Supporting Information

Synthesis-Enabled Conformational Assignment of Natural *N*-Acyl *L*-Phenylalanine Derivatives from Freshwater Sponge–Associated *Micromonospora* sp. MS-62

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Contents

General experimental for Synthesis

Methyl 2-methoxyalkenoate (**10a**–**e**): To a dry, N_2-flushed flask charged with THF (0.18 M with respect to the aldehyde) and diisopropylamine (1.43 equiv) at −78 °C was added *n*-BuLi (2.0 M in hexanes, 1.40 equiv) dropwise. The mixture was stirred for 30 min at −78 °C to generate LDA. Methyl methoxyacetate (**9**, 1.10 equiv) was added and the solution was stirred for 10 min at −78 °C, then the cooling bath was adjusted to −40 °C and stirring continued until the internal temperature reached −40 °C. The corresponding aldehyde **8a**–**e** (1.00 equiv) was added, and the mixture was stirred for 10 min at −40 °C (aldol addition). Methanesulfonyl chloride (1.30 equiv) was then added, the bath was set to 0 °C, and the reaction was stirred to 0 °C (≈40–60 min). The flask was removed from the bath and stirred at rt until the solution turned yellow (≈1–3 h). Triethylamine (4.50 equiv) was added, and the mixture was heated to reflux for 3 h (β-elimination to the α-methoxy enoate). After cooling in an ice bath, the reaction was diluted with EtOAc, and the biphasic mixture was quenched by acidifying the aqueous phase to pH ≈ 1–2 with 5% aq HCl (until both layers changed color). The organic layer was separated, and the aqueous phase was extracted with EtOAc. Combined organics were washed with brine, dried (Na_2SO_4), filtered, and concentrated under reduced pressure to afford crude **10a**–**e**, which were used directly in the next step without further purification.

2-Methoxyalkenoic acid (**7a**–**e**): To a stirred solution of methyl 2-methoxyalkenoate (**10a**–**e**, 0.5 M) in MeOH/H_2O (1:1) was added lithium hydroxide monohydrate (2.50 equiv). The reaction mixture was heated at reflux for 3 h, then cooled in an ice bath. The aqueous layer was acidified with 3 *N* HCl until the pH indicator turned from neutral to acidic. The mixture was extracted with $CHCl_3$, and the combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product (**7a**–**e**) was obtained as a pale solid and used directly in the next step without further purification.

Benzyl (2-methoxyalkenoyl)-*L*-phenylalanine (**11a**–**e**): To a stirred solution of 2-methoxyalkenoic acid (**7a**–**e**, 0.2 M) in CH_2Cl_2 was added *N*-(3-dimethylaminopropyl)-*N'*-ethylcarbodiimide hydrochloride (EDC·HCl, 1.30 equiv), 1-hydroxybenzotriazole monohydrate (1-HOBt·H_2O, 1.20 equiv), and *N,N*-diisopropylethylamine

(DIPEA, 2.00 equiv). The reaction mixture was stirred at room temperature for 20 min, followed by the addition of *L*-phenylalanine benzyl ester hydrochloride (1.05 equiv) and an additional portion of DIPEA (2.00 equiv). The mixture was stirred at room temperature for 24 h and monitored by UPLC–MS. After completion, the reaction was quenched with water and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure to afford crude **11a**–**e** as inseparable E/Z mixtures, which were used directly in the subsequent step without further purification.

N-(2-methoxyalkanoyl)-*L*-phenylalanine (**1**–**5** and **epi-1**–**5**): The dried *E*/*Z* mixture of benzyl (2-methoxyalkenoyl)-*L*-phenylalanine (**11a**–**e**) was dissolved in methanol (0.1 M) and purged with Ar gas. The oxygen dissolved in MeOH solution was removed by high-vacuum and purged with Ar gas. Then the palladium on activated charcoal (10% w/w) was added to the solution and flask was immediately closed with a new rubber stopper. After the solution was degassed completely, inside of flask was substituted by with 3-layered hydrogen balloon. The reaction was stirred overnight at room temperature. Pd powder was filtered through celite and washed once with methanol and EtOAc respectively and concentrated under reduced pressure. Formation of **1**–**5** and **epi-1**–**5** was detected by UPLC-MS and the mixture were isolated by semi-preparative HPLC. The crude reaction mixture was dissolved in a minimal amount of methanol and stored in a refrigerator for at least 24 h to allow the formation of white powdery precipitates. The supernatant was collected and subjected to purification by semi-preparative HPLC using a Phenomenex Luna C18(2) column (250 × 10 mm, 5 µm). Elution was performed with a gradient of acetonitrile/water (0.1% formic acid) from 45% to 65% over 60 min at a flow rate of 4–6 mL min^{-1}, with UV detection at 190 nm.

UHPLC–MS analysis and retention time of compounds: UHPLC analysis was performed on a Phenomenex Luna Omega Polar C18 column (150 × 2.1 mm, 1.6 µm) using a gradient system of acetonitrile/water containing 0.1% formic acid. The elution gradient was programmed from 30% to 90% acetonitrile over 9 min at a flow rate of 0.3 mL min^{-1}. Detection was conducted under standard ESI–MS conditions. UHPLC–MS analysis of the paired *S* and *R* form compounds of C-1' and was carried out under the above chromatographic conditions. The retention times (Rt) are summarized as follows:

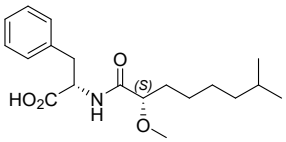
Compounds	***R* form of C-1' (min)**	***S* form of C-1' (min)**
1	9.500	9.667
2	9.599	9.778
3	10.042	10.221
4	9.866	10.072
5	10.656	10.885

Characterization data

Natural P2

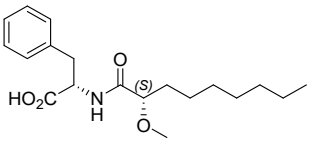
^{1}H NMR (500 MHz, $CDCl_3$ = 7.26) δ 7.30–7.22 (2H, m), 7.18-7.16 (2H, m), 7.00 (1H, d, *J* = 8.0 Hz), 4.93 (1H, dt, *J* = 7.8 and 5.5 Hz), 3.61 (1H, dd, *J* = 7.0 and 4.5 Hz), 3.32 (3H, s), 3.26 (1H, dd, *J* = 14.0 and 5.5 Hz), 3.10 (1H, dd, *J* = 7.8 and 14.3 Hz), 1.63–1.58 (1H, m), 1.53–1.46 (1H, m), 1.33–1.22 (10H, m), 0.89 (3H, t, *J* = 7.0 Hz) ^{13}C NMR (125 MHz, $CDCl_3$ = 77.16) δ 175.0, 173.7, 135.8, 129.5, 128.7, 127.3, 82.4, 58.5, 52.5, 37.7, 32.8, 31.9, 29.5, 29.2, 24.8, 22.8, 14.2.

((*S*)-2-methoxy-7-methoxyoctanoyl)–*L*–phenylalanine



P1 (**1**, 6.6% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) δ 7.28–7.16 (5H, m), 4.74 (1H, dd, *J* = 9.2 and 4.8 Hz), 3.52 (1H, dd, *J* = 6.4 and 4.8 Hz), 3.28 (1H, dd, *J* = 14.0 and 4.8 Hz, estimated due to overlap with solvent), 3.27 (3H, s), 3.02 (1H, dd, *J* = 13.6 and 9.2 Hz), 1.52 (1H, sep, *J* = 6.4 Hz), 1.52–1.38 (2H, m), 1.25–1.11 (6H, m), 0.879 (6H, dd, *J* = 6.4 and 1.2 Hz).^{13}C NMR (100 MHz, CD_3OD = 49.15) δ 175.4, 174.6, 138.6, 130.5, 129.5, 127.9, 83.6, 58.5, 54.1, 40.1, 38.4, 34.1, 29.2, 28.4, 26.1, 23.2. ESI–MS: m/z calcd for $C_{19}H_{30}NO_4$ $[M+H]^+$ 336.22, found 336.15.

((*S*)-2-methoxynonanoyl)–*L*–phenylalanine



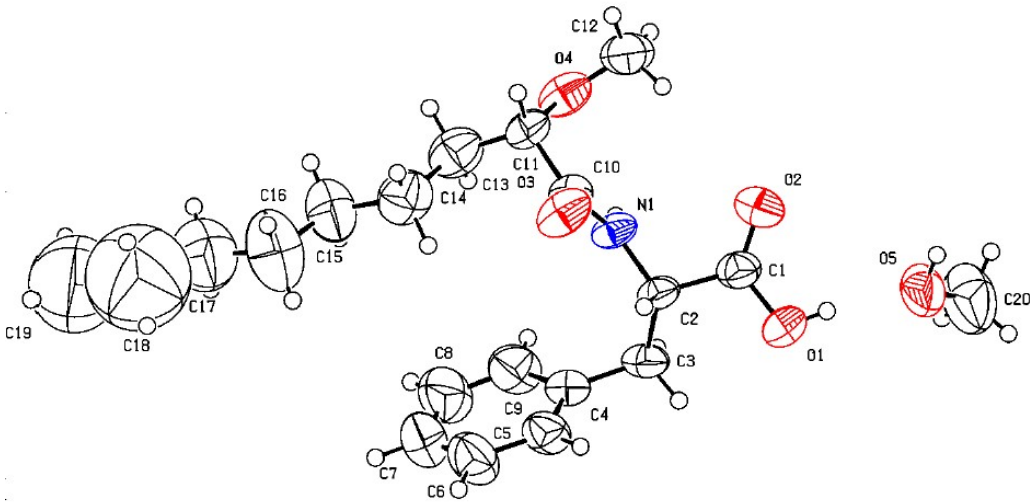
P2 (**2**, 8.3% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) δ 7.27–7.16 (5H, m), 4.76 (1H, dd, *J* = 9.6 and 4.4 Hz), 3.52 (1H, dd, *J* = 7.0 and 5.4 Hz), 3.26 (1H, dd, *J* = 14.0 and 9.4 Hz), 3.27 (3H, s), 3.02 (1H, dd, *J* = 14.0 and 9.6 Hz), 1.54–1.42 (2H, m), 1.34–1.18 (10H, m), 0.90 (3H, t, J = 7.2 Hz). ^{13}C NMR (100 MHz, CD_3OD = 49.15) δ 175.3, 174.8, 138.6, 130.5, 129.5, 127.9, 83.6, 58.5, 54.3, 38.4, 34.1, 33.1, 30.6, 30.4, 25.9, 23.9, 14.6. ESI–MS: m/z calcd for $C_{19}H_{30}NO_4$ $[M+H]^+$ 336.22, found 336.15.

^{1}H NMR (400 MHz, $CDCl_3$ = 7.26) δ 7.32–7.22 (2H, m), 7.19–7.16 (2H, m), 6.95 (1H, d, *J* = 8.8 Hz), 4.91 (dt, 1H, *J* = 7.8 and 6.0 Hz), 3.60 (1H, dd, *J* = 7.0 and 4.4 Hz), 3.32 (3H, s), 3.26 (1H, dd, *J* = 13.8 and 5.4 Hz), (1H, dd, *J* =

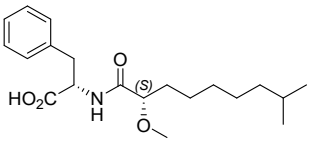
14.2 and 7.4 Hz), 1.65–1.58 (1H, m), 1.54–1.45 (1H, m), 1.31–1.22 (10H, m), 0.88 (3H, t, *J* = 7.0 Hz). ^{13}C NMR (100 MHz, $CDCl_3$ = 77.00) *δ* 174.9, 173.5, 135.6, 129.2, 128.6, 127.2, 82.3, 58.3, 52.4, 37.5, 32.6, 31.8, 29.3, 29.1, 24.7, 22.6, 14.1.

Crystal data and structure refinement for 2P (**2**):

Empirical formula	C20 H33 N O5	
Formula weight	367.47	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 16.744(2) Å	α= 90°.
	b = 5.1551(7) Å	β= 95.926(4)°.
	c = 25.863(4) Å	γ = 90°.
Volume	2220.5(5) Å^3	
Z	4	
Density (calculated)	1.099 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	800	
Crystal size	0.357 x 0.096 x 0.052 mm^3	
Theta range for data collection	2.375 to 28.453°.	
Index ranges	-22<=h<=22, -6<=k<=6, -34<=l<=34	
Reflections collected	40501	
Independent reflections	5577 [R(int) = 0.0779]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6774	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5577 / 23 / 236	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0860, wR2 = 0.2340	
R indices (all data)	R1 = 0.1796, wR2 = 0.3008	
Absolute structure parameter	1.6(6)	
Extinction coefficient	0.012(4)	
Largest diff. peak and hole	0.439 and -0.283 e.Å^{-3}	

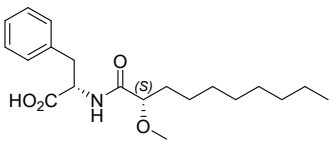


((*S*)-2-methoxy-8-methoxynonanoyl)–*L*–phenylalanine



P3 (**3**, 4.3% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) δ 7.27–7.16 (5H, m), 4.75 (1H, dd, *J* = 8.6 and 3.8 Hz), 3.52 (1H, dd, *J* = 6.8 and 5.2 Hz), 3.28 (1H, dd, *J* = 14.0 and 4.8 Hz, estimated due to overlap with solvent), 3.27 (3H, s), 3.02 (1H, dd, *J* = 14 and 9.2 Hz), 1.52 (1H, sep, *J* = 6.6 Hz), 1.49–1.44 (2H, m), 1.26–1.12 (8H, m), 0.89 (6H, d, *J* = 6.4 Hz). ^{13}C NMR (100 MHz, CD_3OD = 49.15) δ 175.3, 174.7, 138.6, 130.5, 129.5, 127.9, 83.6, 58.5, 54.2, 40.3, 38.4, 34.1, 30.9, 29.3, 28.5, 25.9, 23.2. ESI–MS: m/z calcd for $C_{20}H_{32}NO_4$ $[M+H]^+$ 350.23, found 350.15.

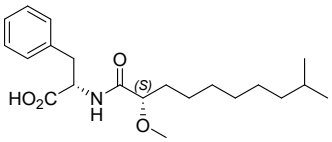
((*S*)-2-methoxydecanoyl)–*L*–phenylalanine



P4 (**4**, 7.6% unoptimized overall isolated yield over four steps): ^{1}H NMR (500 MHz, CD_3OD = 3.31) δ 7.28–7.17 (5H, m), 4.77 (1H, dd, *J* = 9.3 and 4.8 Hz), 3.52 (1H, dd, *J* = 7.0 and 5.5 Hz), 3.29 (1H, dd, *J* = 14.5 and 4.5 Hz), 3.27 (3H, s), 3.02 (1H, dd, *J* = 14 and 9.5 Hz), 1.53–1.41 (2H, m), 1.35–1.11 (12H, m), 0.91 (3H, t, *J* = 7.0 Hz). ^{13}C NMR (125 MHz, CD_3OD = 49.15) δ 175.4, 174.5, 138.5, 130.5, 129.5, 127.9, 83.6, 58.5, 54.1, 38.4, 34.1, 33.2,

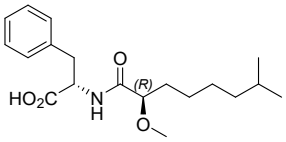
30.7, 30.6, 30.5, 25.9, 23.9, 14.6. ESI–MS: m/z calcd for $C_{20}H_{32}NO_4$ $[M+H]^+$ 350.23, found 350.05.

((*S*)-2-methoxy-9-methoxydecanoyl)–*L*–phenylalanine



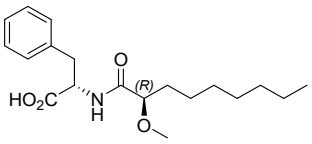
P5 (**5**, 3.0% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) δ 7.28–7.17 (5H, m), 4.77 (1H, dd, *J* =9.6 and 4.4 Hz), 3.52 (1H, dd, *J* = 6.8 and 5.6 Hz), 3.28 (1H, dd, *J* = 14.0 and 4.8 Hz, estimated due to overlap with solvent), 3.27 (3H, s), 3.02 (1H, dd, *J* = 14 and 9.6 Hz), 1.53 (1H, sep, *J* = 6.7 Hz), 1.53–1.42 (2H, m), 1.31–1.14 (10H, m), 0.89 (6H, d, *J* = 6.4 Hz). ^{13}C NMR (100 MHz, CD_3OD = 49.15) δ 175.3, 174.6, 138.6, 130.5, 129.5, 127.9, 83.6, 58.5, 54.2, 40.4, 38.4, 34.1, 30.9, 30.7, 29.3, 28.6, 25.9, 23.2. ESI–MS: m/z calcd for $C_{21}H_{34}NO_4$ $[M+H]^+$ 364.25, found 364.20.

((*R*)-2-methoxy-7-methoxyoctanoyl)–*L*–phenylalanine



epi-P1 (***epi*-1**, 9.0% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) δ 7.30–7.18 (5H, m), 4.72 (1H, dd, *J* = 4.8 Hz), 3.50 (1H, dd, *J* = 7.2 and 5.2 Hz), 3.31 (1H, dd, *J* = 14.0 and 4.8 Hz), 3.14 (3H, s), 3.03 (1H, dd, *J* = 14.2 and 9.8 Hz), 1.63–1.55 (2H, m), 1.50 (1H, sep, *J* = 6.6 Hz), 1.34–1.20 (4H, m), 1.16–1.10 (2H, m), 0.87 (6H, d, *J* = 6.8 Hz). ^{13}C NMR (100 MHz, CD_3OD = 49.15) δ 175.6, 174.5, 138.6, 130.4, 129.6, 128.0, 83.5, 58.6, 54.4, 40.1, 38.1, 34.2, 29.2, 28.4, 26.2, 23.2. ESI–MS: m/z calcd for $C_{19}H_{30}NO_4$ $[M+H]^+$ 336.22, found 336.15.

((*R*)-2-methoxynonanoyl)–*L*–phenylalanine

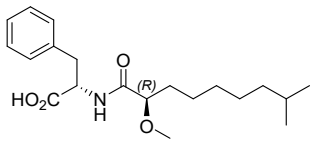


epi-P2 (***epi*-2**, 11.0% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) δ 7.29–7.18 (5H, m), 4.72 (1H, dd, *J* = 9.4 and 4.6 Hz), 3.50 (1H, dd, *J* = 6.8 and 5.2 Hz), 3.30 (1H, dd, *J* = 14.0 and

4.4 Hz), 3.14 (3H, s), 3.03 (1H, dd, *J* = 14.0 and 9.6 Hz), 1.62–1.50 (2H, m), 1.33–1.22 (10H, m), 0.89 (3H, t, *J* = 6.8 Hz). ^{13}C NMR (100 MHz, CD_3OD = 49.15) *δ* 175.5, 174.6, 138.6, 130.4, 129.6, 128.0, 83.5, 58.6, 54.5, 38.1, 34.2, 33.1, 30.6, 30.4, 26.0, 23.8, 14.6. ESI–MS: m/z calcd for $C_{19}H_{30}NO_4$ $[M+H]^+$ 336.22, found 336.10.

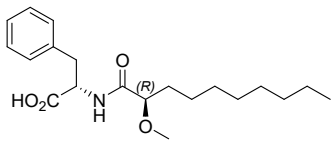
^{1}H NMR (400 MHz, $CDCl_3$ = 7.26) δ 7.32-7.28 (2H, m), 7.24-7.19 (2H, m), 6.90 (1H, d, J = 7.6 Hz), 4.83 (1H, dt, J = 7.6 and 5.6 Hz), 3.55 (1H, dd, J = 7.6 and 4.0 Hz), 3.33 (1H, dd, J = 14.0 and 5.2 Hz), 3.13 (3H, s), 3.10 (1H, dd, J = 14.0 and 7.6 Hz), 1.75-1.67 (1H, m), 1.63-1.54 (1H, m), 1.39-1.24 (10H, m), 0.86 (3H, t, J = 7.0 Hz). ^{13}C NMR (100 MHz, $CDCl_3$ = 77.00) δ 174.7, 173.7, 135.8, 129.2, 128.7, 127.2, 82.3, 58.4, 52.7, 37.1, 32.8, 31.7, 29.3, 29.1, 24.8, 22.6, 14.1.

((*R*)-2-methoxy-8-methoxynonanoyl)–*L*–phenylalanine



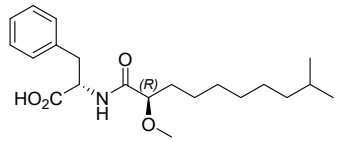
epi-P3 (***epi*-3**, 4.6% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) *δ* 7.30–7.18 (5H, m), 4.70 (1H, dd, *J* = 9.6 and 4.8 Hz), 3.50 (1H, dd, *J* = 6.8 and 5.2 Hz), 3.30 (1H, dd, *J* = 14 and 4.8 Hz), 3.14 (3H, s), 3.03 (1H, dd, *J* = 14 and 9.6 Hz), 1.62–1.56 (2H, m), 1.51 (1H, sep, *J* = 6.6 Hz), 1.34–1.11 (8H, m), 0.87 (6H, d, *J* = 6.4 Hz) ^{13}C NMR (100 MHz, CD_3OD = 49.15) *δ* 175.5, 174.7, 138.6, 130.5, 129.6, 128.0, 83.5, 58.6, 54.5, 40.2, 38.2, 34.2, 30.9, 29.3, 28.5, 26.0, 23.2. ESI–MS: m/z calcd for $C_{20}H_{32}NO_4$ $[M+H]^+$ 350.23, found 350.15.

((*R*)-2-methoxydecanoyl)–*L*–phenylalanine



epi-P4 (***epi*-4**, 8.9% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) *δ* 7.29–7.18 (5H, m), 4.72 (1H, dd, *J* = 9.6 and 4.8 Hz), 3.50 (1H, dd, *J* = 6.8 and 5.2 Hz), 3.30 (1H, dd, *J* = 14.0 and 4.8 Hz), 3.14 (3H, s), 3.03 (1H, dd, *J* = 14 and 9.6 Hz), 1.61–1.49 (2H, m), 1.33–1.22 (12H, m), 0.90 (3H, t, *J* = 6.8 Hz) ^{13}C NMR (100 MHz, CD_3OD = 49.15) *δ* 175.5, 174.6, 138.6, 130.5, 129.6, 128.0, 83.5, 58.6, 54.5, 38.1, 34.2, 33.2, 30.9, 30.7, 30.5, 26.0, 23.9, 14.6. ESI–MS: m/z calcd for $C_{20}H_{32}NO_4$ $[M+H]^+$ 350.23, found 350.05.

((*R*)-2-methoxy-9-methoxydecanoyl)–*L*–phenylalanine



epi-P5 (***epi*-5**, 6.1% unoptimized overall isolated yield over four steps): ^{1}H NMR (400 MHz, CD_3OD = 3.31) δ 7.30–7.18 (5H, m), 4.72 (1H, dd, *J* = 9.6 and 4.8 Hz), 3.50 (1H, dd, *J* = 7.2 and 5.2 Hz), 3.30 (1H, dd, *J* = 14.0 and 4.8 Hz), 3.15 (3H, s), 3.03 (1H, dd, *J* = 14 and 9.6 Hz), 1.62–1.50 (2H, m), 1.52 (1H, sep, *J* = 6.6 Hz), 1.32–1.24 (9H, m), 1.16 (1H, q, *J* = 6.7 Hz), 0.87 (6H, d, *J* = 6.8 Hz). ^{13}C NMR (100 MHz, CD_3OD = 49.15) δ 175.5, 174.6, 138.6, 130.5, 129.6, 128.0, 83.5, 58.6, 54.5, 40.3, 38.1, 34.2, 30.9, 30.7, 29.3, 28.6, 26.0, 23.2. ESI–MS: m/z calcd for $C_{21}H_{34}NO_4$ $[M+H]^+$ 364.25, found 364.15.

Figure S1. The ^{1}H and ^{13}C NMR spectrum of natural P2 in $CDCl_3$

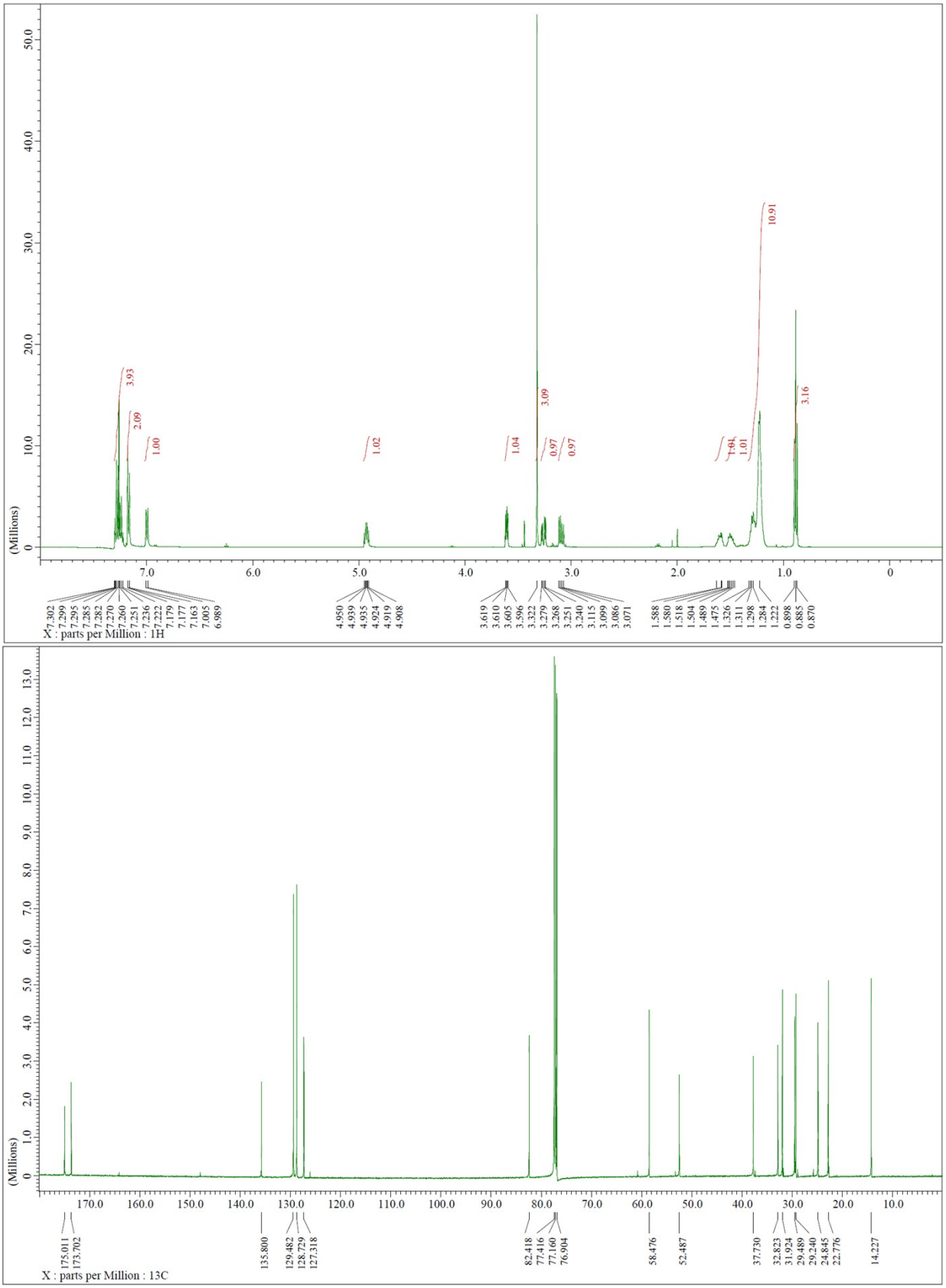


Figure S2. The ^{1}H and ^{13}C NMR spectrum of P1 in MeOD-d_3

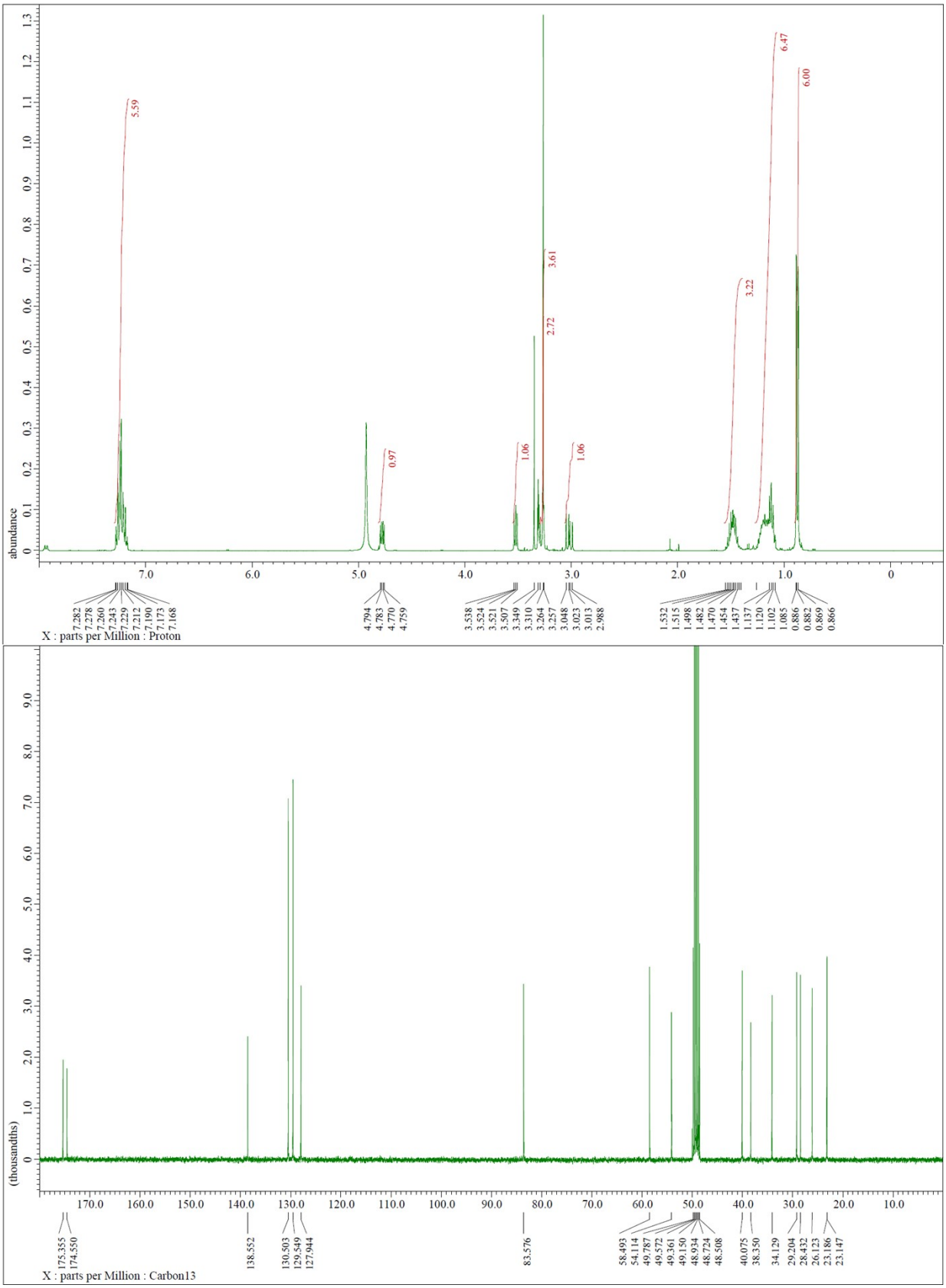


Figure S3. The ^{1}H and ^{13}C NMR spectrum of P2 in MeOD-d_3

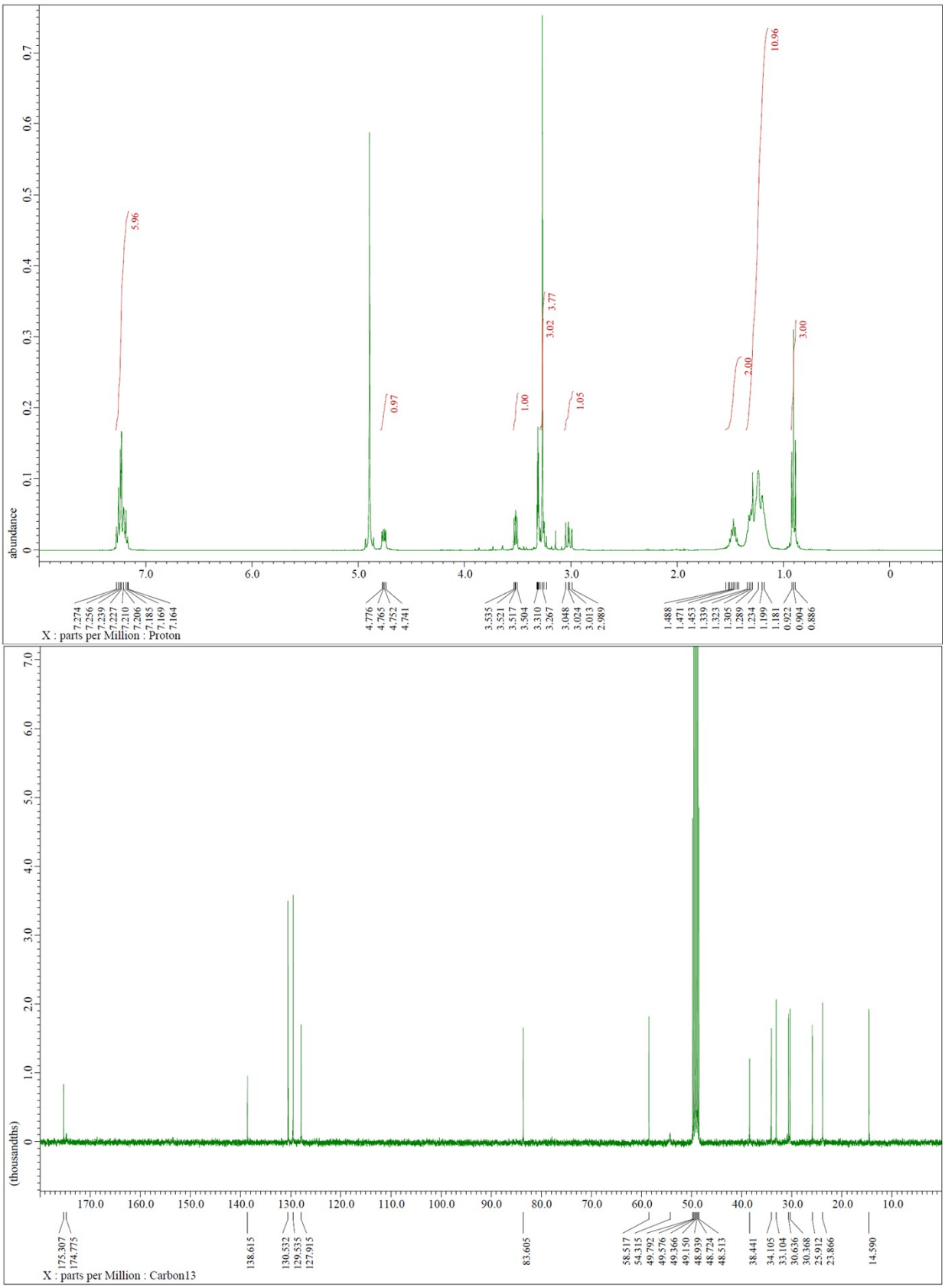


Figure S4. The ^{1}H and ^{13}C NMR spectrum of P2 in $CDCl_3$

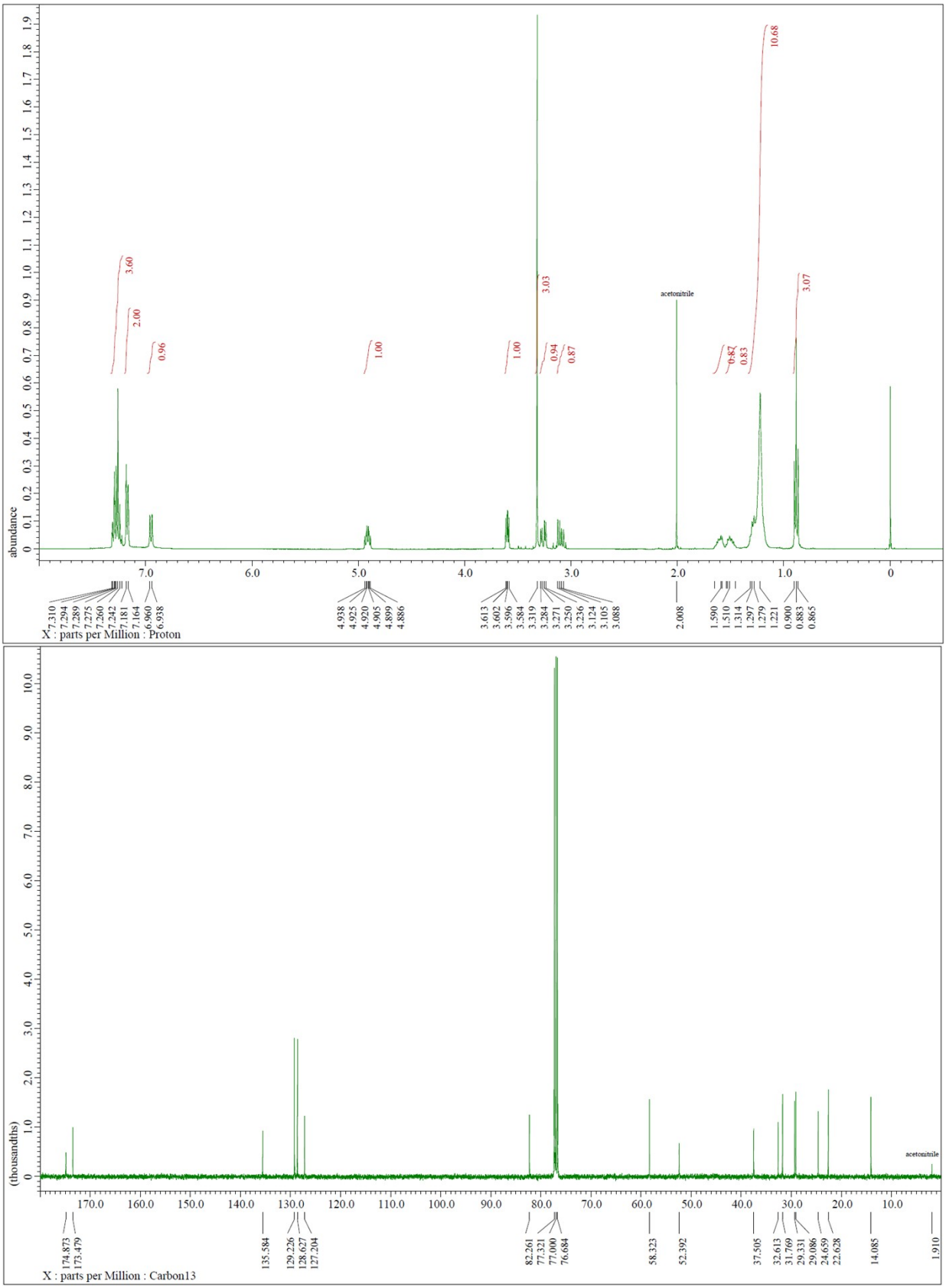


Figure S5. The ^{1}H and ^{13}C NMR spectrum of P3 in MeOD-d_3

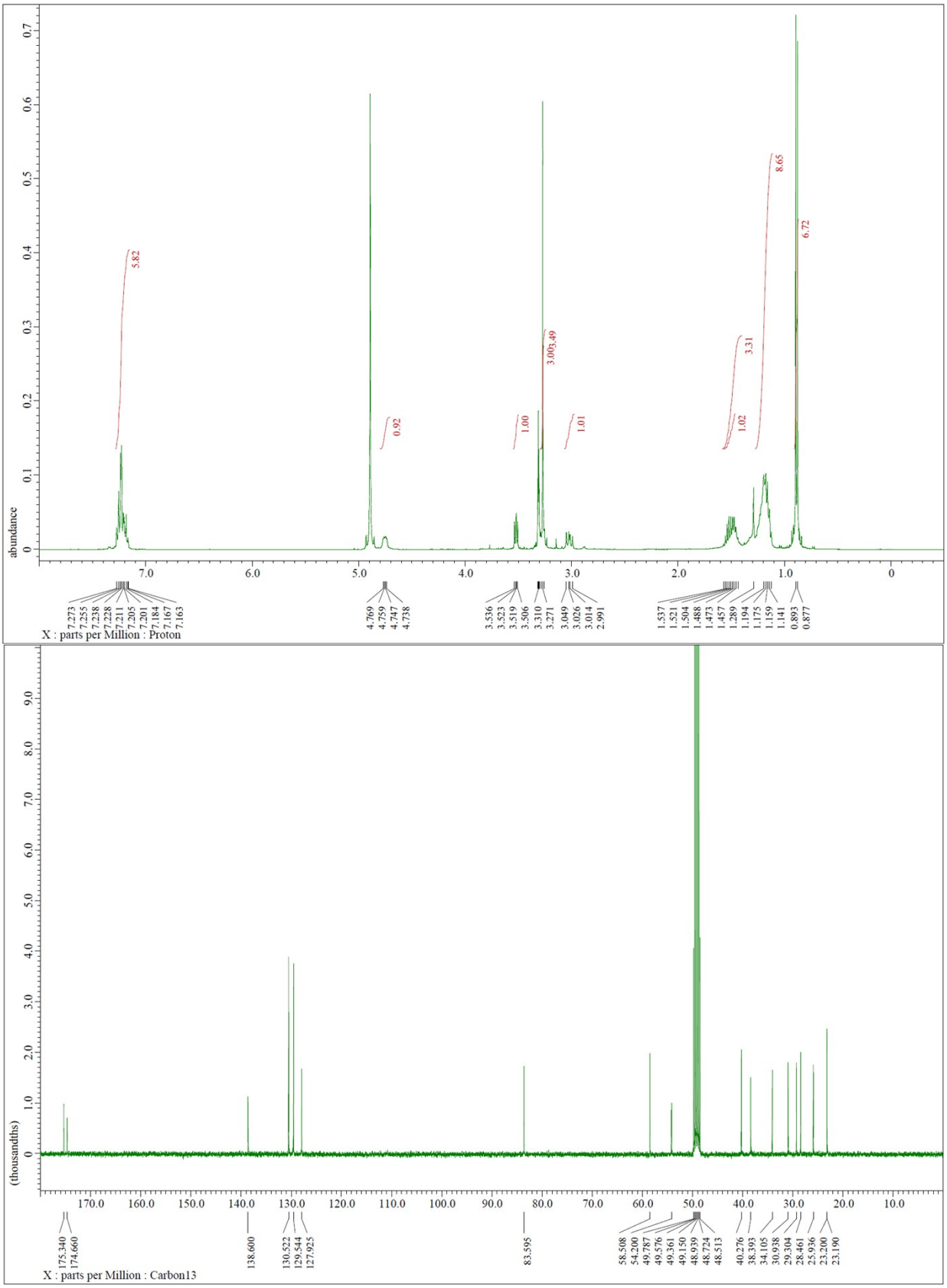


Figure S6. The ^{1}H and ^{13}C NMR spectrum of P4 in MeOD-d_3

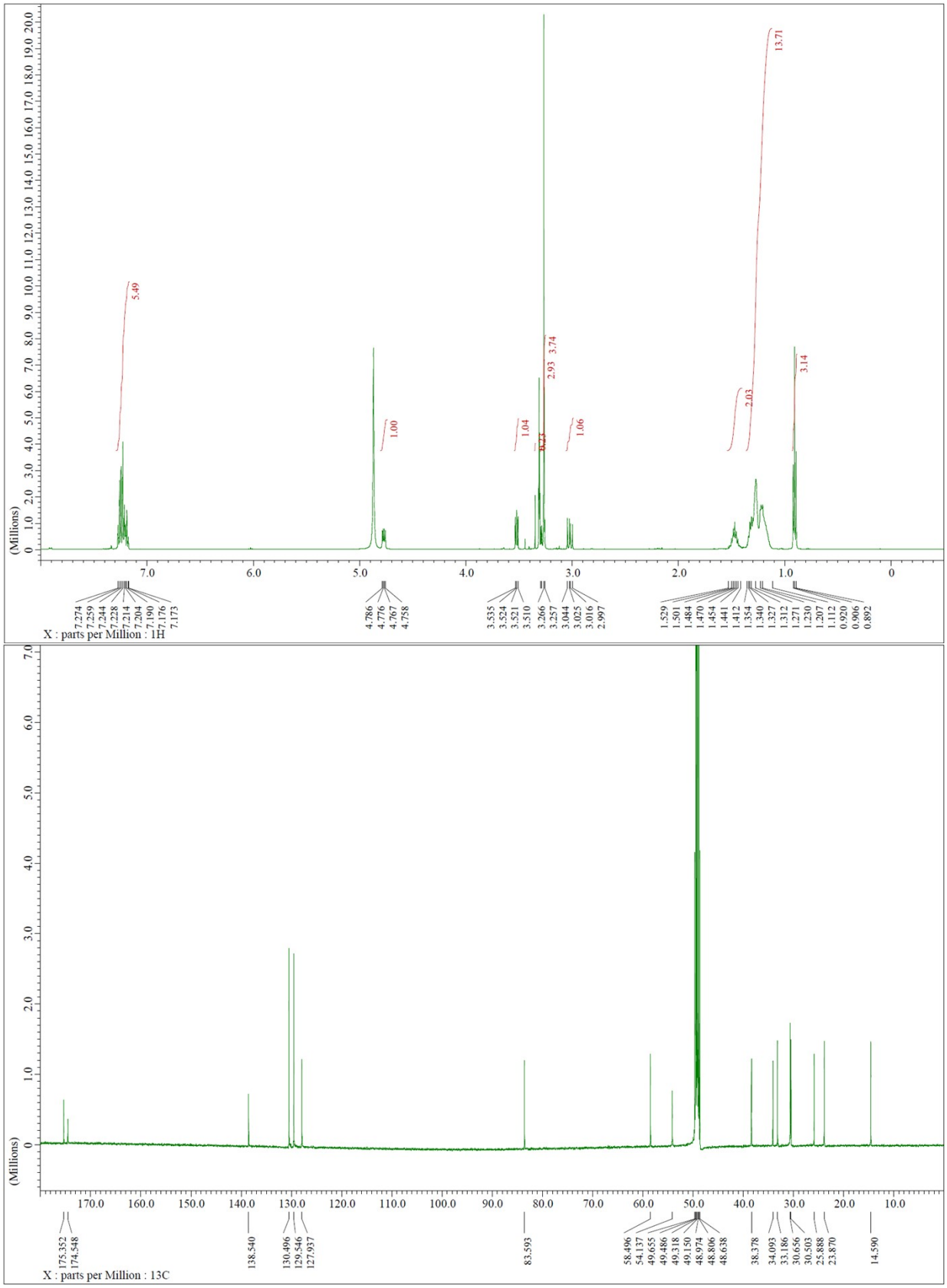


Figure S7. The ^{1}H and ^{13}C NMR spectrum of P5 in MeOD-d_3

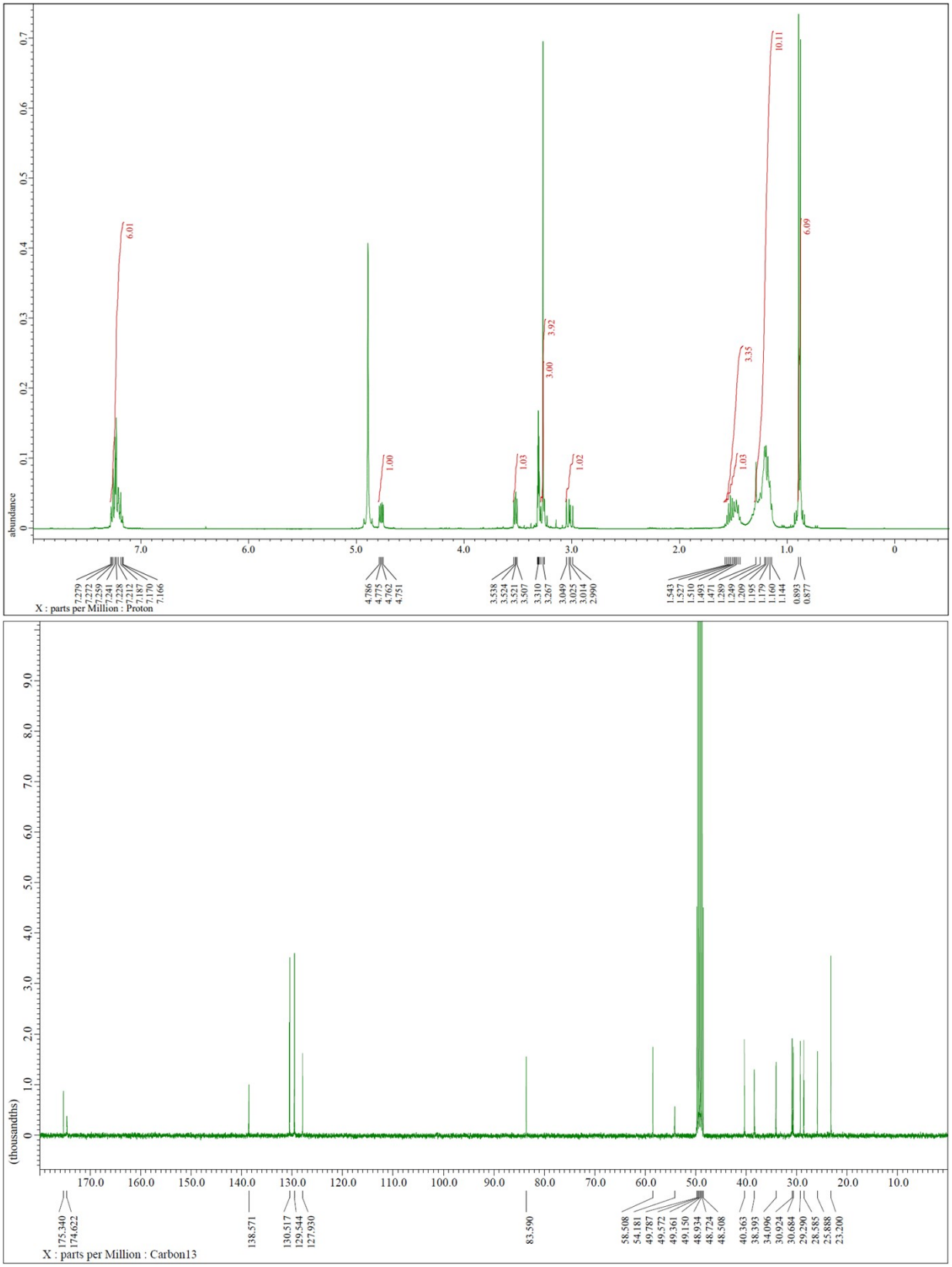


Figure S8. The ^{1}H and ^{13}C NMR spectrum of epi-P1 in MeOD-d_3

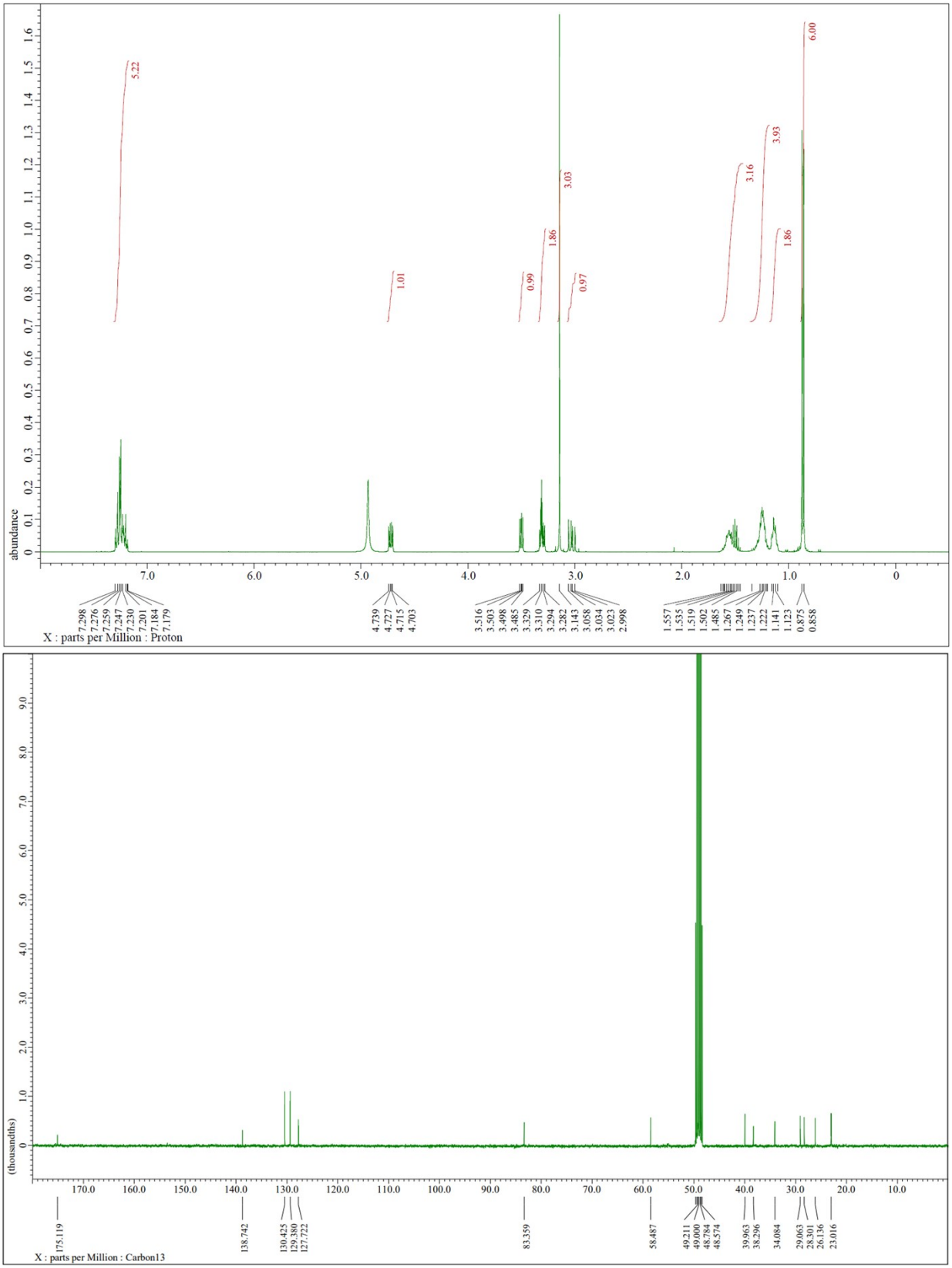


Figure S9. The ^{1}H and ^{13}C NMR spectrum of epi-P2 in MeOD-d_3

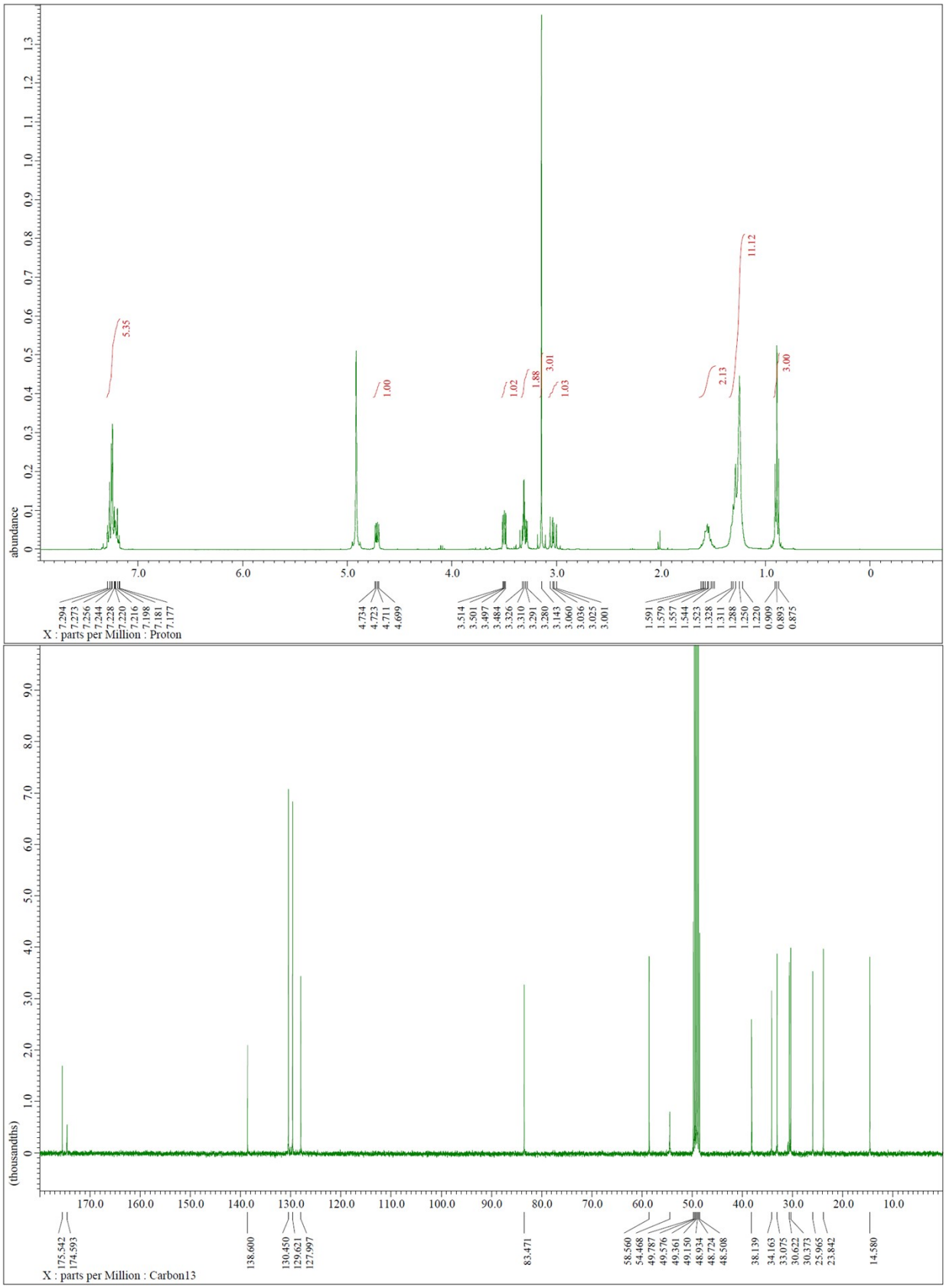


Figure S10. The ^{1}H and ^{13}C NMR spectrum of epi-P2 in $CDCl_3$

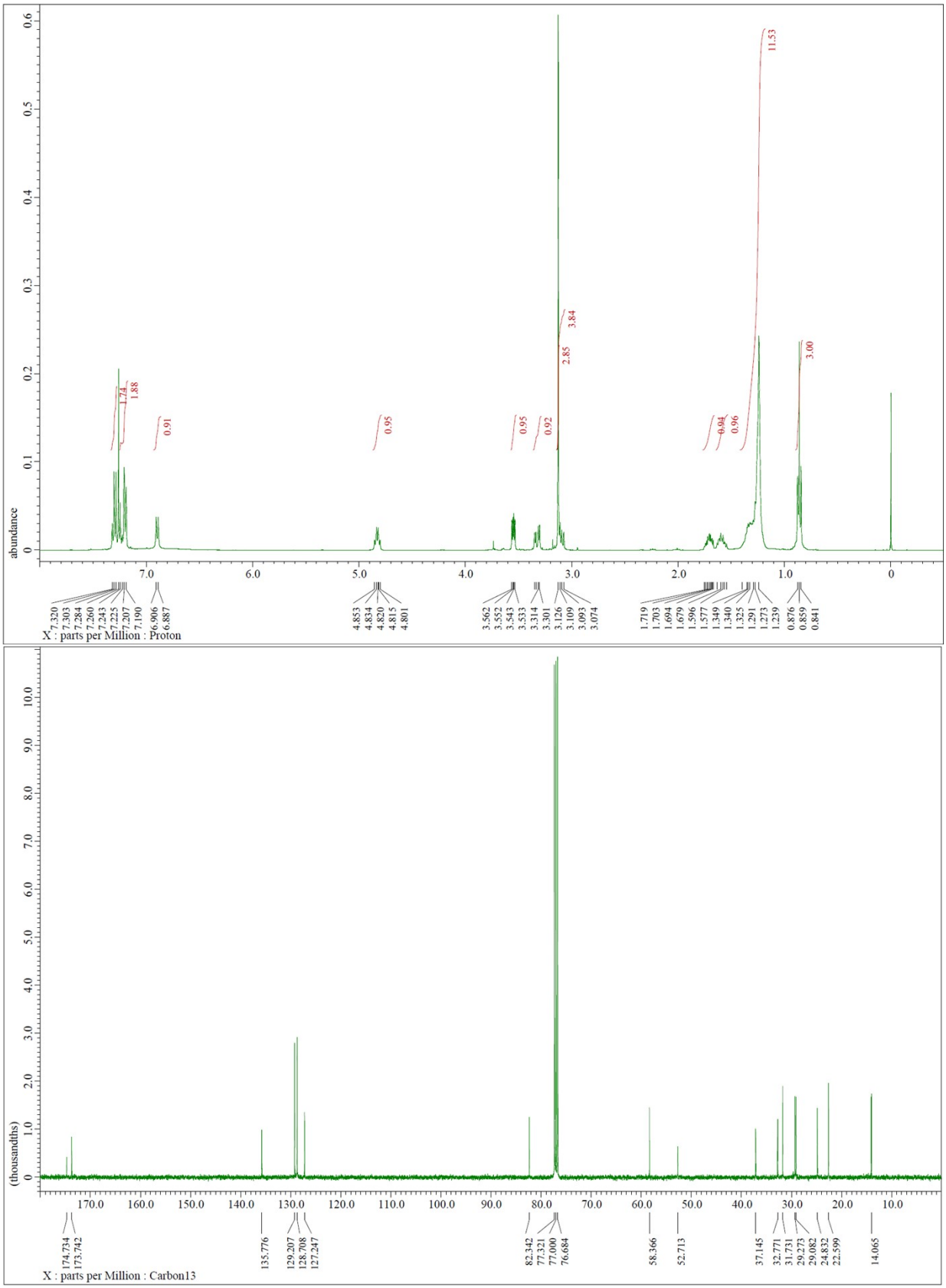


Figure S11. The ^{1}H and ^{13}C NMR spectrum of epi-P3 in MeOD-d_3

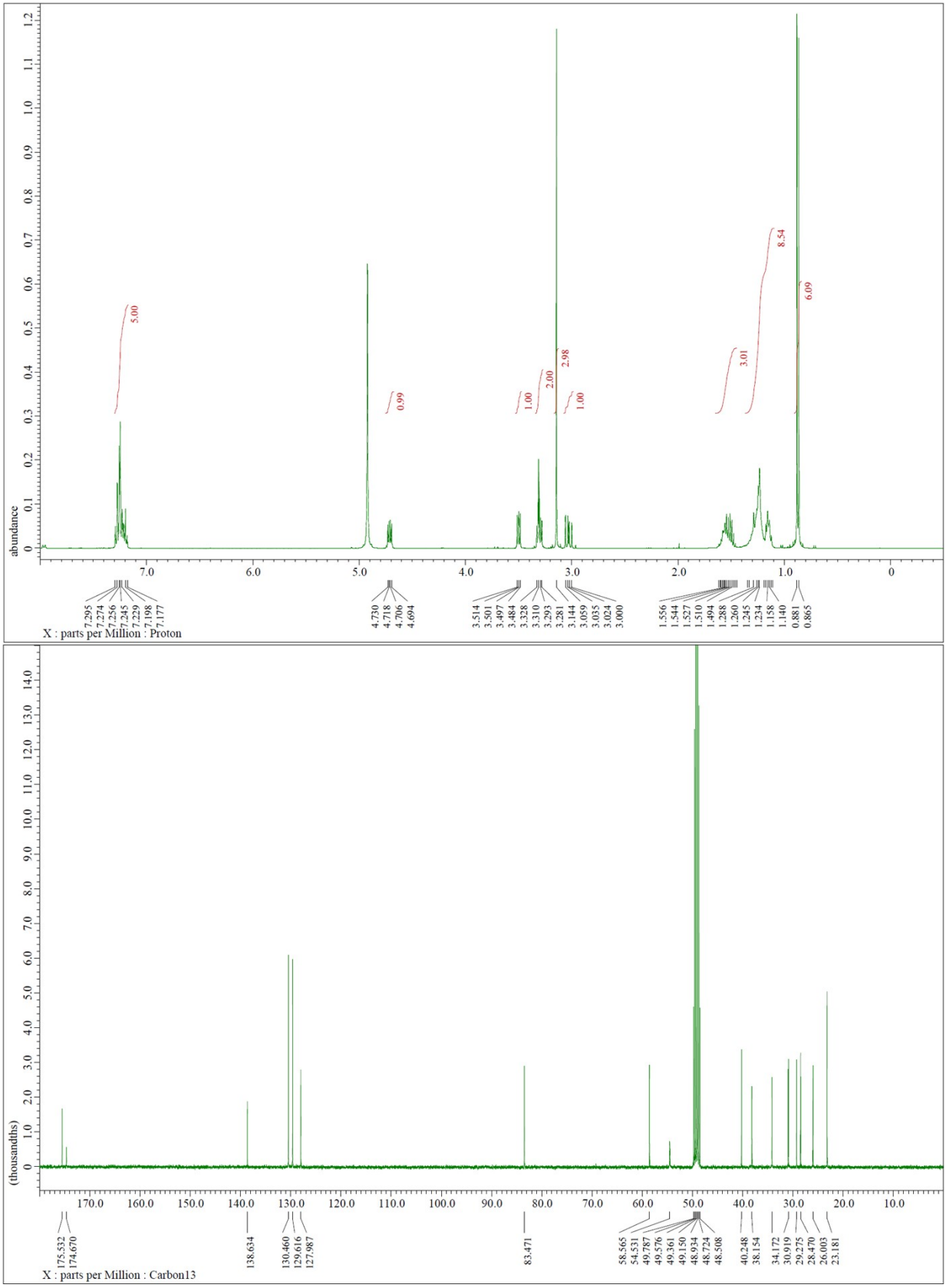


Figure S12. The ^{1}H and ^{13}C NMR spectrum of epi-P4 in MeOD-d_3

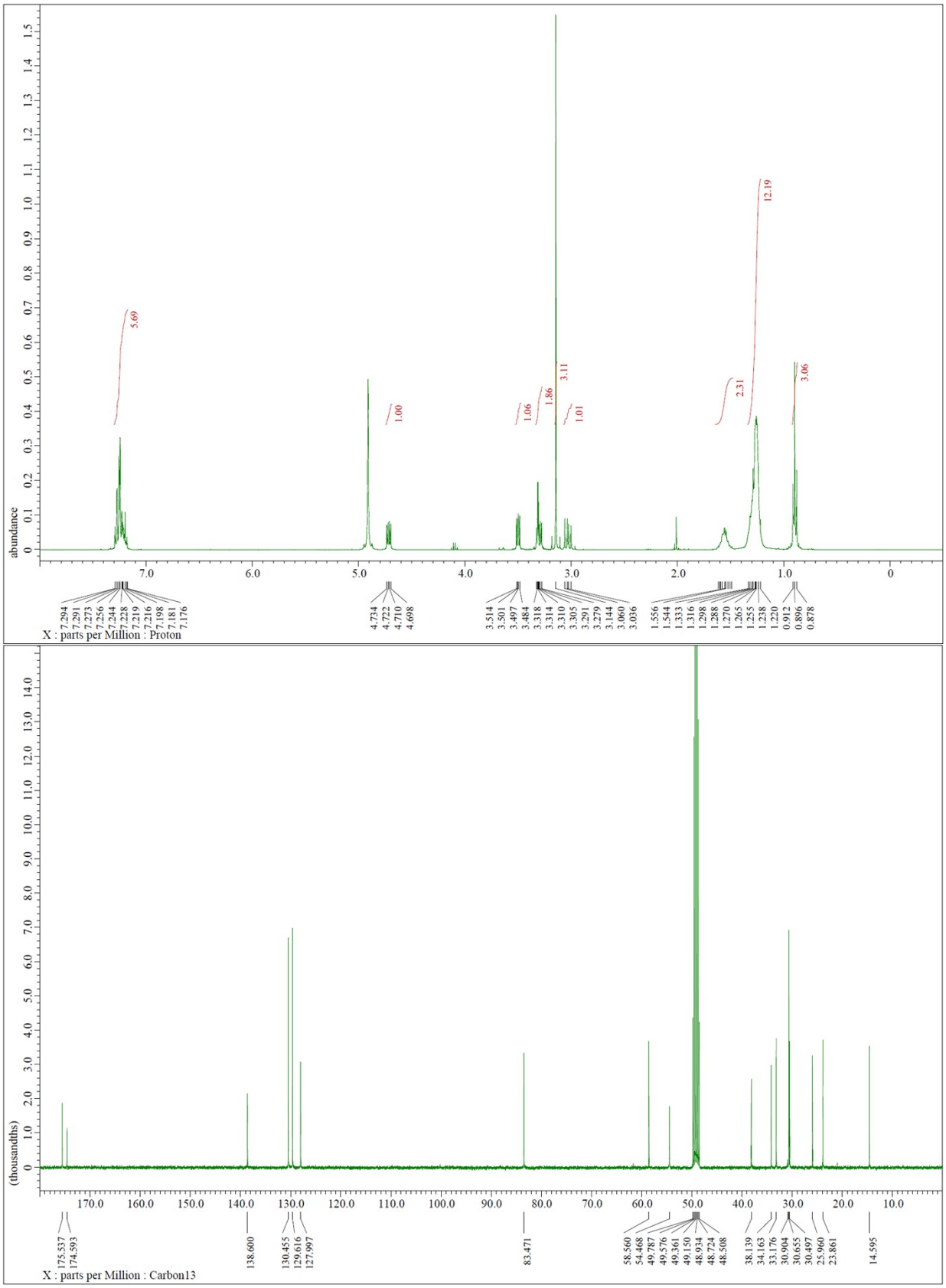


Figure S13. The ^{1}H and ^{13}C NMR spectrum of epi-P5 in MeOD-d_3

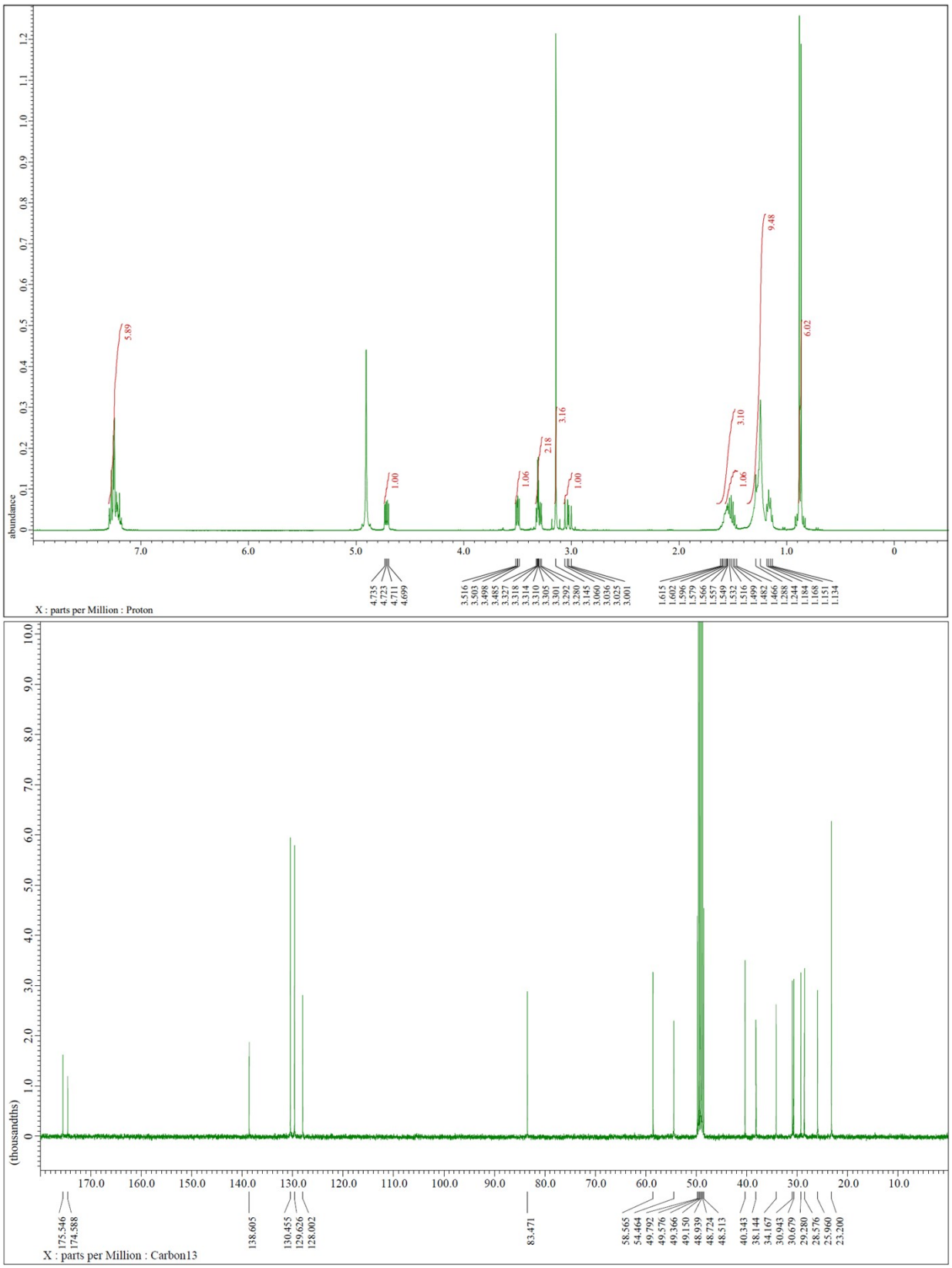


Figure S14. CD spectra of all compounds