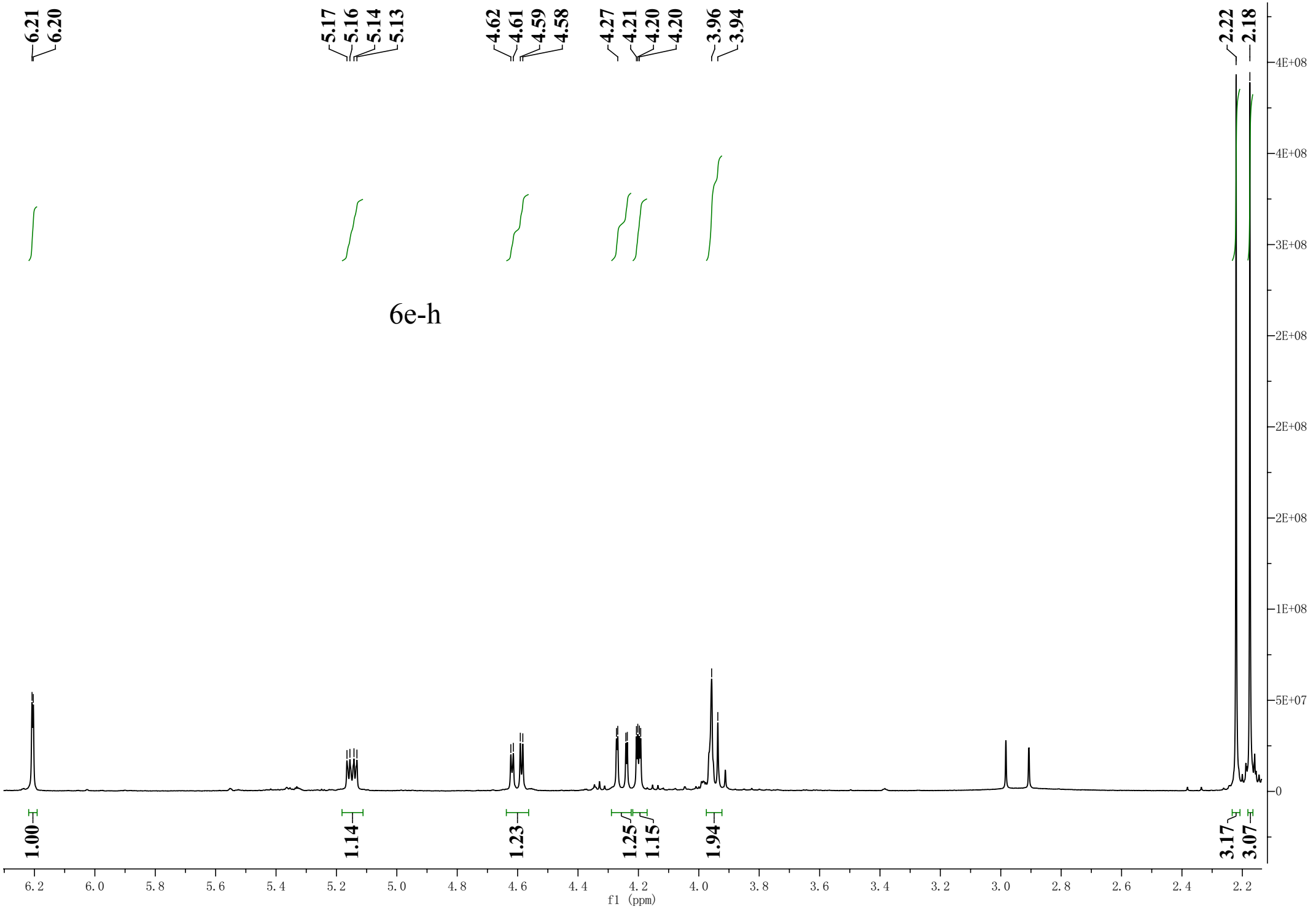
7.49
7.44
7.42
7.41
6.27
6.26
5.39
5.38
5.37
5.12
4.97
4.84
4.44
4.42
4.11
3.86
3.72
3.72
3.55
3.54
3.53
3.53
3.52
2.09
2.00
1.79
1.78
1.11
1.10
6d-h
A (d)
6.27
J(2.58)
H
4.28
4.25
13.25
1.00
1.00
1.17
2.33
1.14
1.13
1.04
1.16
1.28
3.71
1.34
2.80
3.18
5.97
8.76
9.99
f1 (ppm)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5.13
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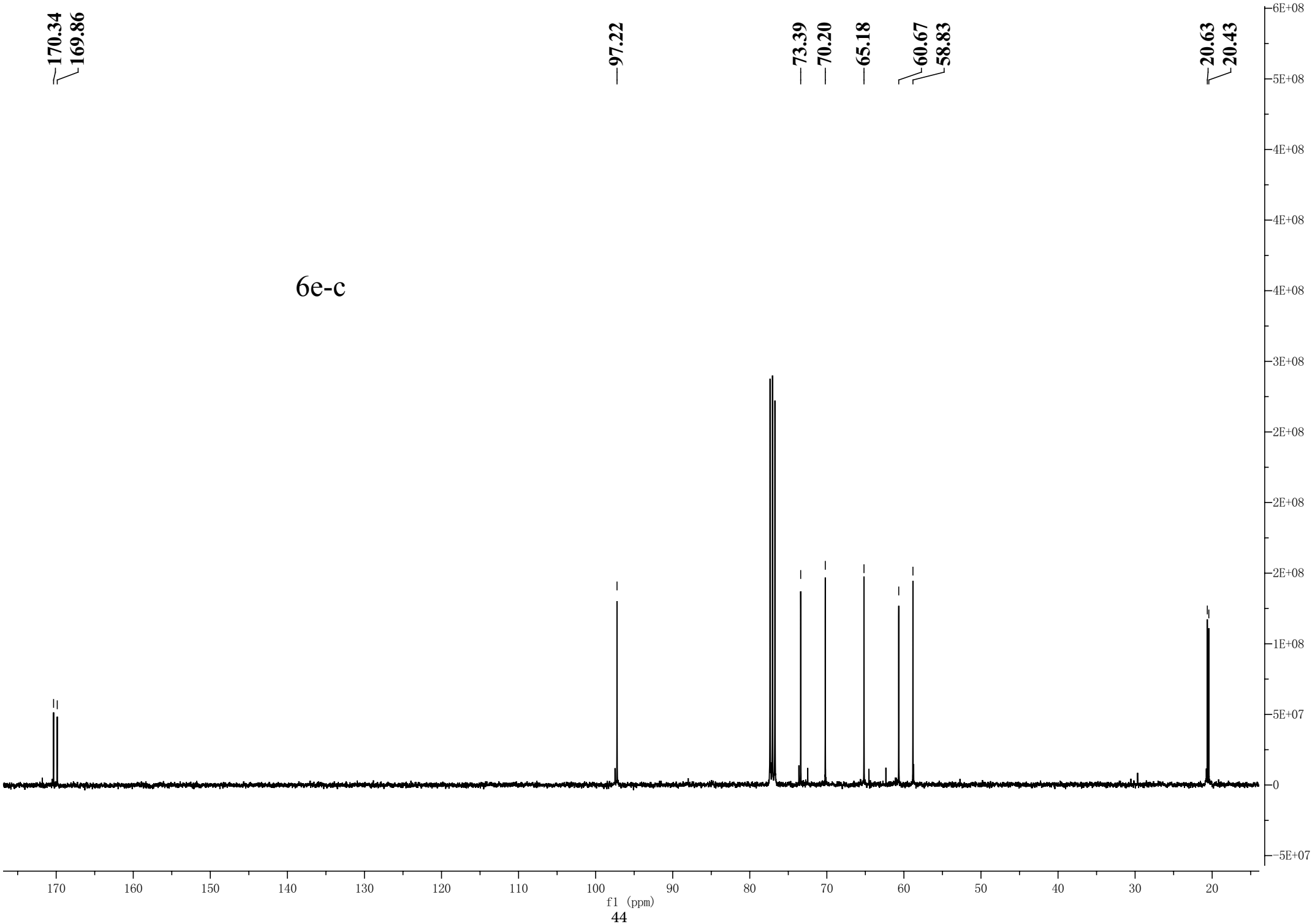
4.61
4.59
4.58
4.27
4.21
4.20
4.20
3.96
3.94
2.22
2.18
6e-h
1.00
1.14
1.23
1.25
1.15
1.94
3.17
3.07
f1 (ppm)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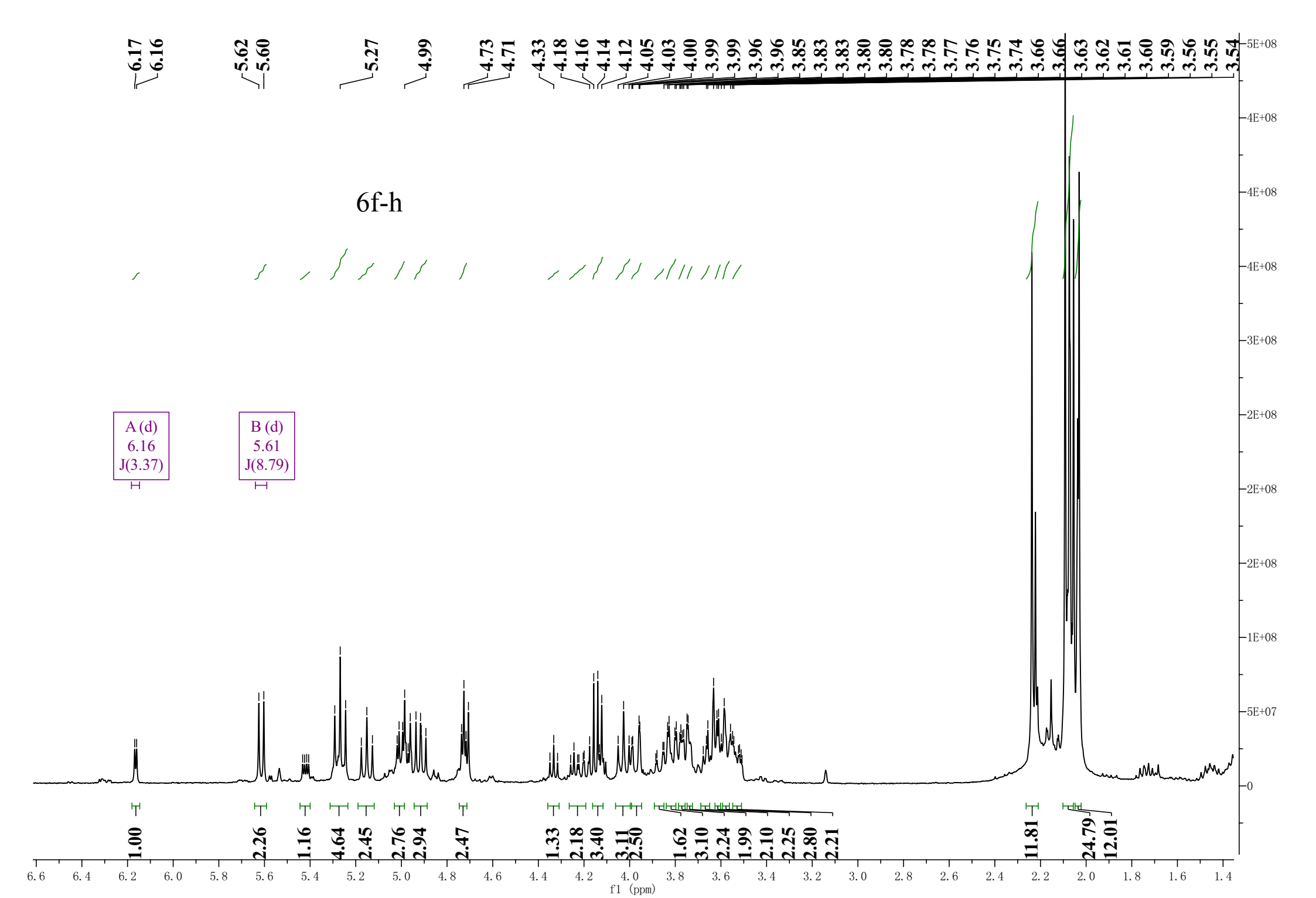
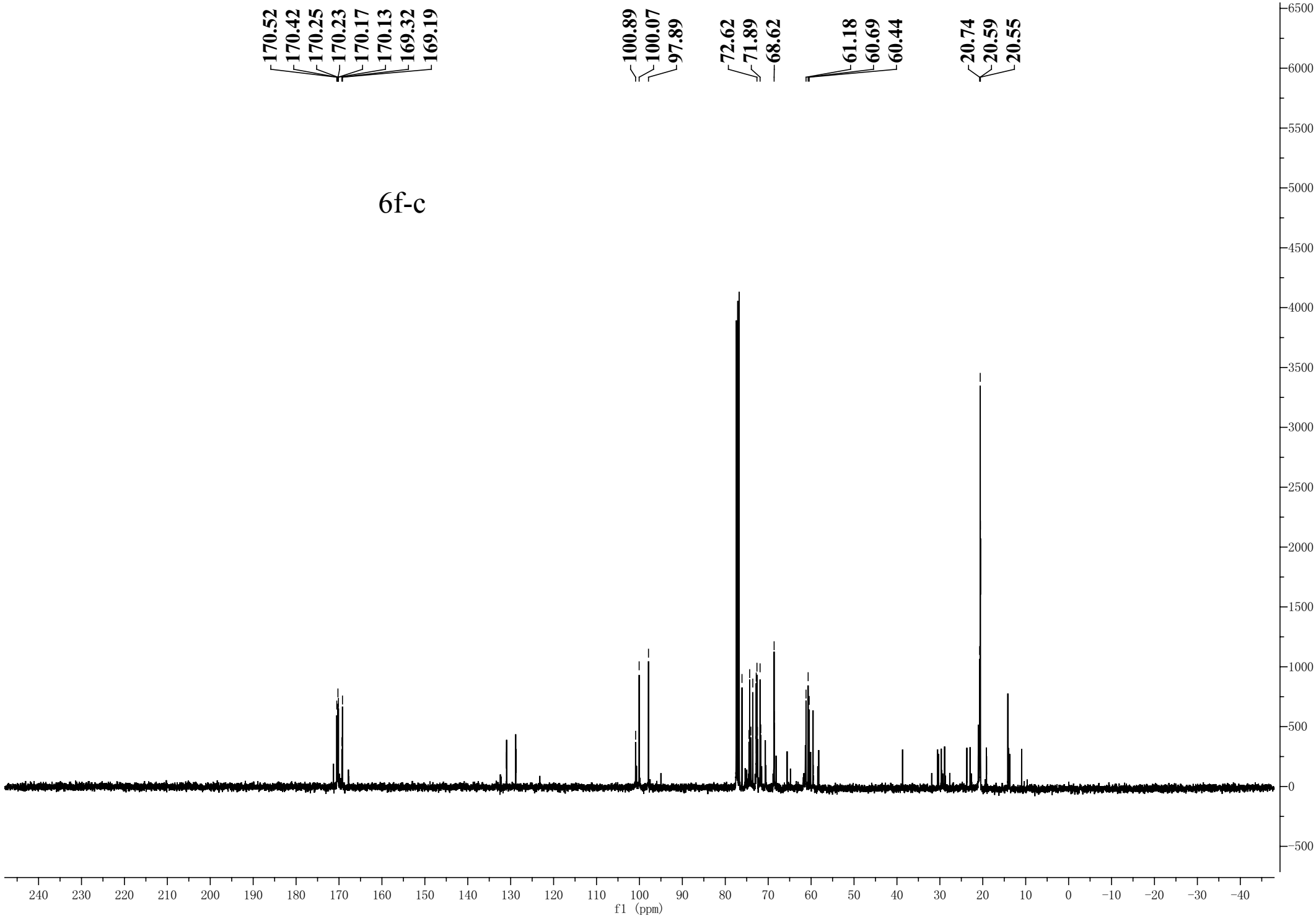
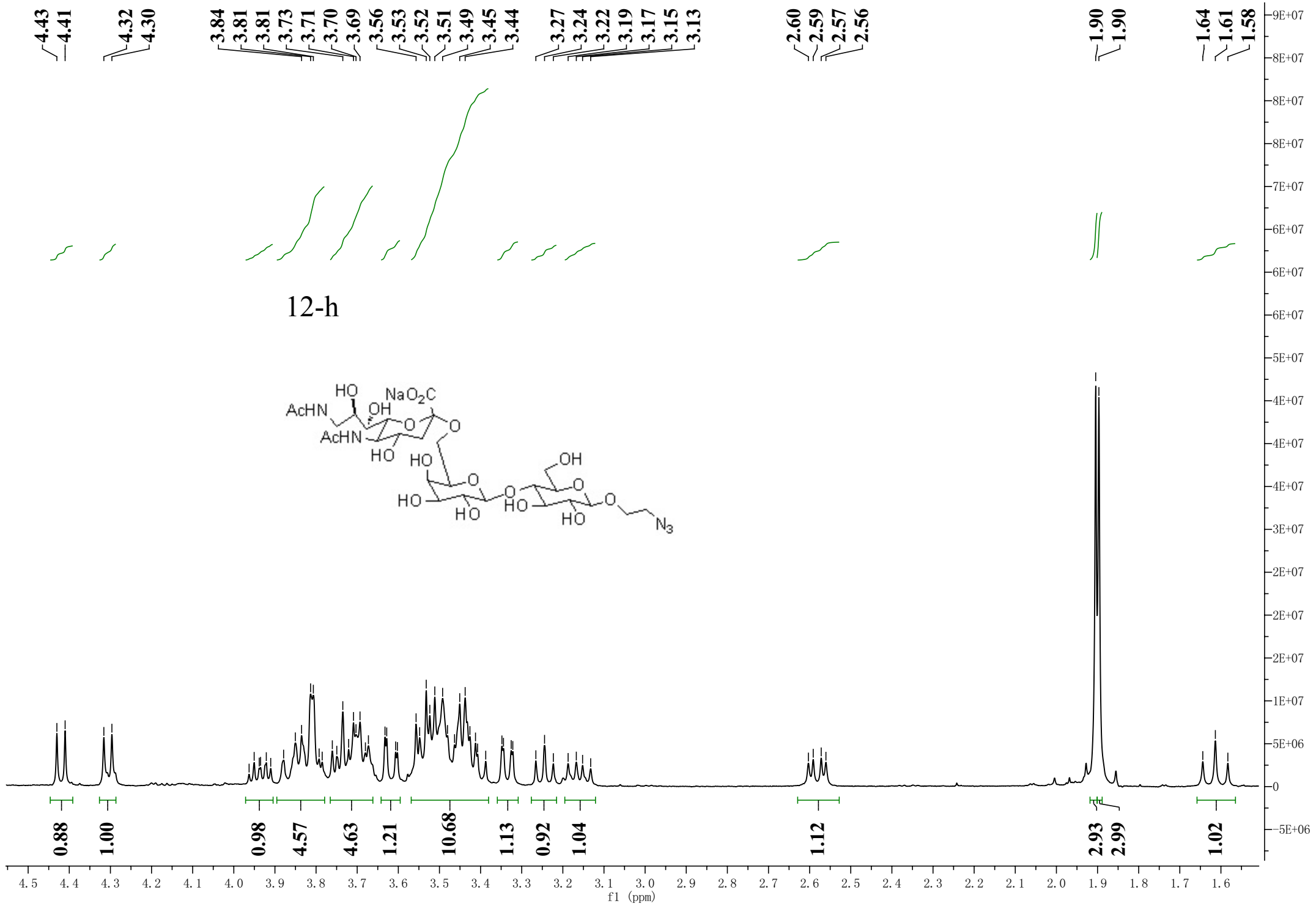
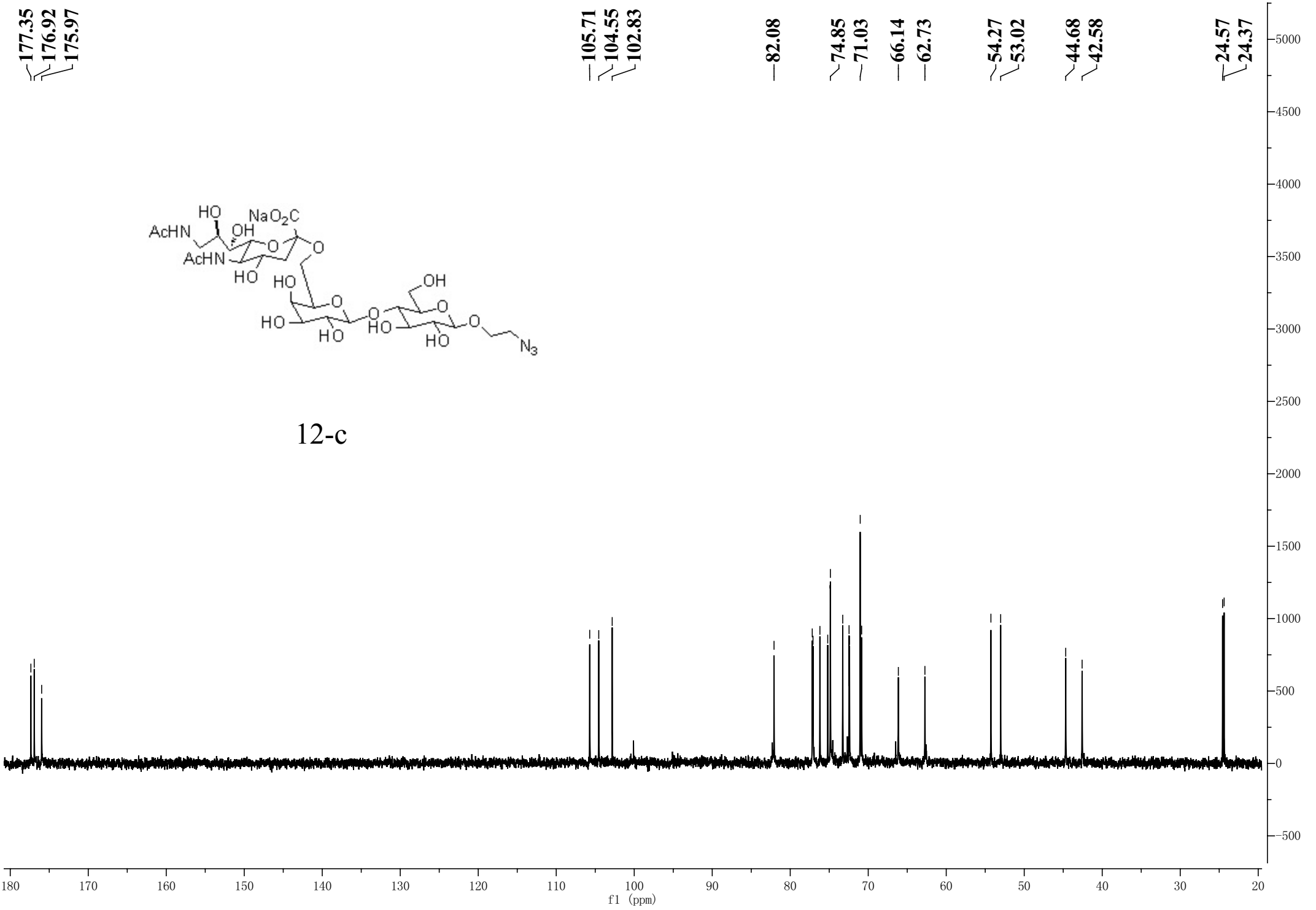
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

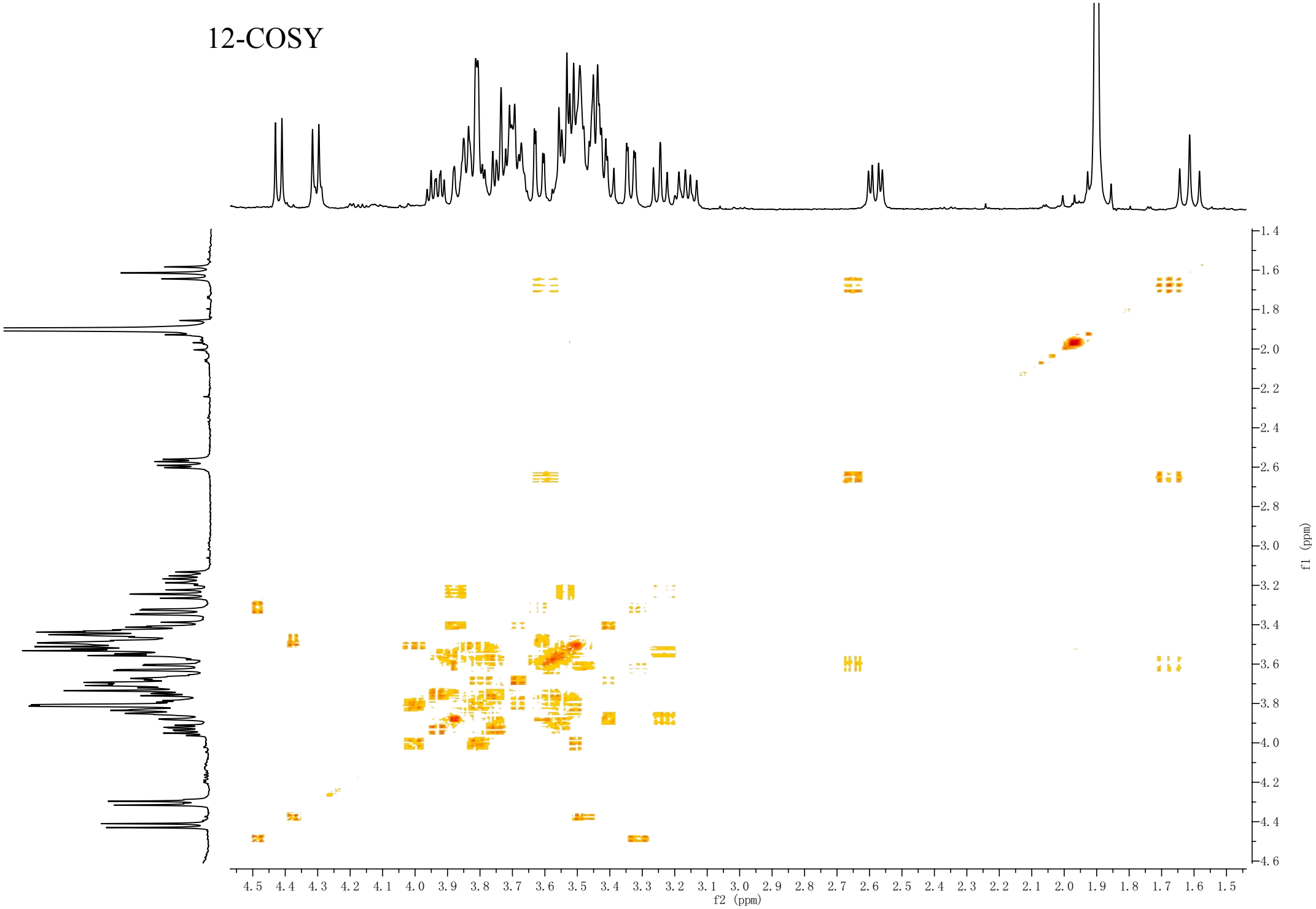

6f-h
A (d)
6.16
J(3.37)
B (d)
5.61
J(8.79)
f1 (ppm)

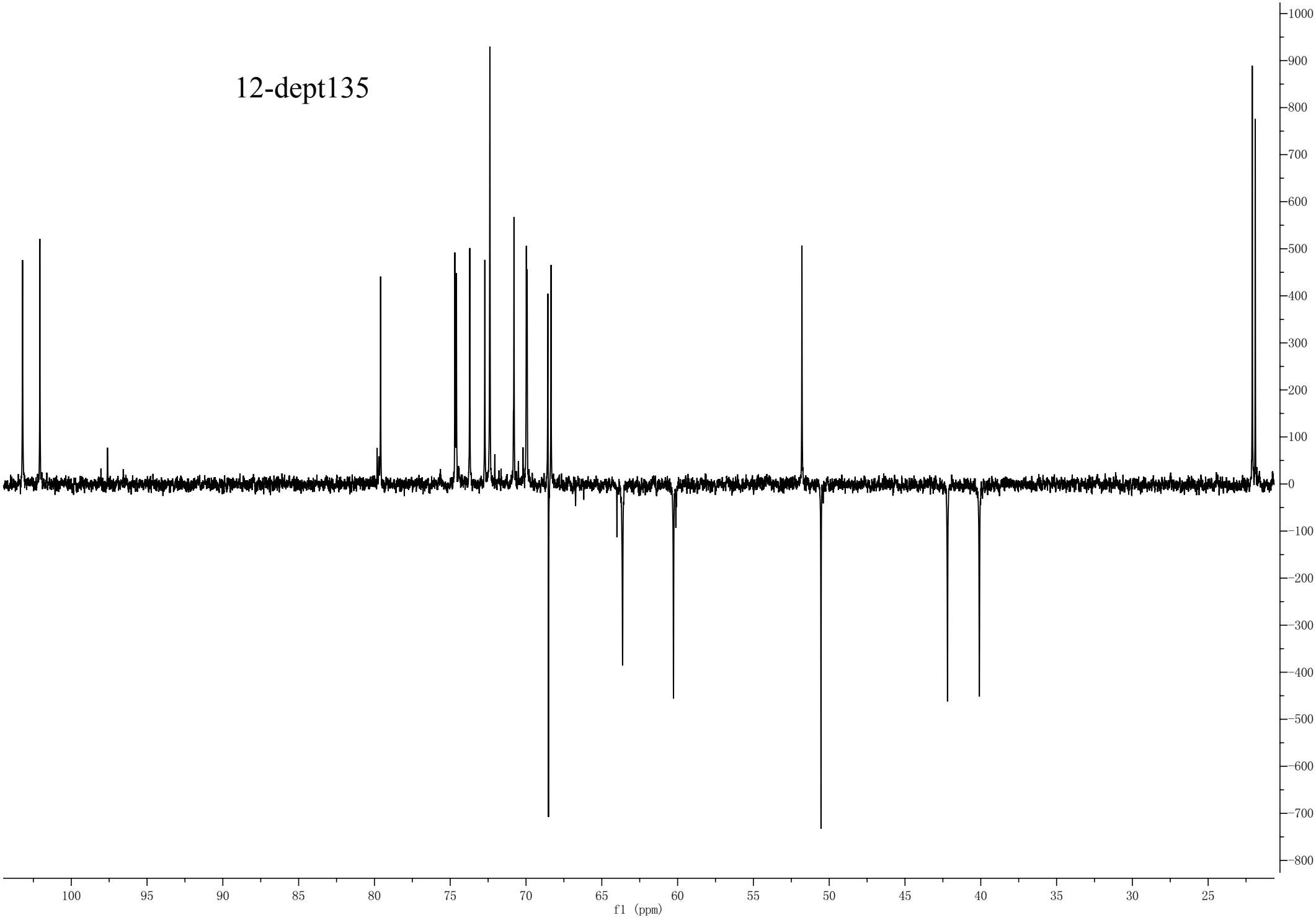

170.52
170.42
170.25
170.23
170.17
170.13
169.32
169.19
100.89
100.07
97.89
72.62
71.89
68.62
61.18
60.69
60.44
20.74
20.59
20.55
6f-c
f1 (ppm)


4.43
4.41
4.32
4.30
3.84
3.81
3.81
3.73
3.71
3.70
3.69
3.56
3.53
3.52
3.51
3.49
3.45
3.44
3.27
3.24
3.22
3.19
3.17
3.15
3.13
2.60
2.59
2.57
2.56
1.90
1.90
1.64
1.61
1.58
12-h
HO
NaO2C
AcHN
OH
O
AcHN
HO
HO
OH
HO
HO
HO
HO
N3
0.88
1.00
0.98
4.57
4.63
1.21
10.68
1.13
0.92
1.04
1.12
2.93
2.99
1.02
f1 (ppm)

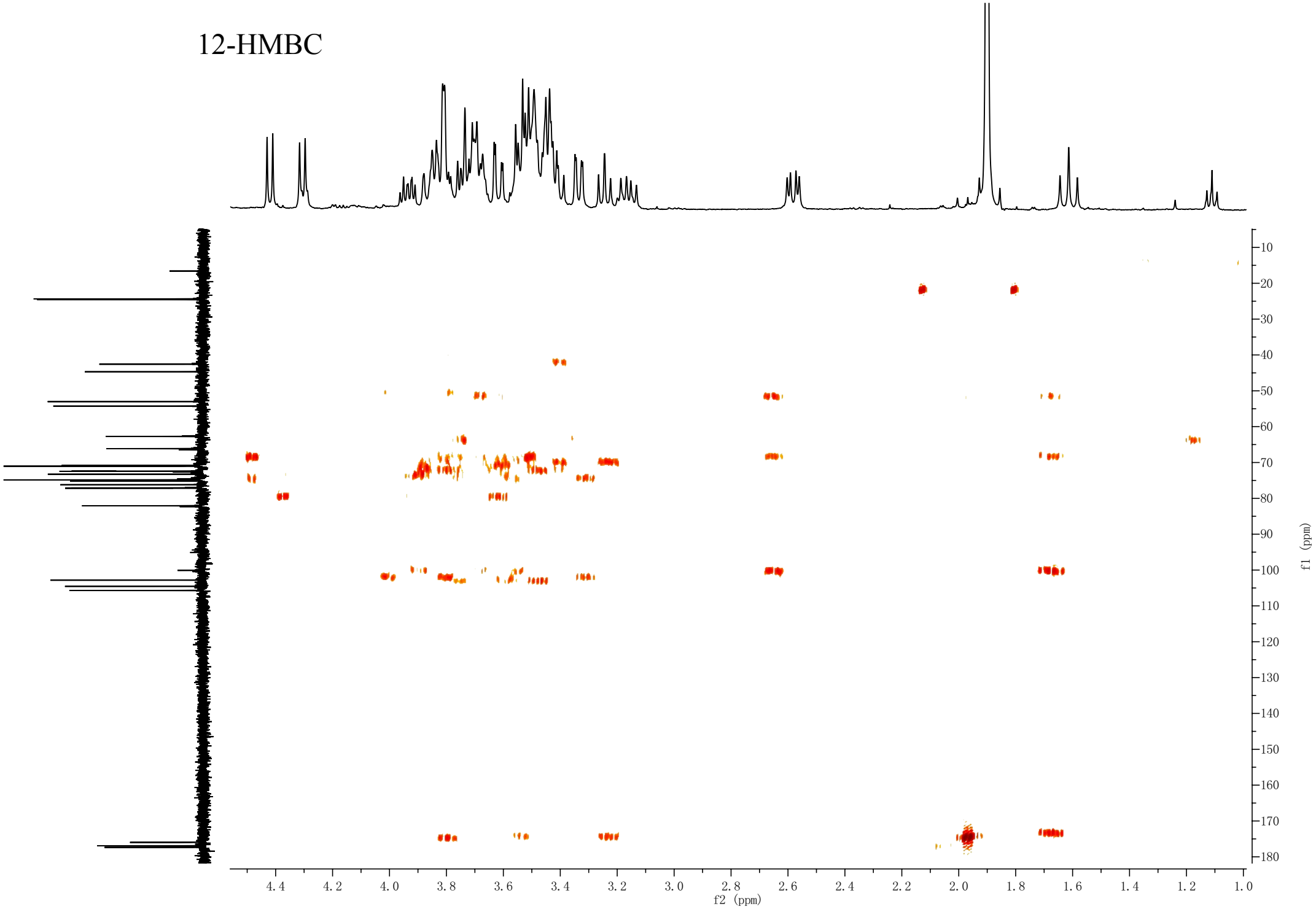

177.35
176.92
175.97
105.71
104.55
102.83
82.08
74.85
71.03
66.14
62.73
54.27
53.02
44.68
42.58
24.57
24.37
HO
NaO2C
AcHN
OH
AcHN
HO
HO
OH
HO
HO
HO
HO
N3
12-c
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

12-COSY

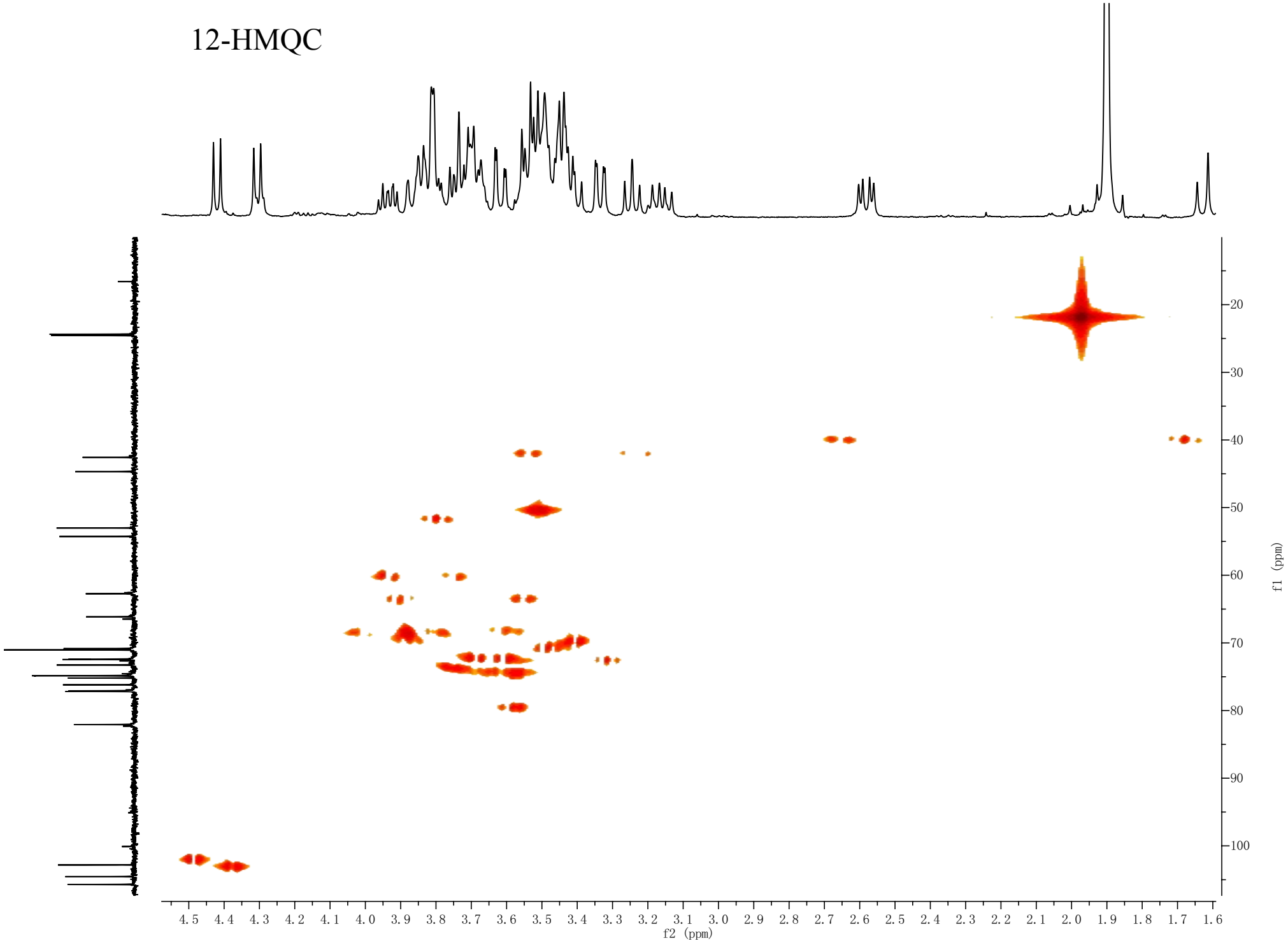



12-dept135
1000
900
800
700
600
500
400
300
200
100
0
−100
−200
−300
−400
−500
−600
−700
−800
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
f1 (ppm)

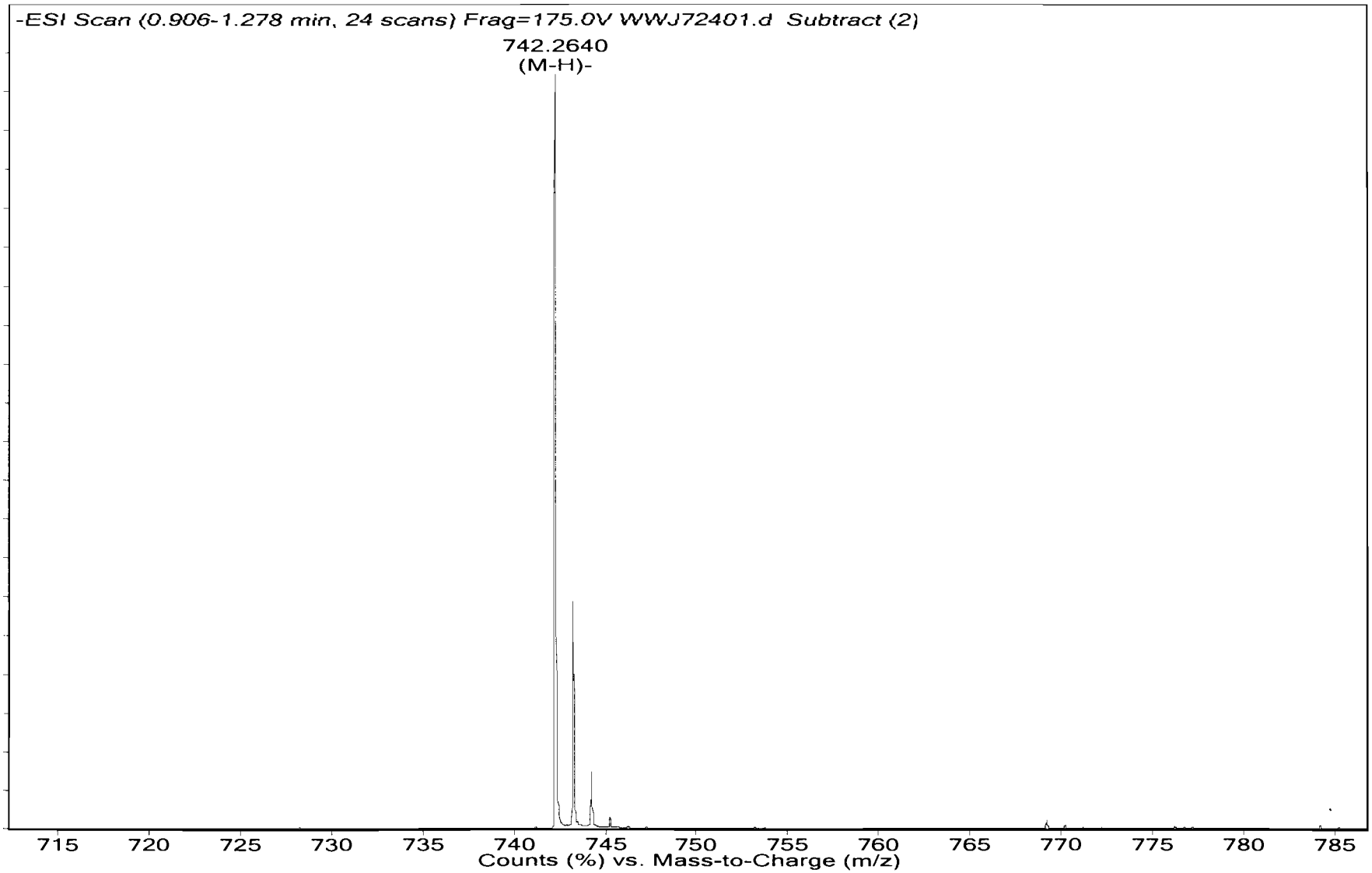
12-HMBC


10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
f1 (ppm)
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
f2 (ppm)

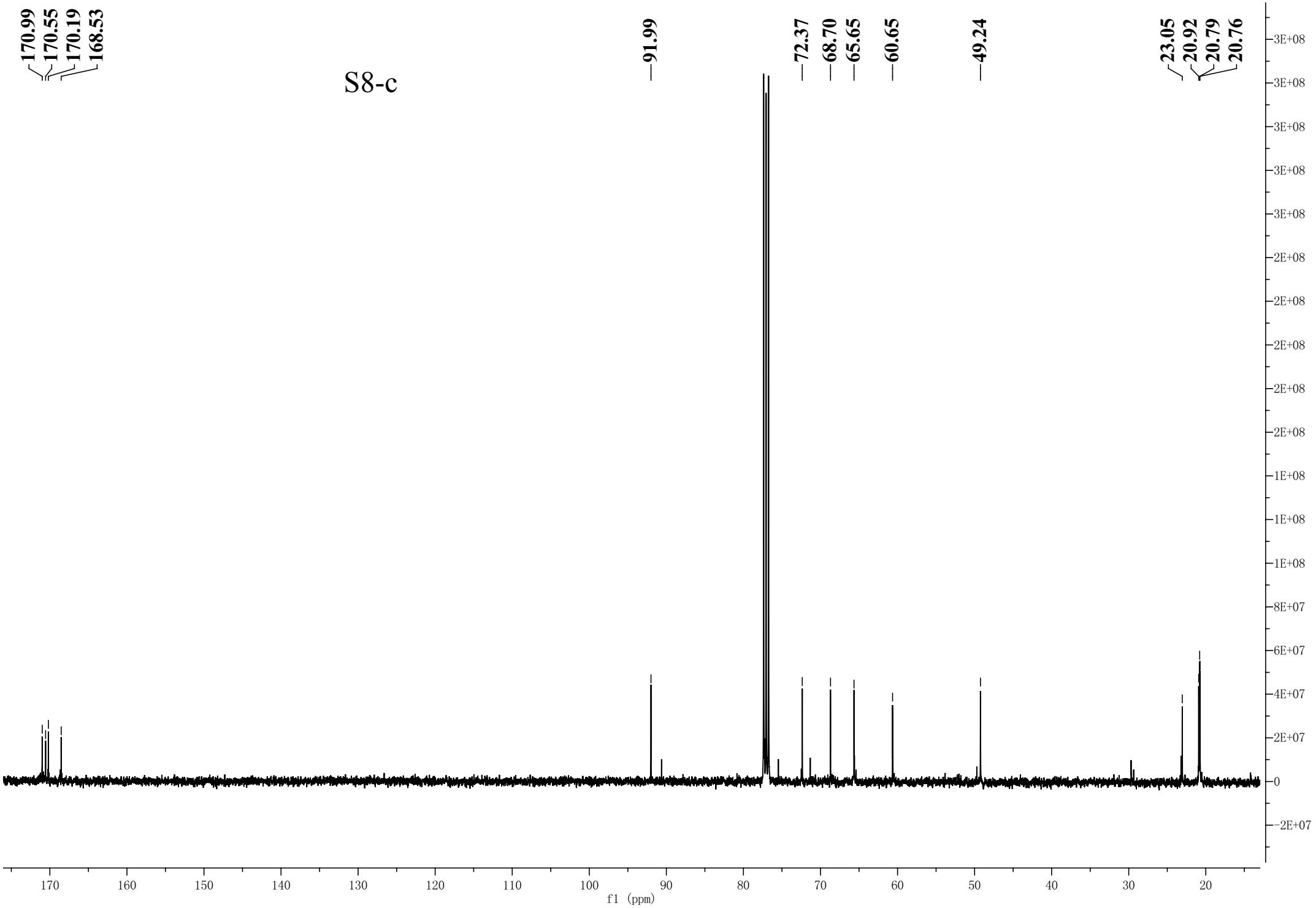
12-HMQC

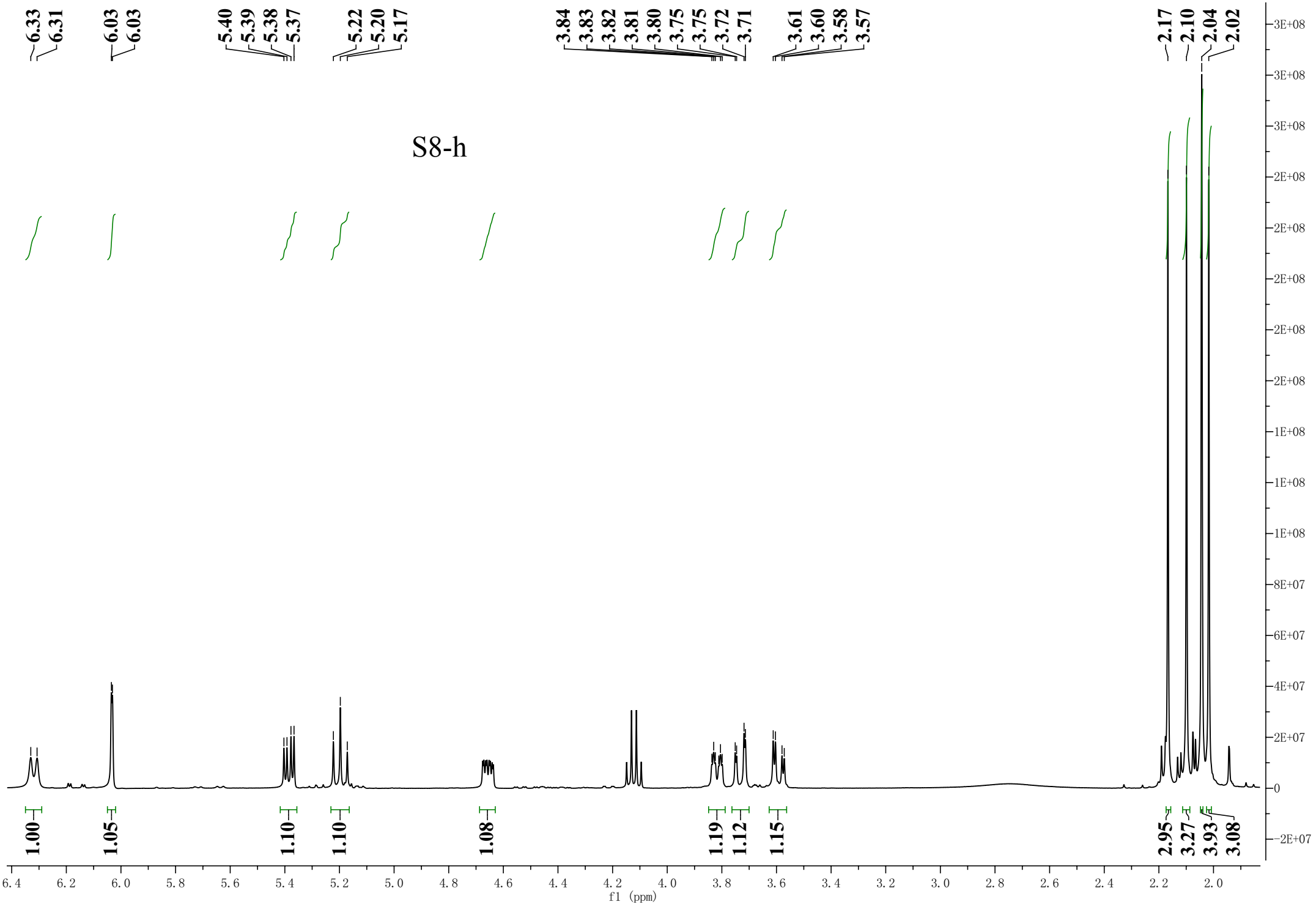

20
30
40
50
60
70
80
90
100
f1 (ppm)
4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f2 (ppm)

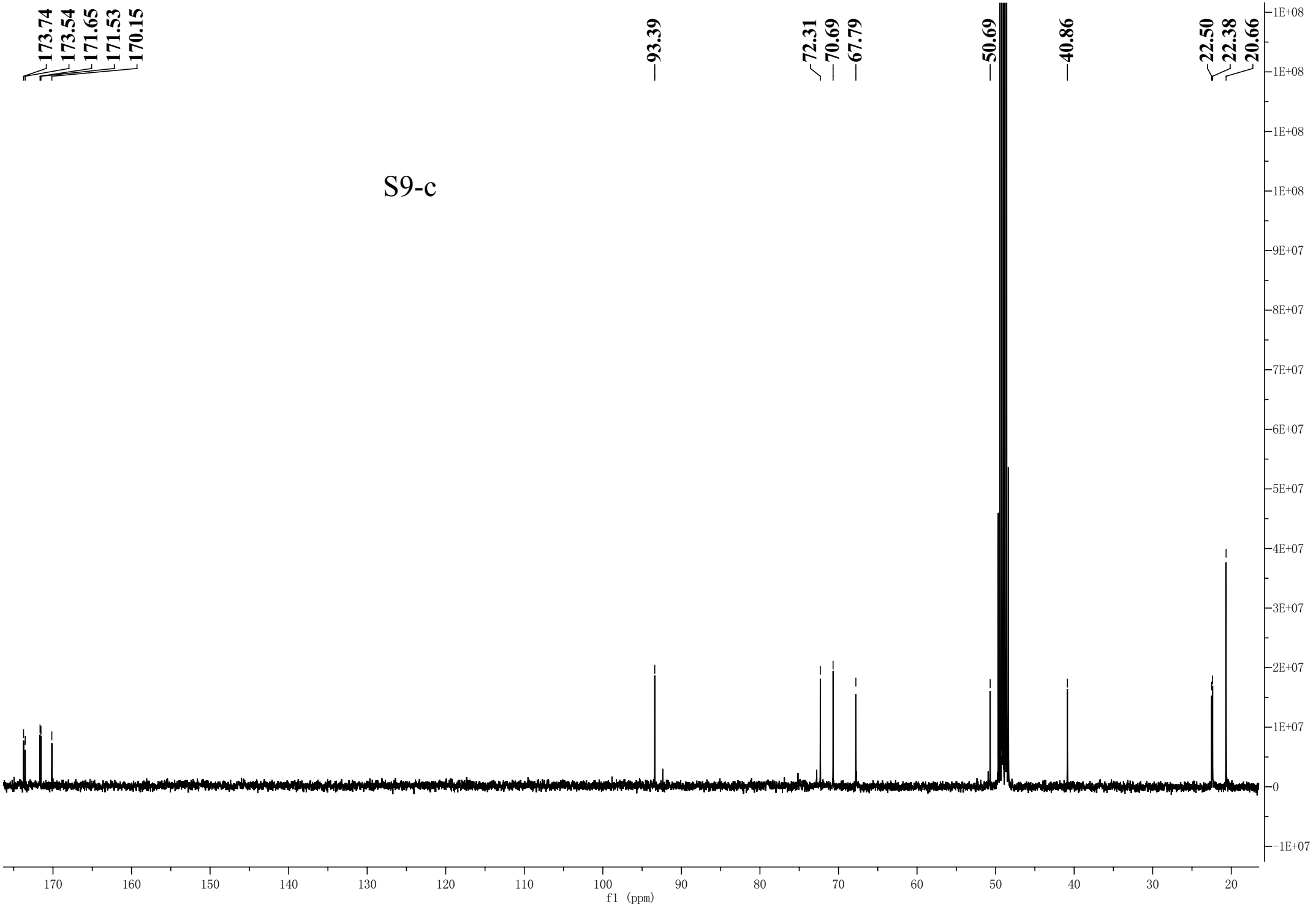
Sample Name	LC/MS	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	WWJ72401.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	11/9/2012 9:59:55 AM

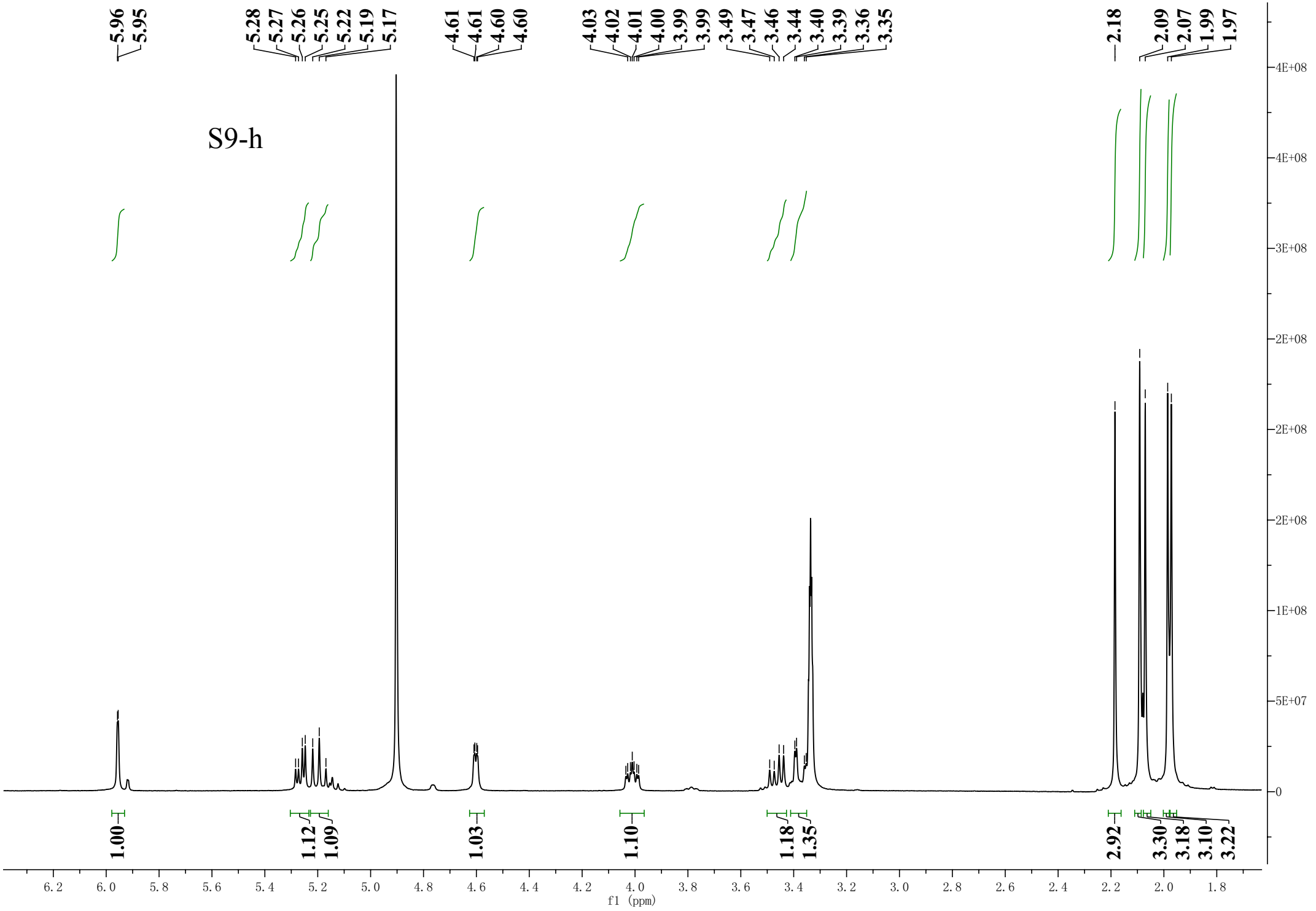


12-MS


S8-c
170.99
170.55
170.19
168.53
91.99
72.37
68.70
65.65
60.65
49.24
23.05
20.92
20.79
20.76
3E+08
2E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


6.33
6.31
6.03
6.03
5.40
5.39
5.38
5.37
5.22
5.20
5.17
3.84
3.83
3.82
3.81
3.80
3.75
3.75
3.72
3.71
3.61
3.60
3.58
3.57
2.17
2.10
2.04
2.02
S8-h
1.00
1.05
1.10
1.10
1.08
1.19
1.12
1.15
2.95
3.27
3.93
3.08
f1 (ppm)


173.74
173.54
171.65
171.53
170.15
93.39
72.31
70.69
67.79
50.69
40.86
22.50
22.38
20.66
S9-c
1E+08
1E+08
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


S9-h
5.96
5.95
5.28
5.27
5.26
5.25
5.22
5.19
5.17
4.61
4.61
4.60
4.60
4.03
4.02
4.01
4.00
3.99
3.99
3.49
3.47
3.46
3.44
3.40
3.39
3.36
3.35
2.18
2.09
2.07
1.99
1.97
1.00
1.12
1.09
1.03
1.10
1.18
1.35
2.92
3.30
3.18
3.10
3.22
f1 (ppm)