Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and investigation of new cyclic molecules using the stilben scaffold

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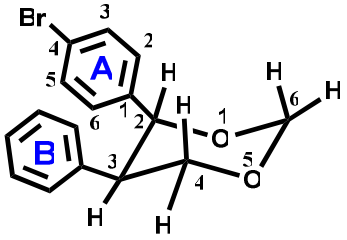
Experimental section.

Substrate (**1, 2, 4**) are commercially available from Sigma-Aldrich, copound (**3**) was synthetized according to literature procedures [Krawczyk,H.;et al, *BioMed Research International* Volume **2014**, Article ID 320895, 8 pages, http://dx.doi.org/10.1155/2014/320895 and (**5**) was prepared according to modyfied literature procedures: [Hattori, T. et al, *Chem. Eur. J.*, 2017, 23, 8196 – 8202]:
Synthesis of (5) THF (100.0 mL), titanium tetrachloride (13.62 g, 7.86 mL, 71.8 mmol) was added dropwise. The mixture was stirred at 0 °C for 0.5 hour and then aldehyde (59.8 mmol) was slowly added. The suspension was refluxed for 24 h under argon, then cooled to 0 °C and diluted with cold water (200 mL). Zinc dust and precipitated stilben were filtered off, washed with distilled water (2x50 ml) and methanol (2x25 ml) and vacuum dried. After recrystallization and hot filtration, pure stilben was obtained. (*E*)-4,4'-dimethoxystilben, crystallized from toluene/ethyl acetate, Yield 68%;. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): 7.41-7.44 (m, 4H, Ar), 6.93 (s, 2H, CH=CH), 6.88-6.91 (m, 4H, Ar), 3.83 (s, 6H, CH_3O). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): 159.2, 130.6, 127.6, 126.3, 114.3, 55.5.

Synthesis of (6); 2 g (3,90 mmol) [(4-bromobenzyl)] triphenylphosphonium bromie in 20 ml distilled water, 326 mg (13.58 mmol) lithium hydroxide were slow sequentially added to a three-necked flask (250 mL) during at for 30 min under nitrogen atmosphere and the mixture was stirred. After 2 min was slow added 660 mg (3.36 mmol) 3,4,5-trimethoxybenzaldehyde.The mixture was stirred at 100 ^{0}C for 24 h. Next was added to mixture of 160 mL of water and extracted with chloroform. The organic layer was dried over anhydrous $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel (hexsane : ethanol 9:1.). Yield 47%, 550 mg; ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): 7.48 (2H, d, *J*=8.5 Hz, H2', H6'); 7.36 (2H, d, *J*=8.5 Hz, H3', H5'); 7.02 (1H, AB spin system, *J*= -16 Hz, Hα); 6.93 (1H, AB spin system, Hβ); 6.73 (2H, s, H2, H6); 3.92 (6H, s, 2-OCH_3); 3.87 (3H, s, -OCH_3). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): 153.42 (C3, C5); 138.19 (C4); 136.15 (C1'); 132.65 (C1); 131.78 (C3',C5'); 129,35 (Cα); 127.85 (C2',C6'); 126.86 (Cβ); 121.25 (C4'); 103.65 (C2,C6); 60.95 (-OCH_3); 56.13 (2-OCH_3). HRMS (ESI): $C_{17}H_{17}O_3NaBr$ (M+Na)+ , calcd *m/z* 371.0259 ; found *m/z* 371.0257.

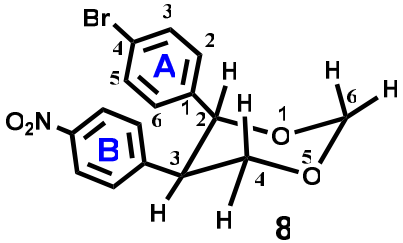
Substrate **(14)** was synthetized according to literature procedures [Krawczyk,H.; et al, *Tetrahedron* **2016**, *72*, 3877).

General procedure of synthesis of compounds (7-11, 15, 16) (Table 1 in the text): (*E*)-stilbenes (**1-6**) or dibenzo[*b*,*f*]oxepin (**14a**) or dibenzo[*b*,*f*]oxepin (**14a**) and 4,4'-diethoxy-1,1'-biphenyl (**14b**) (1 mmol), and paraformaldehyde (1 mmol) in dichloromethane (15 ml), were sequentially added to a three-necked flask (25 mL). The mixture was stirred at for 30 min under nitrogen atmosphere. The reaction flask was capped and nitrogen bubbled through the solution for 30 minutes. Then, boron trifluoride diethyl etherate [$BF_3{\cdot}O(C_2H_5)_2$, 0.25 mL, 2 mmol] was added to the solution and the mixture was stirred at room temperature for 3 h. The solution was poured into methanol (15ml) and washed with water. The organic layer was dried over anhydrous $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel (eluent: CH_2Cl_2). **The procedure of synthesis of compounds** (**12** and **13**) is analogical but without paraformaldehyde.



7

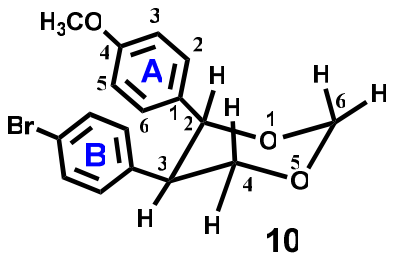
(7): Oil, yield: 80 mg (25%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 5.32 (1H, AB spin system, ^2J = - 6 Hz, H6), 4.99 (1H, AB spin system, H6'), 4.66 (1H, d, ^3J = 10.5 Hz, H2), 3.19 (1H, ddd, ^3J =11 Hz, J= 4.5 Hz, H3), 4.22 (1H, AB spin system, dd, ^2J = -11 Hz, ^3J = 4.5 Hz, H4), 3.91 (AB spin system, t, ^2J = 11 Hz, H4'); **A ring:** 6.88 (1H, d, ^3J = 8.5 Hz, H2,H6), 7.32 (1H, d, H3, H5); **B ring**: 6.99 (2H, d, ^3J = 8.5 Hz, H2, H6), 7.13 (2H, dd, ^3J = 4 Hz, H3, H5), 7.20 (1H, d, H4). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 84.10(C2), 48.72(C3), 71.67(C4), 94.19(C6), **A ring**: 136.19(C1), 130.00(C2,C6), 131.64(C3,C5), 121.10(C4); **B ring**: 138.73(C1), 128.62(C2,C6), 126.99 (C3,C5), 128.18(C4). HRMS (ESI): $C_{16}H_{15}BrO_2Na$+, calcd *m/z* 341.0153; found *m/z* 341.0157.



8

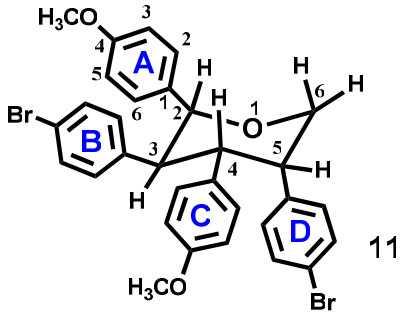
(8): Oil, yield: 73 mg (20%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 5.33 (1H, AB spin system, ^2J = -7 Hz, H6), 5.00 (1H, AB spin system, H6'), 4.68 (1H, d, J = 10 Hz, H2), 3.27 (1H, td, ^3J=11 Hz, ^3J=4.5 Hz, H3). 4.24 (1H, AB spin system, dd, ^2J= -11 Hz, ^3J=4.5 Hz, H4), 3.97 (1H, AB spin system, t, ^2J = - 11 Hz, H4'); **A ring**: 6.98 (2H, d, ^3J = 8.5 Hz, H2,H6), 7.33 (2H, d, H3,H5); **B ring**:

7.17 (2H, d, ^{3}J = 8.5 Hz, H2,H6), 8.09 (2H, d, H3,H5); ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 83.17(C2), 49.47(C3), 71.13(C4), 94.22(C6), **A ring**: 137.77(C1), 128.46(C2,C6), 131.51 (C3,C5), 122.36(C4); **B ring**: 144.34(C1), 129.24(C2,C6), 123.85(C3,C5), 147.22(C4). HRMS (ESI): $C_{16}H_{14}BrNO_4Na$+, calcd *m/z* 386.0004; found *m/z* 386.0001.



10

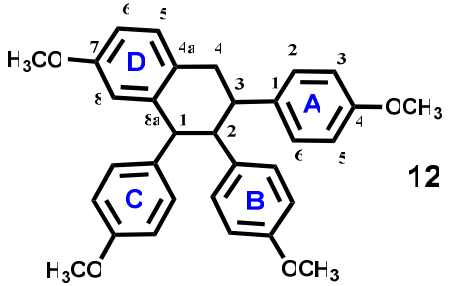
(10): Oil, yield: 87 mg (25%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 5.26 (1H, AB spin system, ^{2}J = -6 Hz, H6), 4.95 (1H, AB spin system, H6'), 4.59 (1H, d, ^{3}J = 10.5 Hz, H2), 3.16 (1H, ddd, ^{3}J= 11 Hz, ^{3}J=4.5 Hz, H3), 4.17 (1H, AB spin system, dd, ^{2}J= -11 Hz, ^{3}J=4.5 Hz, H4), 3.86(1H, AB spin system, t, ^{2}J= -11 Hz, H4'); **A ring**: 7.04 (2H, d, ^{3}J = 8.5 Hz, H2,H6), 6.72 (2H, d, H3,H5), 3.72 (3H, s, OCH_3), **B ring** 6.87 (2H, d, ^{3}J=8.5 Hz, H2, H6), 7.30 (2H, d, H3, H5); ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 83.61(C2), 48.63(C3), 71.73(C4), 94.22(C6), **A ring**: 130.51(C1), 128.22(C2,C6), 113.57 (C3,C5), 159.27(C4), 55.13(s, (C4- OCH_3); **B ring**: 136.37(C1), 129.98(C2,C6), 131.61(C3,C5), 120.99(C4). HRMS (ESI): $C_{17}H_{17}BrO_3Na$+, calcd *m/z* 371.0259; found *m/z* 371.0262.



11

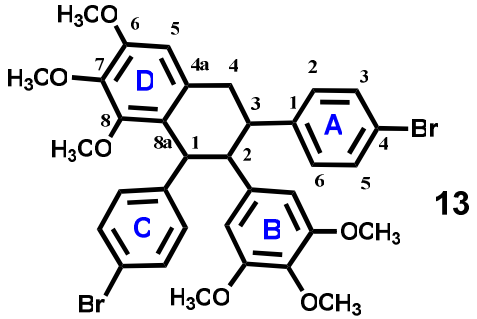
(11): 3,5-bis(4-bromophenyl)-2,4-bis(4-methoxyphenyl)tetrahydro-2H-pyran. White solid, yield: 364 mg (60%), m.p. 119-121 ^{o}C (EtOH). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 4.36 (1H, AB spin system, dd, ^{2}J = -12 Hz, ^{3}J=3.5 Hz, H6), 4.58 (1H, AB spin system, H6'), 4.48 (1H, d, ^{3}J = 9.5 Hz, H2), 3.26 (1H, d, ^{3}J = 10 Hz, H3), 3.78 (1H, d, ^{3}J = 4 Hz, H4), 3.05 (1H, dd, H5); **A ring**: 7.02 (2H, d, ^{3}J = 9 Hz, H2,H6), 6.74 (2H, d, H3,H5), 3.76 (3H, s, OCH_3); **B ring** 6.66 (2H, d, ^{3}J =8.5 Hz, H2, H6), 7.05 (2H, d, H3, H5), **C ring**: 6.52 (2H, s, H2, H6), 6.52 (2H, s, H3, H5); 3.67 (3H, s, OCH_3); **D ring** 7.12 (2H, d, ^{3}J=8.5 Hz, H2,H6), 7.32 (2H, d, H3,H5). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 86.36(C2), 48.11(C3), 50.49(C4), 46.34(C5), 72.63(C6), **A ring**: 132.44(C1),

128.18(C2,C6), 113.50 (C3,C5), 159.01(C4), 55.18 (OCH_3); **B ring**: 138.48(C1), 130.36(C2,C6), 130.92(C3,C5), 119.75(C4); **C ring**: 132.14(C1), 129.76(C2,C6), 113.09(C3,C5), 157.75(C4), 55.00 (OCH_3), **D ring**: 139.74(C1), 132.08(C2,C6), 130.53(C3,C5), 120.50(C4). HRMS (ESI TOF MS ES-): $C_{31}H_{27}Br_2O_3$, calcd *m/z* 605.0327; found *m/z* 605.0318.



12

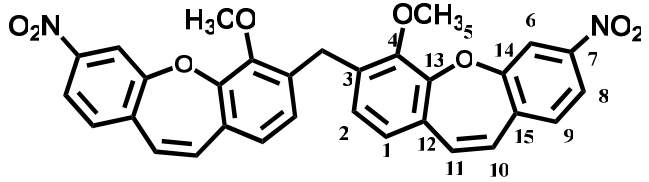
(12): 7-methoxy-1,2,3-tris(4-methoxyphenyl)-1,2,3,4-tetrahydronaphthalene. White solid, yield: 432 mg (90%), m.p. 139-140 °C (EtOH). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): **the ring**: 3.06 (1H, AB spin system, dd ^2J = -16.5 Hz, ^3J=4.5 Hz, H4), 3.18 (1H, AB spin system, dd, ^3J = 11.5 Hz, H4'), 4.18 (1H, d, ^3J = 10.5 Hz, H1), 3.15 (1H, dd, ^3J = 11 Hz, H2), 3.33 (1H, ddd, H3); **A ring**: 6.75 (2H, d, ^3J = 8.5 Hz, H2,H6), 6.66 (2H, d, H3,H5), 3.74 (3H, s, OCH_3); **B ring** 6.68 (2H, d, ^3J =8.5 Hz, H2, H6), 6.52 (2H, d, H3, H5), 3.65 (3H, s, OCH_3); **C ring**: 6.98 (2H, d, ^3J =8.5 Hz, H2, H6), 6.64 (2H, d, H3, H5), 3.70 (3H, s, OCH_3); **D ring** 7.07(1H, d, ^3J =8.5 Hz, H5), 6.34 (1H, d, ^4J = 2.5 Hz, H8), 6.72 (1H, dd, H6), 3.63 (3H, s, OCH_3). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): **the ring**: 55.02(C1), 55.53(C2), 46.35(C3), 39.65(C4); **A ring**: 137.58(C1), 130.19(C2,C6), 113.45(C3,C5), 157.64 (C4), 55.09(OCH_3); **B ring**: 135.18(C1), 129.26(C2,C6), 113.03 (C3,C5), 157.18(C4) 54.91 (OCH_3); **C ring**: 136.82(C1), 128.52 (C2,C6), 113.33 (C3,C5), 157.45(C4),55.06 (OCH_3); **D ring** 129.37 (C4a), 129.06 (C5), 112.07 (C6), 157.75 (C7), 114.86 (C8), 141.45 (C8a), 55.20(OCH_3). HRMS (ESI): $C_{32}H_{32}O_4Na+$, calcd *m/z* 503.2198; found *m/z* 503.2195.



13

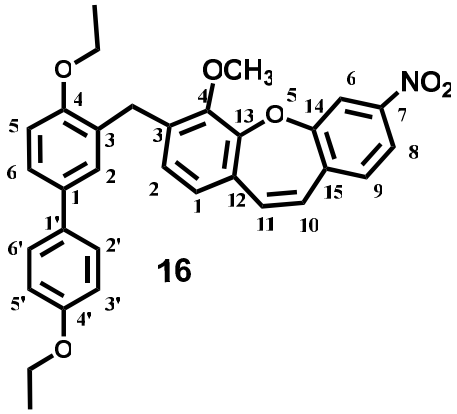
(13): 1,3-bis(4-bromophenyl)-6,7,8-trimethoxy-2-(3,4,5-trimethoxyphenyl)-1,2,3,4-tetrahydronaphthalene. Oil, yield: 594 mg (85%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): **the ring**: 2.92 (1H, dd(AB spin system), ^2J = -17.5 Hz, ^3J = 10 Hz, H4), 3.29 (1H, AB spin system, H4'), 4.28 (1H, d, ^3J = 11 Hz, H1), 3.52 (1H, dd, ^3J = 10.5 Hz H2), 3.33 (1H, dd, H3); **A ring**: 7.39 (2H, d, ^3J = 8.5 Hz, H2, H6), 7.56 (2H, d, H3,

H5); **B ring** 6.44 (2H, s, H2, H6), 3.60 (1H, s, (C3 or C5-OCH_3), 3.82 (1H, s, C3 or C5-OCH_3), 3.81 (1H, s, (C4) OCH_3); **C ring**: 7.35 (2H, d, ^3J = 8.5 Hz, H2,H6), 7.51 (2H, d, H3, H5); **D ring** 5.53 (1H, s, H5), 3.43 (3H, s, C6, OCH_3), 3.19 (3H, s, C8, OCH_3), 3.69 (3H, s, C7, OCH_3). ^{13}C NMR (125 MHz, CDCl3, 298 K): δ (ppm): **the ring**: 57.58(C2), 51.51(C3), 45.69(C1), 34.62(C4); **A ring**: 144.35(C1), 130.07(C2,C6), 131.84(C3,C5), 120.51(C4); **B ring**: 122.09(C1), 104.64(C2,C6), 151.34, 151.41 (C3,C5), 140.46(C4), 60.28(C3 or C5-OCH_3), 55.72(C5 or C3-OCH_3), 60.79 (C4-OCH_3); **C ring**: 144.30(C1), 129.94(C2, C6), 131.58(C3,C5), 120.06(C4); **D ring**: 131.35(C4a), 103.18(C5), 152.90(C6), 141.36(C7), 150.42 (C8), 141.36(C8a), 55.40(C6-OCH_3), 60.67 (C7-OCH_3), 59.84(C8-OCH_3). HRMS (ESI TOF MS ES-, 1.91e^4): $C_{34}H_{34}Br_2O_6$ Na+, calcd *m/z* 721.0600; found *m/z* 721.0598.



15

(15): bis(4-methoxy-7-nitrodibenzo[*b*,*f*]oxepin-3-yl)methane. White solid, above of temerature 123°C decomposition of molecule, yield: 275 mg (100%). ^{1}HNMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): 3.94 (6H, s, OCH_3, OCH_3'), 3.96 (2H, s, CH_2), 6.67 (2H, d, ^3J = 8.5 Hz H2, H2'), 6.83 (2H, d(AB spin system), ^3J = 11.5 Hz, H10,H10'), 6.89 (2H, d, H1, H1'), 6.98 (2H, d(AB spin system), H11, H11'), 7.32 (2H, d, ^3J = 8.5 Hz H9, H9'), 8.01 (2H, dd, ^3J = 8.5 Hz, ^4J =2.5 Hz, H8, H8'), 8.19 (2H, d, H6, H6'). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): 35.37 (CH_2), 56.17(2xOCH_3), 112.97(C1,C1'), 117.49(C6,C6'), 120.07(C8,C8'), 126.56(C2,C2'), 128.65 (C10, C10'), 128.95 (C9, C9'), 129.29 (C12, C12'), 129.35 (C3, C3'), 130.50 (C11, C11'), 137.49(C15, C15'), 145.80 (C13, C13'), 148.54 (C7, C7'), 150.45 (C4, C4'), 157.35 (C14, C14'). HRMS (ESI): $C_{31}H_{22}N_2O_8Na$, calcd *m/z* 573.1274; found *m/z* 573.1277.



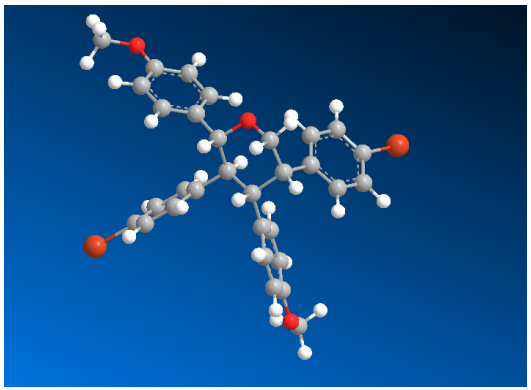
16

(16): 3-((4,4'-diethoxy-[1,1'-biphenyl]-3-yl)methyl)-4-methoxy-7-nitrodibenzo[*b,f*]oxepin. Yellow solid, above of temerature 115 ^{o}C decomposition of molecule, yield 314 mg (60%). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ (ppm): 4.01 (2H, s, CH_2), dibenzo[*b,f*]oxepin ring: 8.20 (1H, d, ^{4}J = 2.5 Hz, H6), 7.99 (1H, dd, ^{3}J = 8.5 Hz, H8), 7.29 (1H, d, H9), 7.15 (1H, d(AB spin system), ^{3}J = 11.5 Hz, H11), 6.97 (1H, d(AB spin system), ^{3}J = 8.5 Hz, H2), 6.93 (1H, d(AB spin system), H1), 6.81(1H, d(AB spin system), H10), 3.95 (3H, s, OCH_3); biphenyl ring: 7.33 (1H, dd, ^{3}J = 8.5 Hz, ^{4}J = 2.5 Hz, H6), 7.25 (2H, d, H2', H6'), 6.96 (1H, d, H2) 6.90 (1H, d, ^{3}J = 8.5 Hz, H5), 6.83 (2H, d, ^{3}J = 8.5 Hz, H3',H5'), 4.09 (2H, q, ^{3}J = 7 Hz, OCH_2), 4.01(2H, q, ^{3}J = 7 Hz, OCH_2), 1.43 (3H, t, CH_3); 1.41 (3H, t, CH_3). ^{13}C NMR (125 MHz, CDCl3, 298 K): δ (ppm): 32.64 (CH_2), dibenzo[*b,f*]oxepin ring: 157.95(C14), 150.16(C4), 148.36(C7), 145,77(C13), 137.81(C15), 131.72(C11), 129.62(C12), 128.81(C3), 128.06(C9), 127.87(C10), 127.35(C2),119.89(C8), 117.46(C6), 113.00(C1), 56.15(OCH_3); biphenyl ring: 157.37(C4'), 155.50(C4), 133.28(C1), 133.05(C1'), 130.55(C3), 127.56(C2) and (C2', C6'), 125.42(C6), 114.60(C3', C5'), 111.27(C5) 63.72(OCH_2), 63.47(OCH_2), 14.96 (CH_3), 14.83(CH_3). HRMS (ESI): $C_{32}H_{29}NO_6Na$, calcd *m/z* 546.1893; found *m/z* 546.1873.

Procedure of synthesis of compound (12) with iodine: (*E*)-stilben (**5**) (1 mmol), and iodine (1mmol) in dichloromethane (15 ml), [and or not paraformaldehyde (1 mmol)] were sequentially added to a three-necked flask (25 mL). The mixture was stirred at room temperature for 20 h under nitrogen atmosphere. The solution was poured into methanol (15ml) and washed with water with $Na_2S_2O_5$ and water. The organic layer was dried over anhydrous $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel (eluent: CH_2Cl_2). Yield 90% (or with paraformaldehyde 70%).

Computational aspects

The optimum ground-state geometry for (**11-13, 15, 16**) compounds were calculated using the density functional theory (DFT). In calculation the B3LYP functional and /6-31G* basis set was employed and the continuum model (PCM; Gaussian 03W) [1,2] was used in order to simulate the effects of the solvent. All the calculations were performed on a server equipped with a 16 quad-core XEON (R) CPU E7310 processor operating at 1.60 GHz. The operating system was Open SUSE 10.3. in $CDCl_3$ as a solvent. Proton and carbon chemical shifts were calculated using GIAO–DFT method. In calculation stages the B3LYP functional and 6-31g* basis set were employed and the Gaussian 03W program was used. The relative chemical shift of a given nucleus *X* in the molecule was defined as δ calc *X* [ppm] = σref*X*– σcalc*X* . For the ^{1}H and ^{13}C spectra, σref *X* is equal to 31.9 and 183.06 ppm respectively, as found on the DFT [B3LYP/6-31g*] geometry of the dual reference standard (TMS).



The calculated coordinates of (**11**) (the part of calculated log file):

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After PCM corrections, the SCF energy is -6567.22609663     a.u.
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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.014114	-3.486809	0.420957
2	6	0	3.180448	-2.656265	1.176172
3	6	0	1.825733	-2.509931	0.878463
4	6	0	1.306710	-3.235425	-0.206629
5	6	0	2.116797	-4.068531	-0.965507
6	6	0	3.480918	-4.197995	-0.658775
7	6	0	0.944023	-1.592850	1.697262
8	6	0	0.466380	-0.326031	0.920335
9	6	0	1.655958	0.492014	0.441231
10	6	0	1.990193	0.531074	-0.918231
11	6	0	3.091977	1.250916	-1.380633
12	6	0	3.877865	1.941870	-0.463172
13	6	0	3.579767	1.922564	0.896897
14	6	0	2.472088	1.198236	1.337207
15	6	0	-0.513687	0.491302	1.805511
16	6	0	-1.679118	-0.414914	2.344022
17	6	0	-1.043835	-1.643275	3.013527
18	8	0	-0.177065	-2.362755	2.143200
19	6	0	-2.768567	-0.755247	1.334610
20	6	0	-1.002802	1.790035	1.184315
21	6	0	-3.872134	0.102851	1.203648
22	6	0	-4.906968	-0.162722	0.308058
23	6	0	-4.842651	-1.313333	-0.473720
24	6	0	-3.771083	-2.194040	-0.365364
25	6	0	-2.742800	-1.909714	0.536386
26	6	0	-1.126692	2.935467	1.988080
27	6	0	-1.599630	4.138740	1.479258
28	6	0	-1.961496	4.234555	0.128162
29	6	0	-1.843649	3.108449	-0.693641
30	6	0	-1.371918	1.906279	-0.159181
31	35	0	-6.256808	-1.692373	-1.712475

32	35	0	5.393996	2.939888	-1.080897
33	8	0	4.192500	-5.038689	-1.465664
34	6	0	5.580758	-5.200911	-1.207196
35	8	0	-2.407519	5.458612	-0.284218
36	6	0	-2.774464	5.613671	-1.648054
37	1	0	5.062034	-3.570299	0.685293
38	1	0	3.607297	-2.108815	2.013213
39	1	0	0.252538	-3.153456	-0.456118
40	1	0	1.716815	-4.632563	-1.802998
41	1	0	1.509392	-1.251348	2.581428
42	1	0	-0.073626	-0.689035	0.037667
43	1	0	1.383101	-0.015497	-1.635239
44	1	0	3.334046	1.271256	-2.437984
45	1	0	4.199789	2.465533	1.602617
46	1	0	2.249422	1.193942	2.400975
47	1	0	0.044281	0.772390	2.710818
48	1	0	-2.160813	0.161806	3.145590
49	1	0	-0.481264	-1.316131	3.904332
50	1	0	-1.806781	-2.358423	3.334978
51	1	0	-3.926275	1.000779	1.813096
52	1	0	-5.750557	0.514154	0.222637
53	1	0	-3.736081	-3.093625	-0.971242
54	1	0	-1.918253	-2.607608	0.630700
55	1	0	-0.842746	2.884059	3.037631
56	1	0	-1.688067	5.020058	2.107749
57	1	0	-2.115144	3.150135	-1.742414
58	1	0	-1.298878	1.047375	-0.819421
59	1	0	5.947276	-5.895010	-1.965625
60	1	0	6.120254	-4.249021	-1.294771
61	1	0	5.757866	-5.625691	-0.210623
62	1	0	-3.089254	6.653155	-1.757201
63	1	0	-1.927036	5.418938	-2.318061
64	1	0	-3.607657	4.952392	-1.919524

The calculated proton and ^{13}C chemical shifts and coupling constants for (**11**):

(11): ^{1}H NMR δ (ppm): **the tetrahydropyran ring**: 4.44 (1H, AB spin system, dd, ^{2}J = -11.7 Hz, ^{3}J=3,4 Hz, H6), 4.61 (1H, AB spin system, ^{3}J=1.1Hz, H6'), 4.52 (1H, d, ^{3}J = 8.1 Hz, H2), 3.27 (1H, d, ^{3}J = 10.6 Hz, H3), 3.79 (1H, d, ^{3}J = 5.1 Hz, H4), 3.01 (1H, dd, H5); **A ring**: 7.39 (2H, d, ^{3}J = 7.1 Hz, H2,H6), 6.86 (2H, d, H3,H5), 3.69 (3H, s, OCH_3); **B ring** 7.02 (2H, d, ^{3}J =7.2 Hz, H2, H6), 7.15 (2H, d, H3, H5), **C ring**: 6.83 (2H, s, H2, H6), 6.66 (2H, s, H3, H5); 3.58 (3H, s, OCH_3); **D ring** 7.60 (2H, d, ^{3}J=7.3 Hz, H2,H6), 7.47 (2H,d, H3,H5).
^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): **the tetrahydropyran ring**: 94.18 (C2), 55.30 (C3), 58.24 (C4), 53.25 (C5), 78.00 (C6), **A ring**: 139.65 (C1), 134.45 (C2,C6), 116.83 (C3,C5), 166.95 (C4), 55.94 (OCH_3); **B ring**148.27 (C1), 136.26 (C2,C6), 136.22 (C3,C5), 143.19 (C4) -different chemical shift compared to the experimental chemical shift; **C ring**: 139.43 (C1), 136.45 (C2,C6), 116.41 (C3,C5), 165.72 (C4), 55.76 (OCH_3), **D ring**: 149.28 (C1), 138.34 (C2,C6), 135.76 (C3,C5), 144.21(C4) -different chemical shift compared to the experimental chemical shift.

The calculated coordinates of (**12**) (the part of calculated log file):

After PCM corrections, the SCF energy is -1539.54534387 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.022958	-1.662770	-0.233083
2	6	0	-0.219428	-0.356852	0.029452
3	6	0	-2.472580	-1.592433	0.221120
4	6	0	-0.924237	0.890833	-0.482207
5	6	0	-3.517873	-1.798896	-0.681583
6	6	0	-4.859315	-1.774525	-0.285514
7	6	0	-5.176937	-1.536799	1.054814
8	6	0	-4.142525	-1.326254	1.978698
9	6	0	-2.817469	-1.356208	1.563457
10	6	0	-1.266898	1.038897	-1.837480
11	6	0	-1.901115	2.182456	-2.305956
12	6	0	-2.216126	3.225986	-1.423251
13	6	0	-1.886144	3.101441	-0.070874
14	6	0	-1.247265	1.941203	0.378486
15	6	0	1.227475	-0.454571	-0.560509
16	6	0	1.877103	-1.833753	-0.404011

17	6	0	1.158163	-2.951038	0.037185
18	6	0	-0.296621	-2.845663	0.435544
19	6	0	3.226373	-1.978340	-0.777376
20	6	0	3.862127	-3.216866	-0.704108
21	6	0	3.145803	-4.336808	-0.254786
22	6	0	1.814545	-4.192602	0.102569
23	6	0	2.104600	0.668252	-0.013021
24	6	0	2.431020	1.783379	-0.798308
25	6	0	3.208822	2.822424	-0.297824
26	6	0	3.684725	2.773592	1.018780
27	6	0	3.370907	1.669821	1.821661
28	6	0	2.590610	0.636342	1.298567
29	8	0	-6.447015	-1.490191	1.560995
30	6	0	-7.530565	-1.675326	0.661600
31	8	0	-2.837773	4.310396	-1.980159
32	6	0	-3.174342	5.396159	-1.128921
33	8	0	5.168672	-3.442798	-1.043962
34	6	0	5.942487	-2.341033	-1.496193
35	8	0	4.440936	3.839929	1.421766
36	6	0	4.948639	3.836895	2.748306
37	1	0	-1.023098	-1.844226	-1.317340
38	1	0	-0.118455	-0.254744	1.118583
39	1	0	-3.288359	-1.984579	-1.728582
40	1	0	-5.634729	-1.940064	-1.025053
41	1	0	-4.401881	-1.141509	3.017165
42	1	0	-2.037947	-1.193300	2.303898
43	1	0	-1.037788	0.245543	-2.545553
44	1	0	-2.165293	2.289449	-3.354090
45	1	0	-2.115580	3.889711	0.637370
46	1	0	-0.992592	1.862382	1.432681
47	1	0	1.132464	-0.281765	-1.642264
48	1	0	-0.380684	-2.739101	1.527951
49	1	0	-0.818461	-3.778902	0.189033
50	1	0	3.766569	-1.101678	-1.115344
51	1	0	3.647723	-5.298440	-0.203548
52	1	0	1.258907	-5.064326	0.442652

53	1	0	2.063082	1.843548	-1.819664
54	1	0	3.459309	3.682586	-0.911789
55	1	0	3.728559	1.600414	2.842942
56	1	0	2.370085	-0.220820	1.930569
57	1	0	-8.437759	-1.588170	1.262432
58	1	0	-7.539906	-0.907060	-0.122847
59	1	0	-7.500933	-2.667209	0.191656
60	1	0	-3.651399	6.142165	-1.767505
61	1	0	-3.876773	5.090391	-0.342365
62	1	0	-2.282597	5.835424	-0.662683
63	1	0	6.939101	-2.737575	-1.699730
64	1	0	5.530023	-1.907994	-2.417016
65	1	0	6.013090	-1.556366	-0.731705
66	1	0	5.515260	4.763875	2.855085
67	1	0	4.139925	3.819403	3.490724
68	1	0	5.615588	2.982595	2.923821

The calculated proton and ^{13}C chemical shifts and coupling constants for (**12**):

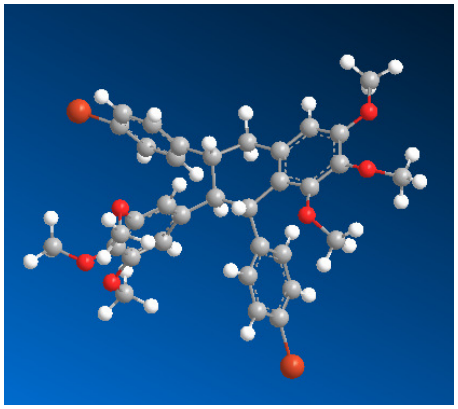
(12): ^{1}H NMR, δ (ppm): **the ring**: 3.00 (1H, AB spin system, dd ^{2}J = -15.9 Hz, ^{3}J=4,0 Hz, H4'), 3.32 (1H, AB spin system, dd, ^{3}J = 10.5 Hz, H4'), 4.33 (1H, d, ^{3}J = 9Hz, H1), 3.15 (1H, dd, ^{3}J = 10 Hz, H2), 3.32 (1H, ddd, H3); **A ring:** 7.09 (2H, d, ^{3}J = 6.9 Hz, H2,H6), 6.81 (2H, d, H3,H5), 3.74 (3H, s, OCH_3); **B ring** 7.05 (2H, d, ^{3}J =7.0 Hz, H2, H6), 6.64 (2H, d, H3, H5), 3.56 (3H, s, OCH_3); **C ring**: 7.30 (2H, d, ^{3}J=6.9 Hz, H2, H6), 6.77 (2H, d, H3, H5), 3.64 (3H, s, OCH_3); **D ring** 7.29 (1H, d, ^{3}J = 6.7 Hz, H5), 6.31(1H, d, ^{4}J =2.5 Hz, H8), 6.89 (1H, dd, H6), 3.46 (3H, s, OCH_3). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): δ (ppm): **the ring**: 62.60 (C1), 63.81 (C2), 53.22 (C3), 45.01 (C4); **A ring**: 146.71 (C1), 136.71 (C2,C6), 116.50 (C3,C5), 165.52 (C4), 55.88 (OCH_3); **B ring**: 143.04 (C1), 135.55 (C2,C6), 116.27 (C3,C5), 165.27 (C4) 55.60 (OCH_3); **C ring**: 144.49 (C1), 134.44 (C2,C6), 116.62 (C3,C5), 165.39 (C4), 55.69 (OCH_3); **D ring** 136.24 (C4a), 134.38 (C5), 119.42 (C6), 165.11 (C7), 115.01 (C8), 150.55 (C8a), 55.44 (OCH_3).

The calculated coordinates of (**13**)(the part of calculated log file):

After PCM corrections, the SCF energy is -6910.77271155 a.u.

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)



Number	Number	Type	X	Y	Z
1	6	0	-0.791635	1.810113	0.161502
2	6	0	-0.183129	0.386706	0.023396
3	6	0	-2.235489	1.888157	-0.309724
4	6	0	-1.048103	-0.691264	0.664257
5	6	0	-3.254329	2.249417	0.580387
6	6	0	-4.584722	2.347317	0.169491
7	6	0	-4.900628	2.078204	-1.158787
8	6	0	-3.914014	1.715501	-2.073056
9	6	0	-2.591240	1.623933	-1.640917
10	6	0	-1.318855	-0.674919	2.035613
11	6	0	-2.126174	-1.658473	2.613146
12	6	0	-2.665688	-2.686070	1.828948
13	6	0	-2.387566	-2.712838	0.448049
14	6	0	-1.584144	-1.719301	-0.121981
15	6	0	1.288629	0.315666	0.567789
16	6	0	2.063287	1.627904	0.466570
17	6	0	1.526947	2.787417	-0.097638
18	6	0	0.102043	2.804675	-0.603494
19	6	0	3.372959	1.679335	1.001586
20	6	0	4.144204	2.847076	0.930896
21	6	0	3.587994	4.001665	0.334553
22	6	0	2.290911	3.962171	-0.168985
23	6	0	2.010241	-0.844077	-0.120642
24	6	0	2.102386	-2.098379	0.494496
25	6	0	2.713612	-3.178916	-0.143813
26	6	0	3.238938	-2.999631	-1.420763
27	6	0	3.161970	-1.766223	-2.063269
28	6	0	2.546779	-0.699351	-1.407269
29	35	0	-6.722644	2.207212	-1.741989
30	35	0	4.087846	-4.472868	-2.309293
31	8	0	4.381932	5.113201	0.343339
32	6	0	3.862300	6.313091	-0.215499
33	8	0	3.796600	0.557678	1.662138
34	6	0	5.099028	0.028977	1.398575

35	8	0	-2.425561	-1.560110	3.953105
36	6	0	-1.869330	-2.585496	4.783930
37	8	0	5.374565	2.885123	1.547741
38	6	0	6.507170	3.097299	0.694792
39	8	0	-3.432290	-3.673547	2.406250
40	6	0	-4.843437	-3.458784	2.291222
41	8	0	-2.956473	-3.742790	-0.243011
42	6	0	-2.740538	-3.807697	-1.646393
43	1	0	-0.770725	2.092542	1.222603
44	1	0	-0.138590	0.174781	-1.052721
45	1	0	-3.008845	2.457246	1.618766
46	1	0	-5.360992	2.627231	0.873929
47	1	0	-4.172954	1.508625	-3.106271
48	1	0	-1.830233	1.339822	-2.363295
49	1	0	-0.926763	0.103222	2.684072
50	1	0	-1.367902	-1.736857	-1.183774
51	1	0	1.230695	0.060169	1.631930
52	1	0	0.072194	2.564605	-1.676957
53	1	0	-0.309015	3.817071	-0.511154
54	1	0	1.843186	4.850094	-0.601222
55	1	0	1.692601	-2.236820	1.491220
56	1	0	2.780132	-4.144255	0.347212
57	1	0	3.576749	-1.638593	-3.057847
58	1	0	2.496611	0.265966	-1.904749
59	1	0	4.652274	7.058150	-0.106416
60	1	0	3.620984	6.190012	-1.278990
61	1	0	2.967189	6.650171	0.322187
62	1	0	5.050917	-1.028174	1.671013
63	1	0	5.345553	0.110383	0.333753
64	1	0	5.861775	0.534781	1.994477
65	1	0	-2.178908	-2.348718	5.804757
66	1	0	-2.246046	-3.572789	4.502125
67	1	0	-0.772639	-2.577363	4.727844
68	1	0	7.384694	3.040842	1.343238
69	1	0	6.572322	2.314103	-0.071637
70	1	0	6.464823	4.077996	0.215101

71	1	0	-5.323631	-4.298178	2.800129
72	1	0	-5.136059	-2.520313	2.777621
73	1	0	-5.152741	-3.443928	1.240205
74	1	0	-3.287128	-4.687421	-1.990831
75	1	0	-3.128224	-2.915911	-2.155316
76	1	0	-1.675813	-3.926223	-1.884395

The calculated proton and ^{13}C chemical shifts and coupling constants for (**13**):

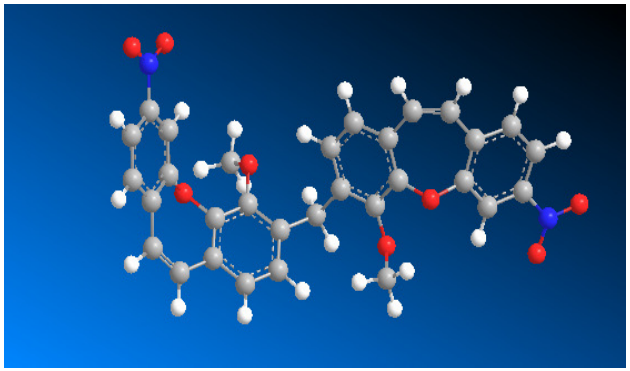
(13): ^{1}H NMR, δ (ppm): **the ring**: 2.38 (1H, dd(AB spin system), ^{2}J = -17.6 Hz, ^{3}J = 10.6 Hz, H4), 2.91 (1H, AB spin system, ^{3}J = 3.4 Hz, H4'), 4.02 (1H, d, ^{3}J = 8.3 Hz, H1), 2.42 (1H, dd, ^{3}J = 10,5 Hz H2), 2.77 (1H, dd, H3); **A ring**: 6.61 (2H, d, ^{3}J = 8.2 Hz, H2, H6), 6.63 (2H, d, H3, H5); **B ring** 5.61 (2H, s, H2, H6), 3.02 (3H, s, (C3 or C5-OCH_3), 3.58 (3H, s, C3 or C5-OCH_3), 3.21 (3H, s, (C4) OCH_3); **C ring**: 6.46 (2H, d, ^{3}J = 8.3 Hz, H2,H6), 6.67 (2H, d, H3, H5); **D ring** 5.74 (1H, s, H5), 3.46 (3H, s, (C6, OCH_3), 2.94 (3H, s, C8, OCH_3), 3.45 (3H, s, C7, OCH_3). ^{13}C NMR, δ (ppm): **the ring**: 54.01 (C2), 41.77 (C3), 46.94 (C1), 34.31(C4); **A ring**: 130.42 (C1), 116.47 (C2,C6) different chemical shift compared to the experimental chemical shift, 118.01 (C3,C5) different chemical shift compared to the experimental chemical shift, 125.36 (C4); **B ring**: 127.27 (C1), 100.15 (C2,C6), 140.95 (C3,C5), 128.90 (C4), 51.42 (C3 or C5-OCH_3), 45.88 (C5 or C3-OCH_3), 50.99 (C4-OCH_3); **C ring**: 136.07 (C1), 116.58 (C2, C6) different chemical shift compared to the experimental chemical shift, 117.64 (C3,C5) different chemical shift compared to the experimental chemical shift, 124.29 (C4); **D ring**: 121.52 (C4a), 93.07(C5), 127.81 (C7), 139.89 (C6), 138.86 (C8), 113.92 (C8a), 45.88 (C6-OCH_3), 50.49 (C7-OCH_3), 50.27 (C8-OCH_3).

The calculated coordinates of (**15**) (the part of calculated log file):

After PCM corrections, the SCF energy is -1905.60044527 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.401806	-0.312384	0.111393
2	6	0	6.050984	-0.789696	-1.047481
3	6	0	5.875866	-2.150950	-1.545045
4	6	0	4.797299	-2.947300	-1.368941
5	6	0	3.571518	-2.643415	-0.633715



6	6	0	3.533980	-1.727601	0.430329
7	8	0	4.708570	-1.182801	0.936772
8	6	0	5.532700	1.002289	0.534164
9	6	0	6.358235	1.857108	-0.195949
10	6	0	7.046184	1.425924	-1.330303
11	6	0	6.885592	0.109198	-1.741020
12	6	0	2.362248	-3.262726	-0.995365
13	6	0	1.172820	-2.945869	-0.350297
14	6	0	1.131165	-2.011896	0.693693
15	6	0	2.339151	-1.410818	1.089431
16	6	0	-0.398393	0.819835	0.858443
17	6	0	-0.909497	-0.482081	0.748316
18	6	0	-2.123221	-0.665650	0.061422
19	6	0	-2.803334	0.441991	-0.466877
20	6	0	-2.298563	1.745863	-0.350356
21	6	0	-1.066674	1.906147	0.309919
22	8	0	-3.957599	0.195382	-1.204239
23	6	0	-5.144111	0.701404	-0.699140
24	6	0	-5.381805	2.092796	-0.691597
25	6	0	-4.346435	3.069598	-1.014134
26	6	0	-3.012107	2.916701	-0.856292
27	6	0	-6.122142	-0.209120	-0.326648
28	6	0	-7.380952	0.274361	0.030317
29	6	0	-7.675546	1.637914	0.023094
30	6	0	-6.674188	2.529364	-0.338330
31	6	0	-0.180182	-1.662132	1.377626
32	7	0	6.513306	3.241156	0.252279
33	8	0	5.903730	3.593761	1.264759
34	8	0	7.243851	3.984081	-0.407841
35	8	0	-2.671486	-1.924025	-0.039263
36	6	0	-2.653515	-2.507562	-1.350283
37	8	0	2.341269	-0.477030	2.101688
38	6	0	2.858609	-0.937137	3.360286
39	7	0	-8.422158	-0.680794	0.408763
40	8	0	-8.140588	-1.881533	0.392376
41	8	0	-9.527632	-0.235335	0.726806

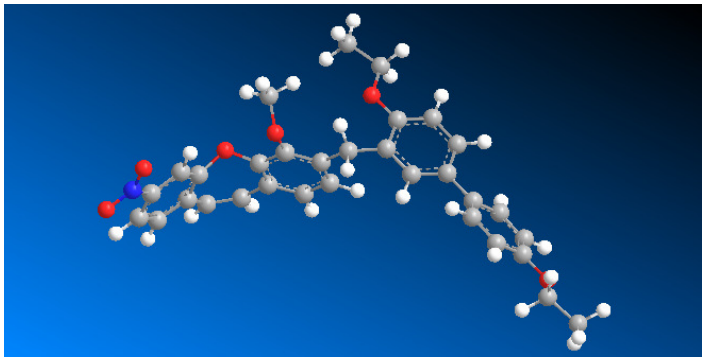
42	1	0	6.662104	-2.508452	-2.206500
43	1	0	4.790090	-3.896118	-1.902342
44	1	0	5.017430	1.343911	1.422087
45	1	0	7.686529	2.113689	-1.867938
46	1	0	7.409167	-0.240907	-2.626201
47	1	0	2.364028	-3.990021	-1.802972
48	1	0	0.254702	-3.443900	-0.648907
49	1	0	0.541037	0.967997	1.381564
50	1	0	-0.650686	2.905299	0.410332
51	1	0	-4.709088	4.050441	-1.314129
52	1	0	-2.388601	3.789606	-1.041451
53	1	0	-5.911318	-1.270323	-0.333000
54	1	0	-8.666218	1.978115	0.296853
55	1	0	-6.884797	3.595143	-0.342353
56	1	0	-0.838273	-2.533514	1.354349
57	1	0	0.014012	-1.423256	2.428109
58	1	0	-3.060927	-3.514589	-1.235991
59	1	0	-3.271678	-1.935291	-2.047144
60	1	0	-1.628328	-2.568824	-1.735594
61	1	0	2.767125	-0.094900	4.049184
62	1	0	2.270765	-1.783349	3.737060
63	1	0	3.909018	-1.228221	3.269280

The calculated proton and ^{13}C chemical shifts and coupling constants for (**15**):

(15): ^{1}H NMR, δ (ppm): 3.85 (3H, s, OCH_3), 3.72 (2H, s, CH_2), 7.18 (2H, d, ^{3}J = 7.7 Hz H2, H2'), 6.18 (2H, d(AB spin system), ^{3}J = 11.5 Hz, H10, H10'), 6.38 (2H, d, H1, H1'), 6.33 (2H, d(AB spin system), H11,H11'), 6.71 (2H, d, ^{3}J = 8.2 Hz H9, H9'), 7.63 (2H, dd, ^{3}J = 8.2 Hz, ^{4}J =1.3 Hz, H8, H8'), 7.70 (2H, d, H6, H6'). ^{13}C NMR, δ (ppm): 23.96 (CH_2), 52.25(2xOCH_3), 112.93(C1,C1'), 107.00(C6,C6'), 108.83(C8,C8'), 115.08(C2,C2'), 116.78 (C10, C10'), 116.82(C9, C9'), 117.96 (C12, C12'), 128.81 (C3, C3'), 124.71 (C11, C11'), 127.96(C15, C15'), 139.08(C13, C13'), 134.89 (C7, C7'), 137.01(C4, C4'), 143.40 (C14, C14').

The calculated coordinates of (**16**) (the part of calculated log file):

After PCM corrections, the SCF energy is -1742.85221598 a.u.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.152267	-0.493797	0.476884
2	6	0	5.487337	-0.962536	1.766123
3	6	0	4.869477	-0.440122	2.980657
4	6	0	3.639517	0.111727	3.093330
5	6	0	2.655451	0.331236	2.036539
6	6	0	3.014687	0.498922	0.688835
7	8	0	4.351281	0.624400	0.321944
8	6	0	5.705647	-1.047522	-0.668410
9	6	0	6.642974	-2.071093	-0.528476
10	6	0	7.031356	-2.547461	0.724071
11	6	0	6.450732	-1.987478	1.854090
12	6	0	1.284194	0.356047	2.344323
13	6	0	0.323505	0.505130	1.350098
14	6	0	0.683625	0.656485	0.005648
15	6	0	2.053086	0.651846	-0.316133
16	6	0	-0.347284	0.777099	-1.108336
17	6	0	-1.689728	1.336643	-0.693292
18	6	0	-2.804721	0.512561	-0.559675
19	6	0	-4.070871	0.997181	-0.180372
20	6	0	-4.180905	2.370650	0.070106
21	6	0	-3.083666	3.225081	-0.052832
22	6	0	-1.838036	2.717127	-0.435186
23	6	0	-5.237590	0.088984	-0.058971
24	6	0	-6.215145	0.279193	0.937368
25	6	0	-7.310471	-0.565925	1.050627
26	6	0	-7.468772	-1.644346	0.166629
27	6	0	-6.509112	-1.855436	-0.830786
28	6	0	-5.415671	-0.992977	-0.932938

29	8	0	-0.712716	3.476051	-0.591823
30	8	0	-8.576563	-2.417366	0.360169
31	6	0	-0.782850	4.877202	-0.313508
32	6	0	0.599670	5.463619	-0.536800
33	6	0	-8.790920	-3.538349	-0.501595
34	6	0	-10.075916	-4.216706	-0.060714
35	8	0	2.446121	0.756271	-1.631371
36	6	0	2.931618	2.051798	-2.013305
37	7	0	7.242467	-2.648475	-1.730832
38	8	0	6.894620	-2.198776	-2.825515
39	8	0	8.064278	-3.557642	-1.588263
40	1	0	5.429146	-0.612689	3.897511
41	1	0	3.294165	0.346894	4.098613
42	1	0	5.424001	-0.674584	-1.644205
43	1	0	7.768610	-3.336887	0.797129
44	1	0	6.737172	-2.351727	2.836749
45	1	0	0.975964	0.236878	3.379940
46	1	0	-0.728236	0.514168	1.618499
47	1	0	0.077294	1.388328	-1.909450
48	1	0	-0.500743	-0.220243	-1.543717
49	1	0	-2.678862	-0.552387	-0.740540
50	1	0	-5.144608	2.794203	0.339257
51	1	0	-3.216016	4.284006	0.137005
52	1	0	-6.101620	1.091199	1.650630
53	1	0	-8.055001	-0.416947	1.827246
54	1	0	-6.605835	-2.672837	-1.536215
55	1	0	-4.698437	-1.158803	-1.732333
56	1	0	-1.520854	5.350692	-0.975893
57	1	0	-1.111085	5.031084	0.723712
58	1	0	0.588302	6.537994	-0.324344
59	1	0	1.332567	4.987369	0.122054
60	1	0	0.918479	5.321121	-1.574508
61	1	0	-8.864995	-3.197162	-1.543768
62	1	0	-7.938395	-4.228601	-0.432285
63	1	0	-10.278108	-5.085044	-0.696775
64	1	0	-9.997326	-4.557165	0.976695

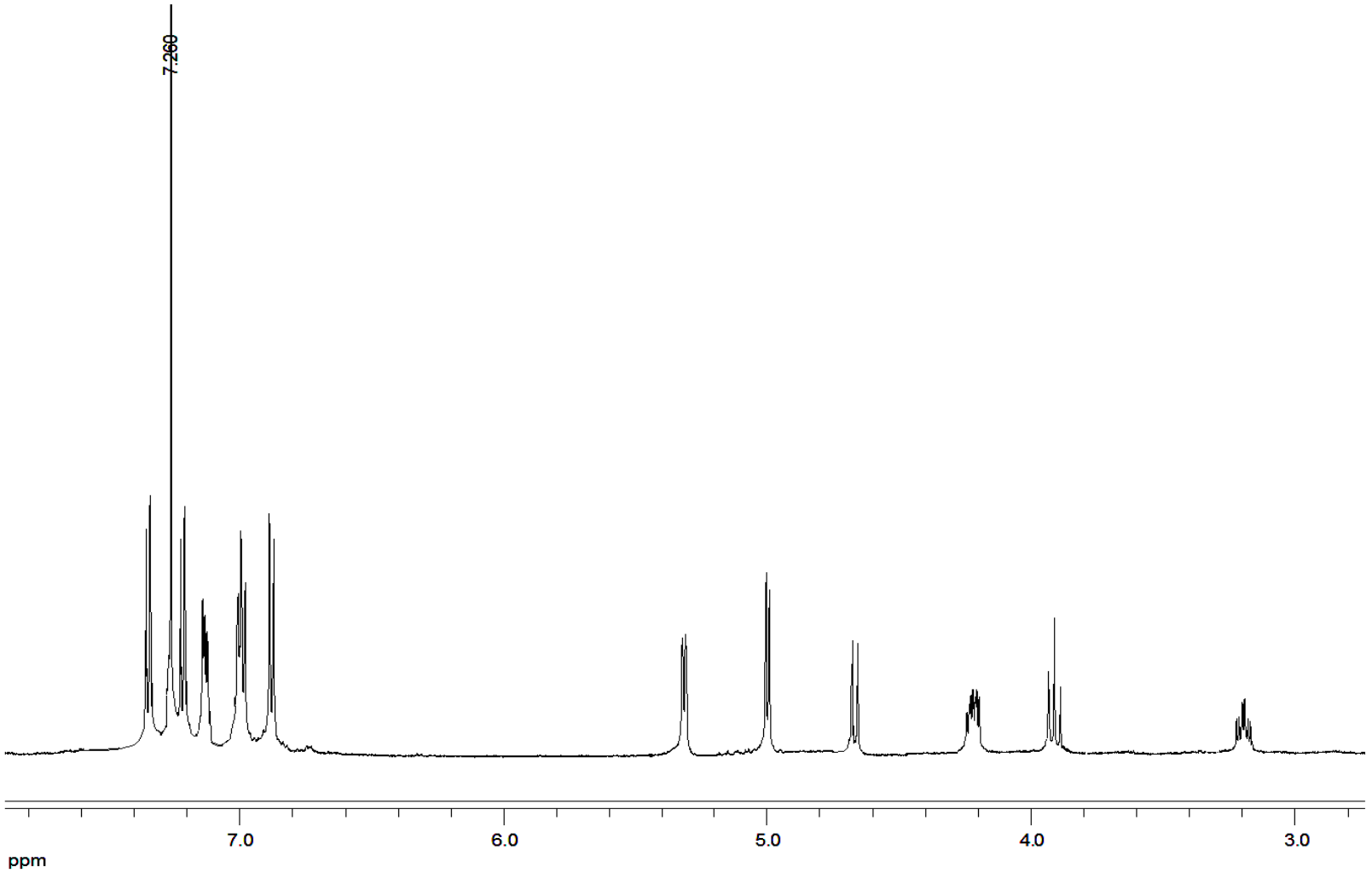
65	1	0	-10.922731	-3.527068	-0.135611
66	1	0	3.161586	1.987031	-3.079253
67	1	0	2.163553	2.817232	-1.848860
68	1	0	3.837666	2.311075	-1.456589

The calculated proton and ^{13}C chemical shifts and coupling constants for (**16**):

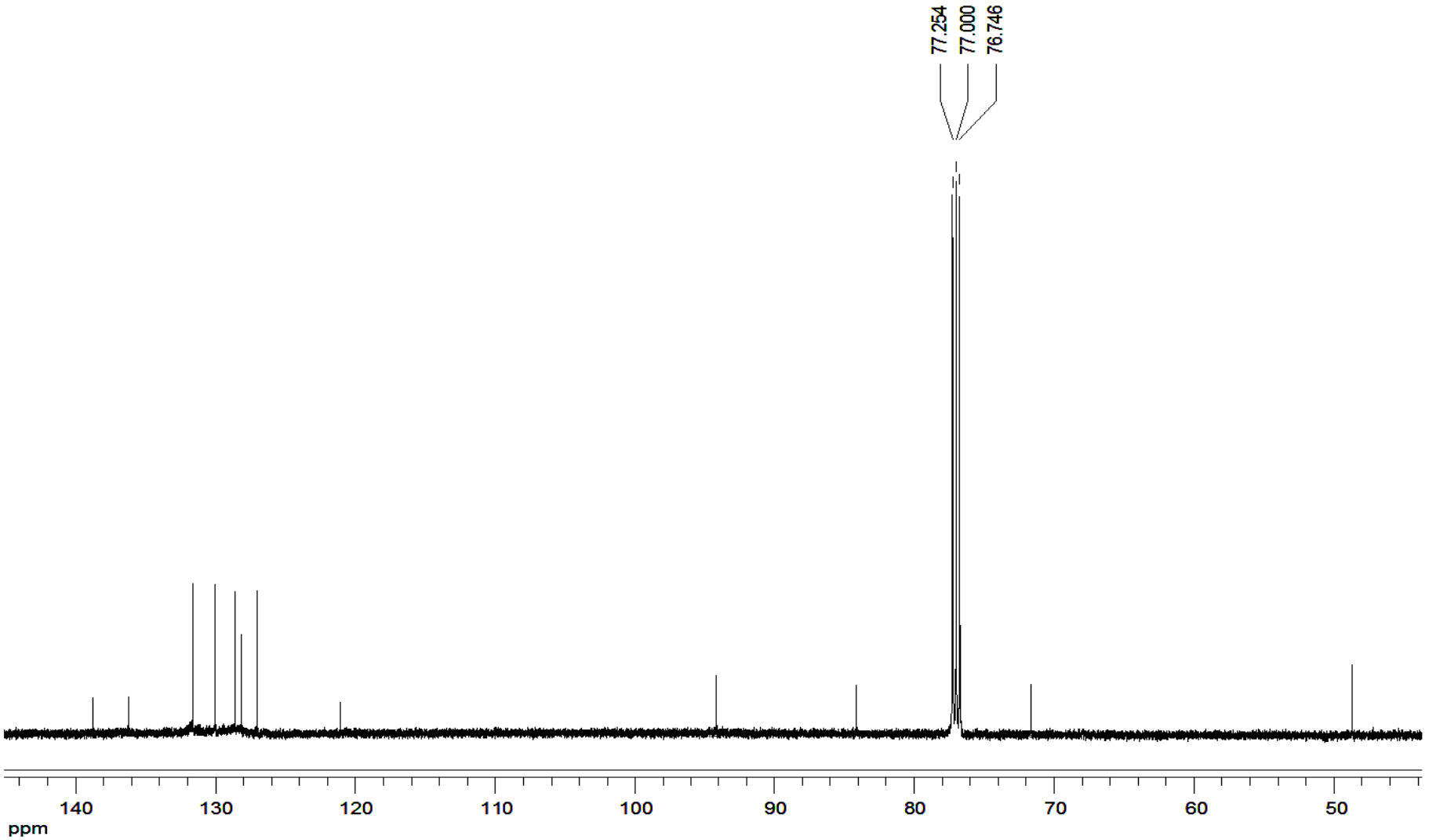
(16): ^{1}H NMR, δ (ppm): 4.20 (2H, s, CH_2), dibenzo[*b,f*]oxepin ring: 8.49 (1H, d, ^{4}J = 2.5 Hz, H6), 8.36 (1H, dd, ^{3}J = 8.5 Hz, H8), 7.41 (H, d, H9), 7.03 (1H, d(AB spin system), ^{3}J = 11.4 Hz, H11), 6.78 (1H, d(AB spin system), ^{3}J = 8.5 Hz, H2), 6.93 (1H, d(AB spin system), H1), 6.84 (1H, d(AB spin system), H10), 4.26 (3H, s, OCH_3); biphenyl ring: 7.68 (1H, dd, ^{3}J = 8.5 Hz, ^{4}J = 2.5 Hz, H6), 7.75 (2H, d, H2',H6'), 7.70 (1H, d, H2) 7.04 (1H, d, ^{3}J = 8.5 Hz, H5), 7.07 (2H, d, ^{3}J = 8.5 Hz, H3'), 7.16 (H5'), 3.97 (2H, q, ^{3}J = 7 Hz, OCH_2), 4.02(2H, q, ^{3}J = 7 Hz, OCH_2), 1.30 (3H, t, CH_3); 1.47 (3H, t, CH_3). ^{13}C NMR, δ (ppm): 36.42 (CH_2), dibenzo[*b,f*]oxepin ring: 164.52 (C14), 157.40 (C4), 155.12(C7), 158.88(C13), 147.60(C15), 143.43(C11), 136.26(C12), 150.47(C3), 133.86(C9), 133.33(C10), 130.02(C2), 126.09(C8), 123.69(C6), 129.74(C1), 62.37(OCH_3); biphenyl ring: 166.08(C4'), 164.24(C4), 141.10(C1), 140.89(C1'), 134.32(C3), 136.66(C2), 132.02(C6), 113.80(C3'), 122.08(C5'), 114.36(C5), 66.67(OCH_2), 66.58(OCH_2), 16.81 (CH_3), 16.63(CH_3).

Copies of ^{1}H NMR and ^{13}C NMR spectra of (7, 8, 10-13, 15, 16)

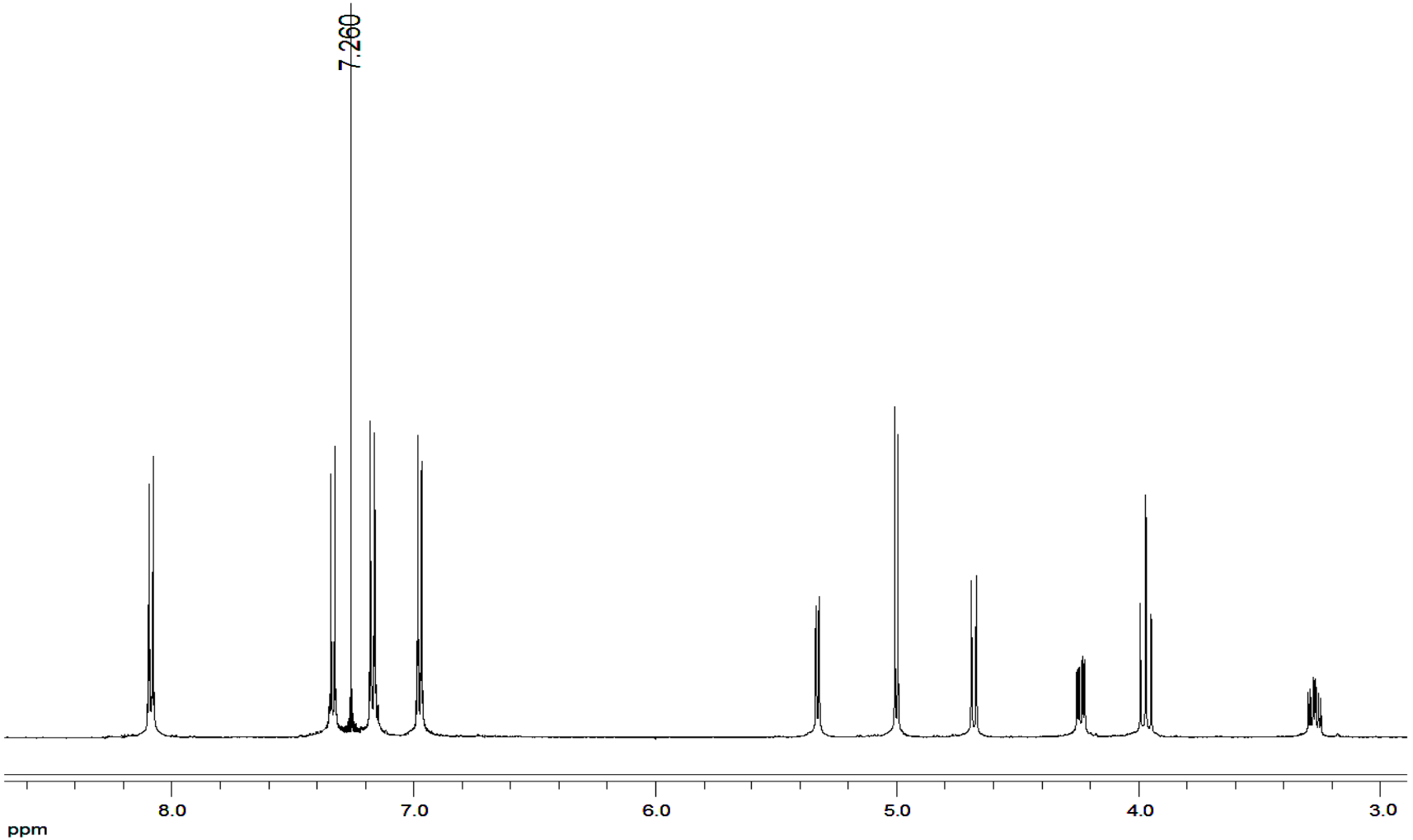
^{1}H NMR of compound (7)



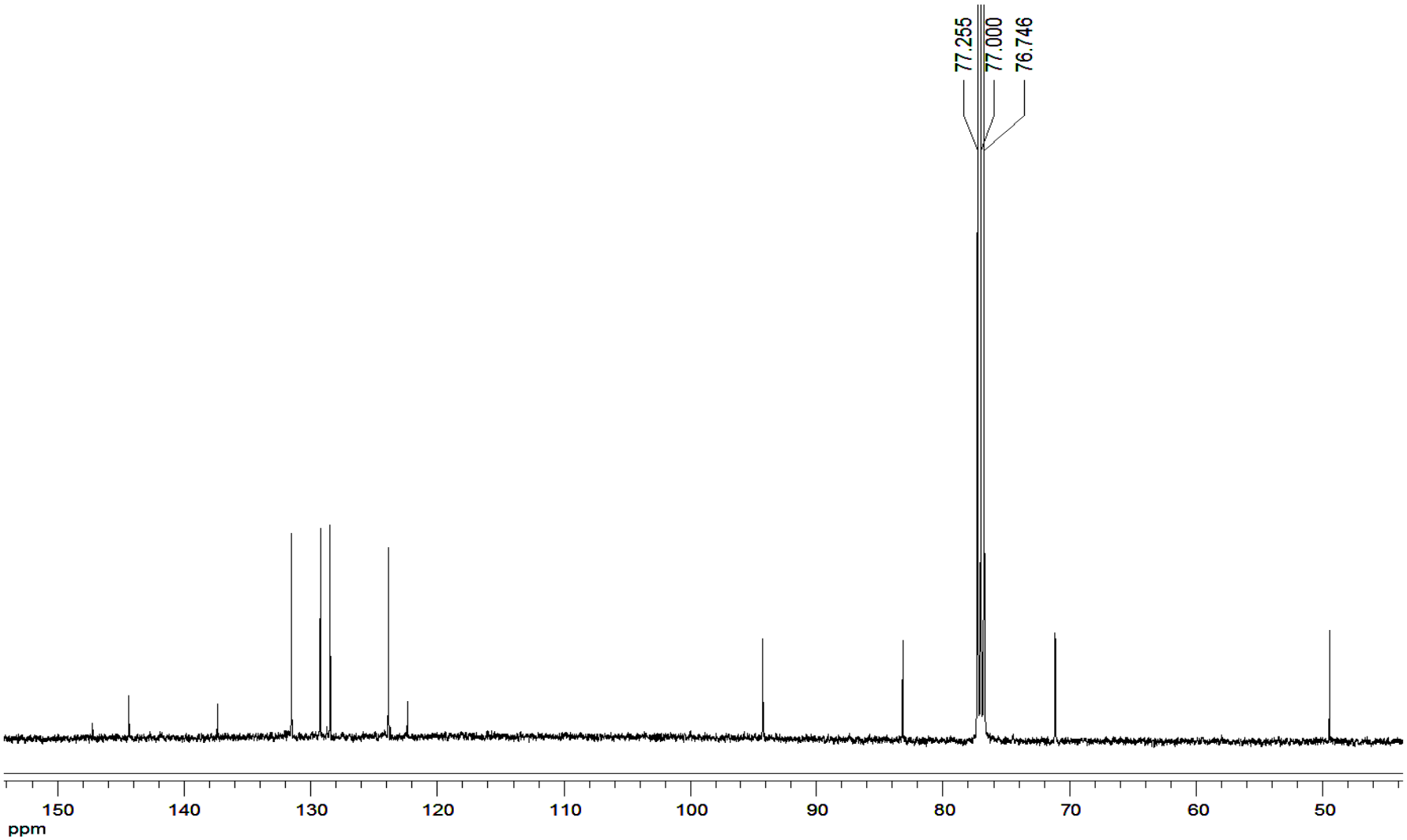
^{13}C NMR of compound (7)



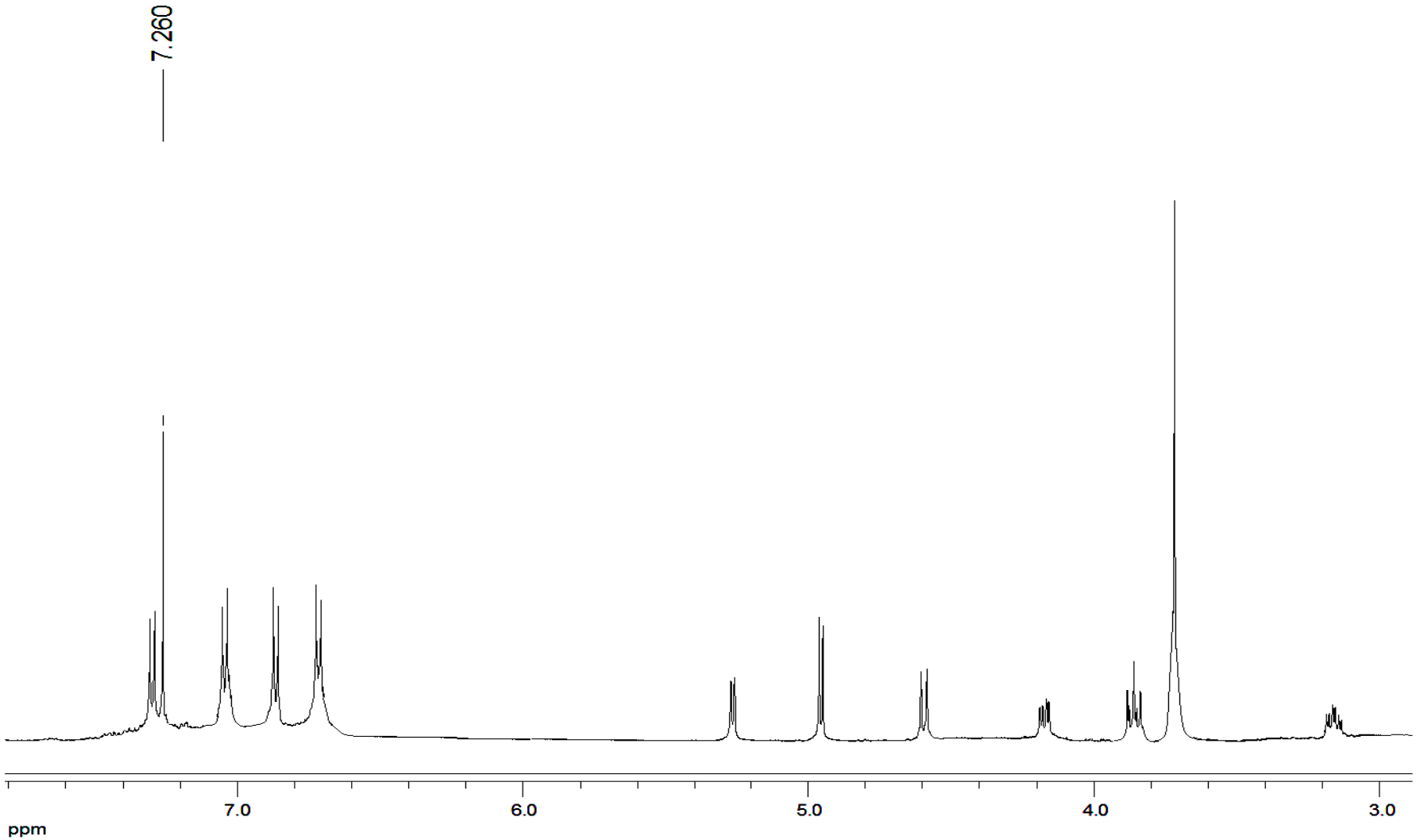
^{1}H NMR of compound (8)



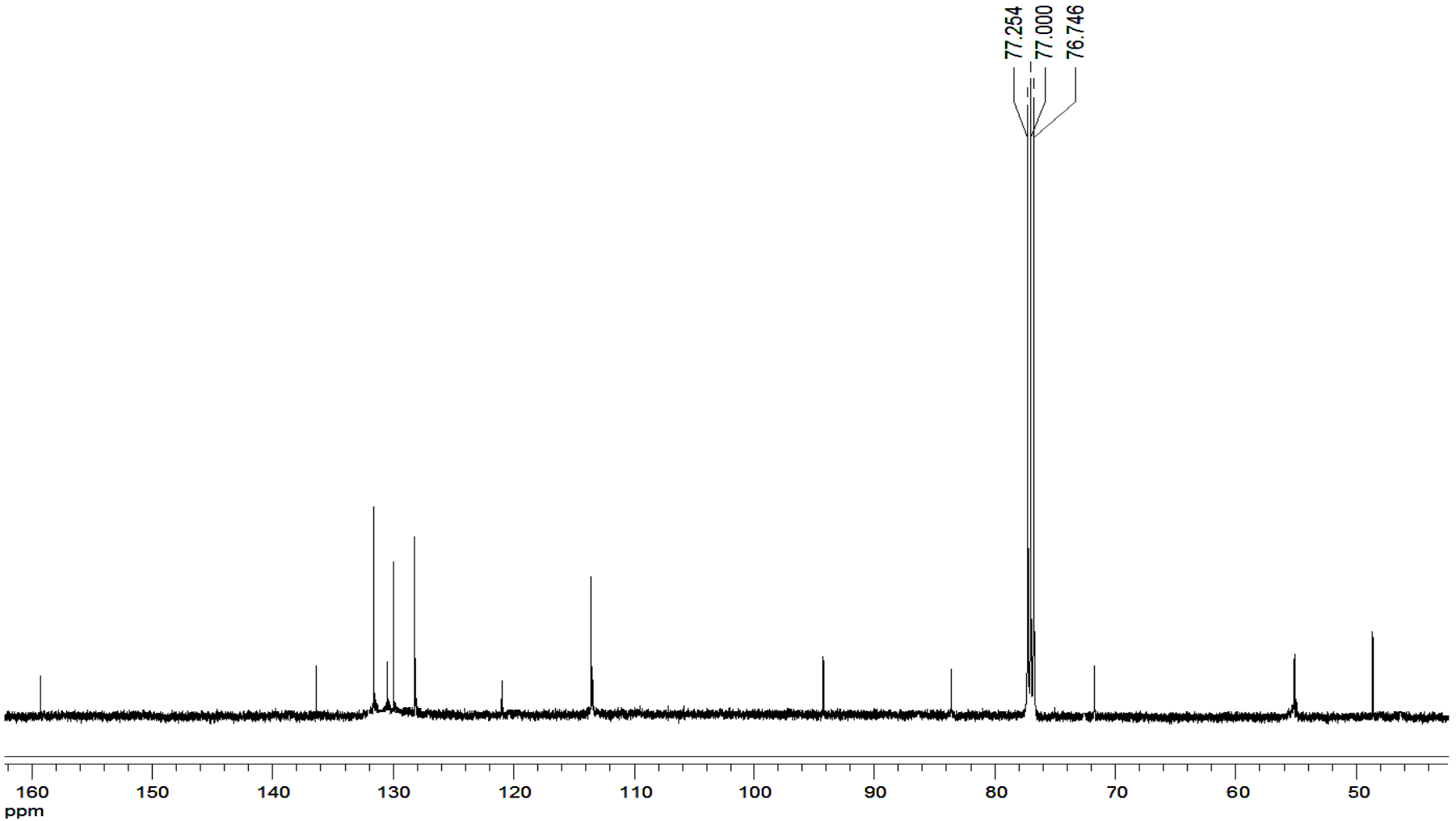
^{13}C NMR of compound (8)



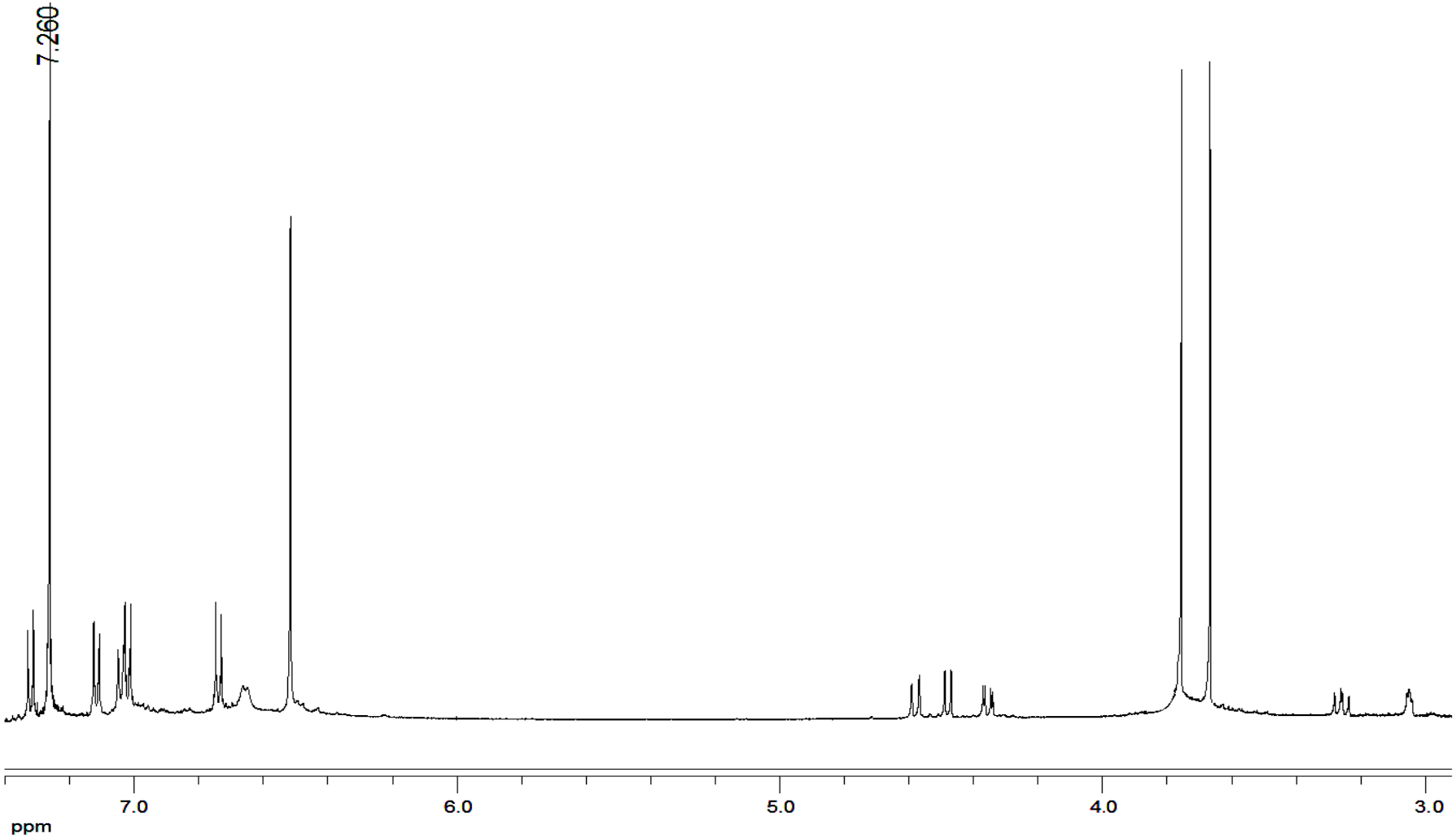
^{1}H NMR of compound (10)



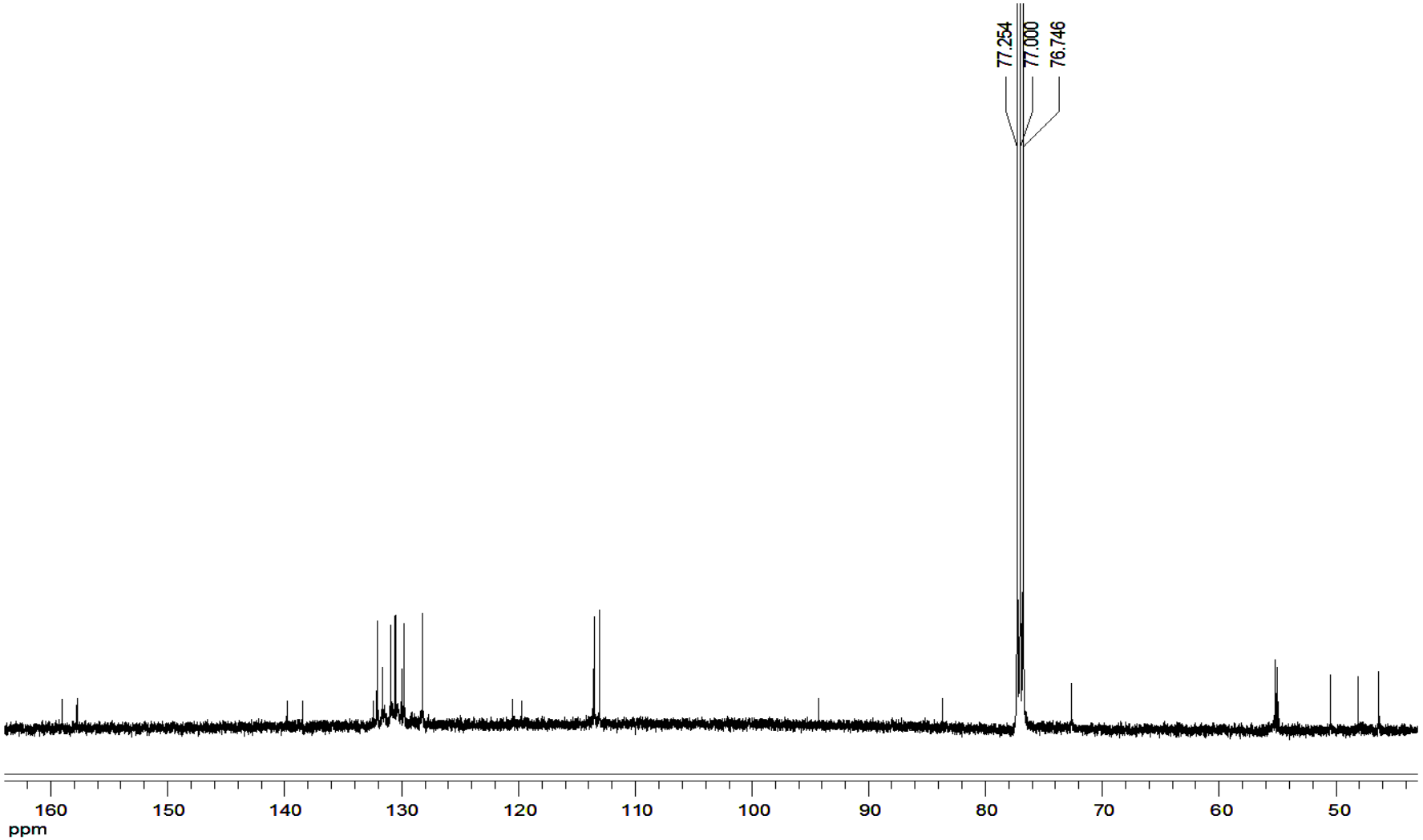
^{13}C NMR of compound (10)



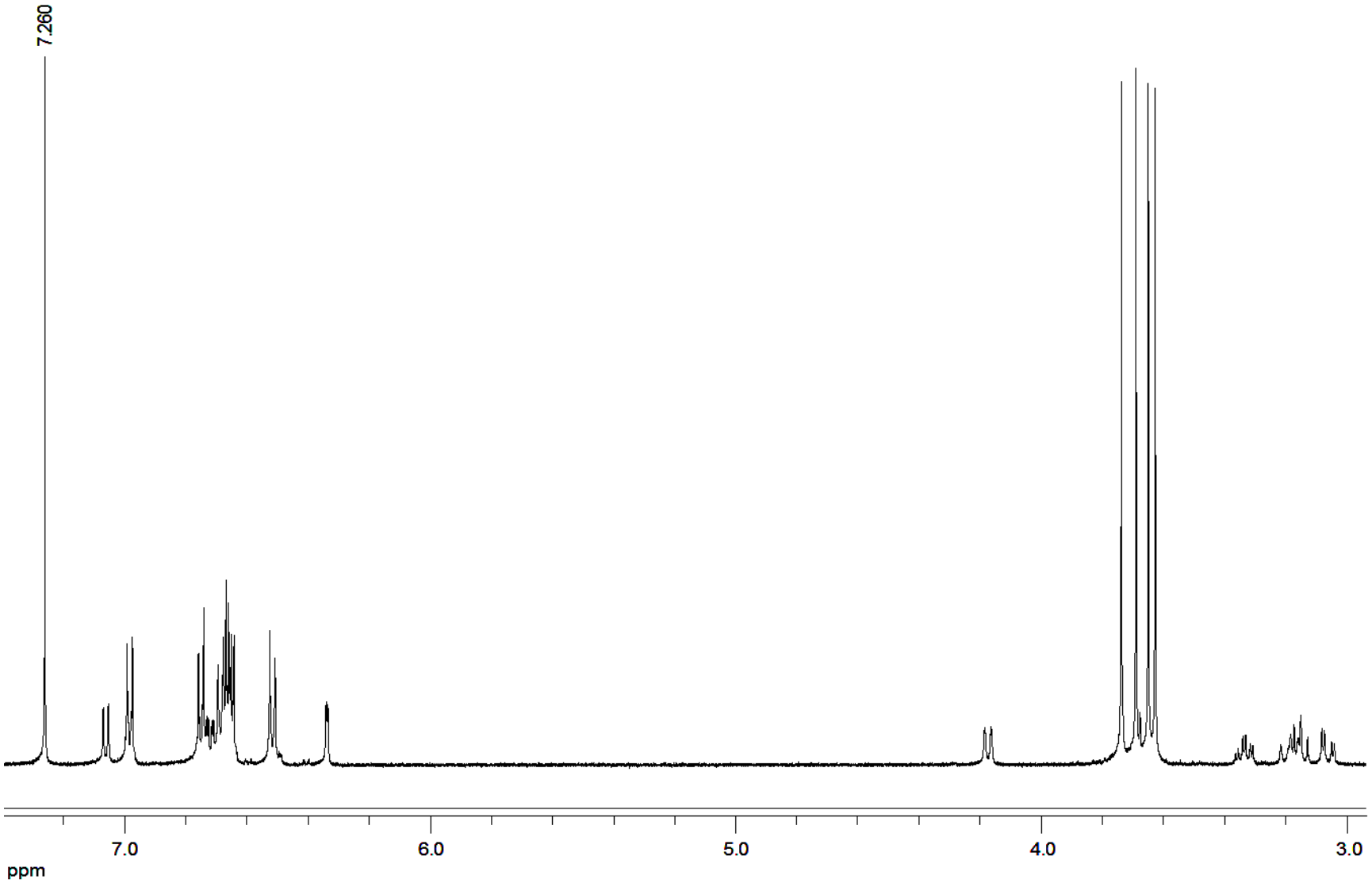
^{1}H NMR of compound (11)



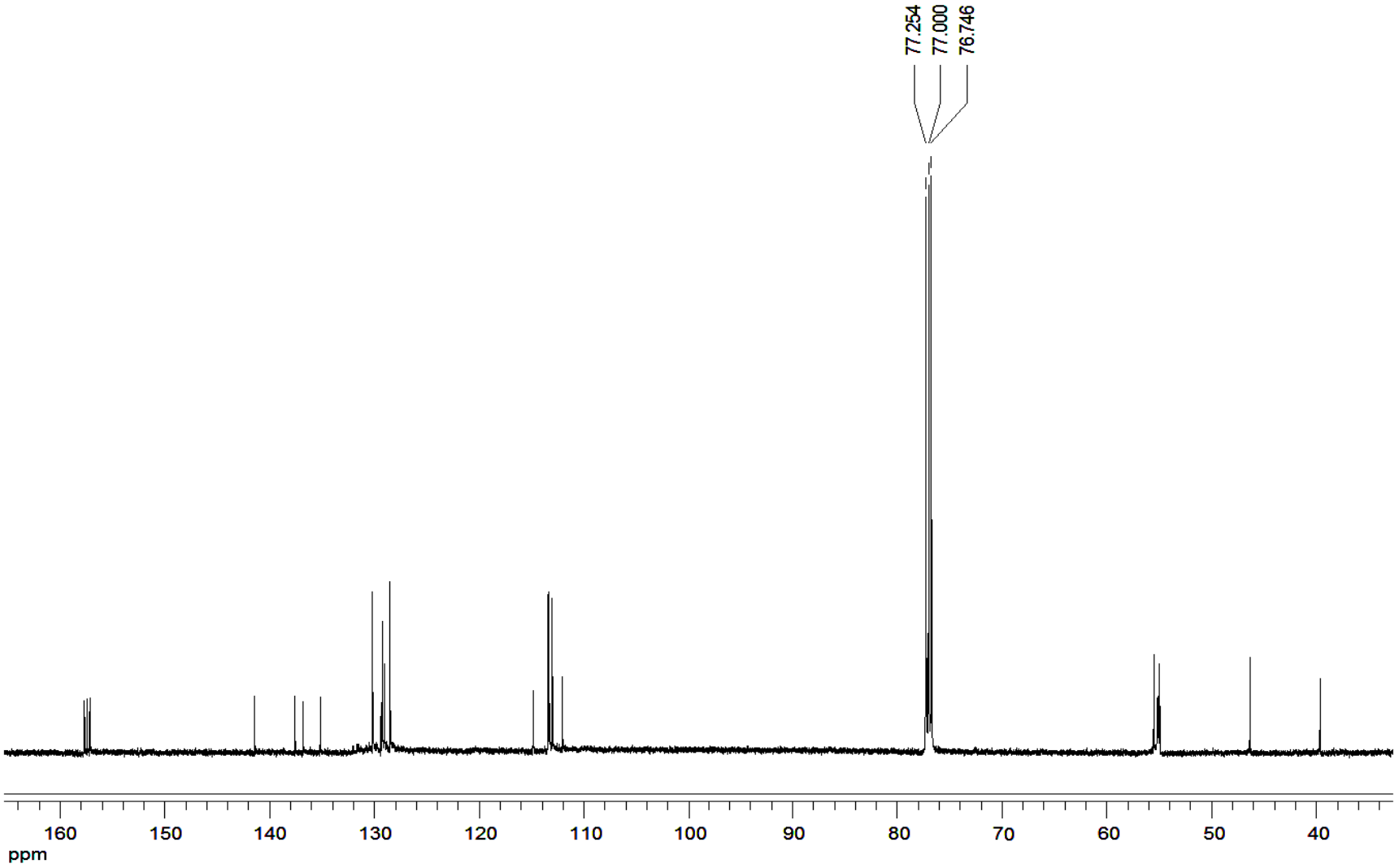
^{13}C NMR of compound (11)



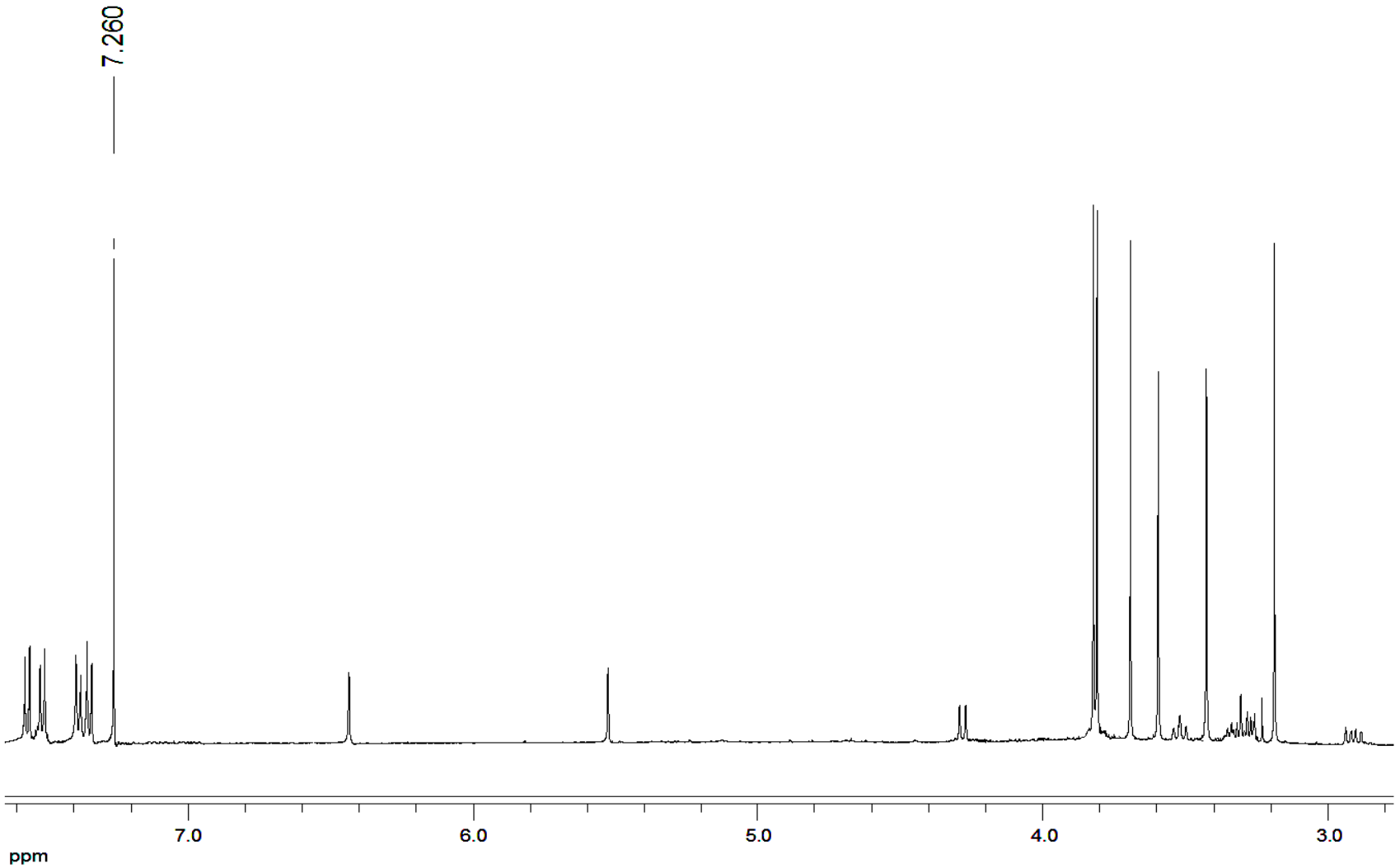
^{1}H NMR of compound (12)



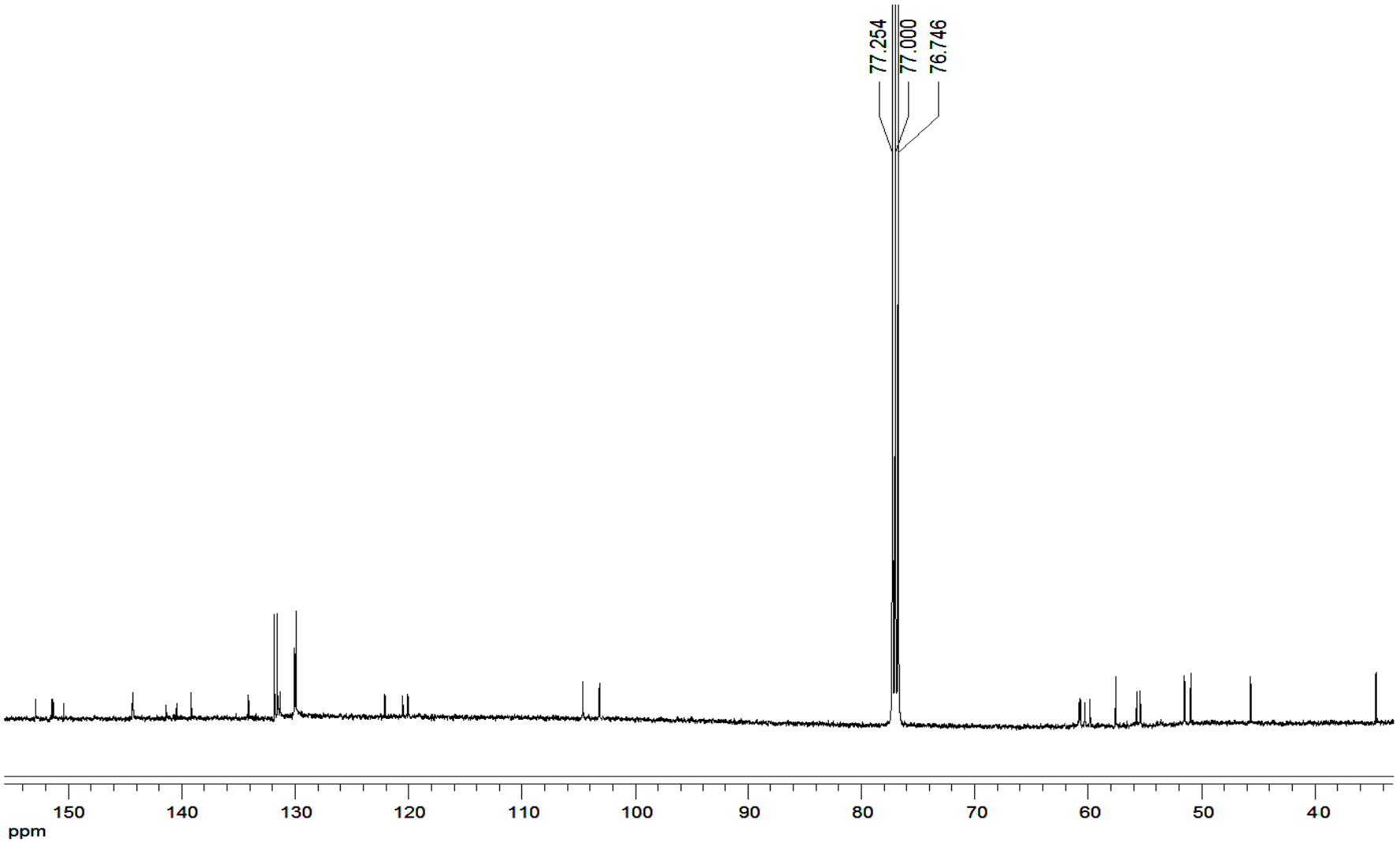
^{13}C NMR of compound (12)



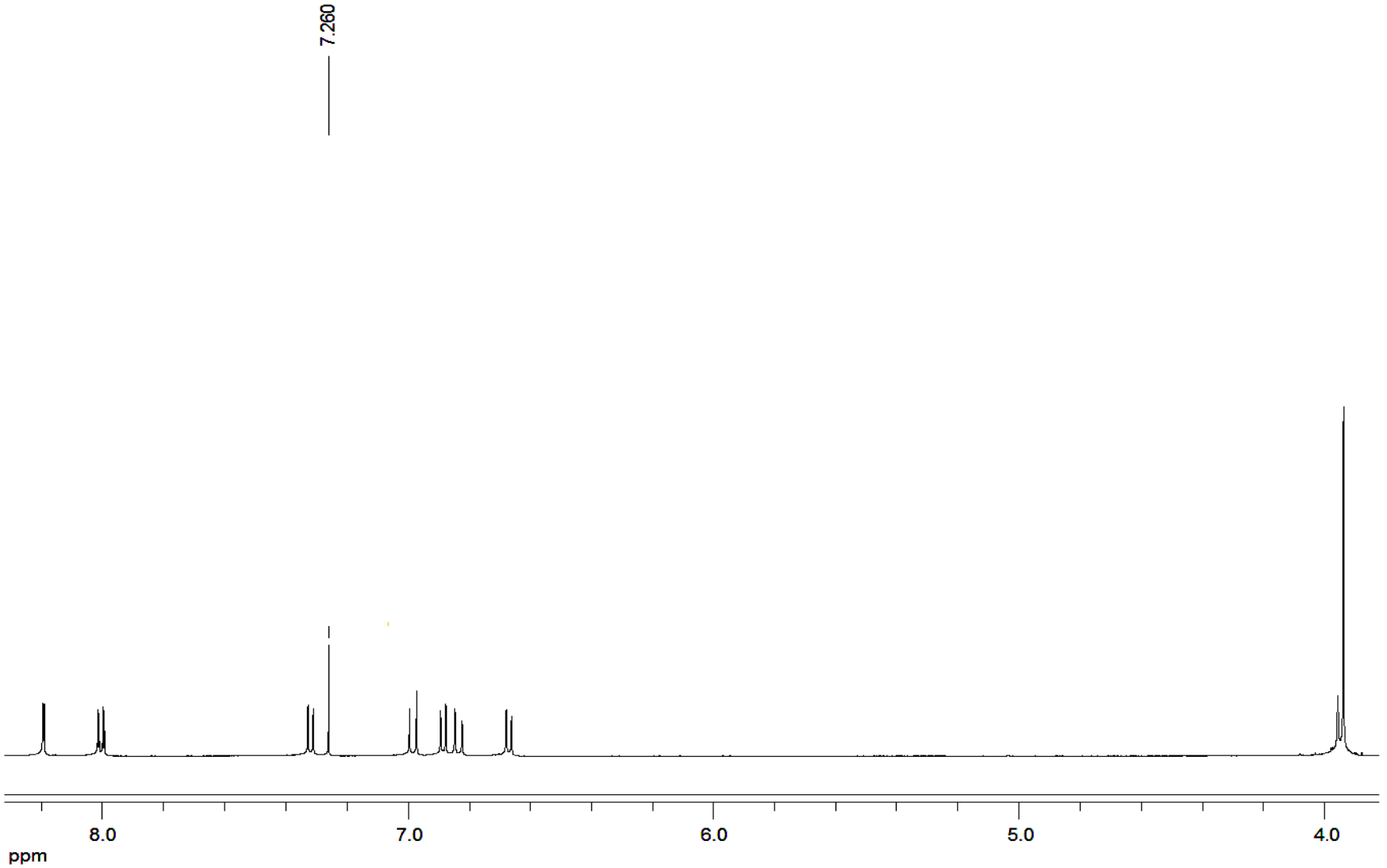
^{1}H NMR of compound (13)



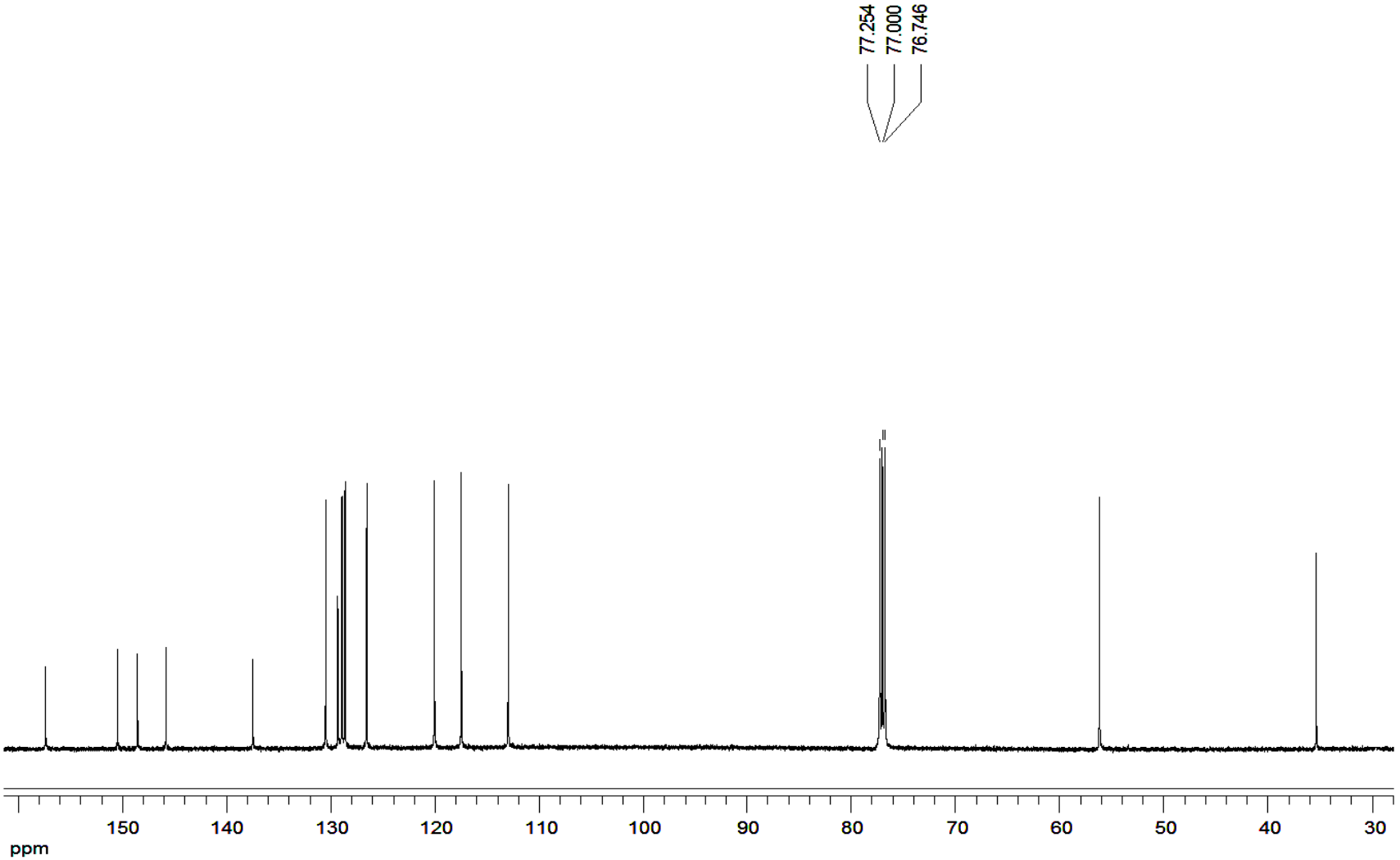
^{13}C NMR of compound (13)



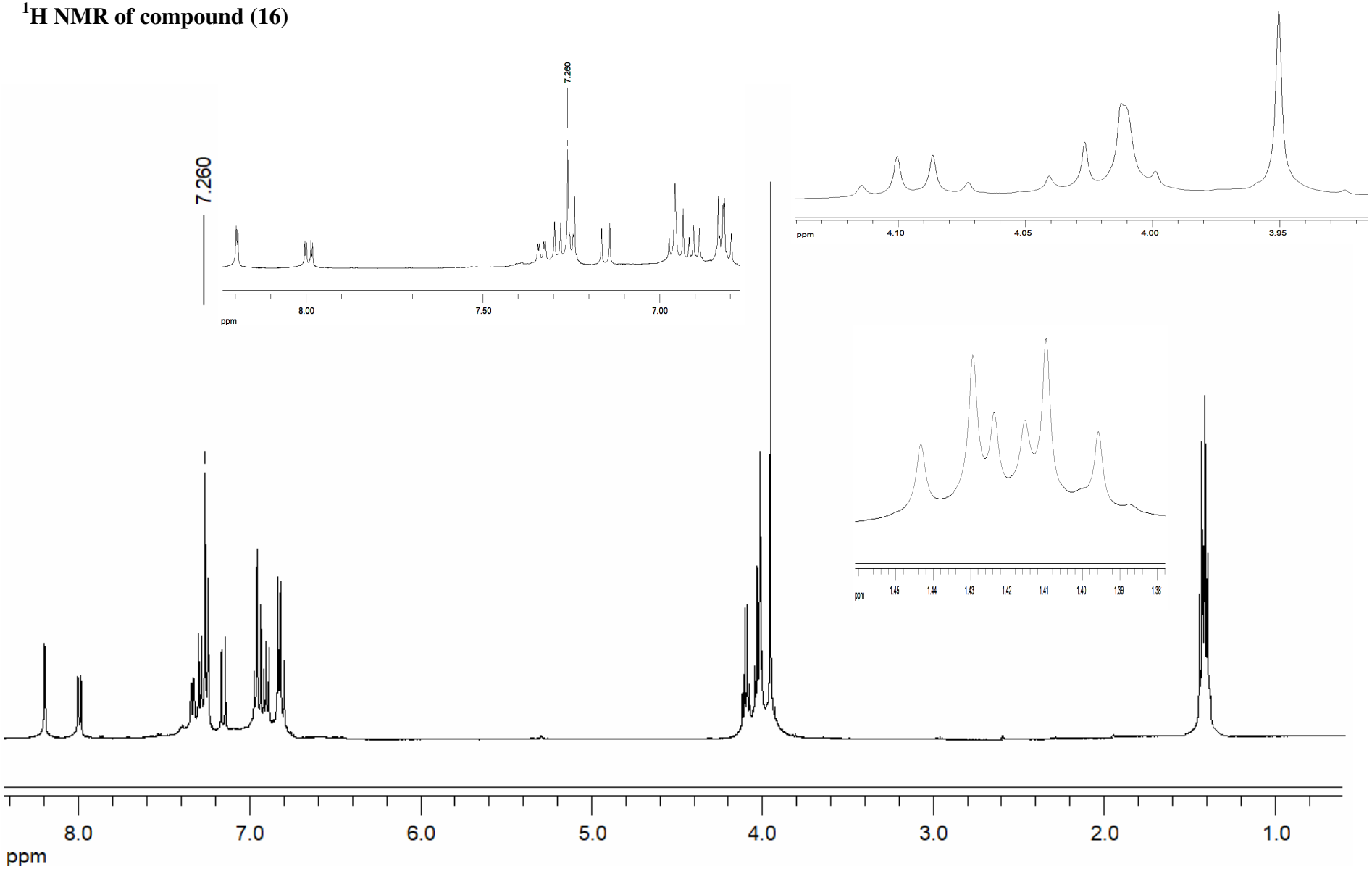
^{1}H NMR of compound (15)



^{13}C NMR of compound (15)



^{1}H NMR of compound (16)



^{13}C NMR of compound (16)