Supporting Information

Metal-free intramolecular [3+2]-cycloaddtion of γ-hydroxy acetylenic ketones with alkynes for the synthesis of naphtho[1,2-c]furan-5-ones and its derivatization via a selective Csp^2-H deuteration reaction

Si-Si Ning,[a] Dan Meng,[a] Jie-Yun Zhang,[a] Shi-Lei Liu,[a] Ni-Ni Zhou,[a] Xiaojie Jin[b] and Hai-Tao Zhu[a]*

[a]Shannxi Key Laboratory of Phytochemistry, College of Chemistry and Chemical Engineering, Baoji University of Arts and Sciences, Baoji 721013, China.

[b]Gansu University Key Laboratory for Molecular Medicine & Chinese Medicine Prevention and Treatment of Major Diseases, Gansu University of Chinese Medicine, Lanzhou 730000, China.

E-mail: zhuht@bjwlxy.edu.cn

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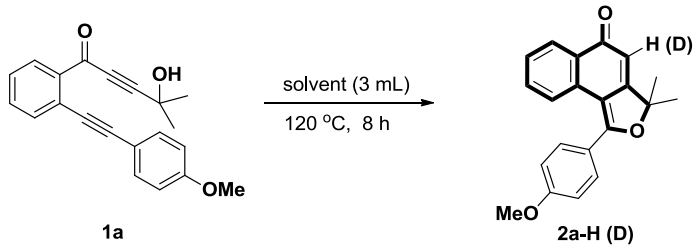
1. Mechanistic investigation

Table S1. Deuteration Experiments



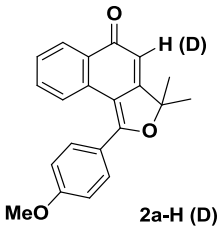
Entry	solvent	yieid	**2a-H : 2a-D**
1	DMSO + 1.0 equiv D_2O	61%	30:70
2	AcOD : D_2O = 1:1	74%	2:98
3	AcOD : H_2O = 1:1	72%	82:18
4	AcOH : D_2O = 1:1	71%	18:82

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.33 (m, 1H), 7.93 – 7.87 (m, 1H), 7.83 – 7.71 (m, 2H), 7.47 – 7.35 (m, 2H), 7.17 – 7.00 (m, 2H), 6.37 (s, 0.30H), 3.93 (s, 3H), 1.68 (s, 6H).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.32 (m, 1H), 8.01 – 7.83 (m, 1H), 7.82 – 7.68 (m, 2H), 7.48 – 7.31 (m, 2H), 7.16 – 6.97 (m, 2H), 6.37 (s, 0.02H), 3.93 (s, 3H), 1.68 (s, 6H).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.32 (m, 1H), 7.96 – 7.84 (m, 1H), 7.86 – 7.72 (m, 2H), 7.50 – 7.32 (m, 2H), 7.12 – 6.99 (m, 2H), 6.37 (s, 0.82H), 3.93 (s, 3H), 1.68 (s, 6H).

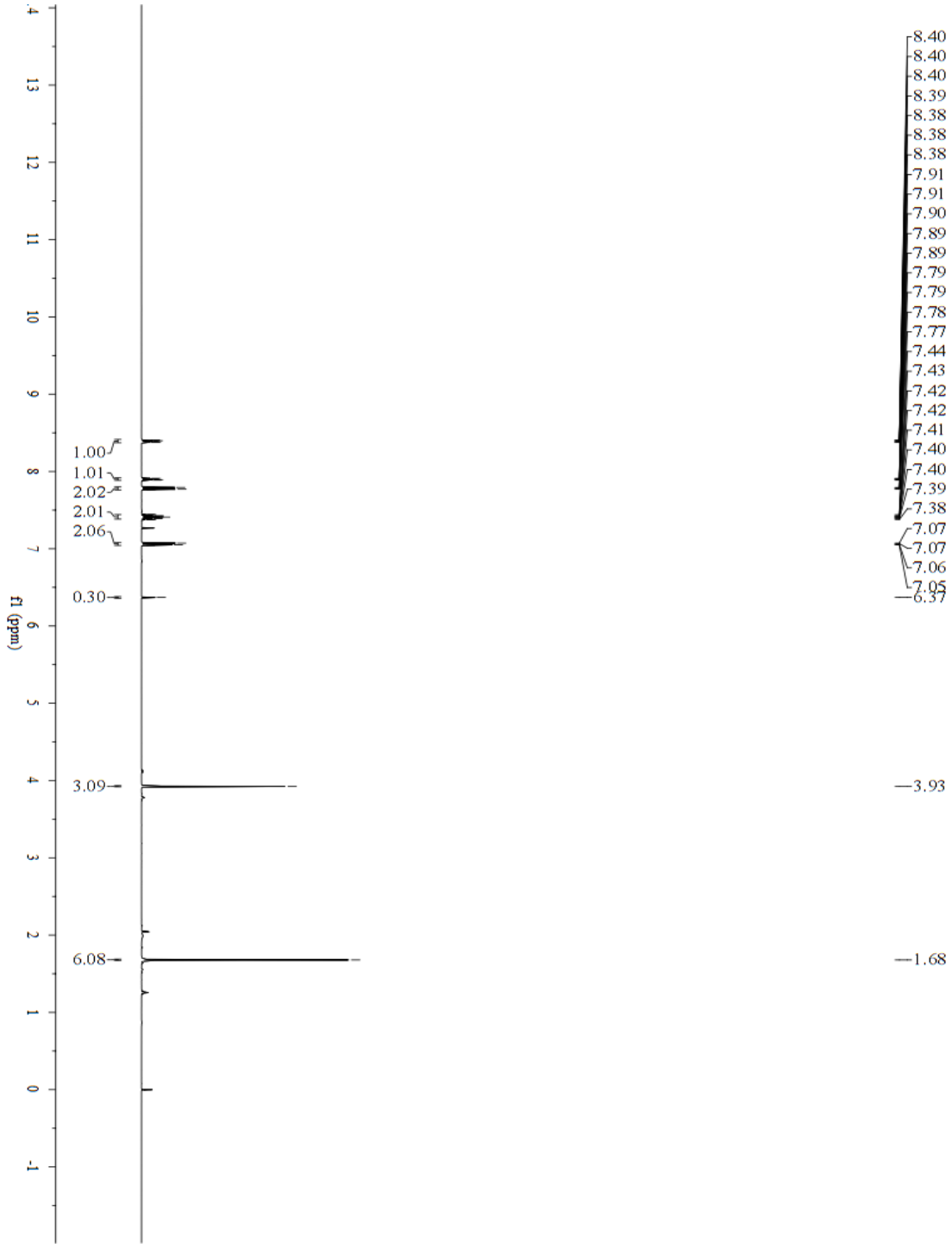
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.33 (m, 1H), 7.96 – 7.86 (m, 1H), 7.82 – 7.73 (m, 2H), 7.46 – 7.33 (m, 2H), 7.12 – 6.95 (m, 2H), 6.37 (s, 0.18H), 3.92 (s, 3H), 1.68 (s, 6H).

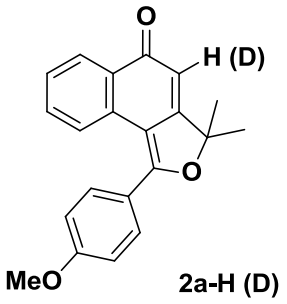


2a-H (D)

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

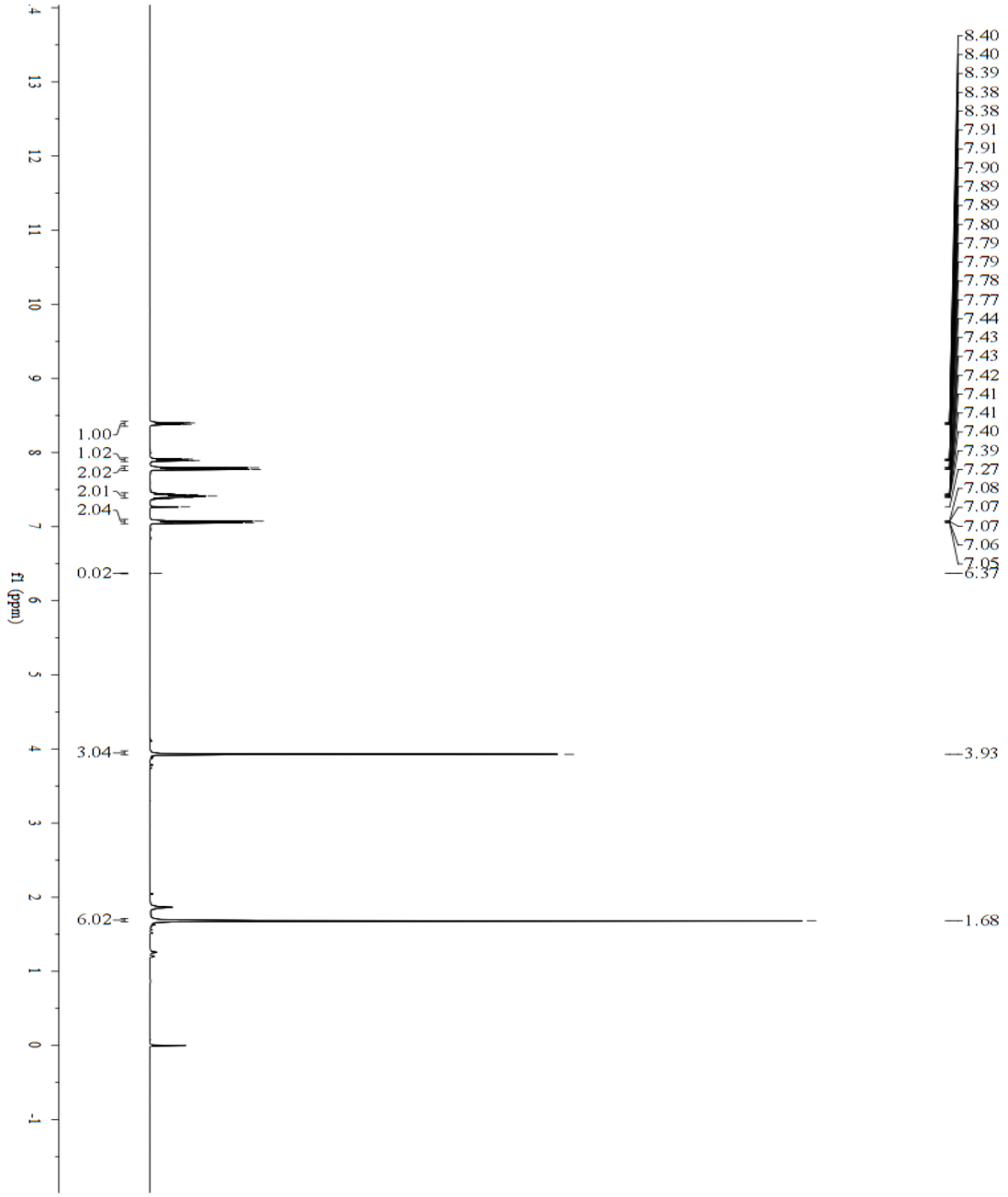
a) DMSO With 1.0 equiv of D_2O
2a-H : 2a-D ; 30 : 70

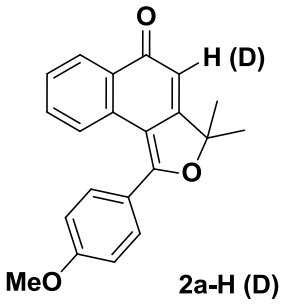




^{1}H NMR (400 MHz, $CDCl_3$)

b) AcOD : D_2O=1:1
2a-H:2a-D ; 2 : 98

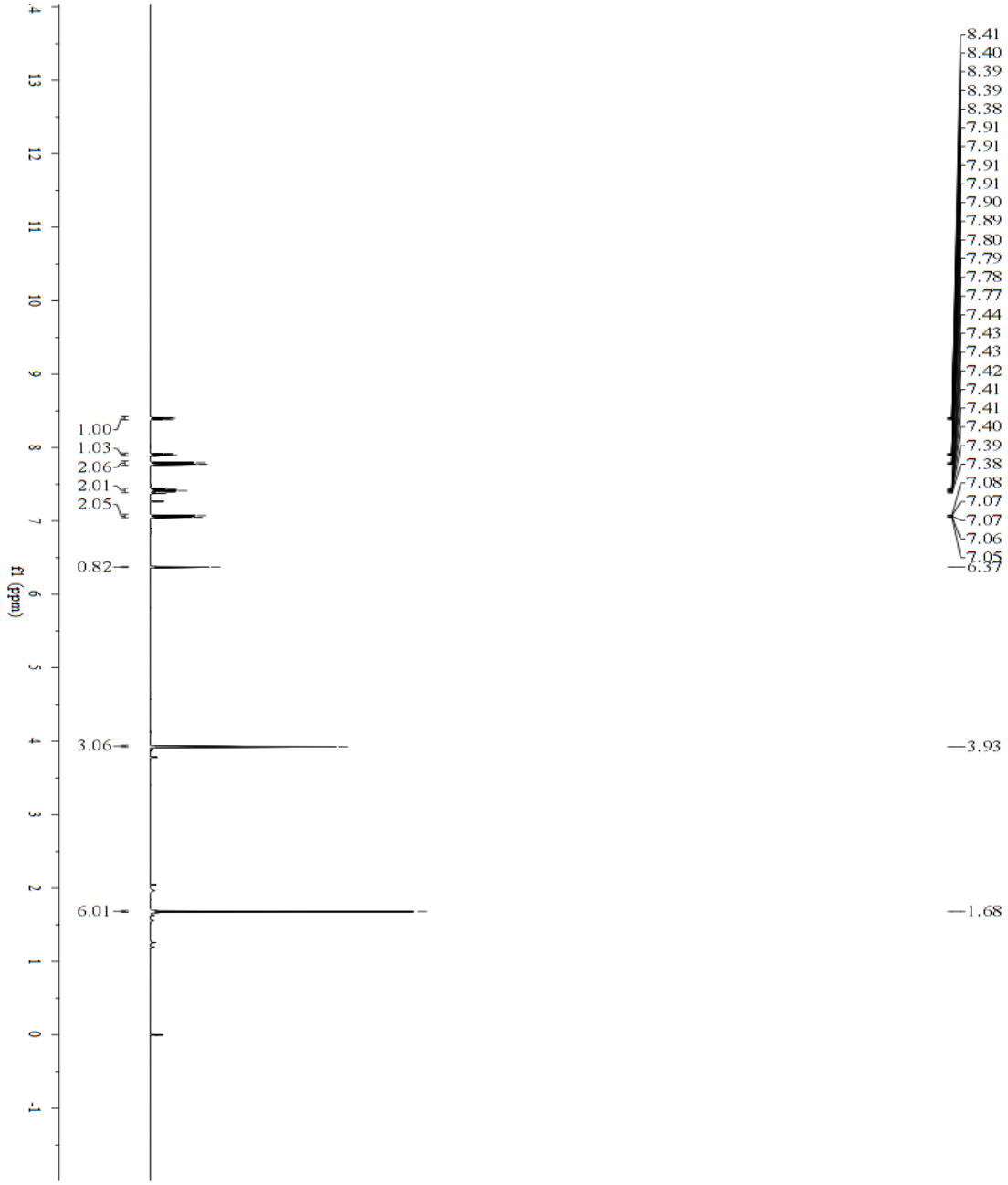


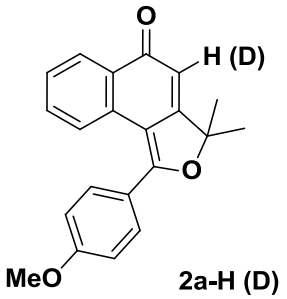


2a-H (D)

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

c) AcOD : H_2O = 1:1
2a-H:2a-D ; 82 : 18

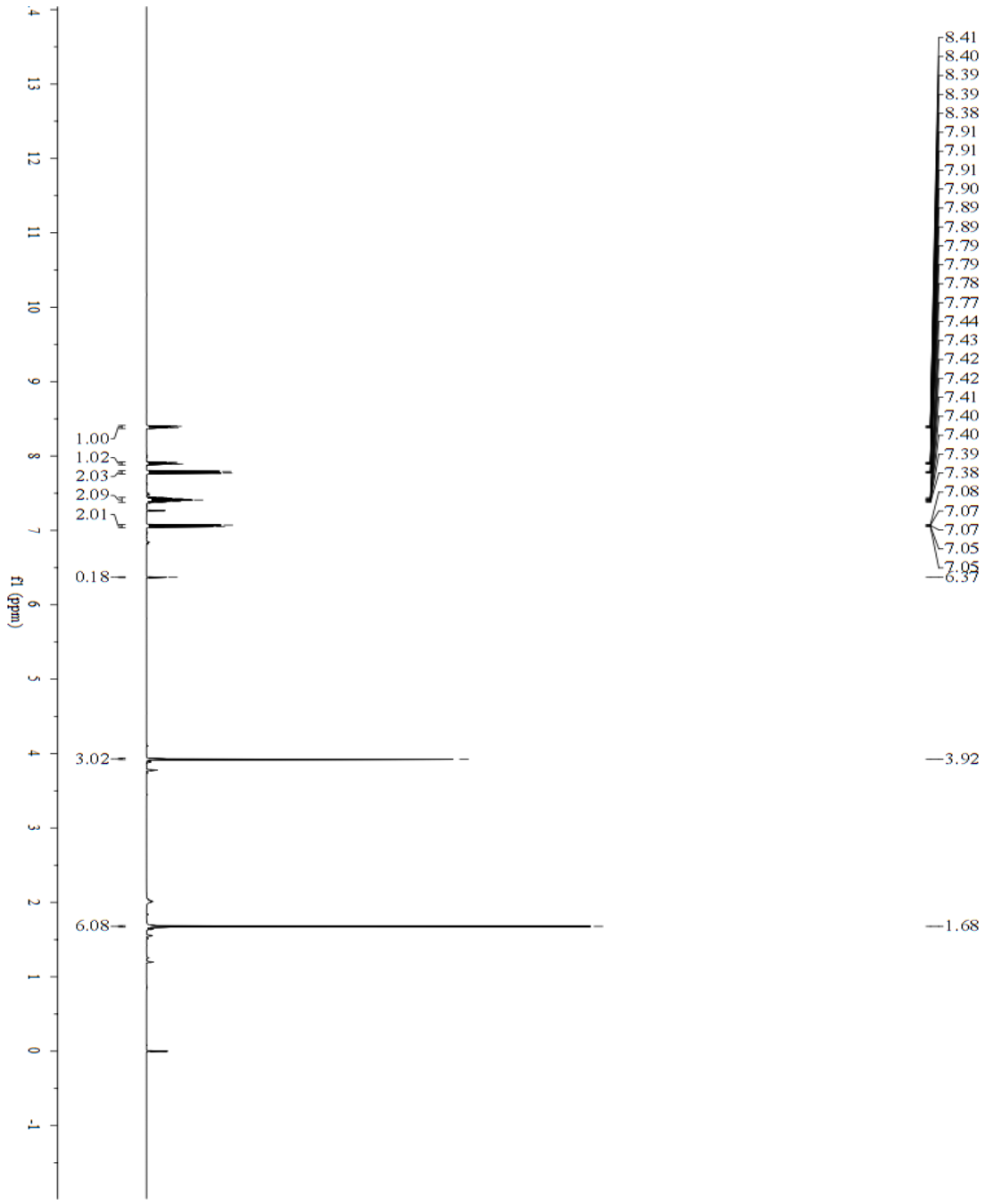




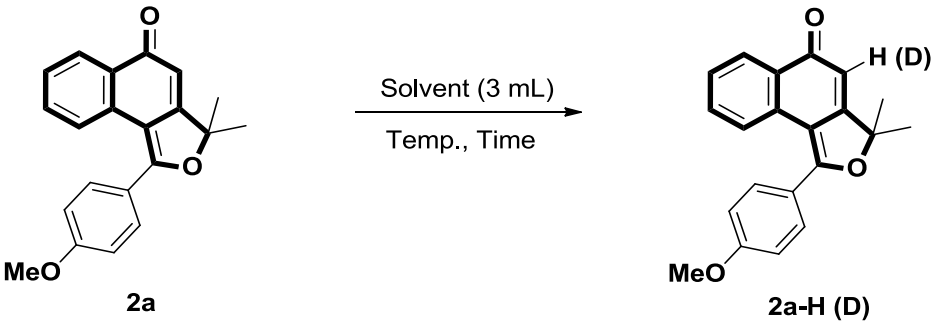
2a-H (D)

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

d) AcOH : D_2O=1:1
2a-H:2a-D ; 18 : 82



2. Table S2. Optimization of the deuteration reaction conditions[a]



entry	solvent	temp. (℃)	time (h)	yieid[b] (%)	**2a-H** : **2a-D**
1	D_2O	120	12	50	66:34
2	AcOD	120	12	91	8:92
3	Ac_2O : D_2O = 1:1	120	12	88	7:93
4	AcOD : D_2O = 1:1	120	4	79	45:55
5	AcOD : D_2O = 1:1	120	12	98	2:98
6	AcOD : D_2O = 1:1	120	24	95	3:97
7	AcOD : D_2O = 1:1	80	12	85	86:14
8	AcOD : D_2O = 1:1	130	12	93	4:96

[a] conditions: **2a-H** (0.2 mmol), solvent (3 mL) or mixed solvent (1.5 mL : 1.5 mL). [b] Isolated yields.

(1) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.40 – 8.36 (m, 1H), 7.93 – 7.85 (m, 1H), 7.81 – 7.72 (m, 2H), 7.47 – 7.33 (m, 2H), 7.12 – 7.00 (m, 2H), 6.36 (s, 0.66H), 3.92 (s, 3H), 1.68 (s, 6H).

(2) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.40 – 8.34 (m, 1H), 7.93 – 7.85 (m, 1H), 7.81 – 7.73 (m, 2H), 7.45 – 7.35 (m, 2H), 7.10 – 7.01 (m, 2H), 6.36 (s, 0.08H), 3.92 (s, 3H), 1.68 (s, 6H).

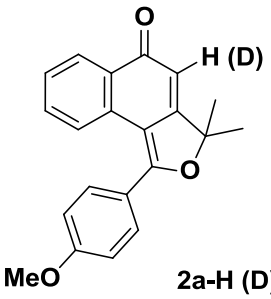
(3) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.42 – 8.34 (m, 1H), 7.92 – 7.85 (m, 1H), 7.81 – 7.74 (m, 2H), 7.46 – 7.35 (m, 2H), 7.10 – 6.99 (m, 2H), 6.36 (s, 0.07H), 3.92 (s, 3H), 1.68 (s, 6H).

(4) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.40 – 8.33 (m, 1H), 7.93 – 7.85 (m, 1H), 7.83 – 7.70 (m, 2H), 7.47 – 7.32 (m, 2H), 7.10 – 7.02 (m, 2H), 6.36 (s, 0.45H), 3.92 (s, 3H), 1.68 (s, 6H).

(6) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.43 – 8.34 (m, 1H), 7.94 – 7.85 (m, 1H), 7.82 – 7.74 (m, 2H), 7.49 – 7.33 (m, 2H), 7.10 – 6.99 (m, 2H), 6.36 (s, 0.03H), 3.92 (s, 3H), 1.68 (s, 6H).

(7) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.40 – 8.36 (m, 1H), 7.93 – 7.85 (m, 1H), 7.81 – 7.72 (m, 2H), 7.47 – 7.34 (m, 2H), 7.09 – 6.98 (m, 2H), 6.36 (s, 0.86H), 3.92 (s, 3H), 1.68 (s, 6H).

(8) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.38 – 8.34 (m, 1H), 7.89 – 7.83 (m, 1H), 7.78 – 7.68 (m, 2H), 7.43 – 7.32 (m, 2H), 7.09 – 6.99 (m, 2H), 6.34 (s, 0.04H), 3.90 (s, 3H), 1.66 (s, 6H).

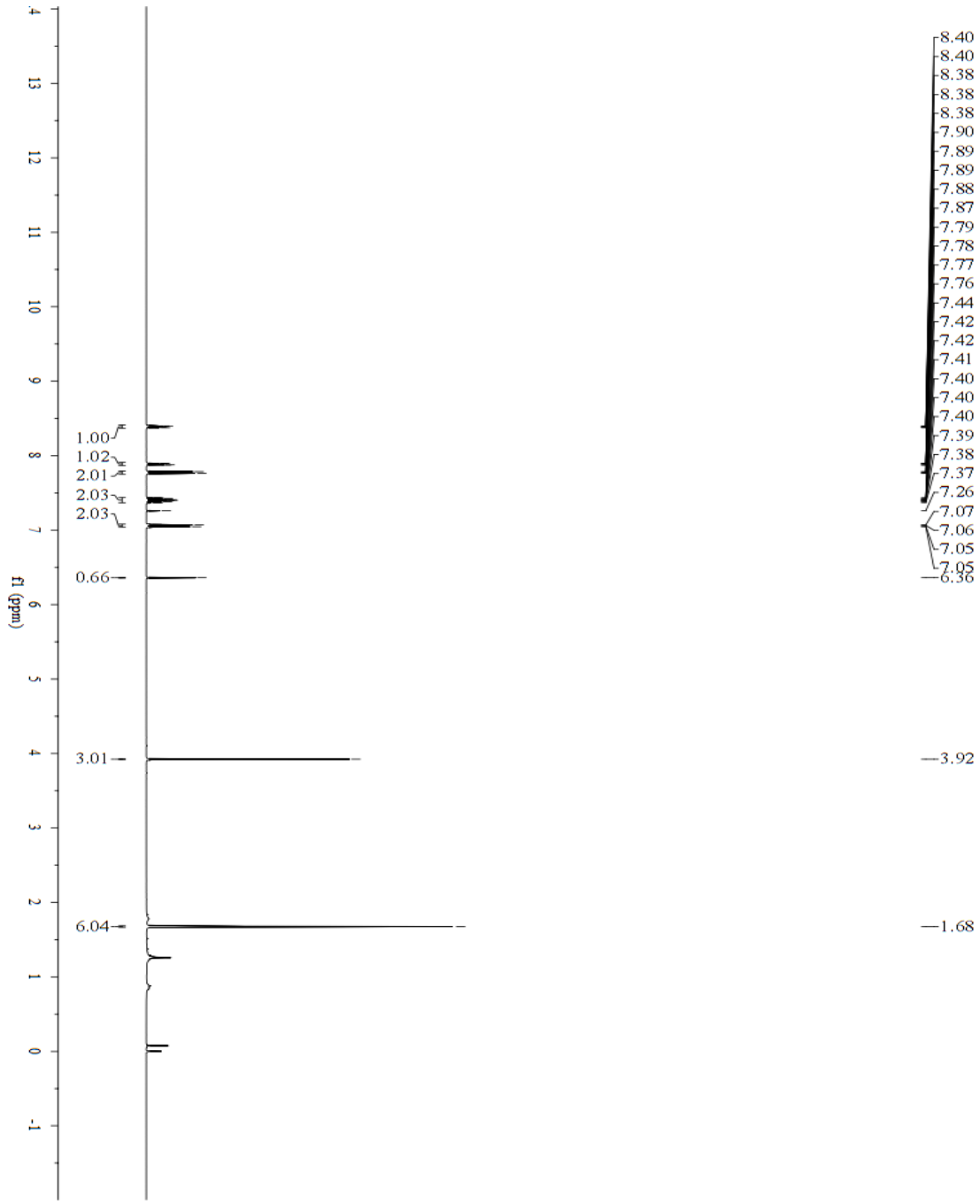


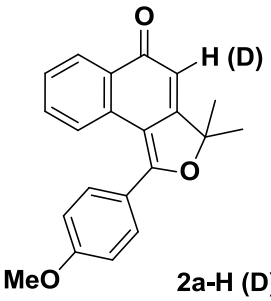
2a-H (D)

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

(1) D_2O

2a-H : 2a-D ; 66 : 34



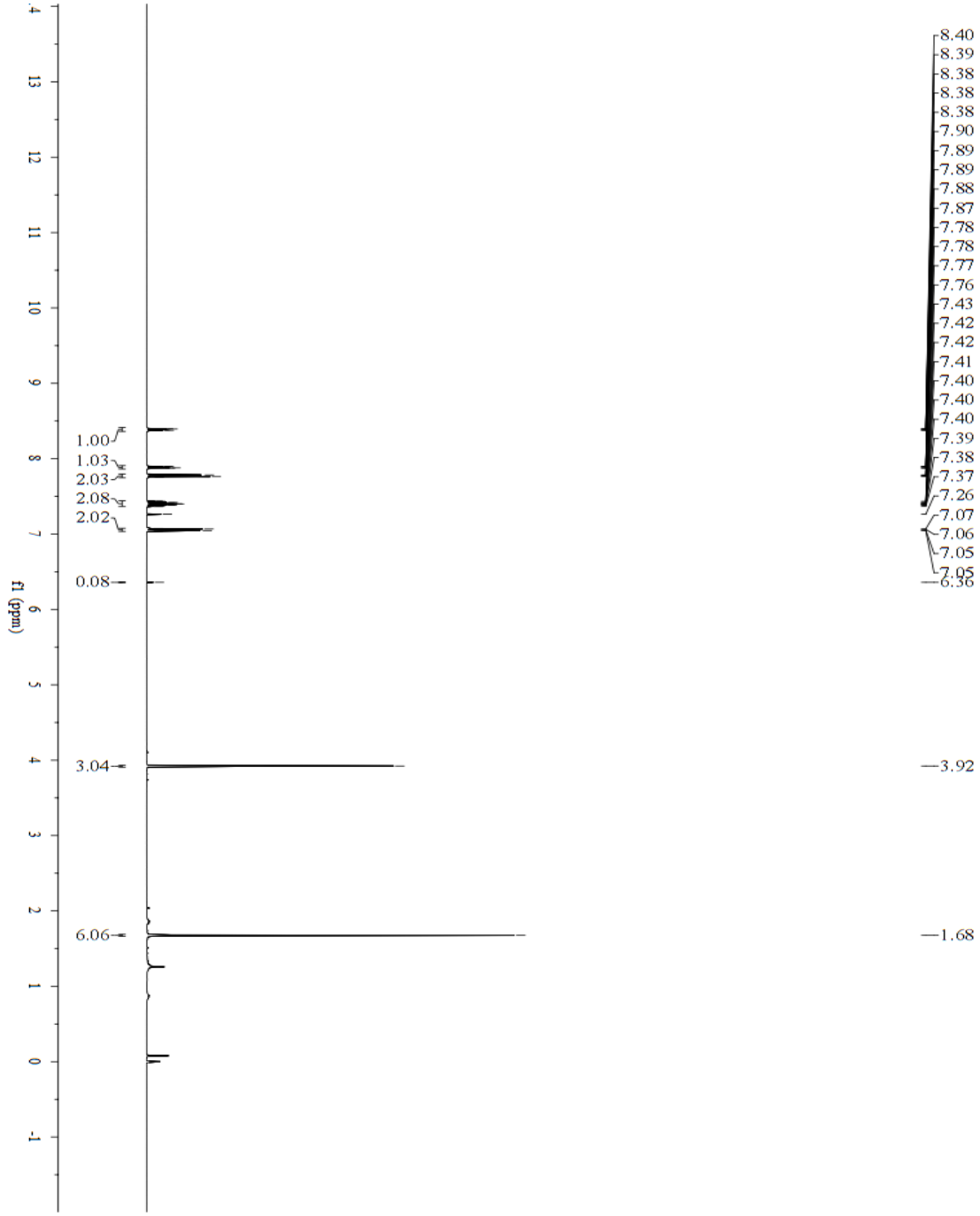


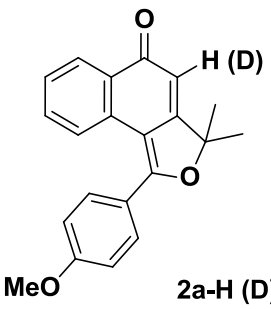
2a-H (D)

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

(2) AcOD

2a-H : 2a-D ; 8 : 92



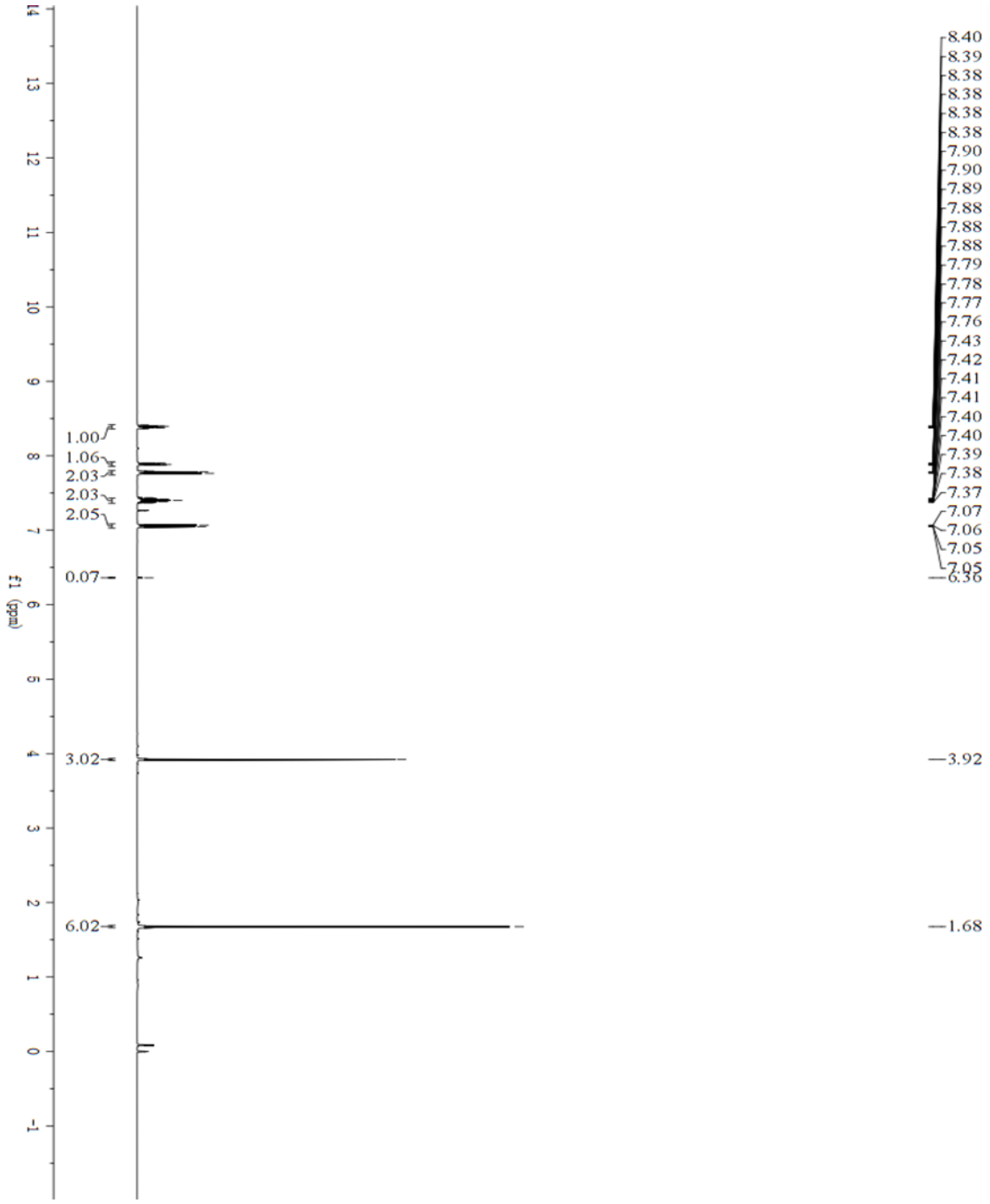


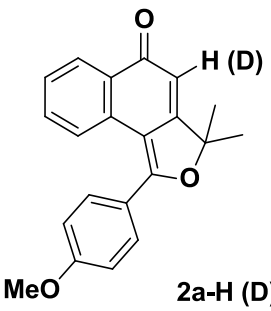
2a-H (D)

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

(3) Ac_2O:D_2O (120 °C)

2a-H : 2a-D ; 7 : 93

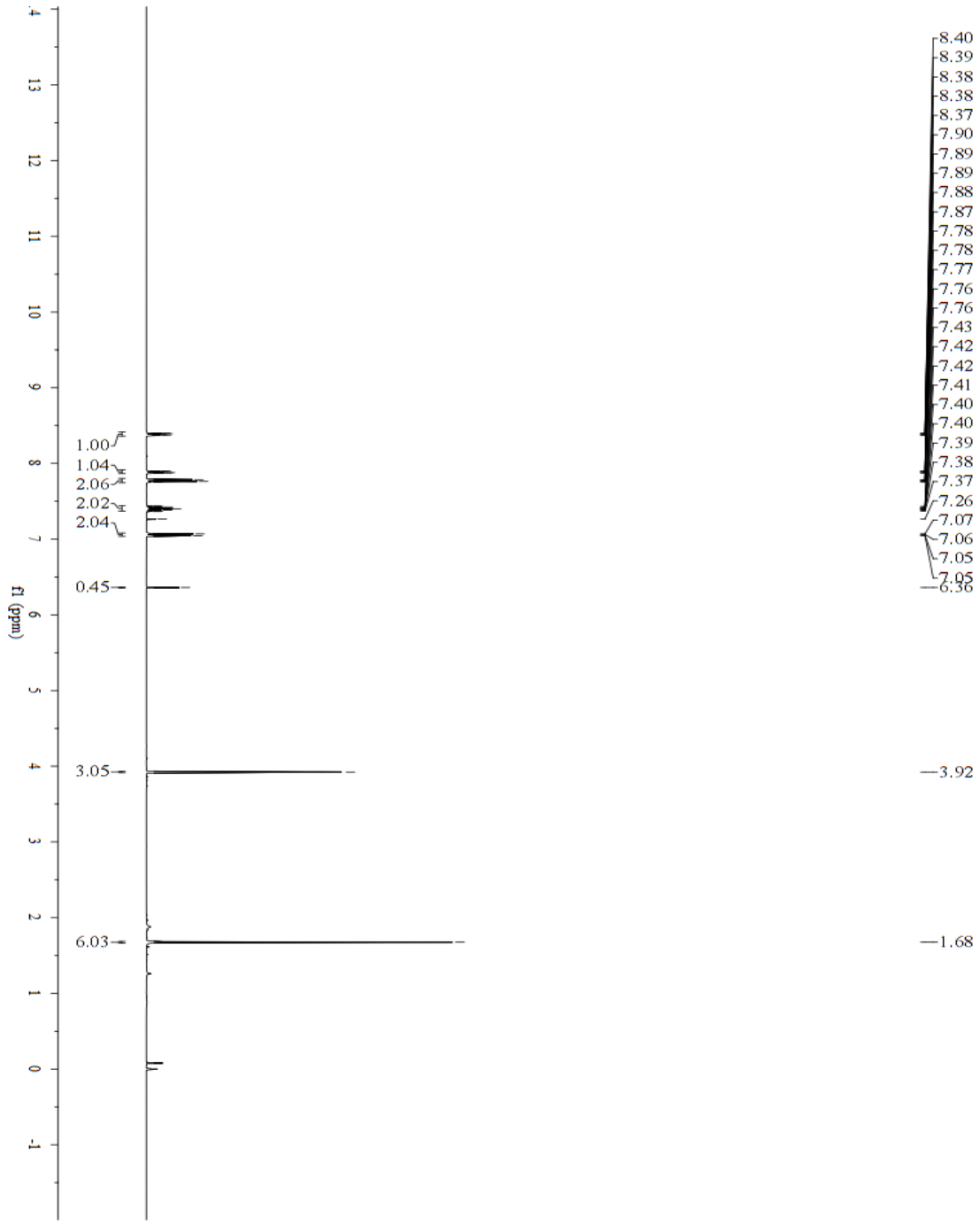


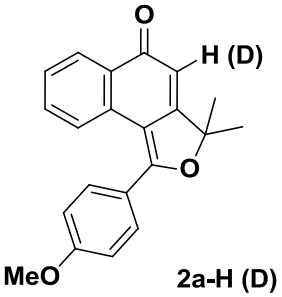


^{1}H NMR (400 MHz, $CDCl_3$)

(4) AcOD:D_2O (4h)

2a-H : 2a-D ; 45 : 55



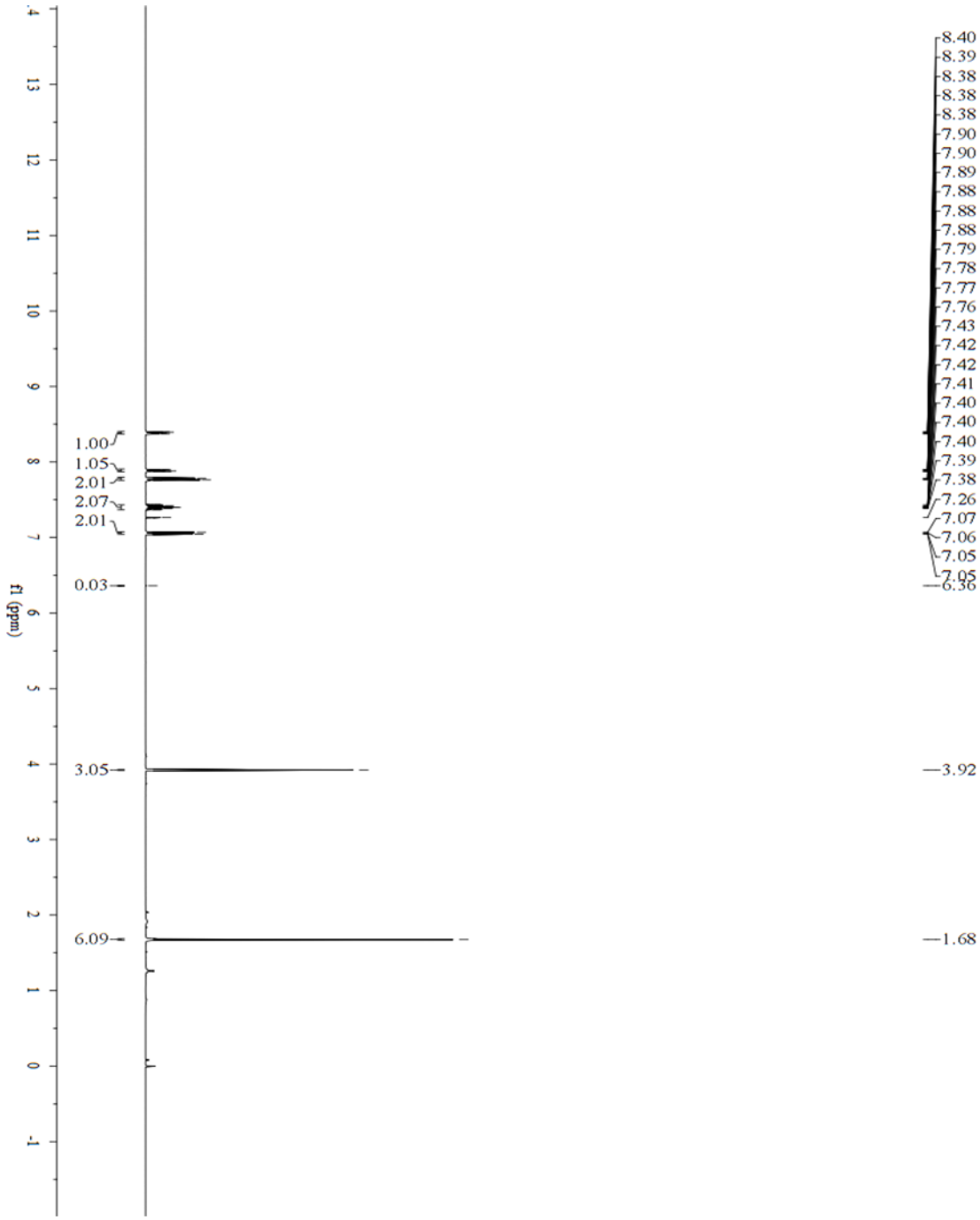


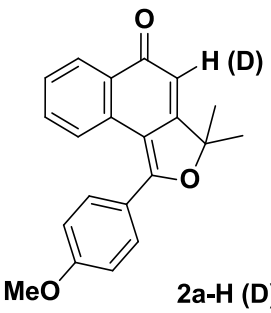
2a-H (D)

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

(6) AcOD:D_2O (24h)

2a-H : 2a-D ; 3 : 97

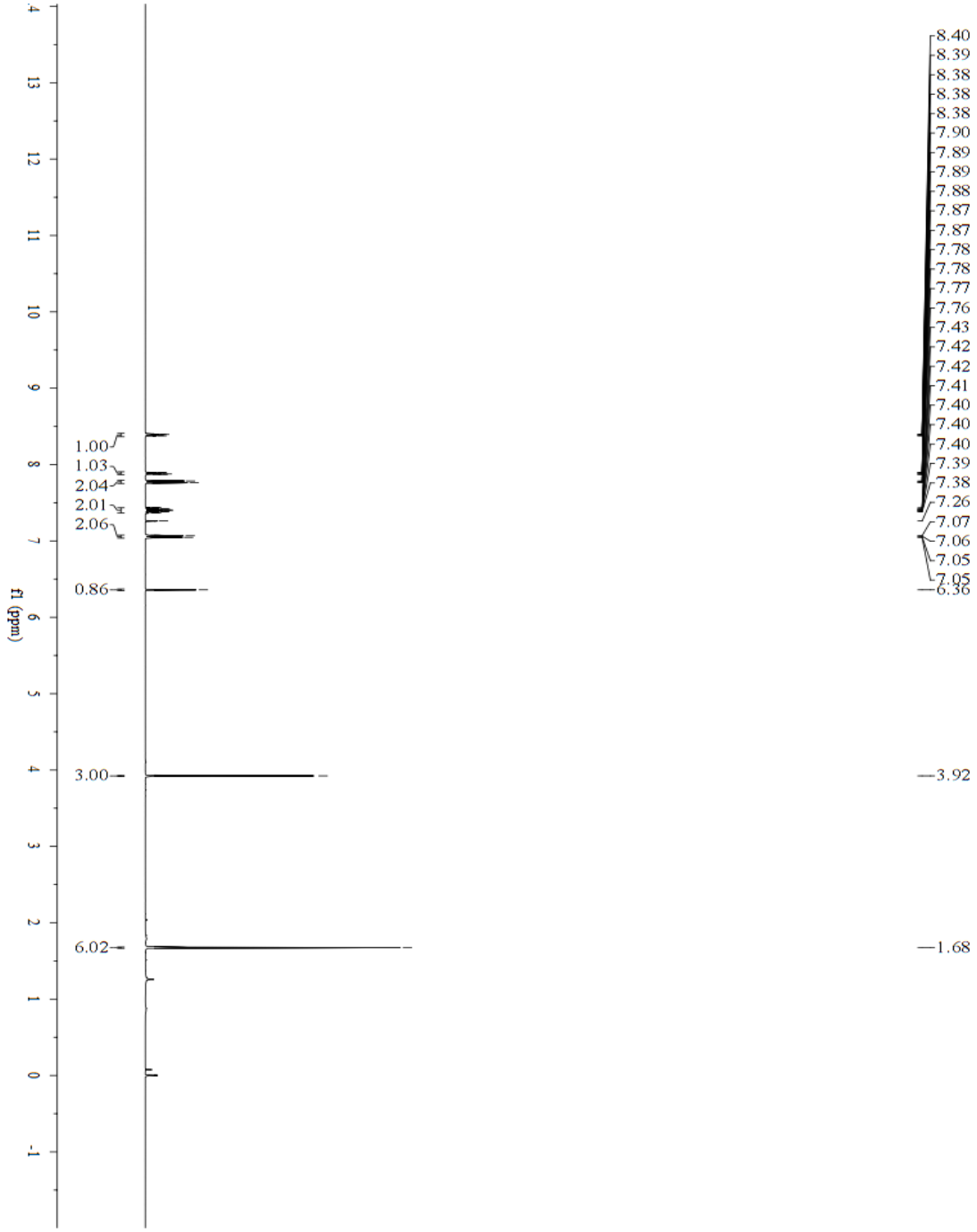


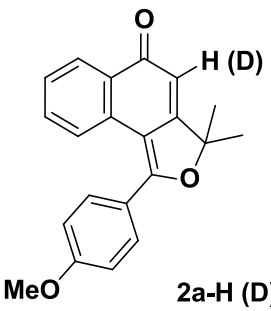


^{1}H NMR (400 MHz, $CDCl_3$)

(7) AcOD:D_2O (80 °C)

2a-H : 2a-D ; 86 : 14

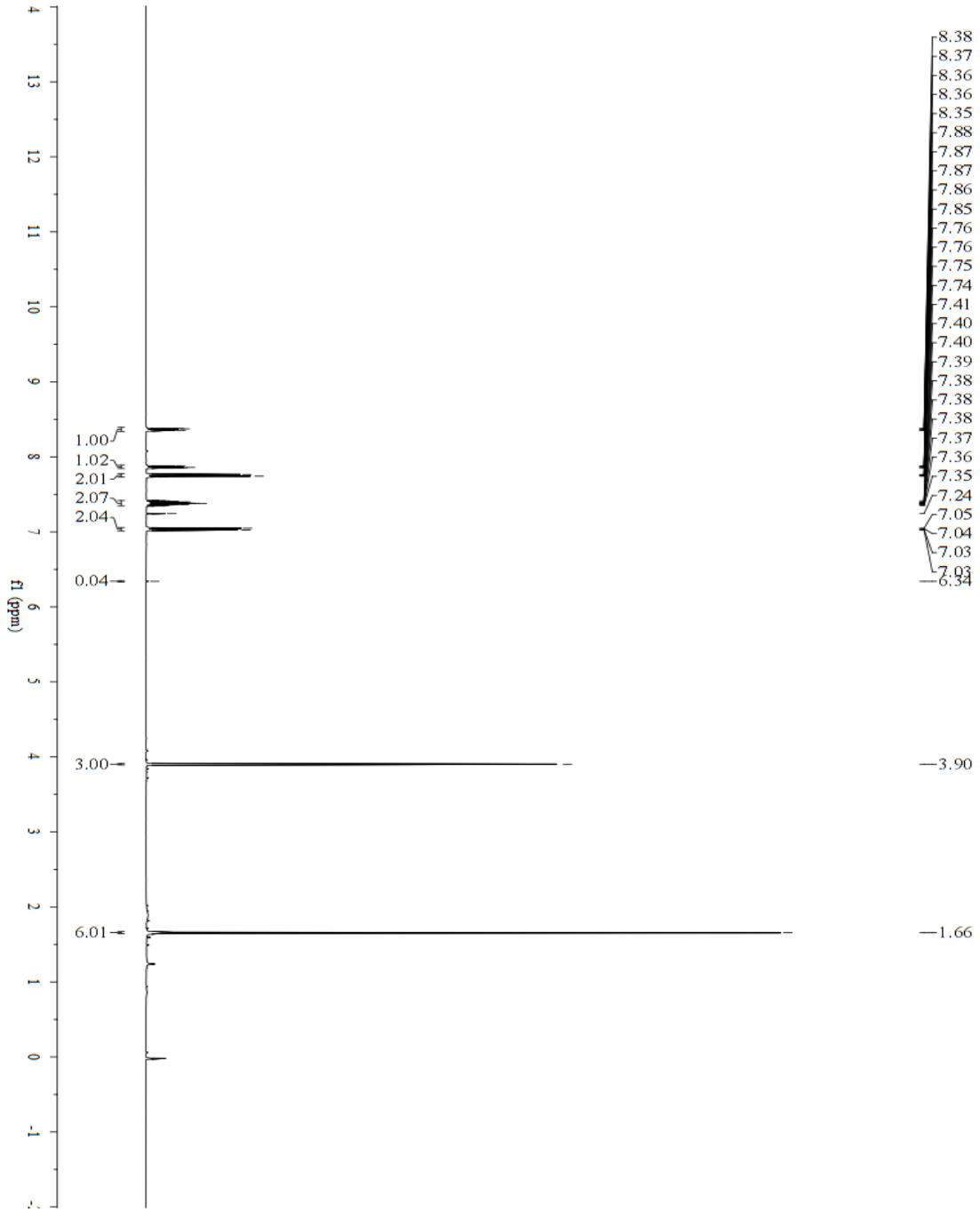




^{1}H NMR (400 MHz, $CDCl_3$)

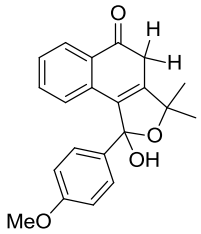
(8) AcOD:D_2O (130 °C)

2a-H : 2a-D ; 4 : 96



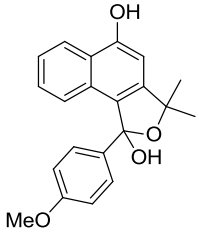
3. DFT calculation data

In cooperation with Xiaojie Jin associate professor coming from College of pharmacy, Gansu University of Chinese Medicine, we carried out a DFT study for revealing the stability of intermediates. In theoretical calculations, the optimal conformation of the molecules was optimized with Gaussian 16 package (Ref1) at B3LYP/6-31G (d,p) computational level. The minimum nature of the structure was confirmed by frequency calculations at the same computational level. The absolute energies of intermediate Int-2 is 4.57 Kcal/mol lower than intermediate Int-1. The structure of intermediates is shown below.



Int-1

-1113.20905333 A.U



Int-2

-1113.21633776 A.U

Ref1: Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

4. The photophysical properties of products

Figure S1. Optical properties of compounds in 1.0 $\times 10^{-5}$ mol/L EtOH solution.

Left: UV−vis absorption spectrum; right: fluorescence emission spectrum.

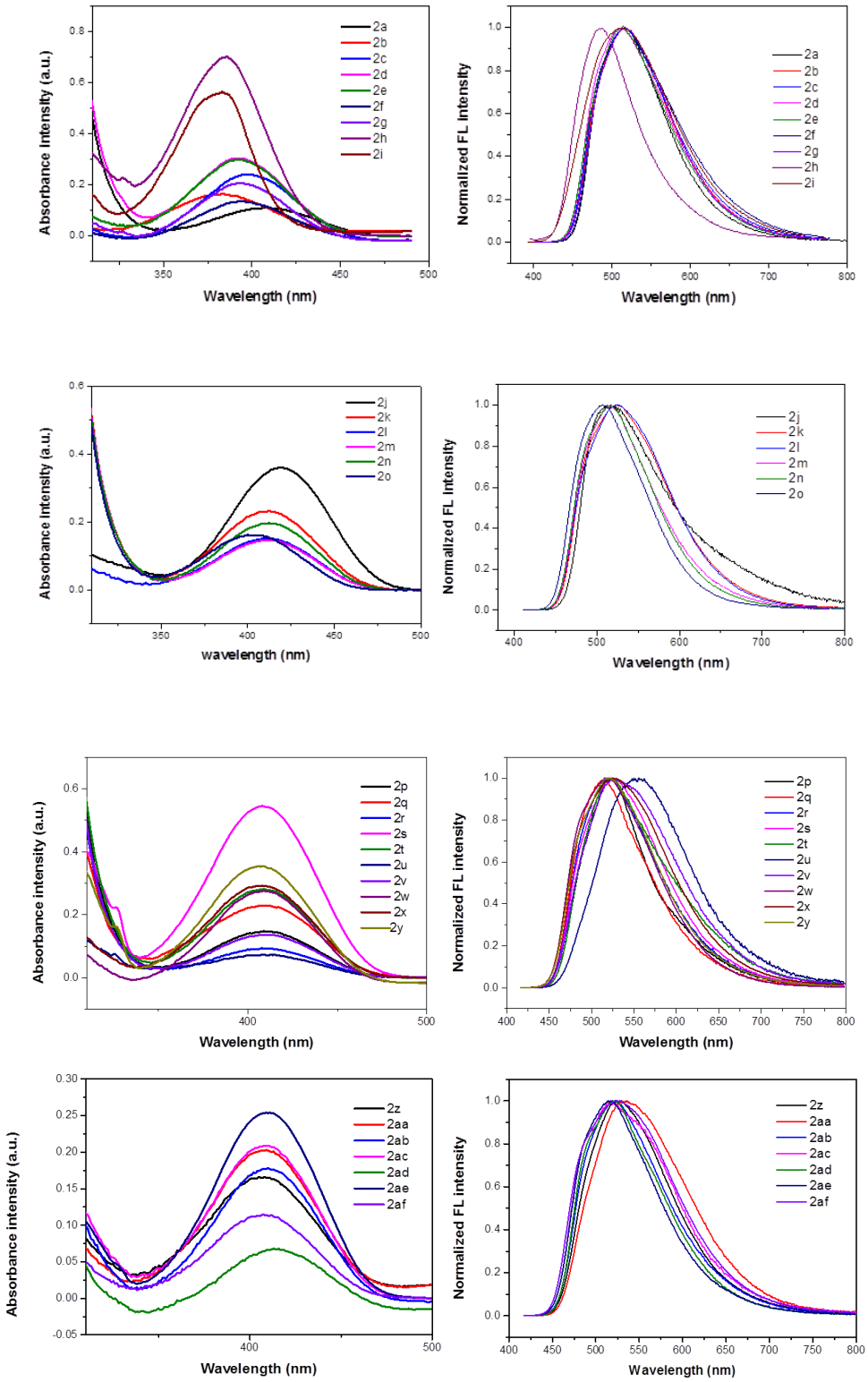


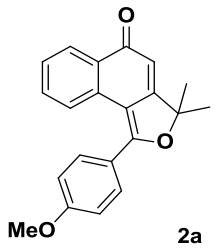
Table S3. photophysical data of all synthesized compounds [a]

Title compound	Solution (nm)		
	λ_{abs}	λ_{em}	Stoke's shift
2a	408	516	108
2b	380	513	133
2c	399	515	116
2d	392	511	119
2e	393	513	120
2f	395	517	122
2g	392	516	124
2h	386	487	101
2i	383	513	130
2j	420	517	97
2k	413	524	111
2l	411	527	116
2m	412	516	104
2n	415	512	97
2o	400	508	108
2p	409	522	113
2q	409	516	107
2r	408	525	117
2s	408	524	116
2t	409	523	114
2u	409	556	147

2v	410	525	115
2w	409	516	107
2x	408	526	118
2y	406	522	116
2z	408	525	117
2aa	409	536	127
2ab	410	522	112
3ac	410	517	107
2ad	413	519	106
2ae	409	514	105
2af	409	524	115

[a] λ_{abs} and λ_{em} refer to optimal absorption wavelength and photoluminescence (PL) peak, respectively

5. Crystallographic data of 2a, 2a′, 6a′,7a and 8 [a]



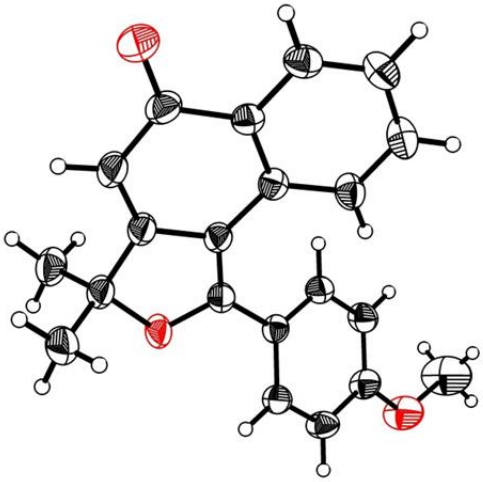
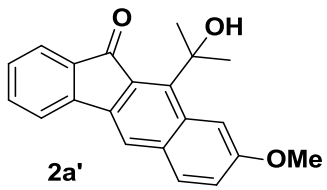


Figure S2. ORTEP diagram of X-ray crystal structure of compounds **2a** (CCDC No. 2048922). The thermal ellipsoids are shown at 35% probability. Colour code: red, oxygen; white, hydrogen; black, carbon. The crystal was grown from CH_2Cl_2 and PE. 20 mg of **2a** was dissolved in CH_2Cl_2/PE mixed solvent (1.5/3.0 mL) and the solvent was evaporated slowly in a cold atmosphere.



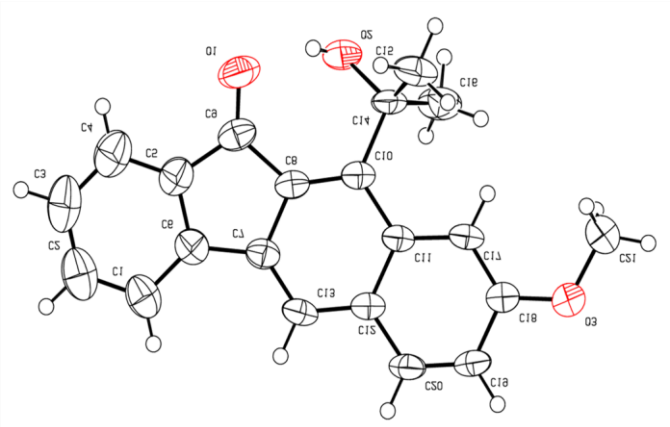


Figure S3. ORTEP diagram of X-ray crystal structure of compounds **2a′** (CCDC No. 2047946). The thermal ellipsoids are shown at 35% probability. Colour code: red, oxygen; white, hydrogen; black, carbon. The crystal was grown from CH_2Cl_2 and PE. 15 mg of **2a′** was dissolved in CH_2Cl_2/PE mixed solvent (1.0/2.0 mL) and the solvent was evaporated slowly in a cold atmosphere.

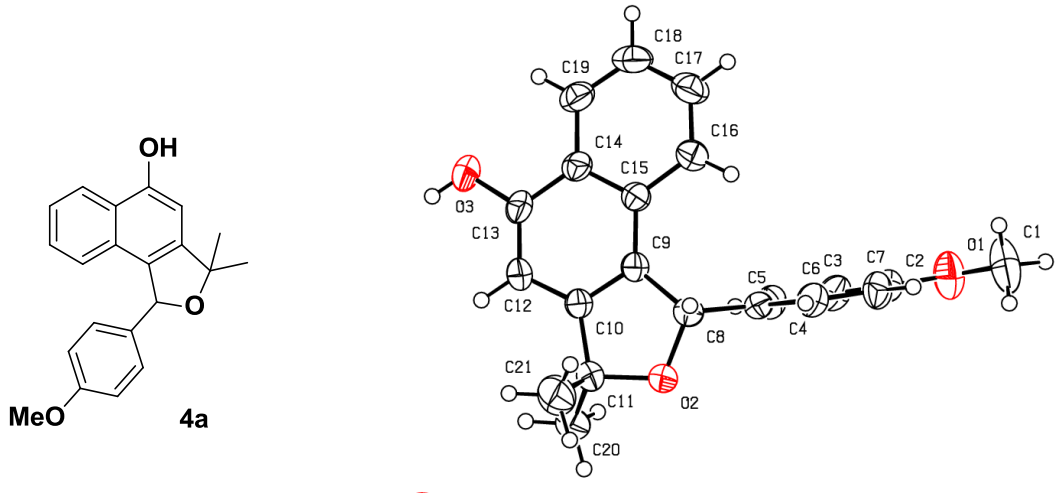


Figure S4. ORTEP diagram of X-ray crystal structure of compounds **4a** (CCDC No. 2047947). The thermal ellipsoids are shown at 35% probability. Colour code: red, oxygen; white, hydrogen; black, carbon. The crystal was grown from CH_2Cl_2 and PE. 15 mg of **4a** was dissolved in CH_2Cl_2/PE mixed solvent (1.5/3.0 mL) and the solvent was evaporated slowly in a cold atmosphere.

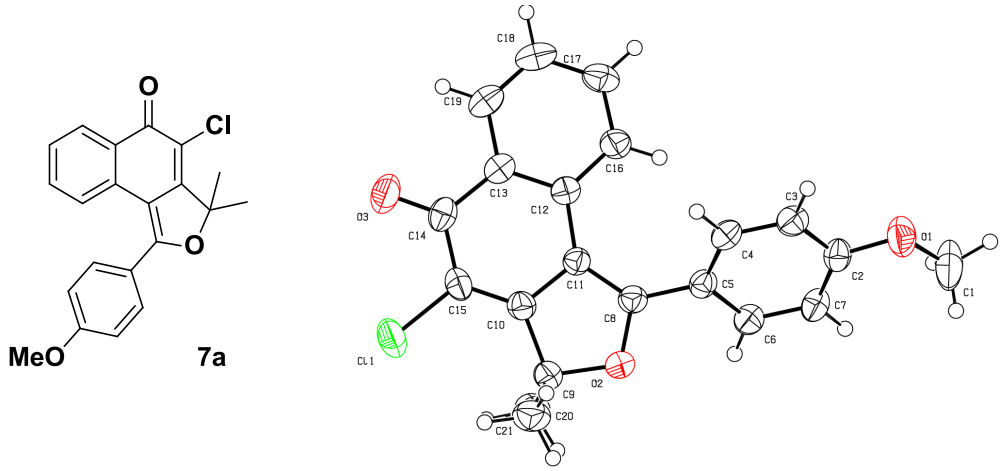
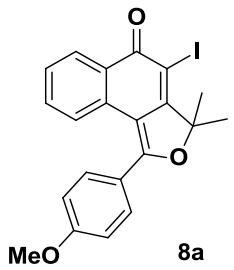


Figure S5. ORTEP diagram of X-ray crystal structure of compounds **7a** (CCDC No. 2047978). The thermal ellipsoids are shown at 35% probability. Colour code: red, oxygen; white, hydrogen; black, carbon; green, chlorine. The crystal was grown from MeOH and PE. 20 mg of **7a** was dissolved in MeOH/PE mixed solvent (2.0/2.0 mL) and the saturated solution was kept in open-air for 7 days to get the crystals.



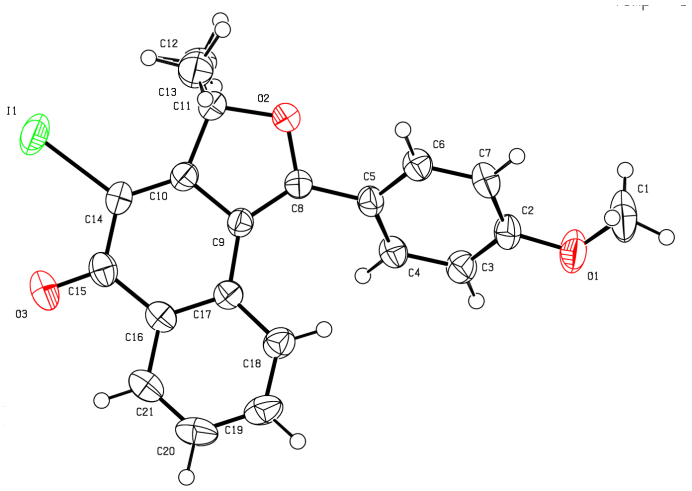
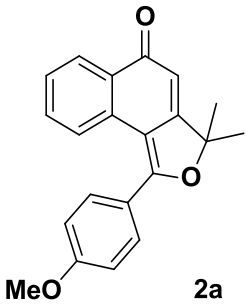


Figure S6. ORTEP diagram of X-ray crystal structure of compounds **8a** (CCDC No. 2047981). The thermal ellipsoids are shown at 35% probability. Colour code: red, oxygen; white, hydrogen; black, carbon; green, iodine. The crystal was grown from CH_2Cl_2 and PE. 20 mg of **8a** was dissolved in CH_2Cl_2/PE mixed solvent (2.0/2.0 mL) and the solvent was evaporated slowly in a cold atmosphere.

Table S4. Single crystal X-ray analysis Data of compounds **2a**, **2a'**, **4a**, **7a** and **8a**

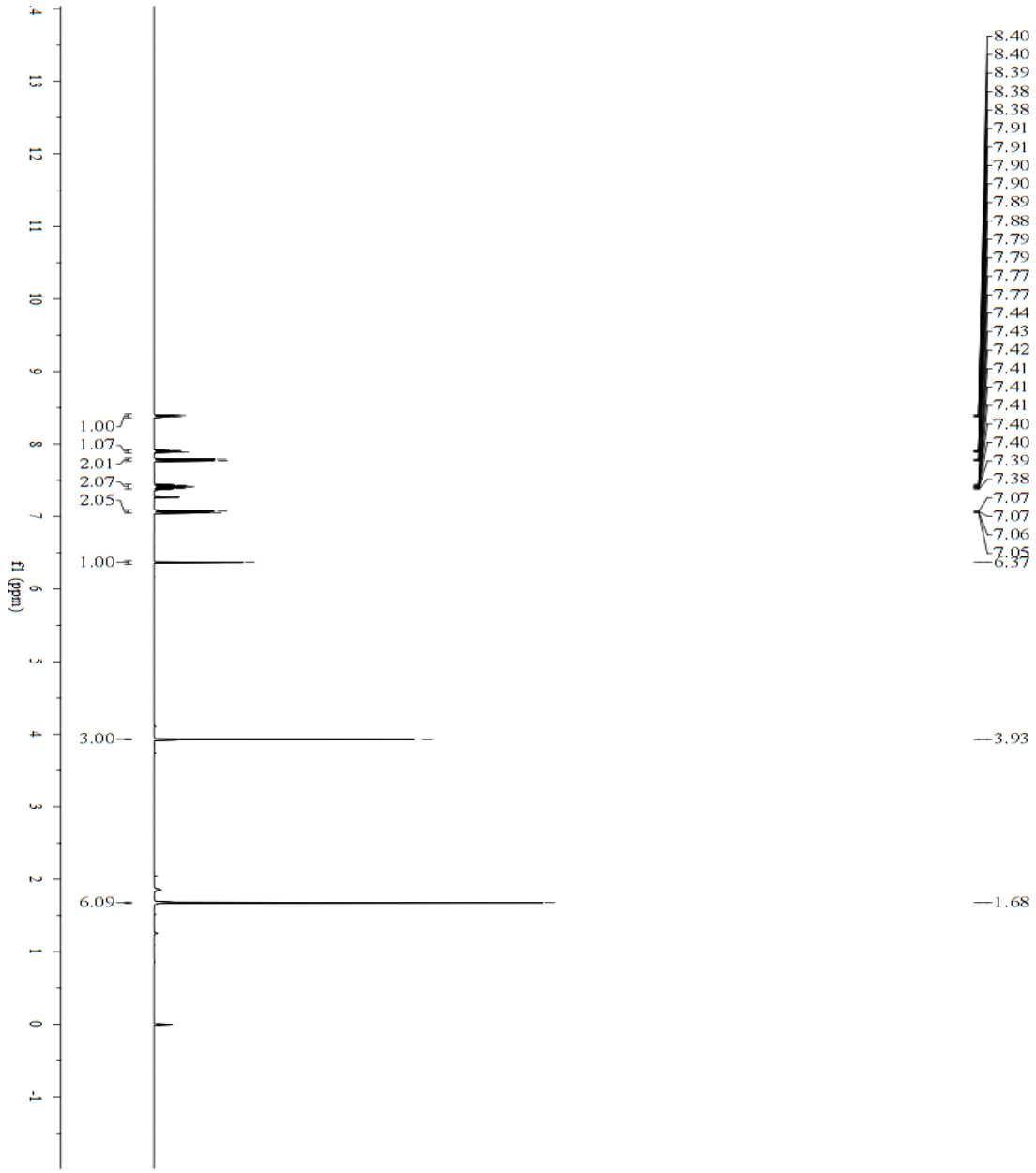
Compound	**2a**	**2a'**	**4a**	**7a**	**8a**
Formula	$C_{21}H_{18}O_3$	$C_{21}H_{18}O_3$	$C_{21}H_{20}O_3$	$C_{21}H_{17}ClO_3$	$C_{21}H_{17}IO_3$
Formula weight	318.35	318.35	320.37	352.80	444.24
Temperature (K)	296	273	293	293	293
Crystal system	triclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	P-1	P121/c1	P-1	P121/n1	P121/n1
a (Å)	8.883(2)	12.113(3)	10.7494(13)	9.7134(13)	9.9035(9)
b (Å)	9.021(2)	8.898(2)	12.6882(15)	10.7377(14)	11.1983(10)
c (Å)	11.529(3)	16.011(4)	14.4376(17)	16.496(2)	16.2555(15)
α (°)	69.035(3)	90	106.113(4)	90	90
β (°)	75.555(4)	111.889(6)	90.491(4)	100.188(4)	101.280(3)
γ (°)	82.063(4)	90	113.104(4)	90	90
$V(Å^3)$	834.2(3)	1601.1(7)	1724.6(4)	1693.4(4)	1767.9(3)
Z	25	4	4	4	4
$D_c/g\ cm^{-3}$	1.2675	1.321	1.234	1.384	1.669
μ/mm^{-1}	0.084	0.087	0.082	0.243	1.828
F(000)	336.1762	672	680	736	880
Crystal size/mm^3	0.02 x 0.01 x 0.01	0.25 x 0.21 x 0.14	0.25 x 0.21 x 0.14	0.25 x 0.21 x 0.13	0.25 x 0.21 x 0.14
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
R(int)	0.0150	0.1959	0.0328	0.0395	0.0326
Total reflections	3279	25003	36614	26152	27294
Independent reflections	2145	3694	7927	3891	4064
θmin< θ < θmax	2.37 to 26.25	2.924 to 27.572	2.963 to 27.558	2.961 to 27.521	2.880 to 27.507
R_1, wR_2 (I>2σ(I))	R_1 = 0.0509, wR_2 = 0.1326	R_1 = 0.0706, wR_2 = 0.1335	R_1 = 0.0471, wR_2 = 0.1117	R_1 = 0.0466, wR_2 = 0.1124	R_1 = 0.0317, wR_2 = 0.0797
R_1, wR_2 (for all data)	R_1 = 0.0763, wR_2 = 0.1482	R_1 = 0.1520, wR_2 = 0.1641	R_1 = 0.0747, wR_2 = 0.1255	R_1 = 0.0735, wR_2 = 0.1257	R_1 = 0.0433, wR_2 = 0.0845
Goodness-of-fit on F^2	1.0157	1.021	1.026	1.021	1.080

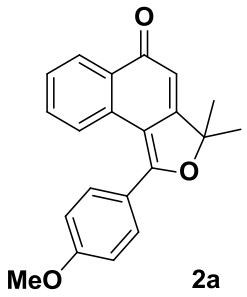
6. ^{1}H NMR and ^{13}C NMR Spectra for Products



2a

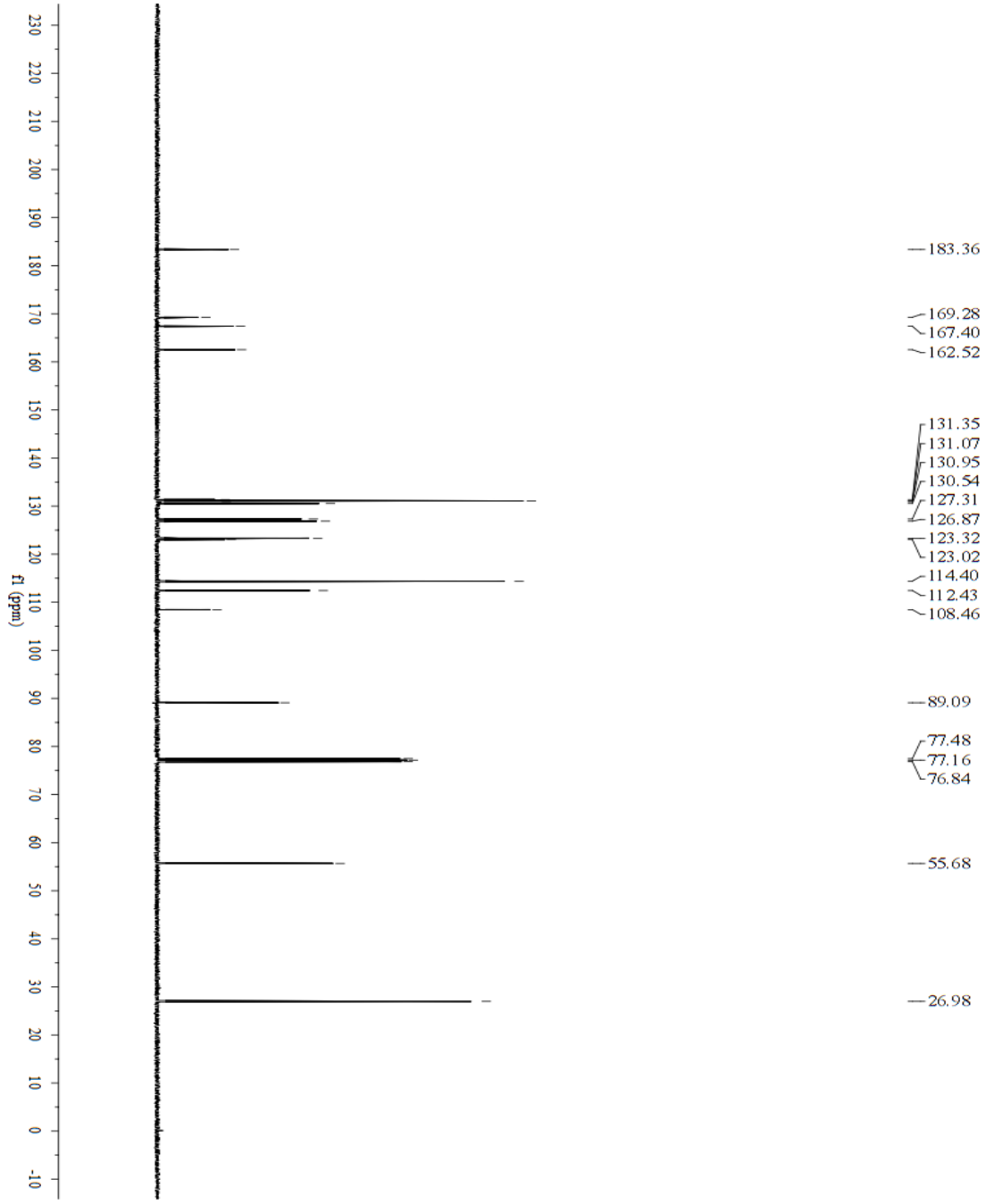
^{1}H NMR (400 MHz, $CDCl_3$)

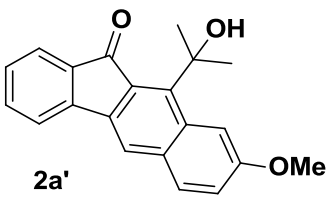




2a

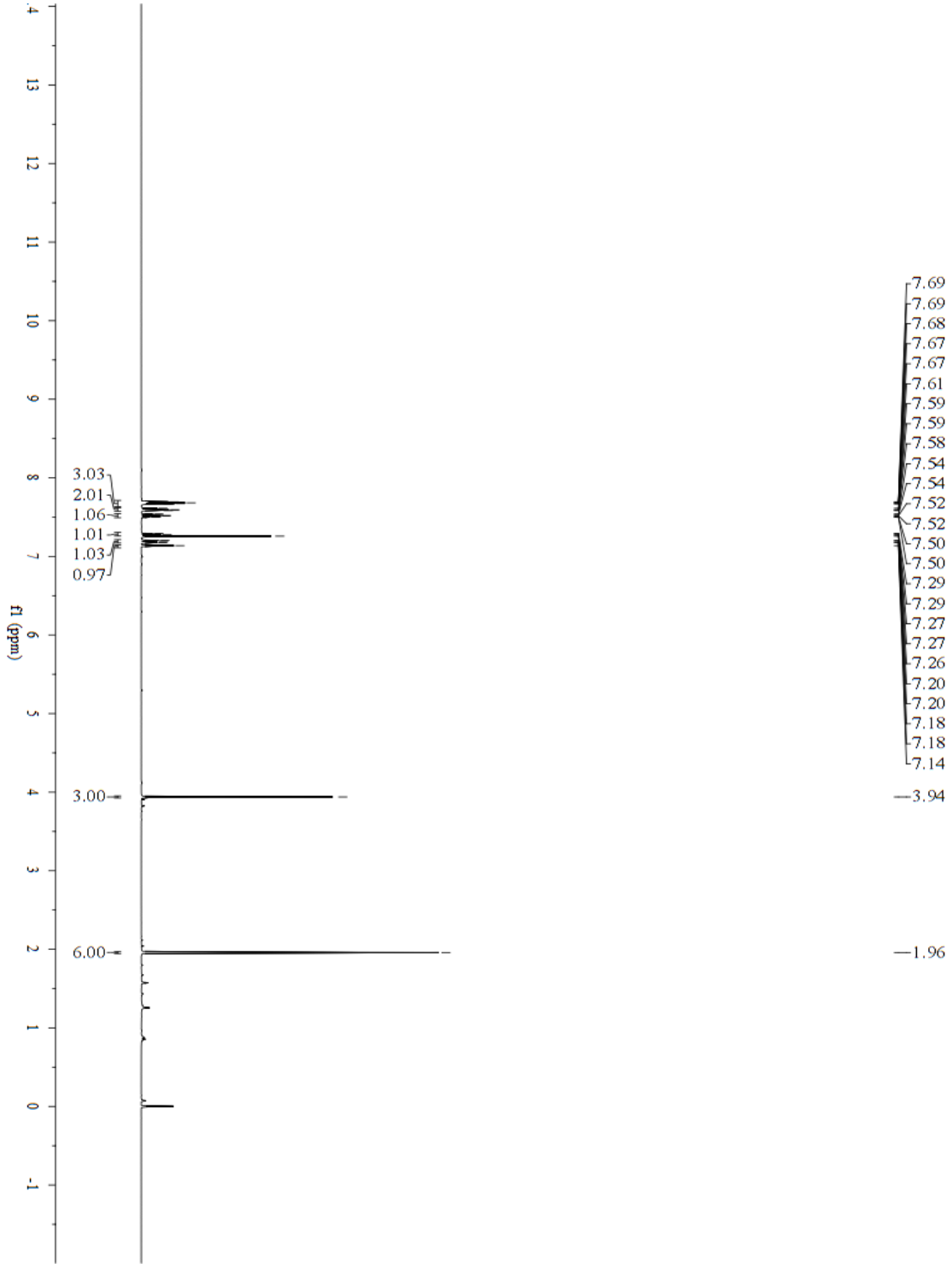
^{13}C {^{1}H}NMR (100 MHz, $CDCl_3$)

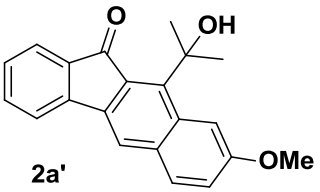




2a'

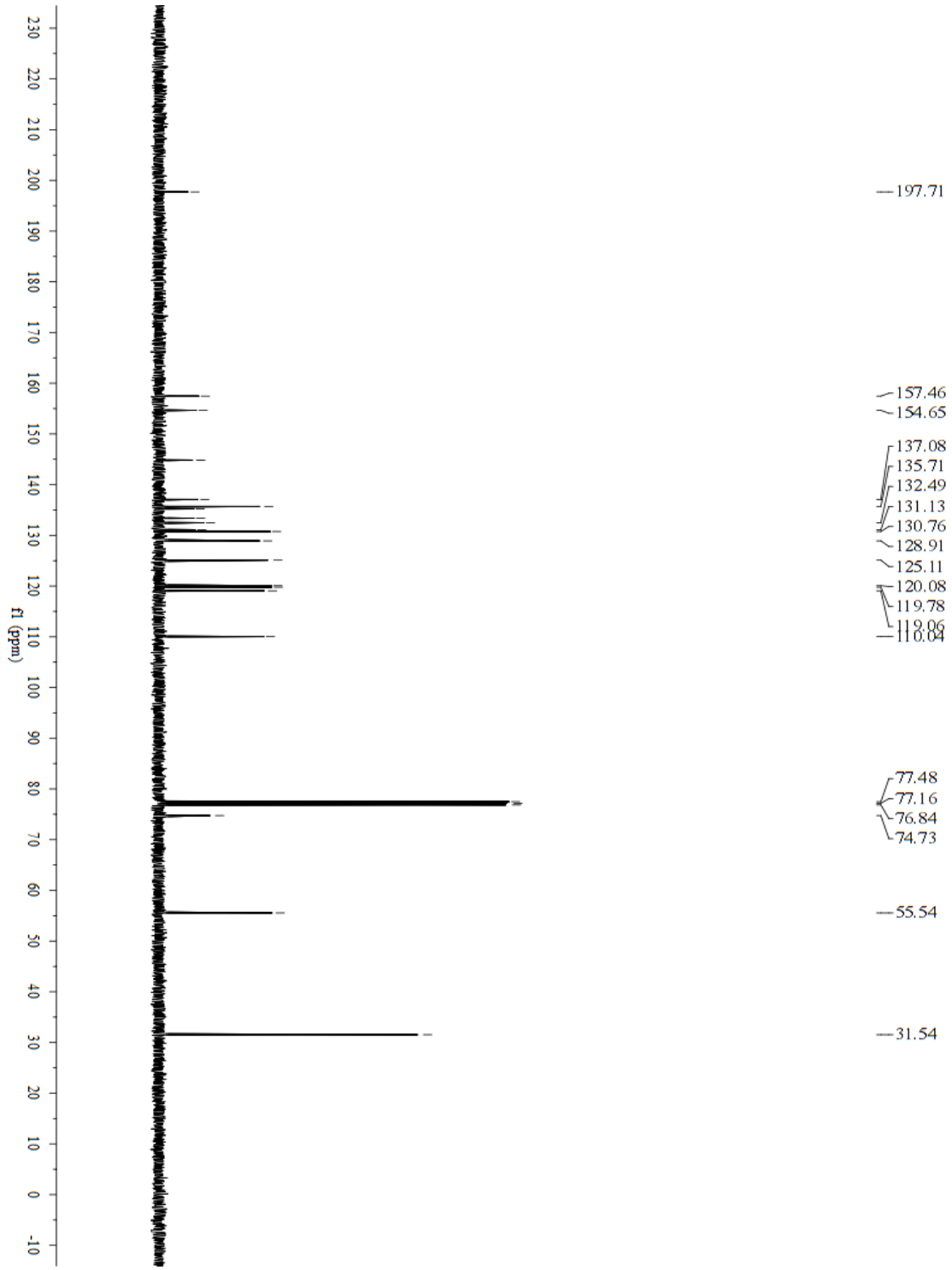
^{1}H NMR (400 MHz, $CDCl_3$)

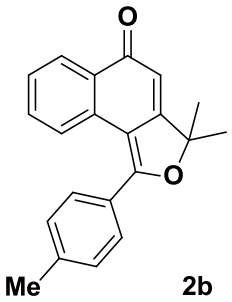




2a'

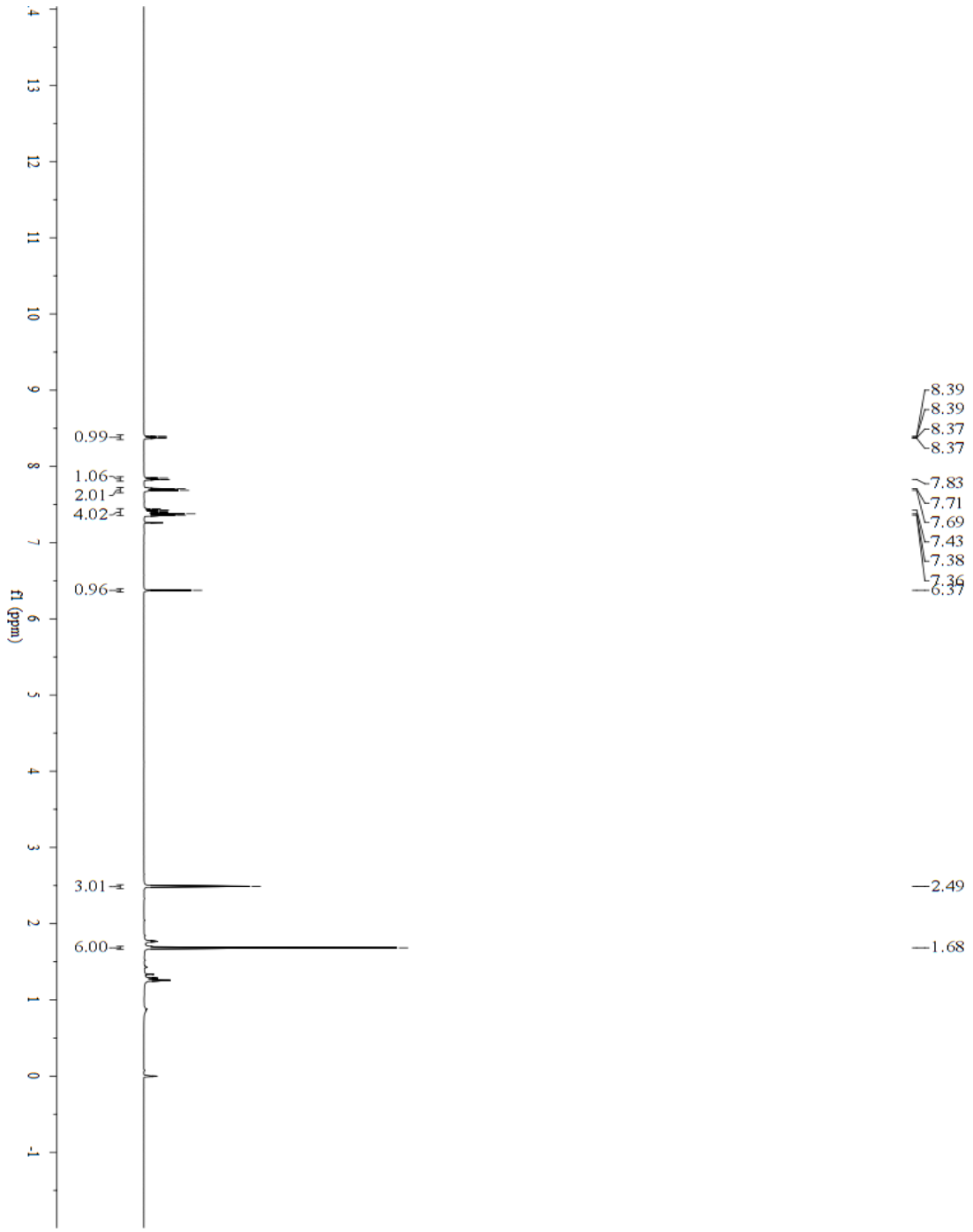
$^{13}C\ \{^{1}H\}$NMR (100 MHz, $CDCl_3$)

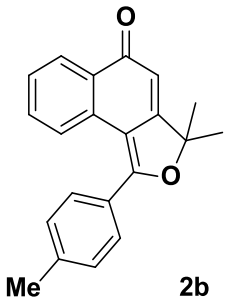




2b

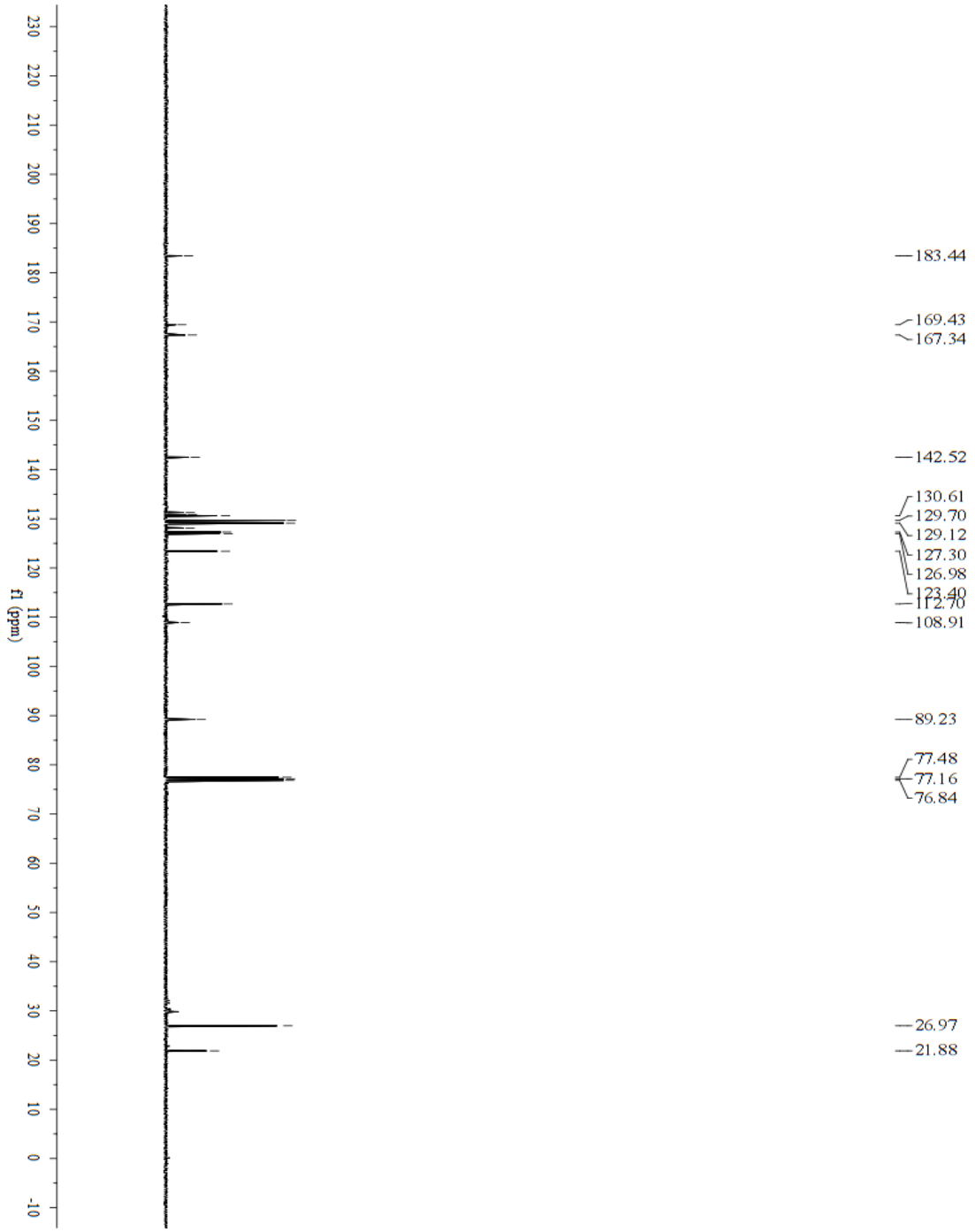
^{1}H NMR (400 MHz, $CDCl_3$)

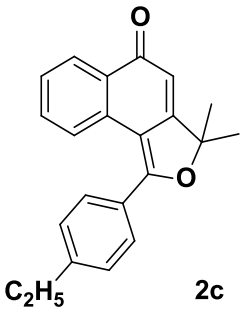




2b

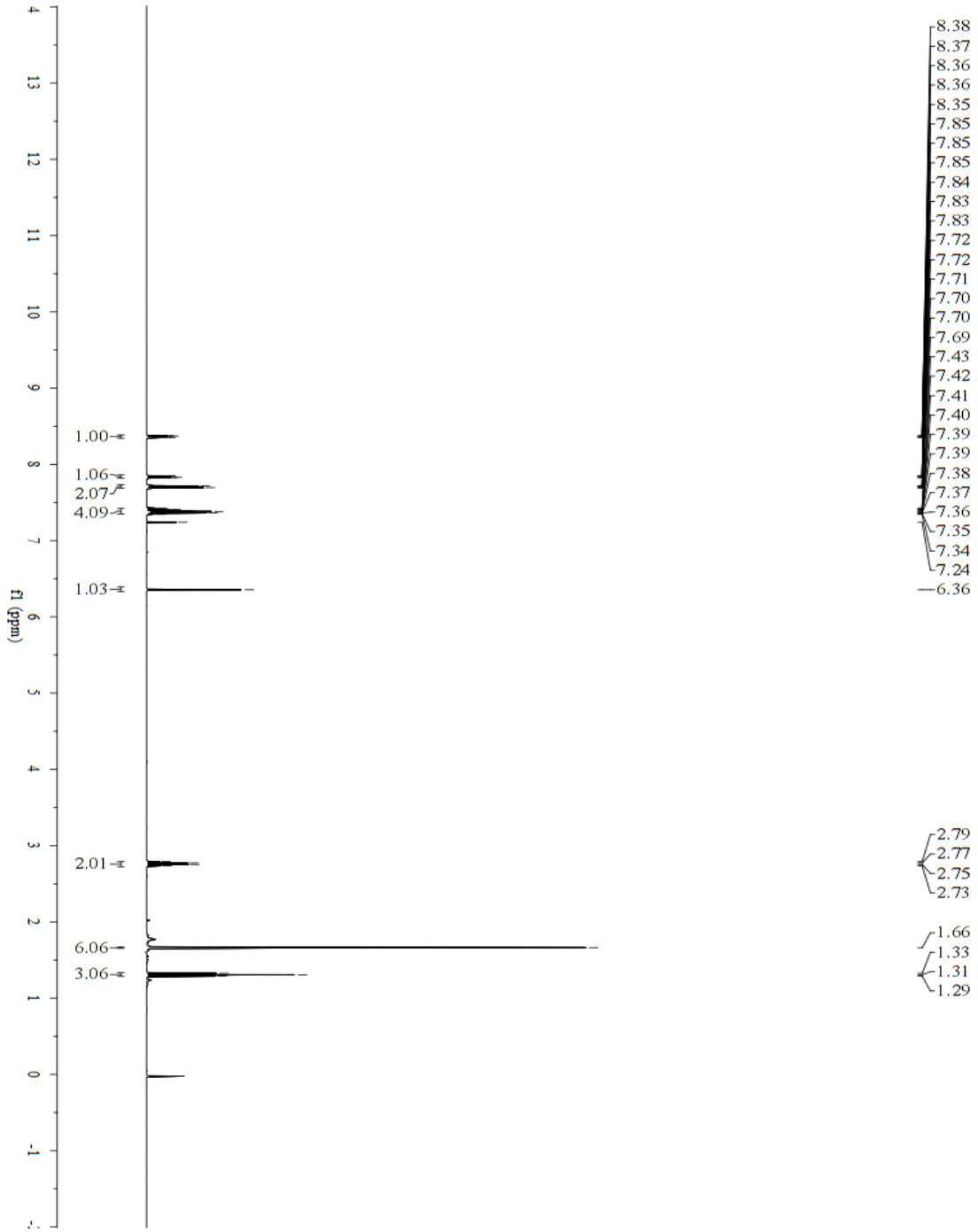
$^{13}C\ \{^{1}H\}$NMR (100 MHz, $CDCl_3$)

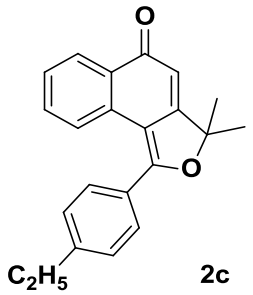




2c

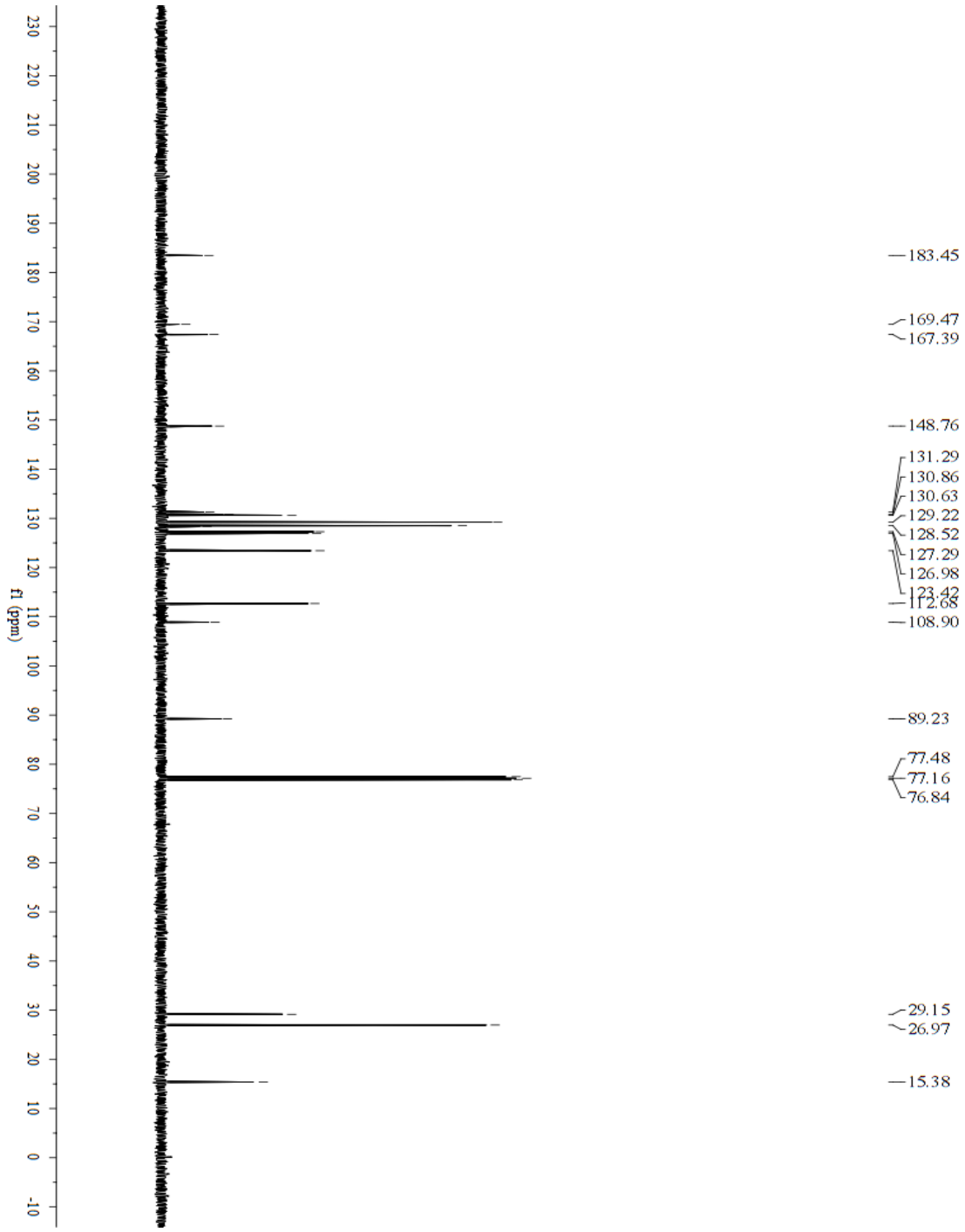
^{1}H NMR (400 MHz, $CDCl_3$)

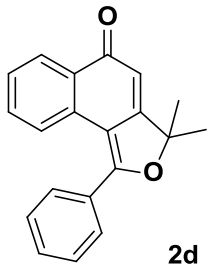




2c

^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)





2d

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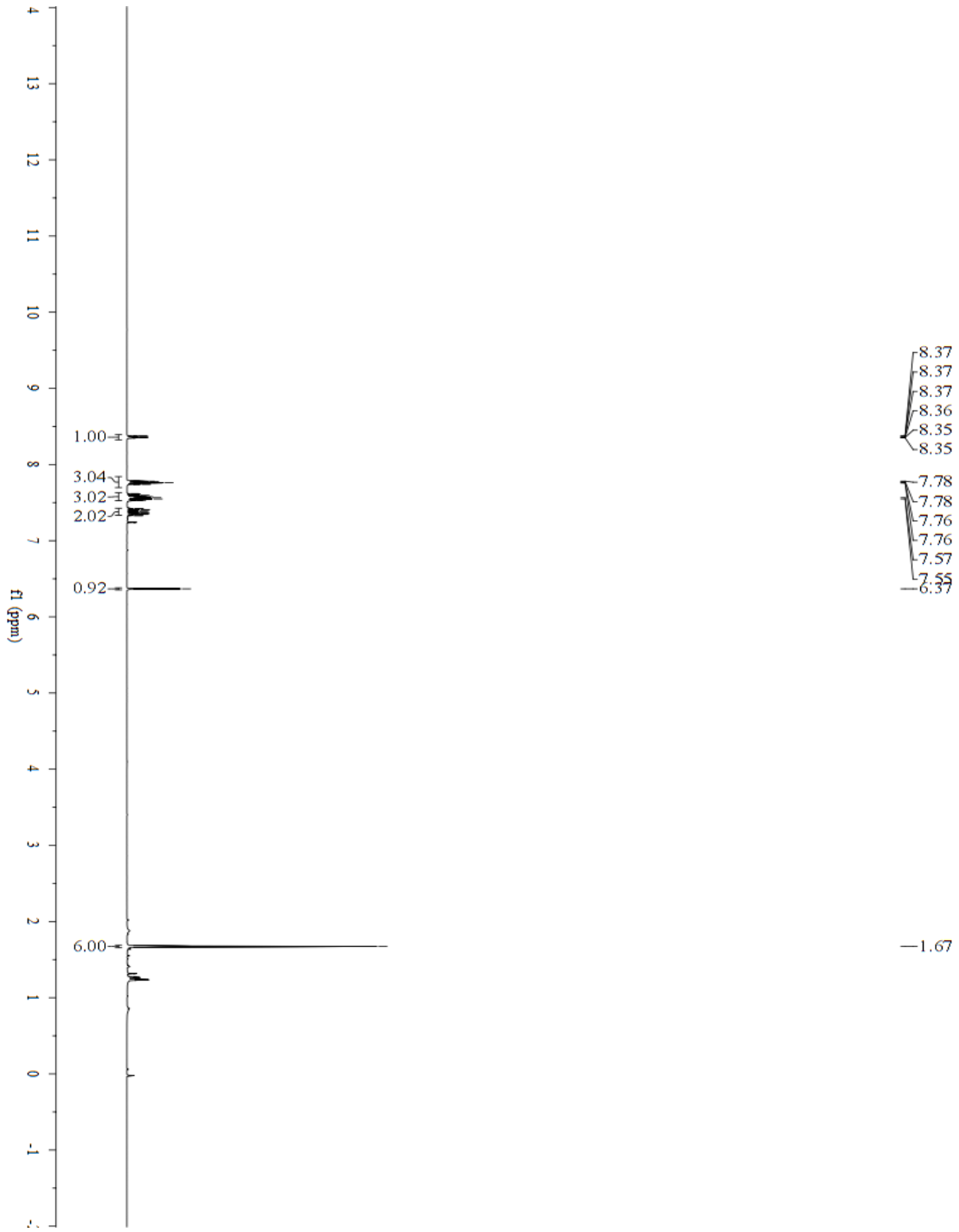

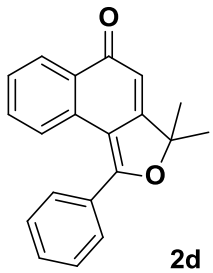

2d

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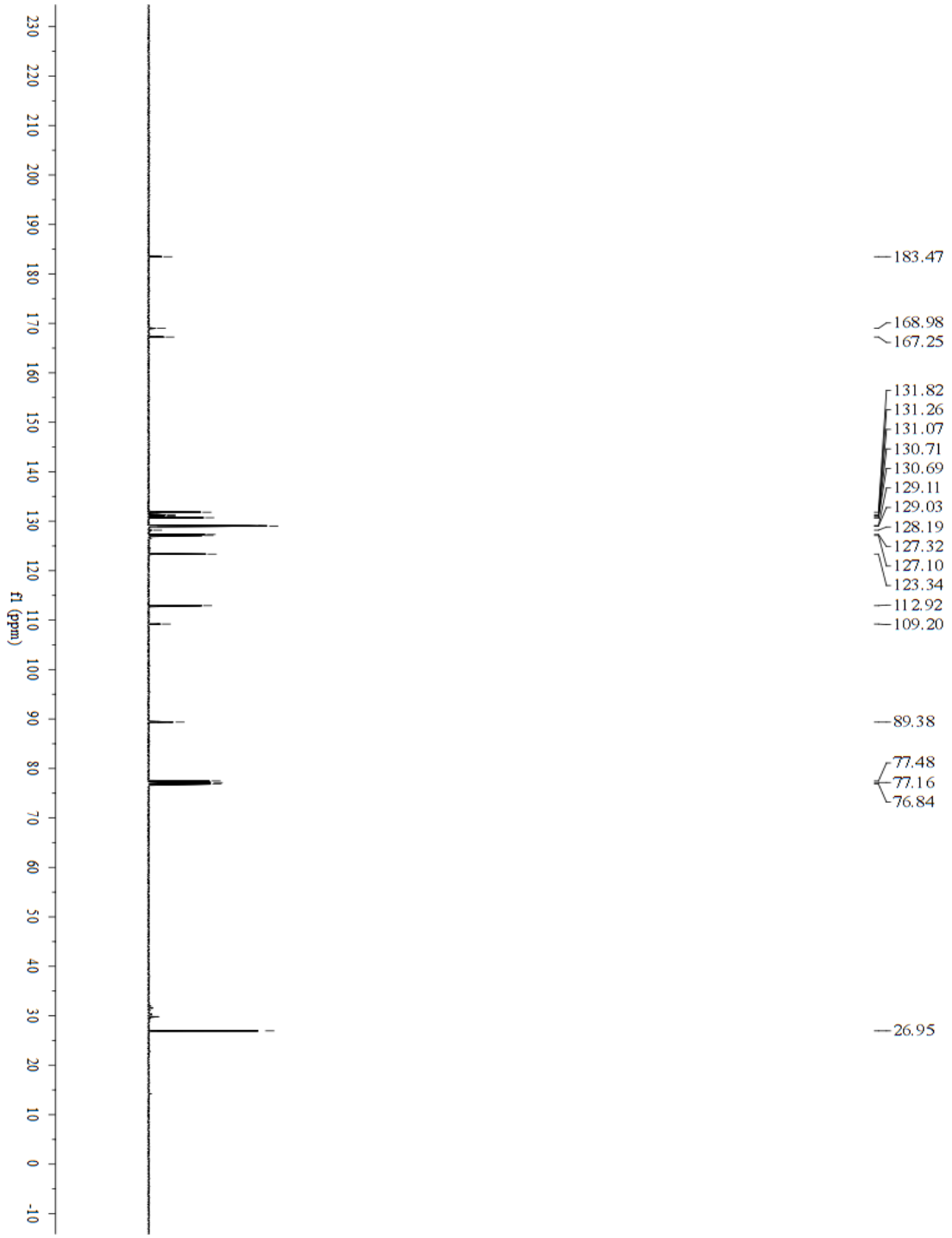
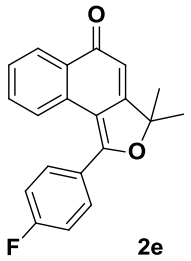
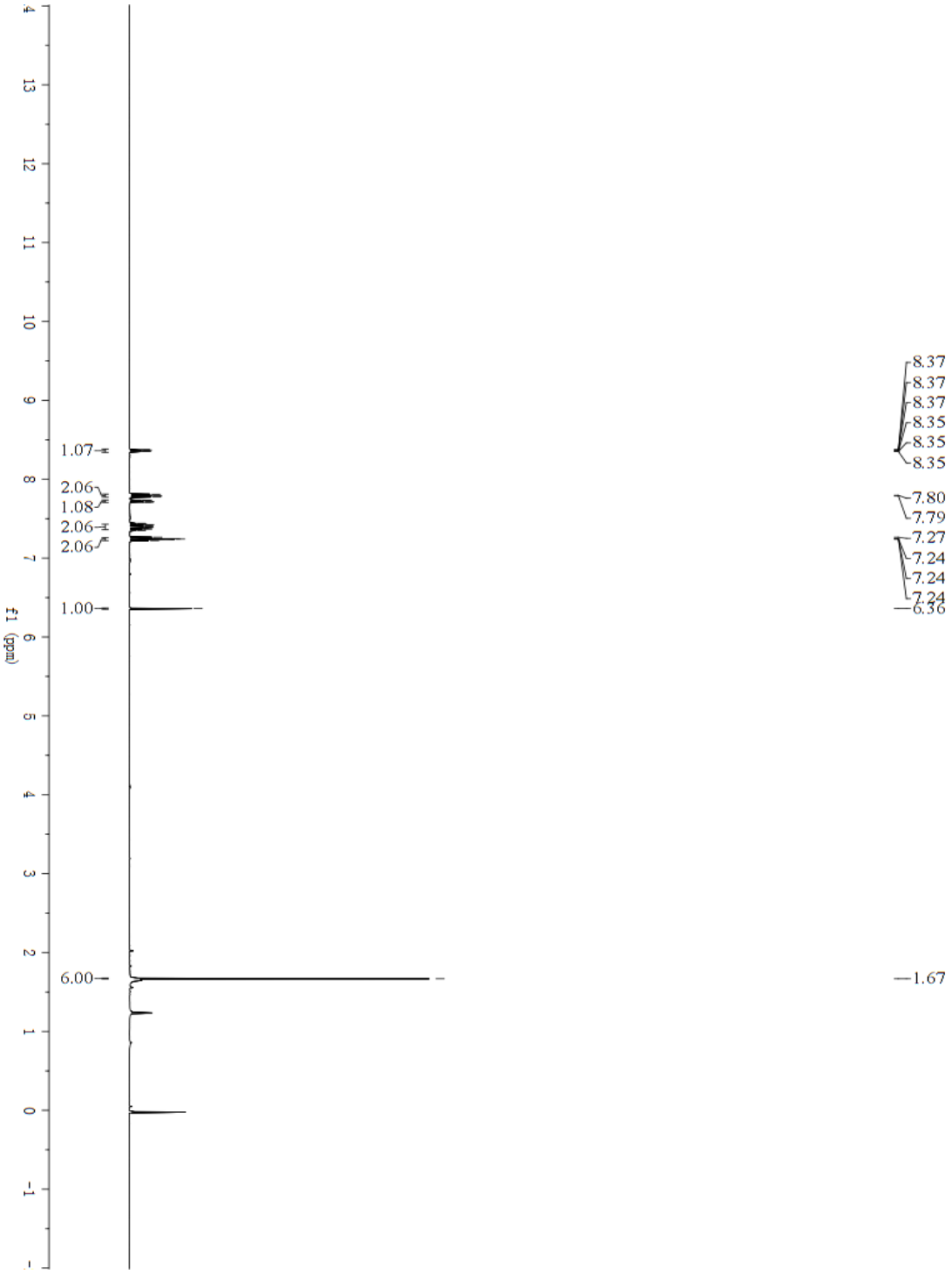
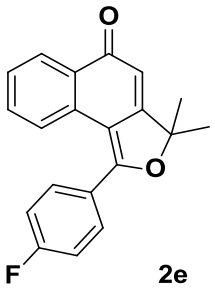




2e

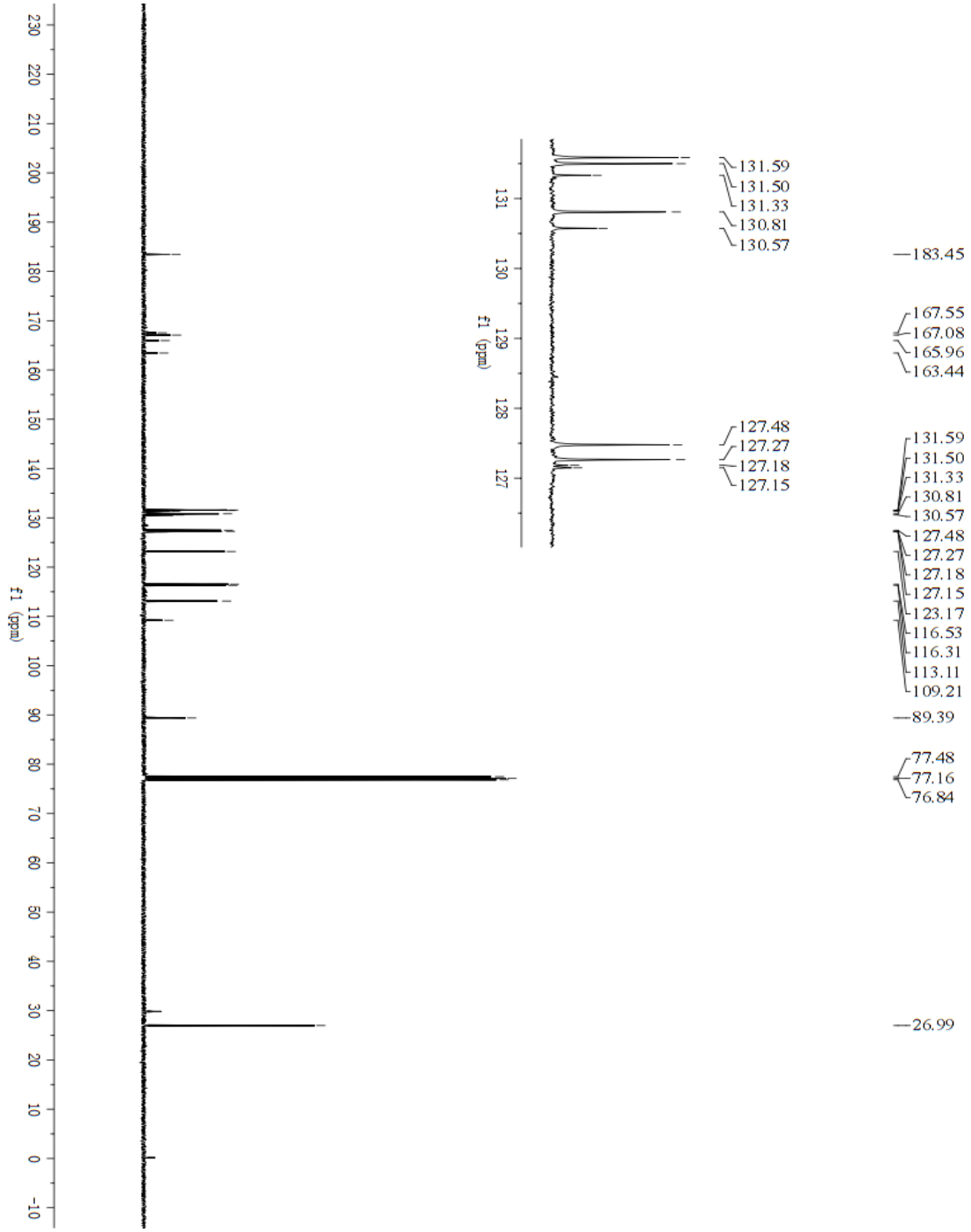
^{1}H NMR (400 MHz, $CDCl_3$)

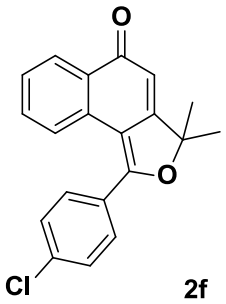




2e

^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)





2f

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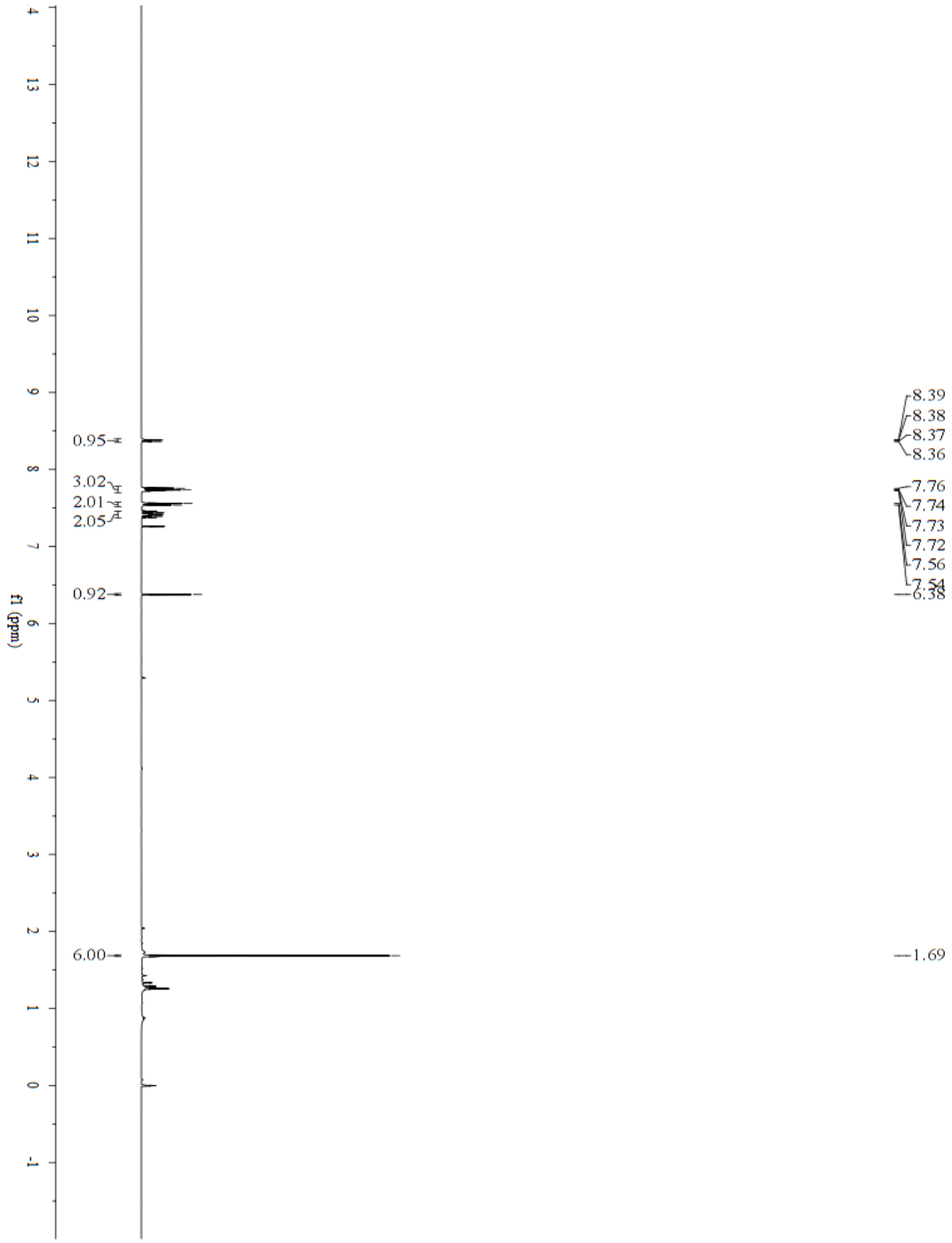
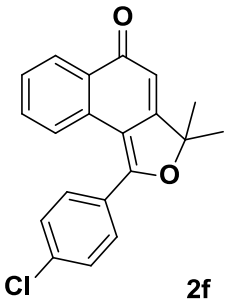
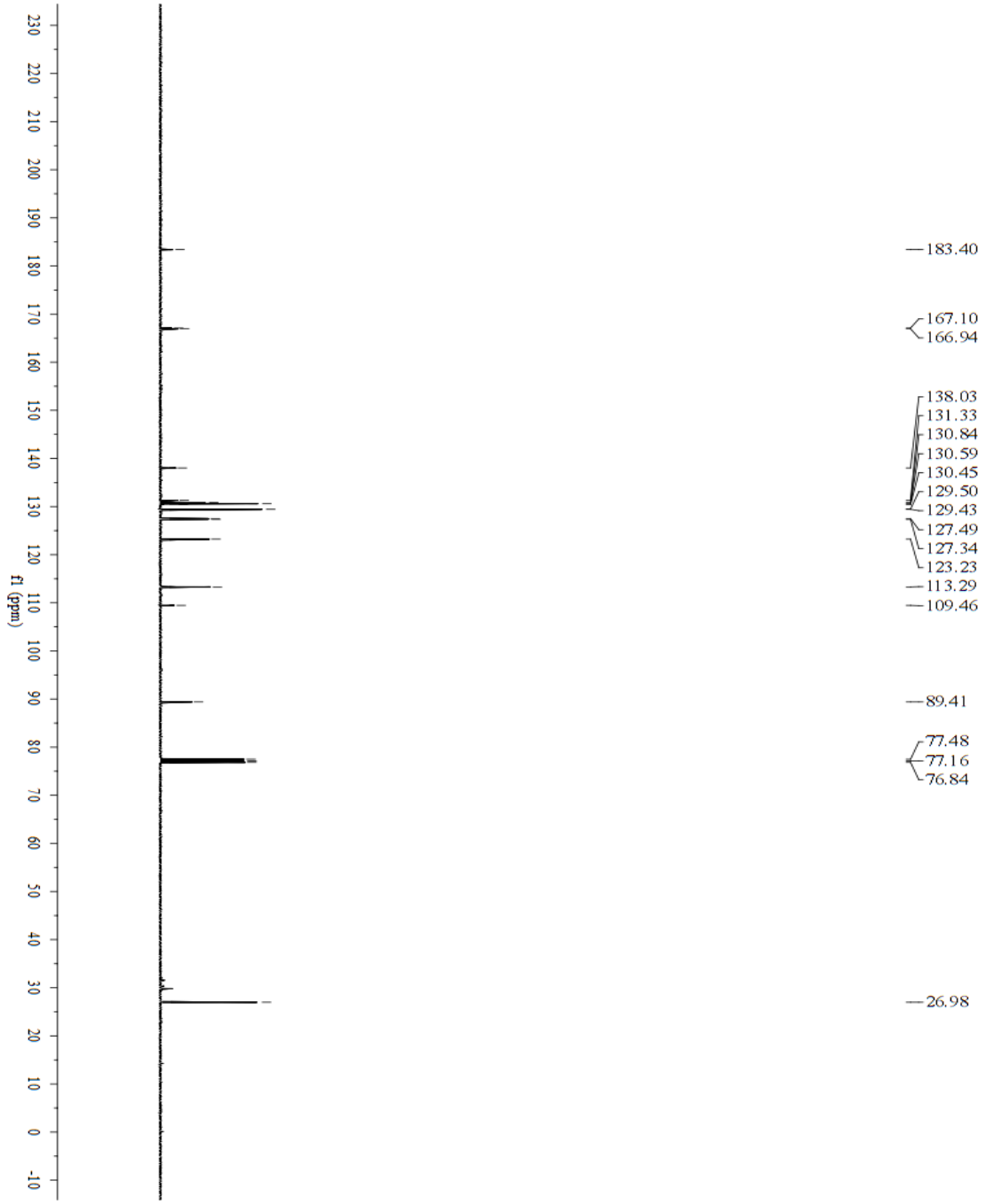
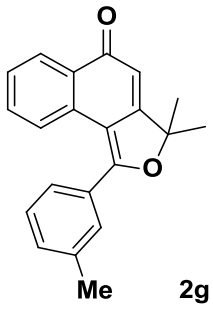




2f

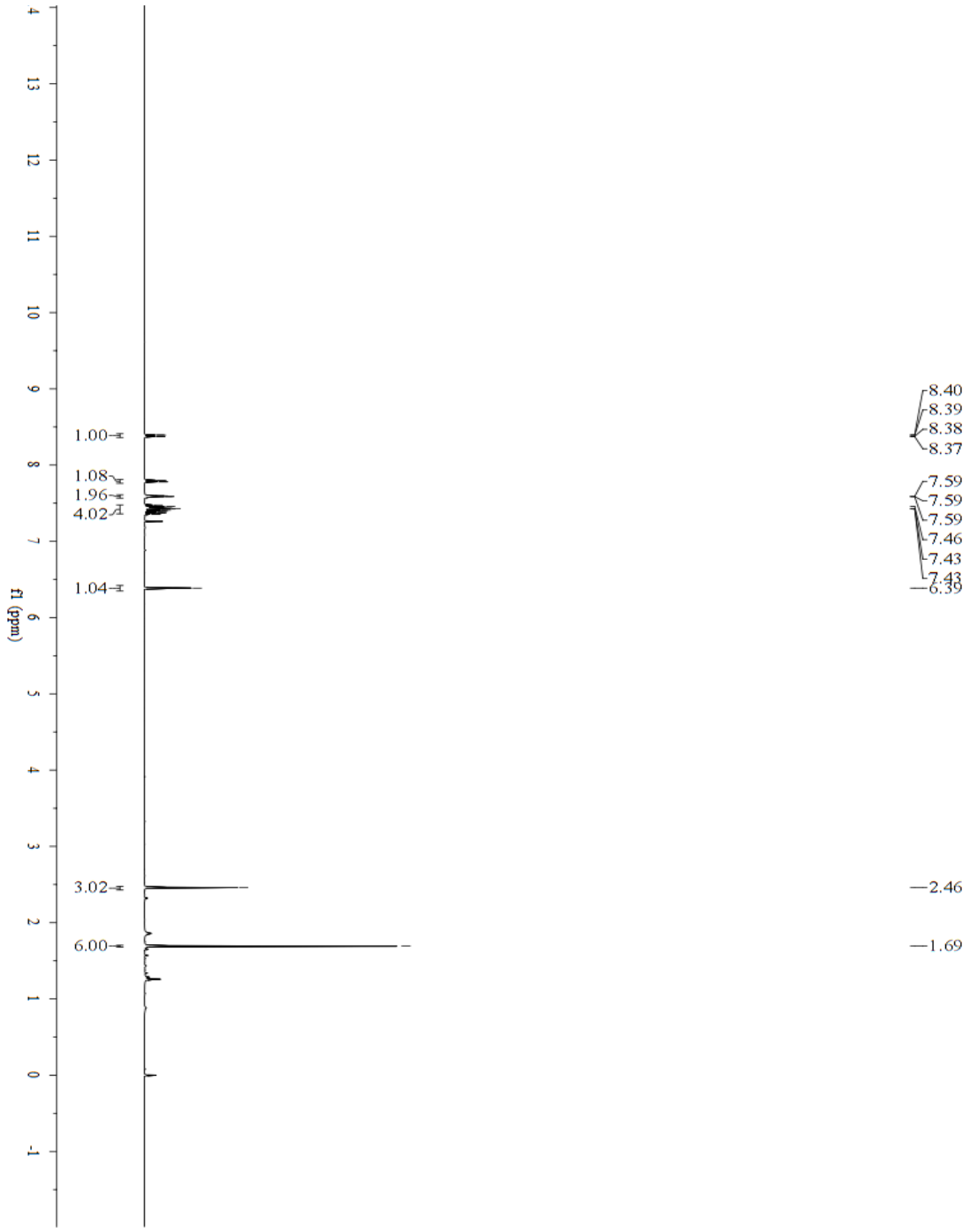
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

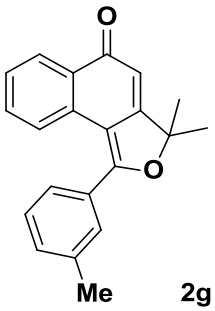




2g

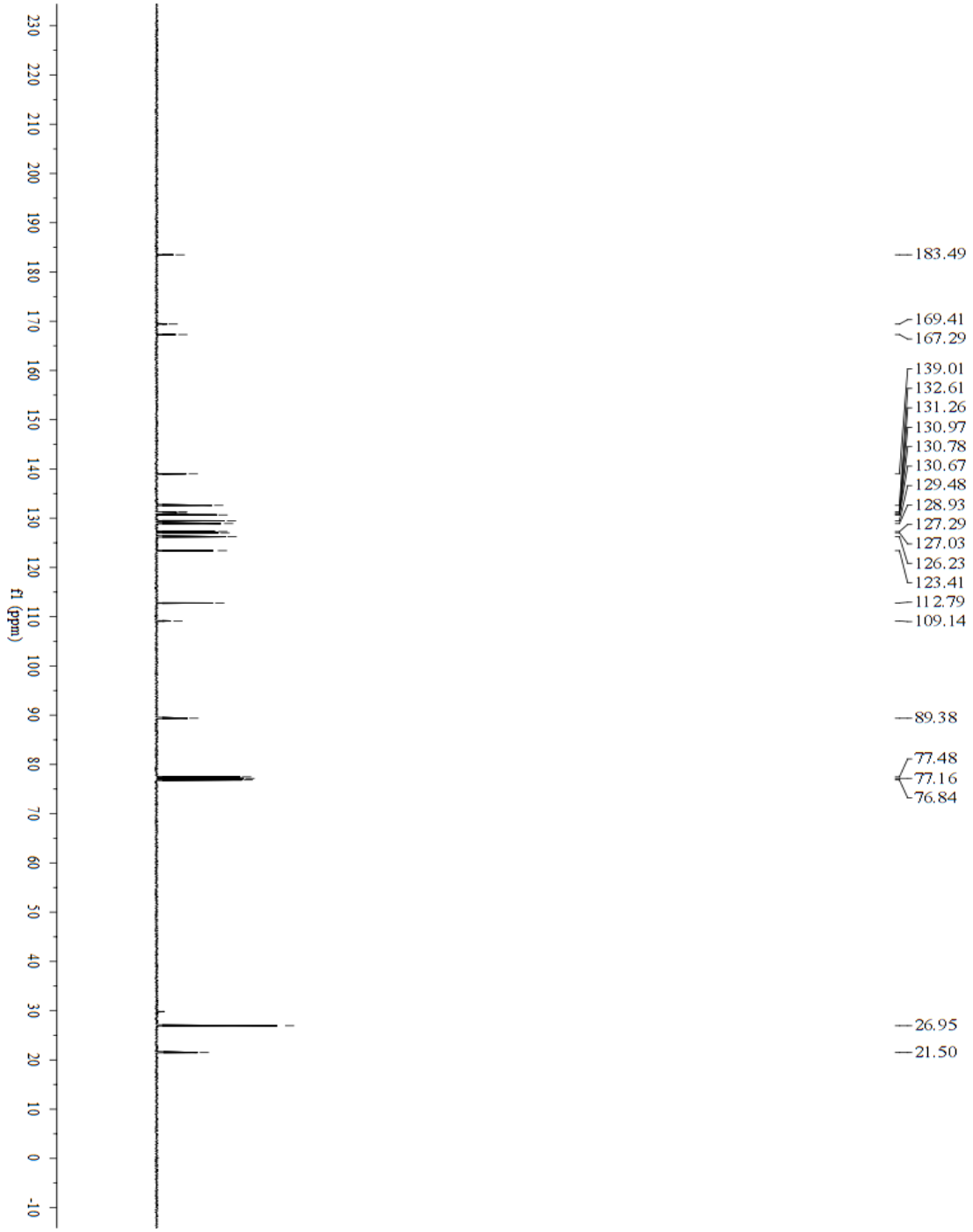
^{1}H NMR (400 MHz, $CDCl_3$)

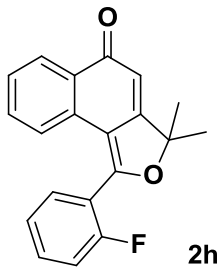




2g

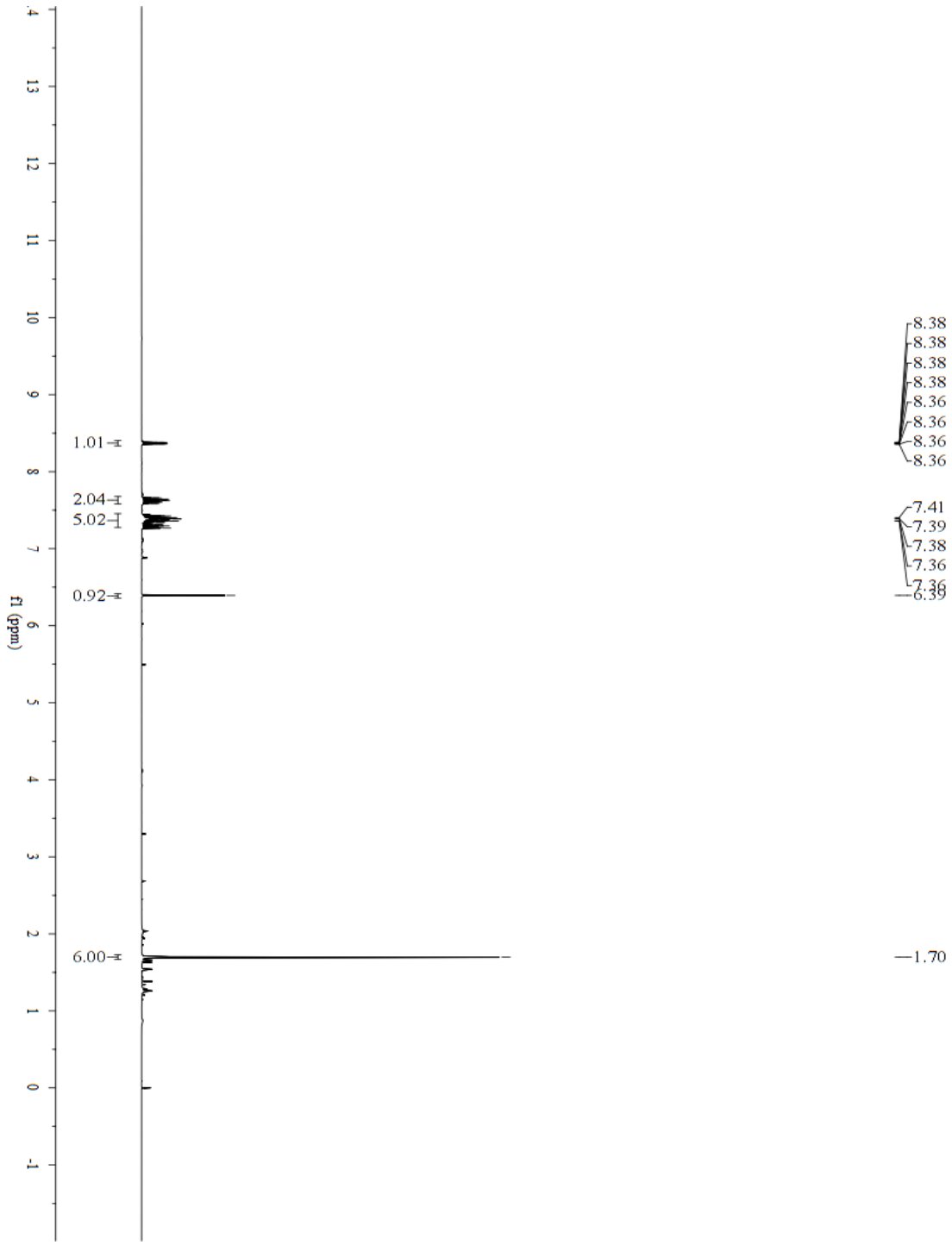
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

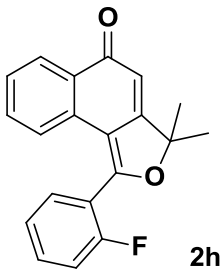




2h

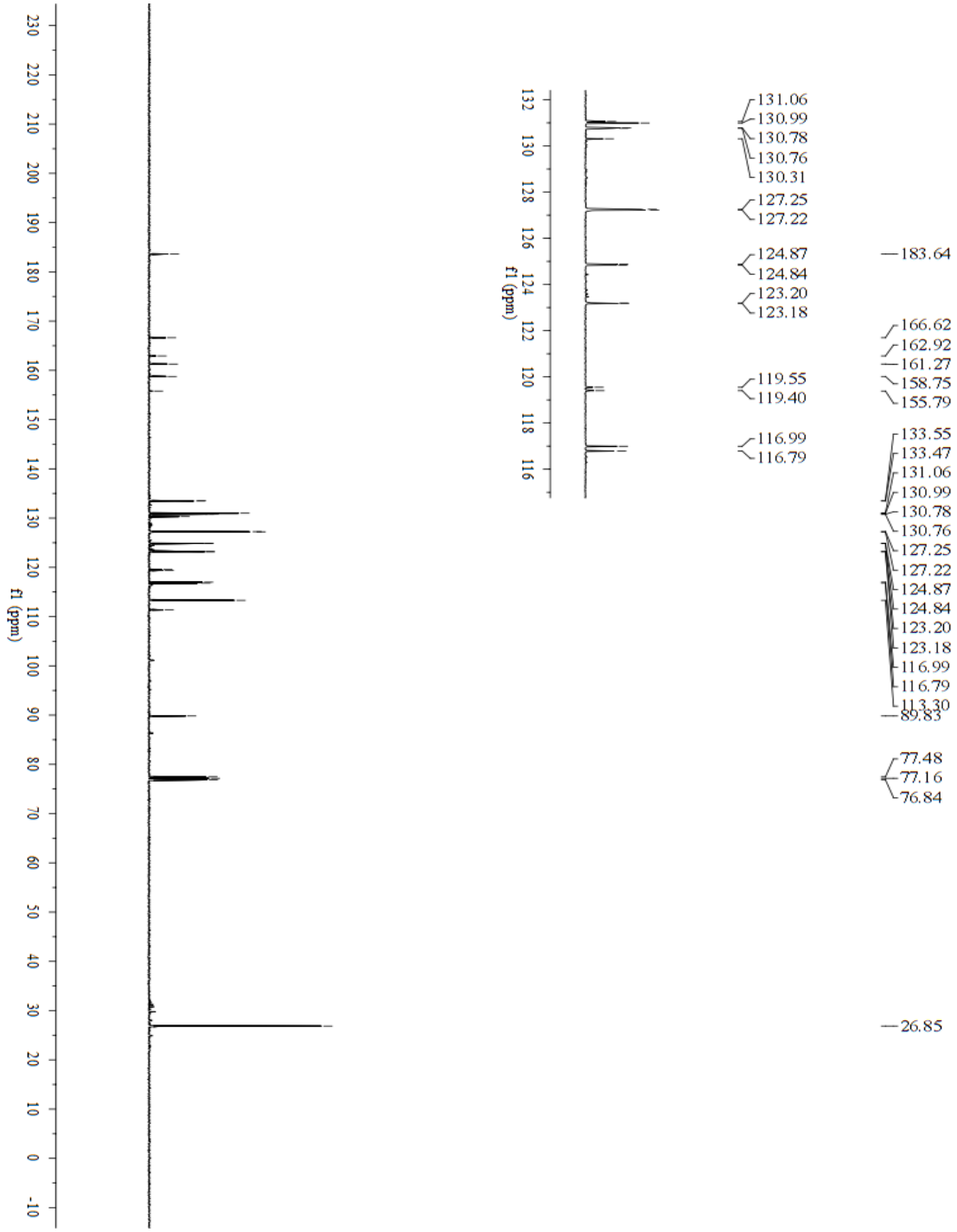
^{1}H NMR (400 MHz, $CDCl_3$)

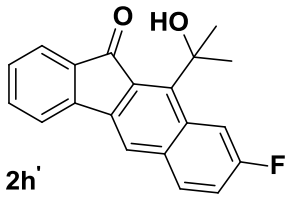




2h

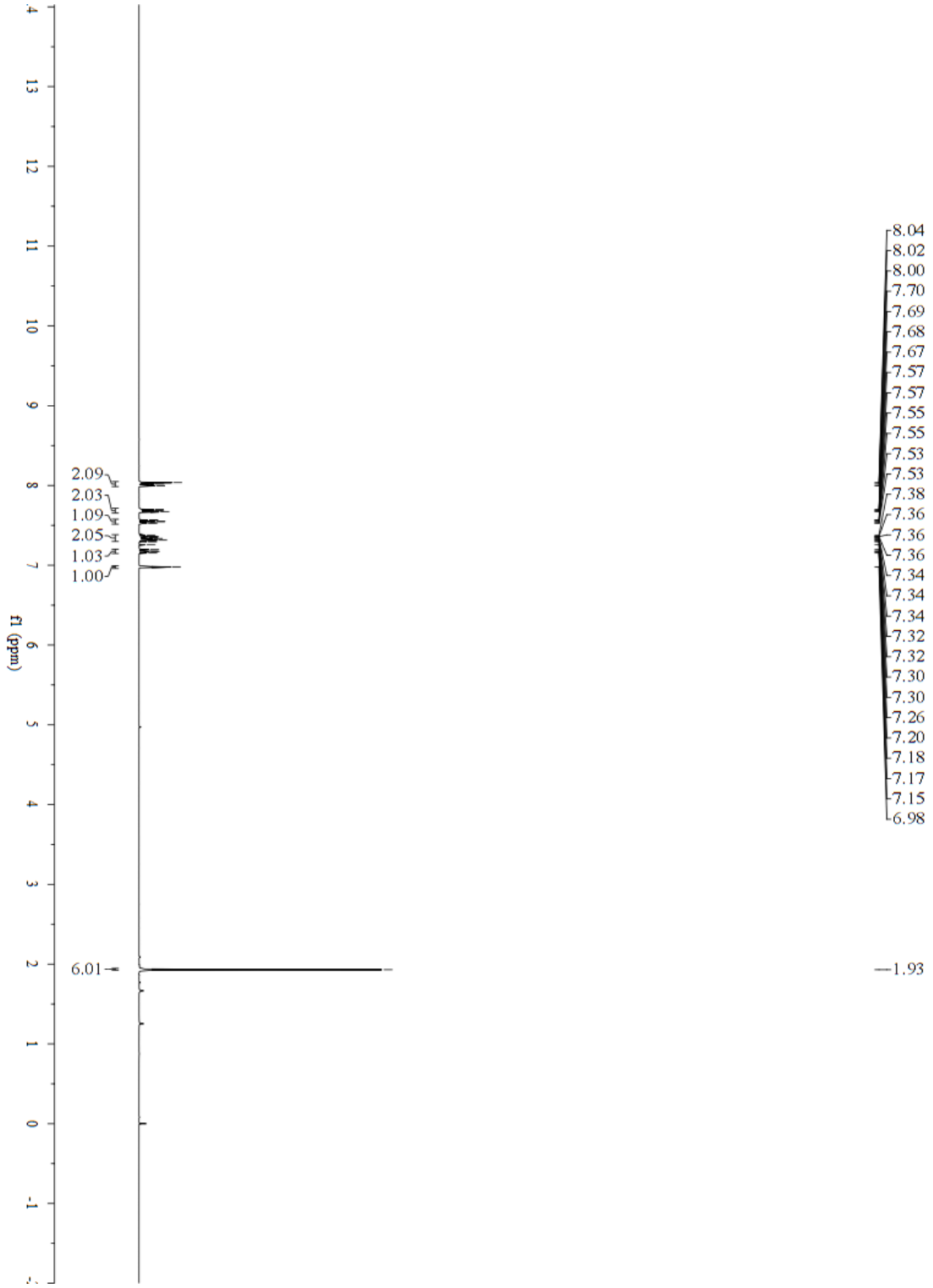
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

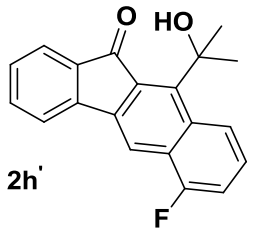




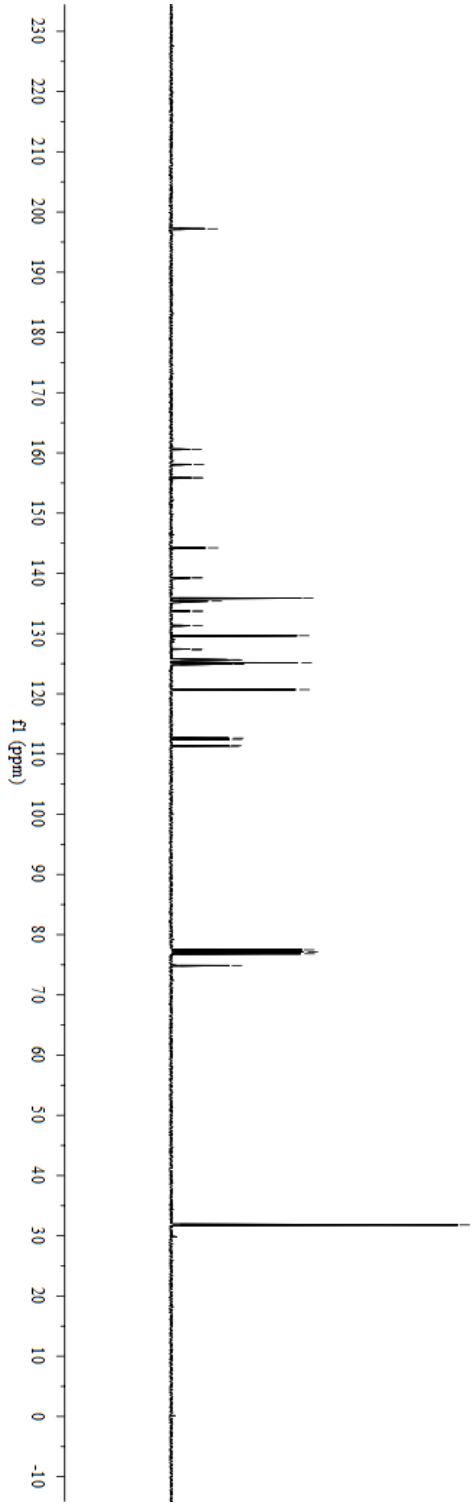
2h'

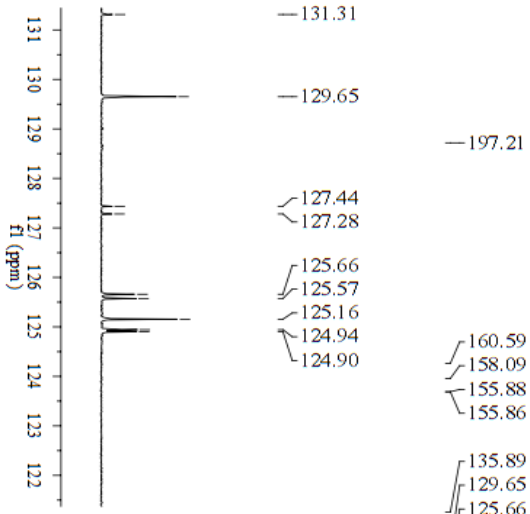
^{1}H NMR (400 MHz, $CDCl_3$)

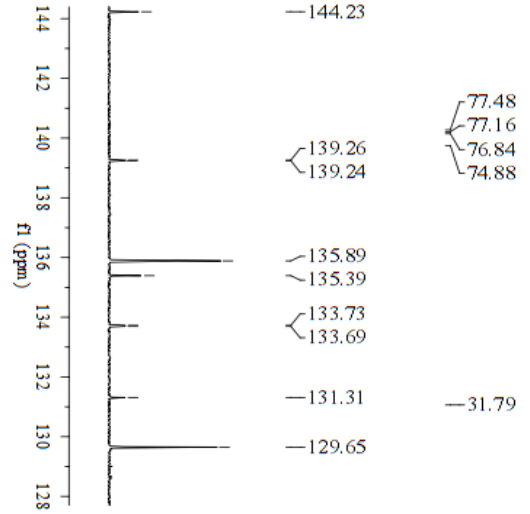


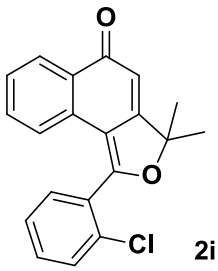


^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)



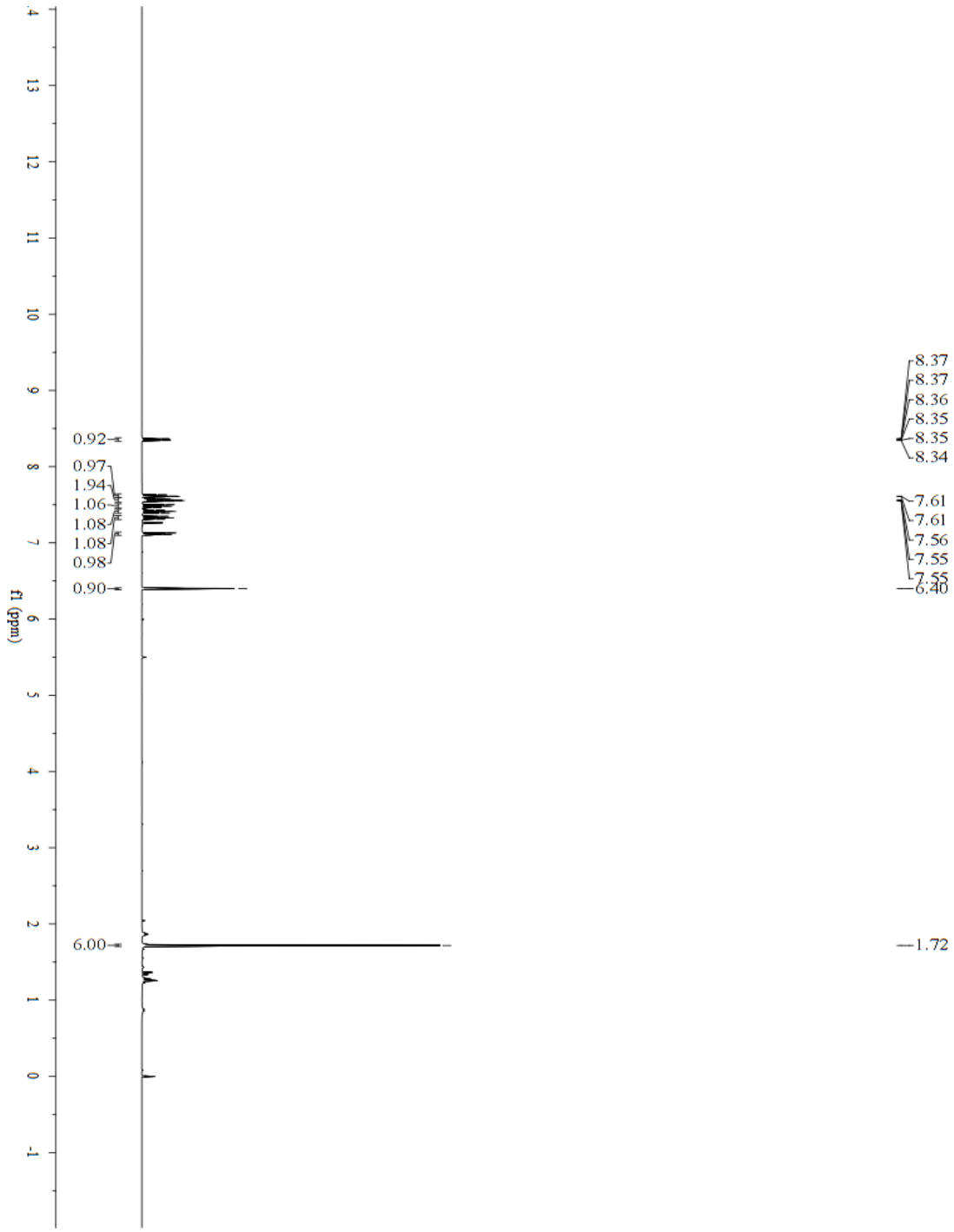


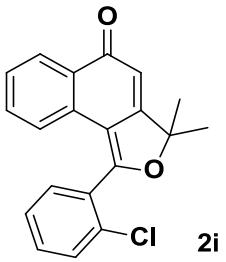




2i

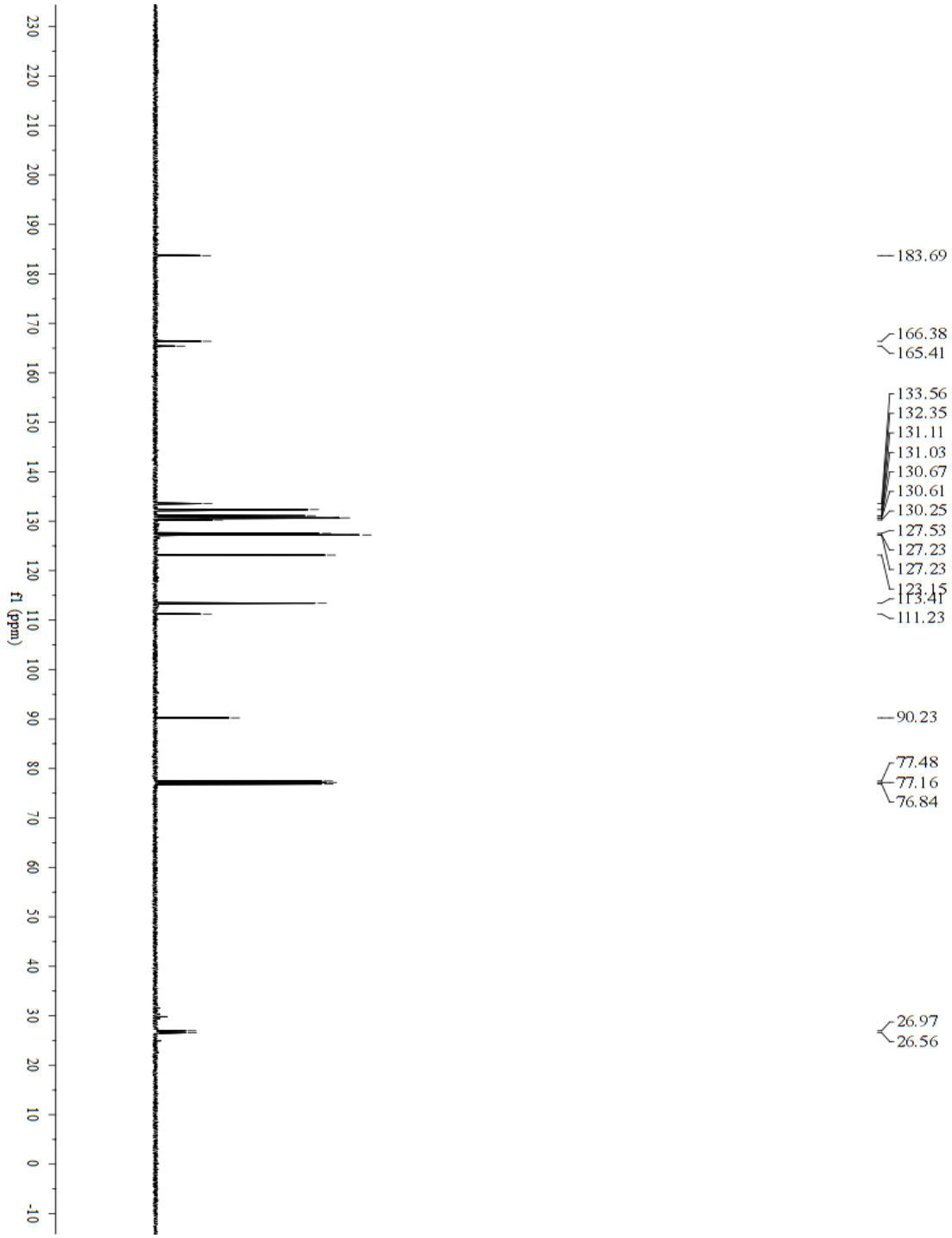
^{1}H NMR (400 MHz, $CDCl_3$)

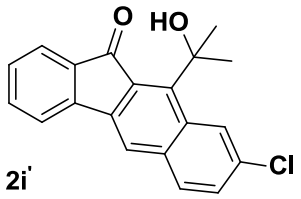




2i

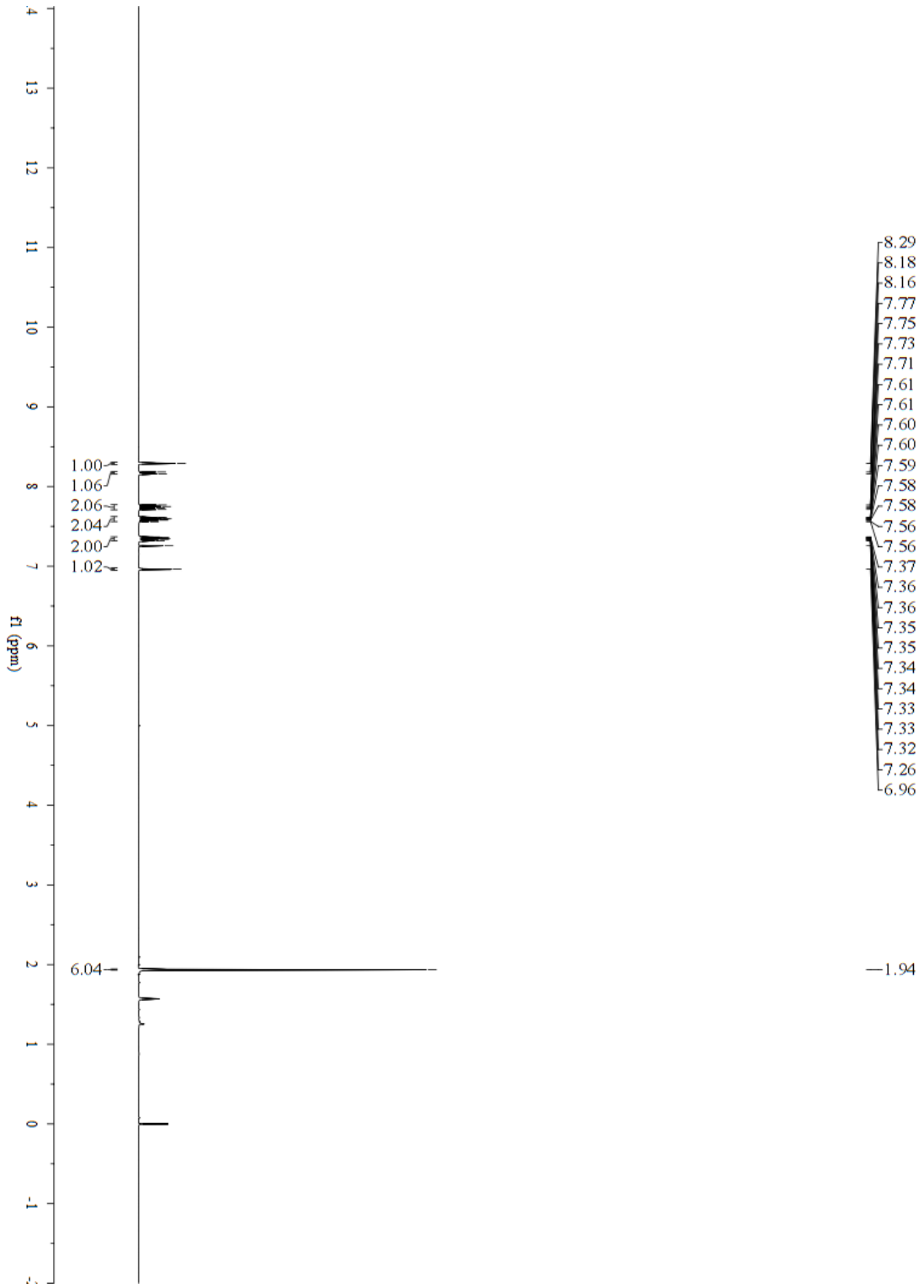
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)

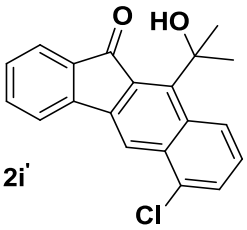




2i'

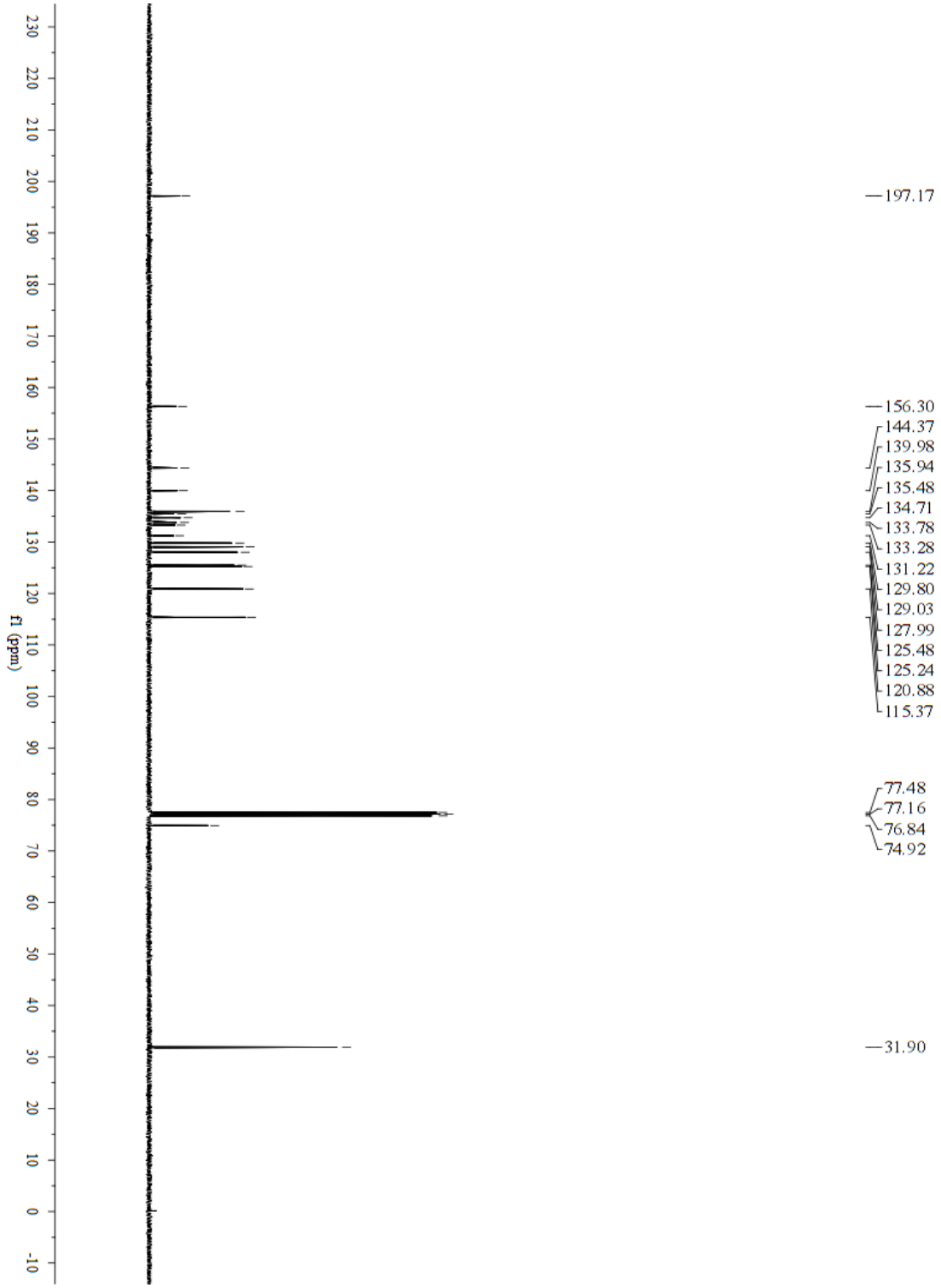
^{1}H NMR (400 MHz, $CDCl_3$)

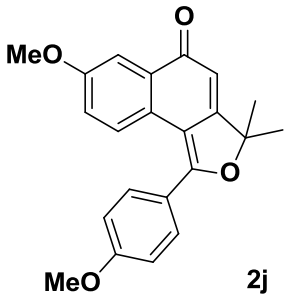




2i'

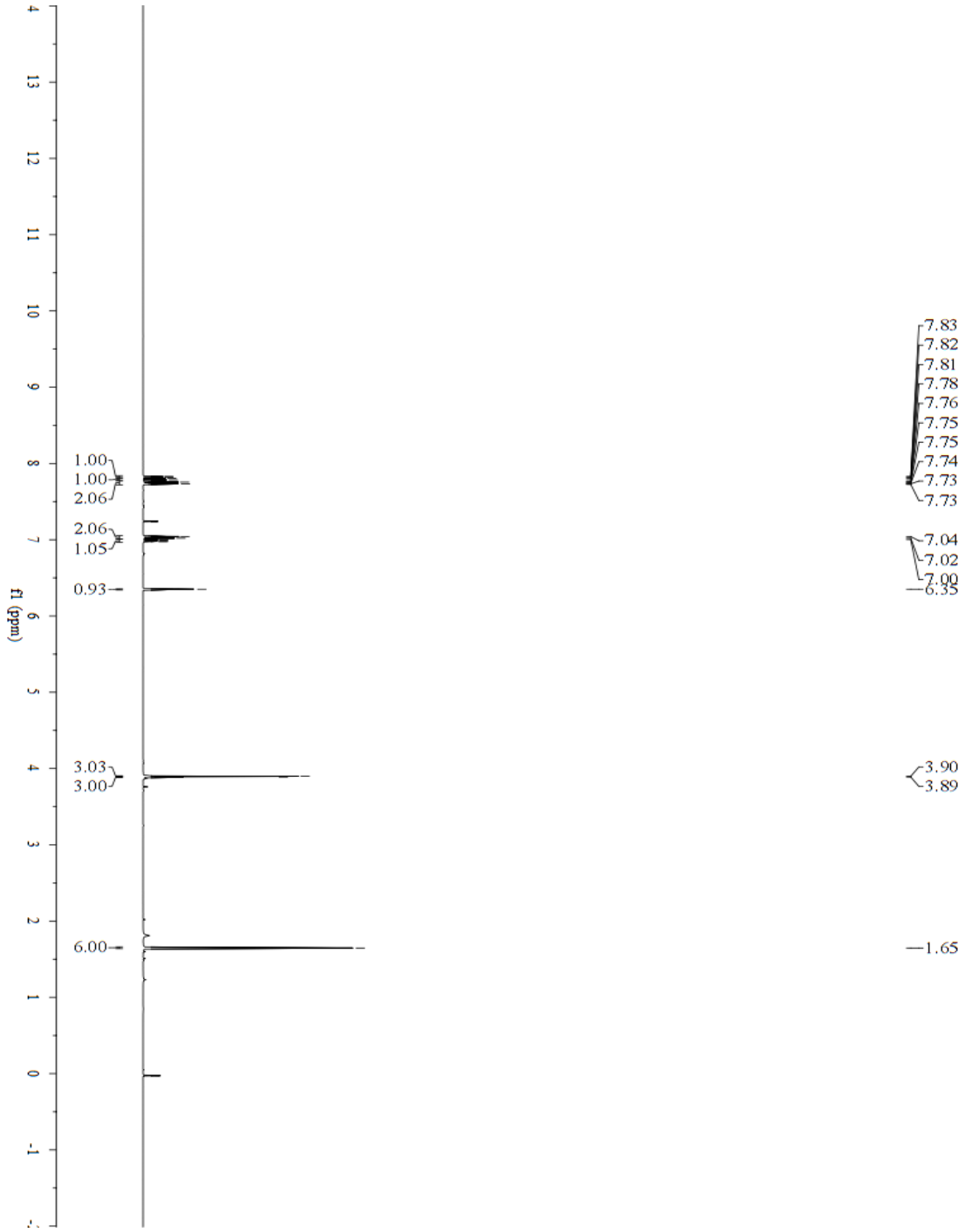
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)

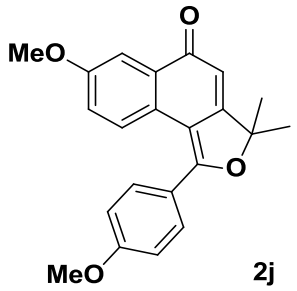




2j

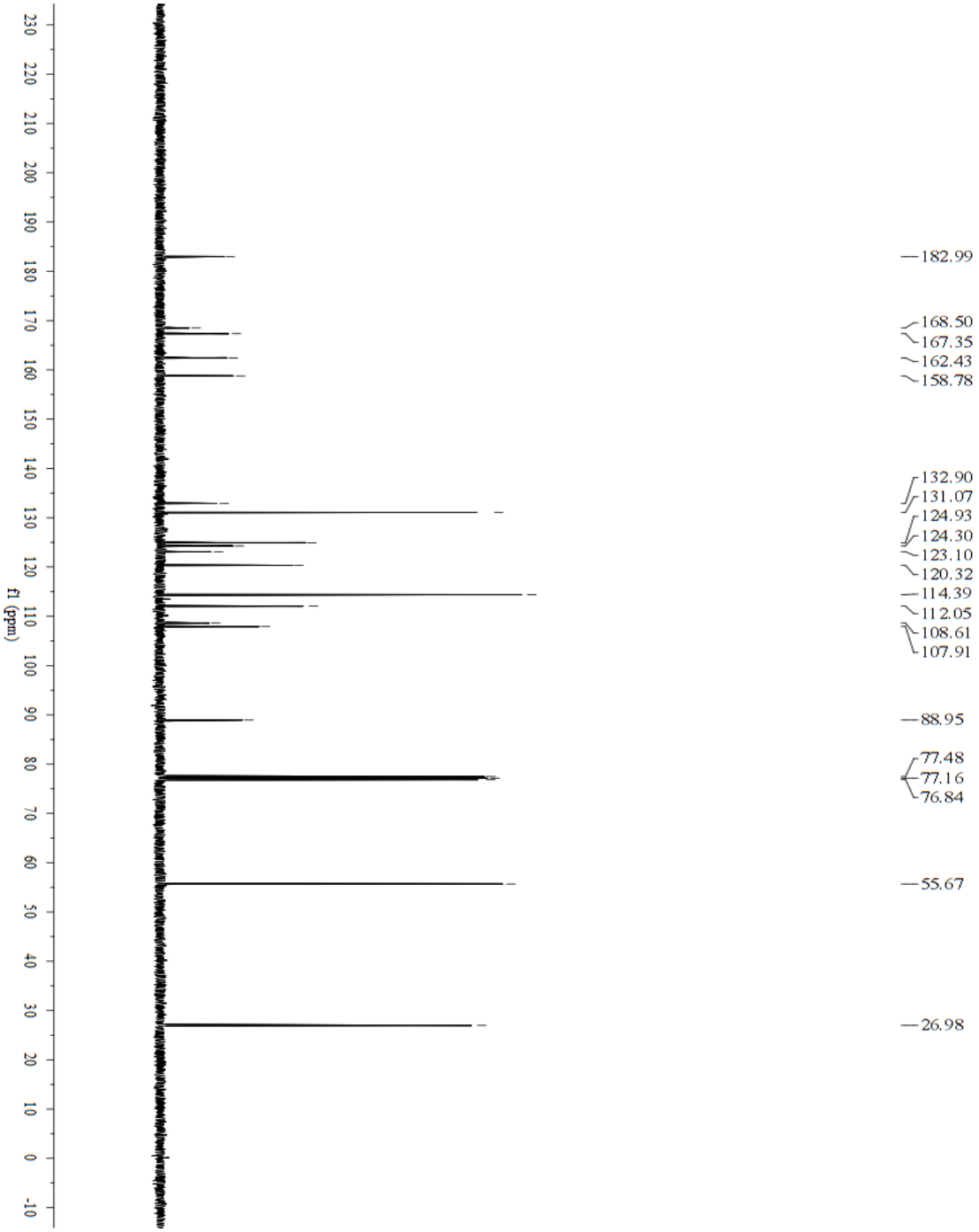
^{1}H NMR (400 MHz, $CDCl_3$)

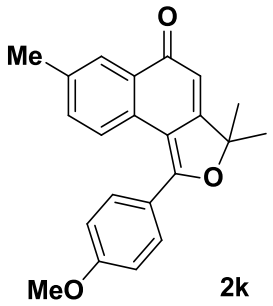




2j

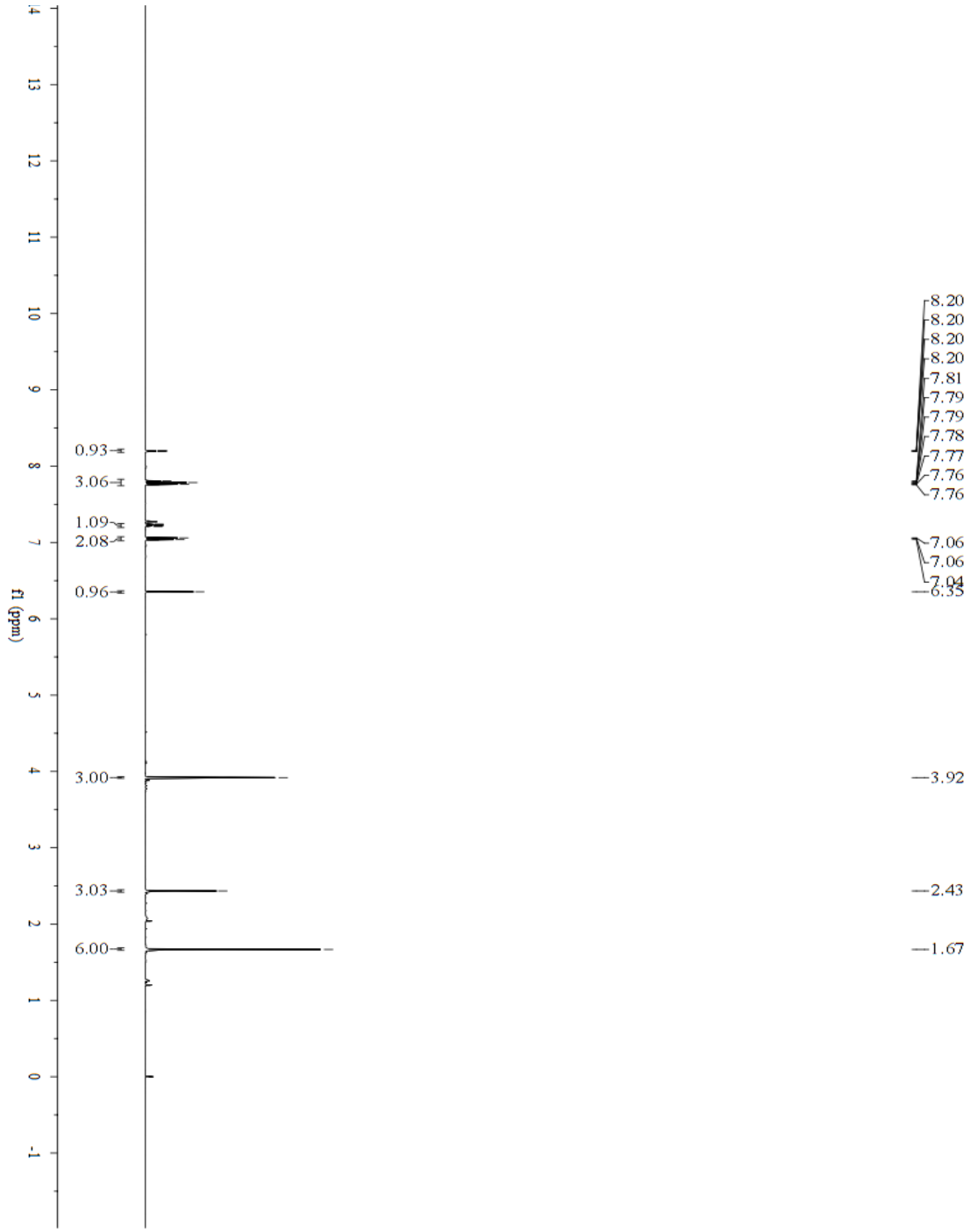
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

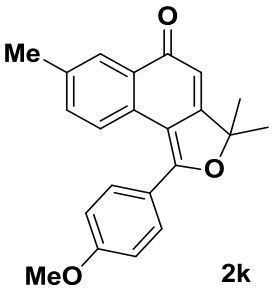




2k

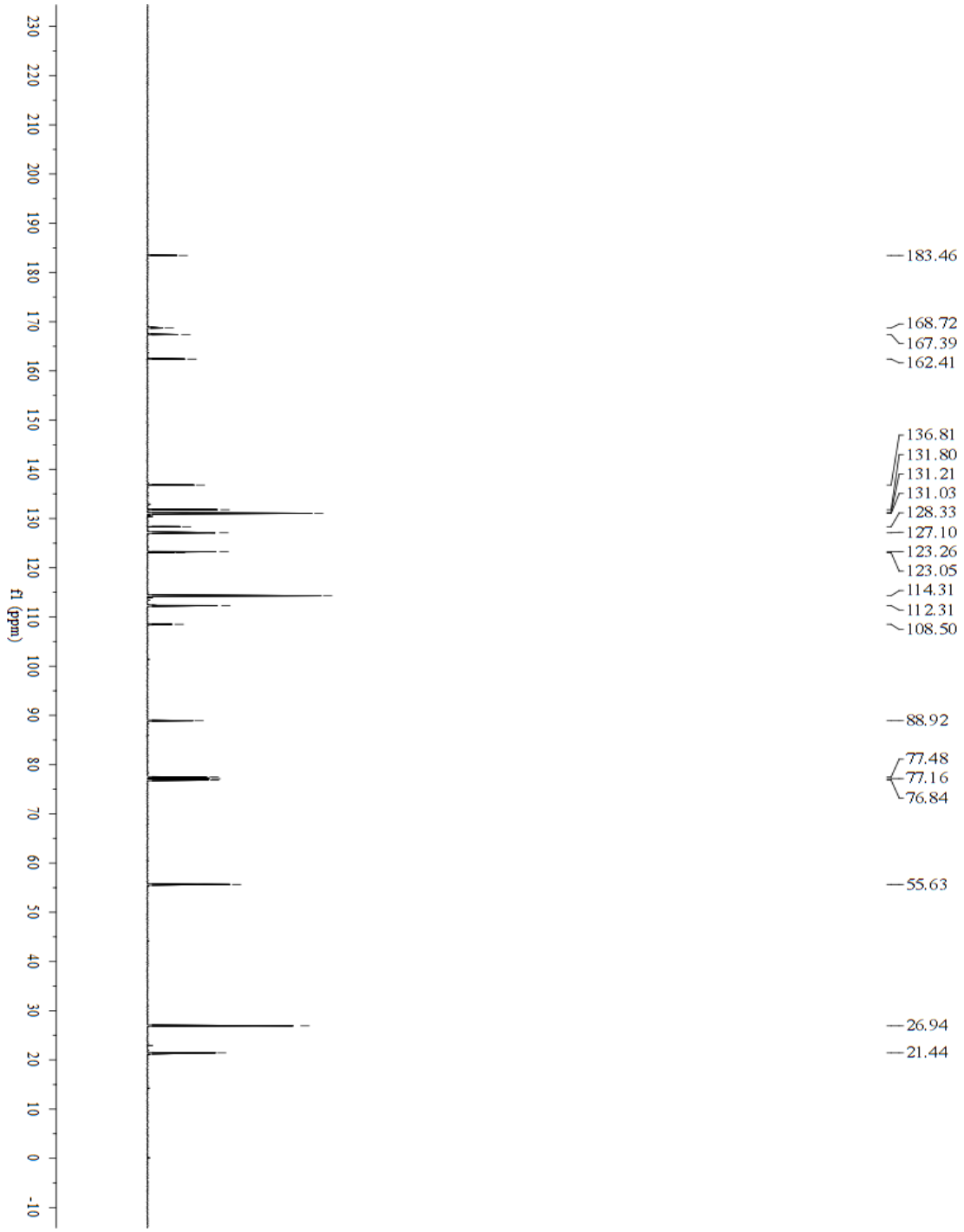
^{1}H NMR (400 MHz, $CDCl_3$)

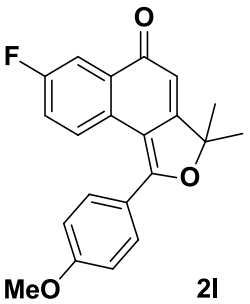




2k

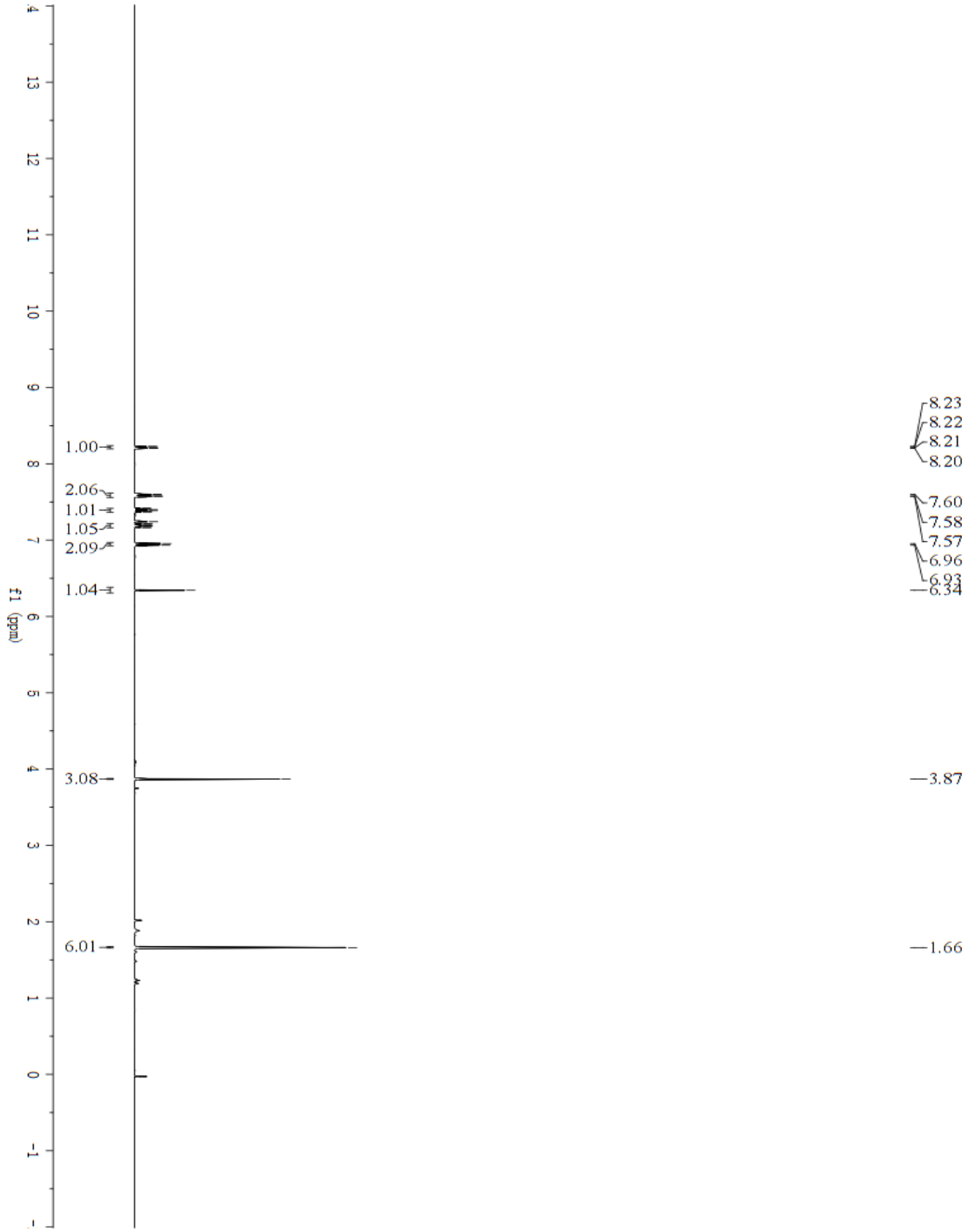
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

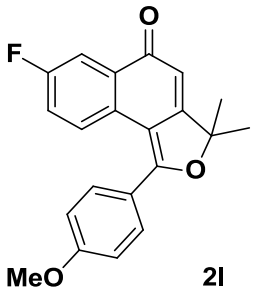




2l

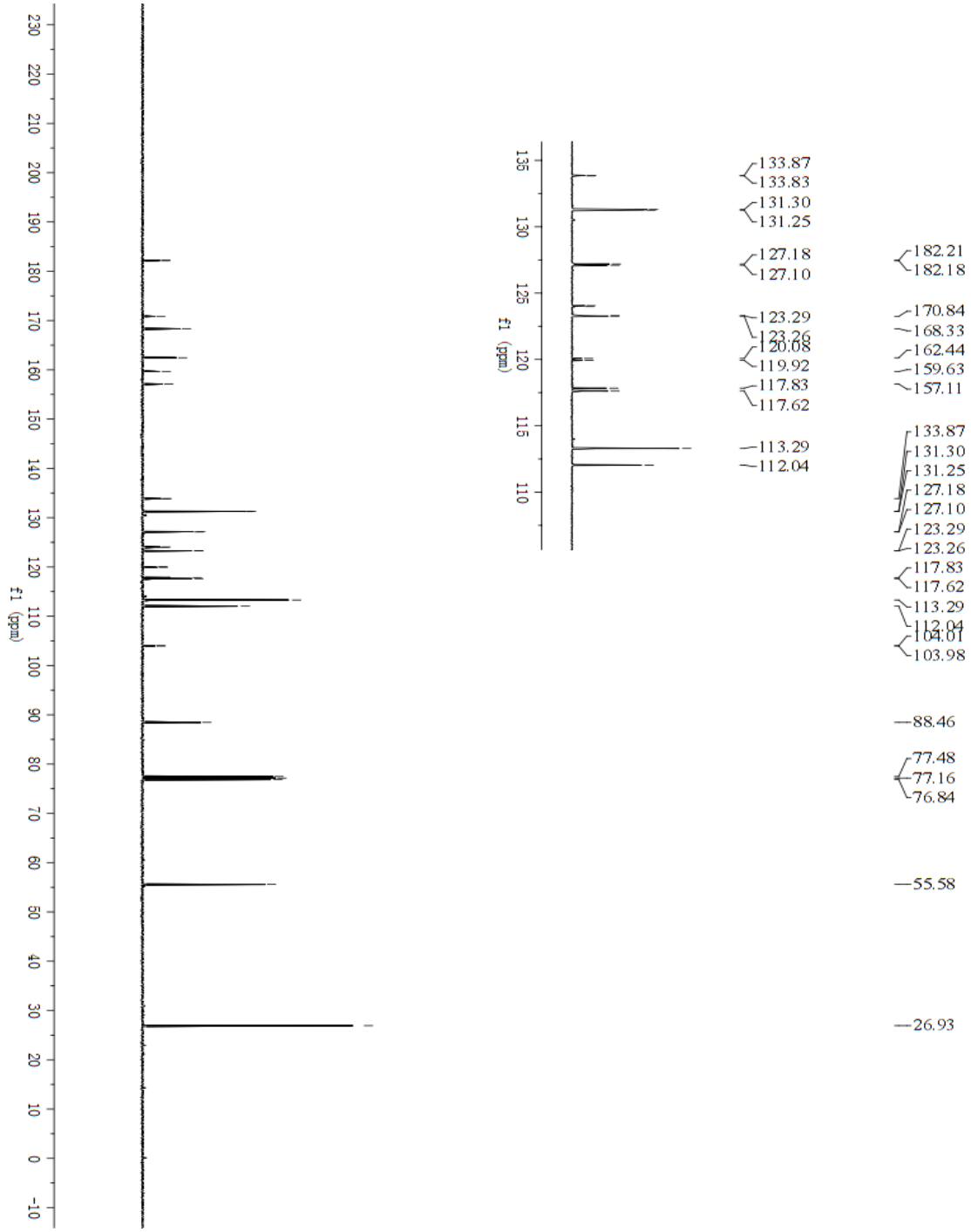
^{1}H NMR (400 MHz, $CDCl_3$)

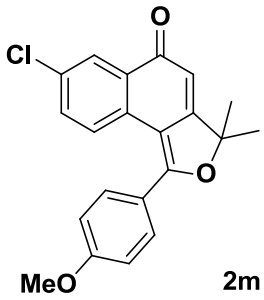




2l

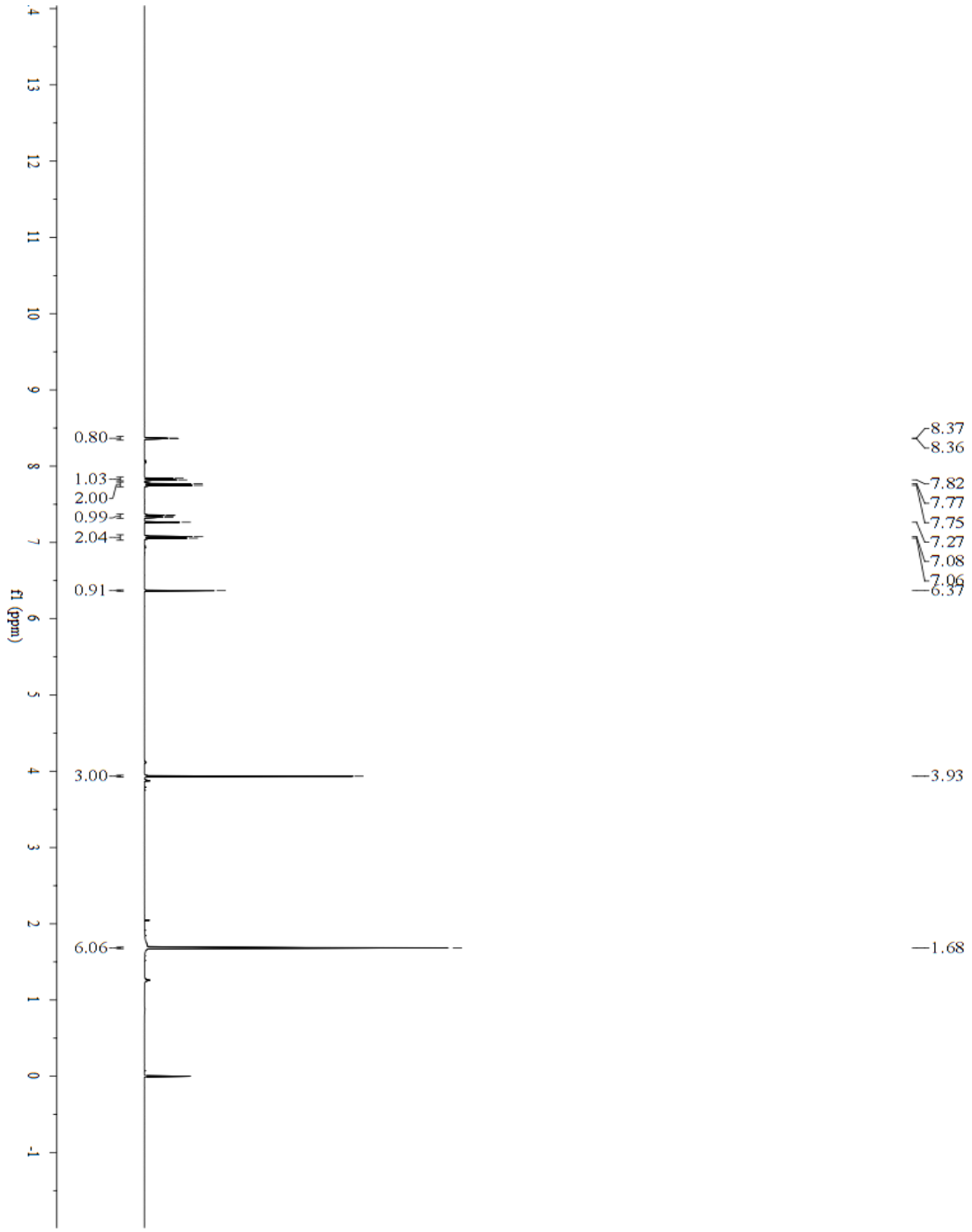
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)

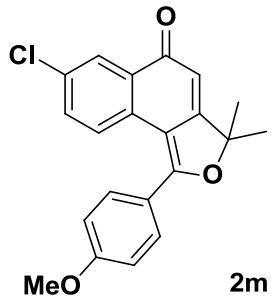




2m

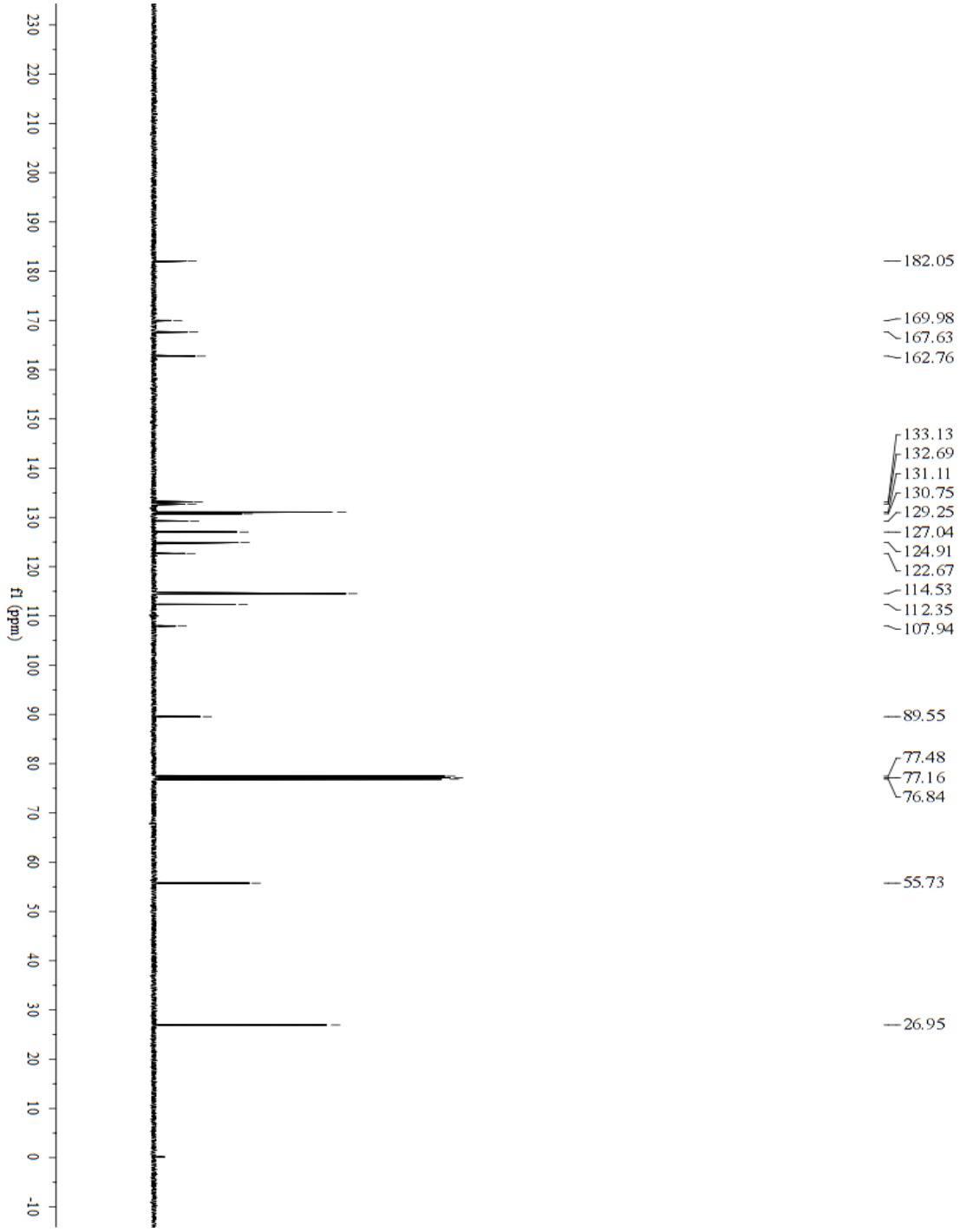
^{1}H NMR (400 MHz, $CDCl_3$)

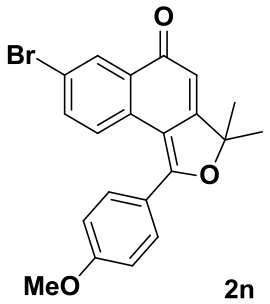




2m

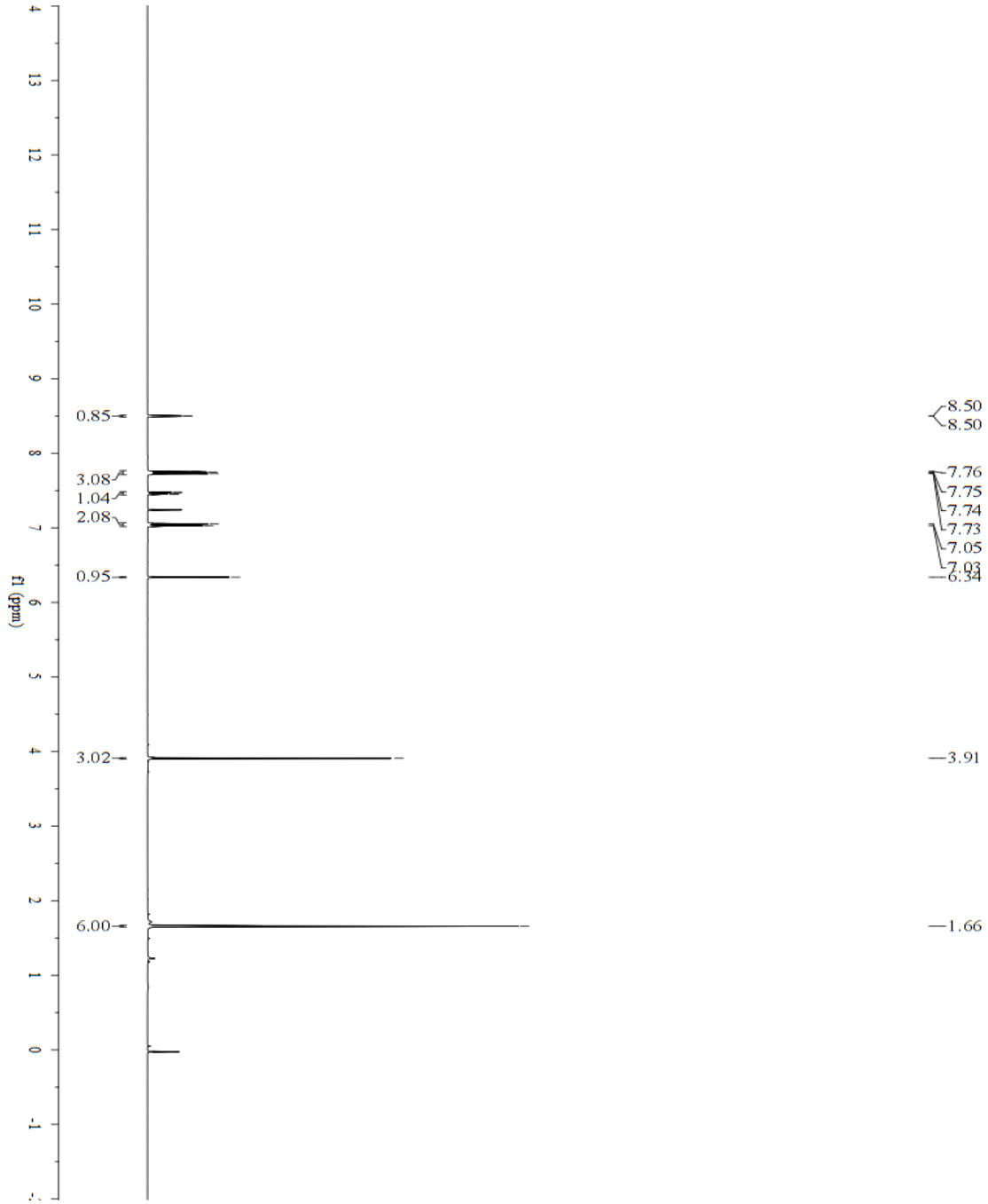
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

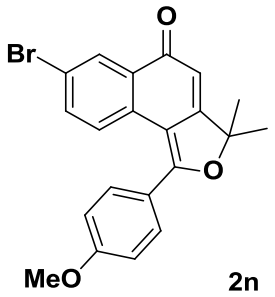




2n

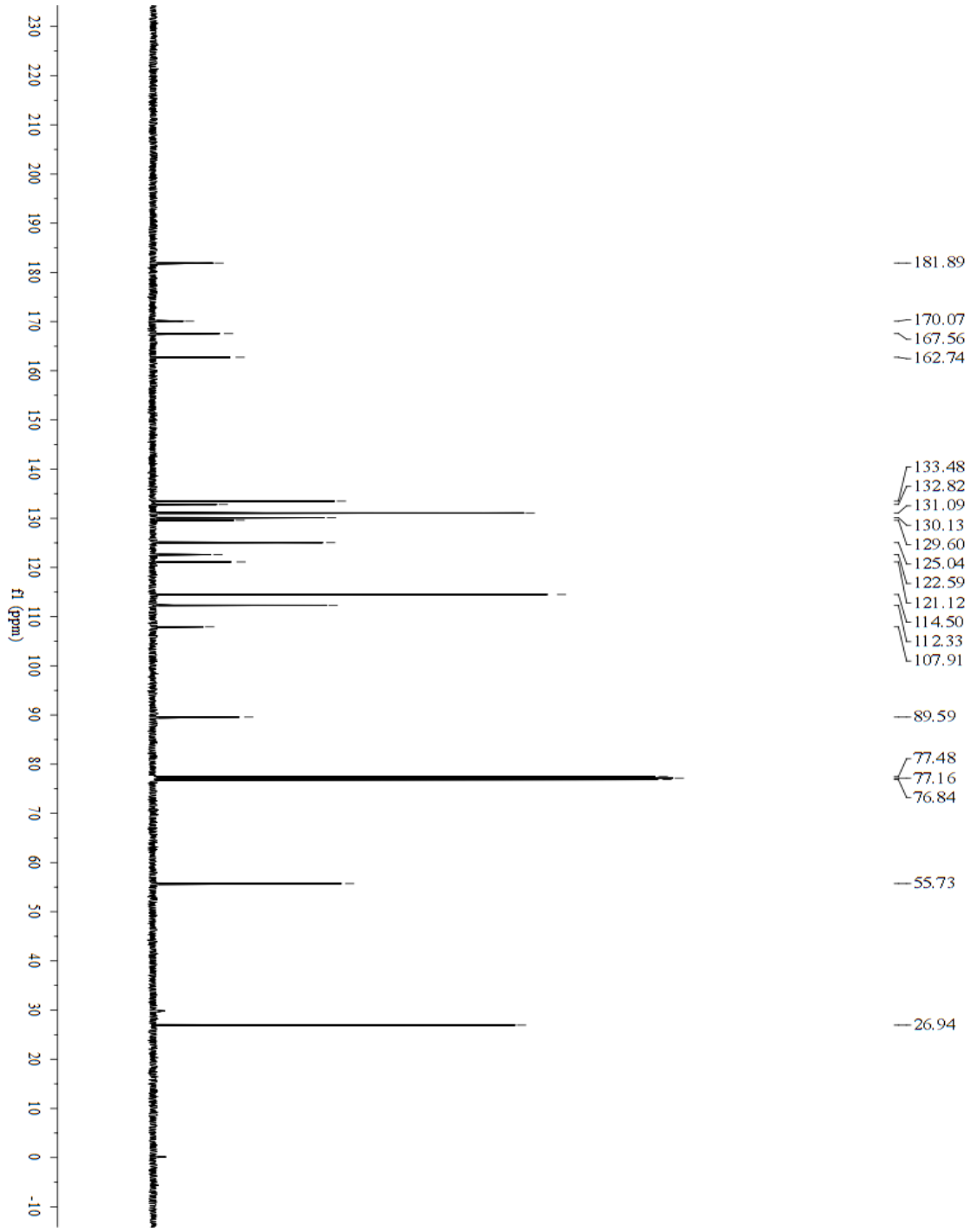
^{1}H NMR (400 MHz, $CDCl_3$)

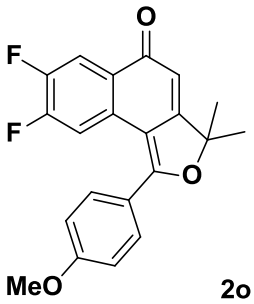




2n

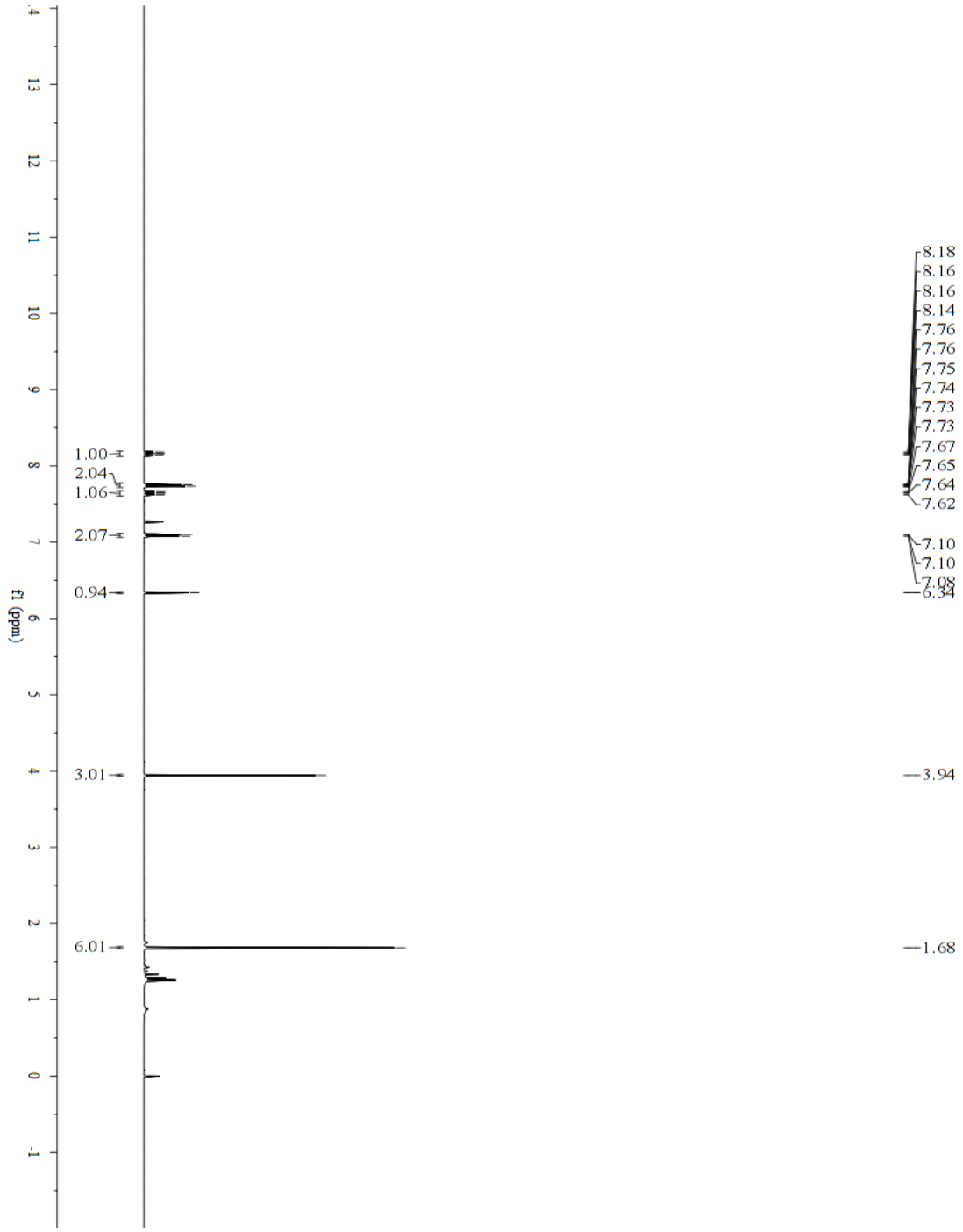
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

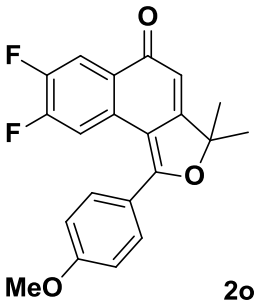




2o

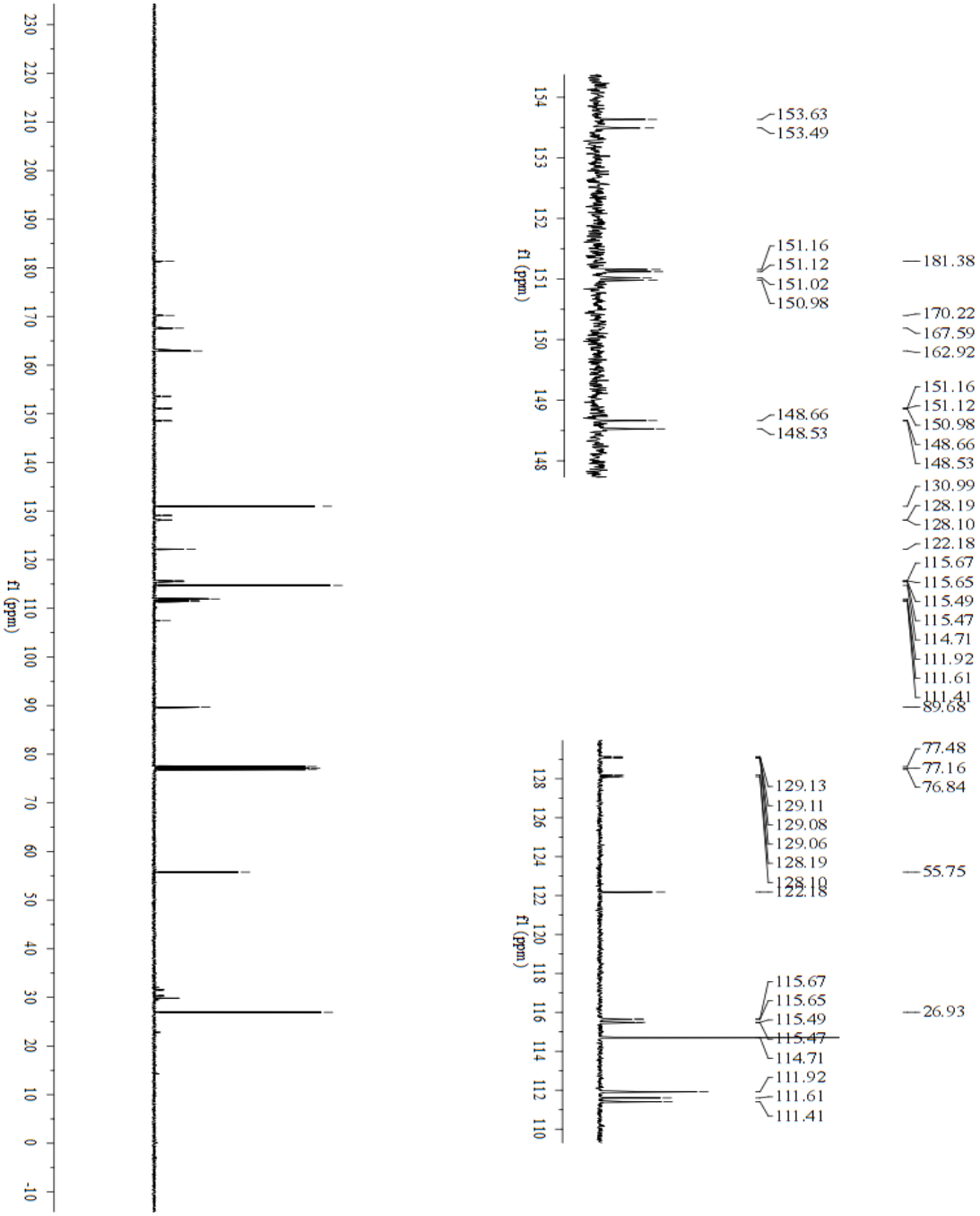
^{1}H NMR (400 MHz, $CDCl_3$)

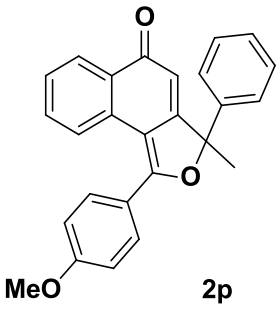




2o

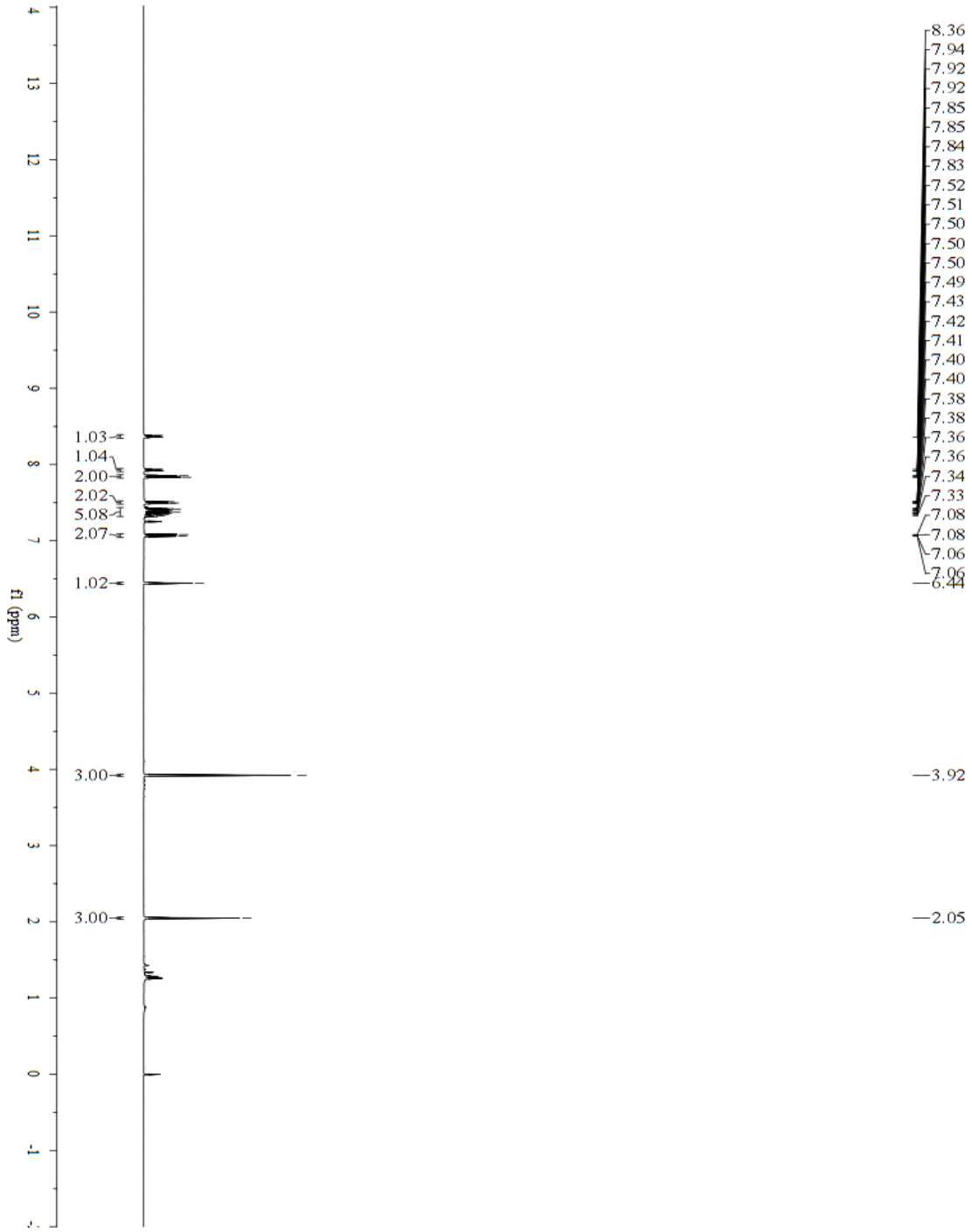
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

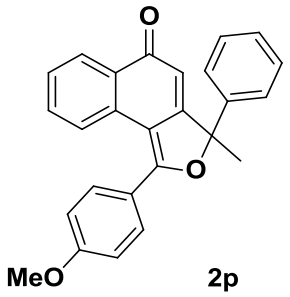




2p

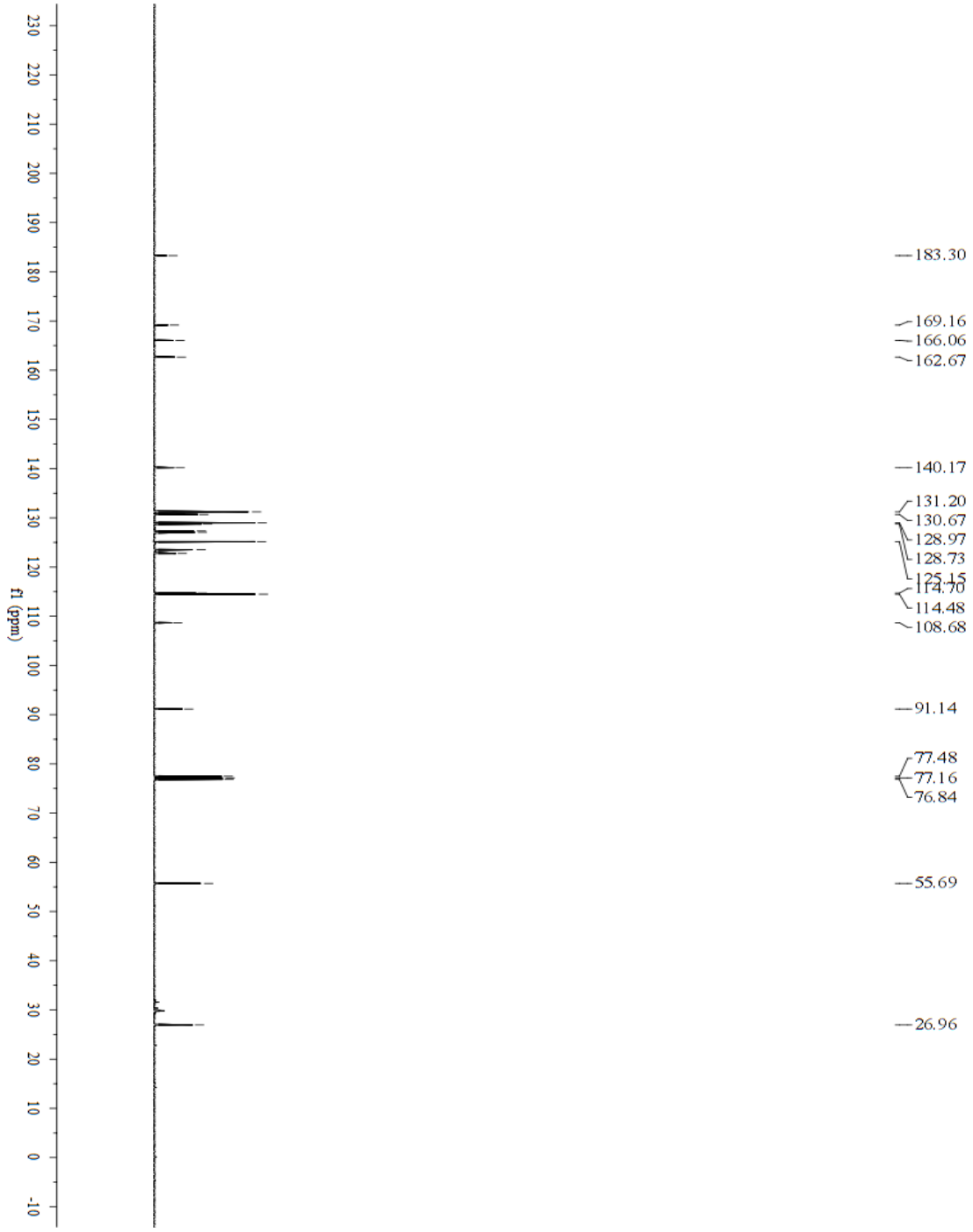
^{1}H NMR (400 MHz, $CDCl_3$)

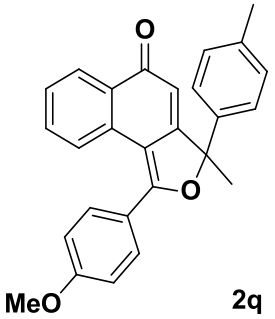




2p

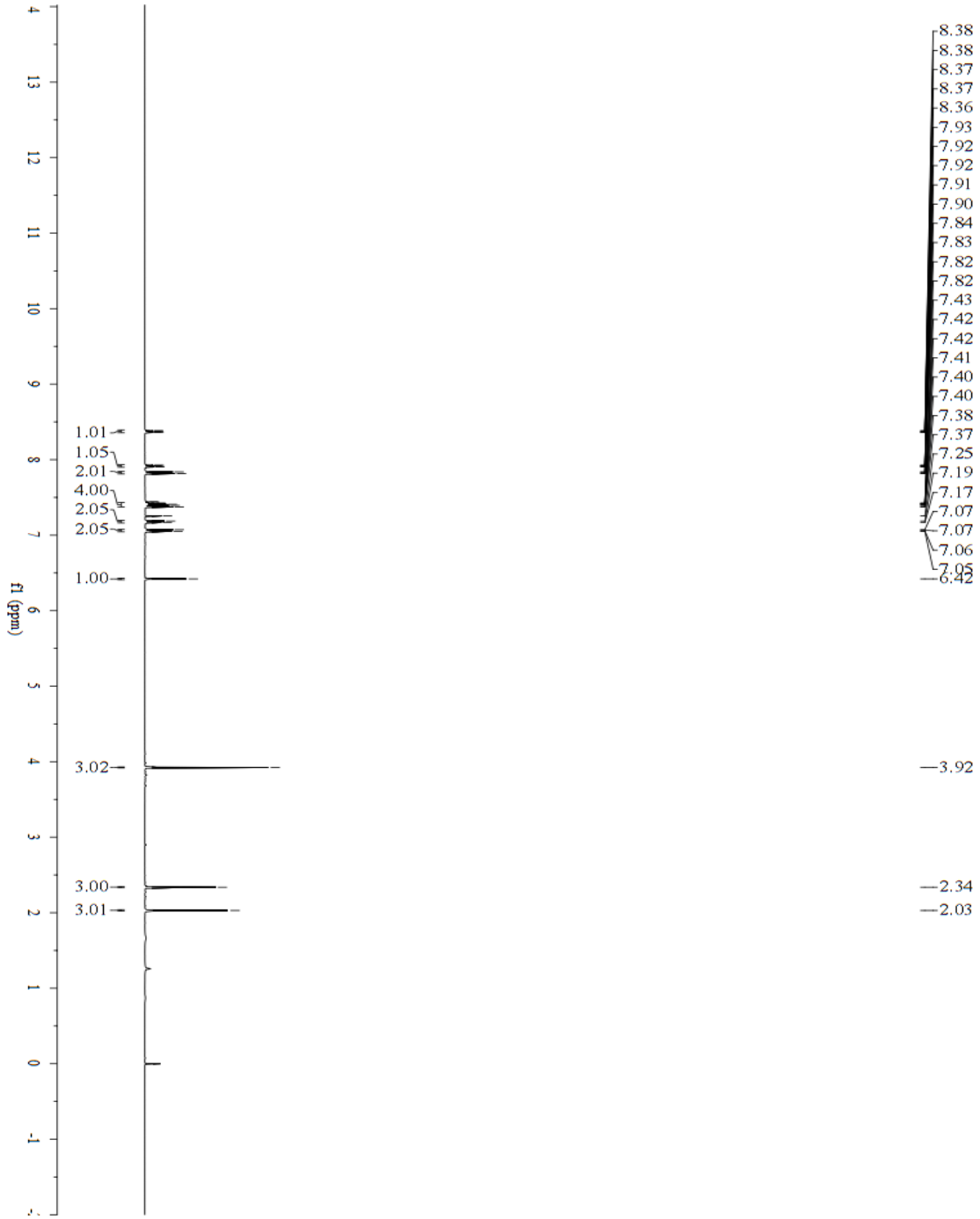
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

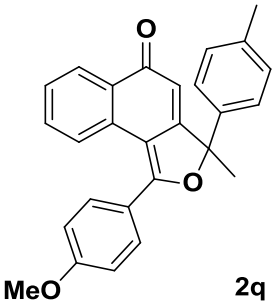




2q

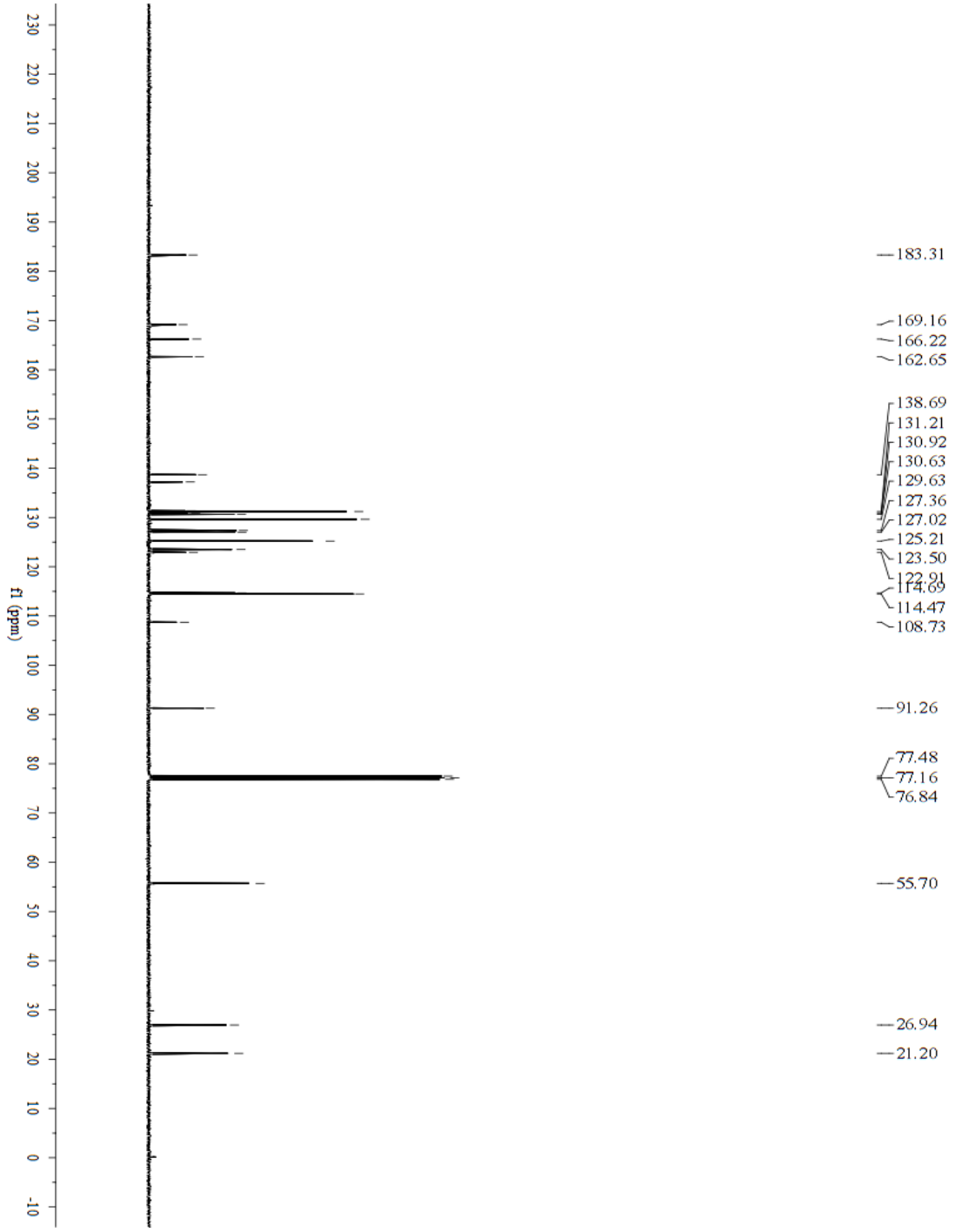
^{1}H NMR (400 MHz, $CDCl_3$)

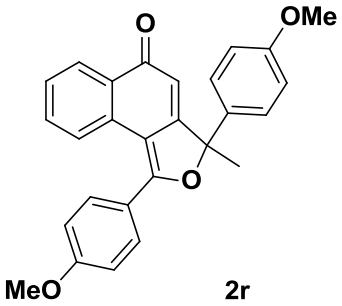




2q

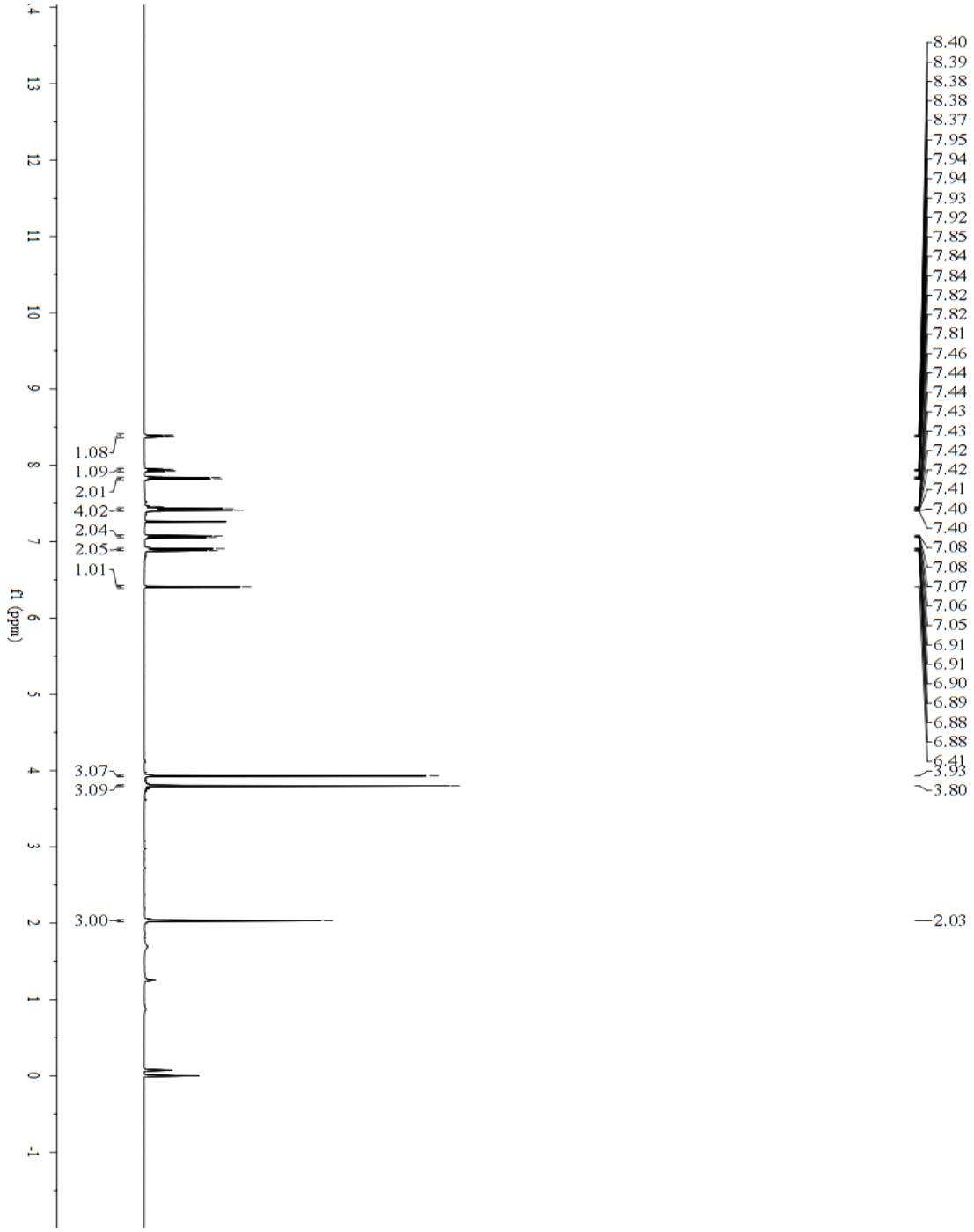
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

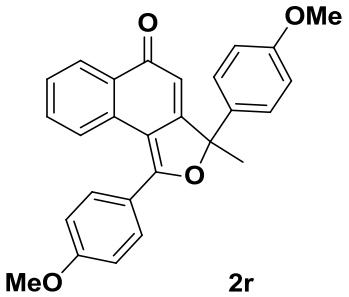




2r

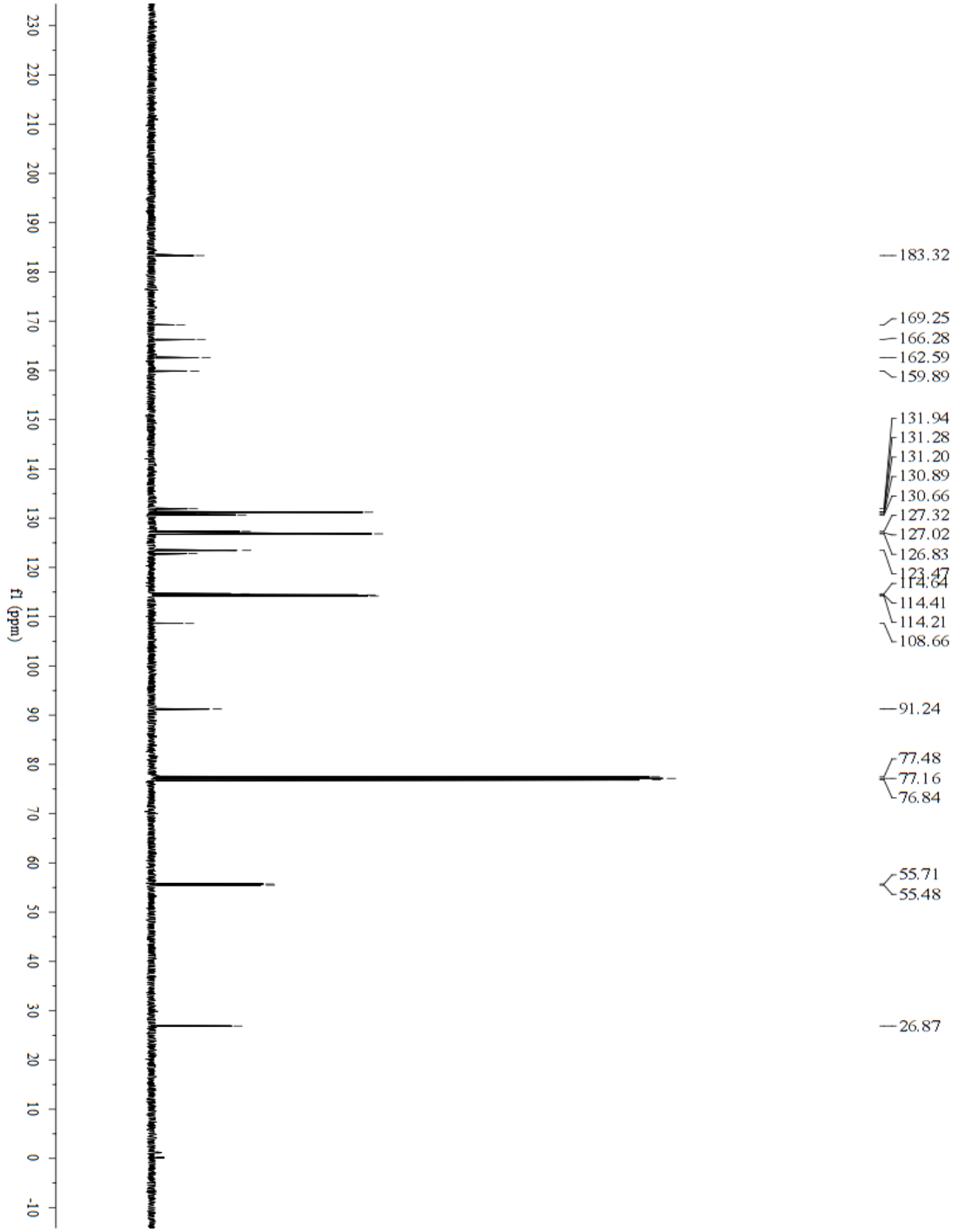
^{1}H NMR (400 MHz, $CDCl_3$)

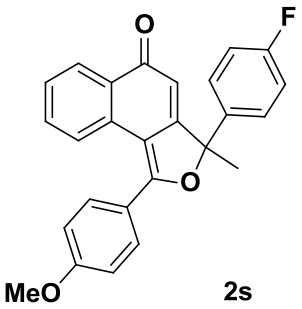




2r

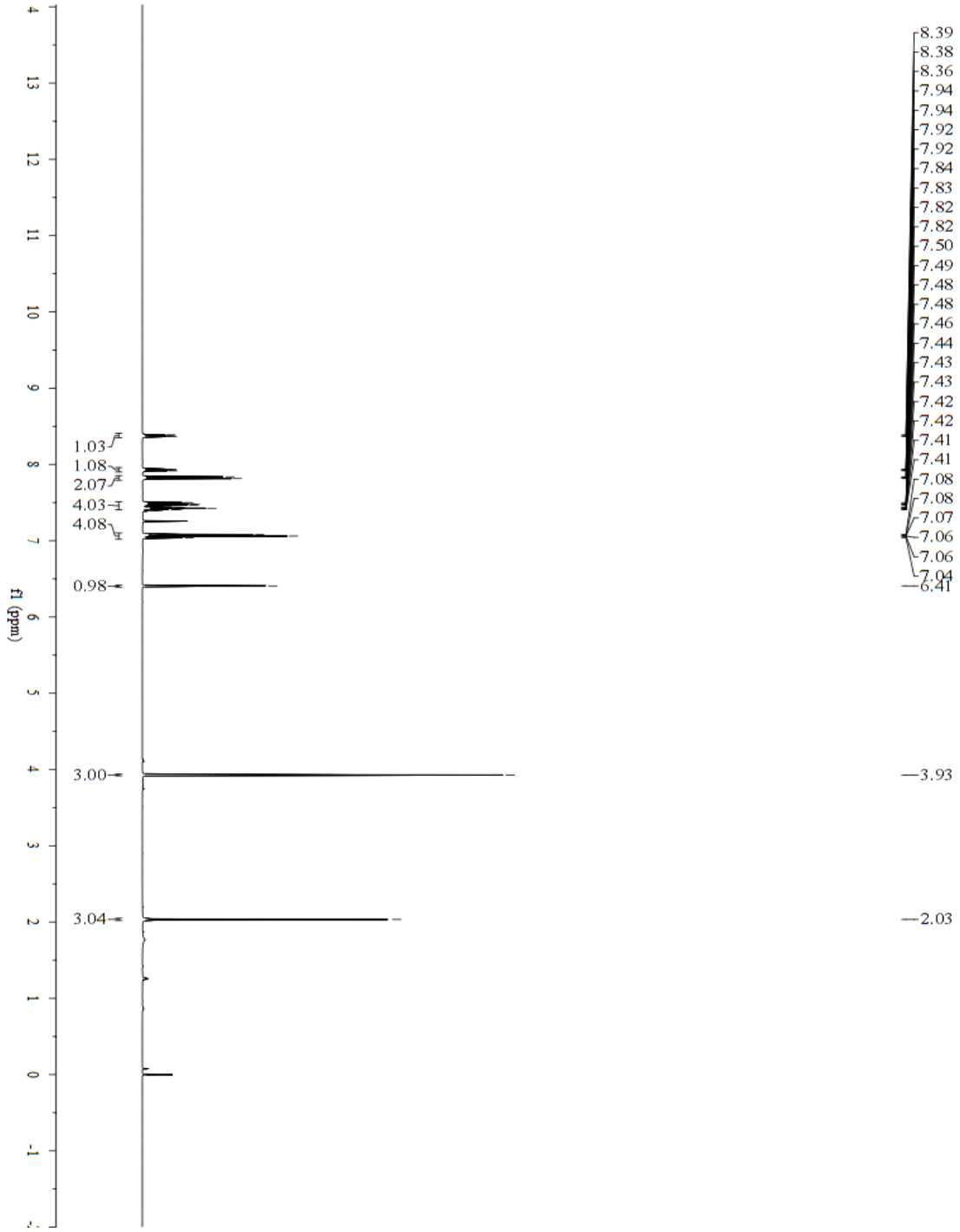
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

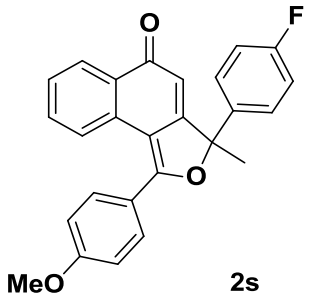




2s

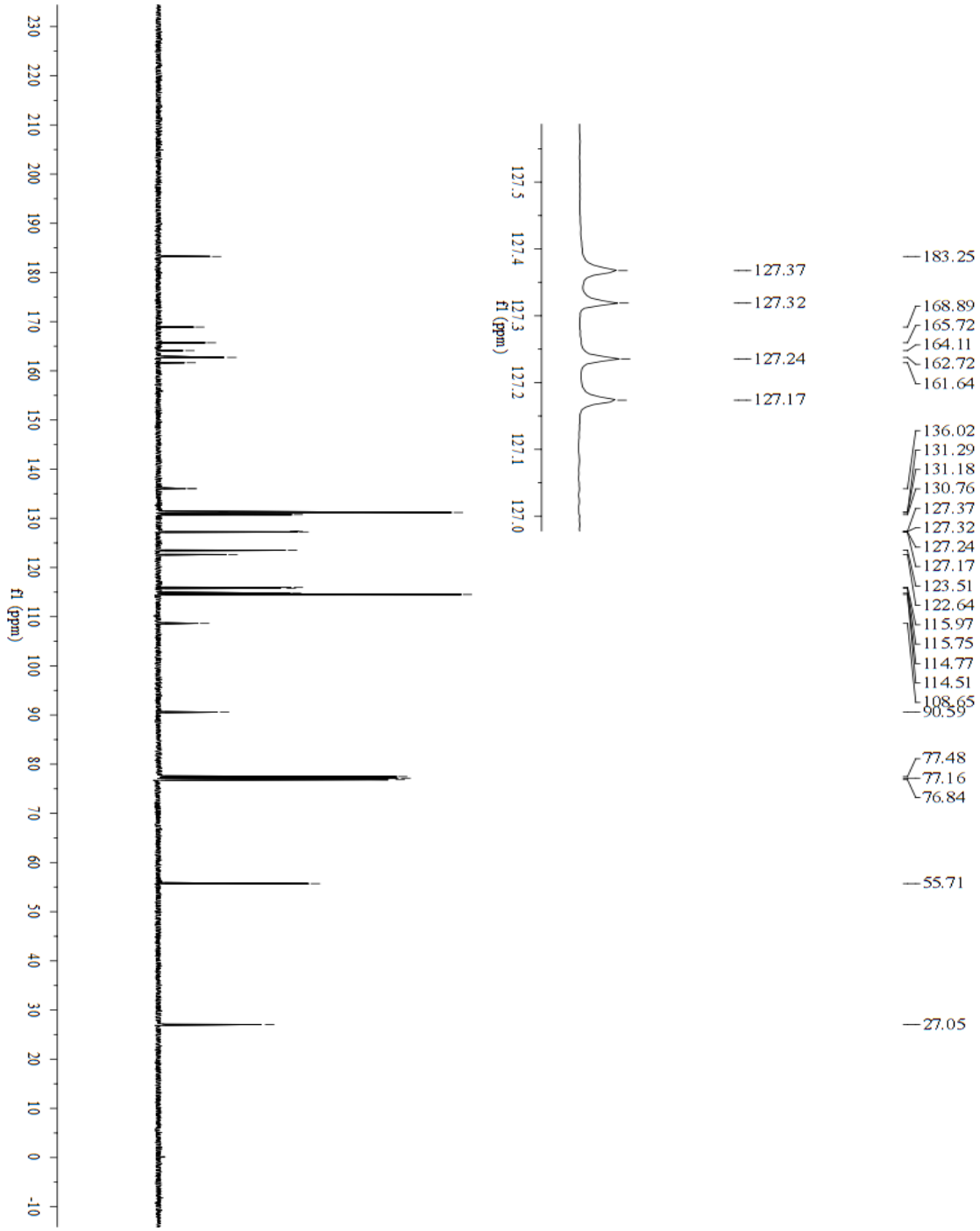
^{1}H NMR (400 MHz, $CDCl_3$)

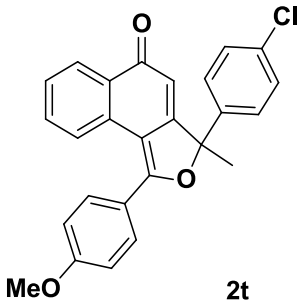




2s

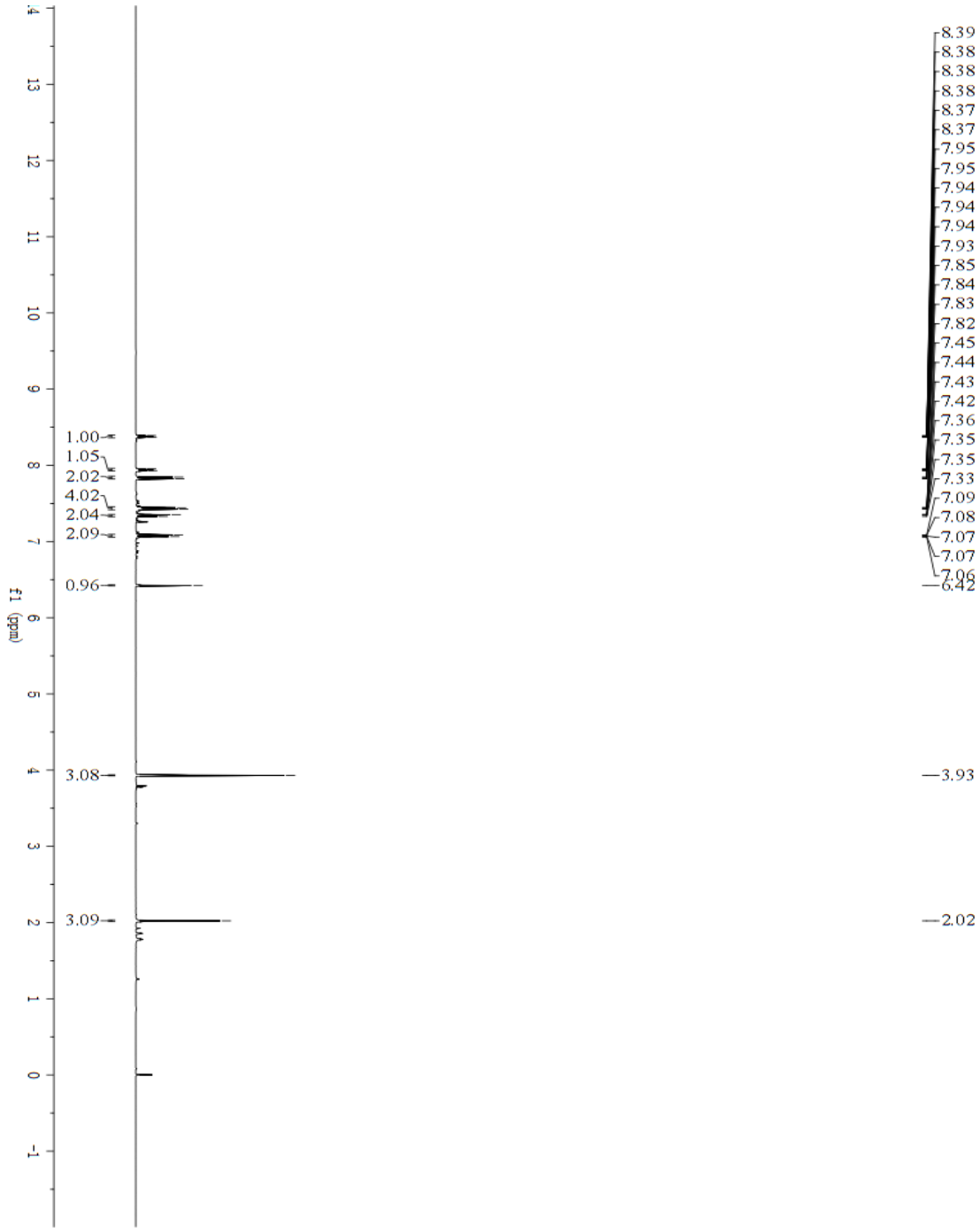
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)

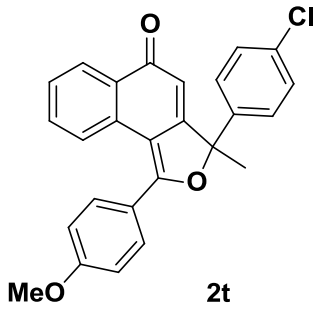




2t

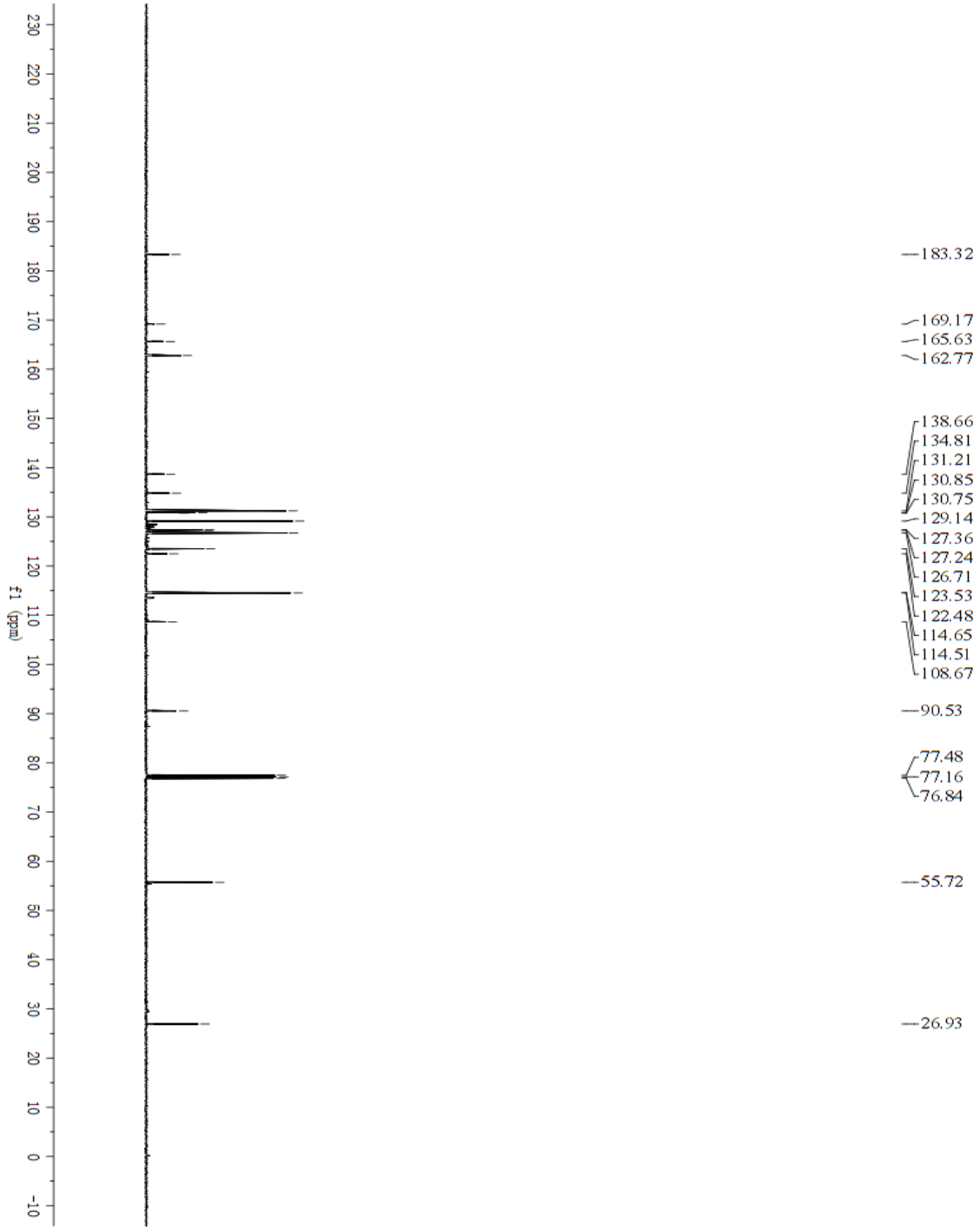
^{1}H NMR (400 MHz, $CDCl_3$)

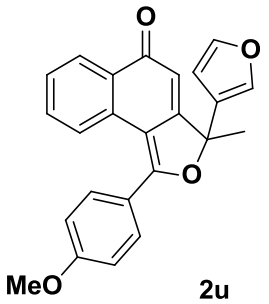




2t

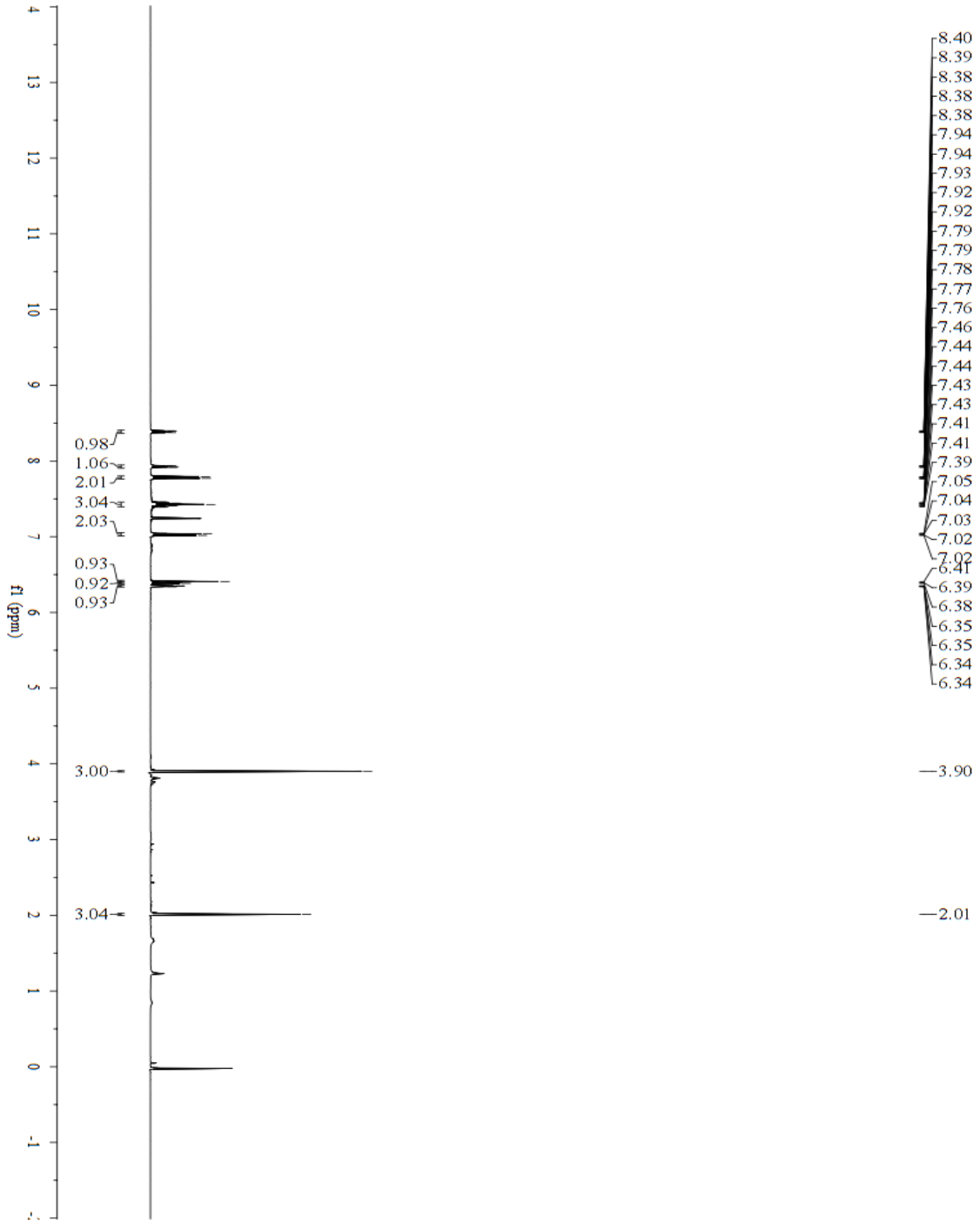
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

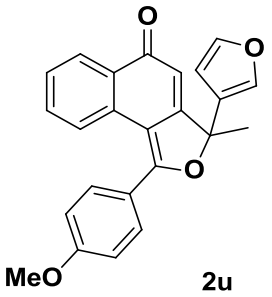




2u

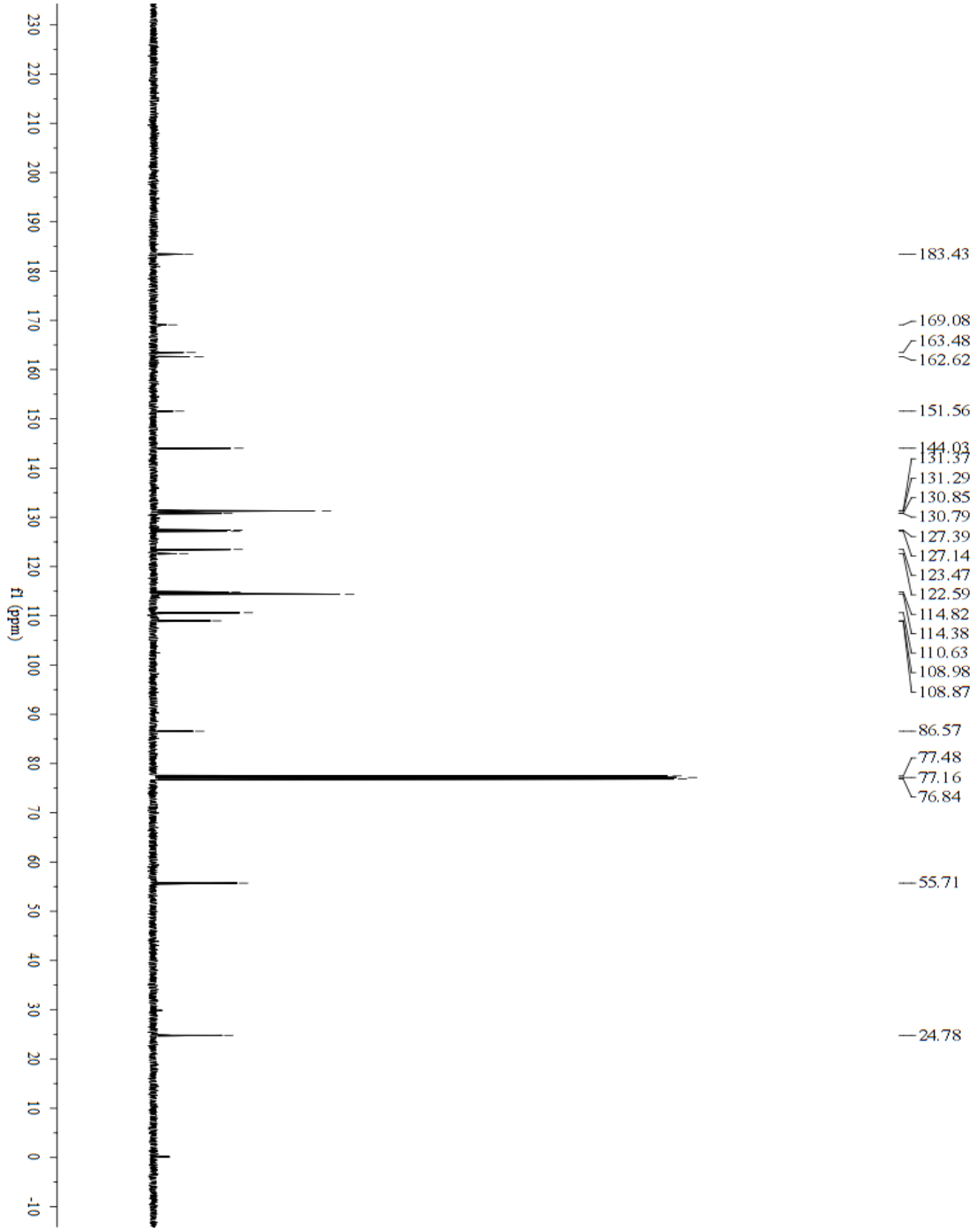
^{1}H NMR (400 MHz, $CDCl_3$)

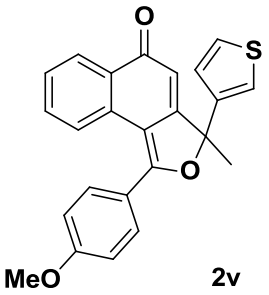




2u

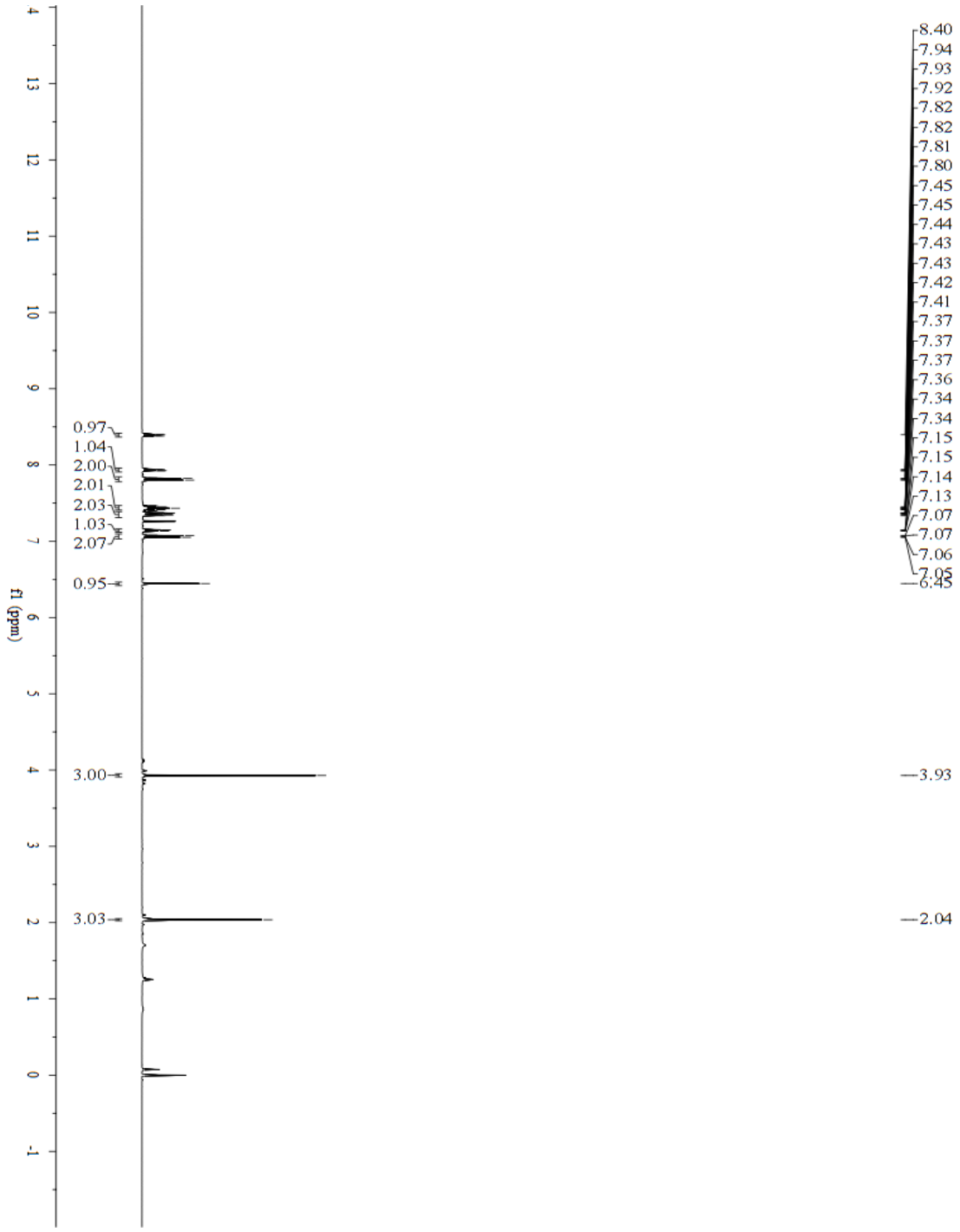
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)

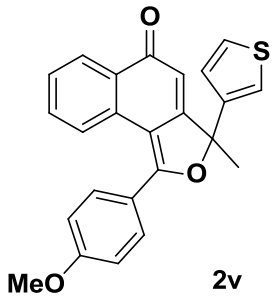




2v

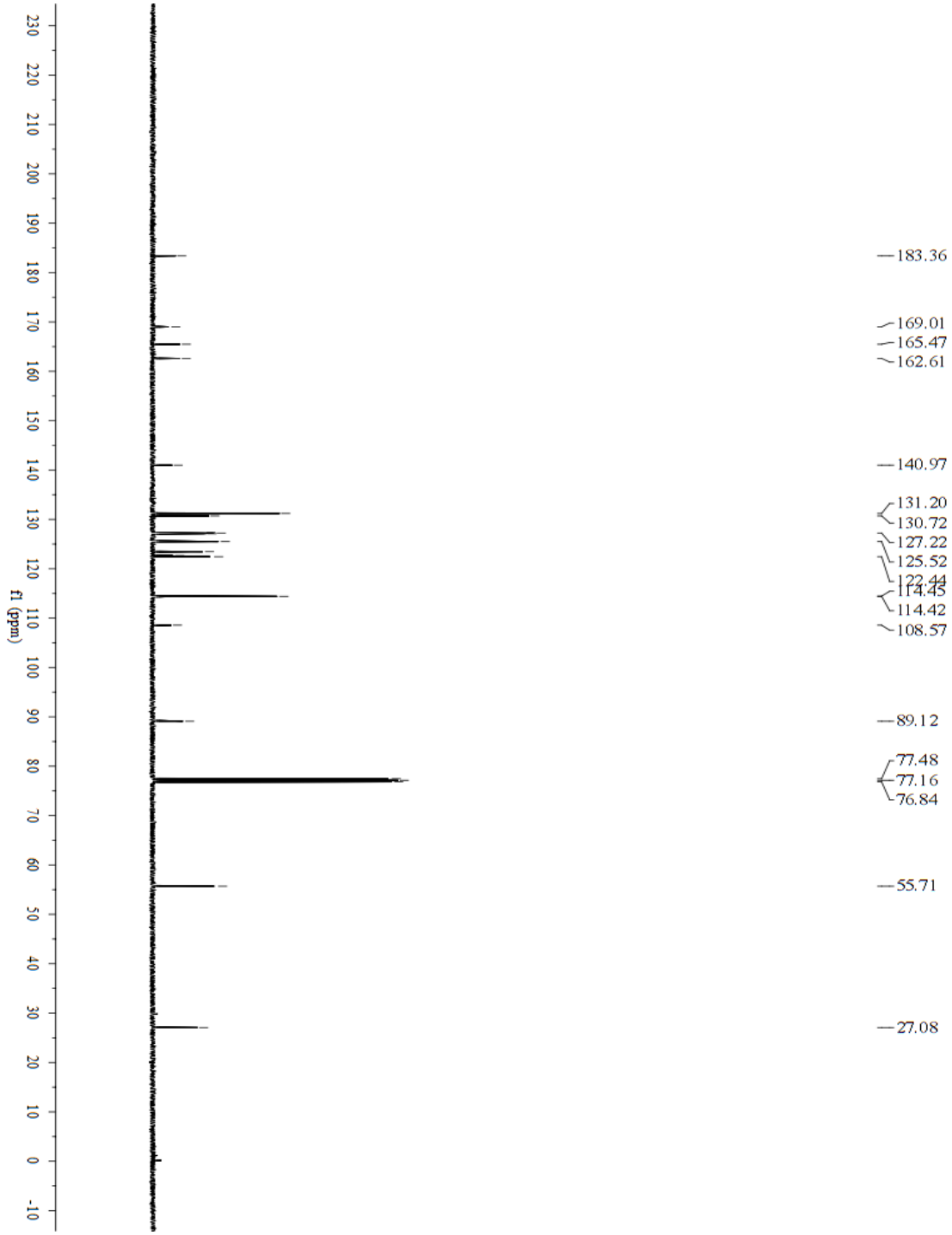
^{1}H NMR (400 MHz, $CDCl_3$)

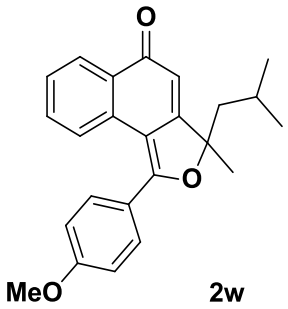




2v

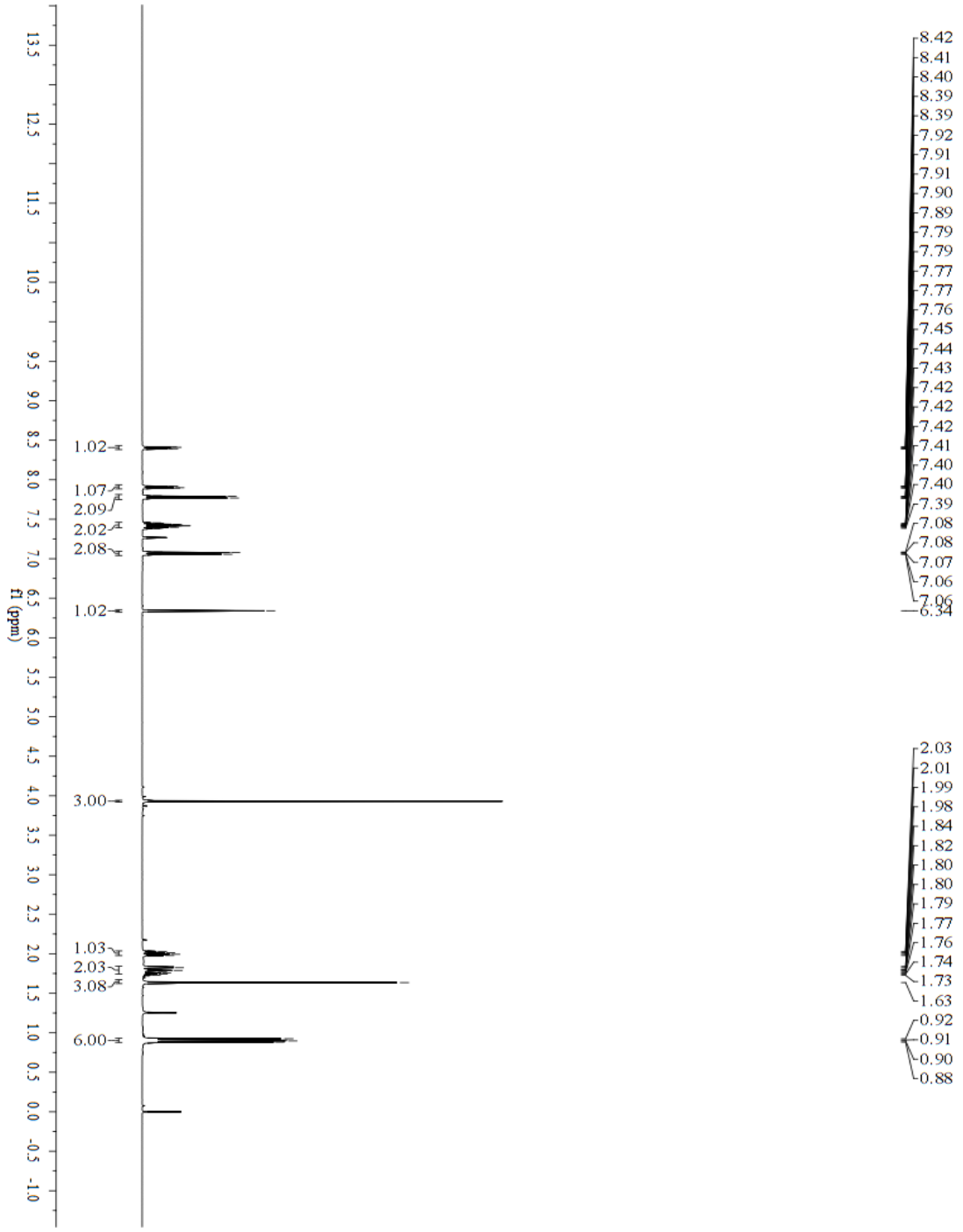
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

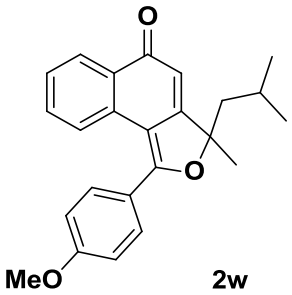




2w

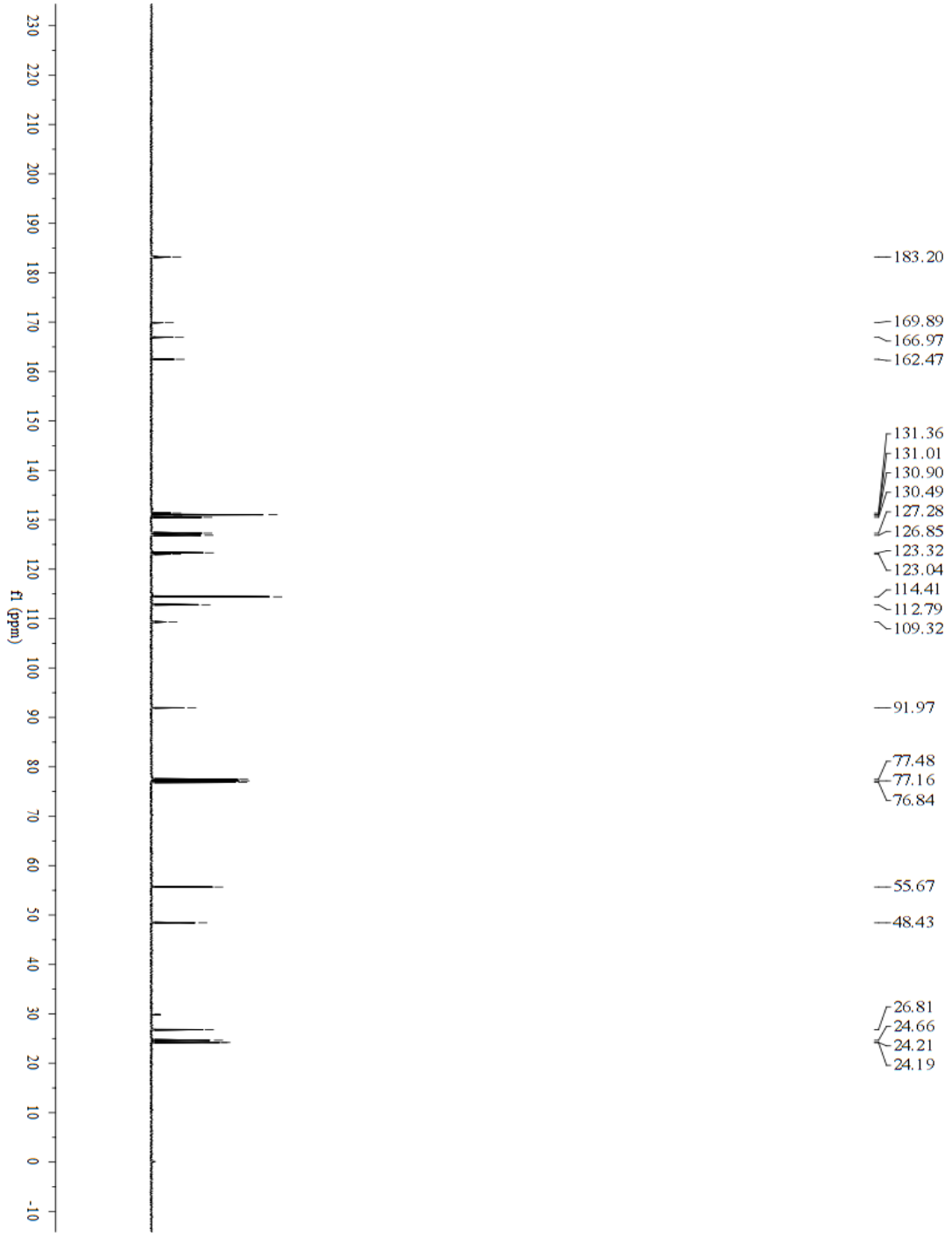
^{1}H NMR (400 MHz, $CDCl_3$)

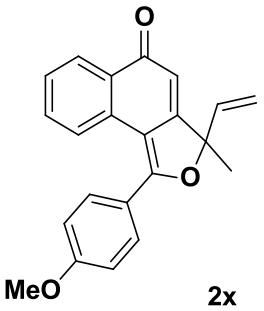




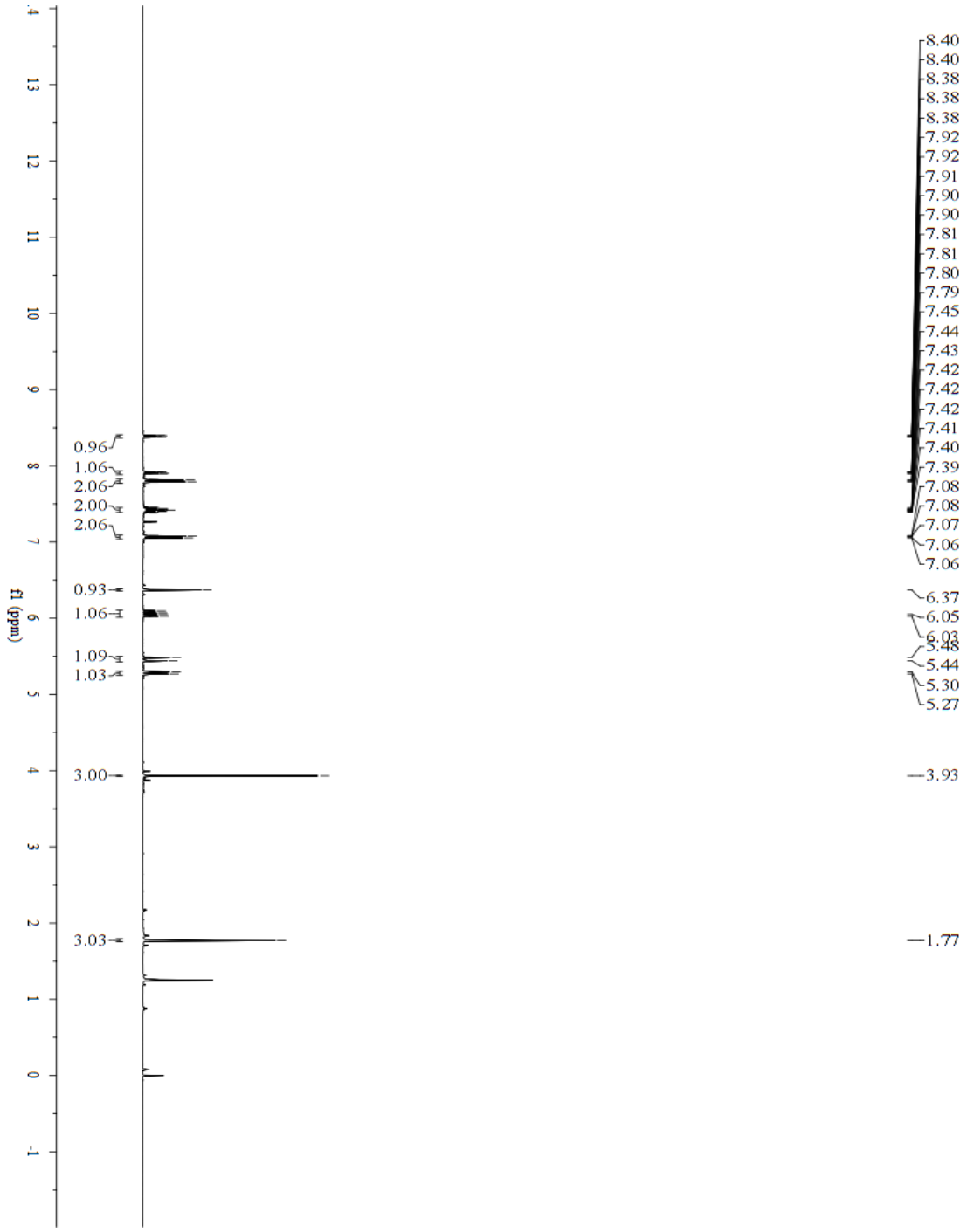
2w

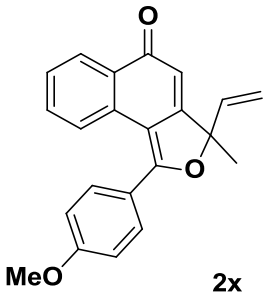
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



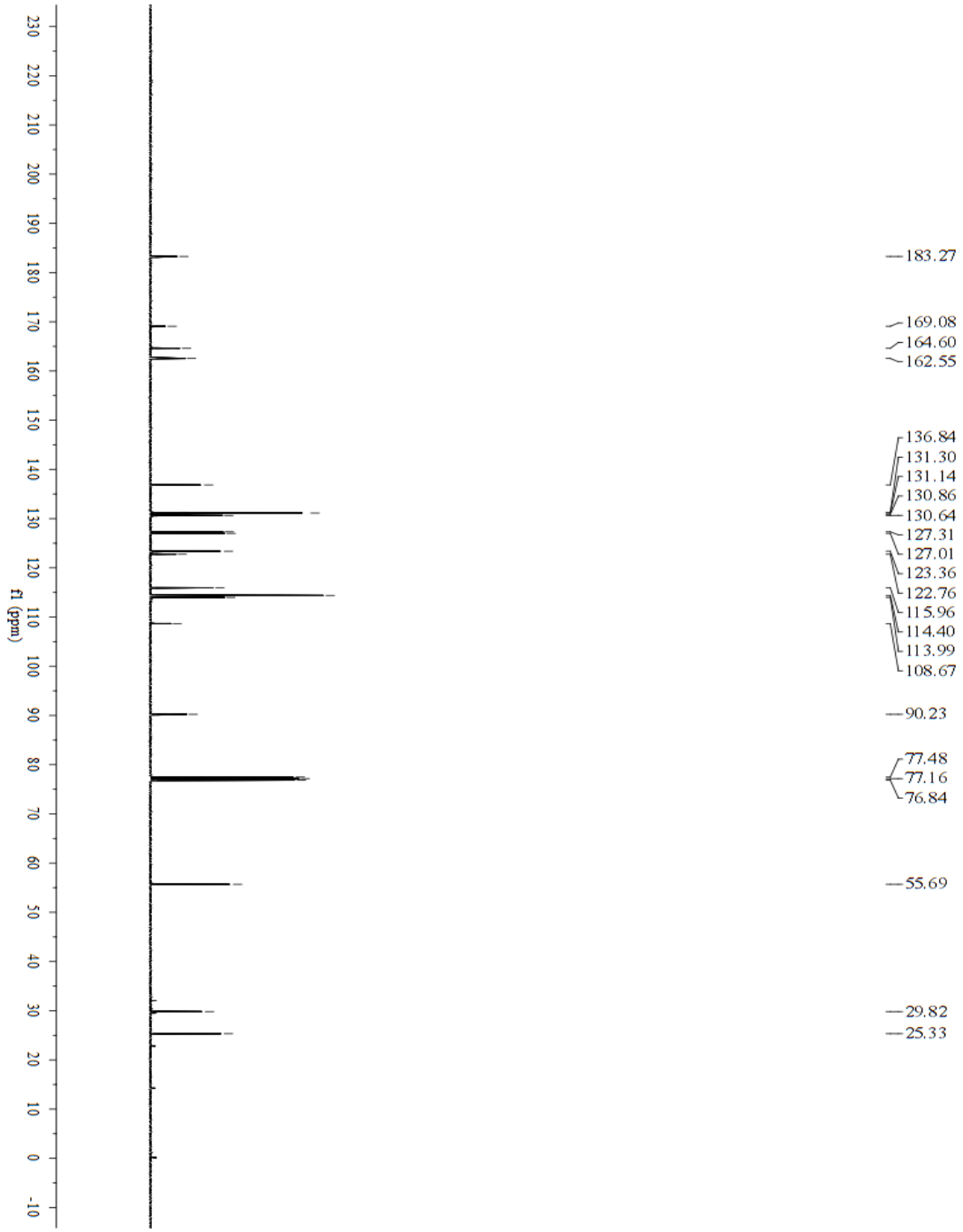


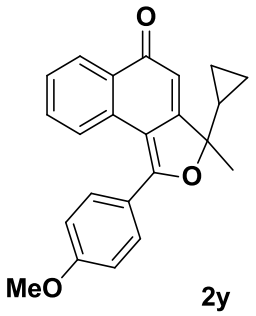
^{1}H NMR (400 MHz, $CDCl_3$)





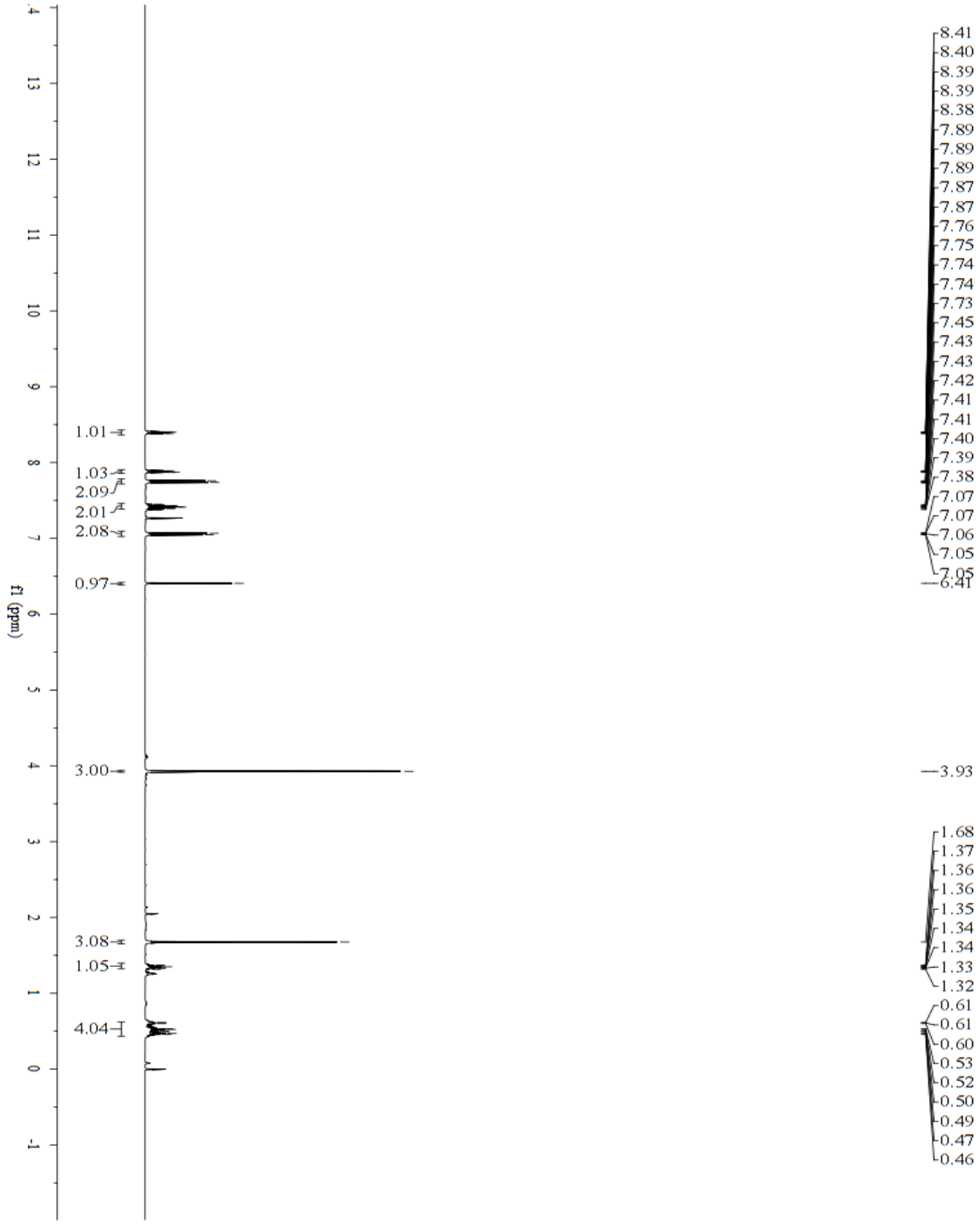
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

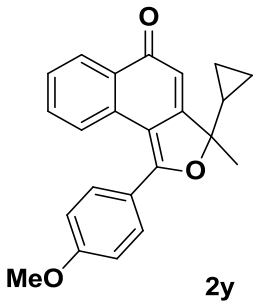




2y

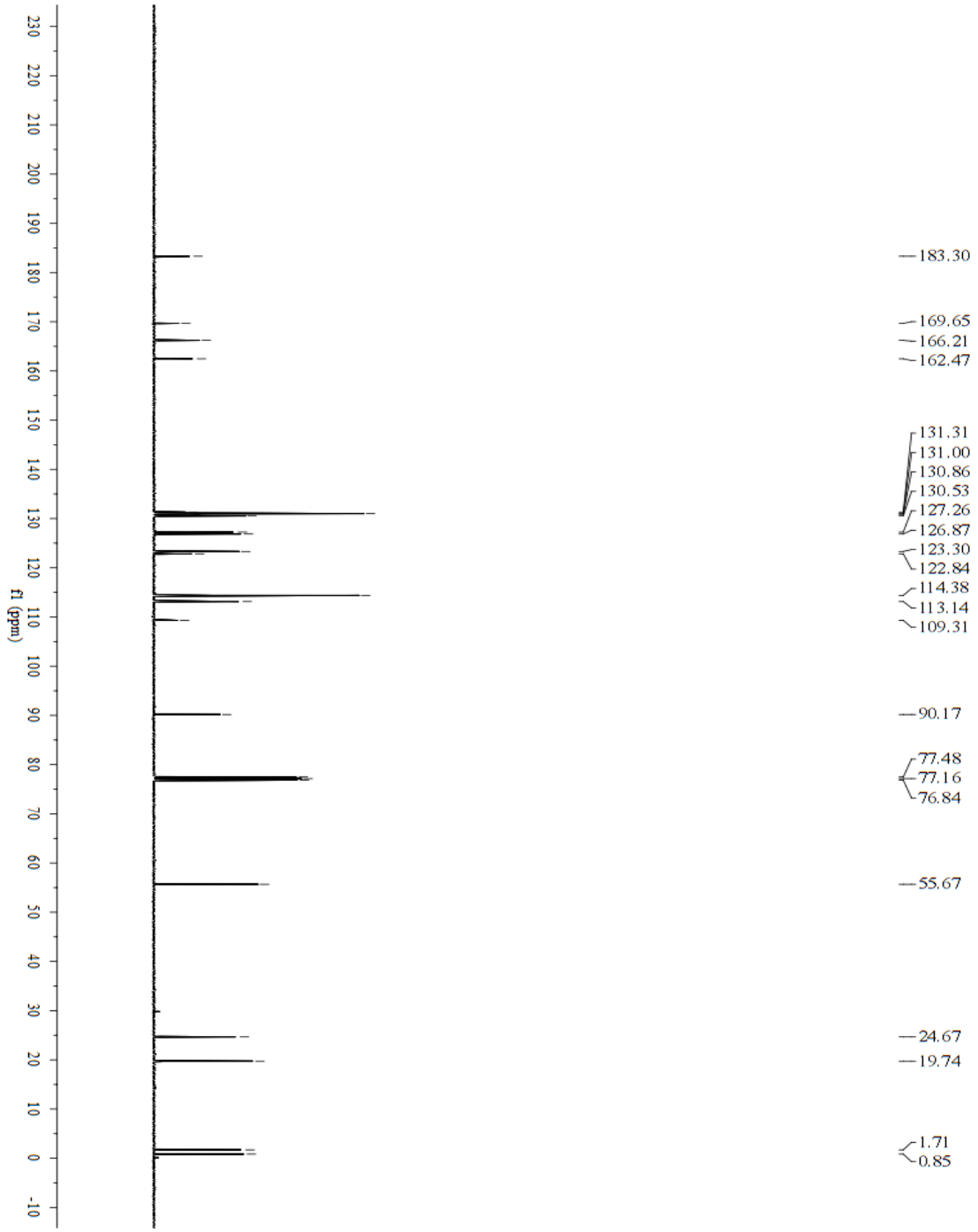
^{1}H NMR (400 MHz, $CDCl_3$)

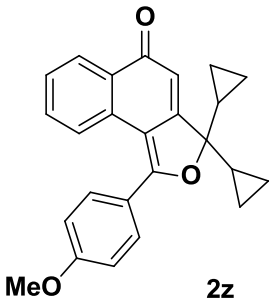




2y

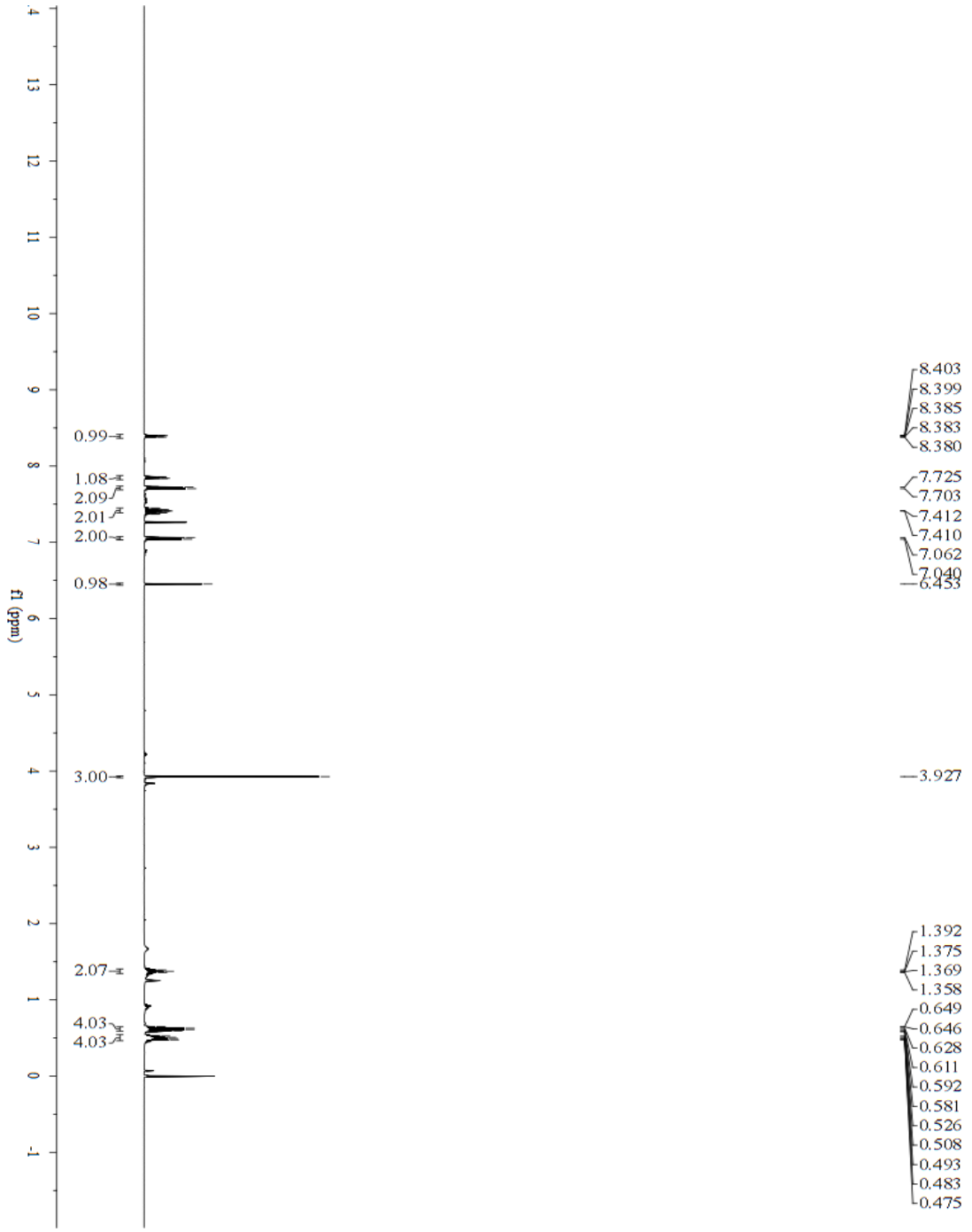
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

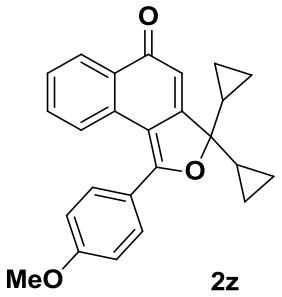




2z

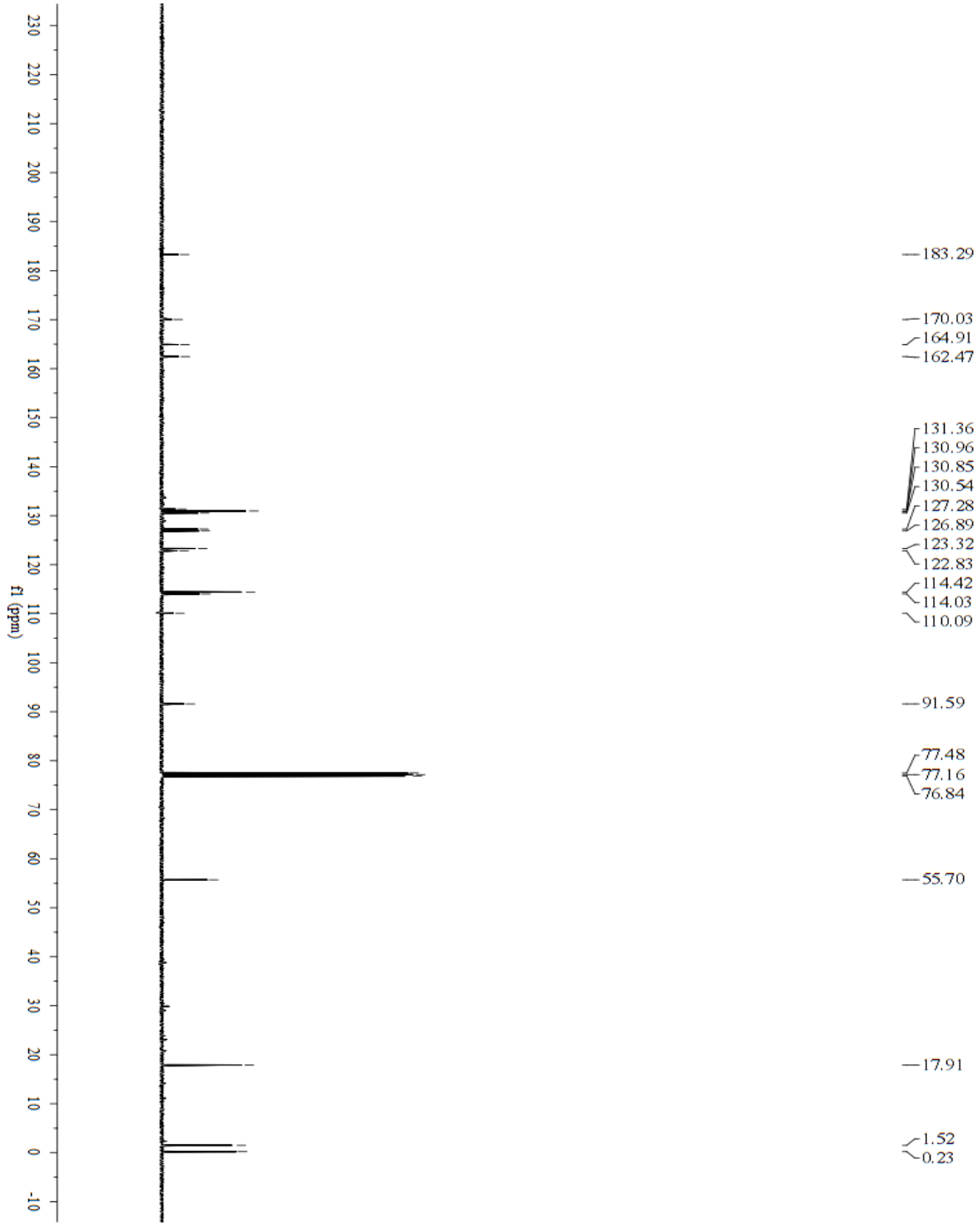
^{1}H NMR (400 MHz, $CDCl_3$)

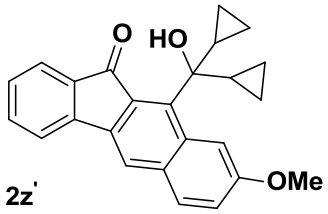




2z

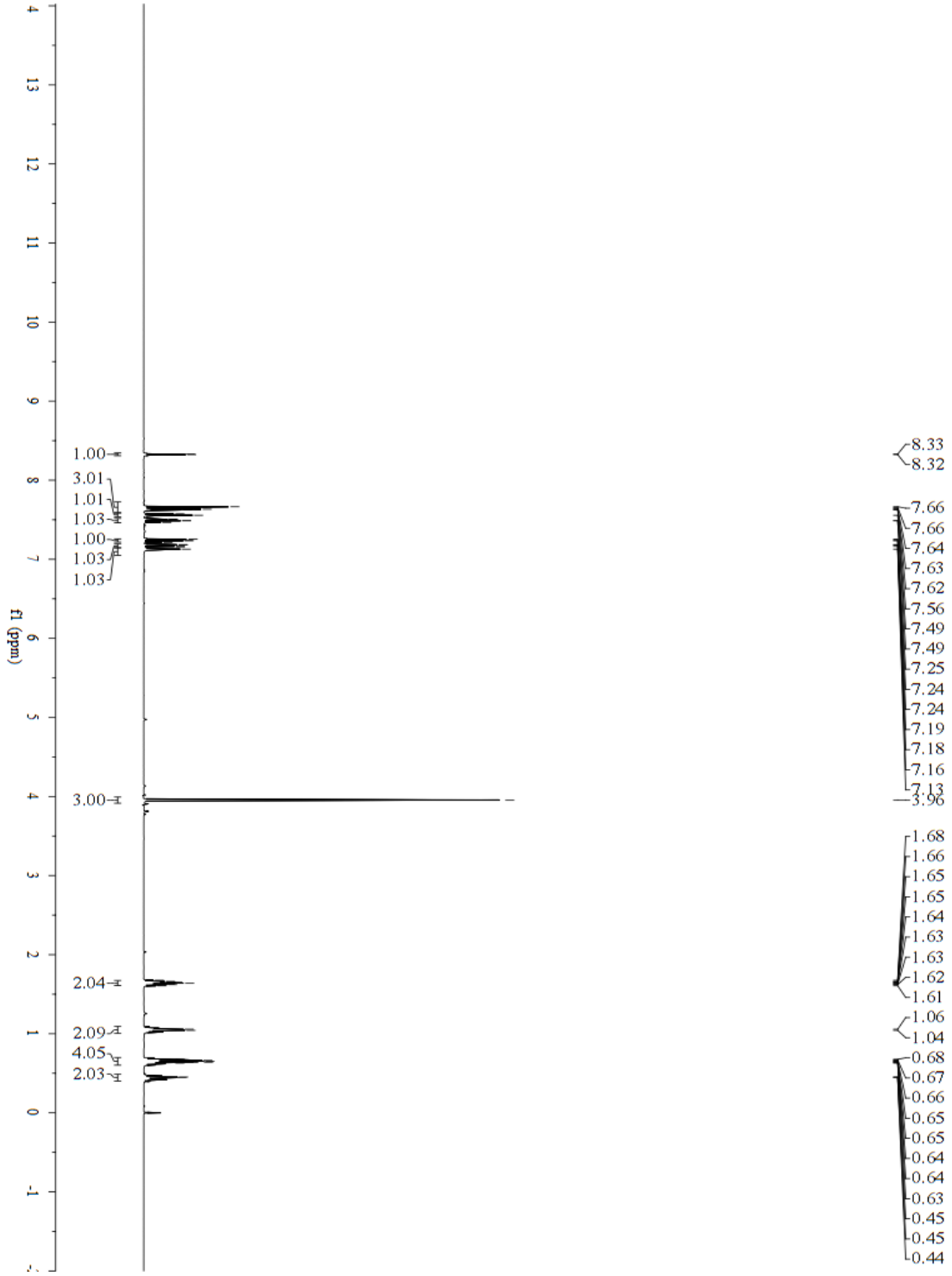
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

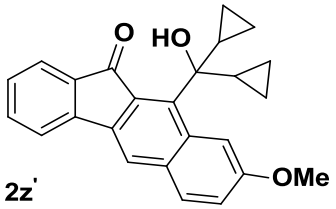




2z'

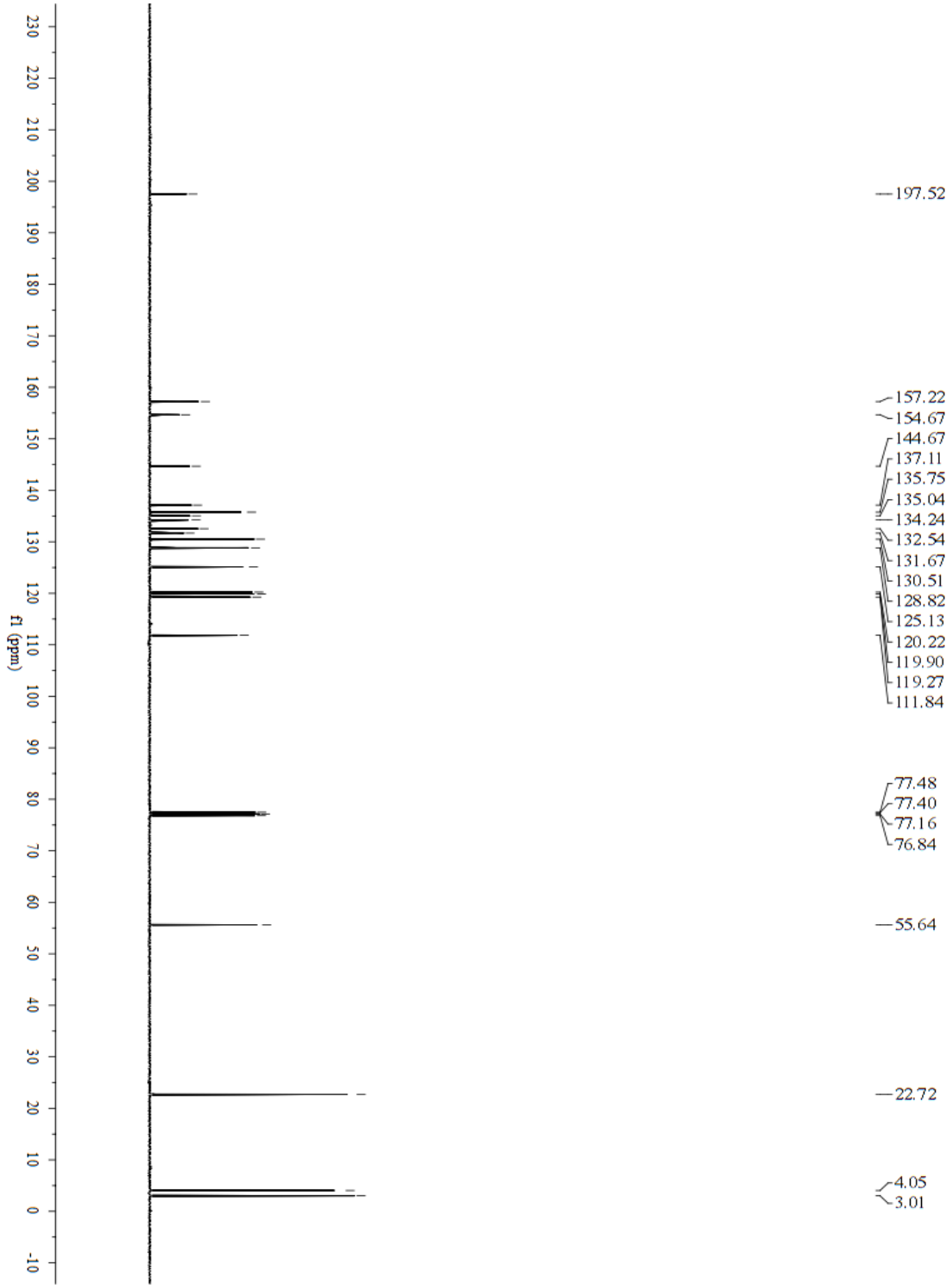
^{1}H NMR (400 MHz, $CDCl_3$)

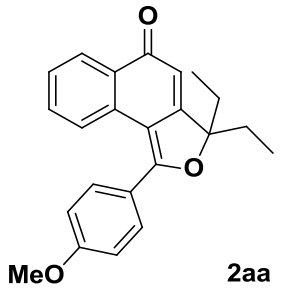




2z'

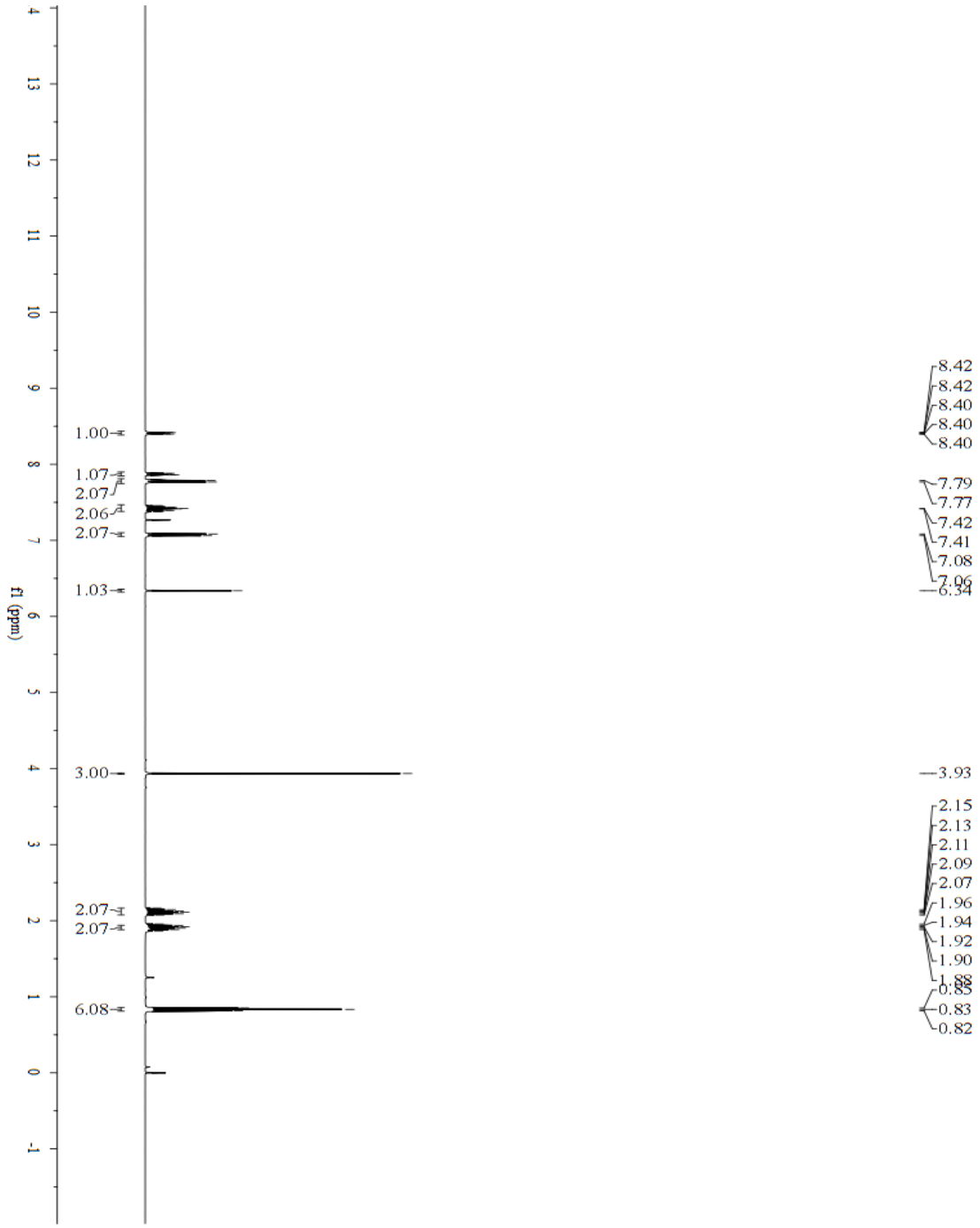
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

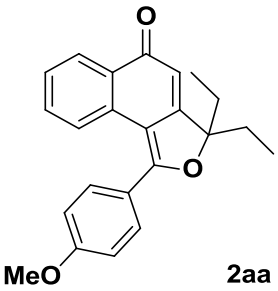




2aa

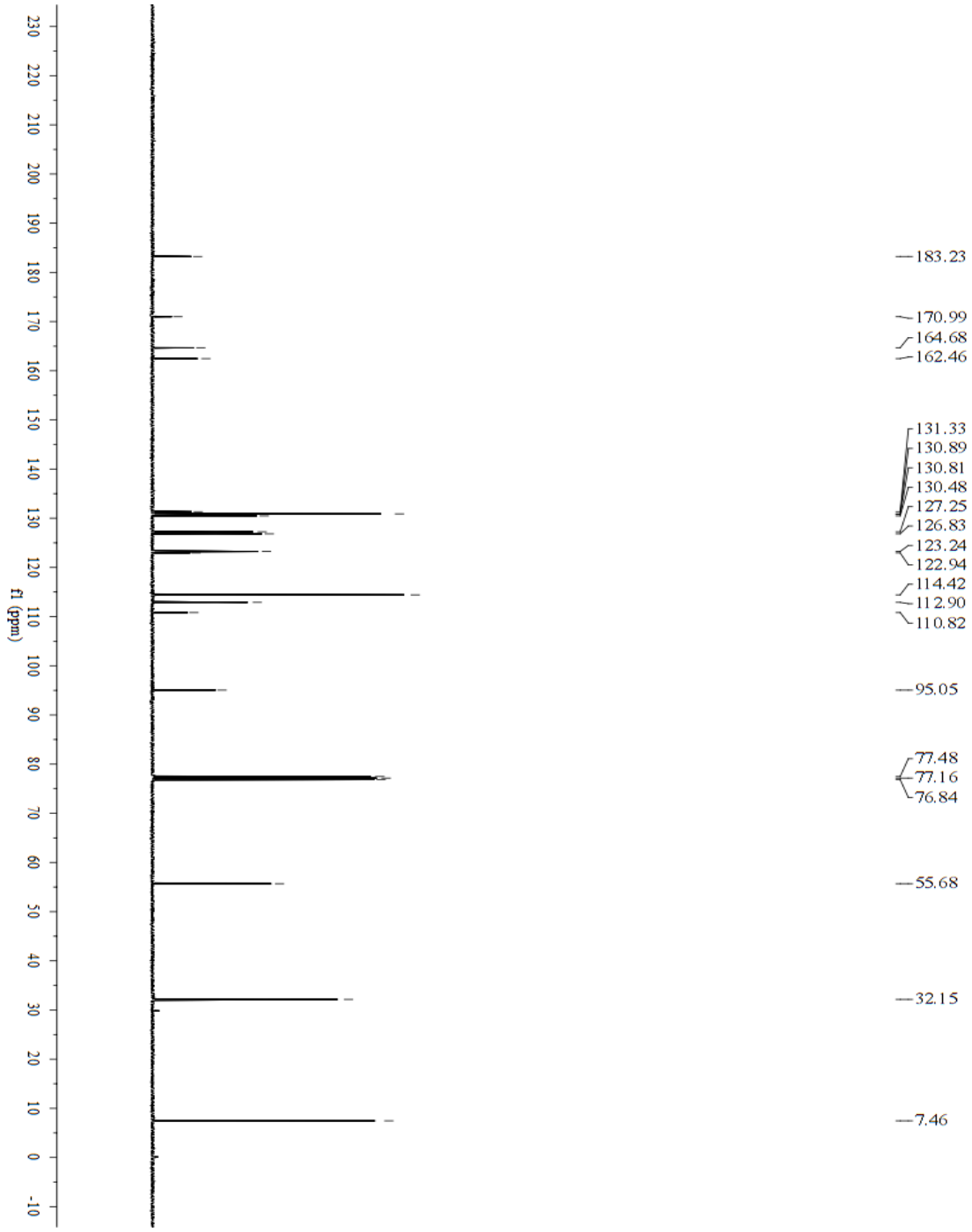
^{1}H NMR (400 MHz, $CDCl_3$)

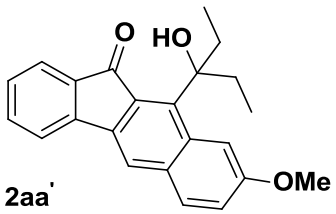




2aa

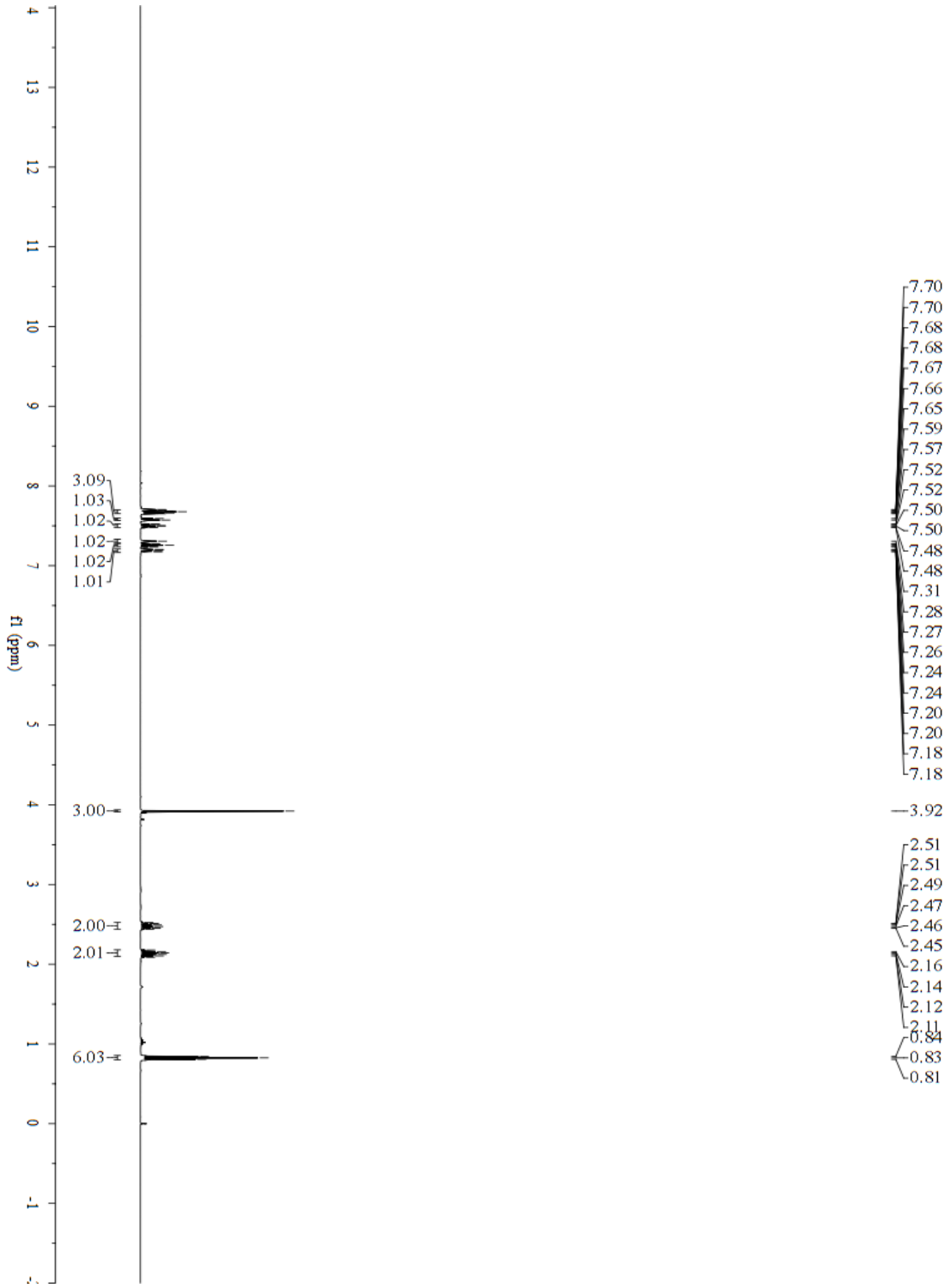
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

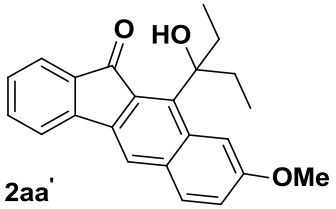




2aa'

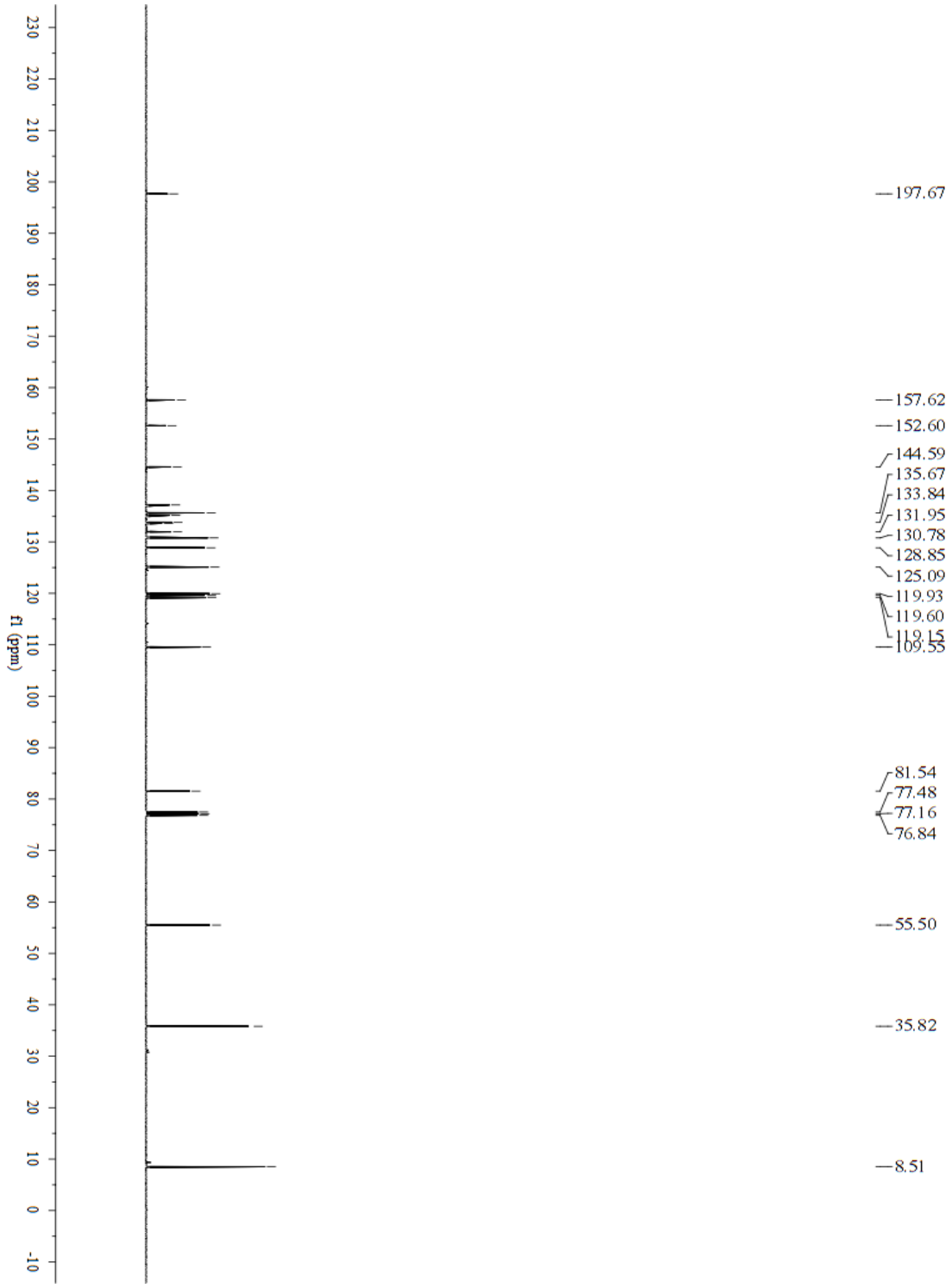
^{1}H NMR (400 MHz, $CDCl_3$)

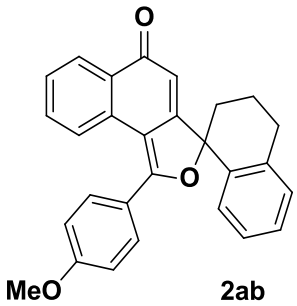




2aa'

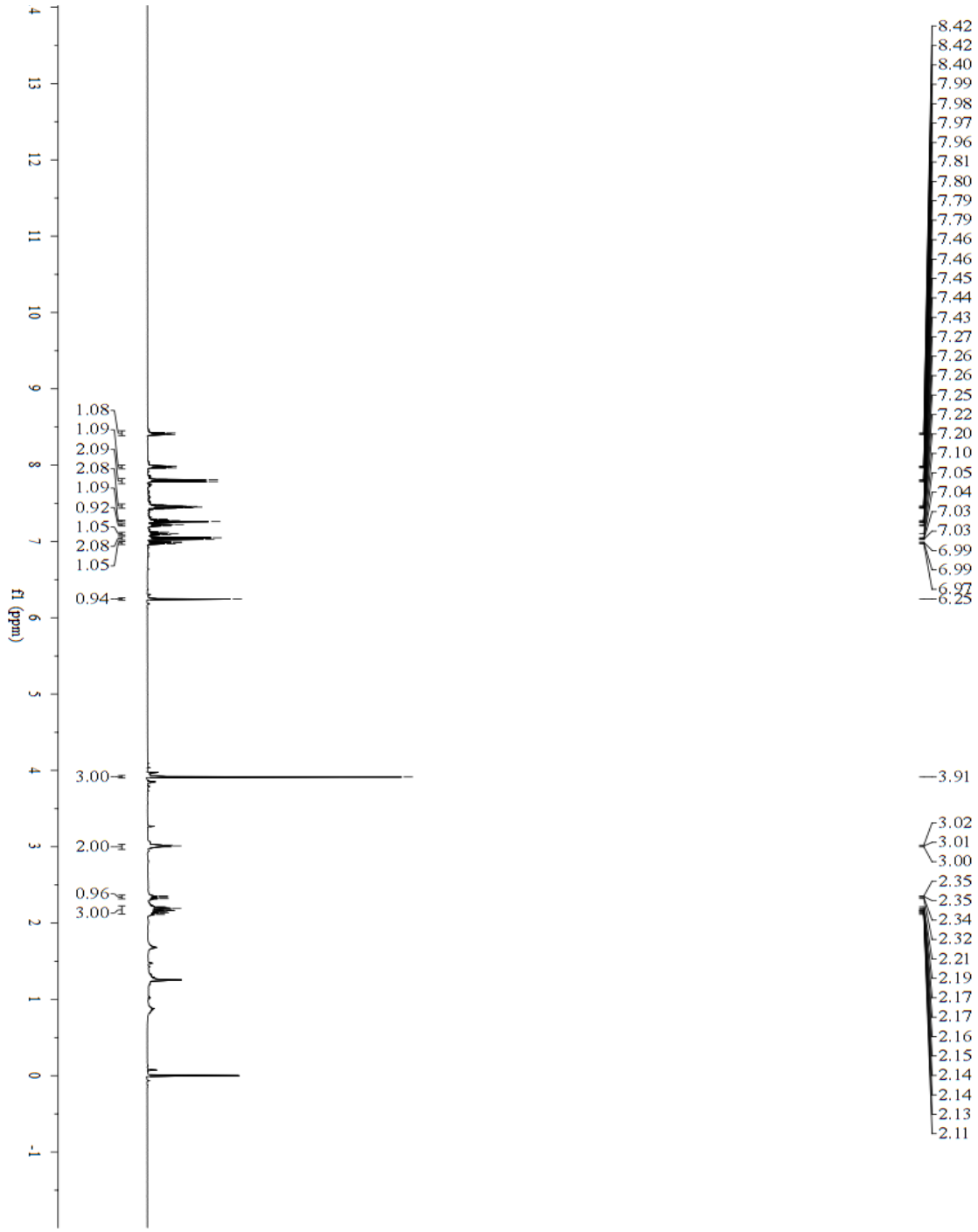
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

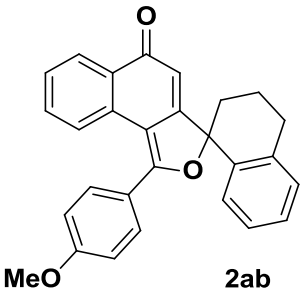




2ab

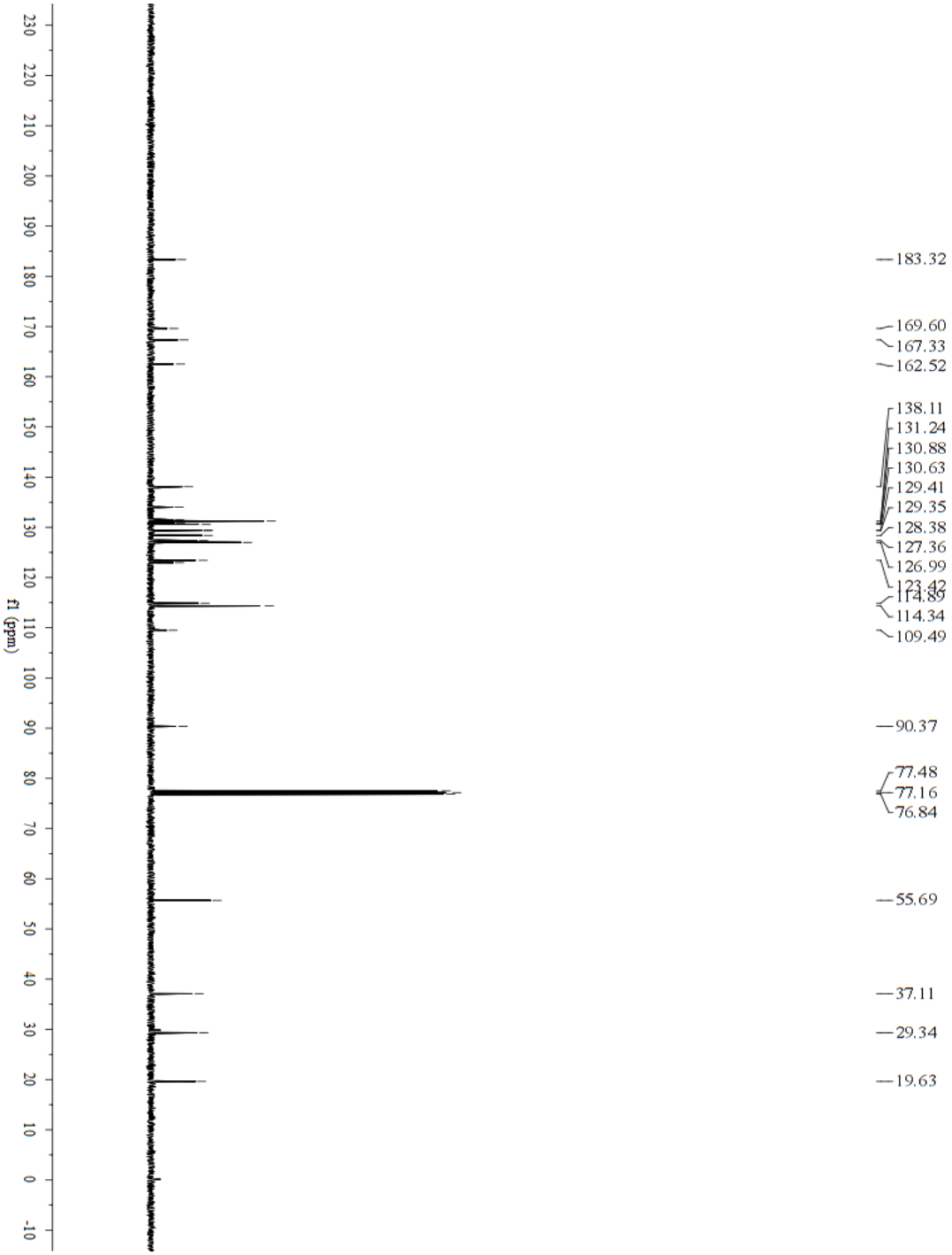
^{1}H NMR (400 MHz, $CDCl_3$)

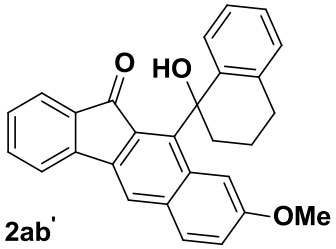




2ab

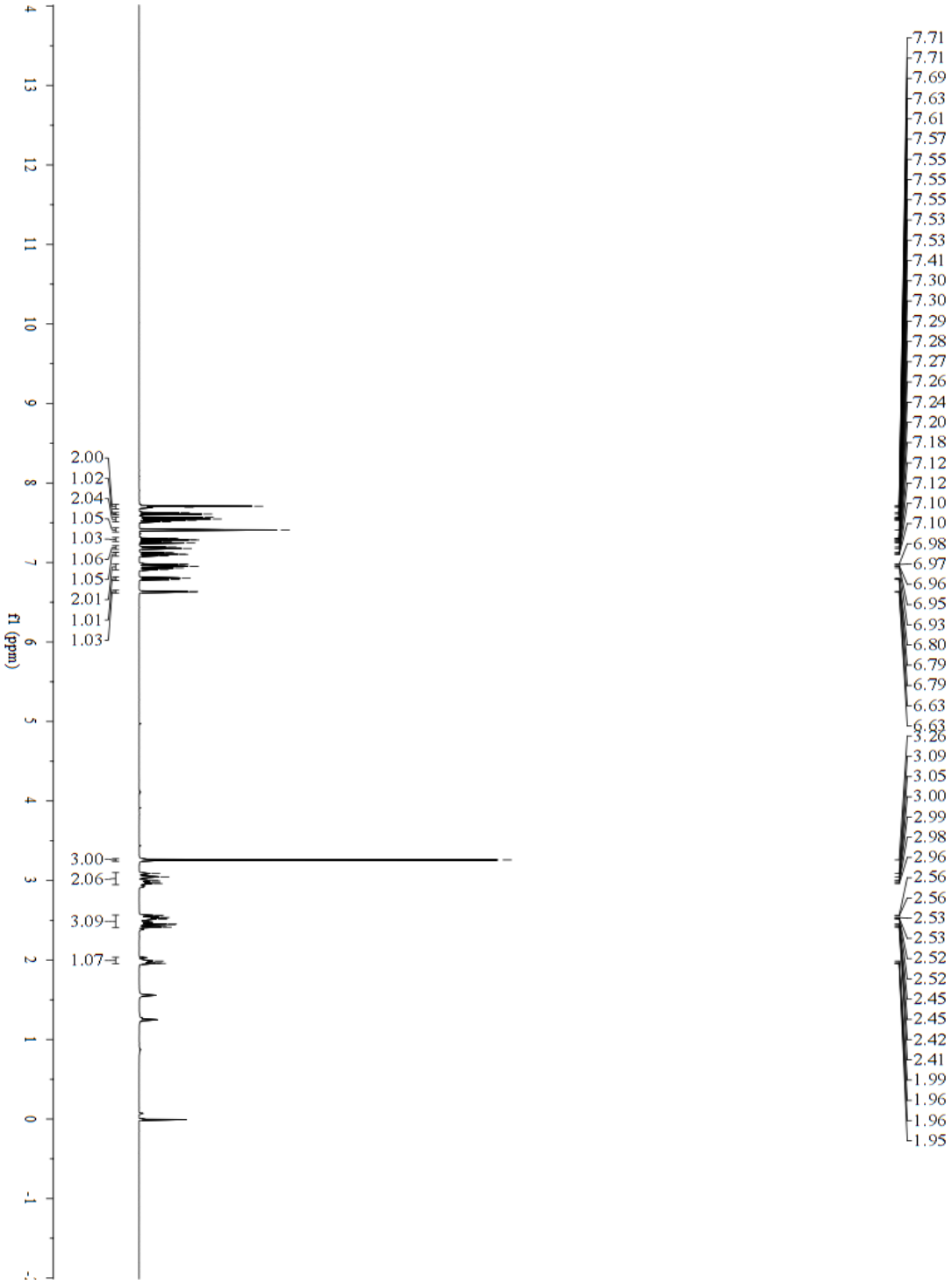
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)

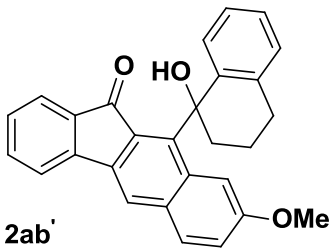




2ab'

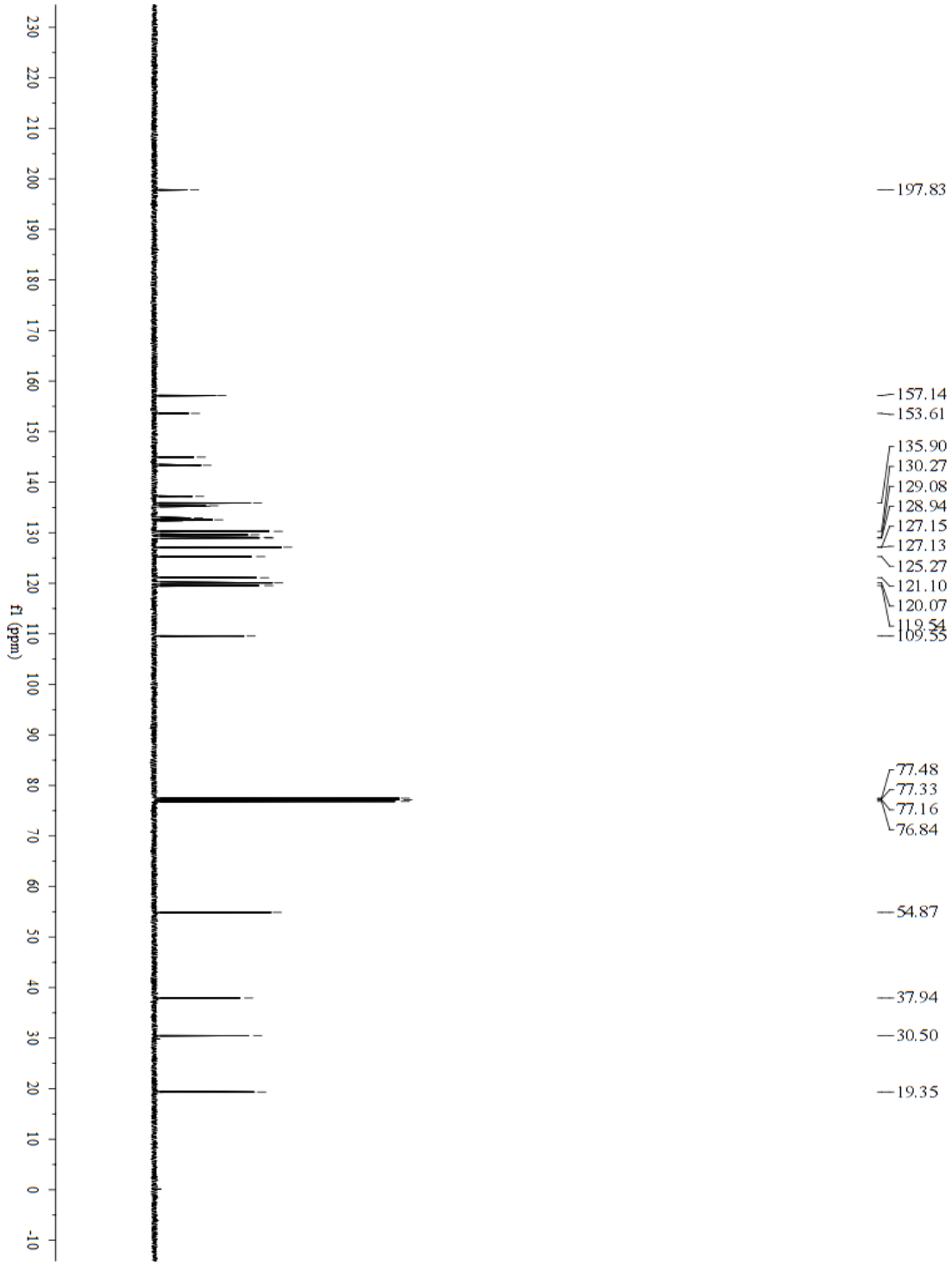
^{1}H NMR (400 MHz, $CDCl_3$)

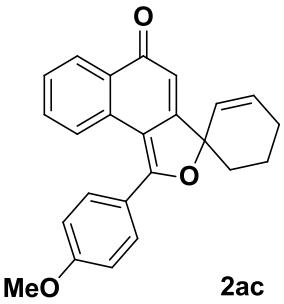




2ab'

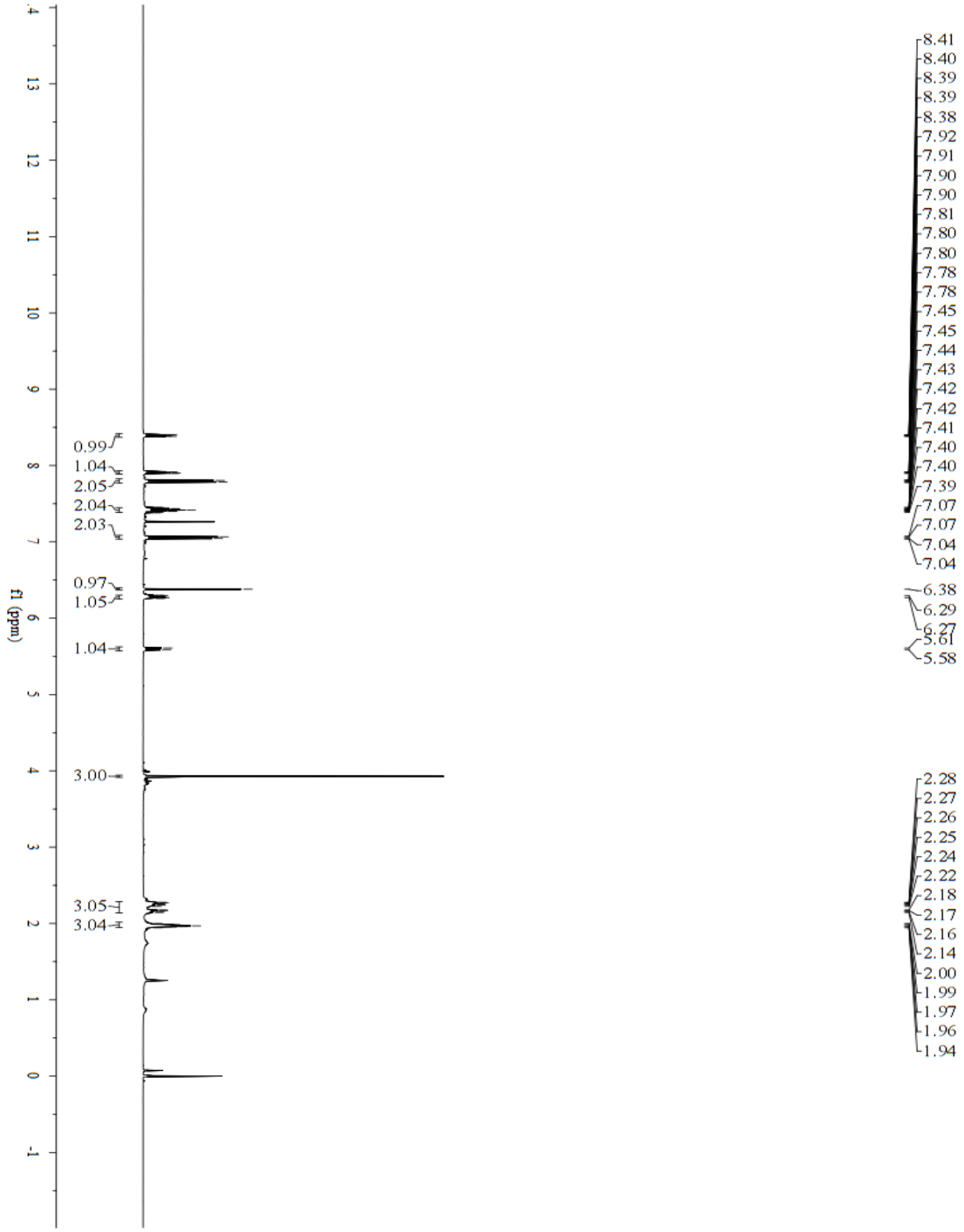
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)

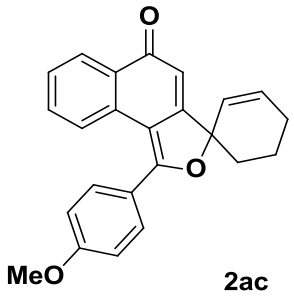




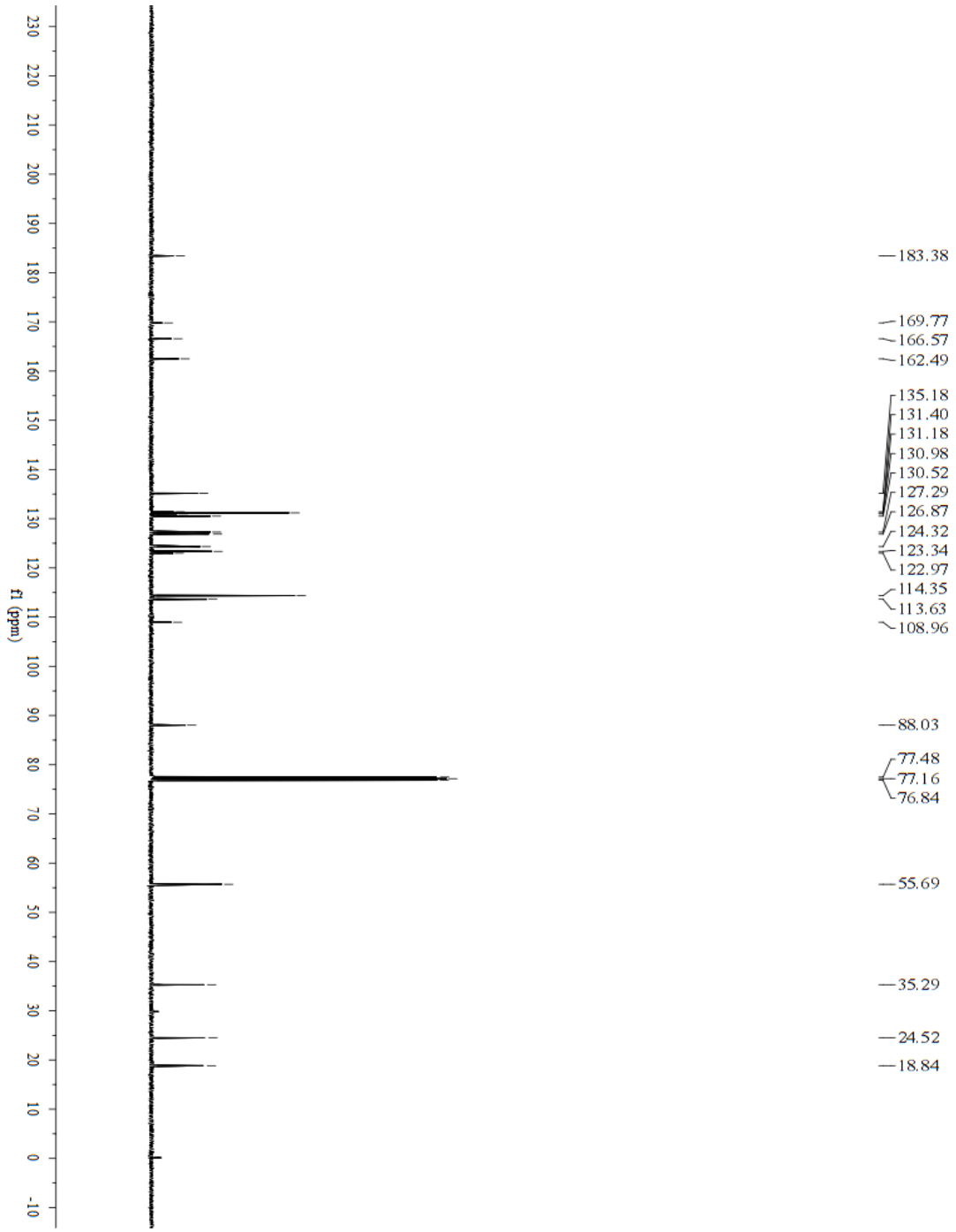
2ac

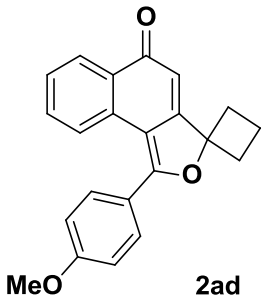
^{1}H NMR (400 MHz, $CDCl_3$)





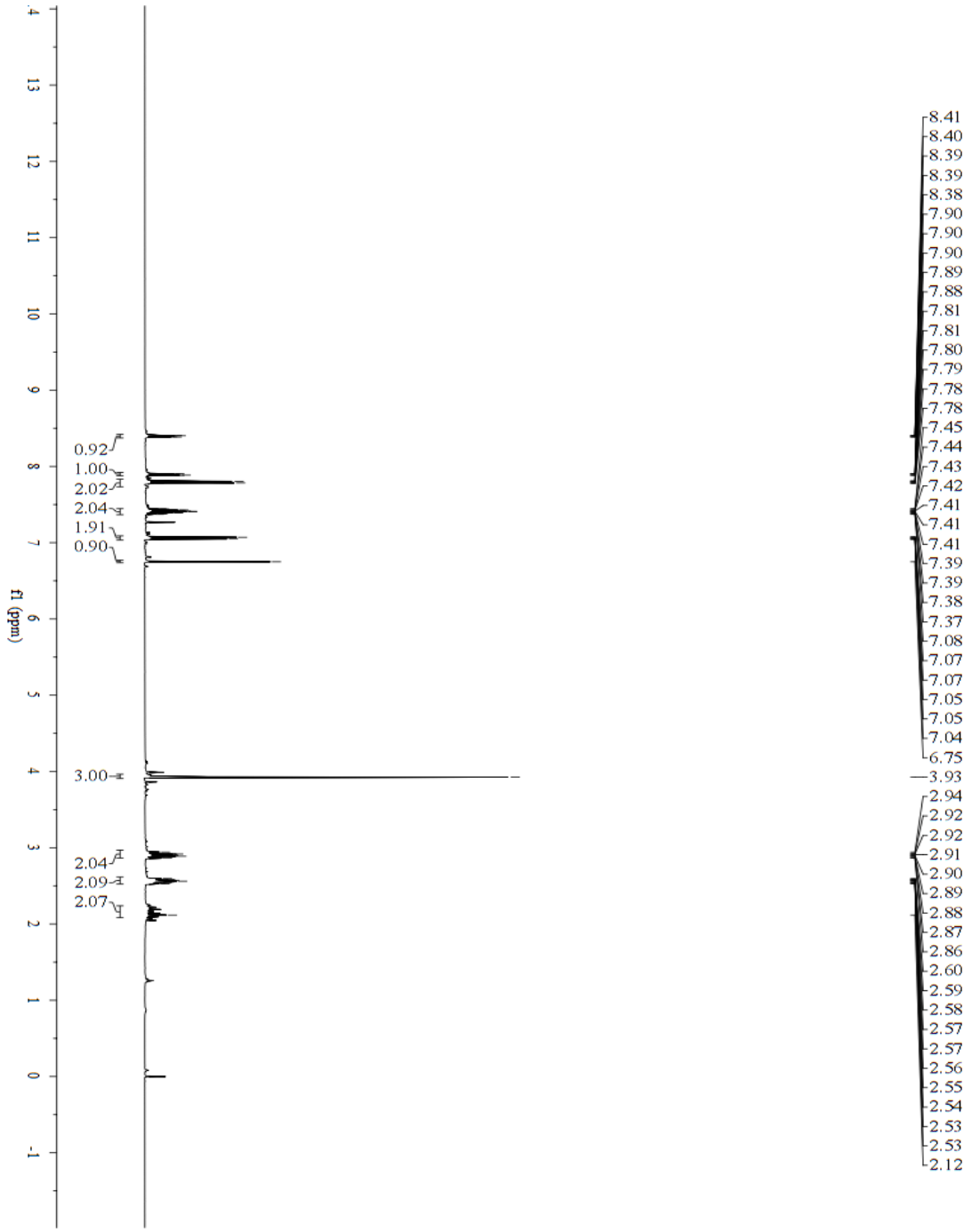
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

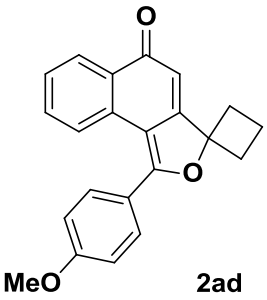




2ad

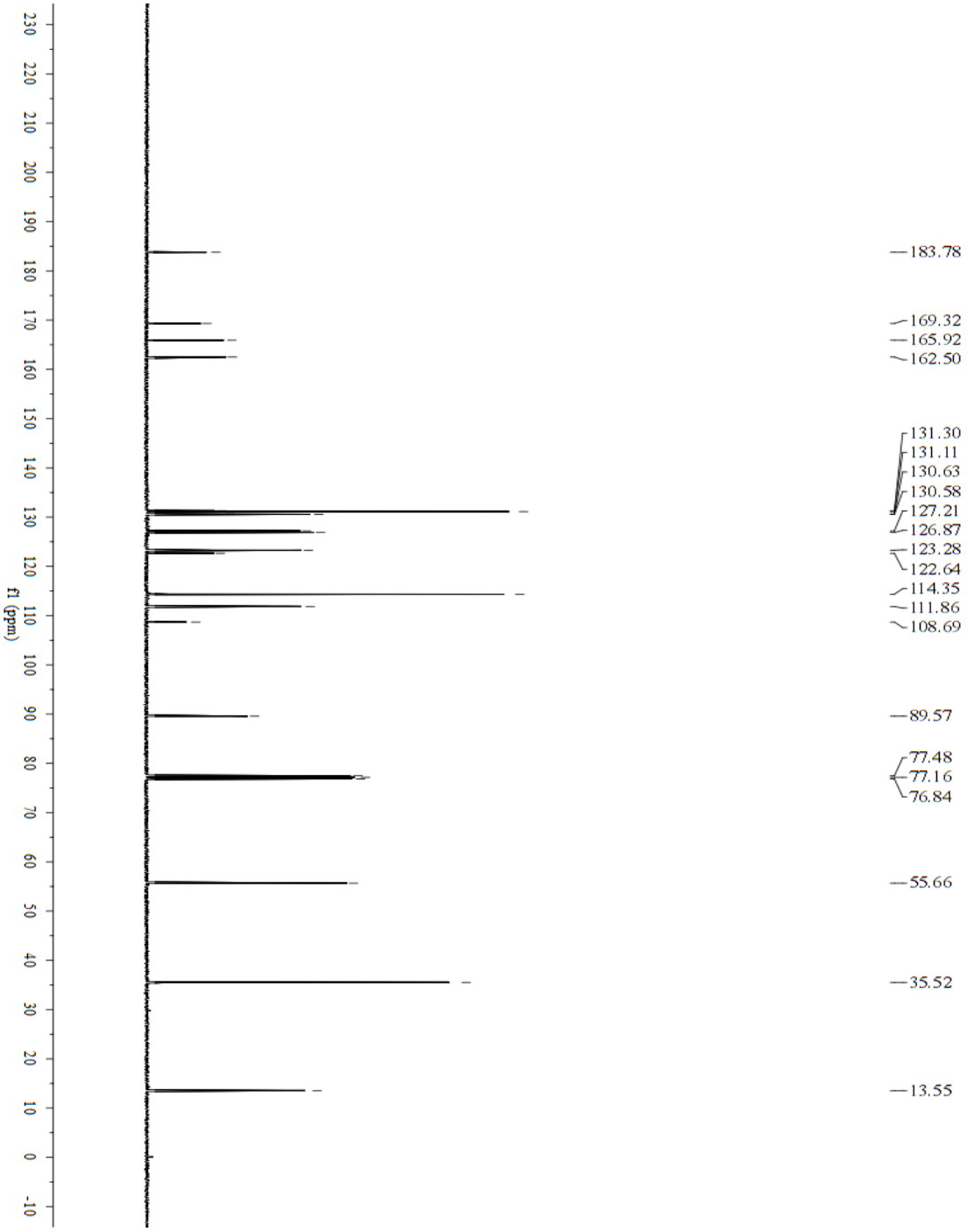
^{1}H NMR (400 MHz, $CDCl_3$)

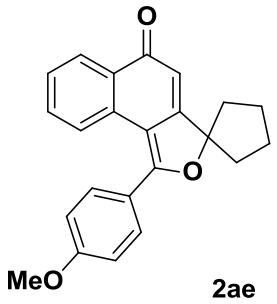




2ad

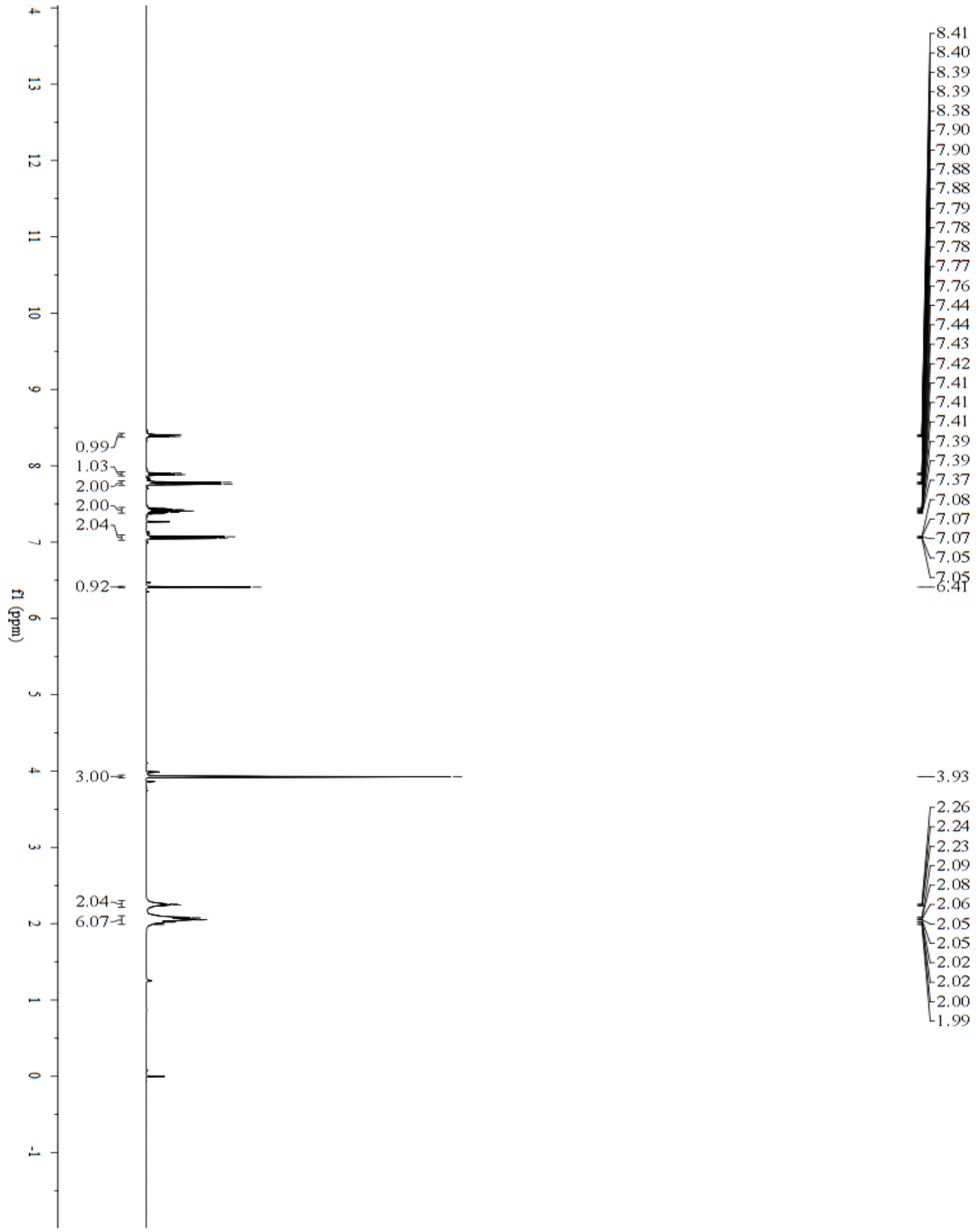
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

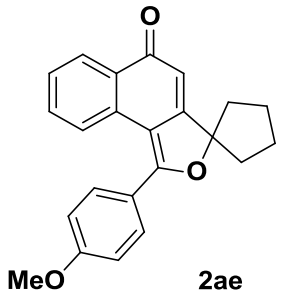




2ae

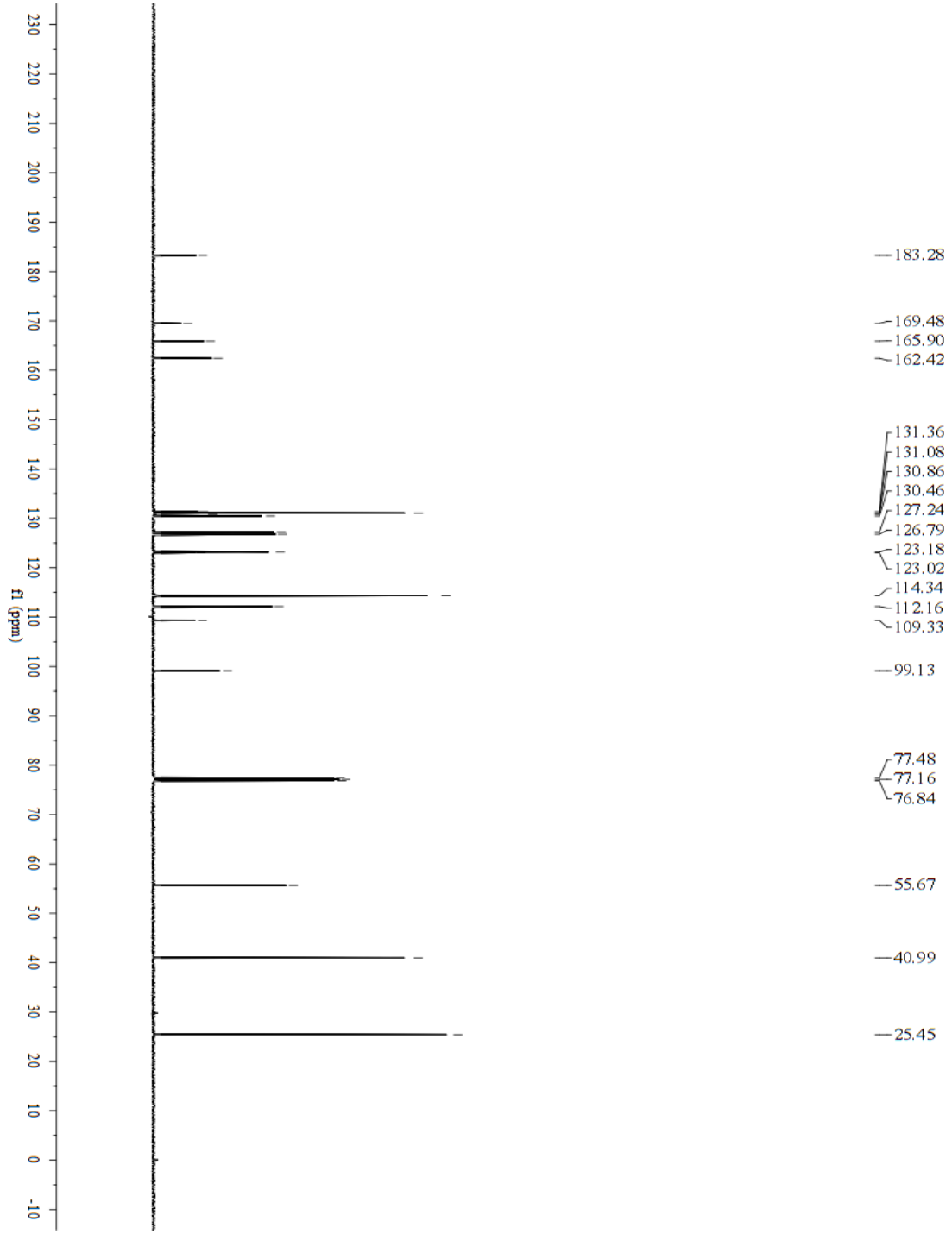
^{1}H NMR (400 MHz, $CDCl_3$)

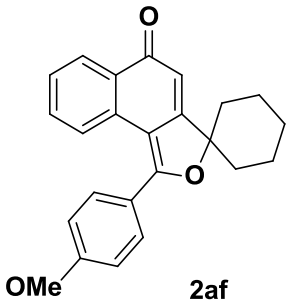




2ae

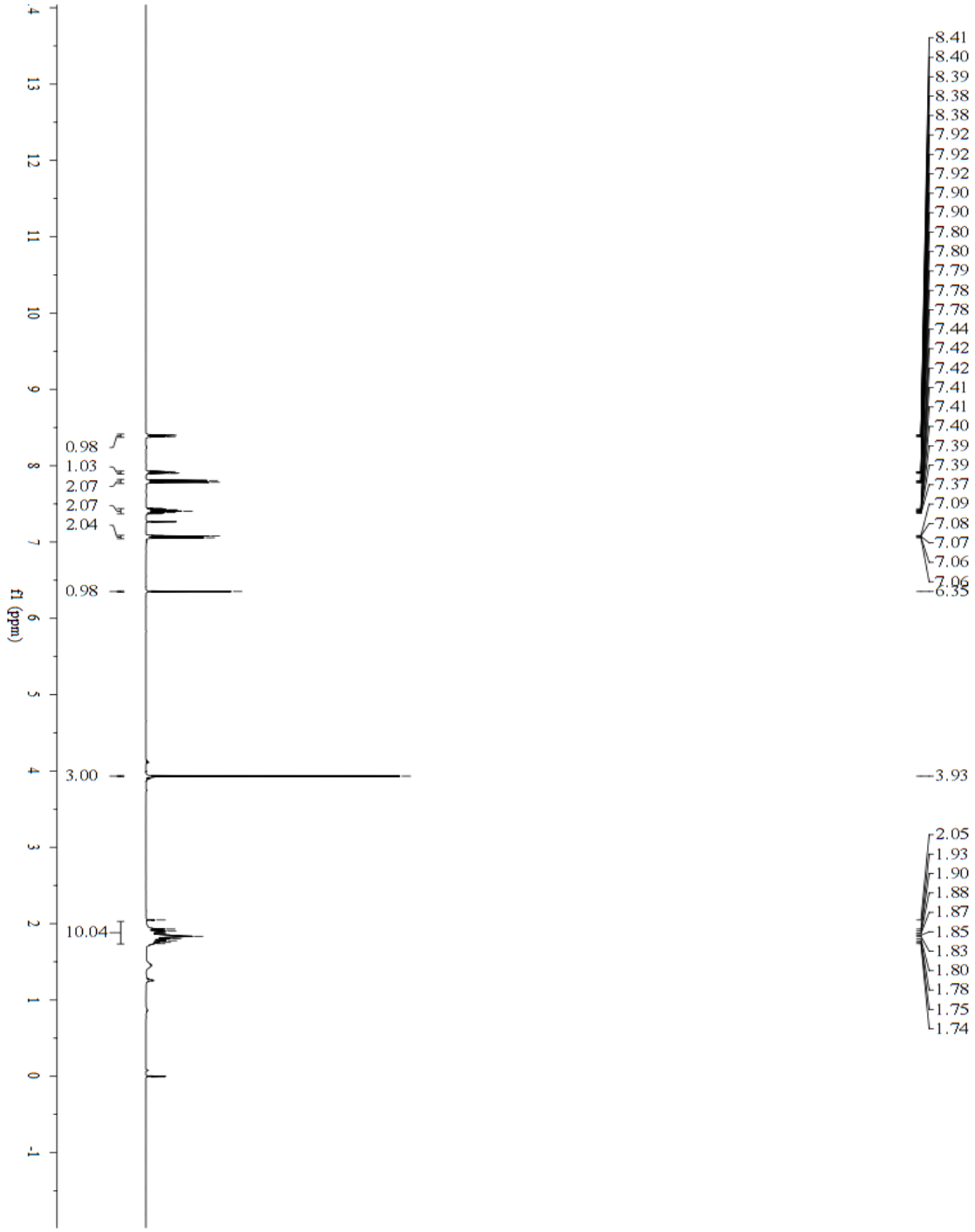
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

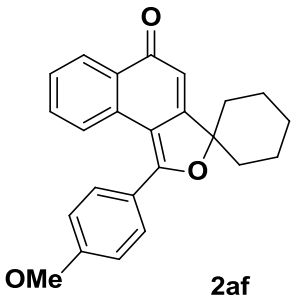




2af

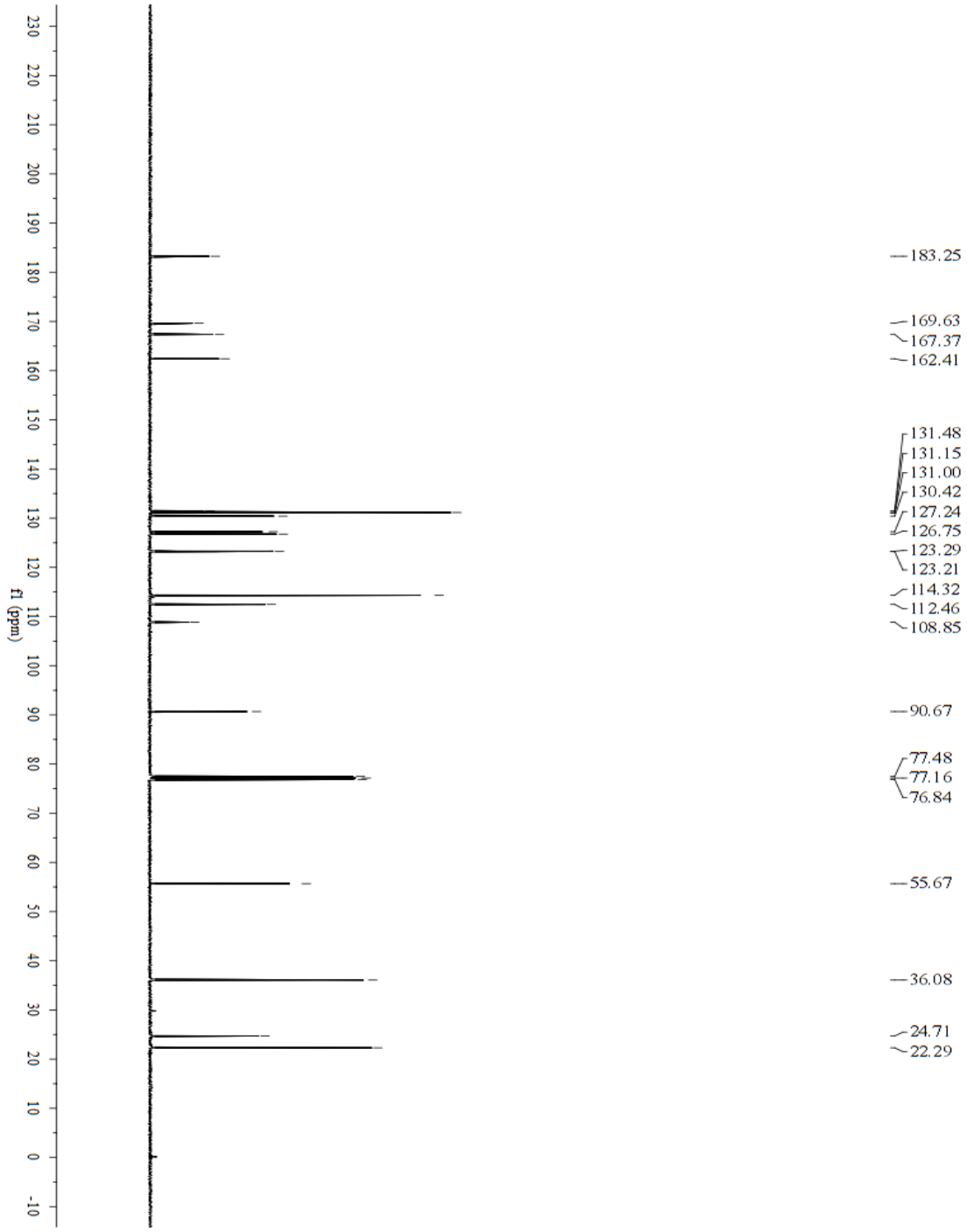
^{1}H NMR (400 MHz, $CDCl_3$)

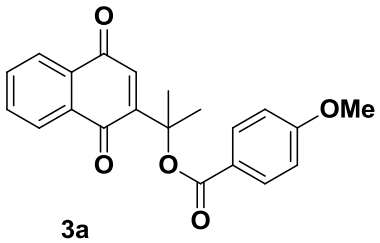




2af

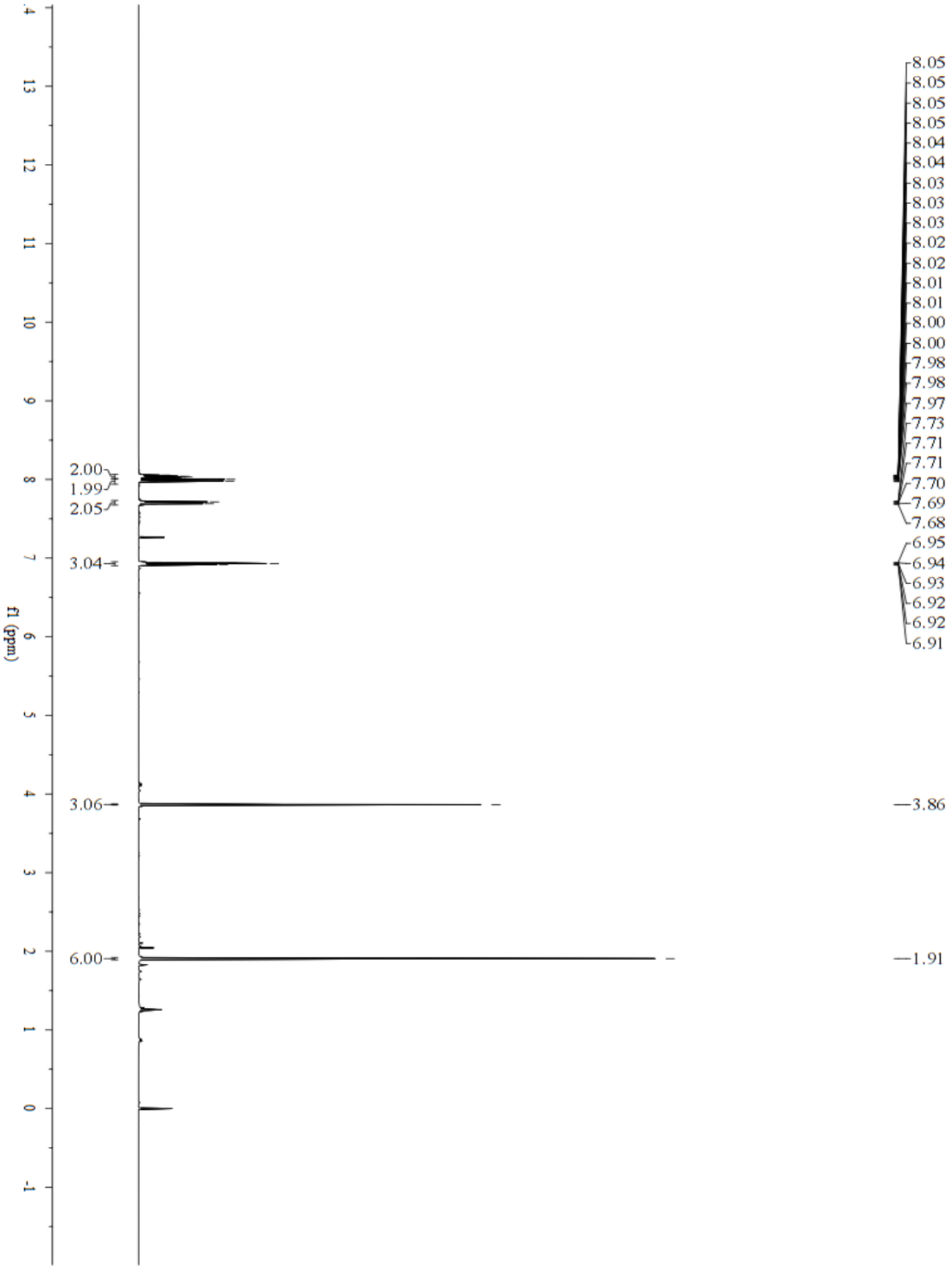
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

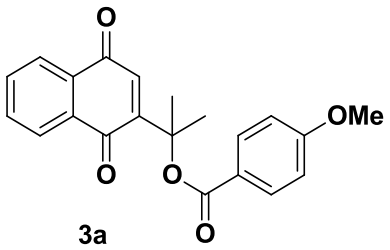




3a

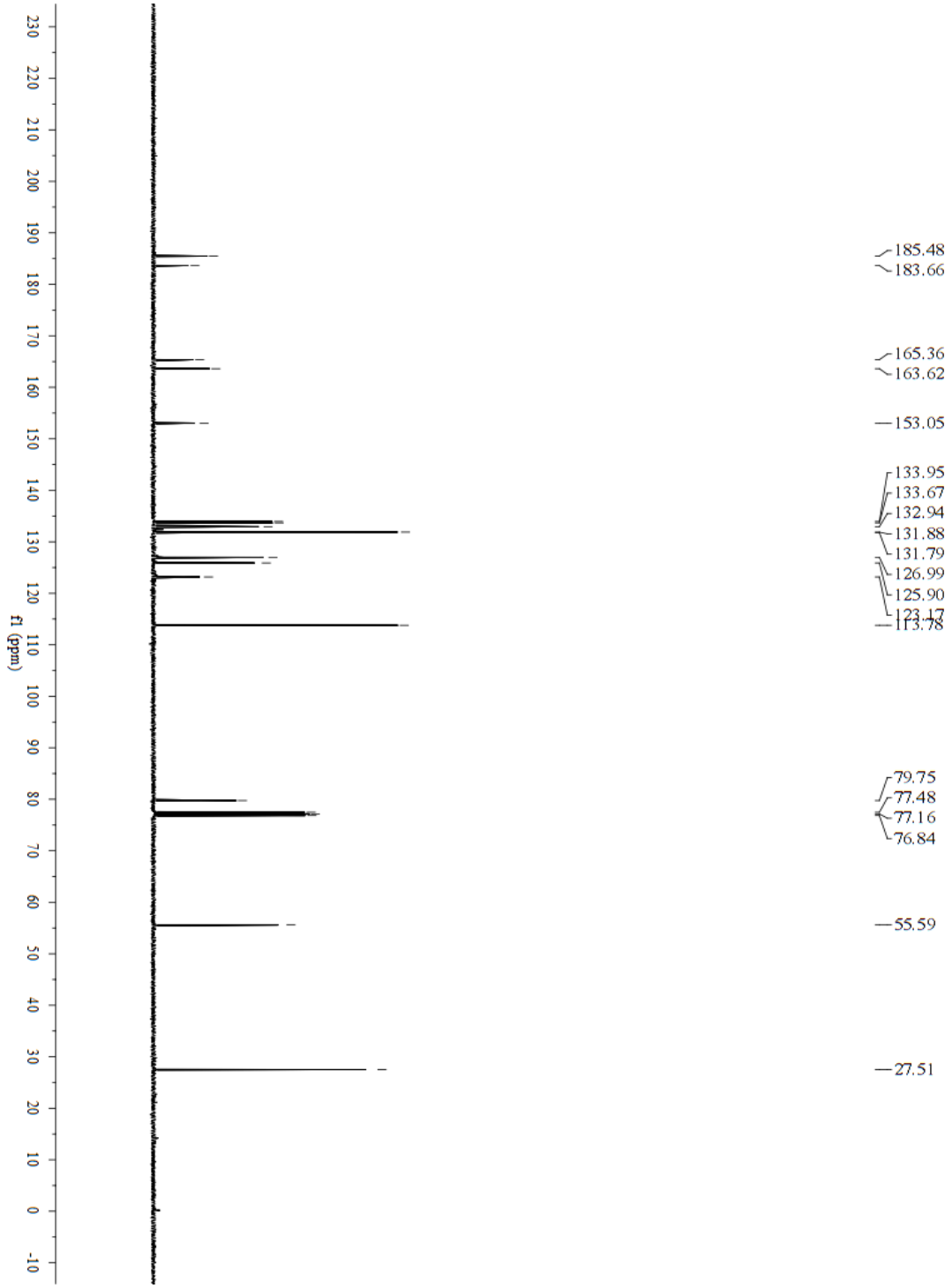
^{1}H NMR (400 MHz, $CDCl_3$)



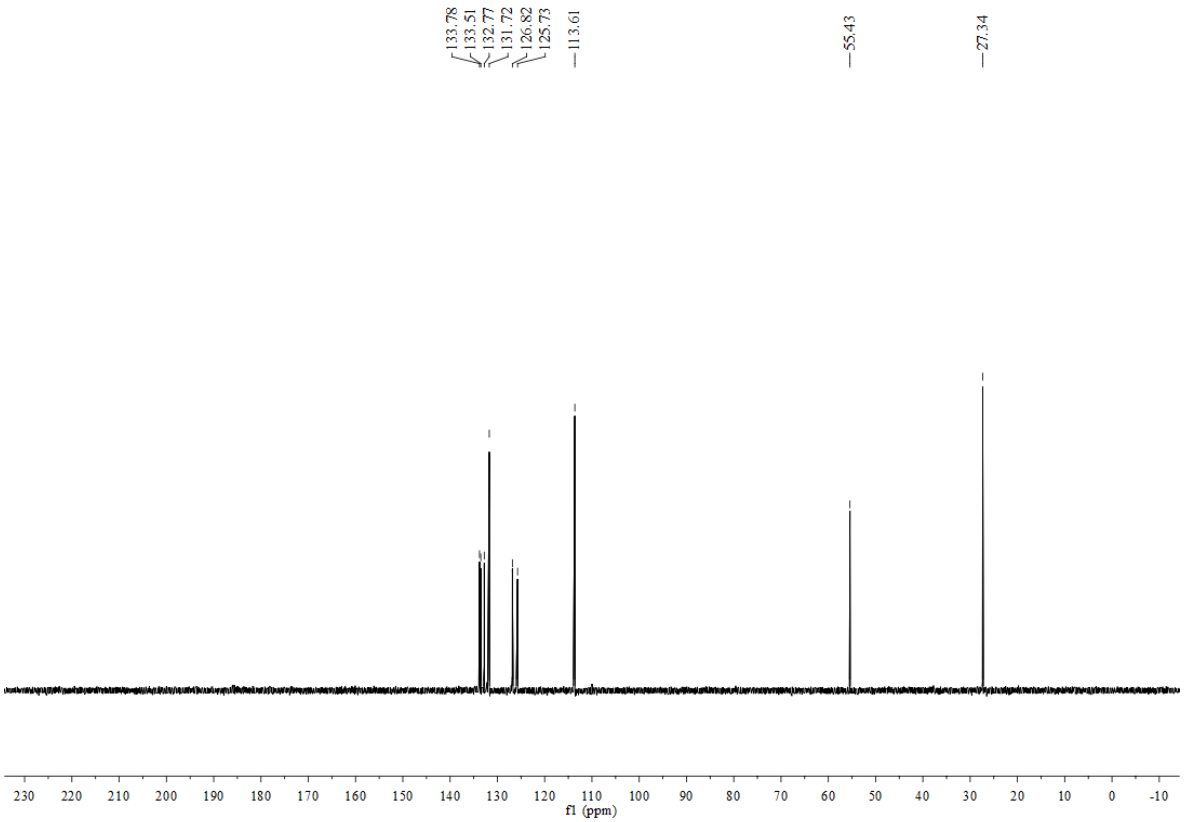


3a

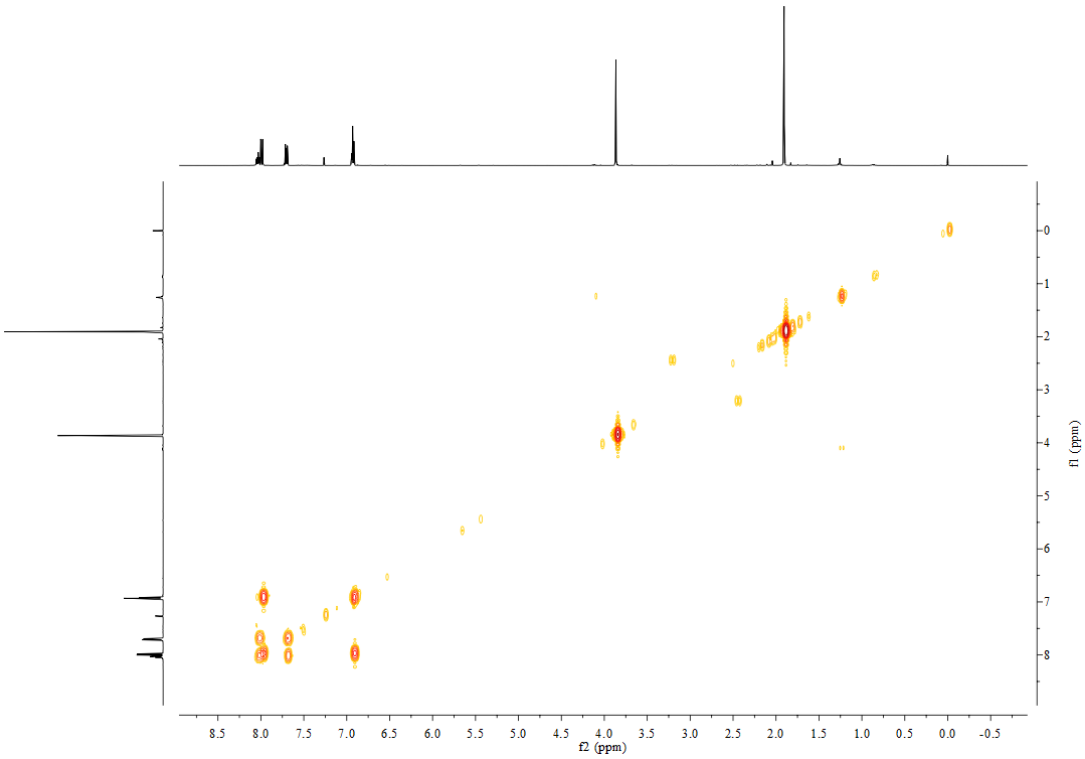
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



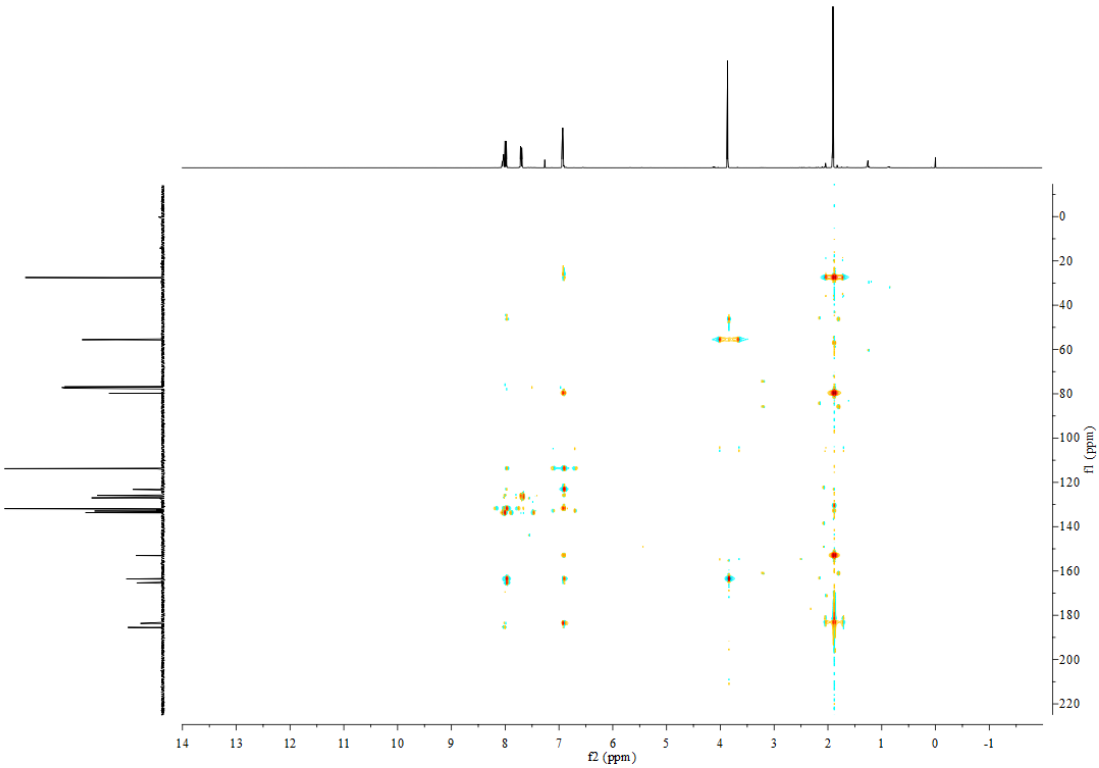
3a-DEPT



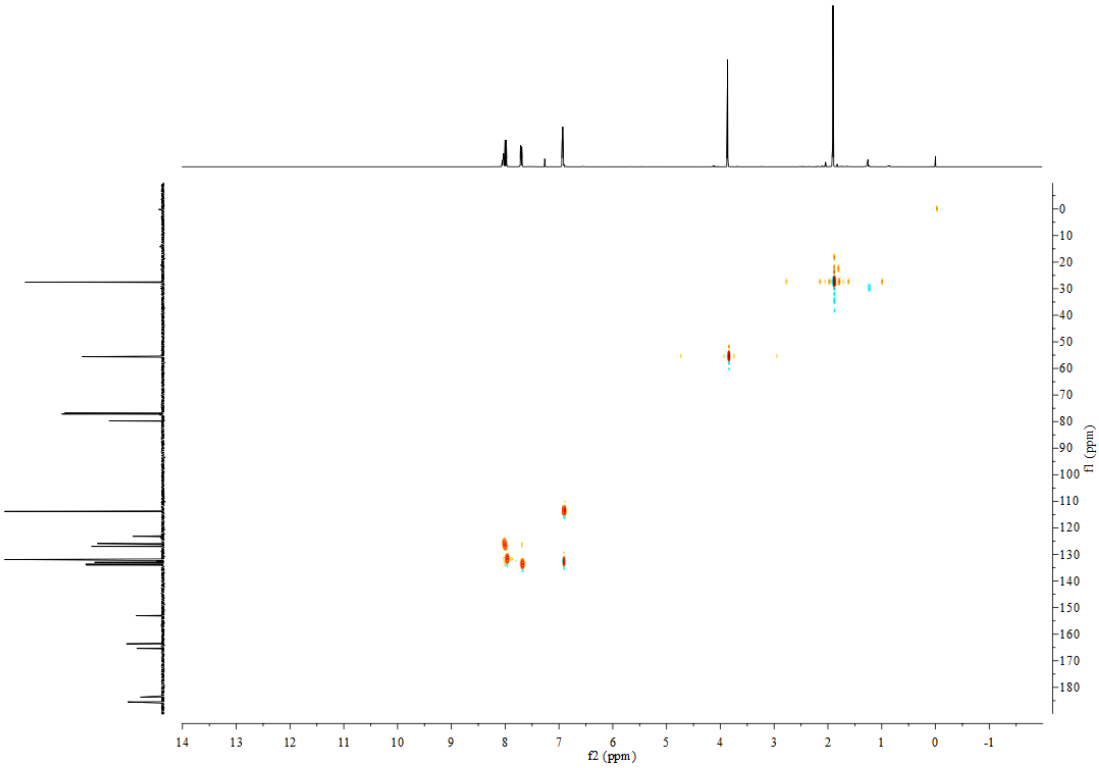
3a- ^{1}H-^{1}H COSY

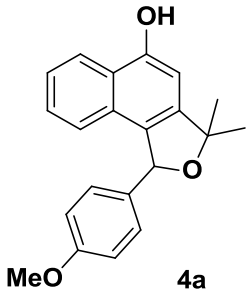


3a- HMBC



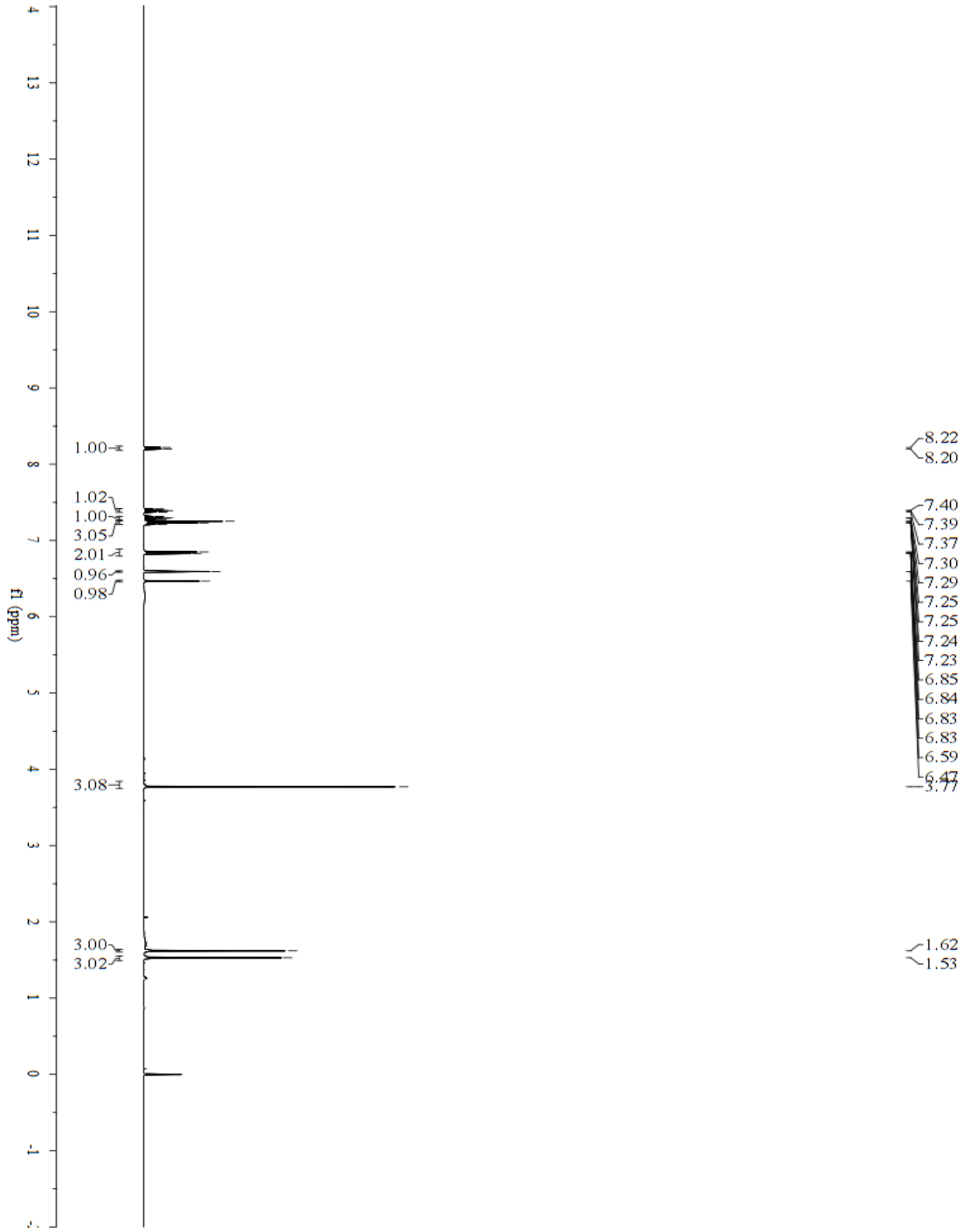
3a- HSQC

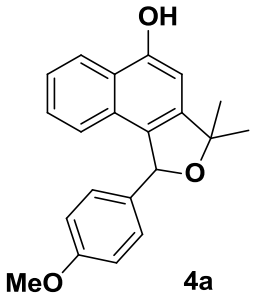




4a

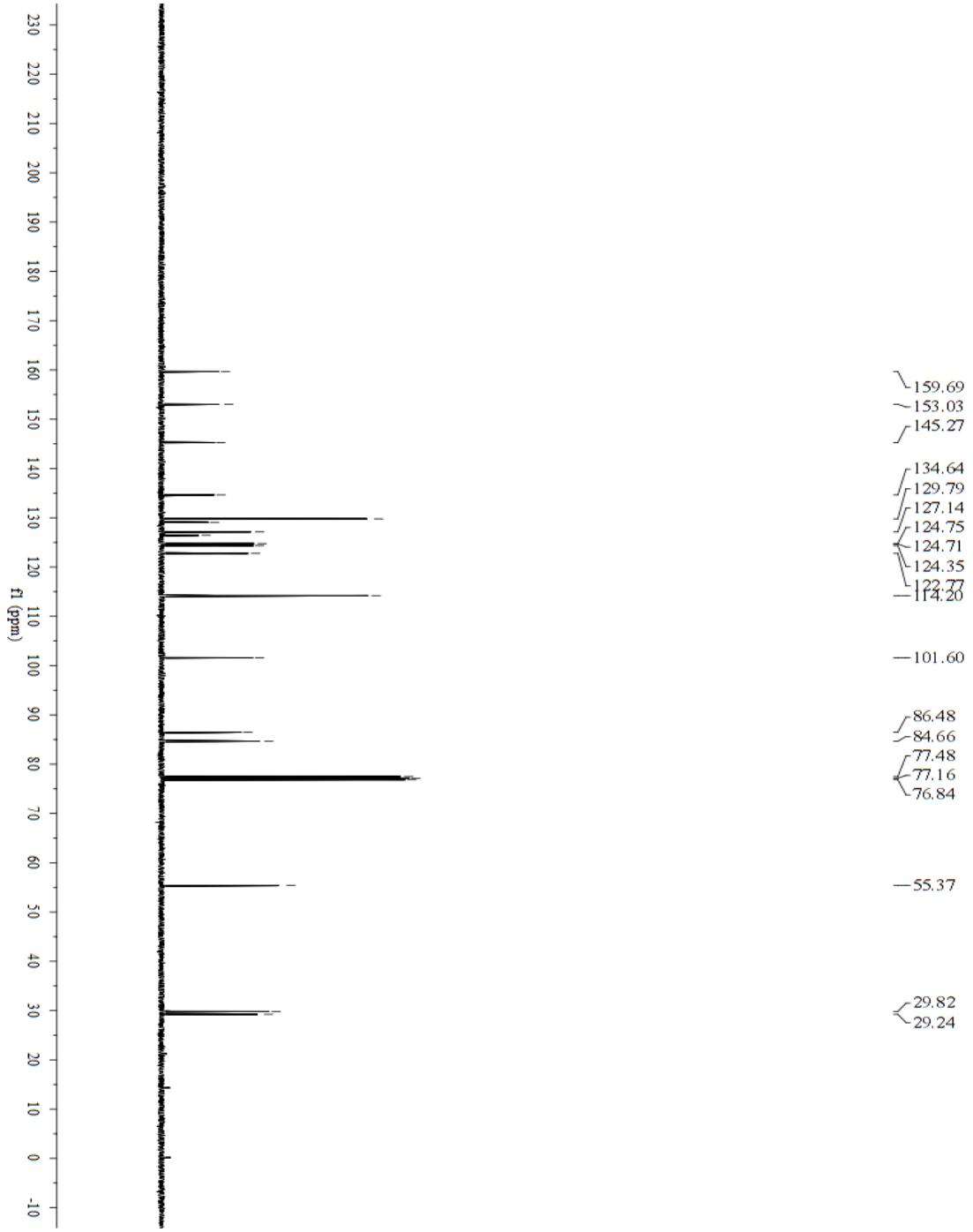
^{1}H NMR (400 MHz, $CDCl_3$)

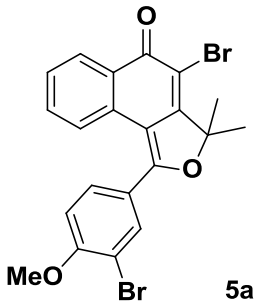




4a

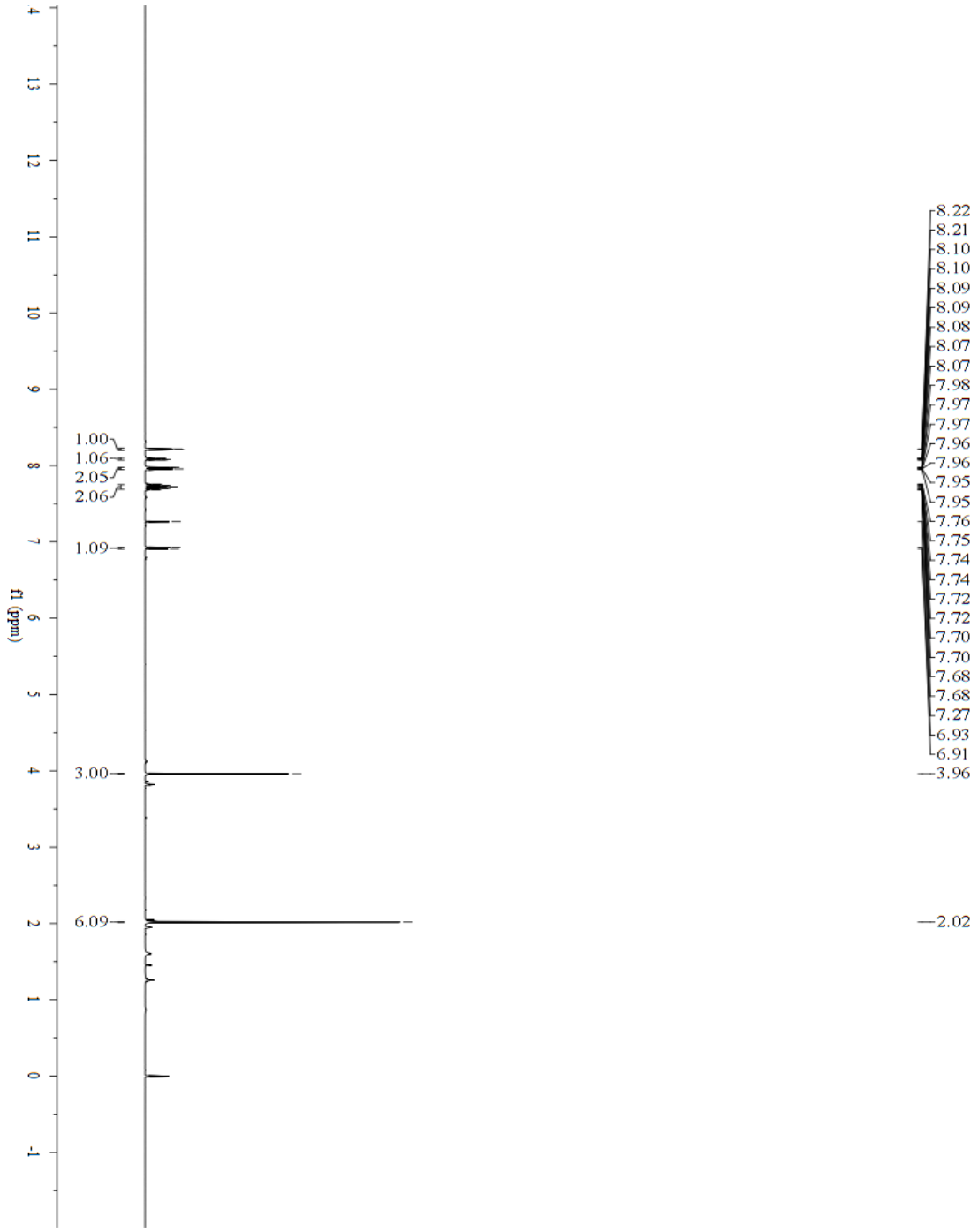
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

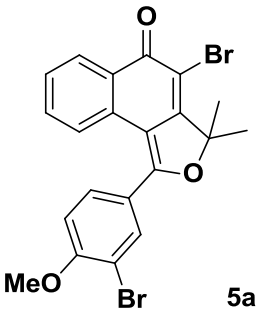




5a

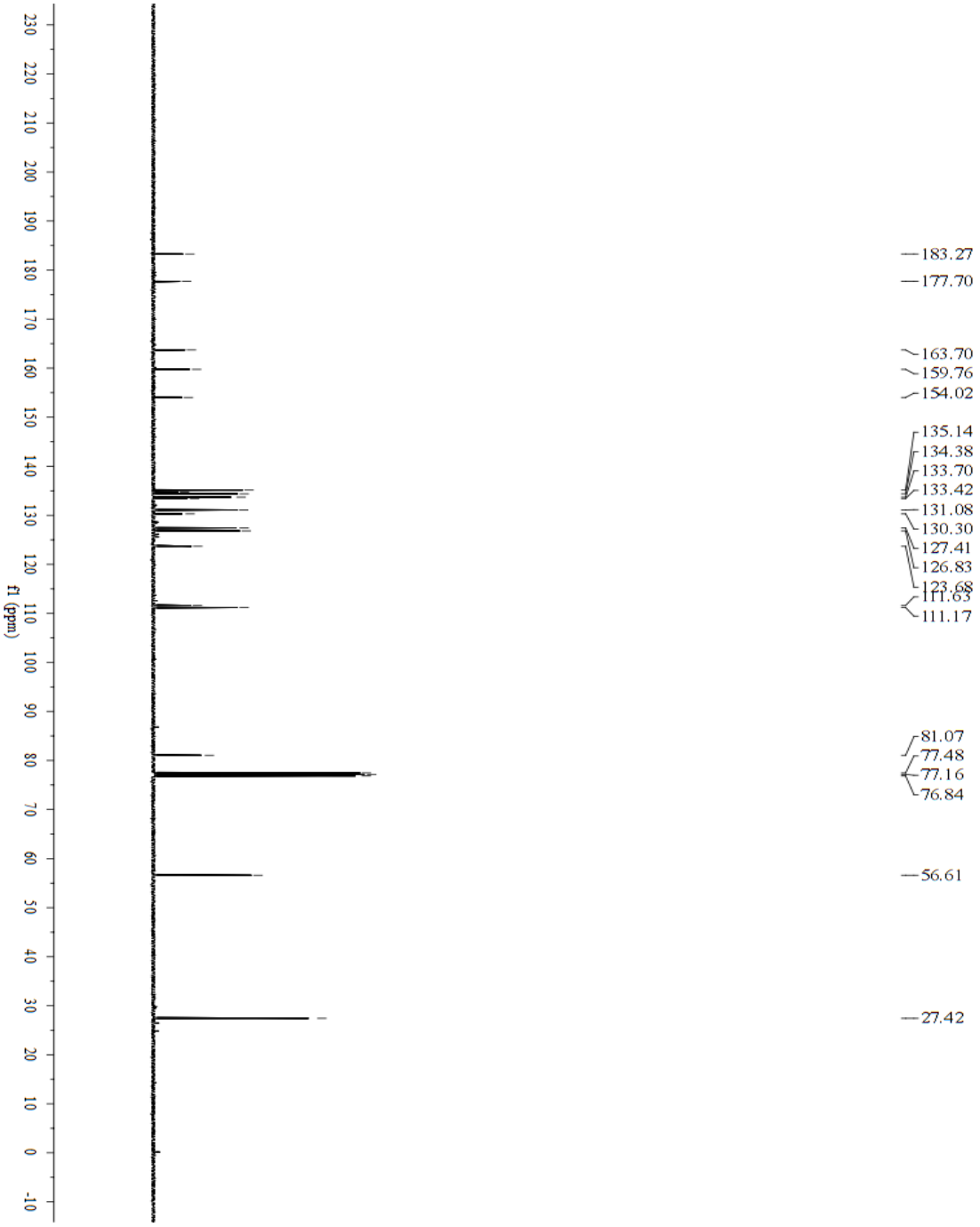
^{1}H NMR (400 MHz, $CDCl_3$)



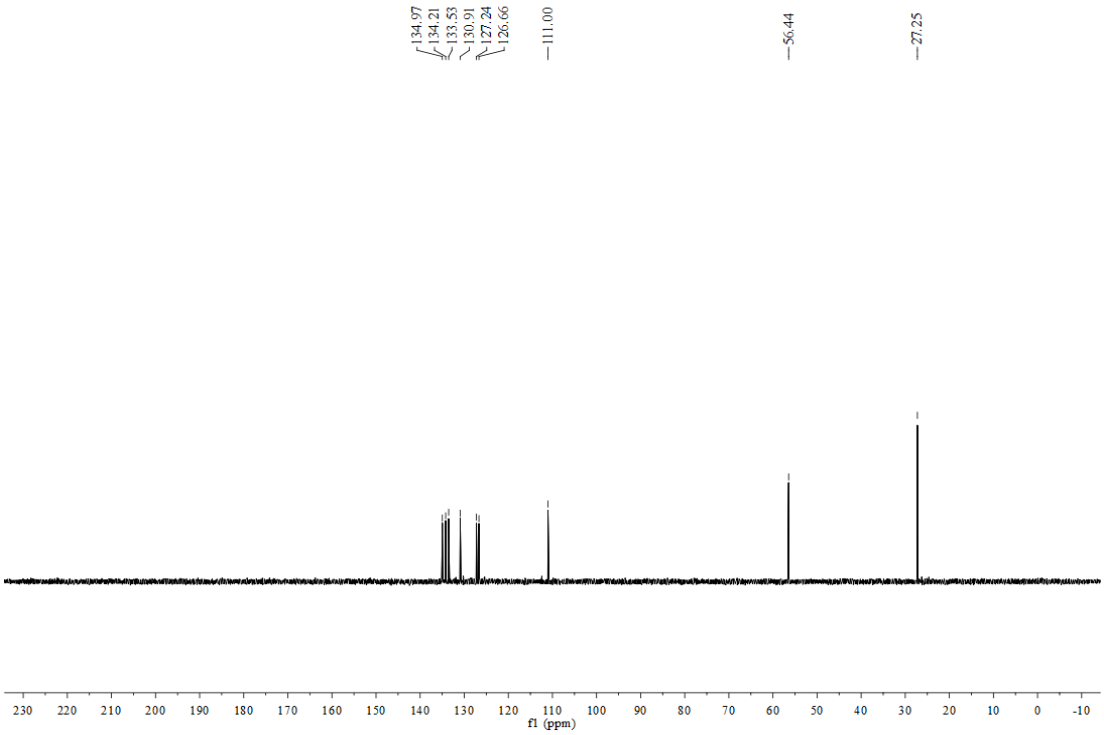


5a

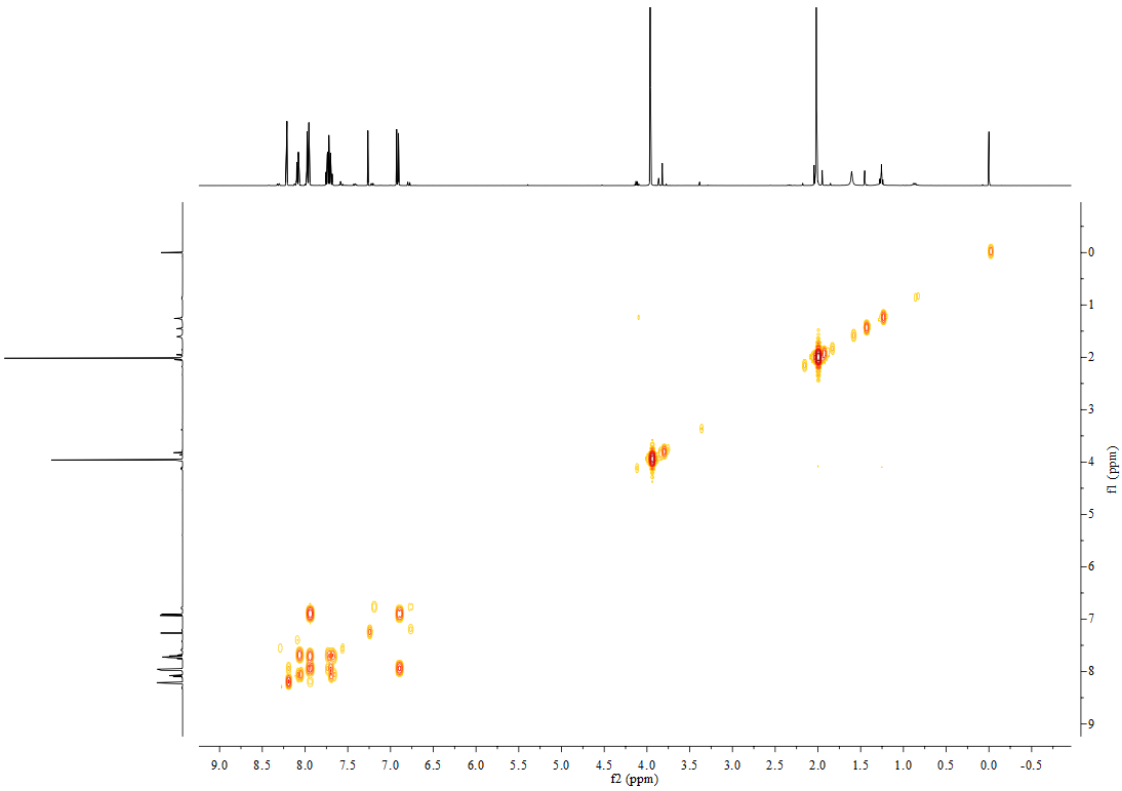
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



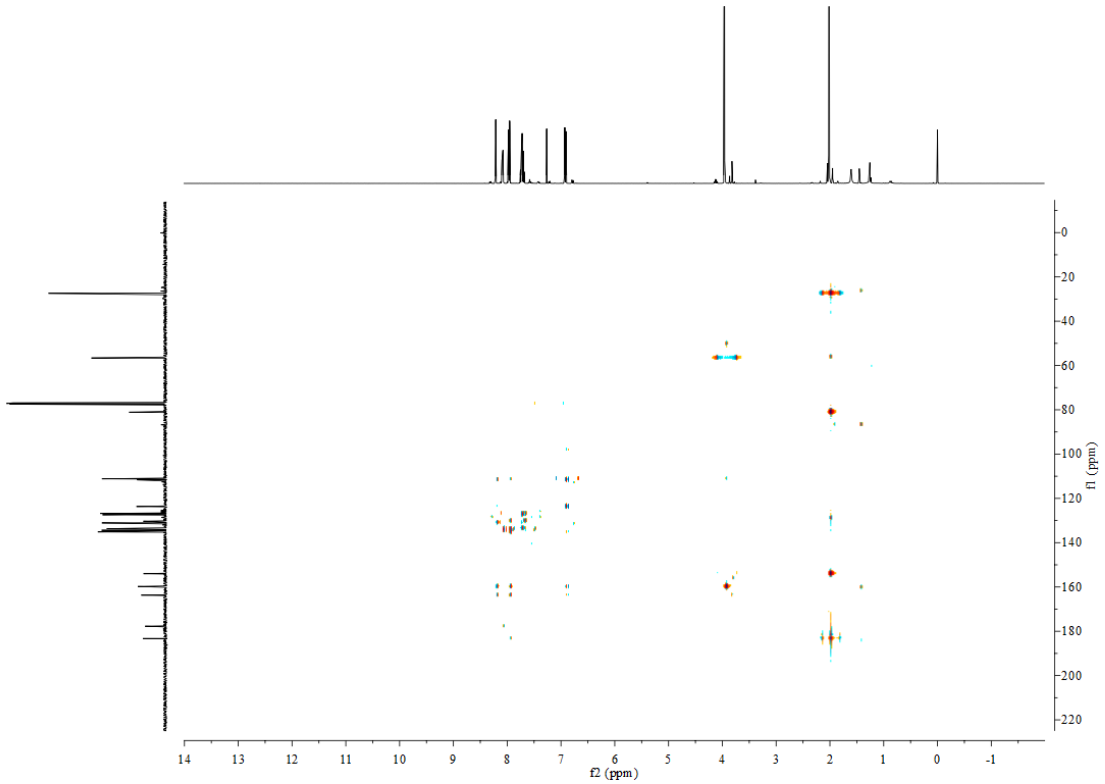
5a-DEPT



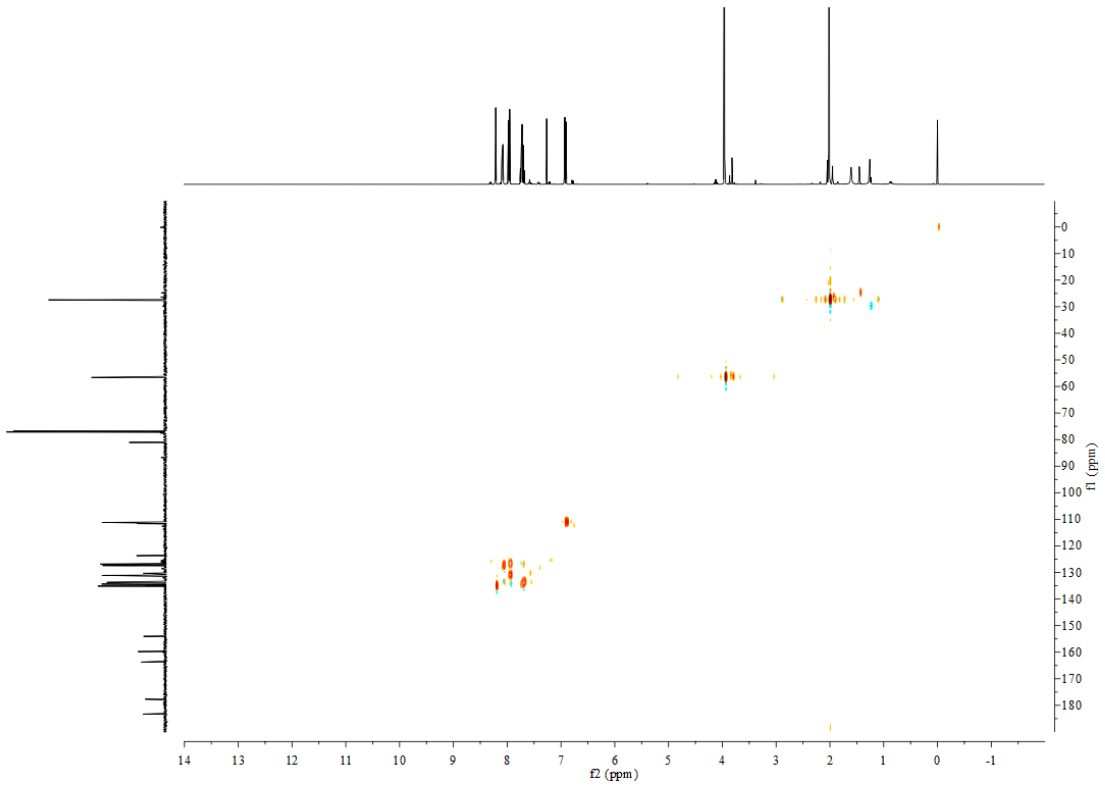
5a- ^{1}H-^{1}H COSY

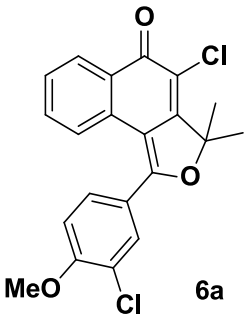


5a- HMBC



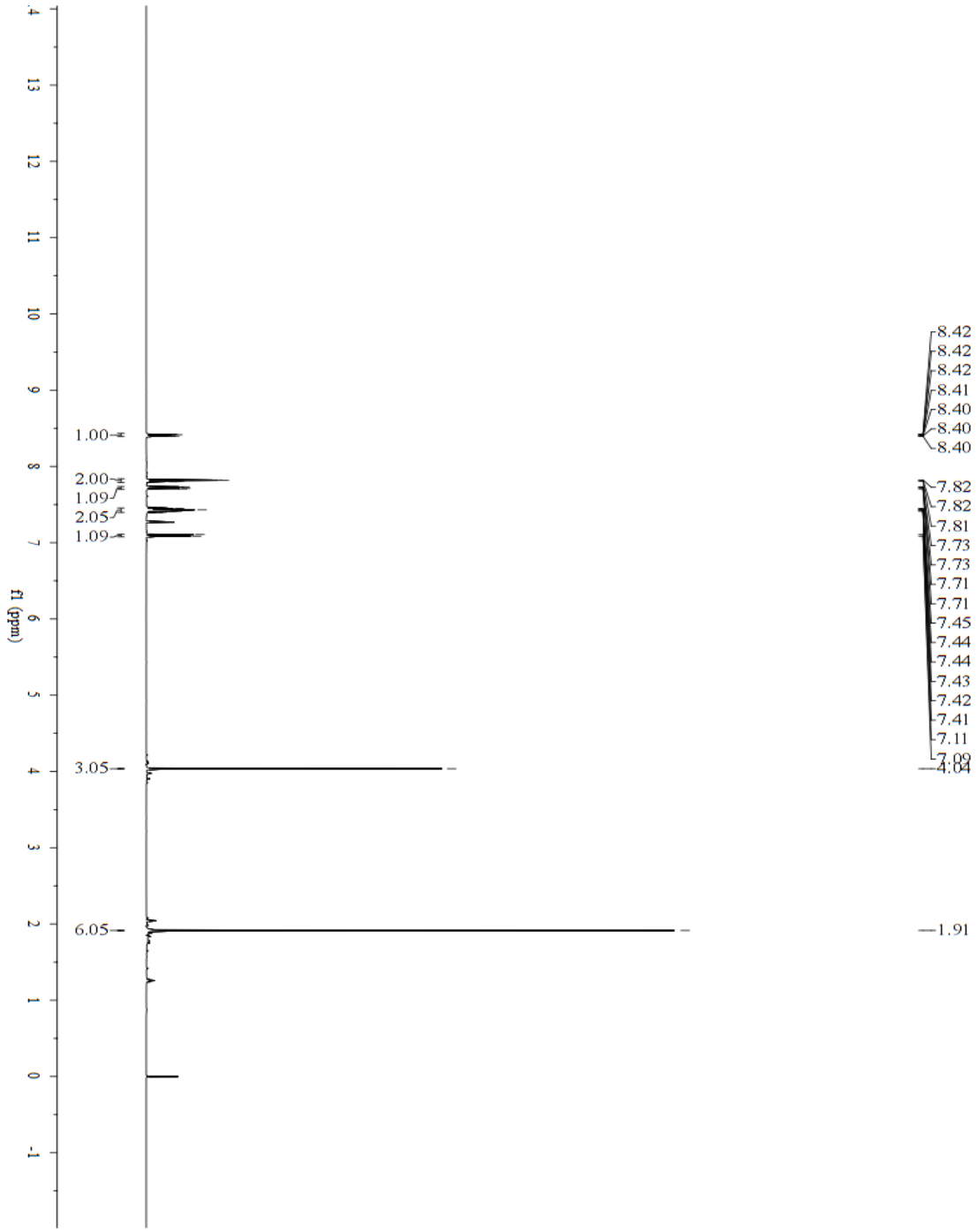
5a- HSQC

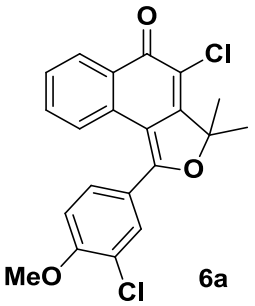




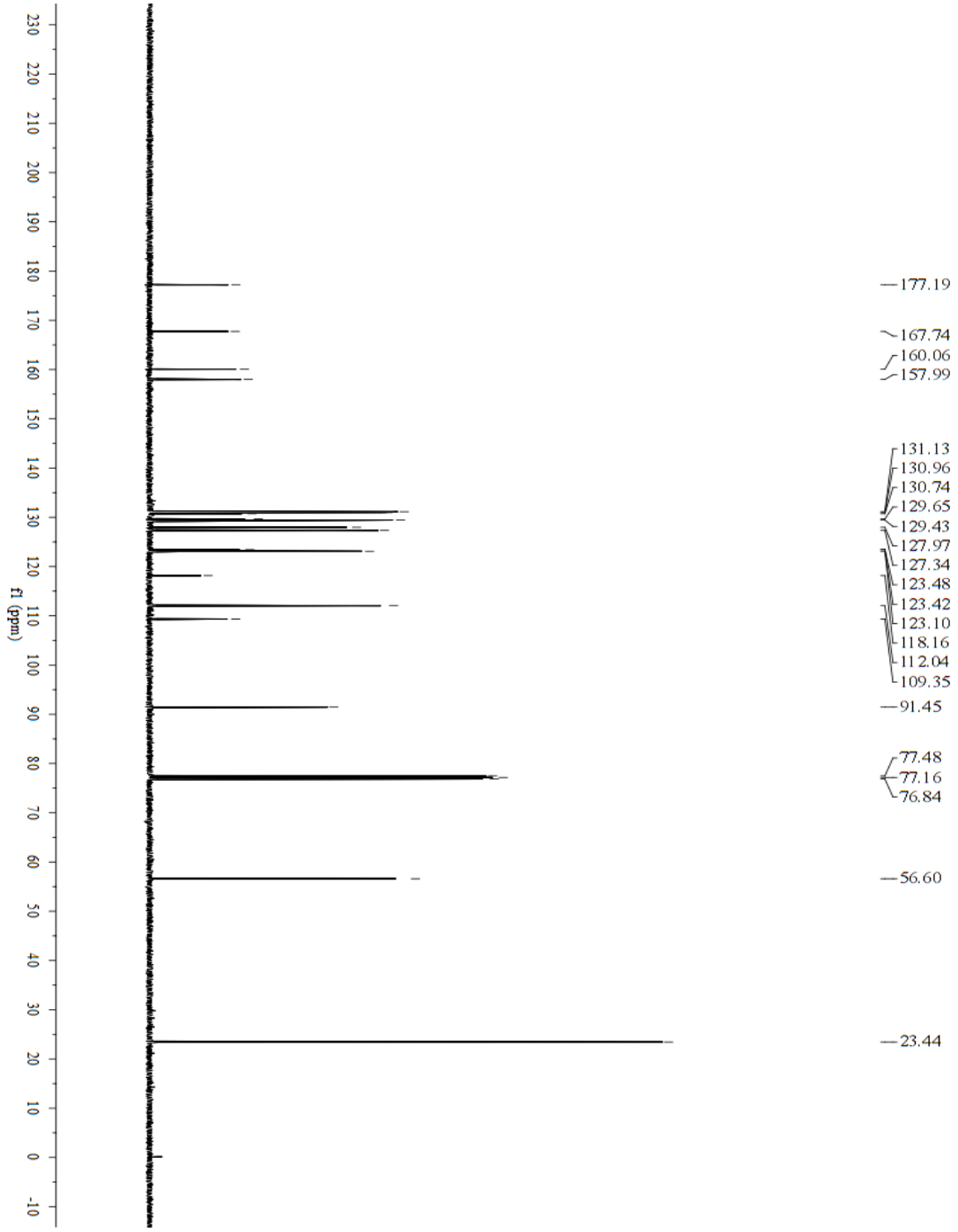
6a

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

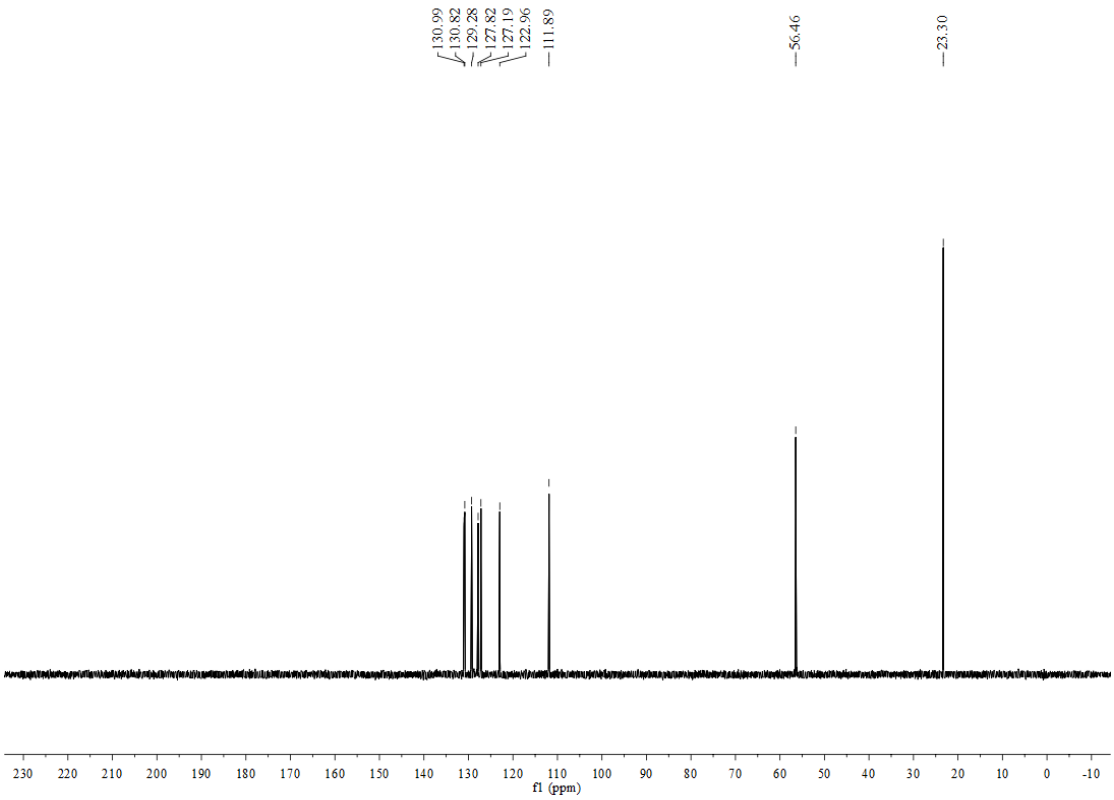




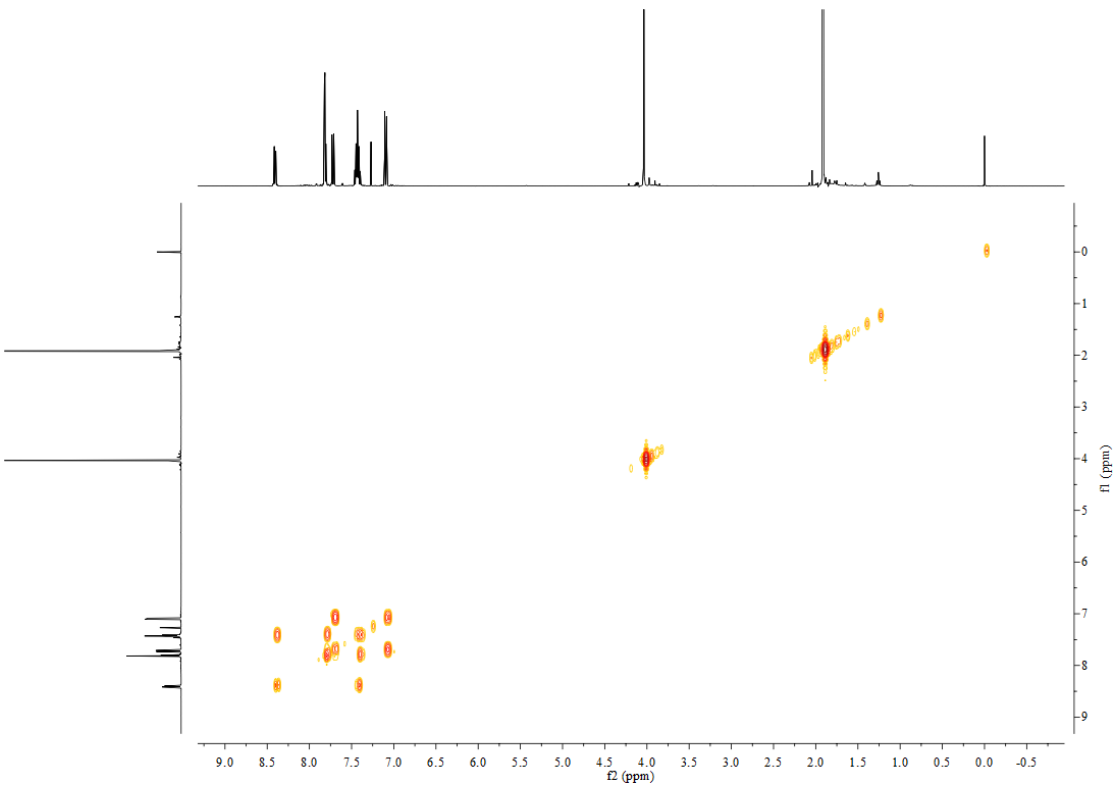
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)



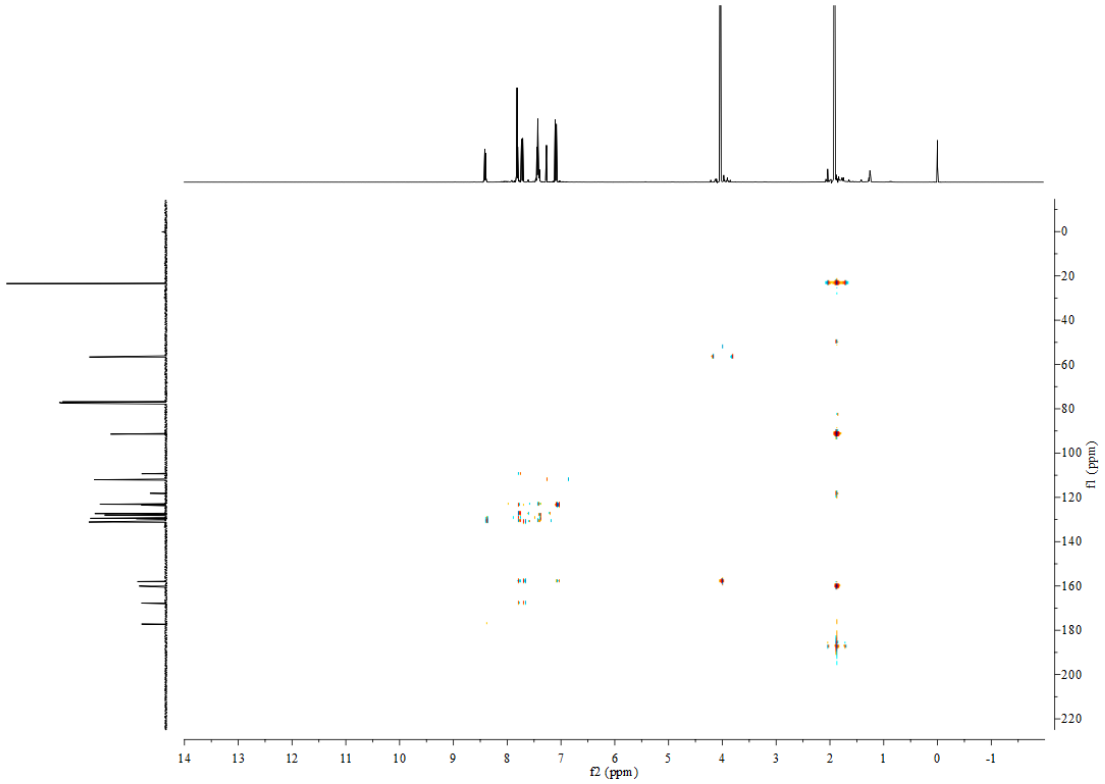
6a-DEPT



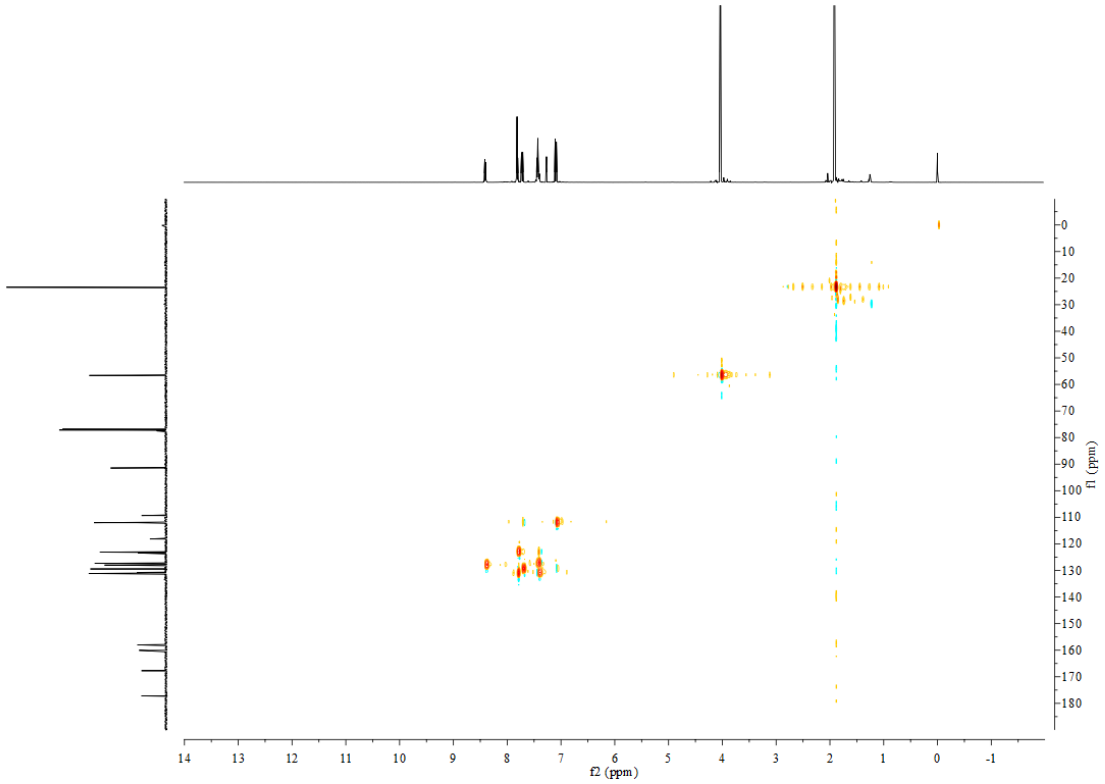
6a- ^{1}H-^{1}H COSY

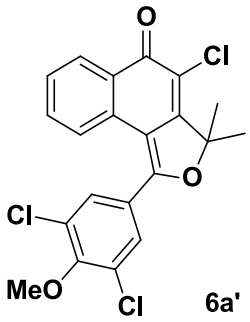


6a- HMBC



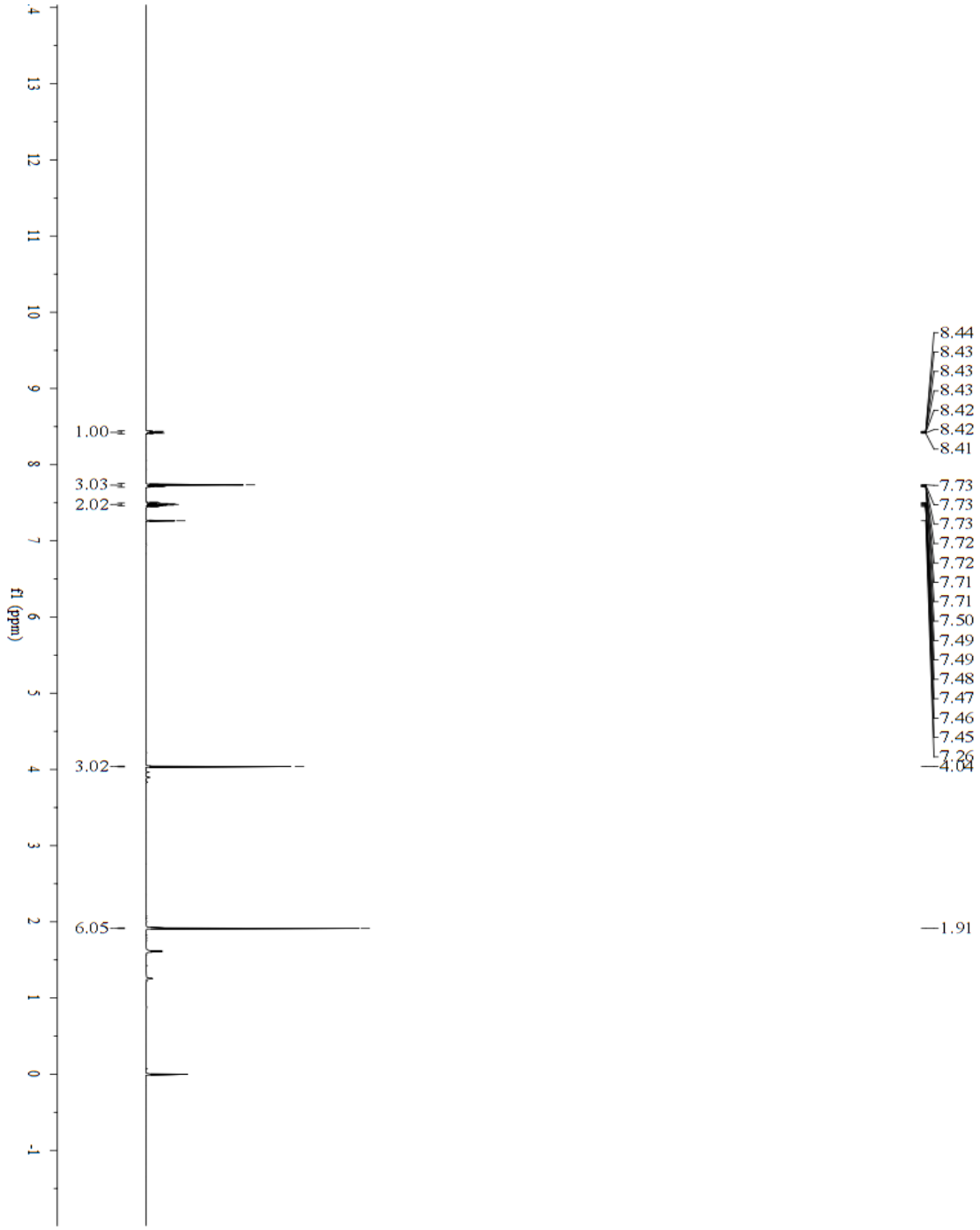
6a- HSQC

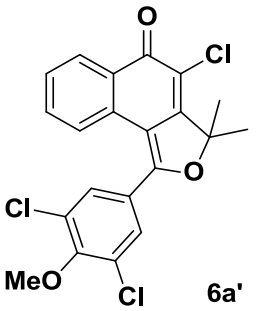




6a'

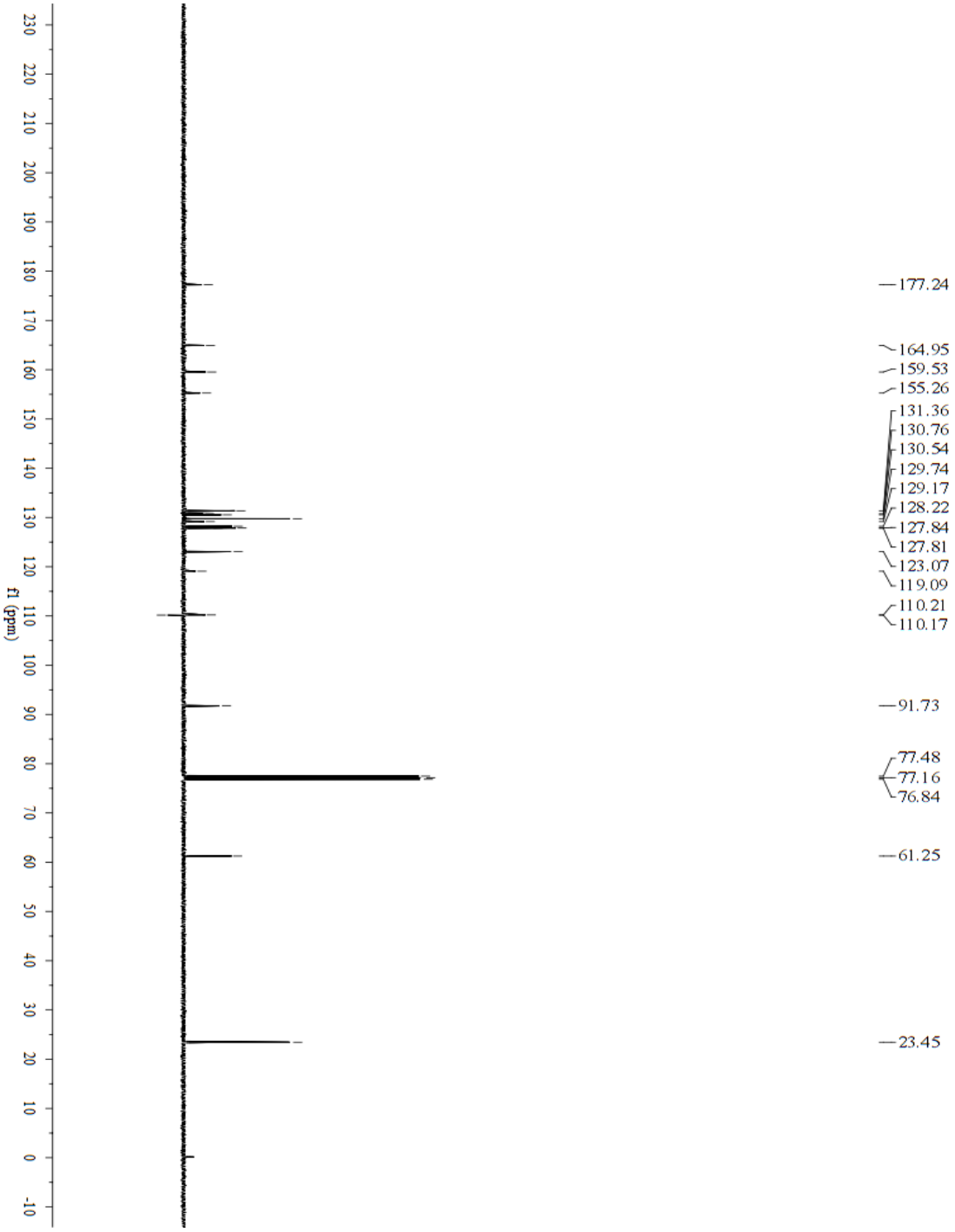
^{1}H NMR (400 MHz, $CDCl_3$)



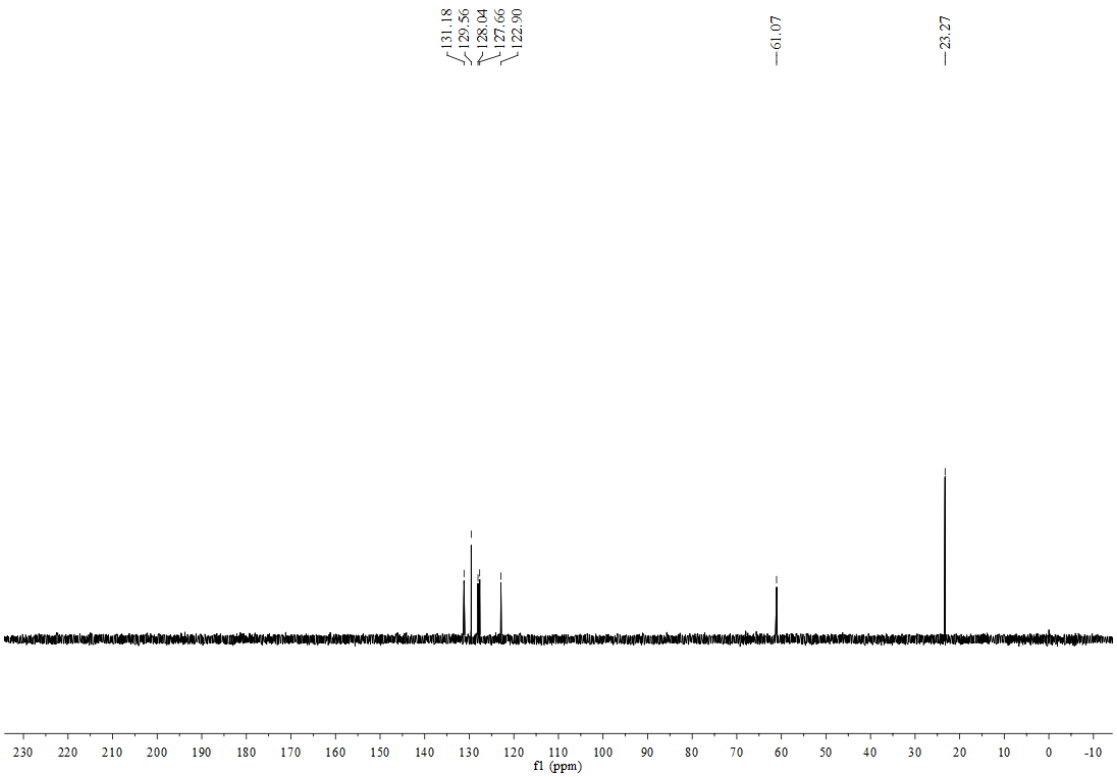


6a'

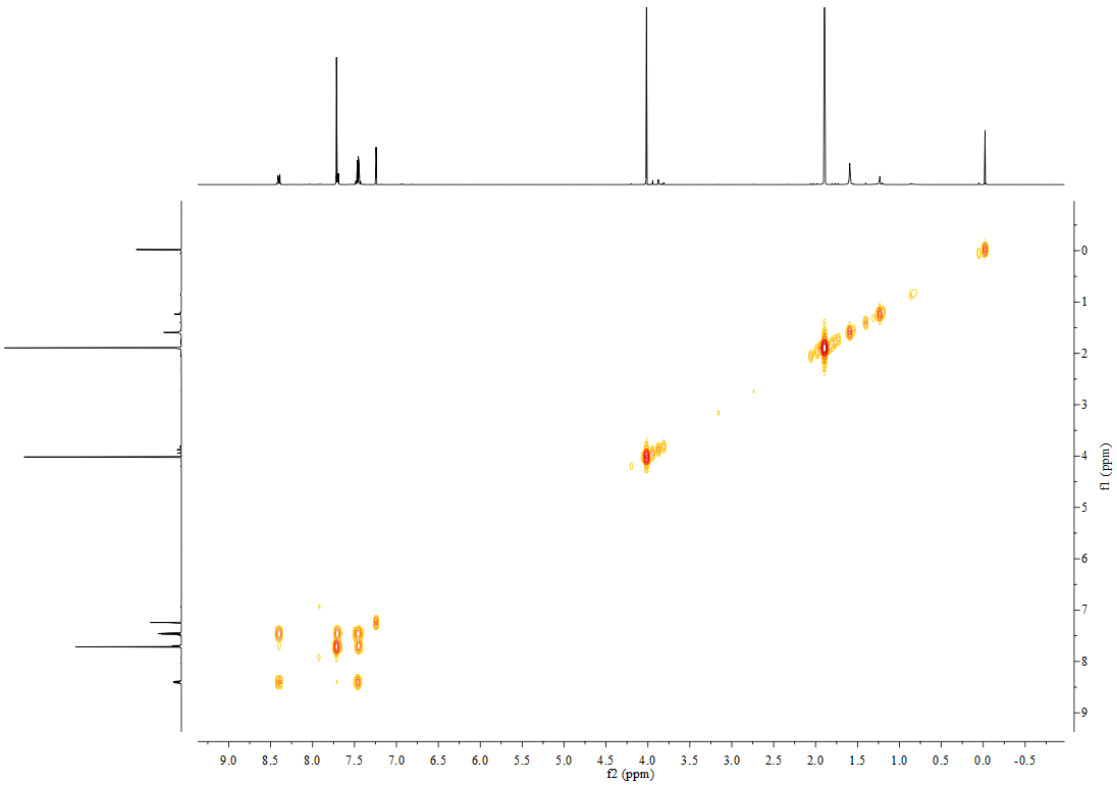
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



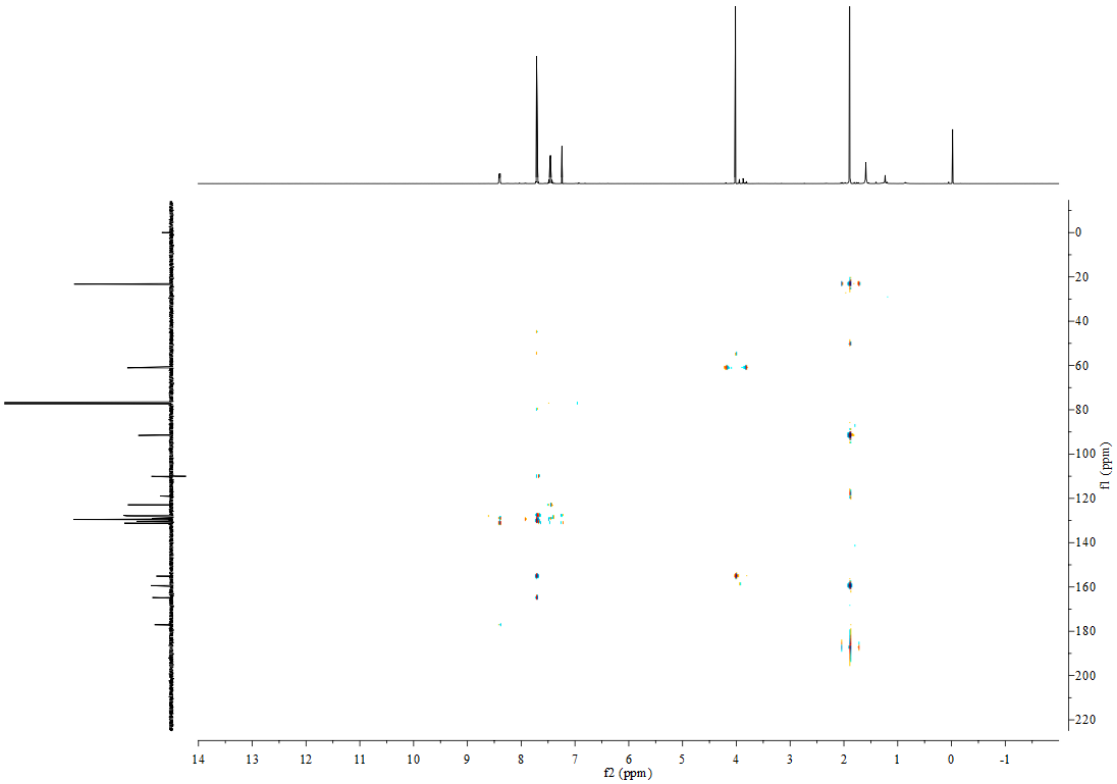
6a'-DEPT



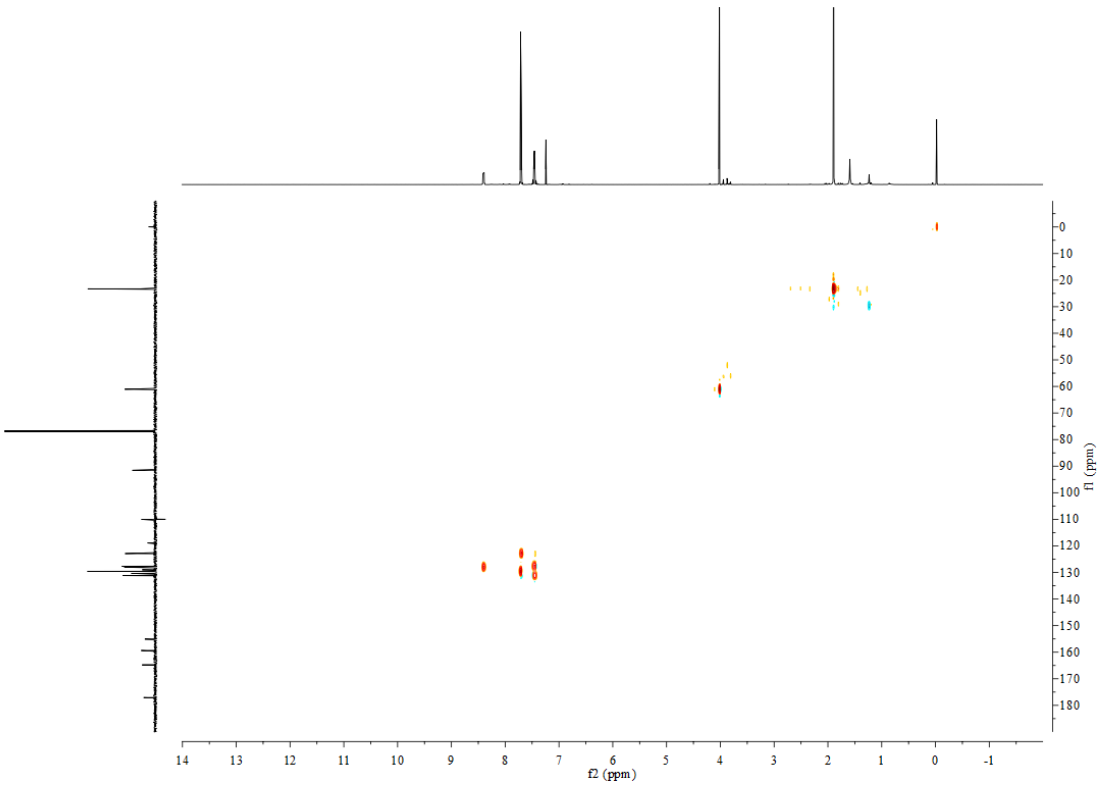
6a'- ^{1}H-^{1}H COSY

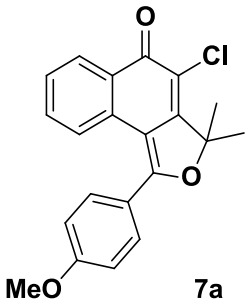


6a'- HMBC



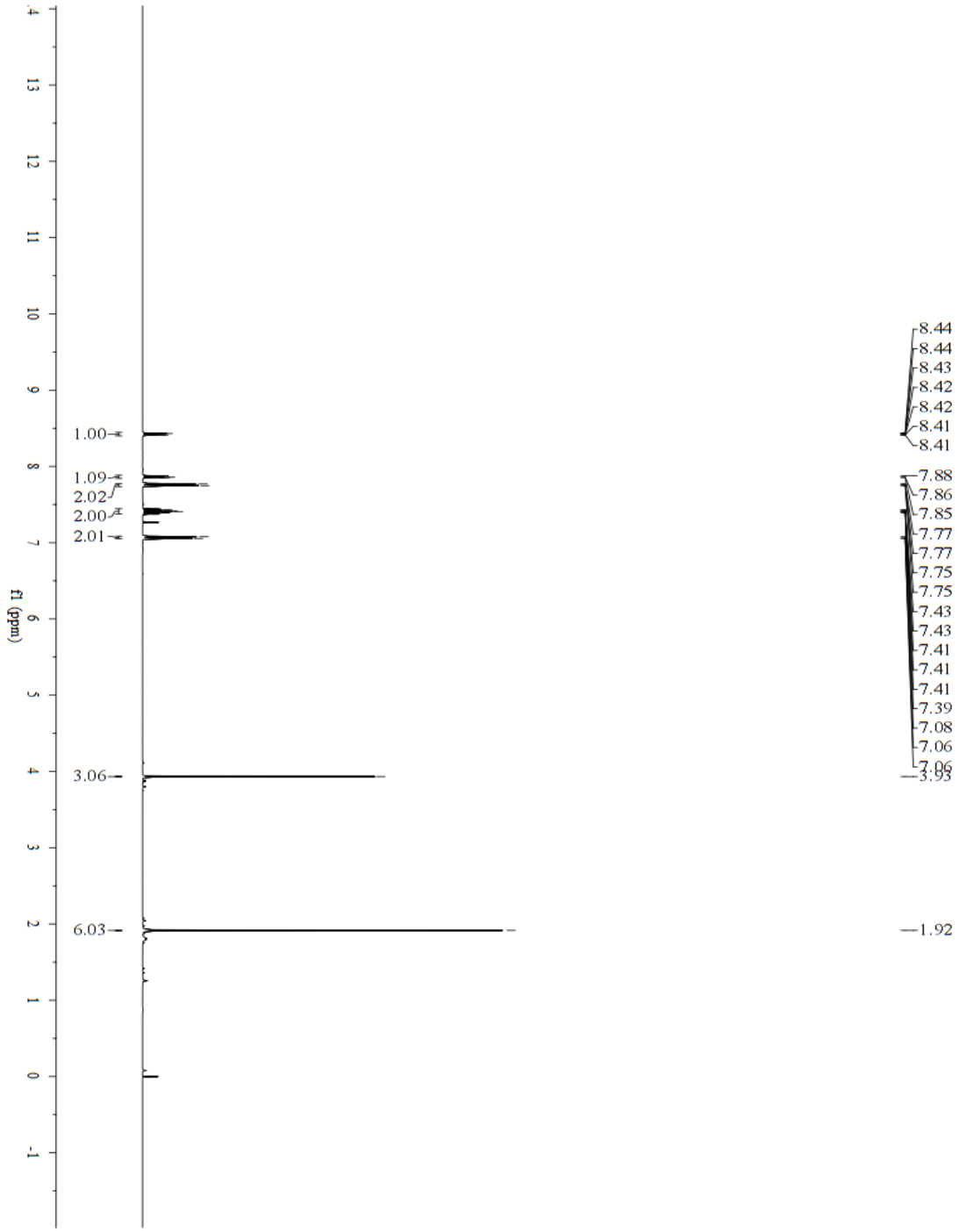
6a'- HSQC

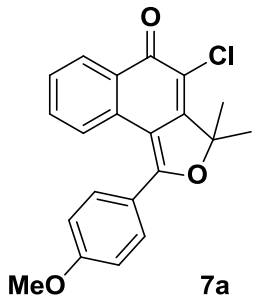




7a

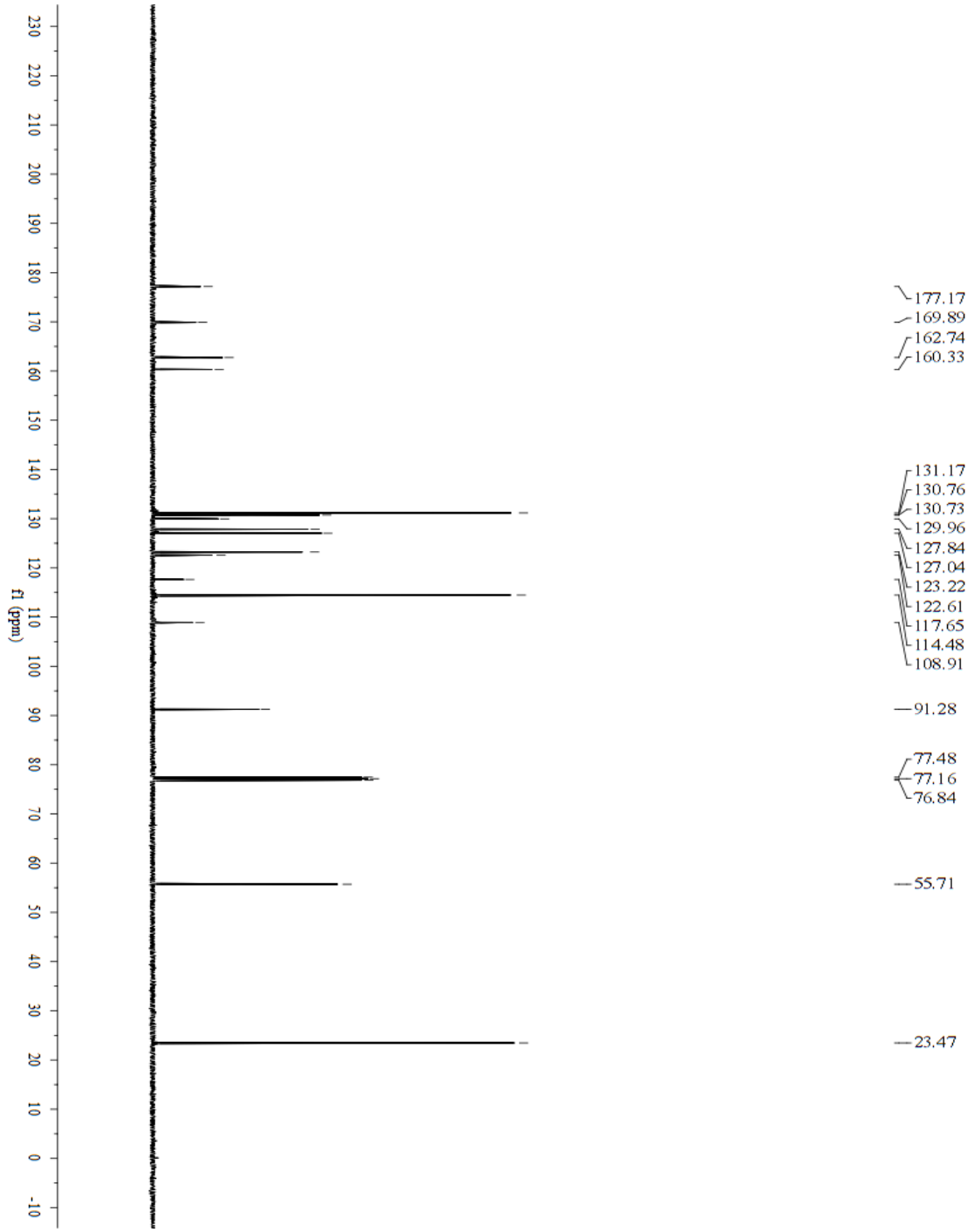
^{1}H NMR (400 MHz, $CDCl_3$)

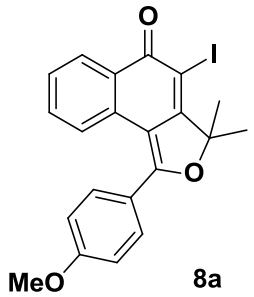




7a

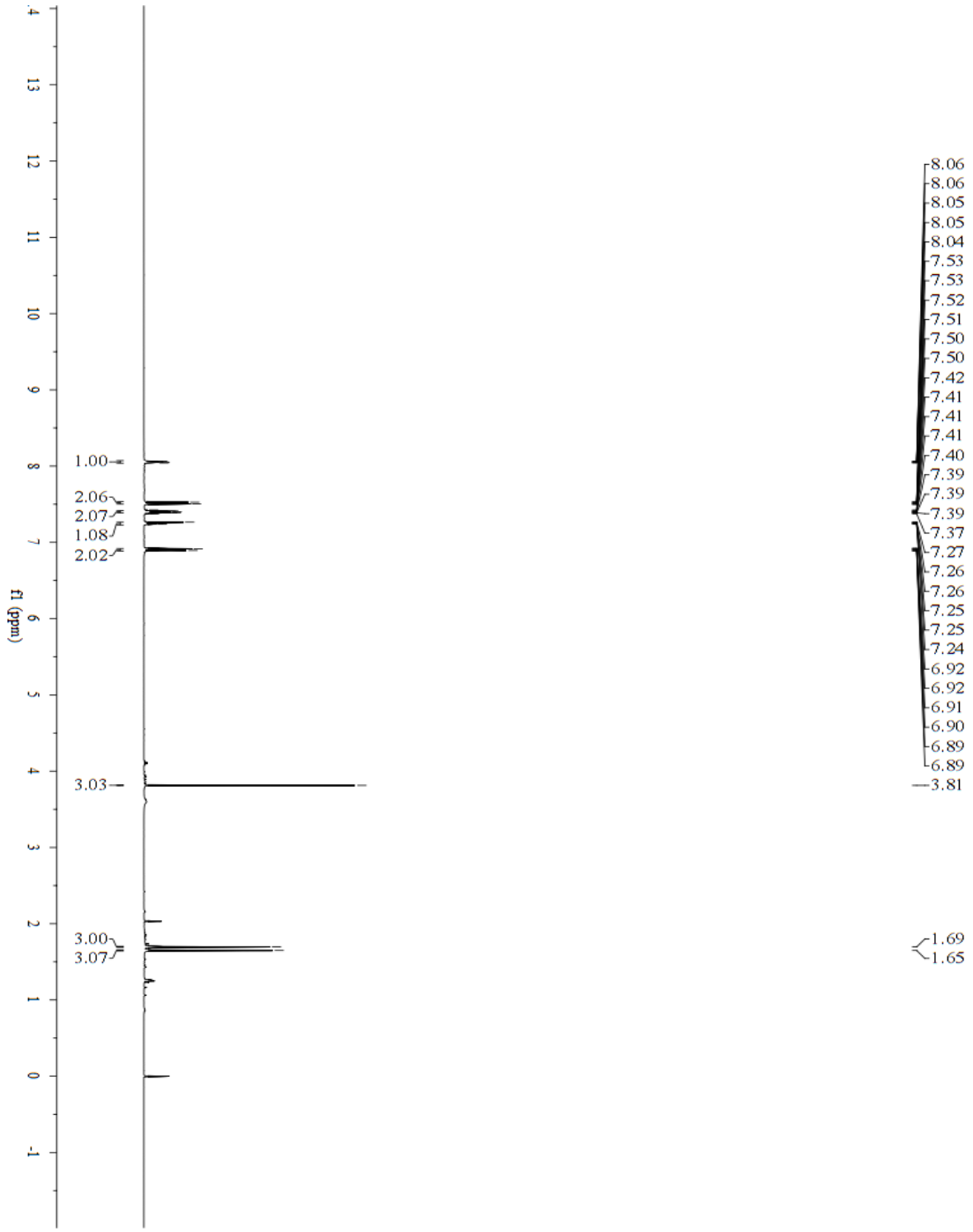
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

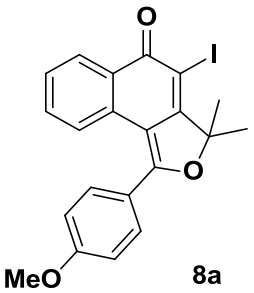




8a

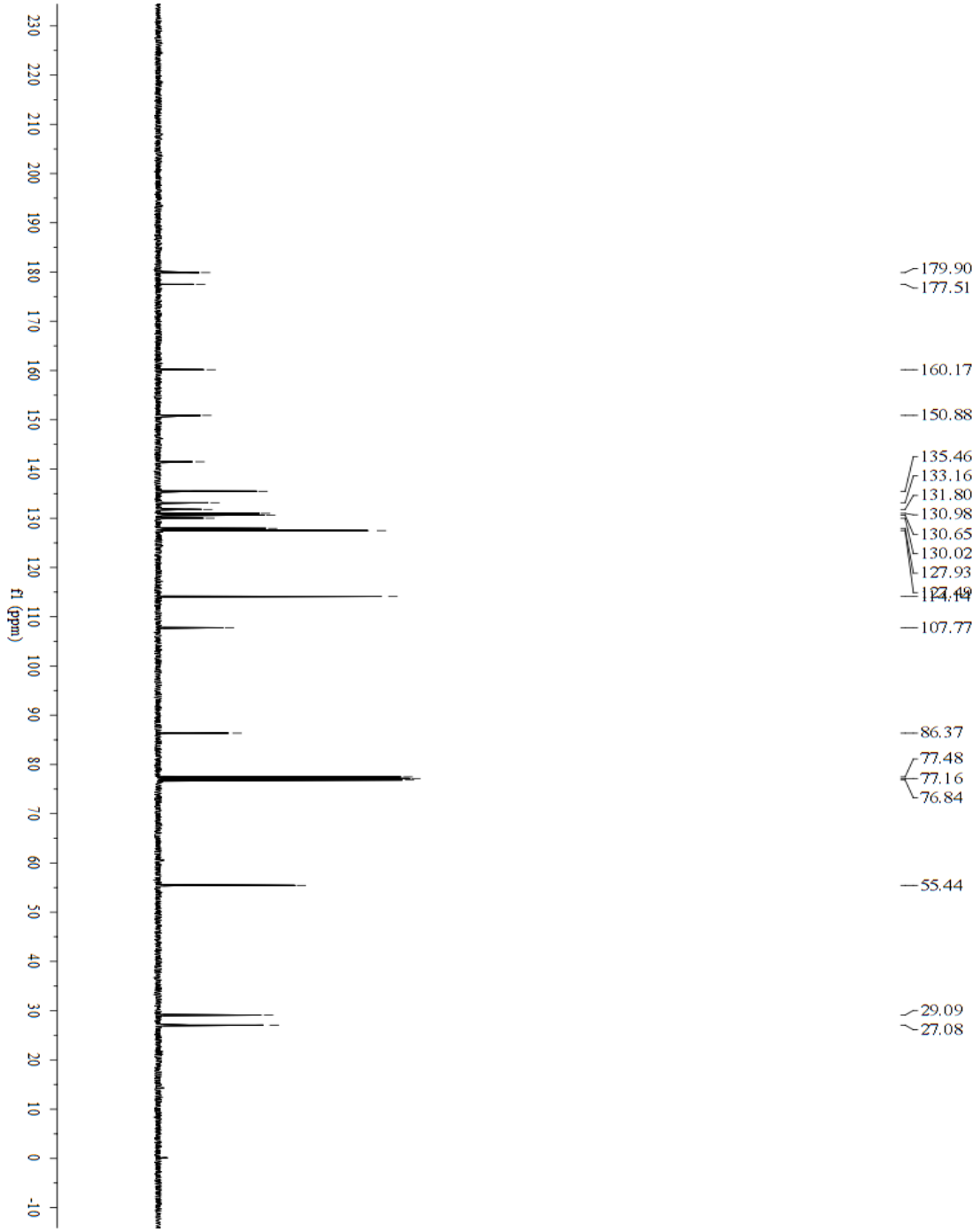
^{1}H NMR (400 MHz, $CDCl_3$)

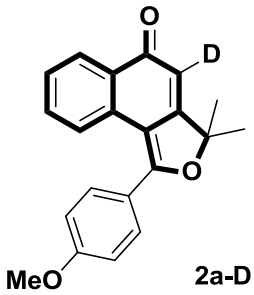




8a

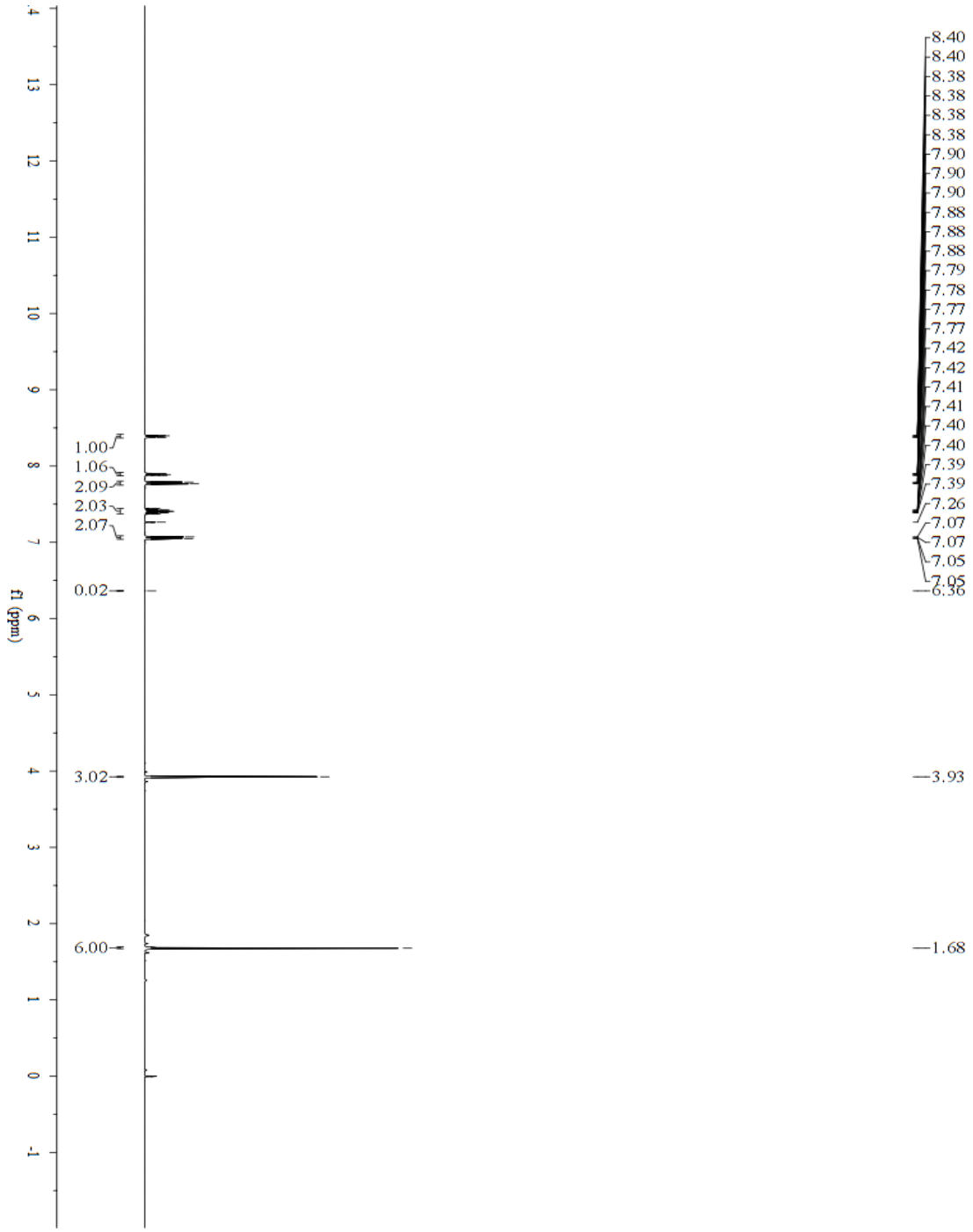
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

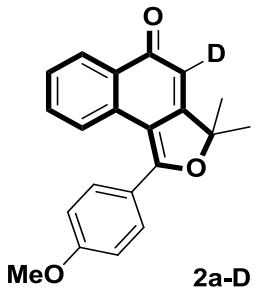




2a-D

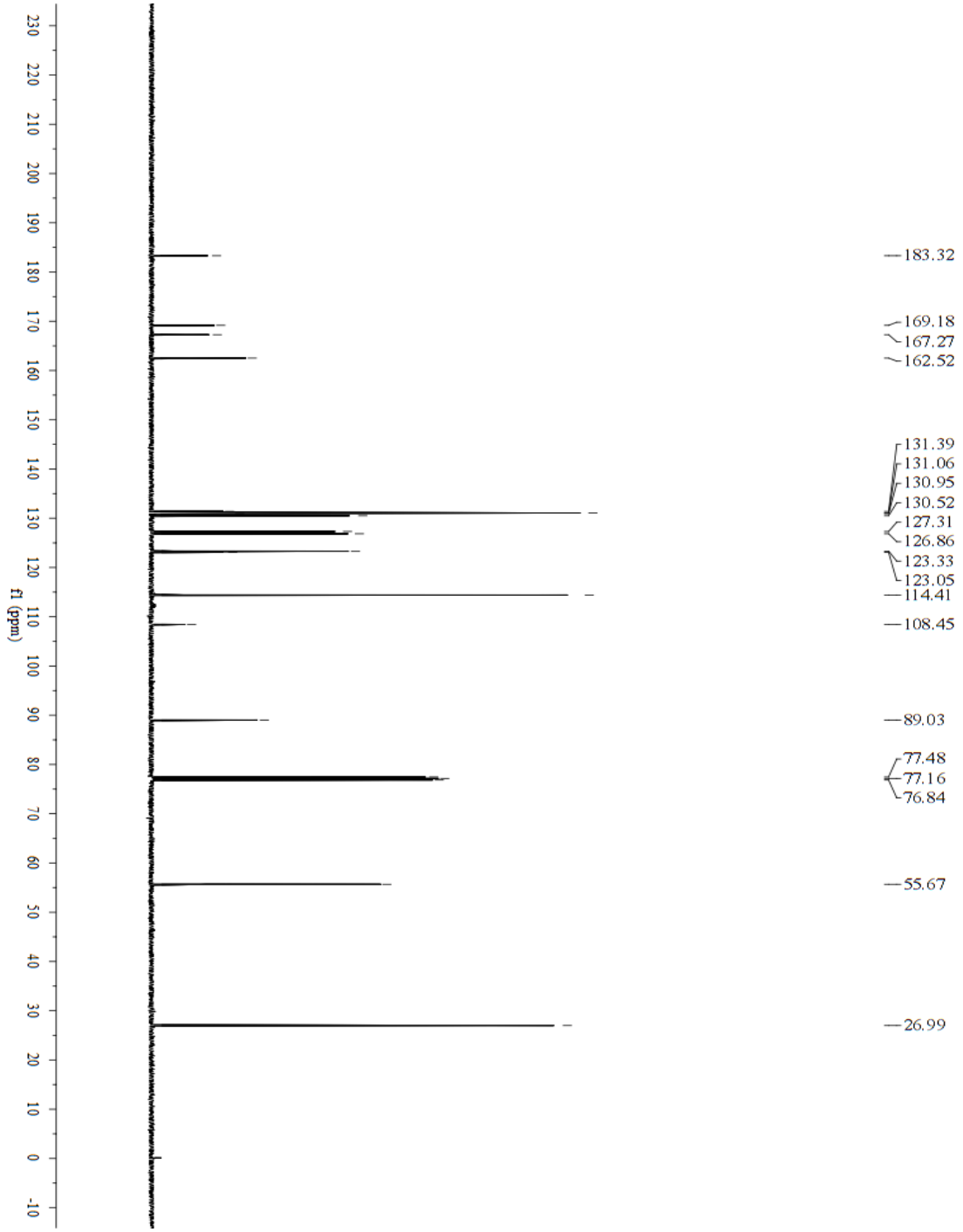
^{1}H NMR (400 MHz, $CDCl_3$)

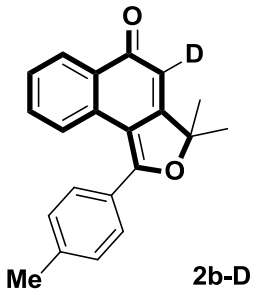




2a-D

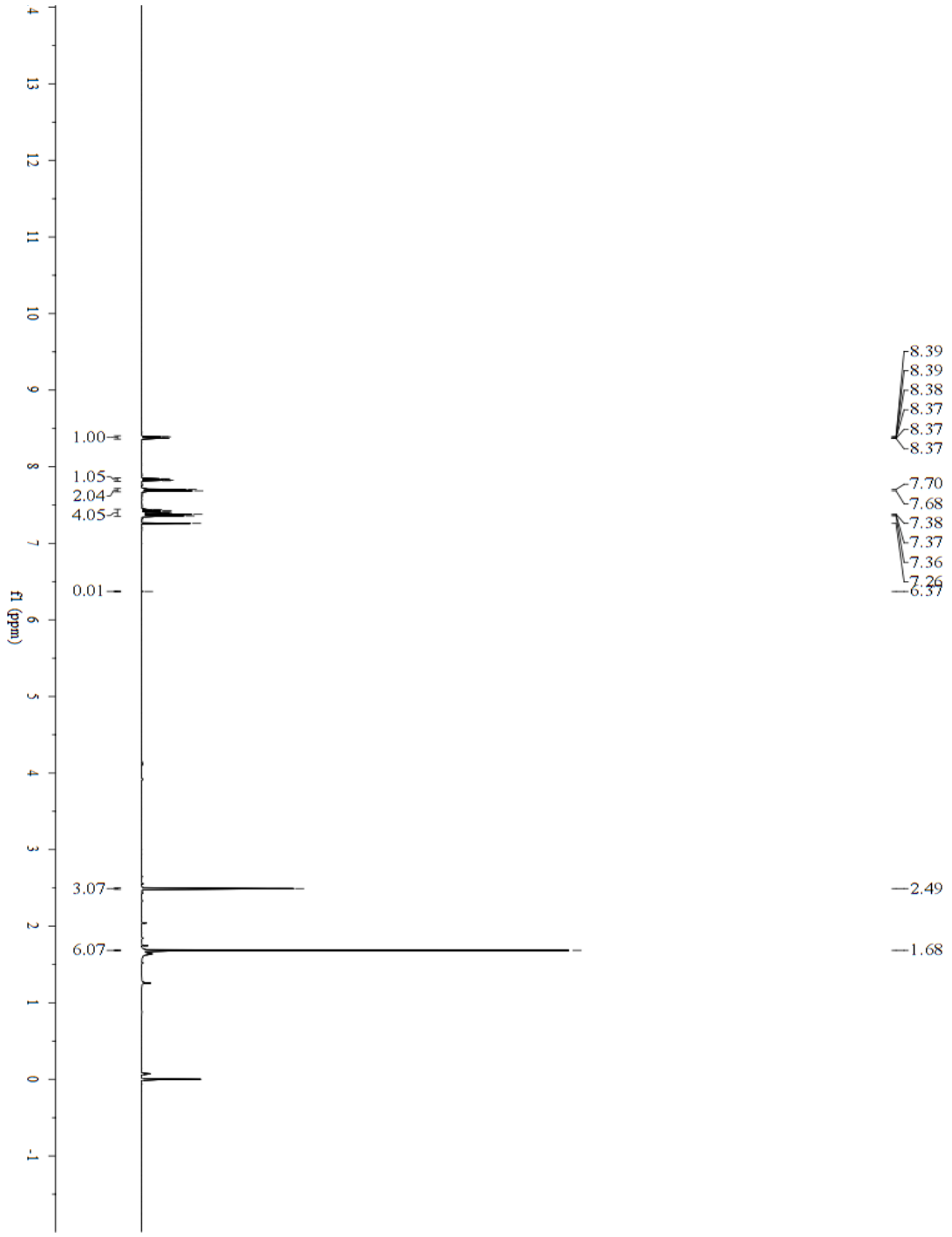
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

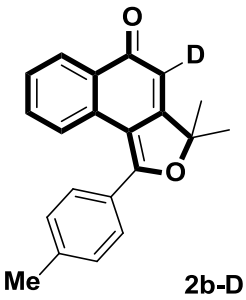




2b-D

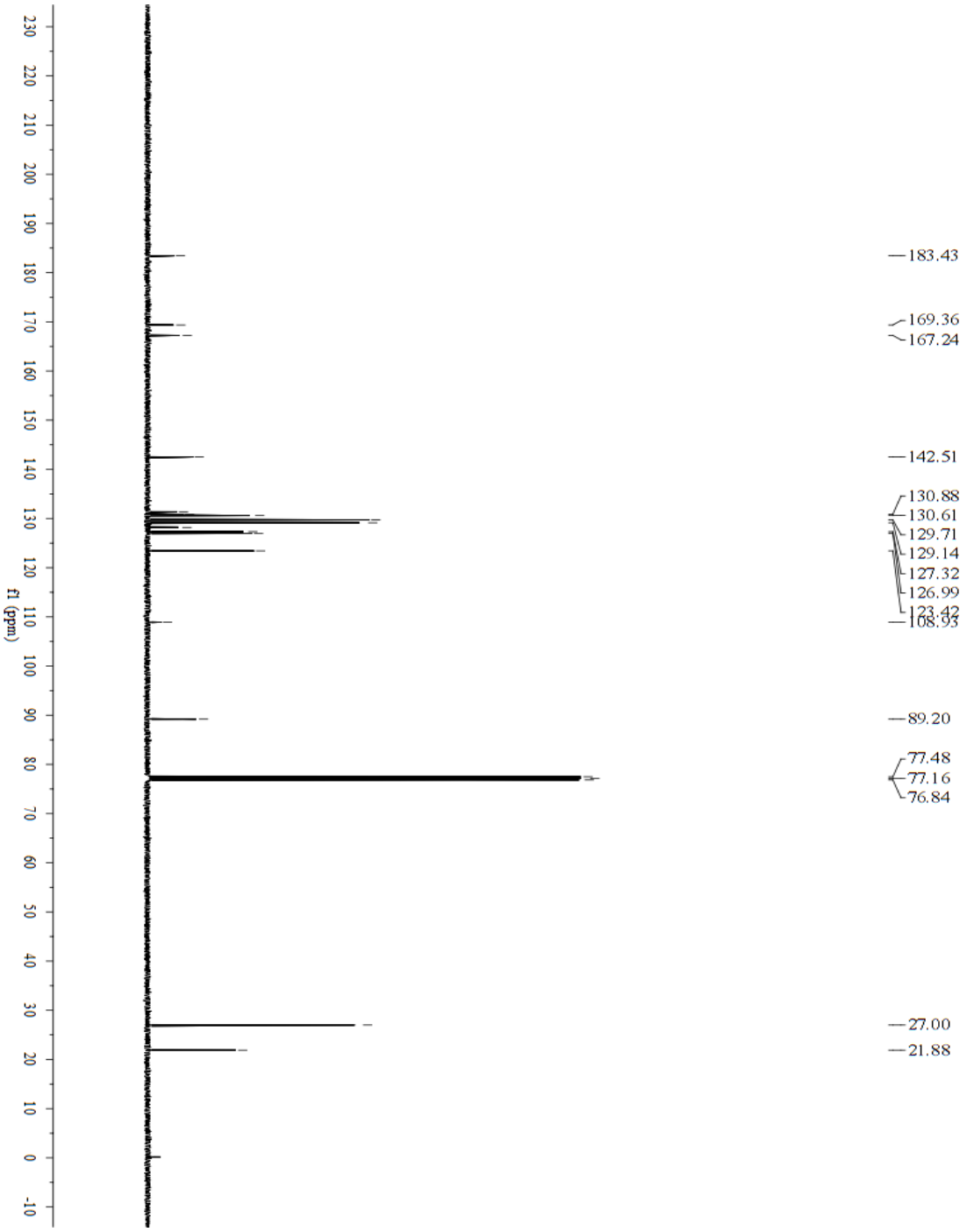
^{1}H NMR (400 MHz, $CDCl_3$)

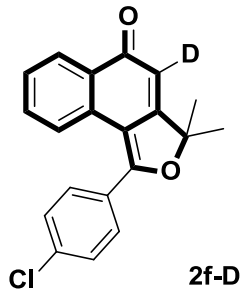




2b-D

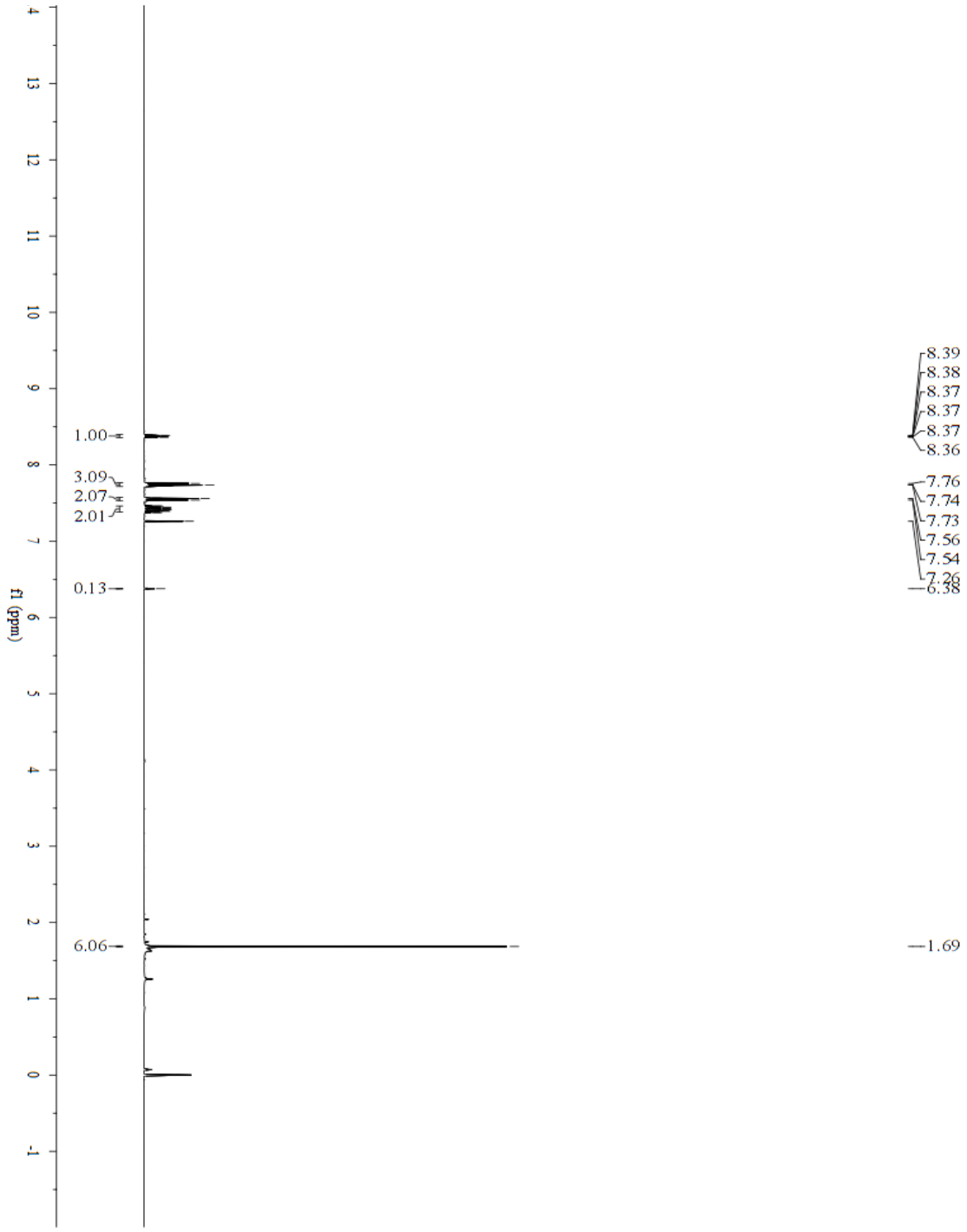
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

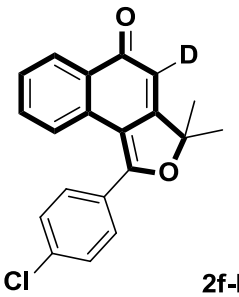




2f-D

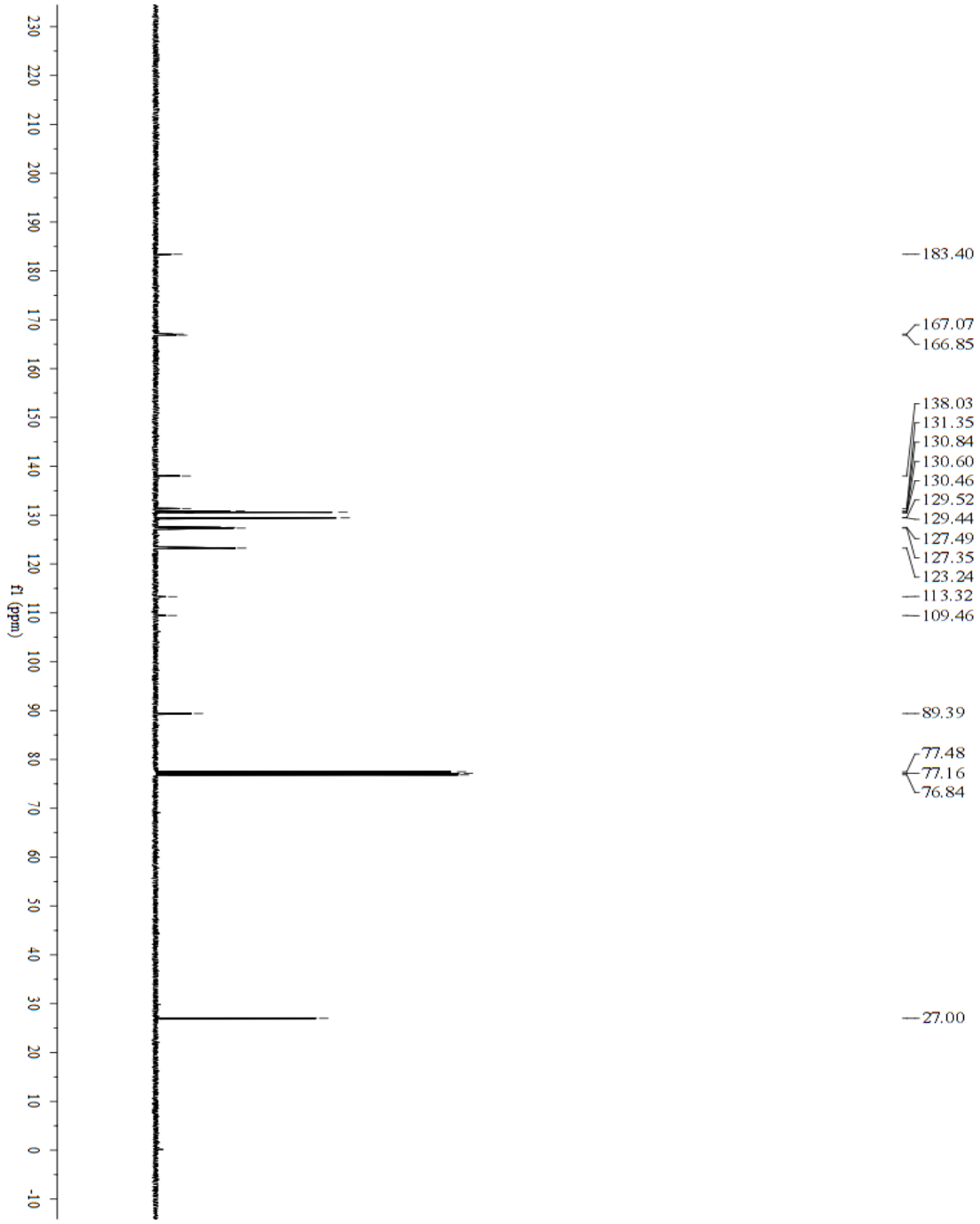
^{1}H NMR (400 MHz, $CDCl_3$)

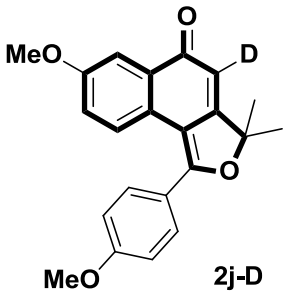




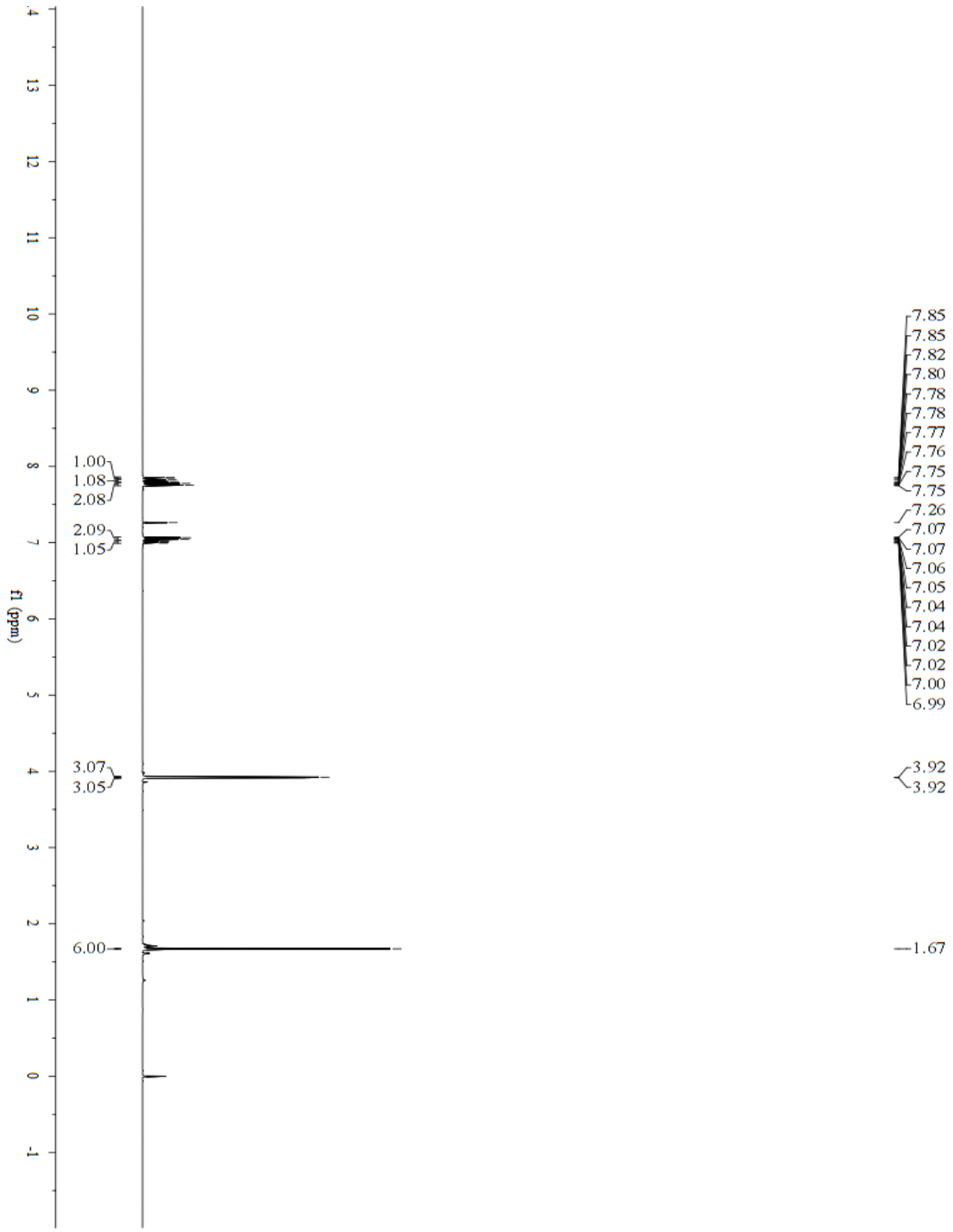
2f-D

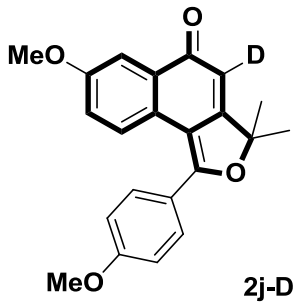
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$)



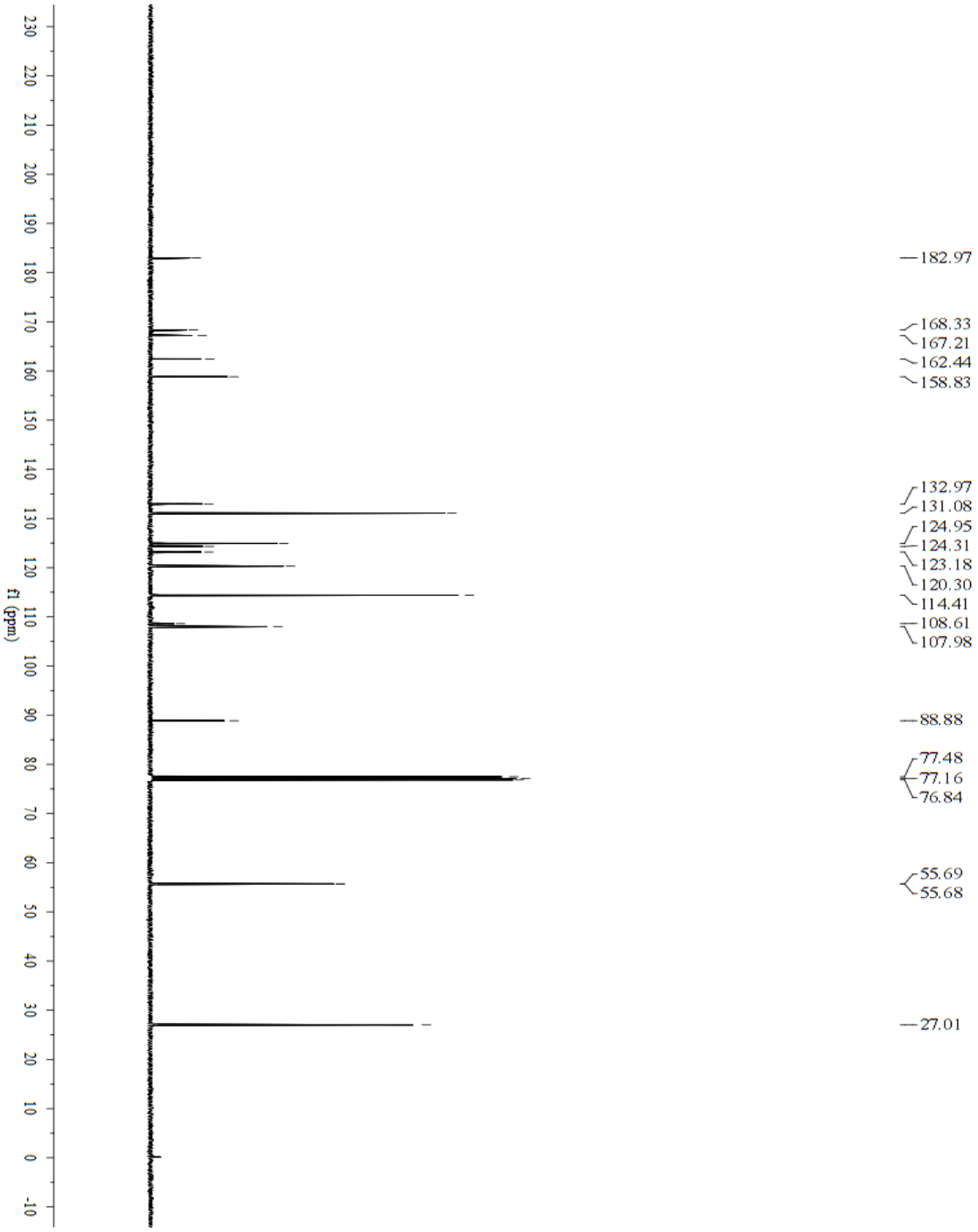


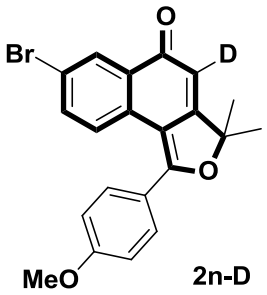
^{1}H NMR (400 MHz, $CDCl_3$)





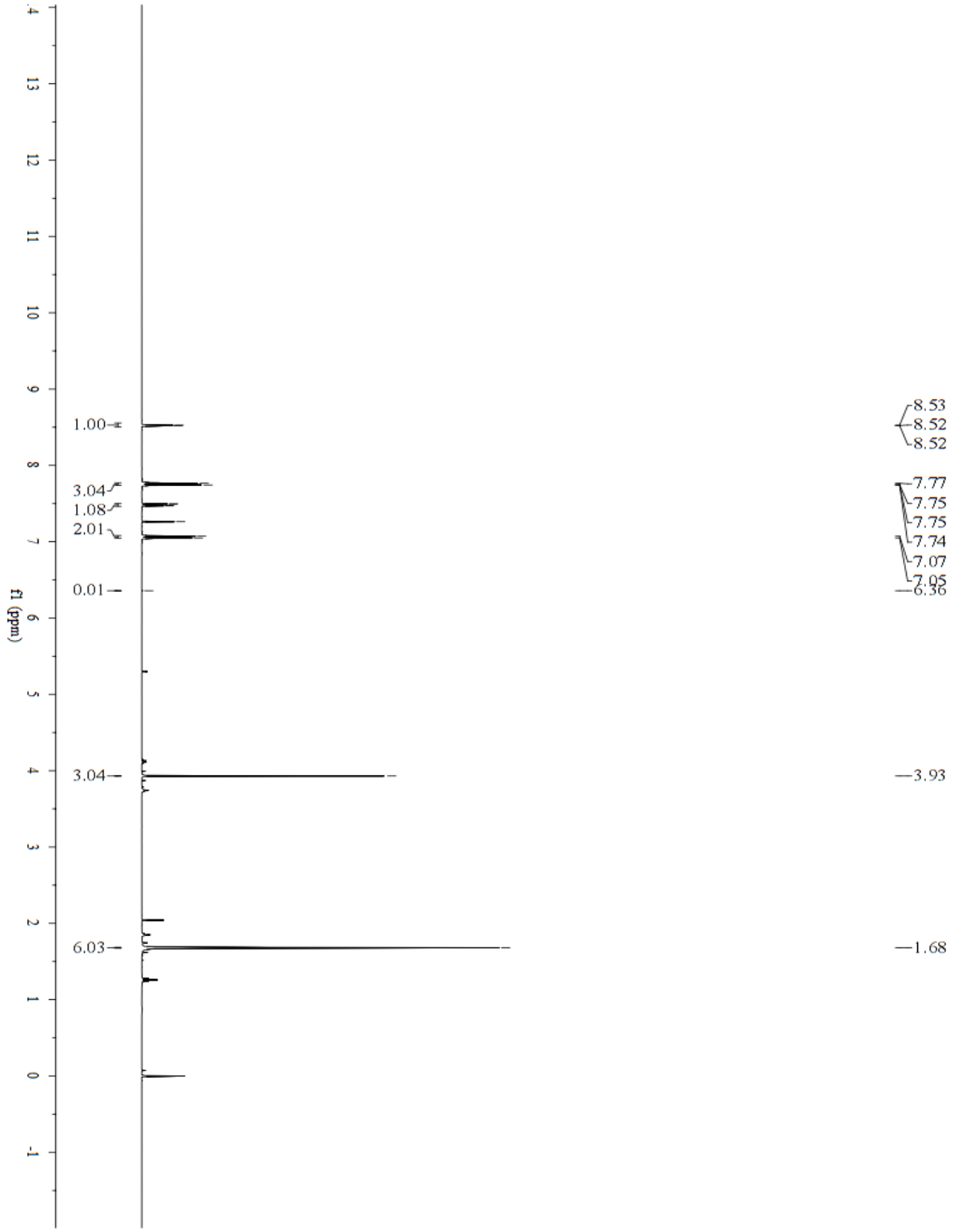
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

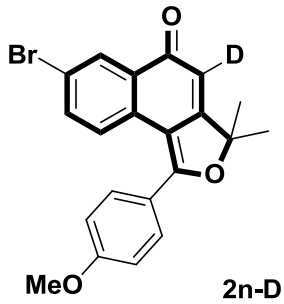




2n-D

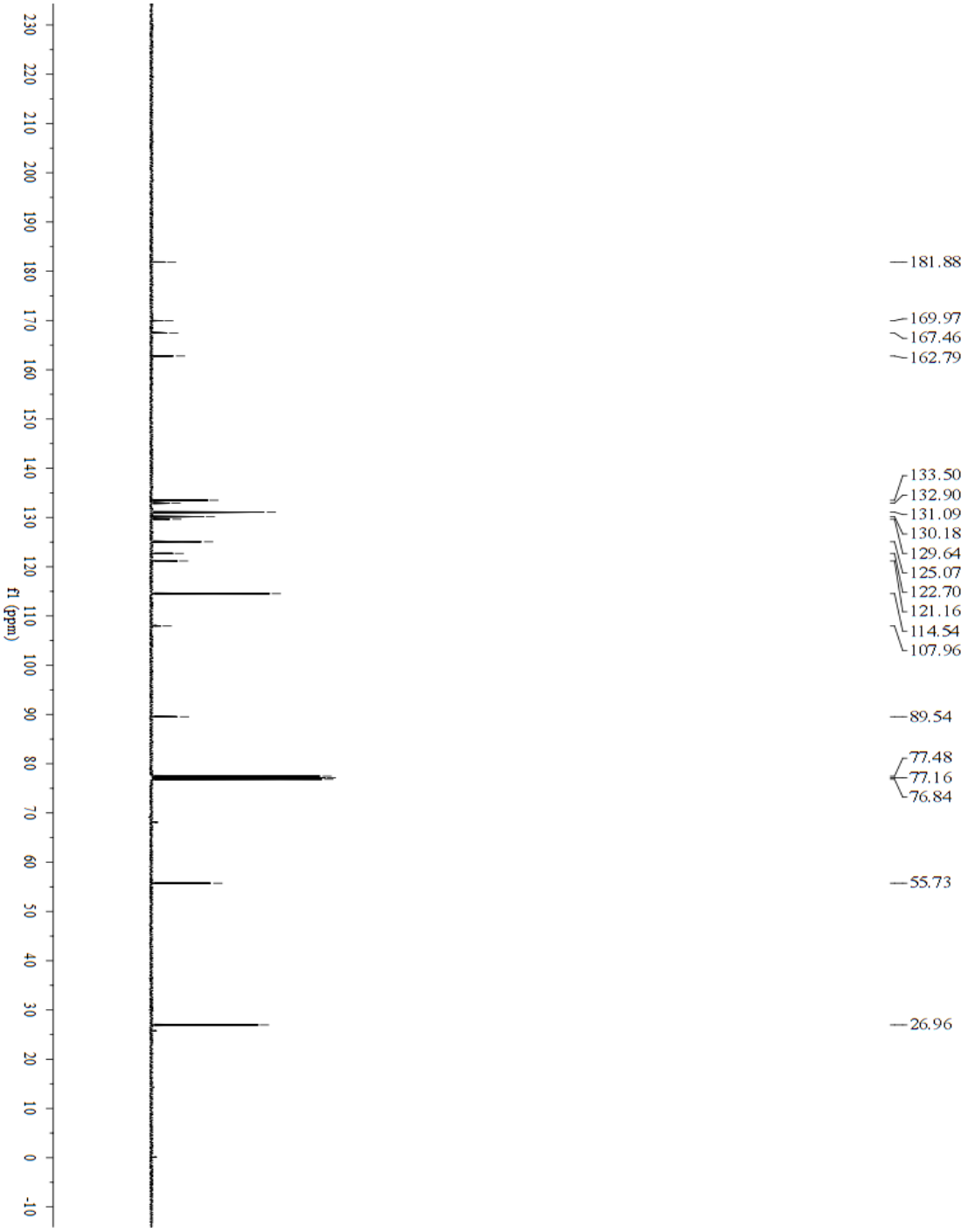
^{1}H NMR (400 MHz, $CDCl_3$)

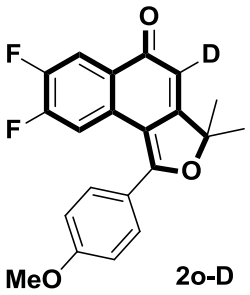




2n-D

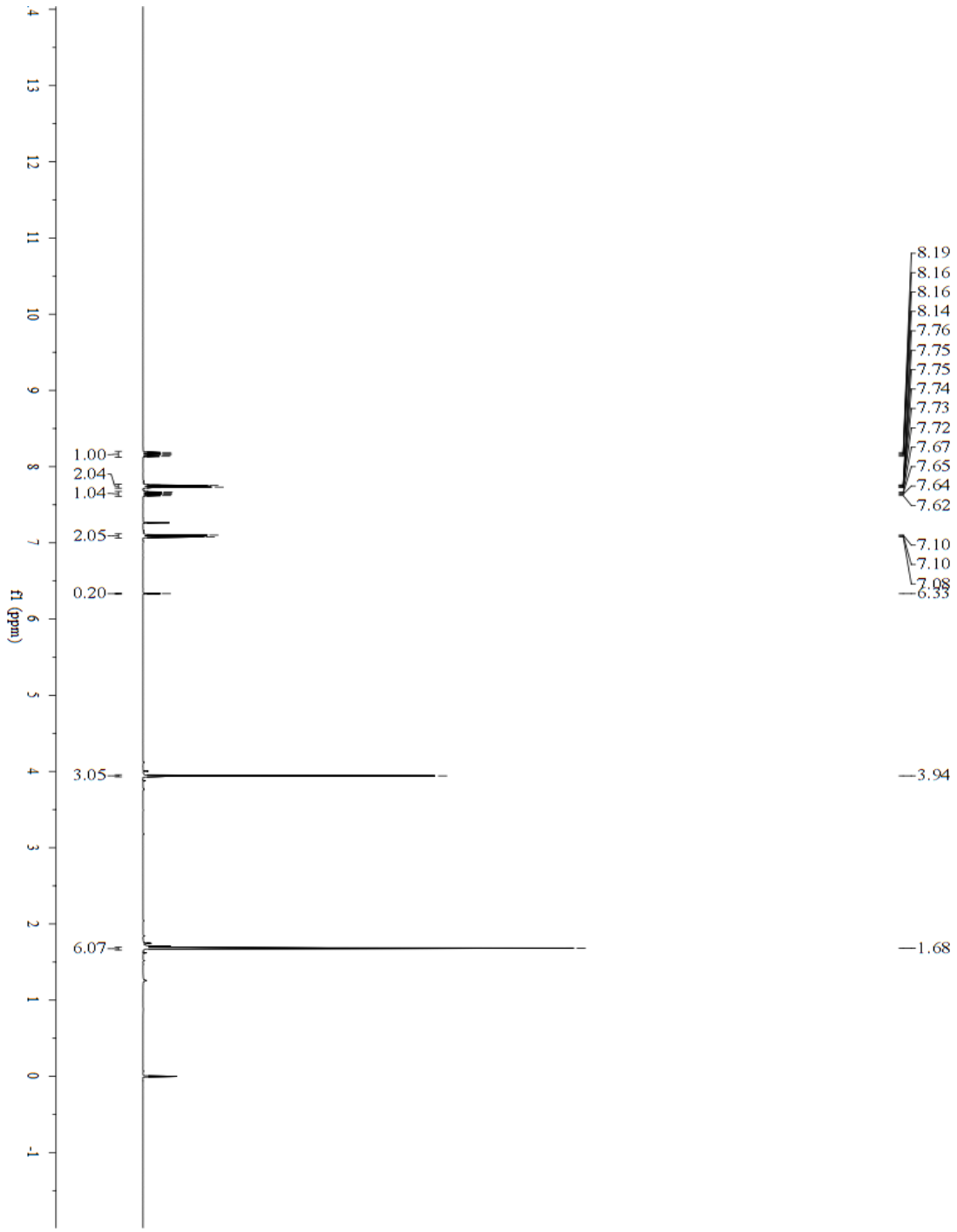
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

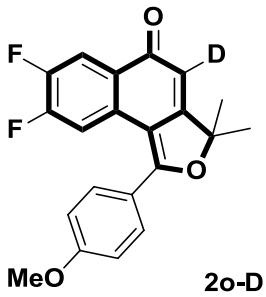




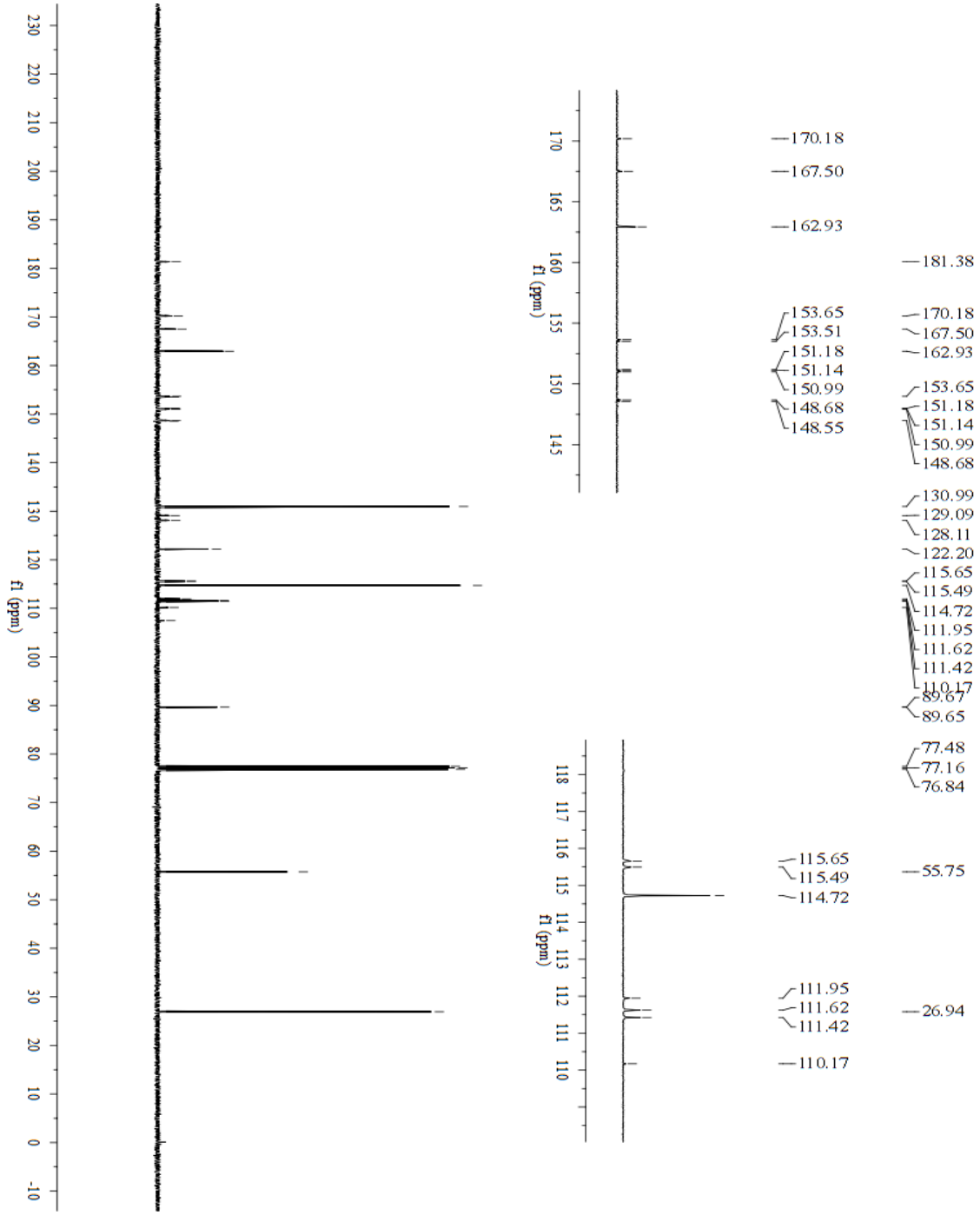
2o-D

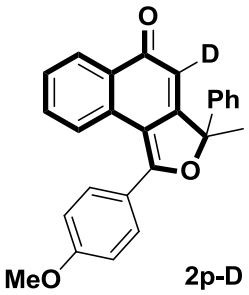
^{1}H NMR (400 MHz, $CDCl_3$)





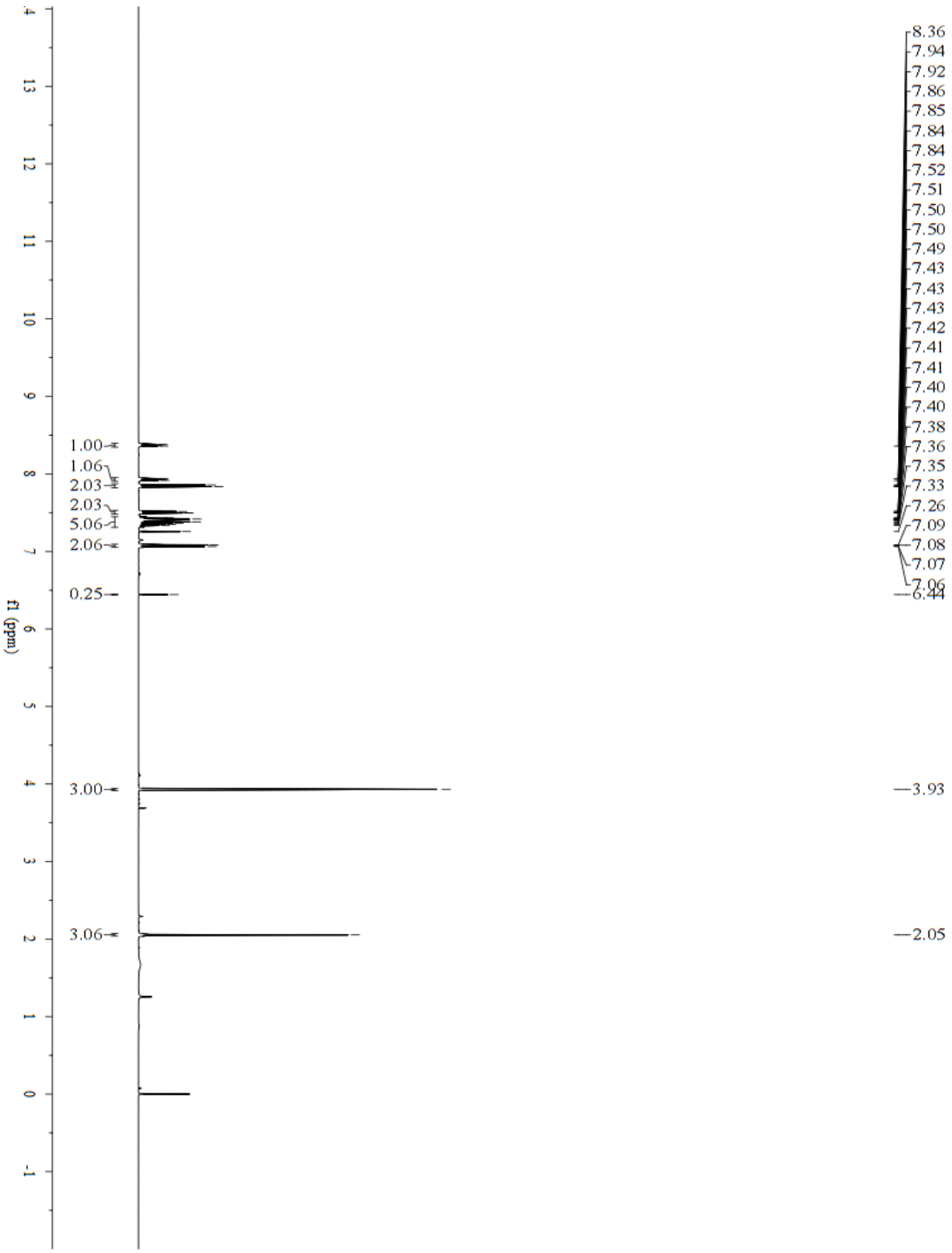
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

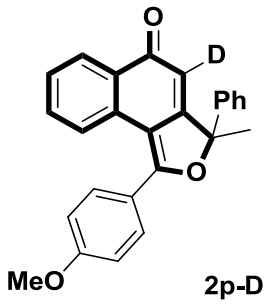




2p-D

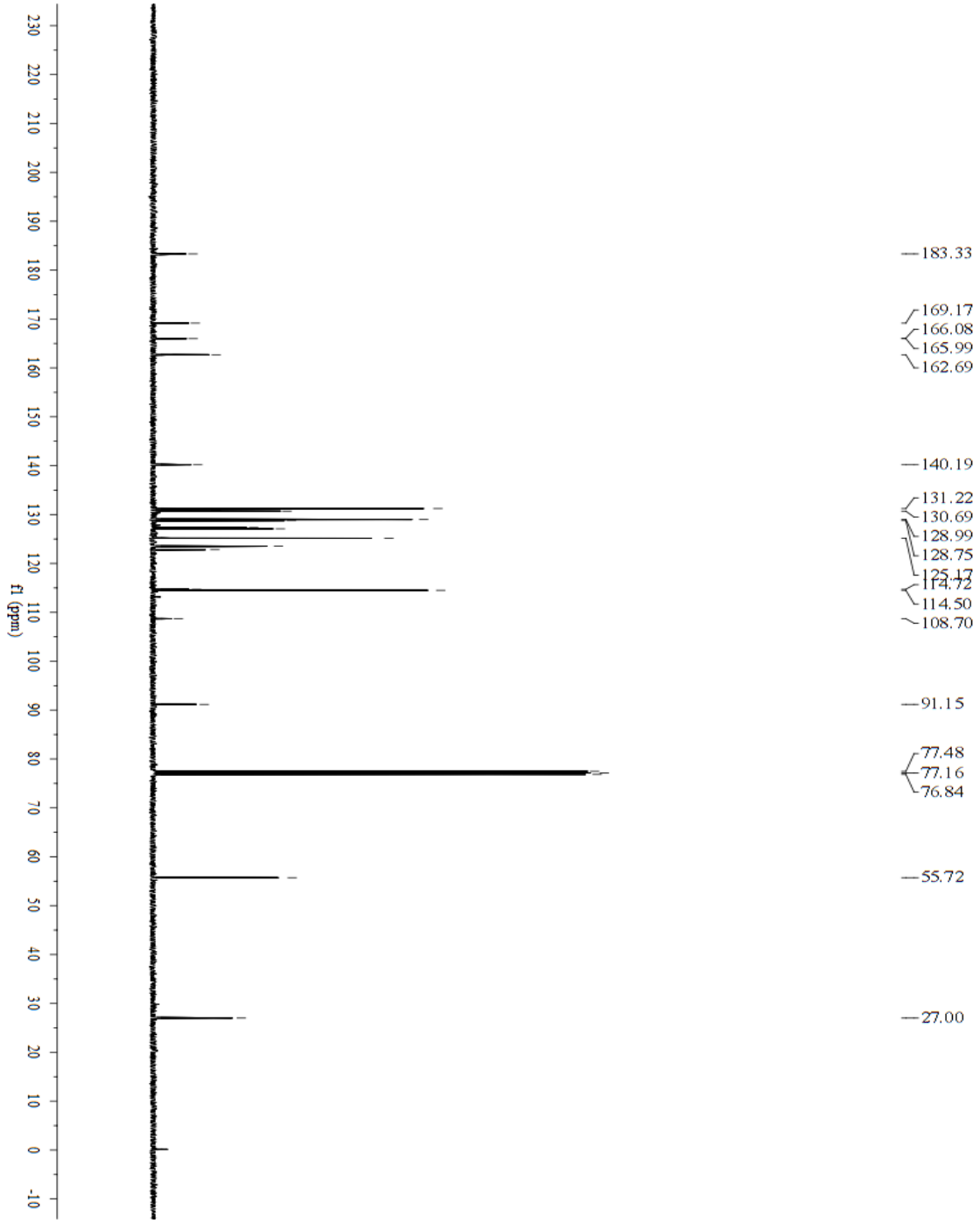
^{1}H NMR (400 MHz, $CDCl_3$)

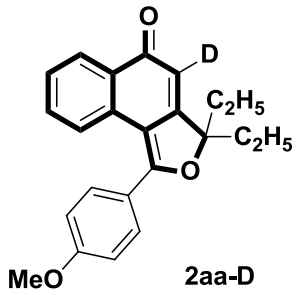




2p-D

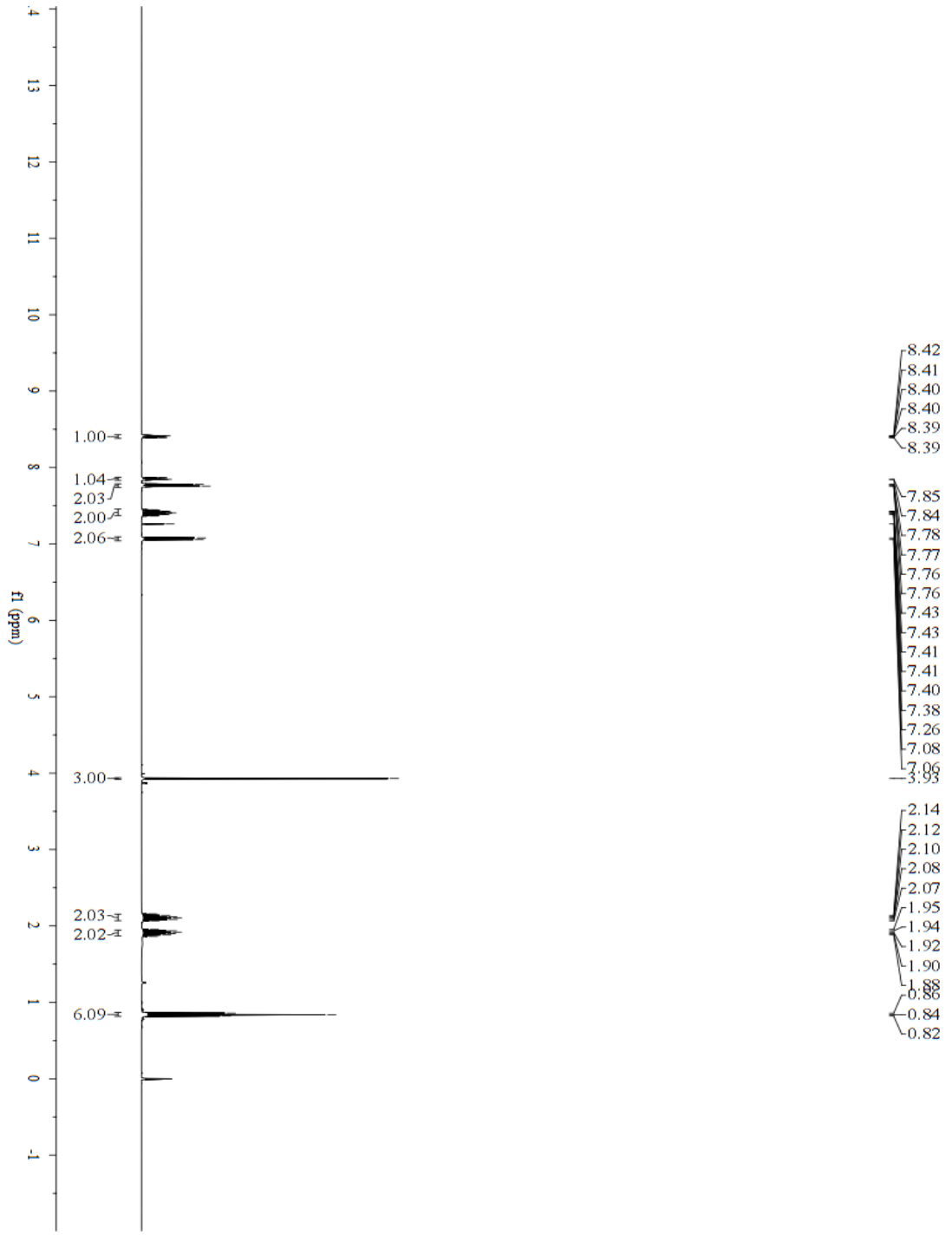
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

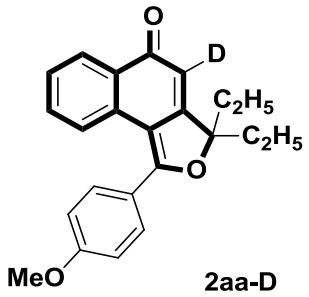




2aa-D

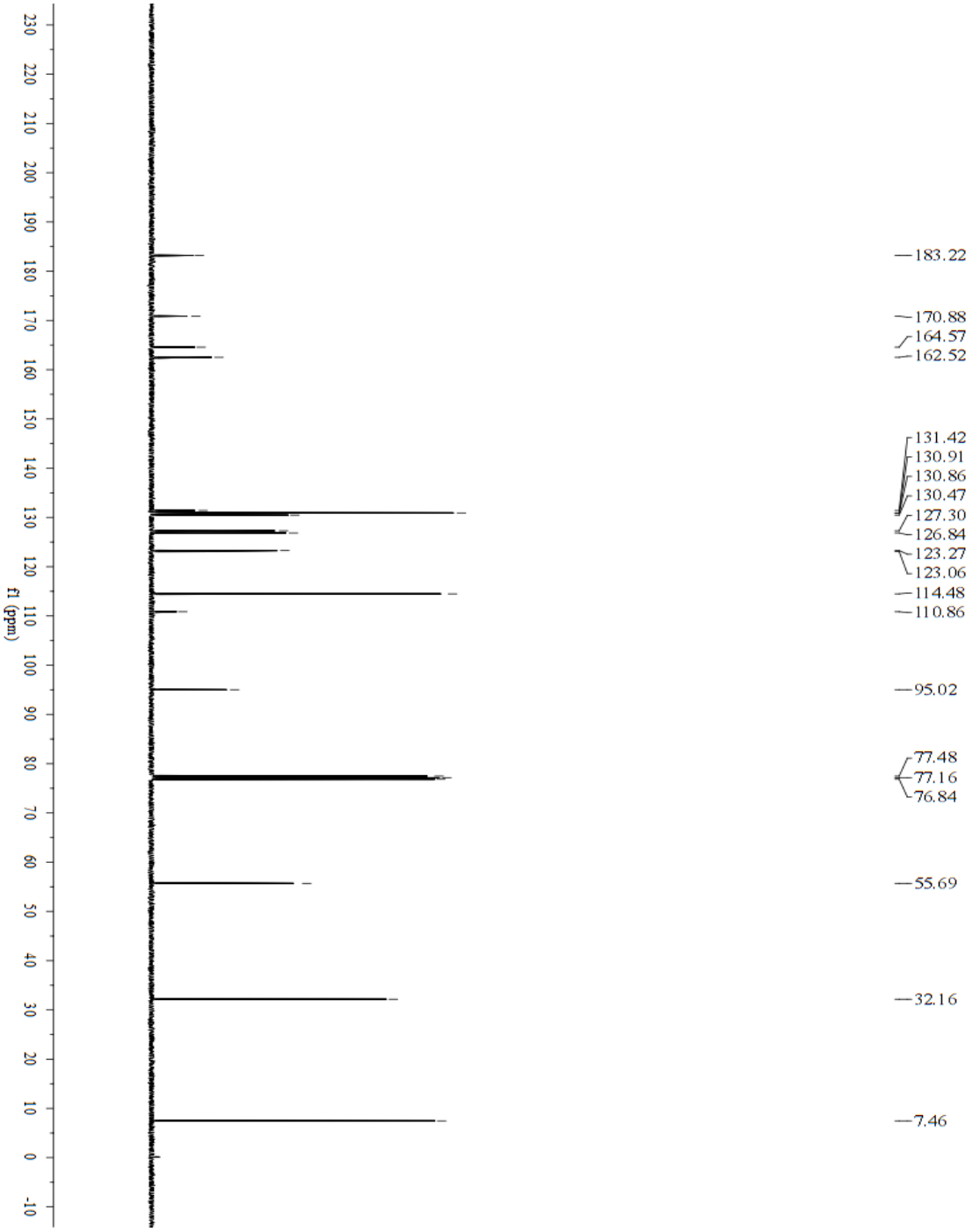
^{1}H NMR (400 MHz, $CDCl_3$)

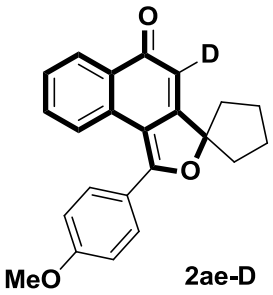




2aa-D

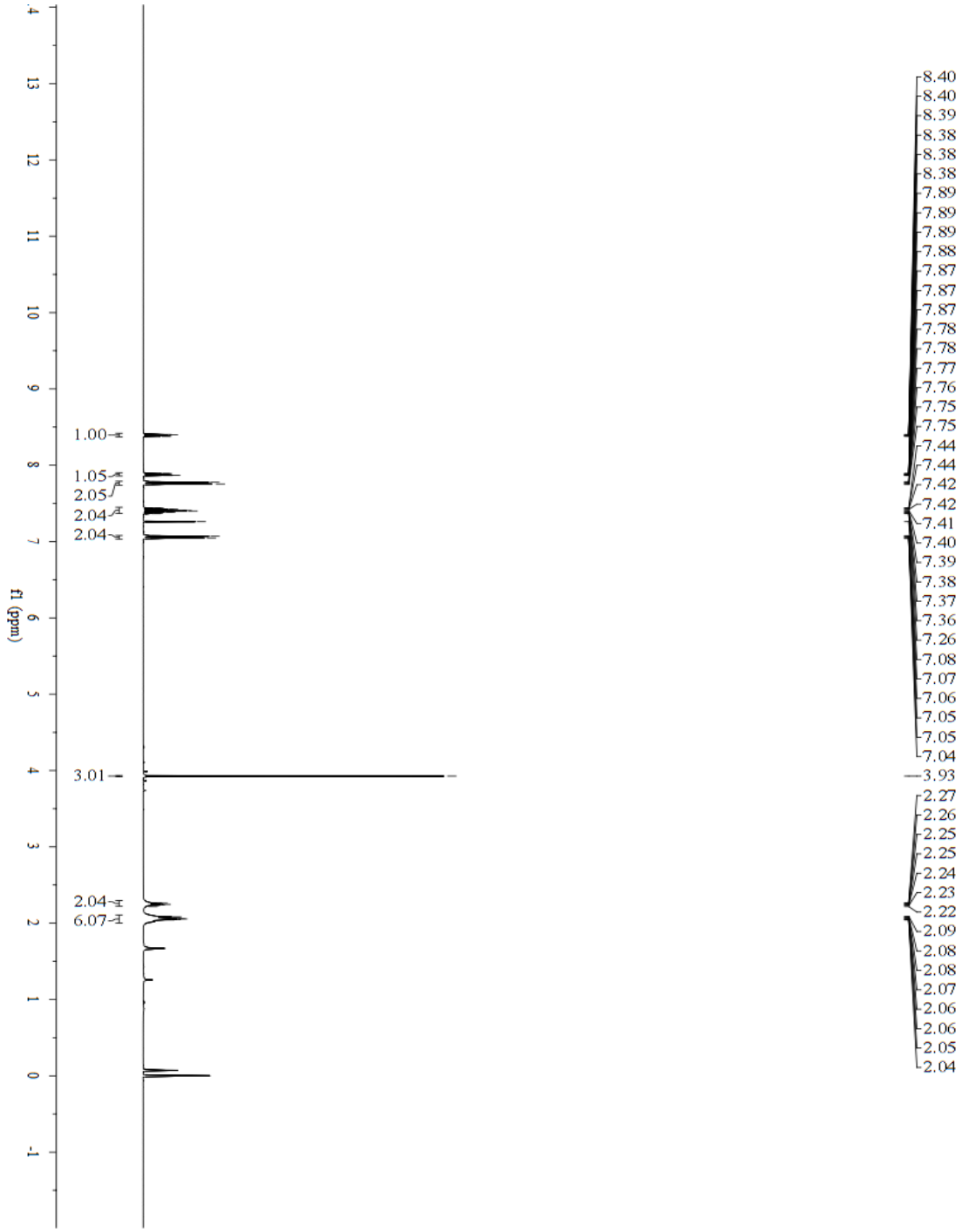
$^{13}C\ \{^1H\}$ NMR (100 MHz, $CDCl_3$)

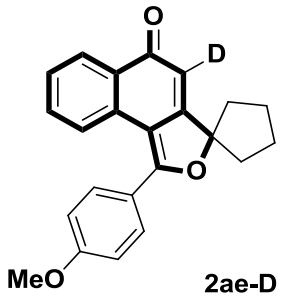




2ae-D

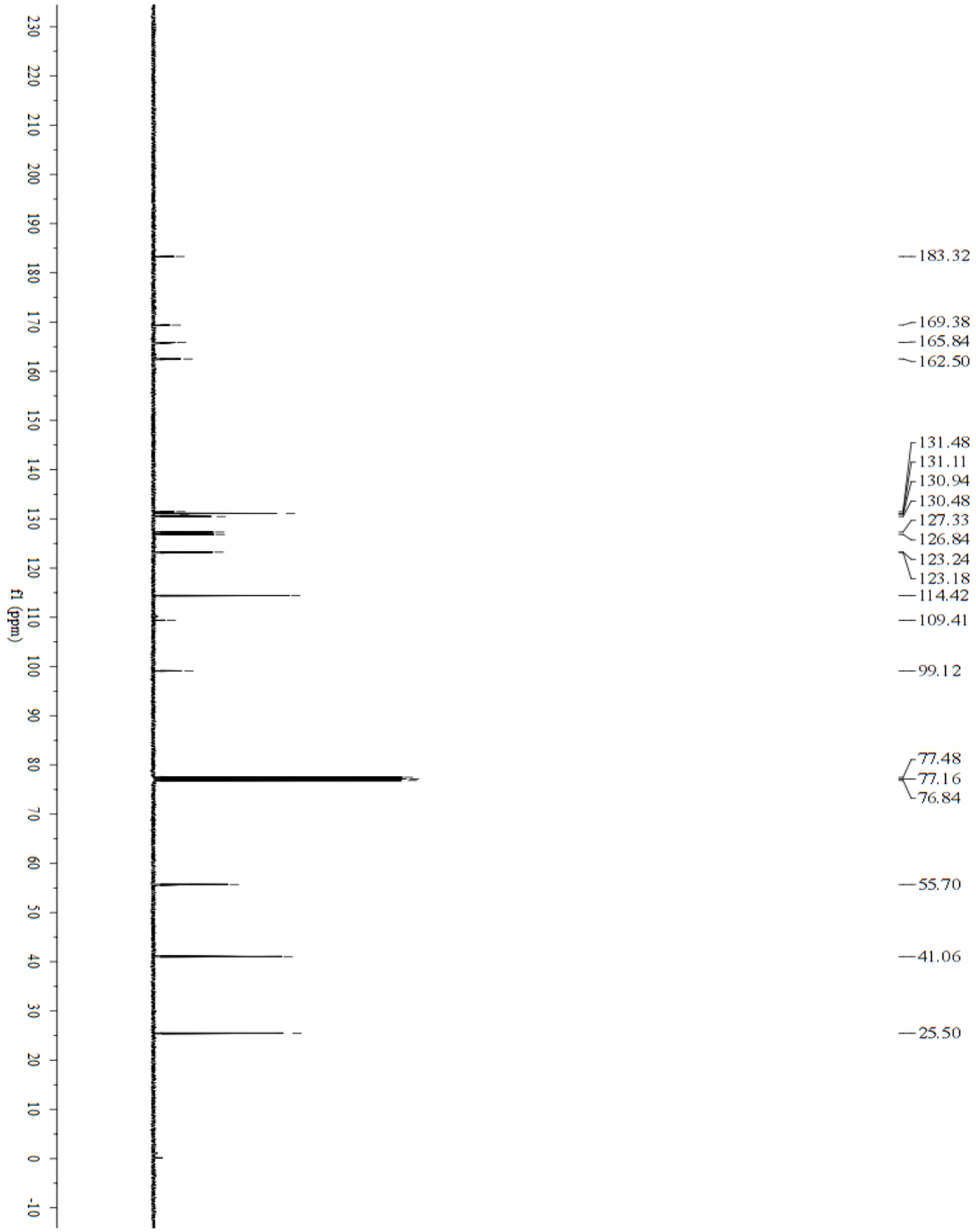
^{1}H NMR (400 MHz, $CDCl_3$)

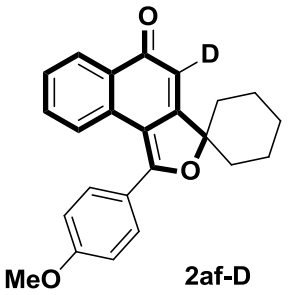




2ae-D

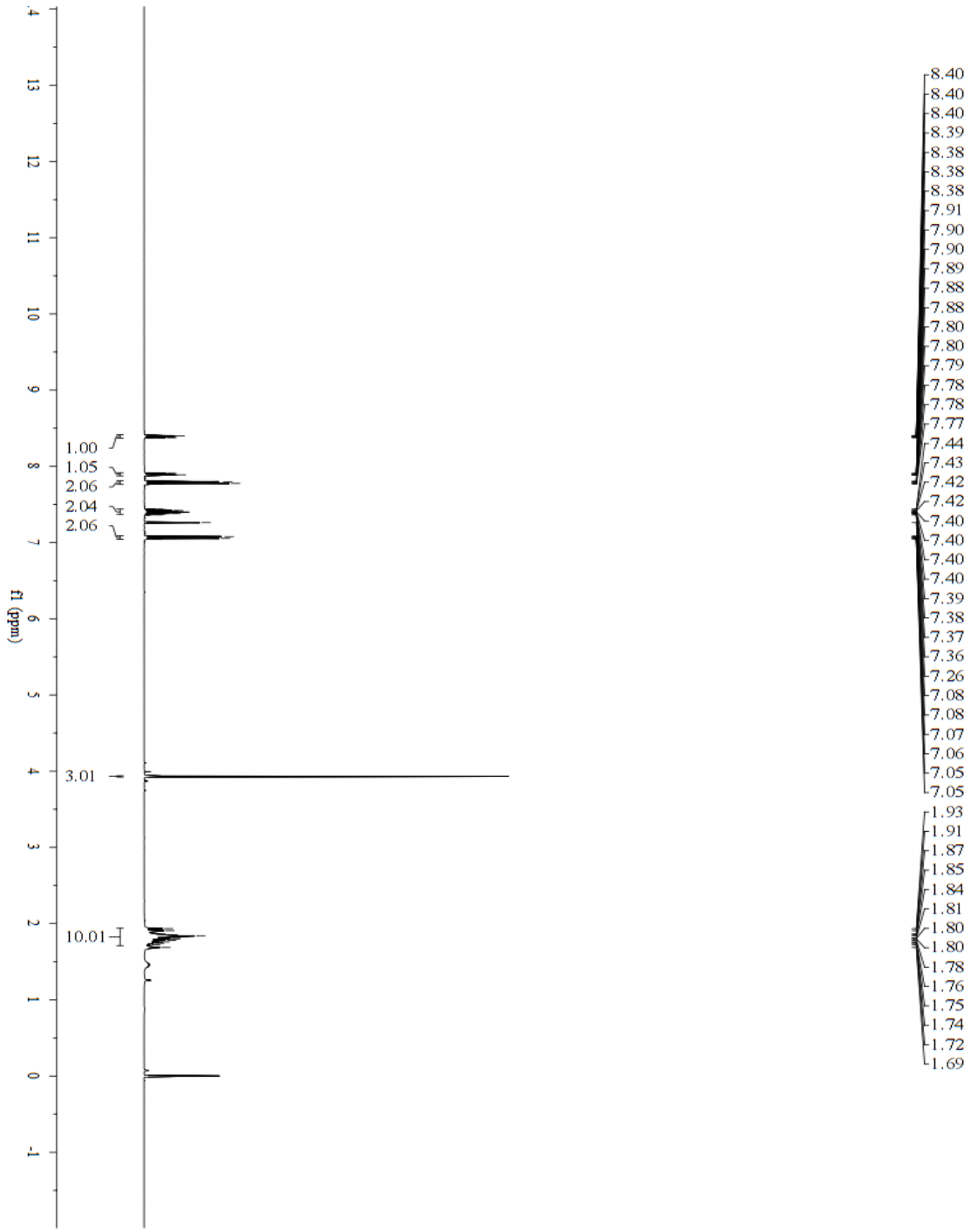
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

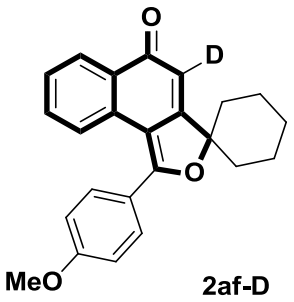




2af-D

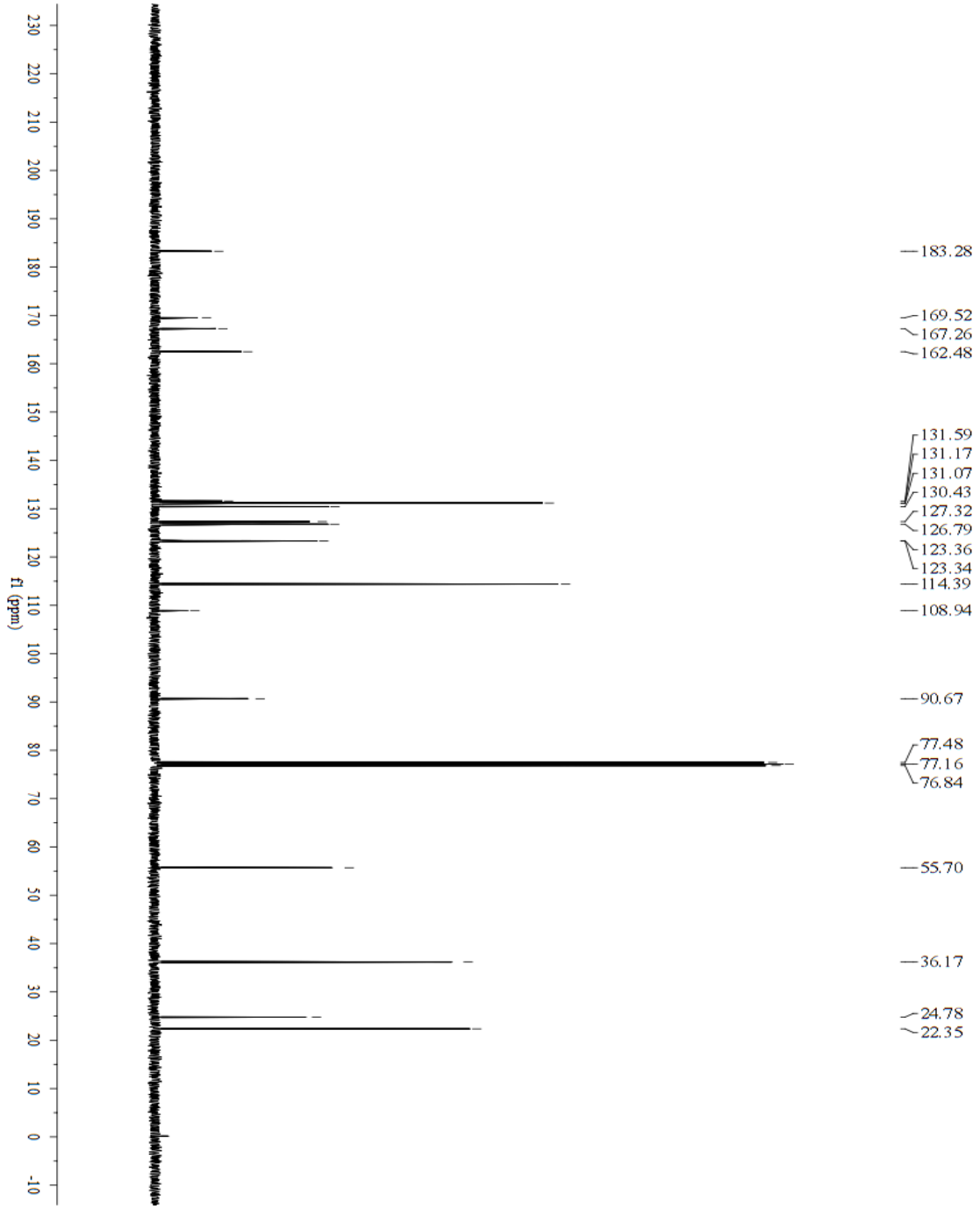
^{1}H NMR (400 MHz, $CDCl_3$)

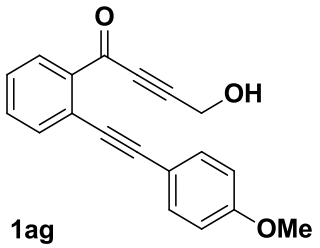




2af-D

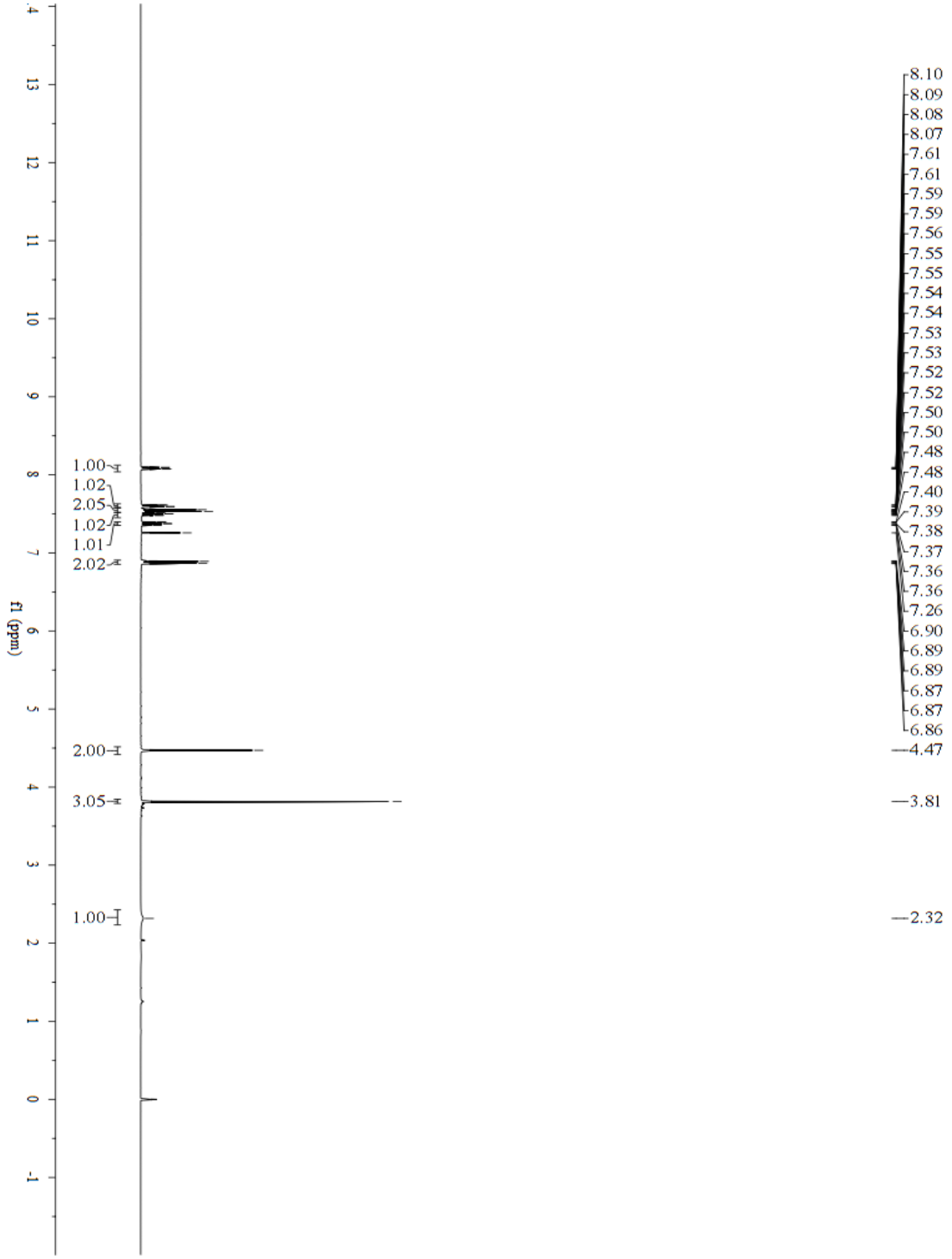
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

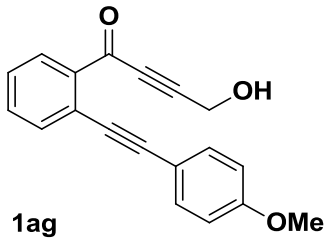




1ag

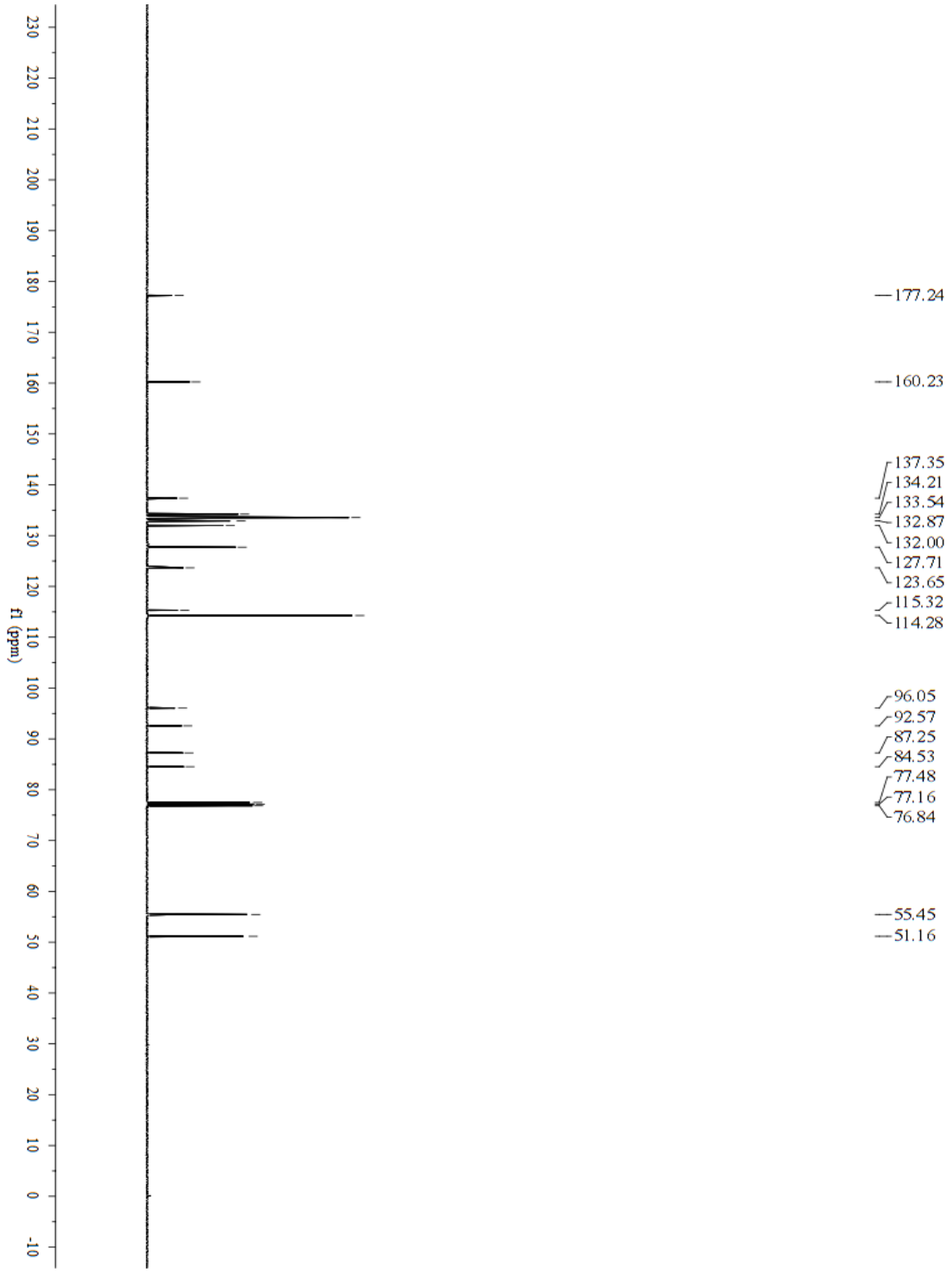
^{1}H NMR (400 MHz, $CDCl_3$)

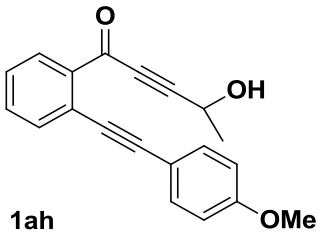




1ag

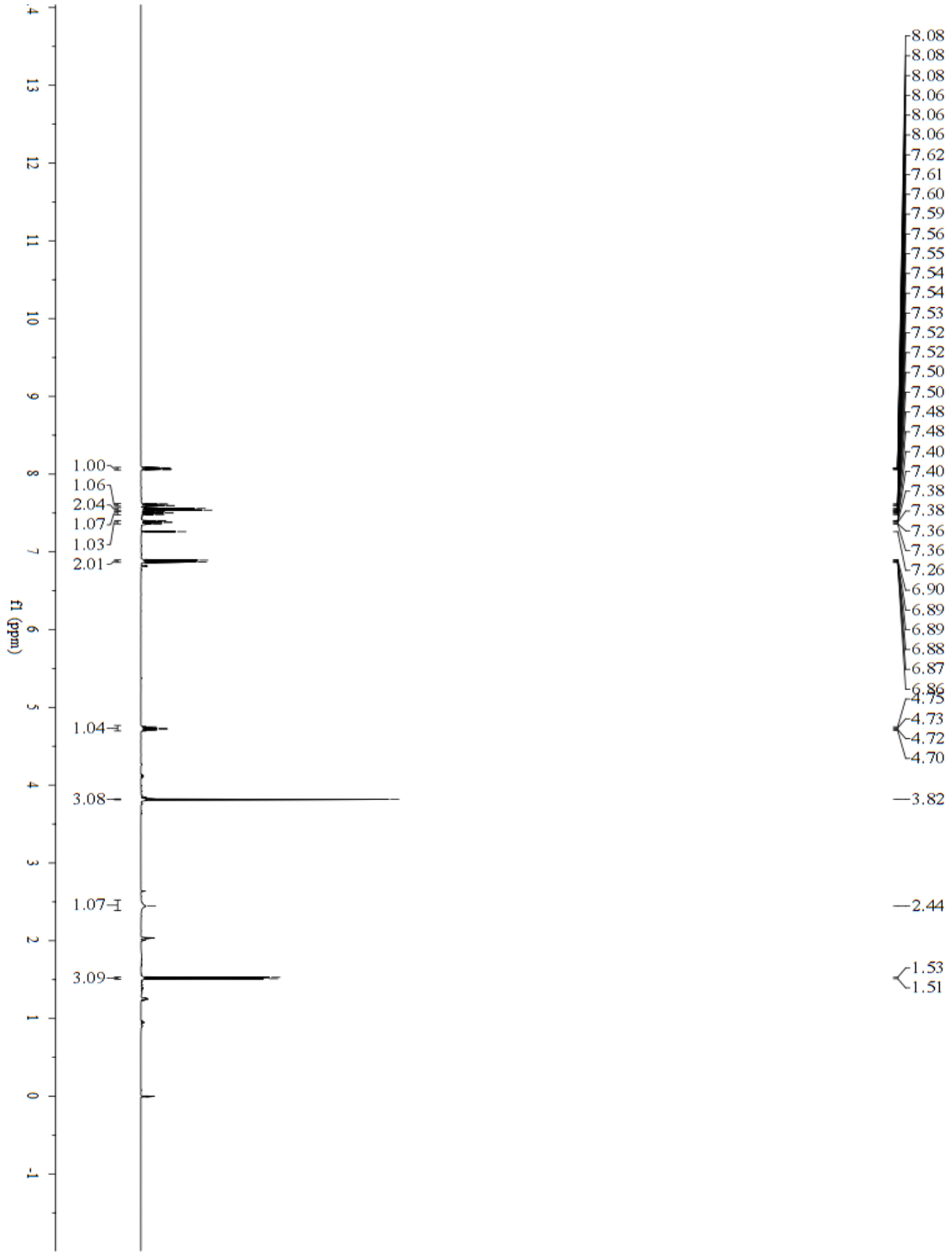
$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)

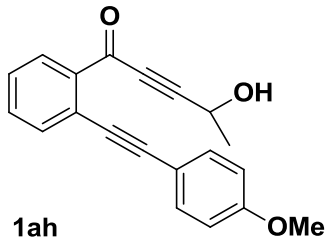


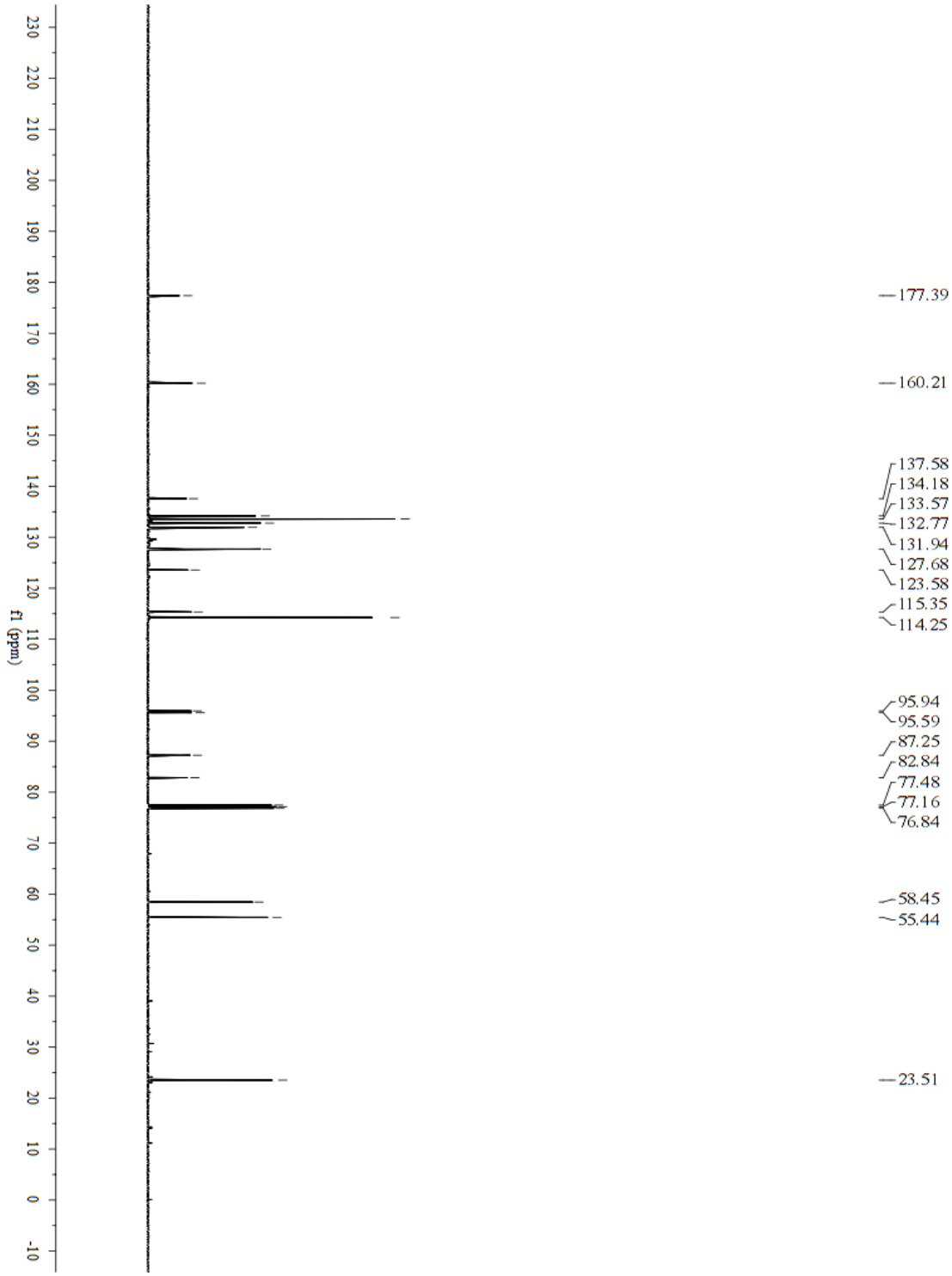


1ah

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





1ah

$^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$)