Supporting Information

For

Iodine-promoted Cyclization of *N*-propynyl amides and *N*-allyl amides *via* Sulfonylation and Sulfenylation

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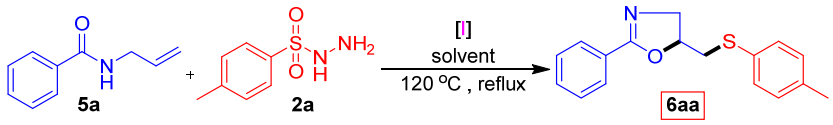
1) General Information

^{1}H, ^{13}C and DEPT NMR spectra were recorded on a 400 MHz Varian Unity Plus or Varian Mercury plus spectrometer or JEOL 400 MHz. The chemical shift (δ) values are reported in parts per million (ppm), and the coupling constants (*J*) are given in Hz. The spectra were recorded using $CDCl_3$ as a solvent. ^{1}H NMR chemical shifts are referenced to tetramethylsilane (TMS) (0 ppm). ^{13}C NMR was referenced to $CDCl_3$ (77.0 ppm). The abbreviations used are as follows: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublet; ddd, doublet of doublet of doublet; dt, doublet of triplets; td, triplet of doublet; m, multiplet. Mass spectra and high-resolution mass spectra (HRMS) was measured using the ESI (FT-MS solariX) at National Sun Yat-Sen University, Kaohsiung, Taiwan or LTQ Orbitrap XL (Thermo Fischer Scientific) at National Chung Hsing University. All IR spectra were obtained as neat films with a Perkin-Elmer Model 2000 FT-IR SYSTEM and selected absorbance are reported in cm^{-1}. Melting points were determined on an EZ-Melt (Automated melting point apparatus). All products reported showed ^{1}H NMR spectra in agreement with the assigned structures. Reaction progress and product mixtures were routinely monitored by TLC using Merck TLC aluminum sheets (silica gel 60 F254). Column chromatography was carried out with 230–400 mesh silica gel 60 (Merck)/neutral alumina and a mixture of hexane/ethyl acetate or hexane as an eluent.

2) Table S1. Optimization of the sulfenylation reaction conditions.[a]



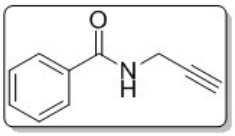
entry	I source (X equiv)	solvent	time (h)	yield (%)
1	I_2 (0.1)	1,2-dichloroethane	48	<10[c]
2	I_2 (0.1)	1,4-dioxane	48	<5[c]
3	I_2 (0.1)	DMSO	48	trace[c]
4	I_2 (0.1)	DMF	48	trace[c]
5	I_2 (0.1)	CH_3CN	48	trace[c]
6	I_2 (0.1)	Toluene	48	15[c]
7	I_2 (0.5)	Toluene	24	32[b]
8[d]	I_2 (0.5)	Toluene	24	24[b]
9	I_2 (0.75)	Toluene	24	48[b]
10	I_2 (1.0)	Toluene	5	65[c]
11	I_2 (1.0)	1,2-dichloroethane	24	53[b]
12	KI (1.0)	Toluene	24	7[b]
13	NaI (1.0)	Toluene	24	7[b]
14	TBAI (1.0)	Toluene	24	4[b]
15	NIS (1.0)	Toluene	24	5[b]
16	NBS (1.0)	Toluene	24	12[b]
17[e]	I_2 (2.0)	Toluene	24	<10[c]
18	KI (2.0)	Toluene	24	4[b]
19	NAI (2.0)	Toluene	24	4[b]
20	TBAI (2.0)	Toluene	24	5[b]
21	-	Toluene	3	0[c]

[a] Reaction conditions: **5a** (1.0 mmol), **2a** (1.5 mmol), iodo source (X equiv), solvent (2.0 mL) at 120 ℃ for 5 h. [b] Determined by GC-MS analysis. [c] Isolated yields. [d] Under O_2. [e] 5-(iodomethyl)-2-phenyl-4,5-dihydrooxazole was isolated as a major product. [c]In the absence of iodine, *S*-(*p*-tolyl) 4-methylbenzenesulfonothioate was isolated as major product and 1,2-di-*p*-tolyldisulfane was isolated as minor product with recovery of **5a**.

3) General Experimental Procedures and Spectral Characterization

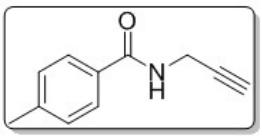
The starting materials **1**(**a**-**o**)[1-9] and **5(a-c)**[10-12] were prepared according to the previously reported literatures.[1-9] The spectra data complies to the reported literature values.[1-9]

***N*-(Prop-2-yn-1-yl)benzamide (1a)**.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.75 (m, 2H), 7.49 (d, *J* = 7.4



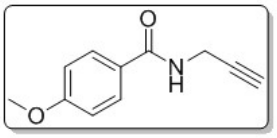
Hz, 1H), 7.45 – 7.36 (m, 2H), 6.67 (s, 1H), 4.24 (dd, *J* = 5.3, 2.6 Hz, 2H), 2.27 (t, *J* = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.18, 133.65, 131.70, 128.52, 127.01, 79.50, 71.71, 29.69.

4-Methyl-*N*-(prop-2-yn-1-yl)benzamide (1b).[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H),



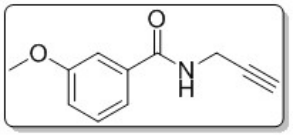
7.25 – 7.19 (m, 2H), 6.55 (s, 1H), 4.23 (dd, *J* = 5.2, 2.6 Hz, 2H), 2.39 (s, 3H), 2.27 (d, *J* = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.08, 142.17, 130.82, 129.18, 127.01, 79.63, 71.64, 29.64, 21.40.

4-Methoxy-*N*-(prop-2-yn-1-yl)benzamide (1c).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.9 Hz, 2H),



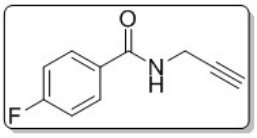
6.91 (d, *J* = 8.9 Hz, 2H), 6.42 (s, 1H), 4.23 (dd, *J* = 5.2, 2.6 Hz, 2H), 3.84 (s, 3H), 2.27 (t, *J* = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.64, 162.35, 128.86, 125.97, 113.74, 79.71, 71.65, 55.37, 29.67.

3-Methoxy-*N*-(prop-2-yn-1-yl)benzamide (1d).[3] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.35 (m, 1H), 7.31



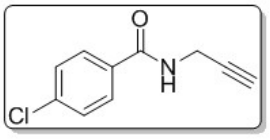
(dd, *J* = 4.2, 2.0 Hz, 2H), 7.08 – 6.98 (m, 1H), 6.68 (s, 1H), 4.23 (dd, *J* = 5.3, 2.6 Hz, 2H), 3.82 (s, 3H), 2.27 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.02, 159.72, 135.11, 129.51, 118.80, 117.91, 112.36, 79.46, 71.70, 55.35, 29.70.

4-Fluoro-*N*-(prop-2-yn-1-yl)benzamide (1e).[3] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.78 (m, 2H), 7.10 (dd,



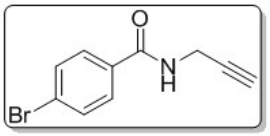
J = 9.6, 7.7 Hz, 2H), 6.67 (s, 1H), 4.23 (dd, *J* = 5.3, 2.6 Hz, 2H), 2.28 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.12, 164.87 (d, *J* = 260.0 Hz), 163.57, 129.42 (d, *J* = 8.8 Hz), 115.59 (d, *J* = 22.0 Hz), 115.48, 79.37, 71.80, 29.76.

4-Chloro-*N*-(prop-2-yn-1-yl)benzamide (1f).[3] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.69 (m, 2H), 7.45 –

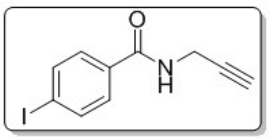


7.37 (m, 2H), 6.46 (s, 1H), 4.24 (dd, *J* = 5.2, 2.6 Hz, 2H), 2.29 (t, *J* = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.08, 138.07, 132.05, 128.87, 128.46, 79.23, 72.01, 29.84.

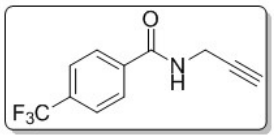
4-Bromo-*N*-(prop-2-yn-1-yl)benzamide (1g).[4] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.63 (m, 2H), 7.60 – 7.54 (m, 2H), 6.43 (s, 1H), 4.24 (dd, *J* = 5.2, 2.6 Hz, 2H), 2.29 (t, *J* = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.17, 132.51, 131.85, 128.62, 126.54, 79.21, 72.04, 29.84.



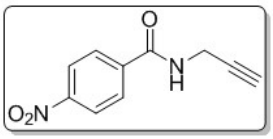
4-Iodo-*N*-(prop-2-yn-1-yl)benzamide (1h).[8] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.75 (m, 2H), 7.54 – 7.46 (m, 2H), 6.33 (s, 1H), 4.24 (dd, *J* = 5.2, 2.6 Hz, 2H), 2.29 (t, *J* = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.30, 137.85, 133.07, 128.57, 98.86, 79.18, 72.10, 29.85.



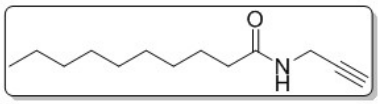
***N*-(Prop-2-yn-1-yl)-4-(trifluoromethyl)benzamide (1i)**.[5] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.1 Hz, 2H), 7.69 (d, *J* = 8.2 Hz, 2H), 6.67 (s, 1H), 4.27 (dd, *J* = 5.2, 2.6 Hz, 2H), 2.30 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.08, 139.20, 133.50 (d, $J_{C,F}$ = 33.0 Hz), 131.00, 128.30, 125.64 (q, $J_{C,F}$ = 3.7 Hz), 123.56 (d, $J_{C,F}$ = 270.0 Hz), 122.20, 72.41, 45.79, 30.08.



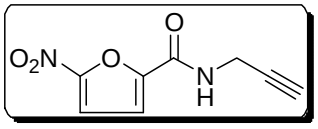
4-Nitro-*N*-(prop-2-yn-1-yl)benzamide (1j).[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (t, *J* = 7.2 Hz, 2H), 7.98 (d, *J* = 8.7 Hz, 2H), 6.56 (s, 1H), 4.34 – 4.25 (m, 2H), 2.33 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.08, 139.20, 131.00, 128.30, 123.87, 123.46, 78.80, 72.41, 30.08.



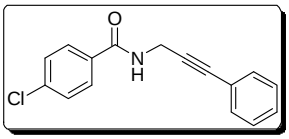
***N*-(Prop-2-yn-1-yl)decanamide (1k)**.[6] ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.86 (s, 1H), 4.05 (dd, *J* = 5.2, 2.6 Hz, 2H), 2.24 – 2.17 (m, 3H), 1.68 – 1.59 (m, 2H), 1.35 – 1.22 (m, 13H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.82, 79.66, 71.40, 36.42, 31.81, 29.24, 25.53, 22.61, 14.05.



5-Nitro-*N*-(prop-2-yn-1-yl)furan-2-carboxamide (1l).[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 3.8 Hz, 1H), 7.31 (d, *J* = 3.8 Hz, 1H), 6.92 (s, 1H), 4.27 (dd, *J* = 5.5, 2.6 Hz, 3H), 2.33 (t, *J* = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.85, 147.36, 116.43, 112.34, 78.19, 72.53, 29.24.

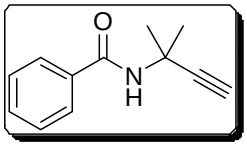


4-Chloro-*N*-(3-phenylprop-2-yn-1-yl)benzamide (1m). The compound was prepared by reported literature protocol.[9] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.7 Hz, 2H), 7.48 – 7.36 (m, 4H), 7.37 – 7.27 (m, 3H), 6.50 (s, 1H), 4.47 (d, *J* = 5.1 Hz, 2H); ^{13}C NMR (100

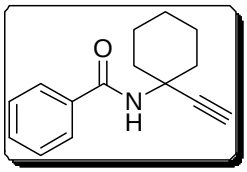


MHz, $CDCl_3$) δ 166.07, 138.02, 132.21, 131.73, 131.47, 128.86, 128.45 (t, *J* = 11.9 Hz), 122.36, 84.41, 83.85, 30.73; HRMS (ESI) calcd for $C_{16}H_{13}NOCl$ $[M+H]^+$: 270.0680 found 270.0677.

***N*-(2-Methylbut-3-yn-2-yl)benzamide (1n)**.[2] ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 2H), 7.52 – 7.39 (m, 3H), 6.26 (s, 1H), 2.39 (s, 1H), 1.77 (s, 7H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.44, 134.79, 131.45, 128.48, 126.84, 87.12, 69.34, 47.99, 28.97.

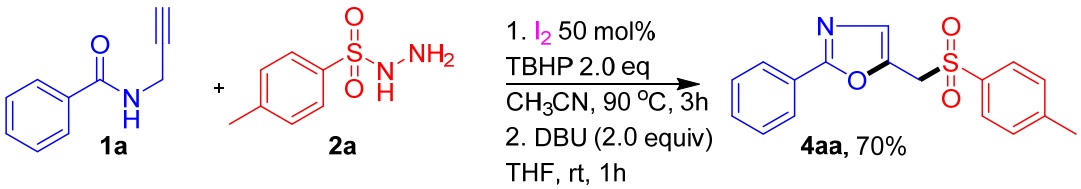


***N*-(1-Ethynylcyclohexyl)benzamide (1o)**.[2] ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.73 (m, 2H), 7.52 – 7.45 (m, 1H), 7.42 (ddd, *J* = 8.3, 4.4, 1.0 Hz, 2H), 6.14 (s, 1H), 2.45 (s, 1H), 2.28 – 2.19 (m, 3H), 2.00 – 1.91 (m, 2H), 1.76 – 1.58 (m, 6H), 1.35 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.30, 134.98, 131.39, 128.47, 126.99 – 126.71, 85.43, 71.48, 52.03, 36.86, 25.21, 22.47.



General Procedure (A) for the Preparation of Sulfonylated Oxazoles

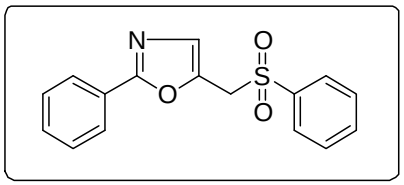
Preparation of 2-Phenyl-5-(tosylmethyl)oxazole (4aa).



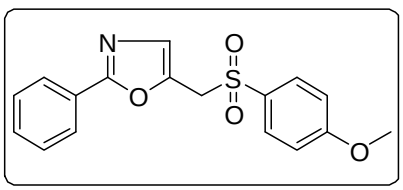
To a stirred solution of *N*-propynyl benzamide **1a** (160 mg, 1.0 equiv) in acetonitrile (2.0 mL) was added tosyllhydrazide **2a** (372 mg, 2.0 equiv), TBHP solution 70% in H_2O (258 µL, 2.0 equiv) and iodine (128 mg, 50 mol %). The reaction mixture was heated to 90 °C. The completion of reaction was monitored by TLC chromatography. After completion, the reaction mixture was cooled to room temperature and added 1 mL of THF followed by the addition of DBU (301 µL, 2.0 equiv). The completion of the reaction was monitored by TLC chromatography. After the completion, the reaction was diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was then given brine wash (2X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was then purified using column chromatography by eluting from hexane to 20% ethyl acetate/hexane to afford pure 2-Phenyl-5-(tosylmethyl)oxazole **4aa** as a light yellow solid (212 mg, 70%); mp 129.3~131.3 ℃; IR $(neat)_{vmax}$: 1596, 1543, 1482, 1322, 1153, 989, 714, 691 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* =

8.0, 1.7 Hz, 2H), 7.60 (d, *J* = 8.3 Hz, 2H), 7.41 – 7.32 (m, 3H), 7.23 (dd, *J* = 8.5, 0.6 Hz, 2H), 6.97 (s, 1H), 4.43 (d, *J* = 0.7 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.76, 145.47, 140.41, 134.89, 130.94, 129.94, 129.51, 128.73, 126.52, 53.87, 21.66; HRMS (ESI) calcd for $C_{17}H_{16}NO_3S$ $[M+H]^+$: 313.0845 found 313.0843.

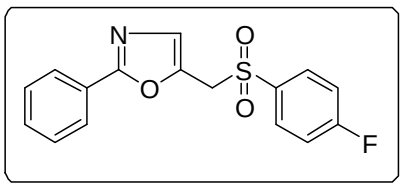
2-Phenyl-5-((phenylsulfonyl)methyl)oxazole (4ab). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a light brown solid (263 mg, 88%); mp 103.5~105.5 ℃; IR (neat)$_{vmax}$: 1607, 1546, 1482, 1448, 1321, 1274, 1158, 1137, 1085, 989, 855, 776, 757 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.78 (m, 4H), 7.65 (dd, *J* = 11.8, 4.3 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 2H), 7.44 (dd, *J* = 8.2, 6.1 Hz, 3H), 7.05 (s, 1H), 4.53 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.83, 134.23, 130.82, 129.72, 129.25, 128.66, 126.36, 53.74; HRMS (ESI) calcd for $C_{16}H_{14}NO_3S$ $[M+H]^+$: 300.0688 found 300. 0687.



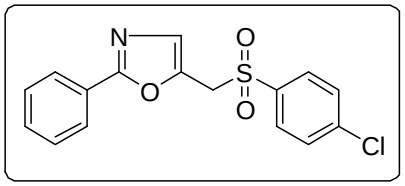
5-(((4-Methoxyphenyl)sulfonyl)methyl)-2-phenyloxazole (4ac). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (312 mg, 95%); mp 140.1~142.1 ℃; IR (neat)$_{vmax}$: 1595, 1545, 1496, 1324, 1262, 1149, 1078, 1024, 989, 836, 715 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 7.6, 2.0 Hz, 2H), 7.63 (d, *J* = 9.0 Hz, 2H), 7.44 – 7.32 (m, 3H), 6.97 (s, 1H), 6.88 (d, *J* = 9.0 Hz, 2H), 4.42 (s, 2H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.13, 162.64, 140.52, 130.79, 129.46, 129.17, 128.73, 126.60, 126.35, 114.39, 55.65, 53.94; HRMS (ESI) calcd for $C_{17}H_{16}NO_4S$ $[M+H]^+$: 330.0794 found 330.0792.



5-(((4-Fluorophenyl)sulfonyl)methyl)-2-phenyloxazole (4ad). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (247 mg, 78%); mp 157.5~159.5 ℃; IR (neat)$_{vmax}$: 1591, 1545, 1492, 1449, 1324, 1292, 1273, 1151, 988, 838, 787, 714 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (ddd, *J* = 13.9, 8.2, 3.3 Hz, 4H), 7.45 (dd, *J* = 5.7, 3.7 Hz, 3H), 7.20 (t, *J* = 8.5 Hz, 2H), 7.07 (s, 1H), 4.53 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.37, 166.09 (d, *J* = 256.0 Hz), 164.81, 139.92, 131.49 (d, *J* = 9.7 Hz), 129.83, 128.80, 126.50, 126.29, 116.72 (d, *J* = 23.0 Hz), 116.49, 53.81. HRMS (ESI) calcd for $C_{16}H_{13}FNO_3S$ $[M+H]^+$: 318.0594 found 318.0593.

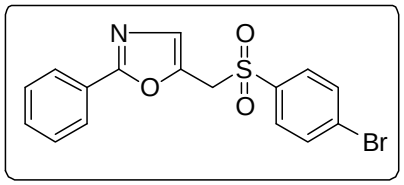


5-(((4-Chlorophenyl)sulfonyl)methyl)-2-phenyloxazole (4ae). Following the general procedure (A) on a



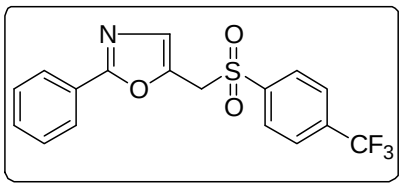
1.0 mmol scale, giving the compound as a yellow solid (167 mg, 50%); mp 143.7~145.7 ℃; IR (neat)$_{vmax}$: 1581, 1475, 1326, 1156, 1090, 989, 830, 634, 547 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.74 (d, *J* = 8.6 Hz, 2H), 7.48 (dd, *J* = 20.5, 8.2 Hz, 7H), 7.10 (s, 1H), 4.53 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.93, 141.24, 139.85, 136.24, 131.08, 130.17–129.54, 129.46–128.03, 128.63, 127.20, 126.35, 53.82; HRMS (ESI) calcd for $C_{16}H_{13}ClNO_3S$ $[M+H]^+$: 334.0297 found 334.0299.

5-(((4-Bromophenyl)sulfonyl)methyl)-2-phenyloxazole (4af). Following the general procedure (A) on a



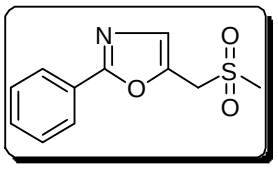
1.0 mmol scale, giving the compound as a brown solid (242 mg, 64%); mp 148.5~150.5 ℃; IR (neat)$_{vmax}$: 1573, 1546, 1481, 1390, 1325, 1155, 1010, 988, 826, 769, 713, 690 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.59 (s, 4H), 7.37 (d, *J* = 7.0 Hz, 3H), 7.01 (s, 1H), 4.45 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.74, 136.77, 132.60, 130.92, 130.23–129.70, 128.84, 126.38, 53.81; HRMS (ESI) calcd for $C_{16}H_{13}BrNO_3S$ $[M+H]^+$: 377.9794 found 377.9791.

2-Phenyl-5-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)oxazole (4ag). Following the general



procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (213 mg, 58%); mp 150.3~152.3 ℃; IR (neat)$_{vmax}$: 1607, 1404, 1322, 1276, 1171, 1138, 1106, 989, 839, 755, 713, 689 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.2 Hz, 2H), 7.78 – 7.66 (m, 4H), 7.42 – 7.31 (m, 3H), 7.05 (s, 1H), 4.50 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.05 , 141.42 - 140.42 (d, $J_{C,F}$ = 200.0 Hz), 139.42 , 131.08 , 130.08 , 129.33 - 129.09 (d, $J_{C,F}$ = 48.0 Hz), 128.85 , 127.81 , 126.57 - 126.18 (q, $J_{C,F}$ = 3.0 Hz), 113.94, 68.81, 53.76, 30.98; HRMS (ESI) calcd for $C_{17}H_{13}F_3NO_3S$ $[M+H]^+$: 368.0562 found 368.0561.

5-((Methylsulfonyl)methyl)-2-phenyloxazole (4ah). Following the general procedure (A) on a 1.0 mmol



scale, giving the compound as a brown solid (76 mg, 32%); mp 118.5~121.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 - 7.92 (m, 2H), 7.54 - 7.38 (m, 3H), 7.30 (s, 1H), 4.44 (s, 2H), 2.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.21, 140.19, 131.11, 130.01, 129.01, 126.78, 126.57, 52.16, 40.16; HRMS (ESI) calcd for $C_{11}H_{12}O_3NS$ $[M + H]^+$: 238.0532

found 238.0537.

2-(*p*-Tolyl)-5-(tosylmethyl)oxazole (4ba). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a white solid (238 mg, 73%); mp 145.5~147.3 ℃; IR (neat)$_{vmax}$: 1597, 1495, 1321, 1153, 1136, 987, 824, 757, 645, 548, 515 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 26.3, 8.2 Hz, 4H), 7.34 – 7.27 (m, 2H), 7.26 – 7.19 (m, 2H), 7.01 (s, 1H), 4.49 (s, 2H), 2.41 (d, *J* = 6.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.34, 141.24, 139.92, 134.87, 129.84, 129.44, 128.59, 126.35, 123.93, 53.84, 21.56; HRMS (ESI) calcd for $C_{18}H_{18}NO_3S$ $[M+H]^+$: 328.1001 found 328.1000.

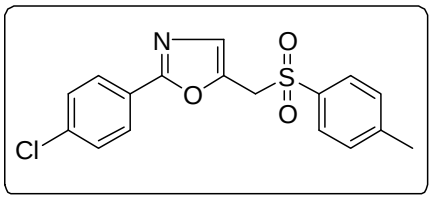
2-(4-Methoxyphenyl)-5-(tosylmethyl)oxazole (4ca). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (216 mg, 63%); mp 131.9~133.7 ℃; IR (neat)$_{vmax}$: 1613, 1496, 1321, 1256, 1153, 988, 839, 757, 645 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.9 Hz, 2H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.00 – 6.89 (m, 3H), 4.48 (s, 2H), 3.86 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.80, 161.63, 145.30, 139.58, 134.84, 129.82, 129.42, 128.59, 128.07, 119.42, 114.13, 55.39, 53.84, 21.61; HRMS (ESI) calcd for $C_{18}H_{18}NO_4S$ $[M+H]^+$: 344.0951 found 344.0949.

2-(3-Methoxyphenyl)-5-(tosylmethyl)oxazole (4da). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (164 mg, 48%); mp 131.2~133.2 ℃; IR (neat)$_{vmax}$: 1597, 1544, 1491, 1321, 1289, 1222, 1086, 1041, 989, 755, 686, 644, 515 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.45 – 7.27 (m, 5H), 7.06 – 6.95 (m, 2H), 4.50 (d, *J* = 0.7 Hz, 2H), 3.85 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.56, 159.78, 145.40, 140.33, 134.84, 129.84, 129.61, 128.58, 127.81, 118.78, 117.20, 111.02, 55.39, 53.80, 21.57; HRMS (ESI) calcd for $C_{18}H_{18}NO_4S$ $[M+H]^+$: 344.0951 found 344.0950.

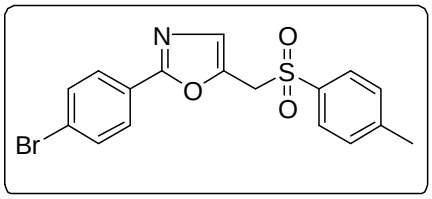
2-(4-Fluorophenyl)-5-(tosylmethyl)oxazole (4ea). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (245 mg, 74%); mp 145.2~147.2 ℃; IR (neat)$_{vmax}$: 1610, 1495, 1322, 1237, 1154, 988,

845, 758, 646, 607, 549 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.72 (m, 2H), 7.63 – 7.56 (m, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.03 (t, *J* = 8.7 Hz, 2H), 6.93 (s, 1H), 4.42 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.41, 164.16 (d, *J* = 250.0 Hz), 162.91, 145.35, 134.78, 129.80, 129.52, 128.47 (d, *J* = 8.0 Hz), 116.01, 115.9 (d, *J* = 22.0 Hz), 53.66, 21.54; HRMS (ESI) calcd for $C_{17}H_{15}FNO_3S$ $[M+H]^+$: 332.0751 found 332.0749.

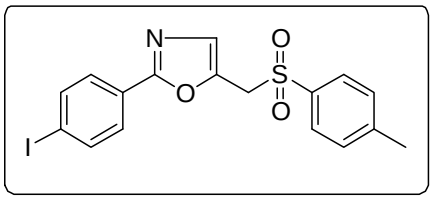
2-(4-Chlorophenyl)-5-(tosylmethyl)oxazole (4fa). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a light yellow solid (174 mg, 50%); mp 167.3~169.3 ℃; IR (neat)$_{vmax}$: 1597, 1481, 1321, 1151, 1135, 1090, 988, 814, 655, 551, 516 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.6 Hz, 2H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.6 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.04 (s, 1H), 4.49 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.78, 145.45, 140.63, 137.07, 134.84, 129.88, 129.56, 129.10, 128.56, 127.67, 125.00, 53.73, 21.62; HRMS (ESI) calcd for $C_{17}H_{15}ClNO_3S$ $[M+H]^+$: 348.0455 found 348.0453.



2-(4-Bromophenyl)-5-(tosylmethyl)oxazole (4ga). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (151 mg, 46%); mp 151.2~153.2 ℃; IR (neat)$_{vmax}$: 1602, 1478, 1402, 1321, 1153, 1010, 988, 834, 756, 645, 611, 549, 514 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 18.2, 8.4 Hz, 4H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.03 (s, 1H), 4.49 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.86, 145.44, 140.58, 134.84, 132.02, 129.85, 128.56, 127.78, 125.60, 125.32, 113.96, 53.76, 30.98, 21.63; HRMS (ESI) calcd for $C_{17}H_{15}BrNO_3S$ $[M+H]^+$: 391.9950 found 391.9947.

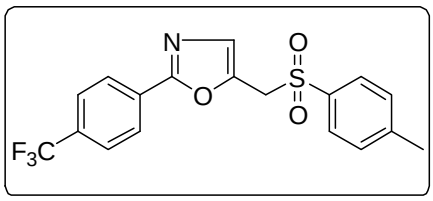


2-(4-Iodophenyl)-5-(tosylmethyl)oxazole (4ha). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (255 mg, 58%); mp 169.4~171.3 ℃; IR (neat)$_{vmax}$: 1600, 1320, 1275, 1153, 1074, 750, 548 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.6 Hz, 2H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 8.6 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 7.03 (s, 1H), 4.49 (d, *J* = 0.4 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.45, 140.62, 137.98, 134.83, 129.82, 128.56, 128.35, 127.78,



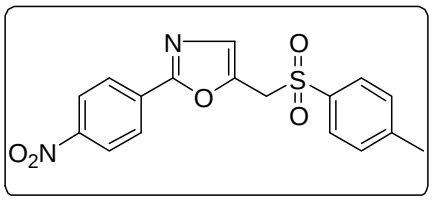
126.10, 97.42, 53.76, 21.64; HRMS (ESI) calcd for $C_{17}H_{15}INO_3S$ $[M+H]^+$: 439.9811 found 439.9808.

5-(Tosylmethyl)-2-(4-(trifluoromethyl)phenyl)oxazole (4ia). Following the general procedure (A) on a



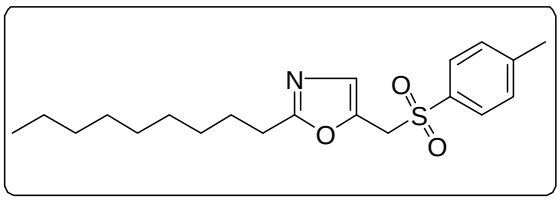
1.0 mmol scale, giving the compound as a white solid (221 mg, 58%); mp 158.2~160.5 ℃ ; IR $(neat)_{vmax}$: 1597, 1416, 1325, 1162, 1135, 1016, 988, 851, 758 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 4H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.08 (s, 1H), 4.52 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.28 , 145.52 , 141.22 , 134.83 , 132.48 ,132.32 (d, $J_{C,F}$ = 32.0 Hz), 132.16, 129.90, 128.54 ,127.57 (d, $J_{C,F}$ = 194.0 Hz), 126.60, 126.30 - 125.29 (q, $J_{C,F}$ = 8.0 Hz), 53.72, 21.60; HRMS (ESI) calcd for $C_{18}H_{15}F_3NO_3S$ $[M+H]^+$: 382.0719 found 382.0716.

2-(4-Nitrophenyl)-5-(tosylmethyl)oxazole (4ja). Following the general procedure (A) on a 1.0 mmol scale,



giving the compound as a yellow solid (143 mg, 40%); mp 176.2~178.5 ℃; IR $(neat)_{vmax}$: 1523, 1339, 1275, 1241, 1069, 859, 645 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 9.0 Hz, 2H), 8.06 (d, *J* = 9.1 Hz, 2H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.34 (dd, *J* = 8.5, 0.6 Hz, 2H), 7.13 (s, 1H), 4.53 (d, *J* = 0.7 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.64, 141.95, 134.83, 132.05, 130.44, 129.98, 128.56, 127.14, 124.15, 53.70, 21.68; HRMS (ESI) calcd for $C_{17}H_{15}N_2O_5S$ $[M+H]^+$: 359.0696 found 359.0694.

2-Nonyl-5-(tosylmethyl)oxazole (4ka). Following the general procedure (A) on a 1.0 mmol scale, giving



the compound as a yellow viscous oil (182 mg, 50%); IR $(neat)_{vmax}$: 1725, 1598, 1561, 1466, 1325, 1154, 1087, 990, 817, 756, 643, 550, 514 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 6.82 (s, 1H), 4.40 (s, 2H), 2.68 (t, *J* = 7.6 Hz, 2H), 2.45 (s, 3H), 1.63 (s, 2H), 1.35 – 1.20 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.43, 140.02, 134.85, 129.95, 128.60, 127.89, 53.52, 31.70, 29.06, 27.88, 26.67, 22.48, 21.50, 13.91; HRMS (ESI) calcd for $C_{26}H_{34}NO_3S$ $[M+H]^+$: 364.1941 found 364.1950.

2-(5-Nitrofuran-2-yl)-5-(tosylmethyl)oxazole (4la). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a brown solid (164 mg, 47%); mp 151.0~153.3 ℃; IR (neat)$_{vmax}$: 1686, 1519, 1353, 1259, 1154, 967, 812, 647 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.39 (dd, *J* = 16.4, 5.9 Hz, 4H), 7.19 – 7.09 (m, 2H), 4.52 (s, 2H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.65, 145.85, 143.09, 142.30, 134.63, 130.39, 130.08, 128.50, 116.78, 113.44, 112.65, 112.32, 53.48, 21.69; HRMS (ESI) calcd for $C_{15}H_{12}N_2NaO_6S$ [M+Na]$^+$: 371.0308 found 371.0306.

2-(4-Chlorophenyl)-5-(phenyl(tosyl)methyl)oxazole (4ma). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (288 mg, 68%); mp 143.9~145.5 ℃; IR (neat)$_{vmax}$: 1710, 1542, 1482, 1455, 1405, 1321, 1148, 1093, 1013, 838, 814, 703, 670, 564 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.8 Hz, 2H), 7.54 – 7.46 (m, 4H), 7.44 – 7.36 (m, 5H), 7.30 – 7.25 (m, 1H), 7.24 – 7.20 (m, 2H), 5.49 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.49, 145.25, 143.97, 136.87, 134.06, 130.28, 129.83–129.40, 129.39–128.68, 128.60, 127.79–127.24, 125.31, 69.05, 21.65; HRMS (ESI) calcd for $C_{23}H_{19}ClNO_3S$ [M+H]$^+$: 424.0768 found 424.0766.

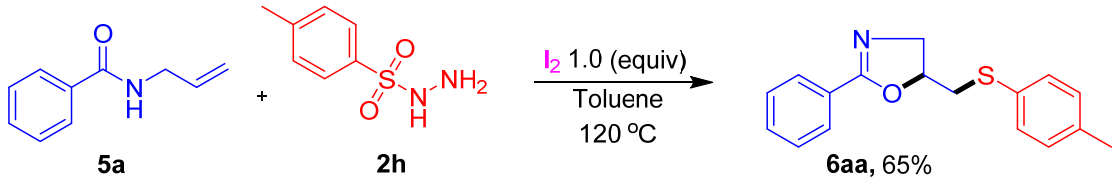
(*E*)-4,4-Dimethyl-2-phenyl-5-(tosylmethylene)-4,5-dihydrooxazole (4na). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a light brown solid (181 mg, 53%); mp 99.7~101.7 ℃; IR (neat)$_{vmax}$: 1674, 1632, 1597, 1321, 1290, 1174, 1150, 1048, 1022, 936, 847, 813, 692, 662, 582 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.91 (m, 1H), 7.90 (d, *J* = 1.4 Hz, 1H), 7.84 (s, 1H), 7.82 (s, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.35 (dd, *J* = 8.6, 0.6 Hz, 2H), 6.21 (s, 1H), 2.44 (s, 3H), 1.86 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.42, 157.55, 144.08, 139.68, 132.27, 129.92, 128.66, 128.12, 127.06, 106.11, 73.19, 26.57, 21.58; HRMS (ESI) calcd for $C_{19}H_{20}NO_3S$ [M+H]$^+$: 342.1158 found 342.1156.

(*E*)-2-Phenyl-4-(tosylmethylene)-3-oxa-1-azaspiro[4.5]dec-1-ene (4oa). Following the general procedure (A) on a 1.0 mmol scale, giving the compound as a yellow solid (191 mg, 50%); mp 30.2~33.7 ℃; IR (neat)$_{vmax}$: 1675, 1625, 1450, 1322, 1278, 1154, 1046, 1022, 692, 661, 588 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.90 (m, 2H), 7.83 (d,

J = 8.3 Hz, 2H), 7.50 (d, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.16 (s, 1H), 2.85 (td, *J* = 13.0, 4.1 Hz, 2H), 2.44 (s, 3H), 2.00 – 1.79 (m, 3H), 1.74 (d, *J* = 13.0 Hz, 2H), 1.68 – 1.51 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.99, 156.56, 143.92, 139.87, 131.97, 129.81, 128.53, 128.11, 126.99, 125.86, 105.87, 34.90, 24.89, 22.27, 21.55; HRMS (ESI) calcd for $C_{22}H_{24}NO_3S$ $[M+H]^+$: 382.1471 found 382.1468.

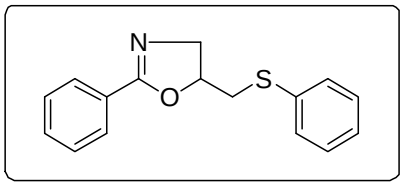
General procedure (B) for preparation of sulfenylated oxazolines

Procedure for the synthesis of 2-Phenyl-5-((*p*-tolylthio)methyl)-4,5-dihydrooxazole (6aa).

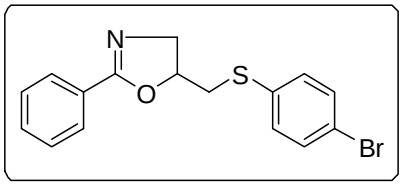


To a stirred solution of *N*-allyl benzamide **5a** (160 mg, 1.0 equiv) in toluene (2.0 mL) was added tosylhydrazide **2a** (280 mg, 1.5 equiv), and iodine (254 mg, 1.0 equiv). The reaction mixture was heated to reflux. The completion of reaction was monitored by TLC chromatography. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was then given brine wash (2X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was then purified using column chromatography using neutral alumina by eluting from hexane to 20% ethyl acetate/hexane to afford pure 2-Phenyl-5-((*p*-tolylthio)methyl)-4,5-dihydrooxazole (**6aa**) as a yellow liquid (184 mg, 65%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.81 (m, 2H), 7.50 – 7.30 (m, 5H), 7.13 – 7.06 (m, 2H), 4.86 – 4.75 (m, 1H), 4.13 (dd, *J* = 15.0, 9.5 Hz, 1H), 3.87 (dd, *J* = 15.0, 6.8 Hz, 1H), 3.27 (dd, *J* = 13.7, 5.5 Hz, 1H), 3.01 (dd, *J* = 13.7, 7.2 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.66, 137.05, 131.46, 131.16, 129.81, 128.51–127.99, 127.52, 78.25, 60.71, 59.54, 39.09, 29.65, 20.99, 7.61; HRMS (ESI) calcd for $C_{17}H_{18}NOS$ $[M+H]^+$: 284.1104 found 284.1112.

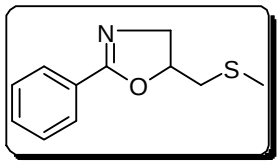
2-Phenyl-5-((phenylthio)methyl)-4,5-dihydrooxazole (6ba). Following the general procedure (B) on a 1.0 mmol scale, giving the compound as a yellow viscous oil (167 mg, 62 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.42 (ddt, *J* = 13.5, 8.5, 7.3 Hz, 5H), 7.32 – 7.19 (m, 3H), 4.90 – 4.79 (m, 1H), 4.16 (dd, *J* = 15.0, 9.5 Hz, 1H), 3.89 (dd, *J* = 15.0, 6.7 Hz, 1H), 3.33 (dd, *J* = 13.7, 5.5 Hz, 1H), 3.07 (dd, *J* = 13.7, 7.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.92, 131.35, 130.33, 129.08, 128.20, 126.79, 78.15, 59.61, 38.47, 29.69; HRMS (ESI) calcd for $C_{16}H_{16}NOS$ $[M+H]^+$: 270.0947 found 270.0952.



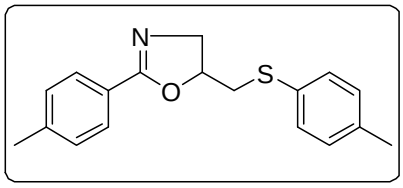
5-(((4-Bromophenyl)thio)methyl)-2-phenyl-4,5-dihydrooxazole (6af). Following the general procedure (B) on a 1.0 mmol scale, giving the compound as a yellow viscous oil (174 mg, 50 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.50 – 7.35 (m, 5H), 7.31 – 7.25 (m, 2H), 4.86 (dd, *J* = 9.5, 5.7 Hz, 1H), 4.16 (dd, *J* = 15.0, 9.5 Hz, 1H), 3.88 (dd, *J* = 15.0, 6.7 Hz, 1H), 3.27 (dd, *J* = 13.9, 5.7 Hz, 1H), 3.10 (dd, *J* = 13.9, 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.98, 131.41, 128.29, 128.07, 120.76, 78.15, 59.54, 38.63; HRMS (ESI) calcd for $C_{16}H_{15}BrNOS$ $[M+H]^+$: 348.0052 found 348.0065.



5-((Methylthio)methyl)-2-phenyl-4,5-dihydrooxazole (6ah). Following the general procedure (B) on a 1.0 mmol scale, giving the compound as a yellow viscous oil (83 mg, 40%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 - 7.91 (m, 2H), 7.51 - 7.45 (m, 1H), 7.45 - 7.37 (m, 2H), 4.97 - 4.80 (m, 1H), 4.19 (dd, *J* = 14.9, 9.4 Hz, 1H), 3.85 (q, *J* = 7.3 Hz, 1H), 2.86 (dd, *J* = 14.2, 6.0 Hz, 1H), 2.77 - 2.63 (m, 1H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.84, 131.45, 128.44, 128.22, 127.73, 79.24, 59.87, 38.66, 16.50; HRMS (ESI) calcd for $C_{11}H_{14}ONS$ $[M + H]^+$: 208.0791 found 208.0788.

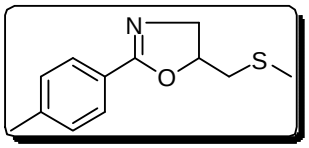


2-(*p*-Tolyl)-5-((*p*-tolylthio)methyl)-4,5-dihydrooxazole (6ba). Following the general procedure (B) on a 1.0 mmol scale, giving the compound as a yellow viscous oil (128 mg, 43 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 4.84 – 4.73 (m, 1H), 4.12 (dd, *J* = 14.9, 9.5 Hz, 1H), 3.85 (dd, *J* = 14.9, 6.8 Hz, 1H), 3.27 (dd, *J* = 13.7, 5.5 Hz, 1H), 3.00 (dd, *J* = 13.7, 7.3 Hz, 1H), 2.38 (d, *J* = 4.9 Hz, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ



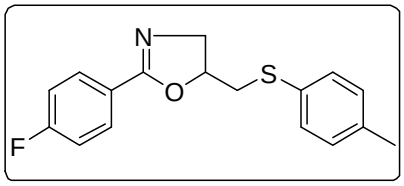
163.81, 141.67, 137.04, 131.14, 129.82, 129.00, 128.09, 124.70, 78.17, 60.66, 59.47, 39.10, 21.52, 21.00, 7.69; HRMS (ESI) calcd for $C_{18}H_{20}NOS$ $[M+H]^+$: 298.1260 found 298.1268.

5-((Methylthio)methyl)-2-(p-tolyl)-4,5-dihydrooxazole (6bh). Following the general procedure (B) on a



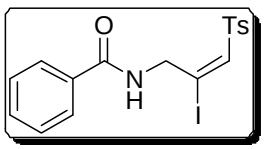
1.0 mmol scale, giving the compound as a yellow viscous oil (100 mg, 45%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 8.2 Hz, 2H), 4.93 - 4.83 (m, 1H), 4.17 (dd, *J* = 14.7, 9.6 Hz, 1H), 3.84 (q, *J* = 7.3 Hz, 1H), 2.86 (dd, *J* = 14.2, 6.0 Hz, 1H), 2.72 (q, *J* = 6.9 Hz, 1H), 2.39 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.94, 141.83, 129.15, 128.18, 124.94, 79.14, 59.82, 38.67, 21.63, 16.50; HRMS (ESI) calcd for $C_{12}H_{16}ONS$ $[M + H]^+$: 222.0947 found 222.0943.

2-(4-Fluorophenyl)-5-((*p*-tolylthio)methyl)-4,5-dihydrooxazole (6ca). Following the general procedure



(B) on a 1.0 mmol scale, giving the compound as a yellow viscous oil (120 mg, 40 %); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.79 (m, 2H), 7.37 – 7.30 (m, 2H), 7.15 – 7.01 (m, 4H), 4.87 – 4.77 (m, 1H), 4.12 (dd, *J* = 15.0, 9.5 Hz, 1H), 3.86 (dd, *J* = 14.9, 6.8 Hz, 1H), 3.26 (dd, *J* = 13.8, 5.6 Hz, 1H), 3.03 (dd, *J* = 13.8, 7.0 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.87, 164.63 (d, *J* = 249.0 Hz), 162.81, 137.14, 131.13, 130.36 (d, *J* = 8.8 Hz), 129.84, 123.76, 115.46 - 115.24 (d, *J* = 22.0 Hz), 78.50, 59.55, 39.12, 29.68, 21.02; HRMS (ESI) calcd for $C_{17}H_{17}FNOS$ $[M+H]^+$: 302.1009 found 302.1018.

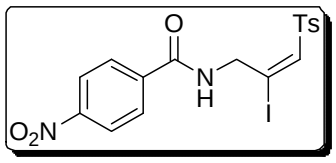
Procedure for the synthesis of (*E*)-*N*-(2-Iodo-3-tosylallyl)benzamide (3aa). To a stirred solution of



N-propynyl benzamide **1a** (160 mg, 1.0 equiv) in acetonitrile (2.0 mL) was added tosyllhydrazide **2a** (372 mg, 2.0 equiv), TBHP solution 70% in H_2O (258 μL, 2.0 equiv) and iodine (128 mg, 50 mol %). The reaction mixture was heated to 90 °C. The completion of reaction was monitored by TLC chromatography. After the completion, the reaction was diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was then given brine wash (2X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was then purified using column chromatography by eluting from hexane to 15% ethyl acetate/hexane to afford pure (*E*)-*N*-(2-Iodo-3-tosylallyl)benzamide ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.80 (m, 4H), 7.57 –

7.43 (m, 3H), 7.41 – 7.36 (m, 2H), 7.17 (t, *J* = 1.1 Hz, 1H), 6.81 (s, 1H), 4.91 (dd, *J* = 6.3, 1.1 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.09, 145.42, 140.69, 136.89, 133.64, 131.93, 130.32, 128.68, 127.68, 127.14, 119.92, 45.47, 21.71; HRMS (ESI) calcd for $C_{17}H_{17}NO_3NIS$ $[M+H]^+$:441.9968 found 441.9982.

Procedure for the synthesis of (*E*)-N-(2-Iodo-3-tosylallyl)-4-nitrobenzamide (3ja). To a stirred solution

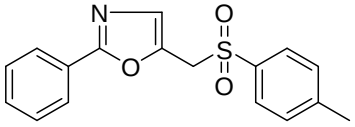


of 4-nitro-N-(prop-2-yn-1-yl)benzamide **3a** (204 mg, 1.0 equiv) in acetonitrile (2.0 mL) was added tosyllhydrazide **2a** (372 mg, 2.0 equiv), TBHP solution 70% in H_2O (258 μL, 2.0 equiv) and iodine (128 mg, 50 mol %). The reaction mixture was heated to 90 °C. The completion of reaction was monitored by TLC chromatography. After the completion, the reaction was diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was then given brine wash (2X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was then purified using column chromatography by eluting from hexane to 15% ethyl acetate/hexane to afford pure (*E*)-*N*-(2-Iodo-3-tosylallyl)-4-nitrobenzamide (**3ja**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.7 Hz, 2H), 8.01 (d, *J* = 8.8 Hz, 2H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.18 (s, 1H), 7.06 (s, 1H), 4.95 (d, *J* = 6.0 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.18, 145.69, 141.13, 139.17, 136.57, 130.40, 128.42, 127.68, 123.92, 117.84, 45.99, 21.75; HRMS (ESI) calcd for $C_{17}H_{16}N_2O_5IS$ $[M+H]^+$: 486.9819 found 486.9834.

4) CCDC 145160-145167, 1473425

Summary of Data CCDC 1465160

Compound Name: 2-Phenyl-5-(tosylmethyl)oxazole

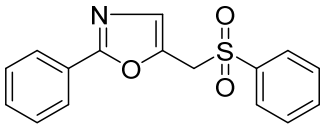


Formula: C_{17} H_{15} N_1 O_3 S_1

Unit Cell Parameters: a 6.0578(6) b 11.1512(14) c 11.9001(15) P-1

Summary of Data CCDC 1465161

Compound Name: 2-Phenyl-5-((phenylsulfonyl)methyl)oxazole

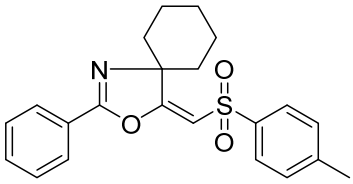


Formula: C_{16} H_{13} N_1 O_3 S_1

Unit Cell Parameters: a 5.8951(3) b 10.7554(8) c 11.3589(8) P-1

Summary of Data CCDC 1465162

Compound Name: (*E*)-2-Phenyl-4-(tosylmethylene)-3-oxa-1-azaspiro[4.5]dec-1-ene



Formula: C_{22} H_{23} N_1 O_3 S_1

Unit Cell Parameters: a 9.8639(12) b 21.953(3) c 10.1344(11) Cc

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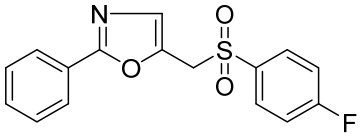
Summary of Data CCDC 1465163

Compound Name: 5-(((4-Fluorophenyl)sulfonyl)methyl)-2-phenyloxazole

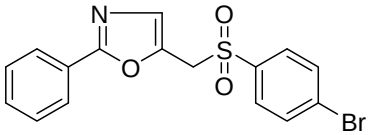


Formula: C_{16} H_{12} F_1 N_1 O_3 S_1

Unit Cell Parameters: a 6.2389(3) b 9.1551(6) c 13.2937(8) P-1

Summary of Data CCDC 1465164

Compound Name: 5-(((4-Bromophenyl)sulfonyl)methyl)-2-phenyloxazole

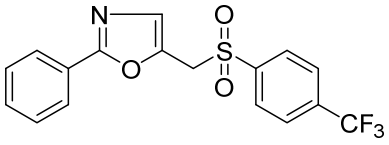


Formula: C_{16} H_{12} Br_1 N_1 O_3 S_1

Unit Cell Parameters: a 6.0573(8) b 9.8062(15) c 13.5008(17) P-1

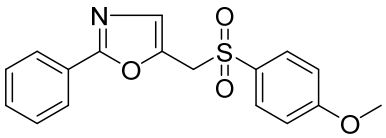
Summary of Data CCDC 1465165

Compound Name: 2-Phenyl-5-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)oxazole



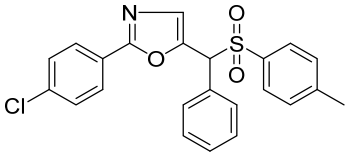
Formula: C_{17} H_{12} F_3 N_1 O_3 S_1
Unit Cell Parameters: a 6.1164(12) b 9.942(3) c 13.652(3) P-1

Summary of Data CCDC 1465166
Compound Name: 5-(((4-Methoxyphenyl)sulfonyl)methyl)-2-phenyloxazole



Formula: C_{17} H_{15} N_1 O_4 S_1
Unit Cell Parameters: a 6.1602(11) b 10.664(2) c 13.258(3) P-1

Summary of Data CCDC 1465167
Compound Name: 2-(4-Chlorophenyl)-5-(phenyl(tosyl)methyl)oxazole



Formula: C_{23} H_{18} Cl_1 N_1 O_3 S_1
Unit Cell Parameters: a 13.752(3) b 8.4132(13) c 19.307(3) P21/c

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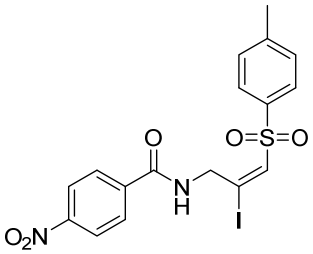
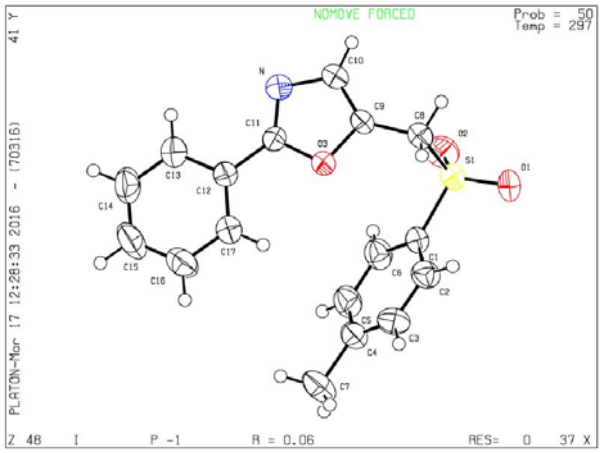
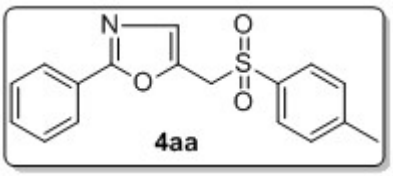
Summary of Data CCDC 1473425
Compound Name: (*E*)-*N*-(2-Iodo-3-tosylallyl)-4-nitrobenzamide



Formula: C_{17} H_{15} I_1 N_2 O_5 S_1
Unit Cell Parameters: a 10.3360(7) b 13.7149(9) c 14.1776(8) P-1

5) X-ray Crystallography Data





Datablock: I

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=6.0578(6) b=11.1512(14) c=11.9001(15)
alpha=71.535(12) beta=86.207(9) gamma=89.004(9)
Temperature: 297 K

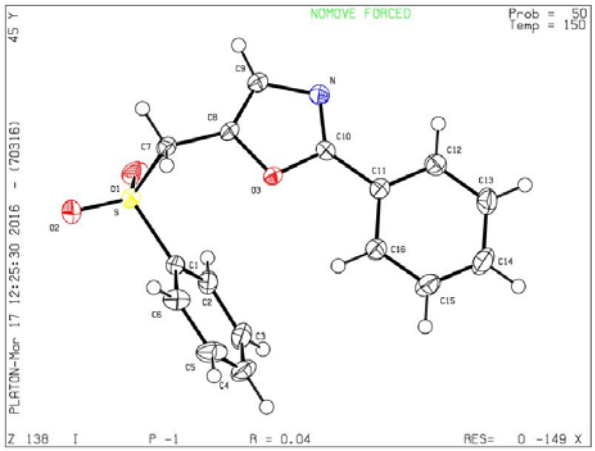
	Calculated	Reported
Volume	760.81(16)	760.81(15)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C17 H15 N O3 S	C17 H15 N O3 S
Sum formula	C17 H15 N O3 S	C17 H15 N O3 S
Mr	313.36	313.36
Dx,g cm-3	1.368	1.368
Z	2	2
Mu (mm-1)	0.224	0.224
F000	328.0	328.0
F000'	328.39	
h,k,lmax	8,15,16	8,13,16
Nref	4138	3490
Tmin,Tmax	0.953,0.982	0.986,1.000
Tmin'	0.904	

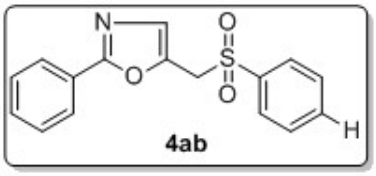
Correction method= # Reported T Limits: Tmin=0.986 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.843 Theta(max)= 29.200

R(reflections)= 0.0604(1988) wR2(reflections)= 0.1440(3490)

S = 0.991 Npar= 199





Datablock: I

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=5.8951(3) b=10.7554(8) c=11.3589(8)
alpha=75.588(3) beta=86.378(2) gamma=81.134(2)
Temperature: 150 K

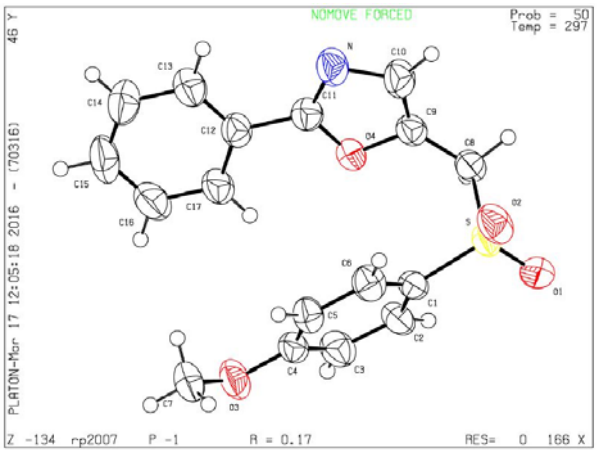
	Calculated	Reported
Volume	688.97(8)	688.97(8)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C16 H13 N O3 S	C16 H13 N O3 S
Sum formula	C16 H13 N O3 S	C16 H13 N O3 S
Mr	299.33	299.33
Dx,g cm-3	1.443	1.443
Z	2	2
Mu (mm-1)	0.244	0.244
F000	312.0	312.0
F000'	312.39	
h,k,lmax	7,13,14	7,13,14
Nref	2821	2809
Tmin,Tmax	0.940,0.964	0.902,0.964
Tmin'	0.900	

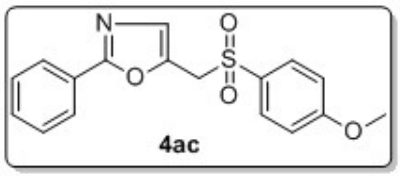
Correction method= # Reported T Limits: Tmin=0.902 Tmax=0.964
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 26.390

R(reflections)= 0.0365(2256) wR2(reflections)= 0.1110(2809)

S = 1.057 Npar= 190



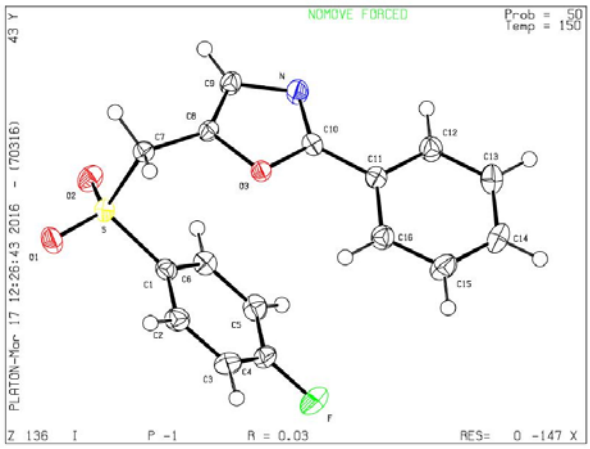


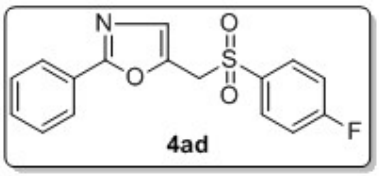
Datablock: rp2007

```
Bond precision:  C-C = 0.0117 A          Wavelength=0.71073

Cell:         a=6.1602(11)       b=10.664(2)       c=13.258(3)
              alpha=103.005(18)  beta=102.402(16)  gamma=106.112(16)
Temperature:  297 K
```

	Calculated	Reported
Volume	778.7(3)	778.7(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H15 N O4 S	C17 H15 N O4 S
Sum formula	C17 H15 N O4 S	C17 H15 N O4 S
Mr	329.36	329.36
Dx,g cm-3	1.405	1.405
Z	2	2
Mu (mm-1)	0.228	0.228
F000	344.0	344.0
F000'	344.41	
h,k,lmax	8,14,18	8,14,16
Nref	4223	3550
Tmin,Tmax	0.914,0.973	0.563,1.000
Tmin'	0.862	

```
Correction method= # Reported T Limits: Tmin=0.563 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.841          Theta(max)= 29.180

R(reflections)= 0.1740( 2033)     wR2(reflections)= 0.4576( 3550)

S = 1.377                 Npar= 208
```



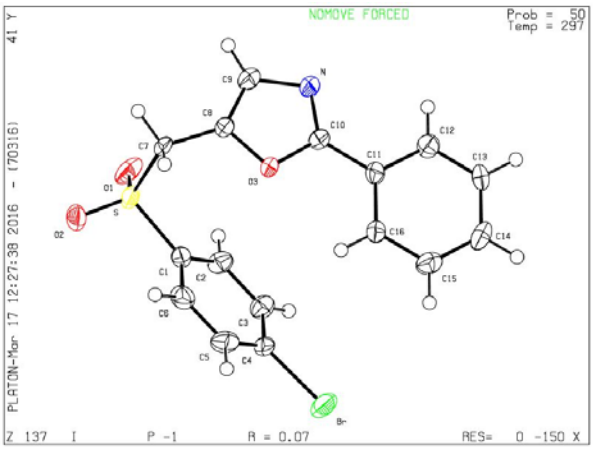


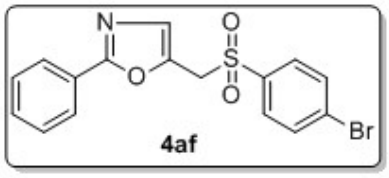
Datablock: I

```
Bond precision:  C-C = 0.0029 A          Wavelength=0.71073

Cell:          a=6.2389(3)       b=9.1551(6)       c=13.2937(8)
               alpha=72.550(2)   beta=81.797(2)    gamma=75.434(2)
Temperature:   150 K
```

	Calculated	Reported
Volume	699.22(7)	699.22(7)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C16 H12 F N O3 S	C16 H12 F N O3 S
Sum formula	C16 H12 F N O3 S	C16 H12 F N O3 S
Mr	317.33	317.33
Dx,g cm-3	1.507	1.507
Z	2	2
Mu (mm-1)	0.255	0.255
F000	328.0	328.0
F000'	328.42	
h,k,lmax	7,11,16	7,11,16
Nref	2885	2880
Tmin,Tmax	0.929,0.967	0.900,0.968
Tmin'	0.898	

```
Correction method= # Reported T Limits: Tmin=0.900 Tmax=0.968
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.440

R(reflections)= 0.0346( 2446)     wR2(reflections)= 0.0933( 2880)

S = 1.026                  Npar= 199
```





Datablock: I

Bond precision: C-C = 0.0083 A Wavelength=0.71073

Cell: a=6.0573(8) b=9.8062(15) c=13.5008(17)
alpha=70.435(13) beta=82.679(10) gamma=82.699(11)
Temperature: 297 K

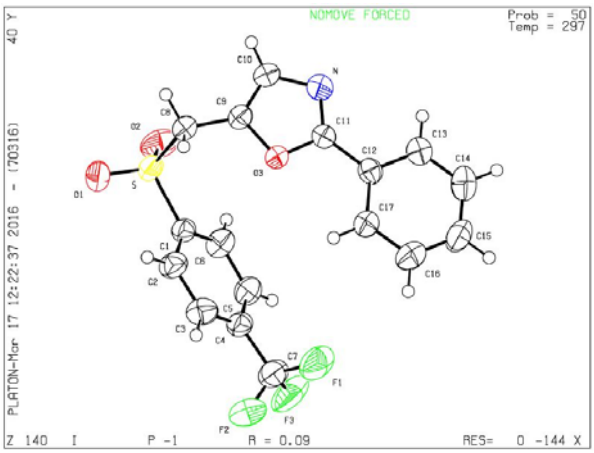
	Calculated	Reported
Volume	746.41(19)	746.41(18)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C16 H12 Br N O3 S	C16 H12 Br N O3 S
Sum formula	C16 H12 Br N O3 S	C16 H12 Br N O3 S
Mr	378.23	378.24
Dx,g cm-3	1.683	1.683
Z	2	2
Mu (mm-1)	2.905	2.905
F000	380.0	380.0
F000'	379.83	
h,k,lmax	8,13,18	8,12,18
Nref	4094	3452
Tmin,Tmax	0.599,0.685	0.969,1.000
Tmin'	0.150	

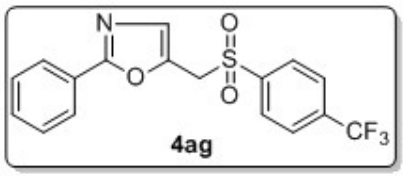
Correction method= # Reported T Limits: Tmin=0.969 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.843 Theta(max)= 29.310

R(reflections)= 0.0719(2269) wR2(reflections)= 0.1985(3452)

S = 1.054 Npar= 199





Datablock: I

Bond precision: C-C = 0.0061 A Wavelength=0.71073

Cell: a=6.1164(12) b=9.942(3) c=13.652(3)
alpha=72.21(2) beta=84.375(18) gamma=87.05(2)
Temperature: 297 K

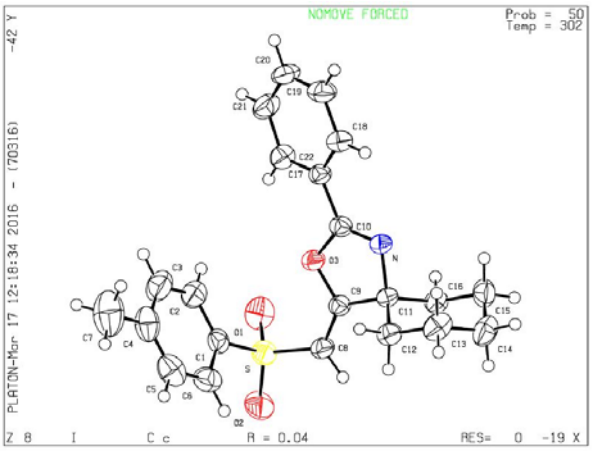
	Calculated	Reported
Volume	786.5(3)	786.5(3)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C17 H12 F3 N O3 S	C17 H12 F3 N O3 S
Sum formula	C17 H12 F3 N O3 S	C17 H12 F3 N O3 S
Mr	367.34	367.34
Dx,g cm-3	1.551	1.551
Z	2	2
Mu (mm-1)	0.256	0.256
F000	376.0	376.0
F000'	376.49	
h,k,lmax	8,13,18	8,13,18
Nref	4262	3584
Tmin,Tmax	0.935,0.950	0.883,1.000
Tmin'	0.840	

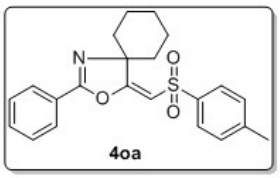
Correction method= # Reported T Limits: Tmin=0.883 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.841 Theta(max)= 29.170

R(reflections)= 0.0895(2191) wR2(reflections)= 0.2694(3584)

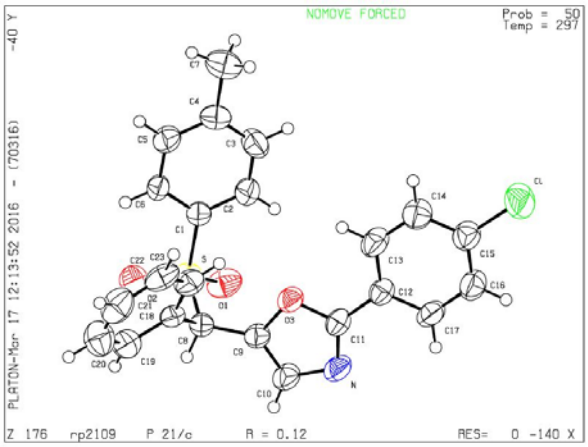
S = 1.070 Npar= 226

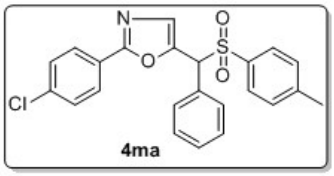




Datablock: I

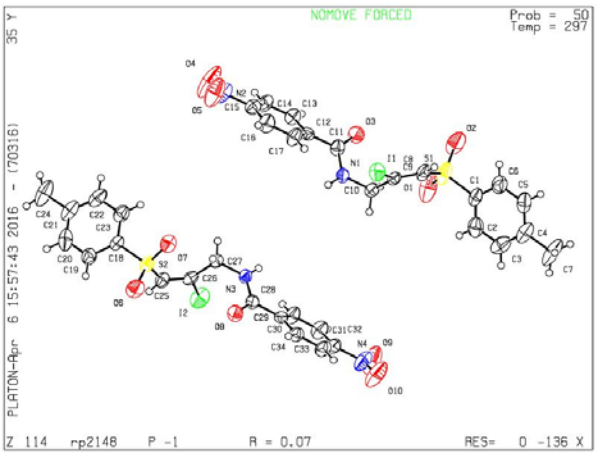
```
Bond precision:  C-C = 0.0036 A          Wavelength=0.71073

Cell:            a=9.8639(12)    b=21.953(3)         c=10.1344(11)
                 alpha=90        beta=115.004(4)     gamma=90
Temperature:     302 K

                 Calculated                  Reported
Volume           1988.9(4)                   1988.8(4)
Space group      C c                         C c
Hall group       C -2yc                      ?
Moiety formula   C22 H23 N O3 S              C22 H23 N O3 S
Sum formula      C22 H23 N O3 S              C22 H23 N O3 S
Mr               381.47                      381.47
Dx,g cm-3        1.274                       1.274
Z                4                           4
Mu (mm-1)        0.184                       0.184
F000             808.0                       808.0
F000'            808.84
h,k,lmax         12,27,12                    12,27,12
Nref             4069[ 2041]                 3891
Tmin,Tmax        0.926,0.948                 0.912,0.948
Tmin'            0.910

Correction method= # Reported T Limits: Tmin=0.912 Tmax=0.948
AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.96      Theta(max)= 26.370

R(reflections)= 0.0352( 3417)     wR2(reflections)= 0.0870( 3891)

S = 1.034                  Npar= 244
```

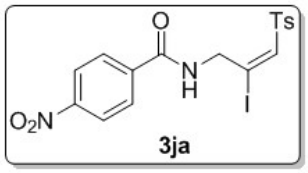




Datablock: rp2109

```
Bond precision:   C-C = 0.0104 A          Wavelength=0.71073

Cell:             a=13.752(3)     b=8.4132(13)        c=19.307(3)
                  alpha=90        beta=110.58(2)      gamma=90
Temperature:      297 K

                  Calculated                  Reported
Volume            2091.2(7)                   2091.2(7)
Space group       P 21/c                      P 21/c
Hall group        -P 2ybc                     -P 2ybc
Moiety formula    C23 H18 Cl N O3 S           C23 H18 Cl N O3 S
Sum formula       C23 H18 Cl N O3 S           C23 H18 Cl N O3 S
Mr                423.89                      423.89
Dx,g cm-3         1.346                       1.346
Z                 4                           4
Mu (mm-1)         0.307                       0.307
F000              880.0                       880.0
F000'             881.44
h,k,lmax          18,11,26                    18,11,25
Nref              5665                        4749
Tmin,Tmax         0.866,0.926                 0.858,1.000
Tmin'             0.850

Correction method= # Reported T Limits: Tmin=0.858 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.838          Theta(max)= 29.193

R(reflections)= 0.1164( 2502)     wR2(reflections)= 0.3860( 4749)

S = 1.131                 Npar= 263
```





Datablock: rp2148

```
Bond precision:  C-C = 0.0114 A          Wavelength=0.71073

Cell:          a=10.3360(7)      b=13.7149(9)      c=14.1776(8)
               alpha=85.839(5)   beta=74.352(6)   gamma=76.639(6)
Temperature:   297 K

                Calculated                Reported
Volume          1882.8(2)                 1882.8(2)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C17 H15 I N2 O5 S         C17 H15 I N2 O5 S
Sum formula     C17 H15 I N2 O5 S         C17 H15 I N2 O5 S
Mr              486.27                    486.27
Dx,g cm-3       1.715                     1.715
Z               4                         4
Mu (mm-1)       1.842                     1.842
F000            960.0                     960.0
F000'           959.01
h,k,lmax        14,18,19                  13,18,19
Nref            10410                     8636
Tmin,Tmax       0.725,0.802               0.831,1.000
Tmin'           0.340

Correction method= # Reported T Limits: Tmin=0.831 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.830          Theta(max)= 29.406

R(reflections)= 0.0698( 5253)     wR2(reflections)= 0.1979( 8636)

S = 1.044                 Npar= 471
```

---

6) References

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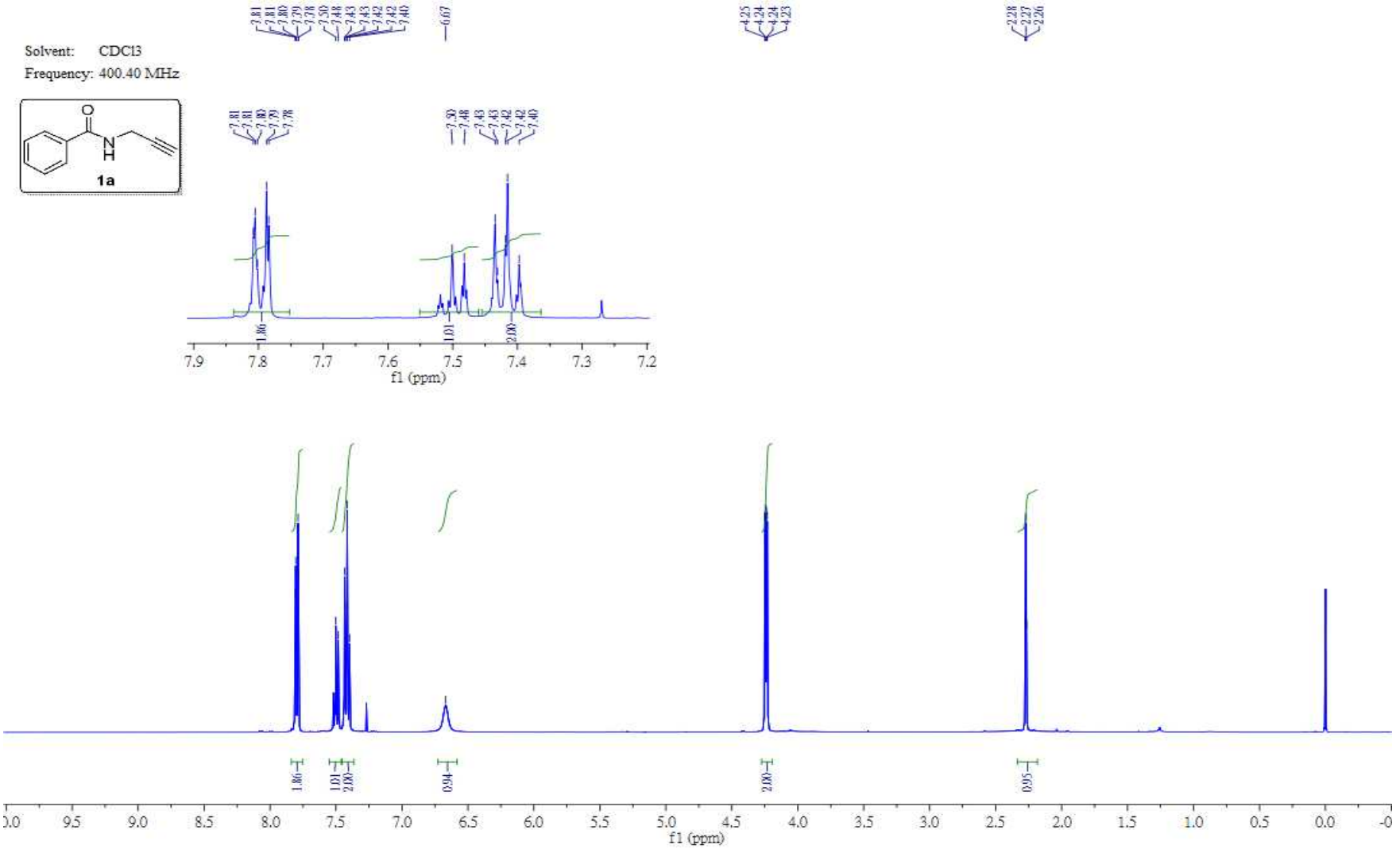
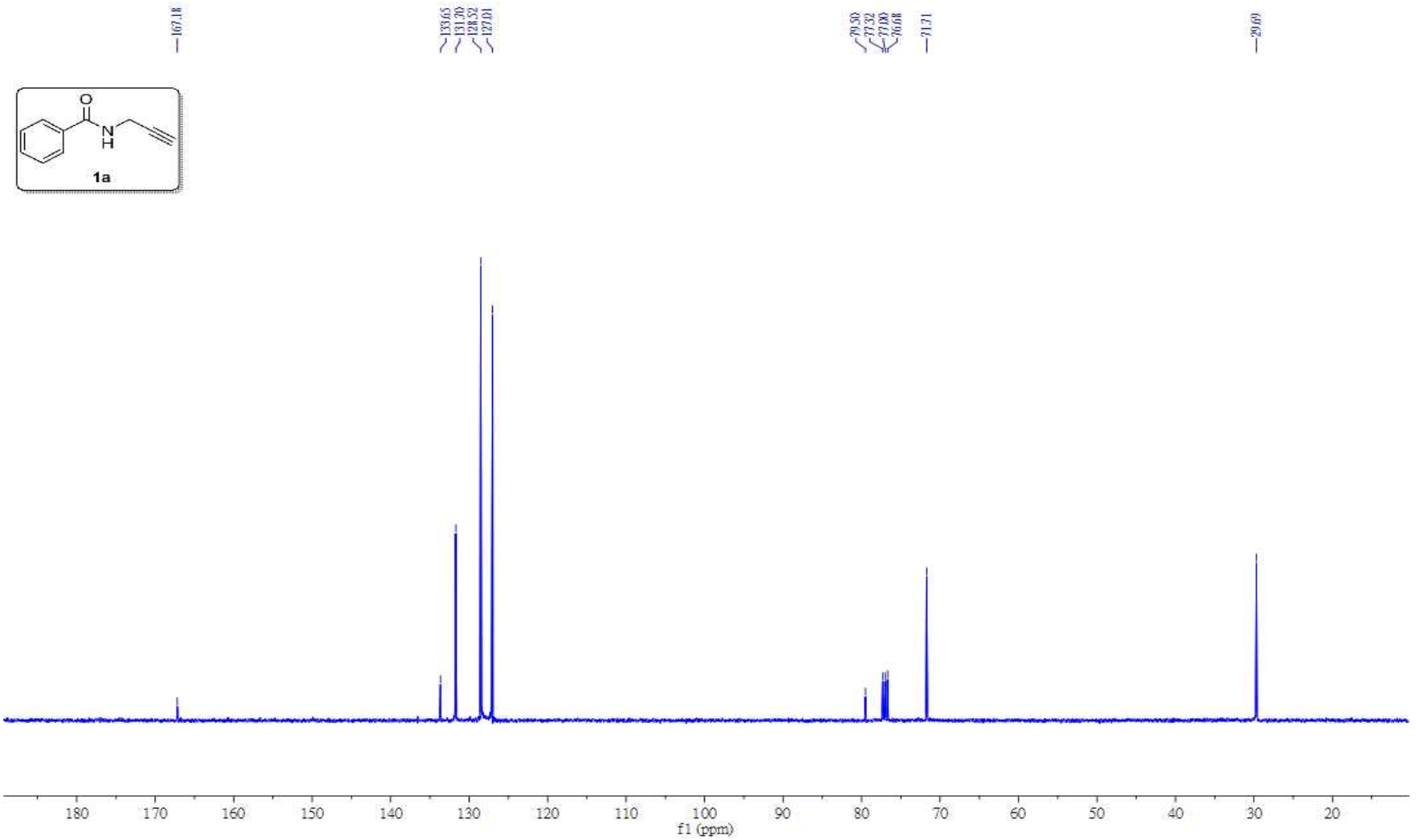
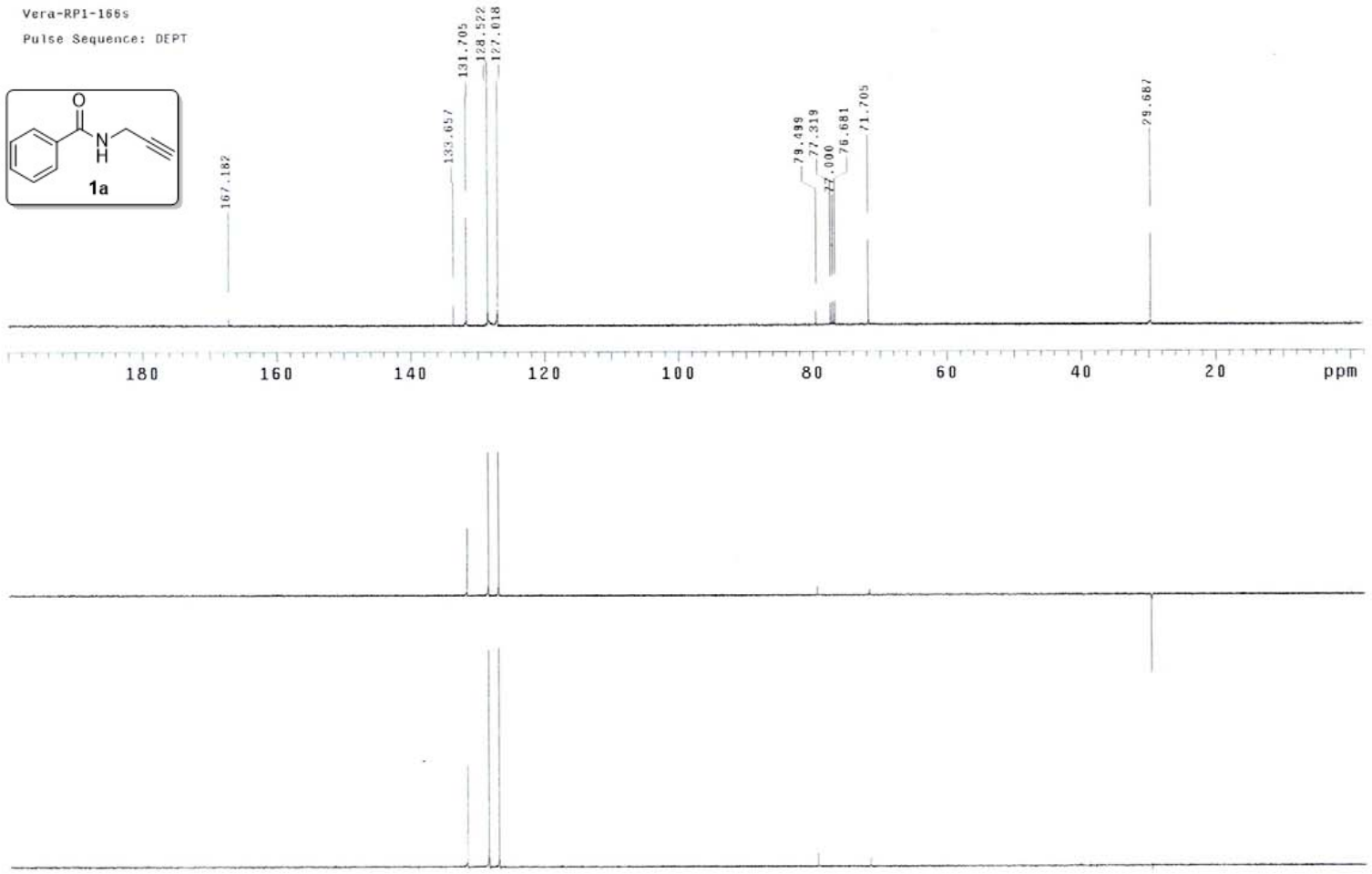
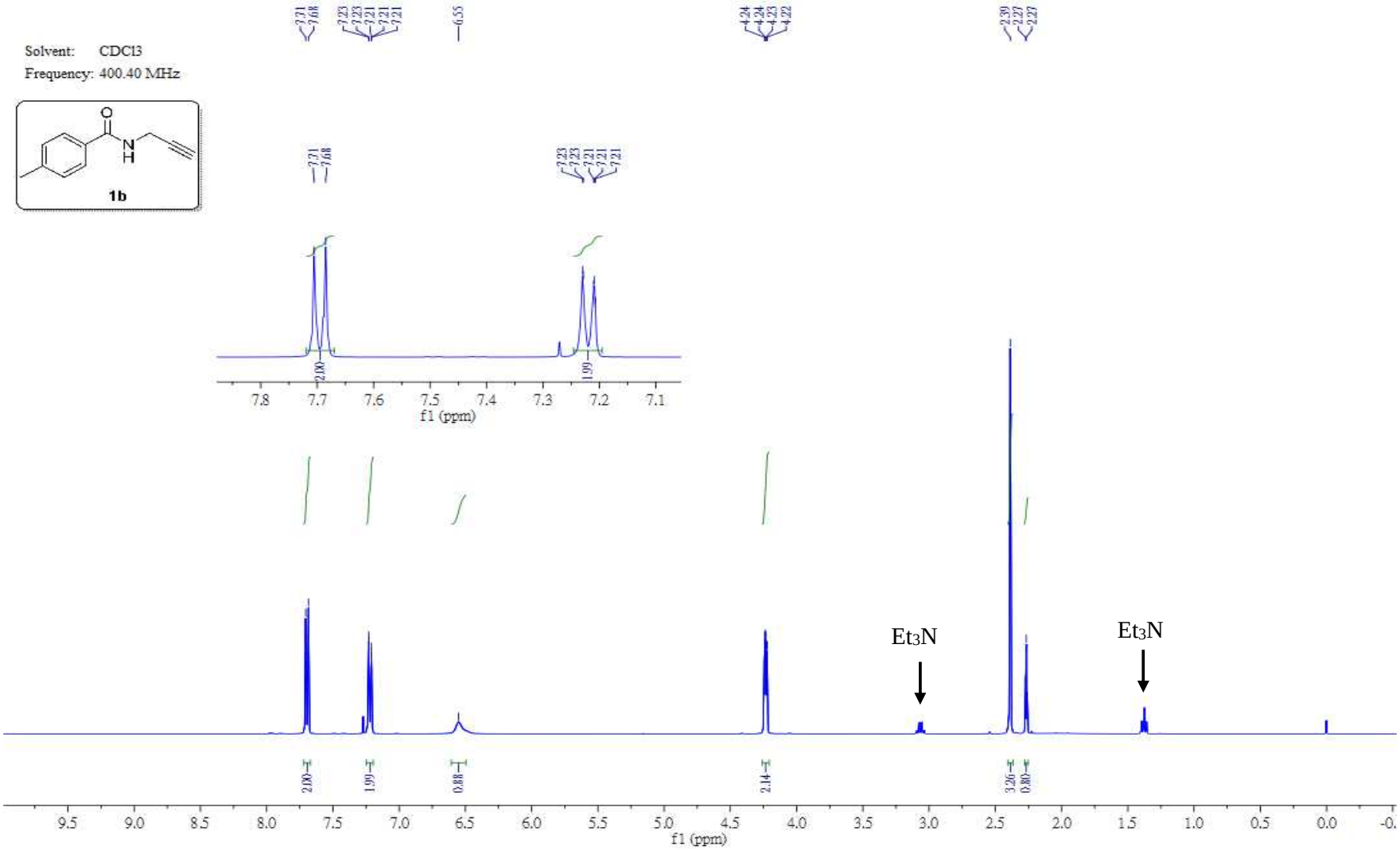
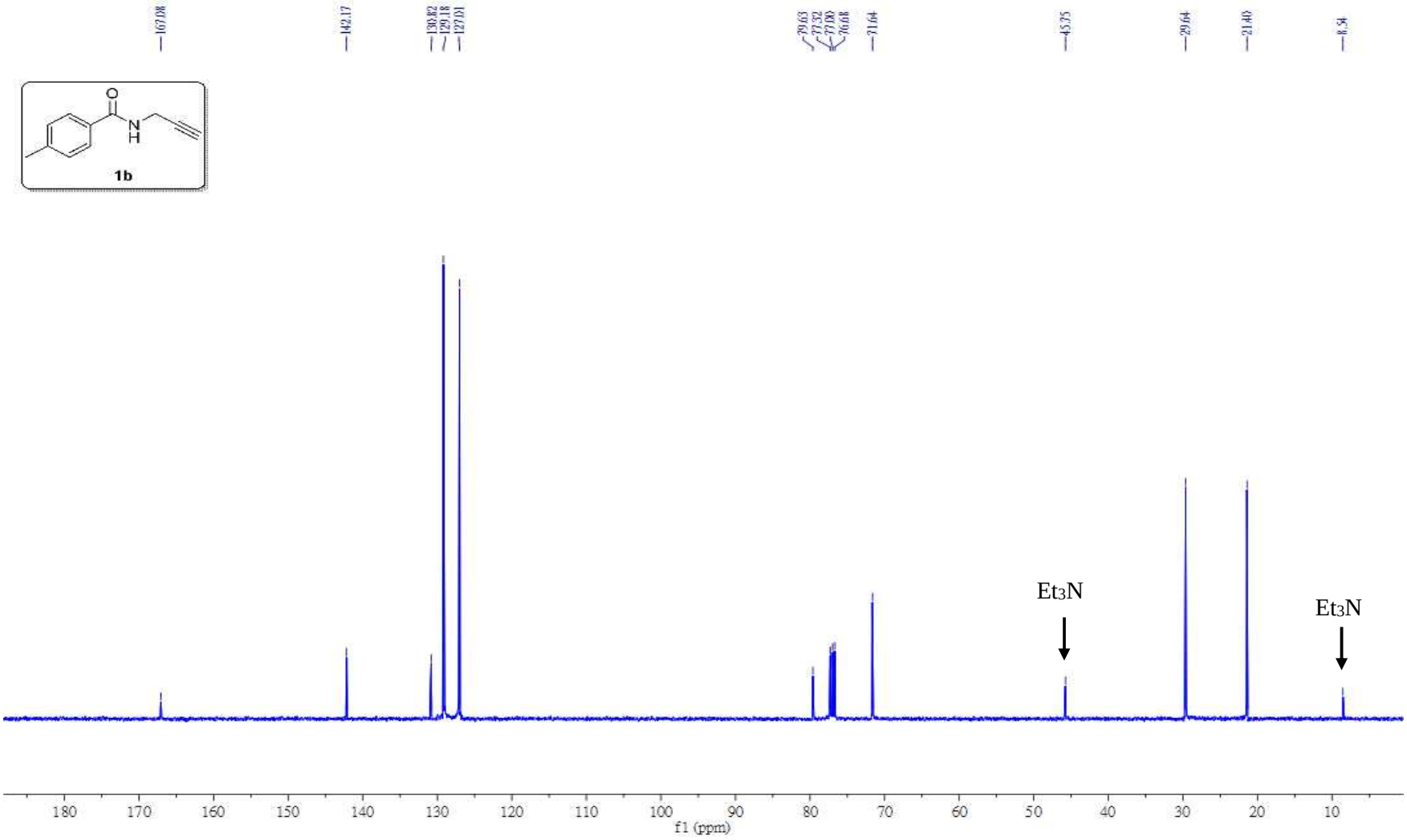
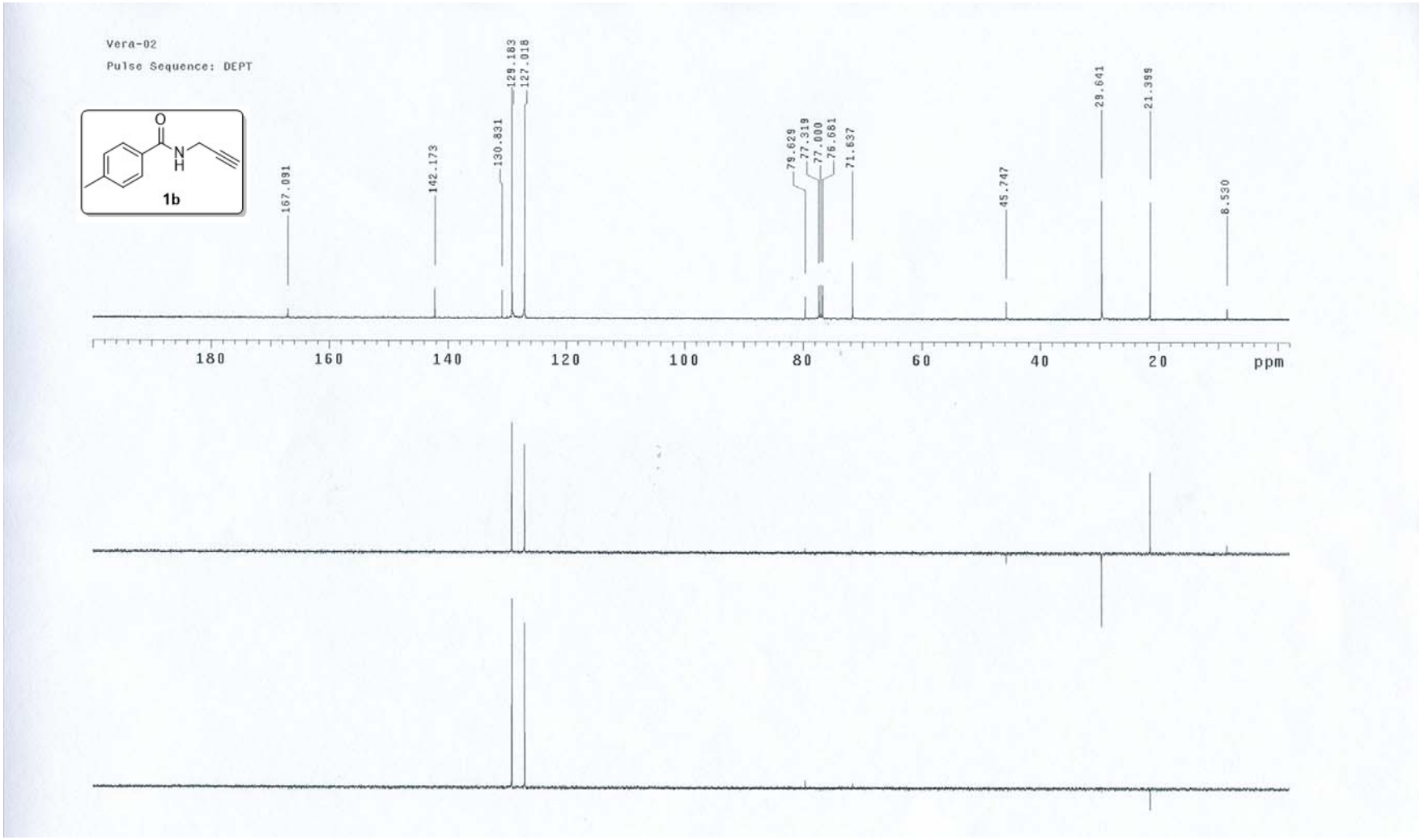

Solvent: CDCl3
Frequency: 400.40 MHz
1a
f1 (ppm)

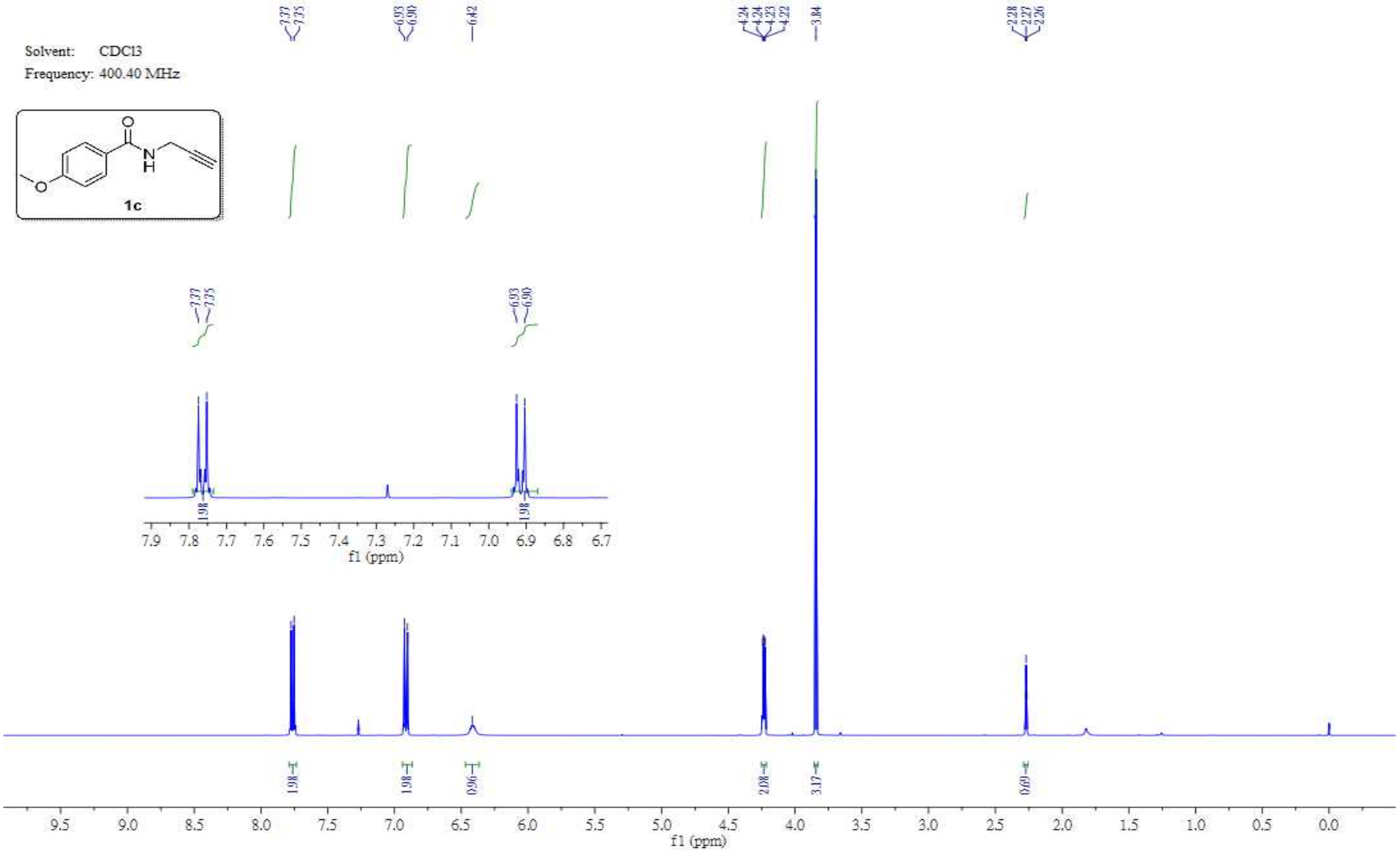

167.18
133.65
131.70
128.52
127.01
79.50
77.32
77.00
76.68
71.71
29.69
O
N
H
1a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

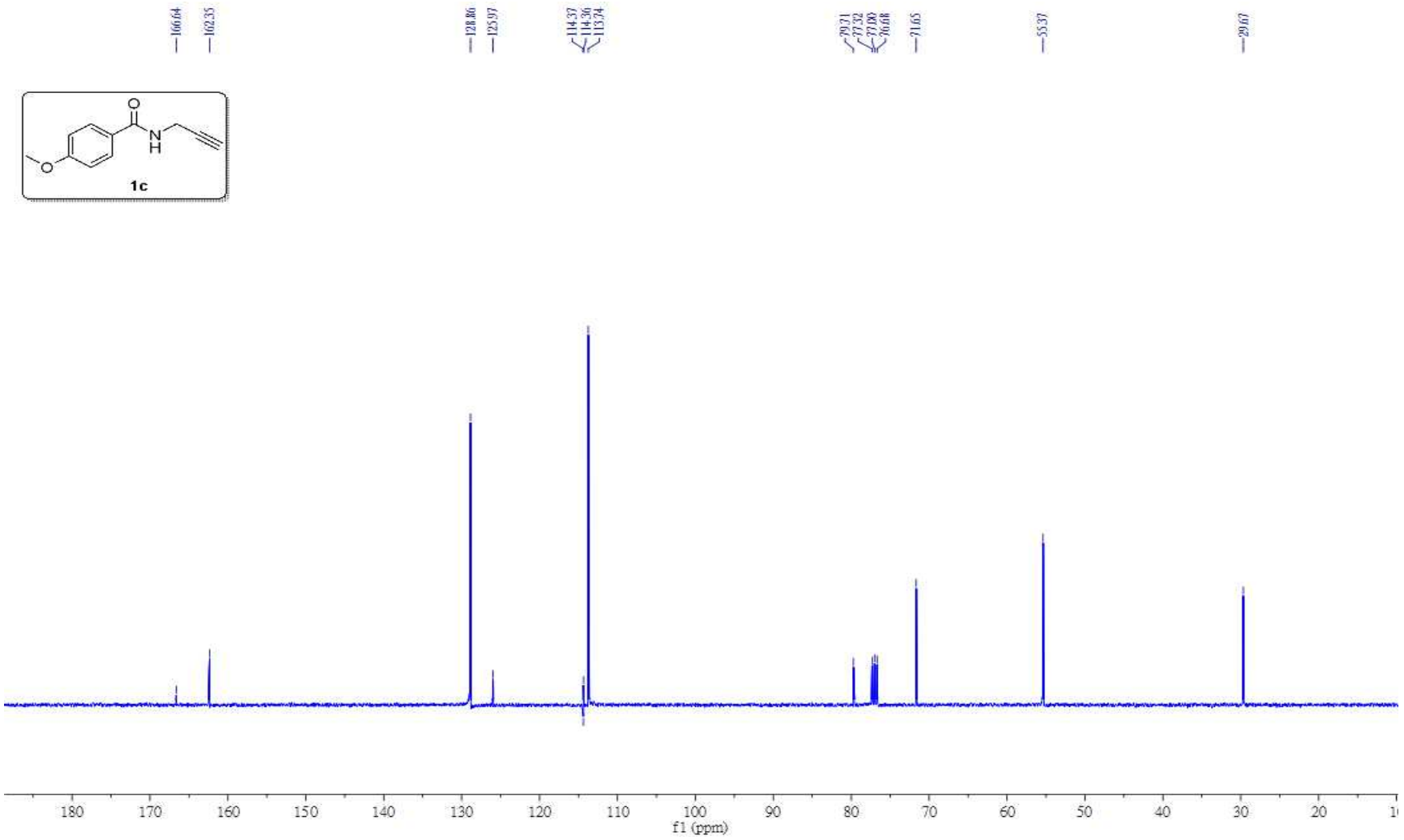

Vera-RP1-166s
Pulse Sequence: DEPT
O
N
H
1a
167.182
133.657
131.705
128.522
127.018
79.499
77.319
77.000
76.681
71.705
29.687
180
160
140
120
100
80
60
40
20
ppm

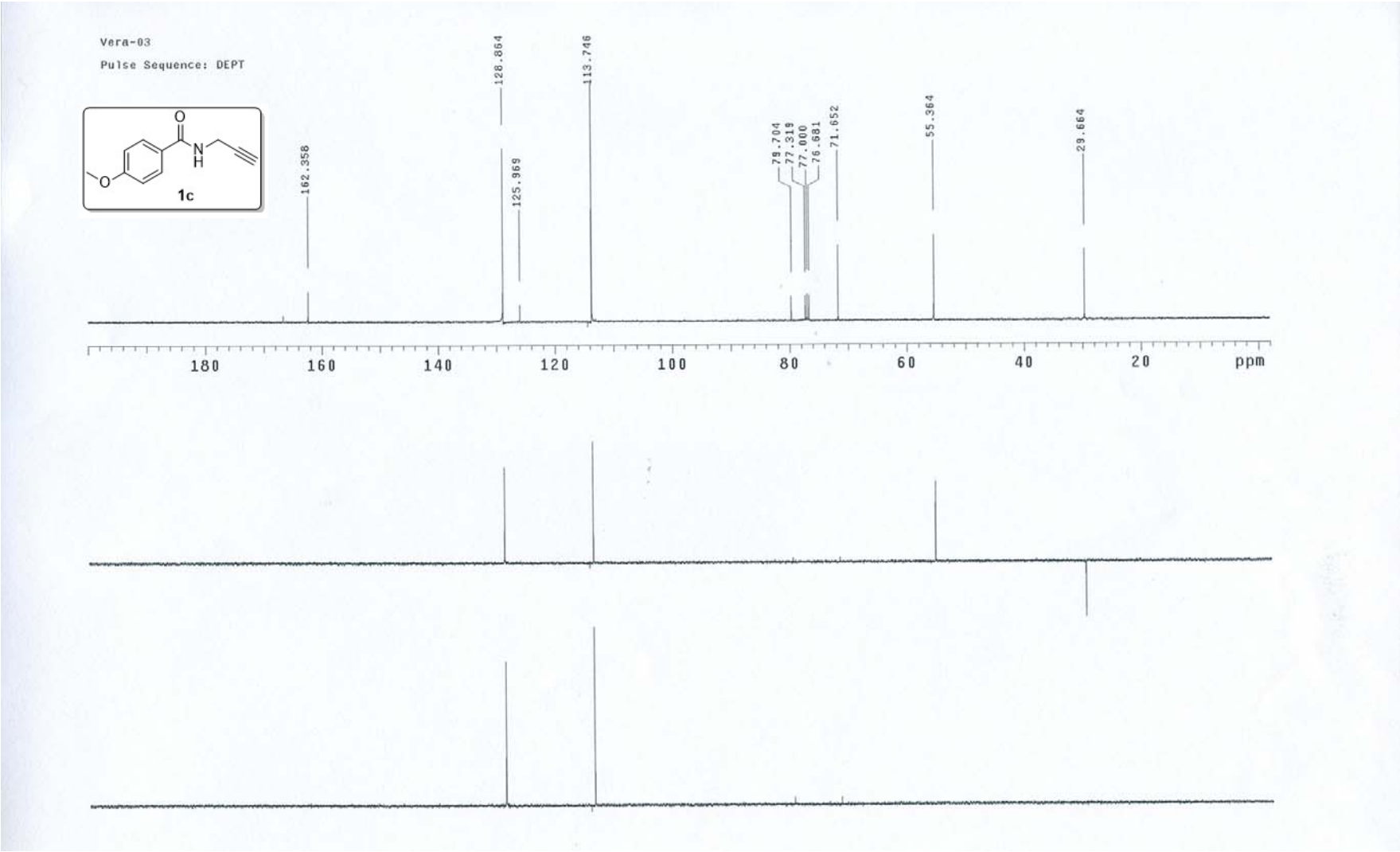

Solvent: CDCl3
Frequency: 400.40 MHz
1b
Et3N
Et3N
f1 (ppm)

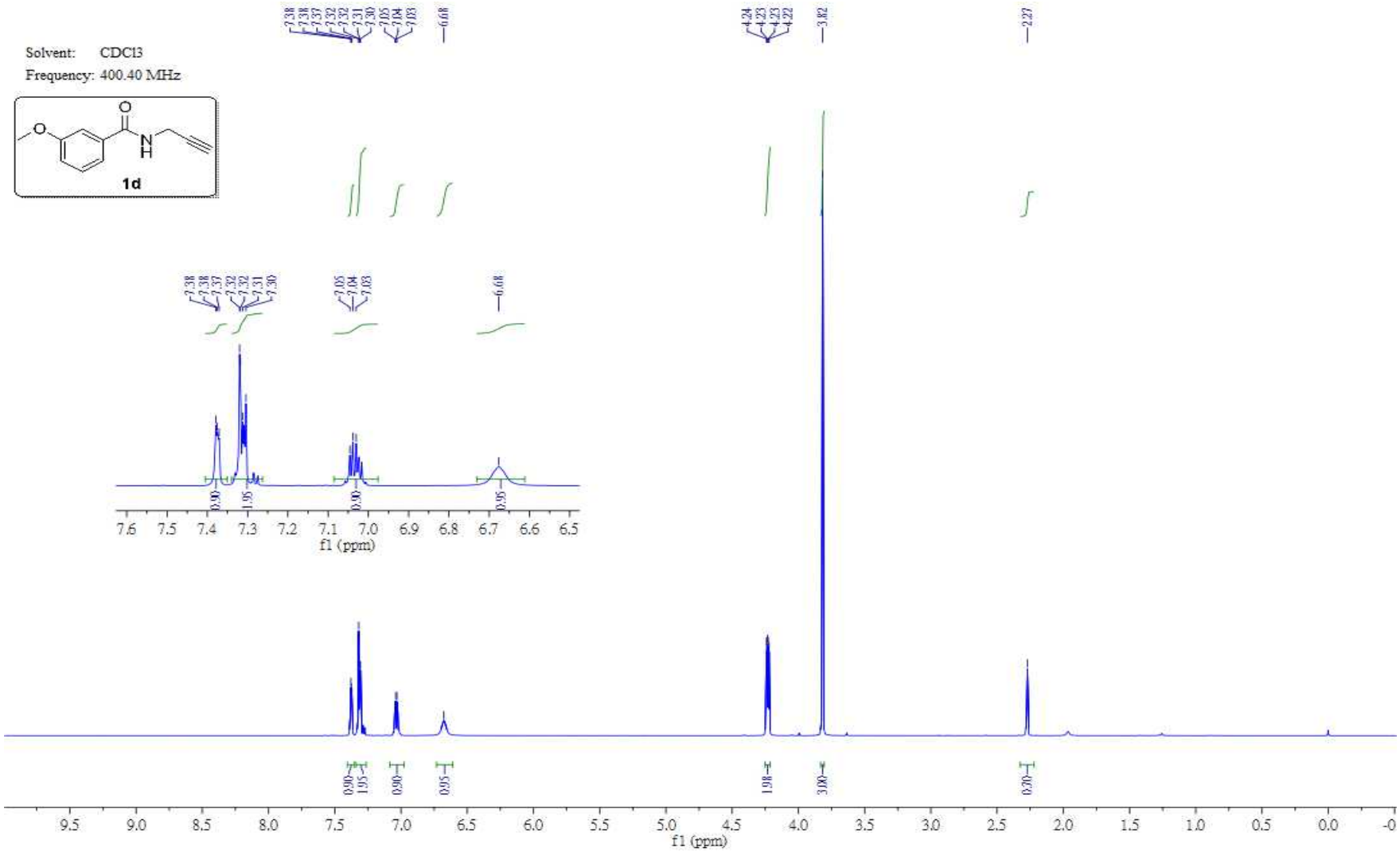

167.08
142.17
130.82
129.18
127.01
79.63
77.32
77.00
76.68
71.64
45.75
29.64
21.40
8.54
O
N
H
1b
Et3N
Et3N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

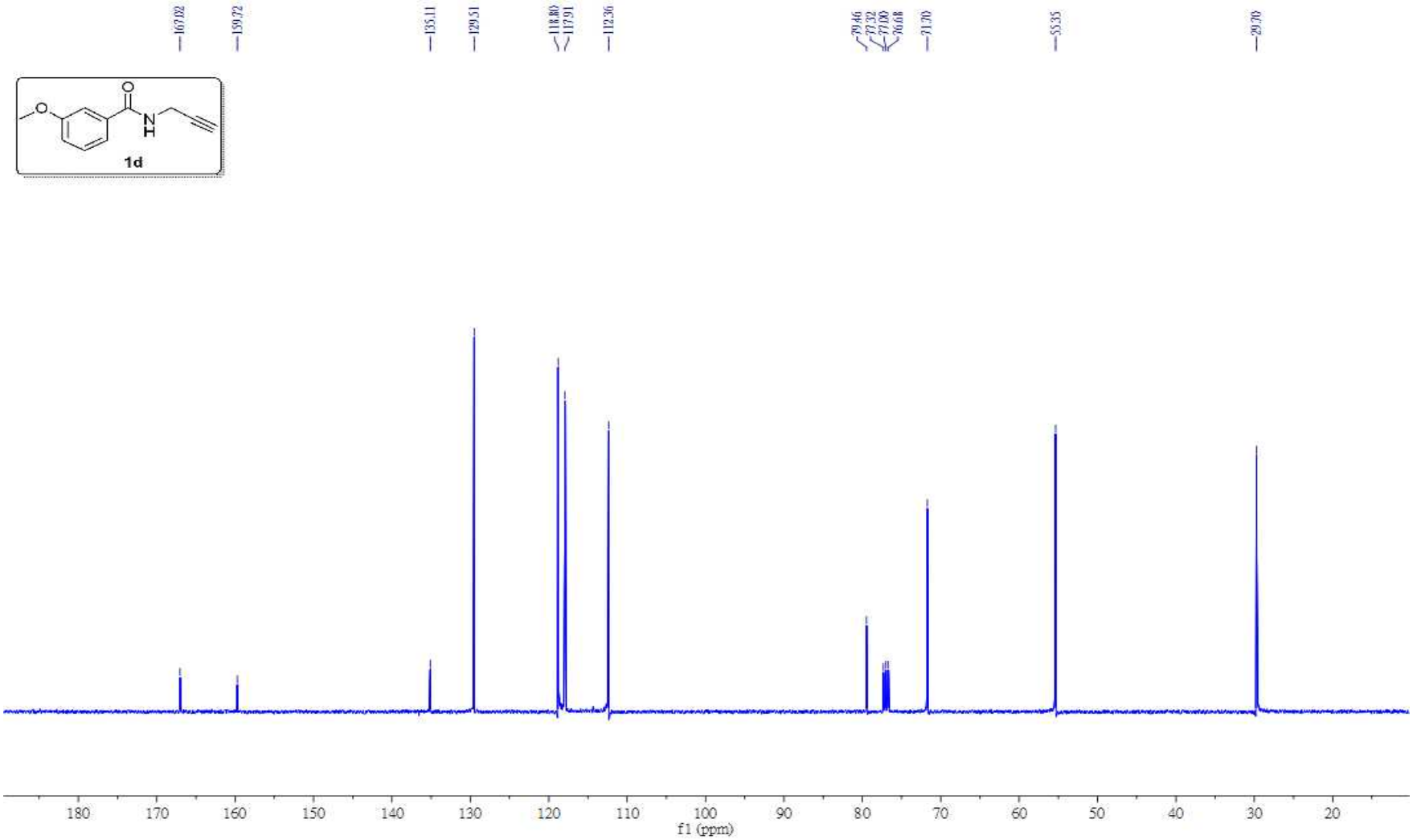

Vera-02
Pulse Sequence: DEPT
1b
167.091
142.173
130.831
129.183
127.018
79.629
77.319
77.000
76.681
71.637
45.747
29.641
21.399
8.530
180
160
140
120
100
80
60
40
20
ppm

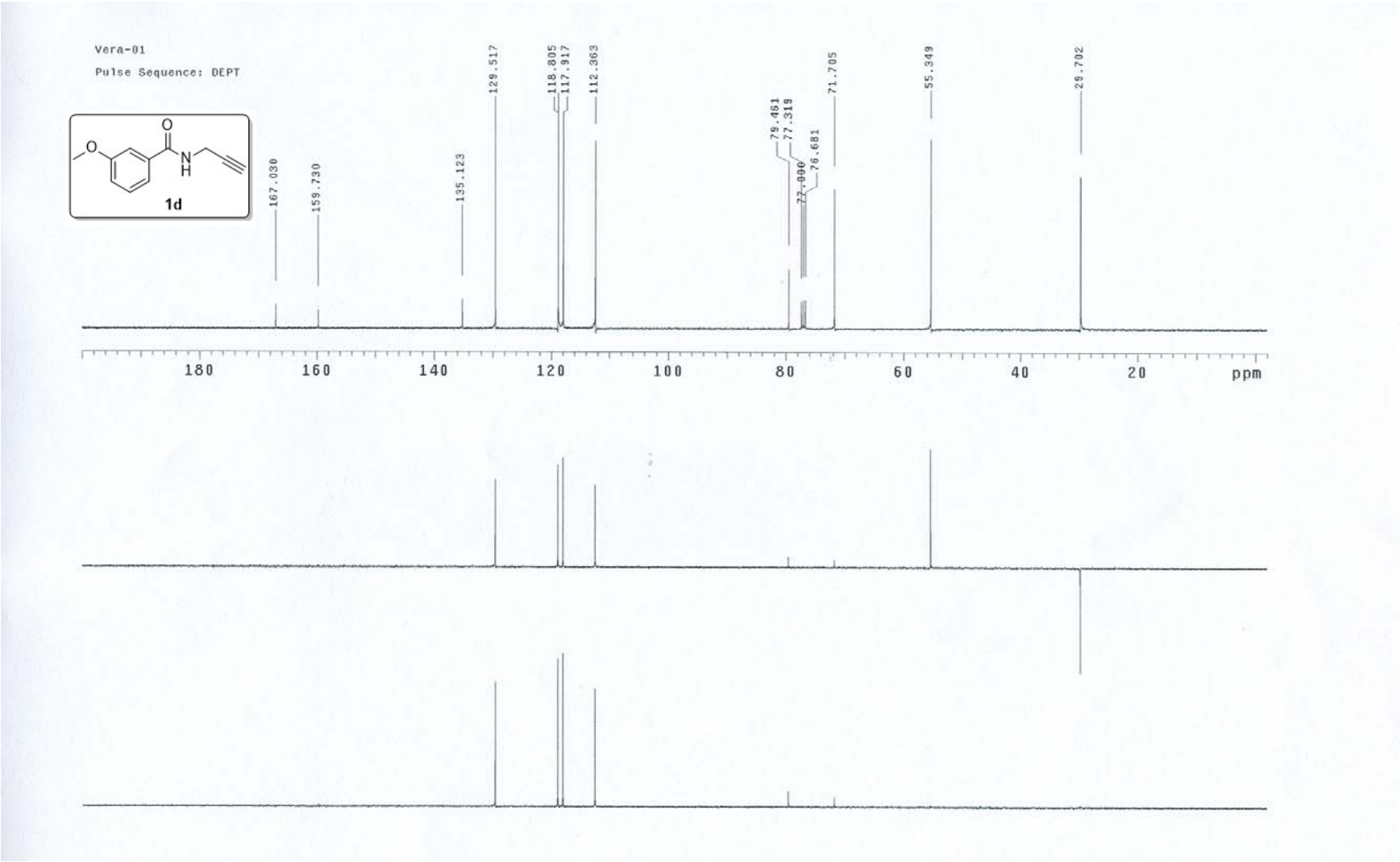

Solvent: CDCl3
Frequency: 400.40 MHz
1c
7.77
7.75
6.93
6.90
6.42
4.24
4.24
4.23
4.22
3.84
2.28
2.27
2.26
1.98
1.98
f1 (ppm)
1.98
1.98
0.96
2.08
3.17
0.69
f1 (ppm)

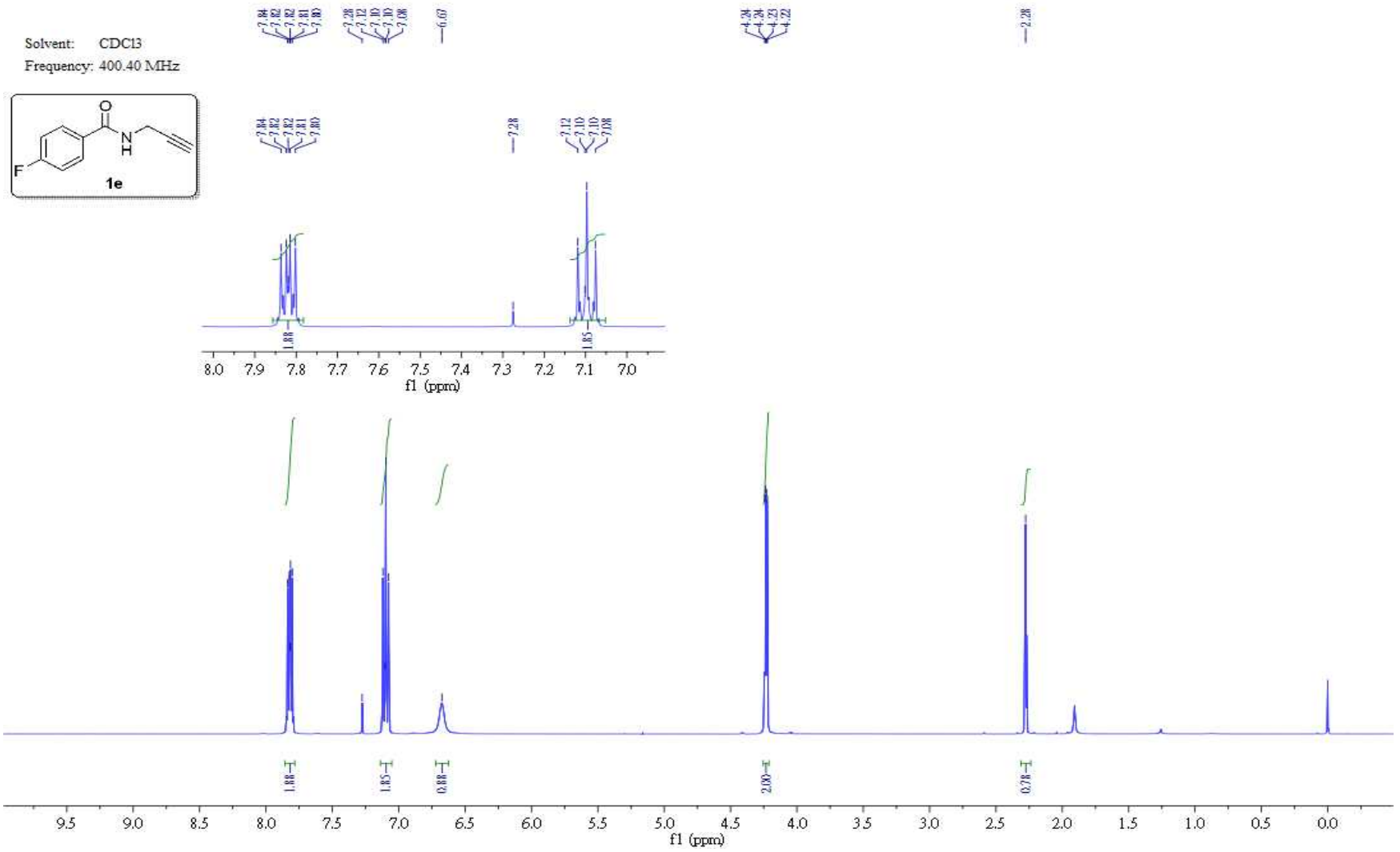

166.64
162.35
128.86
125.97
114.37
114.36
113.74
79.71
77.32
77.00
76.68
71.65
55.37
29.67
1c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

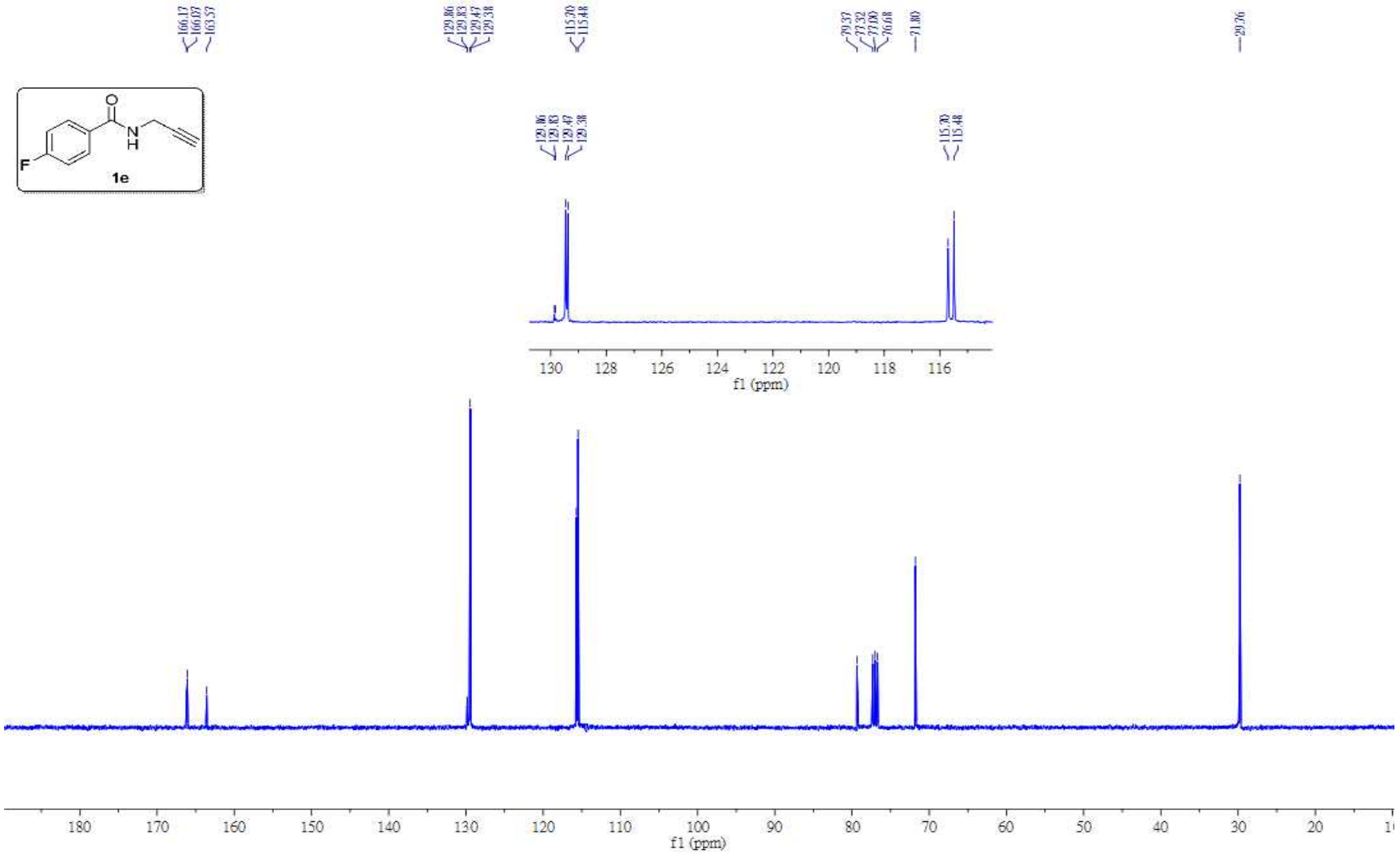

Vera-03
Pulse Sequence: DEPT
1c
162.358
128.864
125.969
113.746
79.704
77.319
77.000
76.681
71.652
55.364
29.664
180
160
140
120
100
80
60
40
20
ppm

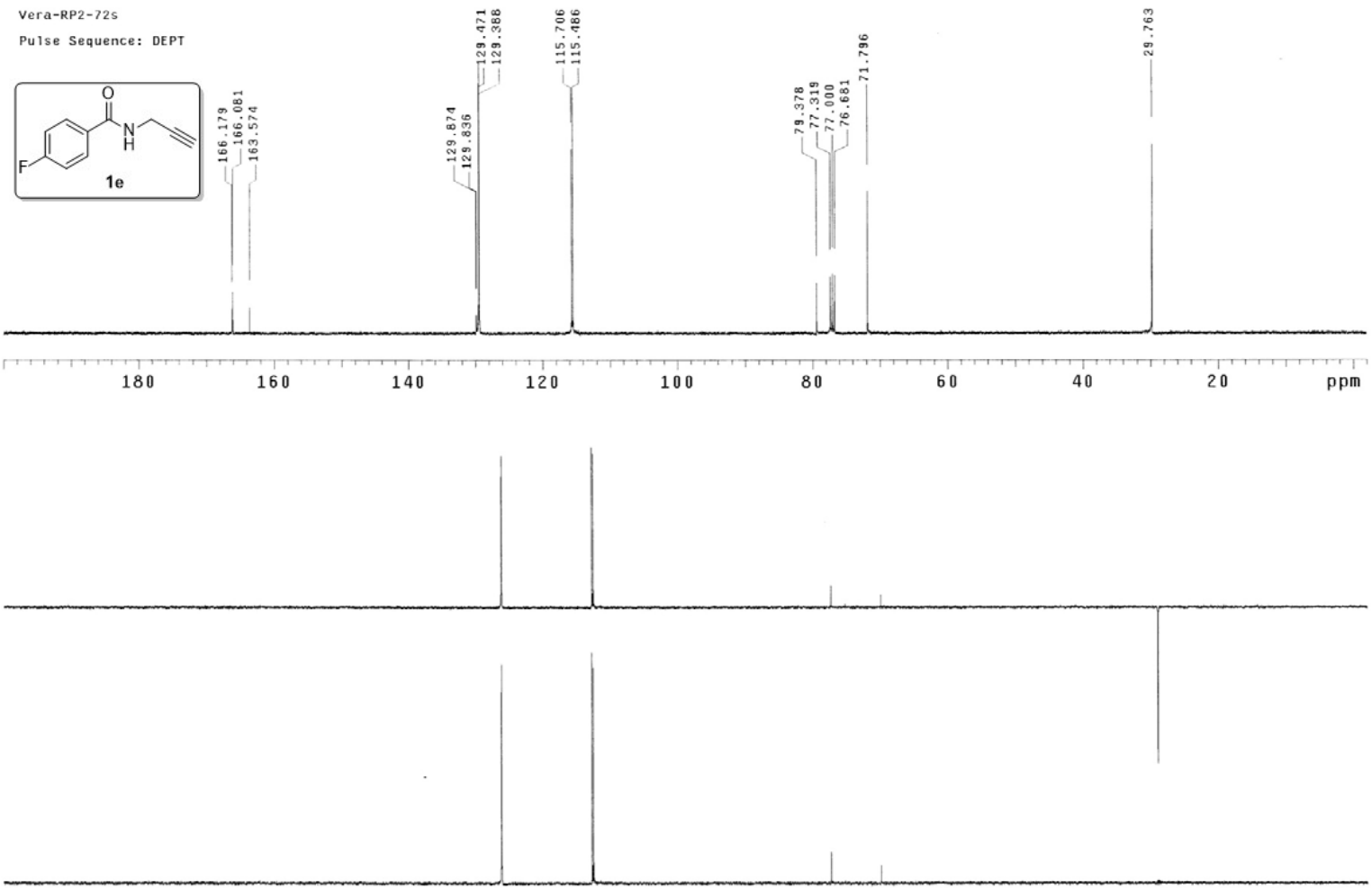

Solvent: CDCl3
Frequency: 400.40 MHz
1d
f1 (ppm)

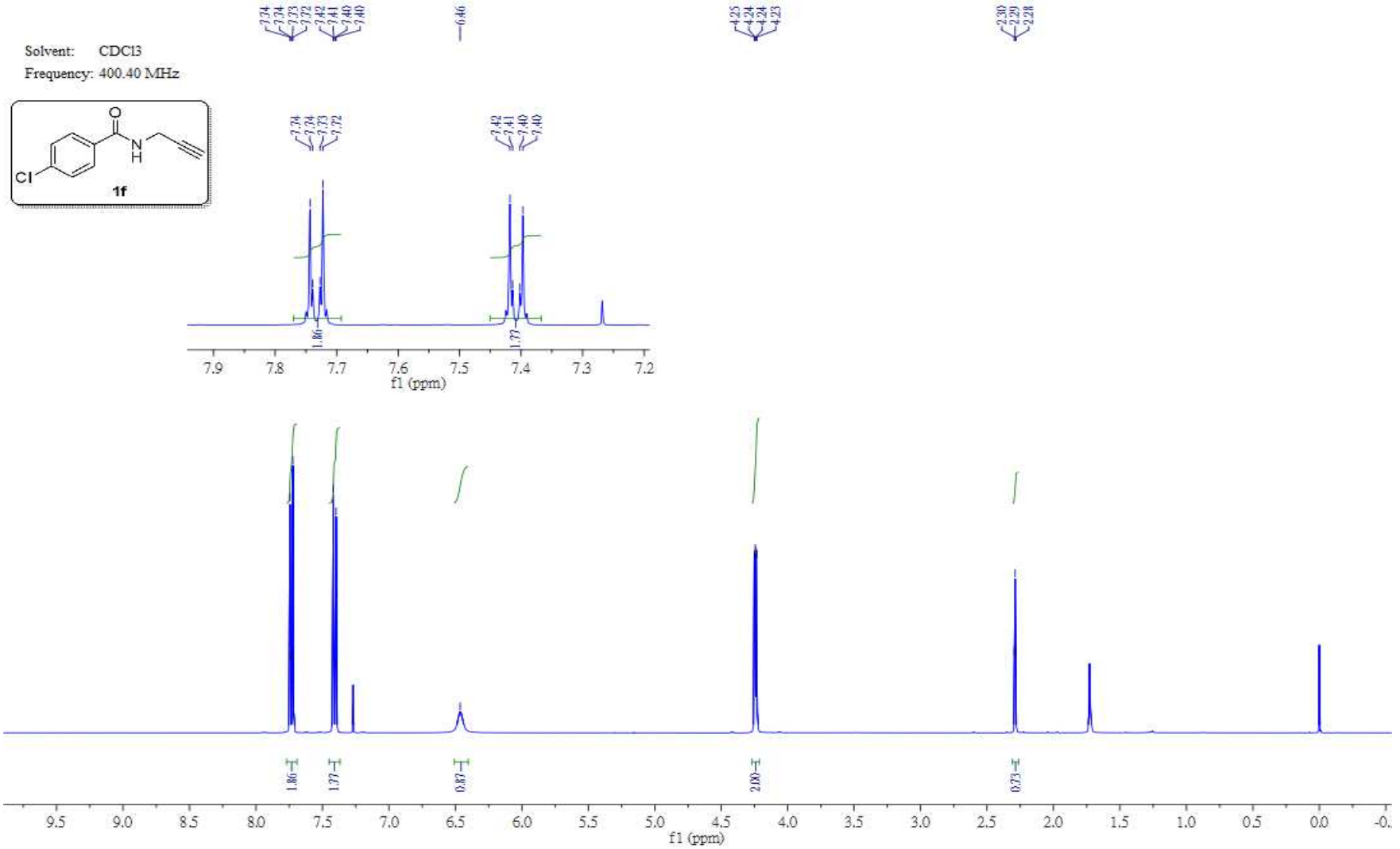

167.02
159.72
135.11
129.51
118.80
117.91
112.36
79.46
77.32
77.00
76.68
71.70
55.35
29.70
1d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

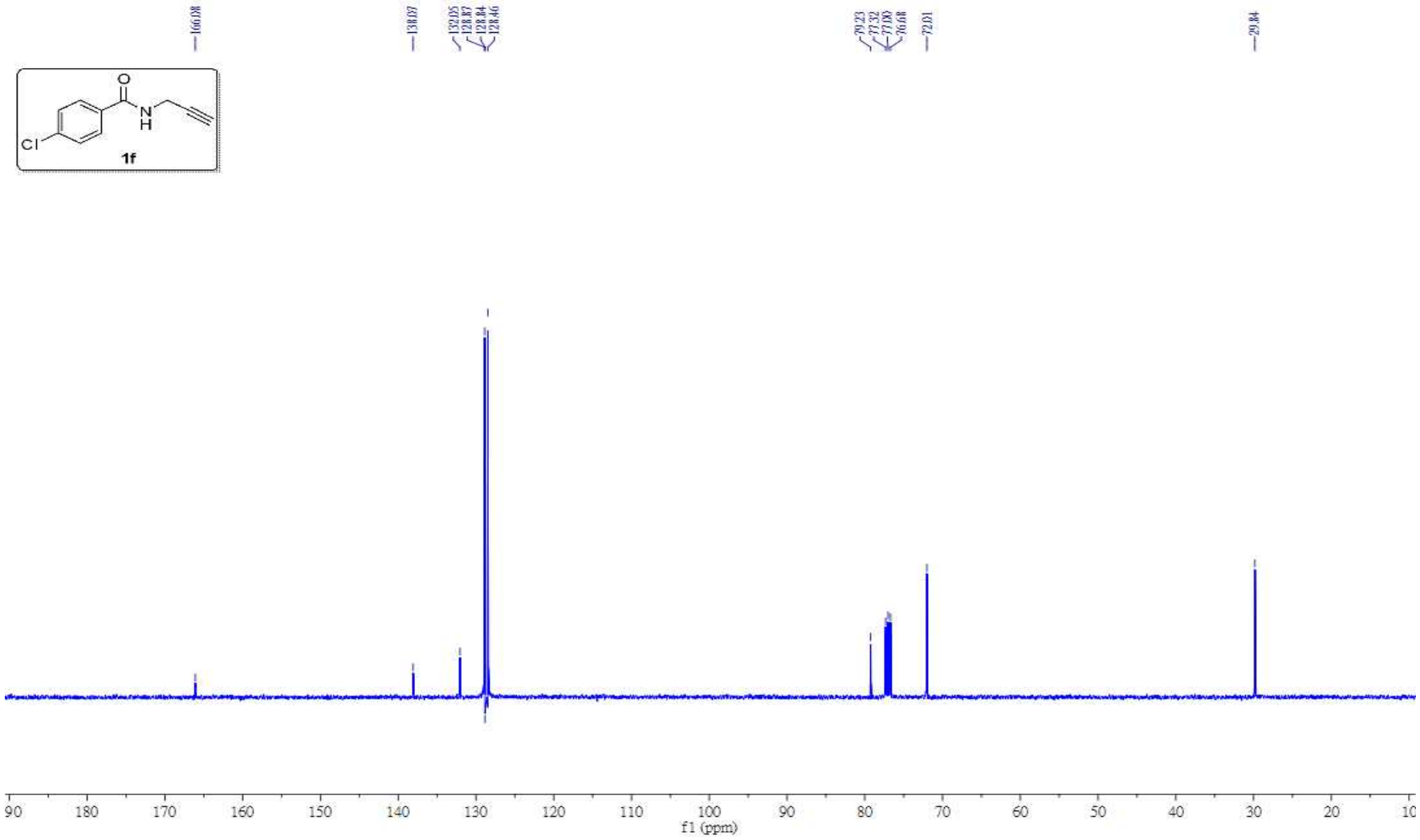

Vera-01
Pulse Sequence: DEPT
1d
167.030
159.730
135.123
129.517
118.805
117.917
112.363
79.461
77.319
77.000
76.681
71.705
55.349
29.702
180
160
140
120
100
80
60
40
20
ppm

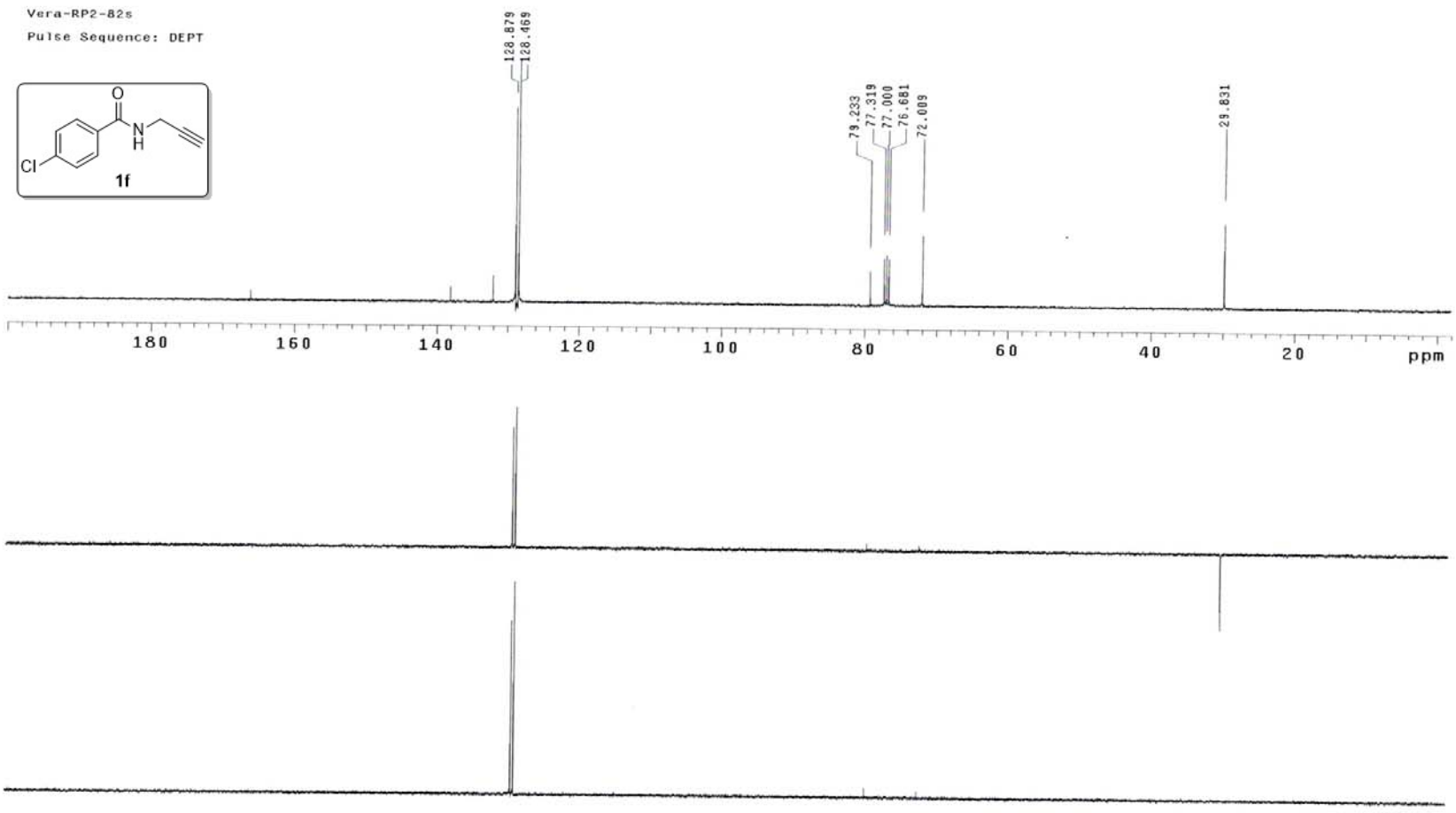

Solvent: CDCl3
Frequency: 400.40 MHz
1e
f1 (ppm)

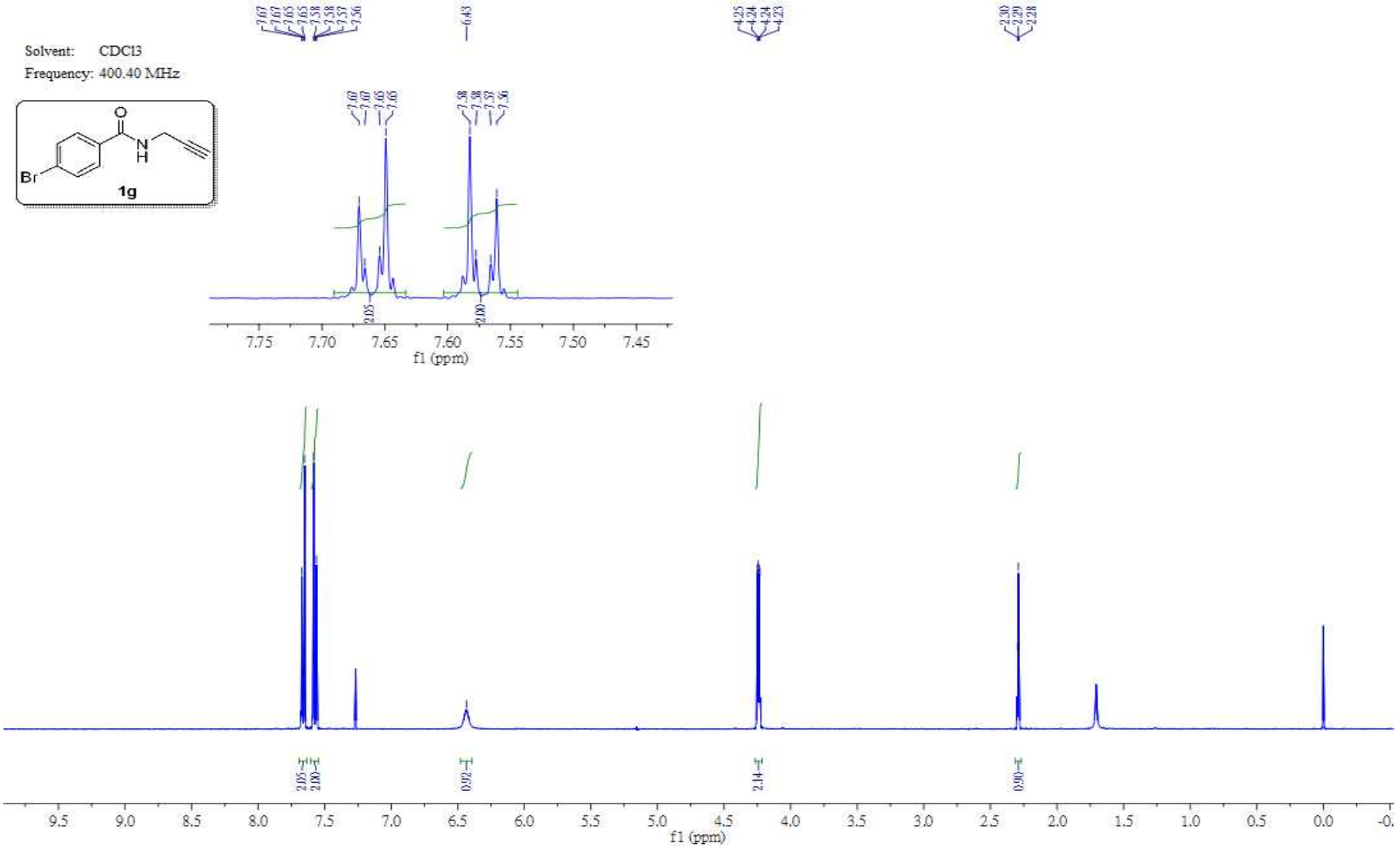

166.17
166.07
163.57
129.86
129.83
129.47
129.38
115.70
115.48
79.37
77.32
77.00
76.68
71.80
29.76
F
O
N
H
1e
f1 (ppm)
f1 (ppm)

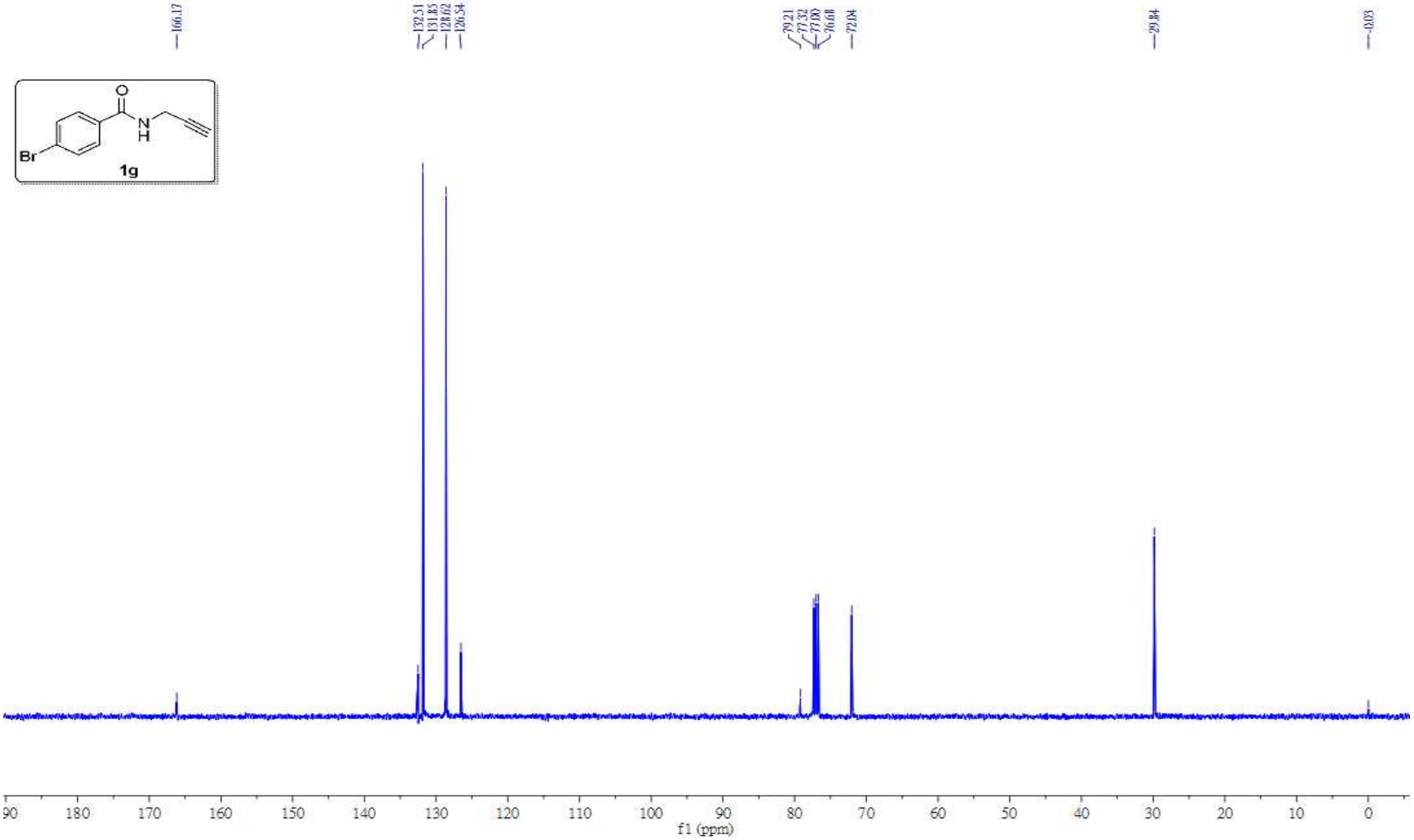

Vera-RP2-72s
Pulse Sequence: DEPT
1e
166.179
166.081
163.574
129.874
129.836
129.471
129.388
115.706
115.486
79.378
77.319
77.000
76.681
71.796
29.763
180
160
140
120
100
80
60
40
20
ppm

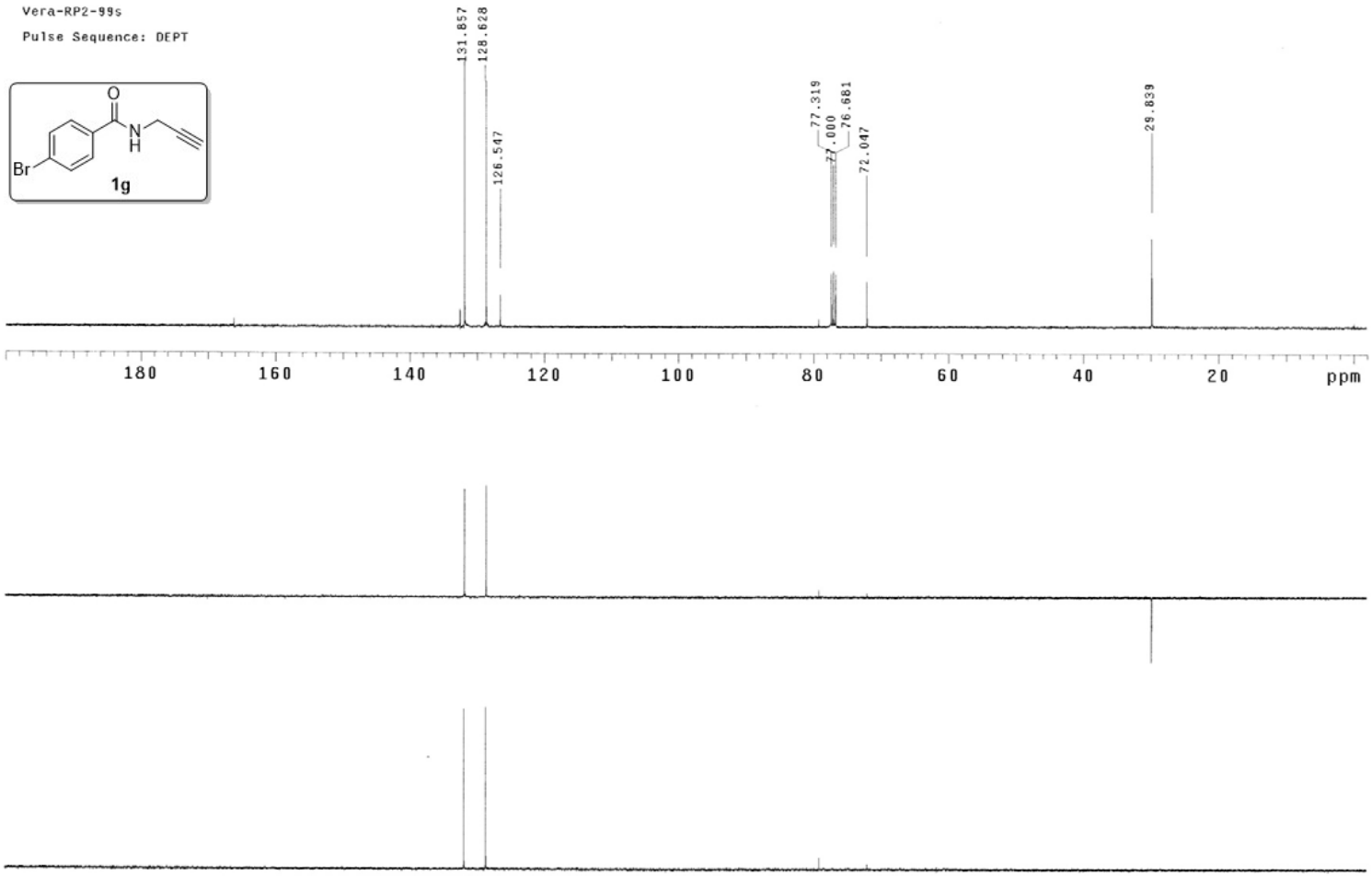

Solvent: CDCl3
Frequency: 400.40 MHz
1f
f1 (ppm)

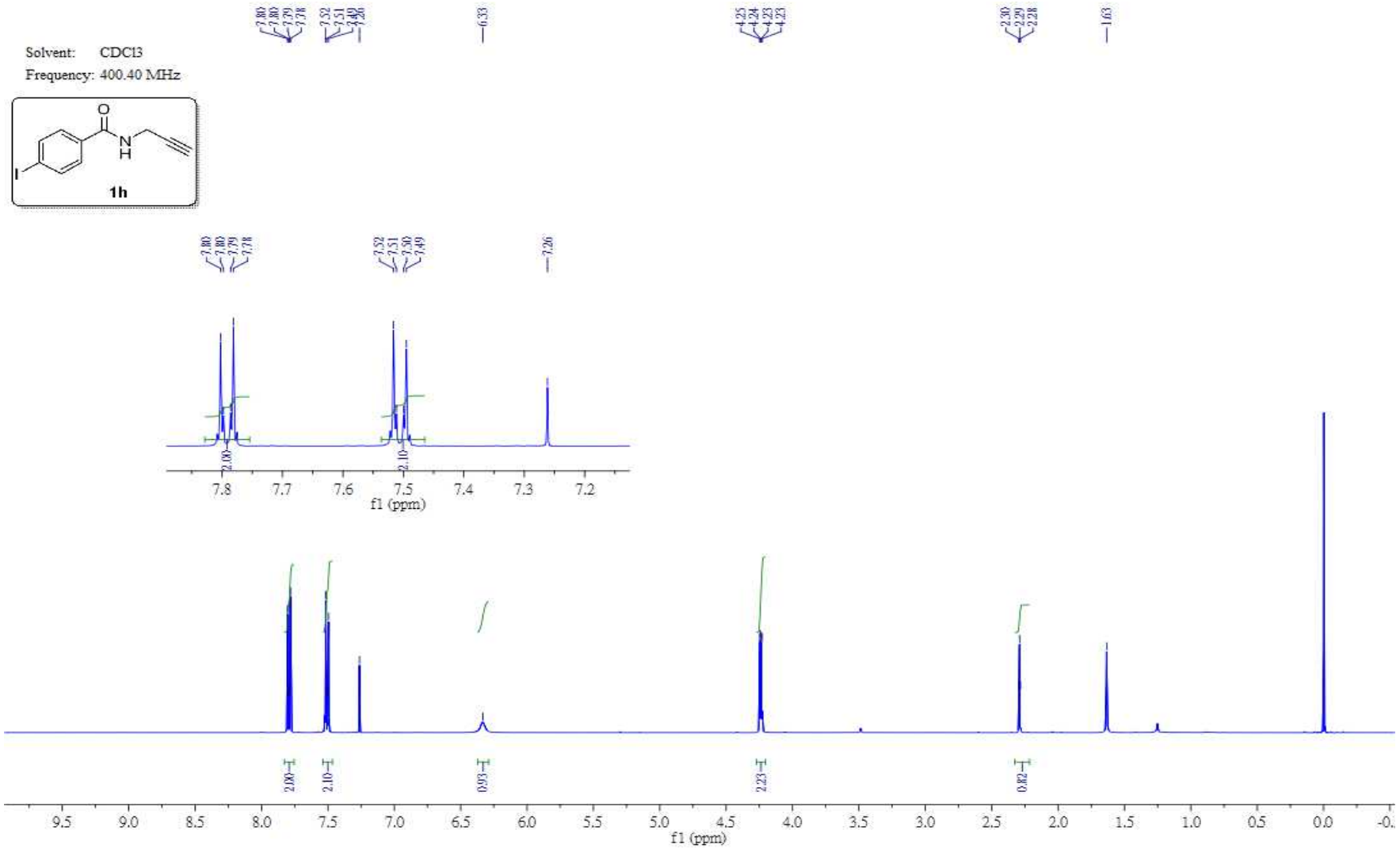

166.08
138.07
132.05
128.87
128.84
128.46
79.23
77.32
77.00
76.68
72.01
29.84
O
N
H
Cl
1f
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

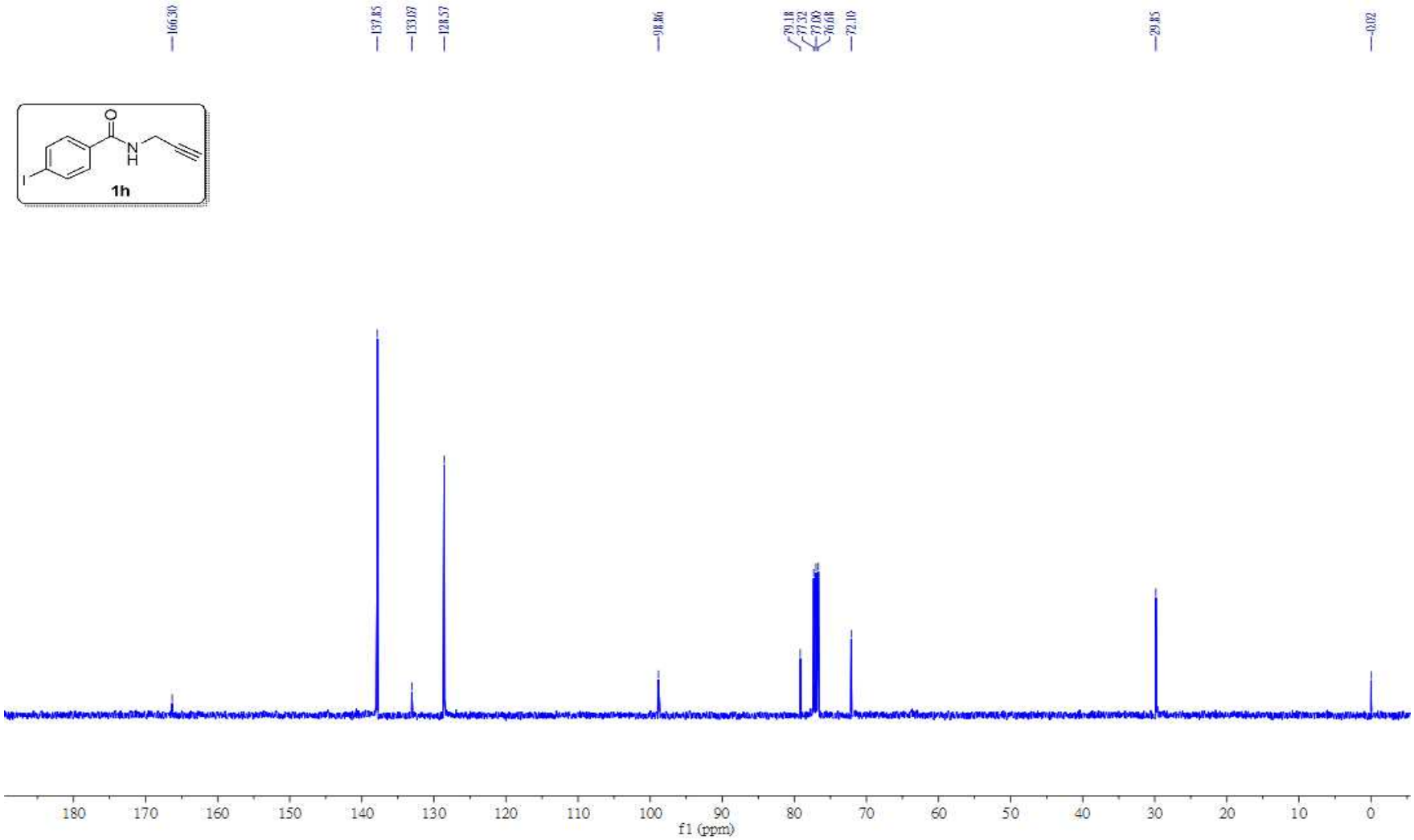

Vera-RP2-82s
Pulse Sequence: DEPT
O
N
H
Cl
1f
128.879
128.469
79.233
77.319
77.000
76.681
72.089
28.831
180
160
140
120
100
80
60
40
20
ppm

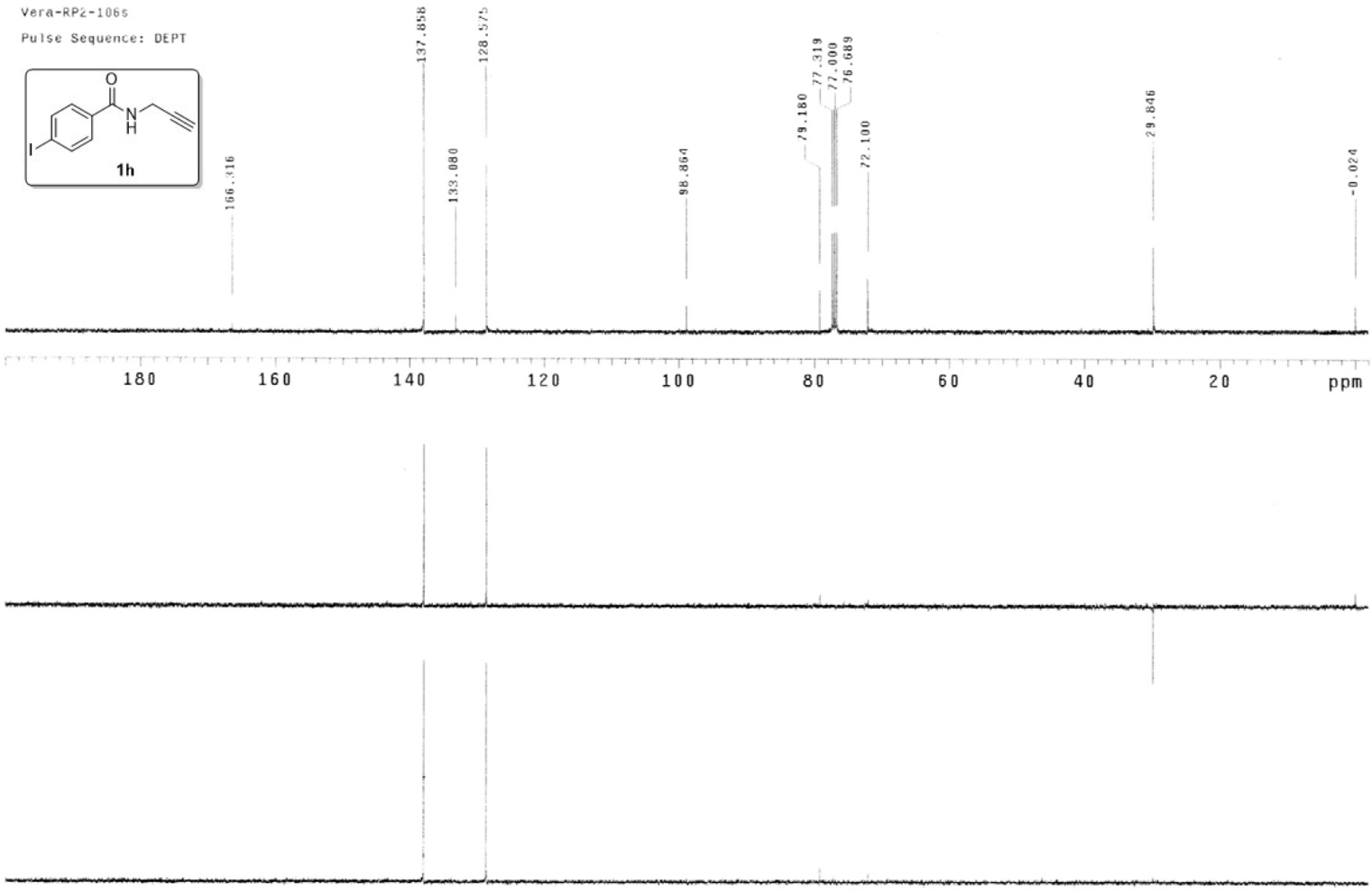

Solvent: CDCl3
Frequency: 400.40 MHz
Br
1g
f1 (ppm)

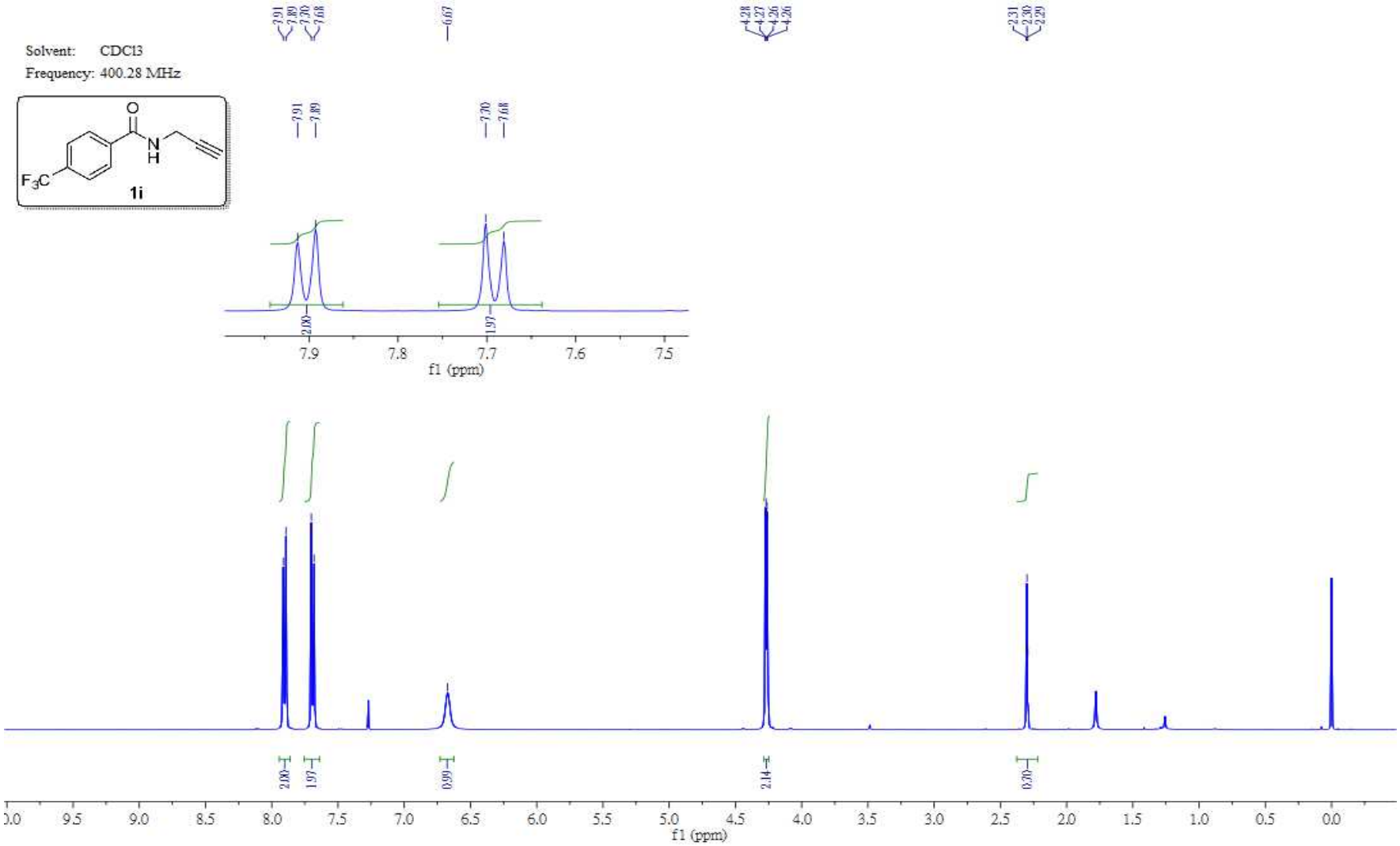

166.17
132.51
131.85
128.62
126.54
79.21
77.32
77.00
76.68
72.04
29.84
0.03
Br
1g
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

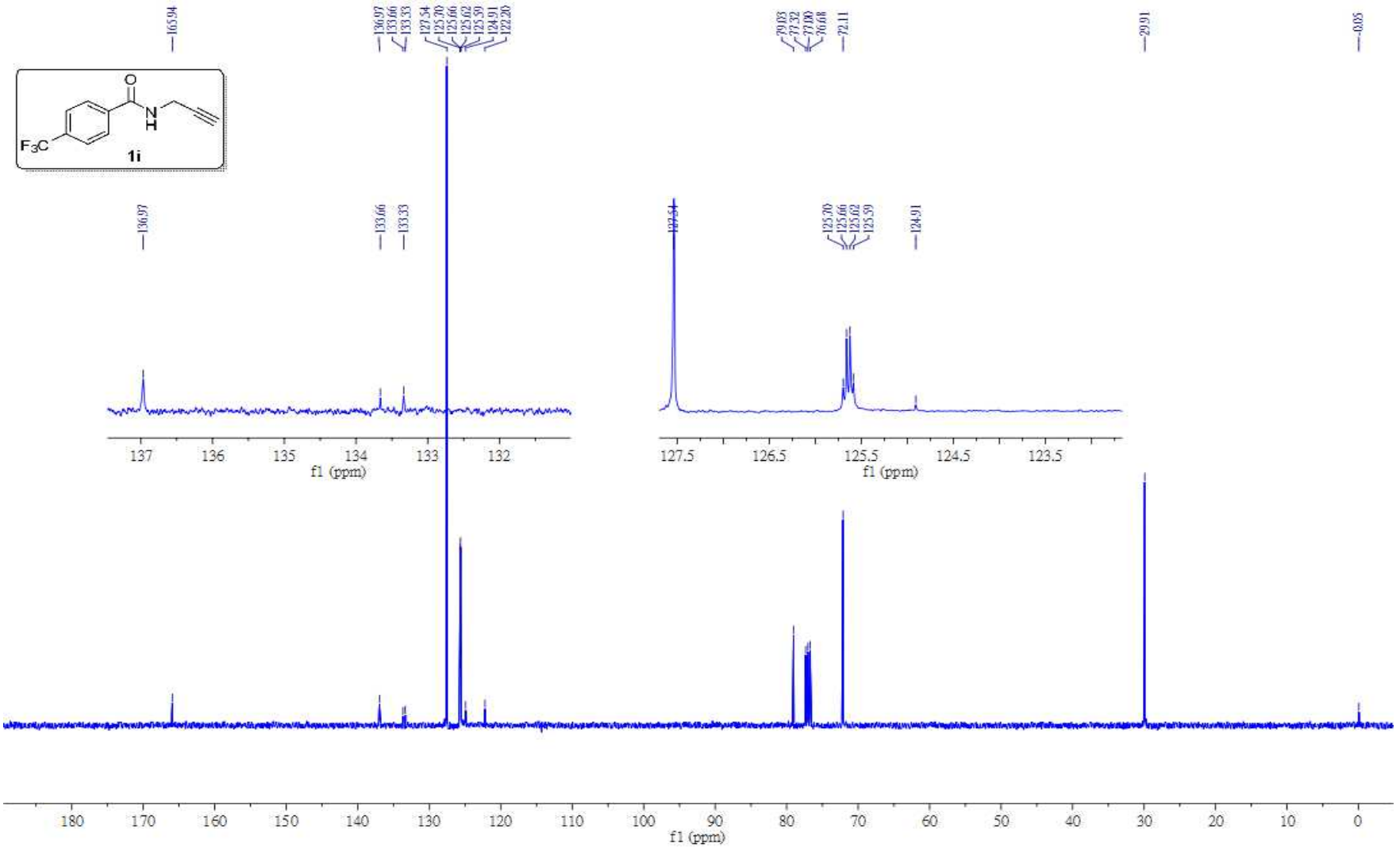

Vera-RP2-99s
Pulse Sequence: DEPT
O
N
H
Br
1g
131.857
128.628
126.547
77.319
77.000
76.681
72.047
29.839
180
160
140
120
100
80
60
40
20
ppm

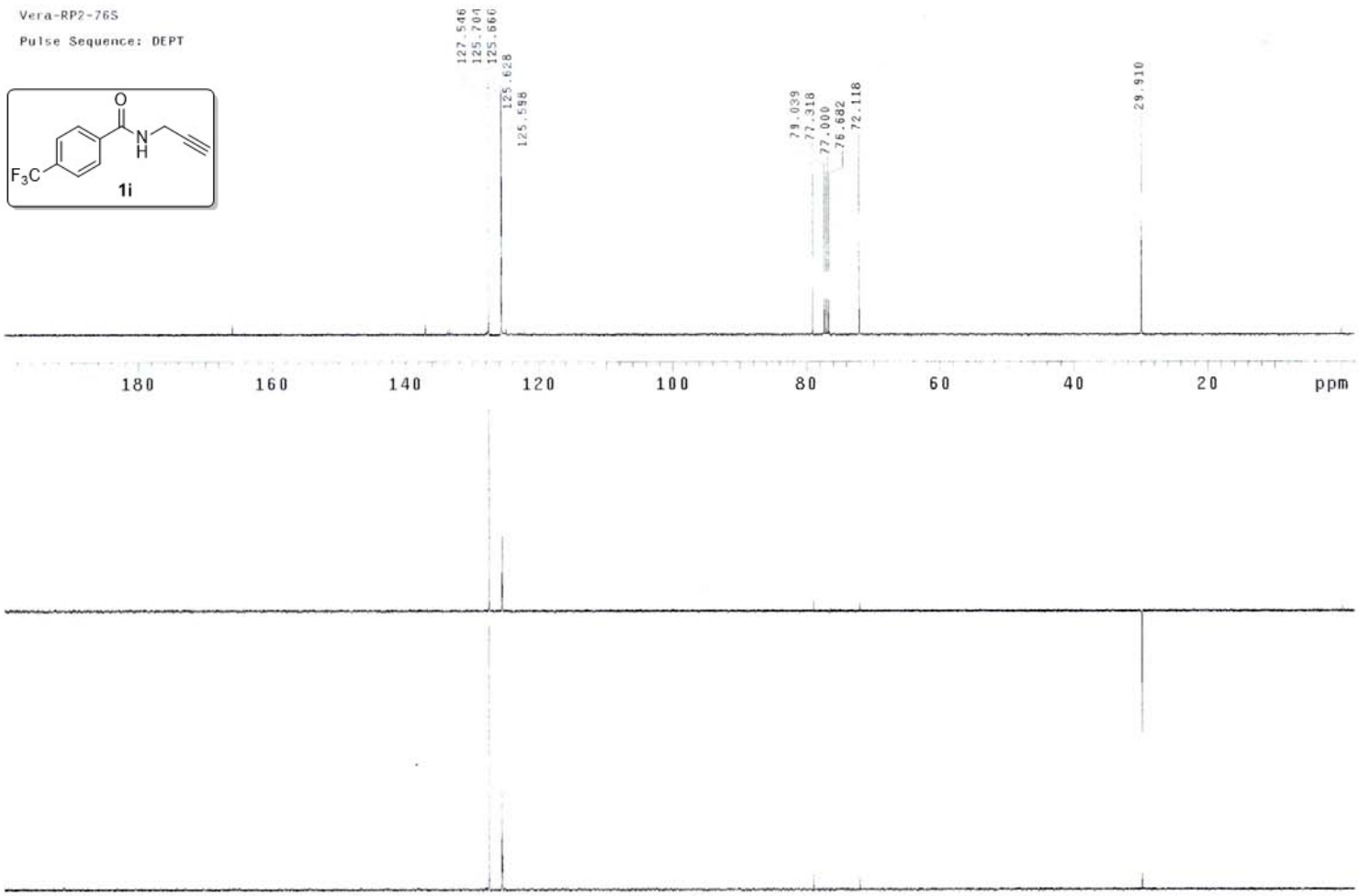

Solvent: CDCl3
Frequency: 400.40 MHz
1h
f1 (ppm)

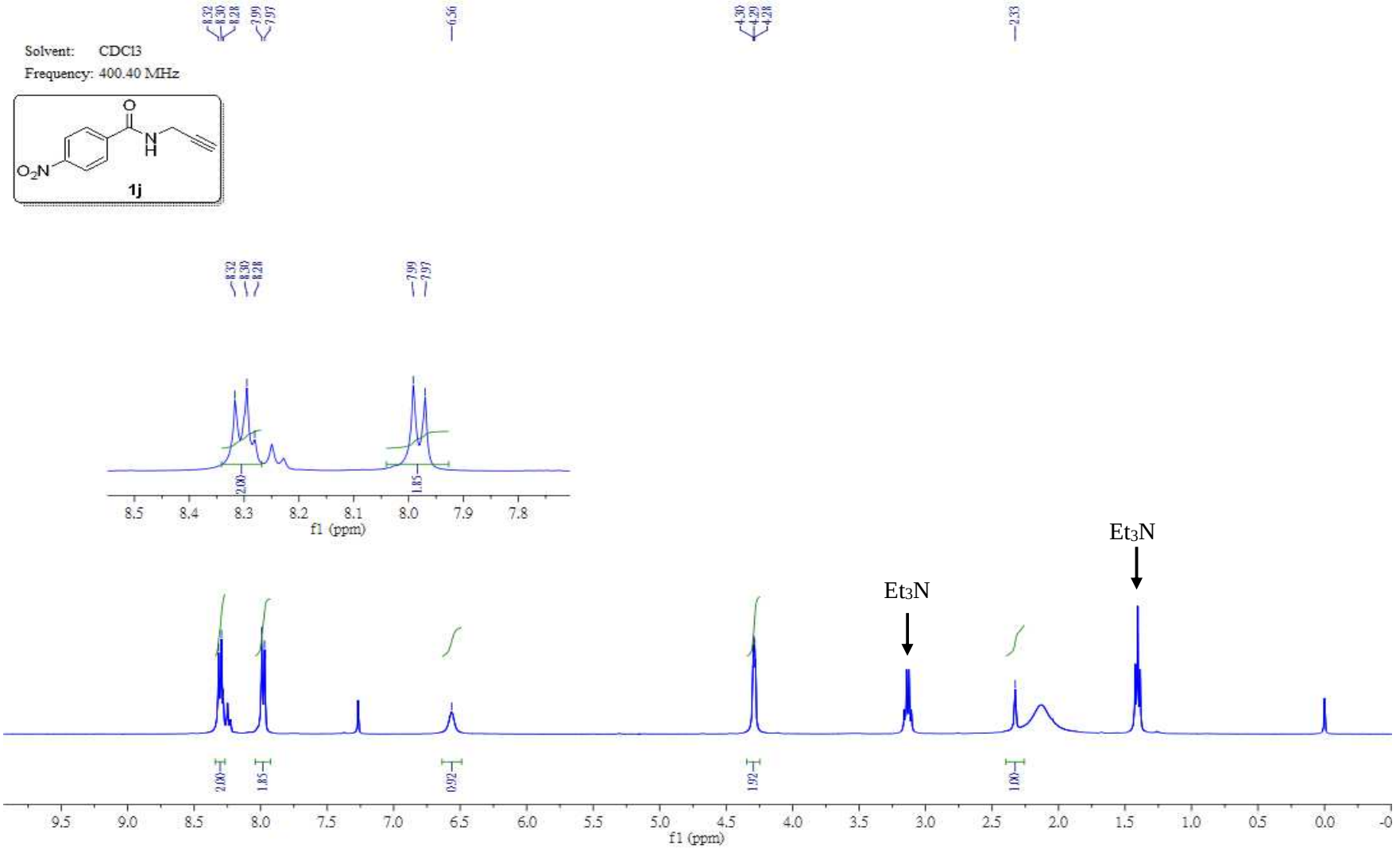

166.30
137.85
133.97
128.57
98.86
79.18
77.32
77.00
76.68
72.10
29.85
0.02
1h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

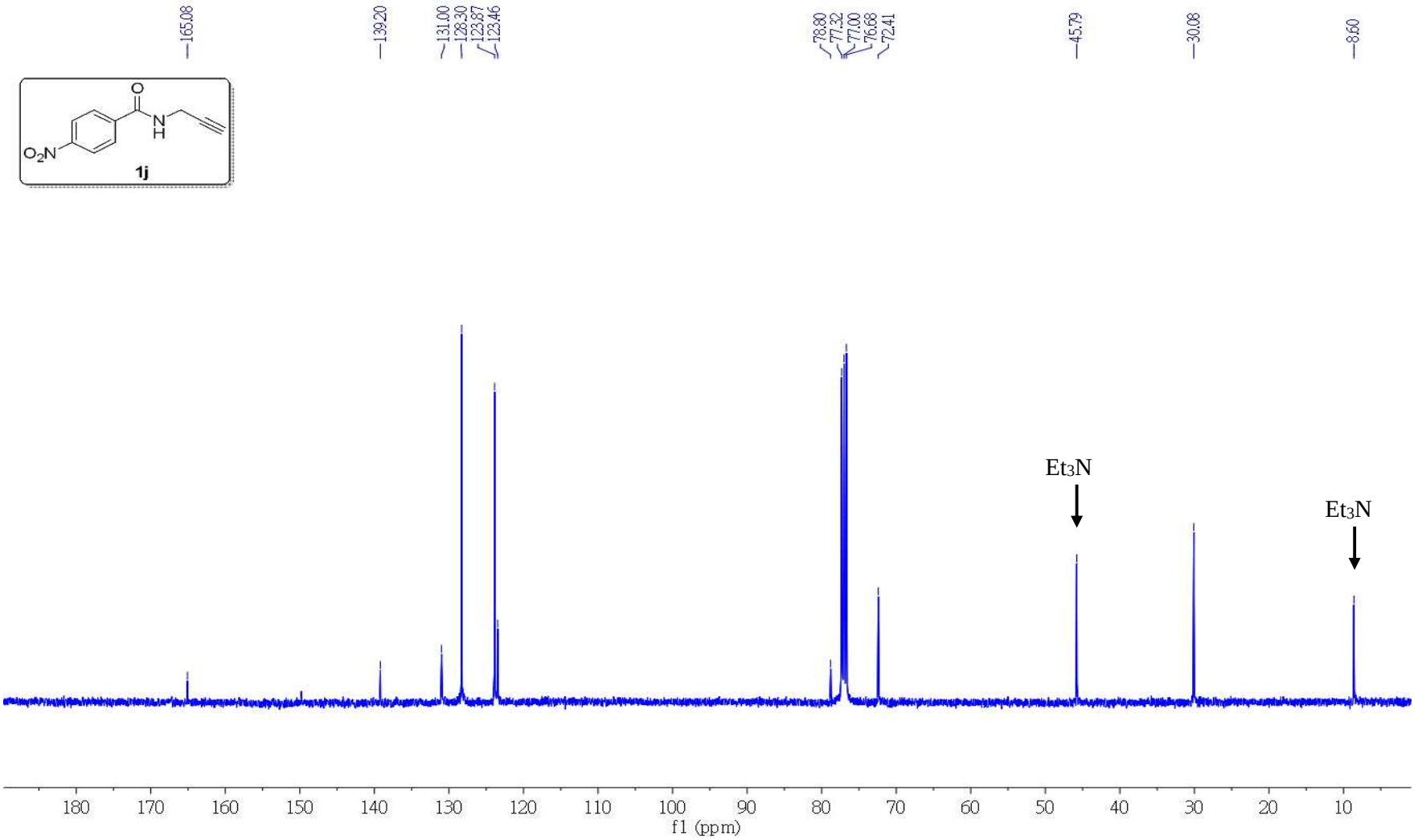

Vera-RP2-106s
Pulse Sequence: DEPT
1h
166.416
137.858
133.080
128.575
98.864
79.180
77.319
77.000
76.689
72.100
29.846
-0.024
180
160
140
120
100
80
60
40
20
ppm

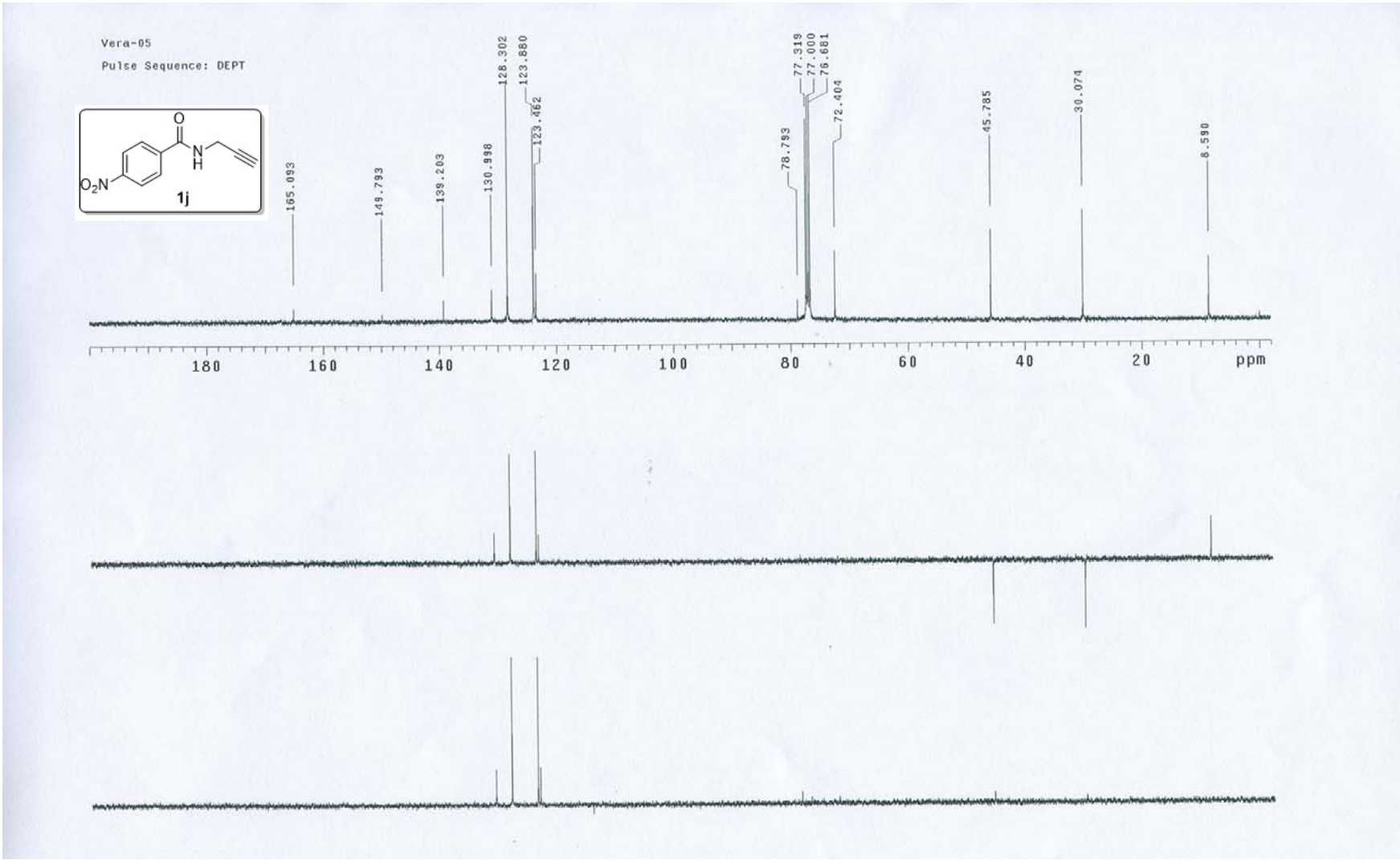

Solvent: CDCl3
Frequency: 400.28 MHz
1i
7.91
7.89
7.70
7.68
6.67
4.28
4.27
4.26
4.26
2.31
2.30
2.29
2.00
1.97
0.99
2.14
0.70
f1 (ppm)

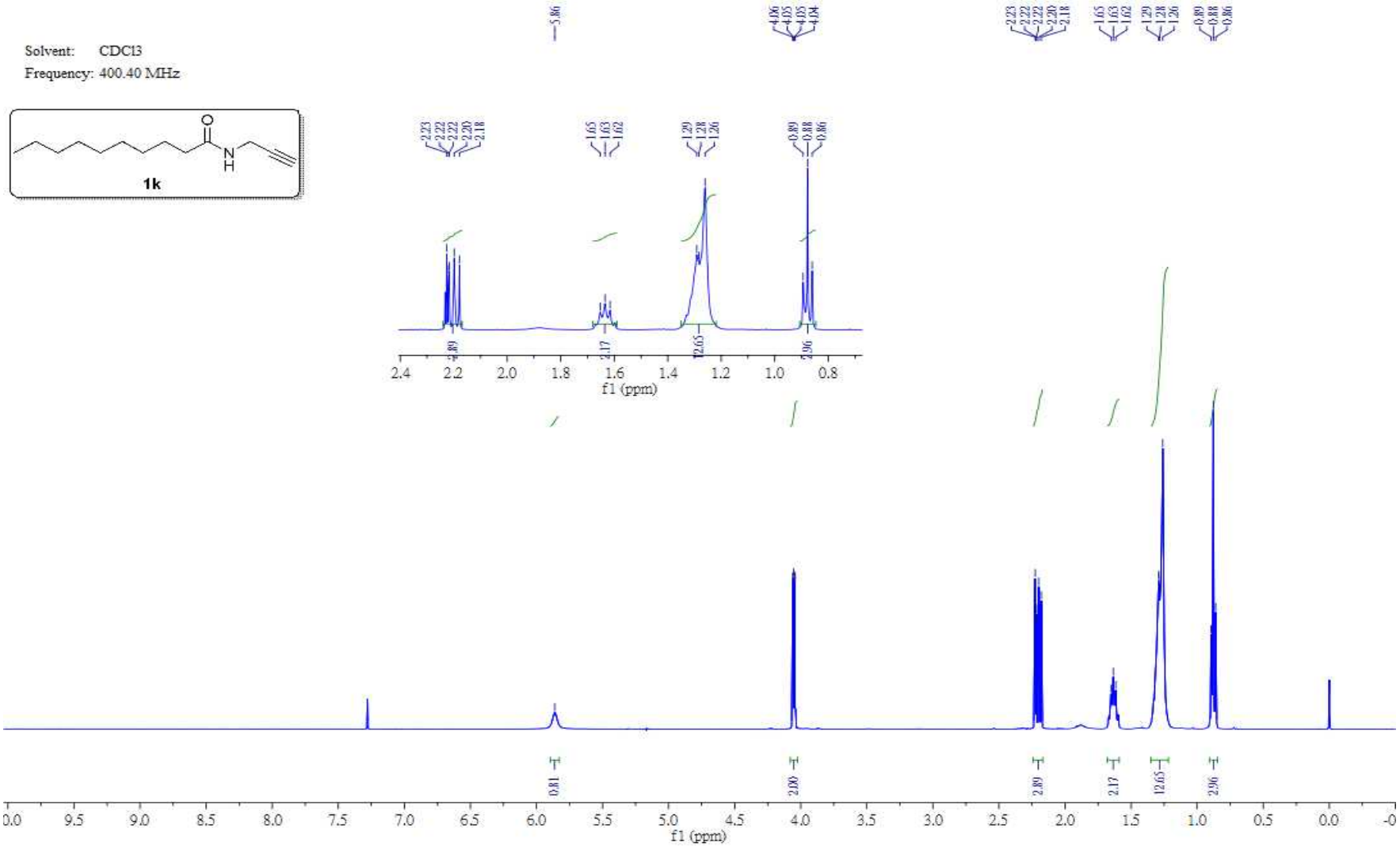

165.94
136.97
133.66
133.33
127.54
125.70
125.66
125.62
125.59
124.91
122.20
79.03
77.32
77.00
76.68
72.11
29.91
0.05
O
N
H
F3C
1i
f1 (ppm)

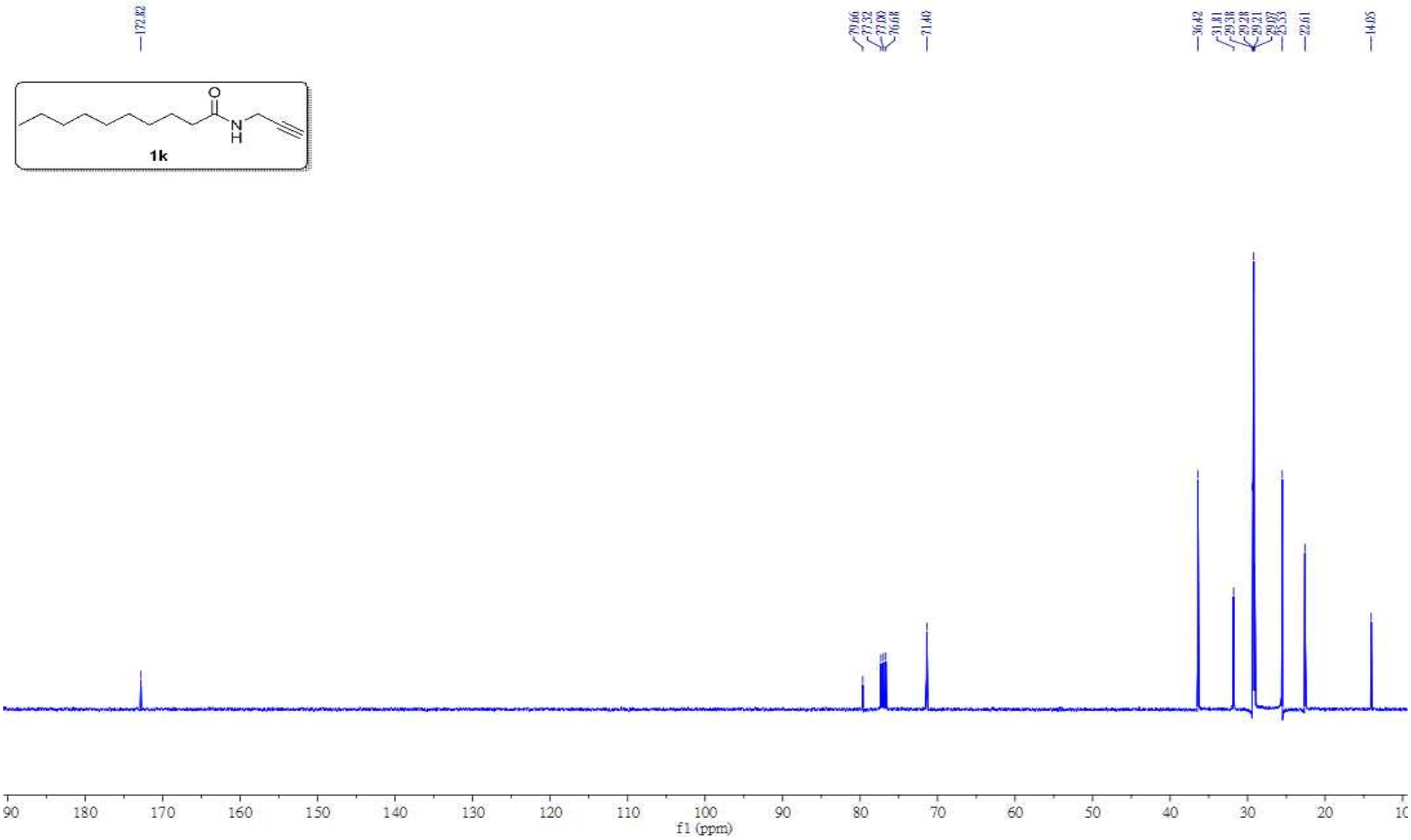

Vera-RP2-76S
Pulse Sequence: DEPT
O
N
H
F3C
1i
127.546
125.704
125.666
125.628
125.598
79.039
77.318
77.000
76.682
72.118
29.910
180
160
140
120
100
80
60
40
20
ppm

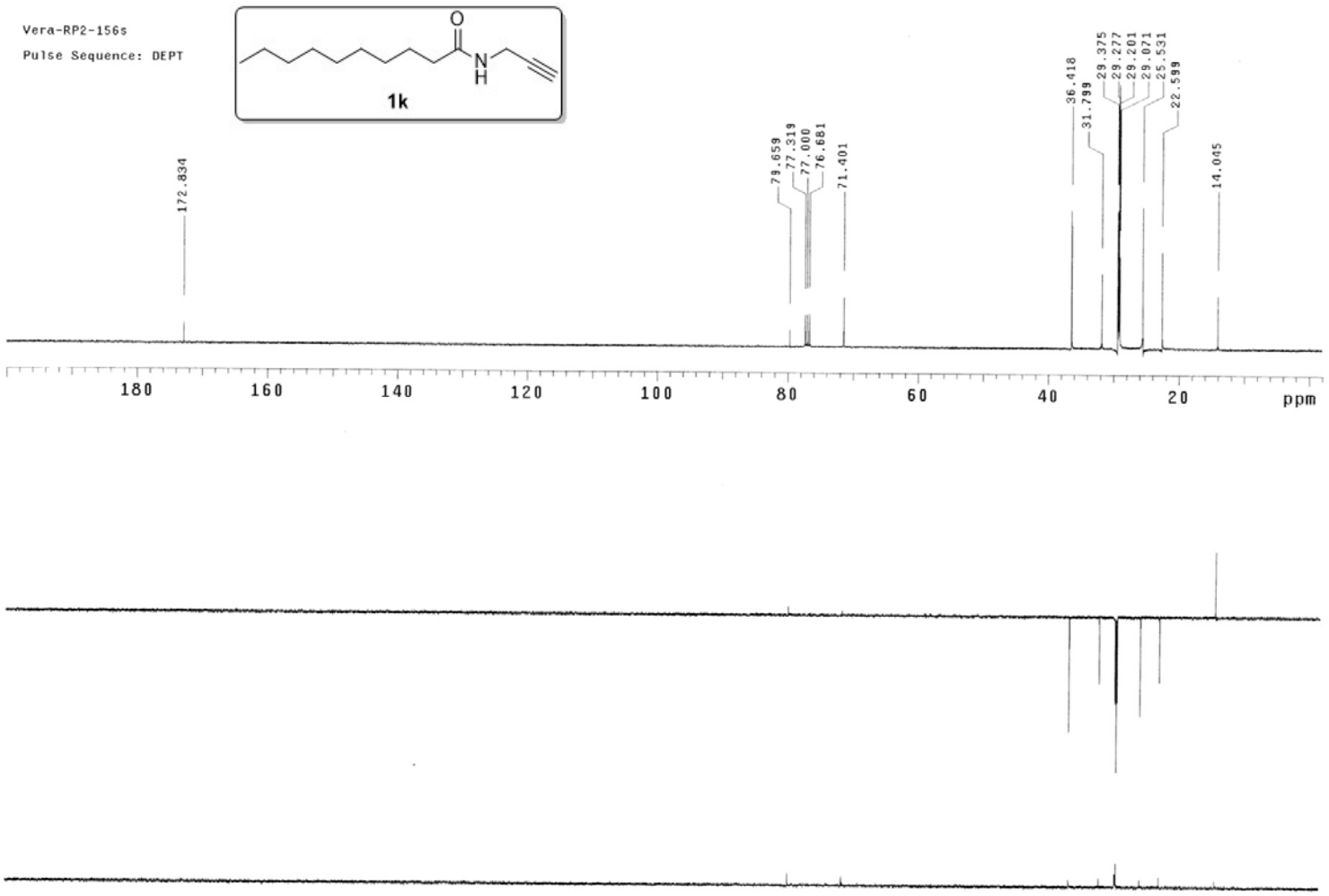

8.32
8.30
8.28
7.99
7.97
6.56
4.30
4.29
4.28
2.33
Solvent: CDCl3
Frequency: 400.40 MHz
O
N
H
O2N
1j
2.00
1.85
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
f1 (ppm)
Et3N
Et3N
2.00
1.85
0.92
1.92
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

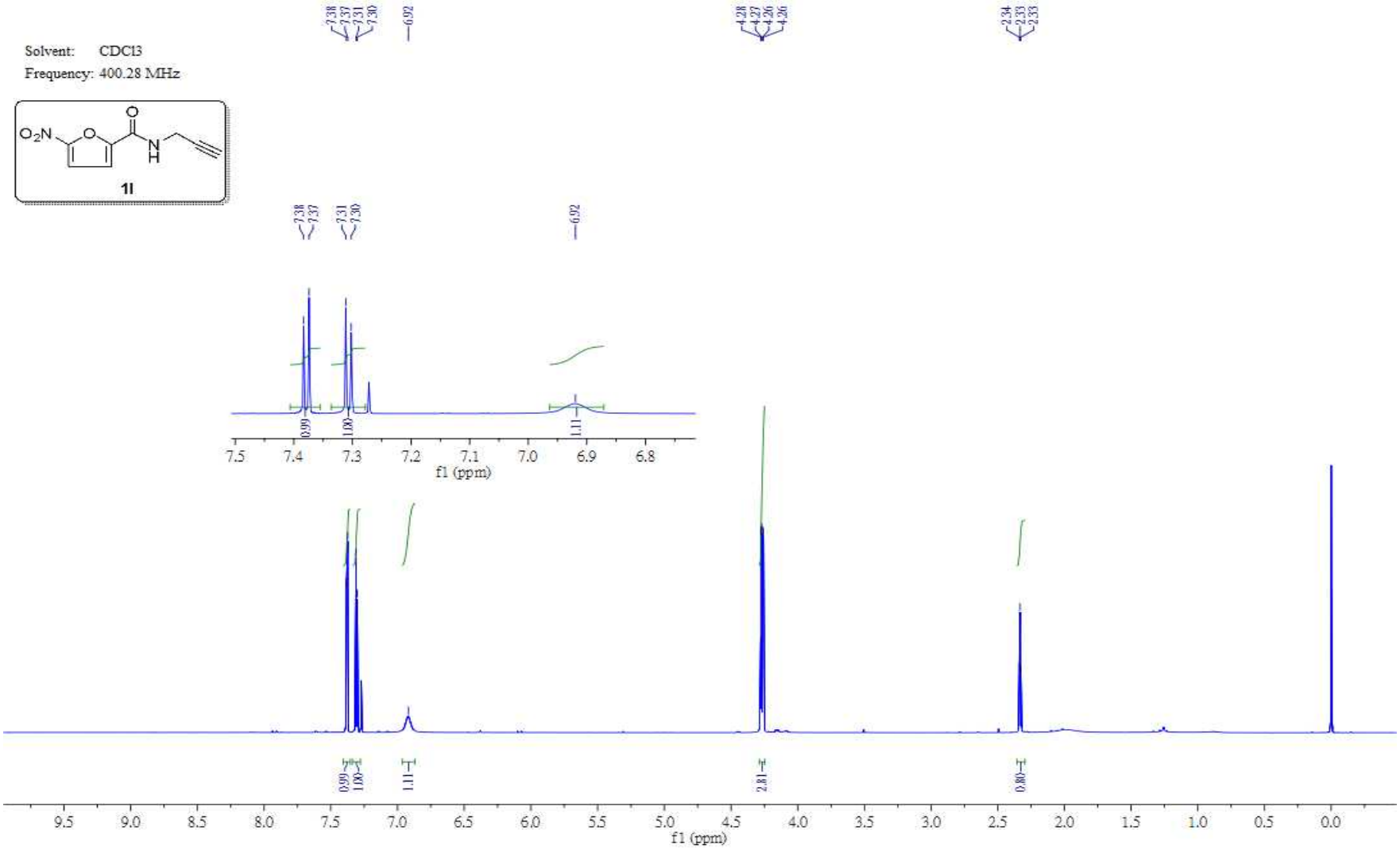

165.08
139.20
131.00
128.30
123.87
123.46
78.80
77.32
77.00
76.68
72.41
45.79
30.08
8.60
O
N
H
O2N
1j
Et3N
Et3N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

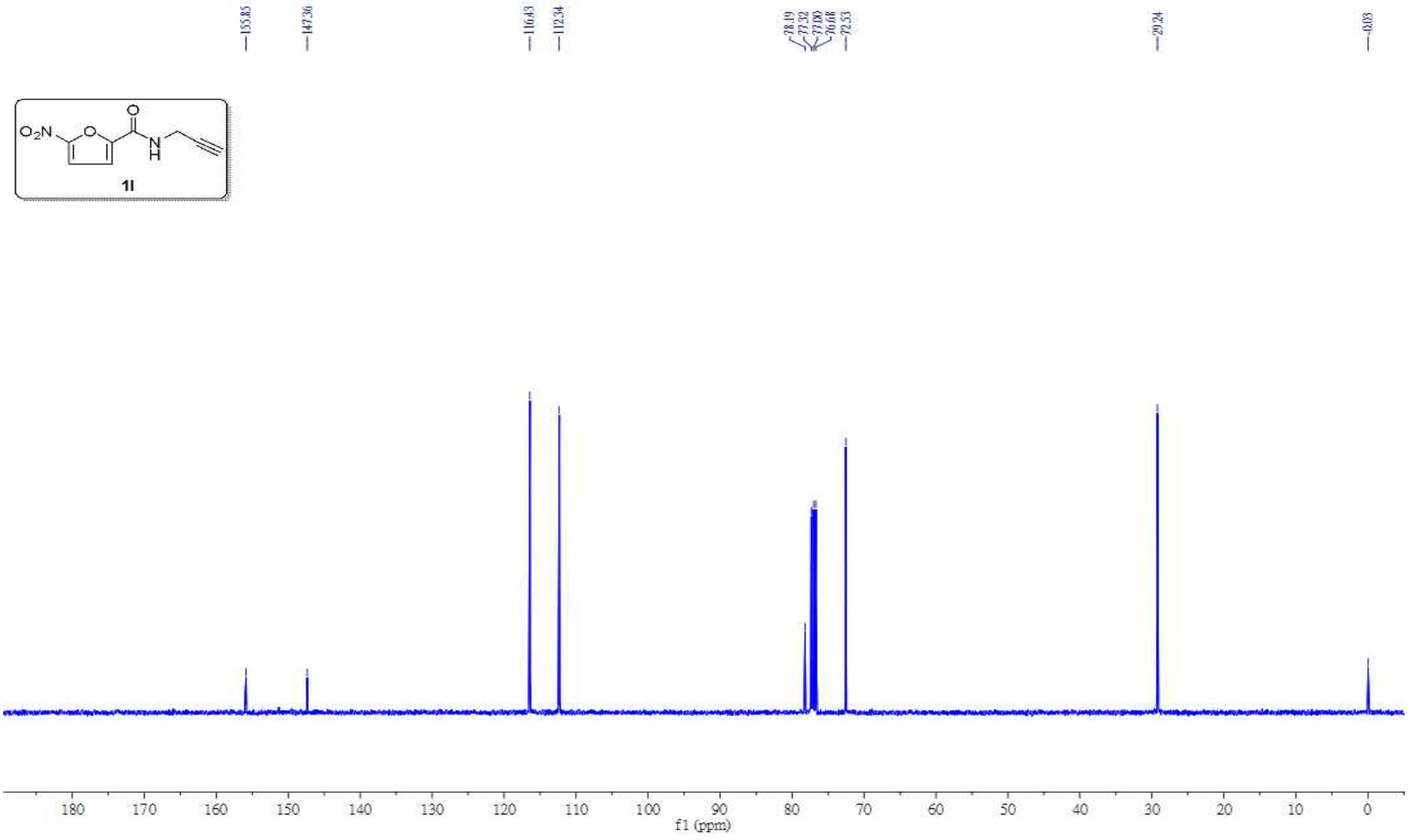

Vera-05
Pulse Sequence: DEPT
1j
165.093
149.793
139.203
130.998
128.302
123.880
123.462
78.793
77.319
77.000
76.681
72.404
45.785
30.074
8.590
180
160
140
120
100
80
60
40
20
ppm

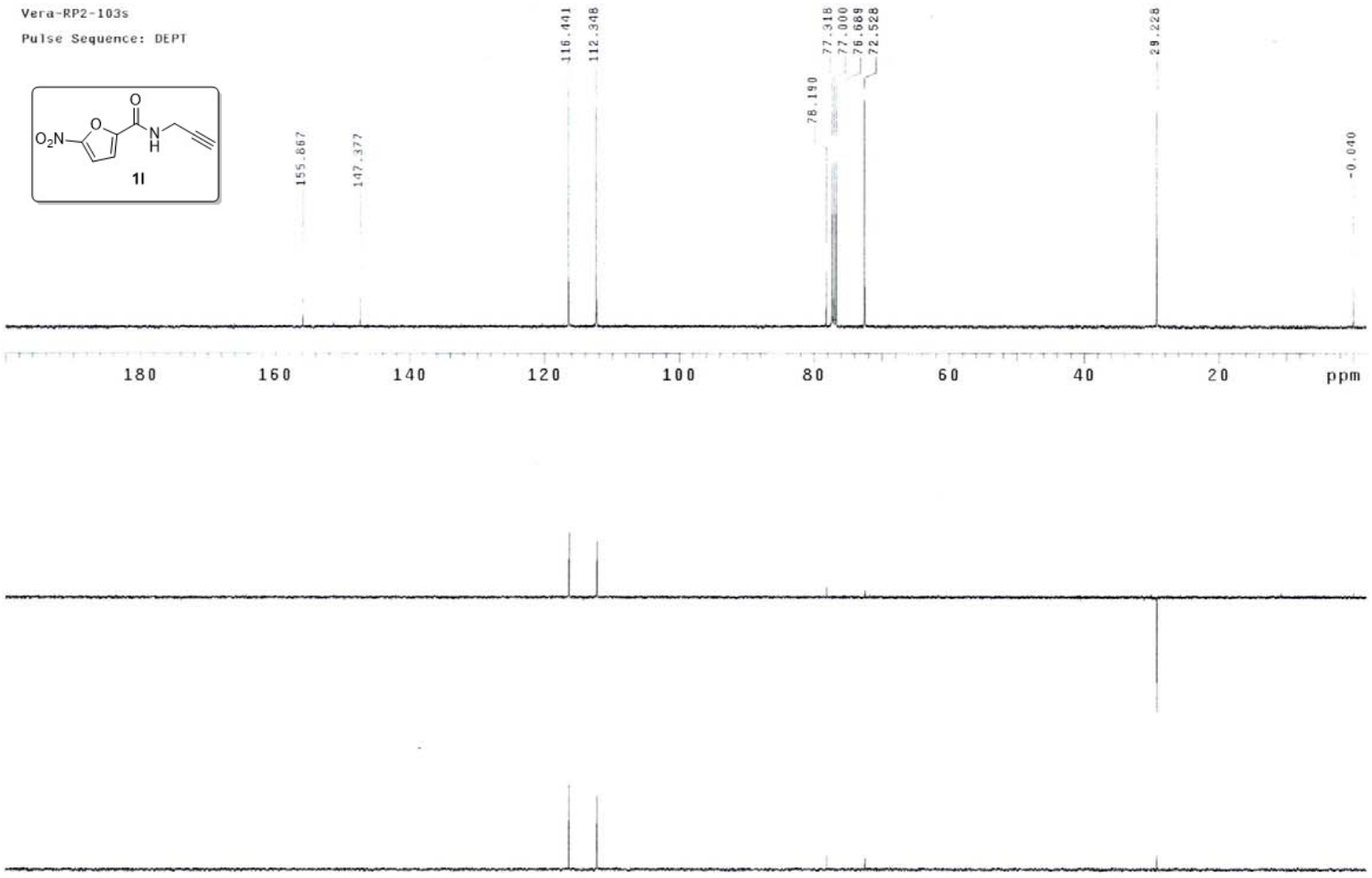

Solvent: CDCl3
Frequency: 400.40 MHz
1k
f1 (ppm)

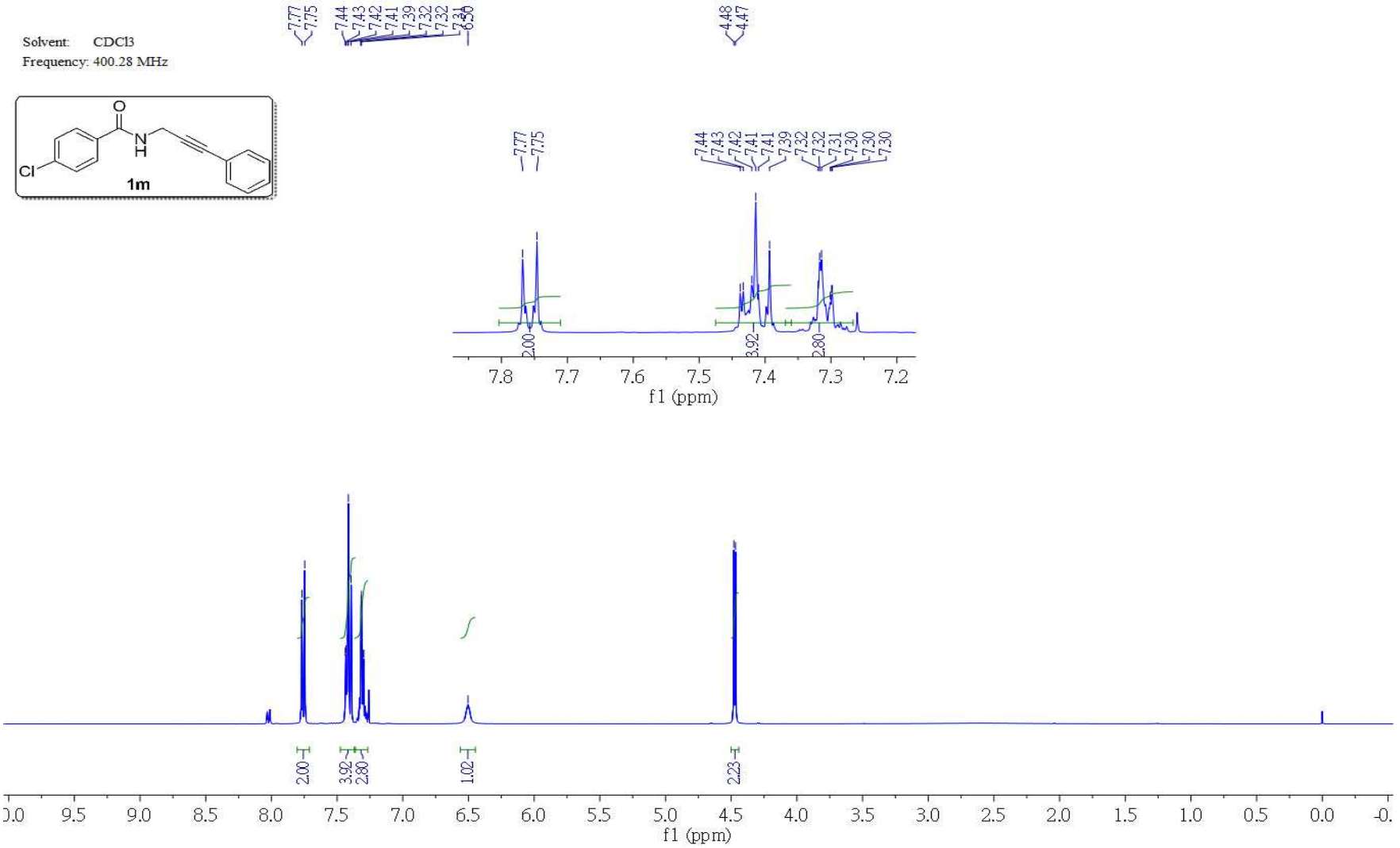

172.82
79.66
77.32
77.09
76.68
71.40
36.42
31.81
29.38
29.28
29.21
29.07
25.53
22.61
14.05
O
N
H
1k
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

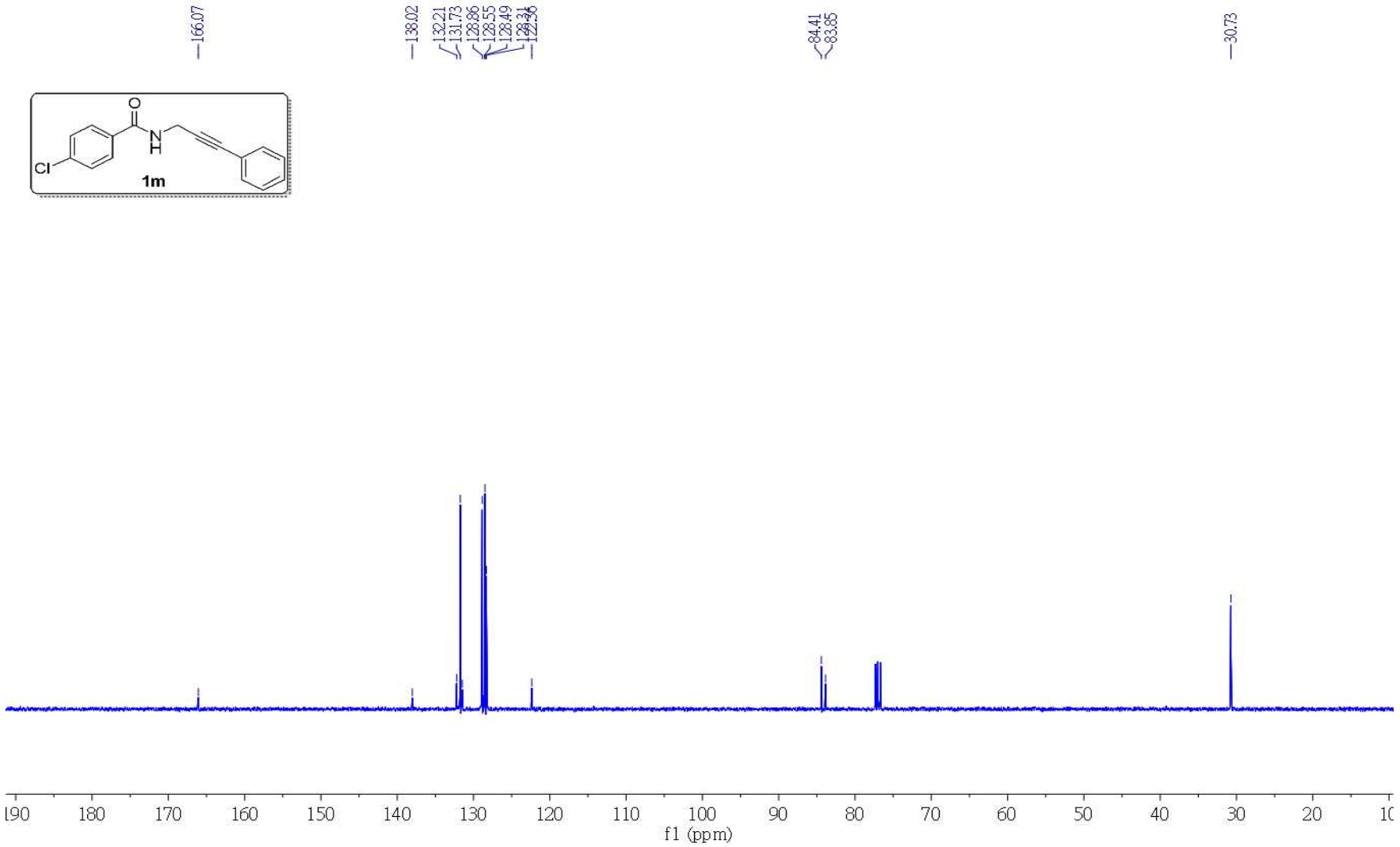

Vera-RP2-156s
Pulse Sequence: DEPT
1k
172.834
79.659
77.319
77.000
76.681
71.401
36.418
31.799
29.375
29.277
29.201
29.071
25.531
22.599
14.045
180
160
140
120
100
80
60
40
20
ppm


Solvent: CDCl3
Frequency: 400.28 MHz
1l
f1 (ppm)

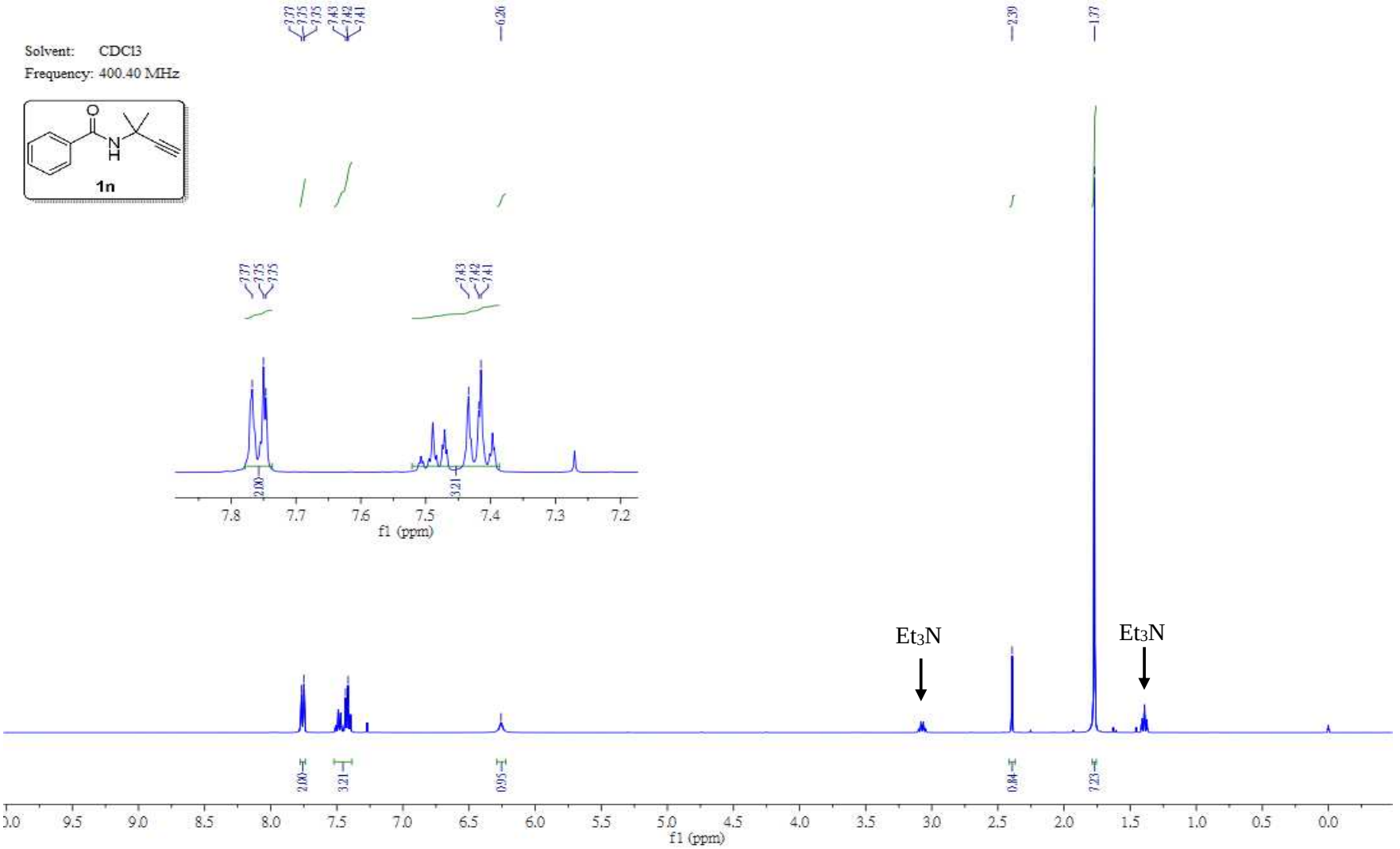

155.85
147.36
116.43
112.34
78.19
77.32
77.00
76.68
72.53
29.24
0.03
O2N
O
O
N
H
1l
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

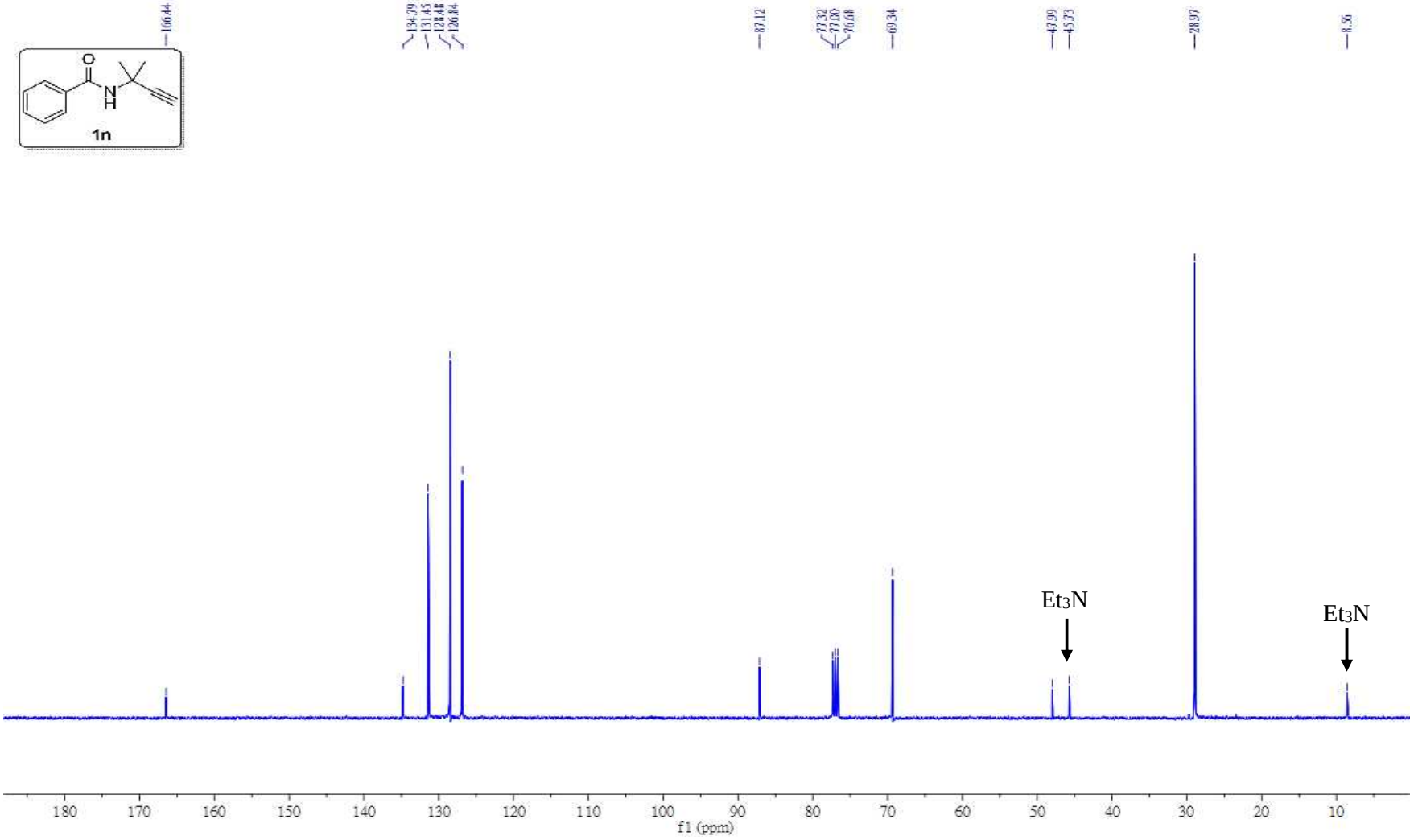

Vera-RP2-103s
Pulse Sequence: DEPT
1l
155.667
147.377
116.441
112.348
78.190
77.318
77.000
76.669
72.528
29.228
-0.040
180
160
140
120
100
80
60
40
20
ppm

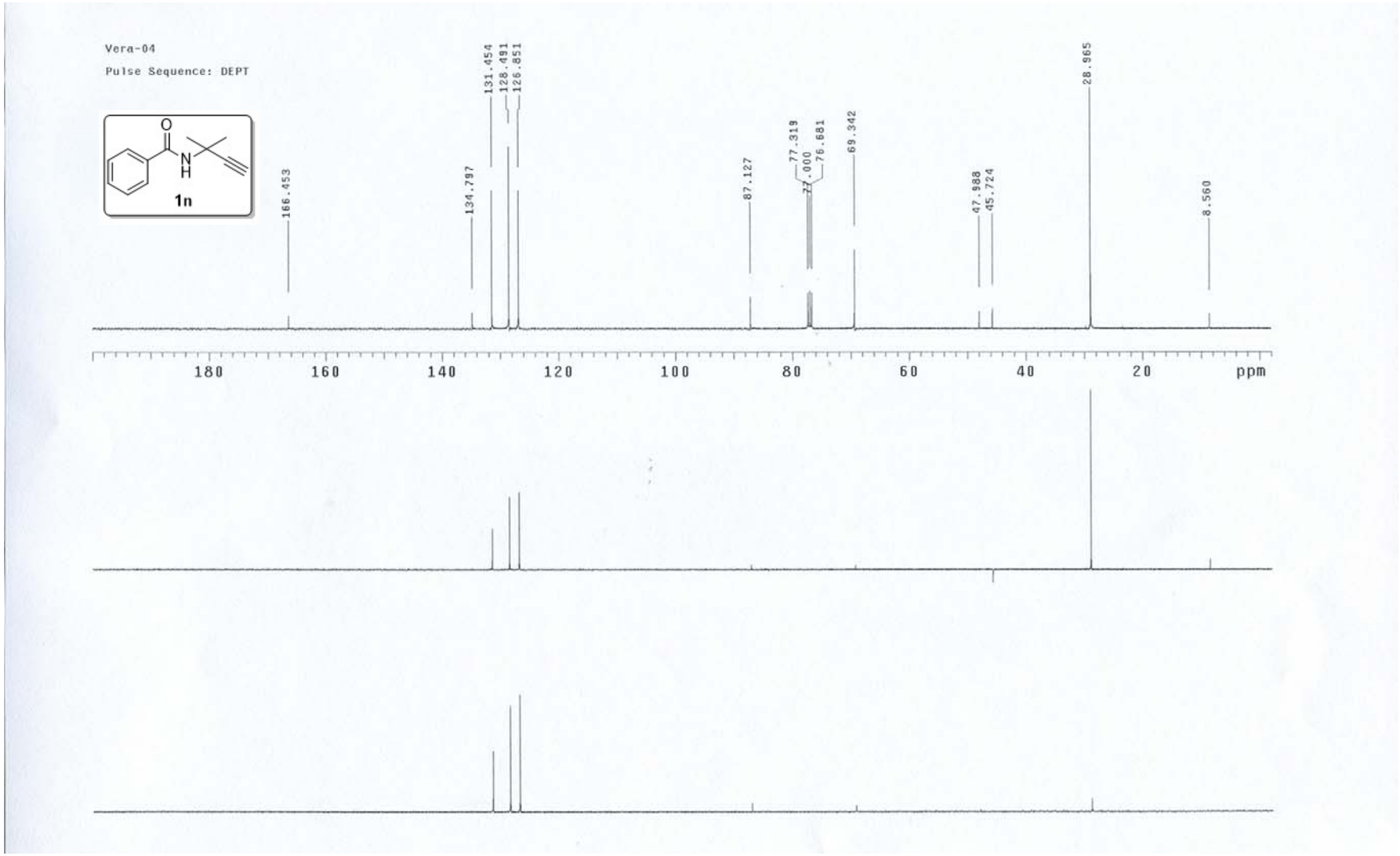

Solvent: CDCl3
Frequency: 400.28 MHz
1m
f1 (ppm)

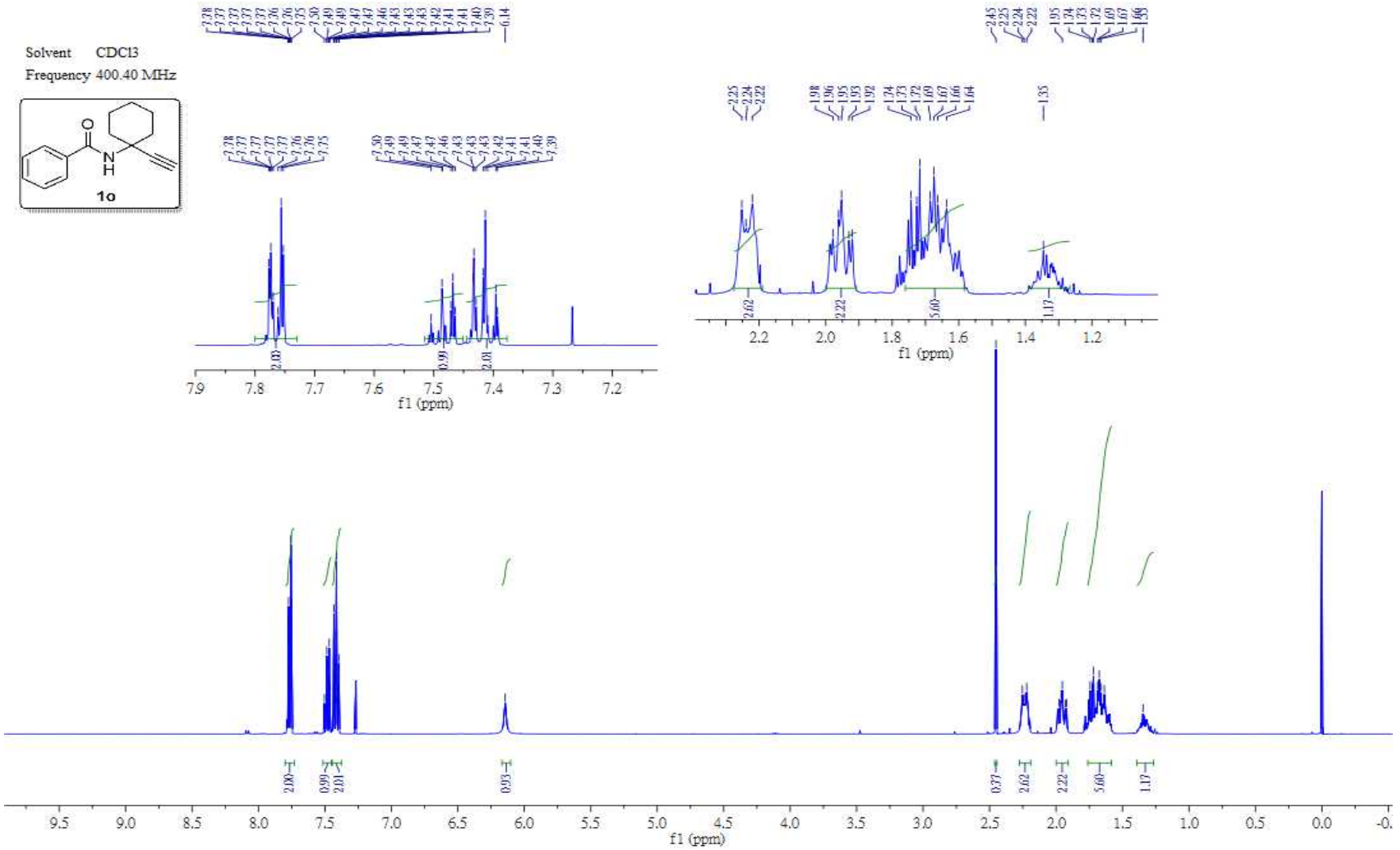

166.07
138.02
132.21
131.73
128.86
128.55
128.49
84.41
83.85
30.73
Cl
O
N
H
1m
f1 (ppm)

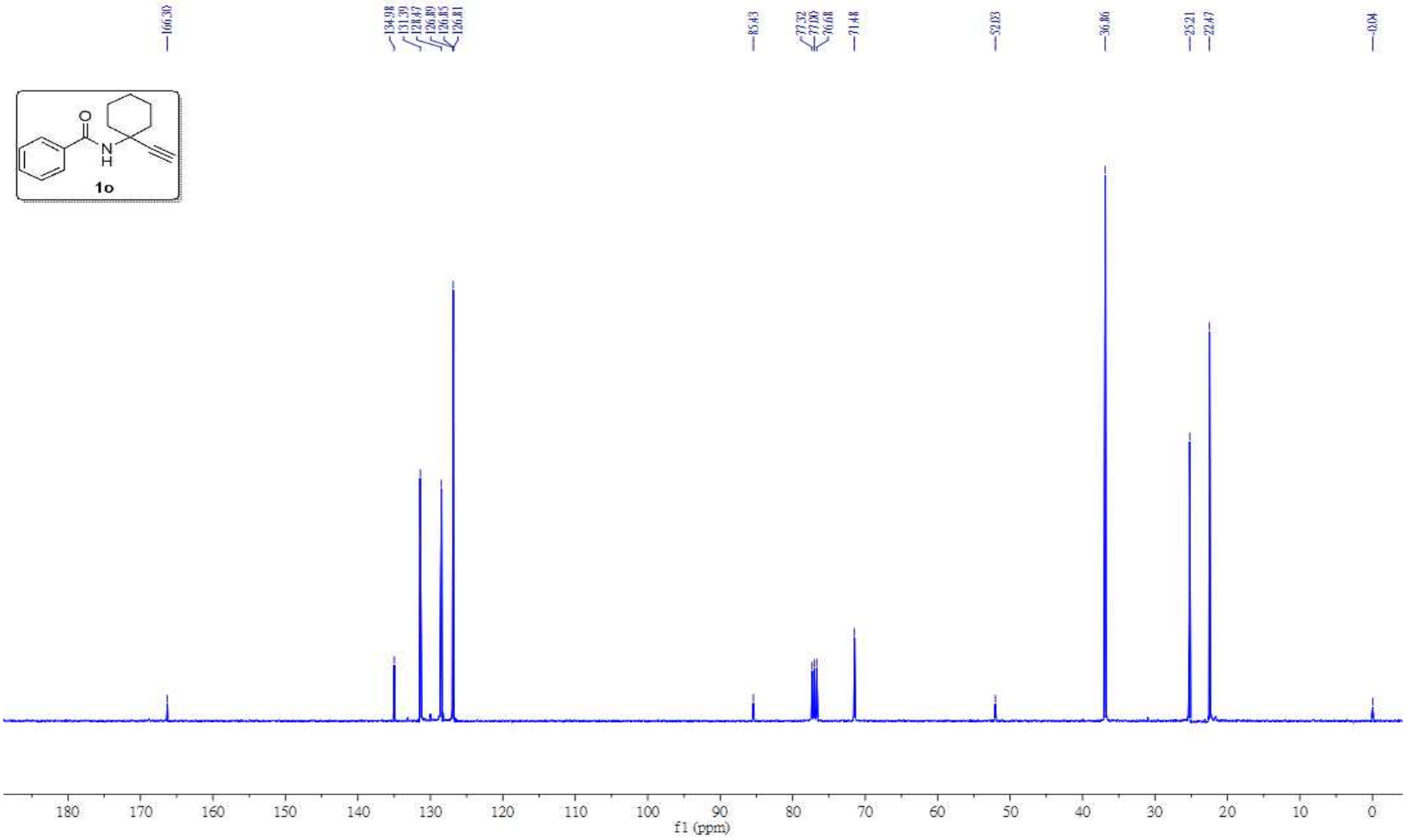

Vera-RP3-03
Pulse Sequence: DEPT
O
N
H
Cl
1m
131.738
128.865
128.547
128.501
128.312
30.722
180
160
140
120
100
80
60
40
20
ppm

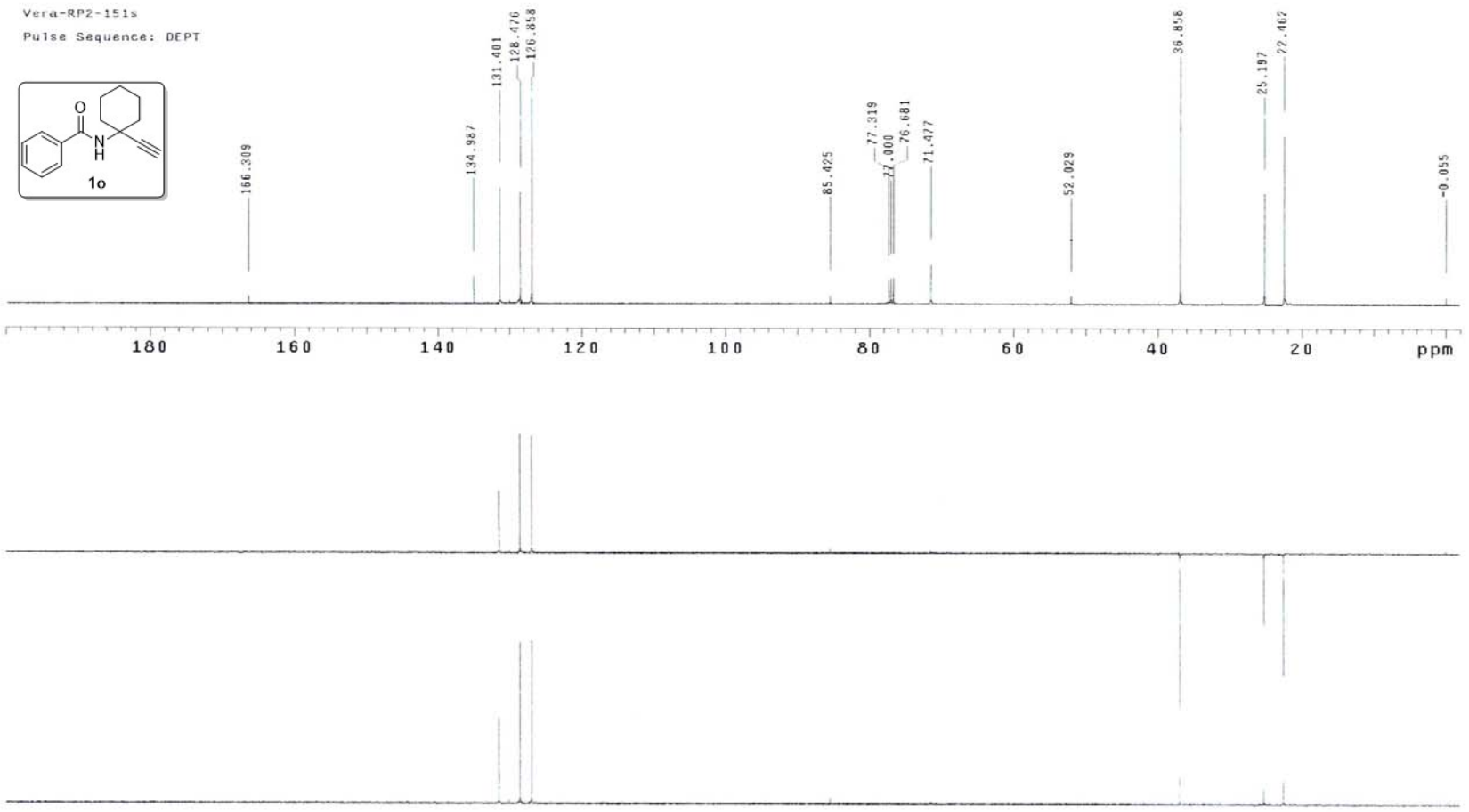

Solvent: CDCl3
Frequency: 400.40 MHz
1n
Et3N
Et3N
f1 (ppm)

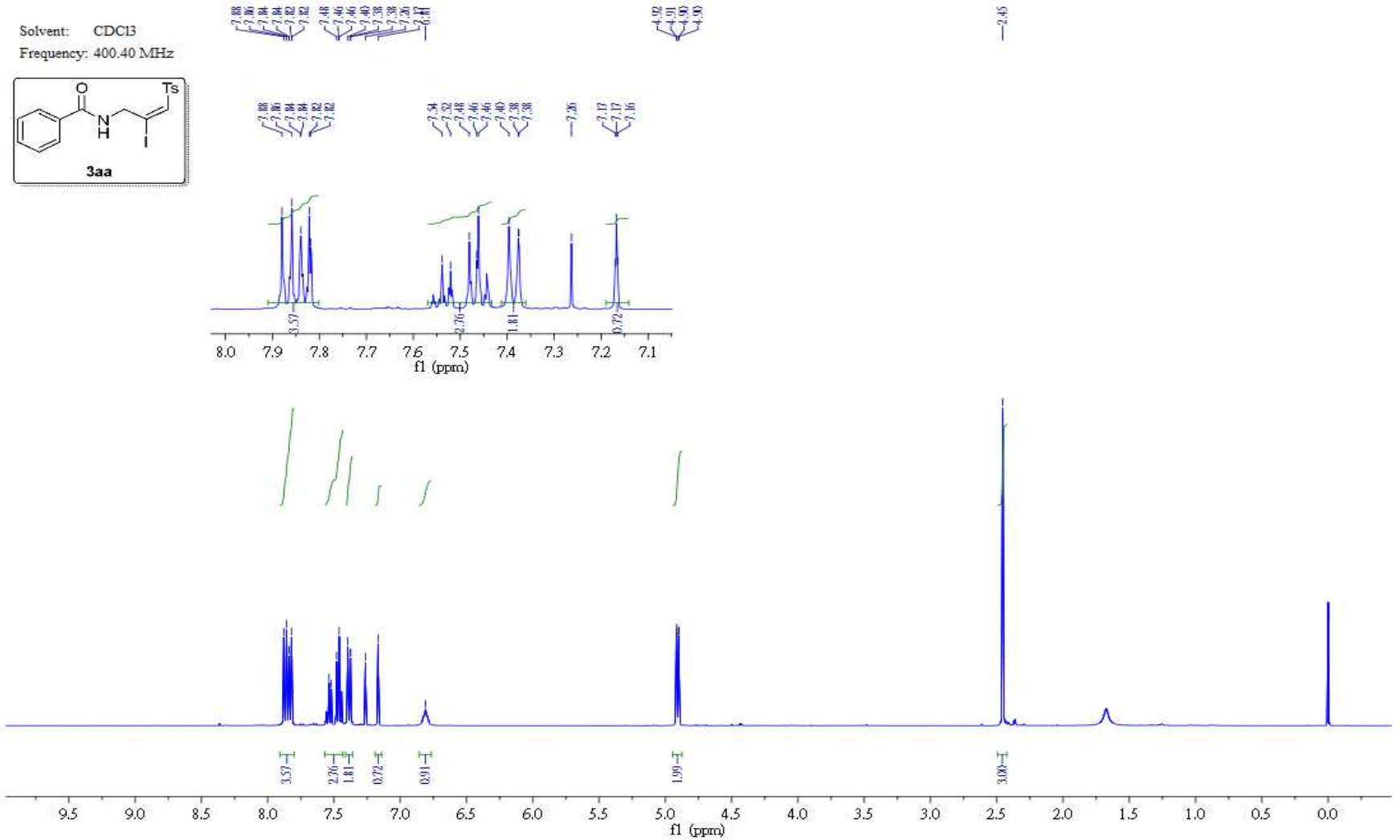

166.44
134.79
131.45
128.48
126.84
87.12
77.32
77.00
76.68
69.34
47.99
45.73
28.97
8.56
O
N
H
1n
Et3N
Et3N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

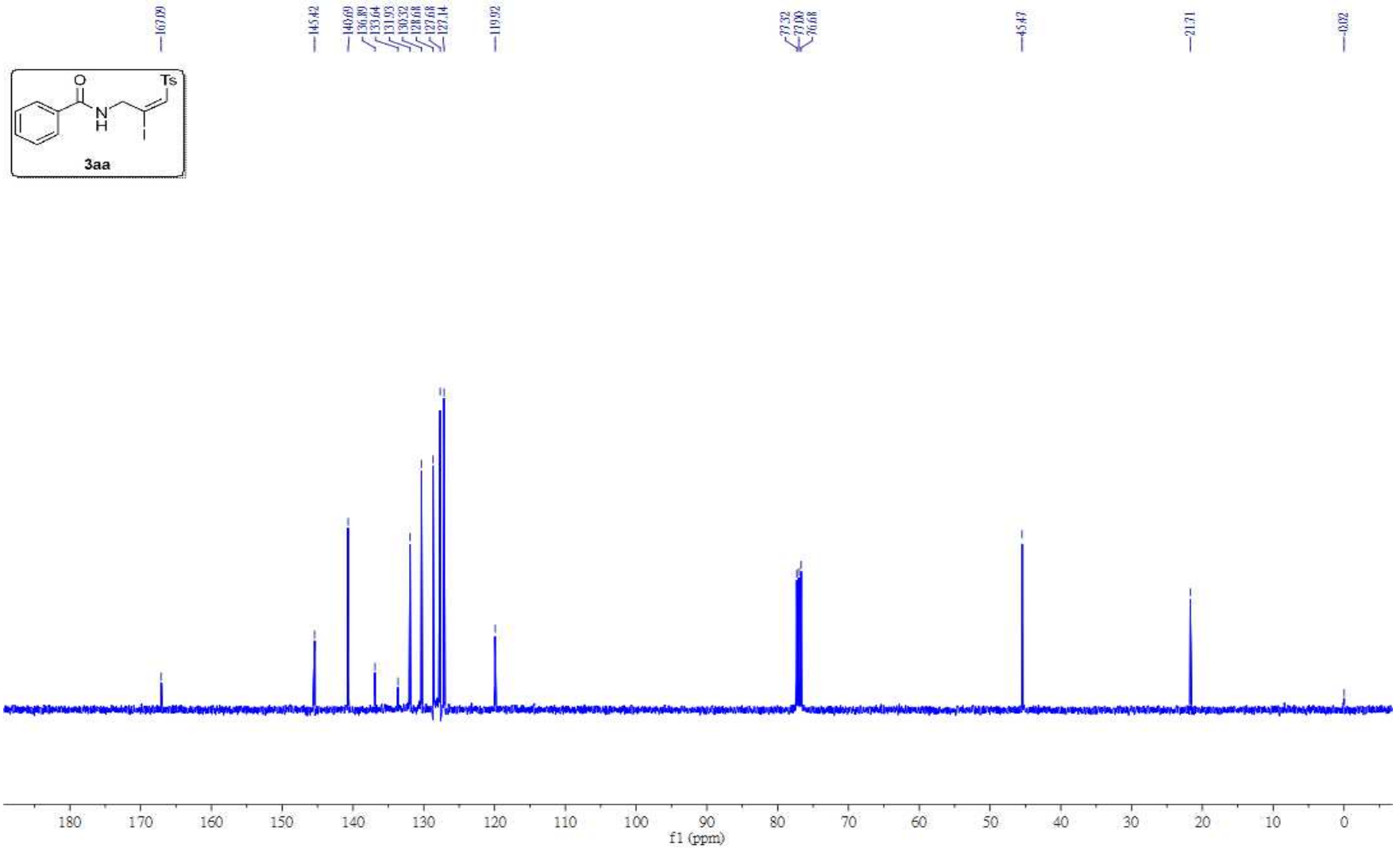

Vera-04
Pulse Sequence: DEPT
1n
166.453
134.797
131.454
128.491
126.851
87.127
77.319
77.000
76.681
69.342
47.888
45.724
28.965
8.560
180
160
140
120
100
80
60
40
20
ppm

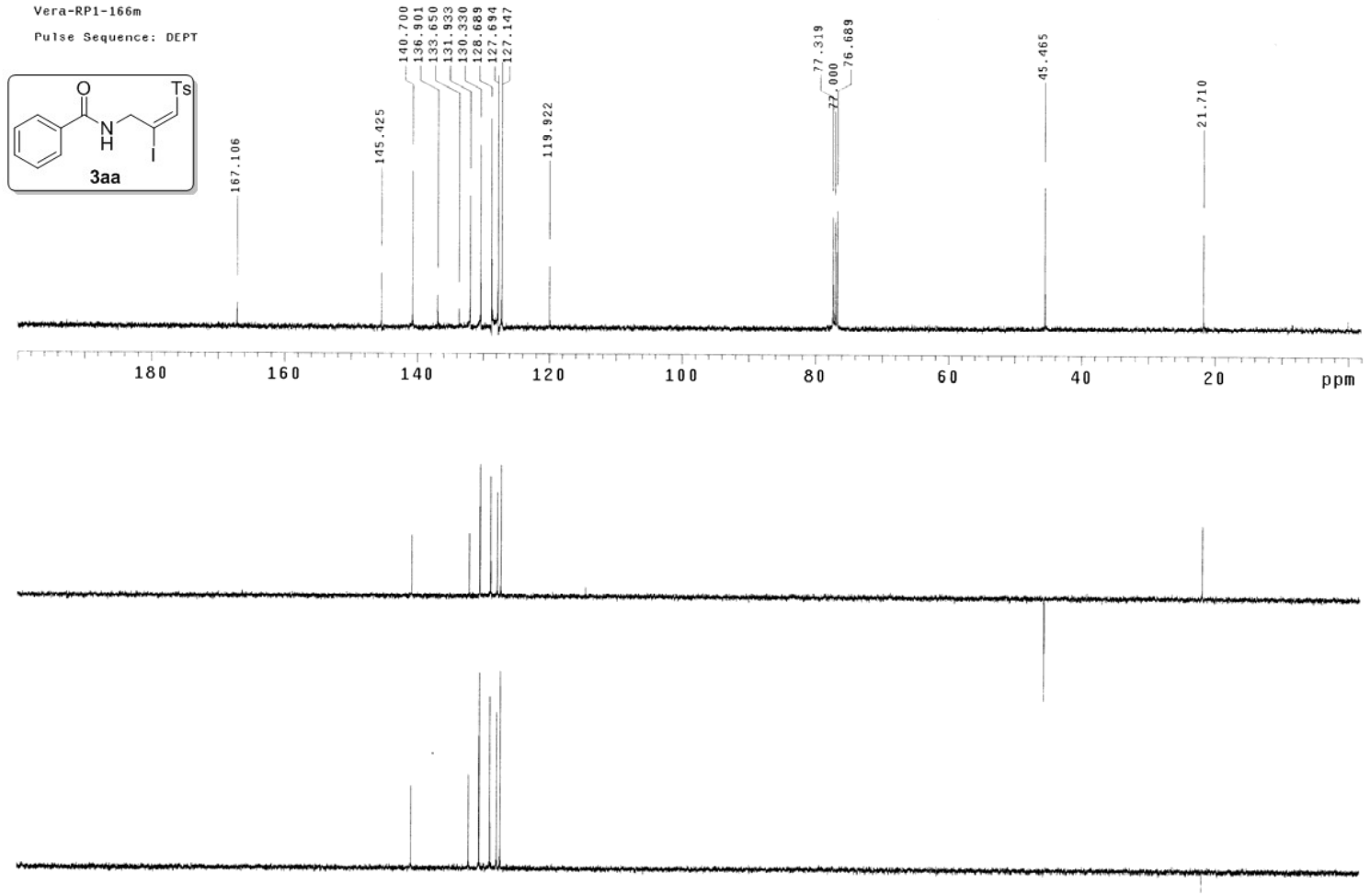

Solvent CDCl3
Frequency 400.40 MHz
1o
f1 (ppm)

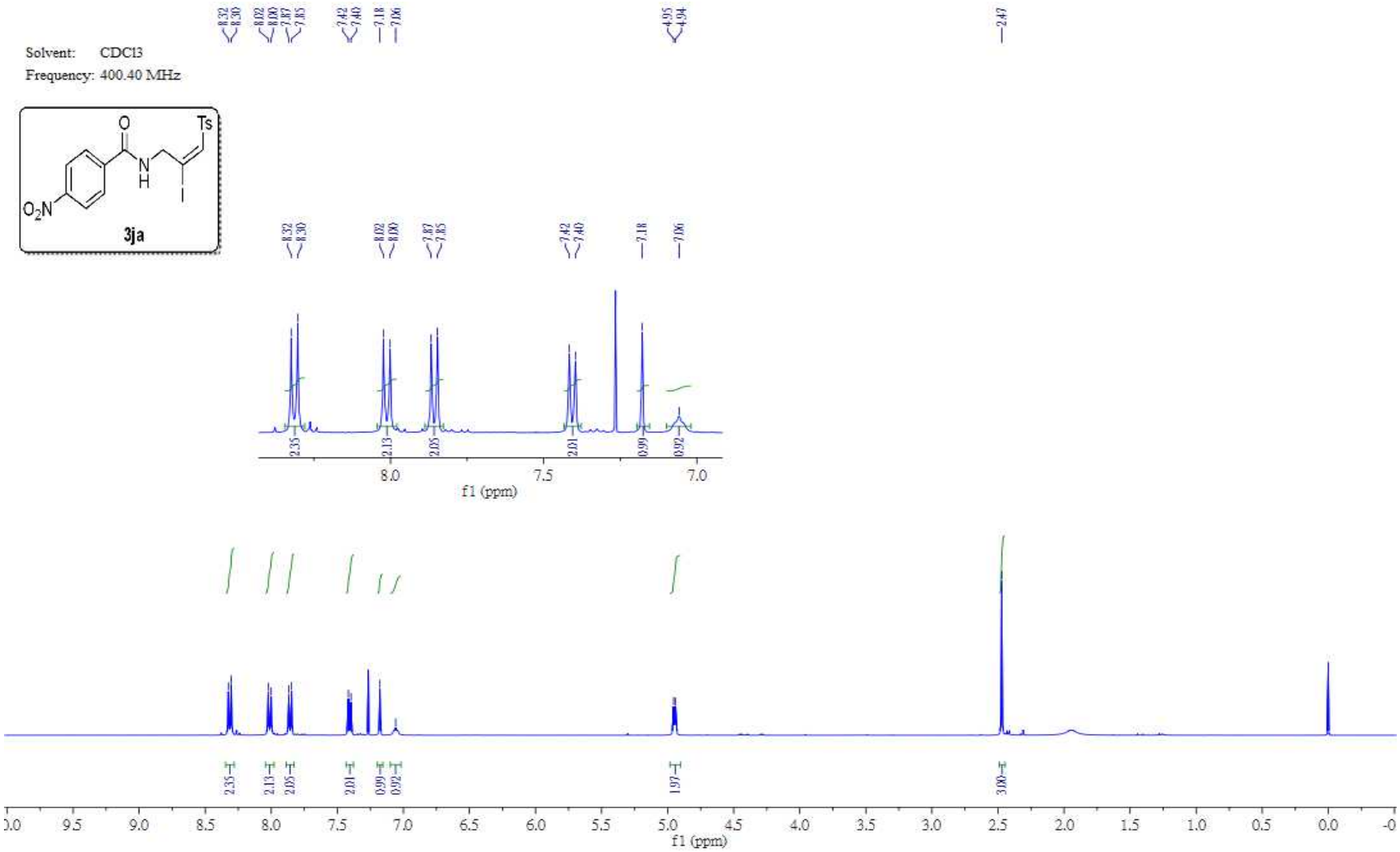

166.30
134.98
131.39
128.47
126.89
126.85
126.81
85.43
77.32
77.00
76.68
71.48
52.03
36.86
25.21
22.47
0.04
O
N
H
1o
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

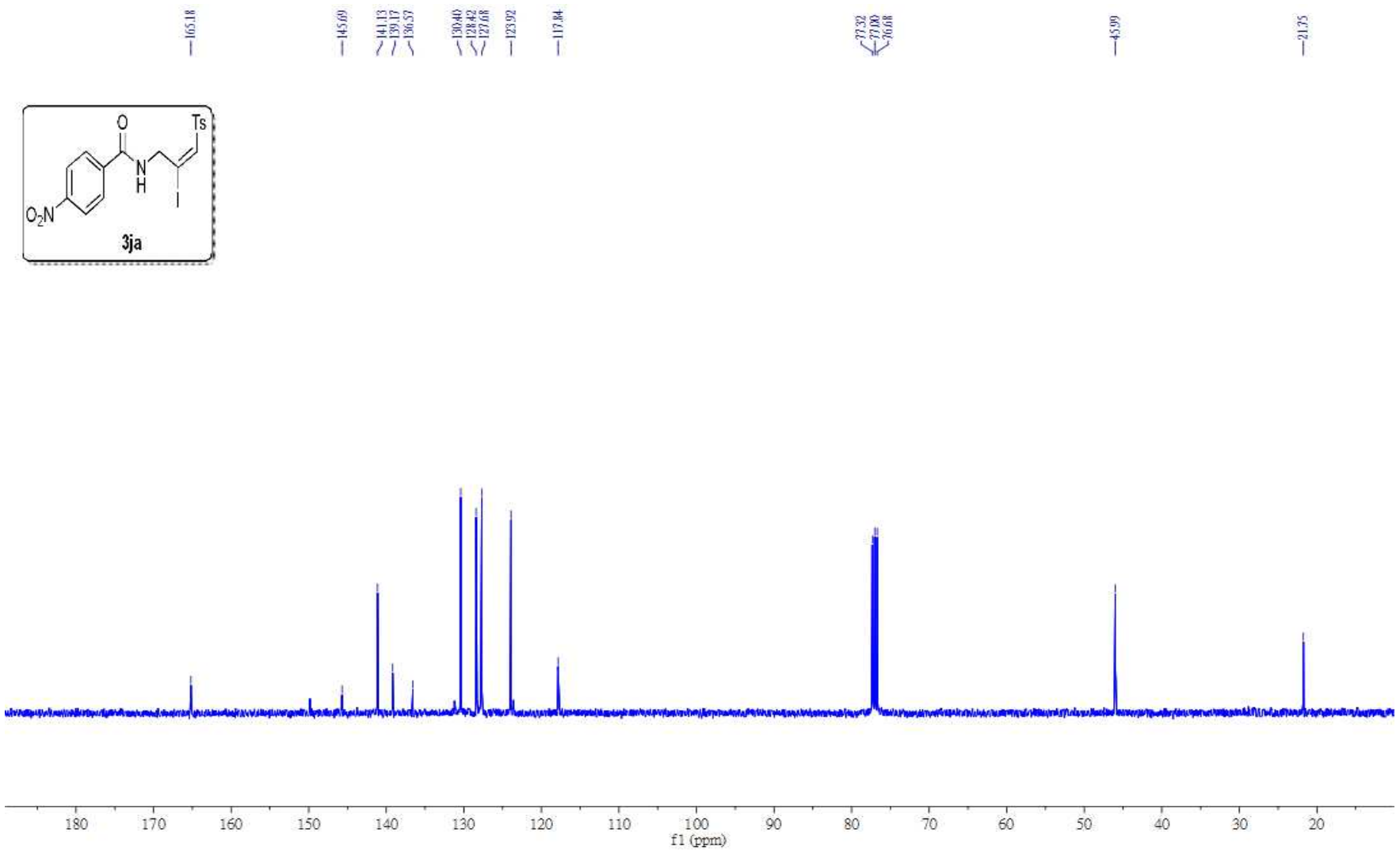

Vera-RP2-151s
Pulse Sequence: DEPT
1o
166.309
134.987
131.401
128.476
126.858
85.425
77.319
77.000
76.681
71.477
52.029
36.858
25.197
22.462
-0.055
180
160
140
120
100
80
60
40
20
ppm

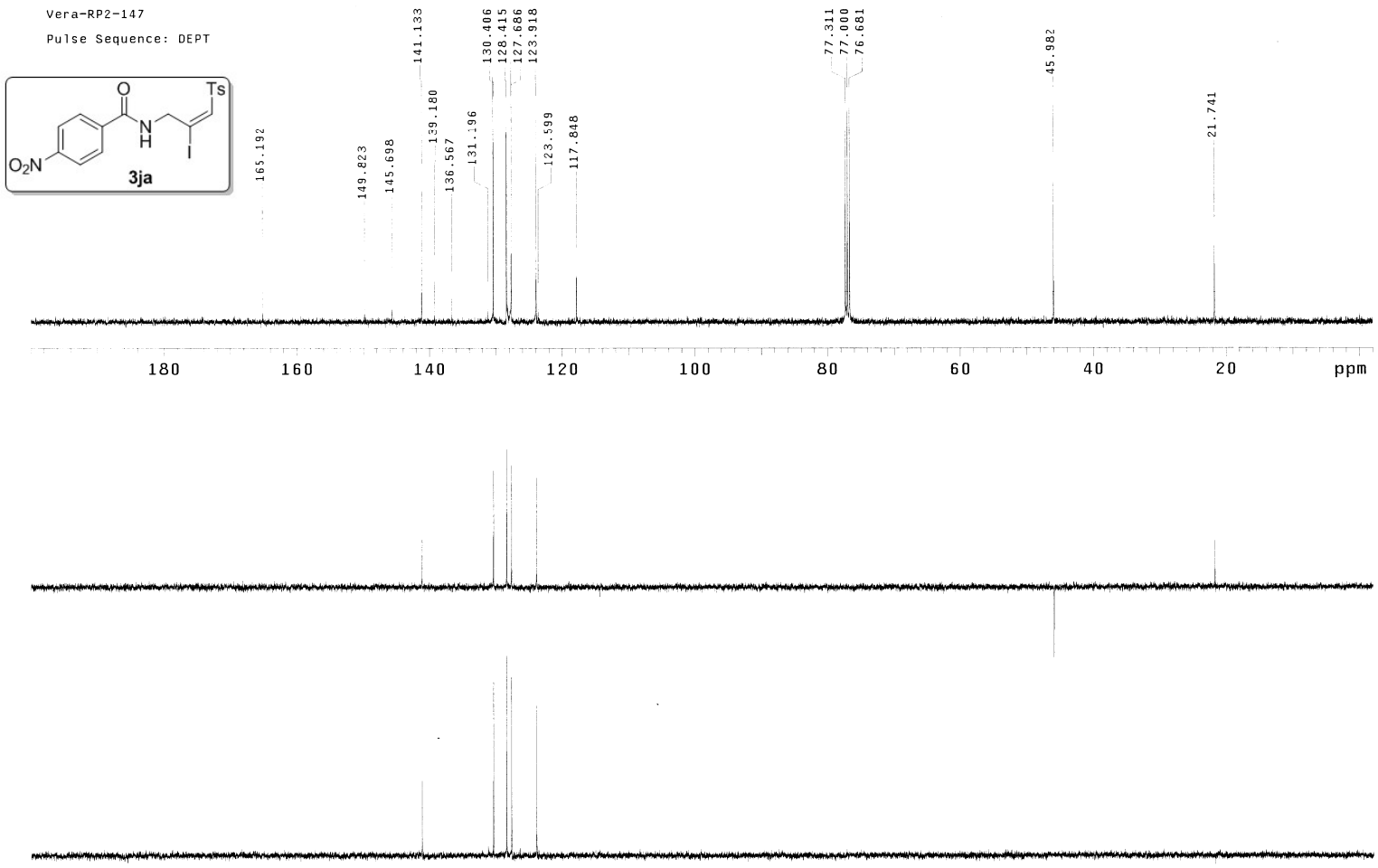

Solvent: CDCl3
Frequency: 400.40 MHz
O
Ts
N
H
I
3aa
f1 (ppm)

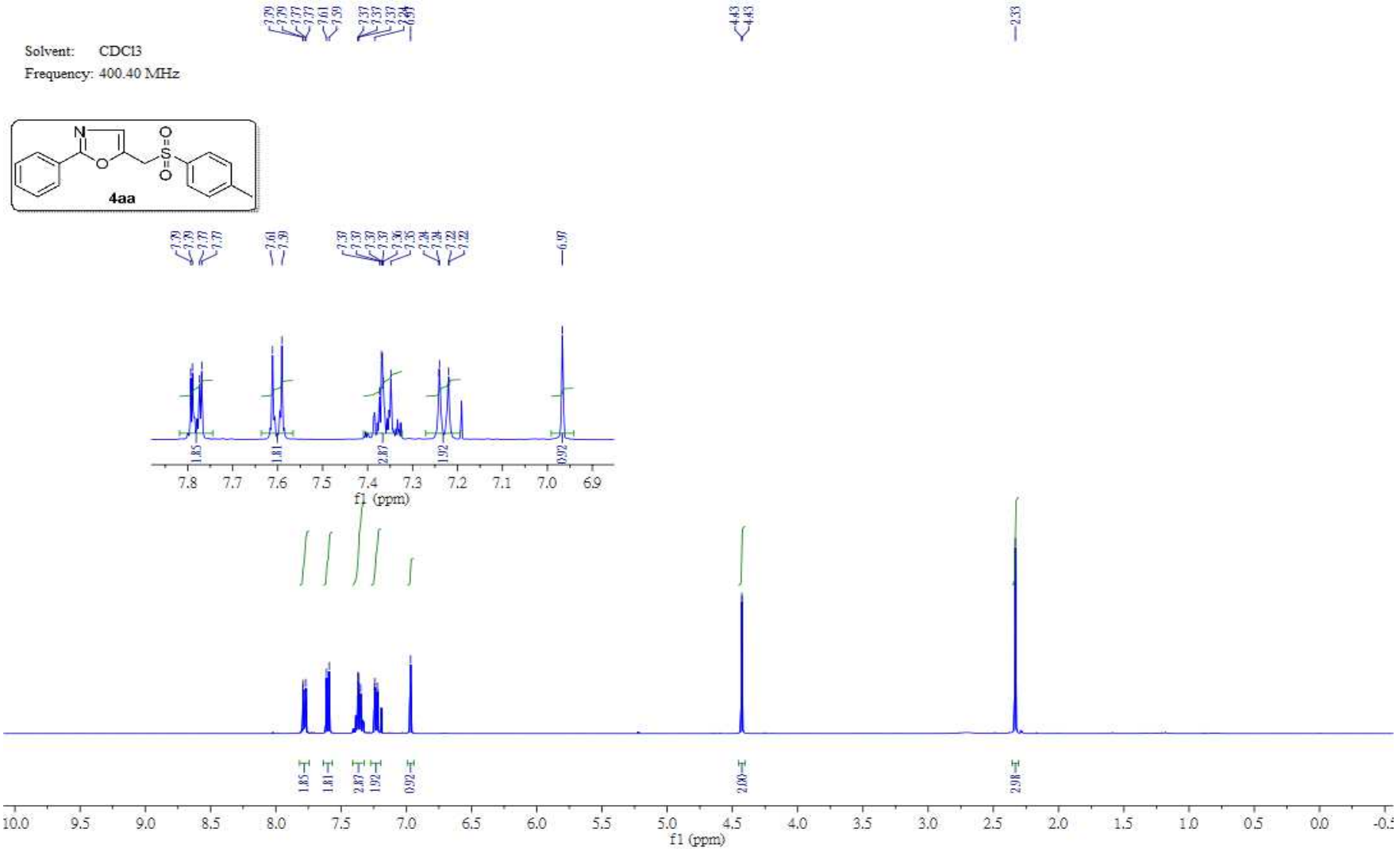

167.09
145.42
140.69
136.89
133.64
131.93
130.32
128.68
127.68
127.14
119.92
77.32
77.00
76.68
45.47
21.71
0.02
O
N
H
Ts
I
3aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

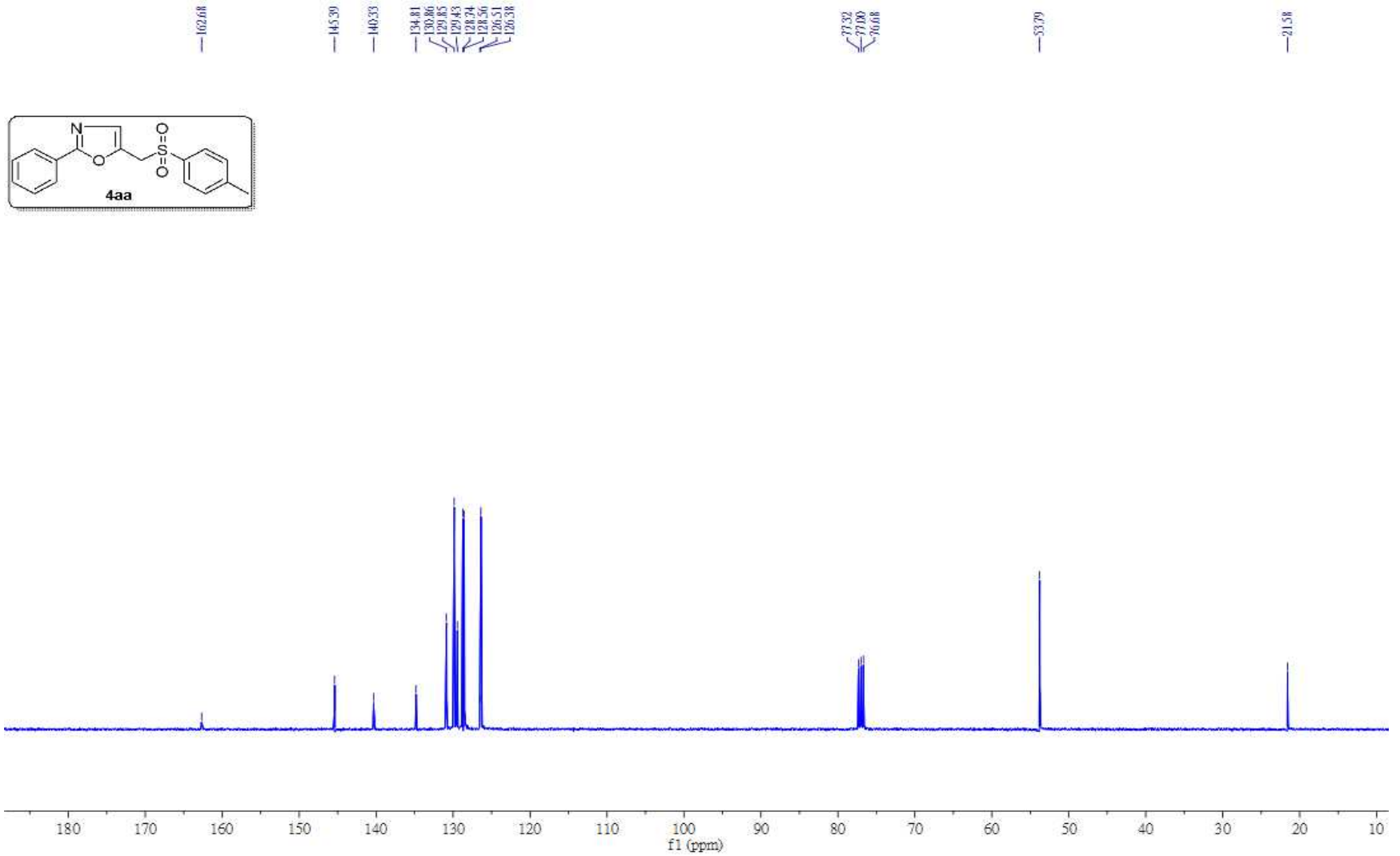

Vera-RP1-166m
Pulse Sequence: DEPT
O
N
H
Ts
I
3aa
167.106
145.425
140.700
136.901
133.650
131.933
130.330
128.689
127.694
127.147
119.922
77.319
77.000
76.689
45.465
21.710
180
160
140
120
100
80
60
40
20
ppm

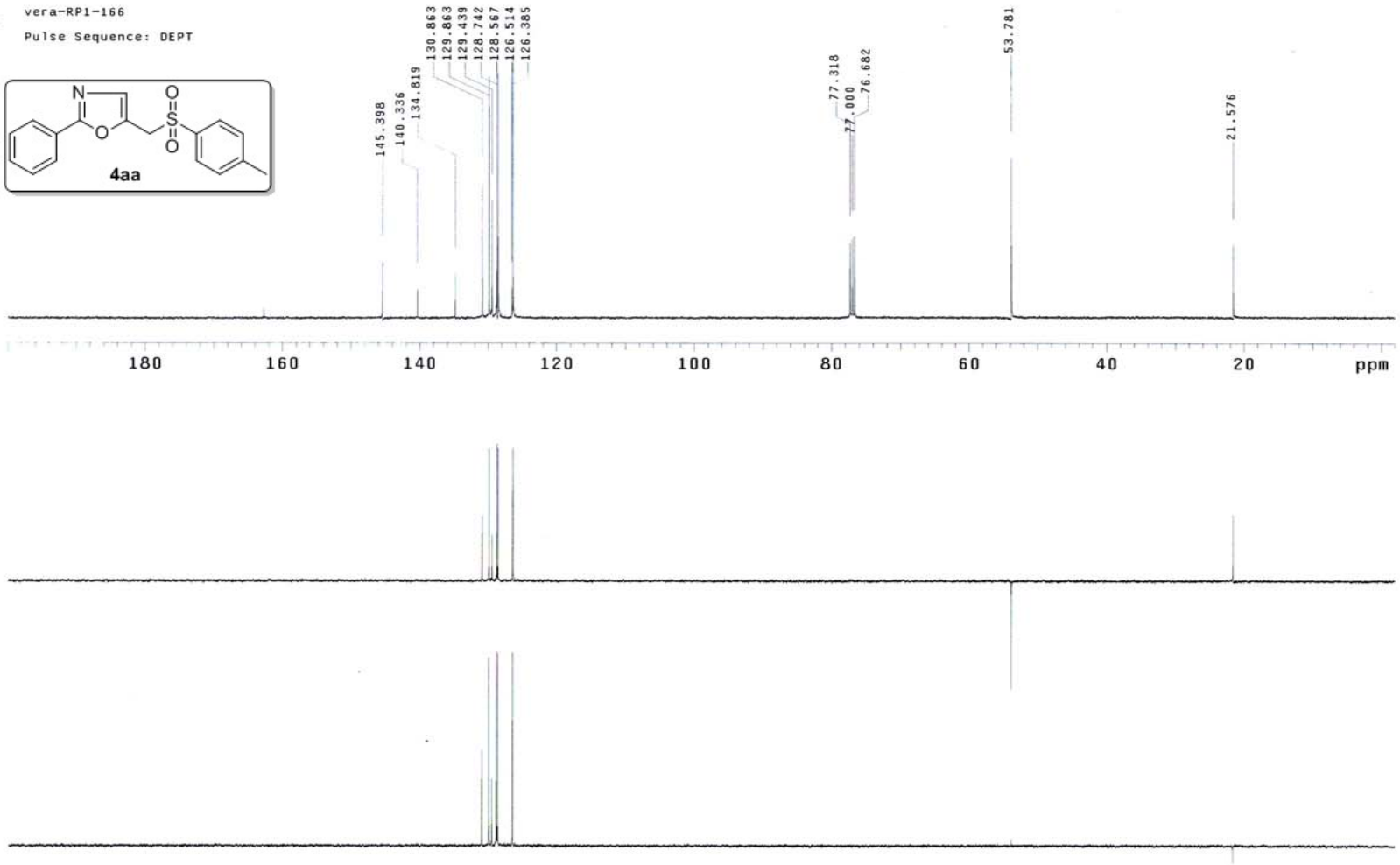

Solvent: CDCl3
Frequency: 400.40 MHz
3ja
f1 (ppm)
f1 (ppm)

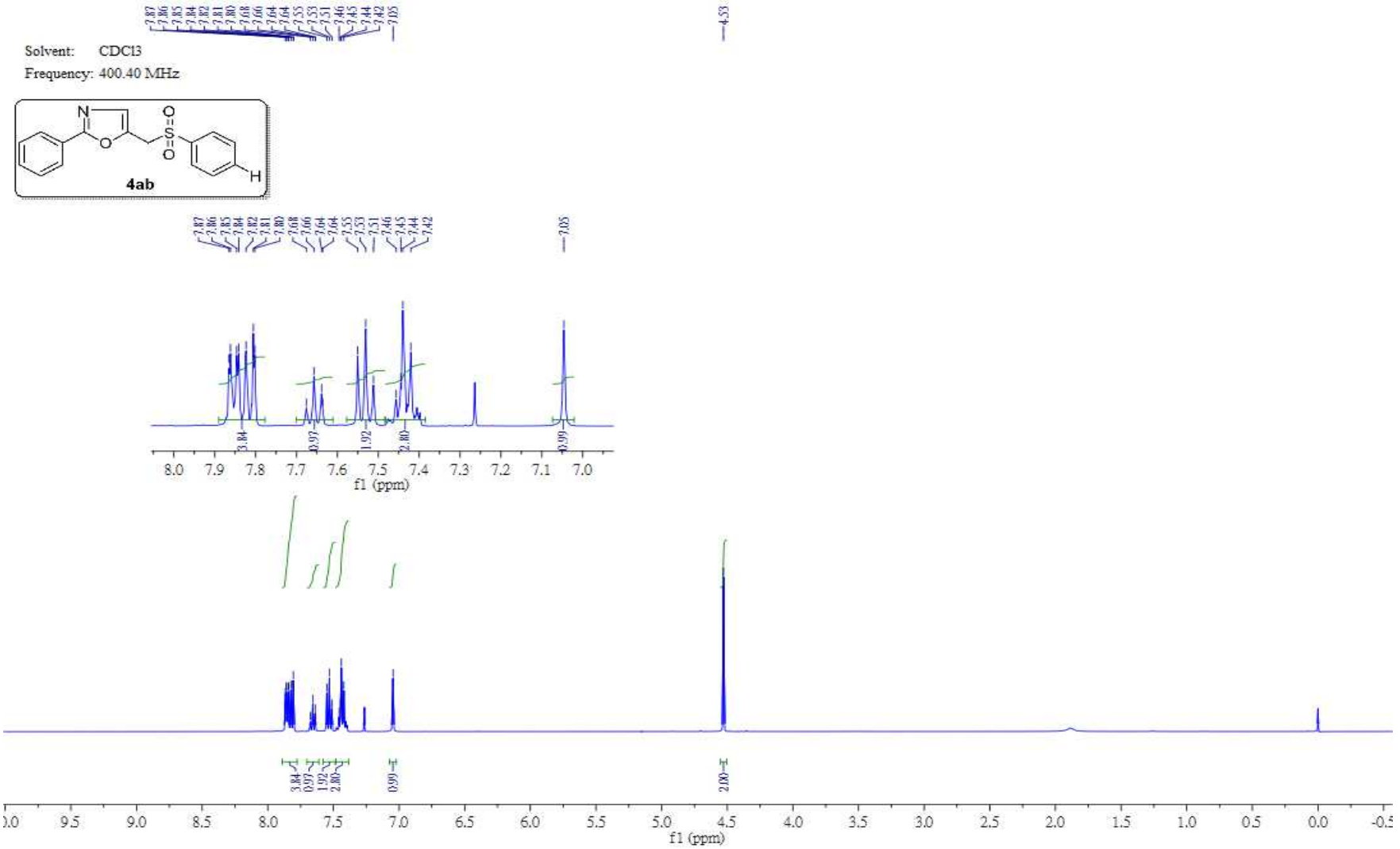

165.18
145.69
141.13
139.17
136.57
130.40
128.42
127.68
123.92
117.84
77.32
77.00
76.68
45.99
21.75
O
Ts
N
H
I
O2N
3ja
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


Vera-RP2-147
Pulse Sequence: DEPT
O
Ts
N
H
I
O2N
3ja
165.192
149.823
145.698
141.133
139.180
136.567
131.196
130.406
128.415
127.686
123.918
123.599
117.848
77.311
77.000
76.681
45.982
21.741
180
160
140
120
100
80
60
40
20
ppm

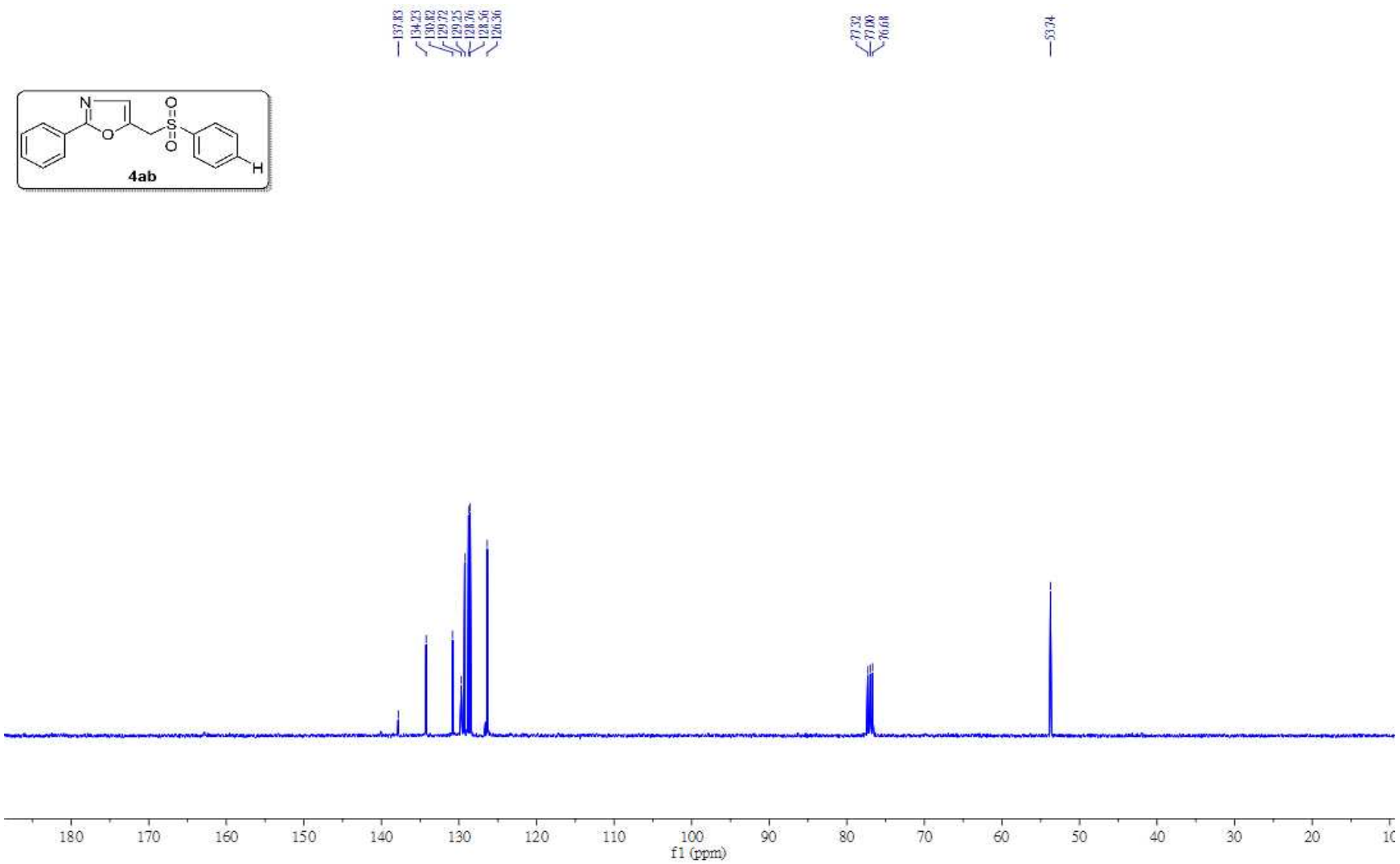

Solvent: CDCl3
Frequency: 400.40 MHz
4aa
f1 (ppm)

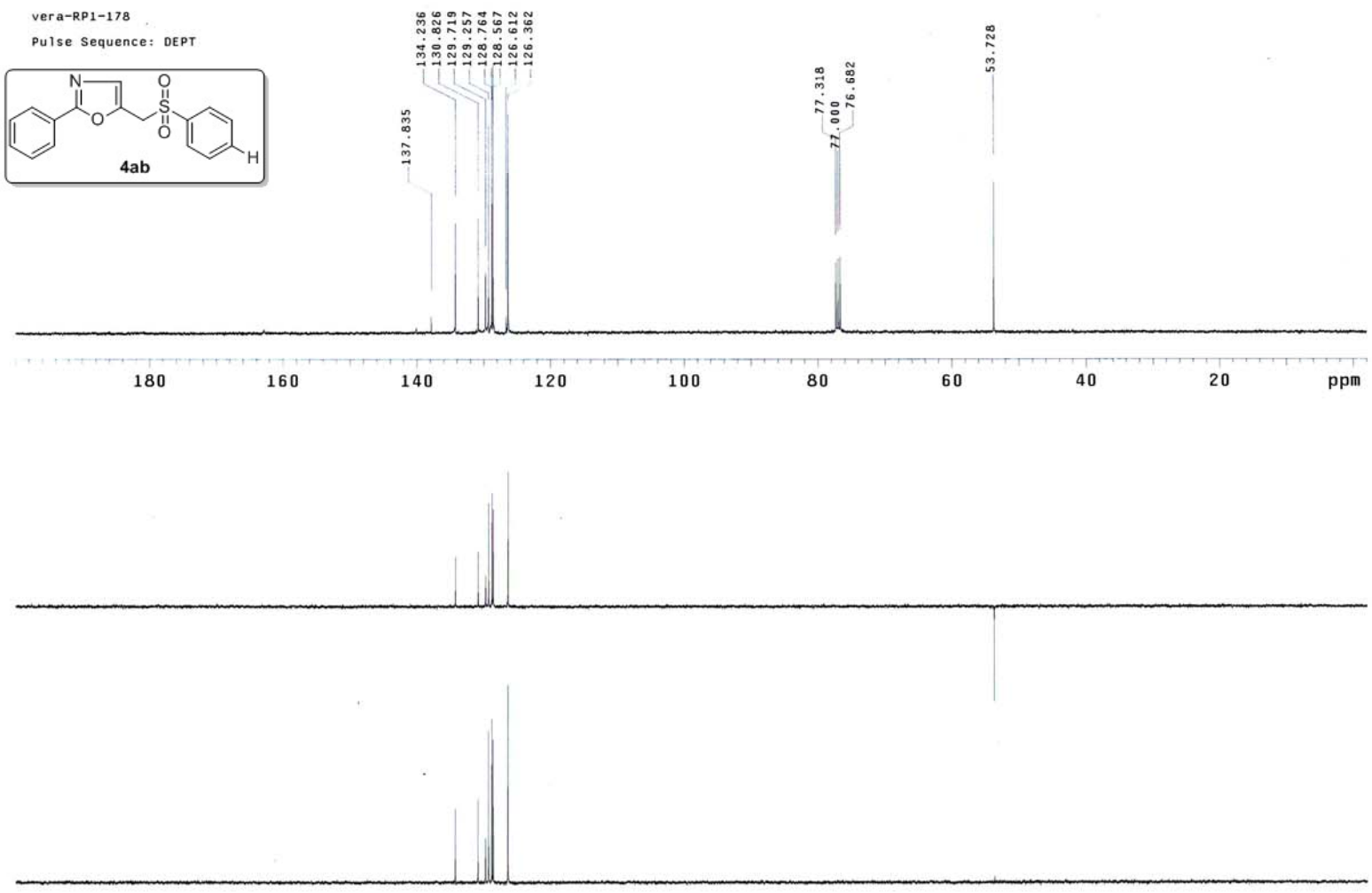

162.68
145.39
140.33
134.81
130.86
129.85
129.43
128.34
128.56
126.51
126.38
77.32
77.00
76.68
53.79
21.58
4aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

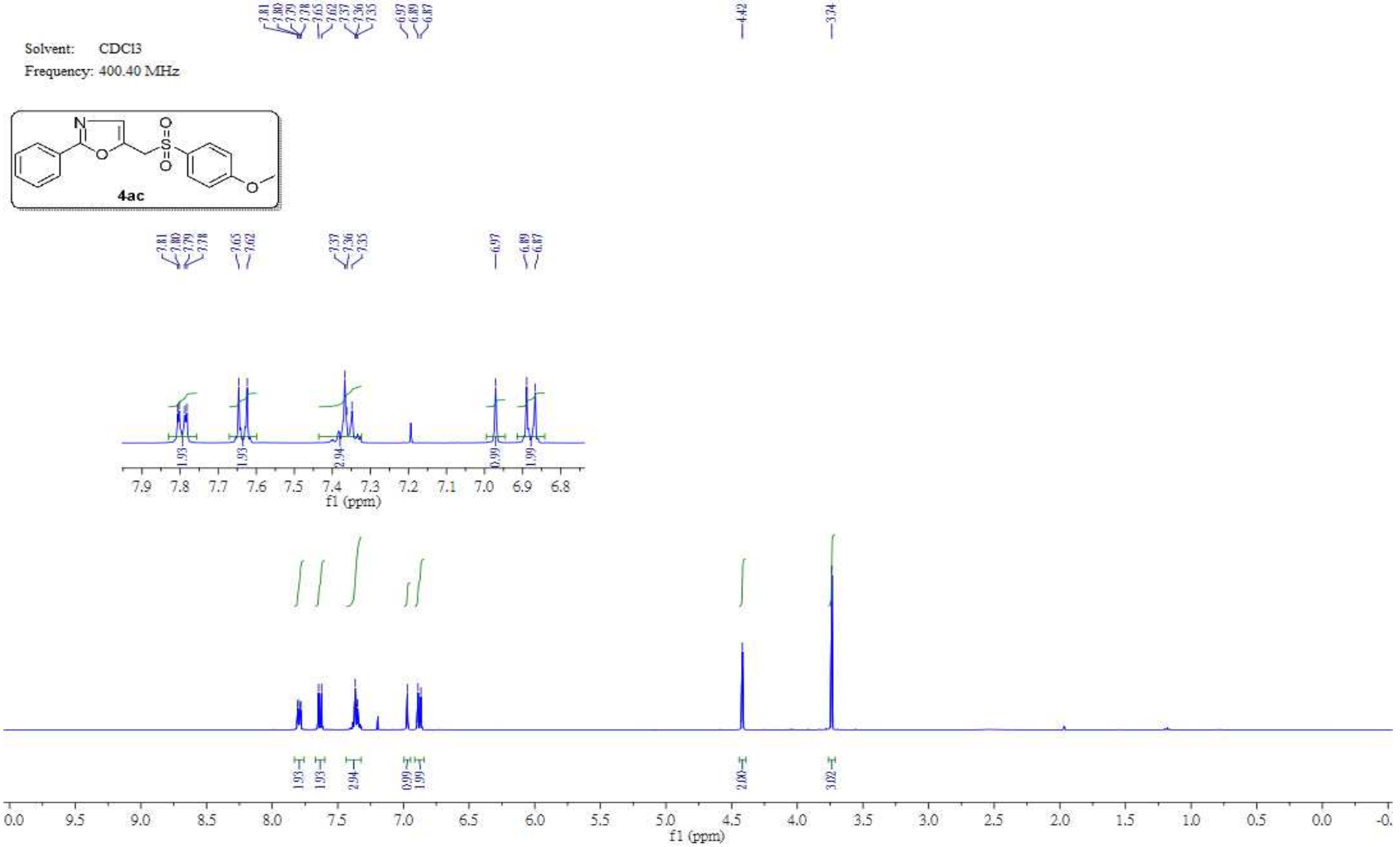

vera-RP1-166
Pulse Sequence: DEPT
4aa
145.398
140.336
134.819
130.863
129.863
129.439
128.742
128.567
126.514
126.385
77.318
77.000
76.682
53.781
21.576
180
160
140
120
100
80
60
40
20
ppm

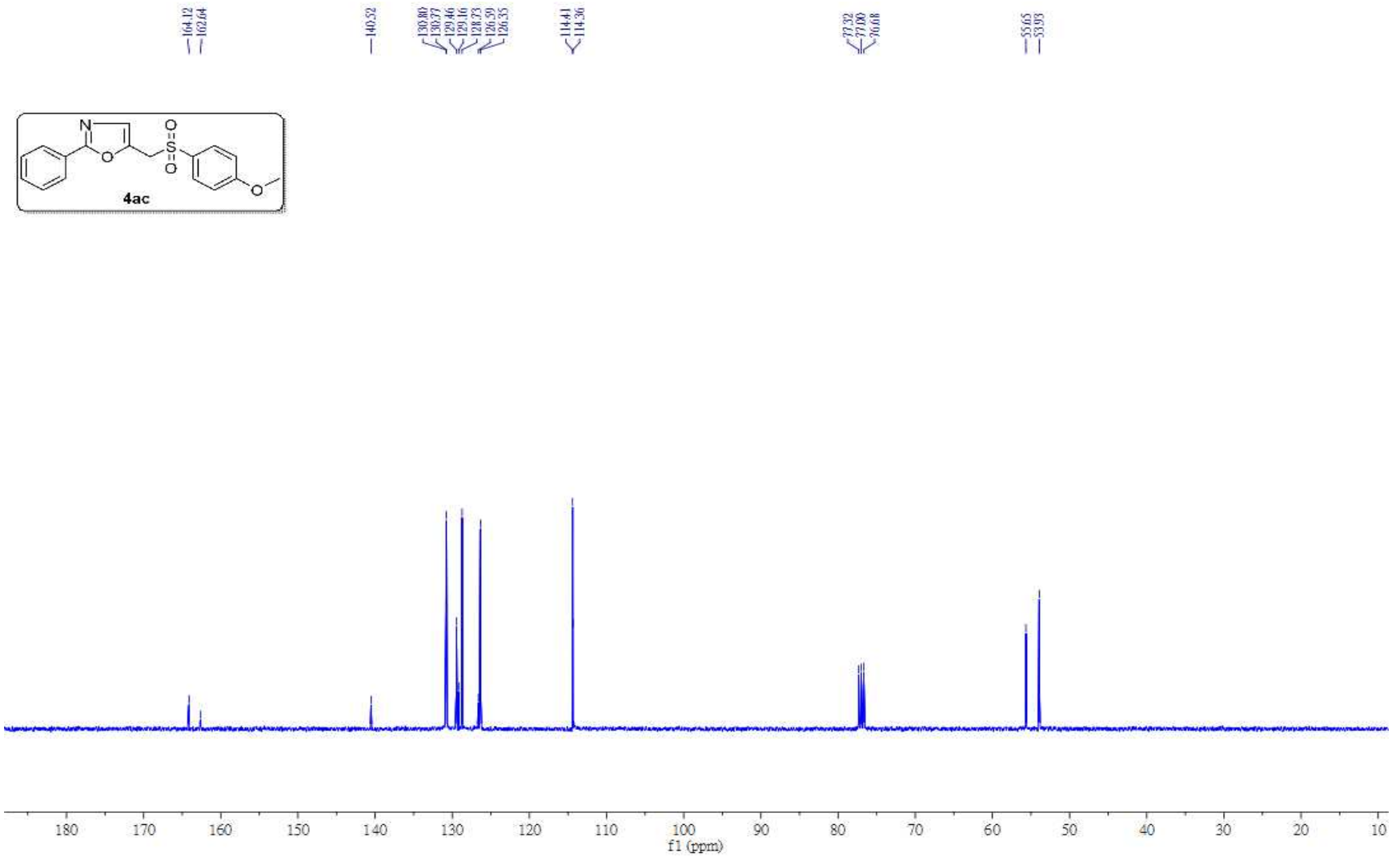

Solvent: CDCl3
Frequency: 400.40 MHz
4ab
f1 (ppm)

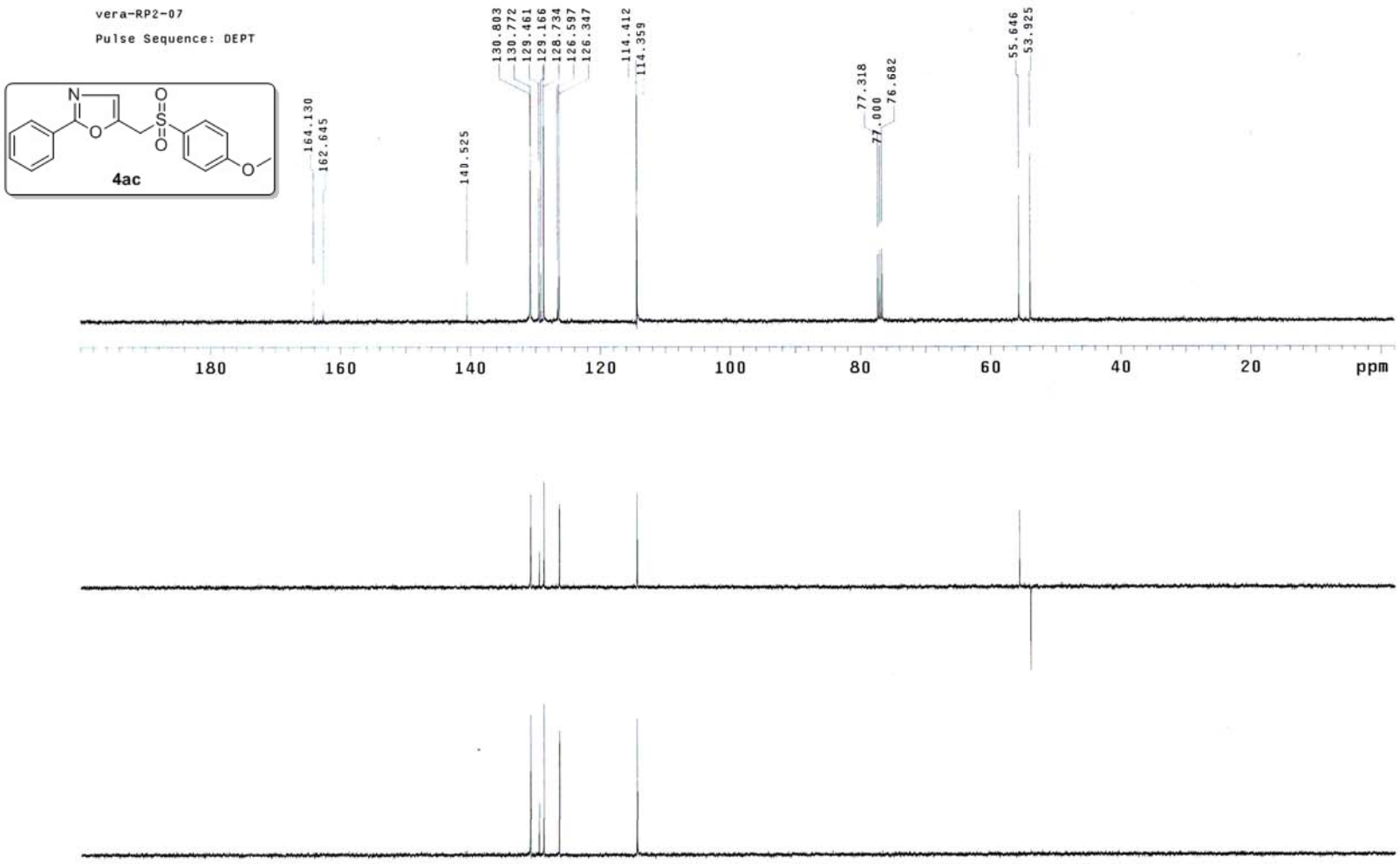
N
O
O
S
O
H
4ab

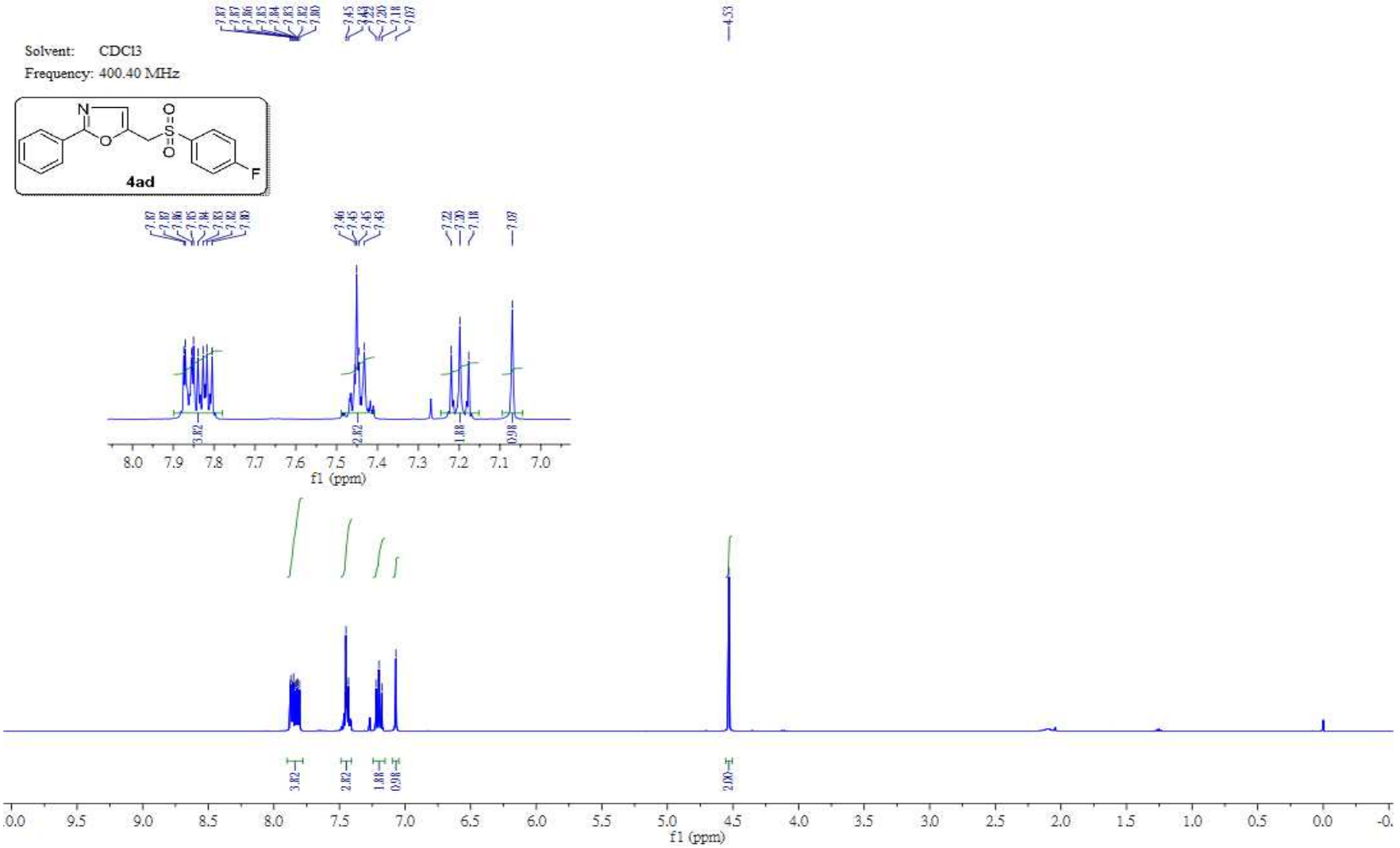

137.83
134.23
130.82
129.72
129.25
128.76
128.56
126.36
77.32
77.00
76.68
53.74
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

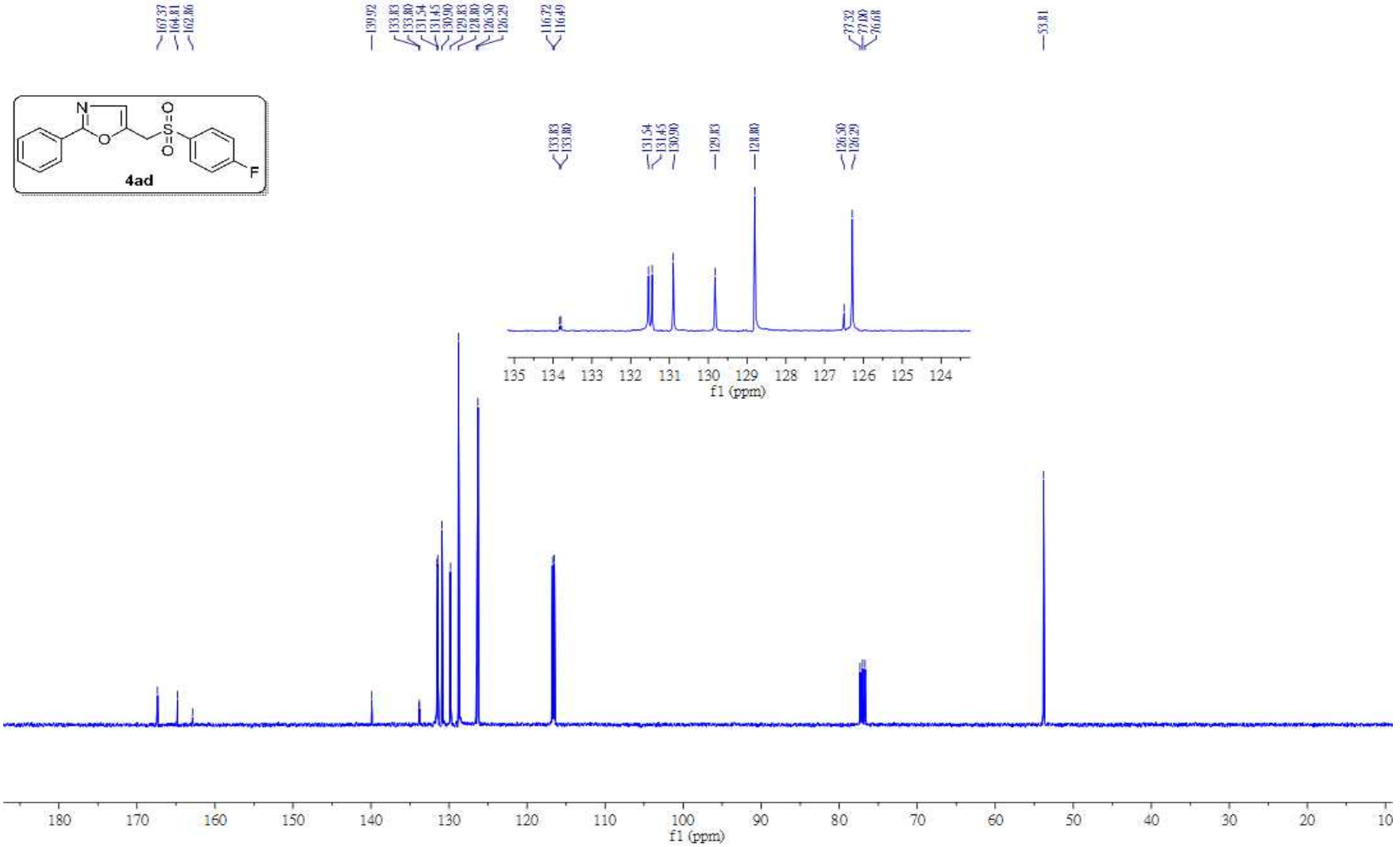

vera-RP1-178
Pulse Sequence: DEPT
4ab
137.835
134.236
130.826
129.719
129.257
128.764
128.567
126.612
126.362
77.318
77.000
76.682
53.728
180
160
140
120
100
80
60
40
20
ppm

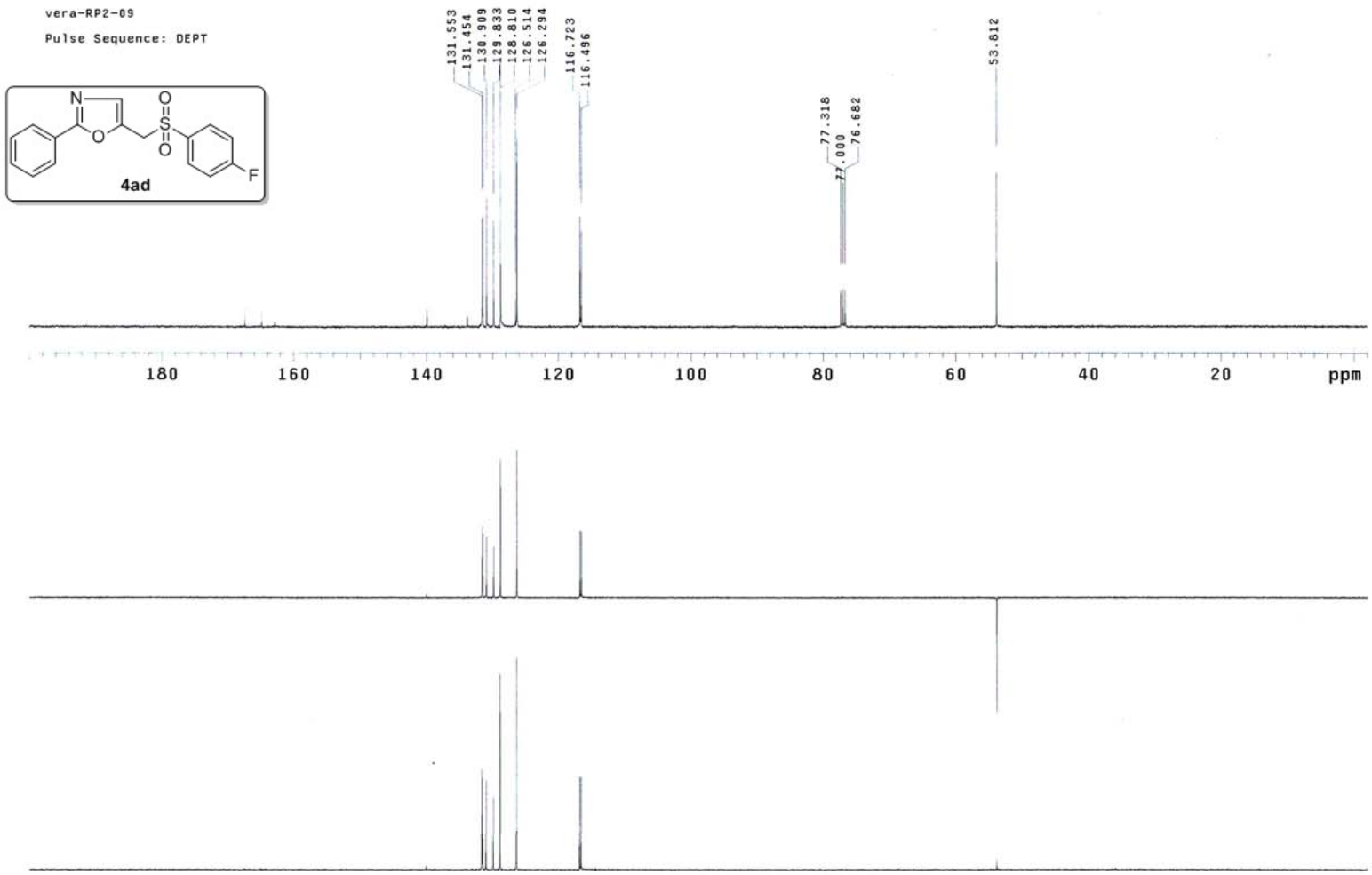

Solvent: CDCl3
Frequency: 400.40 MHz
4ac
f1 (ppm)

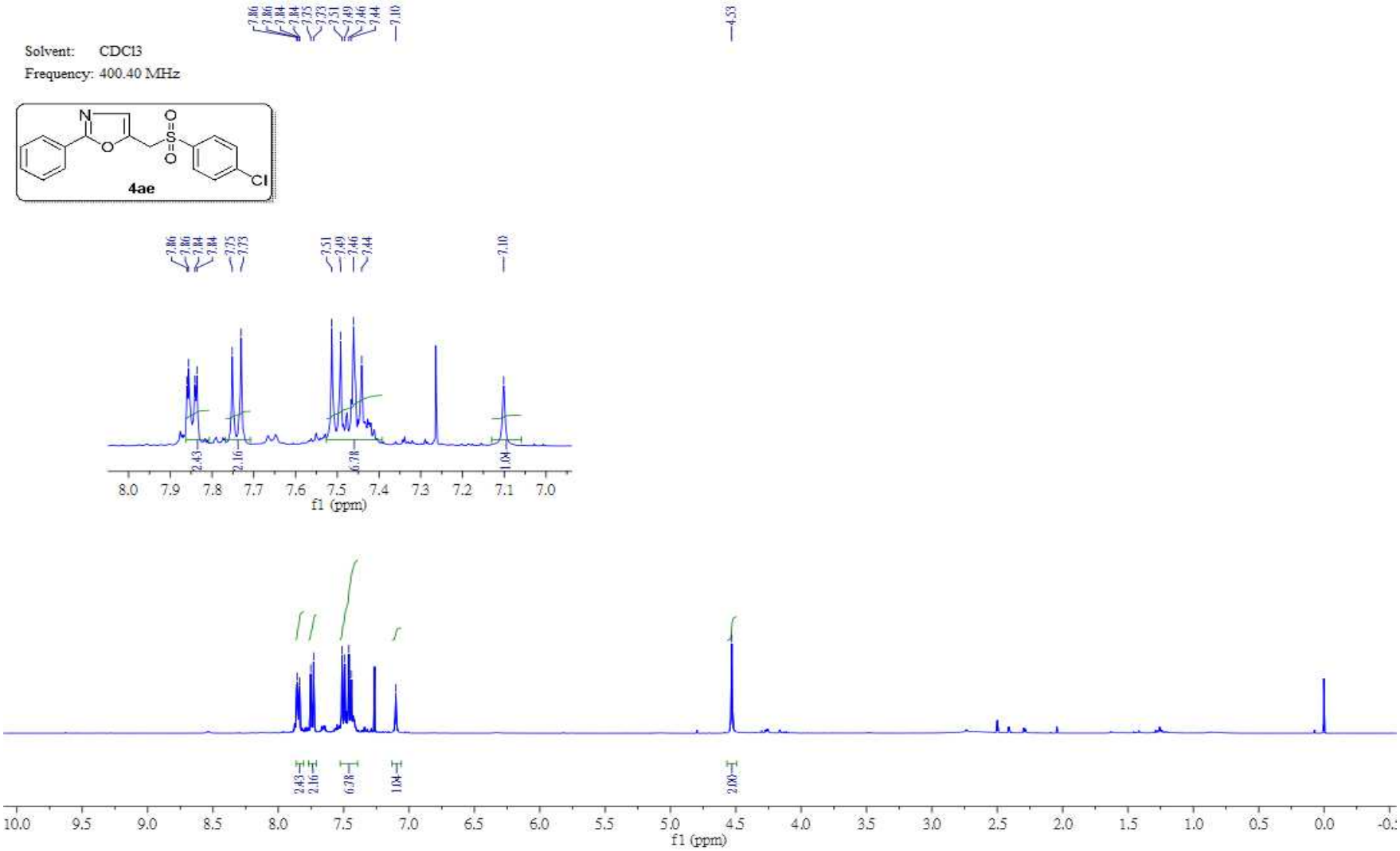

164.12
162.64
140.52
130.80
130.77
129.46
129.16
128.73
126.59
126.35
114.41
114.36
77.32
77.00
76.68
55.65
53.93
4ac
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

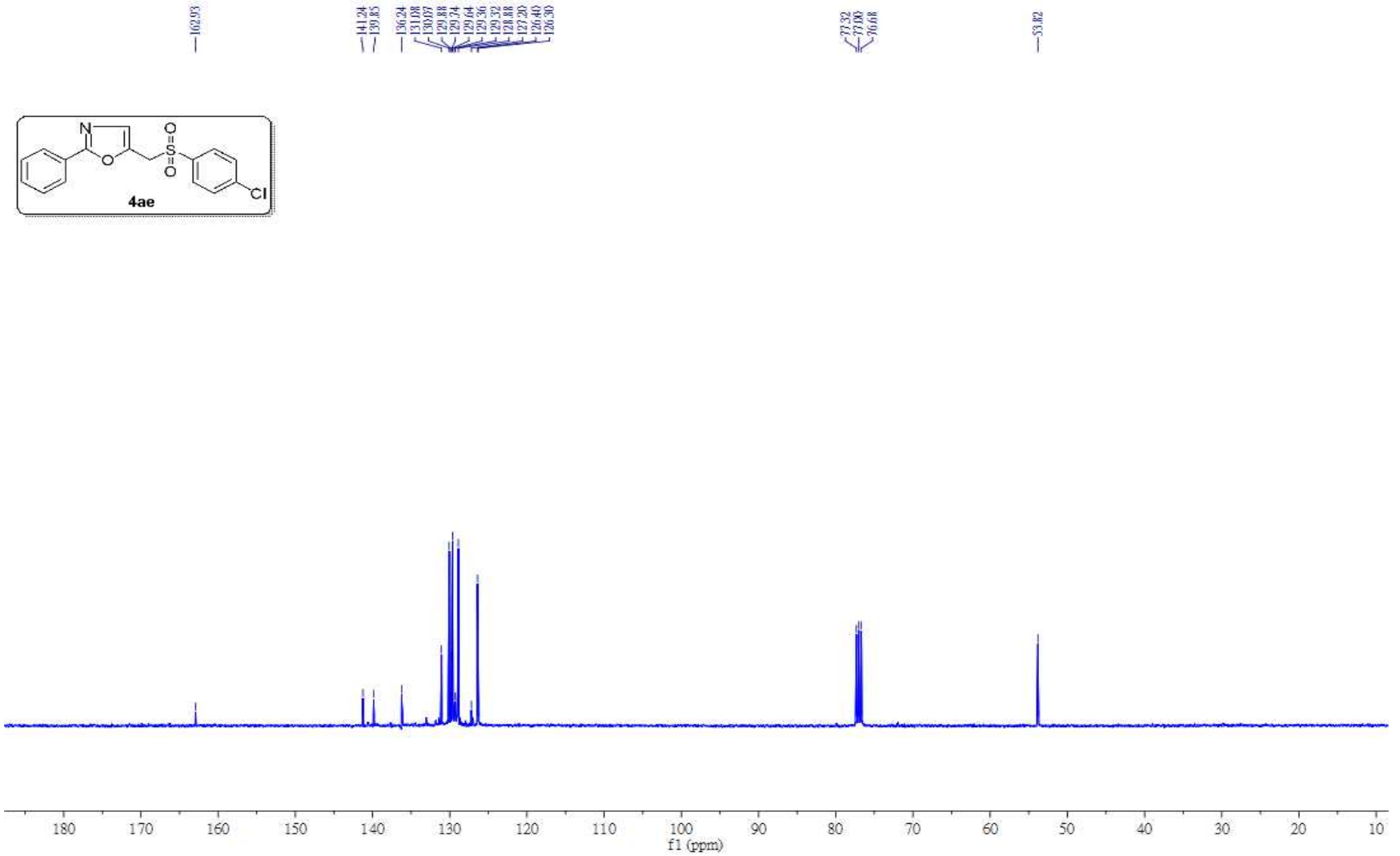

vera-RP2-07
Pulse Sequence: DEPT
4ac
164.130
162.645
140.525
130.803
130.772
129.461
129.166
128.734
126.597
126.347
114.412
114.359
77.318
77.000
76.682
55.646
53.925
180
160
140
120
100
80
60
40
20
ppm

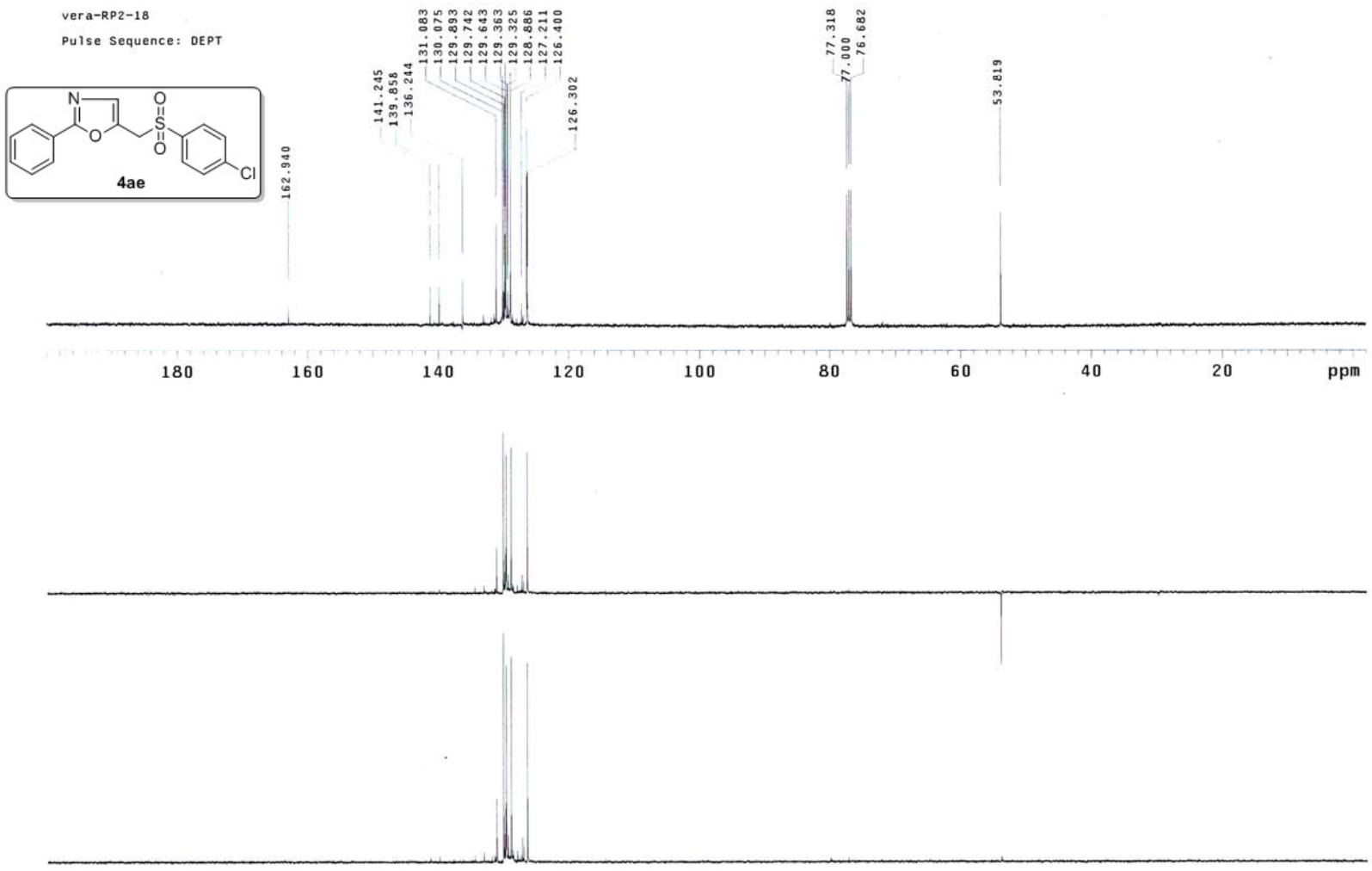

Solvent: CDCl3
Frequency: 400.40 MHz
4ad
f1 (ppm)

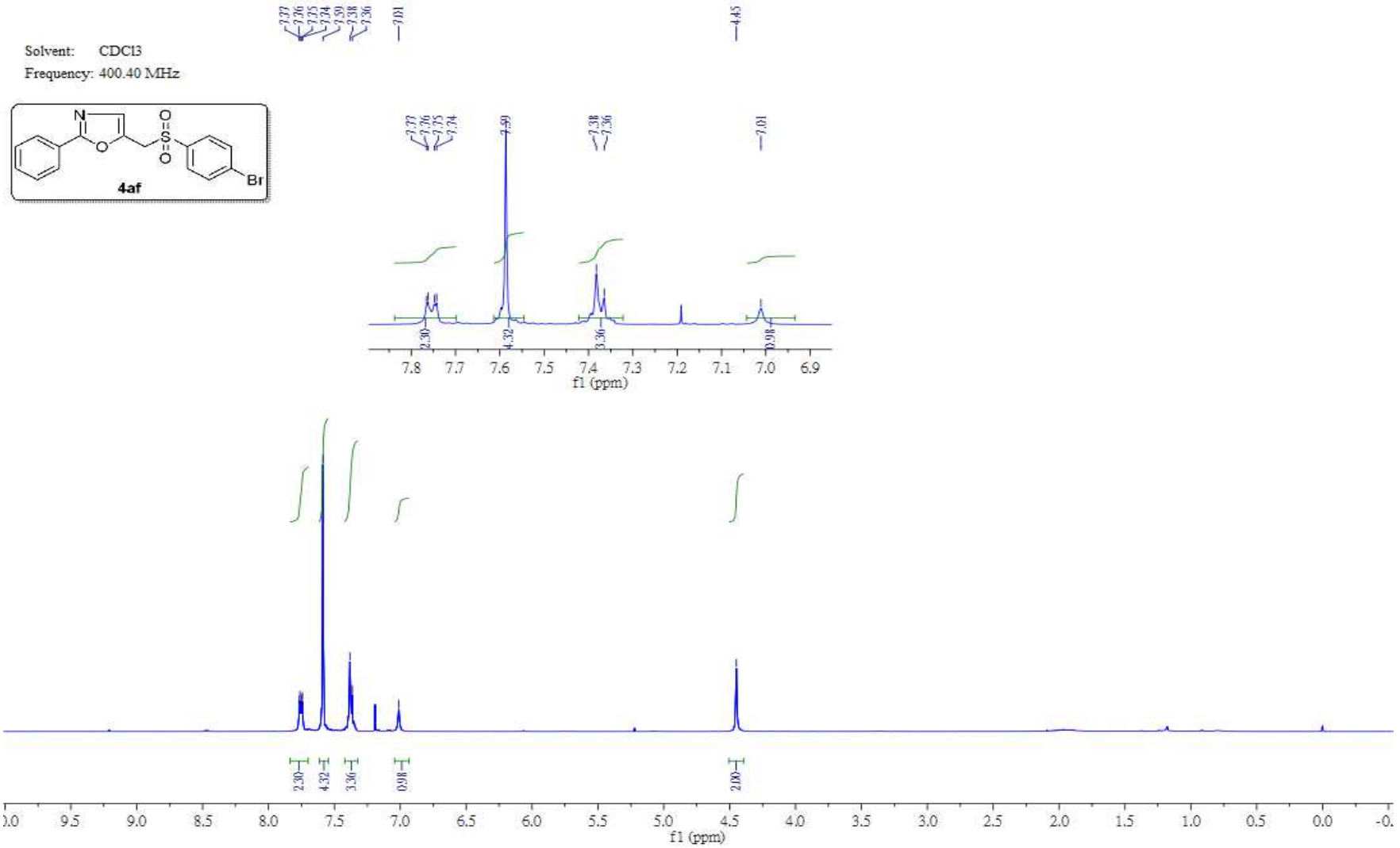

167.37
164.81
162.86
139.92
133.83
133.80
131.54
131.45
130.90
129.83
128.80
126.50
126.29
116.72
116.49
77.32
77.00
76.68
53.81
4ad
F
133.83
133.80
131.54
131.45
130.90
129.83
128.80
126.50
126.29
135 134 133 132 131 130 129 128 127 126 125 124
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


vera-RP2-09
Pulse Sequence: DEPT
4ad
131.553
131.454
130.909
129.833
128.810
126.514
126.294
116.723
116.496
77.318
77.000
76.682
53.812
180
160
140
120
100
80
60
40
20
ppm

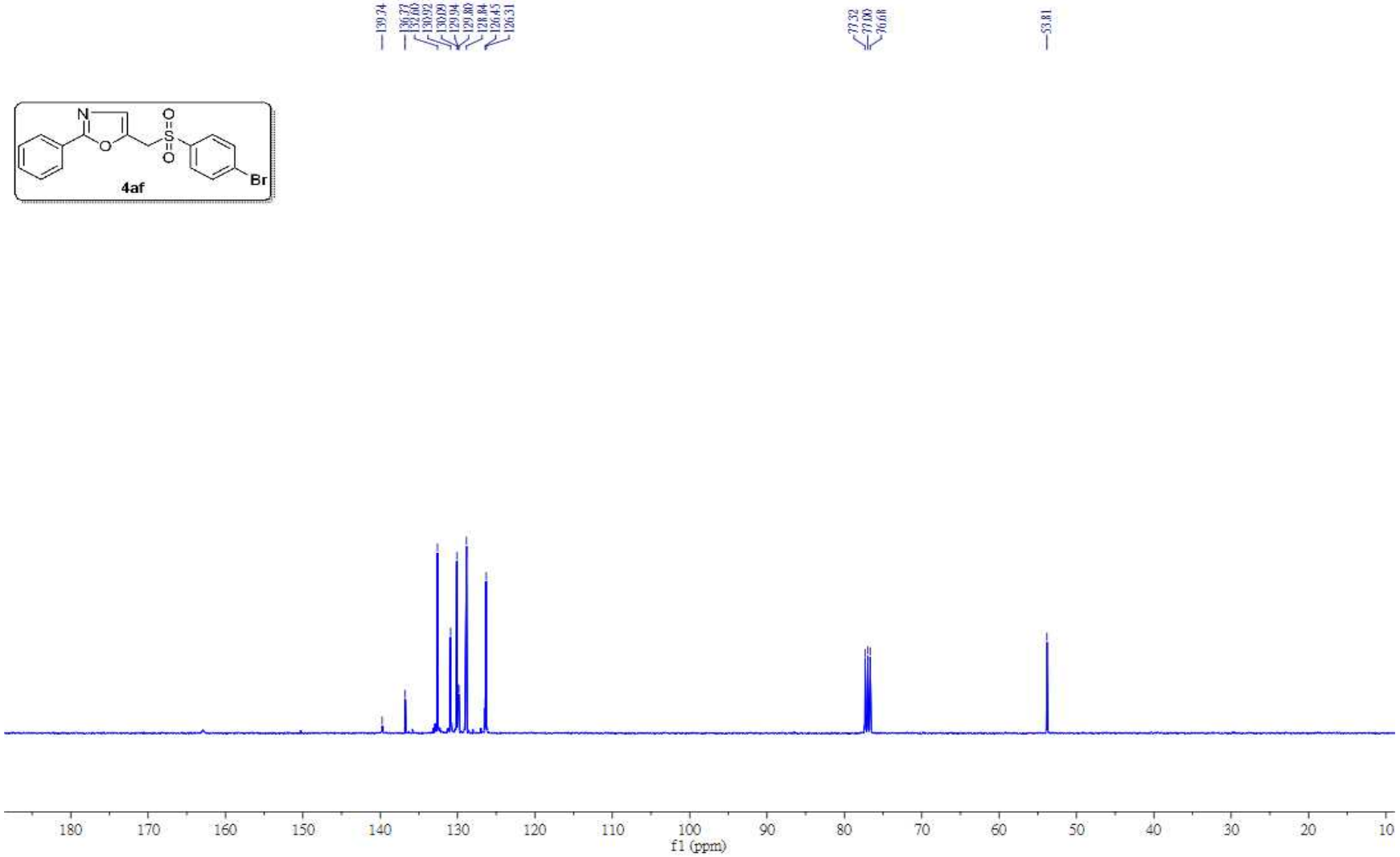

Solvent: CDCl3
Frequency: 400.40 MHz
4ae
f1 (ppm)
f1 (ppm)

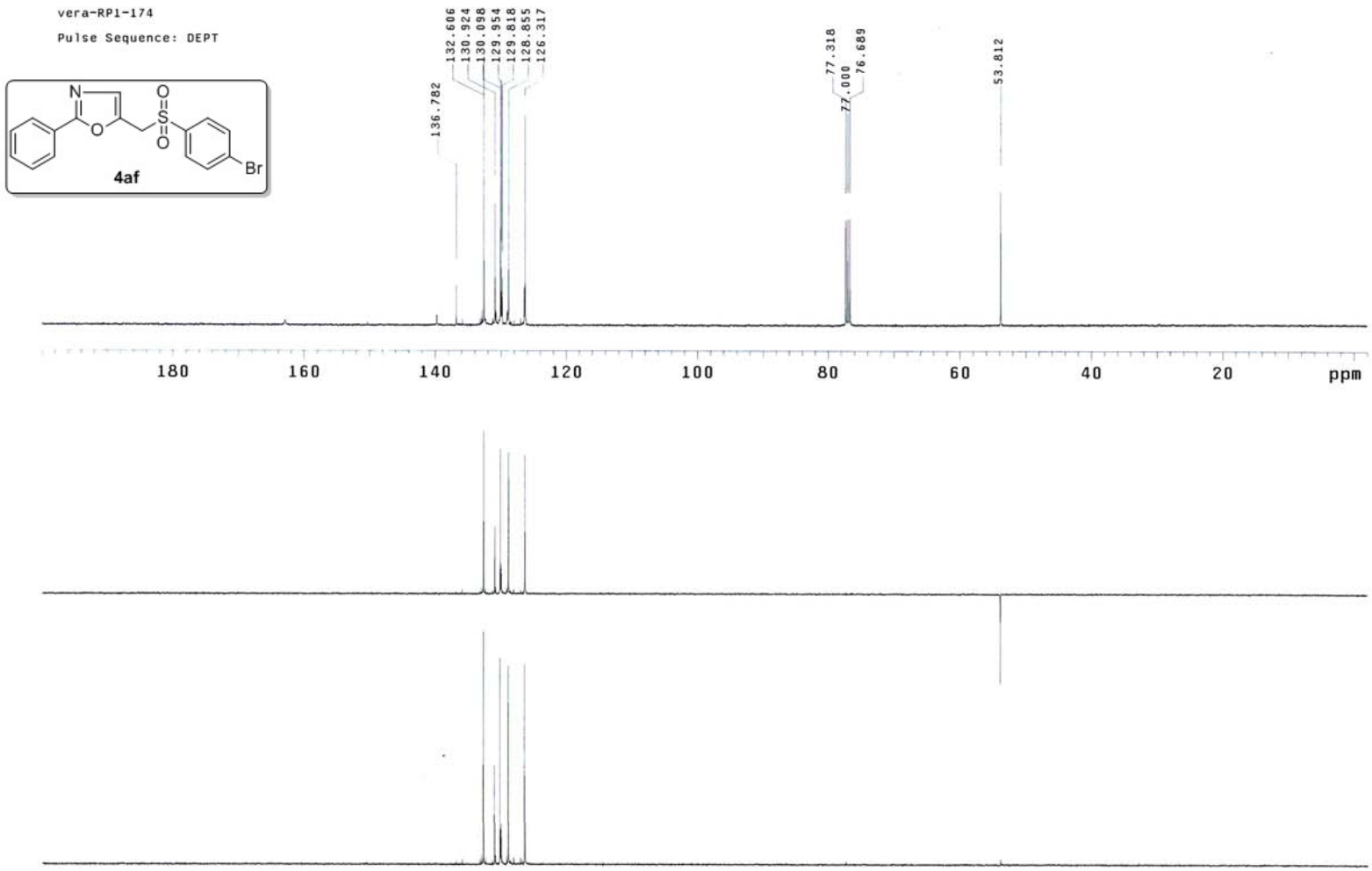

162.93
141.24
139.85
136.24
131.08
130.07
129.88
129.74
129.64
129.36
129.32
128.88
127.20
126.40
126.30
77.32
77.00
76.68
53.82
4ae
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

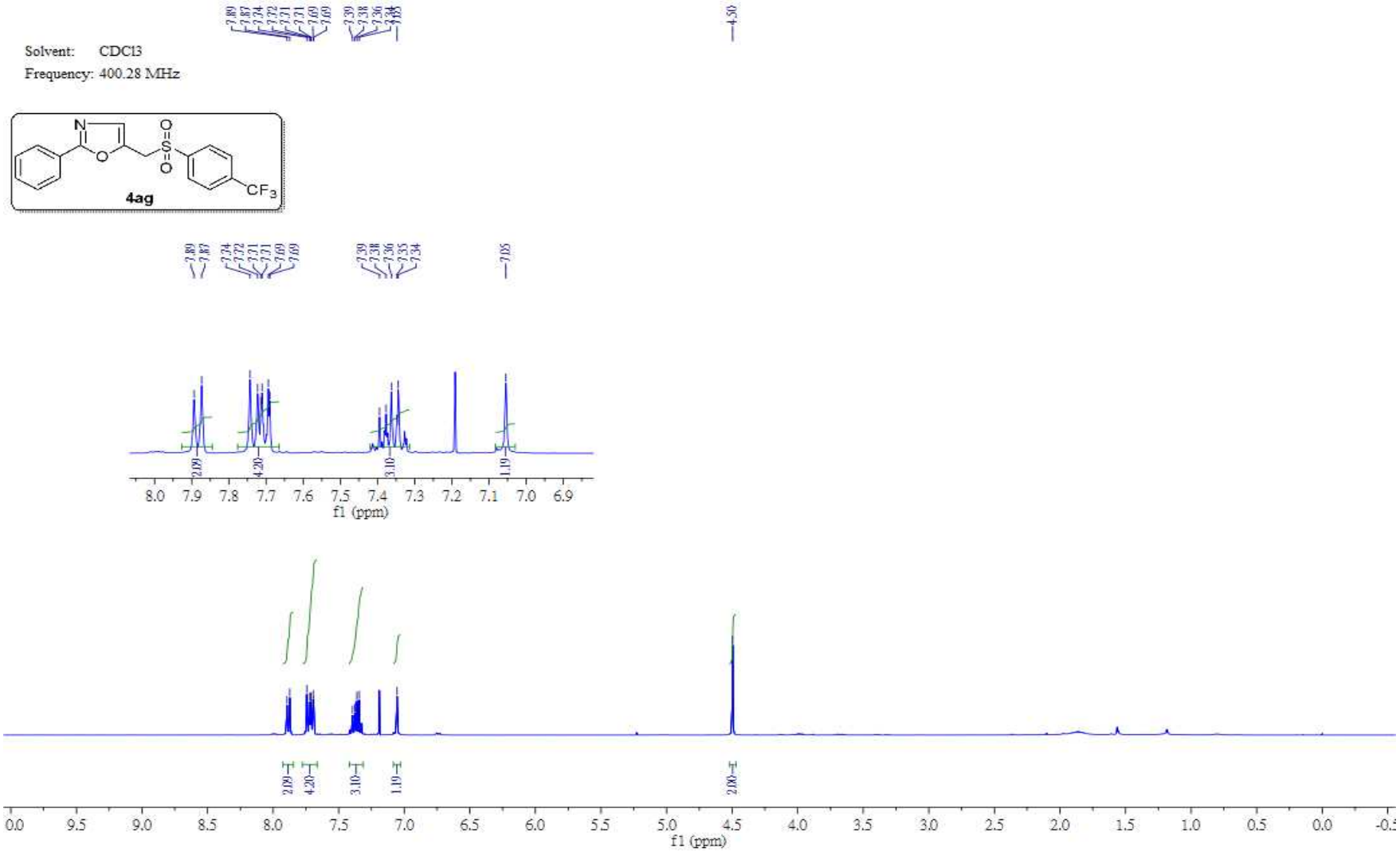

vera-RP2-18
Pulse Sequence: DEPT
4ae
162.940
141.245
139.858
136.244
131.083
130.075
129.893
129.742
129.643
129.363
129.325
128.886
127.211
126.400
126.302
77.318
77.000
76.682
53.819
180
160
140
120
100
80
60
40
20
ppm

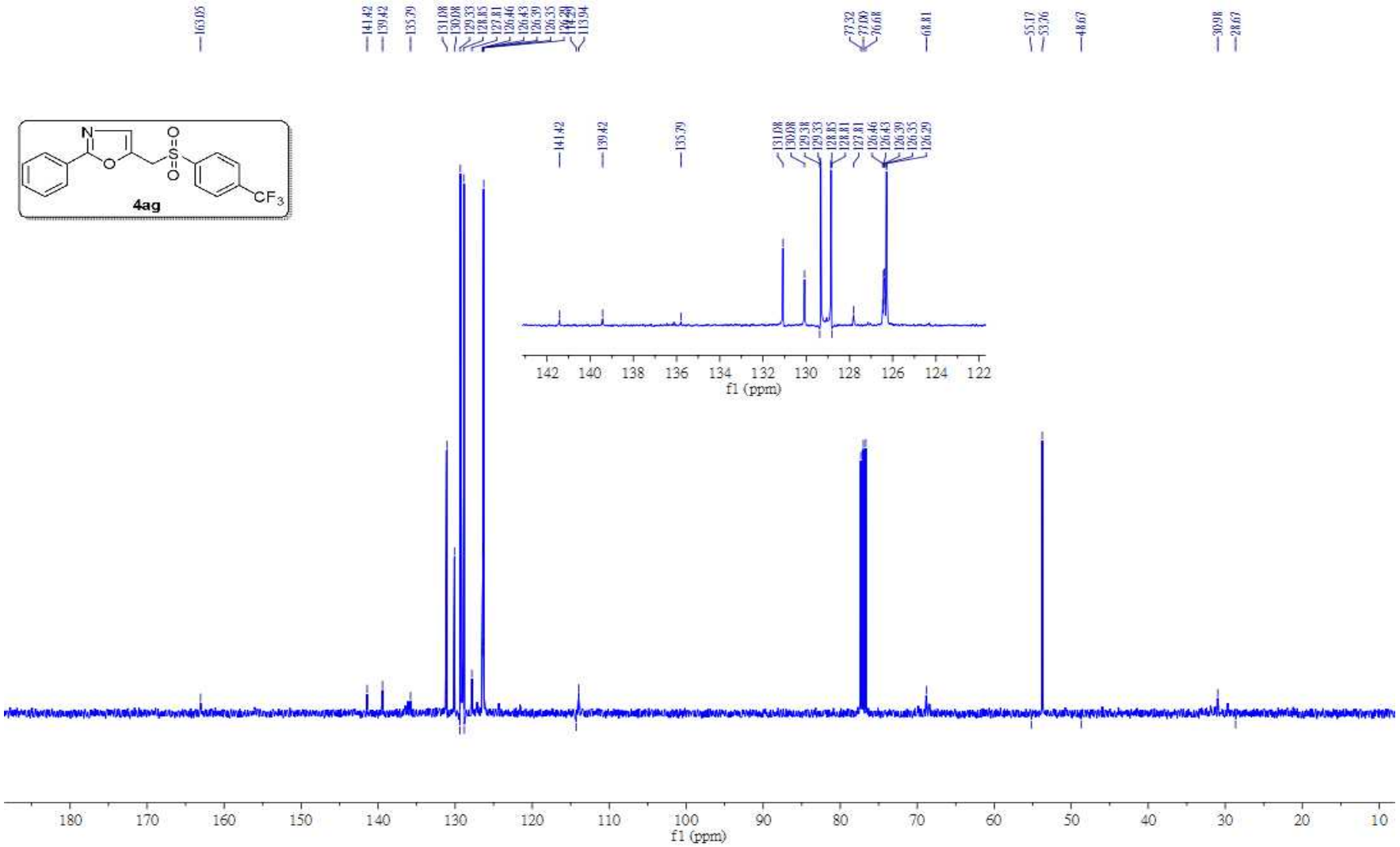

Solvent: CDCl3
Frequency: 400.40 MHz
4af
Br
f1 (ppm)

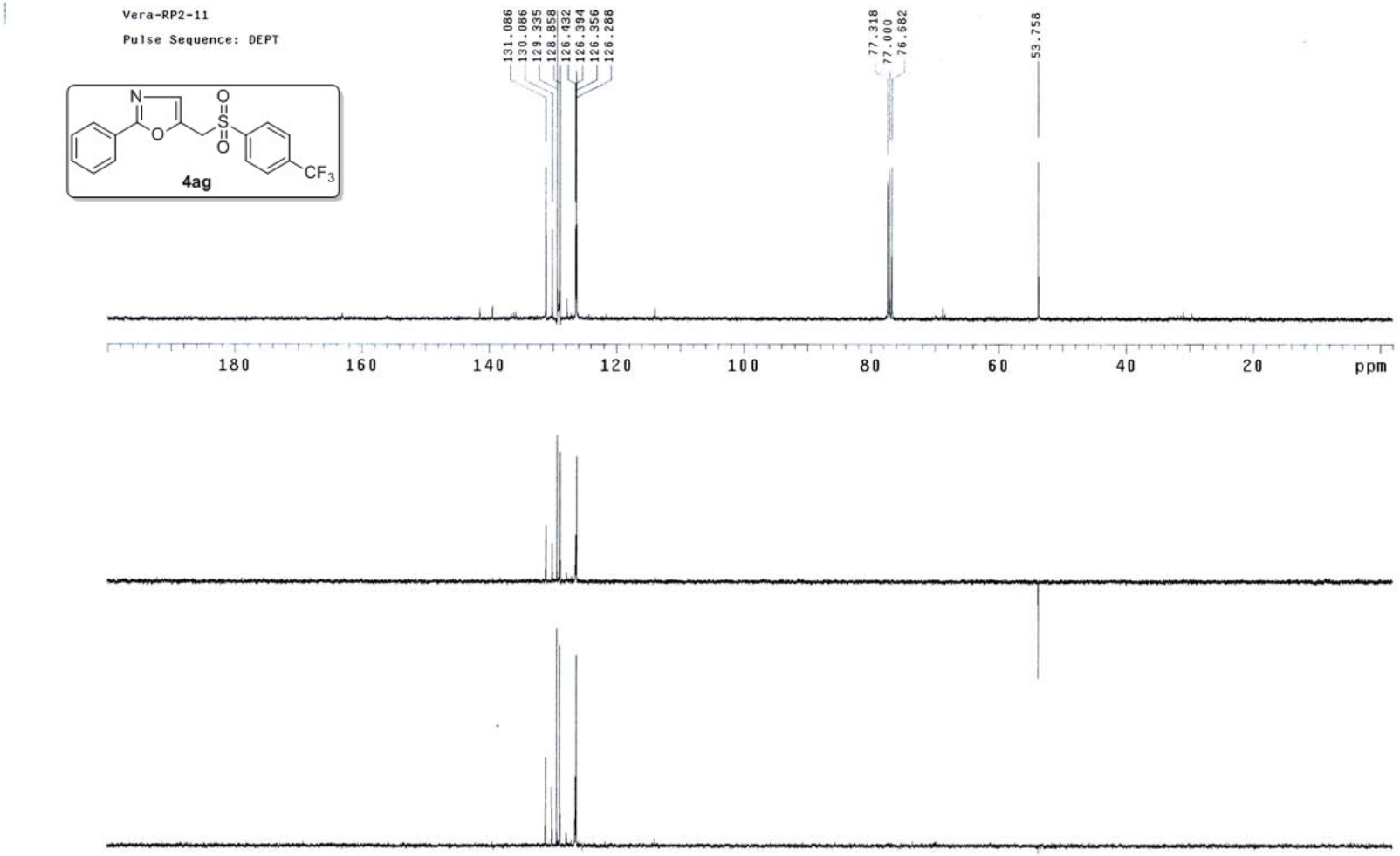
N
O
O
S
O
Br
4af

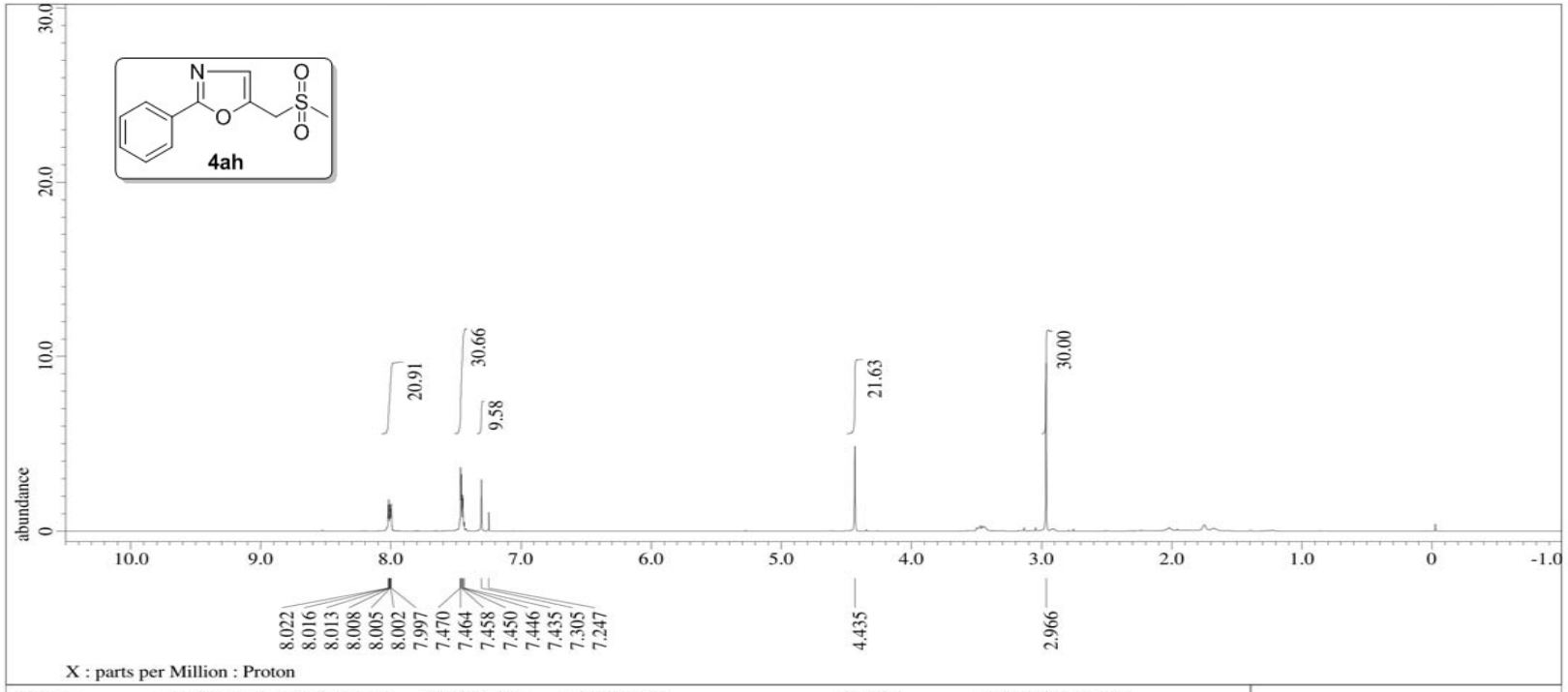

139.74
136.27
132.66
130.92
130.09
129.94
129.80
128.84
126.45
126.31
77.32
77.00
76.68
53.81
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


vera-RP1-174
Pulse Sequence: DEPT
4af
Br
136.782
132.606
130.924
130.098
129.954
129.818
128.855
126.317
77.318
77.000
76.689
53.812
180
160
140
120
100
80
60
40
20
ppm

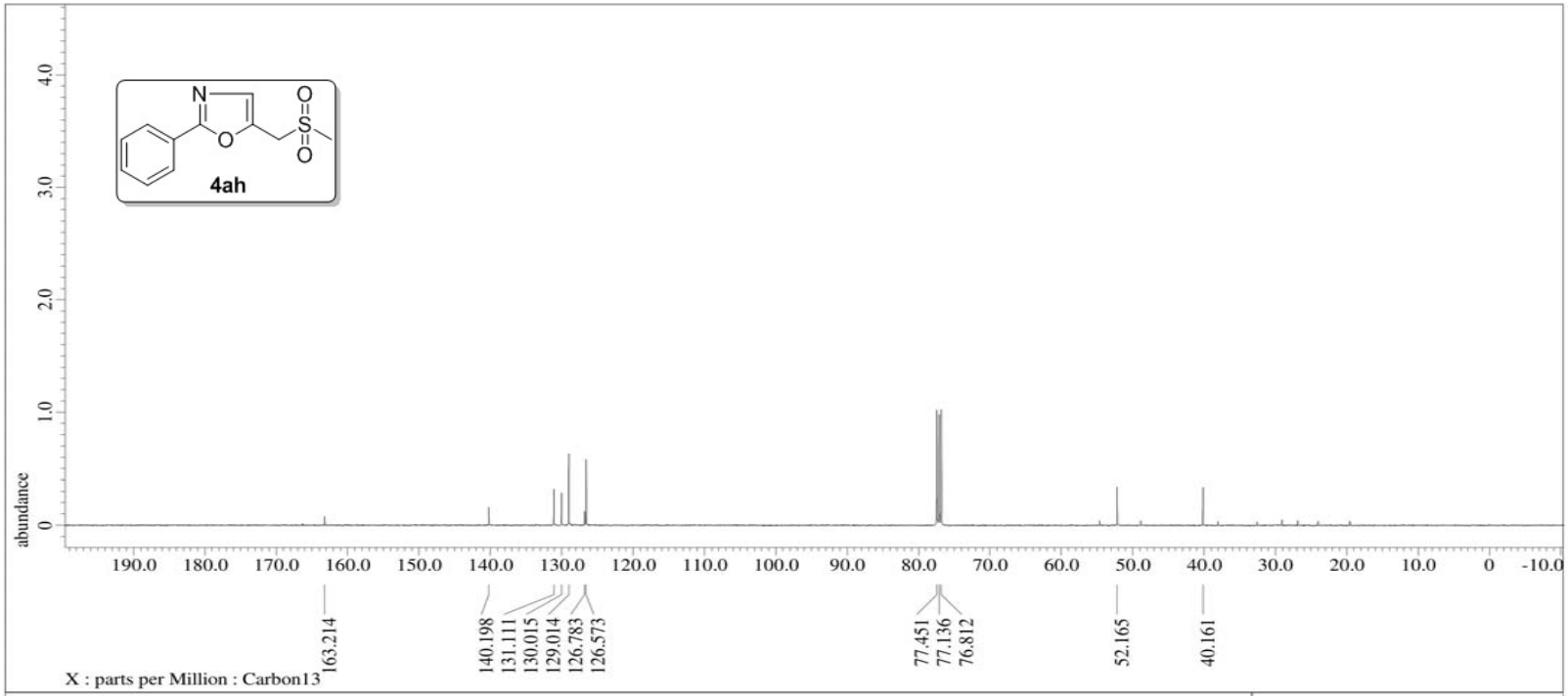

Solvent: CDCl3
Frequency: 400.28 MHz
4ag
f1 (ppm)
f1 (ppm)


163.05
141.42
139.42
135.79
131.08
130.88
129.33
128.85
127.81
126.46
126.43
126.39
126.35
126.29
77.32
77.00
76.68
68.81
55.17
53.76
48.67
30.98
28.67
4ag
CF3
f1 (ppm)
f1 (ppm)

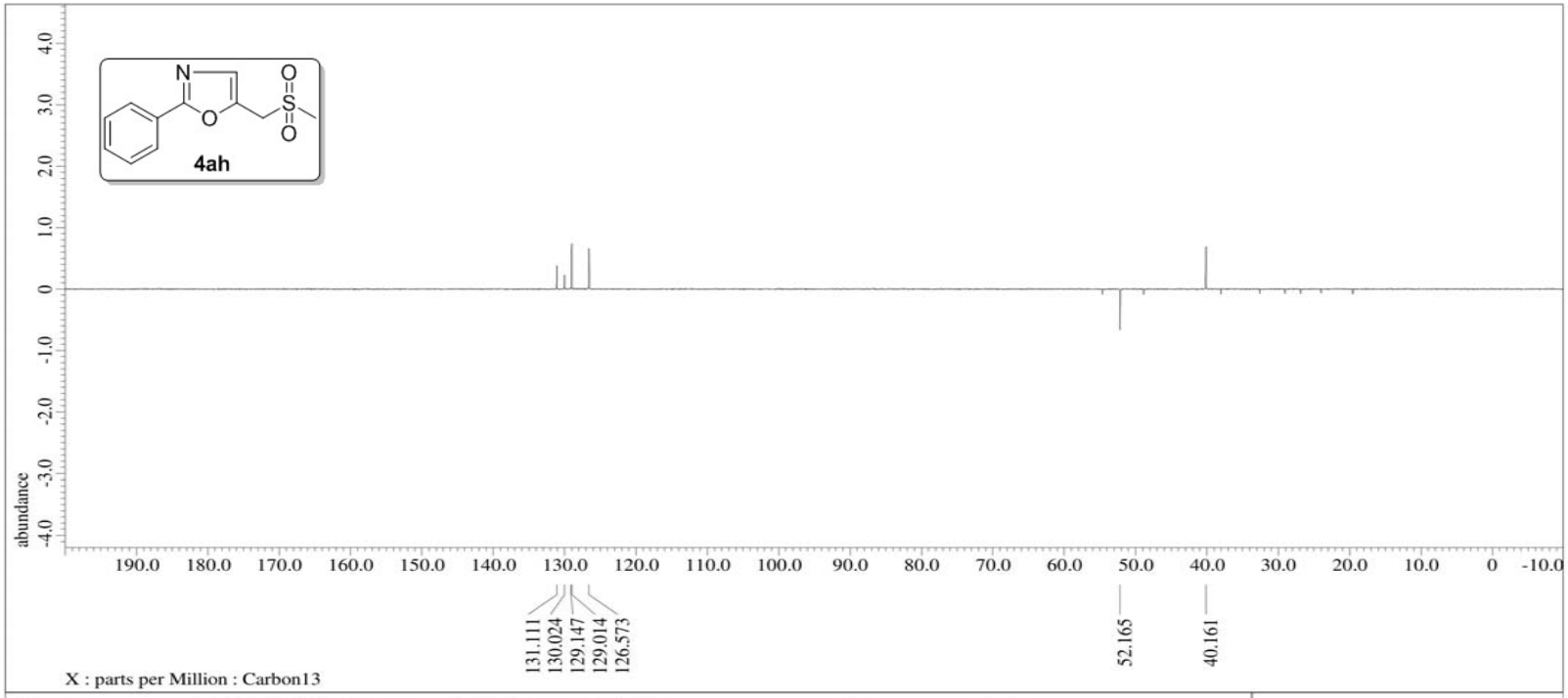

Vera-RP2-11
Pulse Sequence: DEPT
4ag
131.086
130.086
129.335
128.858
126.432
126.394
126.356
126.288
77.318
77.000
76.682
53.758
180
160
140
120
100
80
60
40
20
ppm



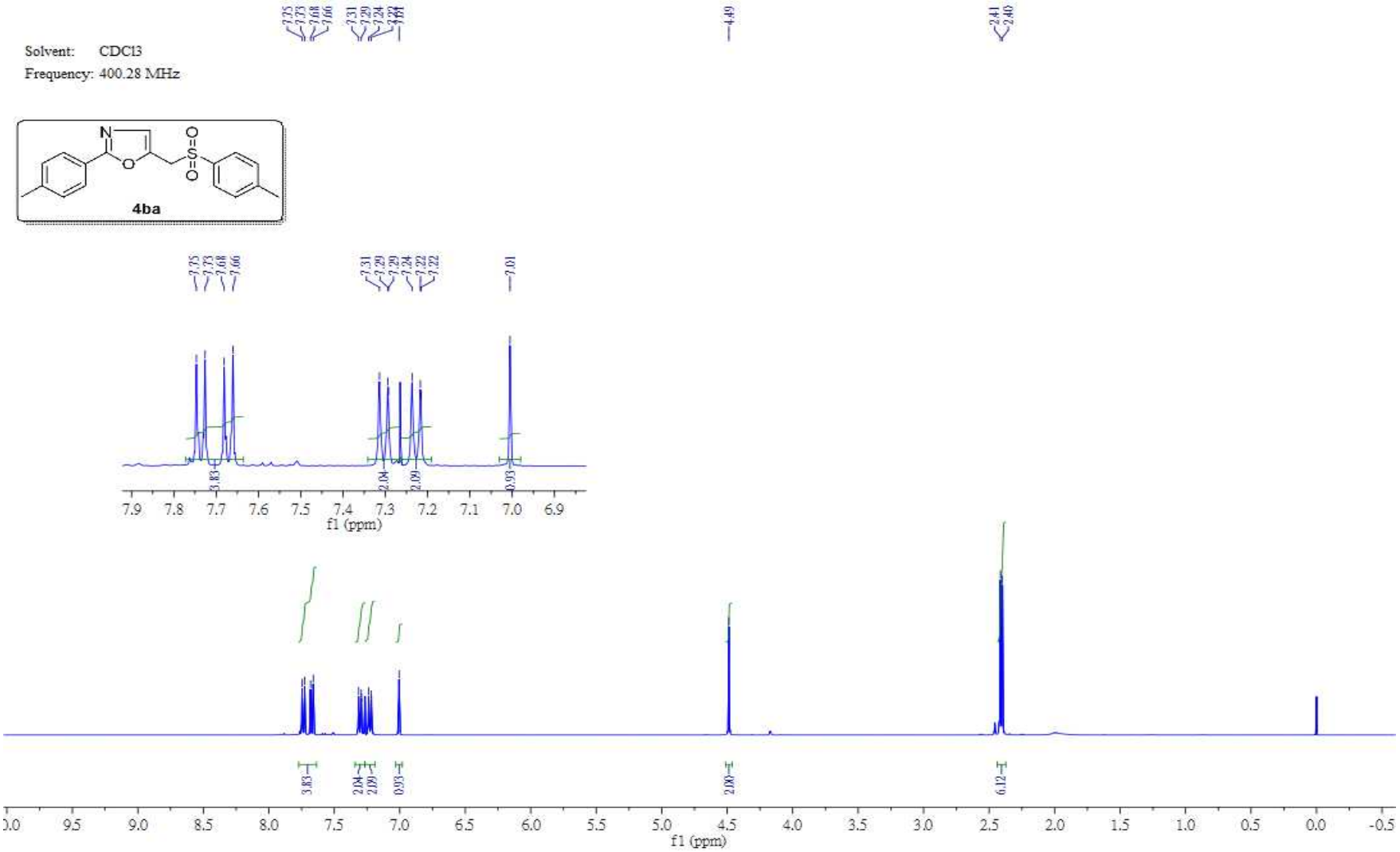
Filename	= VERA-RP3-155_Proton-1-8.jd	Spectrometer	= DELTA2_NMR	Tri_Freq	= 399.78219838[MHz]
Author	= delta			Tri_Offset	= 5[ppm]
Experiment	= proton.jxp	Field_Strength	= 9.389766[T] (400[MHz])	Clipped	= FALSE
Sample_Id	= VERA-RP3-155	X_Acq_Duration	= 2.18365952[s]	Scans	= 24
Solvent	= CHLOROFORM-D	X_Domain	= 1H	Total_Scans	= 24
Creation_Time	= 31-JUL-2016 14:58:11	X_Freq	= 399.78219838[MHz]		
Revision_Time	= 8-AUG-2016 21:43:04	X_Offset	= 5[ppm]	Relaxation_Delay	= 5[s]
Current_Time	= 8-AUG-2016 21:43:55	X_Points	= 16384	Recvr_Gain	= 38
		X_Prescans	= 1	Temp_Get	= 24.8[dC]
Comment	= single_pulse	X_Resolution	= 0.45794685[Hz]	X_90_Width	= 12.795[us]
Data_Format	= 1D COMPLEX	X_Sweep	= 7.5030012[kHz]	X_Acq_Time	= 2.18365952[s]
Dim_Size	= 13107	X_Sweep_Clipped	= 6.00240096[kHz]	X_Angle	= 45[deg]
Dim_Title	= Proton	Irr_Domain	= Proton	X_Atn	= 2.4[dB]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	X_Pulse	= 6.3975[us]
Dimensions	= X	Irr_Offset	= 5[ppm]	Irr_Mode	= Off
Site	= JNM-ECS400	Tri_Domain	= Proton	Tri_Mode	= Off

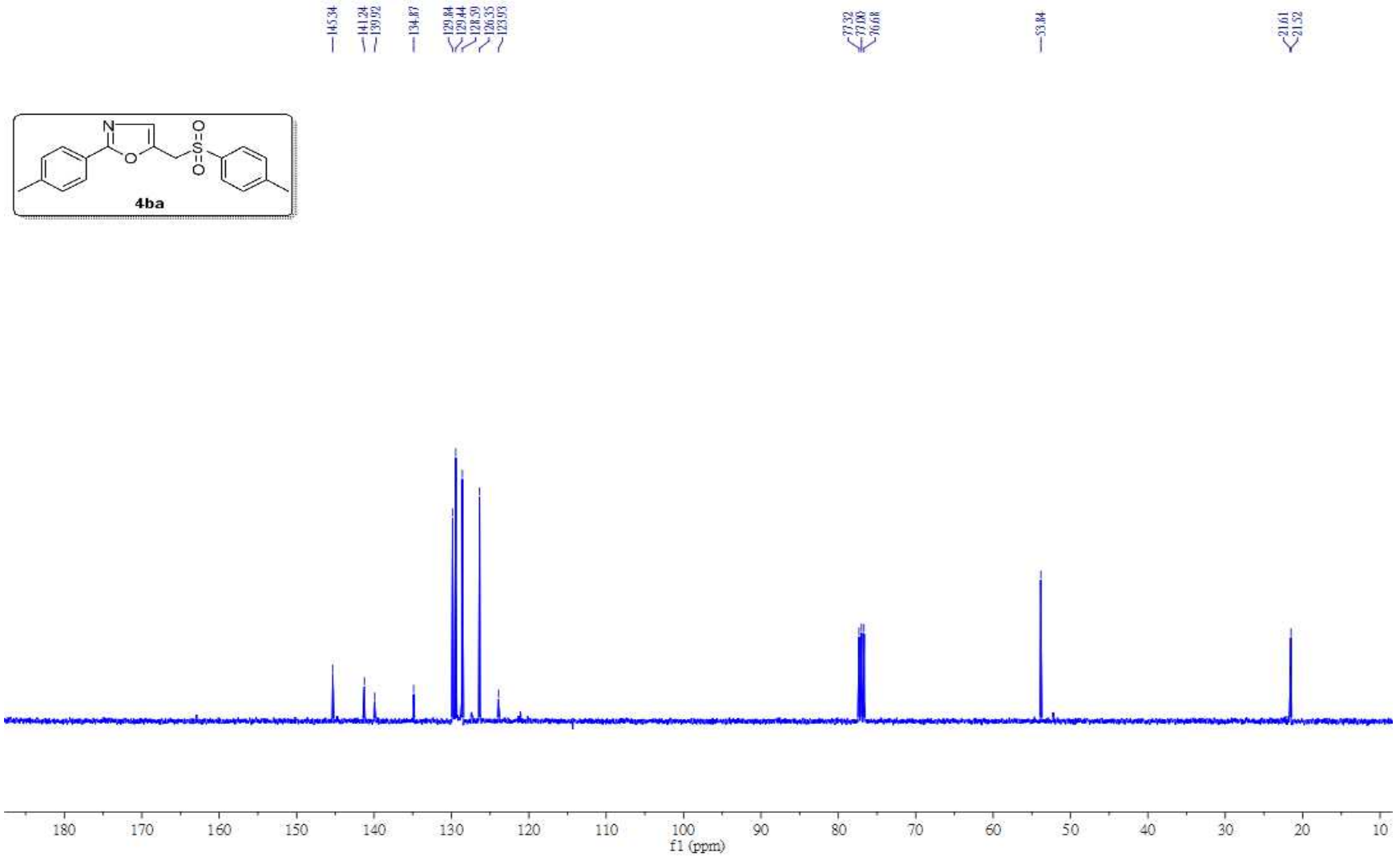


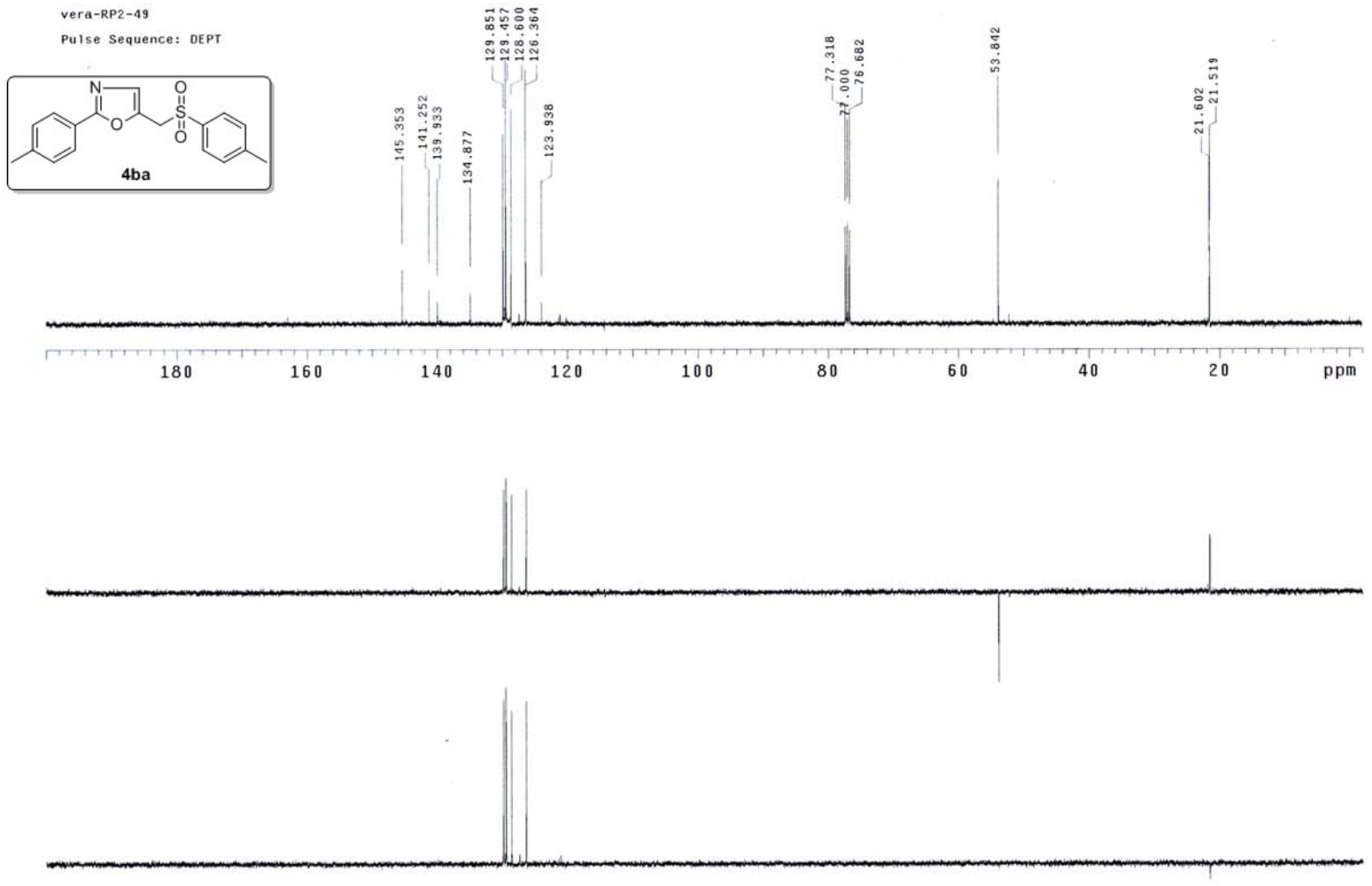
Filename	= VERA-RP3-155_Carbon-1-3.jd	Spectrometer	= DELTA2_NMR	Scans	= 1024
Author	= delta			Total_Scans	= 1024
Experiment	= carbon.jxp	Field_Strength	= 9.389766[T] (400[MHz])		
Sample_Id	= VERA-RP3-155	X_Acq_Duration	= 1.04333312[s]	Relaxation_Delay	= 2[s]
Solvent	= CHLOROFORM-D	X_Domain	= 13C	Recvr_Gain	= 60
Creation_Time	= 31-JUL-2016 15:03:16	X_Freq	= 100.52530333[MHz]	Temp_Get	= 24.9[dC]
Revision_Time	= 8-AUG-2016 21:48:24	X_Offset	= 100[ppm]	X_90_Width	= 10.33[us]
Current_Time	= 8-AUG-2016 21:49:02	X_Points	= 32768	X_Acq_Time	= 1.04333312[s]
		X_Prescans	= 4	X_Angle	= 30[deg]
Comment	= single pulse decoupled gat	X_Resolution	= 0.95846665[Hz]	X_Atn	= 5.3[dB]
Data_Format	= 1D COMPLEX	X_Sweep	= 31.40703518[kHz]	X_Pulse	= 3.44333333[us]
Dim_Size	= 26214	X_Sweep_Clipped	= 25.12562814[kHz]	Irr_Atn_Dec	= 21.473[dB]
Dim_Title	= Carbon13	Irr_Domain	= Proton	Irr_Atn_Noe	= 21.473[dB]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	Irr_Noise	= WALTZ
Dimensions	= X	Irr_Offset	= 5[ppm]	Irr_Pwidth	= 0.115[ms]
Site	= JNM-ECS400	Clipped	= FALSE	Decoupling	= TRUE

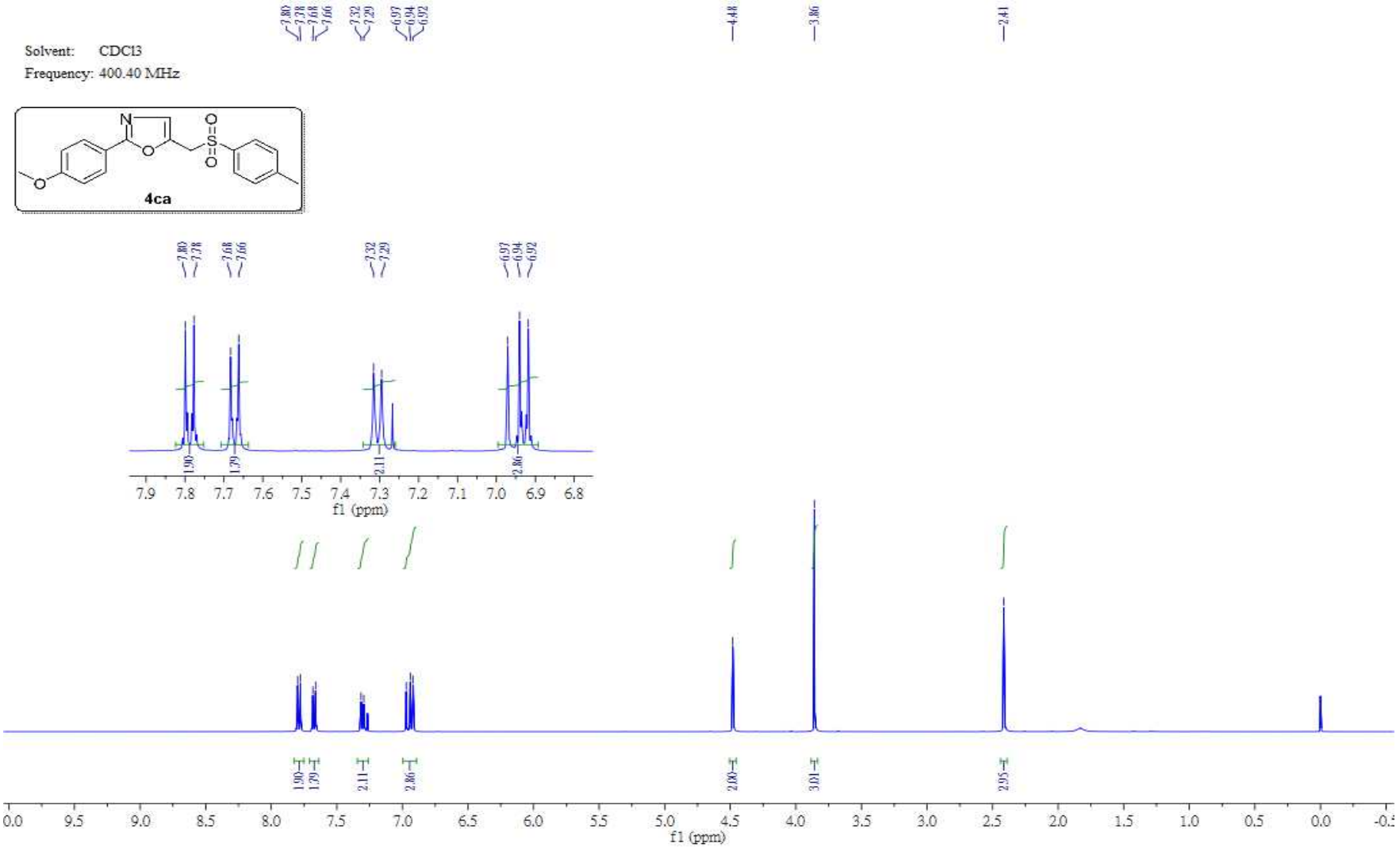


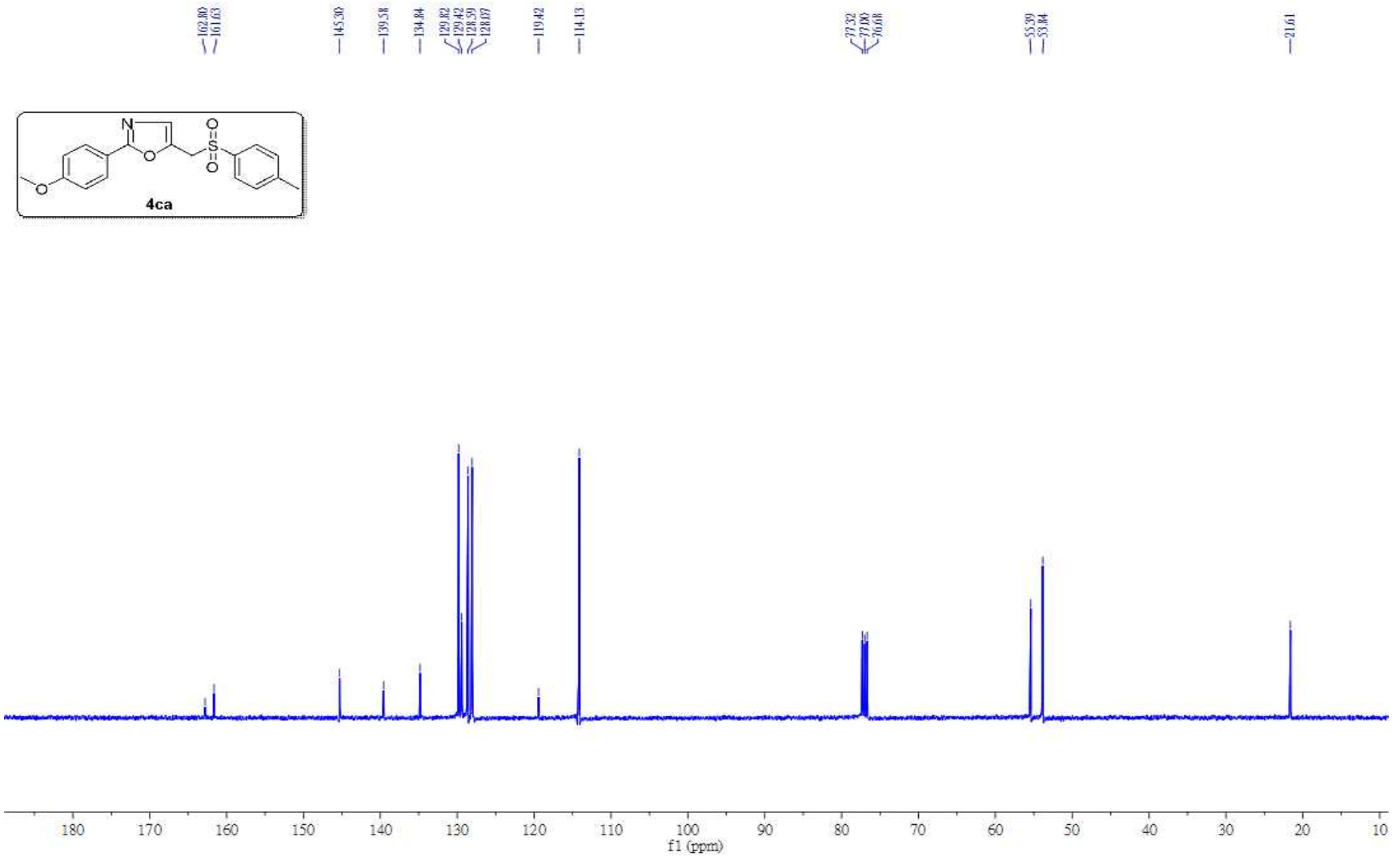
Filename	= VERA-RP3-155_DEPT135deg-1	Spectrometer	= DELTA2_NMR	Scans	= 512
Author	= delta			Total_Scans	= 512
Experiment	= dept.jxp	Field_Strength	= 9.389766[T] (400[MHz])		
Sample_Id	= VERA-RP3-155	X_Acq_Duration	= 1.04333312[s]	Relaxation_Delay	= 2[s]
Solvent	= CHLOROFORM-D	X_Domain	= 13C	Recvr_Gain	= 60
Creation_Time	= 31-JUL-2016 15:57:23	X_Freq	= 100.52530333[MHz]	Temp_Get	= 24.7[dC]
Revision_Time	= 8-AUG-2016 21:52:25	X_Offset	= 100[ppm]	X_Acq_Time	= 1.04333312[s]
Current_Time	= 8-AUG-2016 21:53:08	X_Points	= 32768	X_Atn	= 5.3[dB]
		X_Prescans	= 4	X_Pulse	= 10.33[us]
Comment	= DEPT with decoupling	X_Resolution	= 0.95846665[Hz]	Irr_Atn	= 2.4[dB]
Data_Format	= 1D COMPLEX	X_Sweep	= 31.40703518[kHz]	Irr_Atn_Dec	= 21.473[dB]
Dim_Size	= 26214	X_Sweep_Clipped	= 25.12562814[kHz]	Irr_Noise	= WALTZ
Dim_Title	= Carbon13	Irr_Domain	= Proton	Irr_Pulse	= 12.795[us]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	Irr_Pwidth	= 0.115[ms]
Dimensions	= X	Irr_Offset	= 5[ppm]	Base_Line_Correct	= TRUE
Site	= JNM-ECS400	Clipped	= FALSE	Decoupling	= TRUE

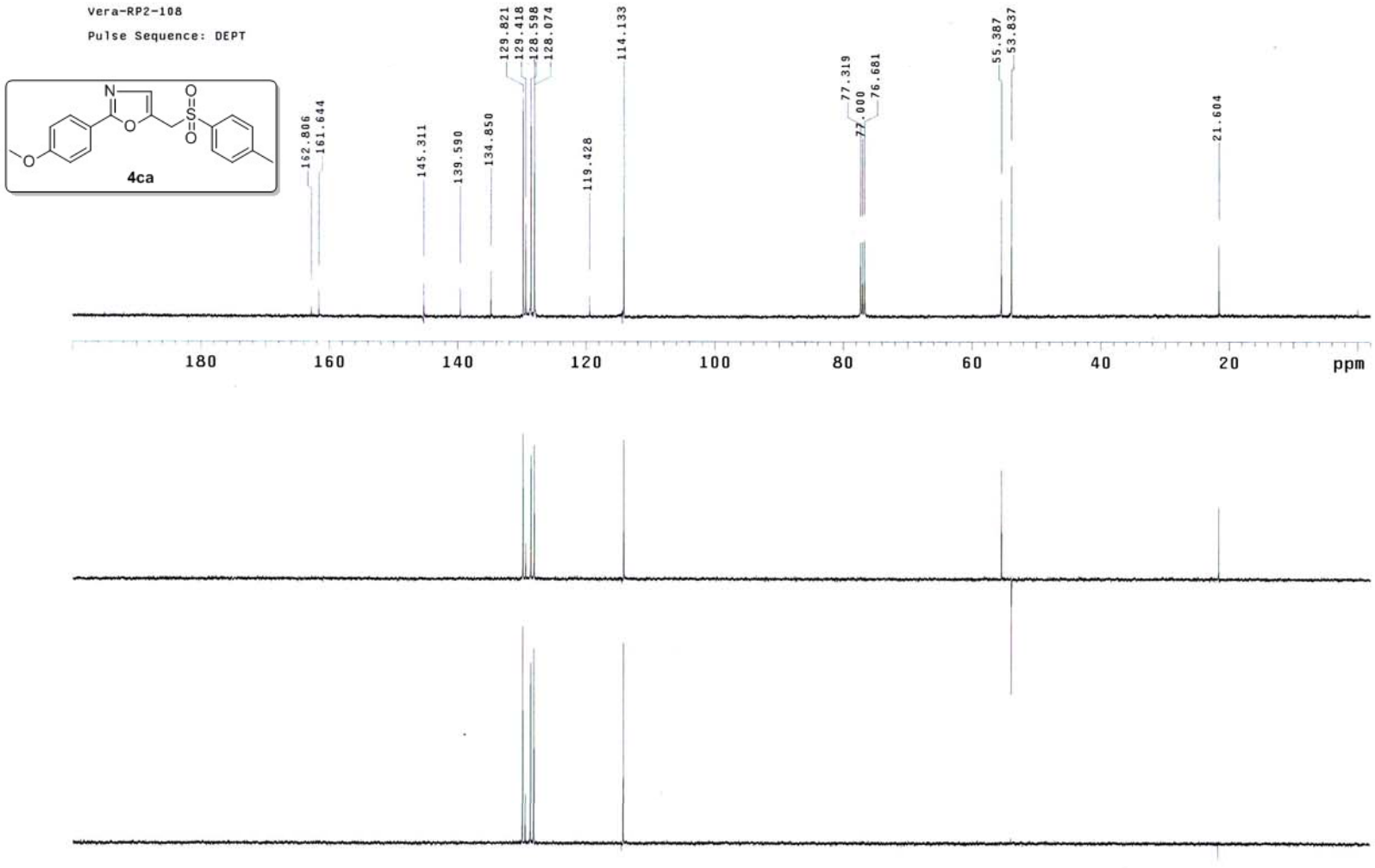

Solvent: CDCl3
Frequency: 400.28 MHz
4ba
f1 (ppm)

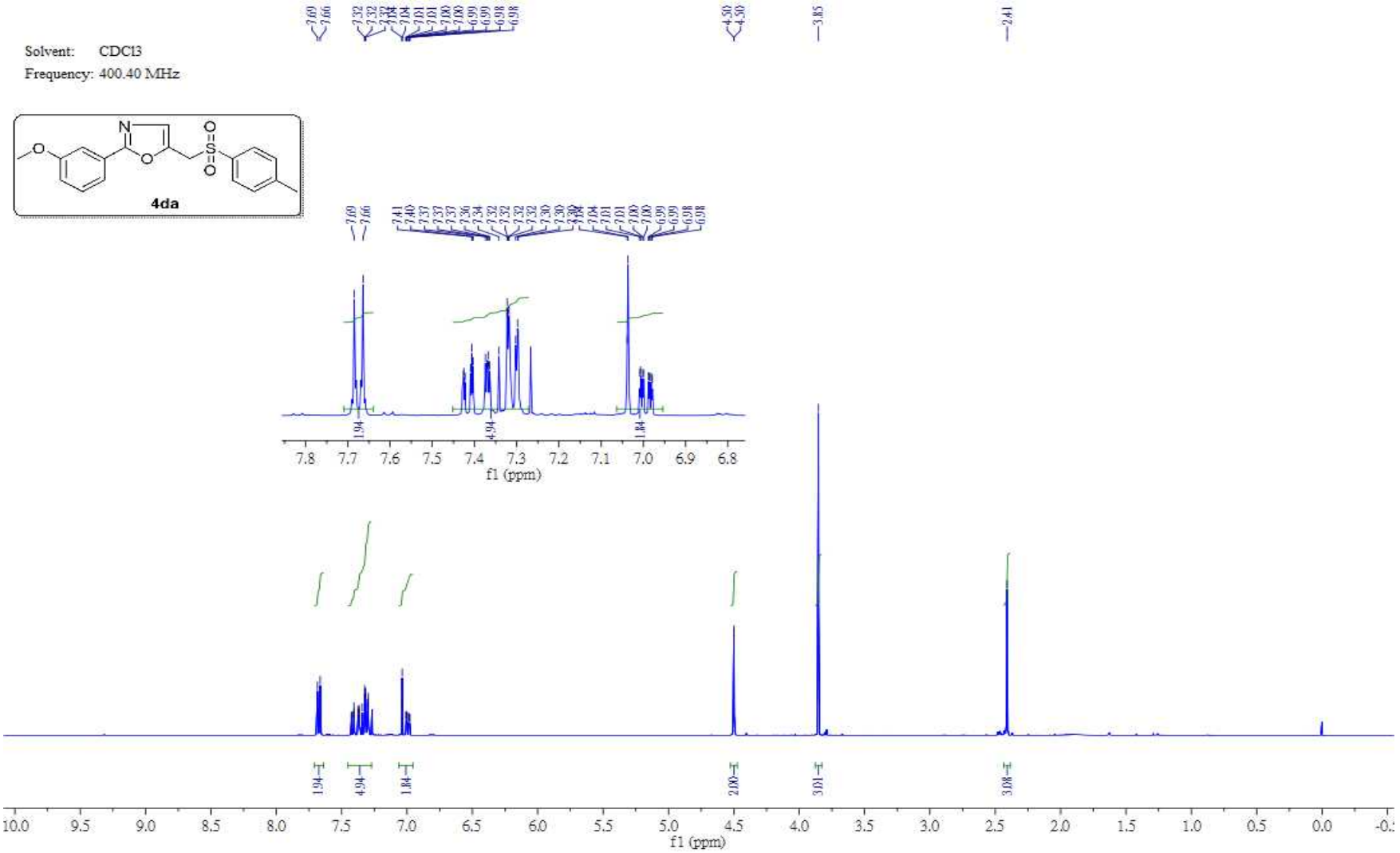

145.34
141.24
139.92
134.87
129.84
129.44
128.59
126.35
123.93
77.32
77.00
76.68
53.84
21.61
21.52
4ba
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

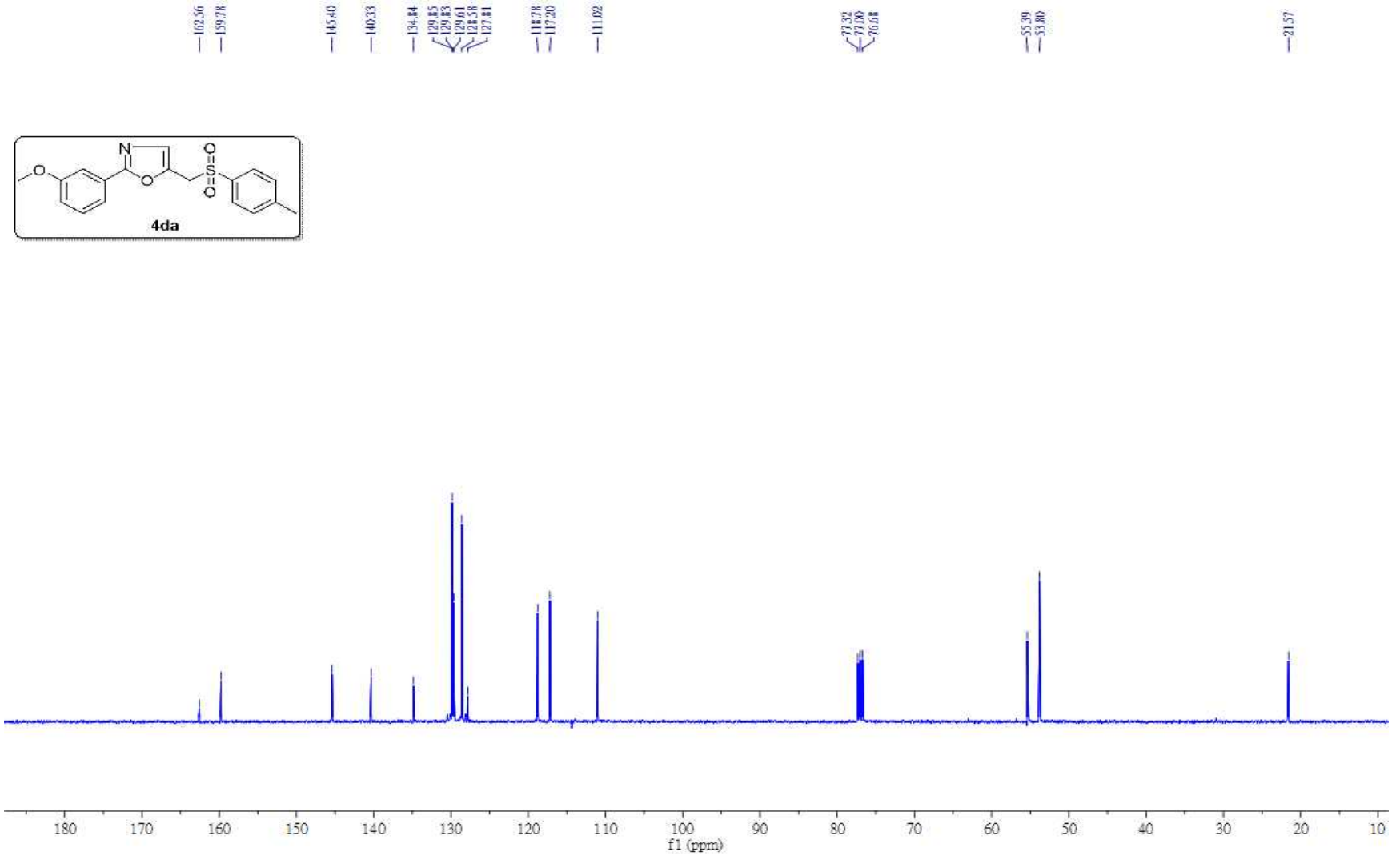

vera-RP2-49
Pulse Sequence: DEPT
4ba
145.353
141.252
139.933
134.877
129.851
129.457
128.600
126.364
123.938
77.318
77.000
76.682
53.842
21.602
21.519
180
160
140
120
100
80
60
40
20
ppm

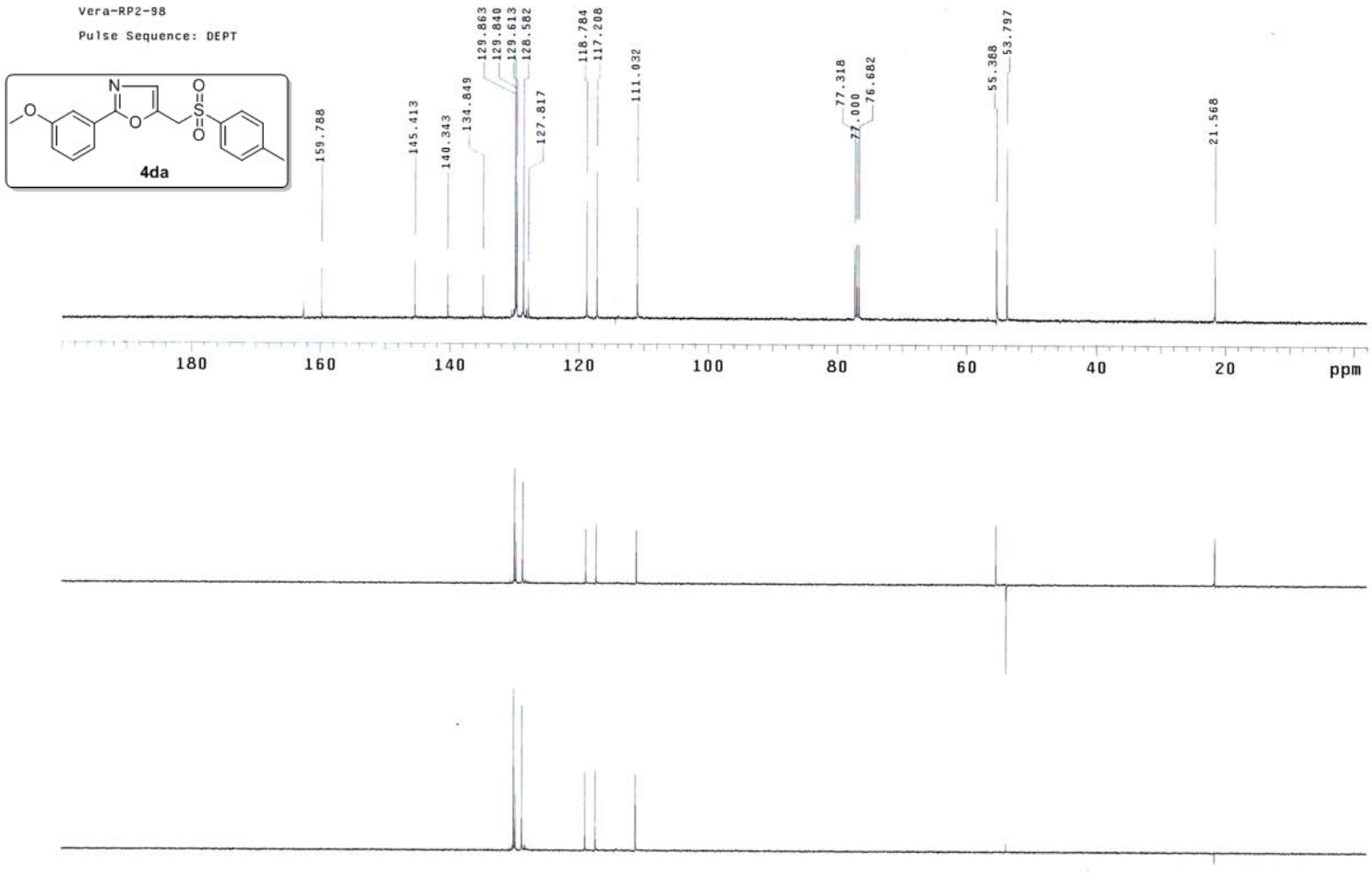

7.80
7.78
7.68
7.66
7.32
7.29
6.97
6.94
6.92
4.48
3.86
2.41
Solvent: CDCl3
Frequency: 400.40 MHz
4ca
1.90
1.79
2.11
2.86
2.00
3.01
2.95
f1 (ppm)

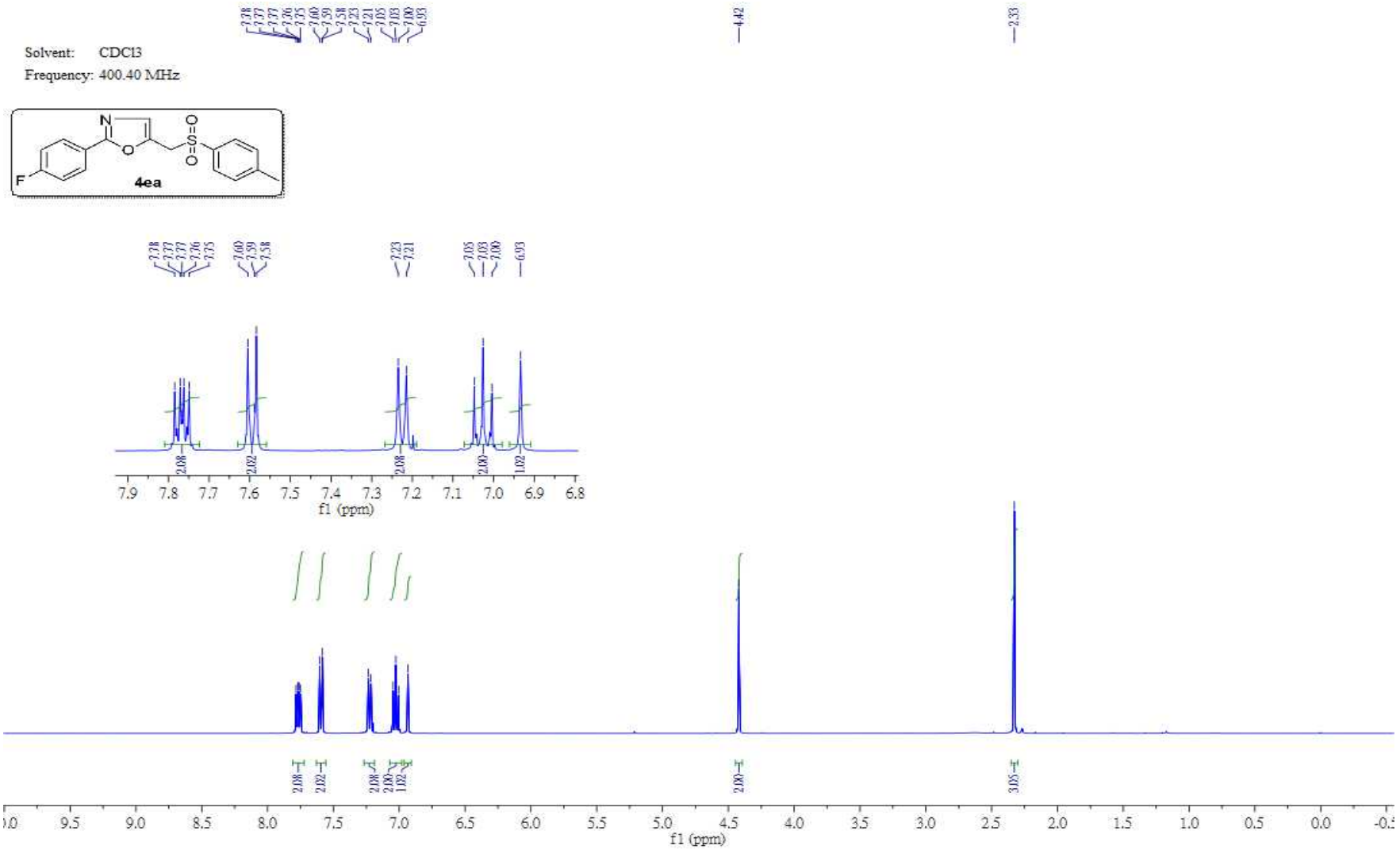

162.80
161.63
145.30
139.58
134.84
129.82
129.42
128.59
128.09
119.42
114.13
77.32
77.00
76.68
55.39
53.84
21.61
4ca
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

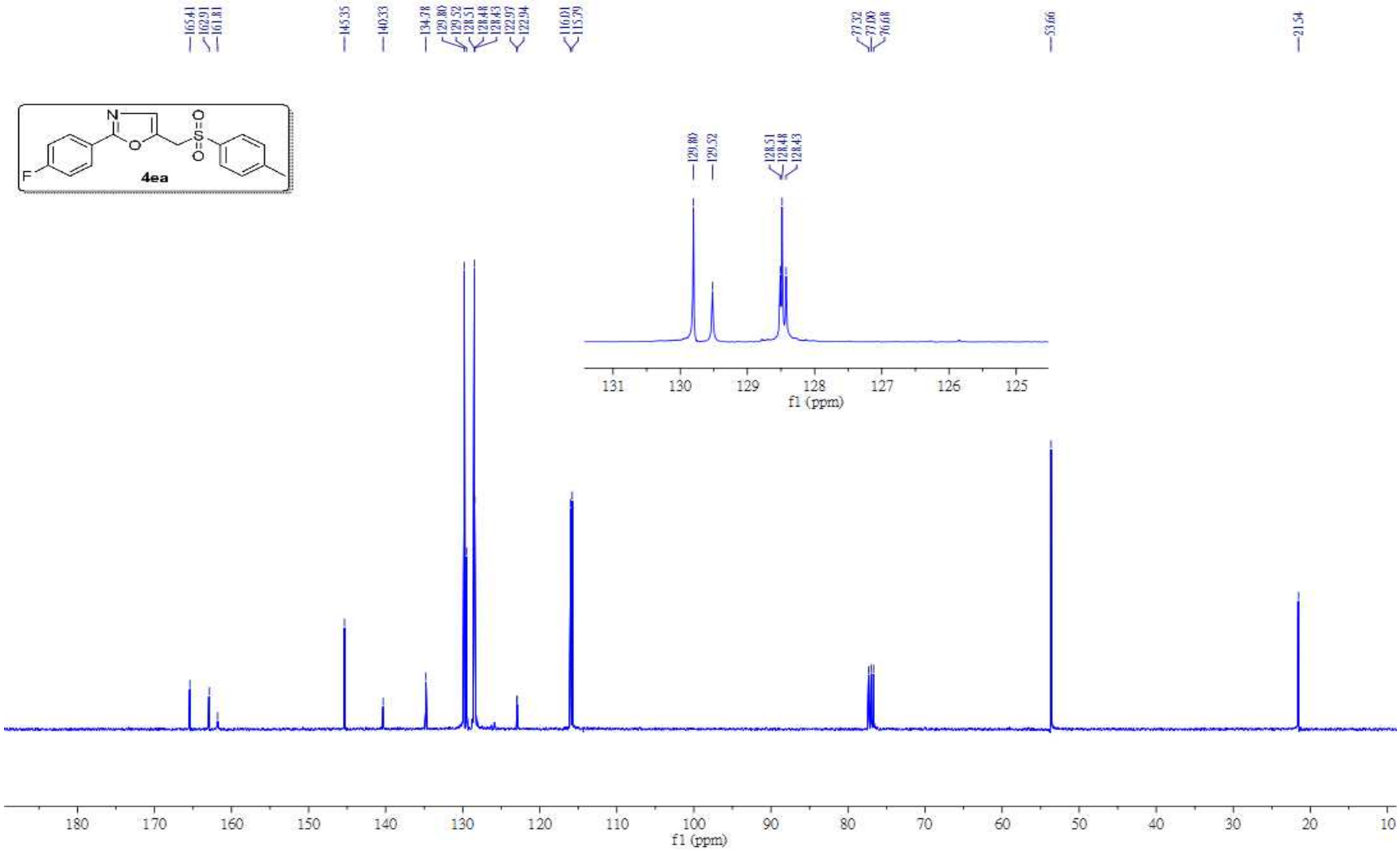

Vera-RP2-108
Pulse Sequence: DEPT
4ca
162.806
161.644
145.311
139.590
134.850
129.821
129.418
128.598
128.074
119.428
114.133
77.319
77.000
76.681
55.387
53.837
21.604
180
160
140
120
100
80
60
40
20
ppm

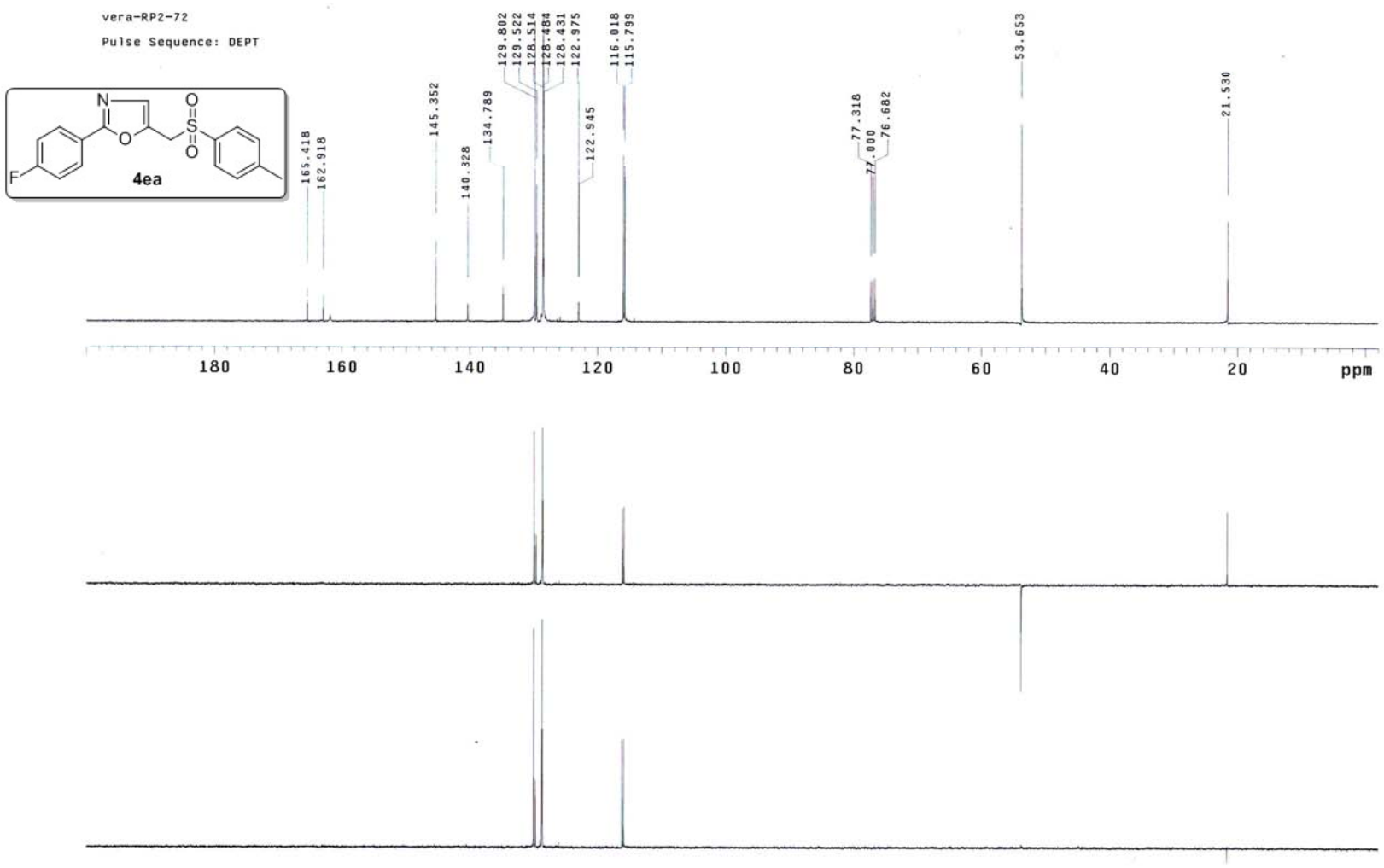

Solvent: CDCl3
Frequency: 400.40 MHz
4da
f1 (ppm)
f1 (ppm)

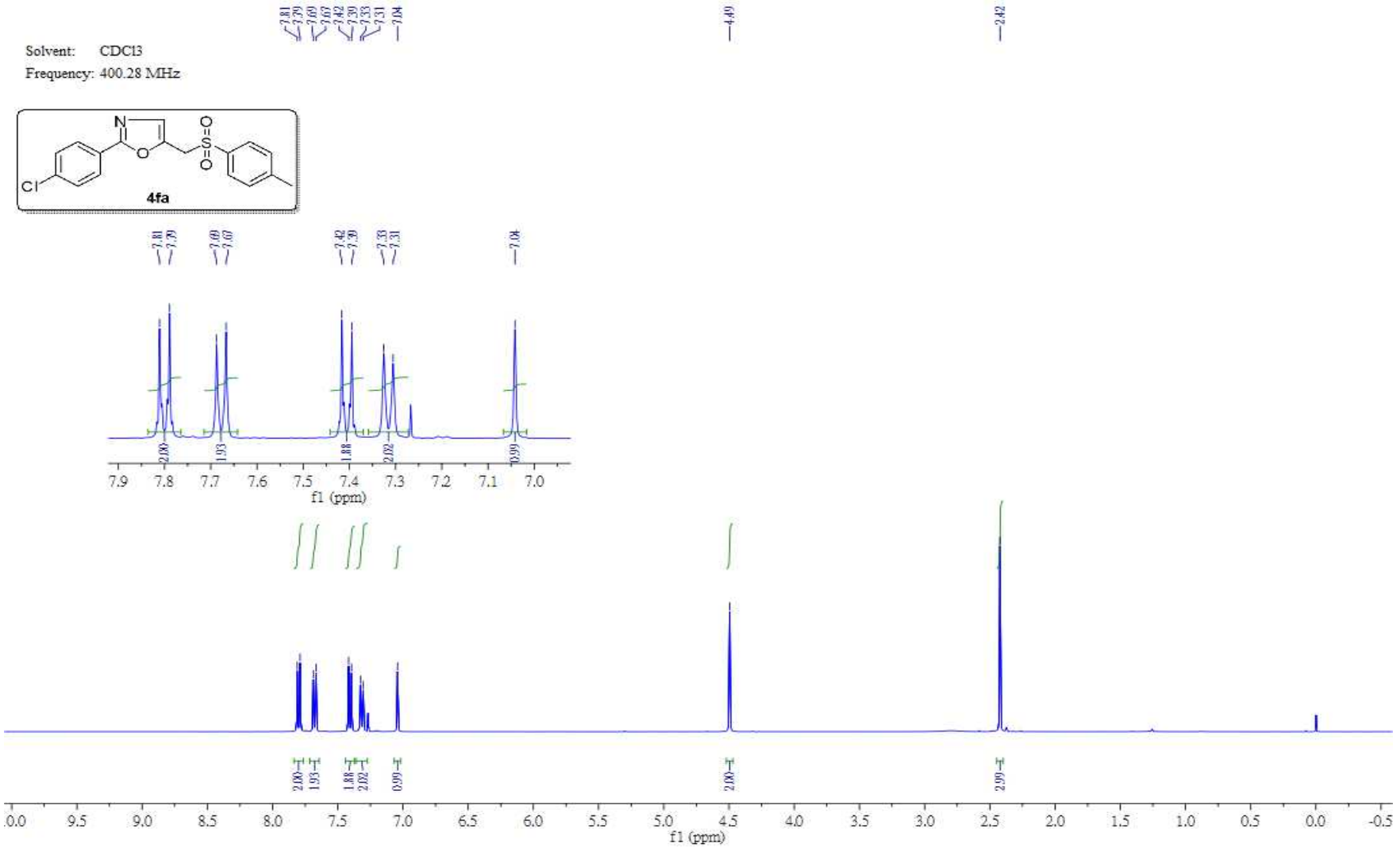

162.56
159.78
145.40
140.33
134.84
129.85
129.83
129.61
128.58
127.81
118.78
117.20
111.02
77.32
77.00
76.68
55.39
53.80
21.57
4da
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

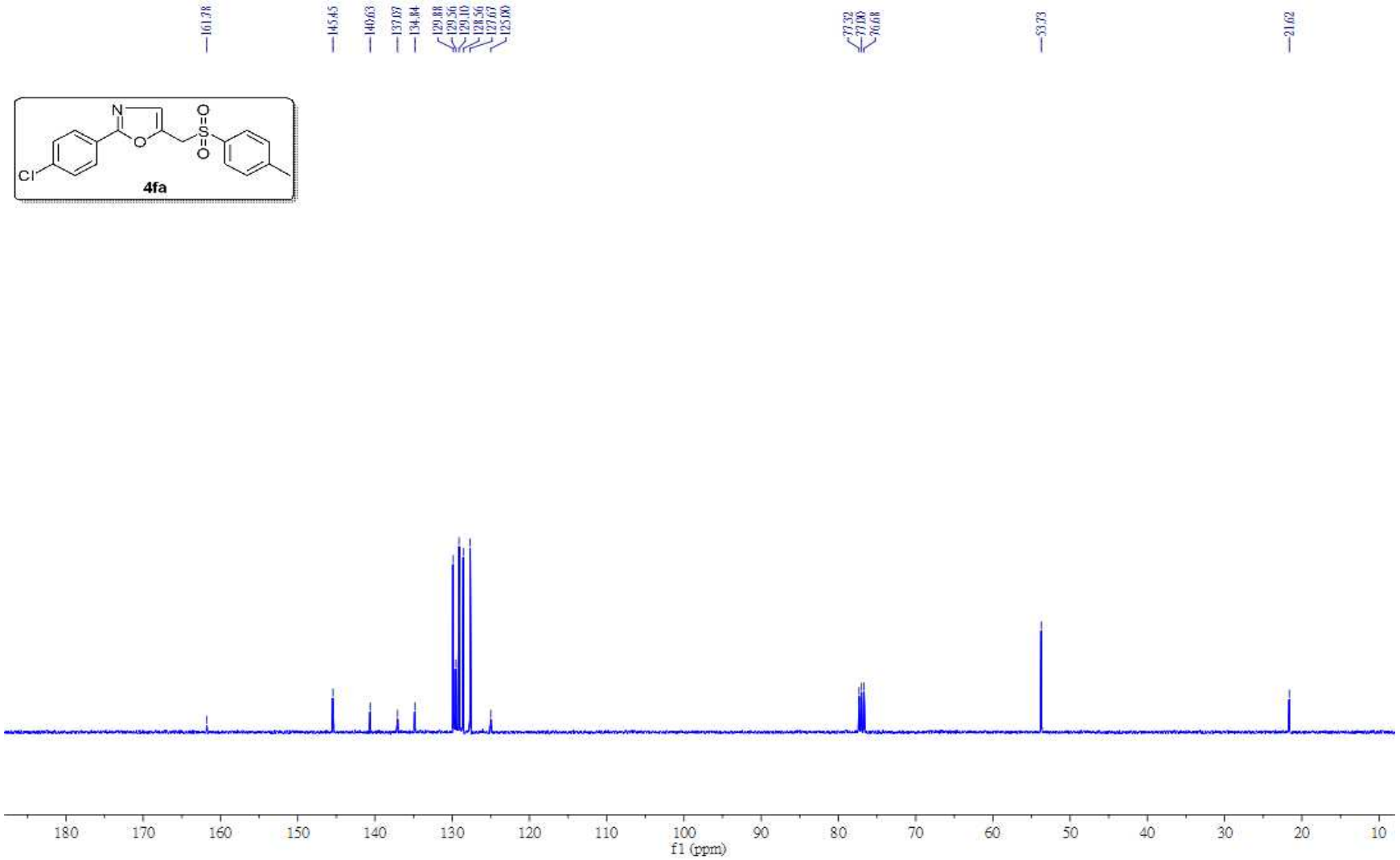

Vera-RP2-98
Pulse Sequence: DEPT
4da
159.788
145.413
140.343
134.849
129.863
129.840
129.613
128.582
127.817
118.784
117.208
111.032
77.318
77.000
76.682
55.388
53.797
21.568
180
160
140
120
100
80
60
40
20
ppm

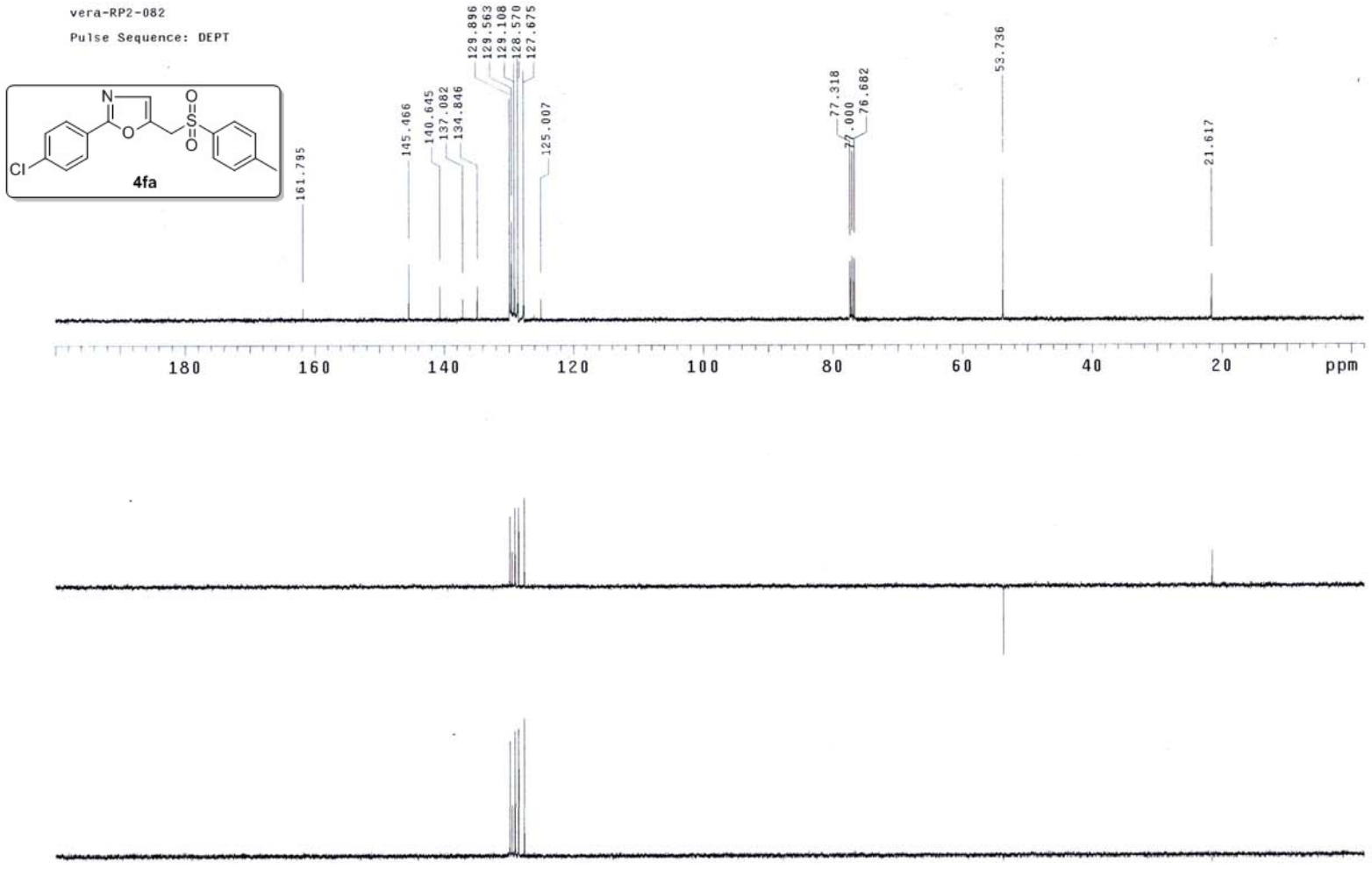

Solvent: CDCl3
Frequency: 400.40 MHz
4ea
f1 (ppm)

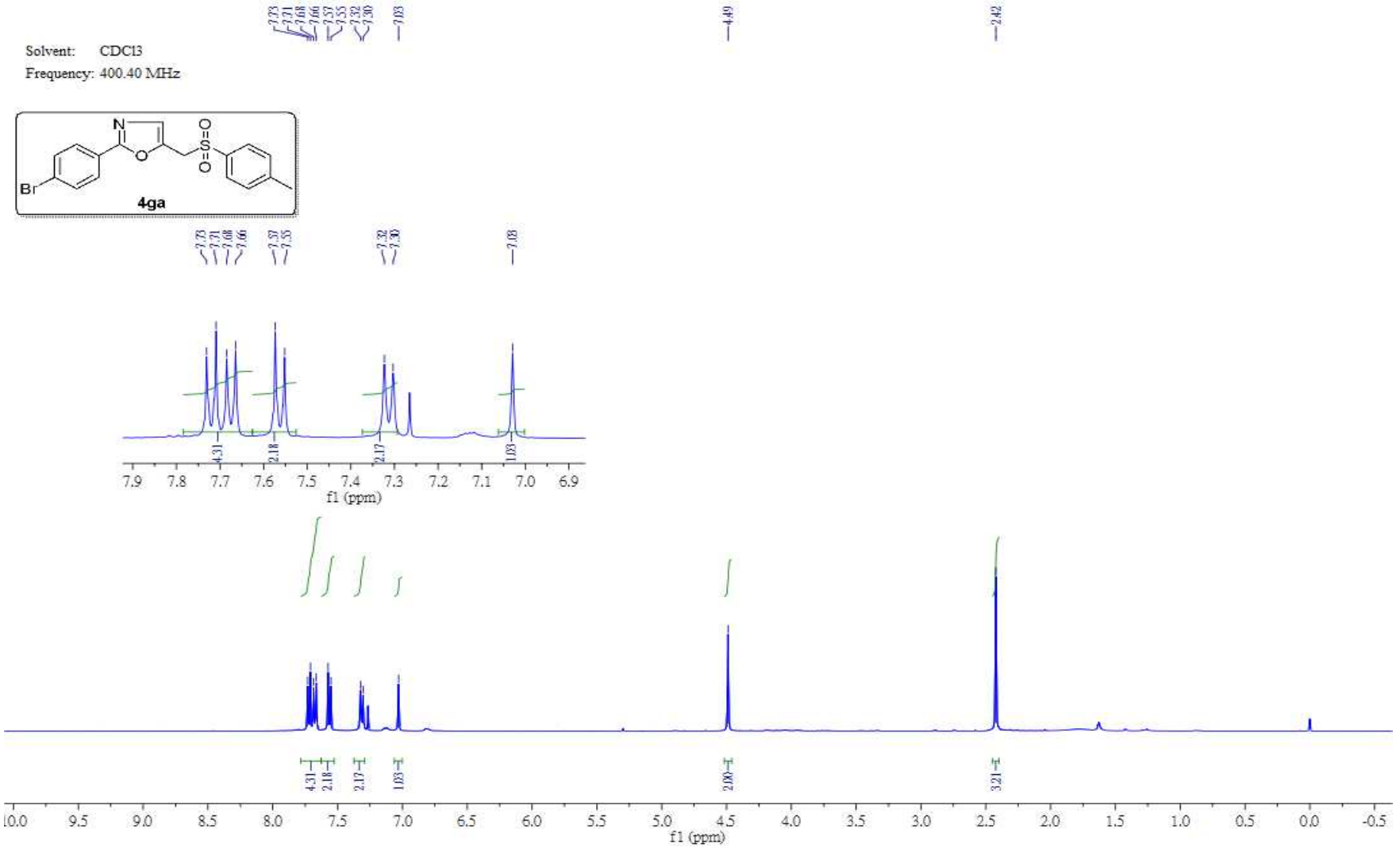

165.41
162.91
161.81
145.35
140.33
134.78
129.80
129.52
128.51
128.48
128.43
122.97
122.94
116.01
115.79
77.32
77.00
76.68
53.66
21.54
4ea
F
N
O
S
O
O
129.80
129.52
128.51
128.48
128.43
131
130
129
128
127
126
125
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

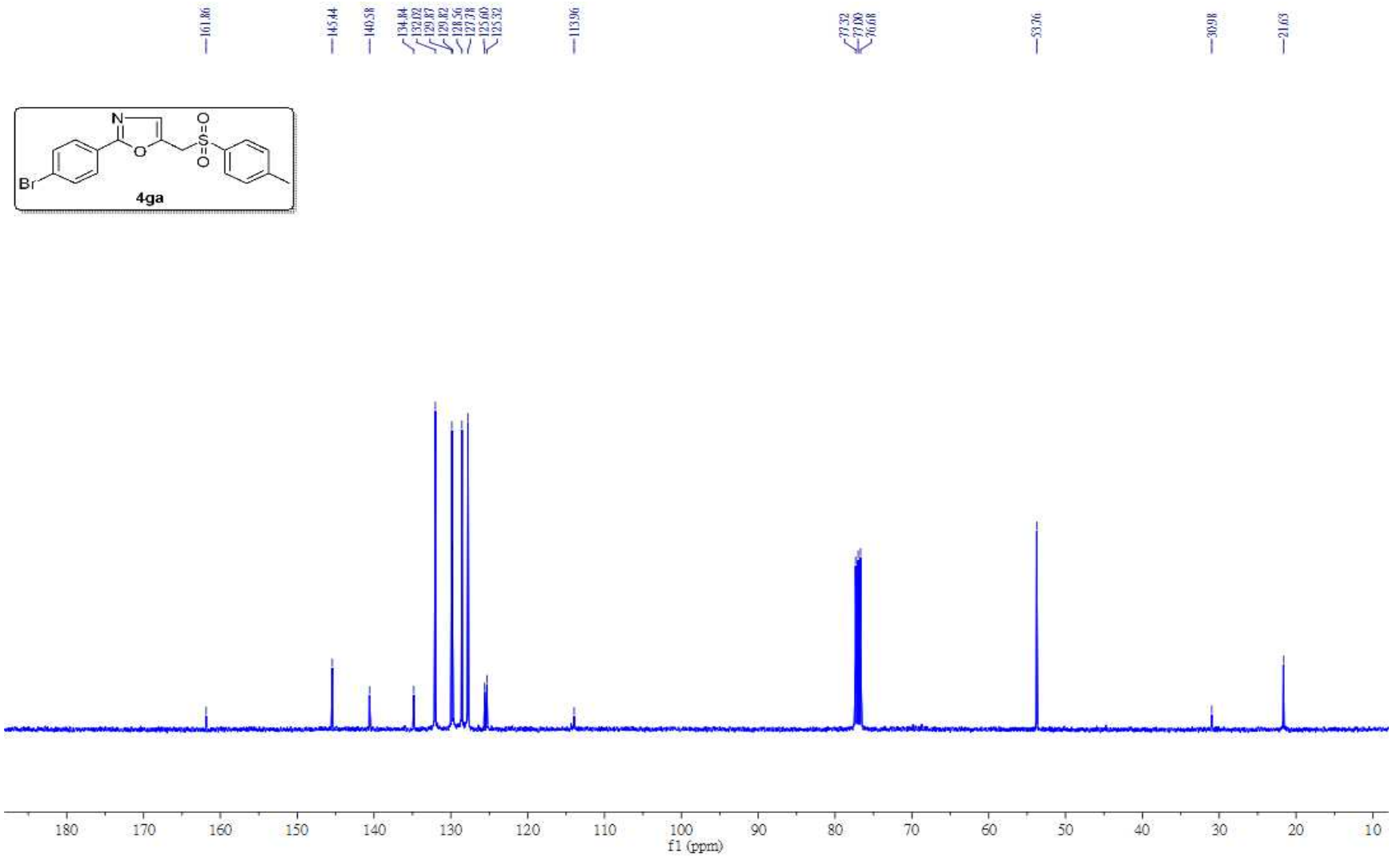

vera-RP2-72
Pulse Sequence: DEPT
4ea
165.418
162.918
145.352
140.328
134.789
129.802
129.522
128.514
128.484
128.431
122.975
122.945
116.018
115.799
77.318
77.000
76.682
53.653
21.530
180
160
140
120
100
80
60
40
20
ppm

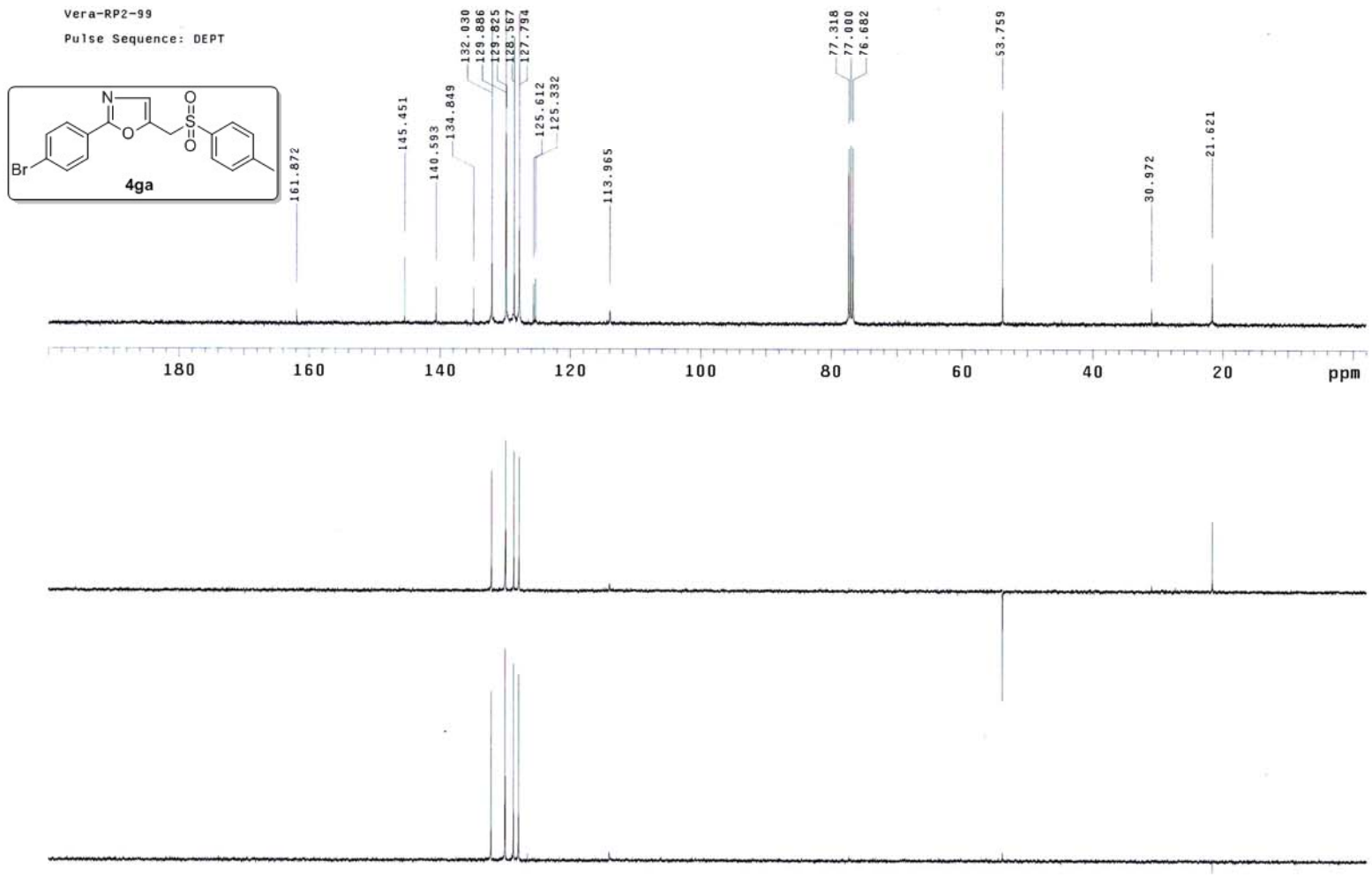

7.81
7.79
7.69
7.67
7.42
7.39
7.33
7.31
7.04
4.49
2.42
Solvent: CDCl3
Frequency: 400.28 MHz
4fa
2.00
1.93
1.88
2.02
0.99
f1 (ppm)
2.00
2.99
f1 (ppm)

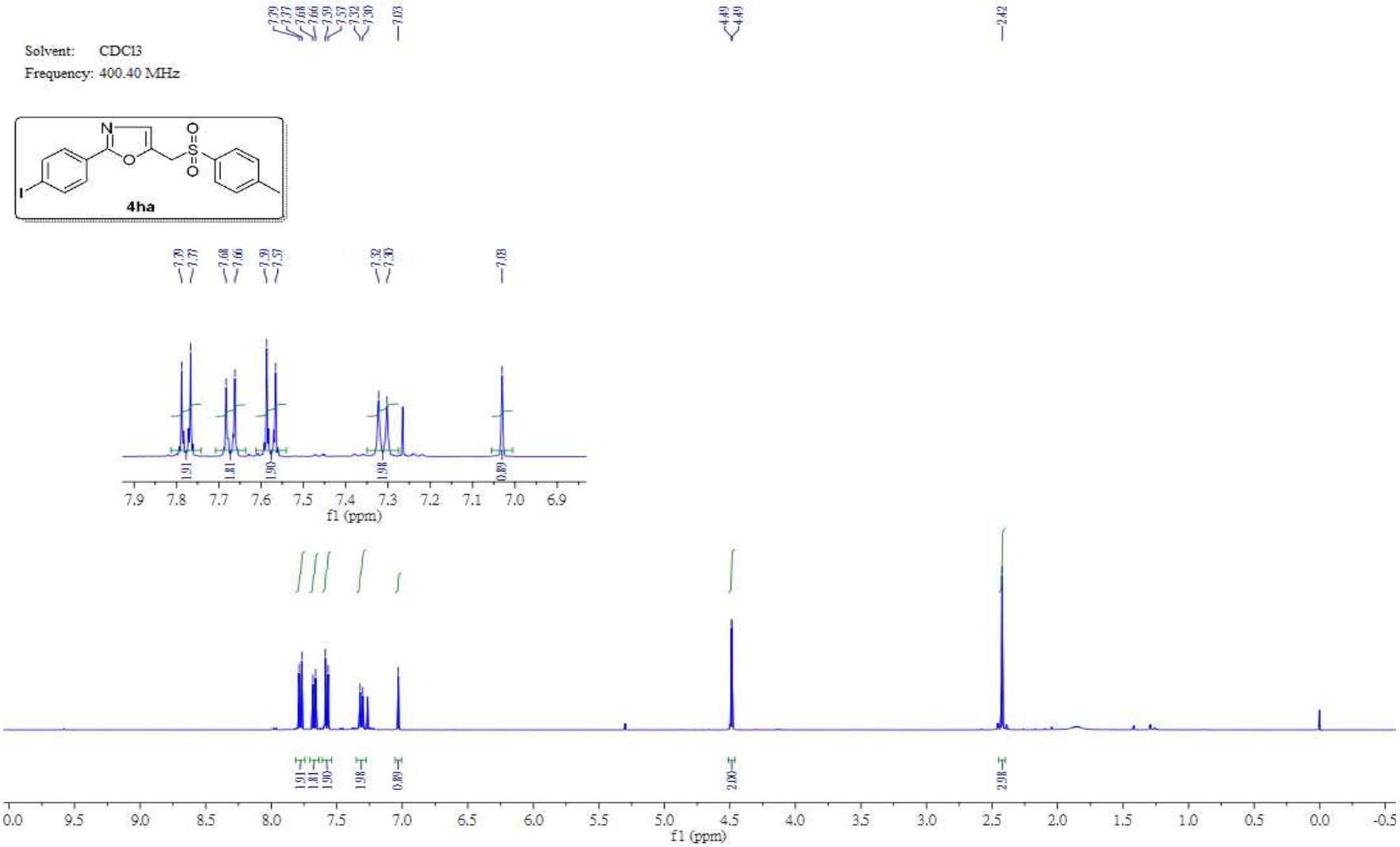

161.38
145.45
140.63
137.07
134.84
129.88
129.56
129.10
128.56
127.67
125.00
77.32
77.00
76.68
53.73
21.62
N
O
O=S=O
Cl
4fa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

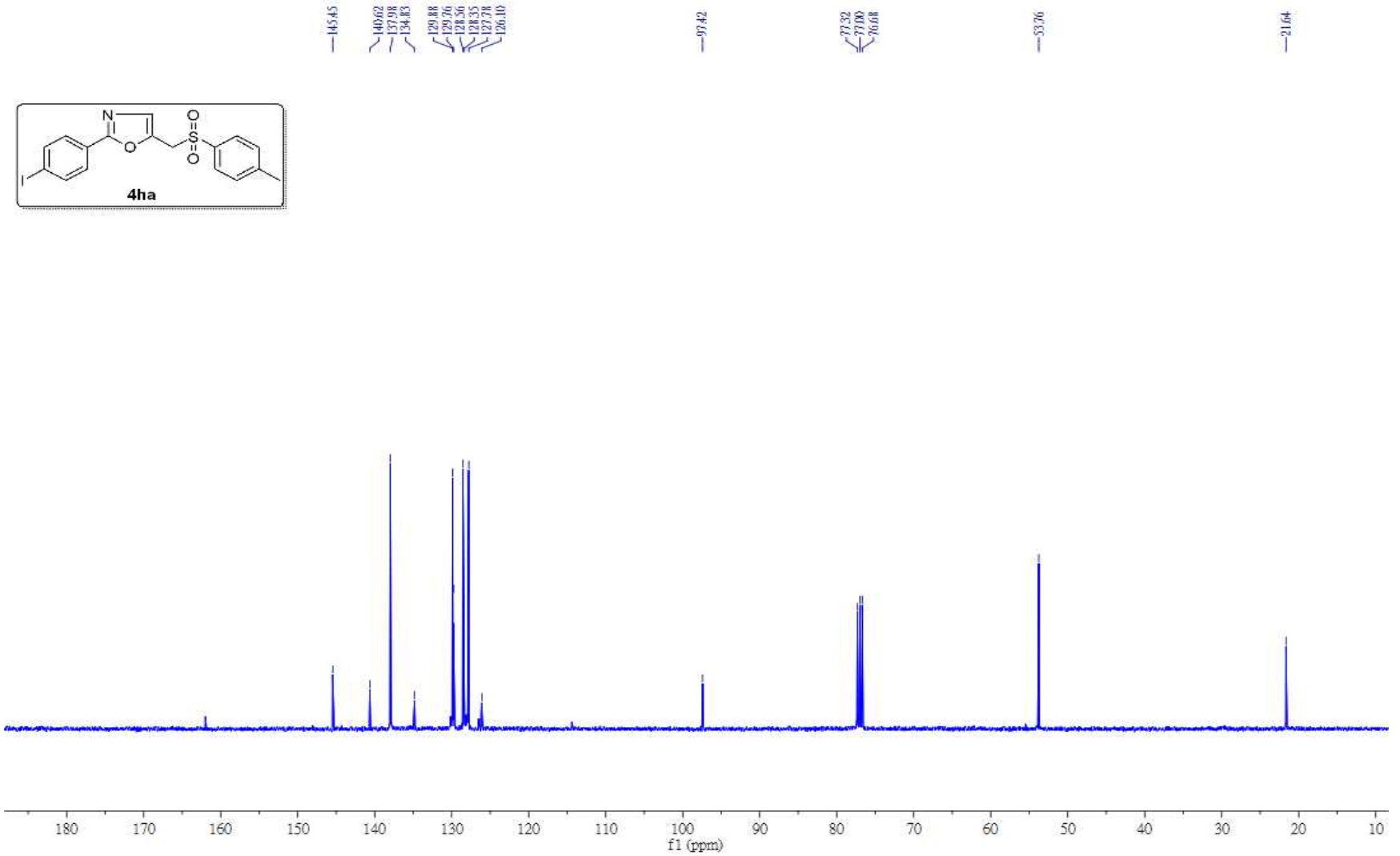

vera-RP2-082
Pulse Sequence: DEPT
4fa
161.795
145.466
140.645
137.082
134.846
129.896
129.563
129.108
128.570
127.675
125.007
77.318
77.000
76.682
53.736
21.617
180
160
140
120
100
80
60
40
20
ppm

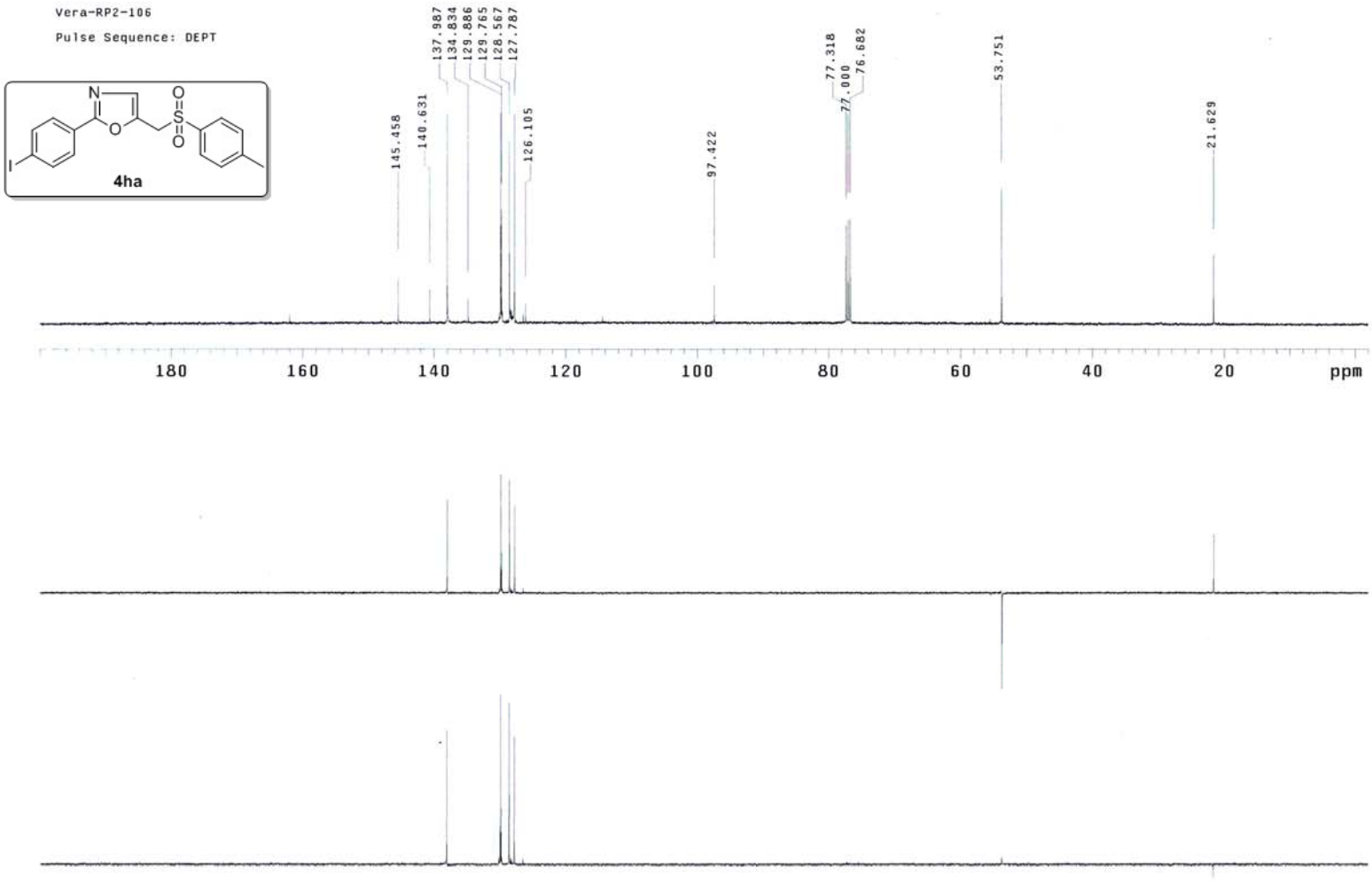

Solvent: CDCl3
Frequency: 400.40 MHz
4ga
f1 (ppm)

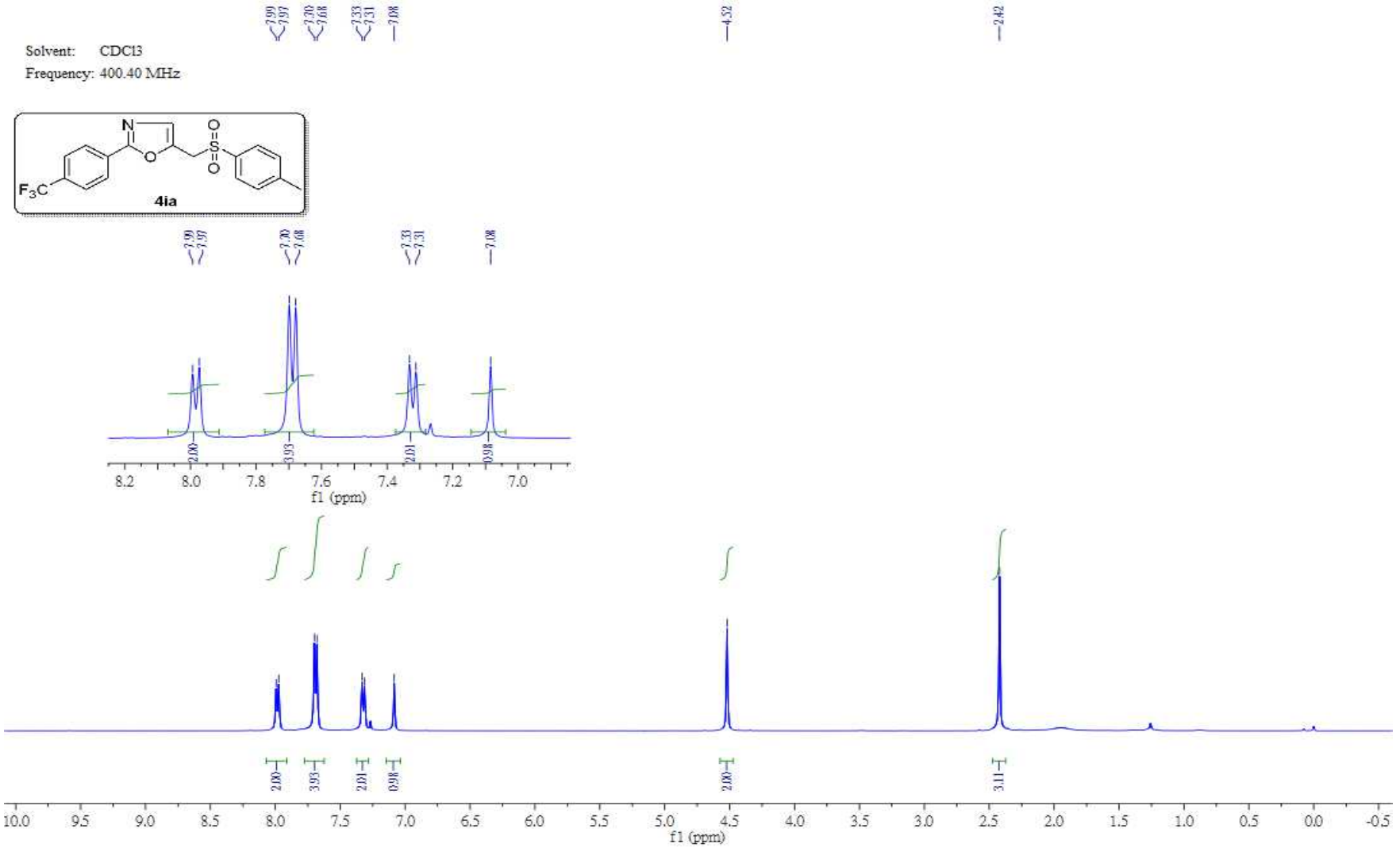

161.86
145.44
140.58
134.84
132.02
129.87
129.82
128.56
127.78
125.60
125.32
113.96
77.32
77.00
76.68
53.76
30.98
21.63
Br
4ga
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

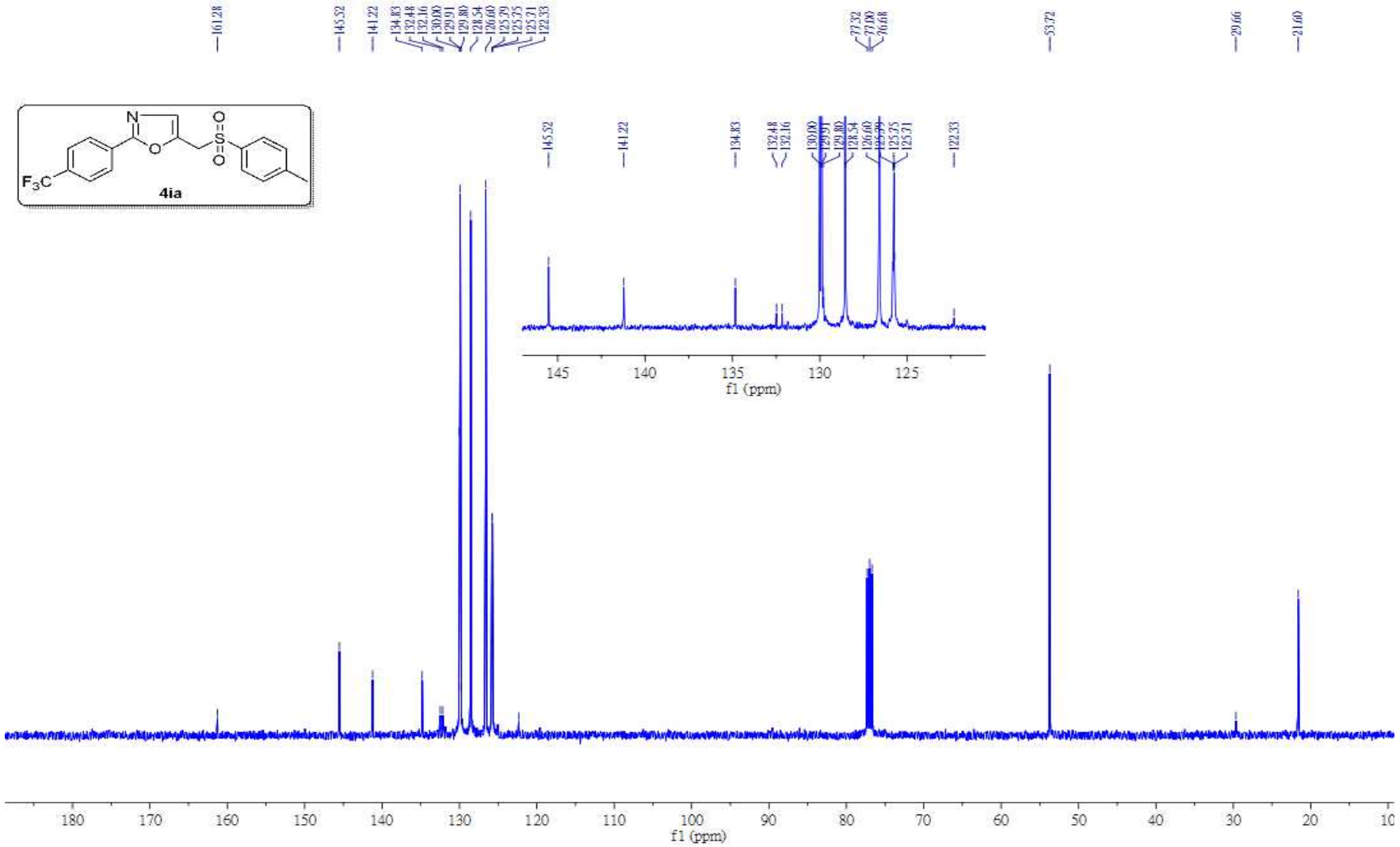

Vera-RP2-99
Pulse Sequence: DEPT
4ga
161.872
145.451
140.593
134.849
132.030
129.886
129.825
128.567
127.794
125.612
125.332
113.965
77.318
77.000
76.682
53.759
30.972
21.621
180
160
140
120
100
80
60
40
20
ppm

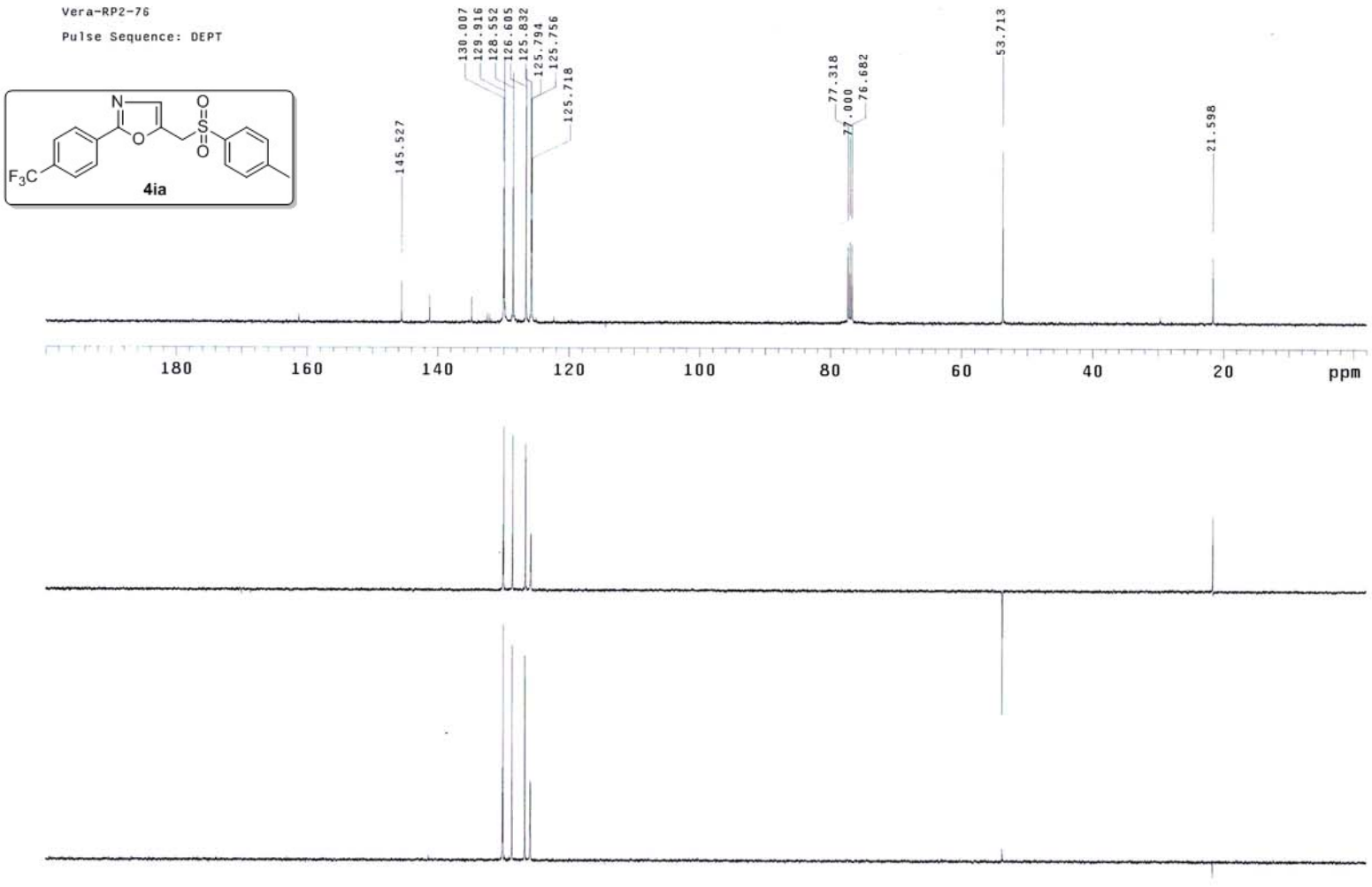

Solvent: CDCl3
Frequency: 400.40 MHz
4ha
f1 (ppm)
f1 (ppm)

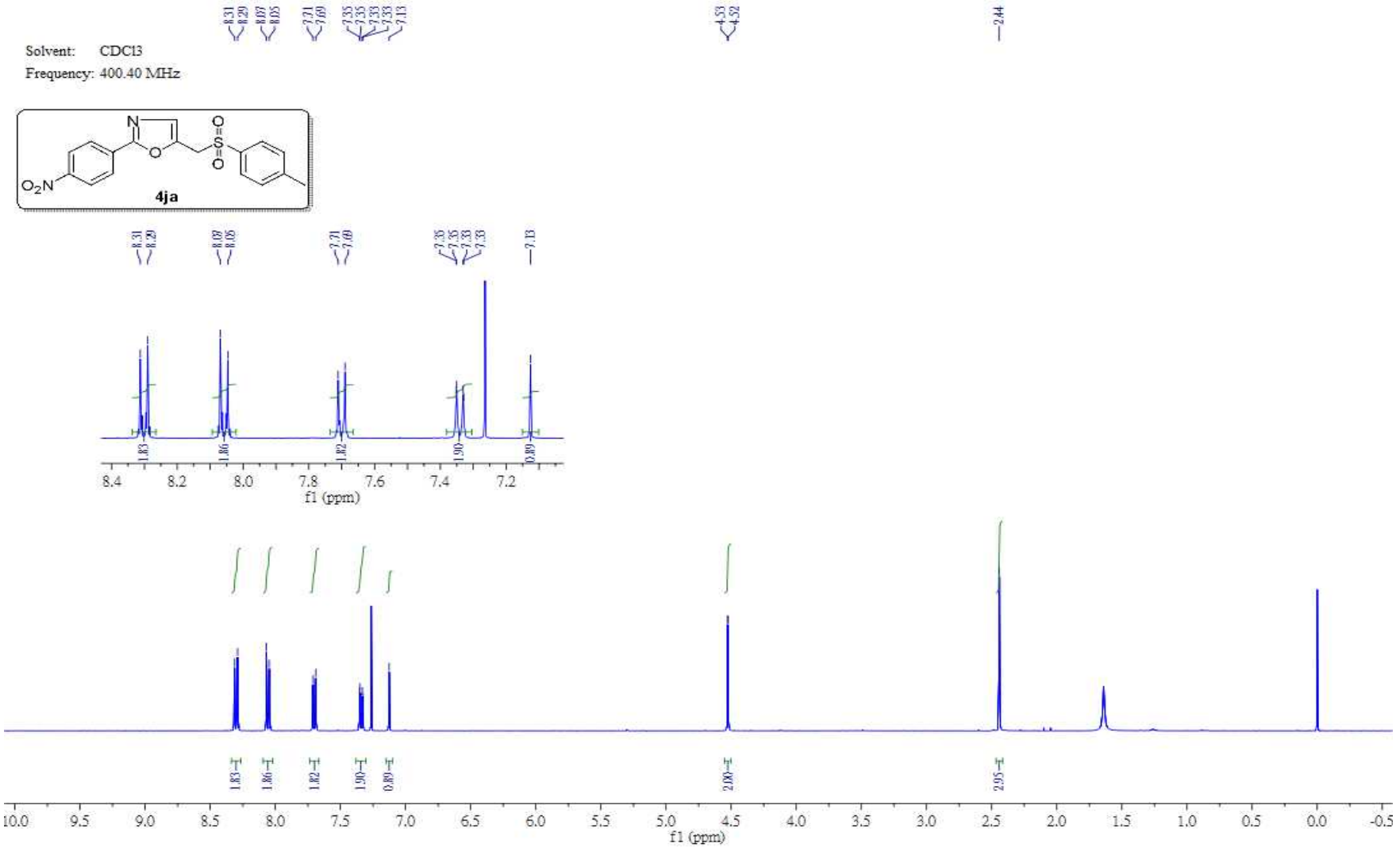

145.45
140.62
137.98
134.83
129.88
129.26
128.56
128.35
127.78
126.10
97.42
77.32
77.00
76.68
53.76
21.64
4ha
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

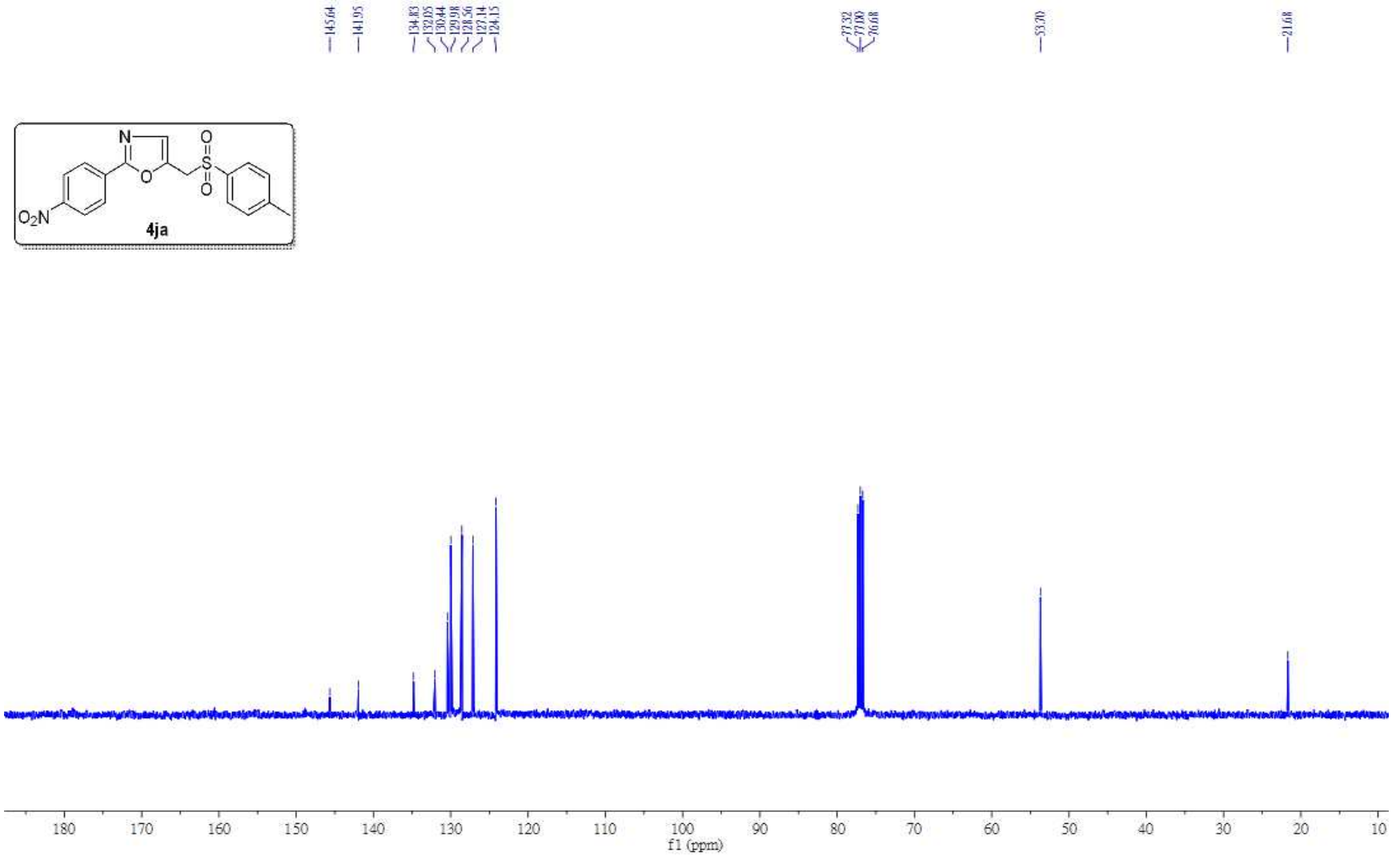

Vera-RP2-106
Pulse Sequence: DEPT
4ha
145.458
140.631
137.987
134.834
129.886
129.765
128.567
127.787
126.105
97.422
77.318
77.000
76.682
53.751
21.629
180
160
140
120
100
80
60
40
20
ppm

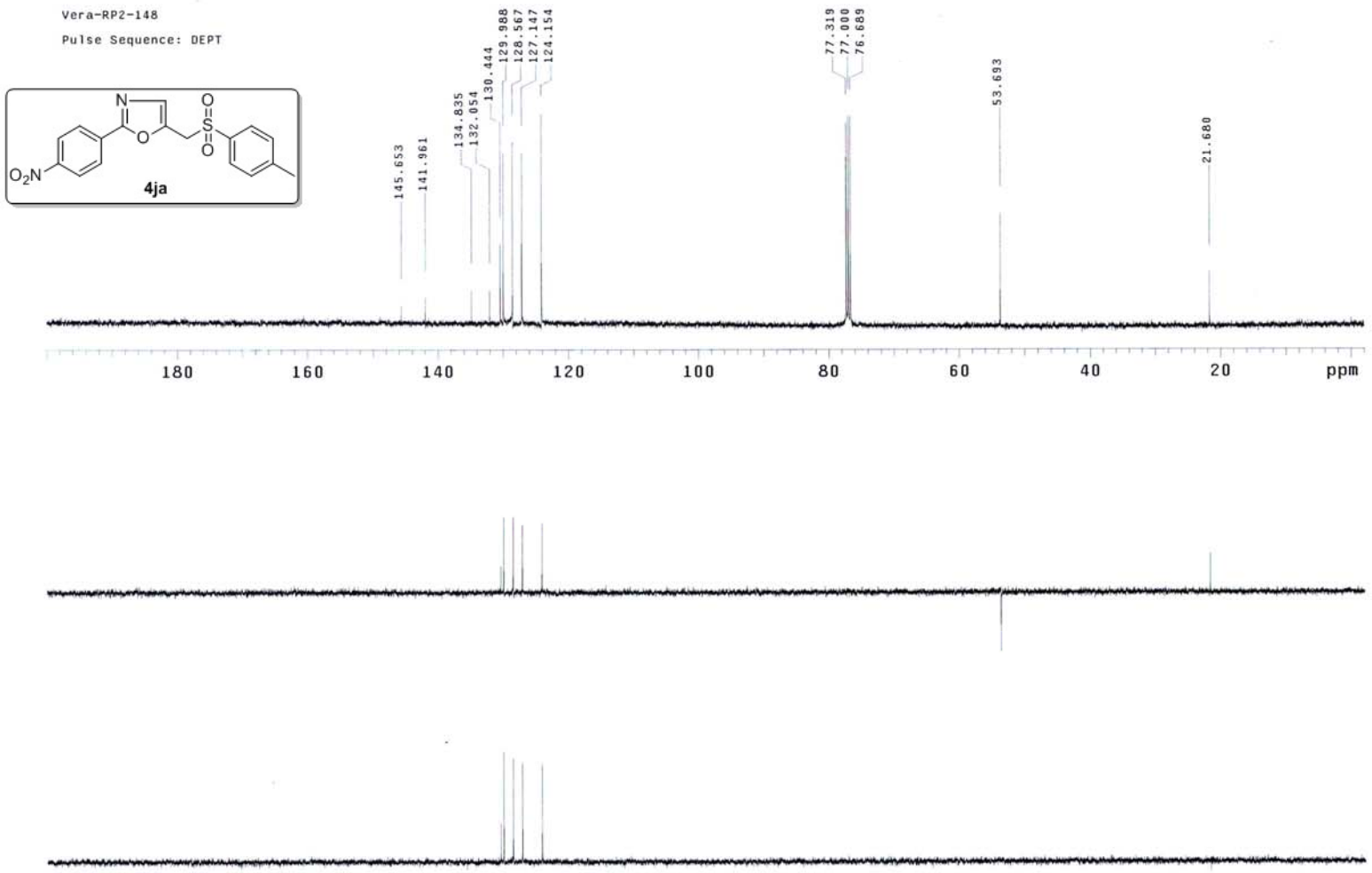

Solvent: CDCl3
Frequency: 400.40 MHz
4ia
f1 (ppm)

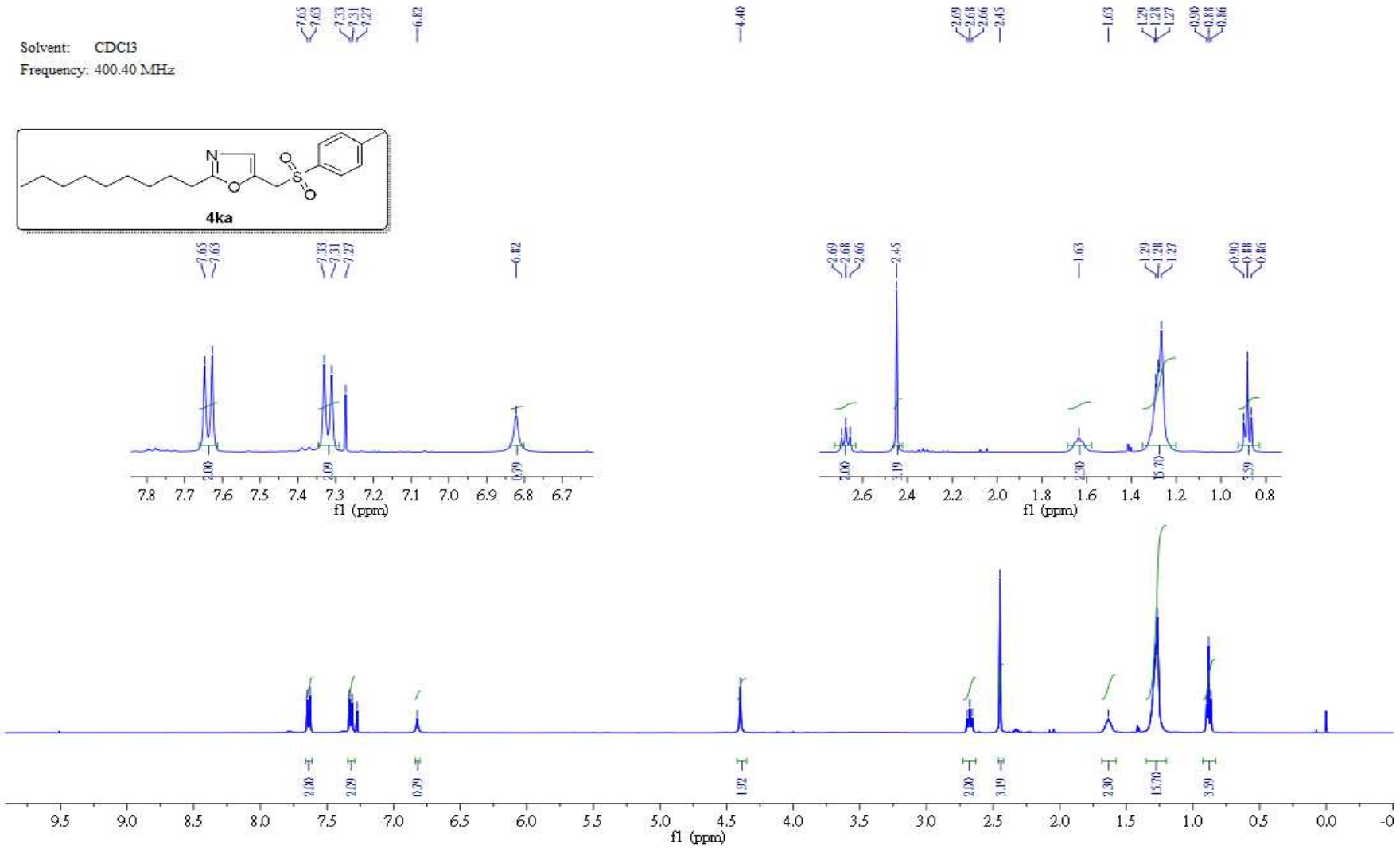

161.28
145.32
141.22
134.83
132.48
132.16
130.00
129.91
129.80
128.54
126.60
125.79
125.75
125.71
122.33
77.32
77.00
76.68
53.72
29.66
21.60
F3C
4ia
f1 (ppm)

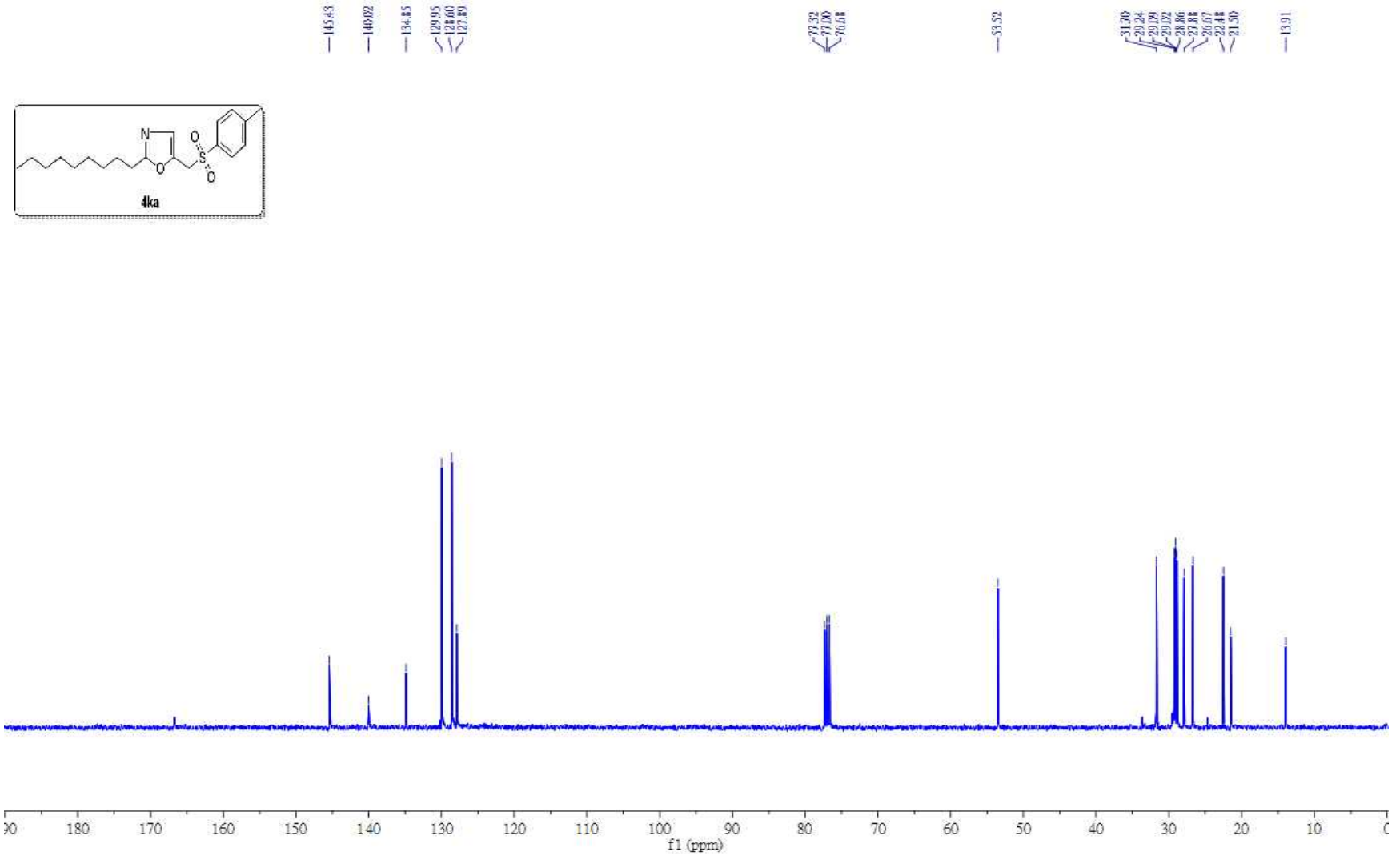

Vera-RP2-76
Pulse Sequence: DEPT
4ia
145.527
130.007
129.916
128.552
126.605
125.832
125.794
125.756
125.718
77.318
77.000
76.682
53.713
21.598
180
160
140
120
100
80
60
40
20
ppm

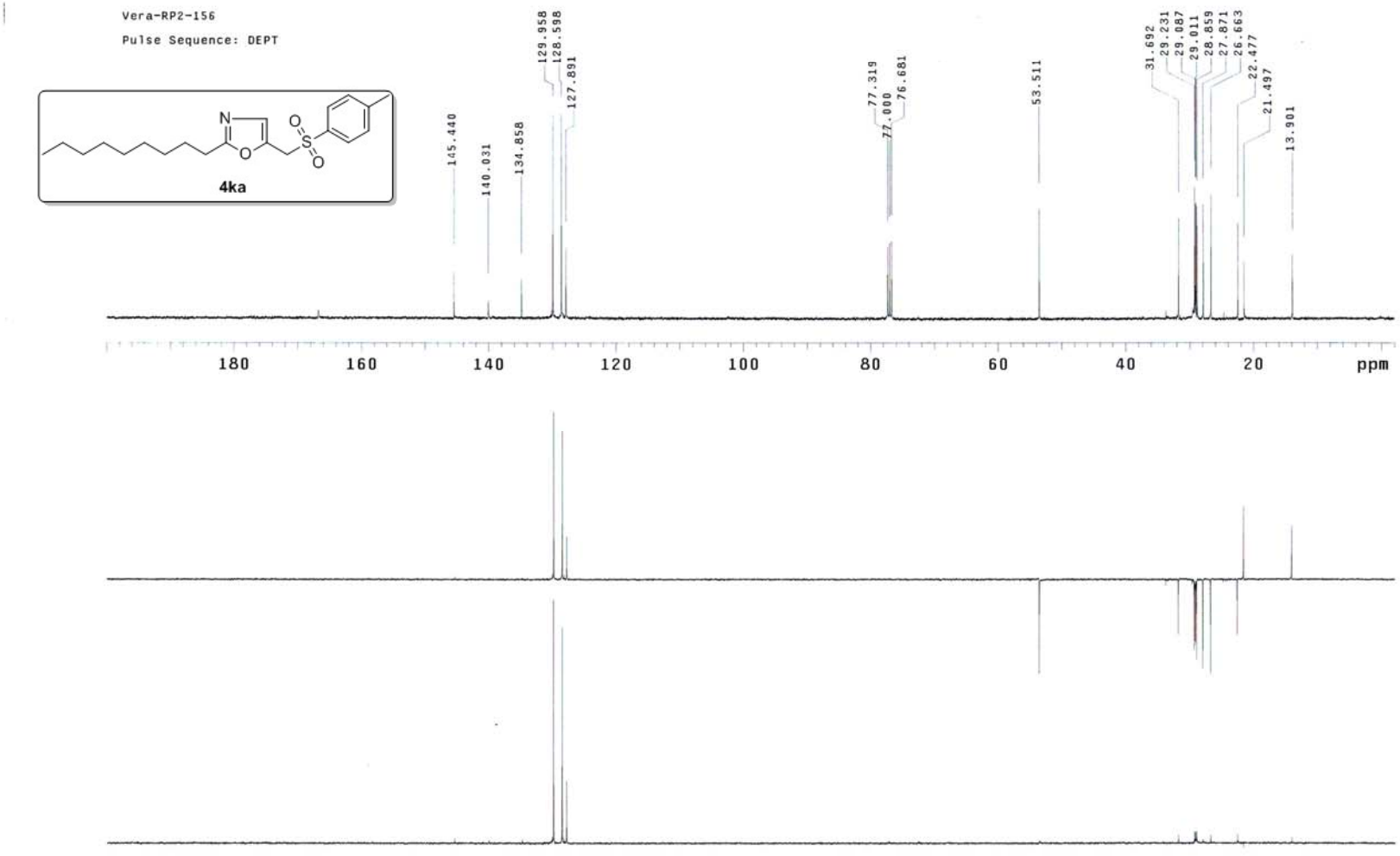

8.31
8.29
8.07
8.05
7.71
7.69
7.35
7.33
7.13
4.53
4.52
2.44
Solvent: CDCl3
Frequency: 400.40 MHz
N
O
O=S=O
O2N
4ja
1.83
1.86
1.82
1.90
0.89
2.00
2.95
f1 (ppm)

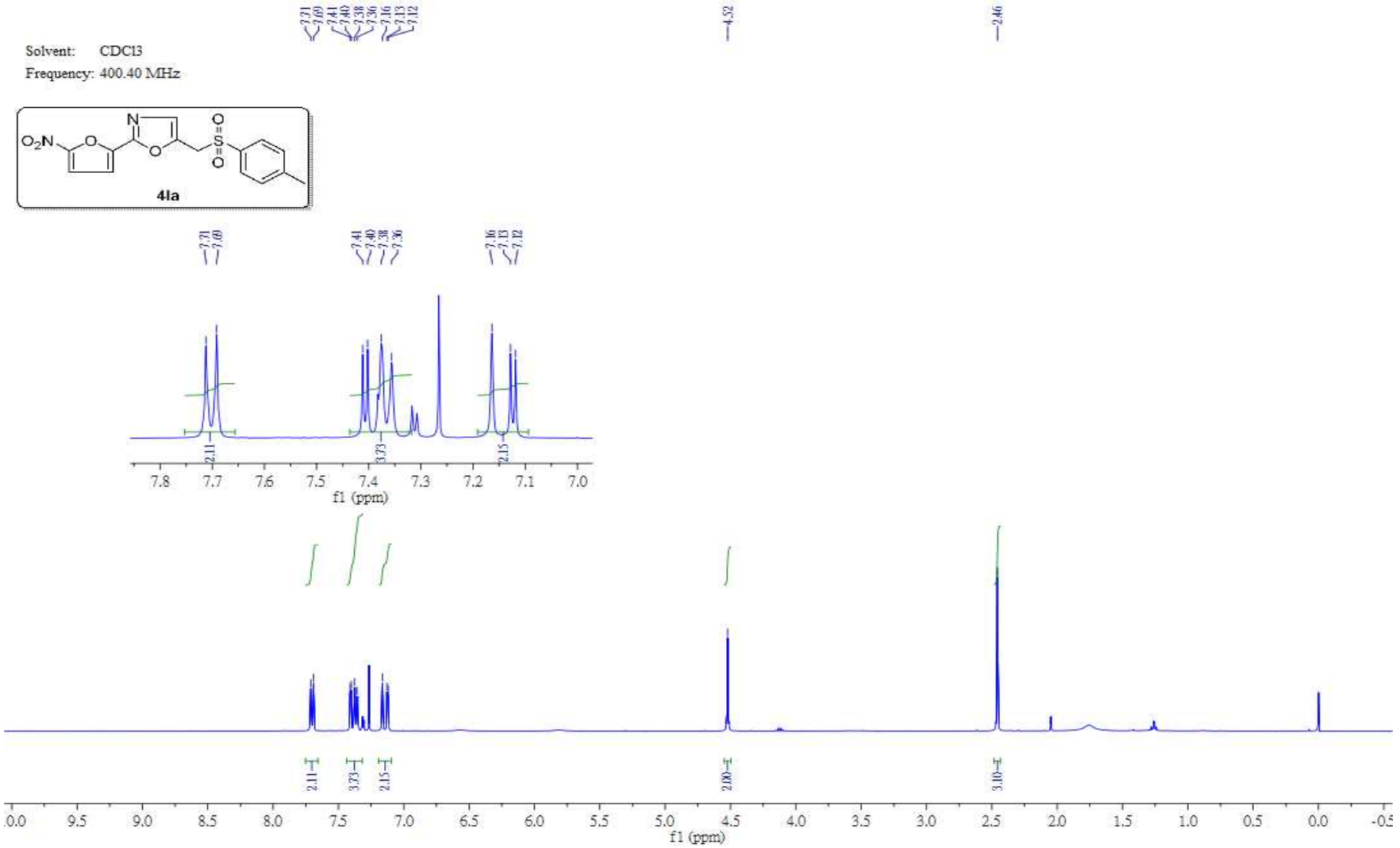

145.64
141.95
134.83
132.05
130.44
129.98
128.56
127.14
124.15
77.32
77.00
76.68
53.70
21.68
N
O
O
S
O
O2N
4ja
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

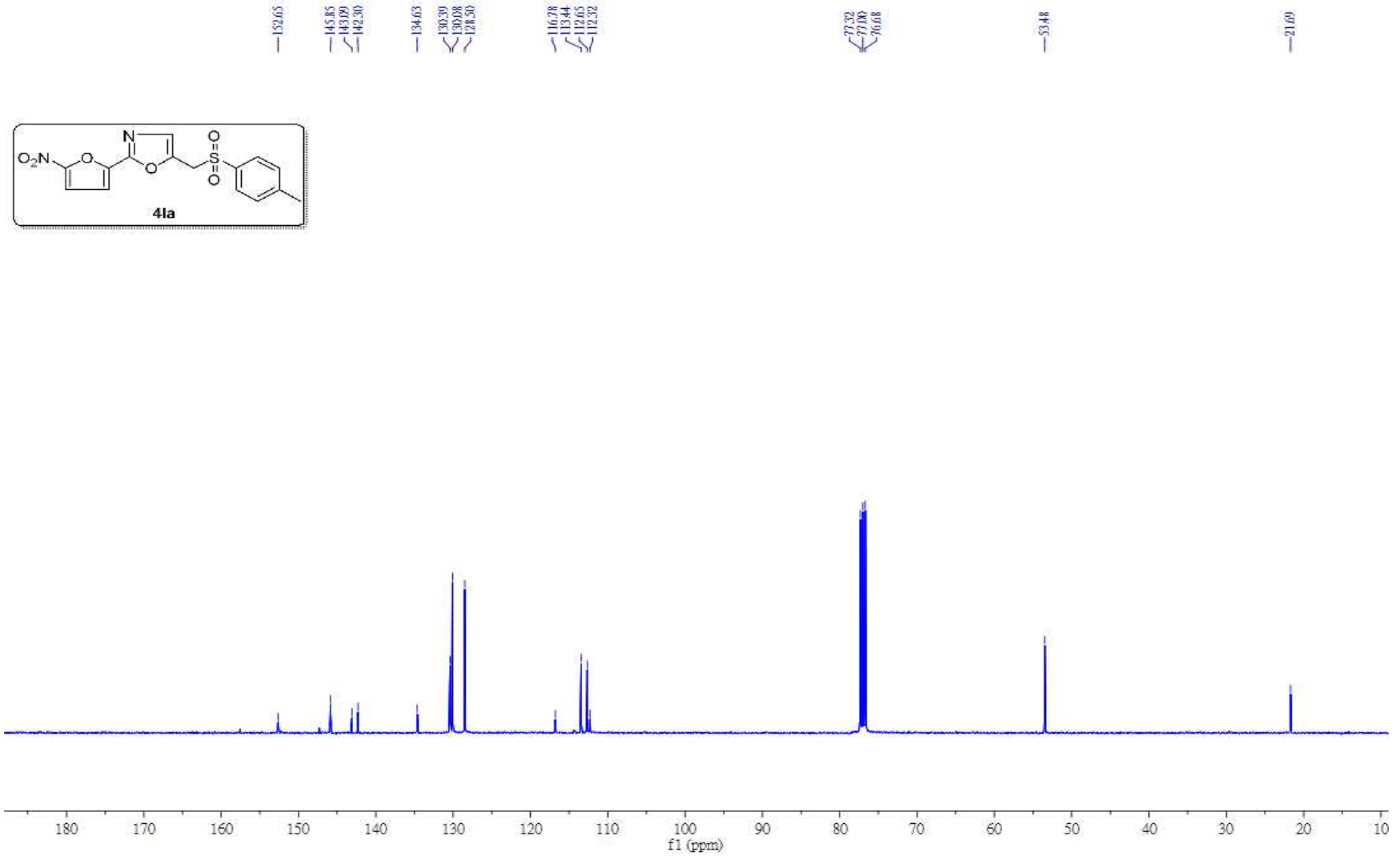

Vera-RP2-148
Pulse Sequence: DEPT
4ja
145.653
141.961
134.835
132.054
130.444
129.988
128.567
127.147
124.154
77.319
77.000
76.689
53.693
21.680
180
160
140
120
100
80
60
40
20
ppm

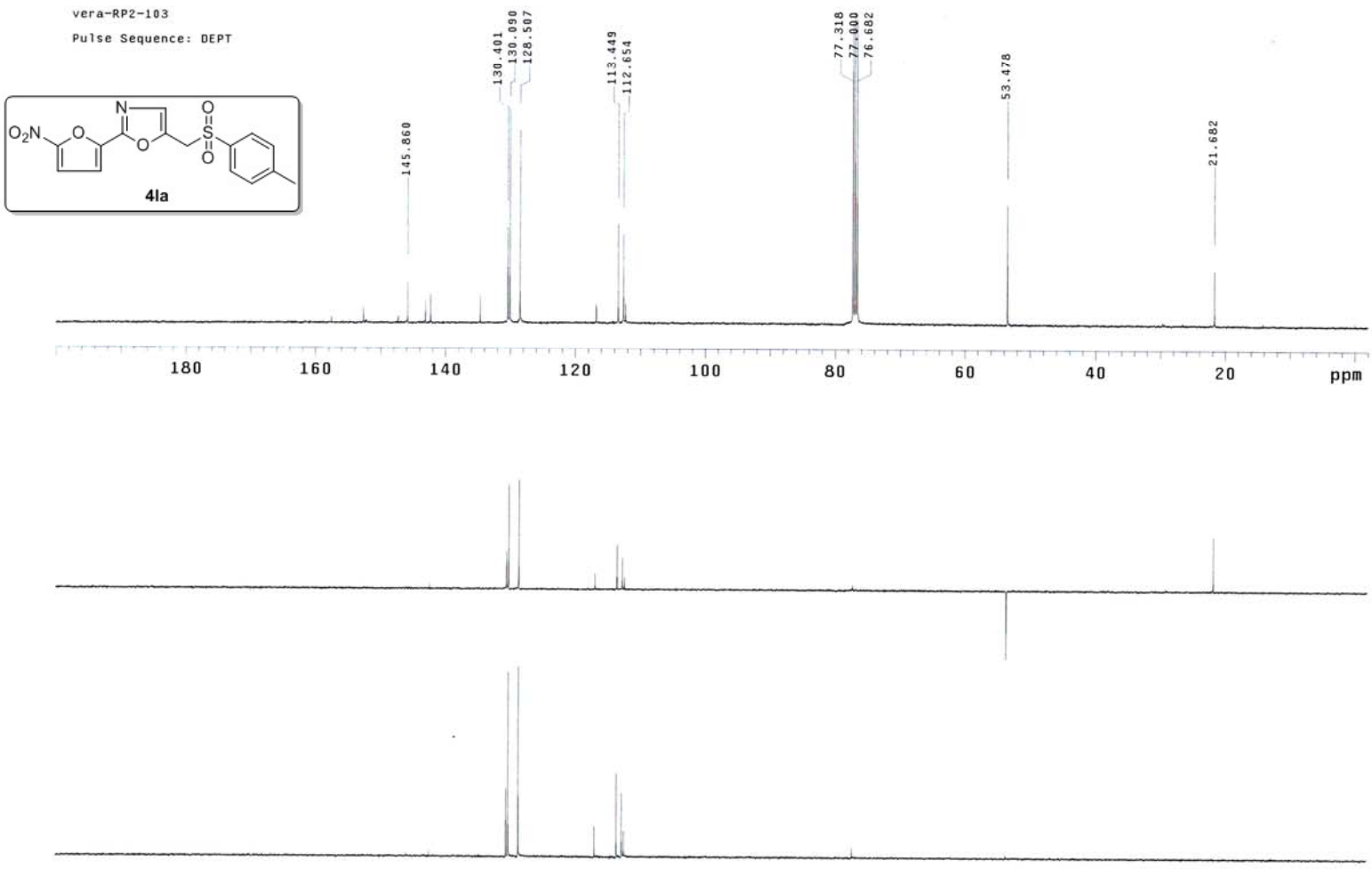

Solvent: CDCl3
Frequency: 400.40 MHz
4ka
f1 (ppm)

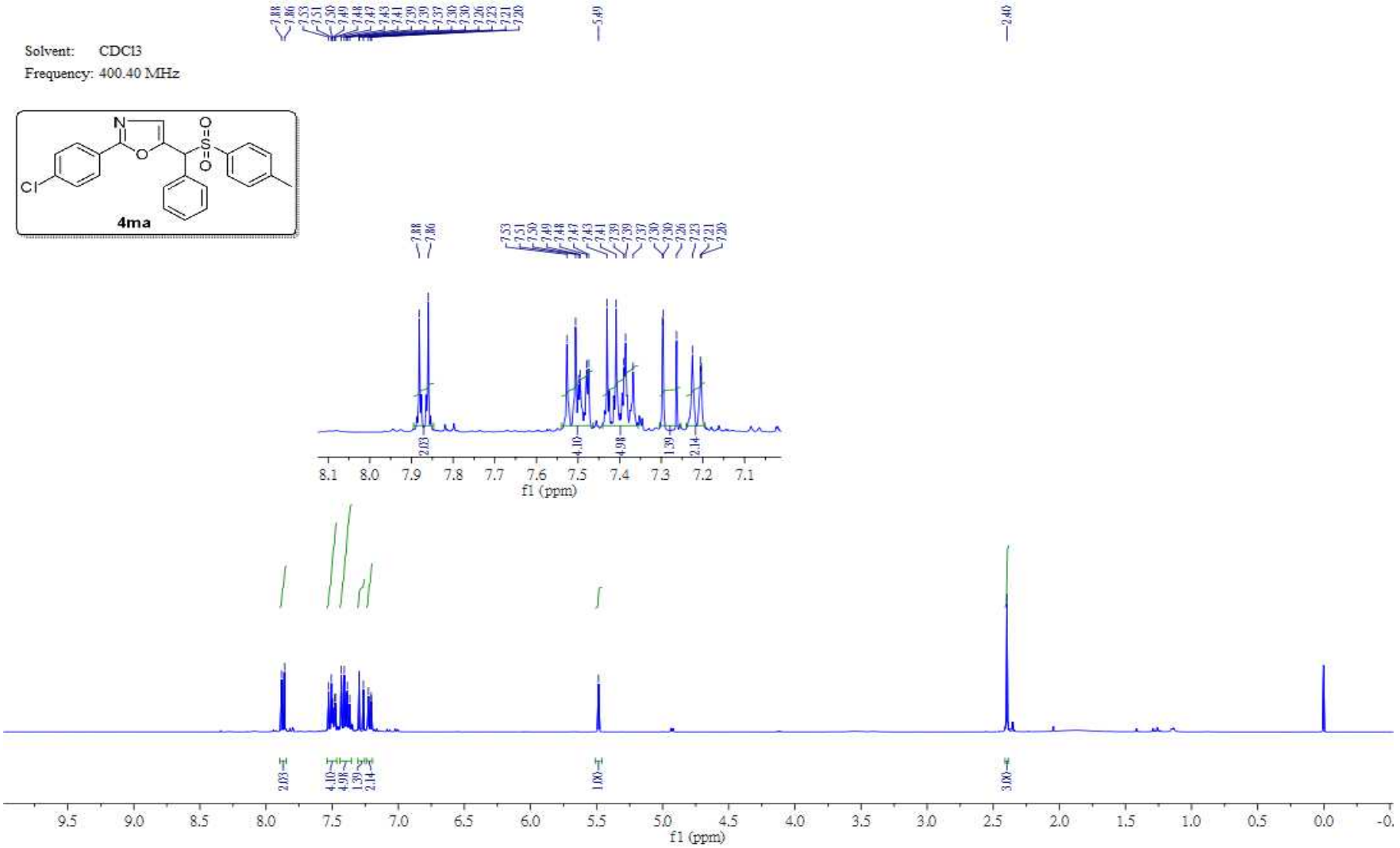

145.43
140.02
134.85
129.95
128.60
127.89
77.32
77.00
76.68
53.52
31.70
29.24
29.09
29.02
28.86
27.88
26.67
22.48
21.50
13.91
4ka
f1 (ppm)

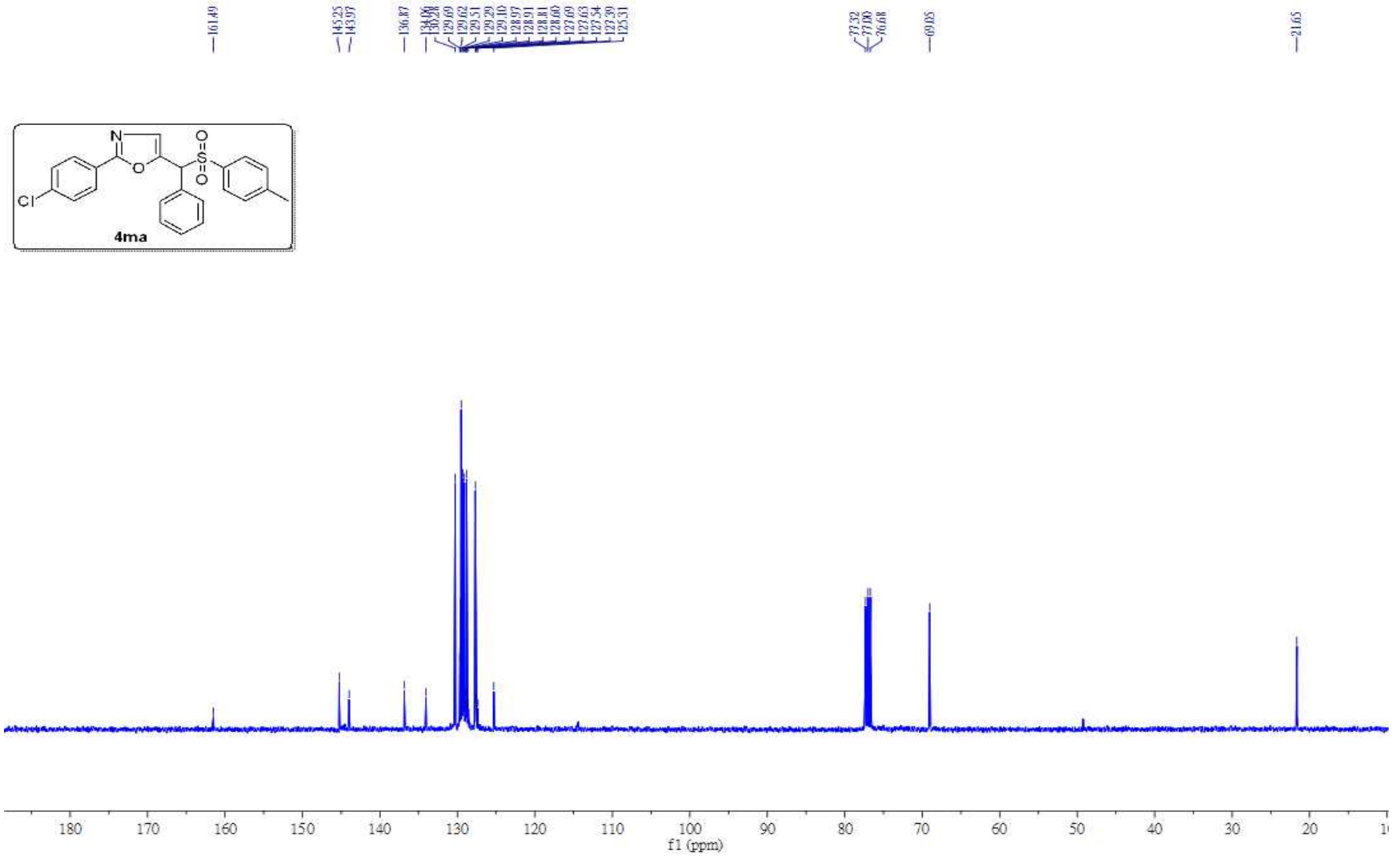

Vera-RP2-156
Pulse Sequence: DEPT
4ka
145.440
140.031
134.858
129.958
128.598
127.891
77.319
77.000
76.681
53.511
31.692
29.231
29.087
29.011
28.859
27.871
26.663
22.477
21.497
13.901
180
160
140
120
100
80
60
40
20
ppm

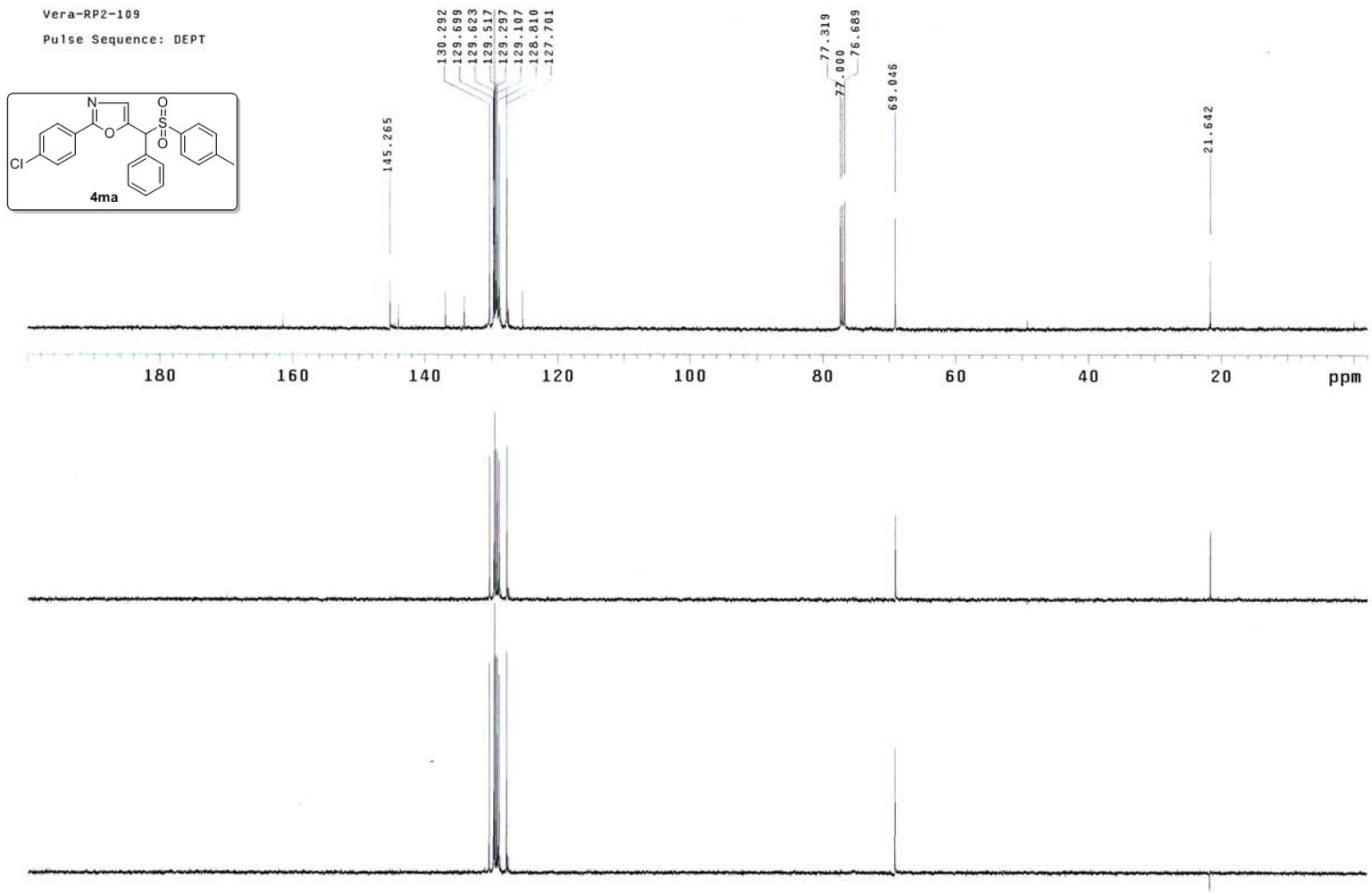

Solvent: CDCl3
Frequency: 400.40 MHz
4la
f1 (ppm)

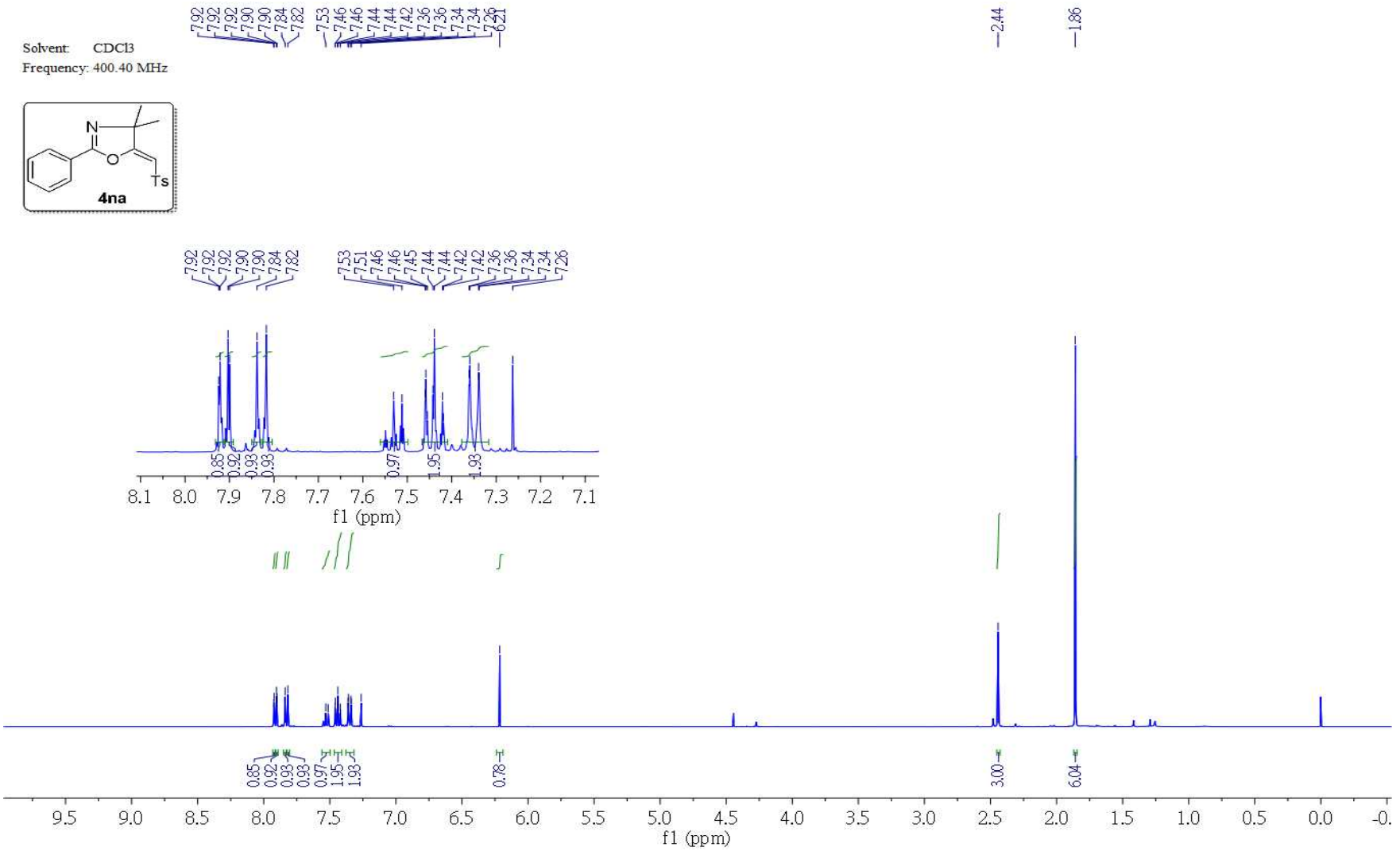

152.65
145.85
143.09
142.30
134.63
130.39
130.08
128.50
116.78
113.44
112.65
112.32
77.32
77.00
76.68
53.48
21.69
4la
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

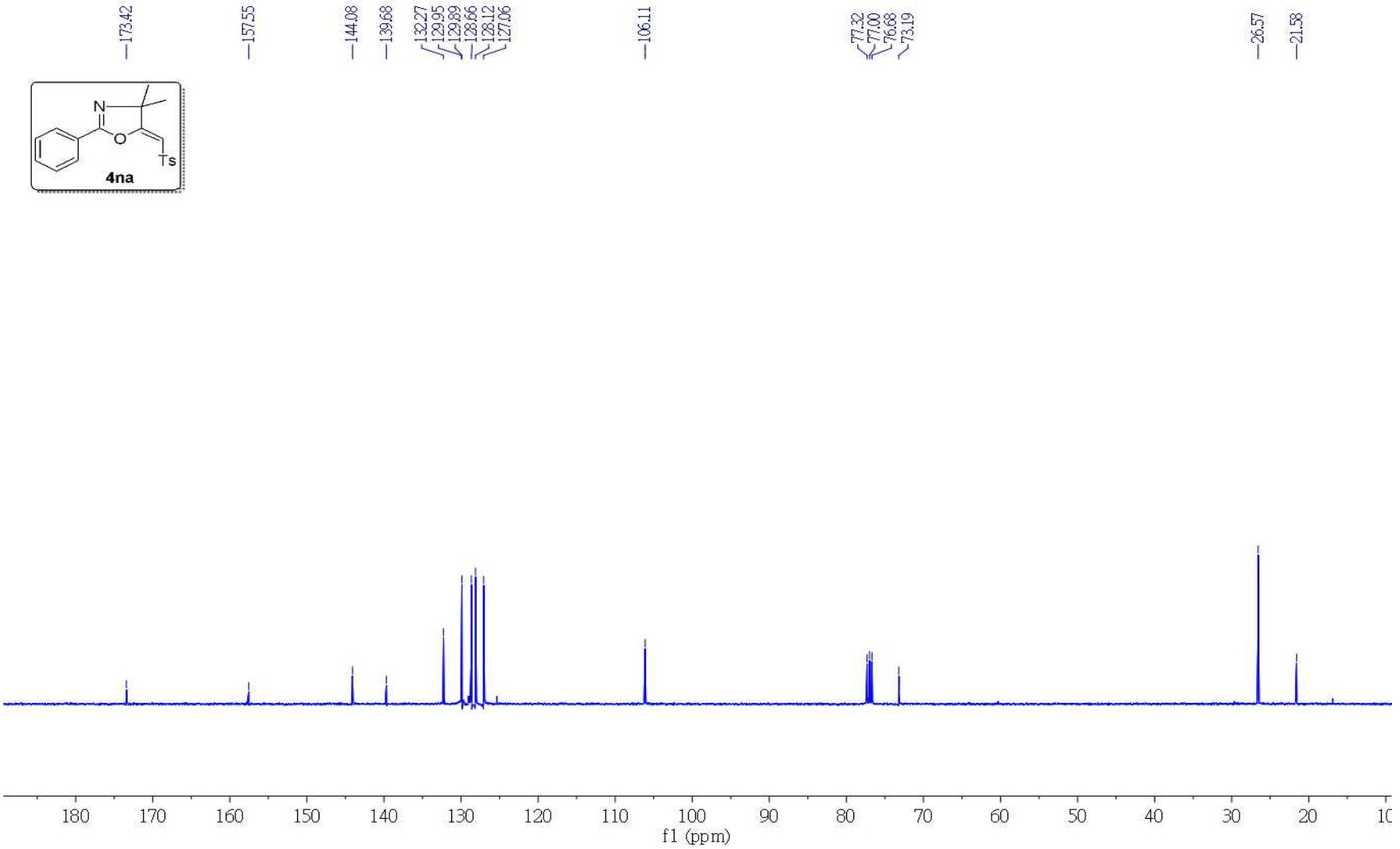

vera-RP2-103
Pulse Sequence: DEPT
4la
145.860
130.401
130.090
128.507
113.449
112.654
77.318
77.000
76.682
53.478
21.682
180
160
140
120
100
80
60
40
20
ppm

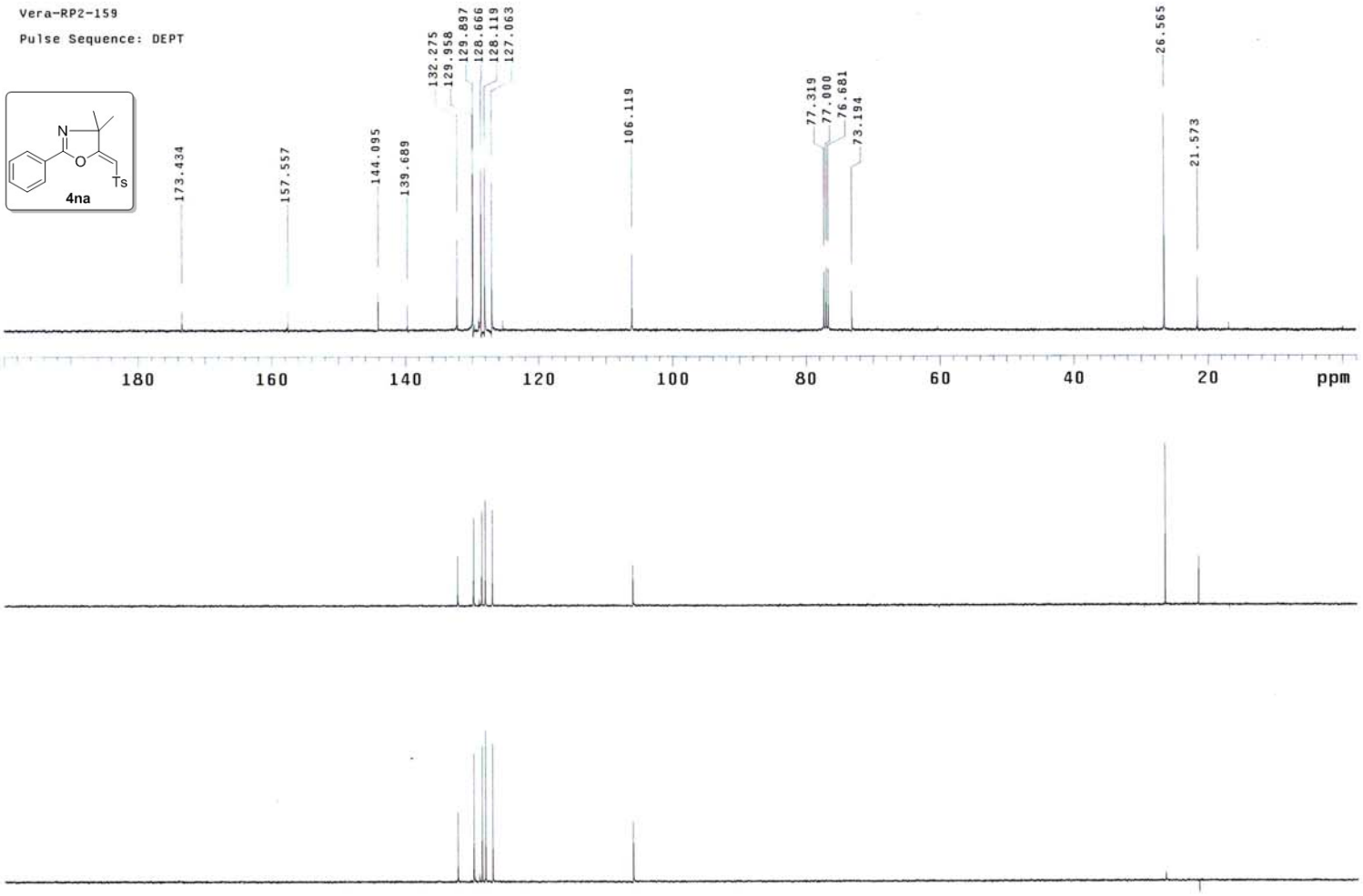

Solvent: CDCl3
Frequency: 400.40 MHz
4ma
f1 (ppm)

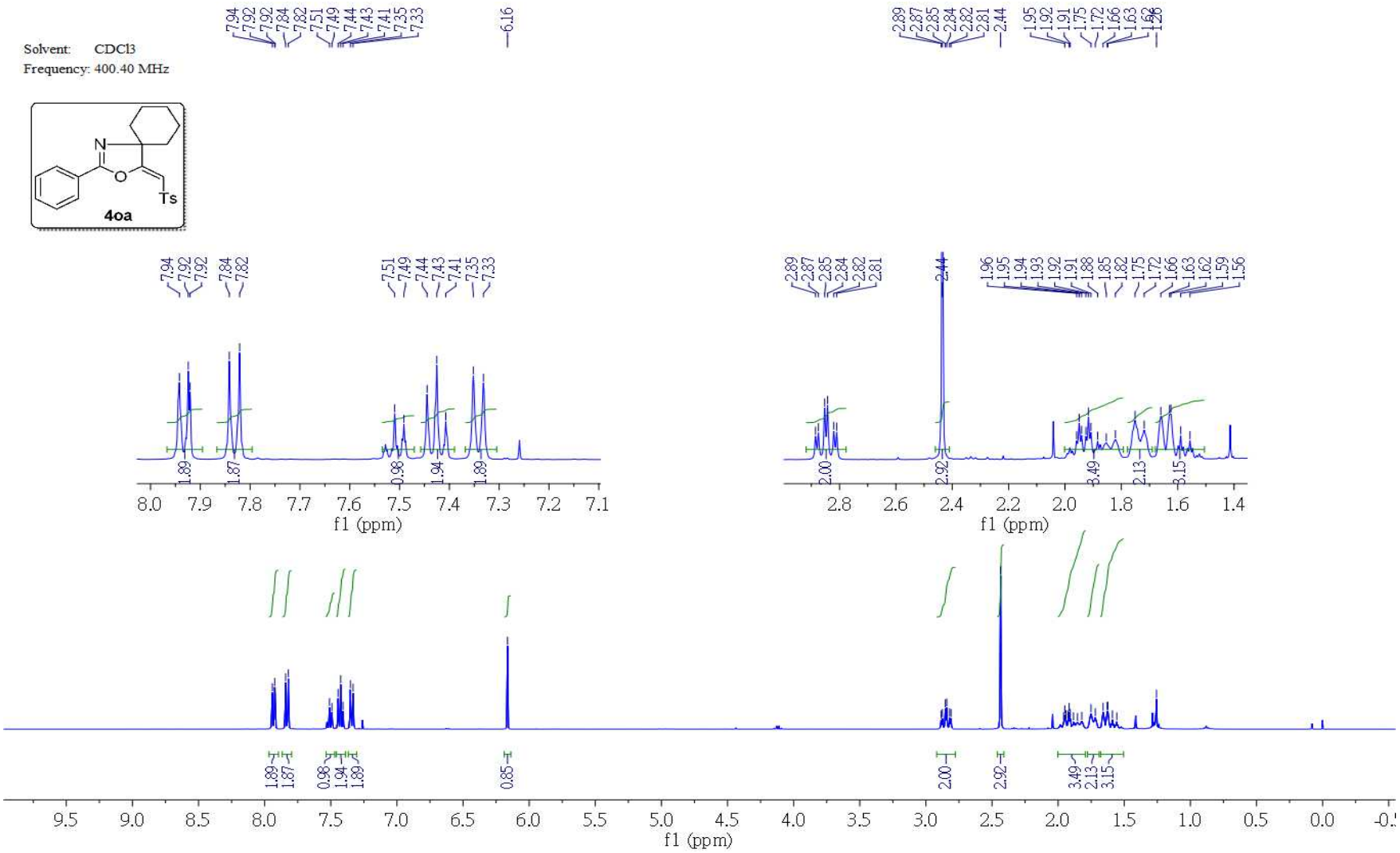

161.49
145.25
143.97
136.87
134.06
130.88
130.28
129.69
129.62
129.51
129.29
129.10
128.97
128.91
128.81
128.66
127.69
127.63
127.54
127.39
125.31
77.32
77.00
76.68
69.05
21.65
Cl
N
O
S
O
O
4ma
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

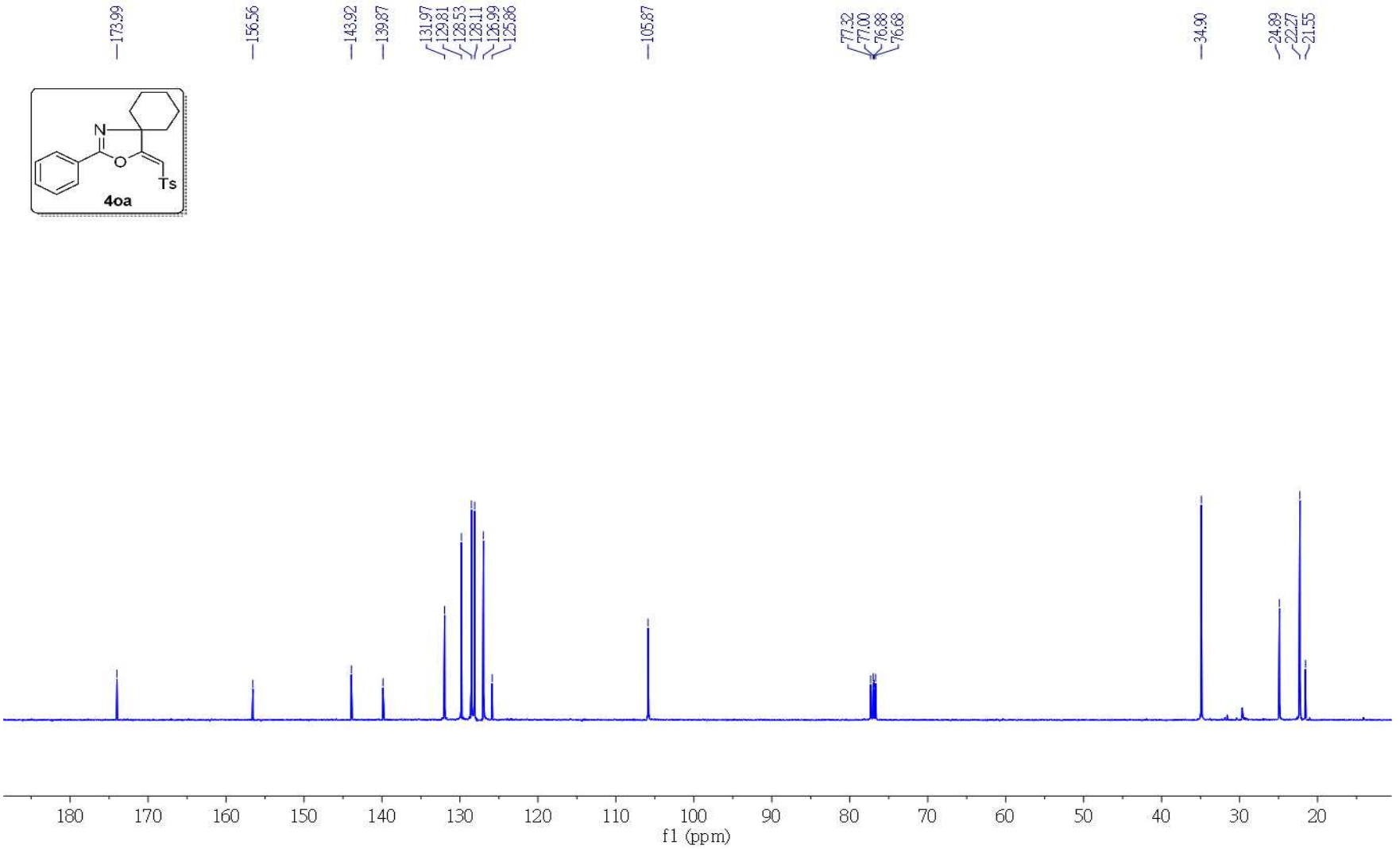

Vera-RP2-109
Pulse Sequence: DEPT
4ma
145.265
130.292
129.699
129.623
129.517
129.297
129.107
128.810
127.701
77.319
77.000
76.689
69.046
21.642
180
160
140
120
100
80
60
40
20
ppm

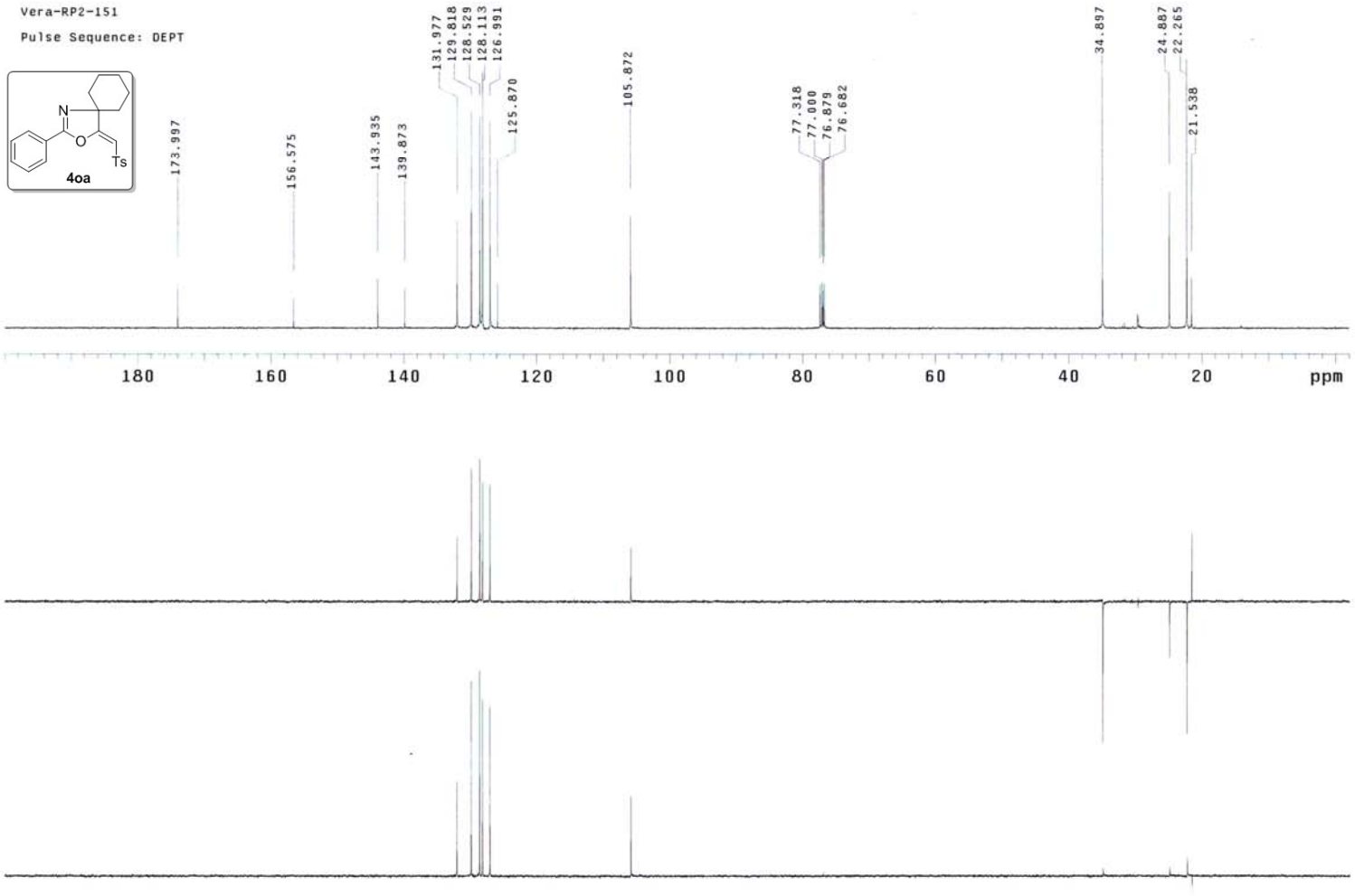

Solvent: CDCl3
Frequency: 400.40 MHz
4na
f1 (ppm)

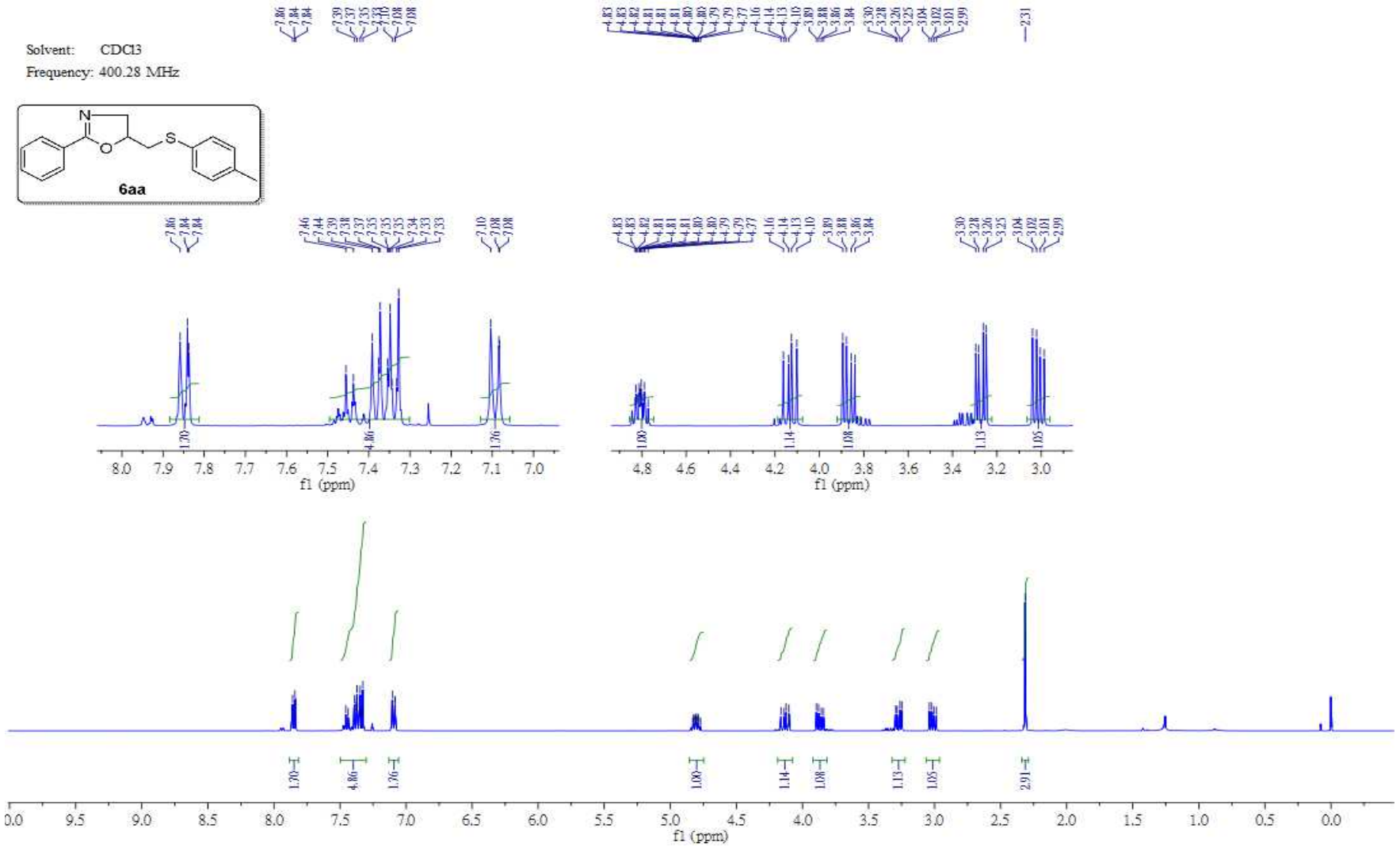

173.42
157.55
144.08
139.68
132.27
129.95
129.89
128.66
128.12
127.06
106.11
77.32
77.00
76.68
73.19
26.57
21.58
N
O
Ts
4na
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

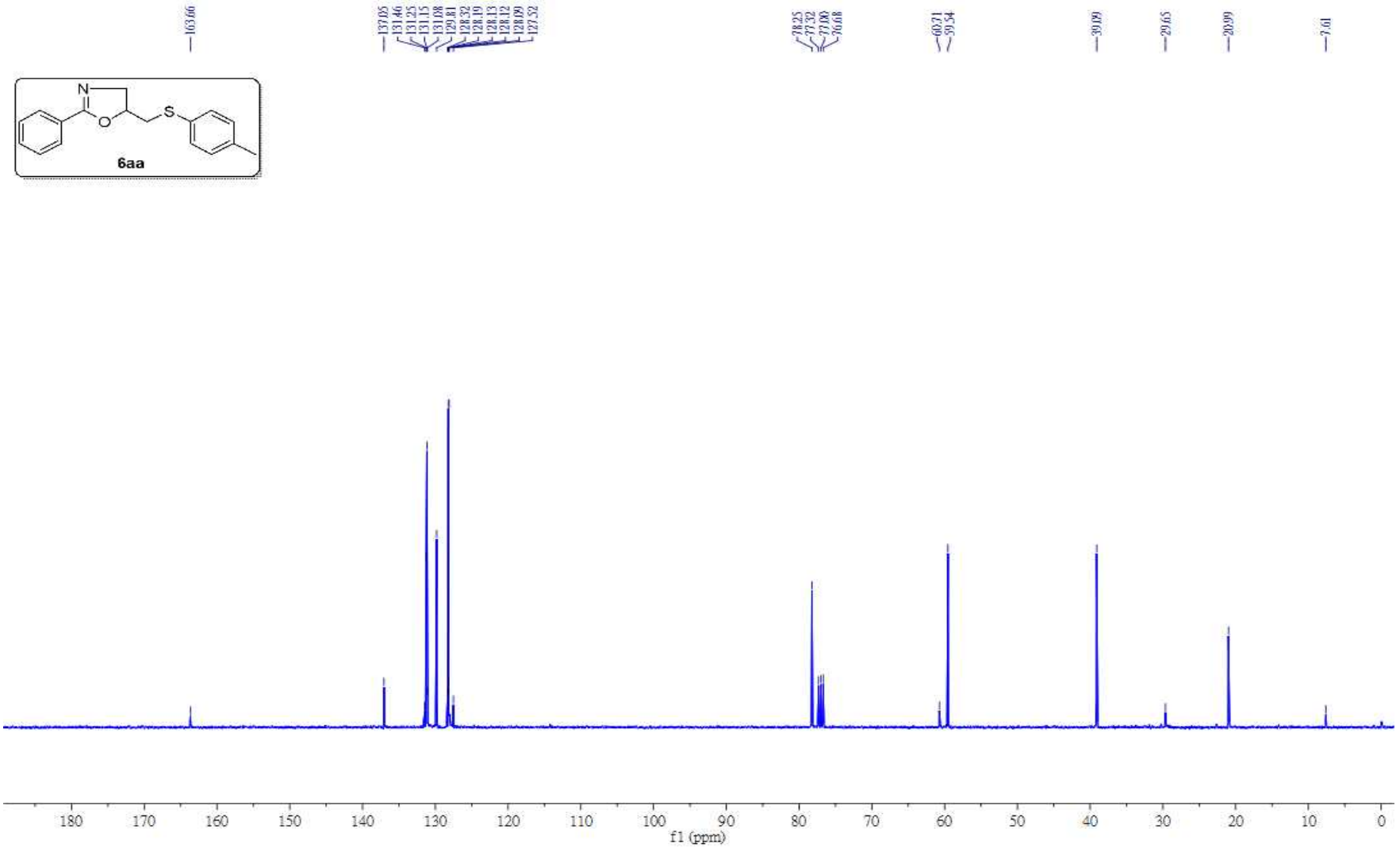

Vera-RP2-159
Pulse Sequence: DEPT
4na
Ts
173.434
157.557
144.095
139.689
132.275
129.958
129.897
128.666
128.119
127.063
106.119
77.319
77.000
76.681
73.194
26.565
21.573
180
160
140
120
100
80
60
40
20
ppm

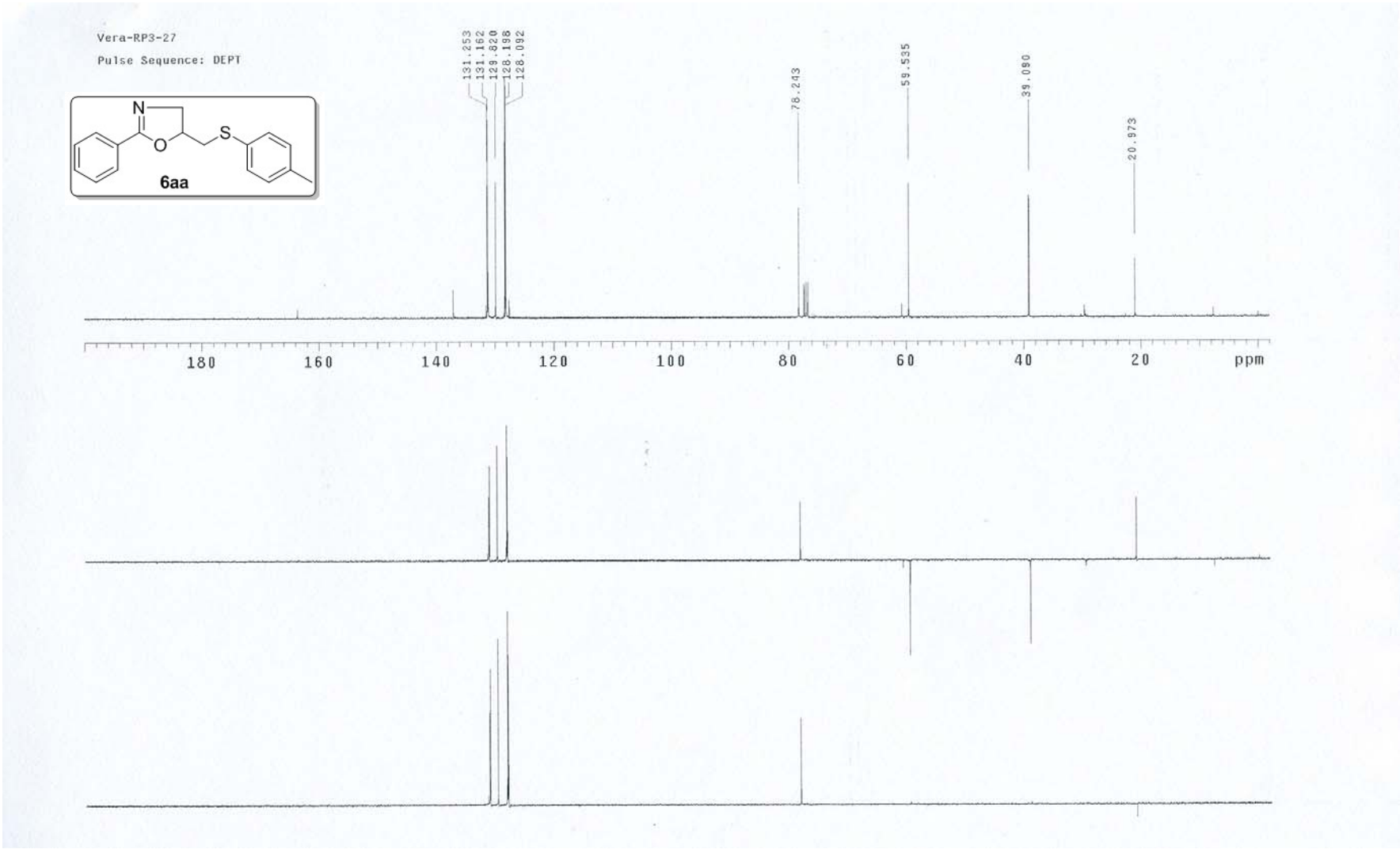

Solvent: CDCl3
Frequency: 400.40 MHz
4oa
f1 (ppm)

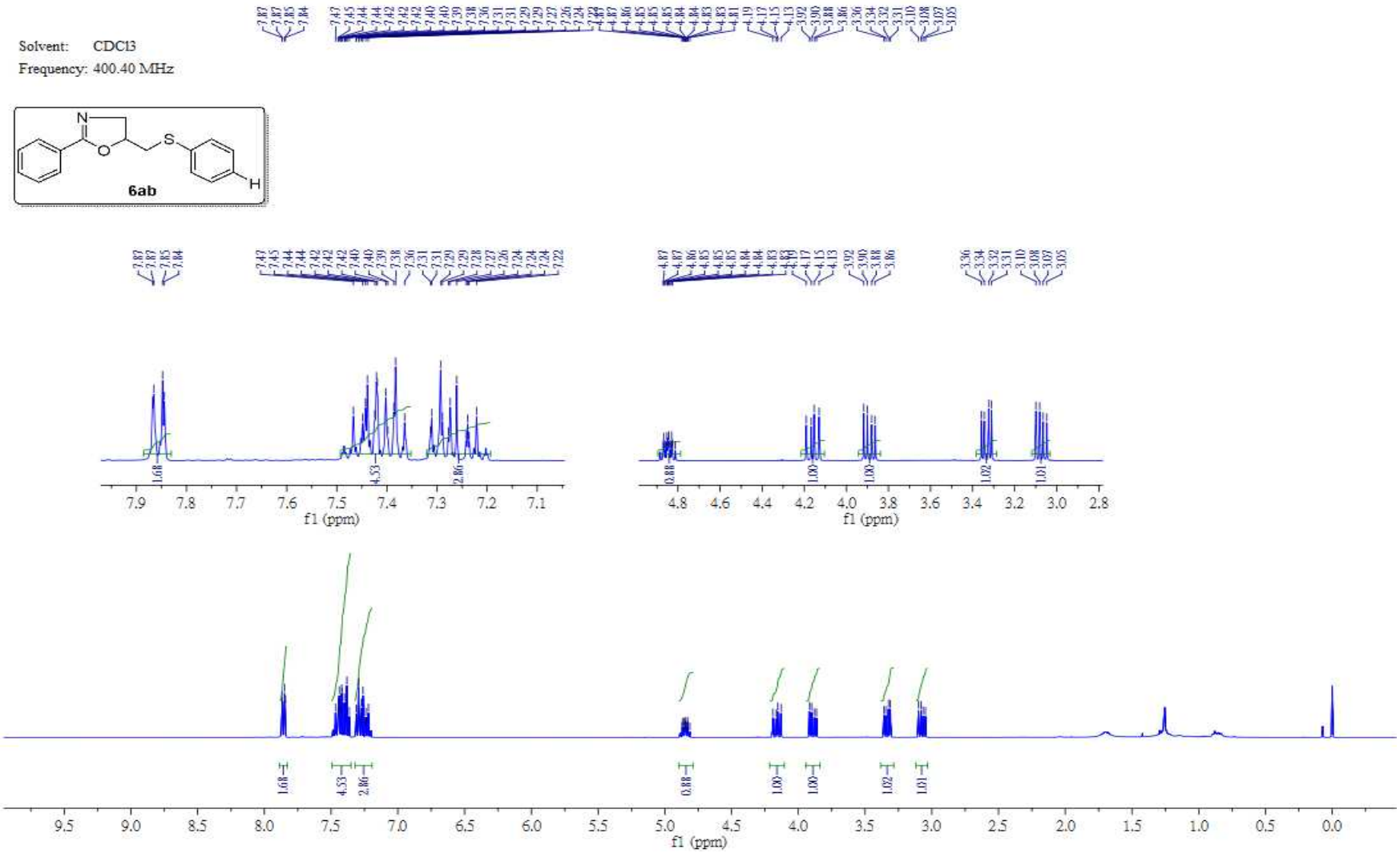

173.99
156.56
143.92
139.87
131.97
129.81
128.53
128.11
126.99
125.86
105.87
77.32
77.00
76.88
76.68
34.90
24.89
22.27
21.55
N
O
Ts
4oa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

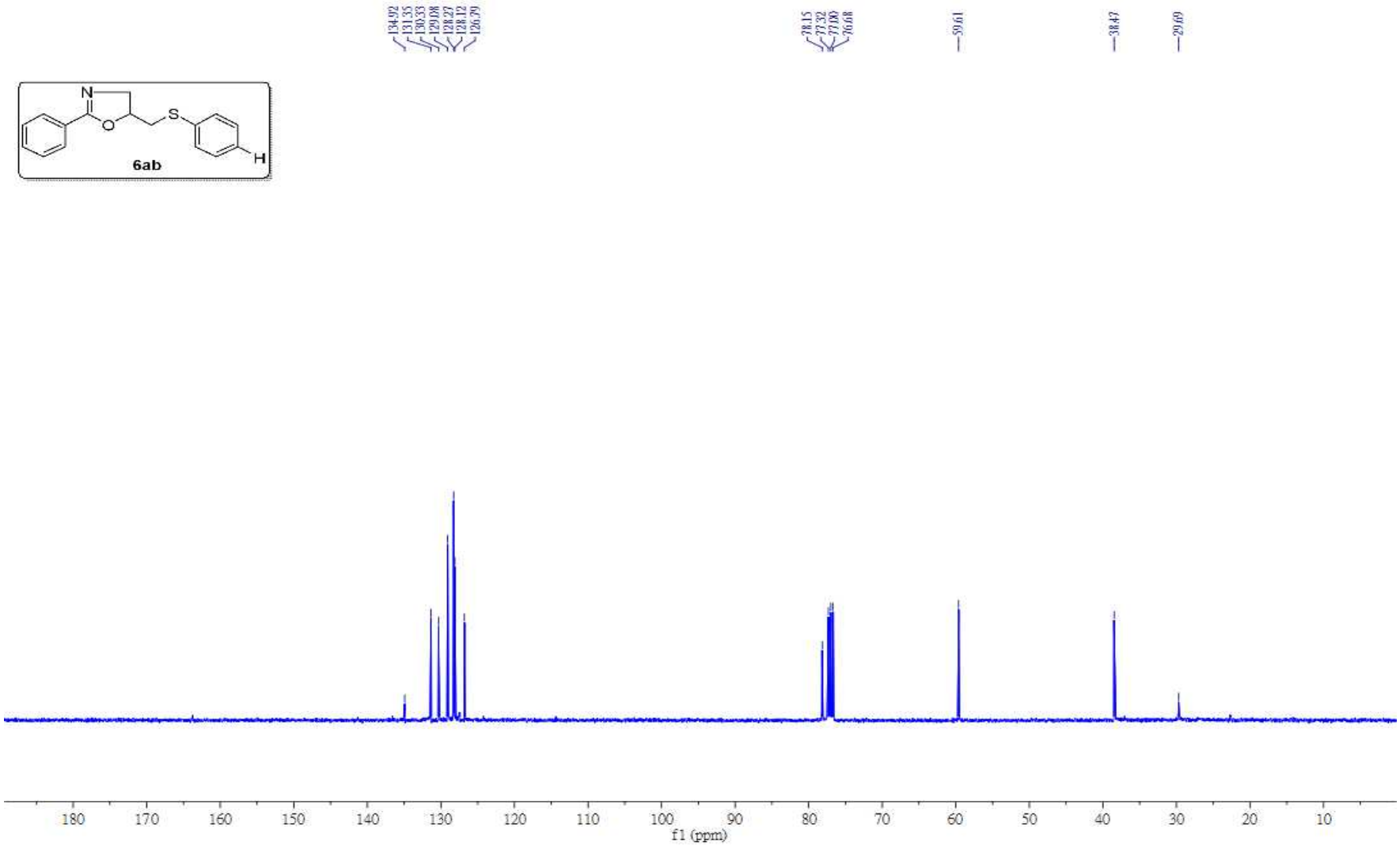

Vera-RP2-151
Pulse Sequence: DEPT
4oa
173.997
156.575
143.935
139.873
131.977
129.818
128.529
128.113
126.991
125.870
105.872
77.318
77.000
76.879
76.682
34.897
24.887
22.265
21.538
180
160
140
120
100
80
60
40
20
ppm

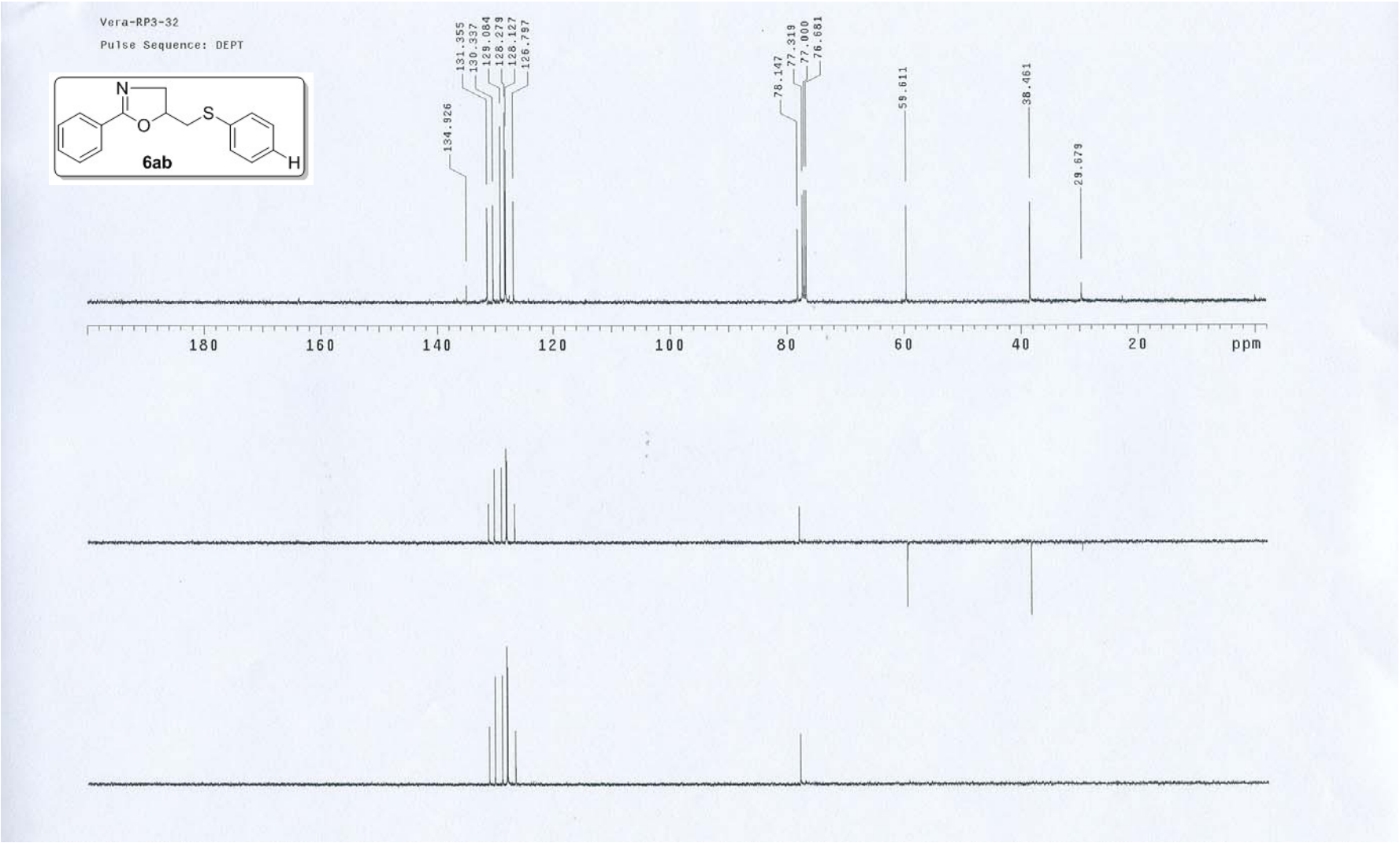

Solvent: CDCl3
Frequency: 400.28 MHz
6aa
f1 (ppm)
f1 (ppm)
f1 (ppm)

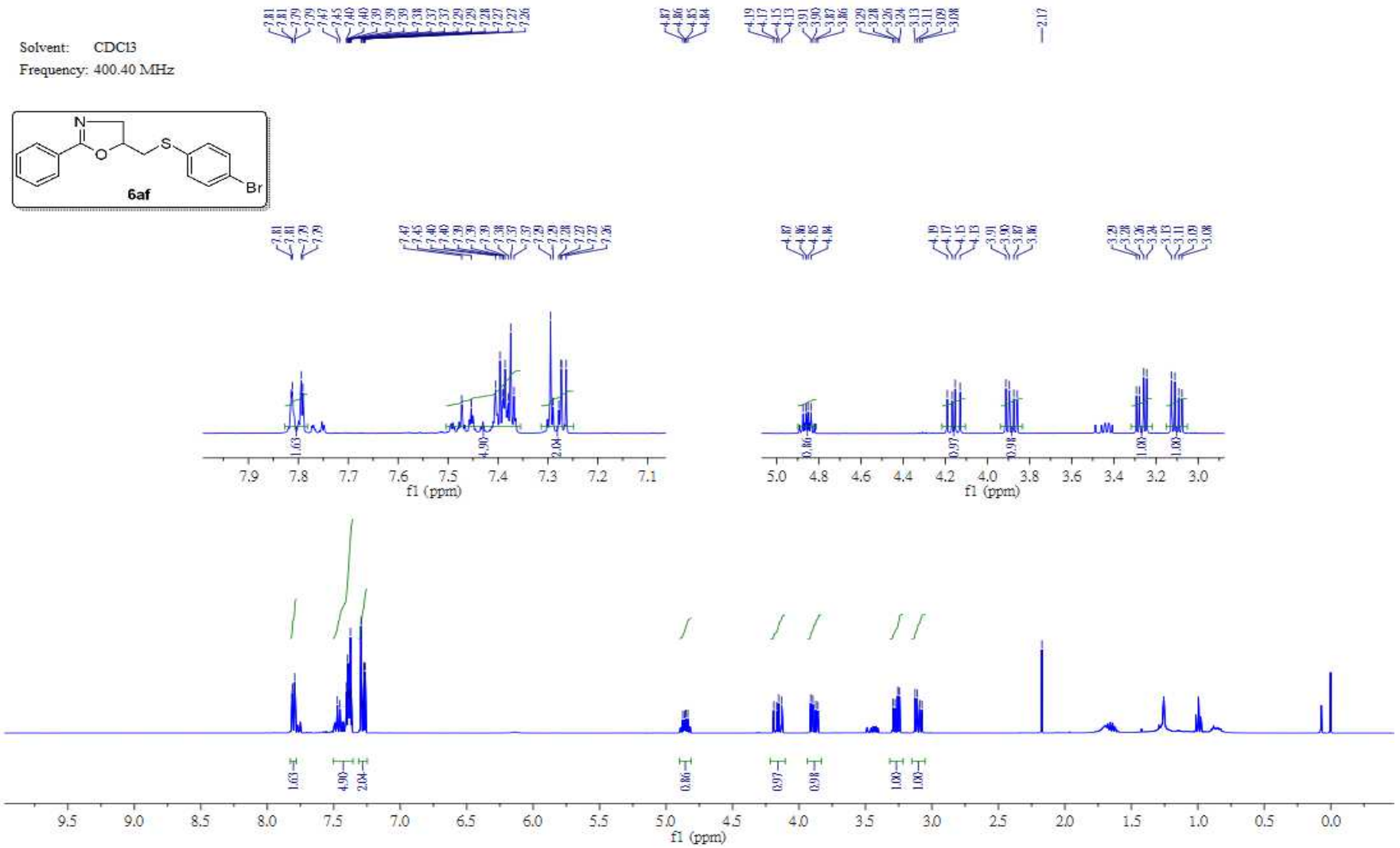

163.66
137.05
131.46
131.25
131.15
131.08
129.81
128.32
128.19
128.13
128.12
128.09
127.52
78.25
77.32
77.00
76.68
60.71
59.54
39.09
29.65
20.99
7.61
6aa
N
O
S
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

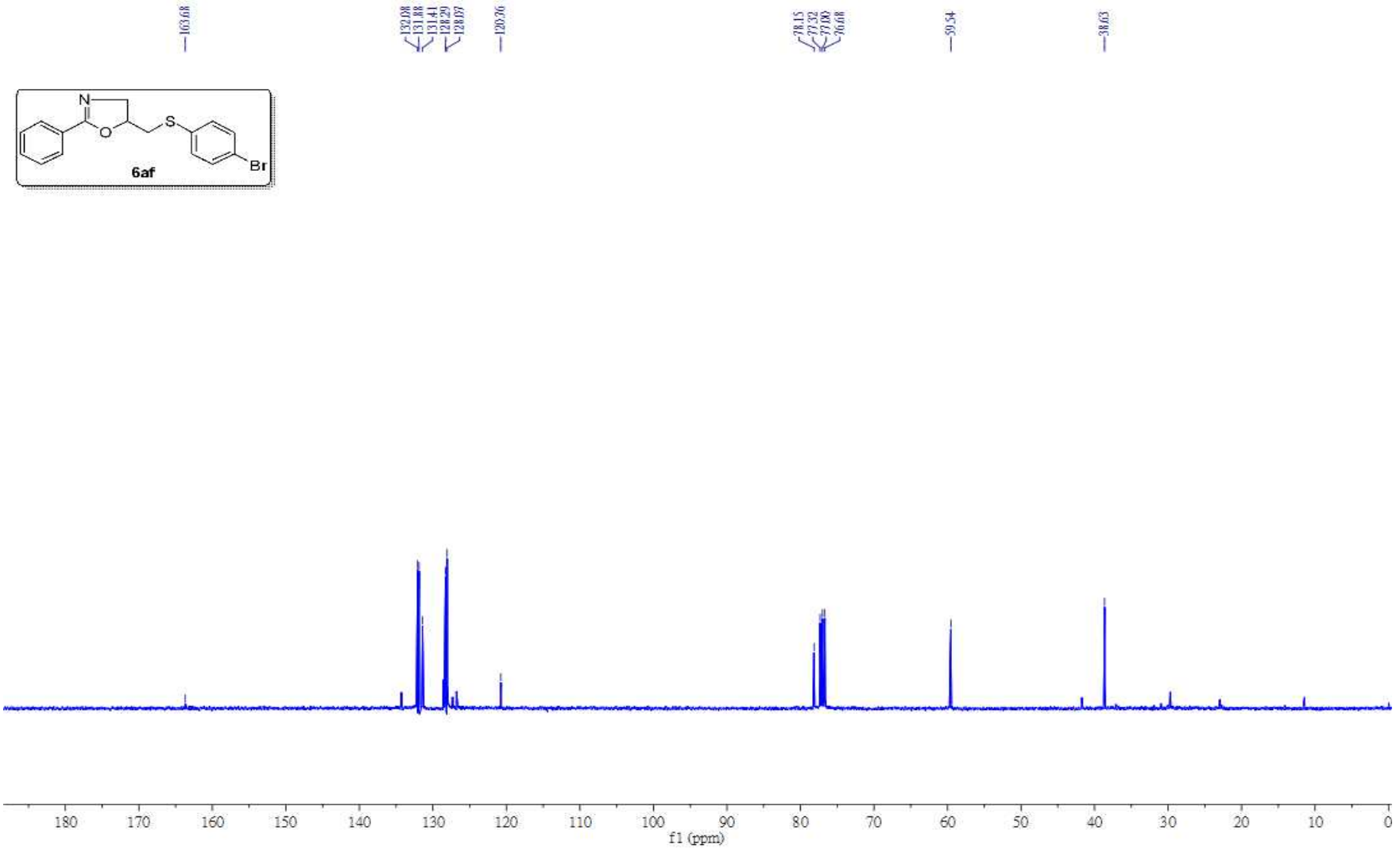

Vera-RP3-27
Pulse Sequence: DEPT
N
O
S
6aa
131.253
131.162
129.820
128.198
128.092
78.243
59.535
39.080
20.973
180
160
140
120
100
80
60
40
20
ppm

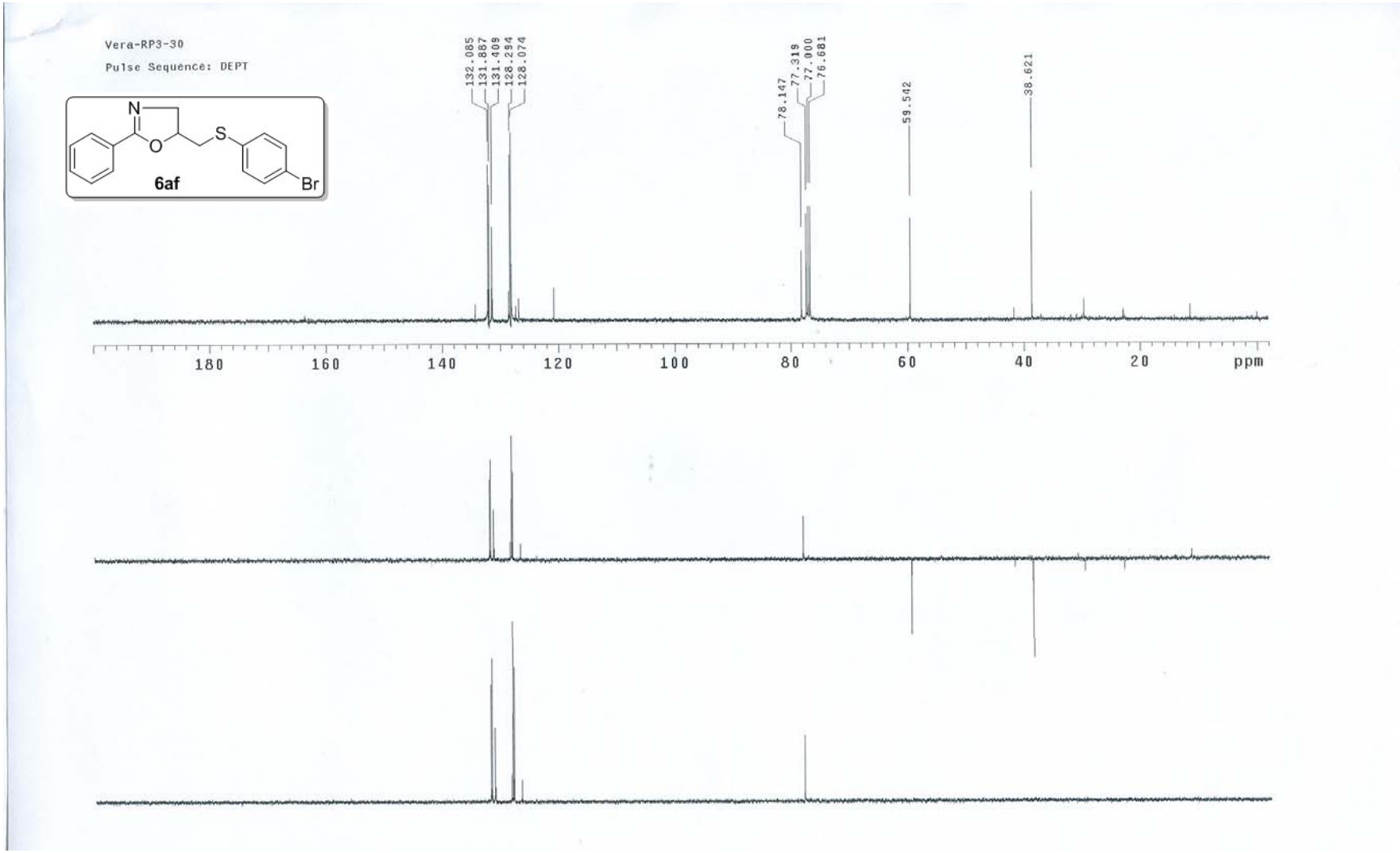

Solvent: CDCl3
Frequency: 400.40 MHz
6ab
f1 (ppm)

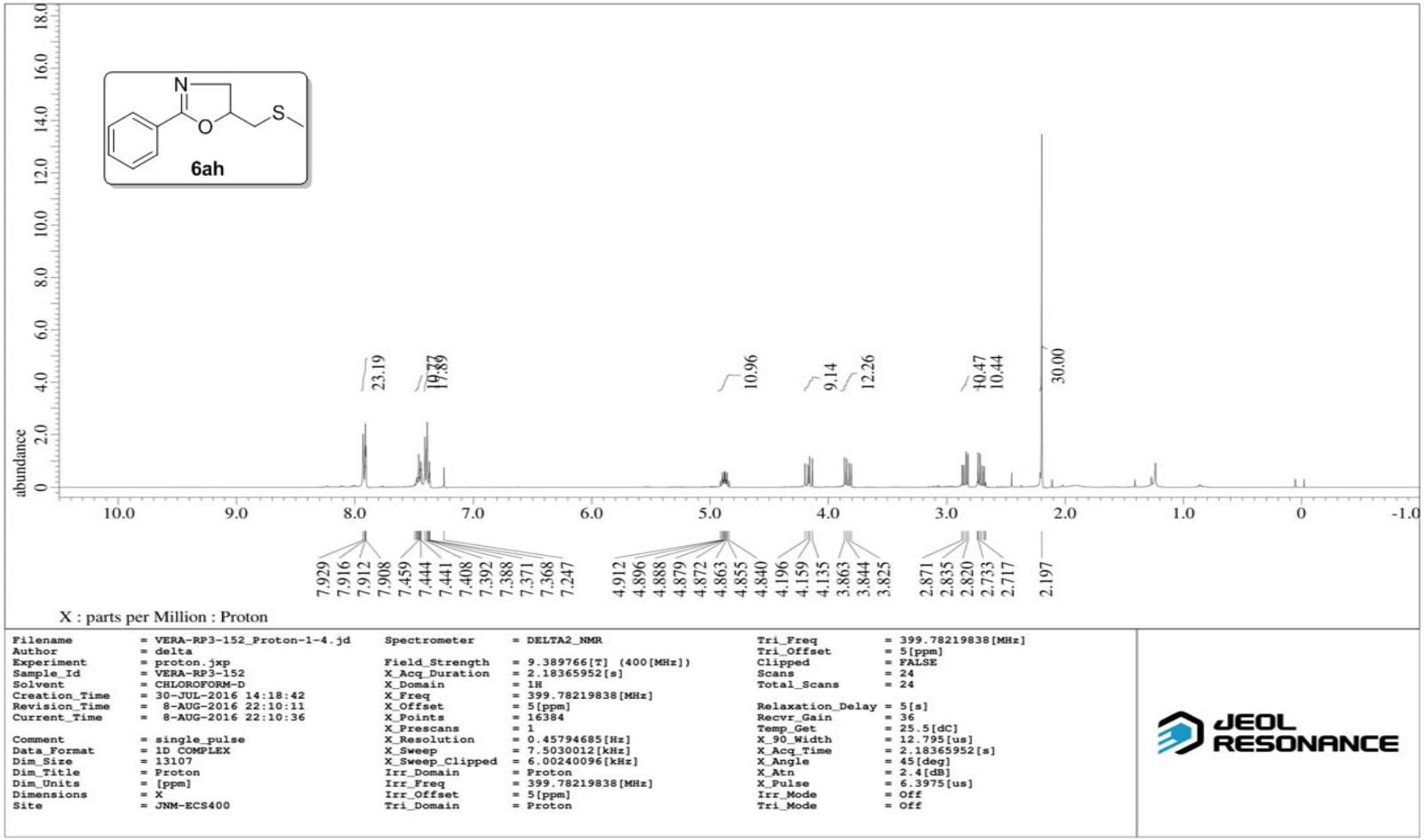

134.92
131.35
130.33
129.08
128.27
128.12
126.79
78.15
77.32
77.00
76.68
59.61
38.47
29.69
N
O
S
H
6ab
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

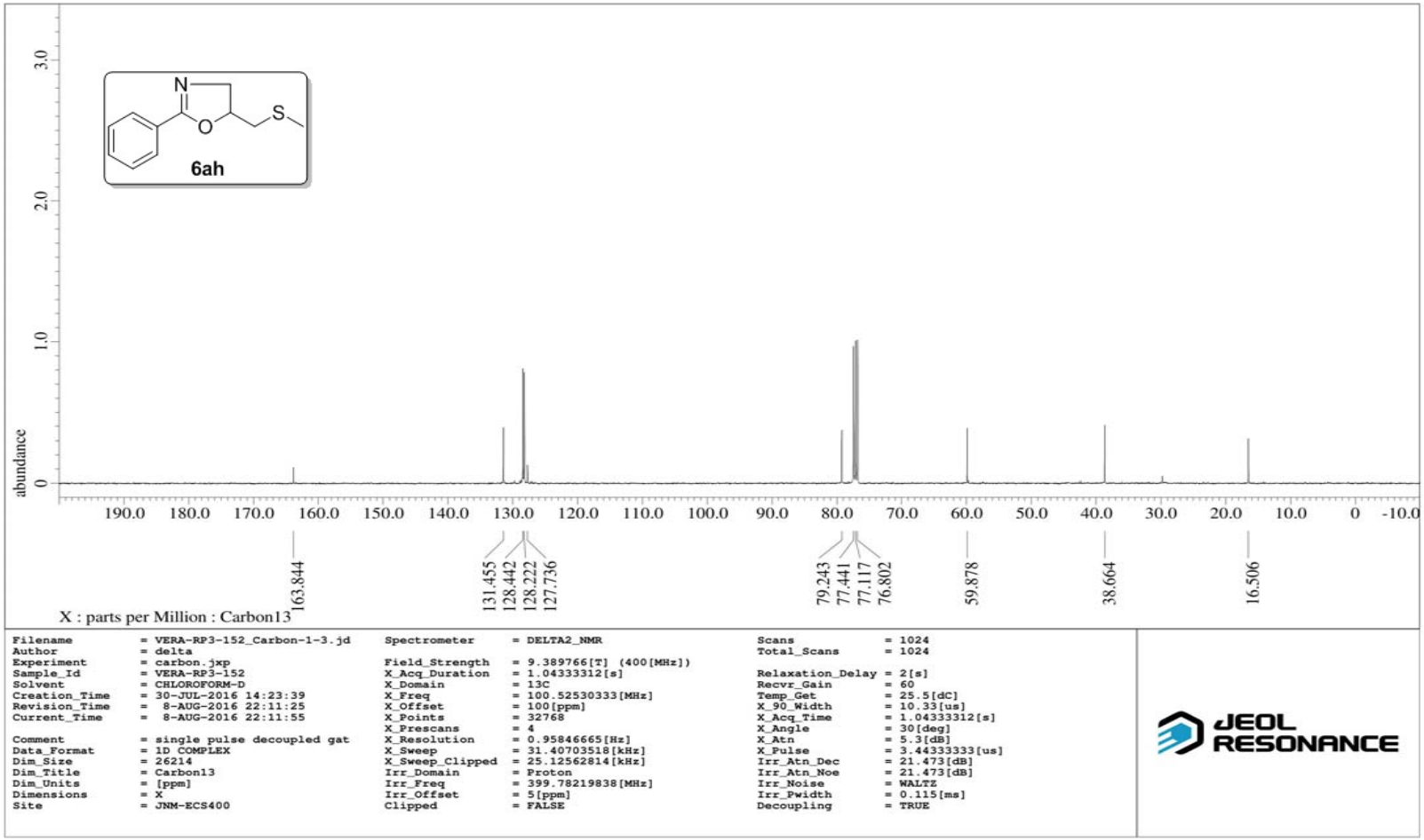

Vera-RP3-32
Pulse Sequence: DEPT
N
O
S
H
6ab
134.926
131.355
130.337
129.084
128.279
128.127
126.797
78.147
77.319
77.000
76.681
59.611
38.461
29.679
180
160
140
120
100
80
60
40
20
ppm


Solvent: CDCl3
Frequency: 400.40 MHz
6af
f1 (ppm)

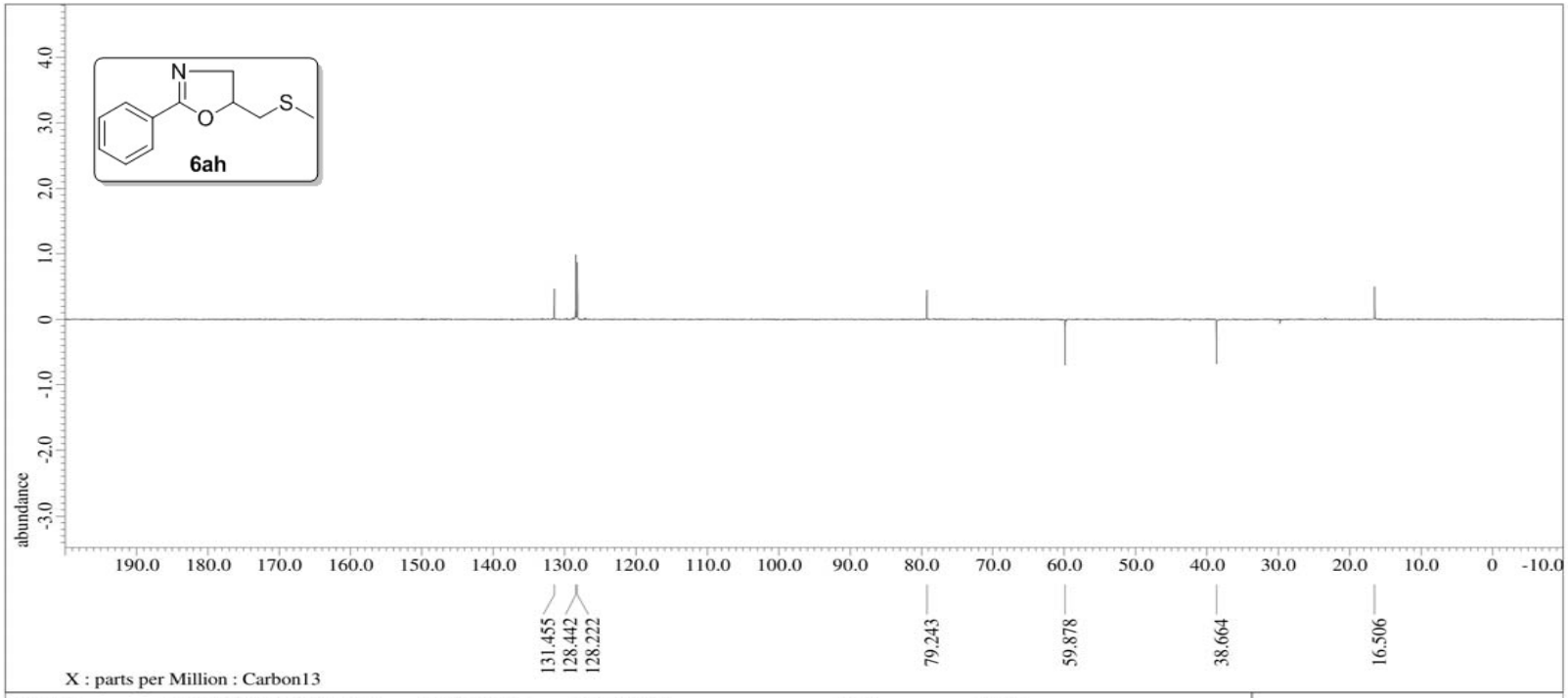

163.68
132.08
131.88
131.41
128.29
128.07
120.36
78.15
77.32
77.00
76.68
59.54
38.63
N
O
S
Br
6af
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Vera-RP3-30
Pulse Sequence: DEPT
N
O
S
Br
6af
132.085
131.887
131.409
128.294
128.074
78.147
77.319
77.000
76.681
59.542
38.621
180
160
140
120
100
80
60
40
20
ppm

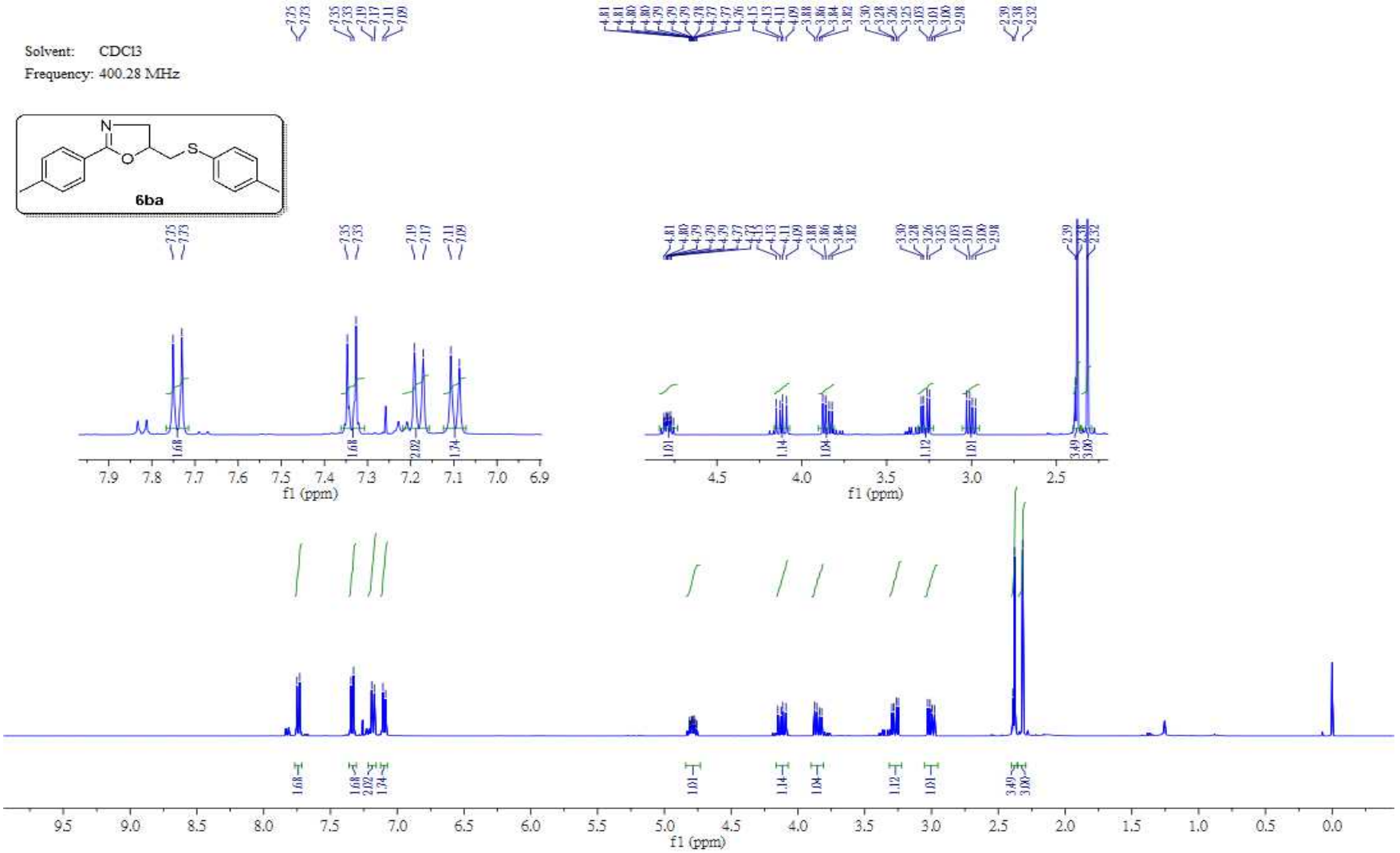

6ah
abundance
23.19
19.77
19.39
10.96
9.14
12.26
10.47
10.44
30.00
7.929
7.916
7.912
7.908
7.459
7.444
7.441
7.408
7.392
7.388
7.371
7.368
7.247
4.912
4.896
4.888
4.879
4.872
4.863
4.855
4.840
4.196
4.159
4.135
3.863
3.844
3.825
2.871
2.835
2.820
2.733
2.717
2.197
X : parts per Million : Proton
Filename = VERA-RP3-152_Proton-1-4.jd
Author = delta
Experiment = proton.jxp
Sample_Id = VERA-RP3-152
Solvent = CHLOROFORM-D
Creation_Time = 30-JUL-2016 14:18:42
Revision_Time = 8-AUG-2016 22:10:11
Current_Time = 8-AUG-2016 22:10:36
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
X_Sweep_Clipped = 6.00240096[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 24
Total_Scans = 24
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 25.5[dC]
X_90_Width = 12.795[us]
X_Acq_Time = 2.18365952[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 6.3975[us]
Irr_Mode = Off
Tri_Mode = Off
JEOL RESONANCE

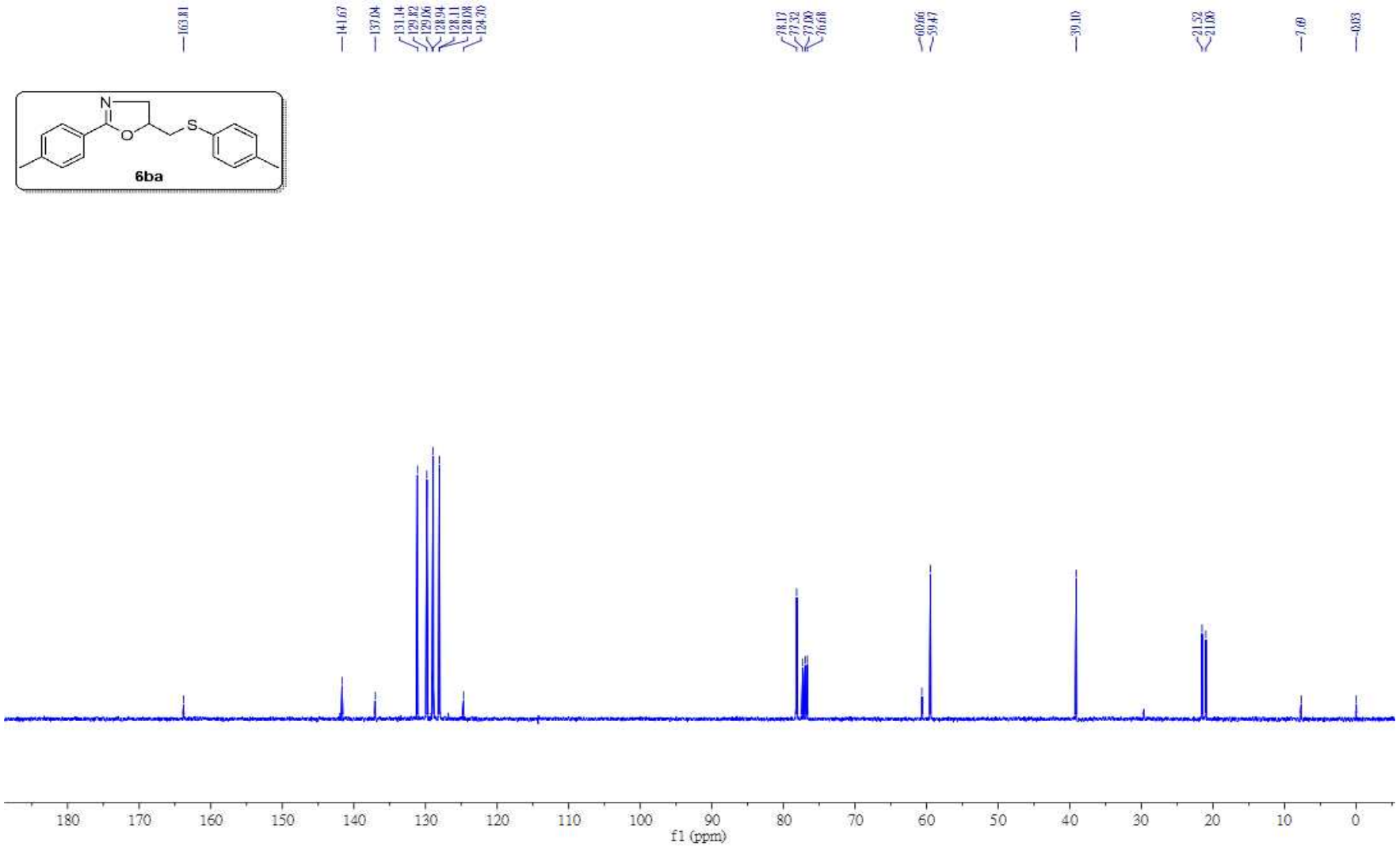


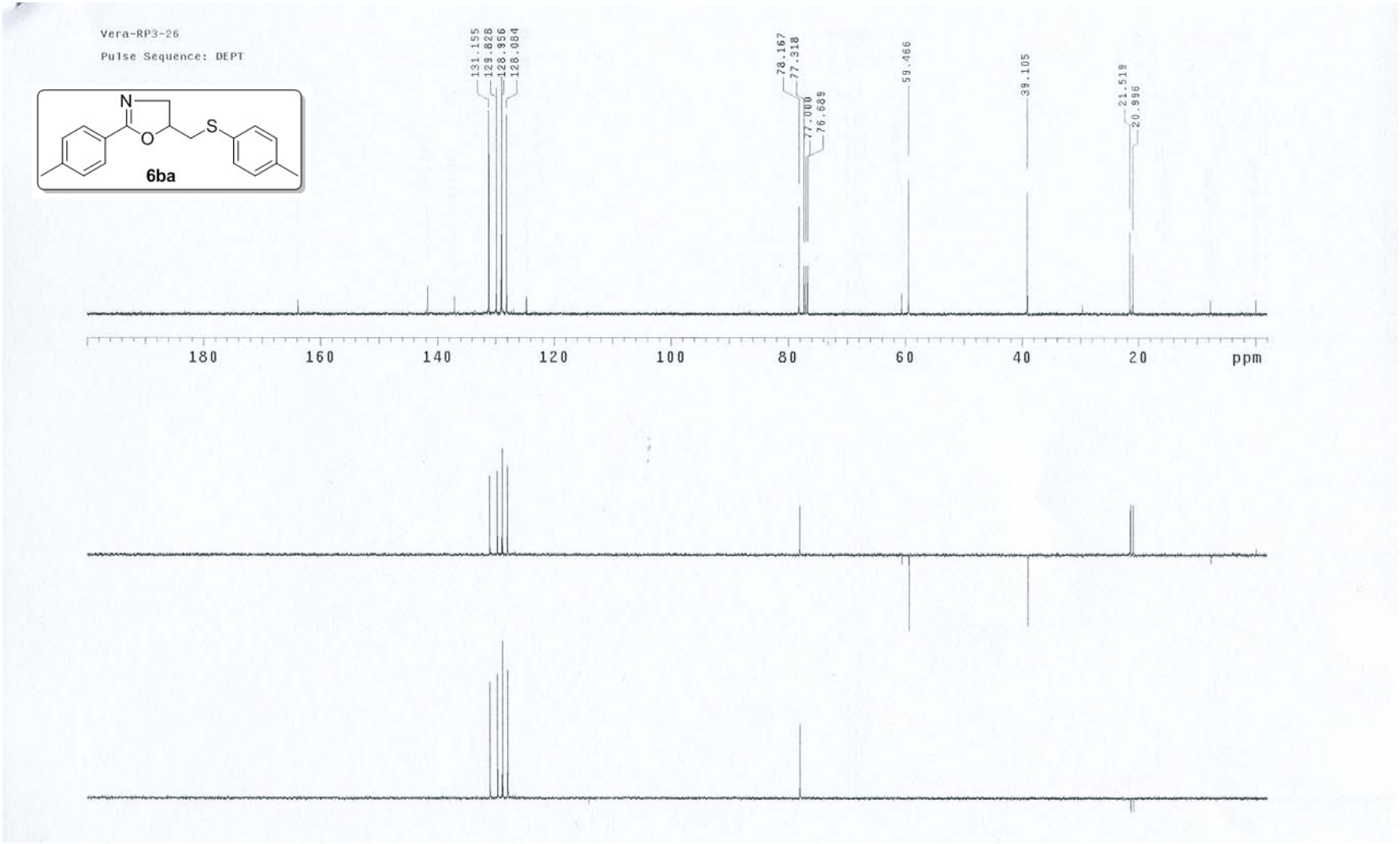
Filename	= VERA-RP3-152_Carbon-1-3.jd	Spectrometer	= DELTA2_NMR	Scans	= 1024
Author	= delta			Total_Scans	= 1024
Experiment	= carbon.jxp	Field_Strength	= 9.389766[T] (400[MHz])		
Sample_Id	= VERA-RP3-152	X_Acq_Duration	= 1.04333312[s]	Relaxation_Delay	= 2[s]
Solvent	= CHLOROFORM-D	X_Domain	= 13C	Recvr_Gain	= 60
Creation_Time	= 30-JUL-2016 14:23:39	X_Freq	= 100.52530333[MHz]	Temp_Get	= 25.5[dC]
Revision_Time	= 8-AUG-2016 22:11:25	X_Offset	= 100[ppm]	X_90_Width	= 10.33[us]
Current_Time	= 8-AUG-2016 22:11:55	X_Points	= 32768	X_Acq_Time	= 1.04333312[s]
		X_Prescans	= 4	X_Angle	= 30[deg]
Comment	= single pulse decoupled gat	X_Resolution	= 0.95846665[Hz]	X_Atn	= 5.3[dB]
Data_Format	= 1D COMPLEX	X_Sweep	= 31.40703518[kHz]	X_Pulse	= 3.44333333[us]
Dim_Size	= 26214	X_Sweep_Clipped	= 25.12562814[kHz]	Irr_Atn_Dec	= 21.473[dB]
Dim_Title	= Carbon13	Irr_Domain	= Proton	Irr_Atn_Noe	= 21.473[dB]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	Irr_Noise	= WALTZ
Dimensions	= X	Irr_Offset	= 5[ppm]	Irr_Pwidth	= 0.115[ms]
Site	= JNM-ECS400	Clipped	= FALSE	Decoupling	= TRUE

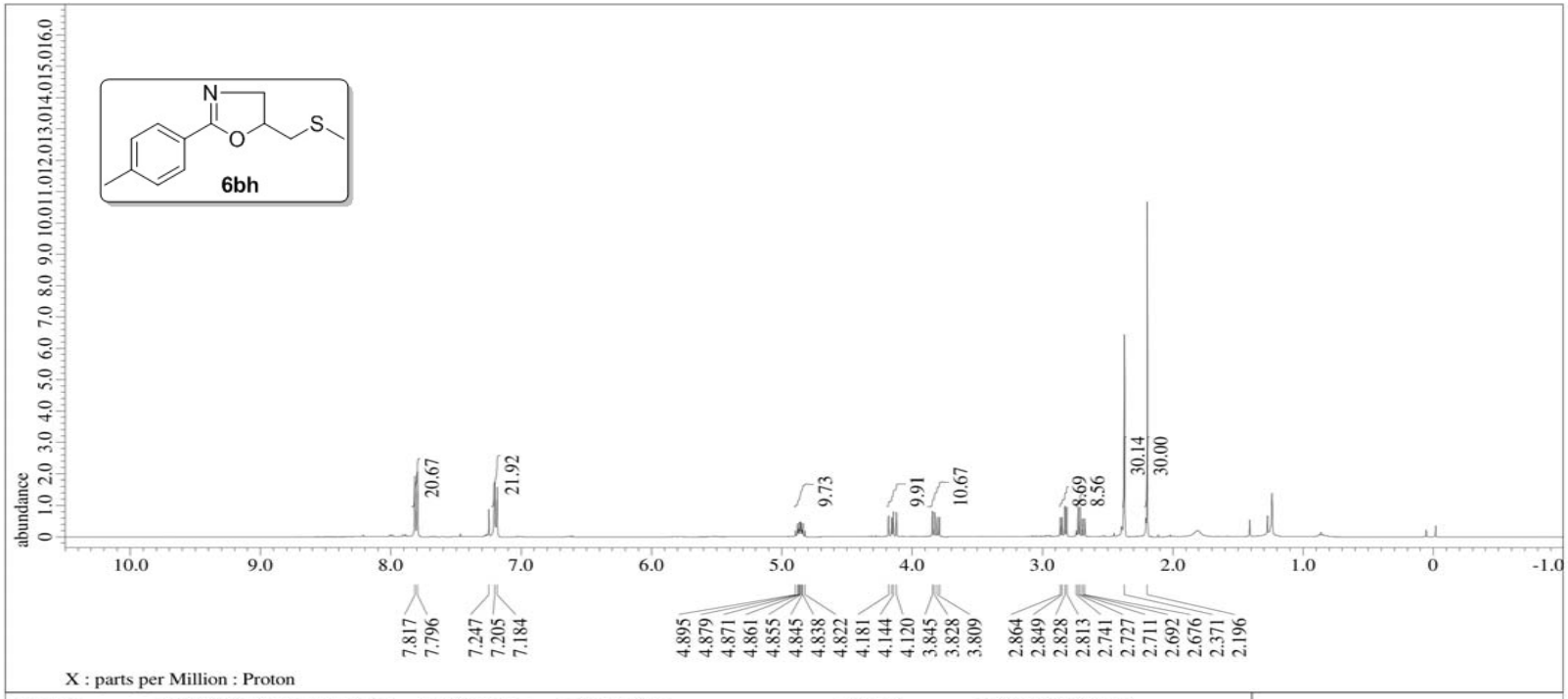


Filename	= VERA-RP3-152_DEPT135deg-1	Spectrometer	= DELTA2_NMR	Scans	= 512
Author	= delta			Total_Scans	= 512
Experiment	= dept.jxp	Field_Strength	= 9.389766[T] (400[MHz])		
Sample_Id	= VERA-RP3-152	X_Acq_Duration	= 1.04333312[s]	Relaxation_Delay	= 2[s]
Solvent	= CHLOROFORM-D	X_Domain	= 13C	Recvr_Gain	= 60
Creation_Time	= 30-JUL-2016 15:17:47	X_Freq	= 100.52530333[MHz]	Temp_Get	= 25.3[dC]
Revision_Time	= 8-AUG-2016 22:14:11	X_Offset	= 100[ppm]	X_Acq_Time	= 1.04333312[s]
Current_Time	= 8-AUG-2016 22:15:02	X_Points	= 32768	X_Atn	= 5.3[dB]
		X_Prescans	= 4	X_Pulse	= 10.33[us]
Comment	= DEPT with decoupling	X_Resolution	= 0.95846665[Hz]	Irr_Atn	= 2.4[dB]
Data_Format	= 1D COMPLEX	X_Sweep	= 31.40703518[kHz]	Irr_Atn_Dec	= 21.473[dB]
Dim_Size	= 26214	X_Sweep_Clipped	= 25.12562814[kHz]	Irr_Noise	= WALTZ
Dim_Title	= Carbon13	Irr_Domain	= Proton	Irr_Pulse	= 12.795[us]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	Irr_Pwidth	= 0.115[ms]
Dimensions	= X	Irr_Offset	= 5[ppm]	Base_Line_Correct	= TRUE
Site	= JNM-ECS400	Clipped	= FALSE	Decoupling	= TRUE

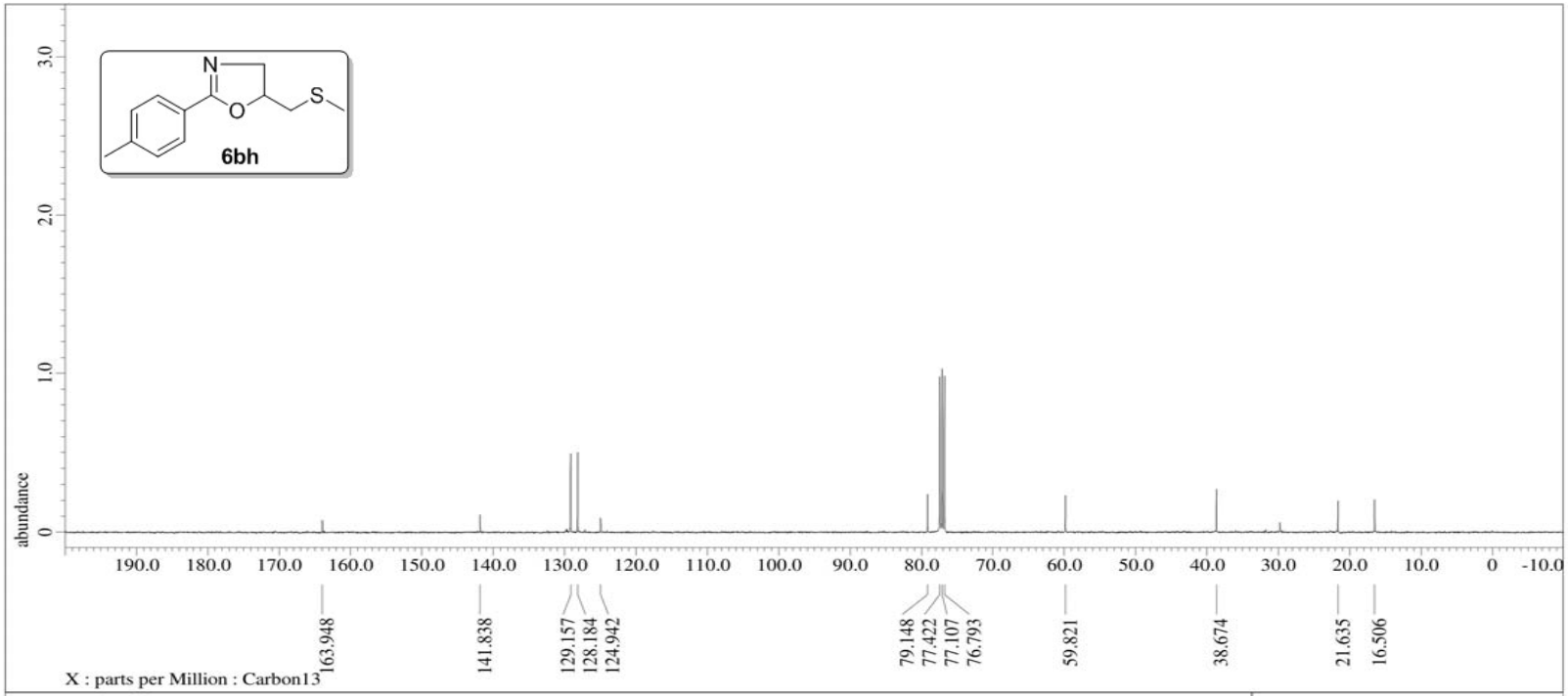

Solvent: CDCl3
Frequency: 400.28 MHz
6ba
f1 (ppm)


163.81
141.67
137.04
131.14
129.82
129.06
128.94
128.11
126.08
124.30
78.17
77.32
77.00
76.68
60.66
59.47
39.10
21.52
21.00
1.00
0.00
N
O
S
6ba
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

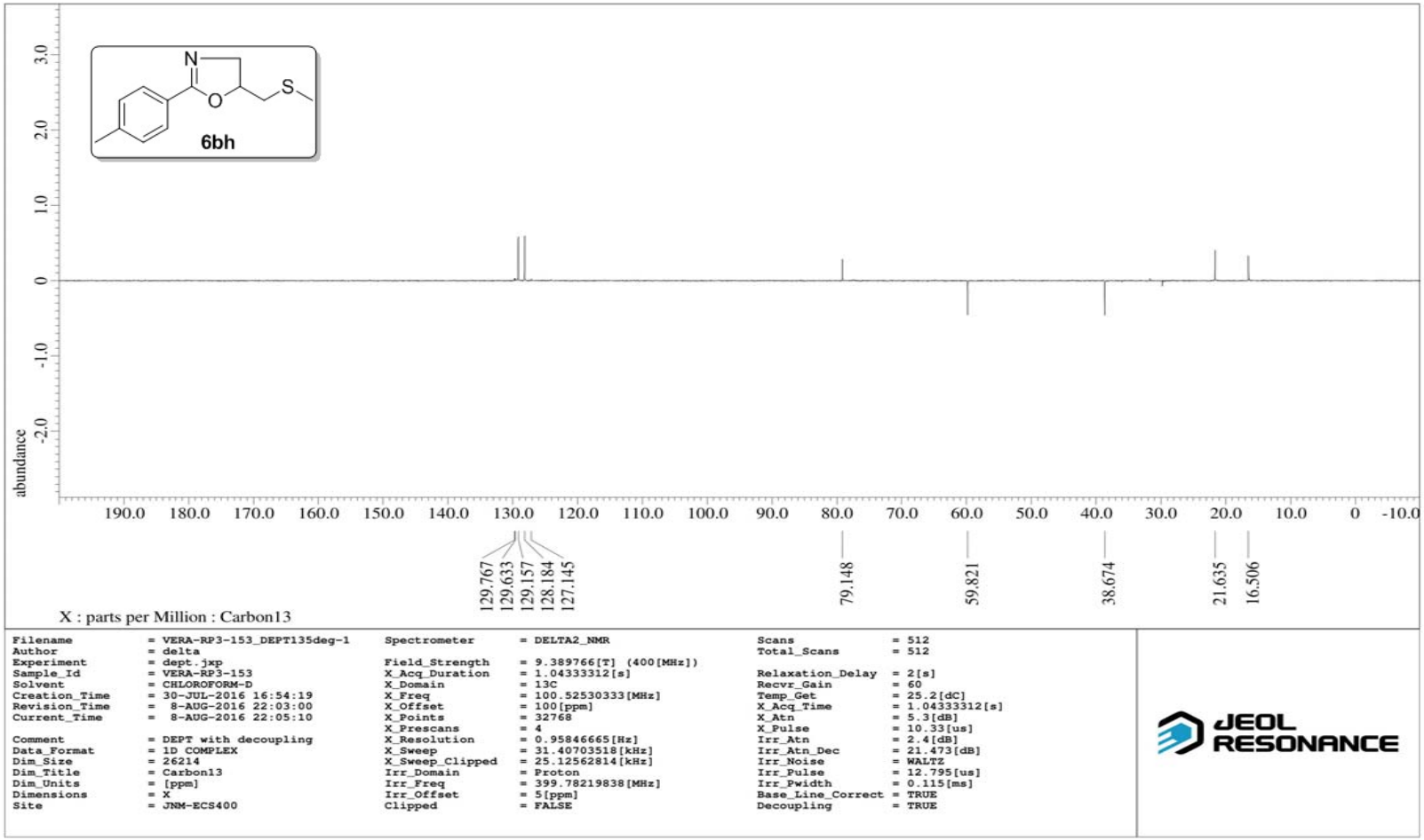

Vera-RP3-26
Pulse Sequence: DEPT
N
O
S
6ba
131.155
129.828
128.956
128.084
78.167
77.318
77.000
76.689
59.466
39.105
21.519
20.996
180
160
140
120
100
80
60
40
20
ppm



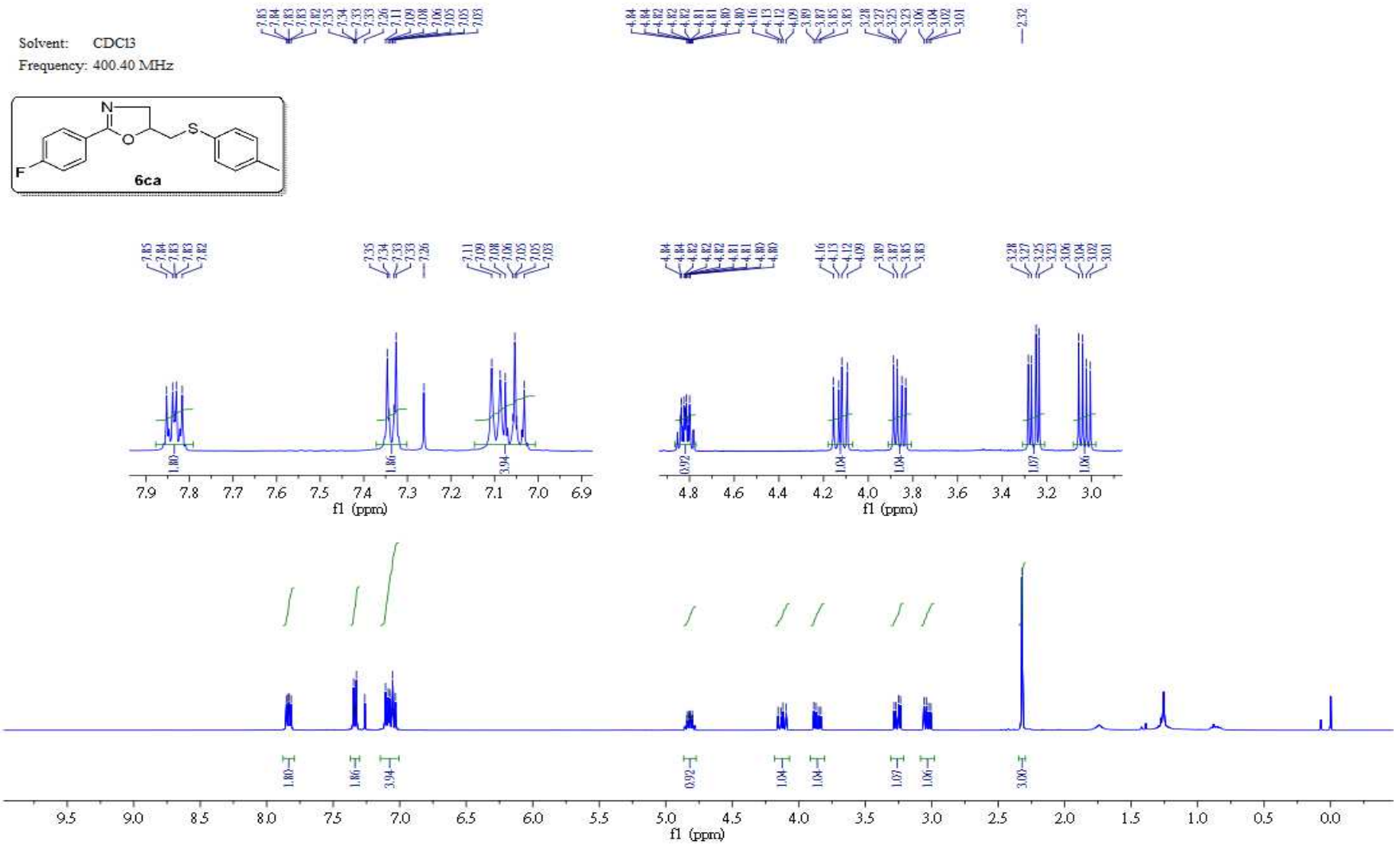
Filename	= VERA-RP3-153_Proton-1-4.jd	Spectrometer	= DELTA2_NMR	Tri_Freq	= 399.78219838[MHz]
Author	= delta			Tri_Offset	= 5[ppm]
Experiment	= proton.jxp	Field_Strength	= 9.389766[T] (400[MHz])	Clipped	= FALSE
Sample_Id	= VERA-RP3-153	X_Acq_Duration	= 2.18365952[s]	Scans	= 24
Solvent	= CHLOROFORM-D	X_Domain	= 1H	Total_Scans	= 24
Creation_Time	= 30-JUL-2016 15:55:15	X_Freq	= 399.78219838[MHz]		
Revision_Time	= 8-AUG-2016 21:58:32	X_Offset	= 5[ppm]	Relaxation_Delay	= 5[s]
Current_Time	= 8-AUG-2016 21:59:04	X_Points	= 16384	Recvr_Gain	= 38
		X_Prescans	= 1	Temp_Get	= 25.4[dC]
Comment	= single_pulse	X_Resolution	= 0.45794685[Hz]	X_90_Width	= 12.795[us]
Data_Format	= 1D COMPLEX	X_Sweep	= 7.5030012[kHz]	X_Acq_Time	= 2.18365952[s]
Dim_Size	= 13107	X_Sweep_Clipped	= 6.00240096[kHz]	X_Angle	= 45[deg]
Dim_Title	= Proton	Irr_Domain	= Proton	X_Atn	= 2.4[dB]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	X_Pulse	= 6.3975[us]
Dimensions	= X	Irr_Offset	= 5[ppm]	Irr_Mode	= Off
Site	= JNM-ECS400	Tri_Domain	= Proton	Tri_Mode	= Off

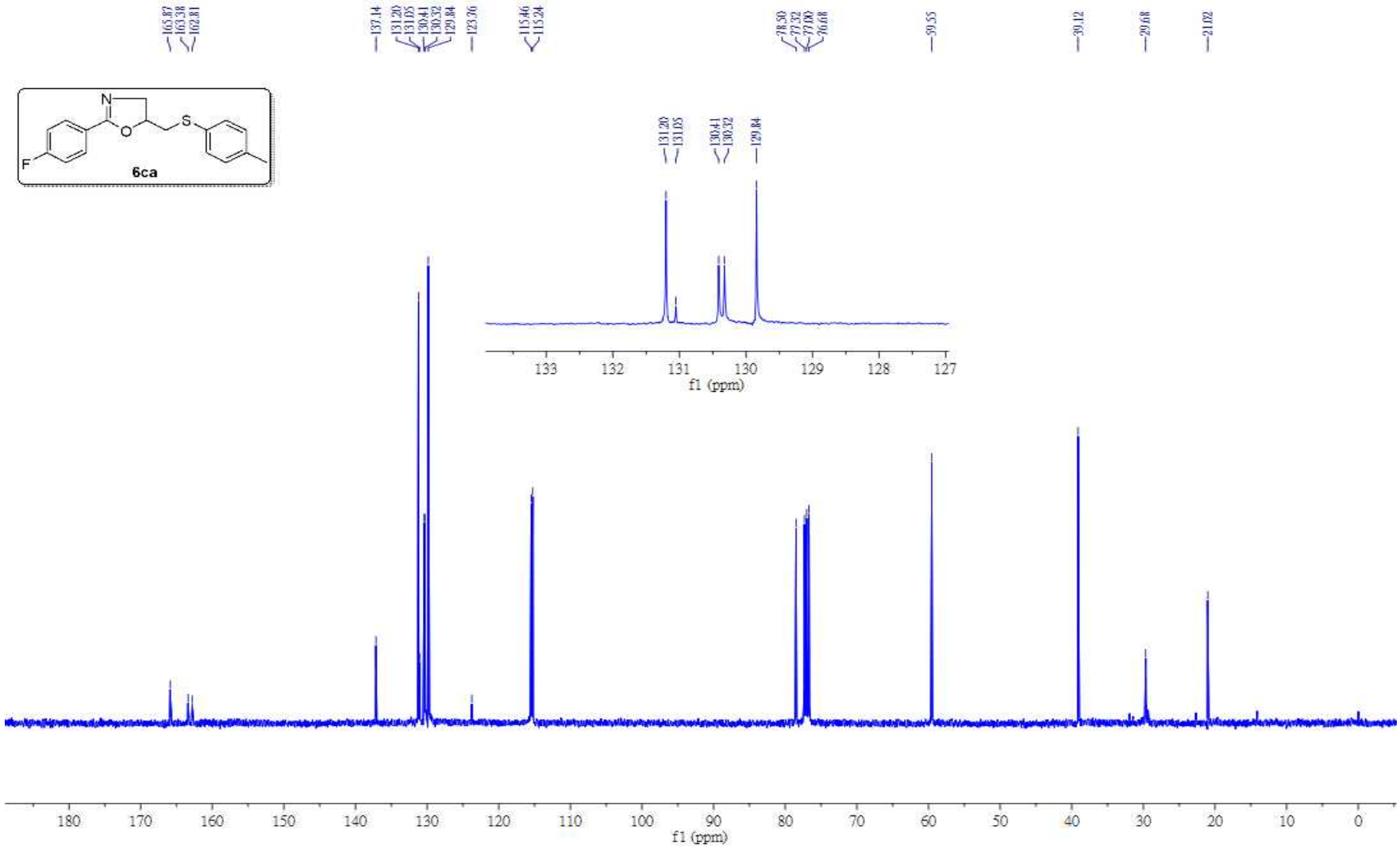


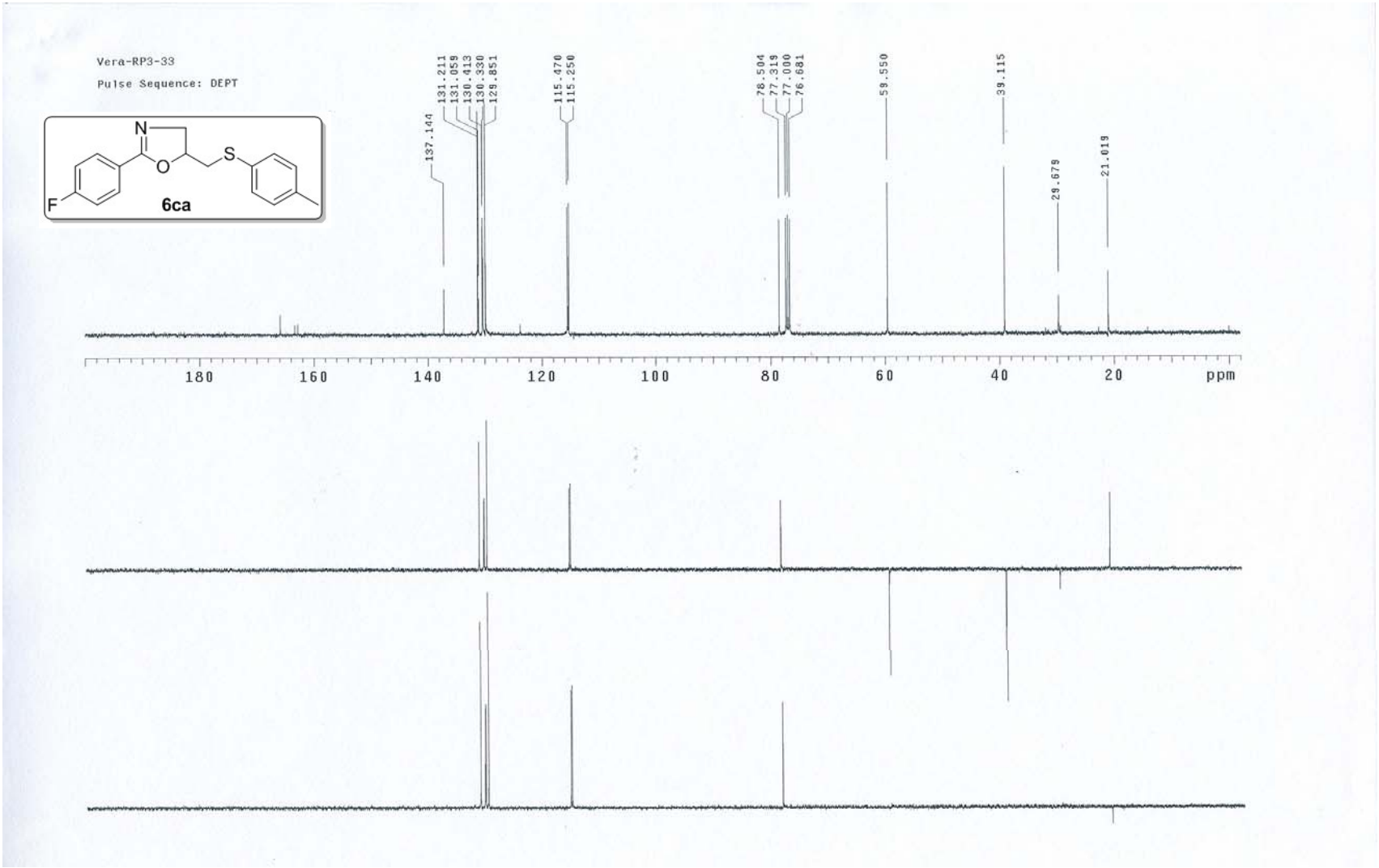
Filename	= VERA-RP3-153_Carbon-1-4.jd	Spectrometer	= DELTA2_NMR	Scans	= 1024
Author	= delta			Total_Scans	= 1024
Experiment	= carbon.jxp	Field_Strength	= 9.389766[T] (400[MHz])		
Sample_Id	= VERA-RP3-153	X_Acq_Duration	= 1.04333312[s]	Relaxation_Delay	= 2[s]
Solvent	= CHLOROFORM-D	X_Domain	= 13C	Recvr_Gain	= 60
Creation_Time	= 30-JUL-2016 16:00:13	X_Freq	= 100.52530333[MHz]	Temp_Get	= 25.5[dC]
Revision_Time	= 8-AUG-2016 22:01:22	X_Offset	= 100[ppm]	X_90_Width	= 10.33[us]
Current_Time	= 8-AUG-2016 22:01:44	X_Points	= 32768	X_Acq_Time	= 1.04333312[s]
		X_Prescans	= 4	X_Angle	= 30[deg]
Comment	= single pulse decoupled gat	X_Resolution	= 0.95846665[Hz]	X_Atn	= 5.3[dB]
Data_Format	= 1D COMPLEX	X_Sweep	= 31.40703518[kHz]	X_Pulse	= 3.44333333[us]
Dim_Size	= 26214	X_Sweep_Clipped	= 25.12562814[kHz]	Irr_Atn_Dec	= 21.473[dB]
Dim_Title	= Carbon13	Irr_Domain	= Proton	Irr_Atn_Noe	= 21.473[dB]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	Irr_Noise	= WALTZ
Dimensions	= X	Irr_Offset	= 5[ppm]	Irr_Pwidth	= 0.115[ms]
Site	= JNM-ECS400	Clipped	= FALSE	Decoupling	= TRUE



Filename	= VERA-RP3-153_DEPT135deg-1	Spectrometer	= DELTA2_NMR	Scans	= 512
Author	= delta			Total_Scans	= 512
Experiment	= dept.jxp	Field_Strength	= 9.389766[T] (400[MHz])		
Sample_Id	= VERA-RP3-153	X_Acq_Duration	= 1.04333312[s]	Relaxation_Delay	= 2[s]
Solvent	= CHLOROFORM-D	X_Domain	= 13C	Recvr_Gain	= 60
Creation_Time	= 30-JUL-2016 16:54:19	X_Freq	= 100.52530333[MHz]	Temp_Get	= 25.2[dC]
Revision_Time	= 8-AUG-2016 22:03:00	X_Offset	= 100[ppm]	X_Acq_Time	= 1.04333312[s]
Current_Time	= 8-AUG-2016 22:05:10	X_Points	= 32768	X_Atn	= 5.3[dB]
		X_Prescans	= 4	X_Pulse	= 10.33[us]
Comment	= DEPT with decoupling	X_Resolution	= 0.95846665[Hz]	Irr_Atn	= 2.4[dB]
Data_Format	= 1D COMPLEX	X_Sweep	= 31.40703518[kHz]	Irr_Atn_Dec	= 21.473[dB]
Dim_Size	= 26214	X_Sweep_Clipped	= 25.12562814[kHz]	Irr_Noise	= WALTZ
Dim_Title	= Carbon13	Irr_Domain	= Proton	Irr_Pulse	= 12.795[us]
Dim_Units	= [ppm]	Irr_Freq	= 399.78219838[MHz]	Irr_Pwidth	= 0.115[ms]
Dimensions	= X	Irr_Offset	= 5[ppm]	Base_Line_Correct	= TRUE
Site	= JNM-ECS400	Clipped	= FALSE	Decoupling	= TRUE


Solvent: CDCl3
Frequency: 400.40 MHz
N
O
S
F
6ca
f1 (ppm)


165.87
163.38
162.81
137.14
131.20
131.05
130.41
130.32
129.84
123.76
115.46
115.24
78.30
77.32
77.00
76.68
39.55
39.12
29.68
21.02
6ca
F
N
O
S
f1 (ppm)
f1 (ppm)


Vera-RP3-33
Pulse Sequence: DEPT
N
O
S
F
6ca
137.144
131.211
131.059
130.413
130.330
129.851
115.470
115.250
78.504
77.319
77.000
76.681
59.550
39.115
29.679
21.019
180
160
140
120
100
80
60
40
20
ppm