Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Electrochemical selective C3-thiolation of quinolines

Dahan Wang,[a] Li Zhang,[b] Fuhong Xiao,*[,a] Guojiang Mao,[c] and and Guo-Jun Deng*[,a]

[a] Key Laboratory of Environmentally Friendly Chemistry and Application of Ministry of Education, Key Laboratory for Green Organic Synthesis and Application of Hunan. Province, College of Chemistry, Xiangtan University, Xiangtan 411105, China.

[b] College of Chemistry and Materials Engineering, Huaihua University, Huaihua 418000, PR China

[c] School of Chemistry and Chemical Engineering, Henan Normal University Xinxiang, 453007, P. R. China

E-mail: fhxiao@xtu.edu.cn; gjdeng@xtu.edu.cn;

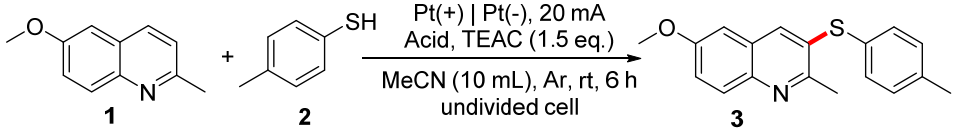
Table of Contents

1. General information

All reactions were carried out under an atmosphere of oxygen unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument using $CDCl_3$ as solvent and TMS as an internal standard. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra (HRMS) was performed on Agilent 6230 TOF LC/MS. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. Most reagents were obtained from commercial suppliers and used without further purification.

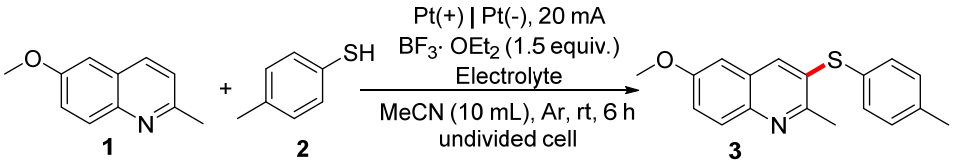
2 Reaction optimization

Table S1 Optimization of acid



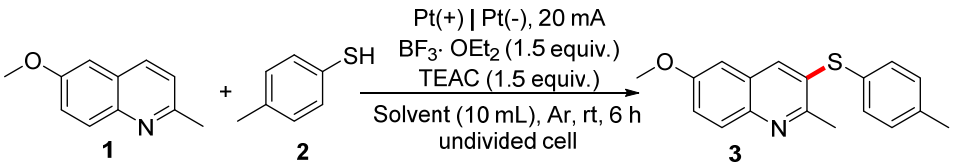
Entry	Acid (equiv.)	Yield (%)
1	none	0
2	AcOH (1.5)	0
3	TFA (1.5)	0
4	$PhCO_2H$ (1.5)	0
5	MsOH (1.5)	0
6	$FeCl_3$ (0.2)	0
7	$Cu(OAc)_2$ (0.2)	0
8	$B(C_6F_5)_3$ (0.2)	0
9	$BF_3{\bullet}OEt_2$ (1.5)	81
10	$BF_3{\bullet}OEt_2$ (2.0)	65
11	$BF_3{\bullet}OEt_2$ (1.0)	73

Table S1 Optimization of electrolyte e



Entry	Electrolyte (equiv.)	Yield (%)
1	*n*-Bu_4NPF_6 (1.5)	0
2	*n*-Bu_4NBF_4 (1.5)	0
3	$LiClO_4$ (1.5)	0
4	TBAI (1.5)	41
5	TBAB (1.5)	56
6	TABC (1.5)	63
7	NH_4Cl (1.5)	trace
8	NaCl (1.5)	35
9	Et_4NClO_4 (1.5)	47
10	TEAC (1.5)	81
11	TEAC (2.0)	80
12	TEAC (1.0)	72

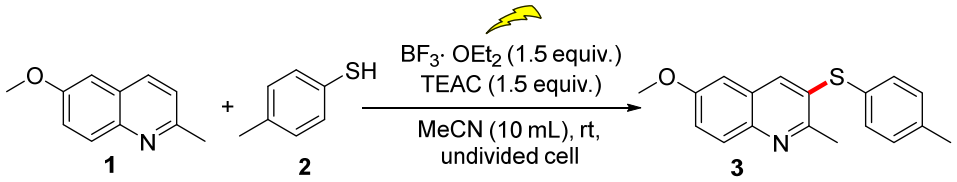
Table S3 Optimization of solvent



Entry	Solvent (mL)	Yield (%)
1	MeOH (10 mL)	0
2	Acetone (10 mL)	22
3	DMF (10 mL)	0
4	DMSO (10 mL)	0
5	THF (10 mL)	0
6	1.4-Dioxane (10 mL)	0

7	DCM (10 mL)	0
8	H_2O (10 mL)	0
9	MeCN (10 mL)	81
10	MeCN/HFIP (8:2 mL)	0
11	MeCN/THF (8:2 mL)	0
12	MeCN/DCM (8:2 mL)	Trace
13	MeCN/DMSO (8:2 mL)	Trace
14	MeCN/Acetone (8:2 mL)	45
15	MeCN/DMF (8:2 mL)	Trace

Table S4 Optimization of electricity amount



Entre	Anode	Cathode	Current (mA)	Time (h)	Yield (%)
1	Pt	Pt	20	6	81
2	Pt	Pt	20	10	81
3	Pt	Pt	20	4	67
4	Pt	Pt	25	6	62
5	Pt	Pt	15	6	51
6	Pt	Pt	15	16	57
7	Pt	C	20	6	none
8	C	C	20	6	none
9	Pt	Fe	20	6	none
10	Pt	Cu	20	6	none

3. cyclic voltammetry experiments

Cyclic voltammograms of substrates in 0.1 M TEAC (MeCN), using a glassy carbon working electrode and Pt wire and Ag/AgNO3 (0.1 M in MeCN) as counter and reference electrodes at a 100 mVs-1 scan rate:

Fig **1**. 6-methoxy-2-methylquinoline (**1a**) (0.1 mM);

Fig **2**. **1a** (0.1 mM) and BF_3•OEt_2 (0.15 mM);

Fig **3.** *p*-toluenethiol (**2a**) (0.25 mM);

Fig **4.** Mixture of **1a** (0.1 mM), *p*-toluenethiol (**2a**) (0. 25 mM) and BF_3•OEt_2 (0.15 mM).

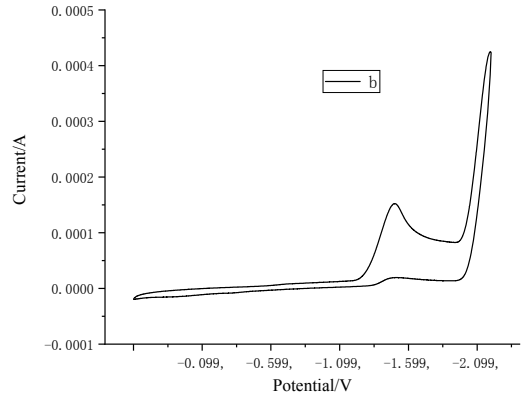


Fig 1

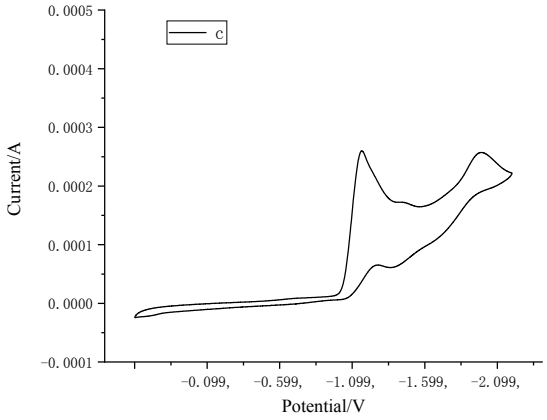


Fig 2

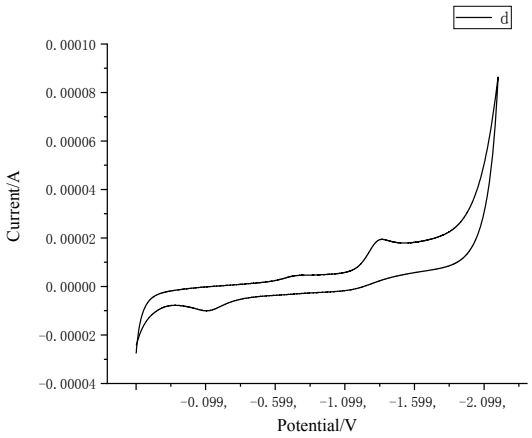


Fig 3

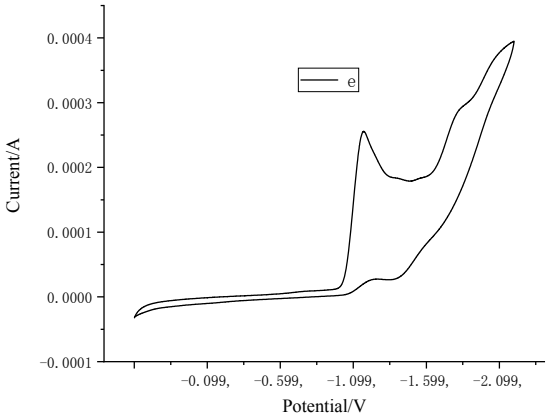
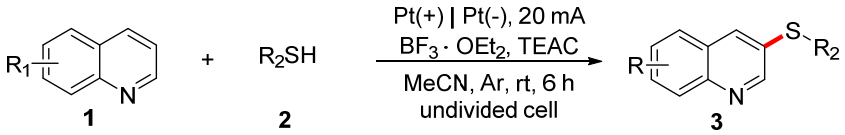


Fig 4

4. General procedure



A 10 mL reaction three-necked flask (Figure S1) was charged with **1** (0.5 mmol), **2** RSH (1.25 mmol) or R_2XXR_2 (0.75 mmol), TEAC (0.5 mmol), the flask was equipped with a reticulated vitreous platinum plate (10 mm x 10 mm x 0.2 mm) anode and a platinum plate (10 mm x 10 mm x 0.2 mm) cathode and then flushed with argon, dry MeCN (10 mL) and BF_3•OEt_2 (0.75 mmol) was added. The electrolysis was carried out at room temperature using a constant current of 20 mA until complete consumption of the substrate. The reaction mixture was concentrated under reduced pressure and the residue was chromatographed through silica gel elutin

with ethyl acetate/hexane to give the desired product.

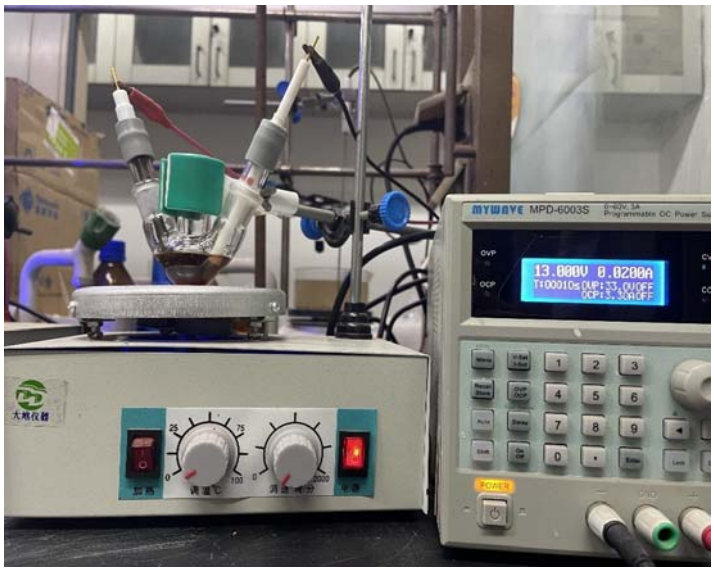
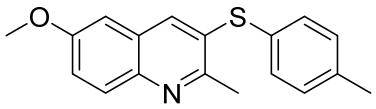


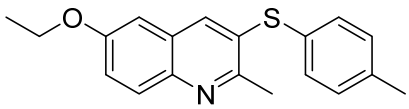
Fig 5. Electrolysis cell for reactions

5. Analytical data for the compounds prepared



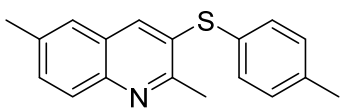
6-Methoxy-2-methyl-3-(*p*-tolylthio)quinoline (**3aa**): 119.4 mg, 81%, yellow solid. Mp: 80 - 82 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 9.2 Hz, 1H), 7.59 (s, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.28 – 7.24 (m, 1H), 7.20 (d, *J* = 7.9 Hz, 2H), 6.83 (d, *J* = 2.8 Hz, 1H), 3.85 (s, 3H), 2.72 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.3, 154.7, 141.9, 138.2, 134.0, 132.6, 131.7, 130.4, 129.6, 128.9, 128.2, 121.4, 104.1, 55.3, 23.4, 21.1. HRMS (ESI) m/z calcd for $C_{18}H_{18}NOS^{+}$ $(M+H)^{+}$ 296.1104, found 296.1114.



6-Ethoxy-2-methyl-3-(*p*-tolylthio)quinoline (3ba): 114.3 mg, 74%, white solid. Mp: 125 - 127 ^{o}C.

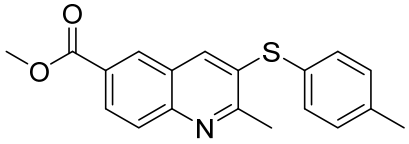
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 9.1 Hz, 1H), 7.56 (s, 1H), 7.32 – 7.22 (m, 3H), 7.18 (d, *J* = 7.9 Hz, 2H), 6.80 (d, *J* = 2.7 Hz, 1H), 4.03 (q, *J* = 7.0 Hz, 2H), 2.71 (s, 3H), 2.36 (s, 3H), 1.42 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 156.7, 154.8, 142.0, 138.2, 134.2, 132.5, 131.6, 130.4, 129.6, 129.1, 128.2, 121.8, 104.9, 63.6, 23.5, 21.1, 14.6. HRMS (ESI) m/z calcd for $C_{19}H_{20}NOS^{+}$ $(M+H)^{+}$ 310.1260, found 310.1273.



2,6-Dimethyl-3-(*p*-tolylthio)quinoline (3ca) : 76.6 mg, 55%, white solid. Mp: 91 – 93 ^{o}C.

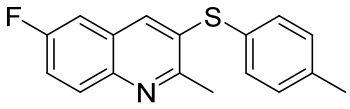
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 8.6 Hz, 1H), 7.62 (s, 1H), 7.46 – 7.40 (m, 1H), 7.36 – 7.24 (m, 3H),

7.17 (d, *J* = 7.9 Hz, 2H), 2.74 (s, 3H), 2.44 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 156.8, 144.6, 138.2, 135.9, 135.1, 132.4, 131.3, 131.2, 130.4, 129.2, 127.9, 127.3, 125.5, 23.7, 21.4, 21.1. HRMS (ESI) m/z calcd for $C_{18}H_{18}NS^+$ (M+H)+ 280.1154, found 280.1167.



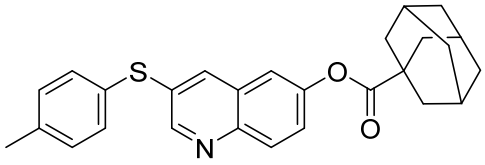
Methyl 2-methyl-3-(*p*-tolylthio)quinoline-6-carboxylate (3da) : 84.2 mg, 56%, yellow solid. Mp: 92 – 94 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 1.9 Hz, 1H), 8.20 – 8.15 (m, 1H), 7.99 (d, *J* = 8.8 Hz, 1H), 7.58 (s, 1H), 7.38 (d, *J* = 7.9 Hz, 2H), 7.28 – 7.25 (m, 2H), 3.94 (s, 3H), 2.80 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.6, 159.4, 147.4, 139.4, 135.9, 134.1, 133.9, 130.8, 129.6, 128.6, 128.2, 127.5, 127.5, 126.5, 52.3, 24.0, 21.3. HRMS (ESI) m/z calcd for $C_{19}H_{18}NO_2S^+$ (M+H)$^+$ 324.1053, found 324.1067.



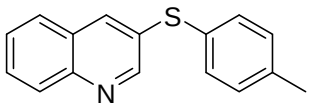
6-Fluoro-2-methyl-3-(*p*-tolylthio)quinoline (3ea) : 79.2 mg, 56%, white solid. Mp: 93 - 95 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.91 (m, 1H), 7.49 (s, 1H), 7.39 – 7.33 (m, 3H), 7.28 – 7.23 (m, 2H), 7.18 – 7.14 (m, 1H), 2.75 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 161.4, 157.6 (d, *J* = 269.0 Hz), , 142.7, 139.0, 133.7, 133.6, 132.8 (d, *J* = 5.1 Hz), 130.7, 130.7 (d, *J* = 9.3 Hz), 127.9, 127.8 (d, *J* = 2.3 Hz), 118.6 (d, *J* = 25.5 Hz), 109.6 (d, *J* = 21.8 Hz), 23.6, 21.2. HRMS (ESI) m/z calcd for $C_{17}H_{15}FNS^+$ (M+H)$^+$ 284.0904, found 284.0918.



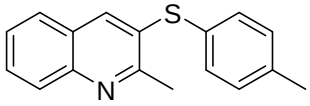
3-(*p*-Tolylthio)quinolin-6-yl adamantane-1-carboxylate (3fa) : 90.1 mg, 42%, white solid. Mp: 141 - 143 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 (d, *J* = 2.2 Hz, 1H), 8.04 (d, *J* = 8.9 Hz, 1H), 7.78 (d, *J* = 2.2 Hz, 1H), 7.39 – 7.31 (m, 4H), 7.19 (d, *J* = 7.9 Hz, 2H), 2.38 (s, 3H), 2.12 – 2.06 (m, 9H), 1.82 – 1.74 (m, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.1, 150.5, 149.5, 144.1, 138.8, 134.1, 133.0, 132.7, 130.6, 130.5, 128.9, 128.6, 124.4, 117.6, 41.1, 38.7, 36.4, 27.8, 21.2. HRMS (ESI) m/z calcd for $C_{27}H_{28}NO_2S^+$ (M+H) $^+$ 430.1835, found 430.1848.



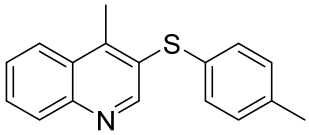
3-(*p*-Tolylthio)quinoline (3ga): 59.0 mg, 47%, yellow oil.[1]

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.78 (d, *J* = 2.3 Hz, 1H), 8.09 – 8.02 (m, 1H), 7.95 (d, *J* = 2.3 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.53 – 7.48 (m, 1H), 7.36 – 7.32 (m, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 151.4, 146.3, 138.3, 135.5, 132.3, 131.2, 130.3, 129.8, 129.2, 129.2, 128.2, 127.1, 127.1, 21.1.



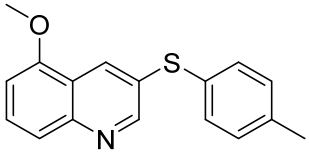
2-Methyl-3-(*p*-tolylthio)quinoline (3ha) : 79.4 mg, 60%, white solid. Mp: 62 - 64 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.95 (m, 1H), 7.70 (s, 1H), 7.65 – 7.53 (m, 2H), 7.46 – 7.37 (m, 1H), 7.33 – 7.27 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 2.77 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.8, 146.0, 138.3, 135.4, 132.6, 131.5, 130.5, 129.0, 128.3, 127.3, 126.6, 126.1, 23.8, 21.2. HRMS (ESI) m/z calcd for $C_{17}H_{16}NS^+$ $(M+H)^+$ 266.0998, found 266.1012.



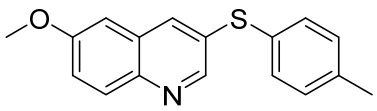
4-Methyl-3-(*p*-tolylthio)quinoline (3ia) : 69 mg, 52%, yellow solid. Mp: 109 - 111 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.76 (s, 1H), 8.09 – 8.02 (m, 2H), 7.73 – 7.67 (m, 1H), 7.61 – 7.56 (m, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 2.82 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 153.7, 146.8, 146.0, 136.9, 131.9, 130.1, 130.0, 129.8, 129.3, 128.1, 126.9, 124.0, 21.0, 16.0. HRMS (ESI) m/z calcd for $C_{17}H_{16}NS^+$ $(M+H)^+$ 266.0998, found 266.1013.



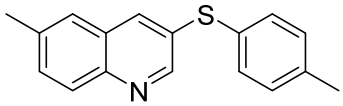
5-Methoxy-3-(p-tolylthio)quinoline (3ja) : 49.1 mg, 35%, yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 (d, *J* = 2.3 Hz, 1H), 8.53 (d, *J* = 2.5 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.57 (t, *J* = 8.1 Hz, 1H), 7.31 – 7.27 (m, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 6.84 (d, *J* = 7.6 Hz, 1H), 3.96 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 154.6, 152.5, 147.3, 137.7, 132.2, 131.4, 131.0, 130.2, 129.5, 129.4, 121.2, 120.6, 104.9, 55.7, 21.1. HRMS (ESI) m/z calcd for $C_{17}H_{16}NOS^+$ $(M+H)^+$ 282.0947, found 282.0965.



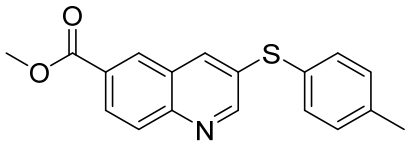
6-Methoxy-3-(*p*-tolylthio)quinoline (**3ka**)**:** 94.1 mg, 67%, yellow solid. Mp: 105 - 107 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 (d, *J* = 2.3 Hz, 1H), 7.93 (d, *J* = 9.2 Hz, 1H), 7.84 – 7.80 (m, 1H), 7.36 – 7.28 (m, 3H), 7.16 (d, *J* = 7.9 Hz, 2H), 6.90 (d, *J* = 2.8 Hz, 1H), 3.87 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 158.1, 148.7, 142.5, 138.2, 134.2, 132.4, 131.6, 130.5, 130.3, 129.8, 129.3, 121.9, 104.4, 55.4, 21.1. HRMS (ESI) m/z calcd for $C_{17}H_{16}NOS^{+}$ $(M+H)^{+}$ 281.0947, found 281.0960.



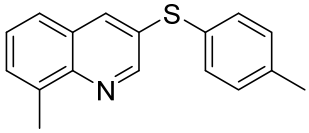
6-Methyl-3-(*p*-tolylthio)quinoline (3la) : 75.5 mg, 57%, white solid. Mp: 68 - 70 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 2.2 Hz, 1H), 7.94 (d, *J* = 8.6 Hz, 1H), 7.86 (d, *J* = 2.2 Hz, 1H), 7.48 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.41 (s, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 2.48 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 150.6, 145.0, 138.1, 137.1, 135.1, 132.1, 131.5, 130.9, 130.3, 130.0, 128.8, 128.2, 125.9, 21.5, 21.1. HRMS (ESI) m/z calcd for $C_{17}H_{16}NS^{+}$ (M+H)+ 266.0998, found 266.1014.



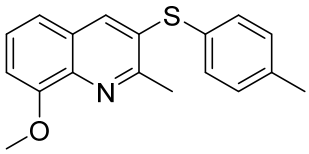
Methyl 3-(*p*-tolylthio)quinoline-6-carboxylate (3ma) : 61.7 mg, 40%, yellow solid. Mp: 93 - 95 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.82 (d, *J* = 2.3 Hz, 1H), 8.40 (d, *J* = 1.9 Hz, 1H), 8.24 – 8.19 (m, 1H), 8.07 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 2.3 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 3.97 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.4, 152.7, 147.9, 139.1, 135.0, 133.4, 133.3, 130.6, 130.0, 129.5, 128.6, 128.5, 128.4, 127.4, 52.4, 21.2. HRMS (ESI) m/z calcd for $C_{18}H_{16}NO_2S^{+}$ $(M+H)^{+}$ 310.0896, found 310.0924.



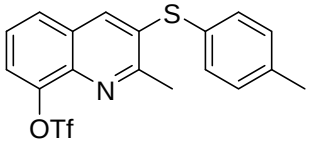
8-Methyl-3-(*p*-tolylthio)quinoline (3na) : 33.1 mg, 25%, yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.78 (d, *J* = 2.3 Hz, 1H), 7.97 (d, *J* = 2.3 Hz, 1H), 7.54 – 7.50 (m, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.36 – 7.32 (m, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 2.77 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 150.4, 145.5, 138.2, 137.1, 136.1, 135.4, 132.3, 130.8, 130.3, 129.6, 128.2, 127.0, 125.2, 21.1, 18.0. HRMS (ESI) m/z calcd for $C_{17}H_{16}NS^{+}$ $(M+H)^{+}$ 266.0998, found 266.1014.



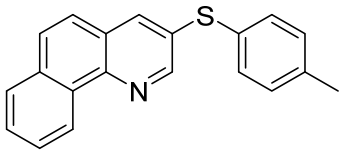
8-Methoxy-2-methyl-3-(*p*-tolylthio)quinoline (3oa) : 45.7 mg, 45%, yellow solid. Mp: 116 - 118 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (s, 1H), 7.36 – 7.26 (m, 3H), 7.21 – 7.13 (m, 3H), 6.97 (dd, *J* = 7.8, 1.2 Hz, 1H), 4.06 (s, 3H), 2.81 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 156.6, 154.6, 138.4, 137.6, 135.0, 132.7, 132.4, 130.5, 128.7, 128.5, 126.2, 118.6, 107.1, 55.9, 24.2, 21.2. HRMS (ESI) m/z calcd for $C_{18}H_{18}NOS^{+}$ $(M+H)^{+}$296.1104, found 296.1121.



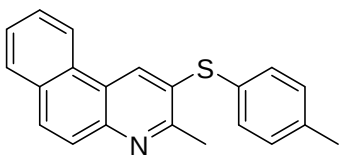
2-Methyl-3-(*p*-tolylthio)quinolin-8-yl trifluoromethanesulfonate (3pa) : 51.6 mg, 25%, yellow solid. Mp: 71 - 73 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.51 (m, 1H), 7.50 – 7.44 (m, 2H), 7.43 – 7.35 (m, 3H), 7.30 – 7.25 (m, 2H), 2.81 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 145.5, 139.6, 138.0, 135.7, 134.3, 131.8, 130.9, 128.9, 127.0, 126.7, 125.4, 120.5, 119.9, 24.0, 21.3. HRMS (ESI) m/z calcd for $C_{18}H_{15}F_3NO_3S_2^{+}$ $(M+H)^{+}$ 414.0440, found 414.0466.



3-(*p*-Tolylthio)benzo[*h*]quinoline (3qa) : 52.9 mg, 35%, yellow solid. Mp: 117 - 119 ^{o}C.

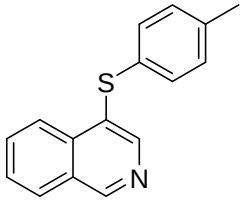
^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.20 (d, *J* = 8.0 Hz, 1H), 8.85 (d, *J* = 2.3 Hz, 1H), 8.01 (d, *J* = 2.3 Hz, 1H), 7.91 – 7.86 (m, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 149.7, 144.6, 138.3, 135.9, 133.4, 132.4, 132.0, 131.2, 130.4, 130.1, 128.5, 128.2, 127.8, 127.3, 126.4, 124.7, 124.2, 21.2. HRMS (ESI) m/z calcd for $C_{20}H_{16}NS^{+}$ $(M+H)^{+}$302.0998, found 302.1013.



3-Methyl-2-(*p*-tolylthio)benzo[*f*]quinoline (3ra) : 74.1 mg, 41%, yellow solid. Mp: 121 - 123 ^{o}C.

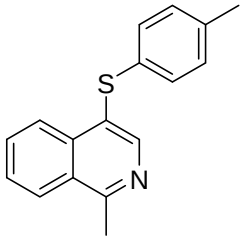
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (s, 1H), 8.28 – 8.22 (m, 1H), 7.92 – 7.83 (m, 3H), 7.61 – 7.53 (m, 2H),

7.31 – 7.26 (m, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 2.79 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.8, 146.0, 137.9, 132.2, 131.7, 131.4, 130.6, 130.6, 130.4, 129.9, 128.9, 128.5, 127.3, 127.0, 126.9, 124.1, 122.3, 23.6, 21.2. HRMS (ESI) m/z calcd for $C_{21}H_{18}NS^+$ $(M+H)^+$316.1154, found 316.1176.



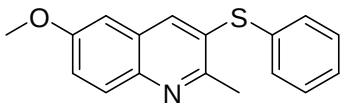
4-(*p*-Tolylthio)isoquinoline (3sa) : 43.9 mg, 35%, yellow oil.[1]

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.19 (s, 1H), 8.56 (s, 1H), 8.27 (dd, *J* = 8.6, 1.2 Hz, 1H), 8.03 – 7.96 (m, 1H), 7.75 – 7.70 (m, 1H), 7.66 – 7.61 (m, 1H), 7.21 – 7.15 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 152.6, 146.8, 137.0, 135.9, 131.3, 131.1, 130.1, 130.0, 128.8, 128.1, 127.7, 127.4, 124.5, 21.0.



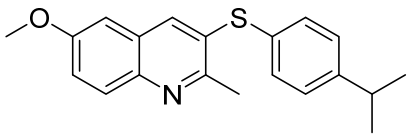
1-Methyl-4-(*p*-tolylthio)isoquinoline (3ta) : 62.3 mg, 47%, yellow solid. Mp: 88 - 90 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.56 (s, 1H), 8.29 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.3 Hz, 1H), 7.71 – 7.65 (m, 1H), 7.63 – 7.57 (m, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 2.97 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 159.8, 147.1, 136.2, 136.2, 132.5, 130.7, 129.8, 128.8, 127.8, 127.4, 126.1, 125.4, 124.4, 22.6, 20.9. HRMS (ESI) m/z calcd for $C_{17}H_{16}NS^+$ $(M+H)^+$266.0998, found 266.1013.



6-Methoxy-2-methyl-3-(phenylthio)quinoline (3ab) : 106.7 mg, 86%, yellow solid. Mp: 105 - 107 ^{o}C.

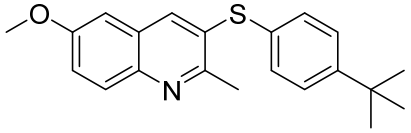
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 9.2 Hz, 1H), 7.74 (s, 1H), 7.36 – 7.27 (m, 6H), 6.86 (d, *J* = 2.8 Hz, 1H), 3.85 (s, 3H), 2.72 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.5, 155.7, 142.4, 136.1, 133.6, 131.4, 130.3, 129.7, 129.5, 128.2, 127.6, 122.0, 104.3, 55.4, 23.5. HRMS (ESI) m/z calcd for $C_{17}H_{16}NOS^+$ $(M+H)^+$282.0947, found 282.0968.



3-((4-Isopropylphenyl)thio)-6-methoxy-2-methylquinoline (3ac) : 132.4 mg, 82%, yellow solid. Mp:

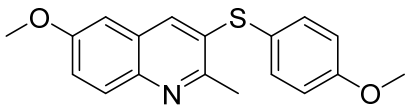
56 - 58 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 9.2 Hz, 1H), 7.65 (s, 1H), 7.35 – 7.23 (m, 5H), 6.84 (d, *J* = 2.8 Hz, 1H), 3.85 (s, 3H), 2.97 – 2.88 (m, 1H), 2.73 (s, 3H), 1.27 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 155.2, 149.0, 142.1, 134.7, 132.4, 131.5, 129.7, 129.6, 128.2, 127.8, 121.6, 104.3, 55.4, 33.7, 23.8, 23.5. HRMS (ESI) m/z calcd for $C_{20}H_{22}NOS^+$ $(M+H)^+$324.1417, found 324.1439.



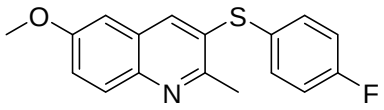
3-((4-(*tert*-butyl)phenyl)thio)-6-methoxy-2-methylquinoline (3ad) : 141.5 mg, 84%, yellow solid. Mp: 76 - 78 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 9.2 Hz, 1H), 7.68 (s, 1H), 7.42 – 7.36 (m, 2H), 7.34 – 7.23 (m, 3H), 6.84 (d, *J* = 2.8 Hz, 1H), 3.84 (s, 3H), 2.73 (s, 3H), 1.33 (s, 9H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 155.3, 151.2, 142.2, 134.9, 131.8, 131.3, 129.7, 129.5, 128.2, 126.6, 121.6, 104.3, 55.4, 34.6, 31.2, 23.6. HRMS (ESI) m/z calcd for $C_{21}H_{24}NOS^+$ $(M+H)^+$338.1573, found 338.1592.



6-Methoxy-3-((4-methoxyphenyl)thio)-2-methylquinoline (3ae) : 94.7 mg, 61%, yellow solid. Mp: 119 - 121 °C.

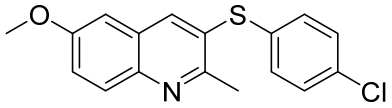
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 9.2 Hz, 1H), 7.47 – 7.42 (m, 2H), 7.37 (s, 1H), 7.26 – 7.21 (m, 1H), 7.01 – 6.96 (m, 2H), 6.79 (d, *J* = 2.8 Hz, 1H), 3.86 (s, 3H), 3.84 (s, 3H), 2.73 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 160.3, 157.4, 153.8, 141.6, 135.9, 133.7, 131.7, 129.6, 128.3, 121.9, 121.2, 115.4, 104.1, 55.4, 55.4, 23.4. HRMS (ESI) m/z calcd for $C_{18}H_{18}NO_2S^+$ $(M+H)^+$312.1053, found 312.1074.



3-((4-Fluorophenyl)thio)-6-methoxy-2-methylquinoline (3af) 97.8 mg, 53%, yellow solid. Mp: 128 - 130 °C.

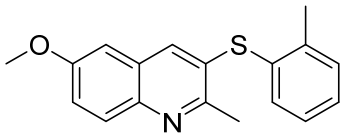
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 9.2 Hz, 1H), 7.57 (s, 1H), 7.44 – 7.36 (m, 2H), 7.31 – 7.25 (m, 1H), 7.09 (t, *J* = 8.6 Hz, 2H), 6.84 (d, *J* = 2.8 Hz, 1H), 3.85 (s, 3H), 2.71 (s, 3H) ^{13}C NMR (100 MHz, Chloroform-*d*) δ 162.7 (d, *J* = 247.3 Hz), 157.5, 154.8, 142.1, 134.6 (d, *J* = 8.3 Hz), 134.4, 131.3, 129.7, 128.2, 128.0 (d, *J* = 3.4 Hz), 121.8, 117.0 (d, *J* = 21.9 Hz), 104.2, 55.41, 23.45. HRMS (ESI) m/z calcd for $C_{17}H_{15}FNOS^+$ $(M+H)^+$300.0853,

found 300.0870.



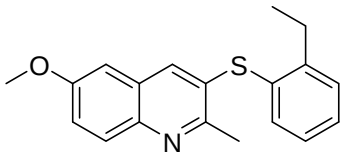
3-((4-Chlorophenyl)thio)-6-methoxy-2-methylquinoline (3ag) : 48.0 mg, 31%, yellow solid. Mp: 64 - 66 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 9.2 Hz, 1H), 7.76 (s, 1H), 7.35 – 7.29 (m, 3H), 7.27 – 7.23 (m, 2H), 6.89 (d, *J* = 2.8 Hz, 1H), 3.87 (s, 3H), 2.71 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.6, 155.7, 142.6, 136.6, 133.7, 132.5, 132.4, 129.8, 129.7, 129.5, 128.2, 122.3, 104.3, 55.5, 23.5. HRMS (ESI) m/z calcd for $C_{17}H_{15}ClNOS^{+}$ $(M+H)^{+}$ 316.0557, found 316.0581.



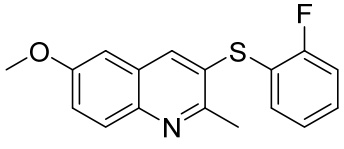
6-Methoxy-2-methyl-3-(*o*-tolylthio)quinoline (3ah) : 101.8 mg, 69%, white solid. Mp: 91 - 93 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 9.2 Hz, 1H), 7.41 (s, 1H), 7.35 – 7.23 (m, 4H), 7.22 – 7.16 (m, 1H), 6.80 (d, *J* = 2.8 Hz, 1H), 3.82 (s, 3H), 2.74 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 154.8, 141.9, 140.5, 133.5, 133.4, 131.6, 130.9, 129.7, 128.6, 128.3, 127.1, 121.5, 104.2, 55.4, 23.4, 20.4. HRMS (ESI) m/z calcd for $C_{18}H_{18}NOS^{+}$ $(M+H)^{+}$ 296.1104, found 296.1123.



3-((2-Ethylphenyl)thio)-6-methoxy-2-methylquinoline (3ai) : 100.4 mg, 65%. yellow solid. Mp: 78 - 80 ^{o}C.

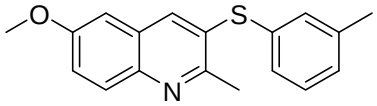
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 9.2 Hz, 1H), 7.43 (s, 1H), 7.39 – 7.31 (m, 2H), 7.26 (ddd, *J* = 6.7, 5.2, 2.3 Hz, 2H), 7.21 – 7.17 (m, 1H), 6.80 (d, *J* = 2.8 Hz, 1H), 3.83 (s, 3H), 2.81 (q, *J* = 7.5 Hz, 2H), 2.74 (s, 3H), 1.23 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 154.8, 146.3, 141.9, 133.8, 133.6, 131.6, 131.0, 129.7, 129.3, 128.8, 128.3, 127.1, 121.5, 104.2, 55.4, 27.1, 23.4, 15.0. HRMS (ESI) m/z calcd for $C_{19}H_{20}NOS^{+}$ $(M+H)^{+}$ 310.1260, found 310.1282.



3-((2-Fluorophenyl)thio)-6-methoxy-2-methylquinoline (3aj) : 76.2 mg, 51%, yellow solid. Mp: 44 -

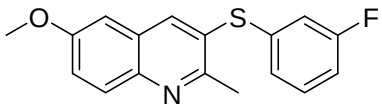
46 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 9.1 Hz, 1H), 7.74 (s, 1H), 7.38 – 7.08 (m, 5H), 6.88 (d, *J* = 2.8 Hz, 1H), 3.87 (s, 3H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 161.4 (d, *J* = 246.3 Hz), 157.6, 155.6, 142.6, 136.2, 133.5, 130.0 (d, *J* = 7.7 Hz), 129.8, 128.6, 128.2, 125.0 (d, *J* = 3.8 Hz), 122.2, 120.7 (d, *J* = 17.9 Hz), 116.2 (d, *J* = 21.9 Hz), 104.3, 55.5, 23.5. HRMS (ESI) m/z calcd for $C_{17}H_{15}FNOS^+$ $(M+H)^+$ 300.0853, found 300.0873.



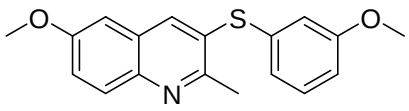
6-Methoxy-2-methyl-3-(*m*-tolylthio)quinoline (3ak) : 103.3 mg, 70%, yellow solid. Mp: 38 - 40 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 9.2 Hz, 1H), 7.73 (s, 1H), 7.33 – 7.22 (m, 2H), 7.21 – 7.10 (m, 3H), 6.88 (d, *J* = 2.8 Hz, 1H), 3.86 (s, 3H), 2.72 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.5, 155.7, 142.4, 139.5, 135.9, 133.2, 132.1, 130.6, 129.7, 129.4, 128.6, 128.6, 128.2, 121.9, 104.3, 55.4, 23.6, 21.3. HRMS (ESI) m/z calcd for $C_{18}H_{18}NOS^+$ $(M+H)^+$ 296.1104, found 296.1122.



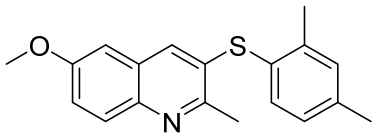
3-((3-Fluorophenyl)thio)-6-methoxy-2-methylquinoline (3al) : 73.4 mg, 50%, yellow solid. Mp: 48 - 50 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 – 7.89 (m, 2H), 7.37 – 7.33 (m, 1H), 7.32 – 7.27 (m, 1H), 7.06 – 7.01 (m, 1H), 6.99 – 6.92 (m, 3H), 3.90 (s, 3H), 2.71 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 163.1 (d, *J* = 247.7 Hz), 157.7, 156.7, 143.1, 138.8, 137.2 (d, *J* = 7.7 Hz), 130.7 (d, *J* = 8.7 Hz), 129.9, 128.2, 128.0, 125.4 (d, *J* = 3.0 Hz), 122.7, 116.6 (d, *J* = 23.0 Hz), 114.1 (d, *J* = 21.1 Hz), 104.5, 55.5, 23.6. HRMS (ESI) m/z calcd for $C_{17}H_{15}FNOS^+$ $(M+H)^+$ 300.0853, found 300.0875.



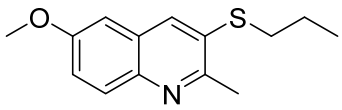
6-Methoxy-3-((3-methoxyphenyl)thio)-2-methylquinoline (3am) : 90.2 mg, 58%. white solid. Mp: 59 - 61 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 9.2 Hz, 1H), 7.80 (s, 1H), 7.33 – 7.23 (m, 2H), 6.93 – 6.82 (m, 4H), 3.87 (s, 3H), 3.76 (s, 3H), 2.72 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 160.3, 157.5, 156.0, 142.6, 136.6, 135.1, 130.3, 129.9, 129.8, 128.2, 123.3, 122.1, 116.3, 113.3, 104.4, 55.4, 55.3, 23.6. HRMS (ESI) m/z calcd for $C_{18}H_{18}NO_2S^+$ $(M+H)^+$ 312.1053, found 312.1073.



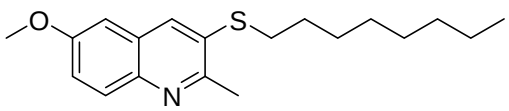
3-((2,4-Dimethylphenyl)thio)-6-methoxy-2-methylquinoline (3an) 97.3 mg, 63%, yellow solid. Mp: 120 - 122 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 9.2 Hz, 1H), 7.29 (d, *J* = 7.9 Hz, 1H), 7.26 – 7.16 (m, 3H), 7.07 – 7.02 (m, 1H), 6.77 (d, *J* = 2.8 Hz, 1H), 3.82 (s, 3H), 2.75 (s, 3H), 2.37 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 154.1, 141.6, 141.3, 139.3, 134.8, 132.2, 131.9, 131.5, 129.7, 128.3, 128.0, 127.2, 121.1, 104.1, 55.4, 23.3, 21.1, 20.4. HRMS (ESI) m/z calcd for $C_{19}H_{20}NOS^+$ $(M+H)^+$ 310.1260, found 310.1281.



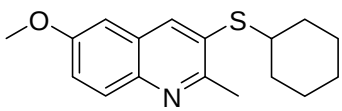
6-Methoxy-2-methyl-3-(propylthio)quinoline (3ao) : 87.7 mg, 71%, yellow solid. Mp: 61 - 63 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 9.1 Hz, 1H), 7.69 (s, 1H), 7.28 – 7.21 (m, 1H), 6.94 (d, *J* = 2.8 Hz, 1H), 3.89 (s, 3H), 2.96 (t, *J* = 7.3 Hz, 2H), 2.70 (s, 3H), 1.77 (h, *J* = 7.4 Hz, 2H), 1.10 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 154.5, 141.0, 132.1, 130.1, 129.6, 128.1, 120.6, 104.0, 55.3, 34.1, 23.3, 21.7, 13.6. HRMS (ESI) m/z calcd for $C_{14}H_{18}NOS^+$ $(M+H)^+$ 248.1104, found 248.1127.



6-Methoxy-2-methyl-3-(octylthio)quinoline (3ap) 125.2 mg, 79%, yellow solid. Mp: 53 - 54 °C.

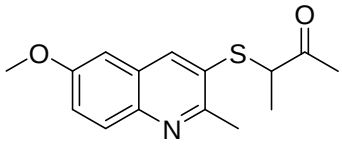
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 9.2 Hz, 1H), 7.69 (s, 1H), 7.26 – 7.20 (m, 1H), 6.94 (d, *J* = 2.8 Hz, 1H), 3.89 (s, 3H), 2.97 (t, *J* = 7.4 Hz, 2H), 2.70 (s, 3H), 1.78 – 1.68 (m, 2H), 1.48 (p, *J* = 7.0 Hz, 2H), 1.34 – 1.23 (m, 8H), 0.90 – 0.86 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 154.4, 141.0, 132.3, 130.0, 129.7, 128.2, 120.6, 104.0, 55.3, 32.1, 31.7, 29.1, 29.0, 28.2, 23.3, 22.6, 14.0. HRMS (ESI) m/z calcd for $C_{19}H_{28}NOS^+$ $(M+H)^+$ 318.1886, found 318.1902.



3-(Cyclohexylthio)-6-methoxy-2-methylquinoline (3aq) : 104.7 mg, 73%. yellow solid. Mp: 73 - 75 °C.

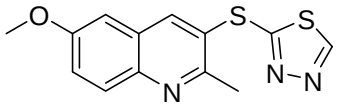
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 – 7.85 (m, 2H), 7.30 – 7.26 (m, 1H), 6.98 (d, *J* = 2.8 Hz, 1H), 3.92 (s, 3H), 3.28 – 3.19 (m, 1H), 2.75 (s, 3H), 2.07 – 2.02 (m, 2H), 1.86 – 1.80 (m, 2H), 1.68 – 1.64 (m, 1H), 1.50 – 1.28 (m, 5H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 156.4, 141.8, 134.7, 130.2, 129.7, 128.1, 121.4, 104.2, 55.5, 45.5, 33.0, 26.0, 25.7, 23.8. HRMS (ESI) m/z calcd for $C_{17}H_{22}NOS^+$ $(M+H)^+$ 288.1417, found 288.1440.



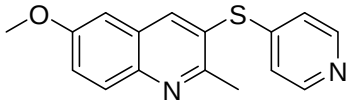
3-((6-Methoxy-2-methylquinolin-3-yl)thio)butan-2-one (3ar) : 48.2 mg, 35%, yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 – 7.84 (m, 2H), 7.32 – 7.28 (m, 1H), 6.98 (d, *J* = 2.8 Hz, 1H), 3.91 (s, 3H), 3.94 – 3.89 (m, 1H) 2.76 (s, 3H), 2.30 (s, 3H), 1.54 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 206.0, 157.6, 155.5, 142.2, 135.4, 129.7, 128.3, 128.1, 122.2, 104.3, 55.5, 51.0, 25.6, 23.7, 16.1. HRMS (ESI) m/z calcd for $C_{15}H_{18}NO_2S^+$ $(M+H)^+$ 276.1053, found 276.1076.



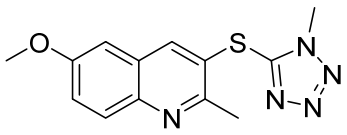
2-((6-Methoxy-2-methylquinolin-3-yl)thio)-1,3,4-thiadiazole (3as) : 46.2 mg, 32%. yellow solid. Mp: 123 - 125 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.03 (s, 1H), 8.40 (s, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.46 – 7.40 (m, 1H), 7.04 (d, *J* = 2.8 Hz, 1H), 3.93 (s, 3H), 2.82 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.9, 157.9, 157.2, 152.4, 144.2, 142.4, 130.0, 128.1, 124.2, 124.2, 104.7, 55.6, 23.7. HRMS (ESI) m/z calcd for $C_{13}H_{12}N_3OS_2^+$ $(M+H)^+$ 290.0416, found 290.0440.



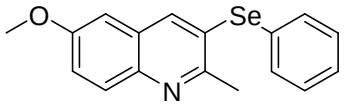
6-Methoxy-2-methyl-3-(pyridin-4-ylthio)quinoline (3at) : 25.4 mg, 18%, yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 – 8.35 (m, 2H), 8.28 (s, 1H), 7.97 (d, *J* = 9.2 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.04 (d, *J* = 2.8 Hz, 1H), 6.95 – 6.89 (m, 2H), 3.94 (s, 3H), 2.72 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 158.4, 157.9, 149.6, 148.7, 144.1, 143.2, 130.1, 128.2, 123.8, 123.3, 120.8, 104.7, 55.6, 23.7. HRMS (ESI) m/z calcd for $C_{16}H_{15}N_2OS^+$ $(M+H)^+$ 283.0900, found 283.0916.

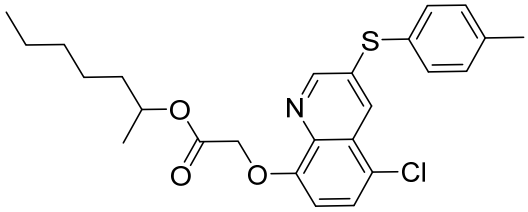


6-Methoxy-2-methyl-3-((1-methyl-1*H*-tetrazol-5-yl)thio)quinoline (3au) : 57.4 mg, 40%, yellow solid. Mp: 123 - 125 ^{o}C.

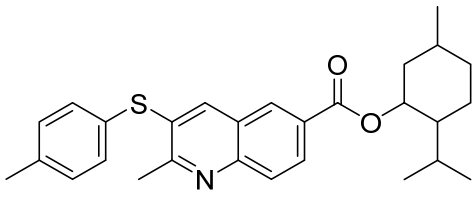
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (s, 1H), 7.91 (d, *J* = 9.2 Hz, 1H), 7.41 – 7.36 (m, 1H), 6.98 (d, *J* = 2.8 Hz, 1H), 4.06 (s, 3H), 3.90 (s, 3H), 2.79 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.9, 155.7, 151.7, 143.7, 140.0, 129.9, 128.1, 123.8, 121.6, 104.6, 55.6, 34.0, 23.7. HRMS (ESI) m/z calcd for $C_{13}H_{14}N_5OS^+$ $(M+H)^+$288.0914, found 288.0933.



6-Methoxy-2-methyl-3-(phenylselanyl)quinoline (3av) : 101.2 mg, 62%, yellow solid. Mp: 79 - 81 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 9.1 Hz, 1H), 7.74 (s, 1H), 7.38 – 7.08 (m, 5H), 6.88 (d, *J* = 2.8 Hz, 1H), 3.87 (s, 3H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.4, 155.9, 142.7, 137.7, 133.9, 129.7, 129.7, 129.0, 128.5, 128.1, 127.4, 121.9, 104.2, 55.4, 25.0. HRMS (ESI) m/z calcd for $C_{17}H_{16}NOSe^+$ $(M+H)^+$330.0392, found 330.0407.



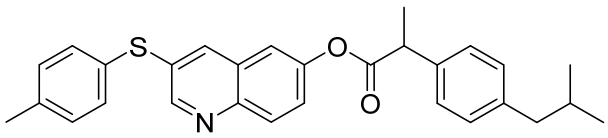
Heptan-2-yl 2-((5-chloro-3-(*p*-tolylthio)quinolin-8-yl)oxy)acetate (4a) : 50.2 mg, 22%, yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.76 (d, *J* = 2.2 Hz, 1H), 8.27 (d, *J* = 2.2 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.40 – 7.36 (m, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 1H), 5.04 – 4.99 (m, 1H), 4.90 (s, 2H), 2.38 (s, 3H), 1.58 – 1.42 (m, 2H), 1.21 (p, *J* = 5.1, 4.5 Hz, 9H), 0.84 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.1, 153.0, 150.2, 138.9, 138.4, 134.3, 133.0, 131.3, 130.5, 128.5, 127.2, 126.8, 122.6, 109.2, 72.7, 66.4, 35.7, 31.5, 24.9, 22.5, 21.2, 19.8, 13.9. HRMS (ESI) m/z calcd for $C_{25}H_{29}ClNO_3S^+$ $(M+H)^+$458.1551, found 458.1566.



2-Isopropyl-5-methylcyclohexyl 2-methyl-3-(*p*-tolylthio)quinoline-6-carboxylate (4b) : 91.6 mg, 41%, yellow oil.

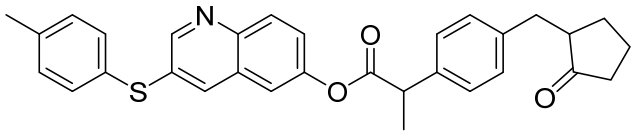
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 1.8 Hz, 1H), 8.24 – 8.16 (m, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.65 (s, 1H), 7.37 (d, *J* = 7.8 Hz, 2H), 7.25 (d, *J* = 8.1 Hz, 2H), 5.04 – 4.93 (m, 1H), 2.80 (s, 3H), 2.42 (s, 3H), 2.12 (dt, *J* =

12.3, 4.0 Hz, 1H), 1.96 (pd, *J* = 6.8, 2.5 Hz, 1H), 1.77 – 1.70 (m, 2H), 1.61 – 1.53 (m, 2H), 1.18 – 1.07 (m, 2H), 0.95 – 0.90 (m, 7H), 0.79 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.6, 159.4, 147.4, 139.1, 134.7, 133.6, 133.6, 130.7, 129.5, 128.4, 128.4, 128.3, 127.8, 126.5, 75.1, 47.2, 40.9, 34.2, 31.4, 26.4, 24.0, 23.5, 22.0, 21.24, 20.8, 16.4. HRMS (ESI) m/z calcd for $C_{28}H_{34}NO_2S^+$(M+H)$^+$ 448.2305, found 448.2319.



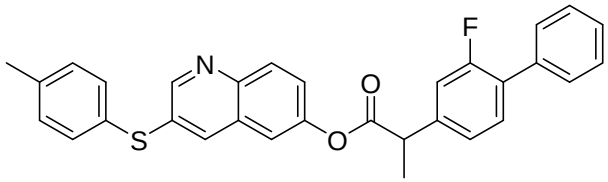
3-(*p*-Tolylthio)quinolin-6-yl 2-(4-isobutylphenyl)propanoate (4c) : 84.2 mg, 37%, yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 2.2 Hz, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.76 (d, *J* = 2.3 Hz, 1H), 7.39 – 7.26 (m, 6H), 7.21 – 7.14 (m, 4H), 4.03 – 3.92 (m, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 2.37 (s, 3H), 1.91 – 1.83 (m, 1H), 1.62 (d, *J* = 7.1 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.1, 150.6, 149.1, 144.1, 141.0, 138.8, 136.9, 134.1, 133.0, 132.8, 130.6, 130.5, 129.6, 128.8, 128.5, 127.2, 124.1, 117.5, 45.2, 45.0, 30.2, 22.4, 21.2, 18.5. HRMS (ESI) m/z calcd for $C_{29}H_{30}NO_2S^+$ (M+H)$^+$ 456.1992, found 456.2016.



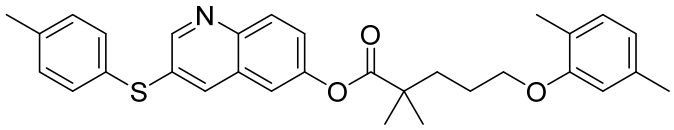
3-(*p*-Tolylthio)quinolin-6-yl 2-(4-((2-oxocyclopentyl)methyl)phenyl)propanoate (4d) : 52.0 mg, 21%, yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.72 (d, *J* = 2.3 Hz, 1H), 8.01 (d, *J* = 9.1 Hz, 1H), 7.77 (d, *J* = 2.3 Hz, 1H), 7.38 – 7.28 (m, 6H), 7.22 – 7.17 (m, 4H), 3.97 (d, *J* = 7.1 Hz, 1H), 3.20 – 3.12 (m, 1H), 2.58 – 2.50 (m, 1H), 2.39 – 2.31 (m, 5H), 2.17 – 2.07 (m, 2H), 2.02 – 1.92 (m, 1H), 1.79 – 1.69 (m, 1H), 1.64 – 1.52 (m, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.0, 150.5, 149.1, 144.1, 139.3, 138.8, 137.5, 134.1, 133.1, 132.9, 130.6, 130.5, 129.4, 128.8, 128.5, 127.6, 124.1, 117.5, 50.9, 45.2, 38.1, 35.2, 29.2, 21.2, 20.5, 18.5. HRMS (ESI) m/z calcd for $C_{31}H_{30}NO_3S^+$ (M+H)$^+$ 496.1941, found 496.1961.



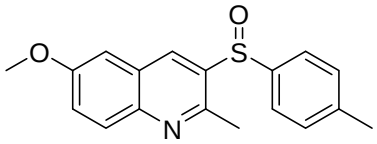
3-(*p*-Tolylthio)quinolin-6-yl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (4e) : 51.7 mg, 21%, white solid. Mp: 95 - 97 ^{o}C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.72 (d, *J* = 2.3 Hz, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 2.3 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.48 – 7.43 (m, 3H), 7.41 – 7.27 (m, 6H), 7.20 (t, *J* = 8.0 Hz, 3H), 4.04 (q, *J* = 7.1 Hz, 1H), 2.37 (s, 3H), 1.68 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.3, 159.8 (d, *J* = 247.2 Hz), 150.5, 149.0, 144.1, 140.9 (d, *J* = 7.6 Hz), 138.9, 135.3, 134.1, 133.1, 133.0, 131.1 (d, *J* = 3.9 Hz), 130.7, 130.5, 128.9 (d, *J* = 2.9 Hz), 128.7, 128.5, 128.5, 128.3, 127.8, 124.0, 123.6 (d, *J* = 3.4 Hz), 117.5, 115.3 (d, *J* = 23.7 Hz), 45.1, 21.2, 18.3. HRMS (ESI) m/z calcd for $C_{31}H_{25}FNO_2S^+$ $(M+H)^+$ 494.1585, found 494.1599.



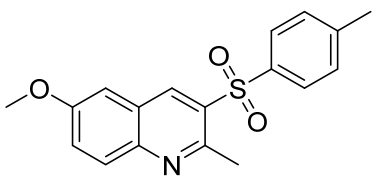
3-(*p*-Tolylthio)quinolin-6-yl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (4f) : 47.4 mg, 19%, yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 (d, *J* = 2.3 Hz, 1H), 8.04 (d, *J* = 8.7 Hz, 1H), 7.77 (d, *J* = 2.3 Hz, 1H), 7.41 – 7.35 (m, 2H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 6.99 (d, *J* = 7.4 Hz, 1H), 6.68 – 6.57 (m, 2H), 4.00 (t, *J* = 5.3 Hz, 2H), 2.38 (s, 3H), 2.29 (s, 3H), 2.16 (s, 3H), 1.94 – 1.84 (m, 4H), 1.40 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.3, 156.7, 150.4, 149.3, 144.0, 138.8, 136.5, 134.1, 133.1, 132.8, 130.6, 130.5, 130.3, 128.8, 128.6, 124.3, 123.5, 120.7, 117.6, 111.8, 67.5, 42.5, 37.1, 25.2, 25.1, 21.4, 21.2, 15.8. HRMS (ESI) m/z calcd for $C_{31}H_{34}NO_3S^+$ $(M+H)^+$ 500.2254, found 500.2270.



6-Methoxy-2-methyl-3-(p-tolylsulfinyl)quinoline (4g) : 40.3 mg, 65%, white solid. Mp: 73 - 75 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 (s, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.46 – 7.40 (m, 1H), 7.28 – 7.21 (m, 3H), 3.95 (s, 3H), 2.52 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.9, 151.1, 144.2, 142.7, 140.0, 137.7, 132.0, 130.2, 129.6, 127.6, 126.8, 124.0, 105.5, 55.6, 22.3, 21.4. HRMS (ESI) m/z calcd for $C_{18}H_{17}NO_2SNa^+$ $(M+Na)^+$ 334.0872, found 334.0892.



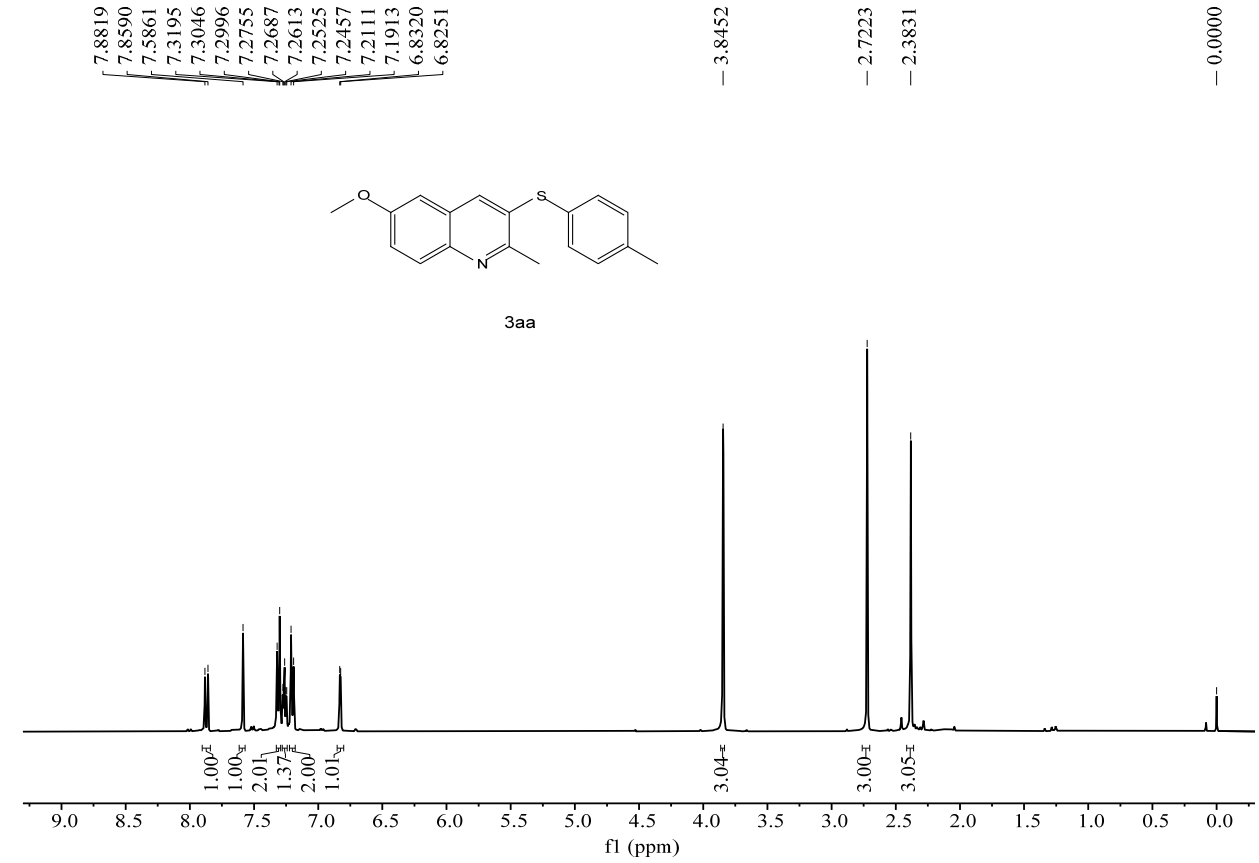
6-Methoxy-2-methyl-3-tosylquinoline (4h) : 46.4 mg, 71%, white solid. Mp: 164 - 166 °C.

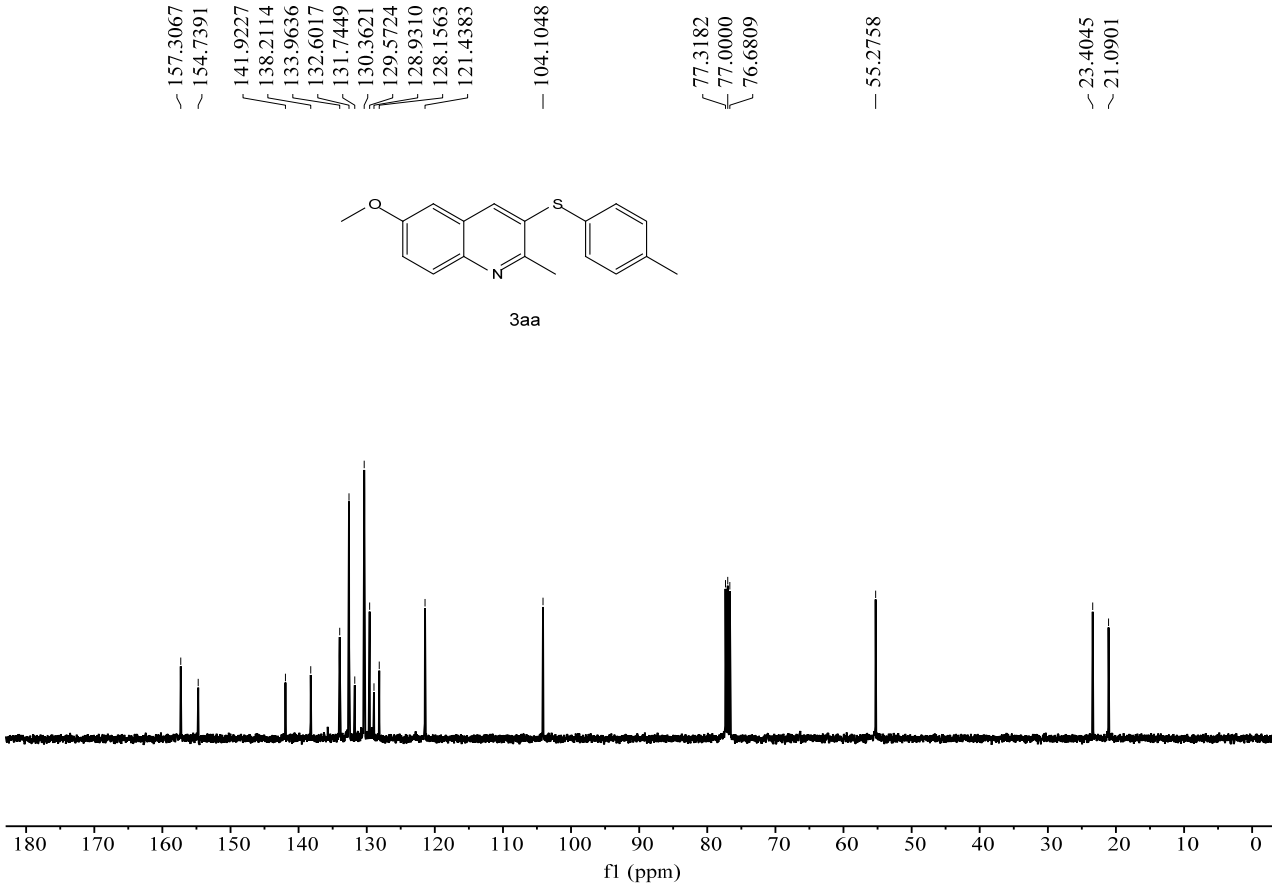
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.94 (s, 1H), 7.93 (d, *J* = 9.2 Hz, 1H), 7.85 – 7.76 (m, 2H), 7.54 – 7.45 (m, 1H),

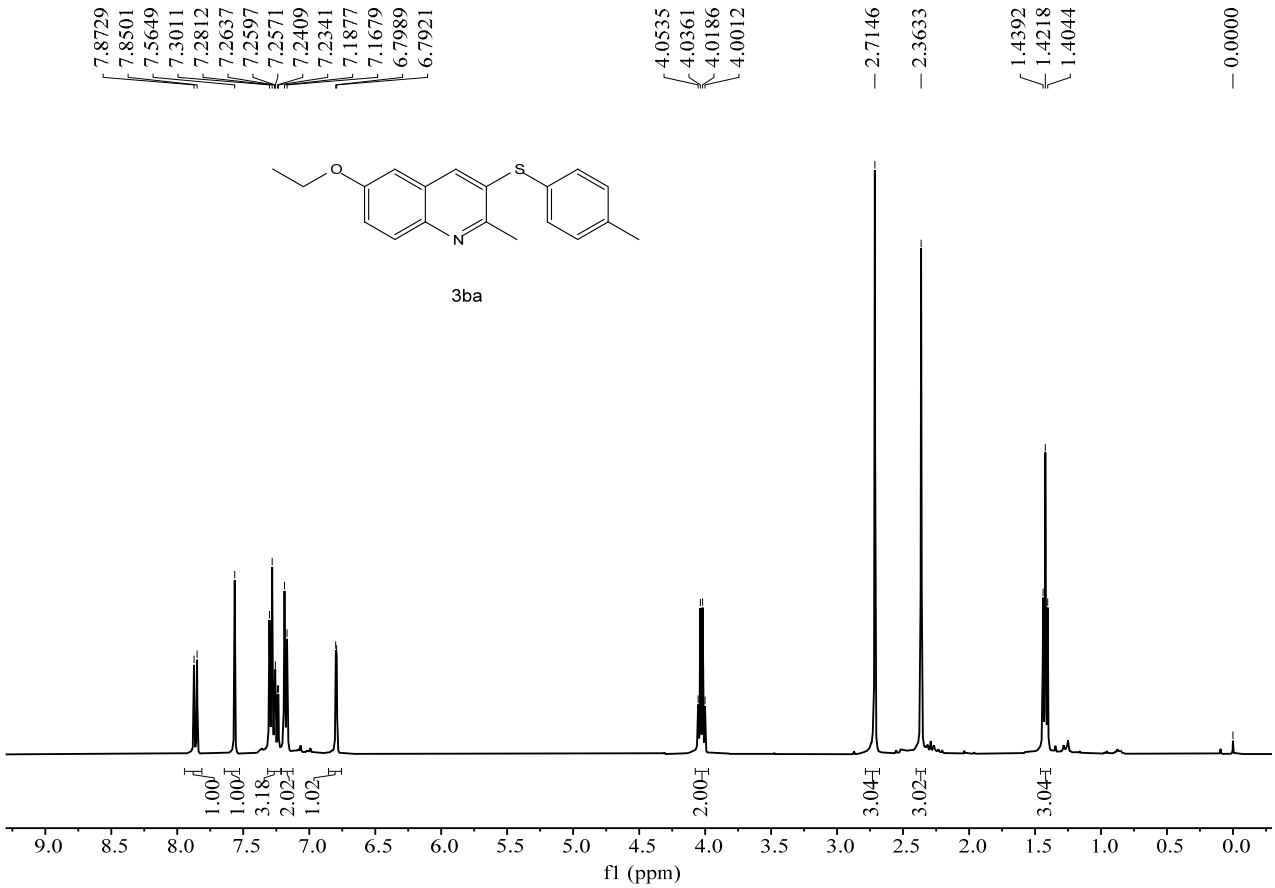
7.32 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 2.8 Hz, 1H), 3.96 (s, 3H), 2.74 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 158.2, 152.5, 145.2, 144.6, 137.6, 137.2, 133.9, 129.9, 129.8, 128.0, 126.7, 125.5, 105.9, 55.7, 23.8, 21.6. HRMS (ESI) m/z calcd for $C_{18}H_{17}NO_3SNa^+$ $(M+Na)^+$350.0821, found 350.0844.

[1] A. Nandy, I. Kazi, S. Guha, G. Sekar, *J. Org. Chem.*, **2021**, *86*, 2570−2581.

6. NMR Spectra for the compounds prepared



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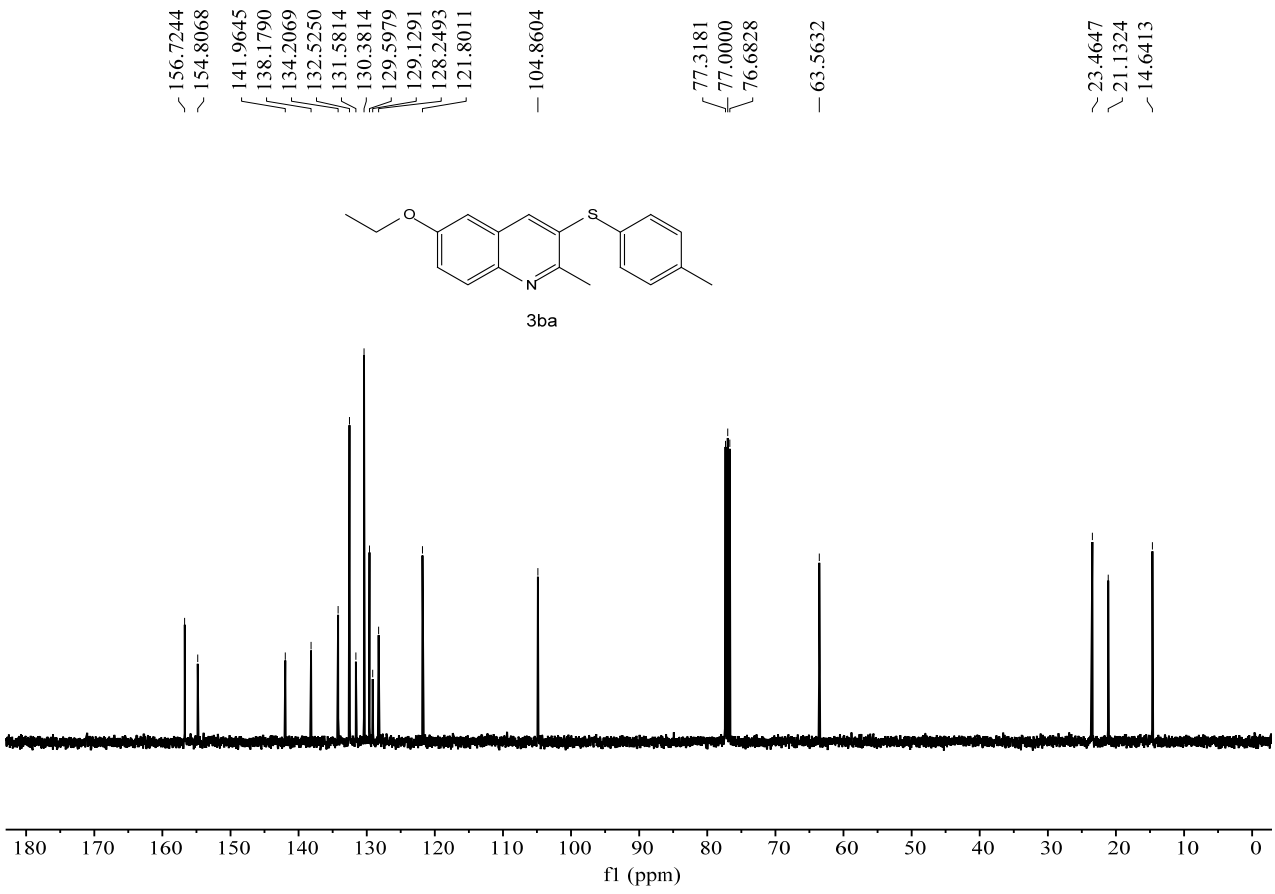
7.1877
7.1679
6.7989
6.7921
4.0535
4.0361
4.0186
4.0012
2.7146
2.3633
1.4392
1.4218
1.4044
0.0000
O
S
N
3ba
1.00
1.00
3.18
2.02
1.02
2.00
3.04
3.02
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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138.1790
134.2069
132.5250
131.5814
130.3814
129.5979
129.1291
128.2493
121.8011
104.8604
77.3181
77.0000
76.6828
63.5632
23.4647
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14.6413
O
S
N
3ba
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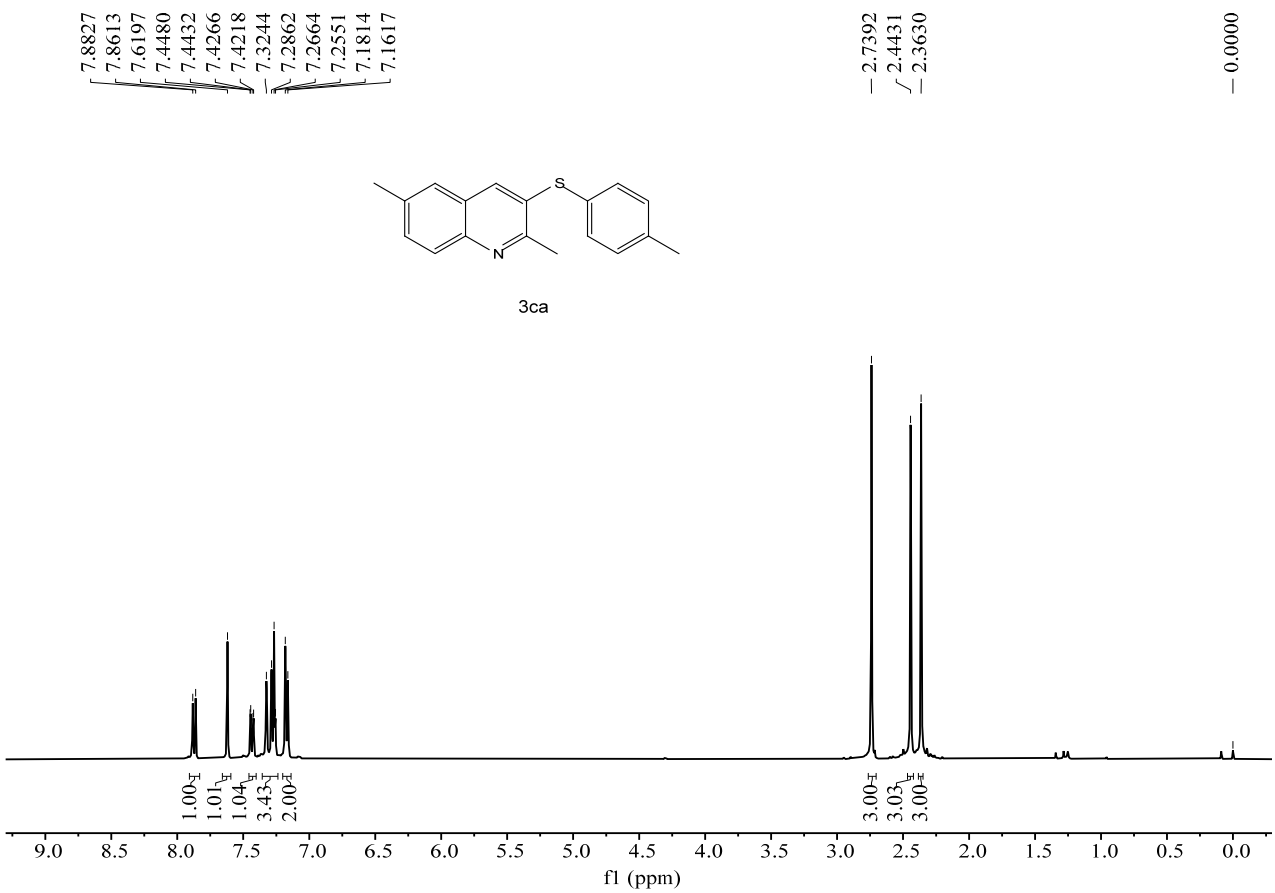
f1 (ppm)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7.4432
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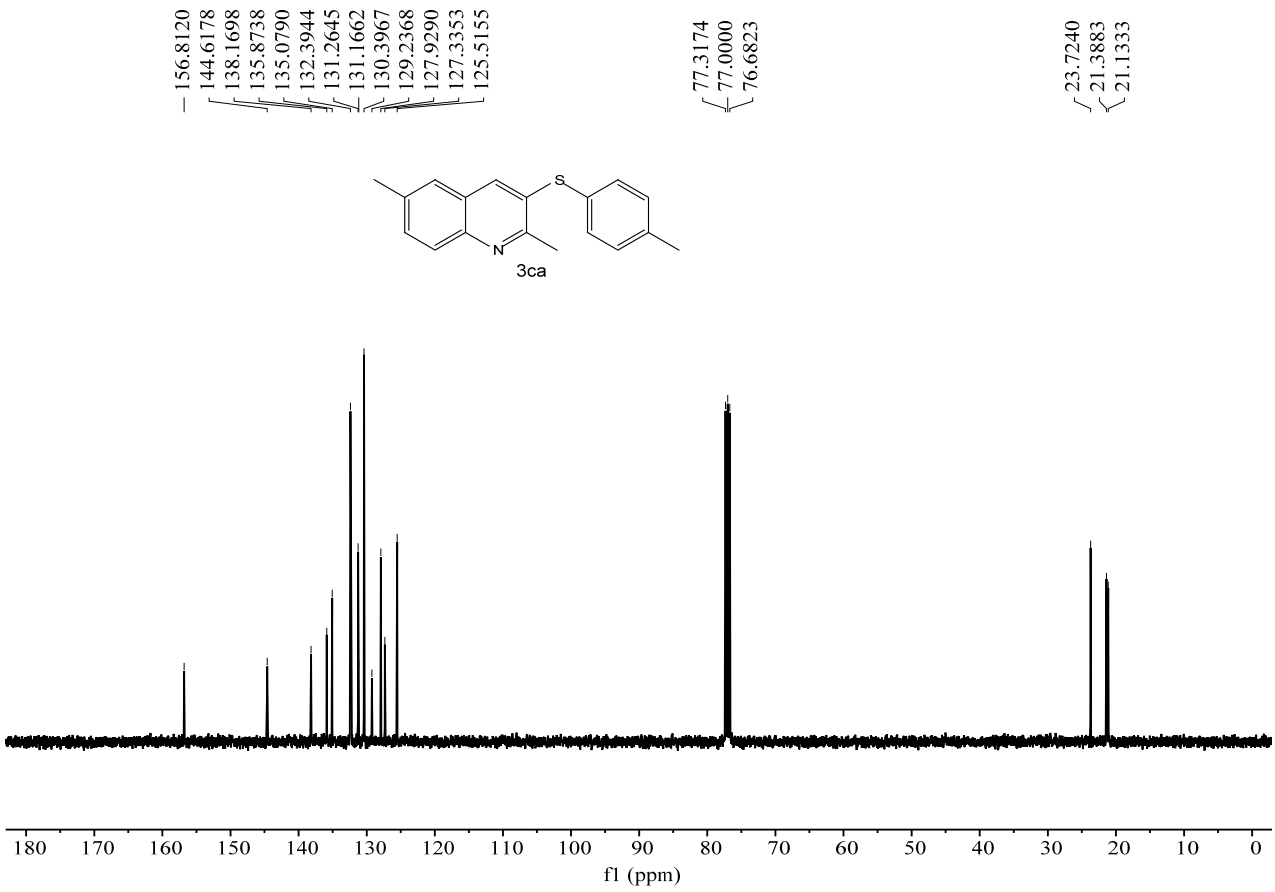
7.4218
7.3244
7.2862
7.2664
7.2551
7.1814
7.1617
2.7392
2.4431
2.3630
0.0000
S
N
3ca
1.00
1.01
1.04
3.43
2.00
3.00
3.03
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.8738
135.0790
132.3944
131.2645
131.1662
130.3967
129.2368
127.9290
127.3353
125.5155
77.3174
77.0000
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23.7240
21.3883
21.1333
S
N
3ca
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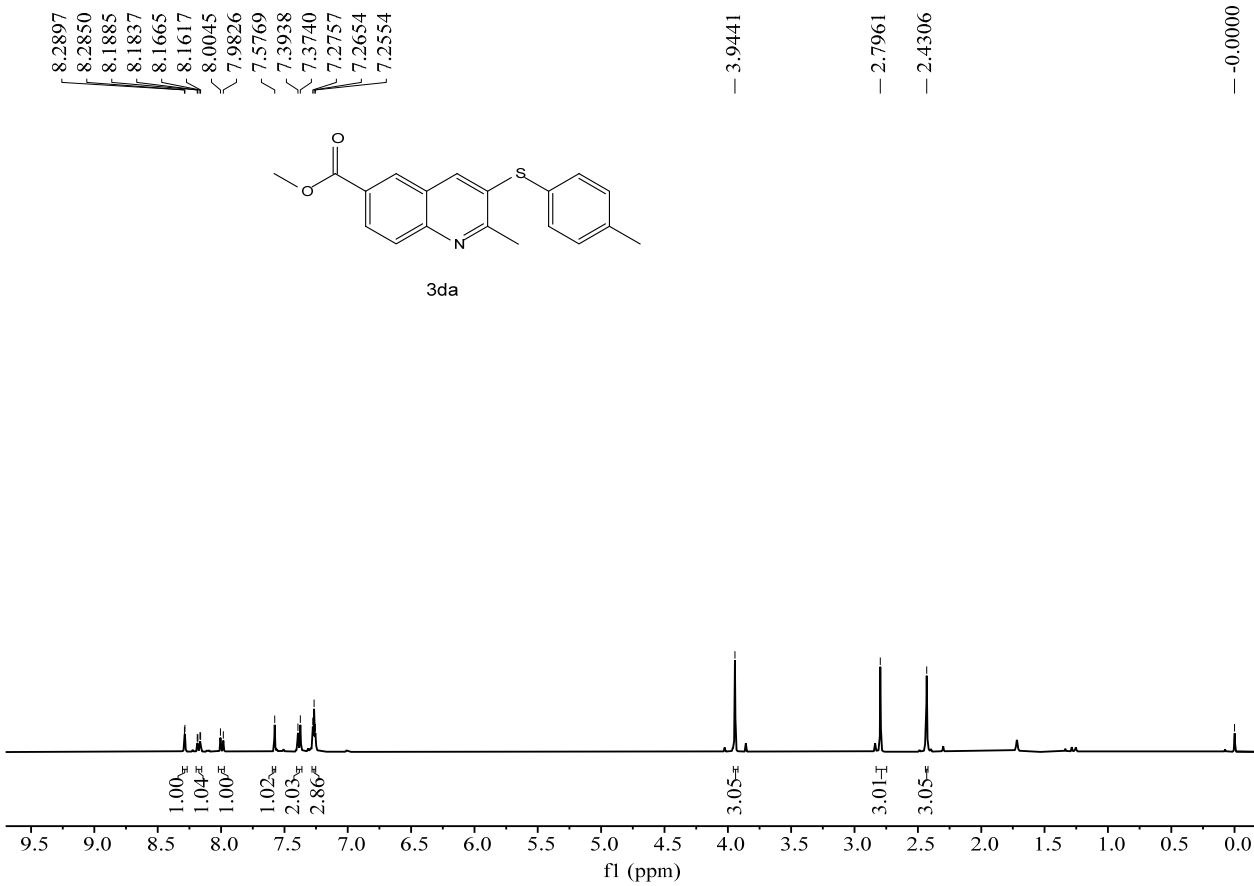
f1 (ppm)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8.1665
8.1617
8.0045
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7.5769
7.3938
7.3740
7.2757
7.2654
7.2554
3.9441
2.7961
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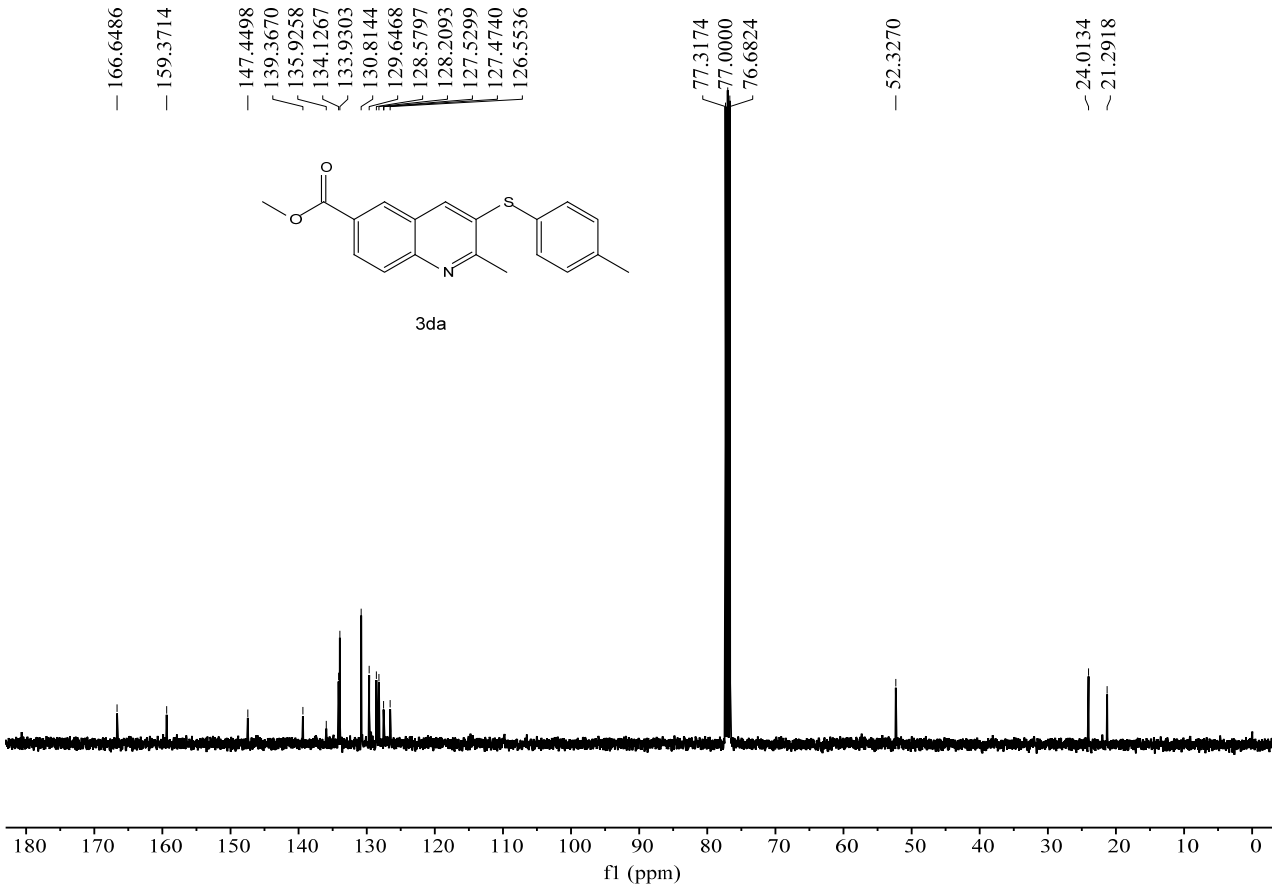
1.00
1.02
2.03
2.86
3.05
3.01
3.05
fl (ppm)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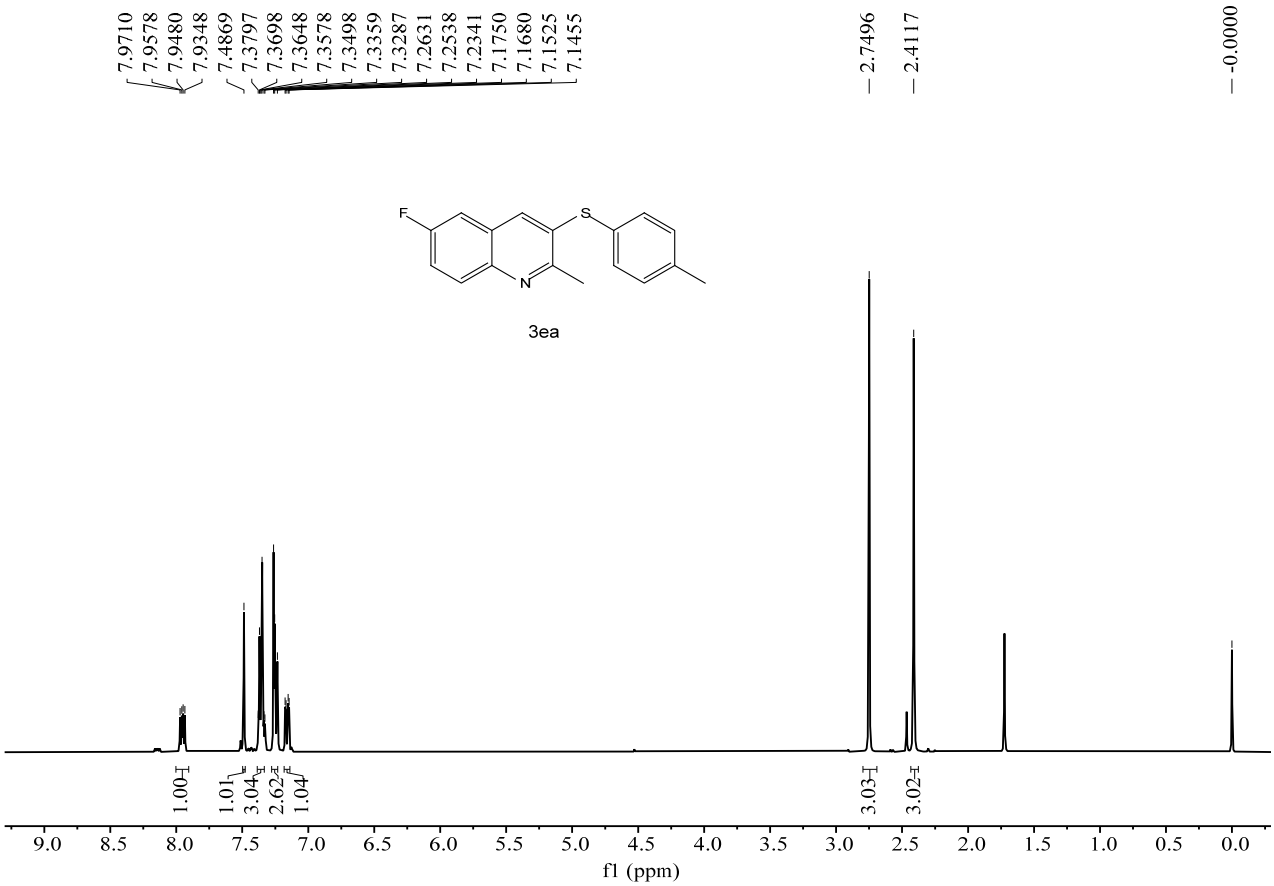
3da
fl (ppm)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7.3287
7.2631
7.2538
7.2341
7.1750
7.1680
7.1525
7.1455
2.7496
2.4117
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F
S
N
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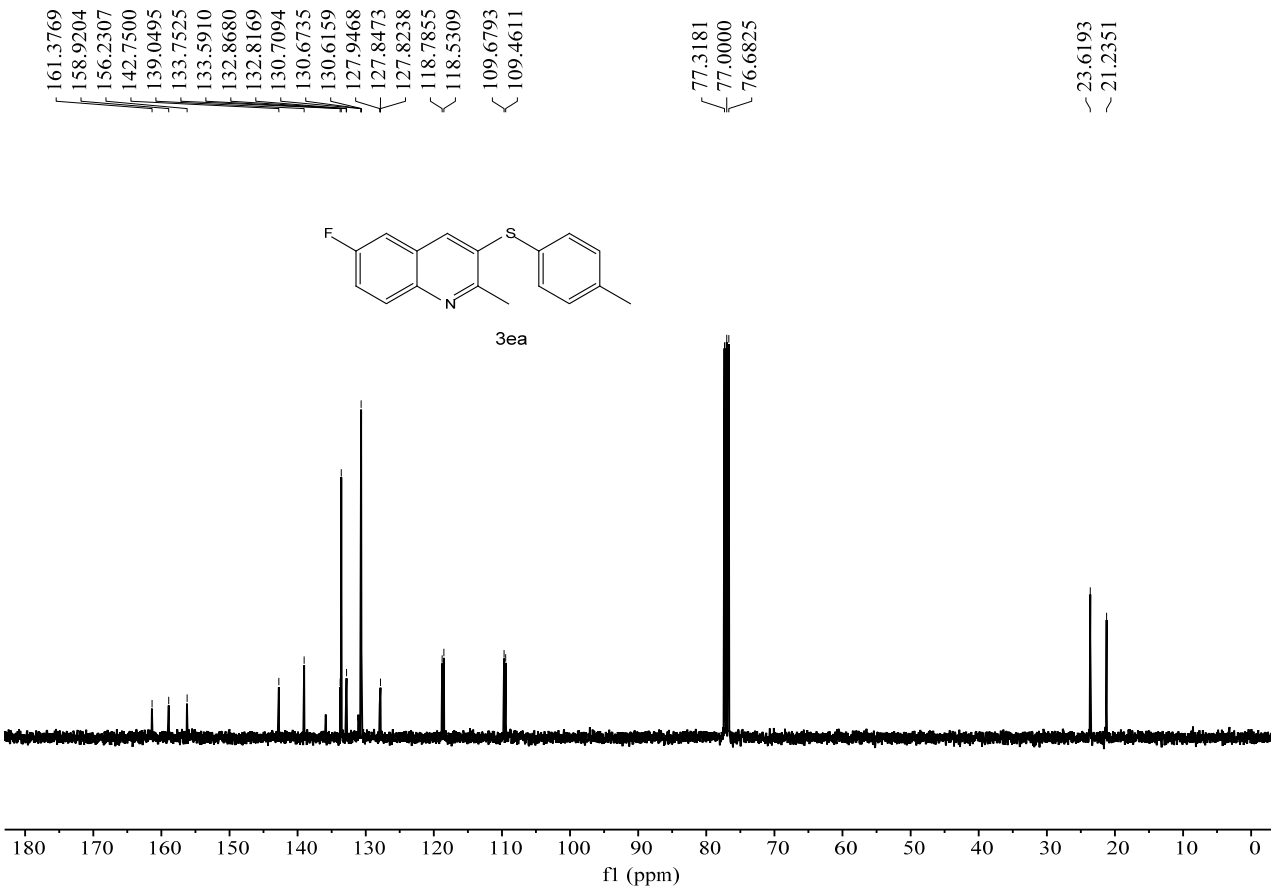
1.00
1.01
3.04
2.62
1.04
3.03
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.8473
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118.5309
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77.3181
77.0000
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S
N
3ea
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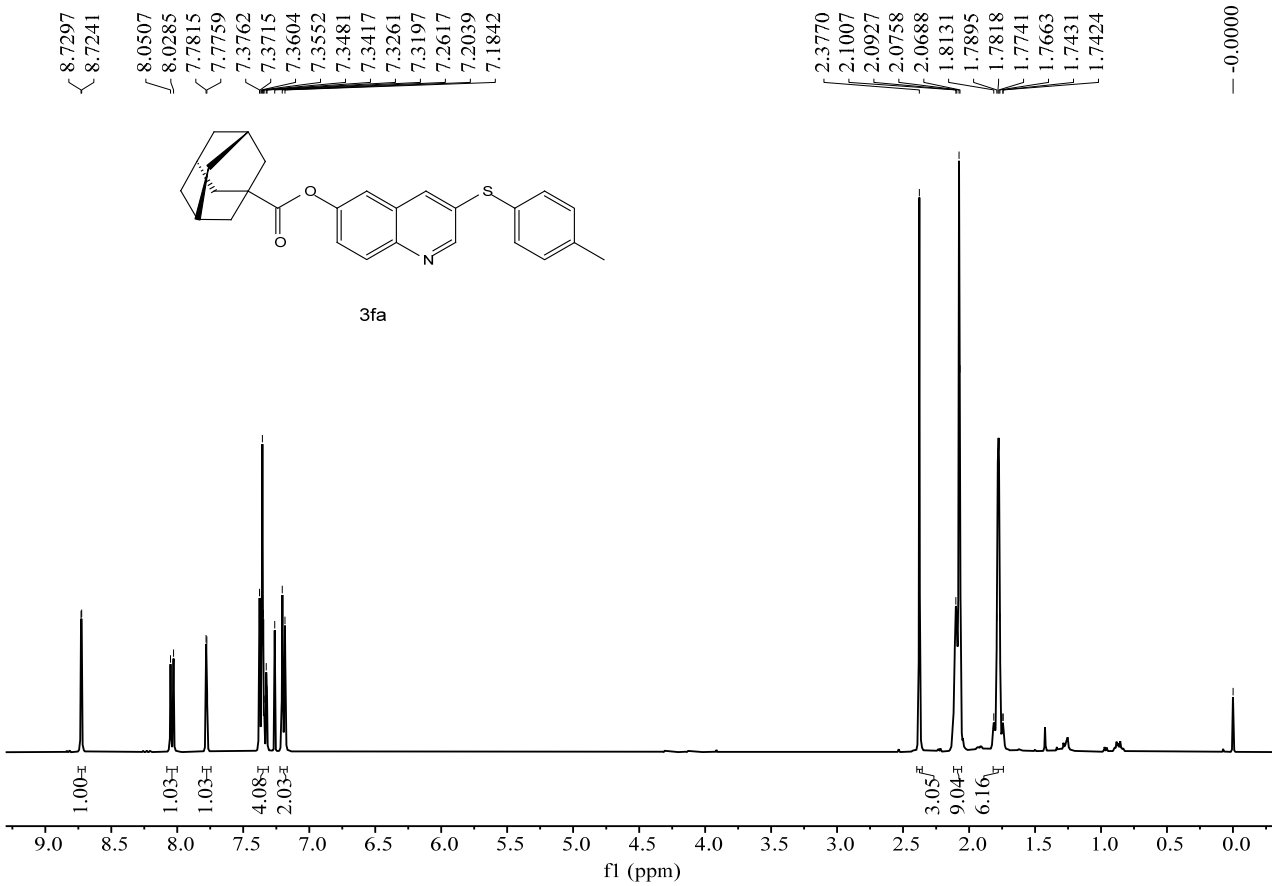
f1 (ppm)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7.3417
7.3261
7.3197
7.2617
7.2039
7.1842
2.3770
2.1007
2.0927
2.0758
2.0688
1.8131
1.7895
1.7818
1.7741
1.7663
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1.7424
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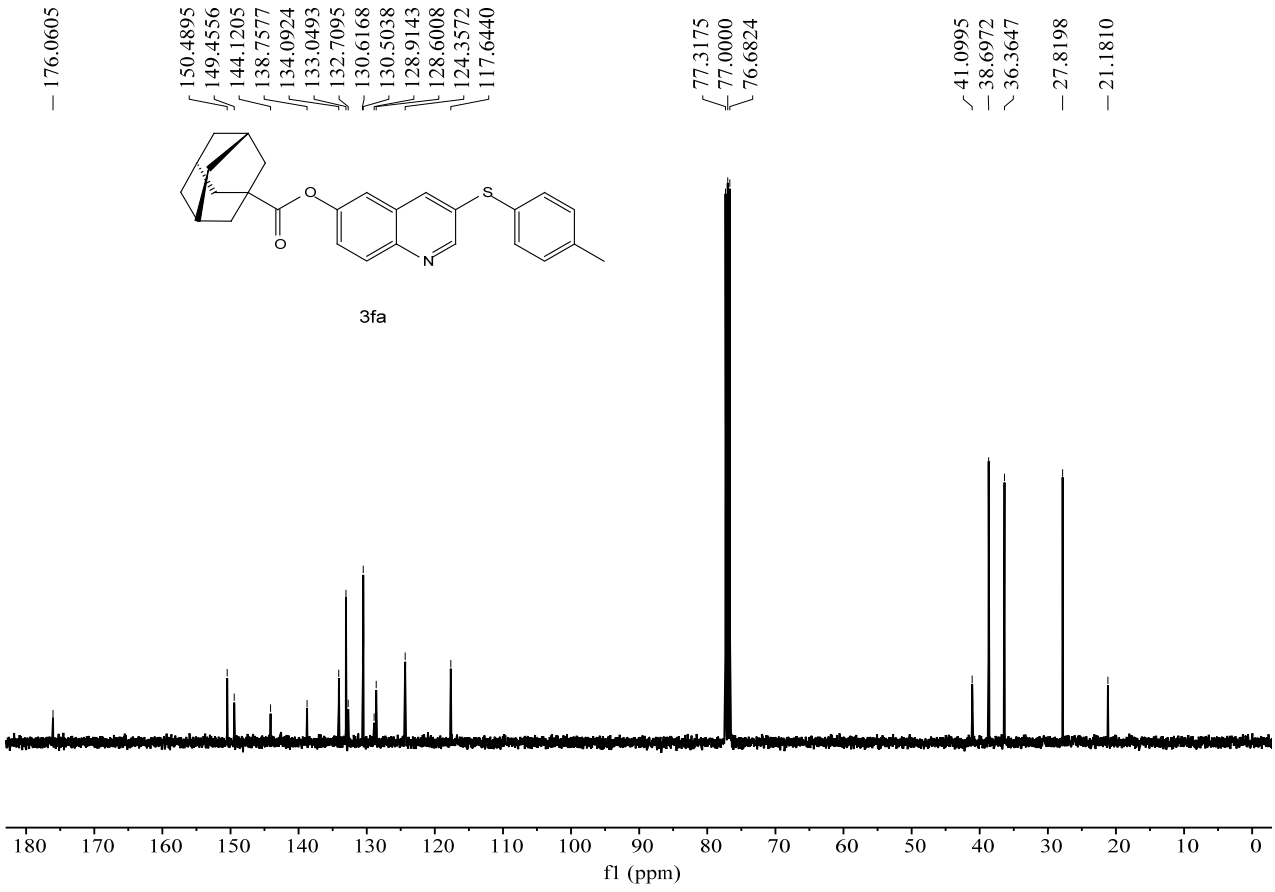
O
S
N
3fa
1.00
1.03
1.03
4.08
2.03
3.05
9.04
6.16
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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S
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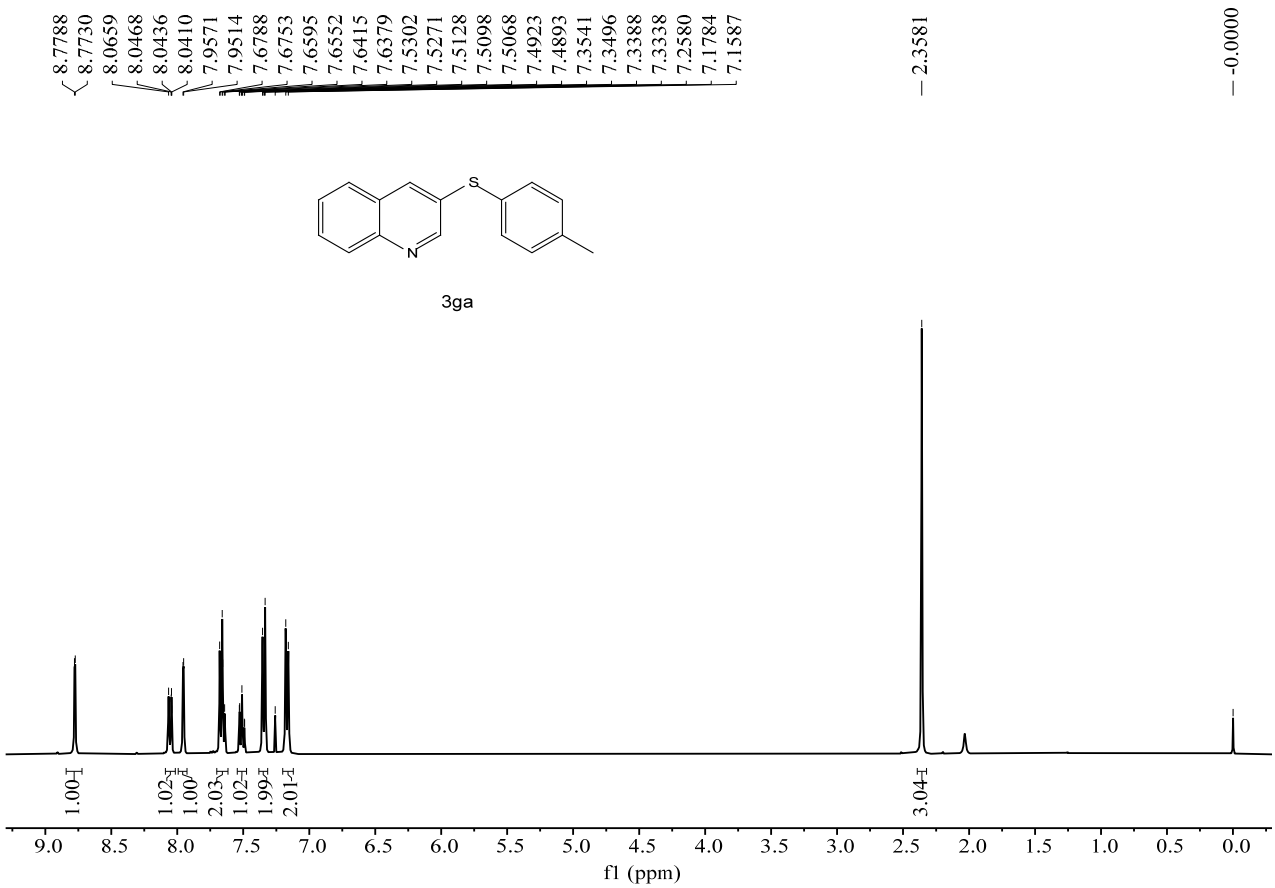
f1 (ppm)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2.01
3.04
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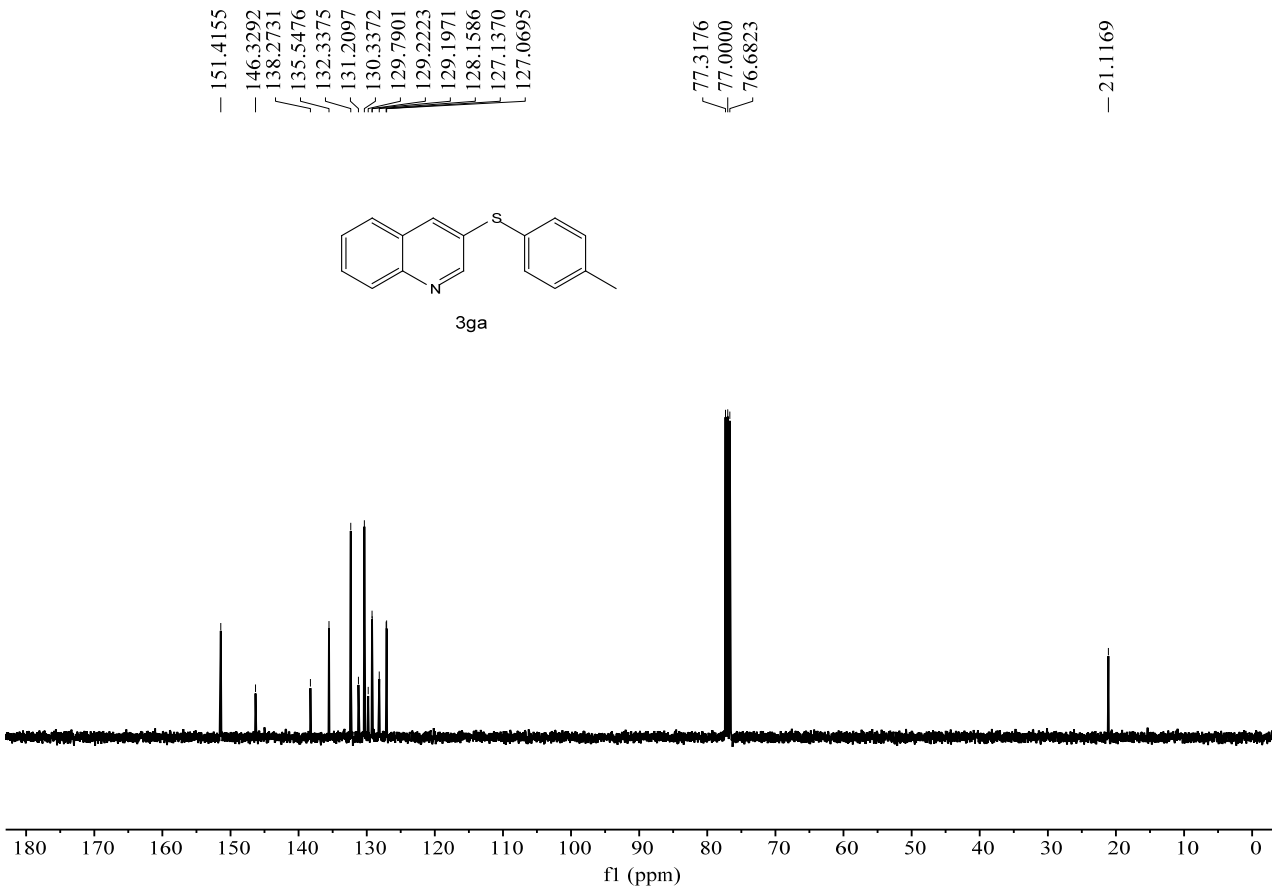
f1 (ppm)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N
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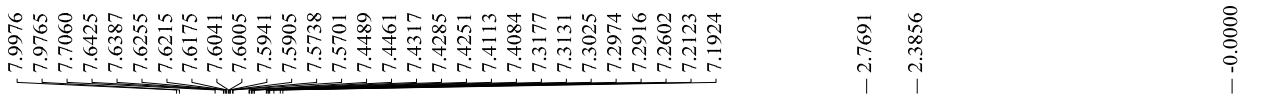
f1 (ppm)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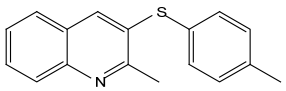
S
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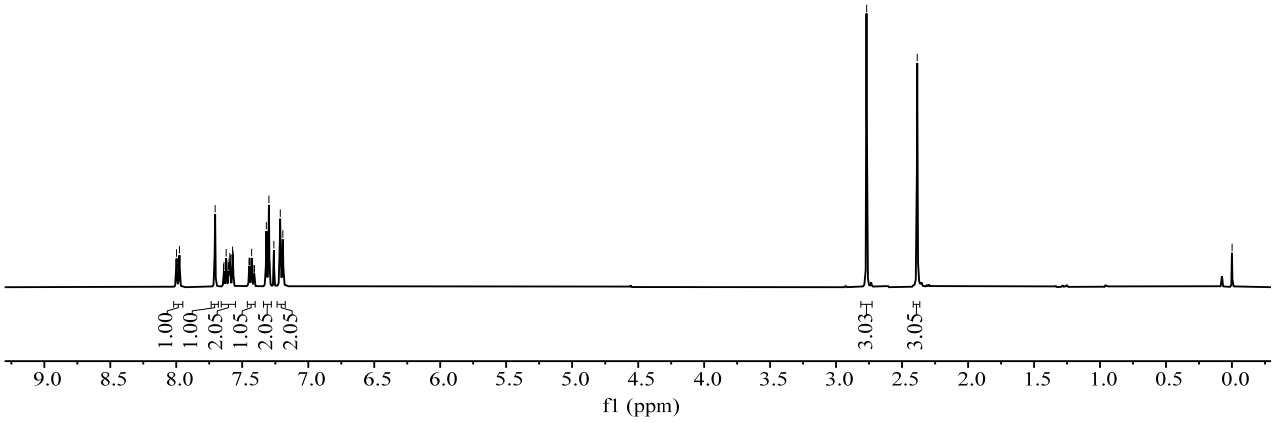
3ha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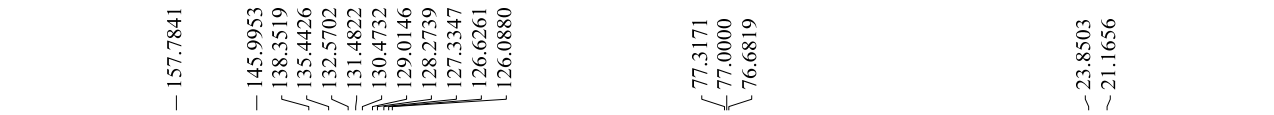
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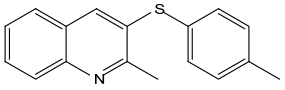
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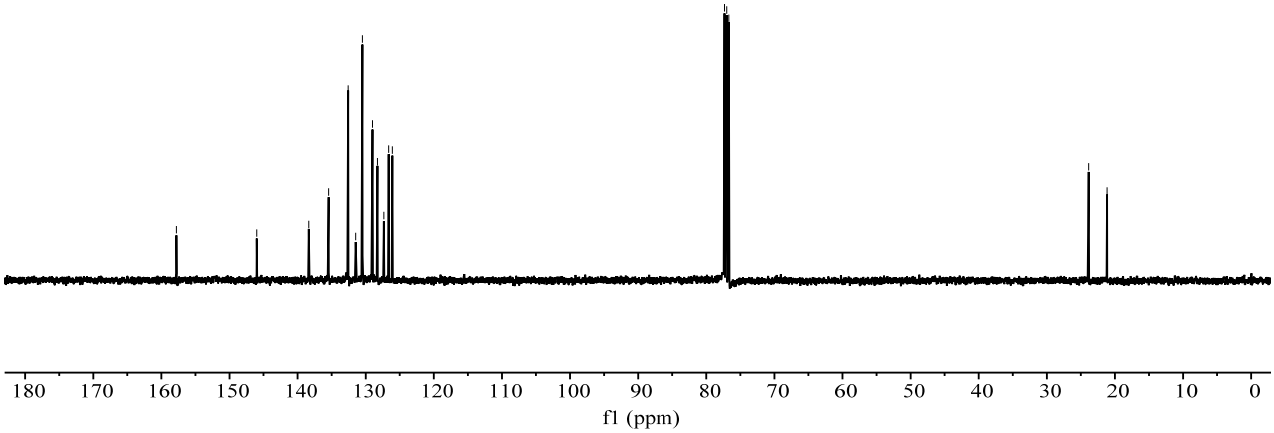
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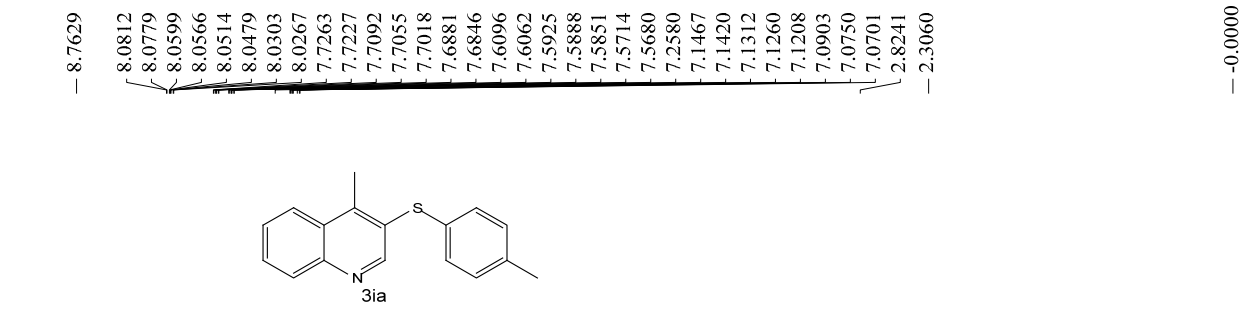
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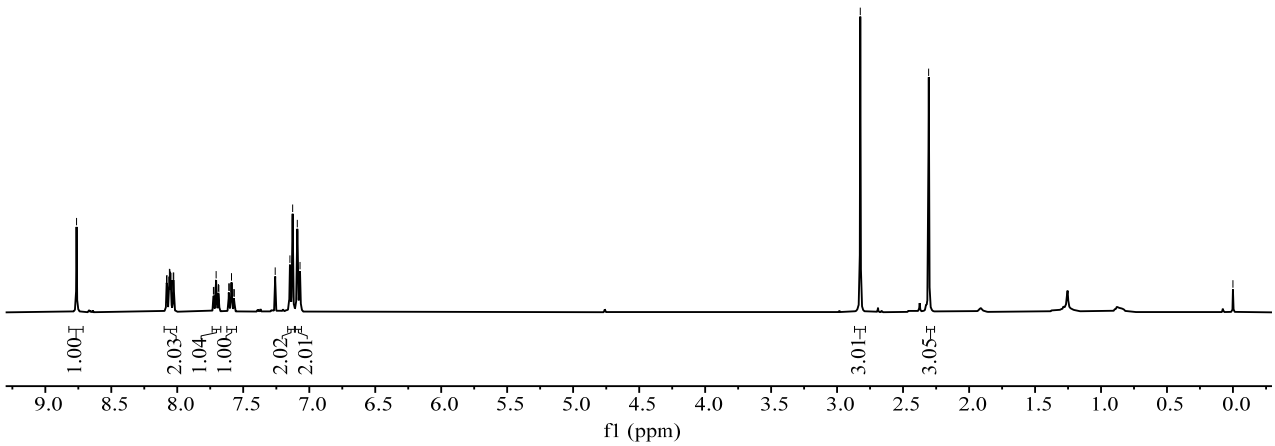
S
N

3ia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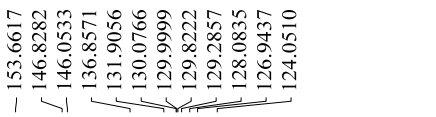
f1 (ppm)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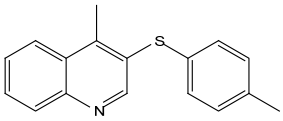
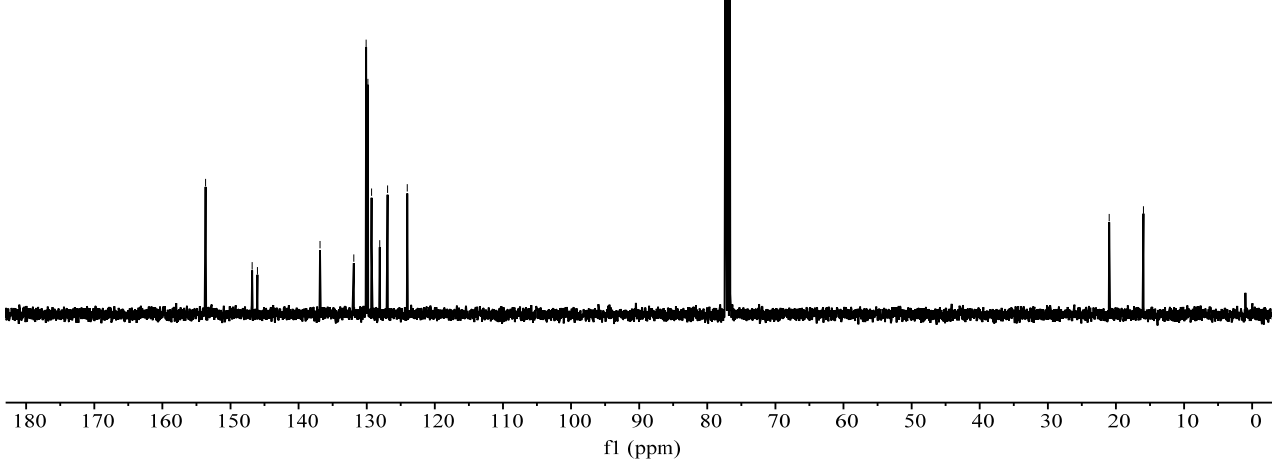
15.9682


S
N

3ia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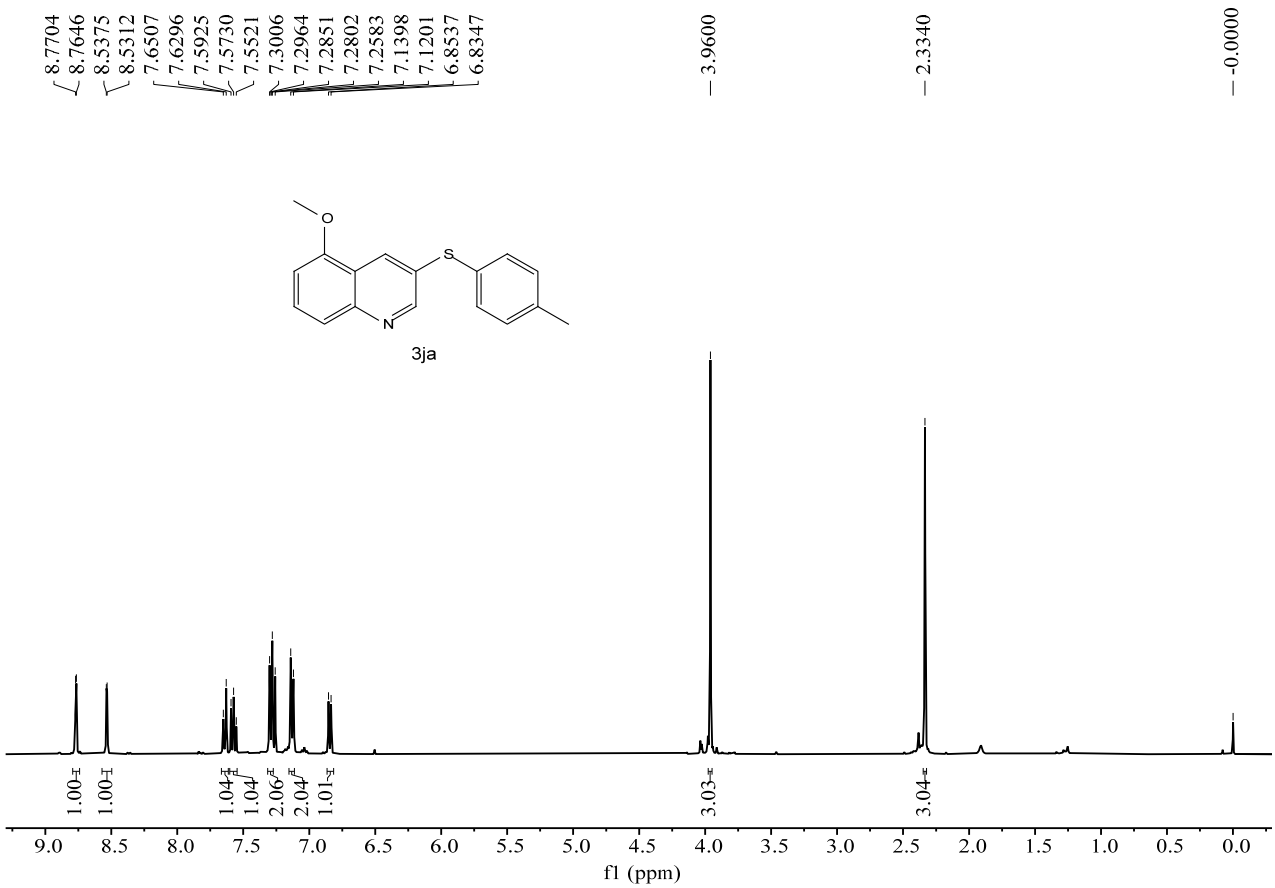
f1 (ppm)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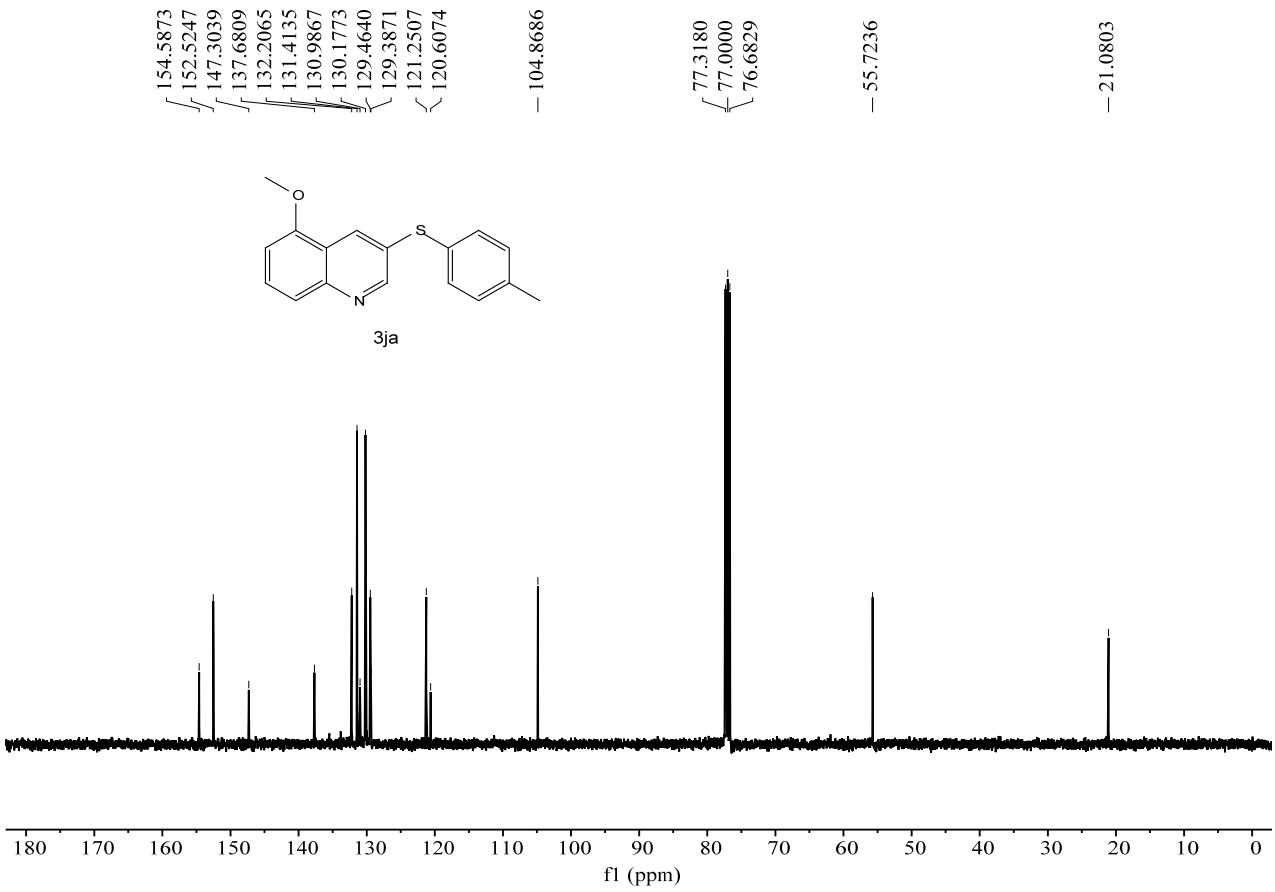
7.2802
7.2583
7.1398
7.1201
6.8537
6.8347
3.9600
2.3340
-0.0000
O
S
N
3ja
1.00
1.00
1.04
1.04
2.06
2.04
1.01
3.03
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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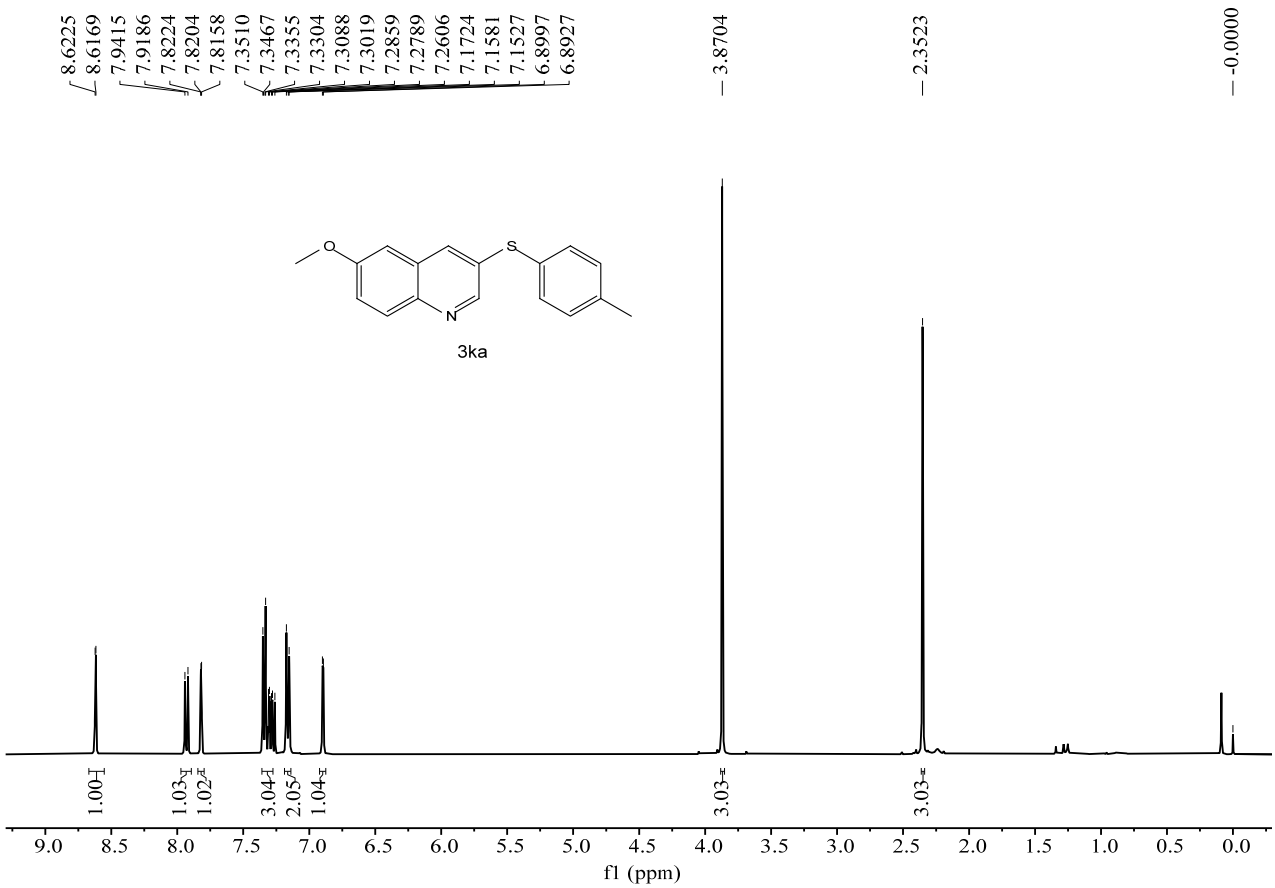
f1 (ppm)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N
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1.00
1.03
1.02
3.04
2.05
1.04
3.03
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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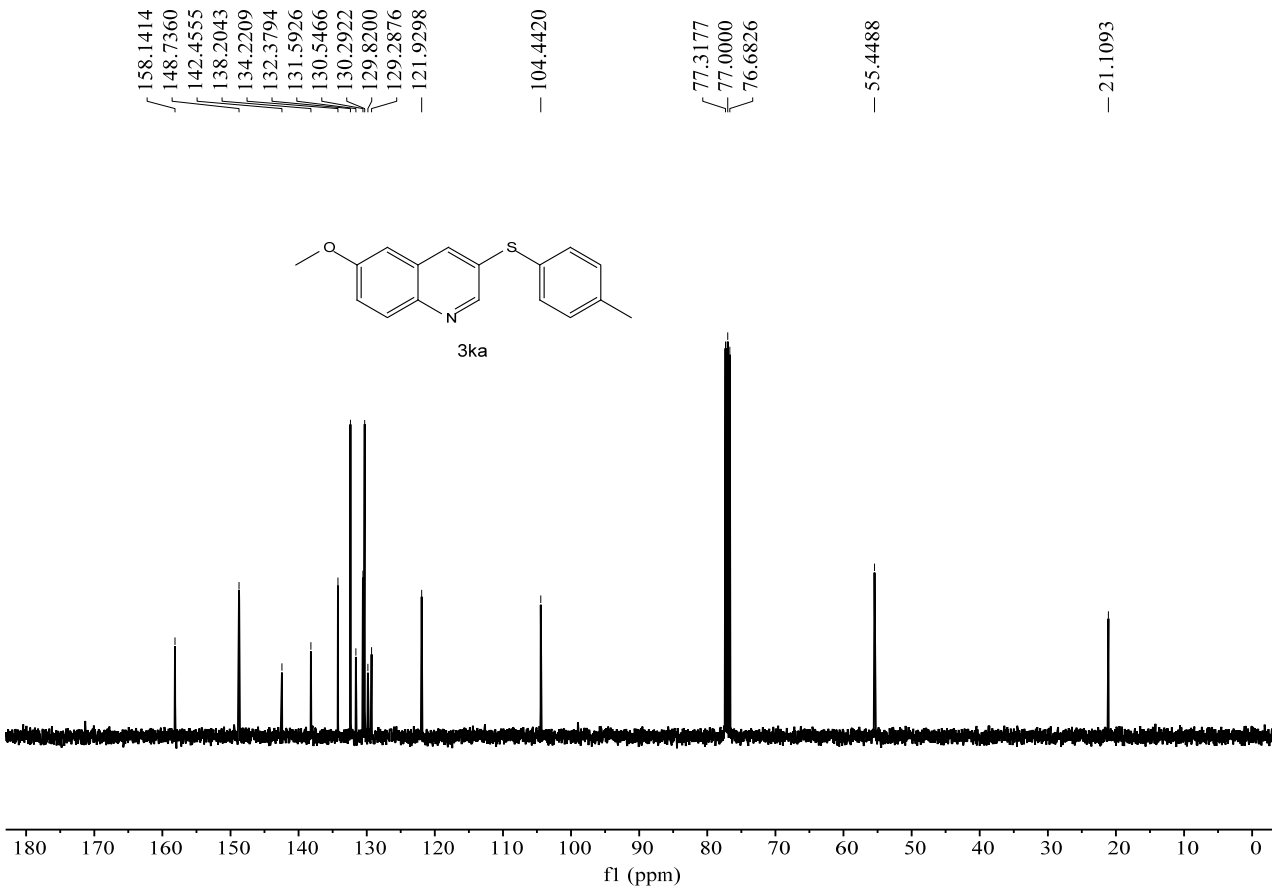
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S
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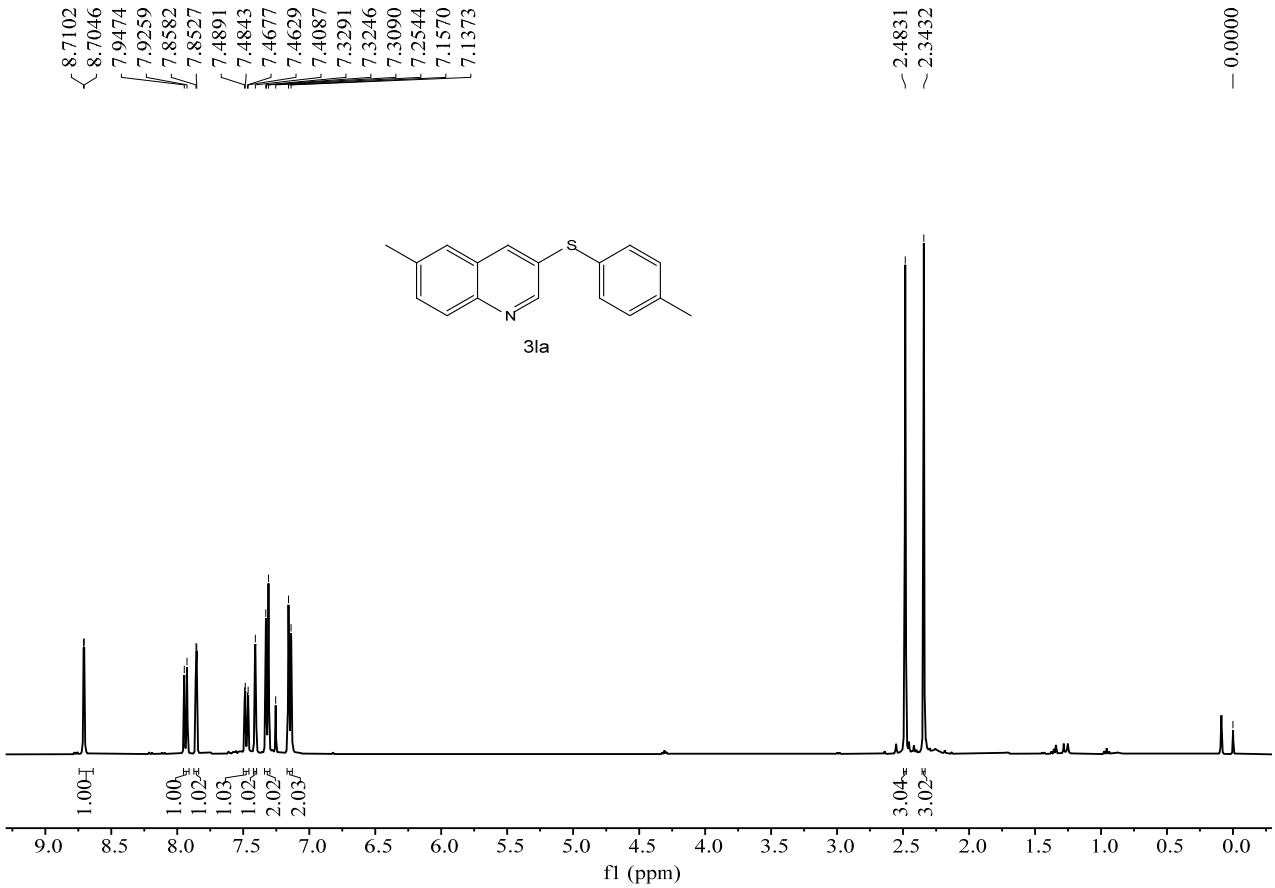
f1 (ppm)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7.3246
7.3090
7.2544
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S
N
3la
1.00
1.00
1.02
1.03
1.02
2.02
2.03
3.04
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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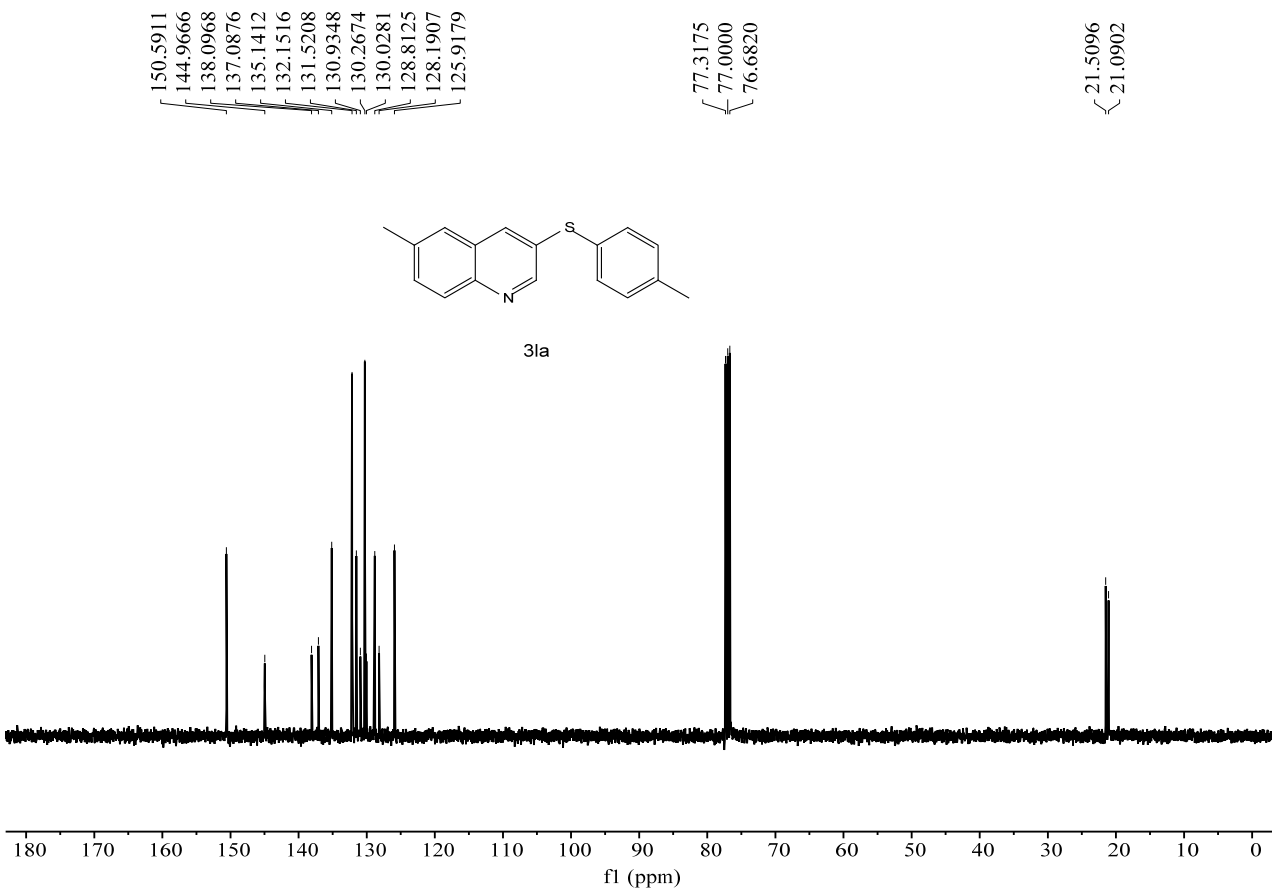
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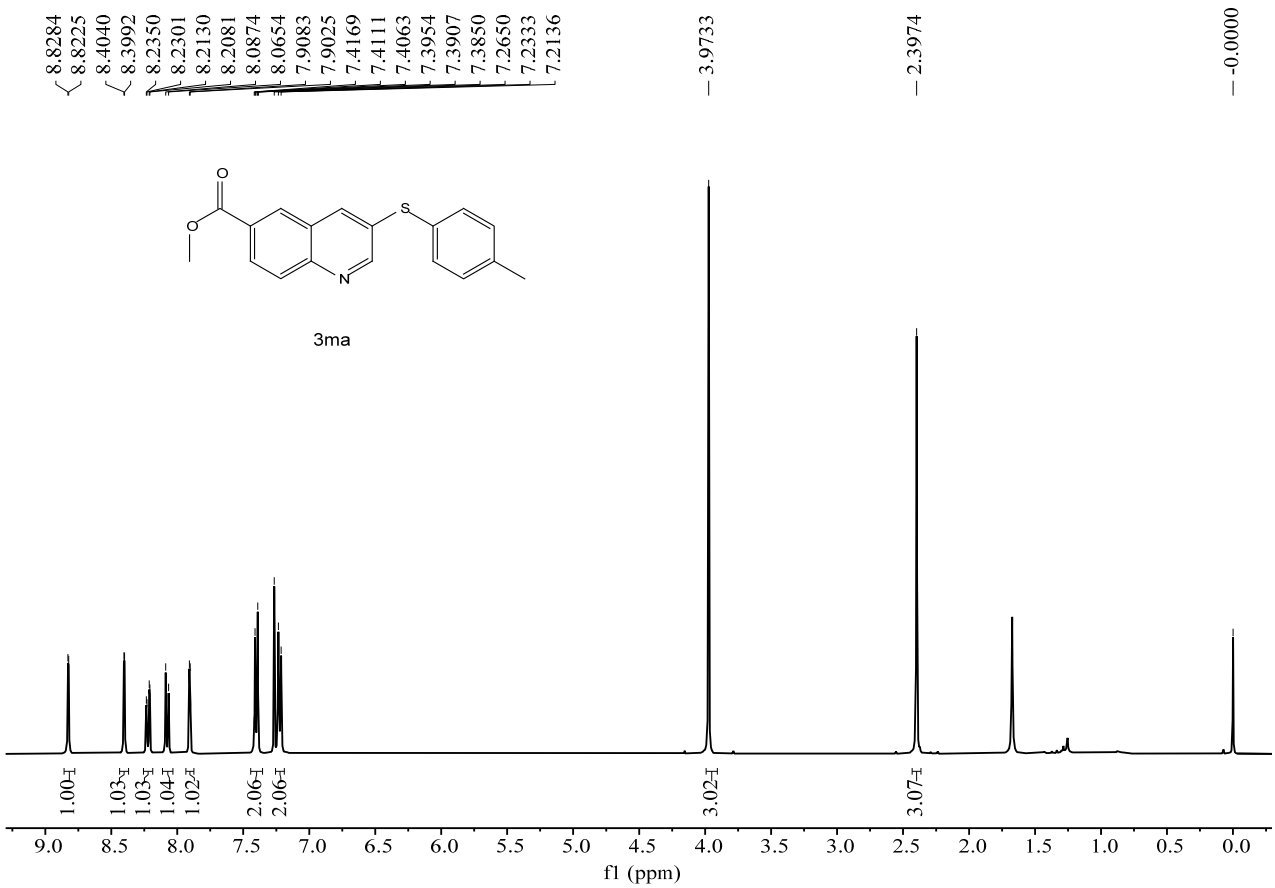
f1 (ppm)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7.4111
7.4063
7.3954
7.3907
7.3850
7.2650
7.2333
7.2136
3.9733
2.3974
-0.0000
O
O
S
N
3ma
1.00
1.03
1.03
1.04
1.02
2.06
2.06
3.02
3.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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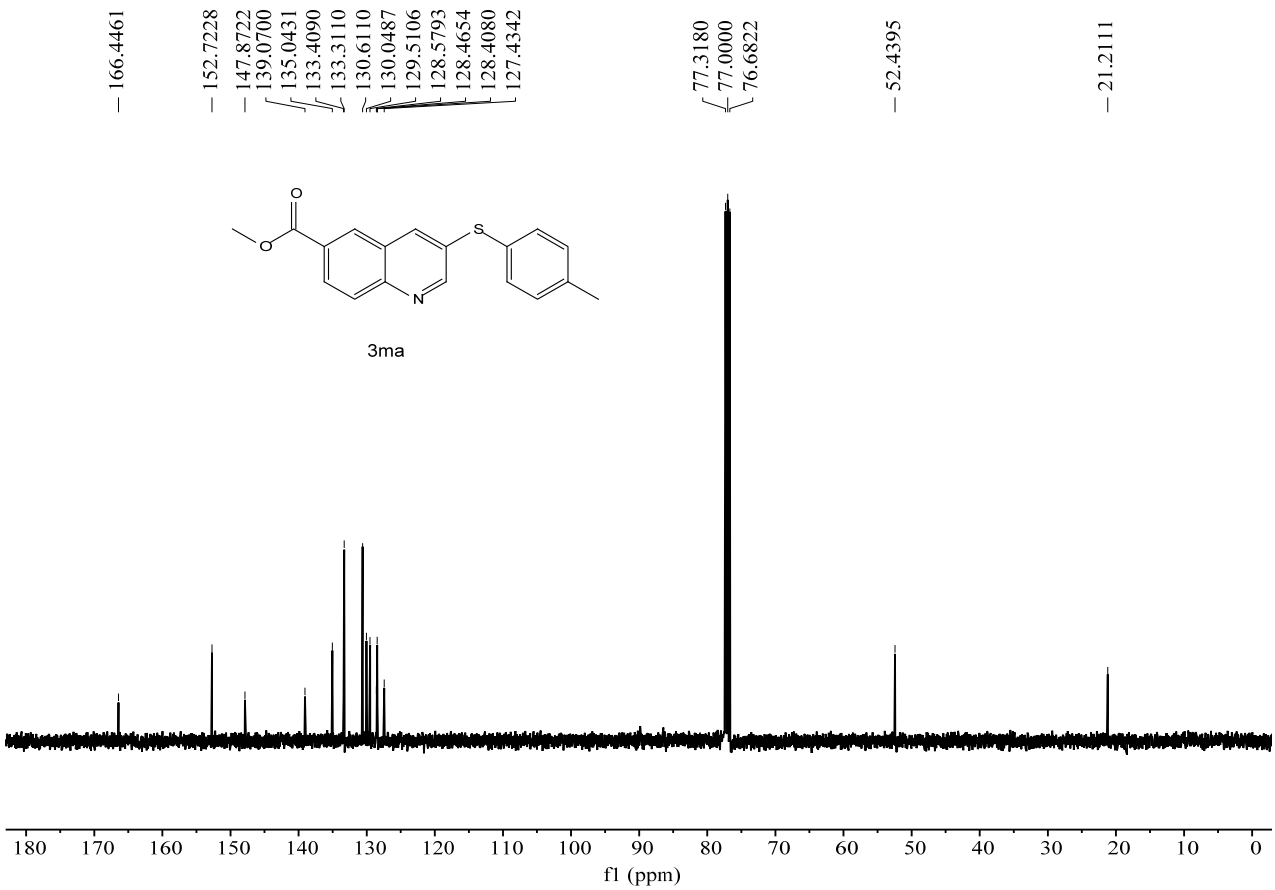
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77.0000
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O
S
N
3ma
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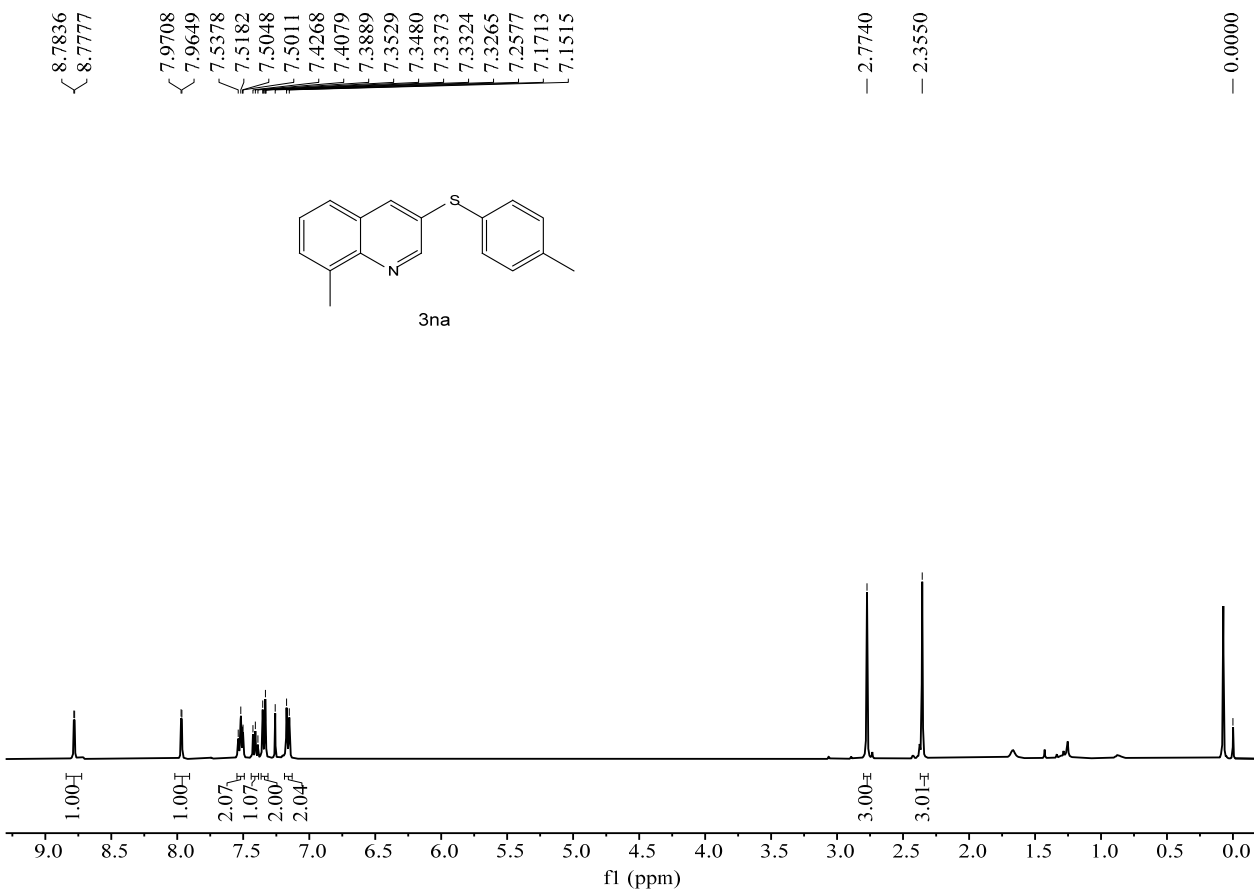
f1 (ppm)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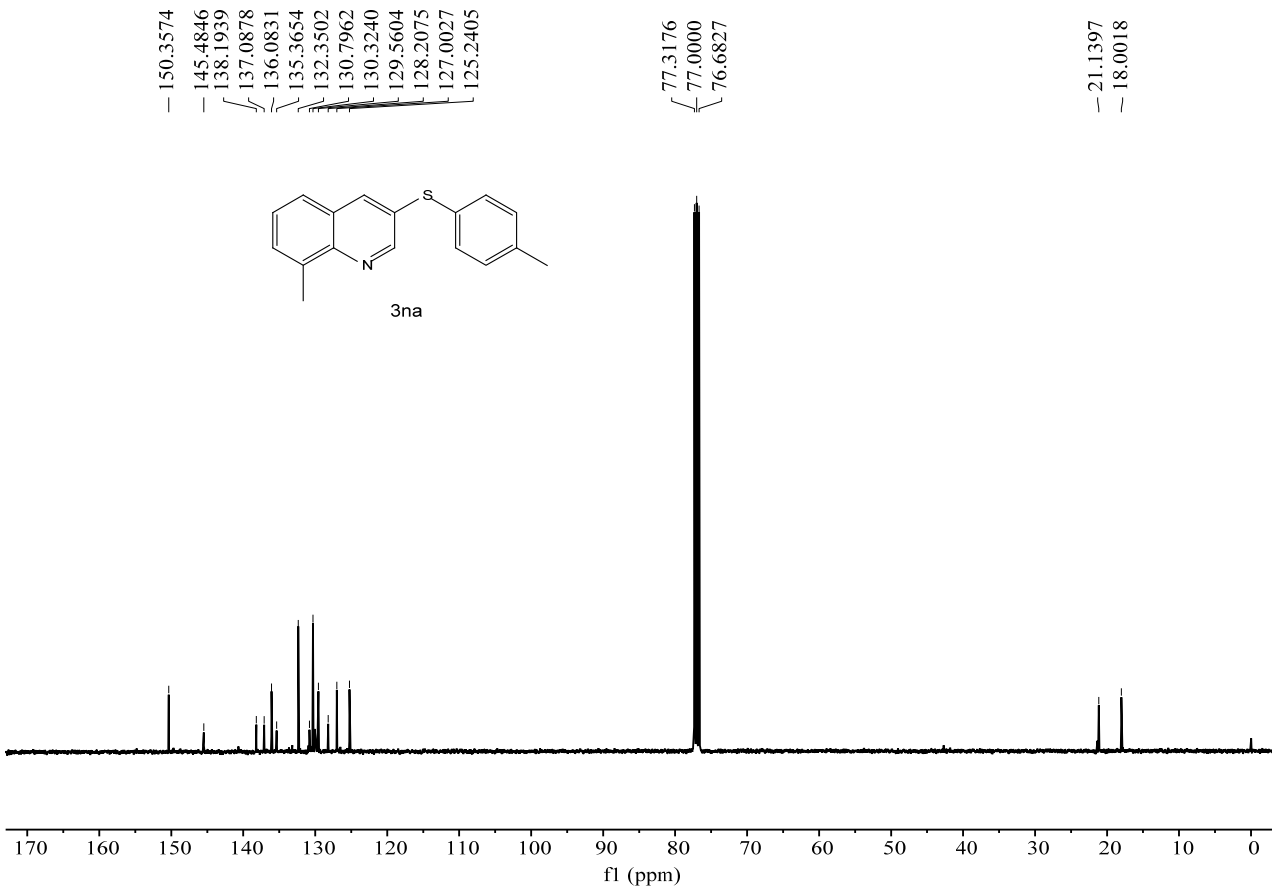
7.3529
7.3480
7.3373
7.3324
7.3265
7.2577
7.1713
7.1515
2.7740
2.3550
0.0000
S
N
3na
1.00
1.00
2.07
1.07
2.00
2.04
3.00
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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N
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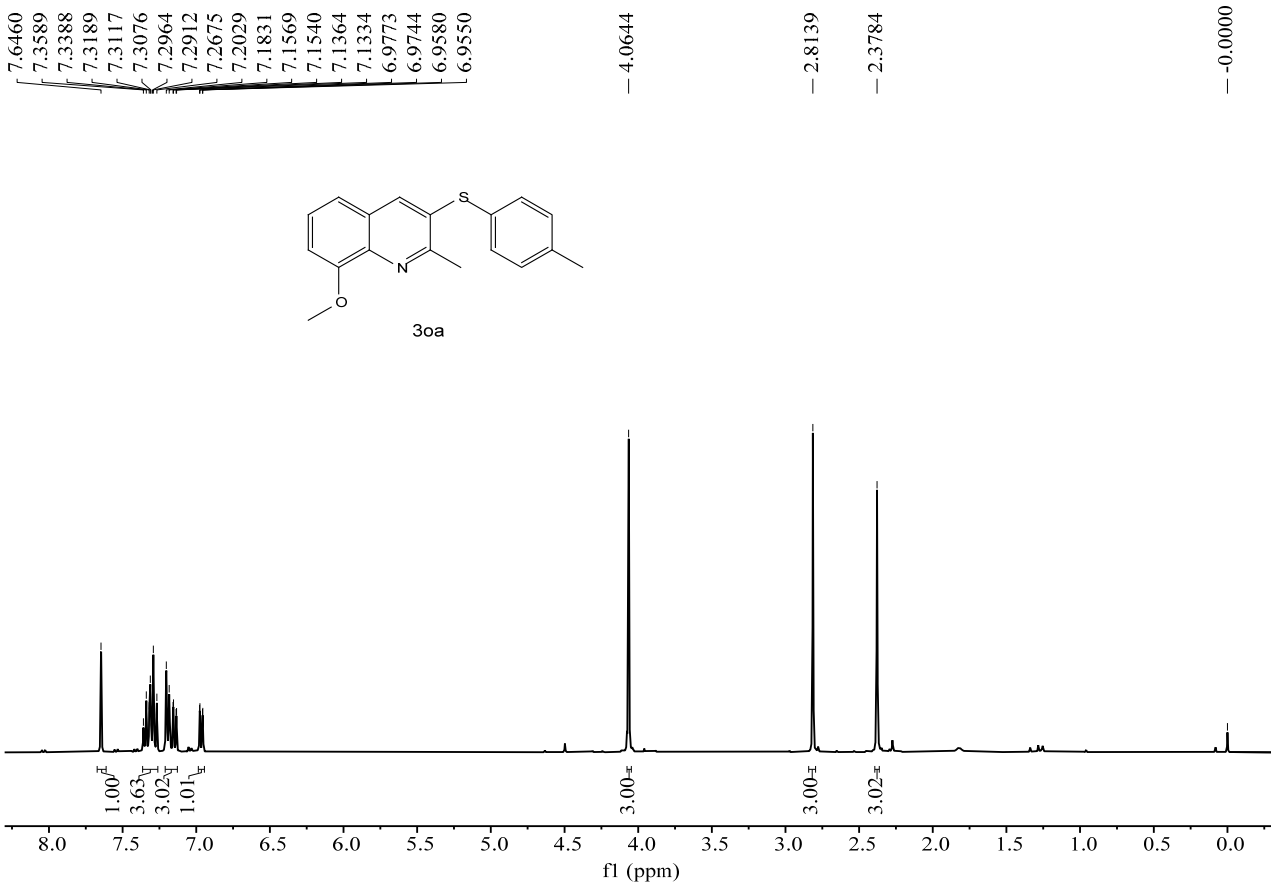
f1 (ppm)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7.1831
7.1569
7.1540
7.1364
7.1334
6.9773
6.9744
6.9580
6.9550
4.0644
2.8139
2.3784
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S
N
O
3oa
1.00
3.63
3.02
1.01
3.00
3.00
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.5
2.0
1.5
1.0
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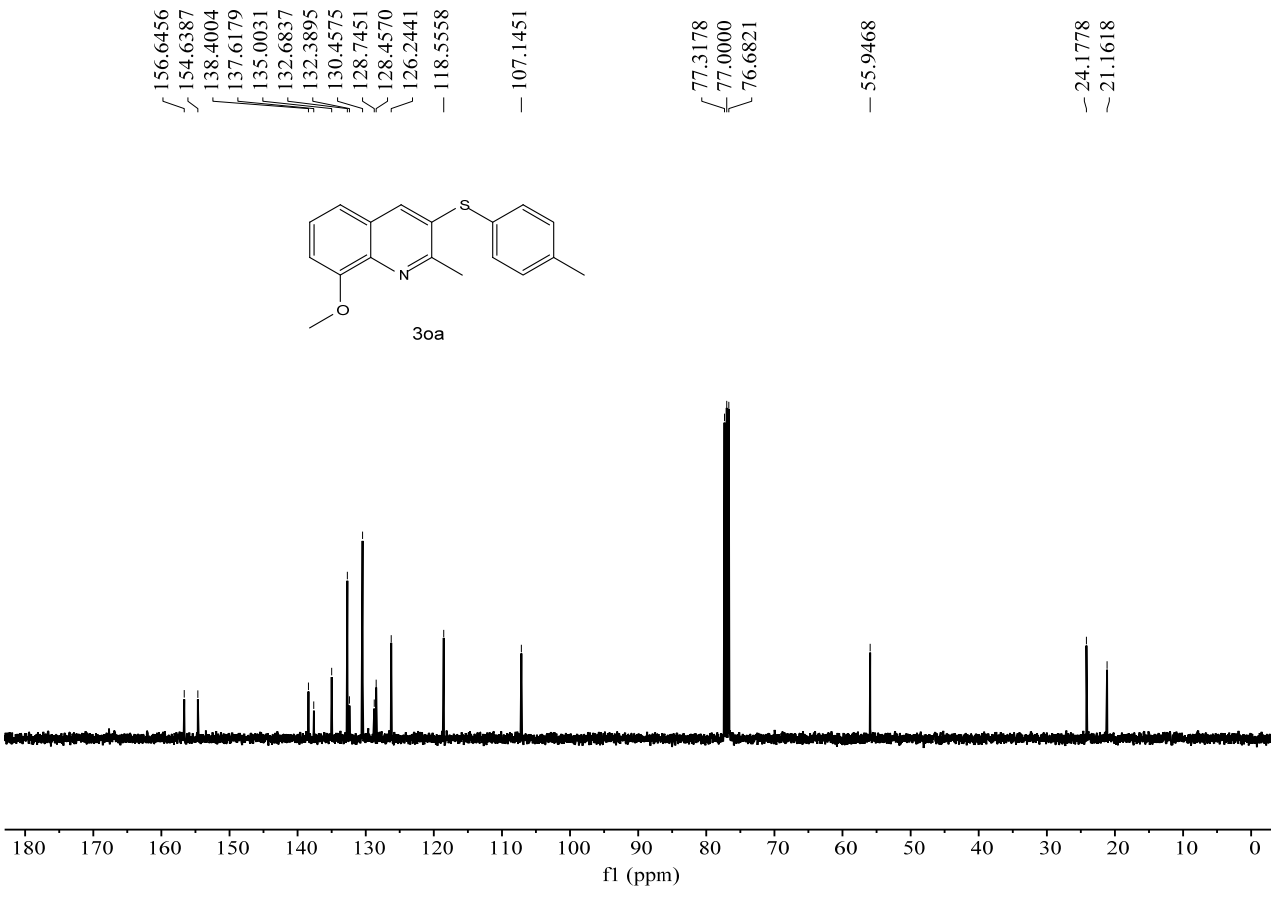
f1 (ppm)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S
N
O
3oa
180
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140
130
120
110
100
90
80
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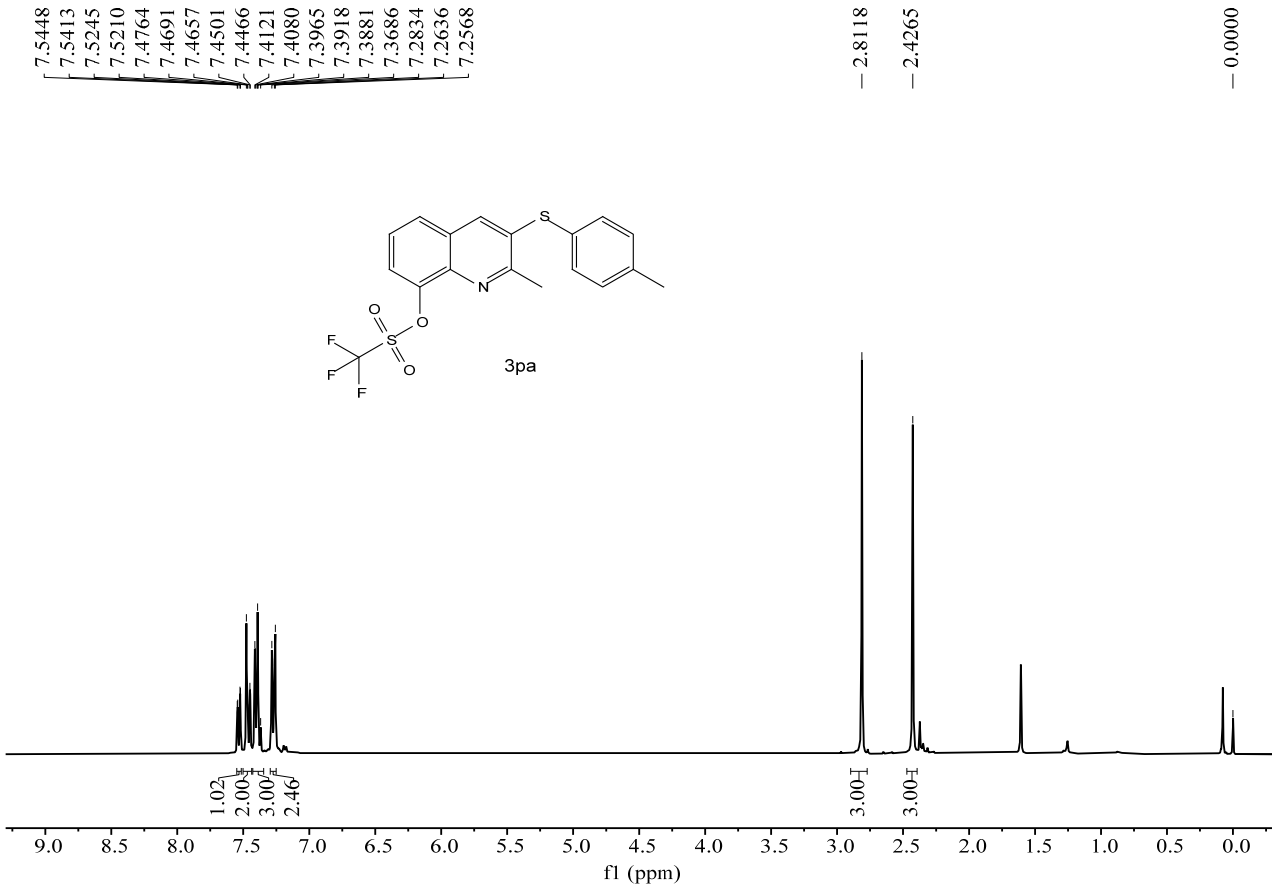
50
40
30
20
10
0
f1 (ppm)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7.4080
7.3965
7.3918
7.3881
7.3686
7.2834
7.2636
7.2568
2.8118
2.4265
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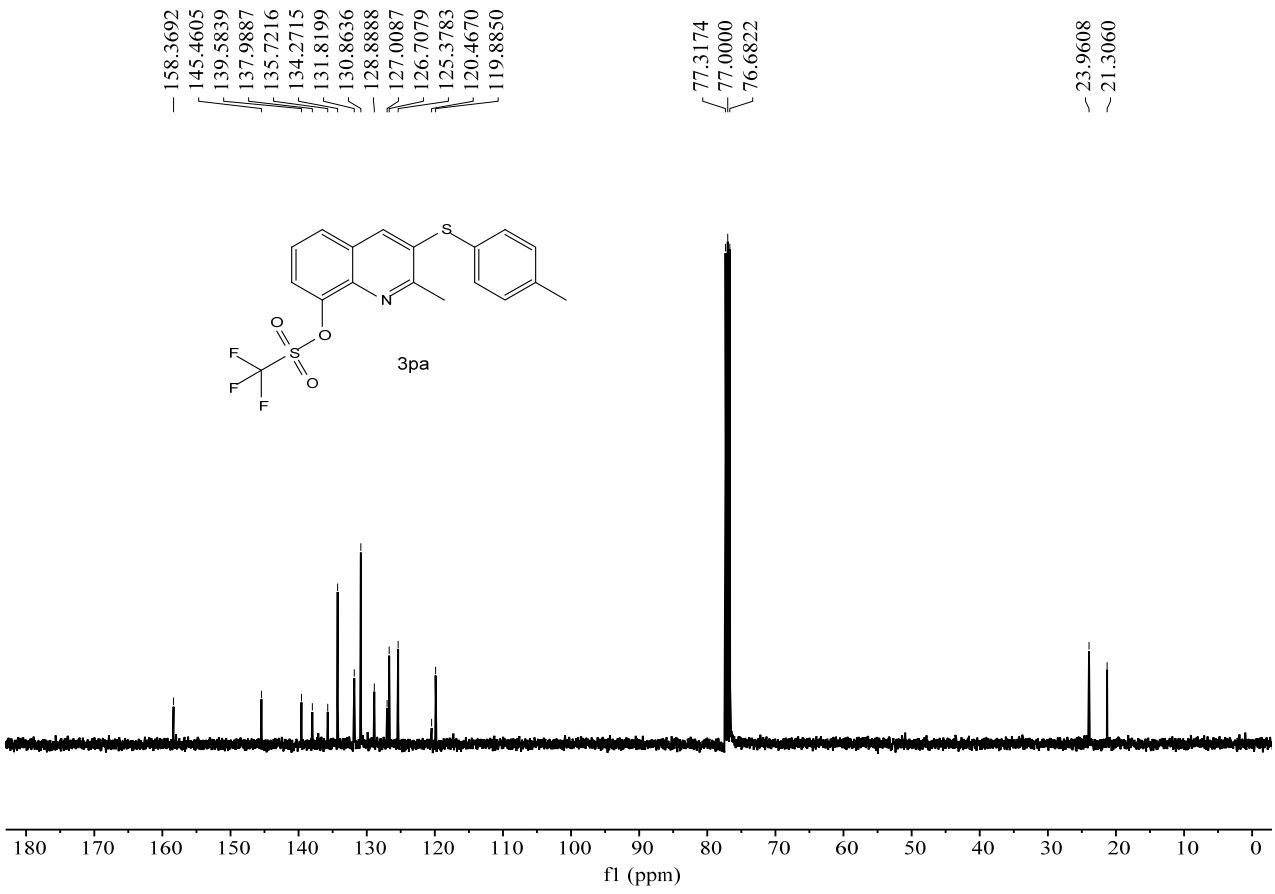
3pa
1.02
2.00
3.00
2.46
3.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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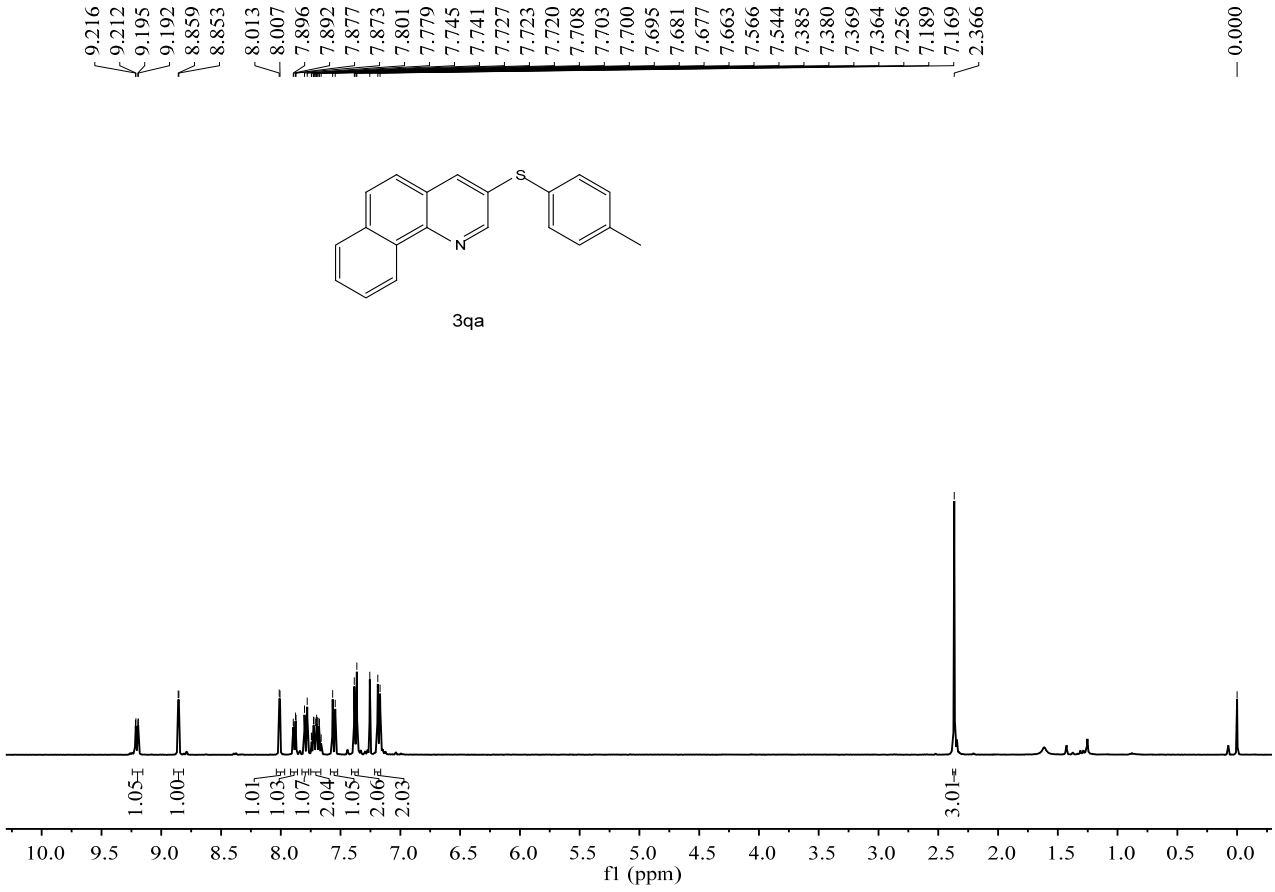
f1 (ppm)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7.741
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7.723
7.720
7.708
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7.700
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7.681
7.677
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7.385
7.380
7.369
7.364
7.256
7.189
7.169
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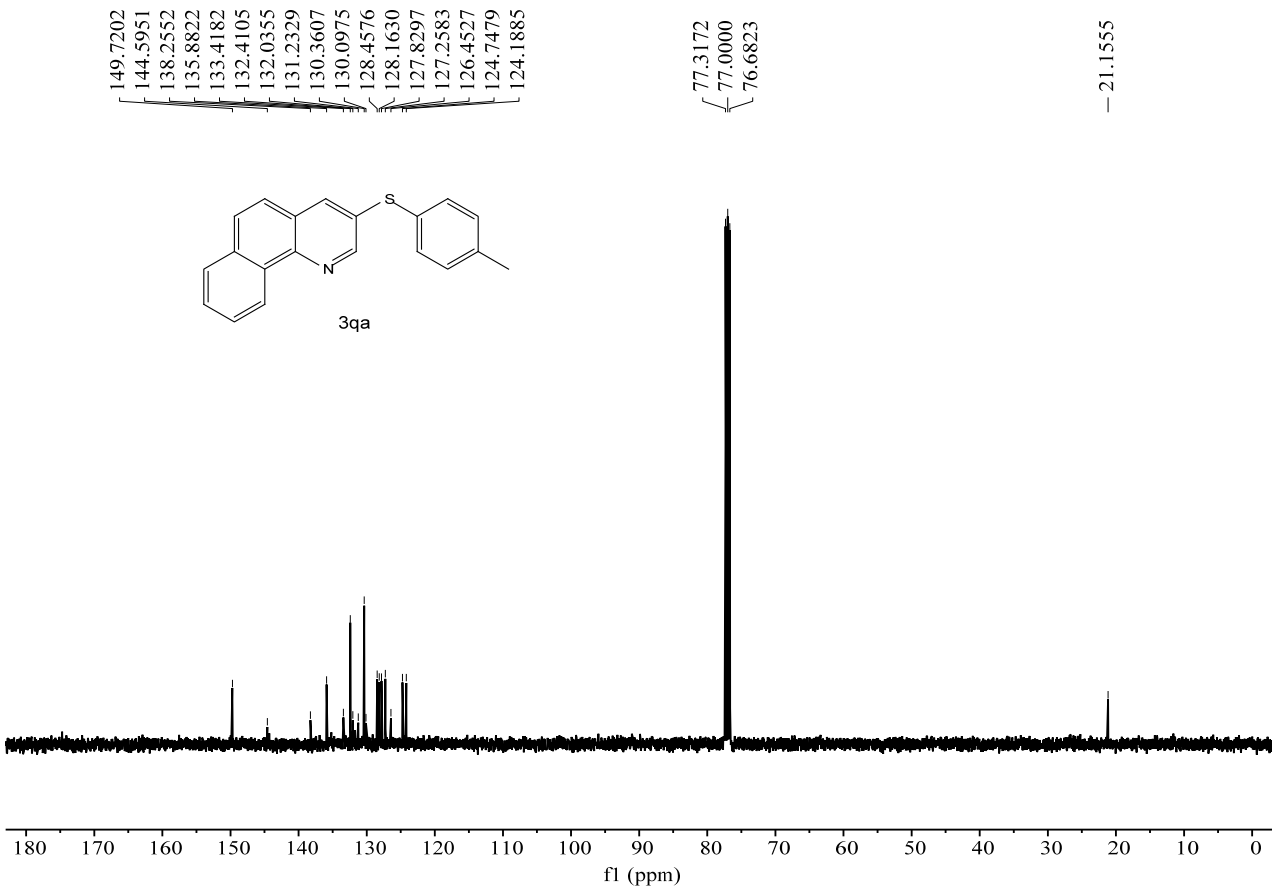
S
N
3qa
1.05
1.00
1.01
1.03
1.07
2.04
1.05
2.06
2.03
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.1885
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S
N
3qa
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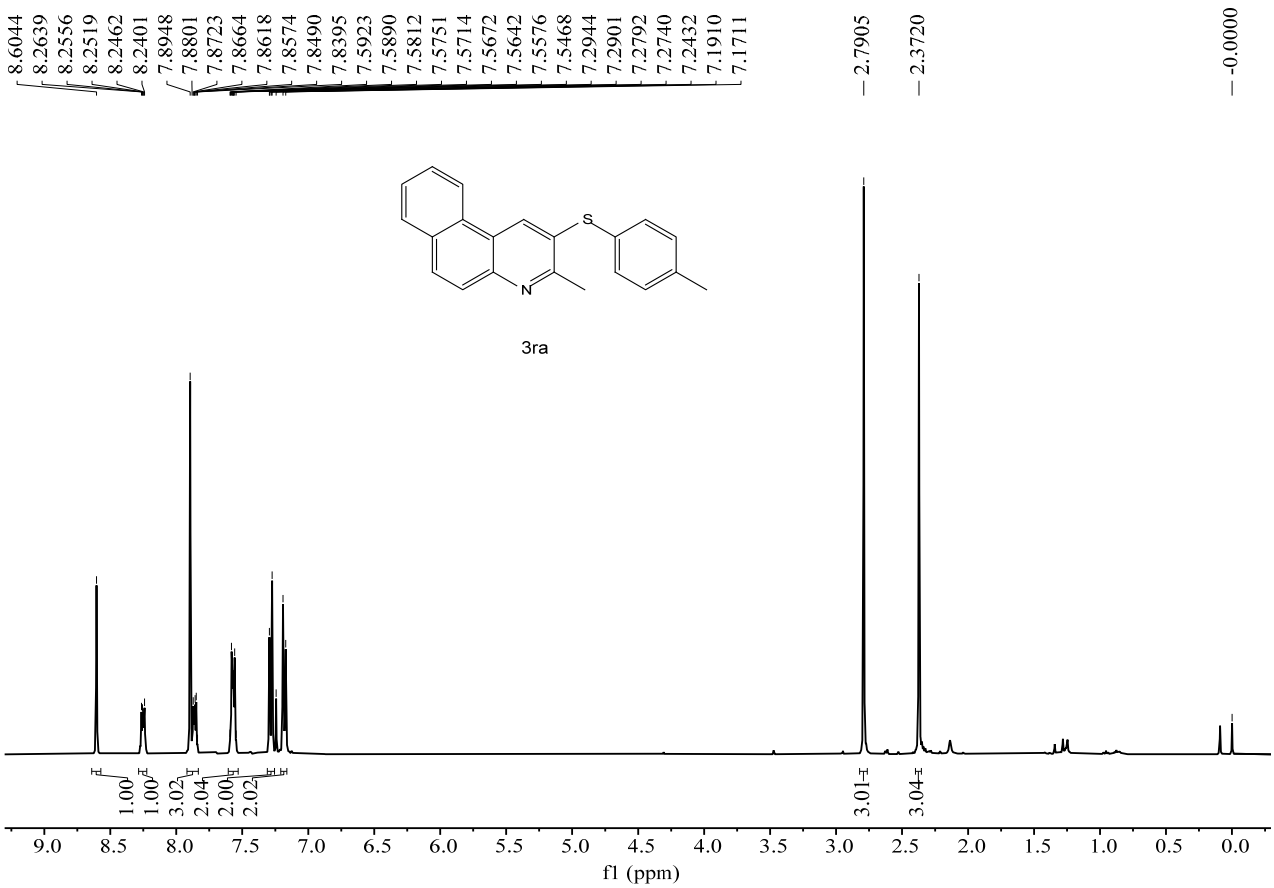
f1 (ppm)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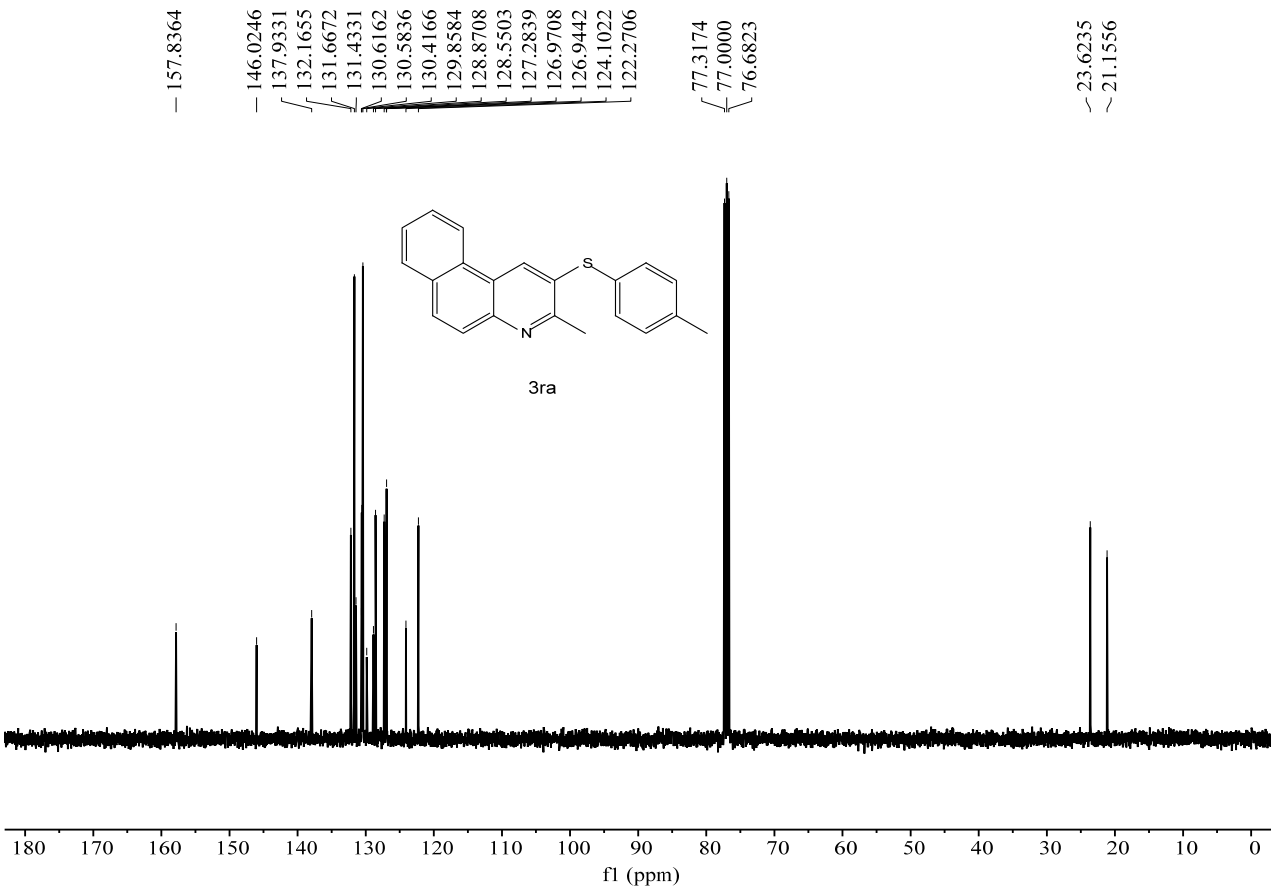
N
3ra
1.00
1.00
3.02
2.04
2.00
2.02
3.01
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.9442
124.1022
122.2706
77.3174
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23.6235
21.1556
S
N
3ra
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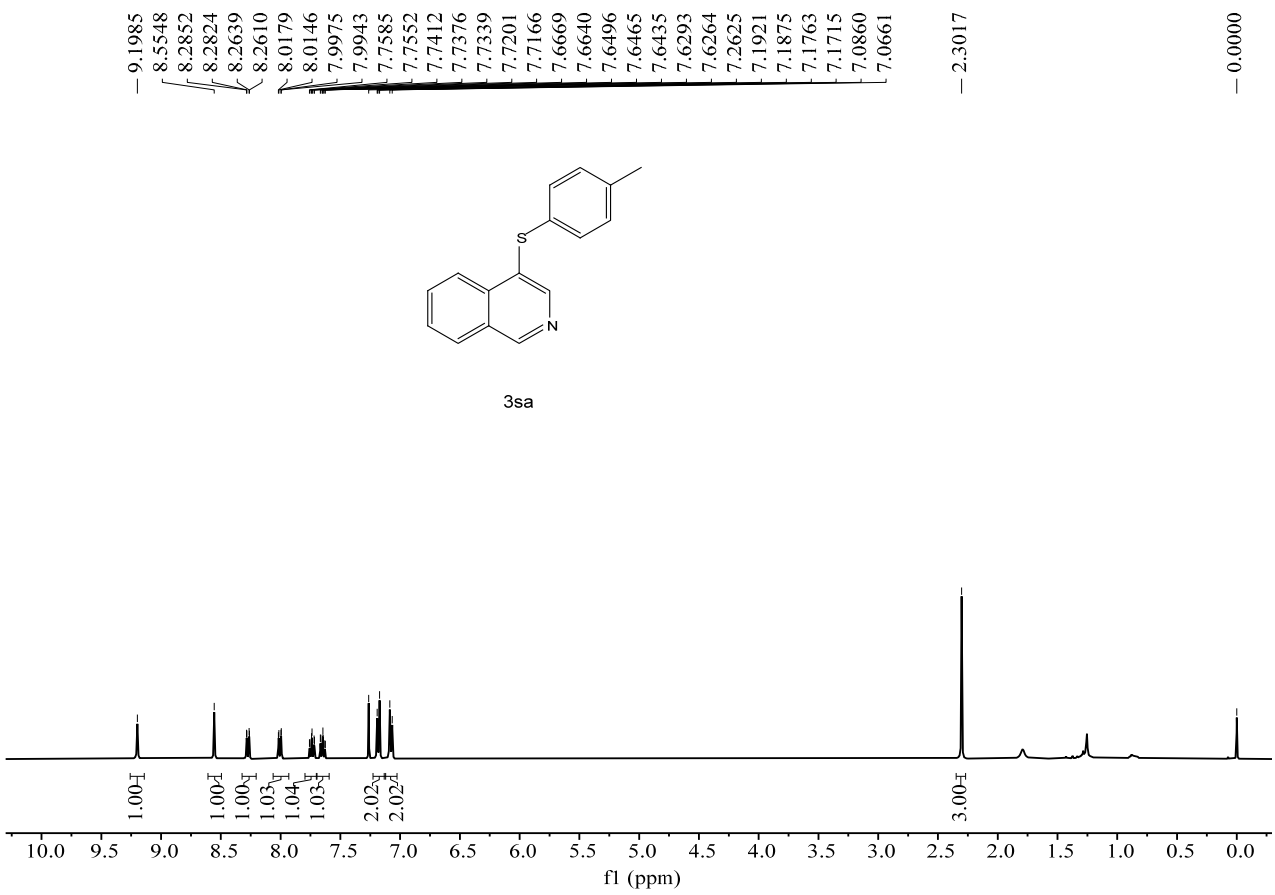
f1 (ppm)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N
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1.00
1.00
1.03
1.04
1.03
2.02
2.02
3.00
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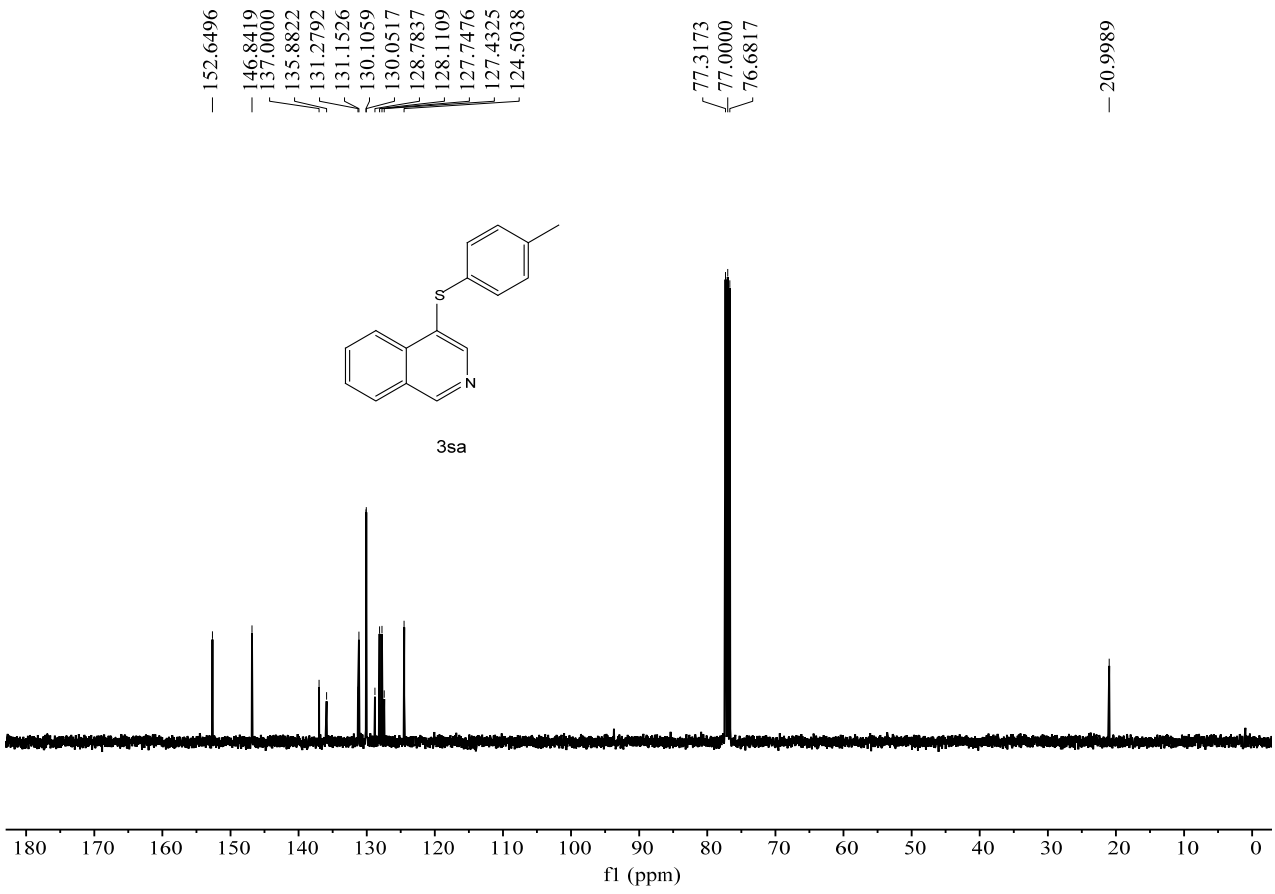
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N
3sa
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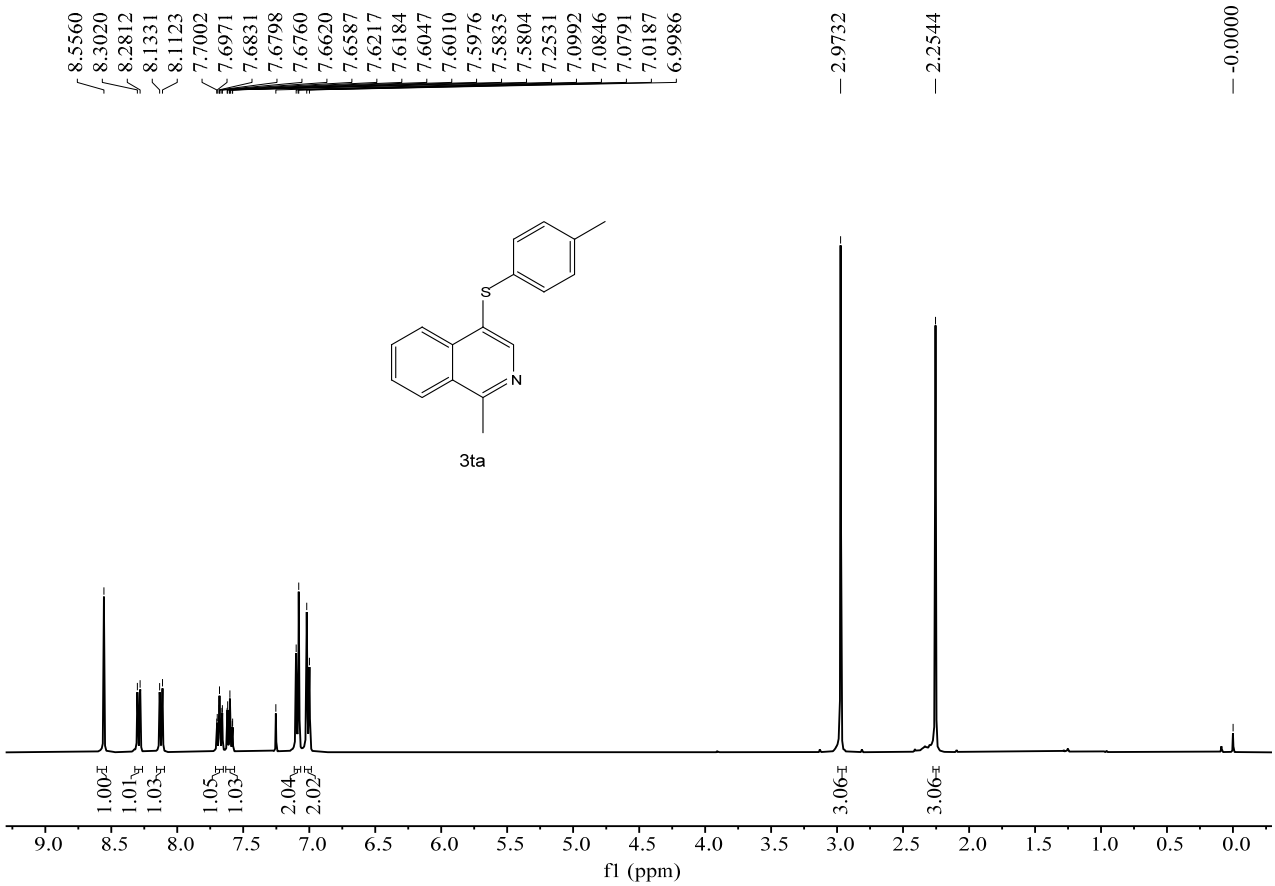
f1 (ppm)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6.9986
2.9732
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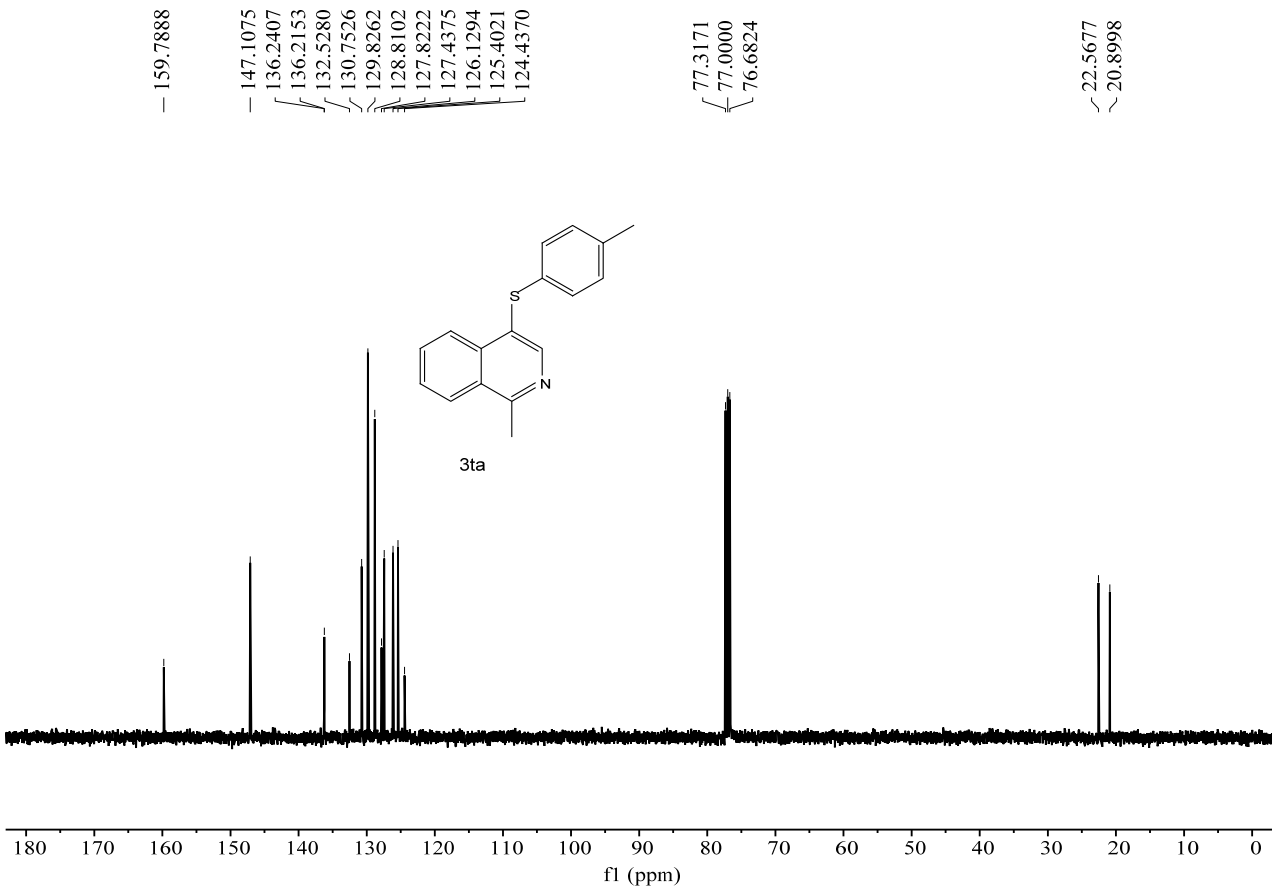
-0.0000
S
N
3ta
1.00
1.01
1.03
1.05
1.03
2.04
2.02
3.06
3.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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N
3ta
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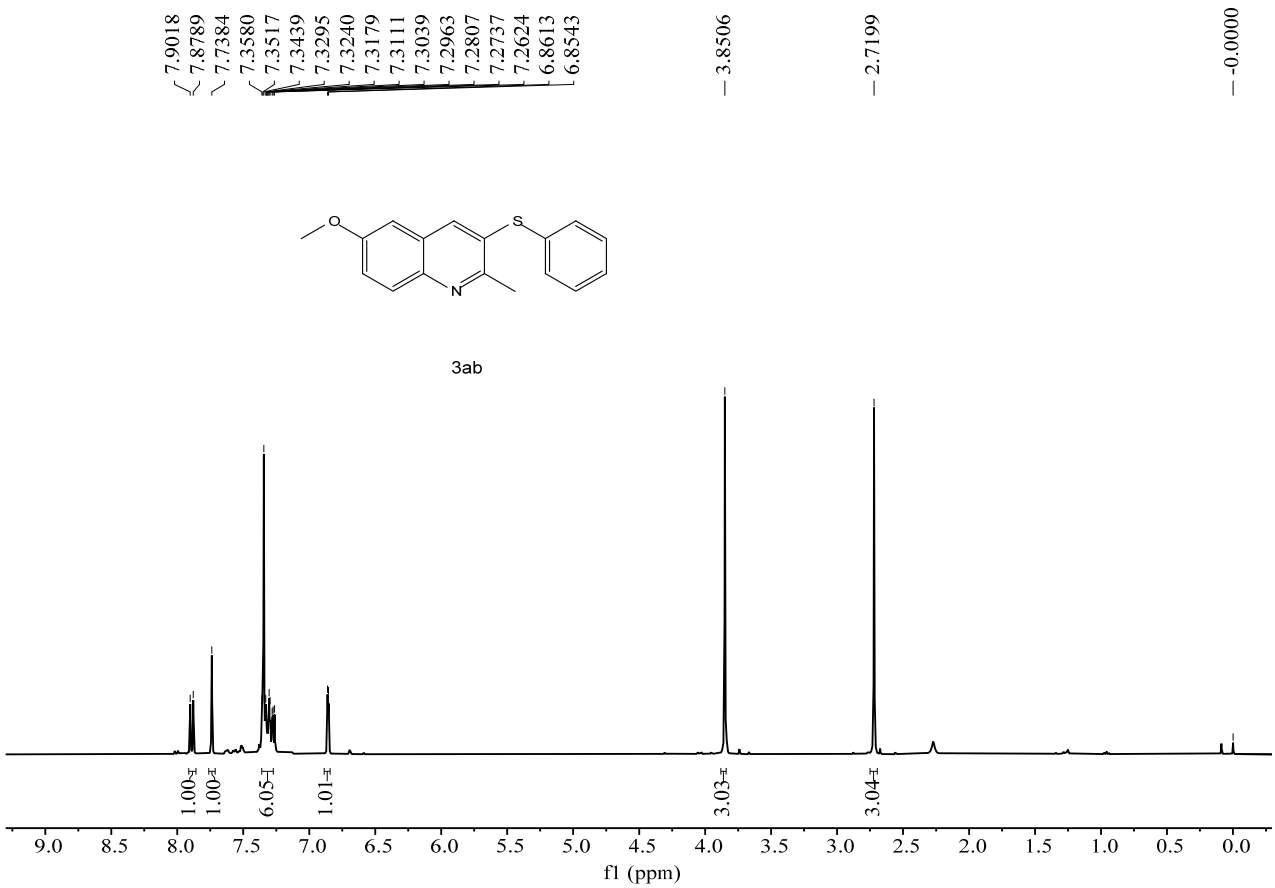
f1 (ppm)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2.7199
-0.0000
O
S
N
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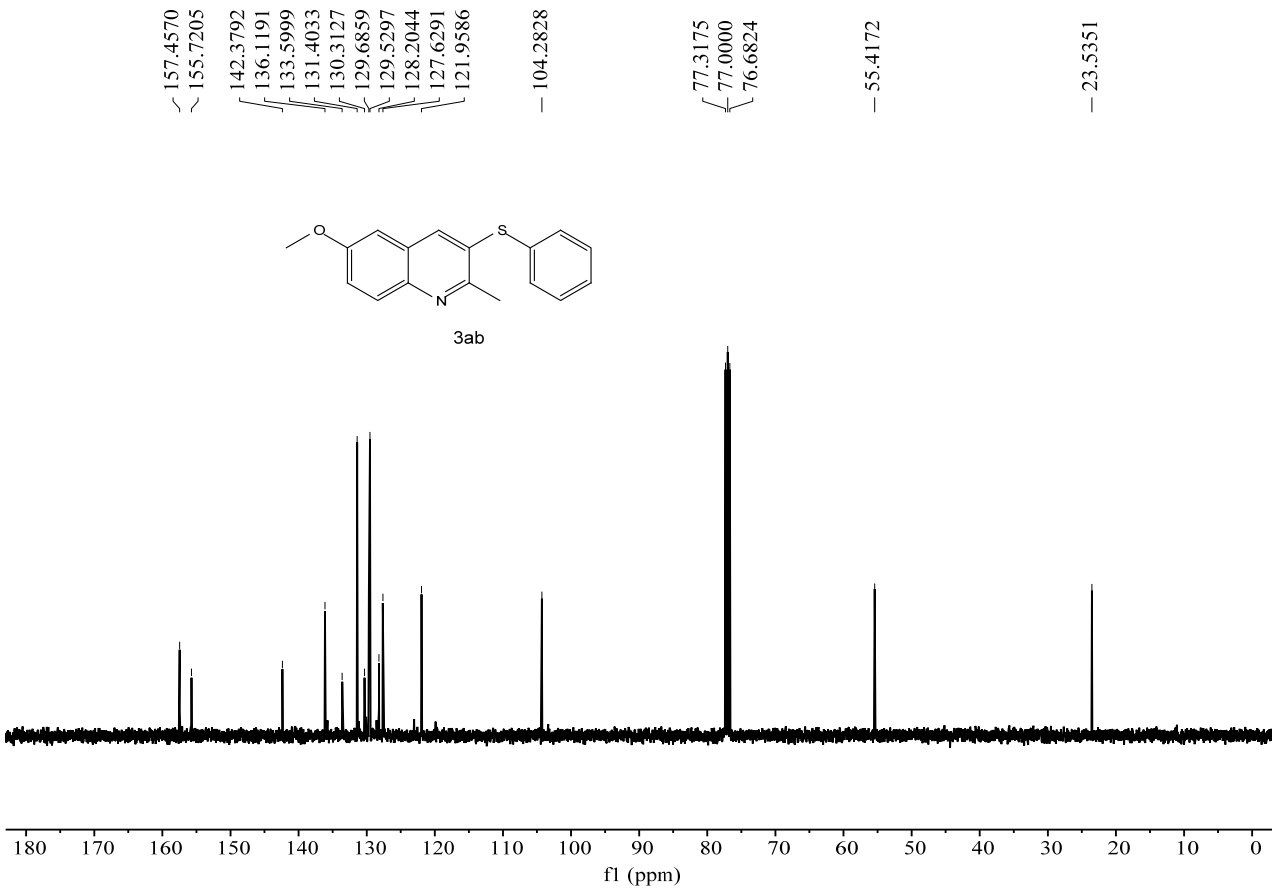
1.00
1.00
6.05
1.01
3.03
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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121.9586
104.2828
77.3175
77.0000
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S
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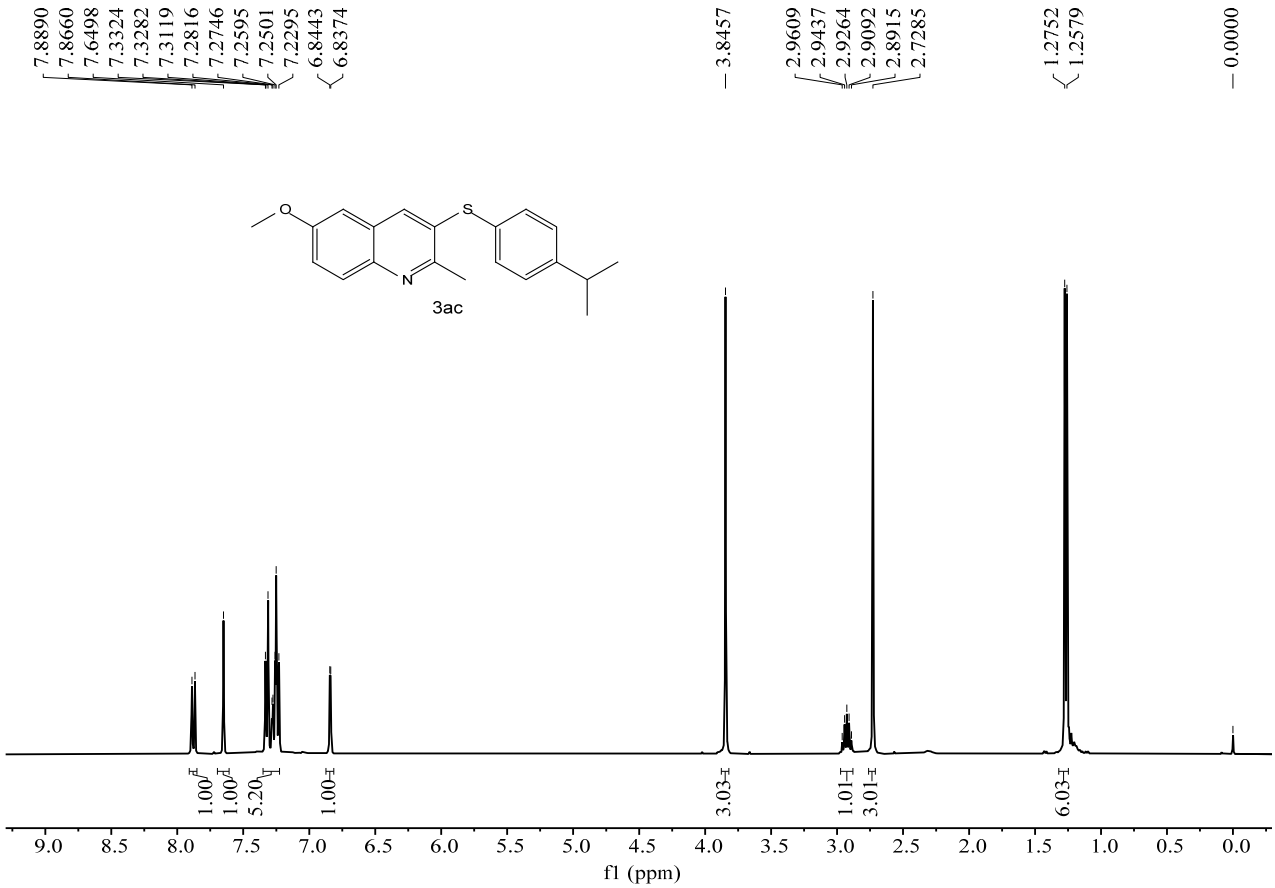
f1 (ppm)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6.8374
3.8457
2.9609
2.9437
2.9264
2.9092
2.8915
2.7285
1.2752
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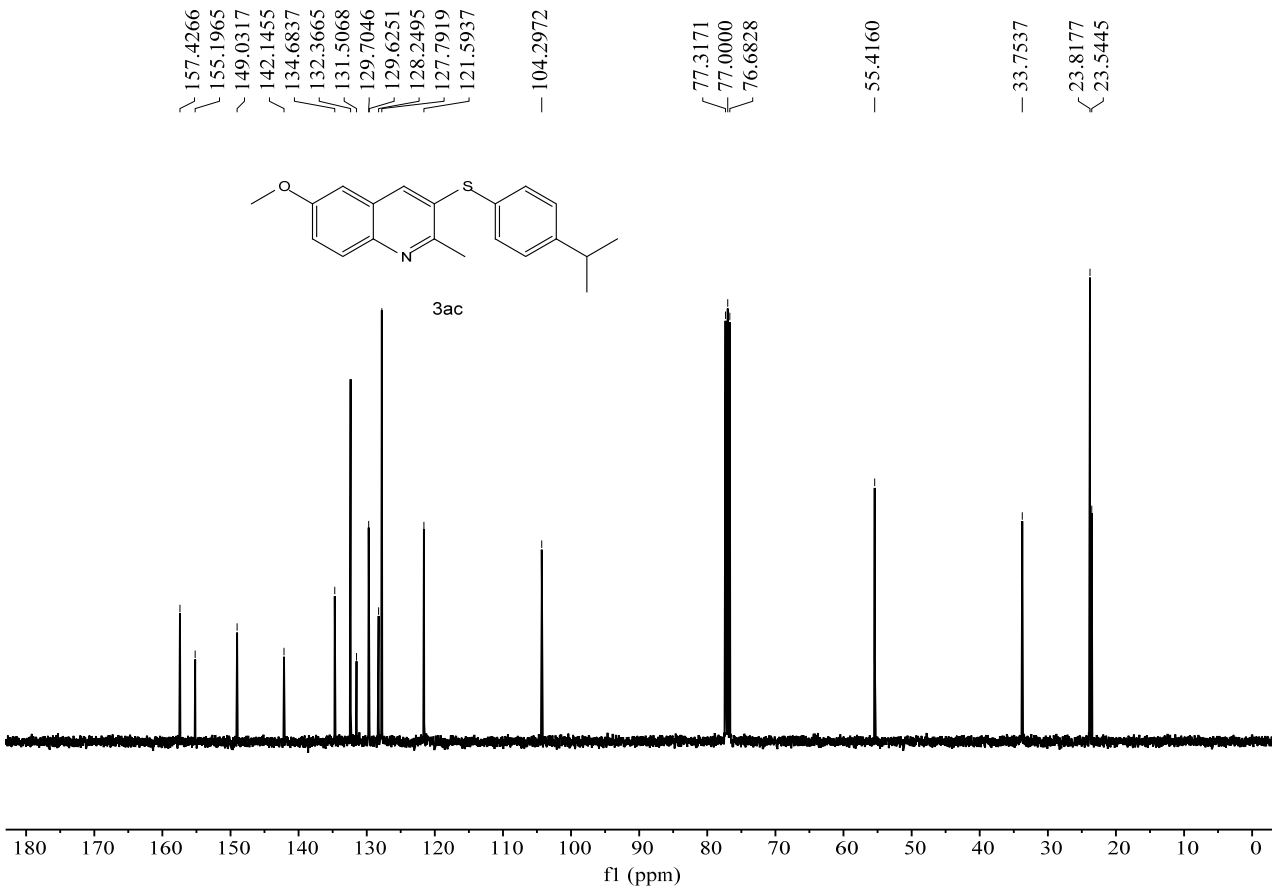
1.00
3.03
1.01
3.01
6.03
fl (ppm)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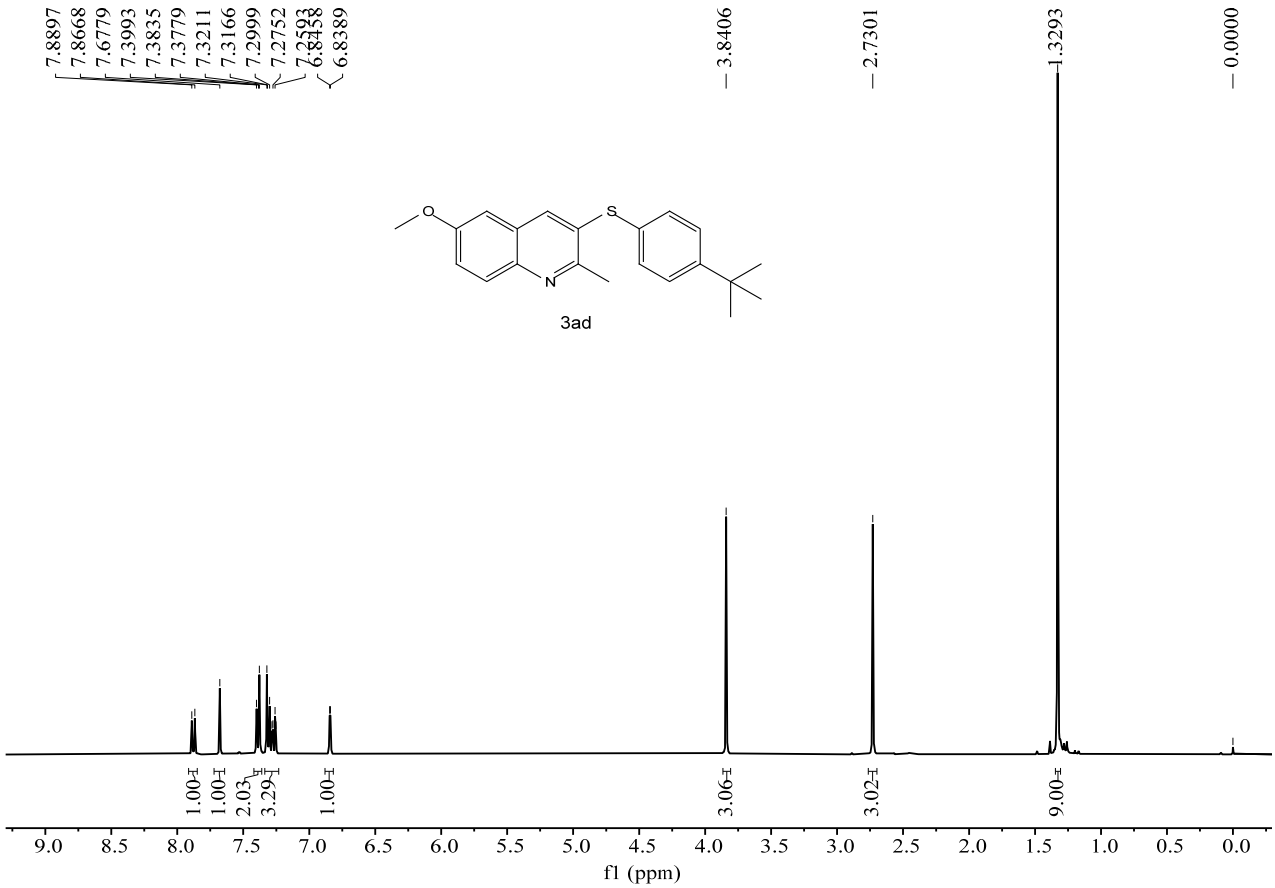
fl (ppm)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6.8458
6.8389
3.8406
2.7301
1.3293
0.0000
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1.00
1.00
2.03
3.29
1.00
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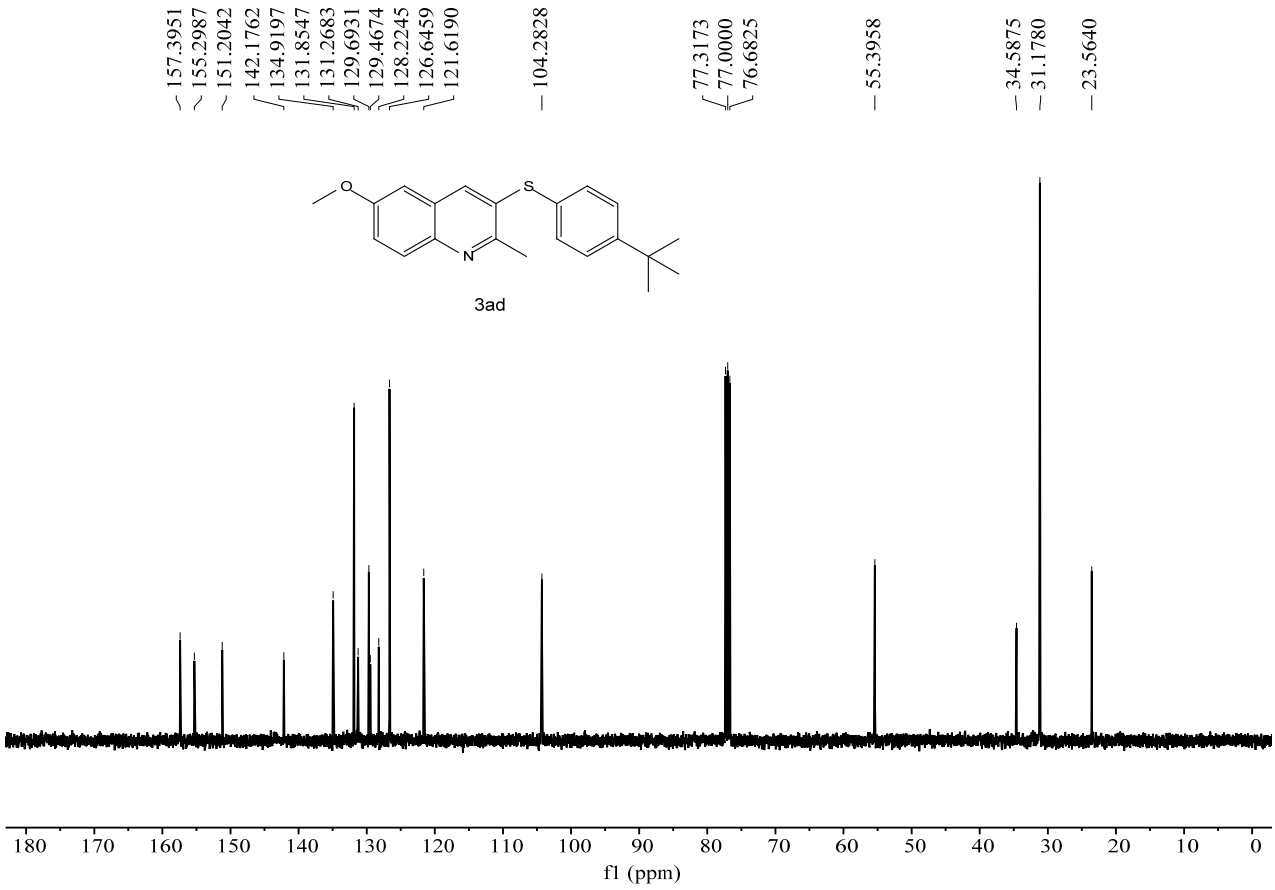
9.00
fl (ppm)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121.6190
104.2828
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23.5640
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S
N
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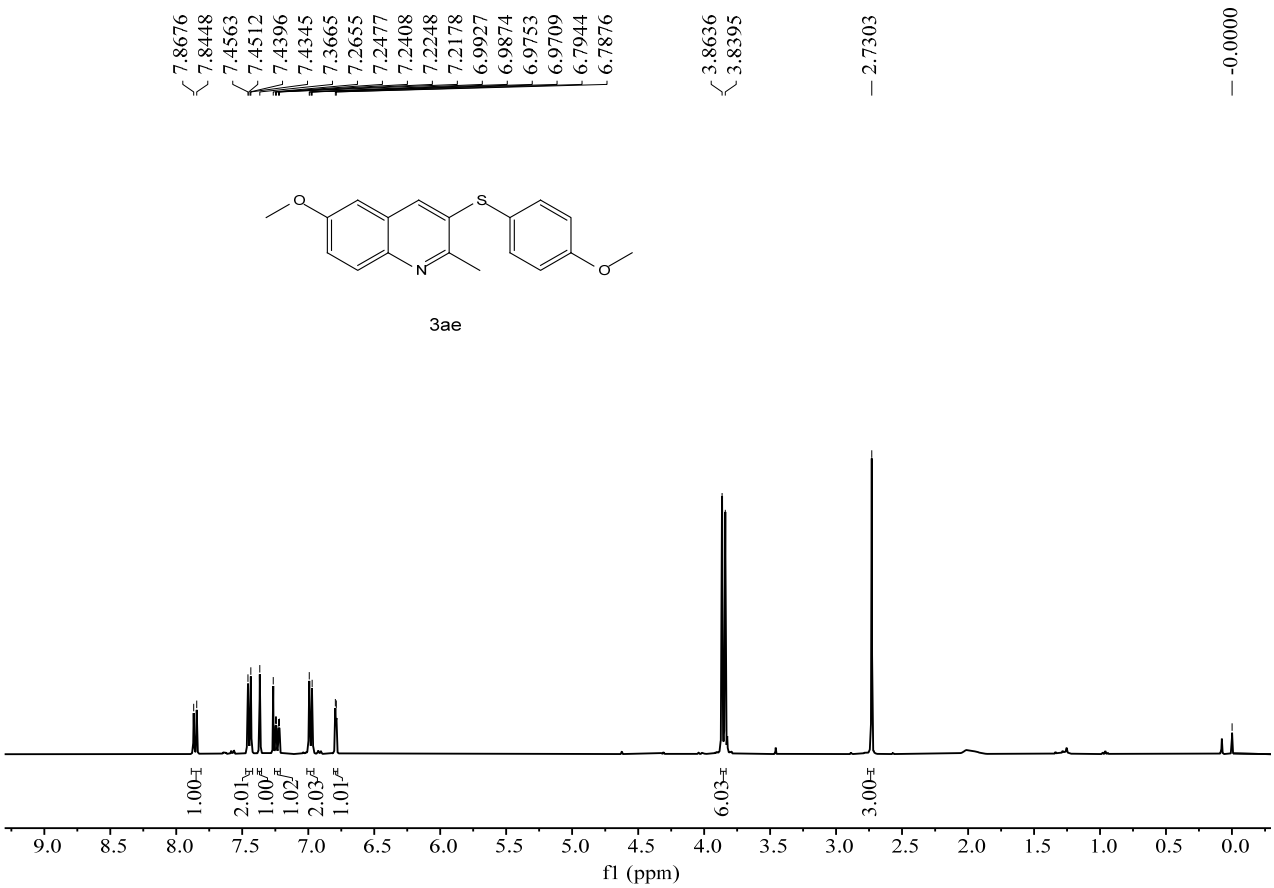
fl (ppm)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6.9927
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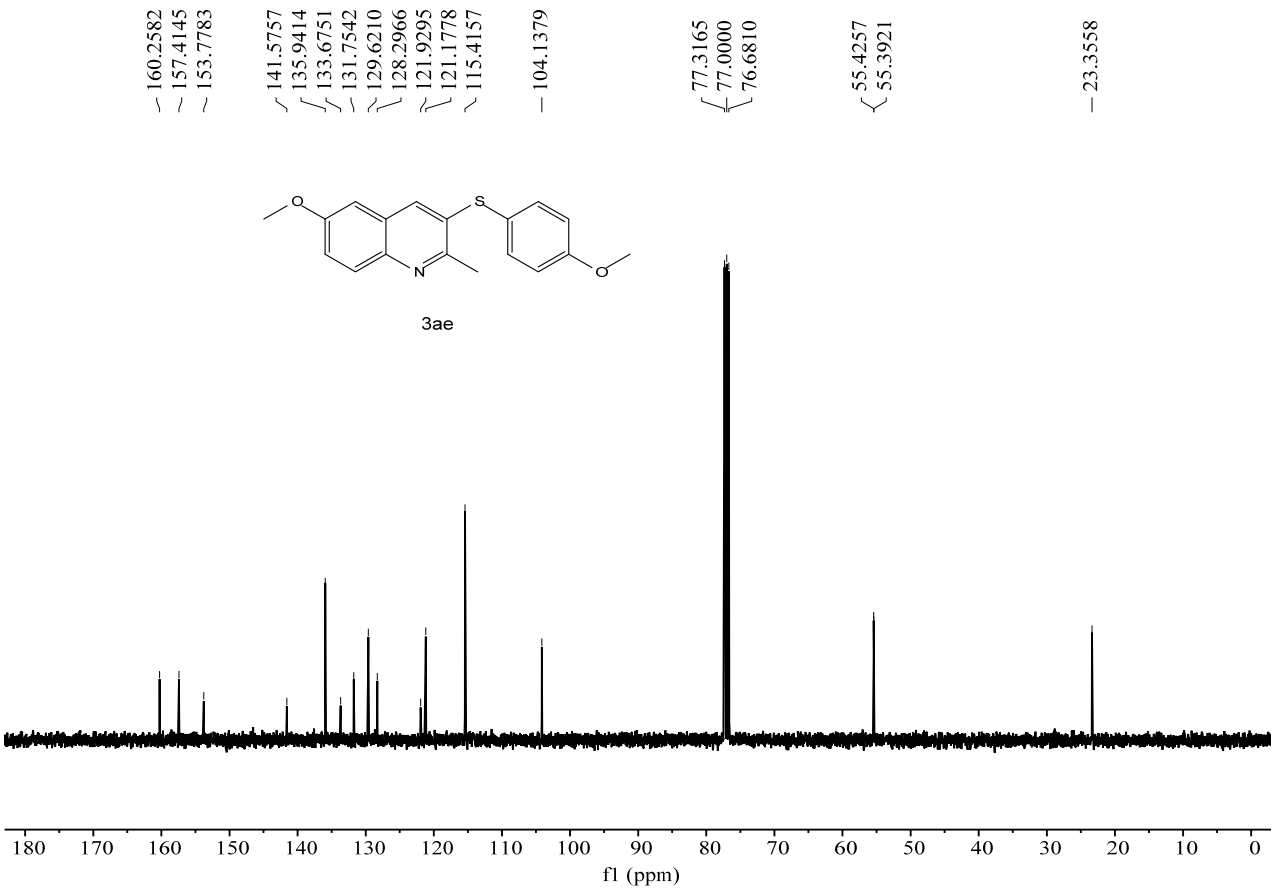
6.9753
6.9709
6.7944
6.7876
3.8636
3.8395
2.7303
-0.0000
O
S
N
O
3ae
1.00
2.01
1.00
1.02
2.03
1.01
6.03
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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76.6810
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N
O
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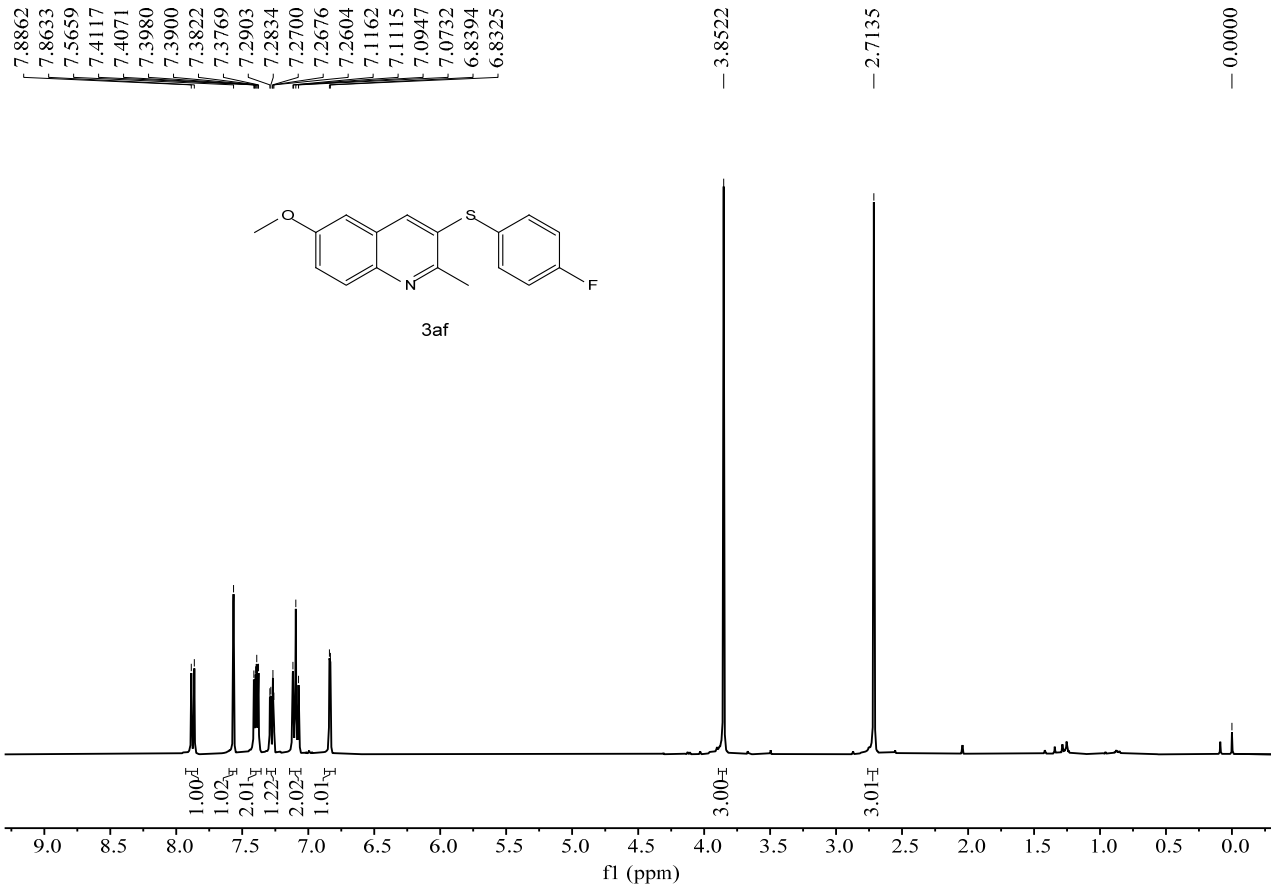
f1 (ppm)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7.2676
7.2604
7.1162
7.1115
7.0947
7.0732
6.8394
6.8325
3.8522
2.7135
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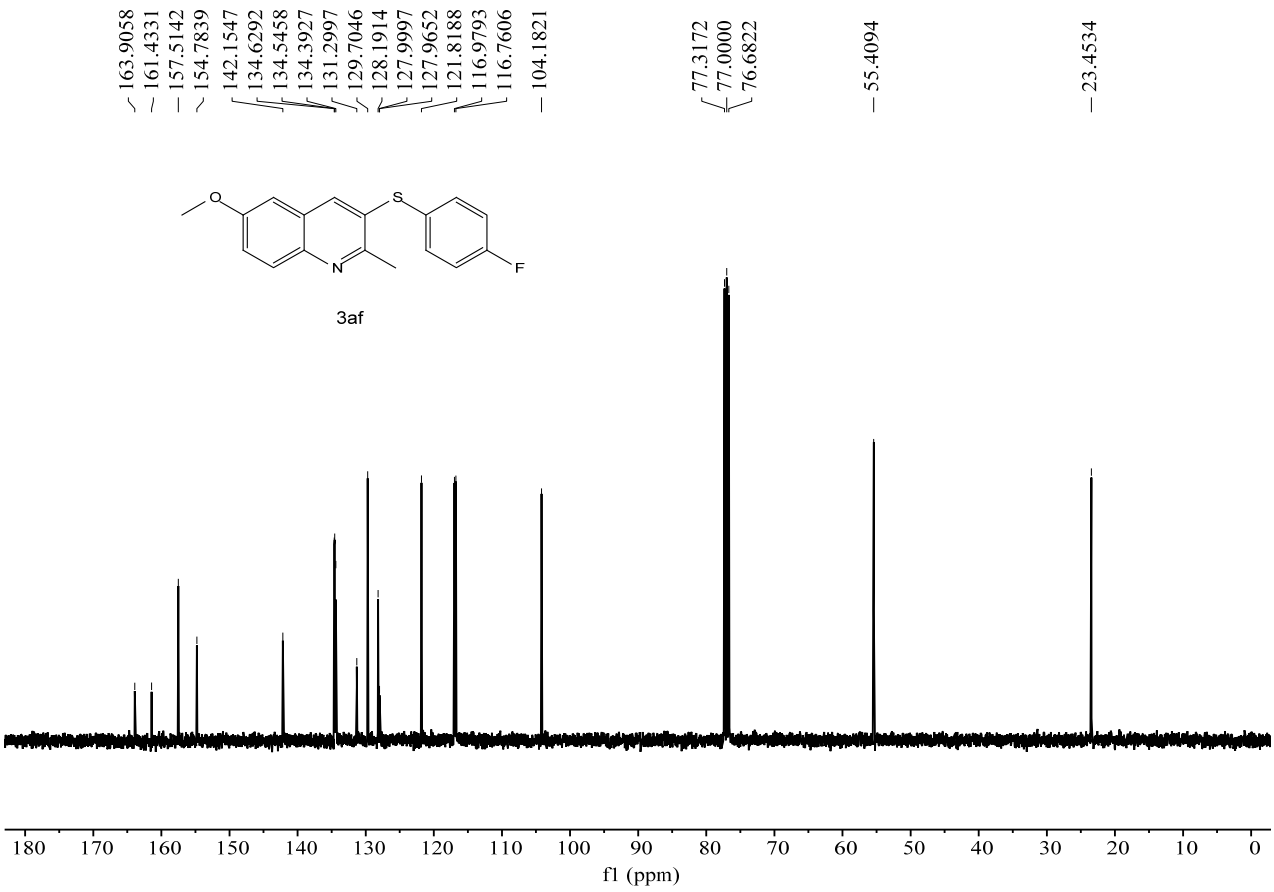
O
S
N
F
3af
1.00
1.02
2.01
1.22
2.02
1.01
3.00
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.9652
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116.7606
104.1821
77.3172
77.0000
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23.4534
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S
N
F
3af
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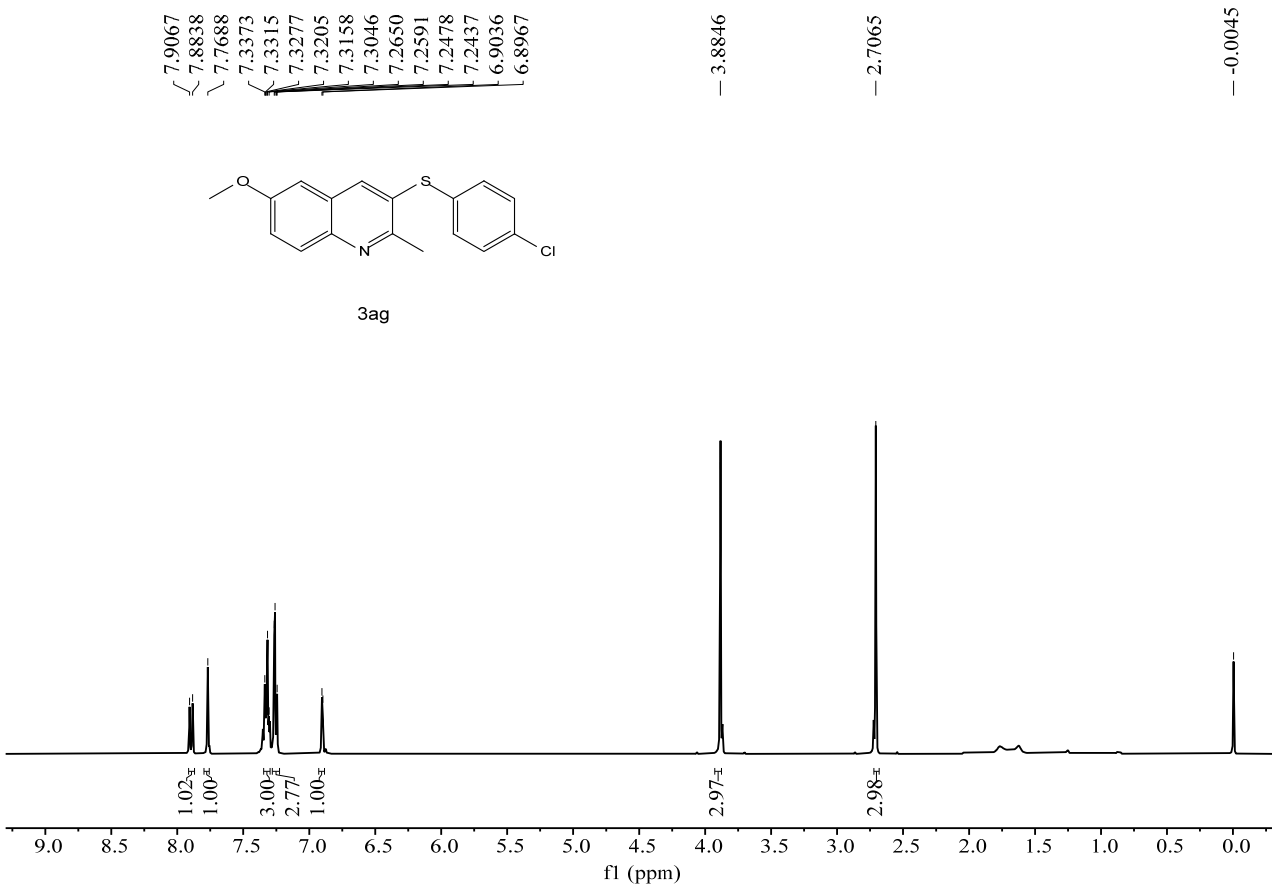
f1 (ppm)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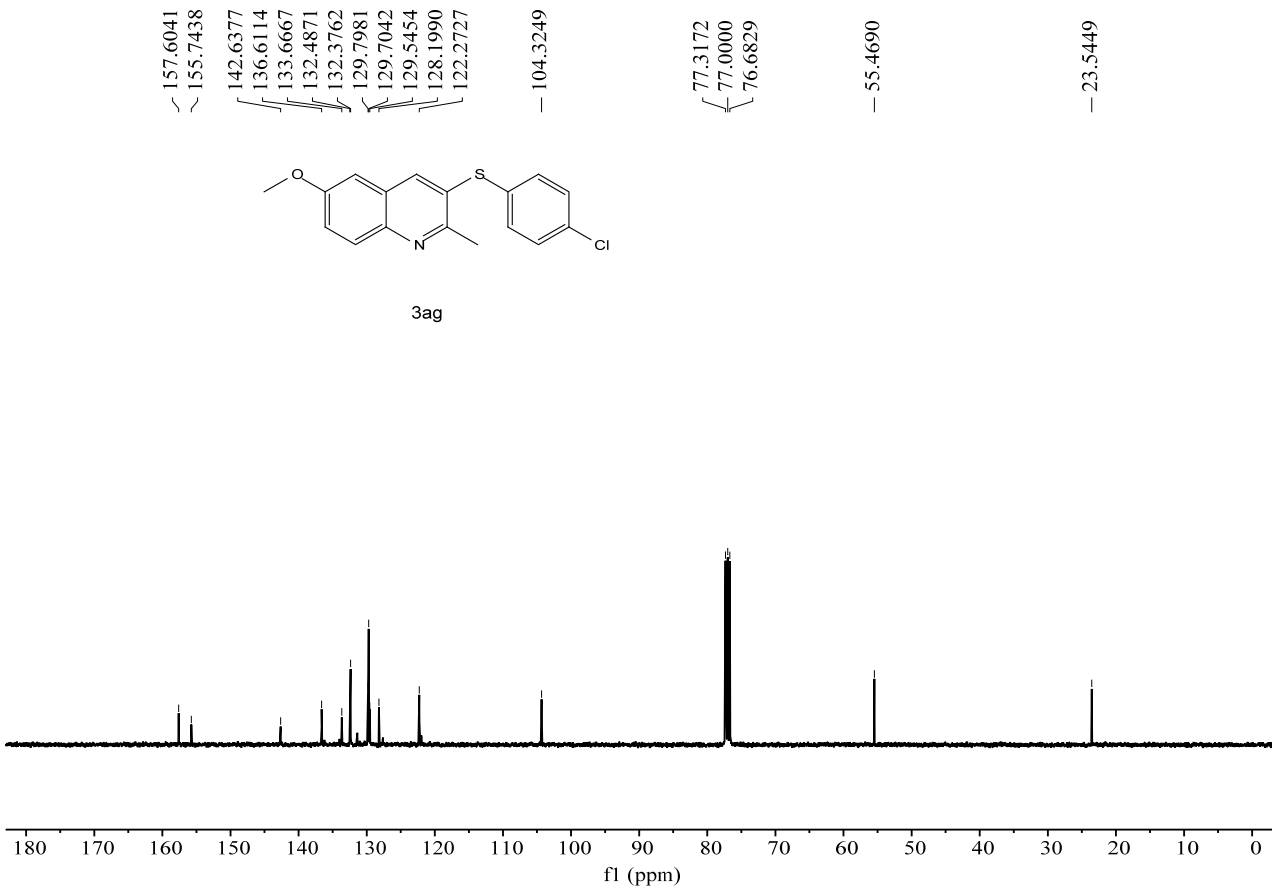
7.2591
7.2478
7.2437
6.9036
6.8967
3.8846
2.7065
-0.0045
O
S
N
Cl
3ag
1.02
1.00
3.00
2.77
1.00
2.97
2.98
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.0000
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O
S
N
Cl
3ag
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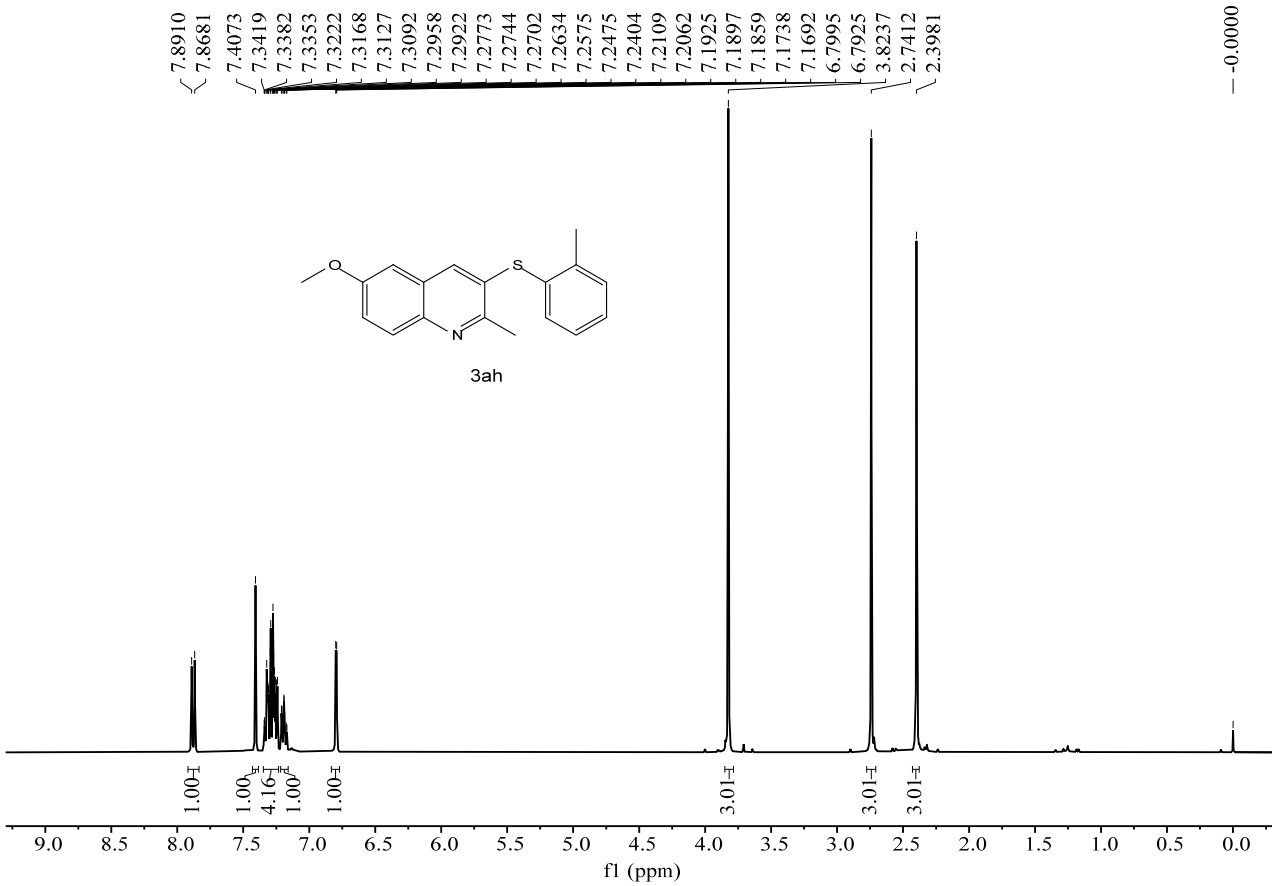
f1 (ppm)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7.2404
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7.2062
7.1925
7.1897
7.1859
7.1738
7.1692
6.7995
6.7925
3.8237
2.7412
2.3981
-0.0000
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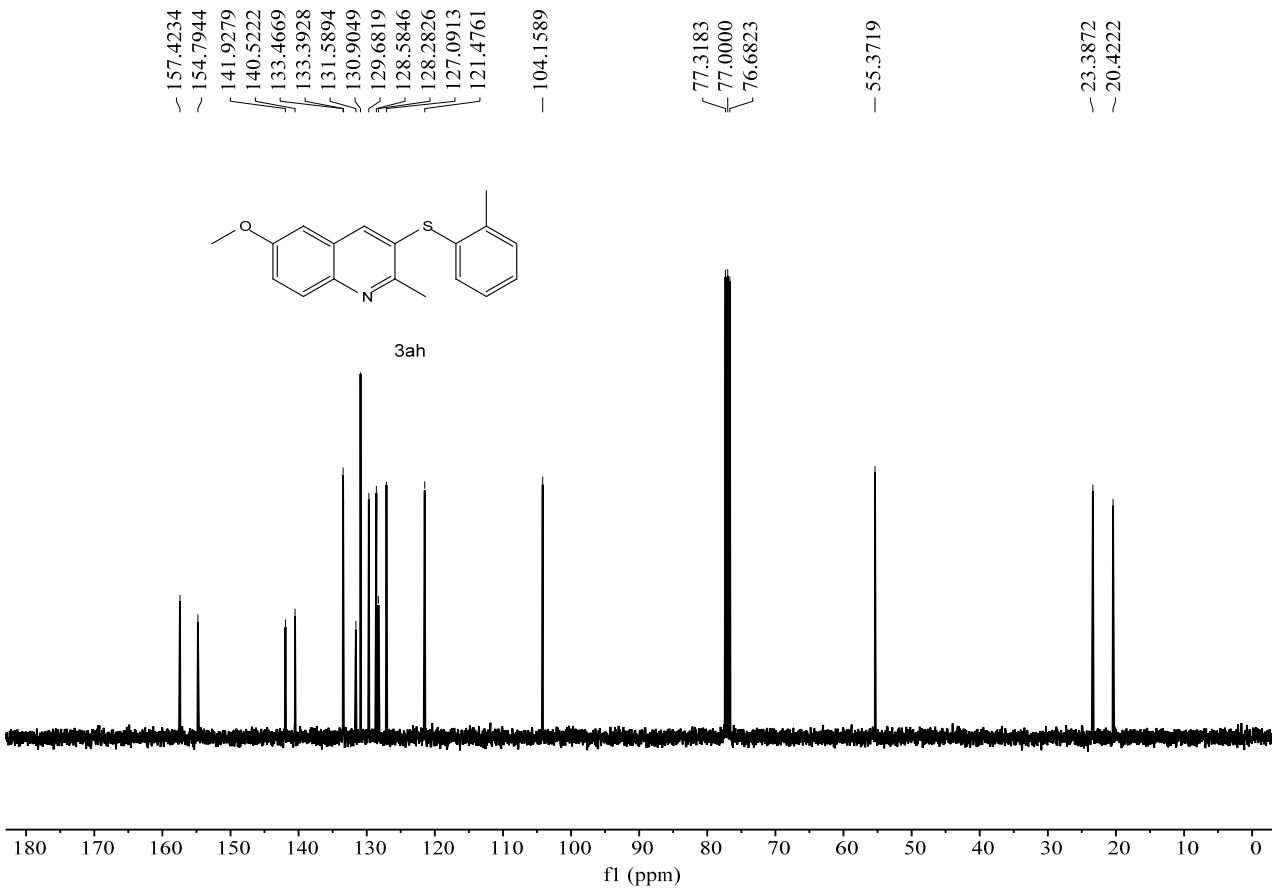
S
N
3ah
1.00
1.00
4.16
1.00
1.00
3.01
3.01
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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S
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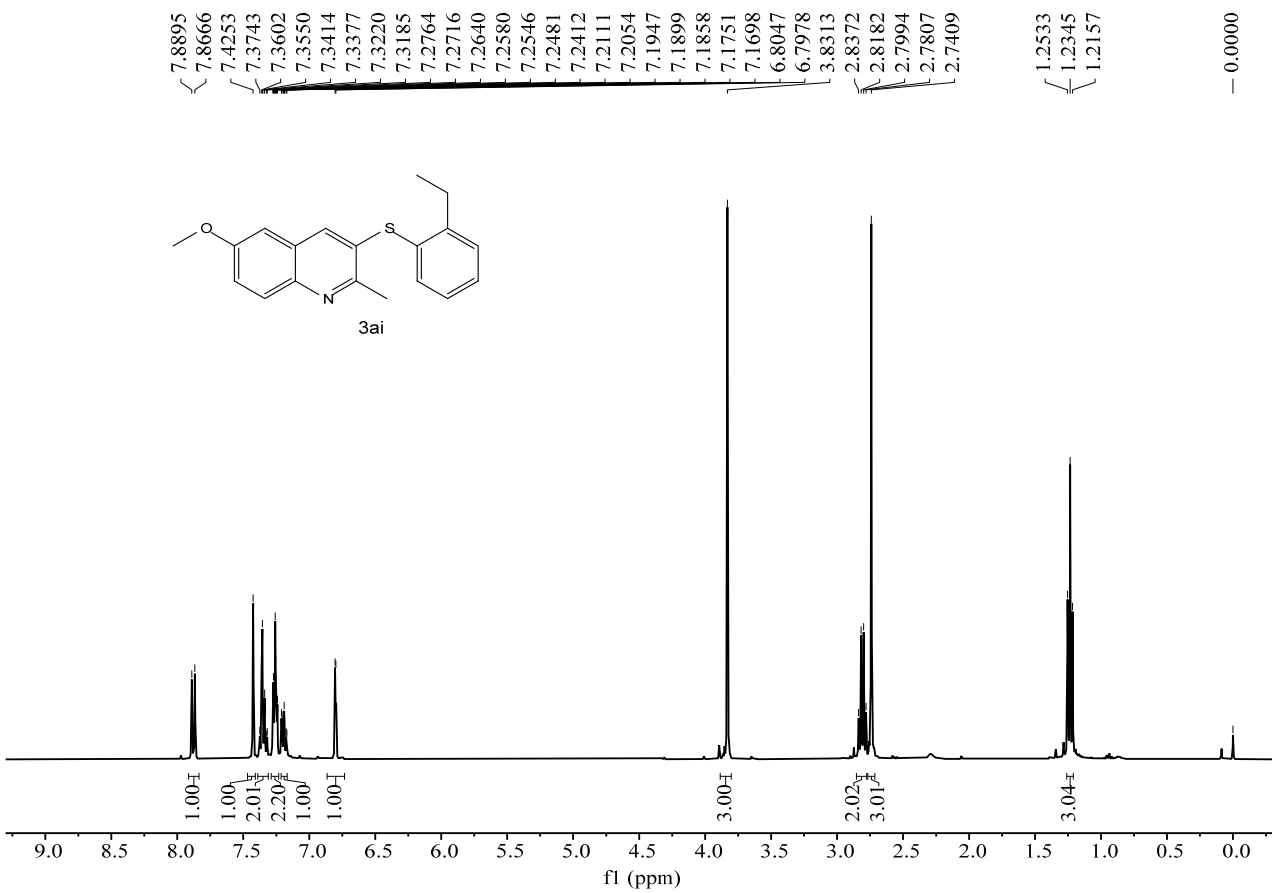
f1 (ppm)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7.2481
7.2412
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1.2157
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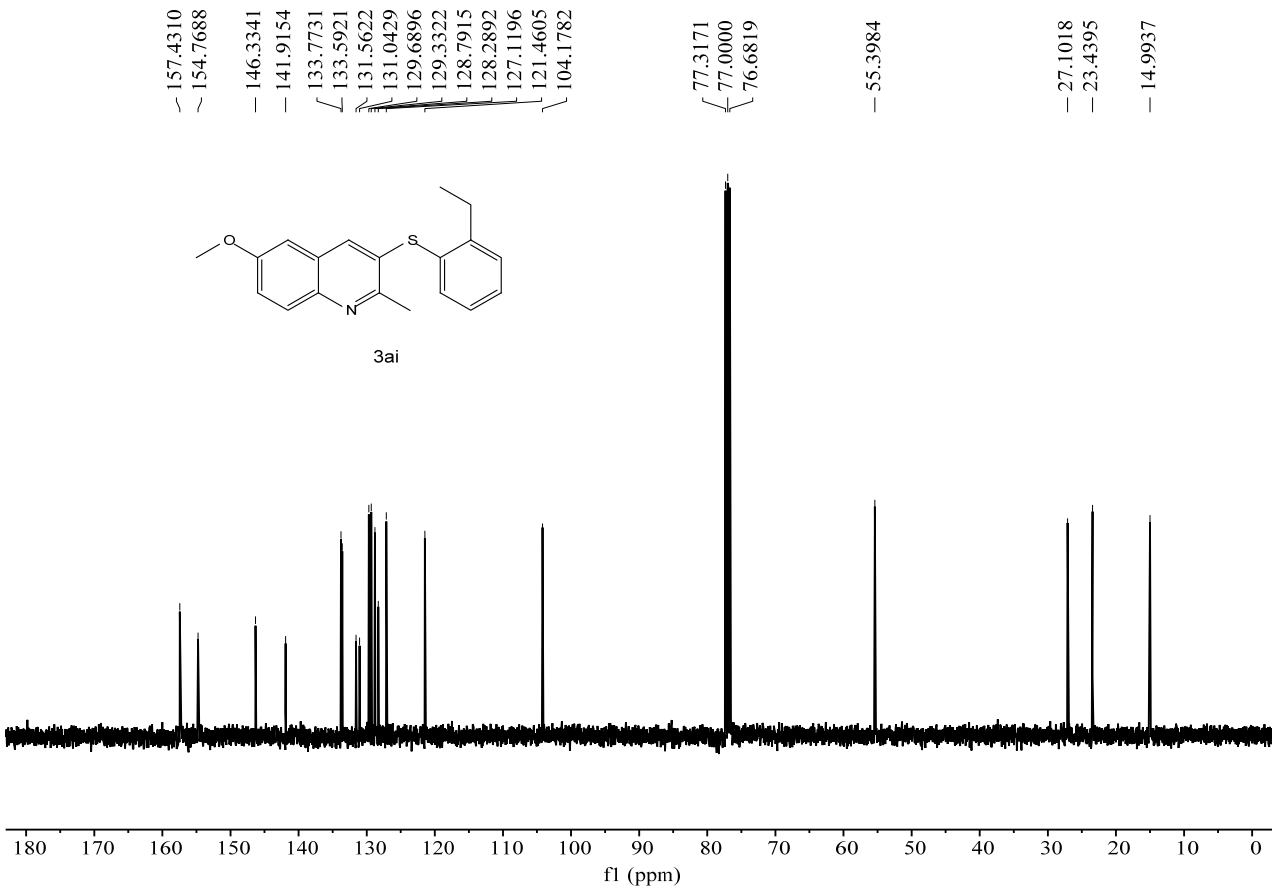
S
N
3ai
1.00
1.00
2.01
2.20
1.00
1.00
3.00
2.02
3.01
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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S
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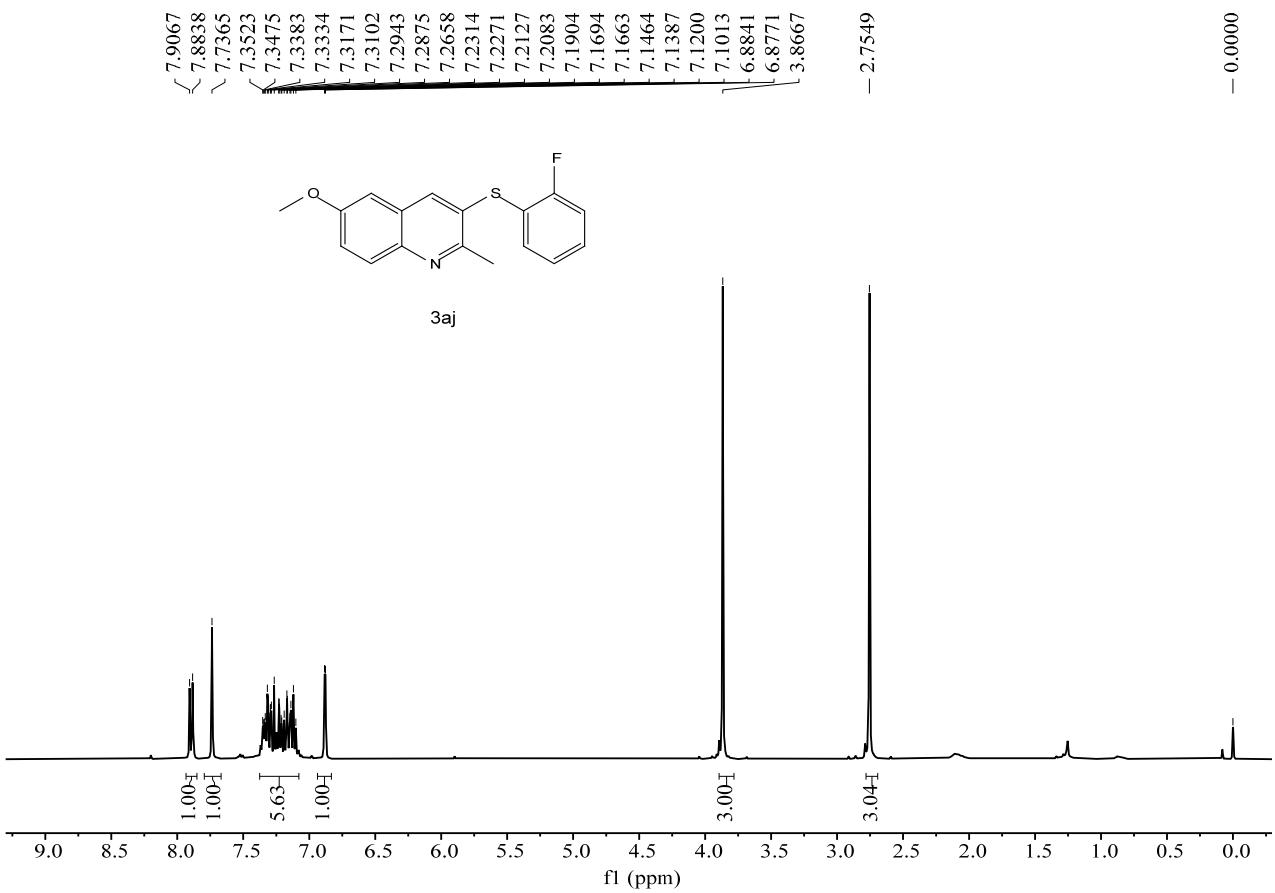
f1 (ppm)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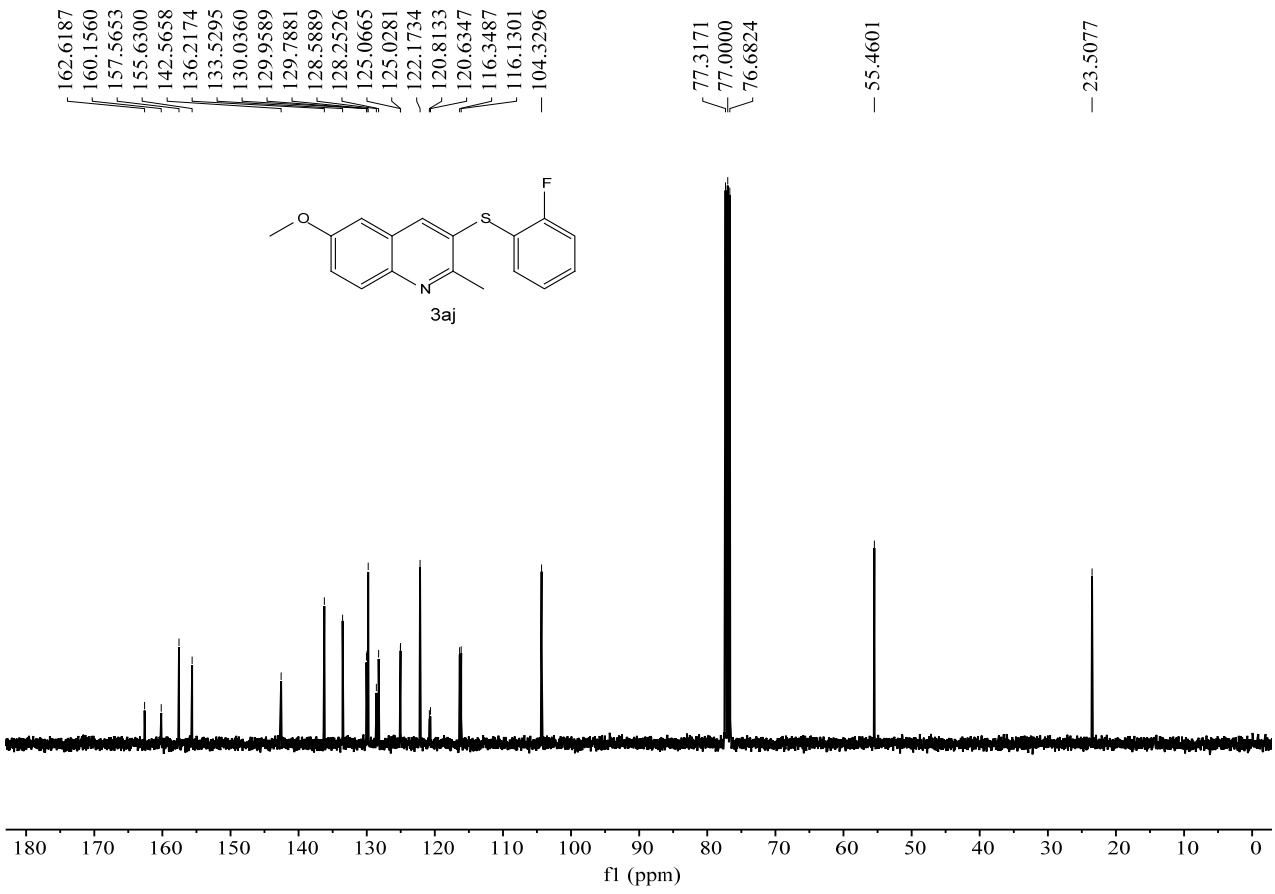
f1 (ppm)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S
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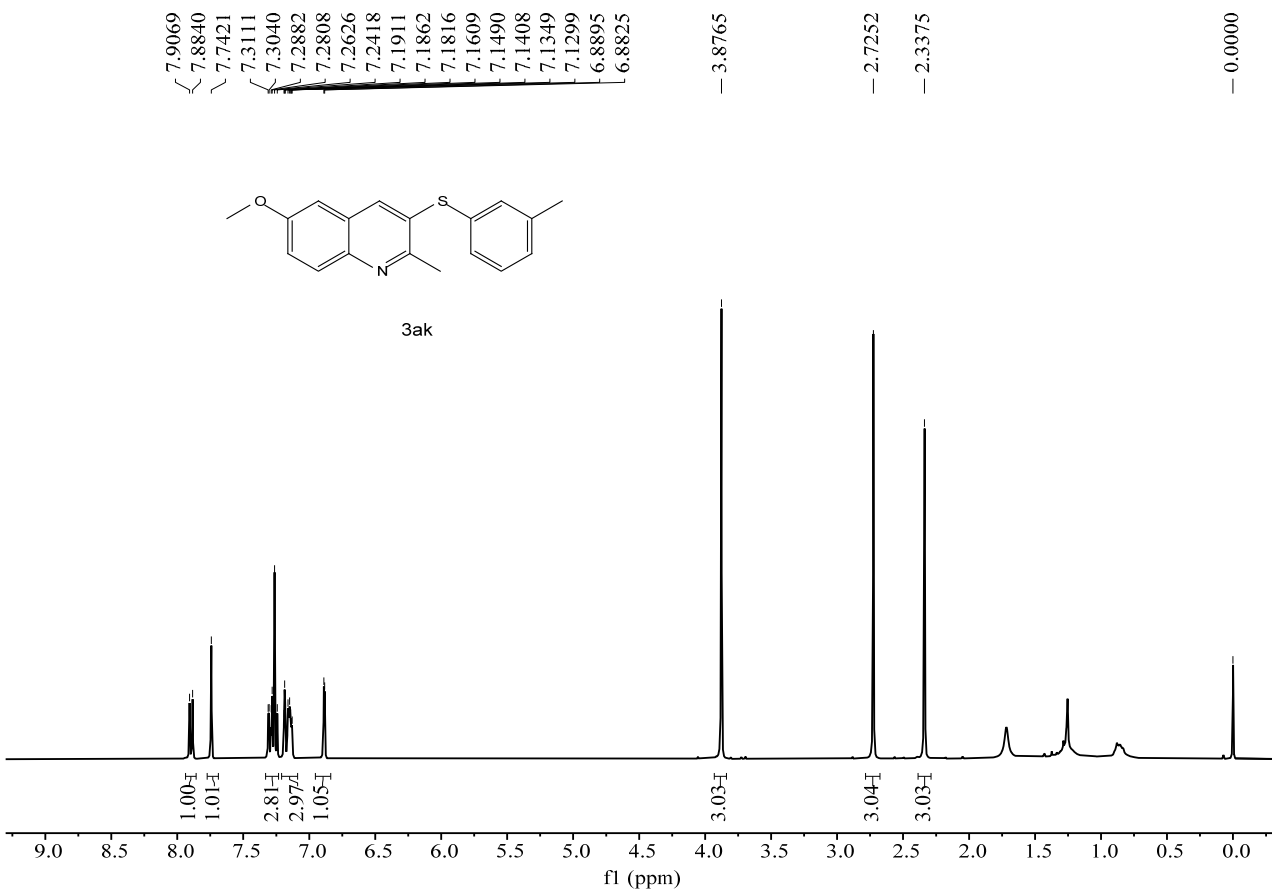
f1 (ppm)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N
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3.03
3.04
3.03
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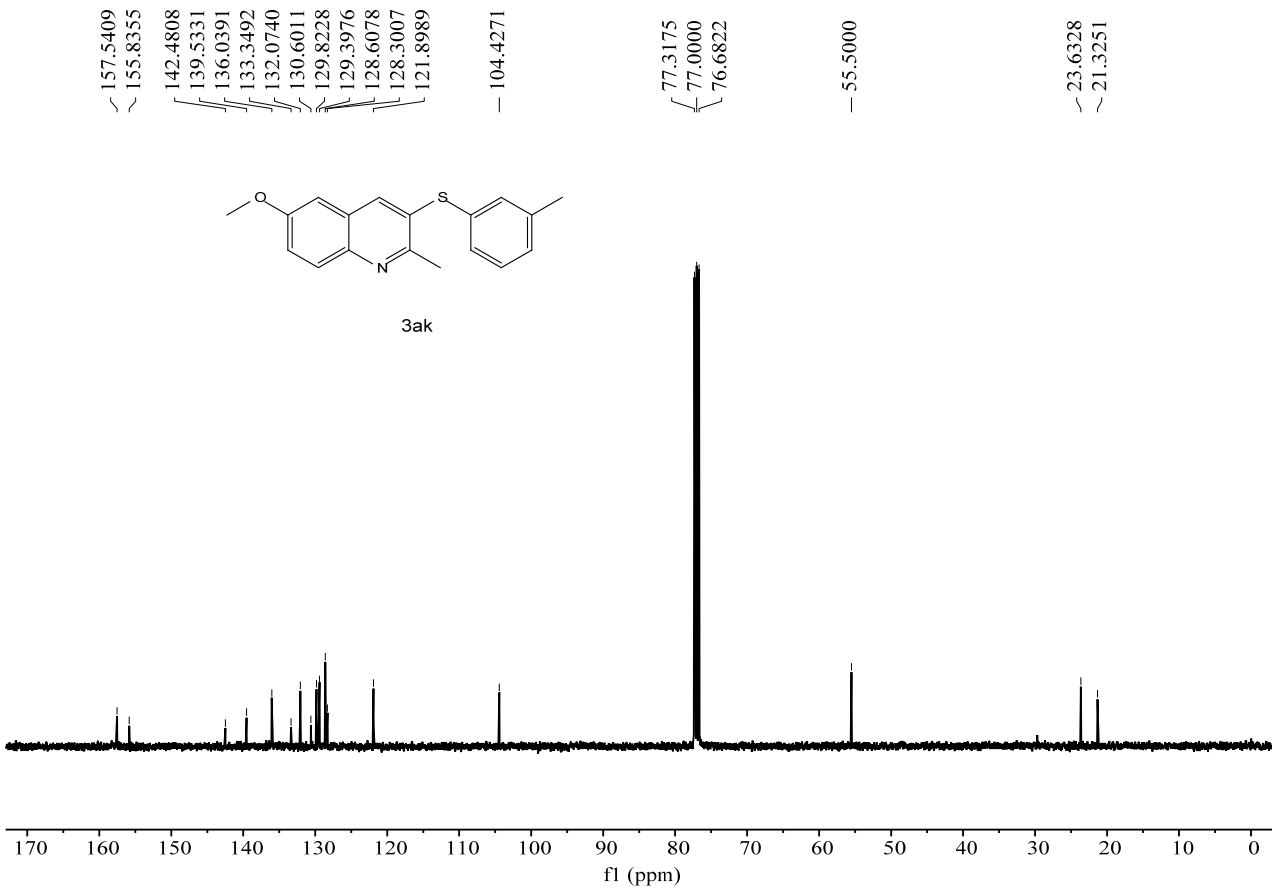
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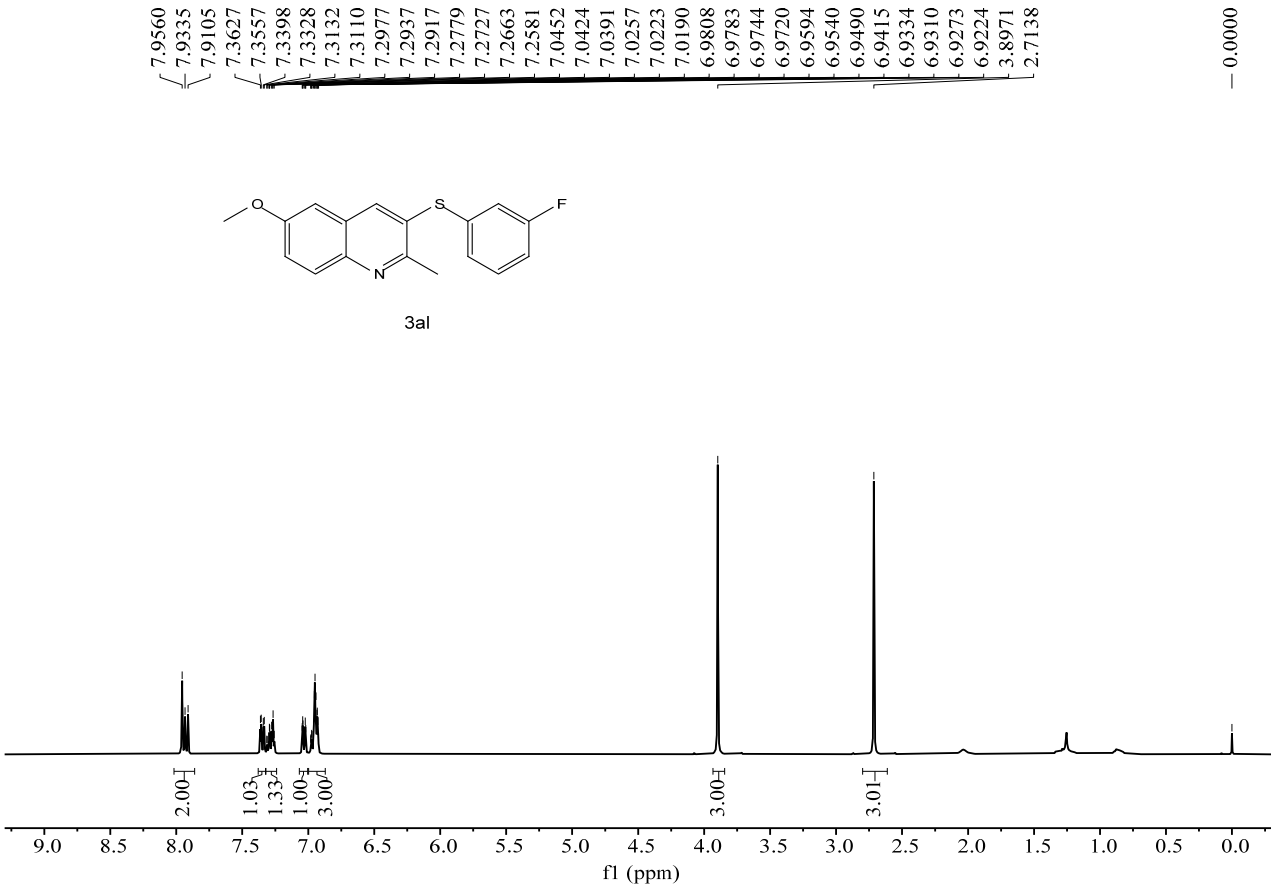
f1 (ppm)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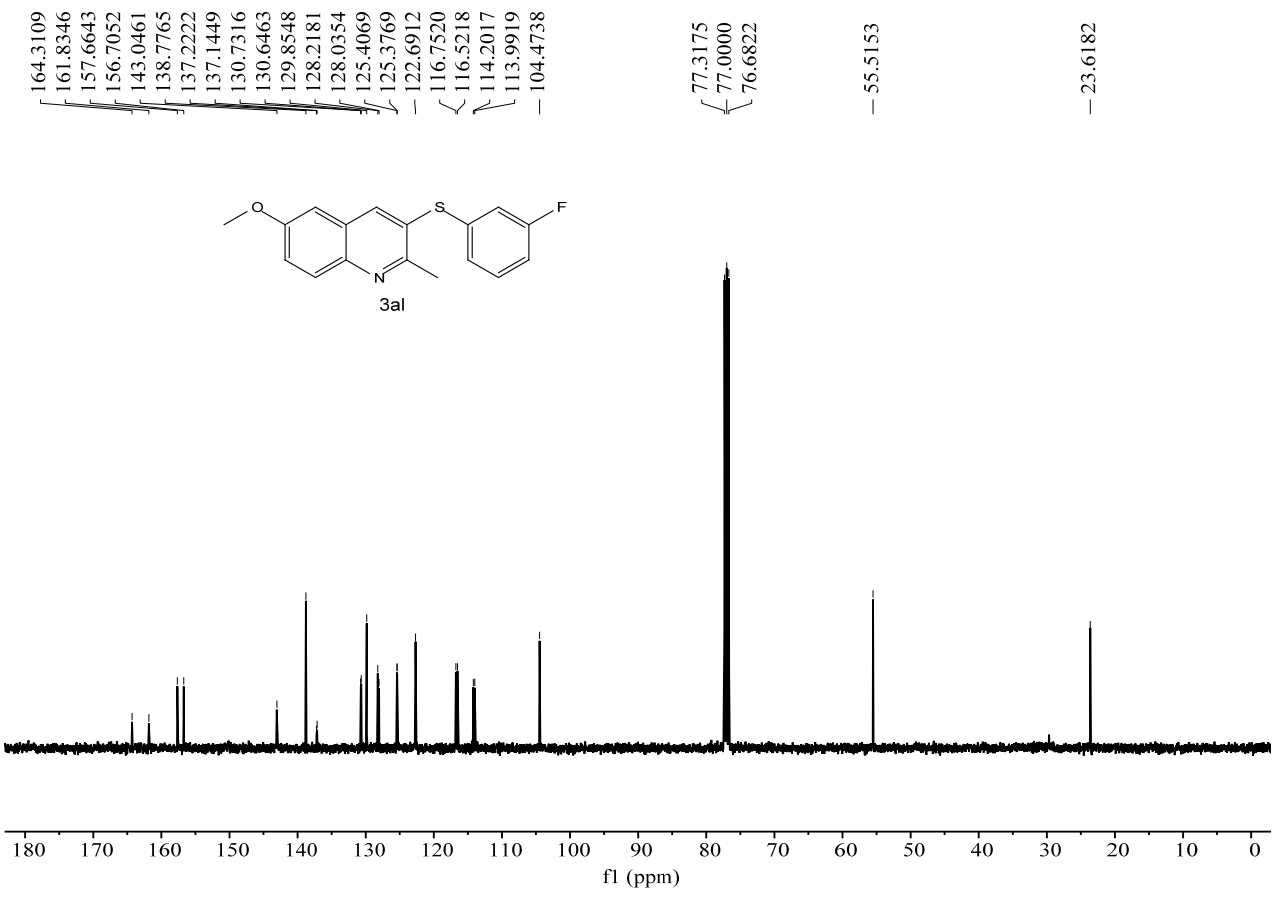
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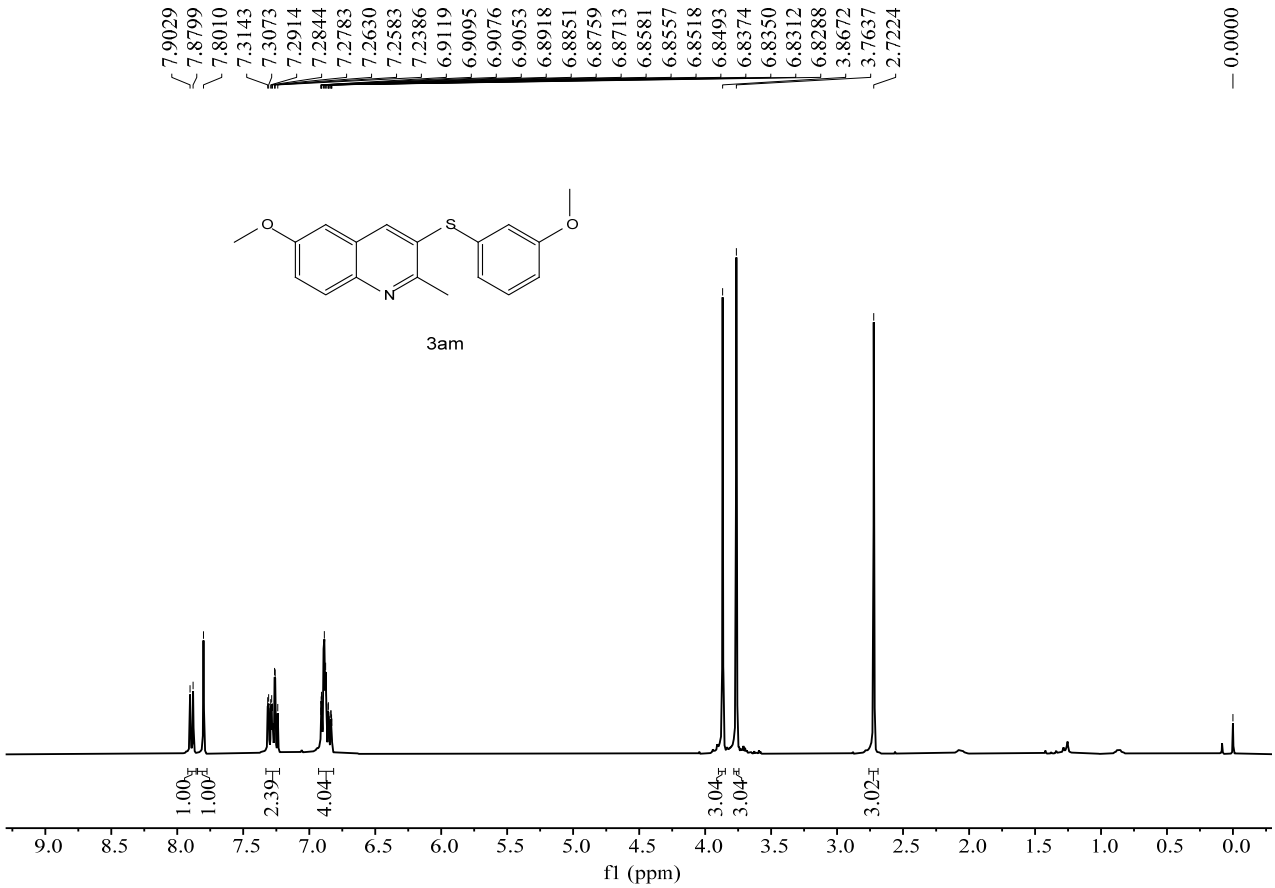
f1 (ppm)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1.00
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4.04
3.04
3.04
3.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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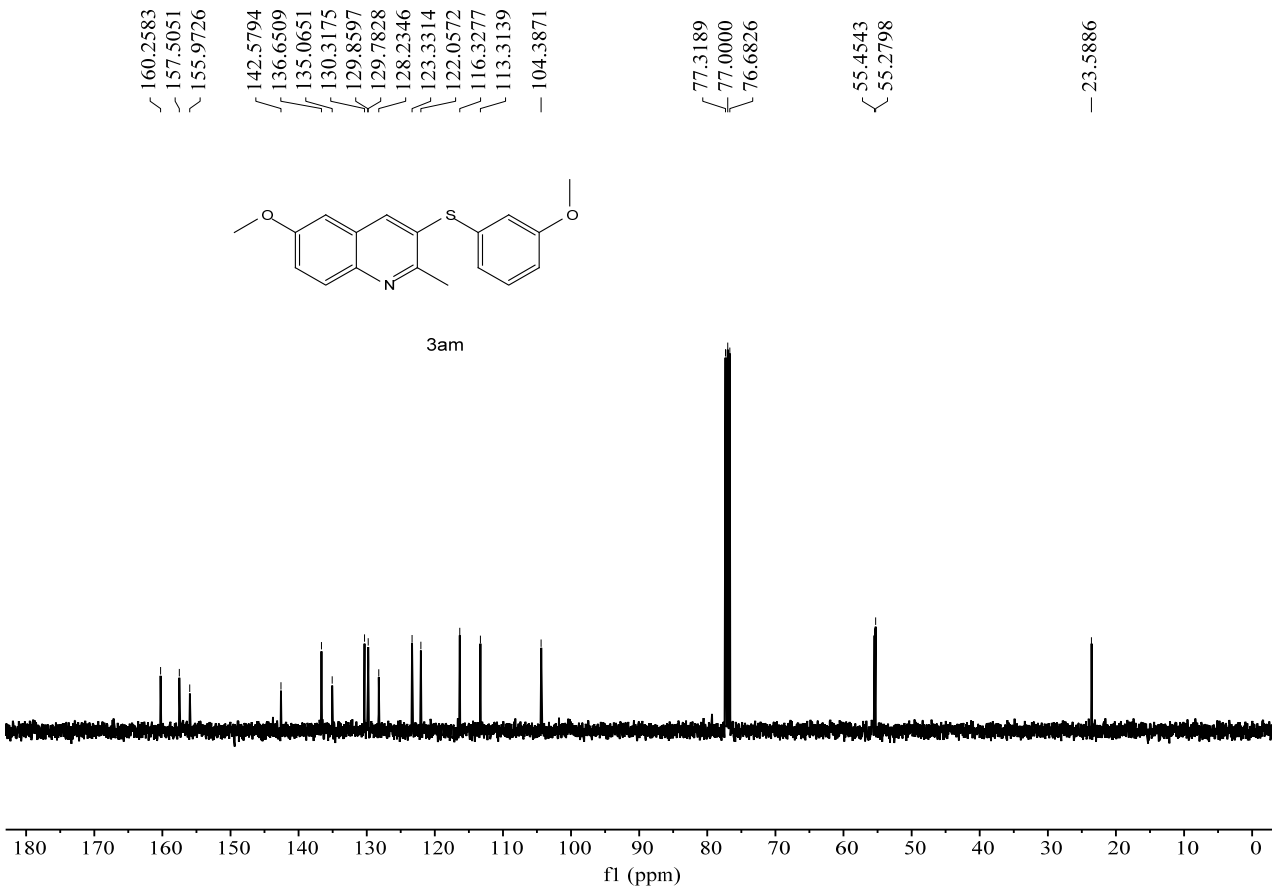
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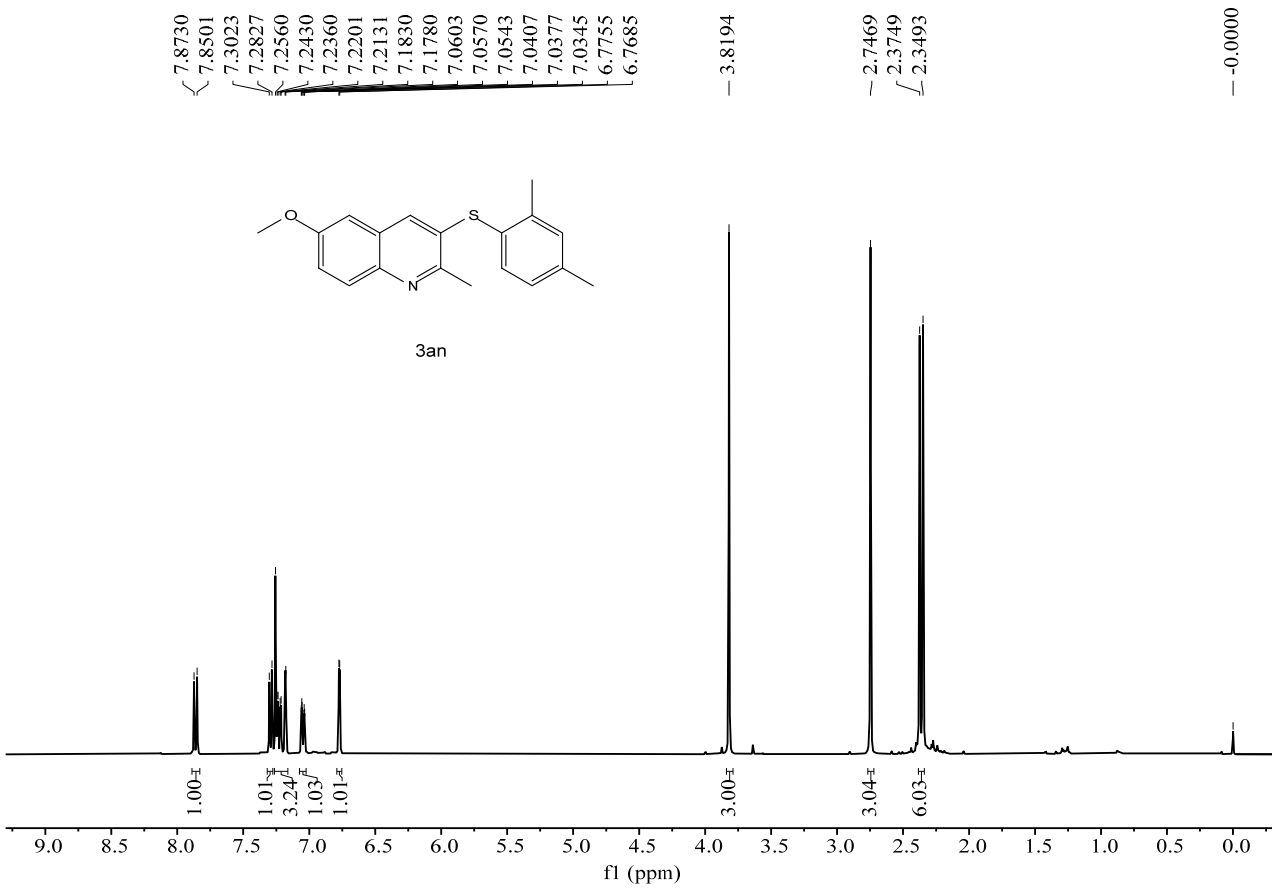
f1 (ppm)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S
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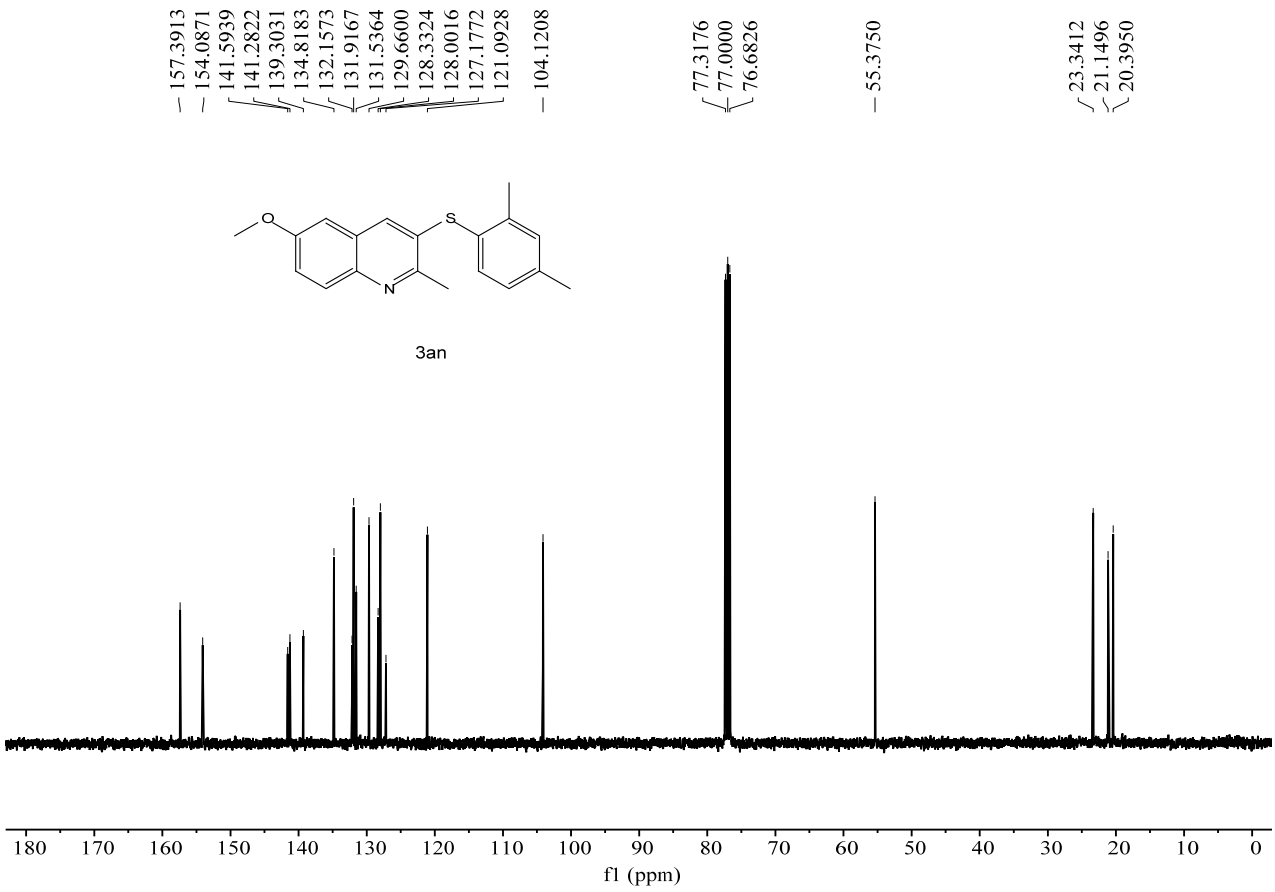
1.01
3.00
3.04
6.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.3324
128.0016
127.1772
121.0928
104.1208
77.3176
77.0000
76.6826
55.3750
23.3412
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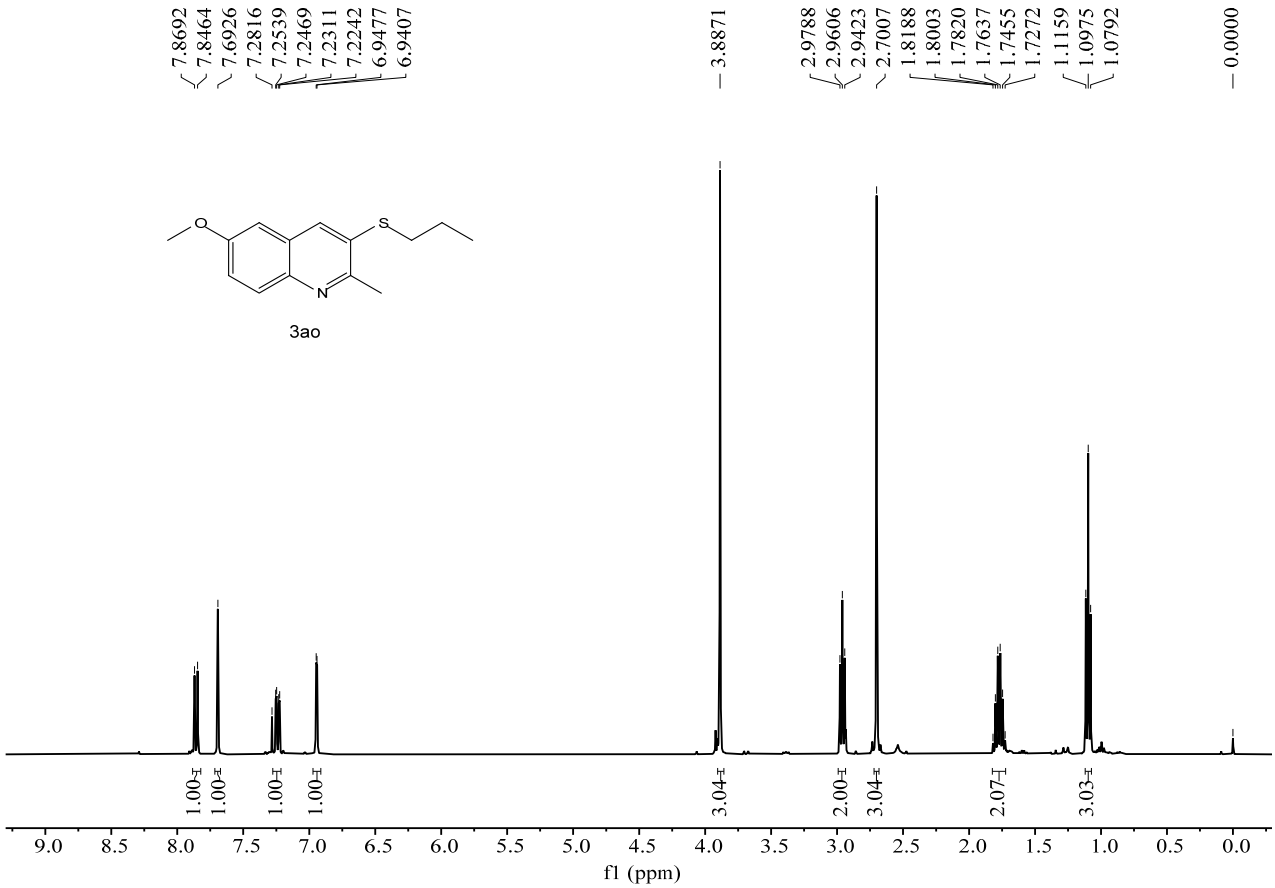
20.3950
O
S
N
3an
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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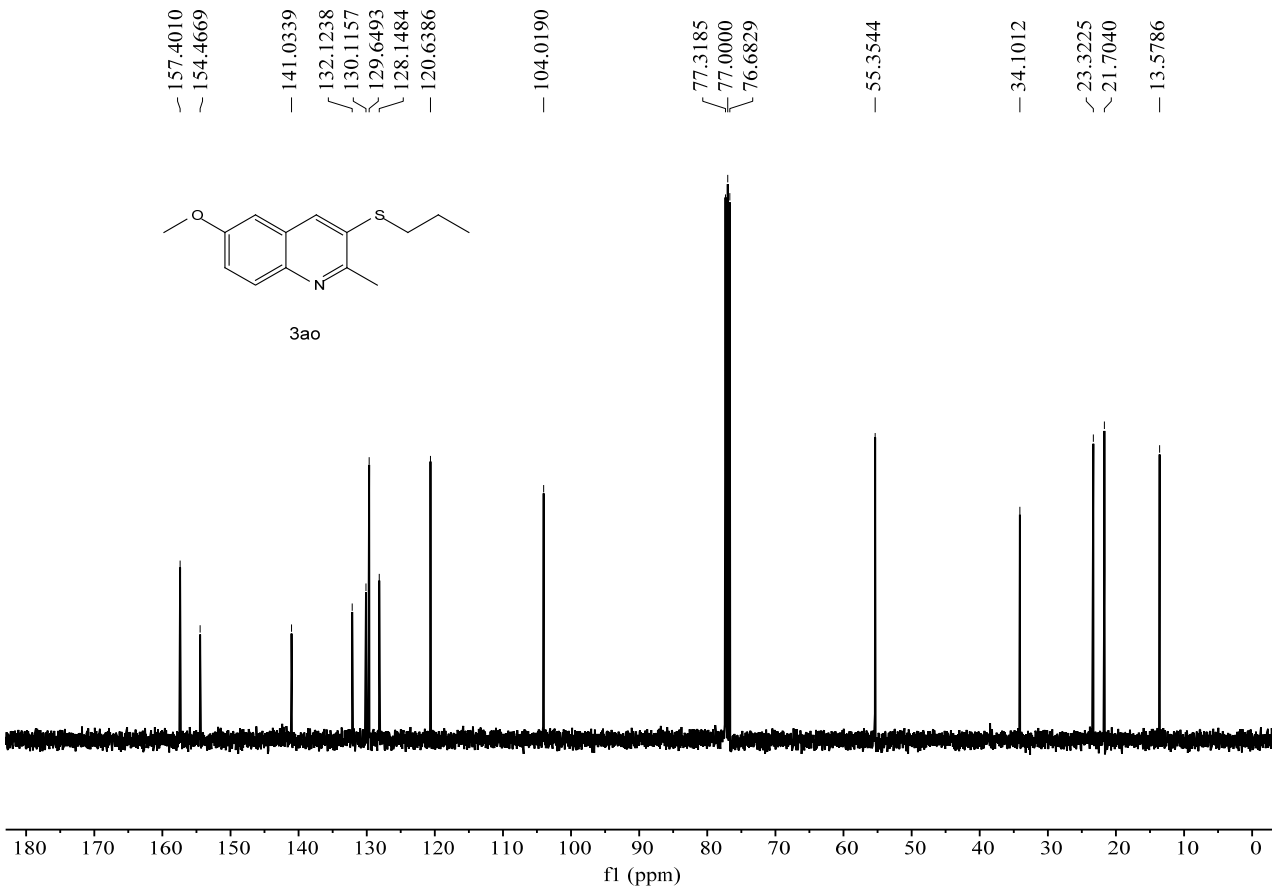
2.9606
2.9423
2.7007
1.8188
1.8003
1.7820
1.7637
1.7455
1.7272
1.1159
1.0975
1.0792
0.0000
O
S
N
3ao
1.00
1.00
1.00
1.00
3.04
2.00
3.04
2.07
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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34.1012
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O
S
N
3ao
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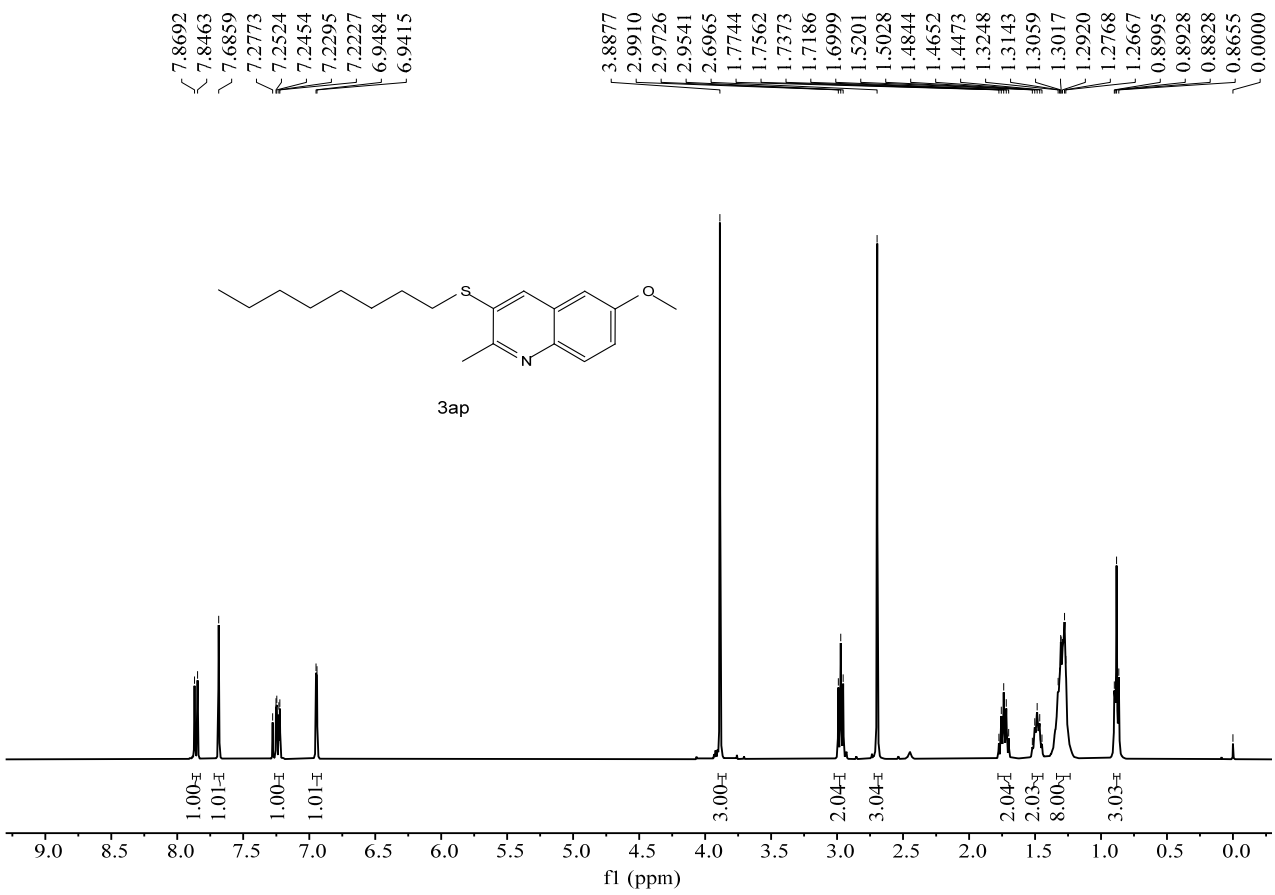
f1 (ppm)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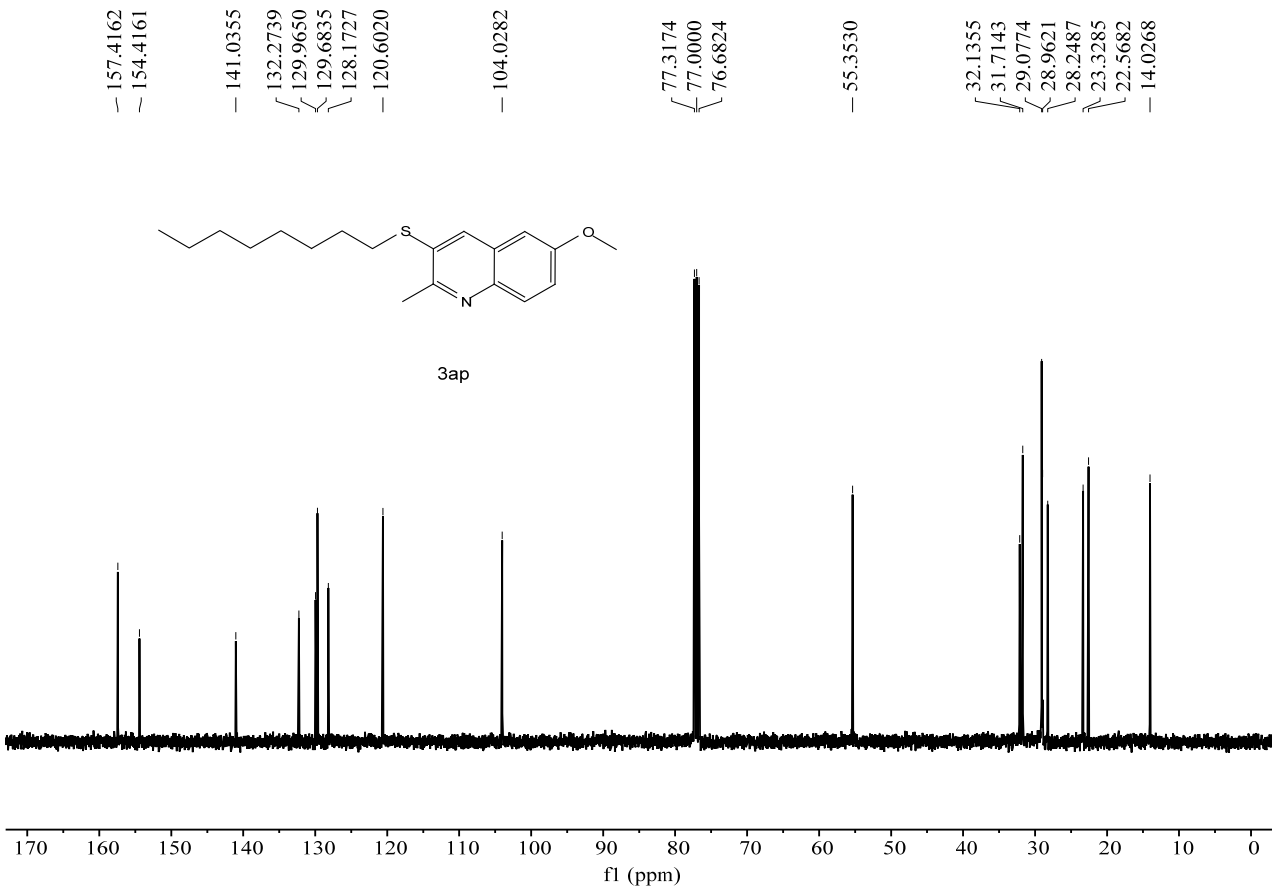
2.9910
2.9726
2.9541
2.6965
1.7744
1.7562
1.7373
1.7186
1.6999
1.5201
1.5028
1.4844
1.4652
1.4473
1.3248
1.3143
1.3059
1.3017
1.2920
1.2768
1.2667
0.8995
0.8928
0.8828
0.8655
0.0000
S
O
N
3ap
1.00
1.01
1.00
1.01
3.00
2.04
3.04
2.04
2.03
8.00
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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32.1355
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S
O
N
3ap
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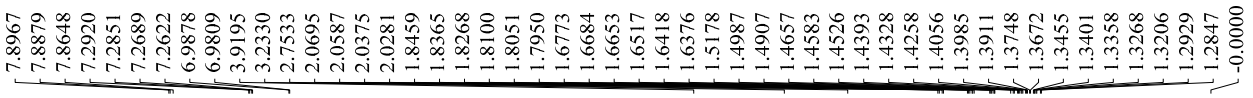
f1 (ppm)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3.2330
2.7533
2.0695
2.0587
2.0375
2.0281
1.8459
1.8365
1.8268
1.8100
1.8051
1.7950
1.6773
1.6684
1.6653
1.6517
1.6418
1.6376
1.5178
1.4987
1.4907
1.4657
1.4583
1.4526
1.4393
1.4328
1.4258
1.4056
1.3985
1.3911
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1.3455
1.3401
1.3358
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1.2929
1.2847
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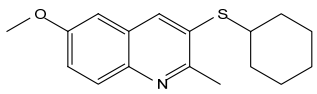
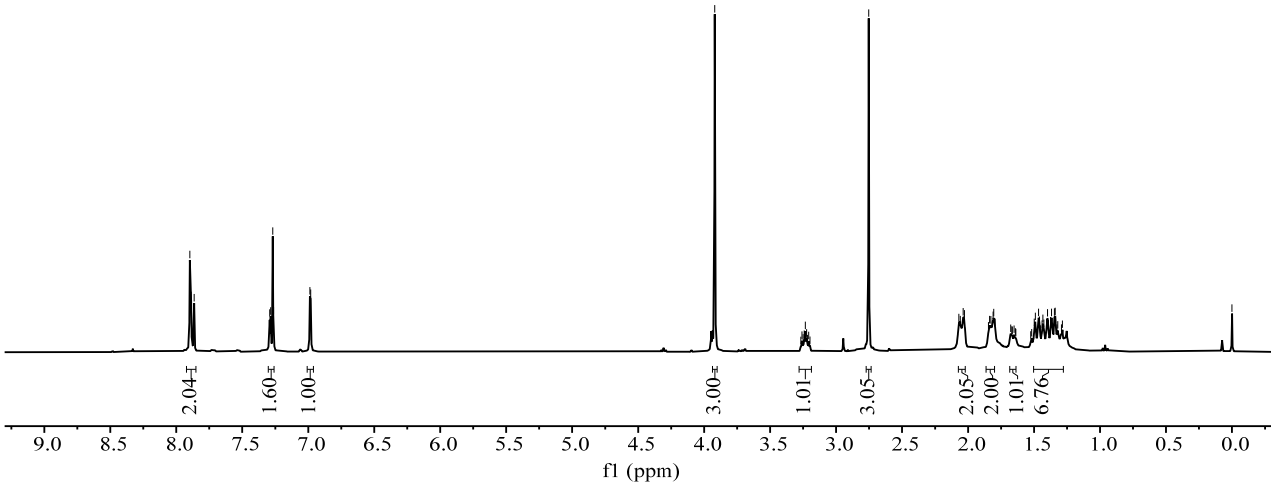

O
S
N

3aq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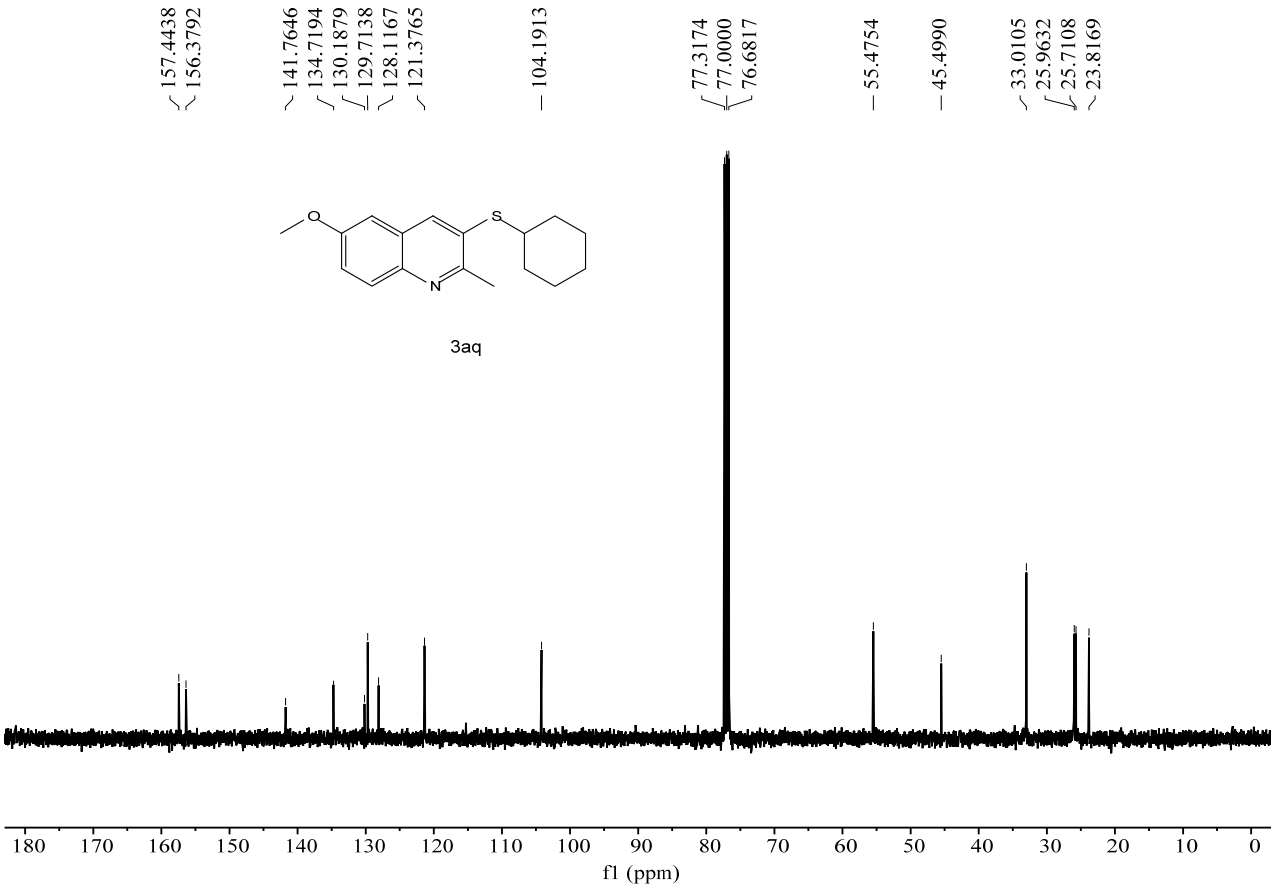
1.60
1.00
3.00
1.01
3.05
2.05
2.00
1.01
6.76
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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45.4990
33.0105
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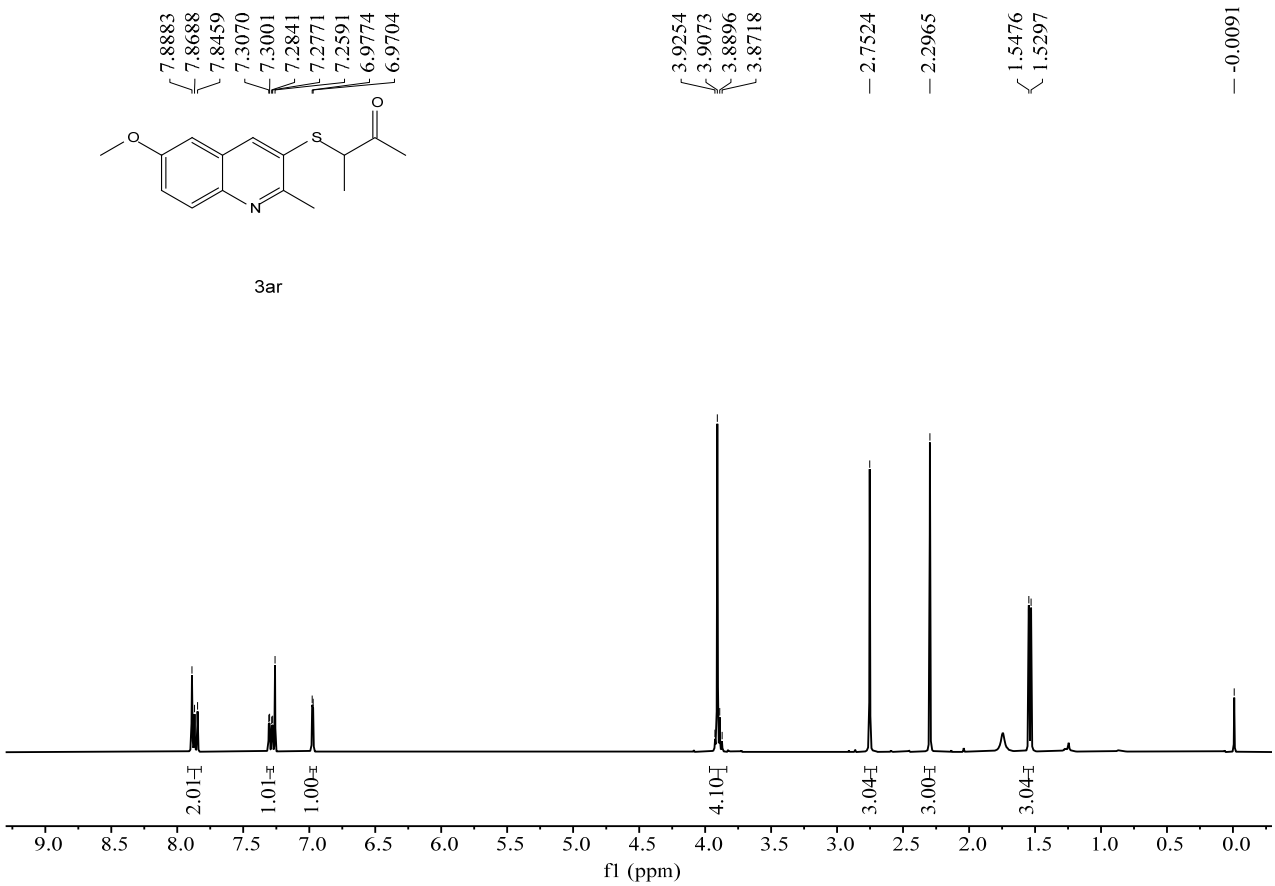
f1 (ppm)

O
S
N

3aq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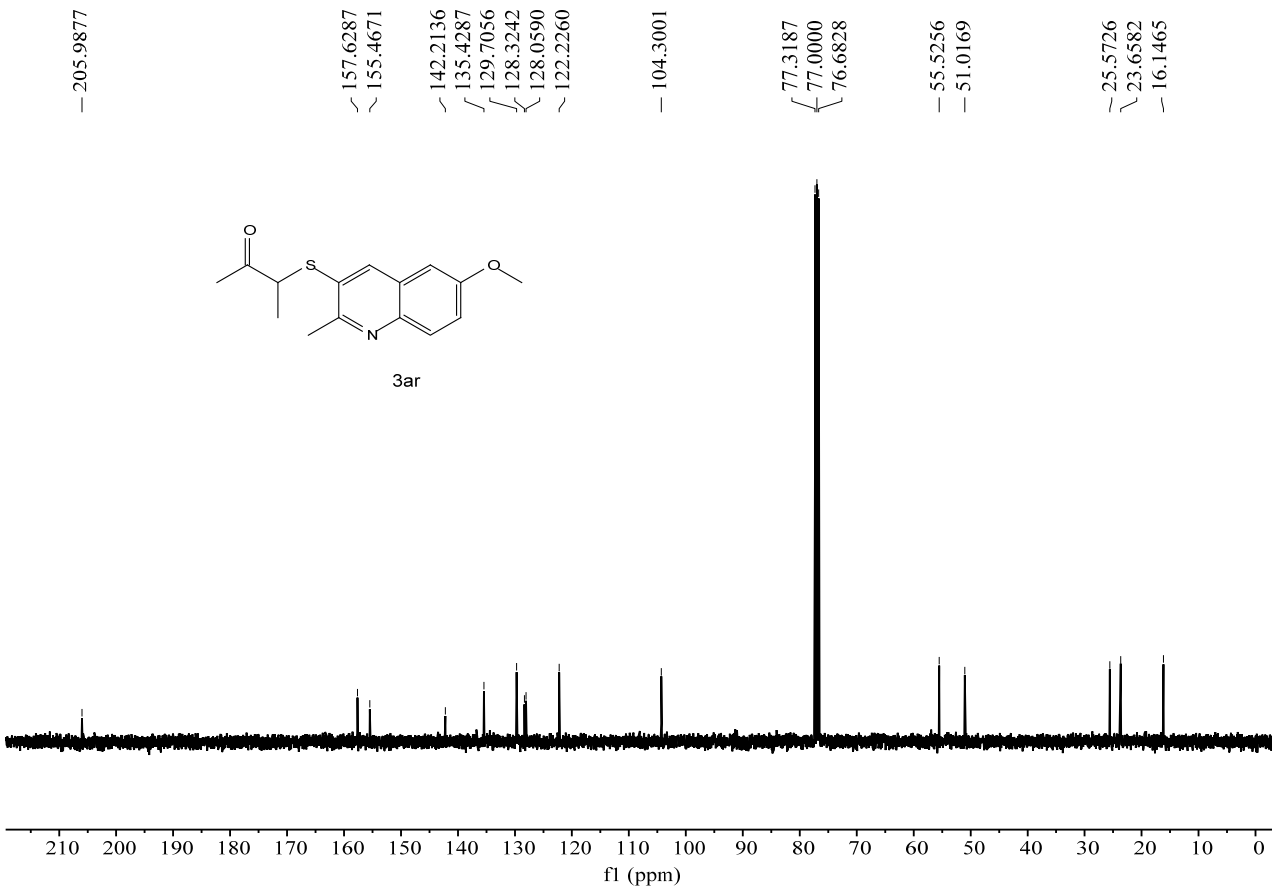
6.9774
6.9704
3.9254
3.9073
3.8896
3.8718
2.7524
2.2965
1.5476
1.5297
-0.0091
O
S
O
N
3ar
2.01
1.01
1.00
4.10
3.04
3.00
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.0000
76.6828
55.5256
51.0169
25.5726
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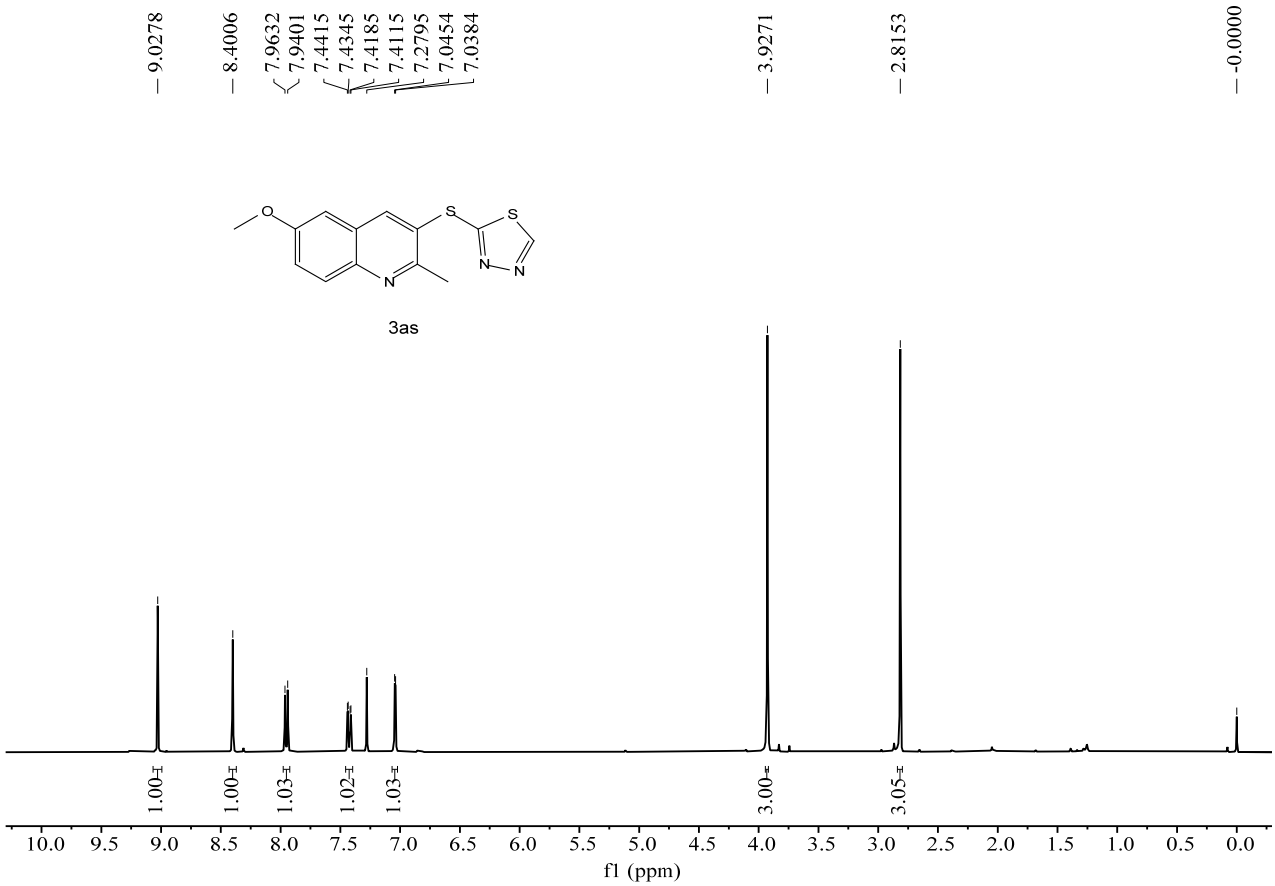
O
S
O
N
3ar
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4345
7.4185
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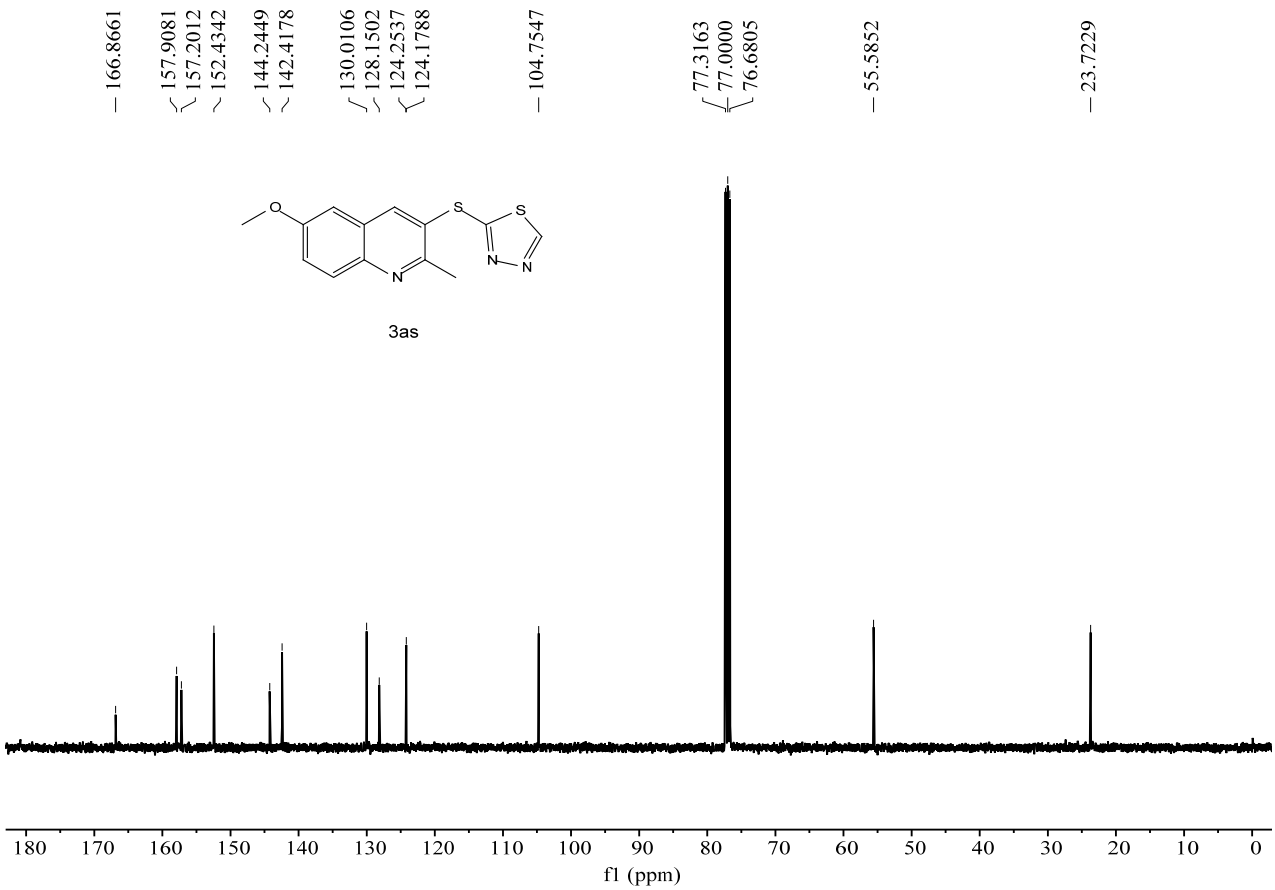
7.0454
7.0384
3.9271
2.8153
-0.0000
3as
1.00
1.00
1.03
1.02
1.03
3.00
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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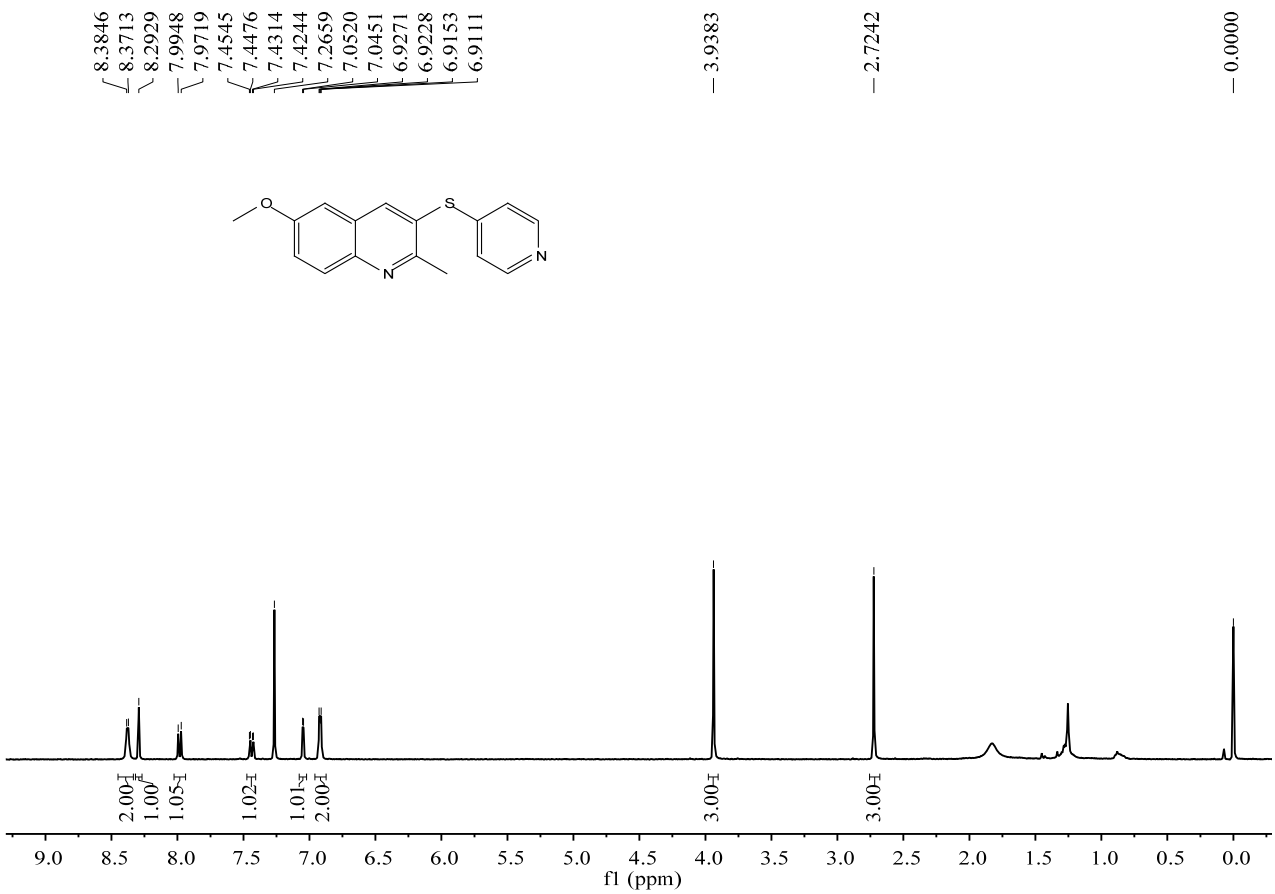
f1 (ppm)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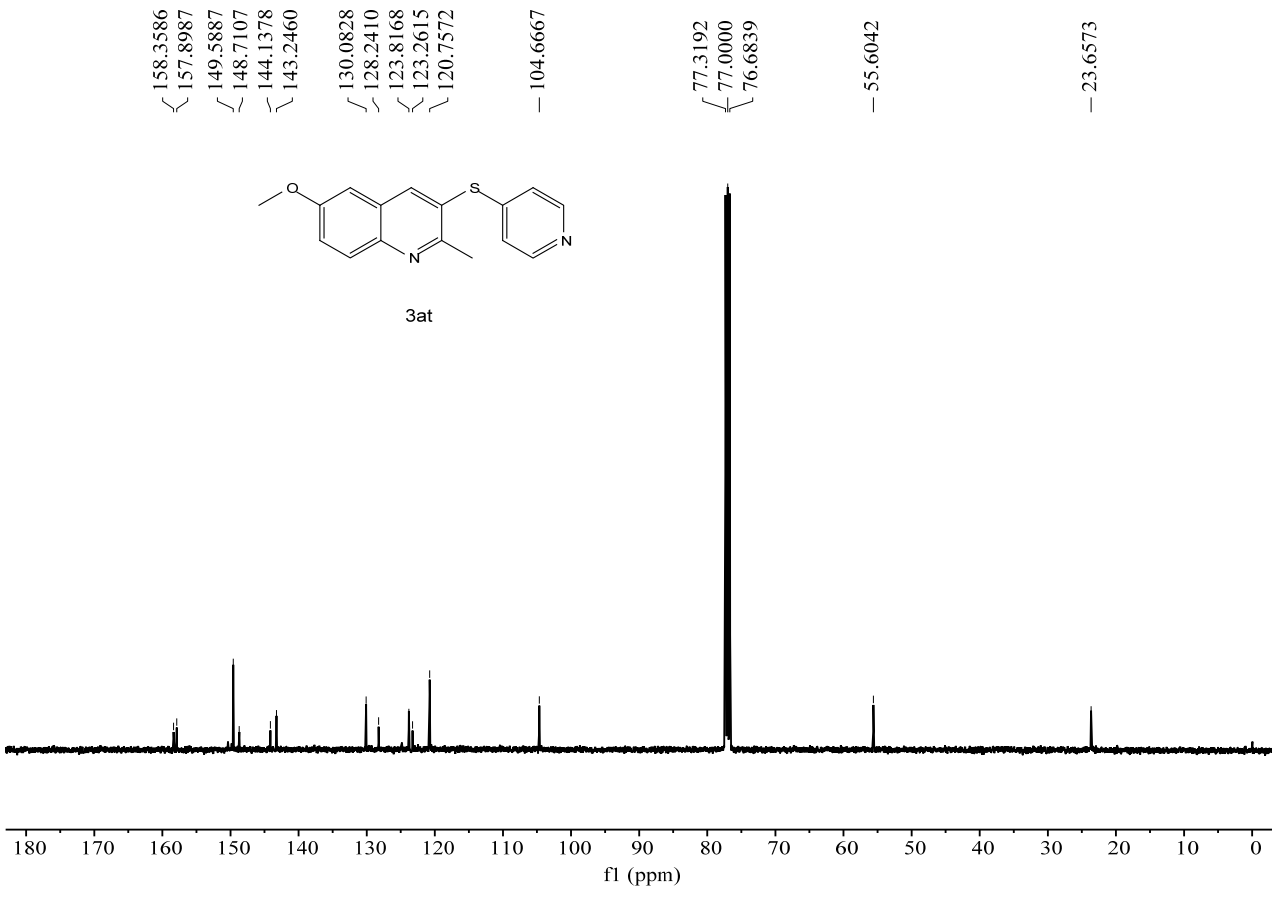
7.4476
7.4314
7.4244
7.2659
7.0520
7.0451
6.9271
6.9228
6.9153
6.9111
3.9383
2.7242
0.0000
O
S
N
N
2.00
1.00
1.05
1.02
1.01
2.00
3.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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123.2615
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104.6667
77.3192
77.0000
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23.6573
O
S
N
N
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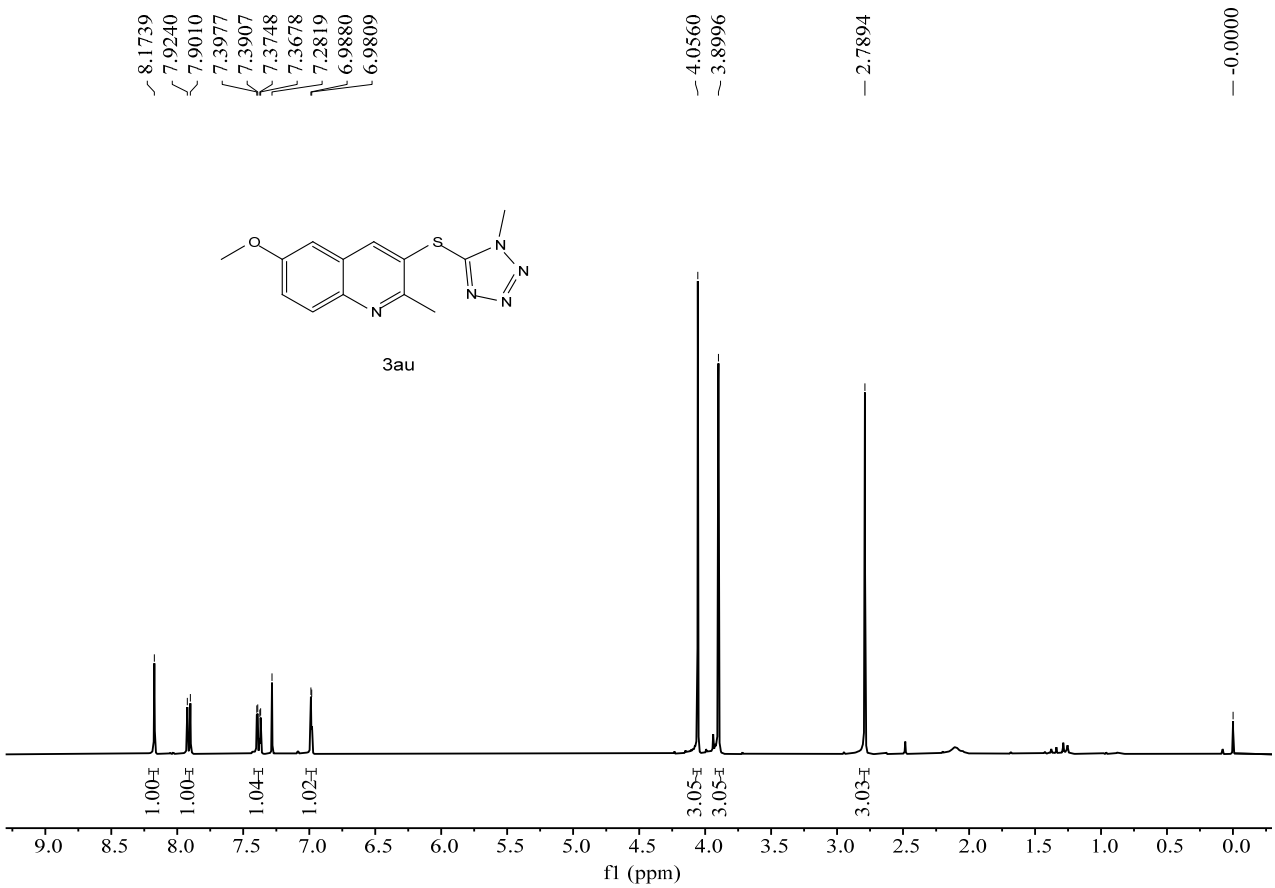
f1 (ppm)

3at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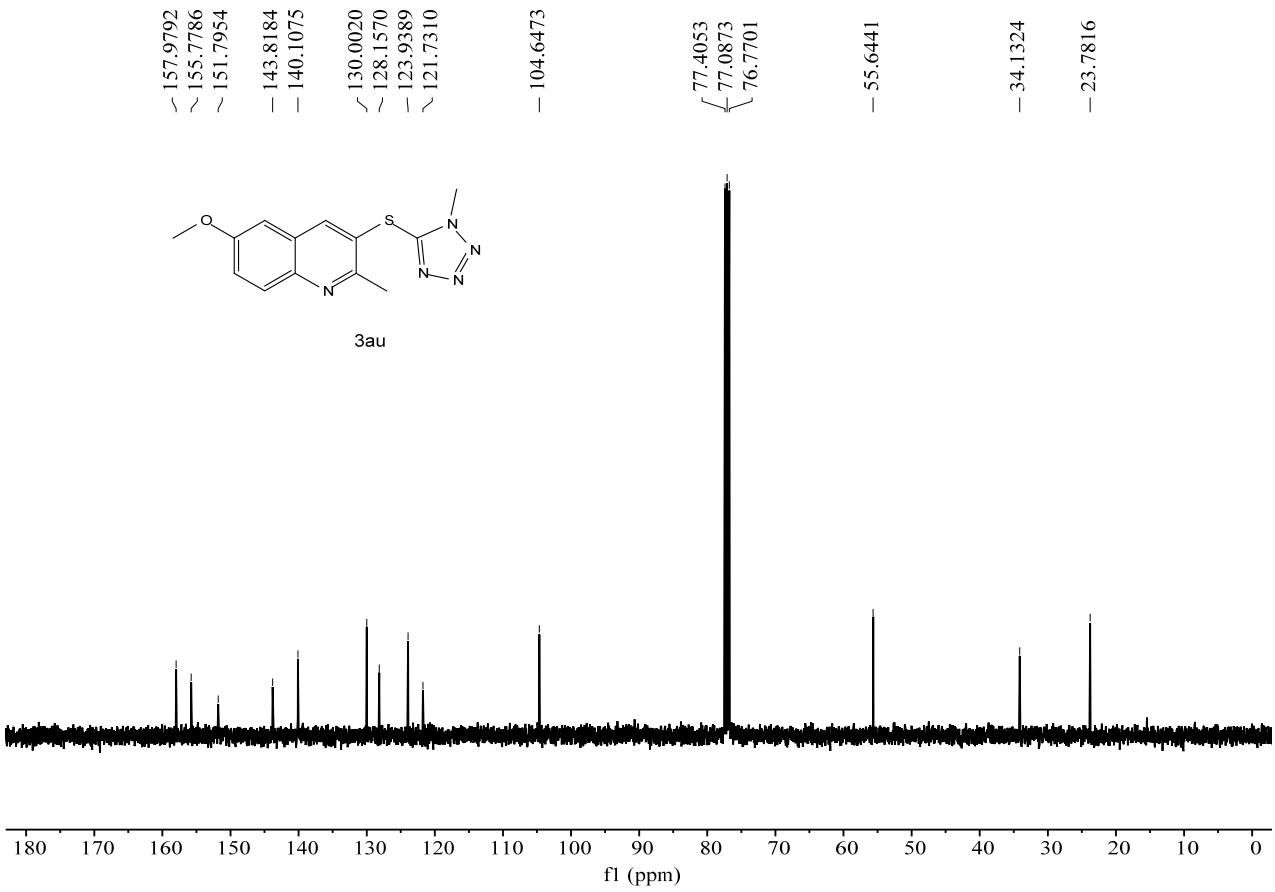
6.9880
6.9809
4.0560
3.8996
2.7894
-0.0000
3au
1.00
1.00
1.04
1.02
3.05
3.05
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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34.1324
23.7816
3au
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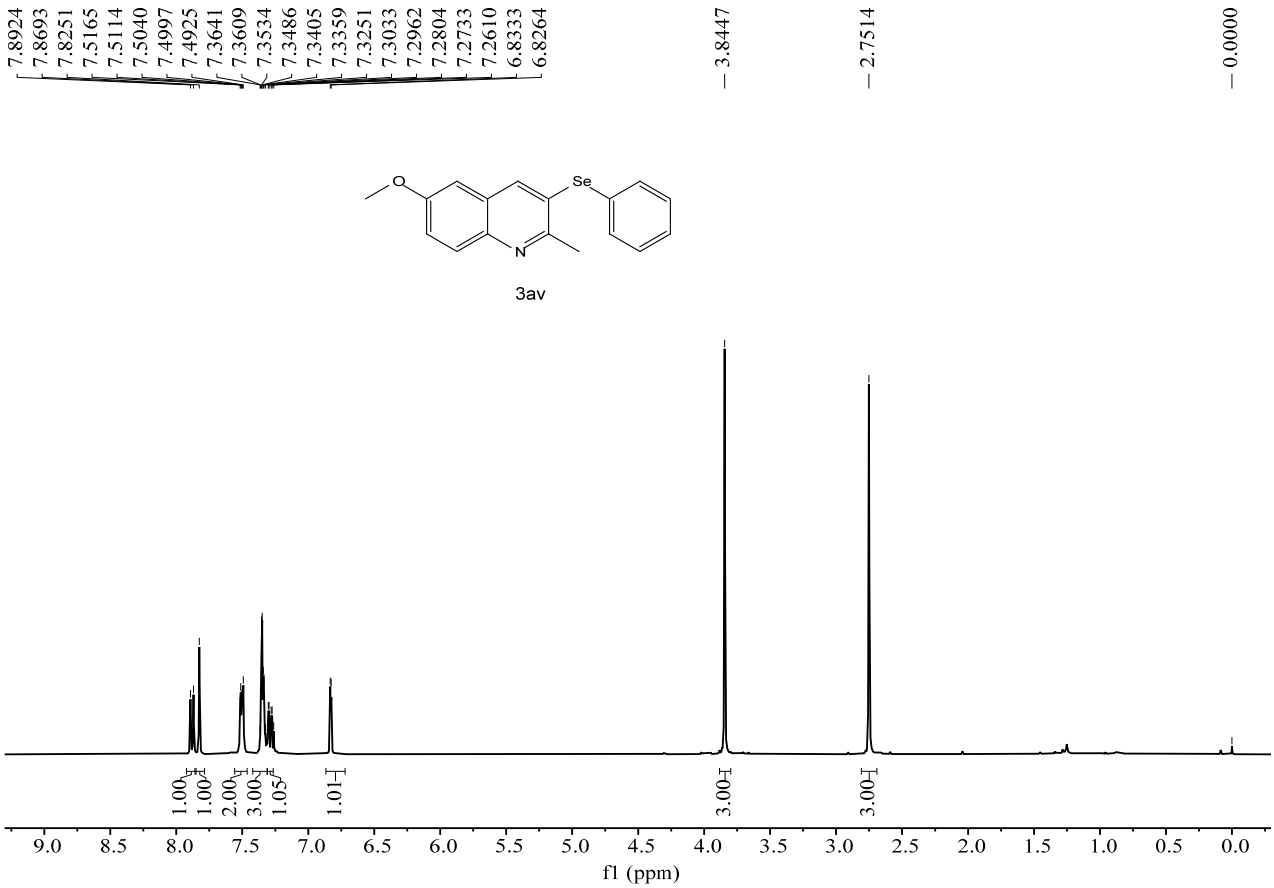
f1 (ppm)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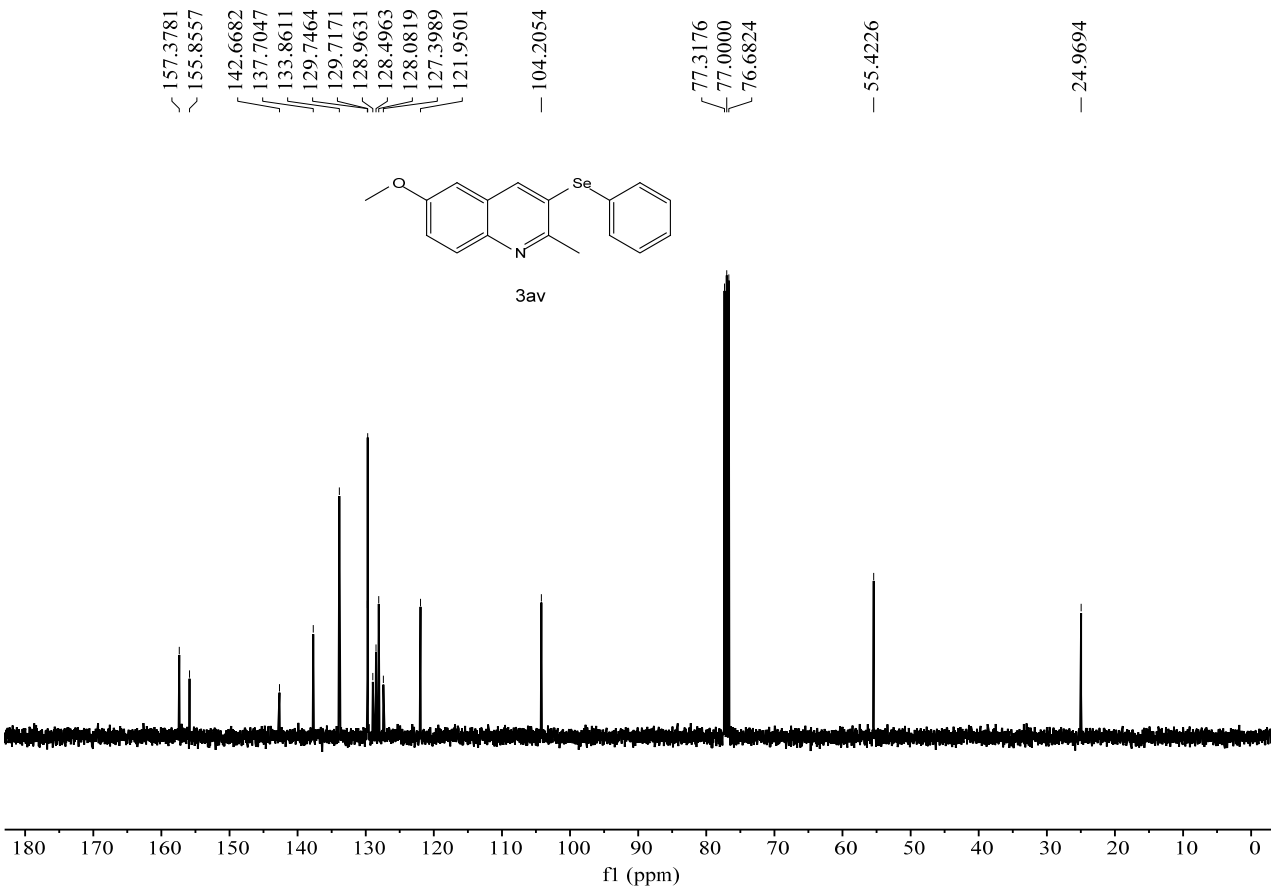
7.3405
7.3359
7.3251
7.3033
7.2962
7.2804
7.2733
7.2610
6.8333
6.8264
3.8447
2.7514
0.0000
O
Se
N
3av
1.00
1.00
2.00
3.00
1.05
1.01
3.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.3176
77.0000
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Se
N
3av
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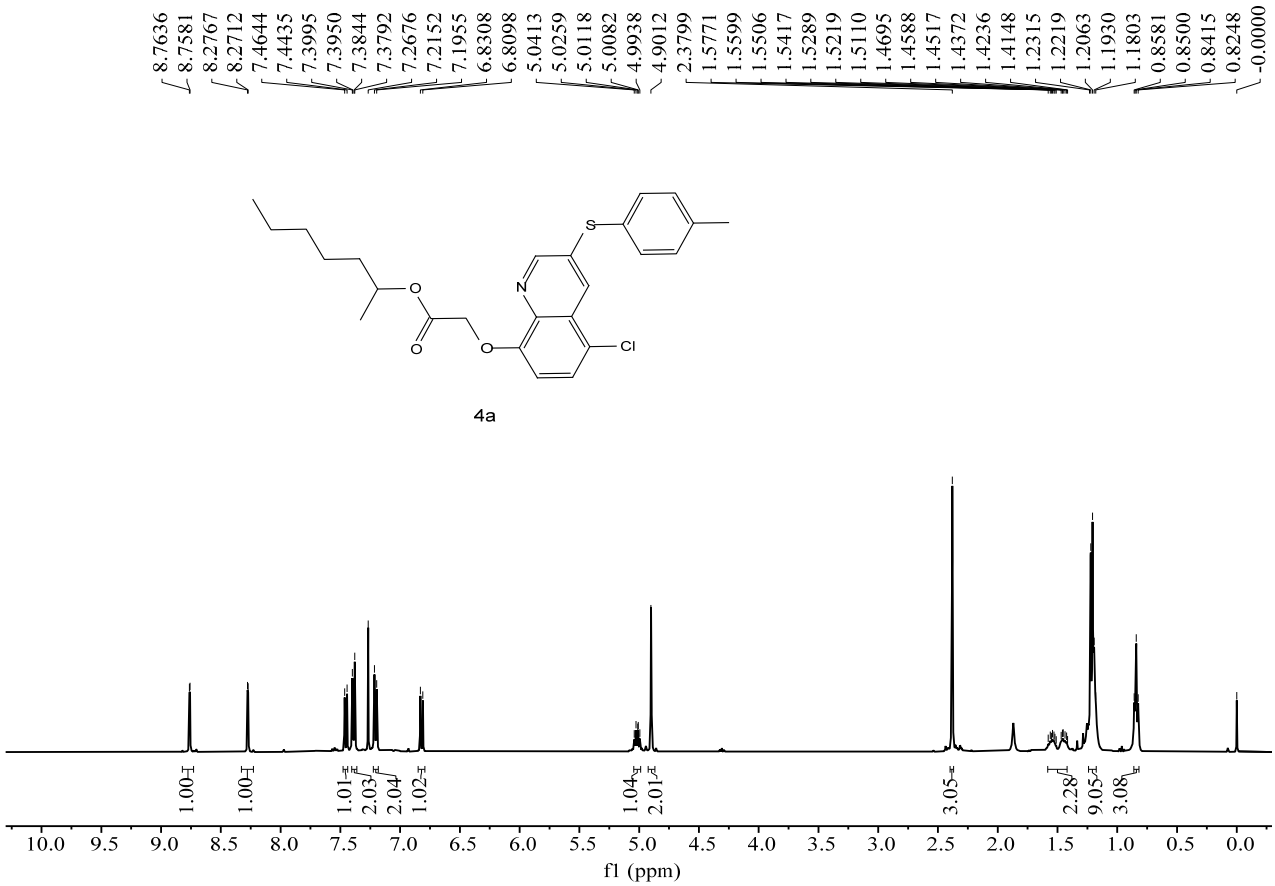
f1 (ppm)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0.8248
-0.0000
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O
O
O
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2.03
2.04
1.02
1.04
2.01
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3.08
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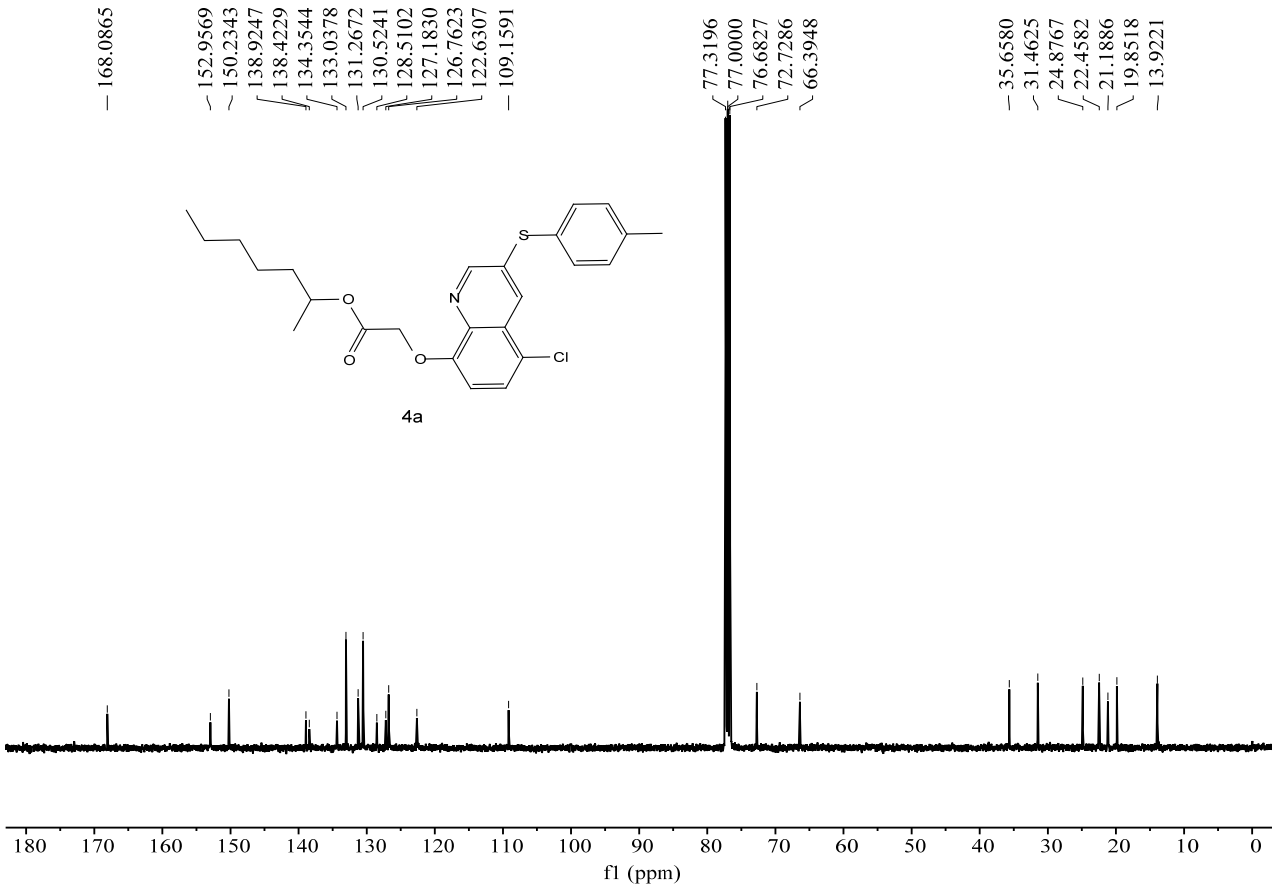
f1 (ppm)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31.4625
24.8767
22.4582
21.1886
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S
N
O
O
O
Cl
4a
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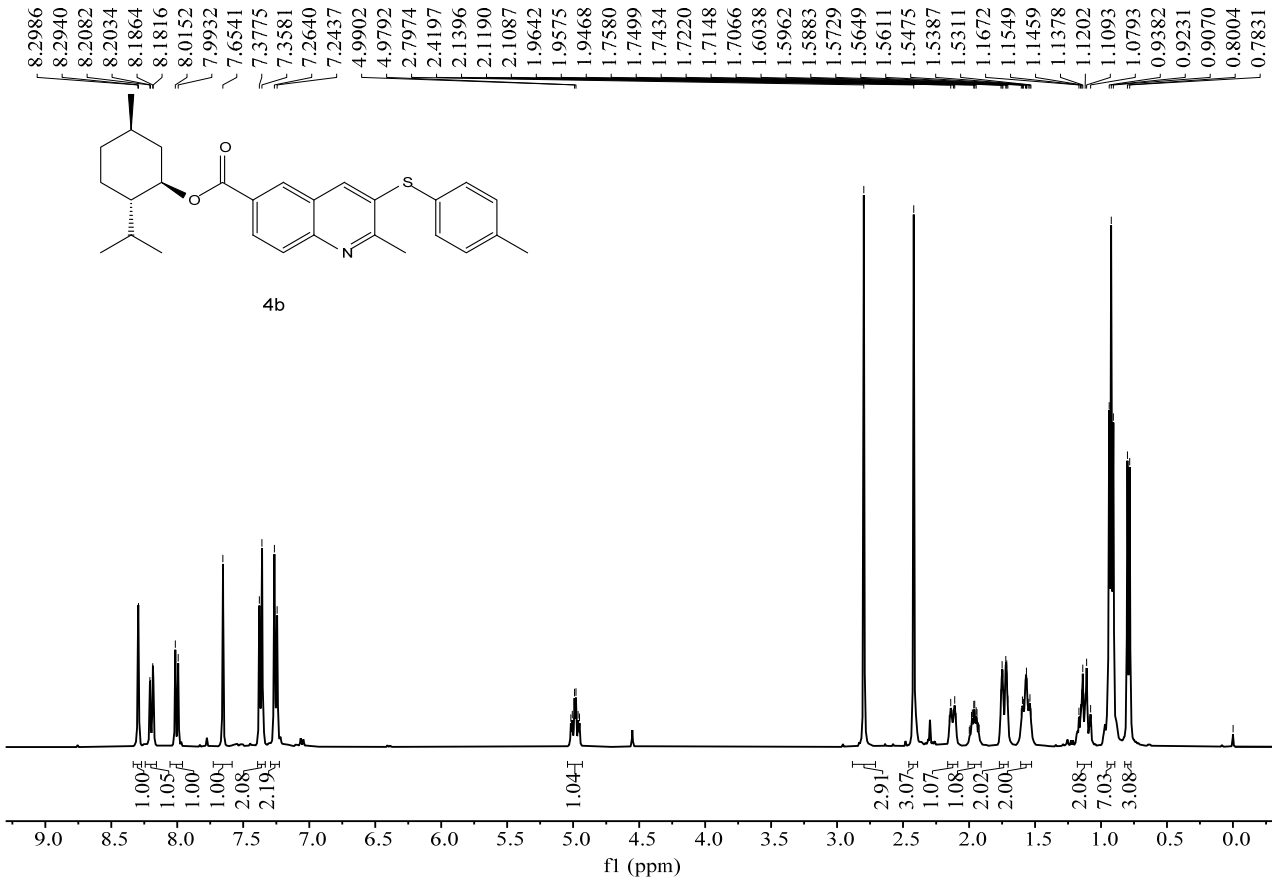
f1 (ppm)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O
O
S
N
4b
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1.00
1.00
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1.08
2.02
2.00
2.08
7.03
3.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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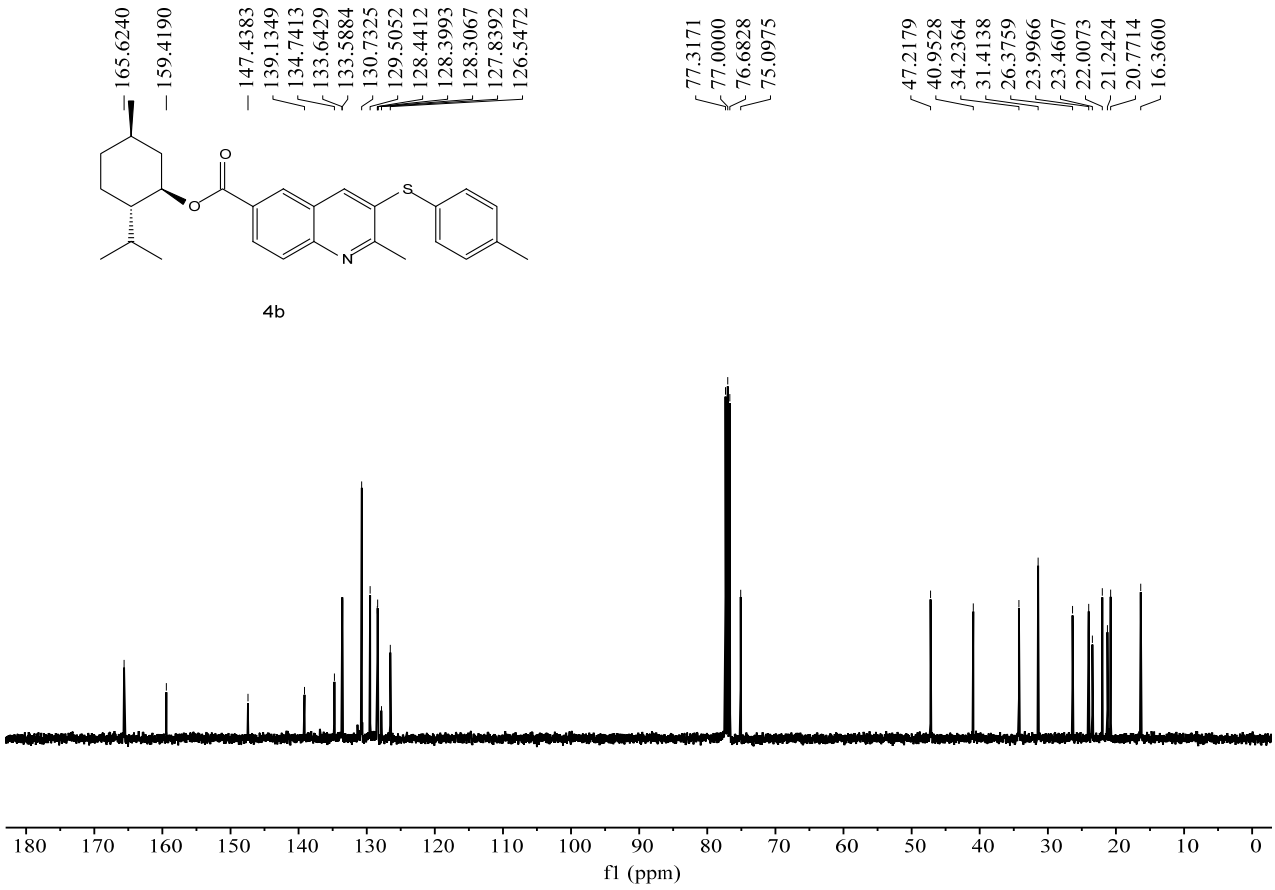
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O
O
S
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4b
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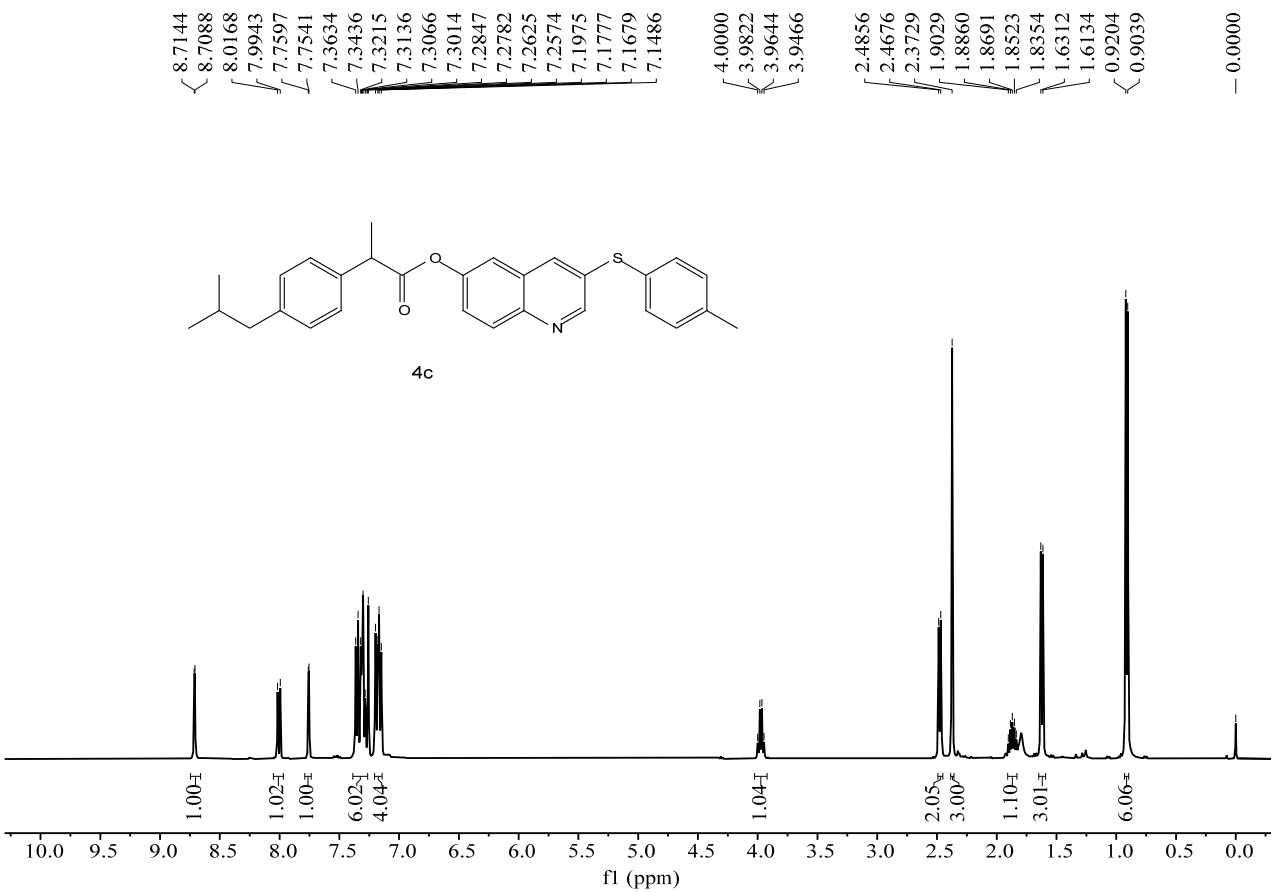
f1 (ppm)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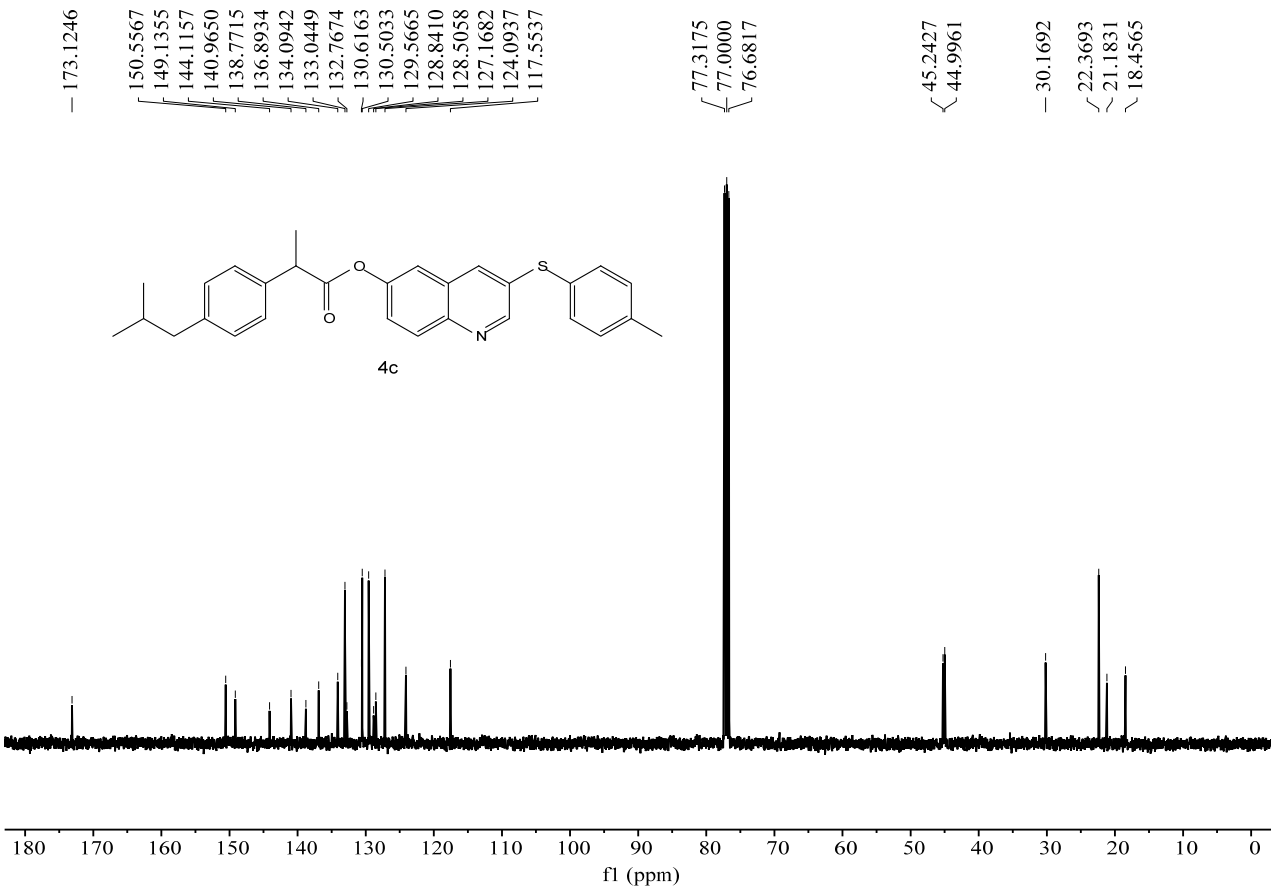
2.4676
2.3729
1.9029
1.8860
1.8691
1.8523
1.8354
1.6312
1.6134
0.9204
0.9039
0.0000
O
O
S
N
4c
1.00
1.02
1.00
6.02
4.04
1.04
2.05
3.00
1.10
3.01
6.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.5033
129.5665
128.8410
128.5058
127.1682
124.0937
117.5537
77.3175
77.0000
76.6817
45.2427
44.9961
30.1692
22.3693
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O
O
S
N
4c
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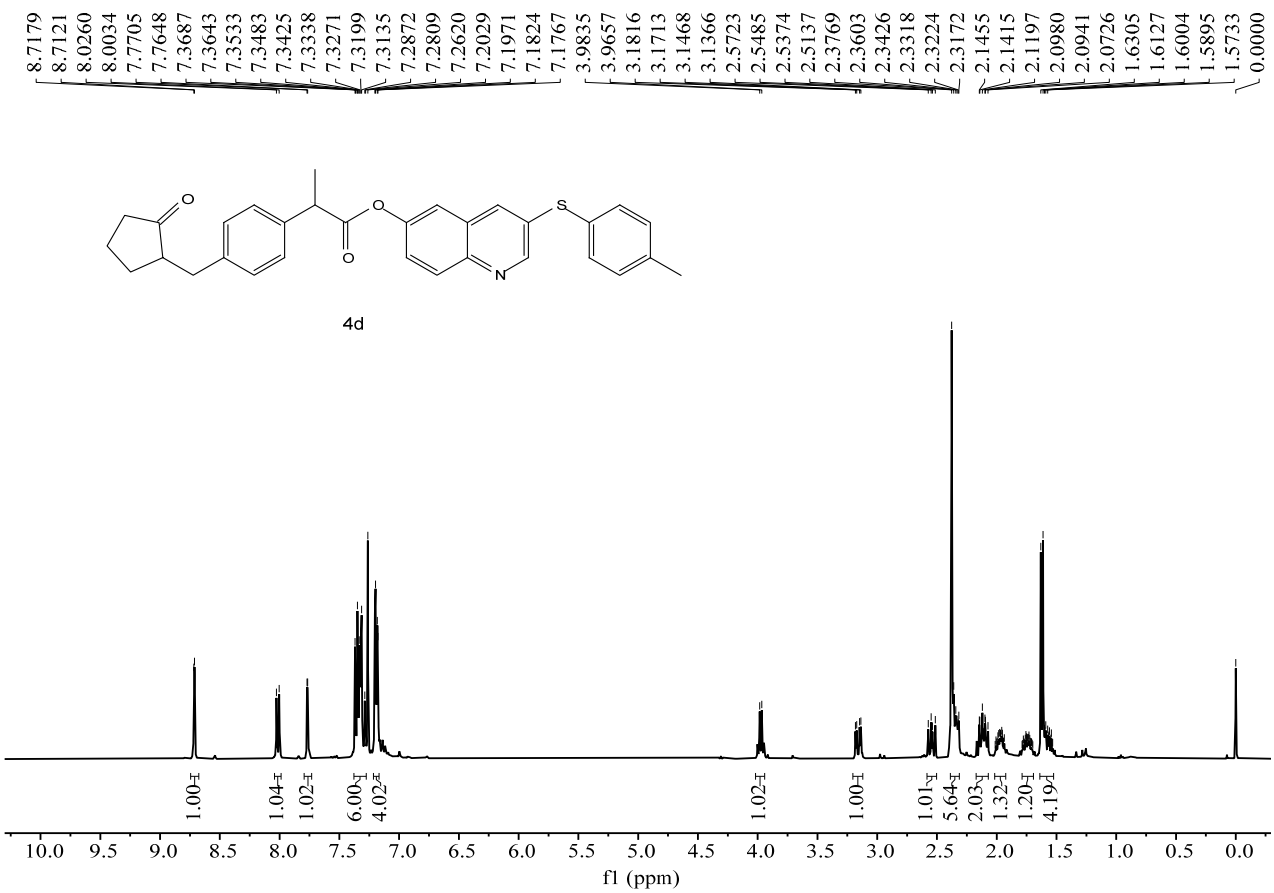
f1 (ppm)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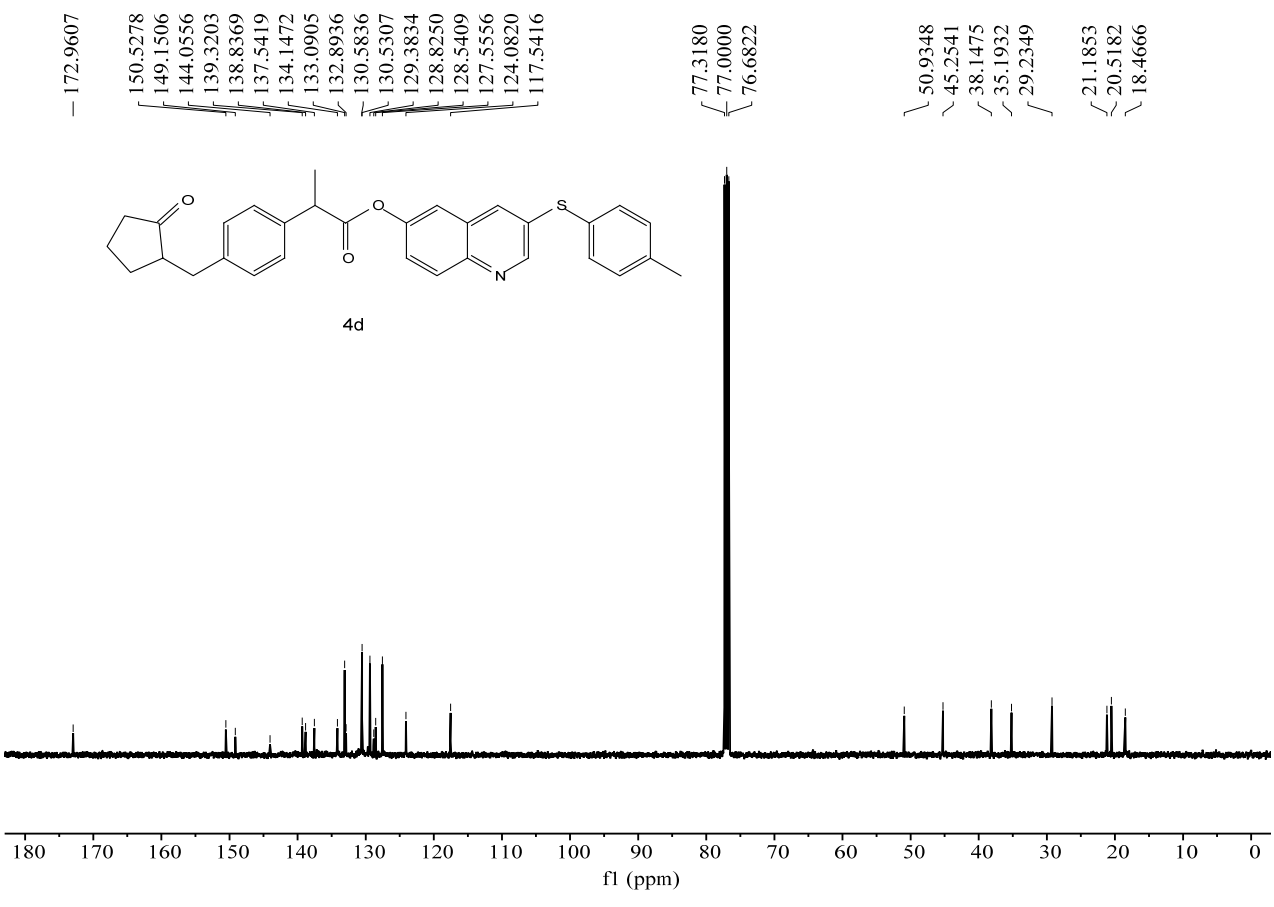
7.3483
7.3425
7.3338
7.3271
7.3199
7.3135
7.2872
7.2809
7.2620
7.2029
7.1971
7.1824
7.1767
3.9835
3.9657
3.1816
3.1713
3.1468
3.1366
2.5723
2.5485
2.5374
2.5137
2.3769
2.3603
2.3426
2.3318
2.3224
2.3172
2.1455
2.1415
2.1197
2.0980
2.0941
2.0726
1.6305
1.6127
1.6004
1.5895
1.5733
0.0000
4d
1.00
1.04
1.02
6.00
4.02
1.02
1.00
1.01
5.64
2.03
1.32
1.20
4.19
fl (ppm)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128.5409
127.5556
124.0820
117.5416
77.3180
77.0000
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20.5182
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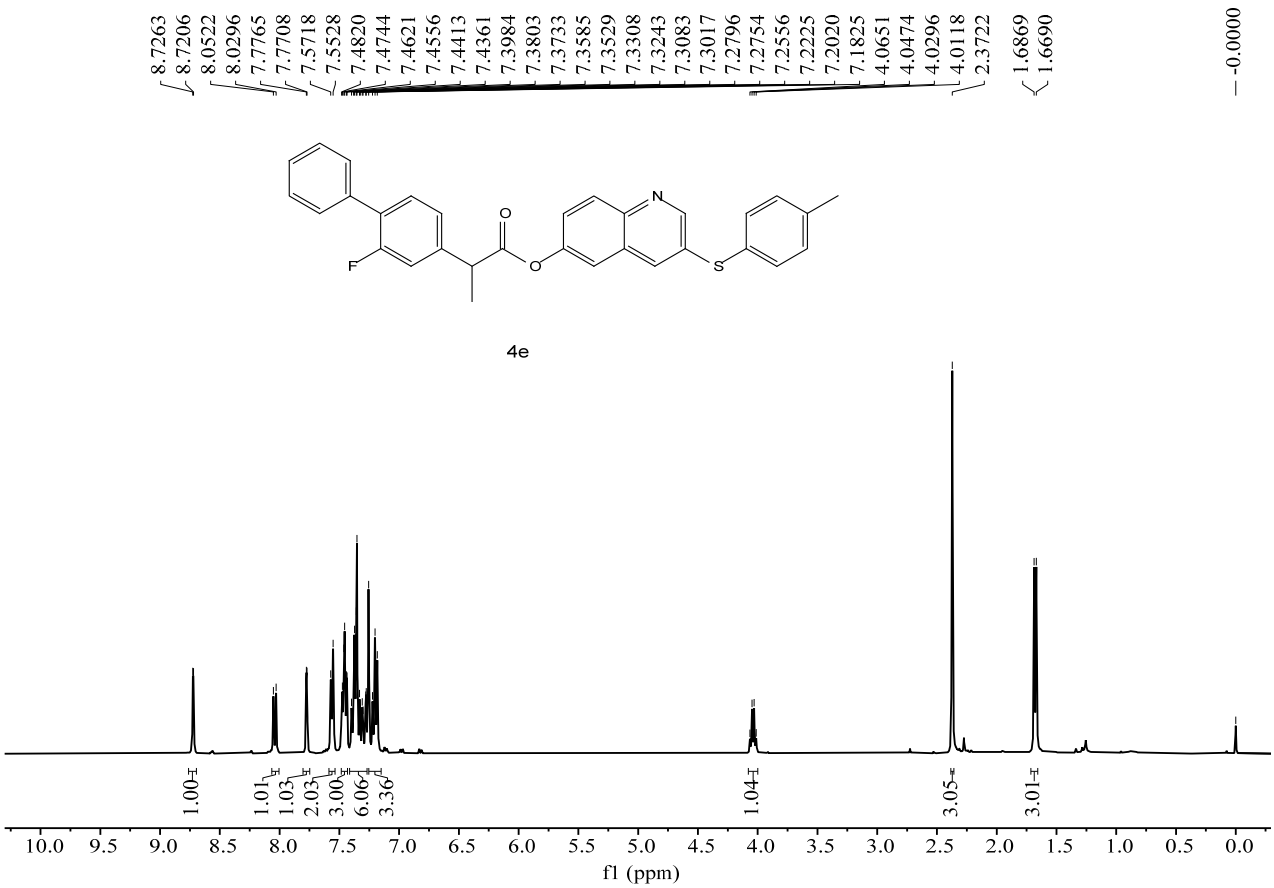
4d
fl (ppm)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7.4556
7.4413
7.4361
7.3984
7.3803
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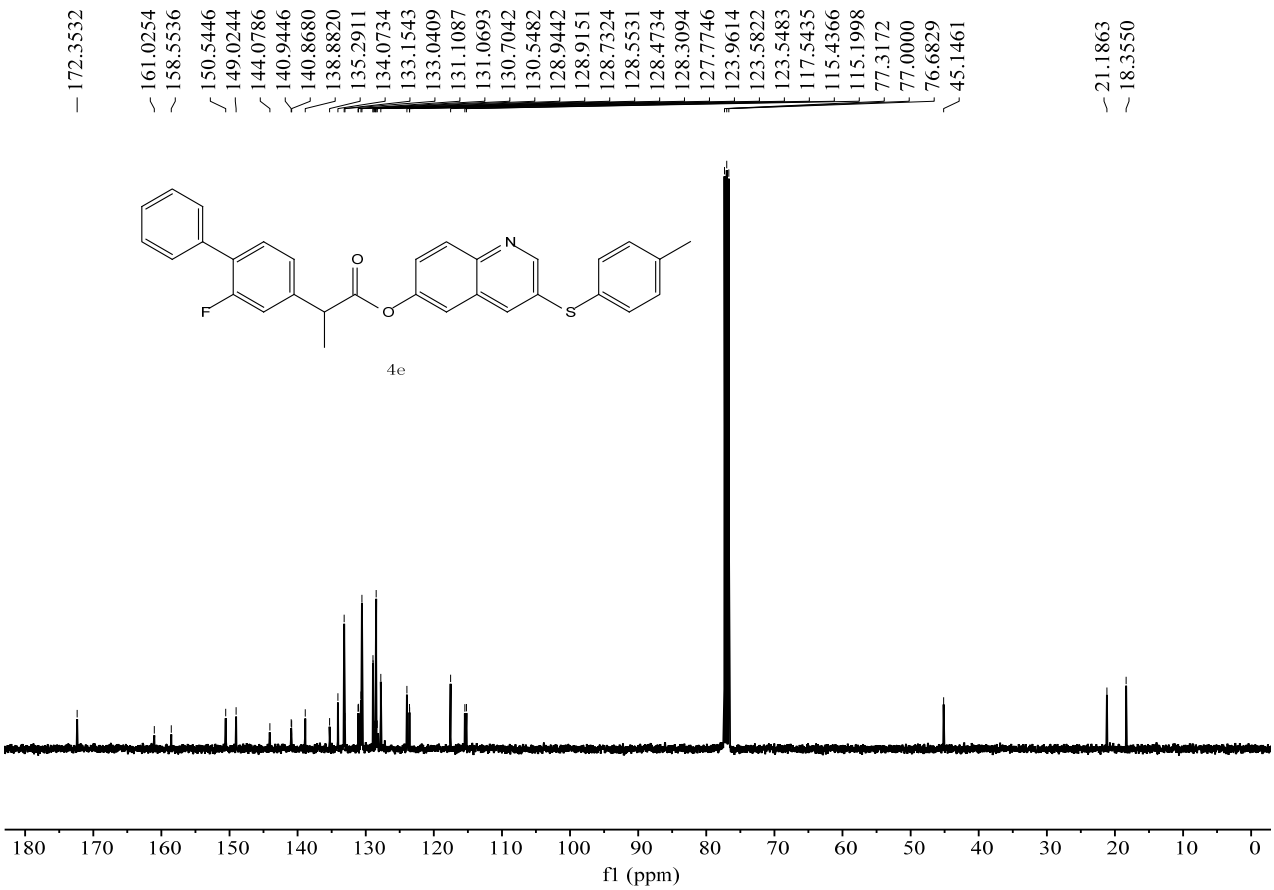
7.3585
7.3529
7.3308
7.3243
7.3083
7.3017
7.2796
7.2754
7.2556
7.2225
7.2020
7.1825
4.0651
4.0474
4.0296
4.0118
2.3722
1.6869
1.6690
0.0000
O
N
F
O
S
4e
1.00
1.01
1.03
2.03
3.00
6.06
3.36
1.04
3.05
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.0693
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130.5482
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128.5531
128.4734
128.3094
127.7746
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123.5822
123.5483
117.5435
115.4366
115.1998
77.3172
77.0000
76.6829
45.1461
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O
N
F
O
S
4e
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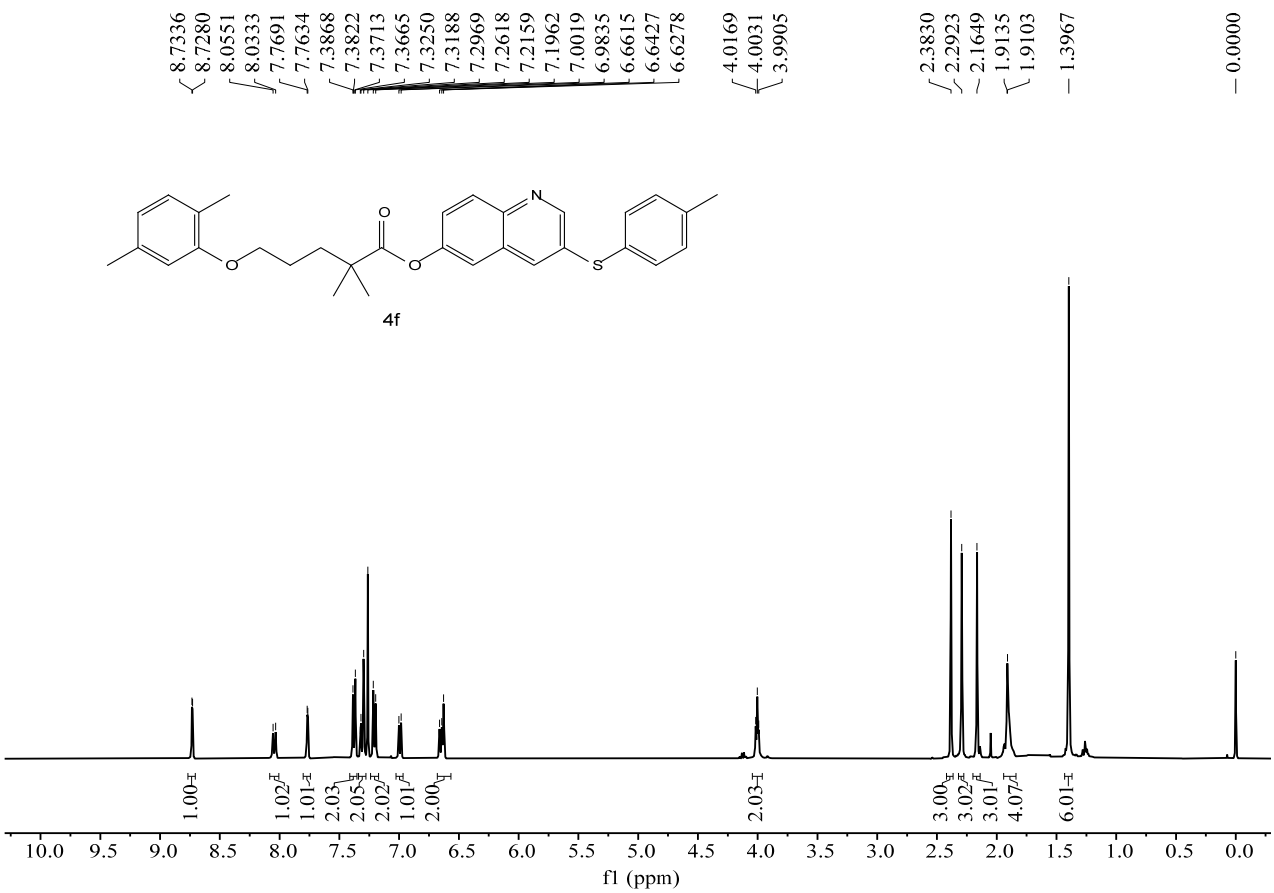
f1 (ppm)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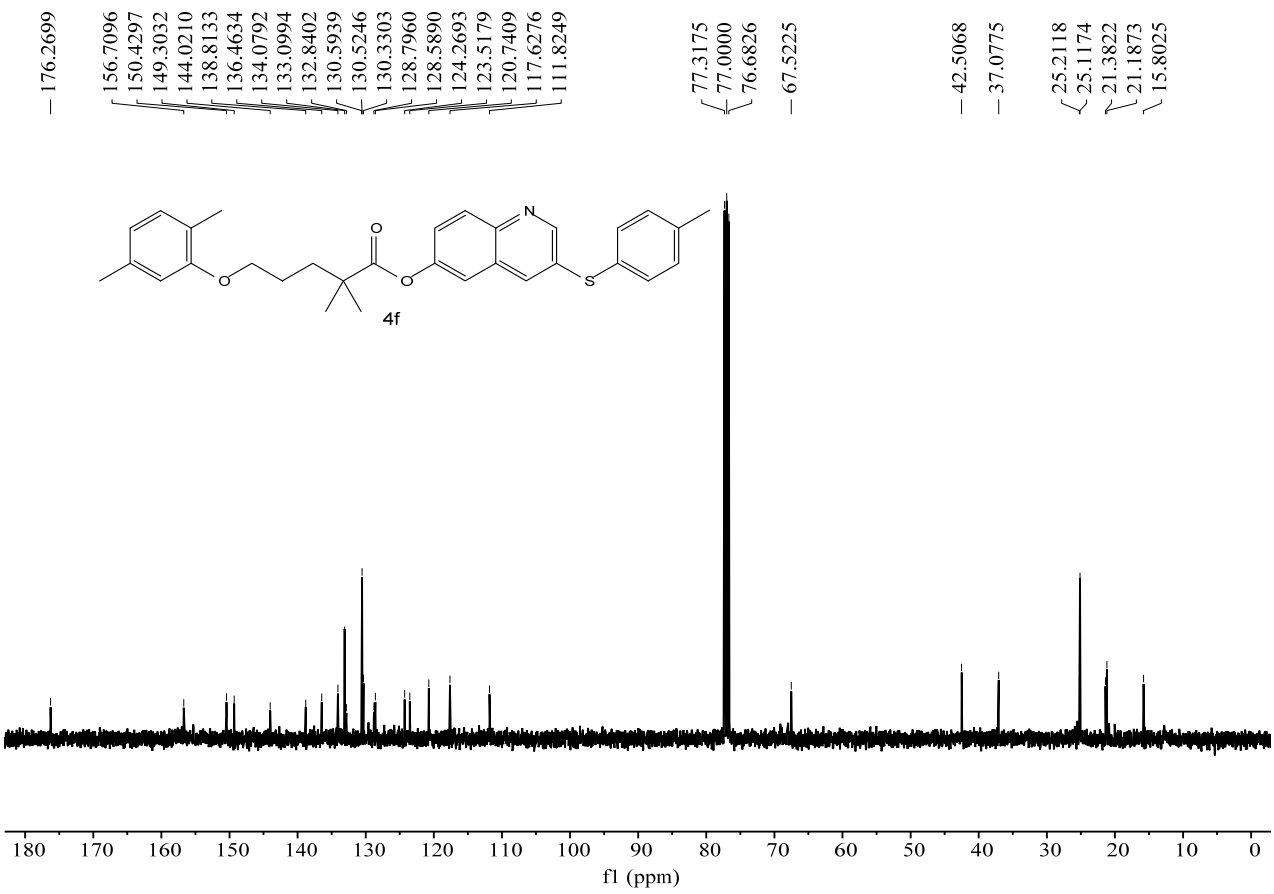
7.3713
7.3665
7.3250
7.3188
7.2969
7.2618
7.2159
7.1962
7.0019
6.9835
6.6615
6.6427
6.6278
4.0169
4.0031
3.9905
2.3830
2.2923
2.1649
1.9135
1.9103
1.3967
0.0000
4f
1.00
1.02
1.01
2.03
2.05
2.02
1.01
2.00
2.03
3.00
3.02
3.01
4.07
6.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.3303
128.7960
128.5890
124.2693
123.5179
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111.8249
77.3175
77.0000
76.6826
67.5225
42.5068
37.0775
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21.3822
21.1873
15.8025
4f
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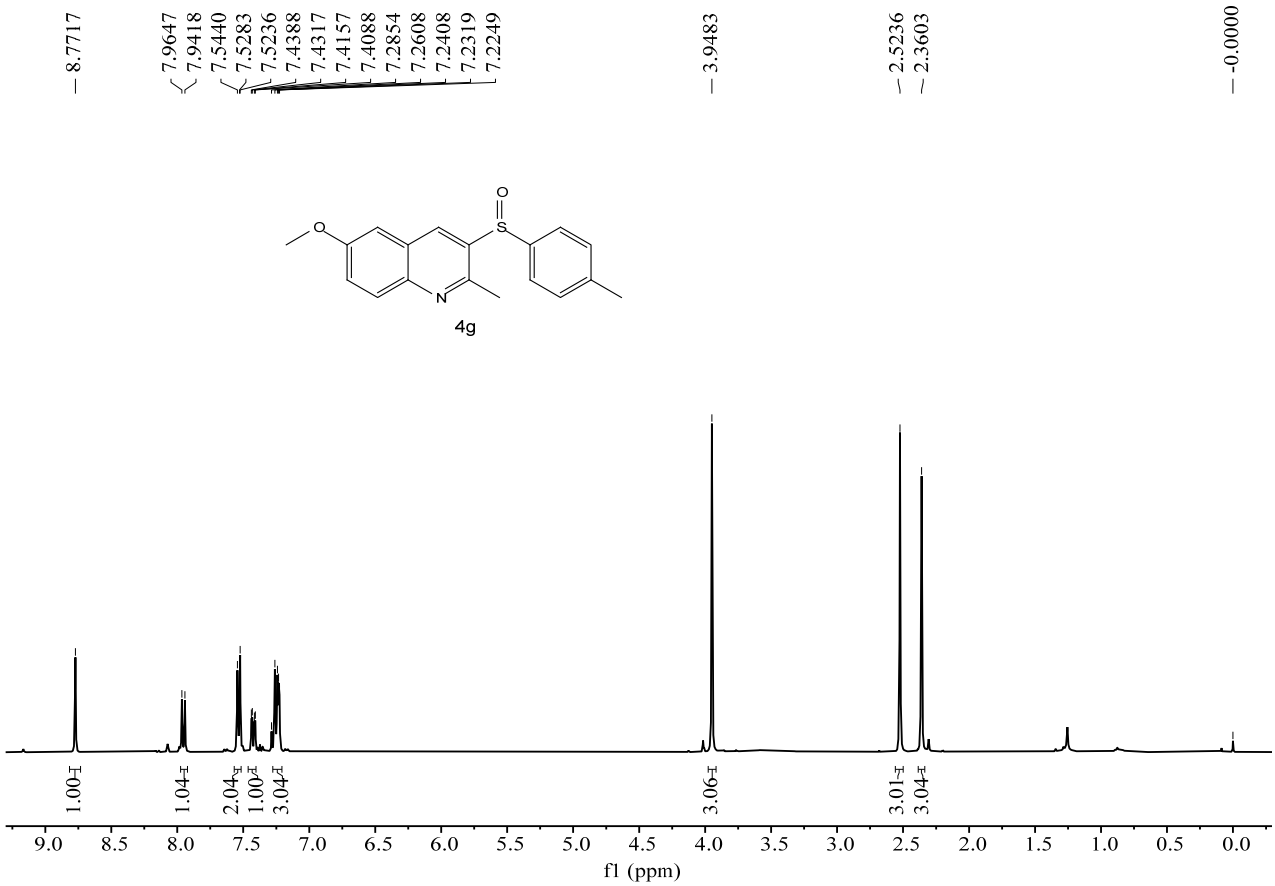
f1 (ppm)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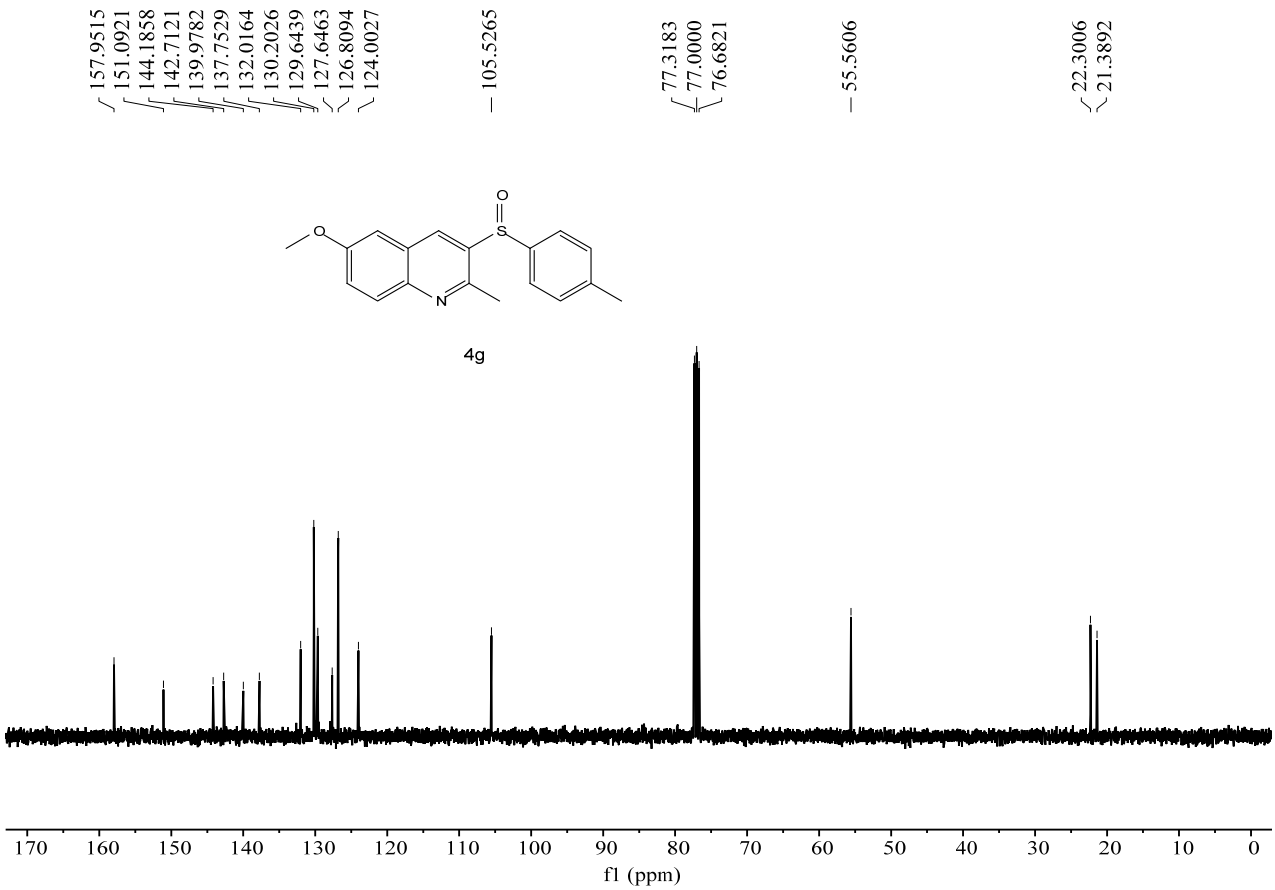
7.2854
7.2608
7.2408
7.2319
7.2249
3.9483
2.5236
2.3603
-0.0000
4g
1.00
1.04
2.04
1.00
3.04
3.06
3.01
3.04
f1 (ppm)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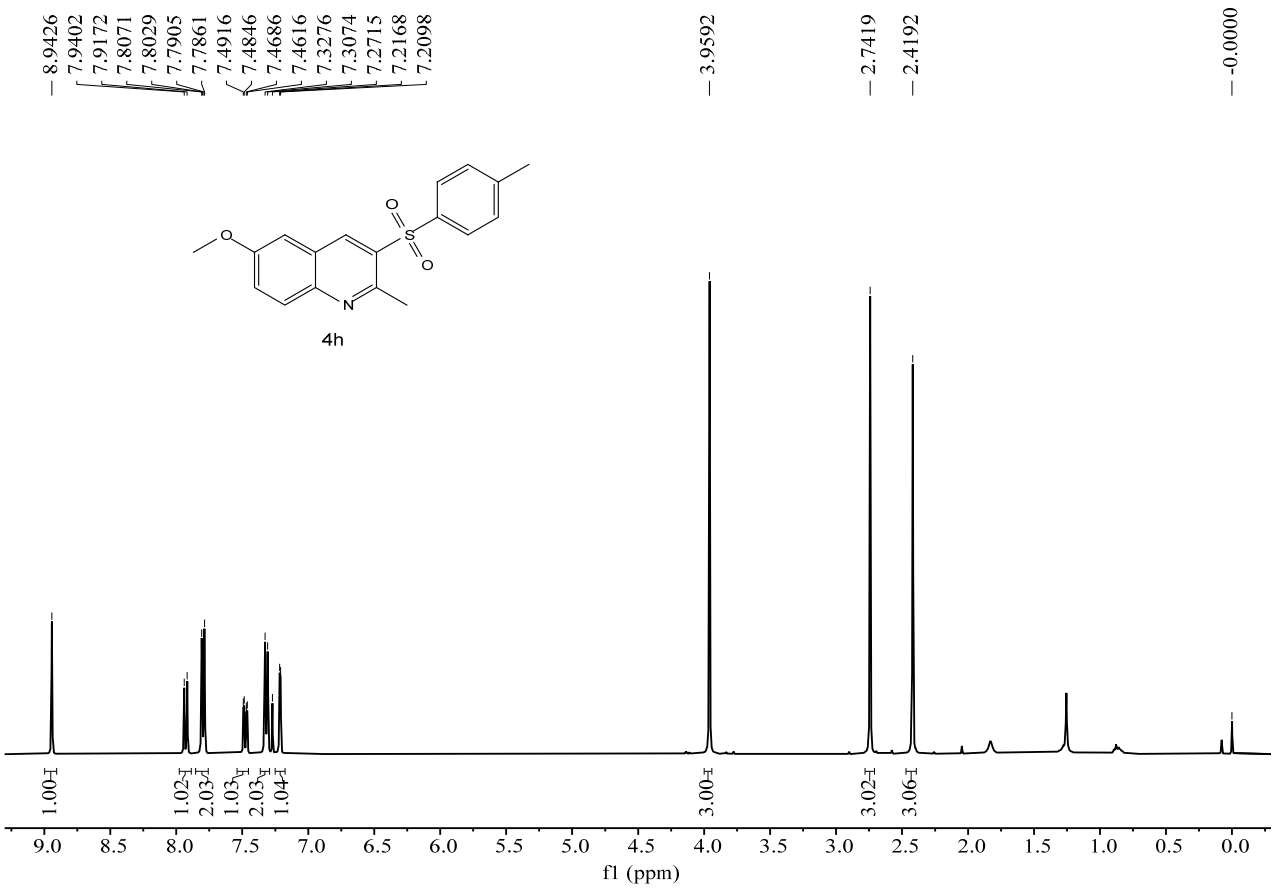
76.6821
55.5606
22.3006
21.3892
4g
f1 (ppm)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7.4616
7.3276
7.3074
7.2715
7.2168
7.2098
3.9592
2.7419
2.4192
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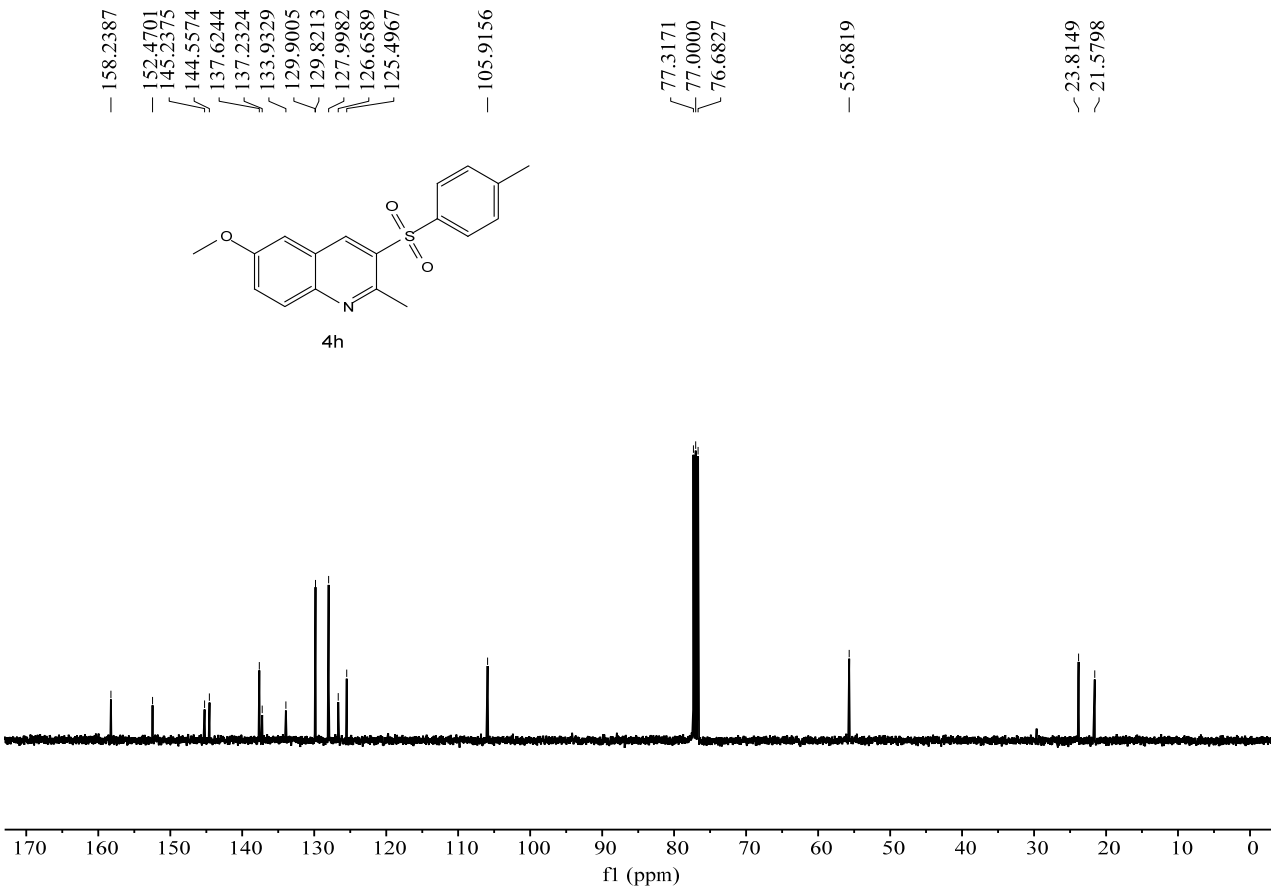
4h
1.00
1.02
2.03
1.03
2.03
1.04
3.00
3.02
3.06
fl (ppm)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125.4967
105.9156
77.3171
77.0000
76.6827
55.6819
23.8149
21.5798
4h
fl (ppm)