Supporting Information

Radical Cascade Cyclization of Chalcone Skeleton Enynes with Sulfonylhydrazides: Access to *meta*-sulfonyl Functionalized Pyridines

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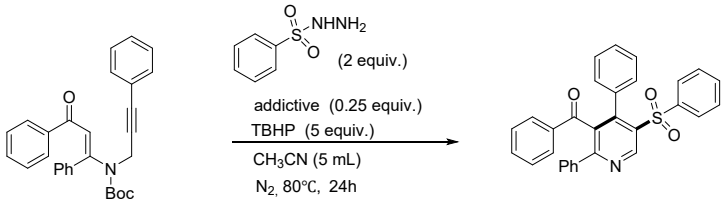
Ⅰ. Genernal information

Chemicals and anhydrous solvents were purchased from commercial suppliers and used as received. Uncommercial available substrates were synthesized according to literatures. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR spectra were recorded on a JEOL-500 M (500 MHz) spectrometer. Chemical shifts were calibrated using residual undeuterated solvent as an internal reference ($CDCl_3$: 7.26 ppm ^{1}H NMR, 77.0 ppm ^{13}C NMR). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), br (broad singlet). The highresolution mass spectra (HR-MS) were obtained on a Sciex Triple TOF 5600. X-ray diffraction of single crystal was performed on Bruker D8 venture and Bruker D8 QUEST diffractometer. All GC analysis was performed on Shimadzu GC-2014 and Shimadzu QP 2010 GC-MS. The sealed-tubes utilized were microwave vials (7.5 or 10 mL) with septum caps were purchased from Biotage or sealed-tubes with Teflon caps (15 mL) were purchased from Synthware. The reaction temperature was controlled by using oil baths.

Ⅱ. Experimental section

1) Reaction conditions optimization

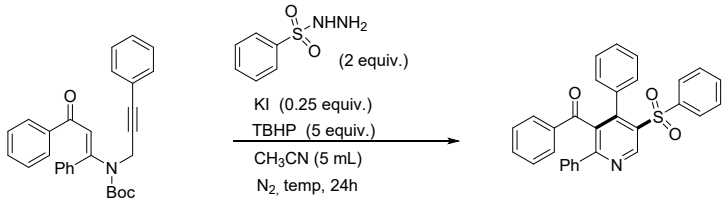
Table S1. Screening of Additive



Entry[a]	Solvent	mL	Oxidant[b]	Additive	Temp	Time	System	Yield[c]
1	CH_3CN	5 mL	TBHP (5 equiv)	KI (0.25 equiv)	80℃	24h	N_2	75%
2	CH_3CN	5 mL	TBHP (5 equiv)	I_2 (0.25 equiv)	80℃	24h	N_2	59%
3	CH_3CN	5 mL	TBHP (5 equiv)	CuI(0.25 equiv.)	80℃	24h	N_2	Trace

[a]reaction conditions: 1a (0.2 mmol, 1.0 equiv.), $PhSO_2NHNH_2$ (0.4 mmol, 2.0 equiv.), KI (0.05 mmol, 0.25 equiv.), Oxidant[b]: TBHP (0.8mmol, 4 equiv., 6.0 M solution in decane), CH_3CN (5 mL) at 80℃ under N_2 for 24h. [b]Isolated yields.

Table S2. Screening of reaction temperatures

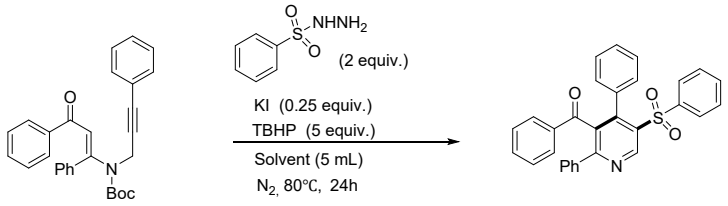


1a 3a

Entry[a]	Solvent	mL	Oxidant	Additive	Temp	Time	System	Yield[b]
3	CH_3CN	5 mL	TBHP (5 equiv)	KI (0.25 equiv)	90℃	24h	N_2	68%
4	CH_3CN	5 mL	TBHP (5 equiv)	KI (0.25 equiv)	80℃	24h	N_2	75%
5	CH_3CN	5 mL	TBHP (5 equiv)	KI (0.25 equiv)	70℃	24h	N_2	62%

[a]reaction conditions: 1a (0.2 mmol, 1.0 equiv.), $PhSO_2NHNH_2$ (0.4 mmol, 2.0 equiv.), KI (0.05 mmol, 0.25 equiv.), [b]Oxidant: TBHP (0.8mmol, 5 equiv.), CH_3CN (5 mL) at 80℃ under N_2 for 24h. [b]Isolated yields.

Table S3. Screening of solvents.

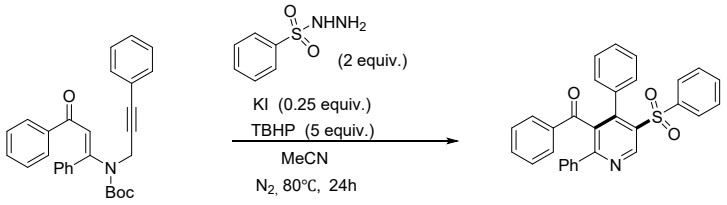


1a 3a

Entry[a]	Solvent	mL	Oxidant	Additive	Temp	Time	System	Yield[b]
6	CH_3CN	5 mL	TBHP	KI	80℃	24h	N_2	75%
7	CH_3OH	5 mL	TBHP	KI	80℃	24h	N_2	53%
8	CH_3CN+H_2O	4:1	TBHP	KI	80℃	24h	N_2	49%
9	CH_3CH_2OH	5 mL	TBHP	KI	80℃	24h	N_2	40%
10	THF	5 mL	TBHP	KI	80℃	24h	N_2	42%
11	Toluene	5 mL	TBHP	KI	80℃	24h	N_2	56%
12	DMF	5 mL	TBHP	KI	80℃	24h	N_2	39%
13	H_2O	5 mL	TBHP	KI	80℃	24h	N_2	36%
14	DMSO	5 mL	TBHP	KI	80℃	24h	N_2	18%

[a]reaction conditions: 1a (0.2 mmol, 1.0 equiv.), $PhSO_2NHNH_2$ (0.4 mmol, 2.0 equiv.), KI (0.05 mmol, 0.25 equiv.), Oxidant: TBHP (0.8mmol, 5 equiv.), CH_3CN (5 mL) at 80℃ under N_2 for 24h. [b]Isolated yields.

Table S4. Screening of the Solvent Dosage

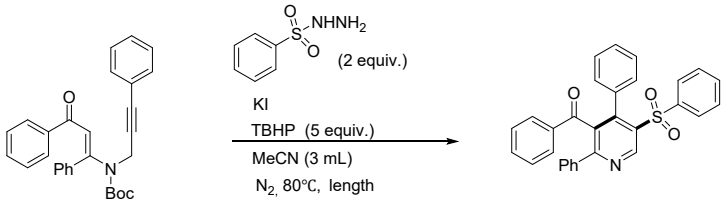


1a 3a

Entry[a]	Solvent	mL	Oxidant	Additive	Temp	Time	System	Yield[b]
15	CH_3CN	3 mL	TBHP	KI	80℃	24h	N_2	82%
16	CH_3CN	2 mL	TBHP	KI	80℃	24h	N_2	70%

[a]reaction conditions: 1a (0.2 mmol, 1.0 equiv.), $PhSO_2NHNH_2$ (0.4 mmol, 2.0 equiv.), KI (0.05 mmol, 0.25 equiv.), Oxidant: TBHP (0.8mmol, 5 equiv.), CH_3CN (3 mL) at 80℃ under N_2 for 24h. [b]Isolated yields.

Table S5. Screening of the KI Dosage & reaction time length

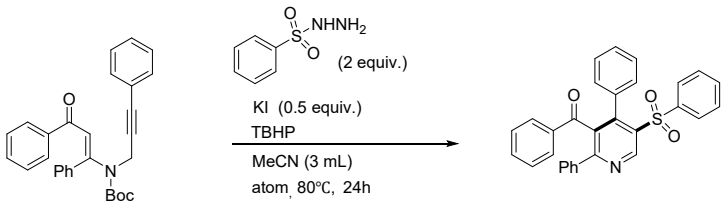


1a 3a

Entry[a]	Solvent	mL	Oxidant	Additive	Temp	Time	System	Yield[b]
17	CH_3CN	3 mL	TBHP	KI (0.25 equiv.)	80℃	24h	N_2	82%
18	CH_3CN	3 mL	TBHP	KI (0.5 equiv.)	80℃	24h	N_2	84%
19	CH_3CN	3 mL	TBHP	KI (0.5 equiv.)	80℃	12h	N_2	59%

[a]reaction conditions: 1a (0.2 mmol, 1.0 equiv.), $PhSO_2NHNH_2$ (0.4 mmol, 2.0 equiv.), KI (0.1 mmol, 0.5 equiv.), Oxidant: TBHP (0.8mmol, 5 equiv.), CH_3CN (3 mL) at 80℃ under N_2 for 24h. [b]Isolated yields.

Table S6. Screening of the TBHP Dosage & atmosphere.



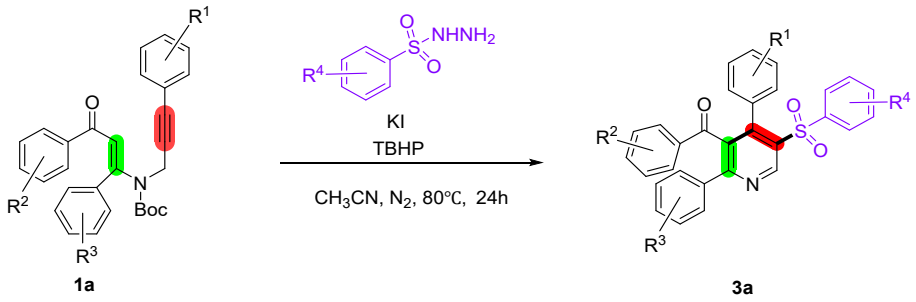
1a 3a

Entry[a]	Solvent	mL	Oxidant	Additive	Temp	Time	System	Yield[b]
19	CH_3CN	3 mL	TBHP (4 equiv.)	KI	80℃	24h	N_2	91%
20	CH_3CN	3 mL	TBHP (5 equiv.)	KI	80℃	24h	N_2	86%
21	CH_3CN	3 mL	TBHP (4 equiv.)	KI	80℃	24h	Air	60%

22	CH_3CN	3 mL	TBPB	KI	80°C	24h	N_2	68%
23	CH_3CN	3 mL	AIBN	KI	80°C	24h	N_2	Trace
24	CH_3CN	3 mL	$K_2S_2O_8$	KI	80°C	24h	N_2	None

[a]reaction conditions: 1a (0.2 mmol, 1.0 equiv.), $PhSO_2NHNH_2$ (0.4 mmol, 2.0 equiv.), KI (0.1 mmol, 0.5 equiv.), Oxidant: TBHP (0.8 mmol, 4 equiv.), CH_3CN (3 mL) at 80°C under N_2 for 24h. [b]Isolated yields.

2) General procedure for 3-sulfonyl poly-substituted pyridine

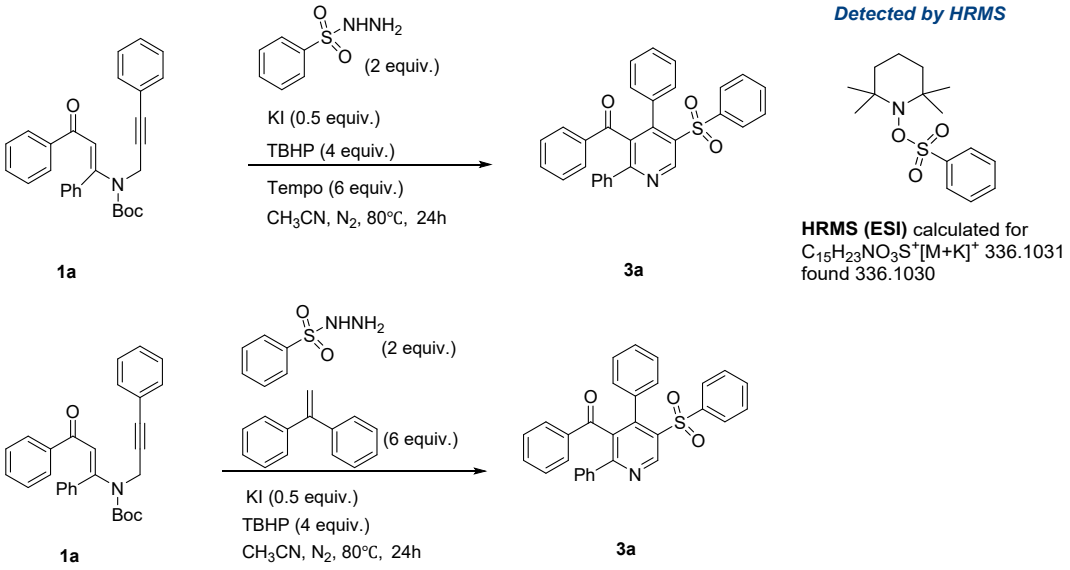


In this section, our group took tert-butyl (Z)-(3-oxo-1,3-diphenylprop-1-en-1-yl) (3-phenylprop-2-yn-1-yl) carbamate (**1a**) as a standard operational substrate. The synthesis methods for all the substrates are all derived from the articles previously reported by our research group. [1] Under nitrogen atmosphere, a Schlenk tube was equipped with a rubber septum and magnetic stir bar and charged with 1,5-enyne (**1a**, 0.2 mmol, 88.00 mg), Benzene sulfonohydrazide (0.4 mmol, 68.82 mg), TBHP (0.8 mmol, 72.06 mg), KI (0.1 mmol, 16.51 mg), 3 mL anhydrous CH_3CN as the solvent. The resulting mixture was cooled to 0 ºC and degassed via a vacuum evacuation and back filled with high pressure nitrogen under 0 ºC. Then this Schlenk tube with nitrogen balloon was returned to room temperature and then heated in a oil bath at 80 ºC for 24 h. After the reaction was completed, the reaction mixture was cooled to room temperature. Then the mixture was extracted with chloroform and saturated NaOH solution for three times. All the organic layers were combined and concentrated under vacuum to remove extra solvent and then purified by chromatography (petroleum ether: ethyl acetate = 5:1) to afford the desired product.

For 2.5 mmol scale of this reaction, 1,5-enyne (1a, 2.5 mmol, 1093 mg), Benzene sulfonohydrazide (5.0 mmol, 860.2 mg) and TBHP (10 mmol, 900.70 mg), KI (1.25 mmol, 207.34 mg) and anhydrous CH_3CN (40 mL) were added into an Schlenk flask in order. Then, the reaction mixture was cooled to 0 ºC and degassed via a vacuum evacuation and back filled with high pressure nitrogen under 0 ºC. Then the reaction flask was returned to room temperature and placed to a magnetic stirrer equipped with oil bath. Then the reaction flask was heated to 80 ºC and stirred for 36 h. After the reaction was finished, the mixture was extracted with chloroform and saturated NaOH solution for three times. All the organic layers were combined and concentrated under vacuum to remove solvent. The residue was purified by column chromatography (petroleum ether: ethyl acetate = 5:1) to afford the crude product, and

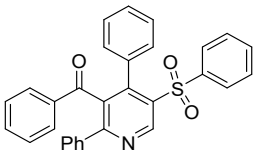
recrystallization with ethanol to give the desired product **3a** (0.98 g, 82% yield).

3) Control experiments



Radical scavengers	Yield of 3a (%)
Tempo	0
1,1-DiPhenylethylene	22

Ⅲ. Detail descriptions for products



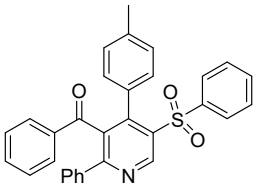
(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)(phenyl)methanone

White solid was obtained in 91% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.56 (d, *J* = 7.0 Hz, 2H), 7.43 (d, *J* = 7.1 Hz, 1H), 7.34 (d, *J* = 7.7 Hz, 4H), 7.28 (s, 2H), 7.23 (d, *J* = 8.0 Hz, 4H), 7.16 (t, *J* = 7.7 Hz, 2H), 7.11 (t, *J* = 7.6 Hz, 1H), 6.94 (dt, *J* = 27.1, 7.5 Hz, 2H), 6.81 (d, *J* = 7.8 Hz, 1H), 6.59 (d, *J* = 7.7 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.17, 160.58, 149.33, 148.59, 139.91, 137.82, 136.85, 135.88, 134.41, 133.52, 133.13, 131.49, 130.27, 129.70, 129.20, 129.01, 128.65, 128.44, 128.42, 128.26, 127.79, 127.17.

HRMS (ESI) calculated for $C_{30}H_{21}NO_3S^+[M+H]^+$ 476.1314 found 476.1327.



3b

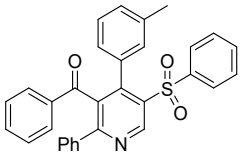
phenyl(2-phenyl-5-(phenylsulfonyl)-4-(p-tolyl)pyridin-3-yl)methanone

White solid was obtained in 83% isolated yield.

1H NMR (500 MHz, Chloroform-d) δ 9.74 (s, 1H), 7.58 – 7.51 (m, 2H), 7.48 – 7.41 (m, 1H), 7.38 – 7.32 (m, 3H), 7.29 – 7.25 (m, 5H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.17 (t, *J* = 7.7 Hz, 2H), 6.82 – 6.66 (m, 3H), 6.49 (d, *J* = 7.8 Hz, 1H), 2.22 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.28, 160.47, 149.30, 148.98, 139.97, 138.41, 137.83, 136.87, 136.02, 134.73, 133.50, 133.12, 130.19, 129.69, 129.22, 129.06, 128.54, 128.42, 128.24, 127.85, 127.53, 21.18.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1459.



3c

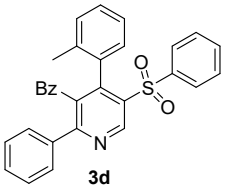
phenyl(2-phenyl-5-(phenylsulfonyl)-4-(m-tolyl)pyridin-3-yl)methanone

White solid was obtained in 61% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.69 (s, 1H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.29 (d, *J* = 7.5 Hz, 2H), 7.24 – 7.16 (m, 7H), 7.11 (t, *J* = 7.7 Hz, 2H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.77 (d, *J* = 8.7 Hz, 1H), 6.60 (d, *J* = 7.3 Hz, 1H), 6.38 (s, 1H), 6.19 (s, 1H), 1.91 (d, *J* = 57.8 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.25, 160.54, 149.26, 148.85, 139.98, 137.82, 134.49, 133.50, 132.97, 131.38, 130.65, 129.72, 129.22, 129.05, 128.45, 128.22, 127.93, 127.18, 126.83, 21.07.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1467.



3d

phenyl(2-phenyl-5-(phenylsulfonyl)-4-(o-tolyl)pyridin-3-yl)methanone

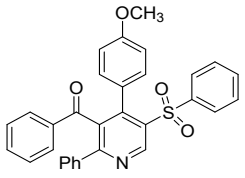
White solid was obtained in 42% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.60 (d, *J* = 6.8 Hz, 2H), 7.51 (tq, *J* = 5.8, 3.8, 3.2 Hz, 1H), 7.38 – 7.27 (m, 11H), 7.16 (t, *J* = 7.7 Hz, 2H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.7 Hz, 1H), 6.68 (s, 1H), 6.50 (d, *J*

= 7.7 Hz, 1H), 1.54 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.33, 160.60, 149.26, 148.60, 139.91, 138.12, 137.83, 136.87, 136.07, 134.40, 133.14, 131.55, 130.18, 129.73, 129.32, 129.21, 129.03, 128.66, 128.45, 128.41, 128.27, 128.13, 127.82, 127.19, 126.82, 126.60, 126.20, 21.05.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1470.



3e

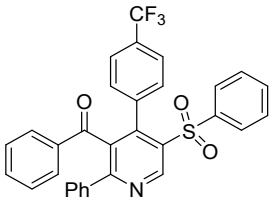
(4-(4-methoxyphenyl)-2-phenyl-5-(phenylsulfonyl)pyridin-3-yl)(phenyl)methanone

White solid was obtained in 88% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.67 (s, 1H), 7.51 – 7.46 (m, 2H), 7.38 (tt, *J* = 6.9, 1.8 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.21 (dd, *J* = 6.2, 2.9 Hz, 6H), 7.19 (s, 1H), 7.14 – 7.10 (m, 2H), 6.71 (d, *J* = 8.5 Hz, 1H), 6.42 (s, 3H), 3.64 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.33, 160.45, 159.65, 149.25, 148.85, 139.97, 137.66, 136.87, 136.39, 134.98, 133.56, 133.18, 131.68, 129.77, 129.25, 129.04, 128.62, 128.46, 128.32, 127.81, 123.58, 112.55, 55.18,.

HRMS (ESI) calculated for $C_{31}H_{23}NO_4S^+$ $[M+H]^+$506.1348 found 506.1350.



3f

phenyl(2-phenyl-5-(phenylsulfonyl)-4-(4-(trifluoromethyl)phenyl)pyridin-3-yl)methanone

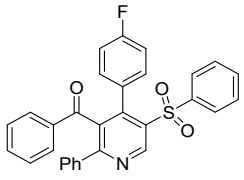
Yellow solid was obtained in 58% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.57 (dd, *J* = 7.5, 1.9 Hz, 2H), 7.51 – 7.45 (m, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.35 – 7.26 (m, 6H), 7.26 (s, 4H), 7.19 (t, *J* = 7.6 Hz, 3H), 6.99 – 6.86 (m, 1H), 6.83 – 6.70 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 194.89, 160.80, 149.37, 146.99, 139.74, 137.57, 136.65, 135.45, 135.25, 134.26, 133.92, 133.48, 129.99, 129.25, 129.01, 128.88, 128.55, 128.48, 127.65, 123.77.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -62.88.

HRMS (ESI) calculated for $C_{31}H_{20}F_3NO_3S^+$ $[M+H]^+$ 544.1189 found 544.1180.



3g

(4-(4-fluorophenyl)-2-phenyl-5-(phenylsulfonyl)pyridin-3-yl)(phenyl)methanone

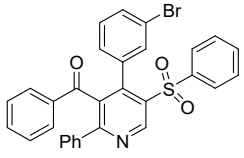
White solid was obtained in 62% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.75 (s, 1H), 7.59 – 7.53 (m, 2H), 7.48 (p, *J* = 4.3 Hz, 1H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.37 – 7.30 (m, 2H), 7.30 (d, *J* = 4.4 Hz, 6H), 7.26 (s, 1H), 7.20 (t, *J* = 7.6 Hz, 2H), 6.82 (s, 1H), 6.65 (s, 2H), 6.57 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 194.96, 160.82, 149.46, 146.70, 137.75, 136.78, 134.20, 133.79, 133.55, 132.68, 131.63, 129.87, 129.22, 129.01, 128.87, 128.74, 128.51, 128.44, 127.77.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -111.74.

HRMS (ESI) calculated for $C_{30}H_{20}FNO_3S^+$ $[M+H]^+$ 494.1221 found 494.1225.



3h

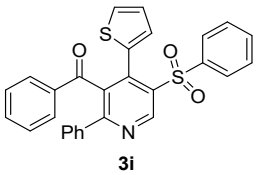
(4-(3-bromophenyl)-2-phenyl-5-(phenylsulfonyl)pyridin-3-yl)(phenyl)methanone

White solid was obtained in 61% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.56 (d, *J* = 7.2 Hz, 2H), 7.40 – 7.30 (m, 8H), 7.28 (d, *J* = 7.8 Hz, 3H), 7.20 (t, *J* = 7.7 Hz, 2H), 6.89 (d, *J* = 27.5 Hz, 2H), 6.70 (d, *J* = 23.4 Hz, 1H), 6.57 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.09, 160.95, 149.59, 146.83, 137.88, 136.91, 134.33, 133.92, 133.68, 132.81, 131.76, 130.00, 129.35, 129.14, 129.00, 128.87, 128.64, 128.57, 127.90.

HRMS (ESI) calculated for $C_{30}H_{20}BrNO_3S^+$ $[M+H]^+$ 556.0420 found 556.0423.



3i

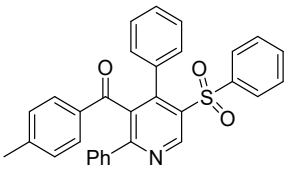
phenyl(2-phenyl-5-(phenylsulfonyl)-4-(thiophen-2-yl)pyridin-3-yl)methanone

Yellow solid was obtained in 71% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.56 – 7.50 (m, 2H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 7.7 Hz, 3H), 7.38 (d, *J* = 7.4 Hz, 3H), 7.33 – 7.24 (m, 6H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.15 (d, *J* = 5.1 Hz, 1H), 6.71 (d, *J* = 4.2 Hz, 2H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.06, 160.95, 149.62, 141.95, 139.62, 137.80, 136.98, 136.62, 135.53, 133.66, 133.27, 132.75, 130.28, 129.75, 129.19, 129.16, 129.08, 128.75, 128.44, 128.33, 127.74, 126.07.

HRMS (ESI) calculated for $C_{28}H_{19}NO_3S_2^+$ $[M+H]^+$ 482.0879 found 482.0877.



4a

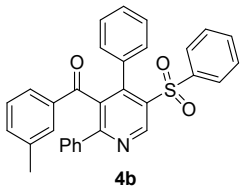
(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)(p-tolyl)methanone

White solid was obtained in 72% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.57 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.44 (td, *J* = 6.5, 3.0 Hz, 1H), 7.29 – 7.22 (m, 9H), 7.12 (t, *J* = 7.5 Hz, 1H), 6.94 (dd, *J* = 19.8, 7.7 Hz, 4H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.59 (d, *J* = 7.7 Hz, 1H), 2.26 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 194.68, 160.47, 149.22, 148.53, 144.65, 139.93, 137.91, 136.03, 134.45, 134.36, 133.11, 131.53, 130.28, 130.00, 129.67, 129.22, 129.19, 129.03, 128.64, 128.40, 127.79, 127.15, 126.82, 21.64.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1474.



4b

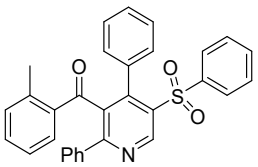
(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)(m-tolyl)methanone

White solid was obtained in 74% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.76 (d, *J* = 4.0 Hz, 1H), 7.62 – 7.52 (m, 2H), 7.44 (ddd, *J* = 8.7, 5.1, 2.8 Hz, 1H), 7.38 – 7.32 (m, 1H), 7.31 – 7.27 (m, 2H), 7.25 – 7.20 (m, 4H), 7.17 (q, *J* = 7.3 Hz, 2H), 7.12 (tdd, *J* = 7.5, 3.6, 1.5 Hz, 2H), 7.06 (dd, *J* = 8.5, 7.4 Hz, 1H), 6.94 (t, *J* = 7.7 Hz, 2H), 6.85 (d, *J* = 7.1 Hz, 1H), 6.60 – 6.48 (m, 1H), 2.20 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.33, 160.60, 149.26, 148.60, 139.91, 138.12, 137.83, 136.87, 136.07, 134.40, 133.14, 131.55, 130.18, 129.73, 129.32, 129.21, 129.03, 128.66, 128.45, 128.41, 128.27, 128.13, 127.82, 127.19, 126.82, 126.60, 126.20, 21.05.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1475.



4c

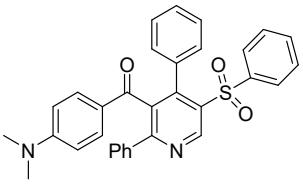
(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)(o-tolyl)methanone

White solid was obtained in 60% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.73 (s, 1H), 7.59 (dd, *J* = 7.3, 2.4 Hz, 2H), 7.43 (q, *J* = 4.3 Hz, 1H), 7.31 (d, *J* = 6.6 Hz, 3H), 7.23 (d, *J* = 4.4 Hz, 4H), 7.21 – 7.16 (m, 2H), 7.11 (t, *J* = 7.7 Hz, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.96 – 6.84 (m, 3H), 6.73 – 6.56 (m, 2H), 2.04 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 196.10, 160.80, 149.15, 140.34, 139.94, 138.08, 134.44, 133.10, 132.45, 131.84, 131.61 (d, *J* = 10.5 Hz), 129.95, 129.61, 129.12, 128.65, 128.41, 128.29, 127.79, 126.97, 125.31, 21.06.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1469.



4d

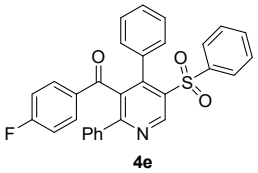
(4-(dimethylamino)phenyl)(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)methanone

White solid was obtained in 36% isolated yield.

^{1}H NMR (500 MHz, Chloroform-d) δ 9.72 (s, 1H), 7.66 – 7.57 (m, 2H), 7.43 (t, *J* = 6.3 Hz, 1H), 7.24 (q, *J* = 9.4, 6.6 Hz, 9H), 7.11 (t, *J* = 7.5 Hz, 1H), 6.96 (dt, *J* = 11.5, 7.7 Hz, 2H), 6.89 (d, *J* = 7.8 Hz, 1H), 6.61 (d, *J* = 7.7 Hz, 1H), 6.34 (d, *J* = 8.7 Hz, 2H), 2.95 (s, 6H).

^{13}C NMR (126 MHz, Chloroform-d) δ 192.22, 160.42, 153.37, 148.80, 148.37, 140.09, 138.32, 136.59, 134.19, 132.98, 131.86, 131.62, 130.16, 130.03, 129.44, 129.15, 128.60, 128.25, 128.19, 127.76, 127.00, 126.65, 125.15, 110.26, 39.85.

HRMS (ESI) calculated for $C_{32}H_{26}N_2O_3S^+$ $[M+H]^+$ 519.1737 found 519.1738.



4e

(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)(4-fluorophenyl)methanone

White solid was obtained in 82% isolated yield.

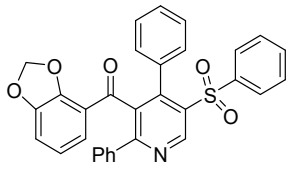
^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.58 – 7.52 (m, 2H), 7.45 (tt, *J* = 6.1, 2.7 Hz, 1H), 7.40 – 7.36 (m, 2H), 7.31 – 7.21 (m, 7H), 7.14 (td, *J* = 7.6, 1.4 Hz, 1H), 6.97 (q, *J* = 8.1 Hz, 2H), 6.88 – 6.77 (m, 3H), 6.59 (d,

J = 7.7 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 193.59, 166.69, 164.64, 160.53, 149.50, 148.52, 139.86, 137.80, 135.49, 134.45, 133.35, 133.18, 131.74, 131.66, 131.46, 130.29, 129.87, 129.81, 129.15, 128.68, 128.56, 128.49, 127.81, 127.27, 126.94, 115.69, 115.52.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -103.33.

HRMS (ESI) calculated for $C_{30}H_{20}FNO_3S^+$ $[M+H]^+$ 494.1221 found 494.1218.



4f

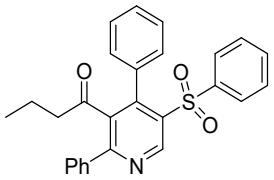
benzo[d][1,3]dioxol-4-yl(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)methanone

White solid was obtained in 73% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.74 (s, 1H), 7.57 (dd, *J* = 7.6, 1.9 Hz, 2H), 7.44 (tt, *J* = 5.8, 2.7 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.24 (d, *J* = 5.8 Hz, 4H), 7.18 – 7.11 (m, 1H), 6.99 (q, *J* = 7.8 Hz, 2H), 6.92 – 6.84 (m, 3H), 6.58 (dd, *J* = 16.9, 8.1 Hz, 2H), 5.92 (s, 2H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 192.94, 160.38, 152.20, 149.22, 148.46, 147.93, 139.89, 137.95, 135.82, 134.33, 133.11, 131.89, 131.54, 130.26, 129.93, 129.67, 129.13, 128.64, 128.43, 128.41, 127.77, 127.17, 126.87, 126.82, 107.74, 107.59, 101.91.

HRMS (ESI) calculated for $C_{31}H_{21}NO_5S^+$ $[M+H]^+$ 520.1145 found 520.1147.



4g

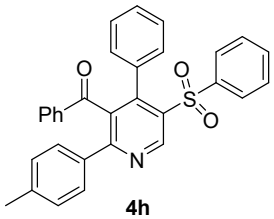
1-(2,4-diphenyl-5-(phenylsulfonyl)pyridin-3-yl)butan-1-one

White solid was obtained in 51% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.67 (s, 1H), 7.60 – 7.55 (m, 2H), 7.46 (q, *J* = 7.3, 6.6 Hz, 4H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.26 (d, *J* = 5.3 Hz, 4H), 7.18 (t, *J* = 7.6 Hz, 2H), 6.87 (d, *J* = 7.5 Hz, 2H), 1.92 (t, *J* = 7.0 Hz, 2H), 1.08 – 1.00 (m, 2H), 0.36 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 204.88, 159.18, 148.74, 147.00, 139.89, 138.36, 137.88, 134.29, 133.17, 131.48, 130.09, 129.91, 129.68, 129.19, 128.80, 128.68, 128.66, 127.77, 127.37, 46.78, 16.04, 12.82.

HRMS (ESI) calculated for $C_{27}H_{23}NO_3S^+$ $[M+H]^+$ 442.1426 found 442.1430.



4h

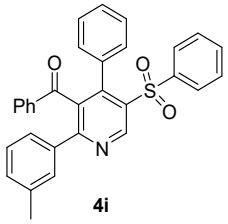
phenyl(4-phenyl-5-(phenylsulfonyl)-2-(p-tolyl)pyridin-3-yl)methanone

White solid was obtained in 70% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.74 (s, 1H), 7.47 (d, *J* = 7.9 Hz, 2H), 7.43 (ddd, *J* = 8.7, 5.2, 2.5 Hz, 1H), 7.38 – 7.33 (m, 3H), 7.25 – 7.21 (m, 4H), 7.17 (t, *J* = 7.7 Hz, 2H), 7.12 – 7.04 (m, 3H), 6.92 (dt, *J* = 22.9, 6.3 Hz, 2H), 6.81 (d, *J* = 7.8 Hz, 1H), 6.56 (d, *J* = 7.7 Hz, 1H), 2.26 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.42, 160.65, 149.32, 148.44, 139.95, 136.91, 135.61, 135.05, 134.01, 133.48, 133.07, 131.54, 130.23, 130.11, 129.21, 129.14, 129.04, 128.62, 128.37, 128.26, 127.76, 127.15, 126.78, 21.22.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1471.



4i

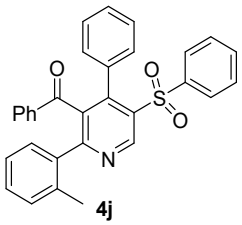
phenyl(4-phenyl-5-(phenylsulfonyl)-2-(m-tolyl)pyridin-3-yl)methanone

White solid was obtained in 72% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.75 (s, 1H), 7.43 (dt, *J* = 8.3, 2.7 Hz, 2H), 7.38 – 7.32 (m, 3H), 7.29 (dt, *J* = 7.2, 1.9 Hz, 1H), 7.26 – 7.20 (m, 4H), 7.18 (t, *J* = 7.7 Hz, 2H), 7.11 (qd, *J* = 6.3, 5.1, 3.5 Hz, 3H), 6.94 (dt, *J* = 17.2, 7.4 Hz, 2H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.57 (d, *J* = 7.5 Hz, 1H), 2.25 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.23, 160.84, 149.29, 148.49, 139.89, 138.22, 137.76, 136.90, 135.86, 134.27, 133.48, 133.11, 131.51, 130.49, 130.23, 130.05, 129.93, 129.00, 128.63, 128.42, 128.23, 127.77, 127.16, 126.83, 126.16, 21.25.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1474.



4j

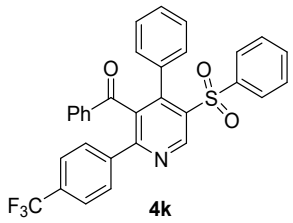
phenyl(4-phenyl-5-(phenylsulfonyl)-2-(o-tolyl)pyridin-3-yl)methanone

White solid was obtained in 63% isolated yield.

^{1}H NMR (500 MHz, Chloroform-d) δ 9.76 (d, J = 4.1 Hz, 1H), 7.63 – 7.51 (m, 2H), 7.43 (t, J = 6.7 Hz, 1H), 7.35 (d, J = 7.6 Hz, 1H), 7.29 (d, J = 6.8 Hz, 2H), 7.24 (d, J = 13.9 Hz, 4H), 7.14 (dt, J = 18.8, 7.6 Hz, 4H), 7.05 (t, J = 7.5 Hz, 1H), 6.94 (t, J = 7.7 Hz, 2H), 6.85 (d, J = 8.7 Hz, 1H), 6.56 (t, J = 9.6 Hz, 1H), 2.22 (d, J = 30.2 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.36, 160.64, 149.32, 148.49, 139.93, 138.09, 137.94, 136.87, 136.00, 134.36, 133.11, 131.57, 130.48, 130.17, 129.95, 129.66, 129.29, 129.18, 129.01, 128.64, 128.41, 128.24, 128.10, 127.79, 127.15, 126.81, 126.58, 21.03.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1469.



4k

phenyl(4-phenyl-5-(phenylsulfonyl)-2-(4-(trifluoromethyl)phenyl)pyridin-3-yl)methanone

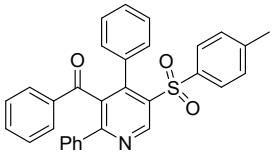
White solid was obtained in 46% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.45 (tt, *J* = 5.5, 3.0 Hz, 1H), 7.41 – 7.32 (m, 3H), 7.23 (d, *J* = 2.1 Hz, 4H), 7.22 – 7.17 (m, 2H), 7.15 – 7.09 (m, 1H), 6.94 (t, *J* = 7.7 Hz, 2H), 6.88 (s, 1H), 6.53 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 194.99, 159.08, 149.51, 148.74, 141.24, 139.68, 136.69, 136.24, 135.15, 133.90, 133.28, 131.24, 130.19, 129.62, 129.04, 128.71, 128.63, 128.46, 127.85, 126.93, 125.42, 125.39.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -63.08.

HRMS (ESI) calculated for $C_{31}H_{20}F_3NO_3S^+$ $[M+H]^+$ 544.1189 found 544.1183.



5a

(2,4-diphenyl-5-tosylpyridin-3-yl)(phenyl)methanone

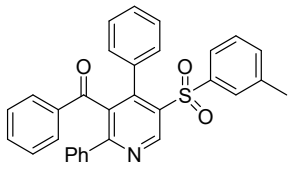
White solid was obtained in 75% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.73 (s, 1H), 7.59 – 7.52 (m, 2H), 7.39 – 7.32 (m, 3H), 7.32 – 7.23 (m, 3H), 7.21 – 7.14 (m, 2H), 7.16 – 7.09 (m, 3H), 7.03 (d, J = 8.1 Hz, 2H), 6.99 (s, 1H), 6.92 (s, 1H), 6.83 (s, 1H), 6.62 (d,

J = 7.8 Hz, 1H), 2.35 (s, 3H) .

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.29, 160.47, 149.31, 148.98, 139.98, 138.41, 137.84, 136.88, 136.02, 134.74, 133.50, 133.13, 130.20, 129.69, 129.22, 129.07, 128.54, 128.42, 128.24, 127.86, 127.54, 21.19.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1472.



5b

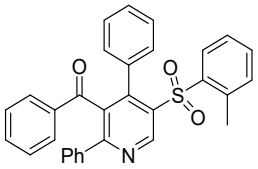
(2,4-diphenyl-5-(m-tolylsulfonyl)pyridin-3-yl)(phenyl)methanone

White solid was obtained in 73% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.69 (s, 1H), 7.50 (dd, J = 7.8, 1.8 Hz, 2H), 7.31 – 7.26 (m, 3H), 7.24 – 7.19 (m, 3H), 7.18 (d, J = 7.1 Hz, 1H), 7.13 – 7.04 (m, 5H), 6.89 (d, J = 13.6 Hz, 3H), 6.79 (d, J = 6.8 Hz, 1H), 6.51 (d, J = 7.6 Hz, 1H), 2.13 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.15, 160.32, 149.07, 148.81, 139.58, 138.83, 137.54, 136.86, 136.02, 134.82, 134.10, 133.60, 131.43, 130.34, 129.85, 129.27, 129.07, 128.64, 128.50, 128.42, 128.32, 126.79, 125.04, 21.06.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1466.



5c

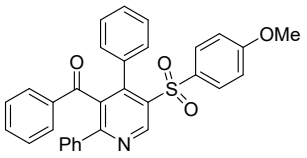
(2,4-diphenyl-5-(o-tolylsulfonyl)pyridin-3-yl)(phenyl)methanone

White solid was obtained in 48% isolated yield

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.63 – 7.54 (m, 2H), 7.37 – 7.32 (m, 3H), 7.28 (ddt, J = 9.7, 6.5, 3.6 Hz, 5H), 7.17 (t, J = 7.7 Hz, 2H), 7.12 (d, J = 7.6 Hz, 1H), 7.05 – 6.99 (m, 2H), 6.84 (t, J = 7.7 Hz, 3H), 6.50 (d, J = 7.7 Hz, 1H), 2.37 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.28, 160.37, 149.92, 148.28, 137.93, 137.73, 136.89, 136.79, 135.69, 134.20, 133.54, 133.30, 131.93, 131.23, 129.72, 129.63, 129.27, 129.03, 128.44, 128.34, 128.28, 127.11, 126.73, 126.06, 20.01.

HRMS (ESI) calculated for $C_{31}H_{23}NO_3S^+$ $[M+H]^+$ 490.1471 found 490.1474.



5d

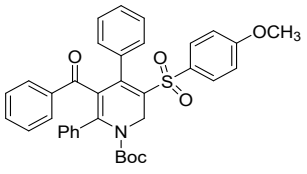
(5-((4-methoxyphenyl)sulfonyl)-2,4-diphenylpyridin-3-yl)(phenyl)methanone

White solid was obtained in 83% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.73 (s, 1H), 7.55 (dd, J = 7.3, 2.0 Hz, 2H), 7.38 – 7.28 (m, 3H), 7.27 (d, J = 6.7 Hz, 3H), 7.20 – 7.09 (m, 5H), 7.04 (d, J = 8.3 Hz, 1H), 6.94 (s, 1H), 6.87 – 6.82 (m, 1H), 6.68 (d, J = 8.6 Hz, 3H), 3.80 (s, 3H).

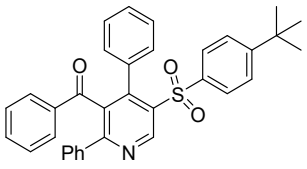
^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.32, 163.37, 160.33, 149.28, 148.36, 137.97, 136.95, 135.86, 134.96, 133.49, 131.77, 131.49, 130.40, 130.19, 129.64, 129.22, 129.05, 128.47, 128.42, 128.26, 127.14, 126.86, 113.90, 55.63.

HRMS (ESI) calculated for $C_{31}H_{23}NO_4S^+$ $[M+H]^+$506.1420 found 506.1407.



5d'

HRMS (ESI) calculated for $C36H_{33}NO_6S^+$ $[M+H]^+$608.2048 found 608.2051.



5e

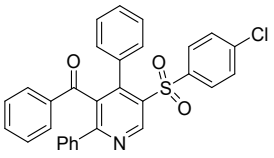
(5-((4-(tert-butyl)phenyl)sulfonyl)-2,4-diphenylpyridin-3-yl)(phenyl)methanone

White solid was obtained in 72% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.75 (s, 1H), 7.58 – 7.54 (m, 2H), 7.36 – 7.32 (m, 3H), 7.30 – 7.25 (m, 3H), 7.23 – 7.20 (m, 2H), 7.19 – 7.14 (m, 4H), 7.09 (tt, J = 7.3, 1.3 Hz, 1H), 6.94 – 6.85 (m, 3H), 6.53 (d, J = 7.8 Hz, 1H), 1.27 (s, 9H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.33, 160.44, 157.12, 149.24, 148.33, 137.95, 136.87, 136.75, 135.81, 134.73, 133.49, 131.64, 130.16, 129.61, 129.18, 129.03, 128.38, 128.31, 128.23, 127.64, 126.99, 125.65, 35.05, 30.92.

HRMS (ESI) calculated for $C_{34}H_{29}NO_3S^+$ $[M+H]^+$ 532.1996 found 532.1998.



5f

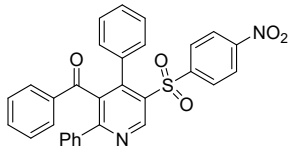
(5-((4-chlorophenyl)sulfonyl)-2,4-diphenylpyridin-3-yl)(phenyl)methanone

White solid was obtained in 60% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.75 (s, 1H), 7.56 (d, J = 6.6 Hz, 2H), 7.34 (dd, J = 7.6, 3.1 Hz, 3H), 7.30 – 7.26 (m, 3H), 7.17 (dd, J = 12.1, 6.9 Hz, 7H), 7.07 – 7.01 (m, 1H), 6.94 (s, 1H), 6.86 – 6.77 (m, 1H), 6.70 – 6.62 (m, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.05, 160.85, 149.31, 148.53, 139.99, 138.41, 137.75, 136.84, 135.97, 134.19, 133.61, 131.50, 130.39, 130.11, 129.84, 129.32, 129.27, 129.08, 128.95, 128.69, 128.49, 128.34, 127.28, 127.00.

HRMS (ESI) calculated for $C_{30}H_{20}ClNO_3S^+$ $[M+H]^+$ 510.0935 found 510.0943.



5g

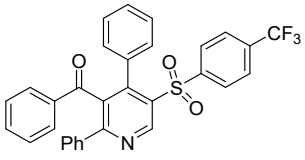
(5-((4-nitrophenyl)sulfonyl)-2,4-diphenylpyridin-3-yl)(phenyl)methanone

White solid was obtained in 66% isolated yield.

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 8.05 (d, J = 8.2 Hz, 2H), 7.57 (d, J = 7.3 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 7.37 – 7.32 (m, 3H), 7.29 (d, J = 7.3 Hz, 2H), 7.21 – 7.14 (m, 3H), 6.99 – 6.93 (m, 3H), 6.82 (s, 1H), 6.62 (s, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 194.83, 161.51, 150.11, 149.44, 148.46, 145.52, 137.67, 136.71, 135.99, 133.73, 133.33, 131.32, 130.26, 130.00, 129.27, 129.18, 129.04, 128.96, 128.54, 128.39, 127.39, 123.68.

HRMS (ESI) calculated for $C_{30}H_{20}N_2O_5S^+$ $[M+H]^+$ 521.1129 found 521.1131.



5h

(2,4-diphenyl-5-((4-(trifluoromethyl)phenyl)sulfonyl)pyridin-3-yl)(phenyl)methanone

White solid was obtained in 45% isolated yield.

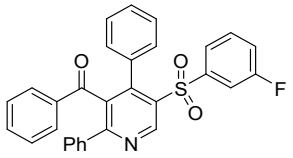
^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.79 (s, 1H), 7.57 (d, J = 7.1 Hz, 2H), 7.48 (d, J = 6.9 Hz, 2H), 7.41 – 7.32 (m, 5H), 7.29 (d, J = 8.0 Hz, 3H), 7.18 (t, J = 7.3 Hz, 2H), 7.14 (t, J = 7.5 Hz, 1H), 6.94 (p, J = 6.9 Hz, 2H), 6.82 (d,

J = 7.9 Hz, 1H), 6.56 (d, J = 7.6 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 194.92, 161.13, 149.34, 148.57, 143.34, 137.63, 136.73, 136.01, 133.82, 133.69, 131.34, 130.28, 129.94, 129.29, 129.10, 128.74, 128.53, 128.38, 127.29, 125.72.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -63.21.

HRMS (ESI) calculated for $C_{31}H_{20}F_3NO_3S^+$ $[M+H]^+$ 544.1189 found 544.1189.



5i

(5-((3-fluorophenyl)sulfonyl)-2,4-diphenylpyridin-3-yl)(phenyl)methanone

White solid was obtained in 59% isolated yield

^{1}H NMR (500 MHz, Chloroform-*d*) δ 9.68 (s, 1H), 7.50 (dd, J = 7.7, 1.9 Hz, 2H), 7.32 – 7.26 (m, 3H), 7.24 – 7.18 (m, 4H), 7.13 – 7.04 (m, 5H), 6.91 (dt, J = 30.8, 7.6 Hz, 2H), 6.76 (dt, J = 7.9, 2.2 Hz, 2H), 6.56 (d, J = 7.9 Hz, 1H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 195.06, 162.83, 160.92, 160.82, 149.27, 148.61, 137.72, 136.80, 135.92, 134.09, 133.63, 131.32, 130.55, 130.49, 130.30, 130.05, 129.85, 129.24, 129.05, 128.75, 128.49, 128.33, 127.23, 126.97, 123.63, 120.58, 120.42, 115.48, 115.28.

^{19}F NMR (471 MHz, Chloroform-*d*) δ -109.72.

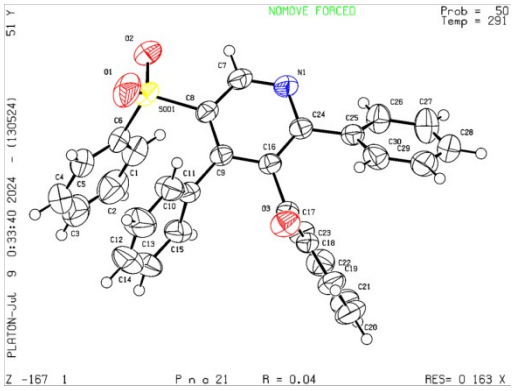
HRMS (ESI) calculated for $C_{30}H_{20}FNO_3S^+$ $[M+H]^+$ 494.1221 found 494.1218.

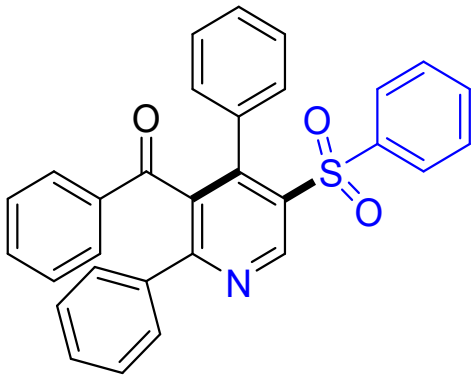
Ⅳ. Crystal data

Adequate crystals 3a was obtained by crystallization from DCM/PE (4:1) at room temperature (25 ℃).

The crystal X-ray diffraction of 3a was measured at a low temperature of 273 K. A Bruker - AXS Venture diffractometer equipped with an IμS source and a Photon III area detector was used, with Cu - Kα radiation having

a wavelength of λ = 1.54178 Å. A white needle - shaped crystal was fixed on a Kapton® loop and then cooled to 112 K in a cold nitrogen stream provided by an OXFORD Crysosystems 800. Data collection and reduction were accomplished using the Bruker AXS APEX 3 software.[2] The SADABS method was applied to perform absorption corrections.[3] The assignment of space groups was determined by inspecting systematic absences, analyzing E - statistics, and successively refining the structures. The structures were solved via the SHELXT program.[4] Subsequently, least - squares refinement on F2 was carried out, followed by difference Fourier synthesis using SHELXL - 2018 for further refinement. In the final calculation of the structure factors, all hydrogen atoms were placed at idealized positions and were assumed to move along with their neighboring atoms, with relative isotropic displacement coefficients. The thermal parameters of all non - hydrogen atoms were refined anisotropically until convergence was achieved.





Crystal data and structure refinement for **3a**. CCDC Number =**2407604**

Bond precision: C-C = 0.0047 A Wavelength=1.54178

Cell: a=11.3681(12) b=12.4428(12) c=17.3170(19)
alpha=90 beta=90 gamma=90
Temperature: 291 K

	Calculated	Reported
Volume	2449.5(4)	2449.5(4)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C30 H21 N O3 S	C30 H21 N O3 S
Sum formula	C30 H21 N O3 S	C30 H21 N O3 S
Mr	475.54	475.54
Dx,g cm-3	1.289	1.289
Z	4	4
Mu (mm-1)	1.431	1.431
F000	992.0	992.0
F000'	996.10	
h,k,lmax	13,14,20	13,14,20
Nref	4469[2314]	4262
Tmin,Tmax	0.756,0.740	0.485,0.753
Tmin'	0.685	

Correction method= # Reported T Limits: Tmin=0.485 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.95 Theta(max)= 68.105

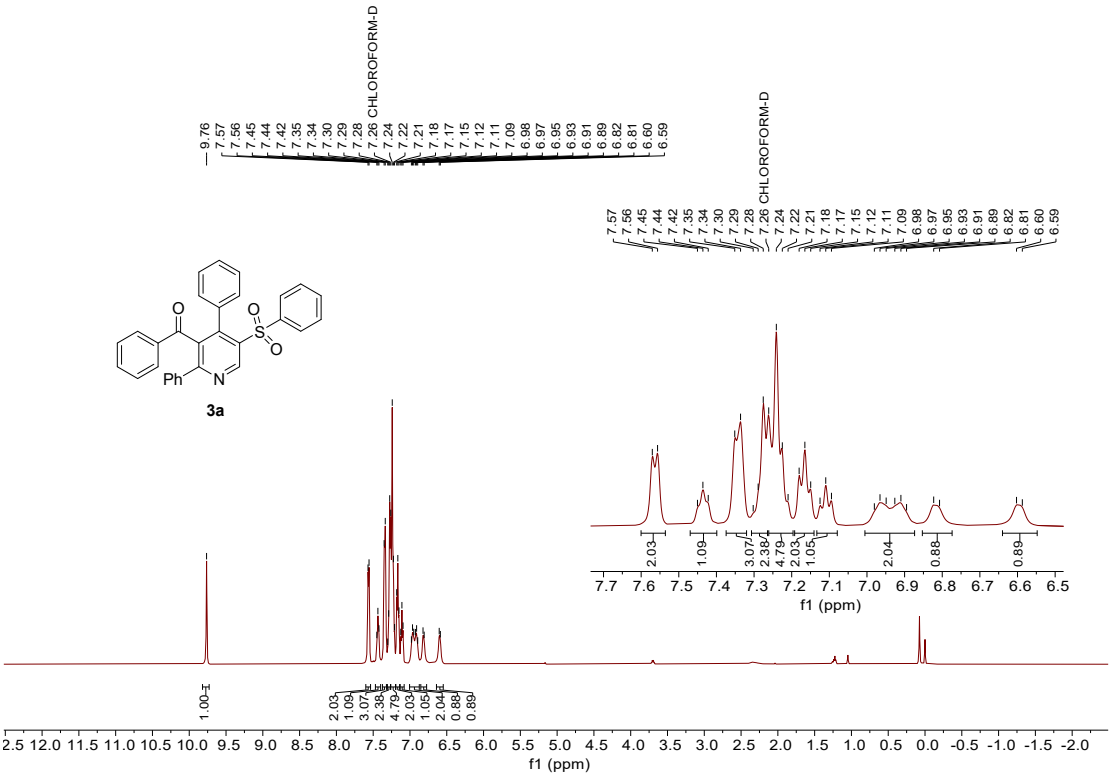
R(reflections)= 0.0377(4147) wR2(reflections)= 0.0966(4262)

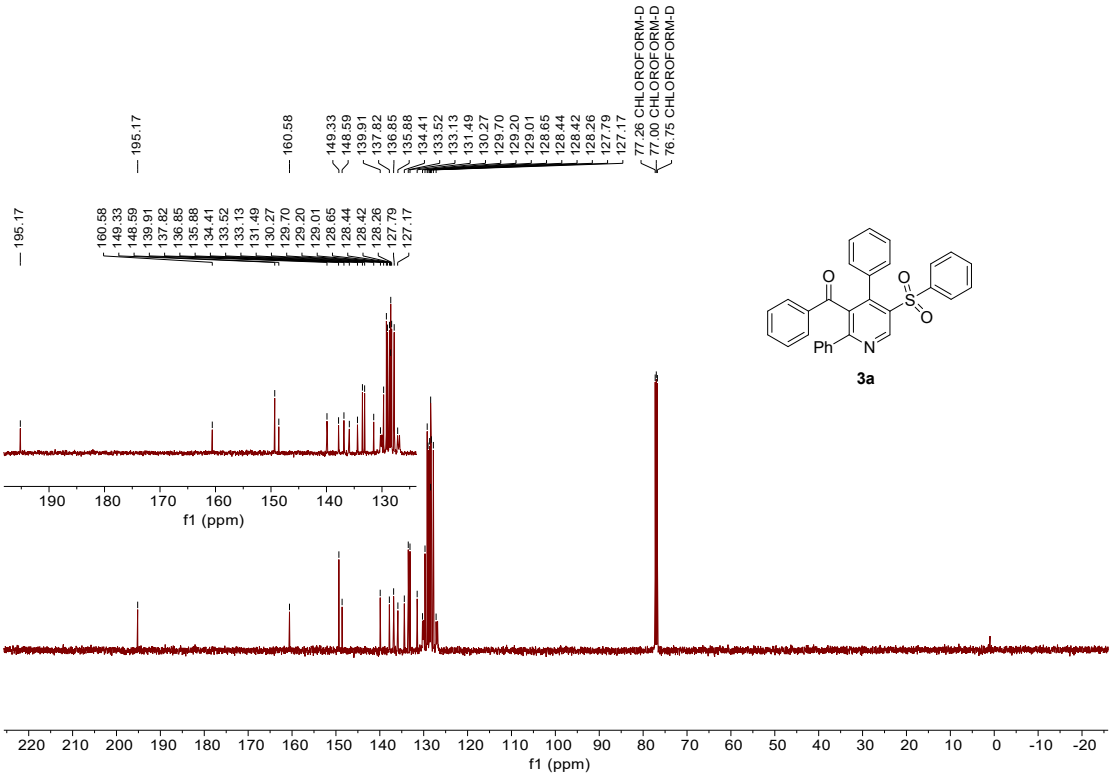
S = 1.058 Npar= 316

Ⅴ. Reference

1. Tongyan Yu, Hairui Ni, Siyan Fan, Jing Jiang, Siliang You, and Chao Deng, *Org. Lett*., 2024, **26**, 10729
2. Bruker, APEX3, Bruker Nano，Inc., Madison, Wisconsin, WI，USA, 20019.
3. G. M. Sheldrick. Acta Cryst., 2015, C71:3-8.
4. Bruker (2019). APEX3 (v2019.1-0) Bruker AXS Inc., Madison, Wisconsin, USA.

Ⅵ. ^{1}H NMR and ^{13}C NMR spectra

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127.17
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77.00 CHLOROFORM-D
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f1 (ppm)
Ph
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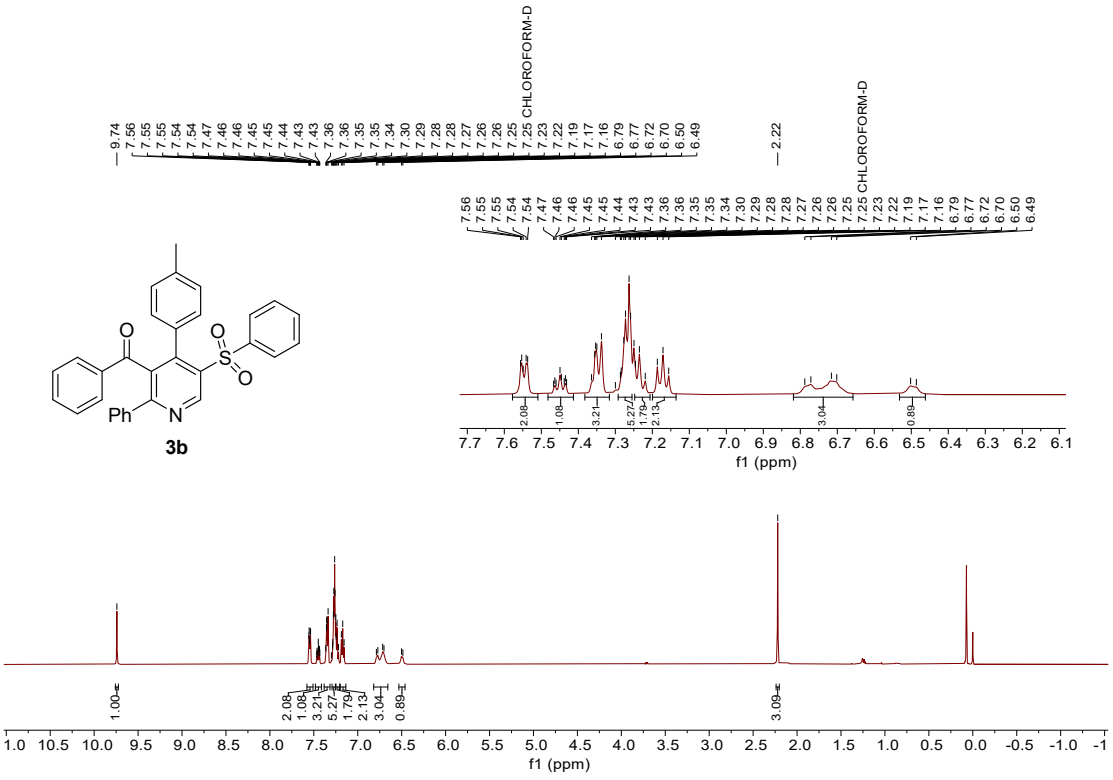
O
S
3a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f1 (ppm)
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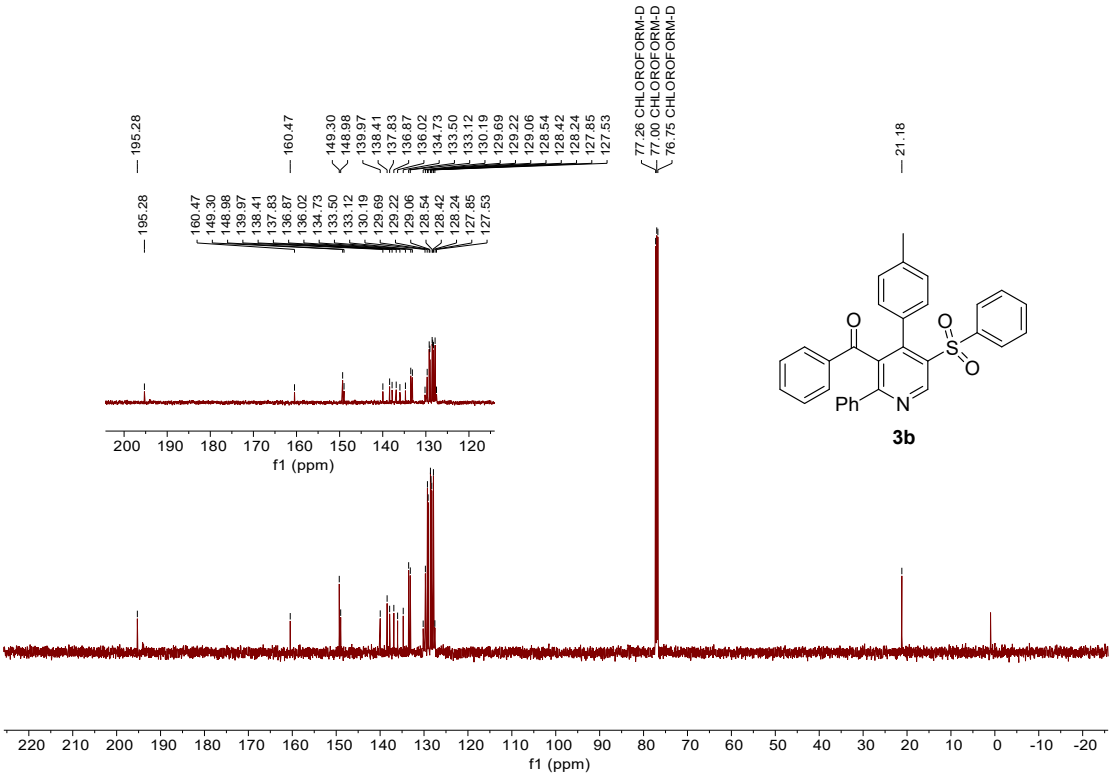
O
S
3b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f1 (ppm)
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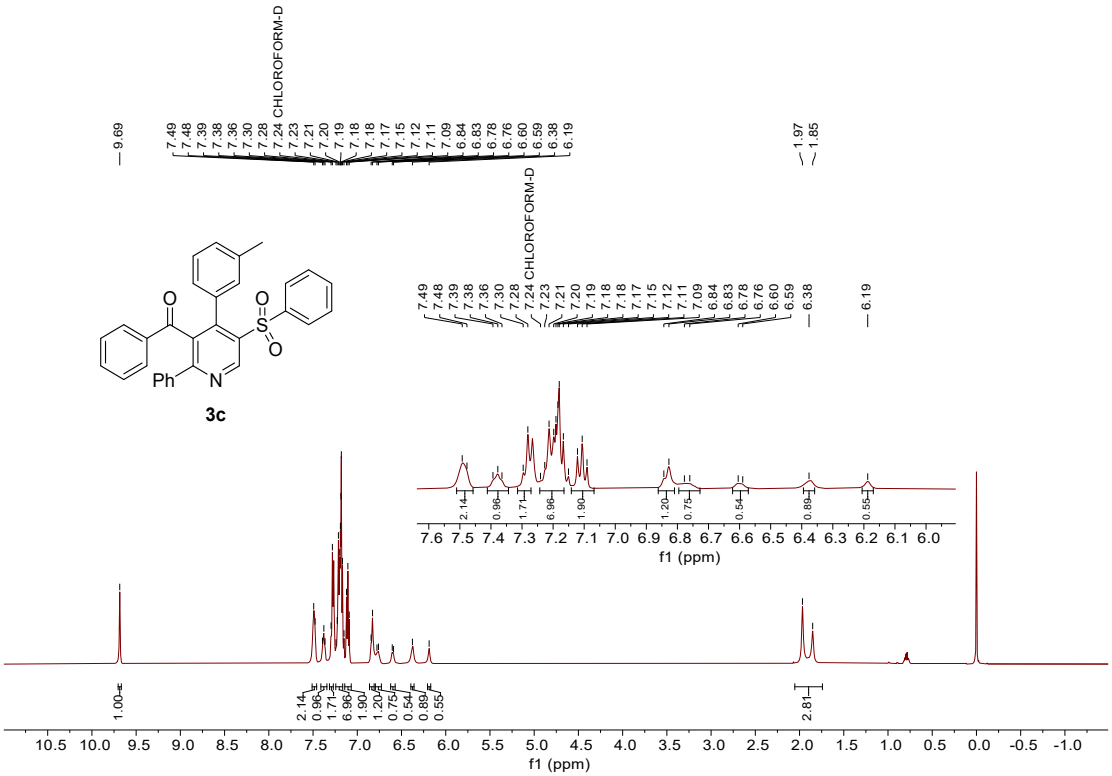
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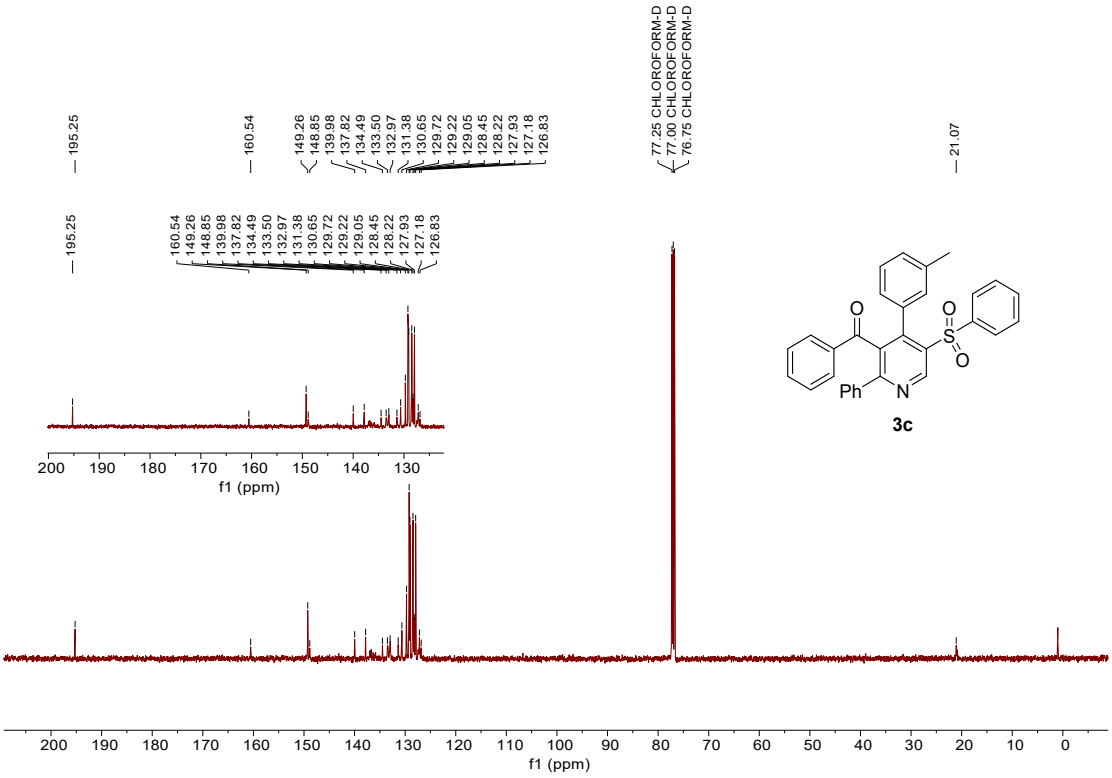
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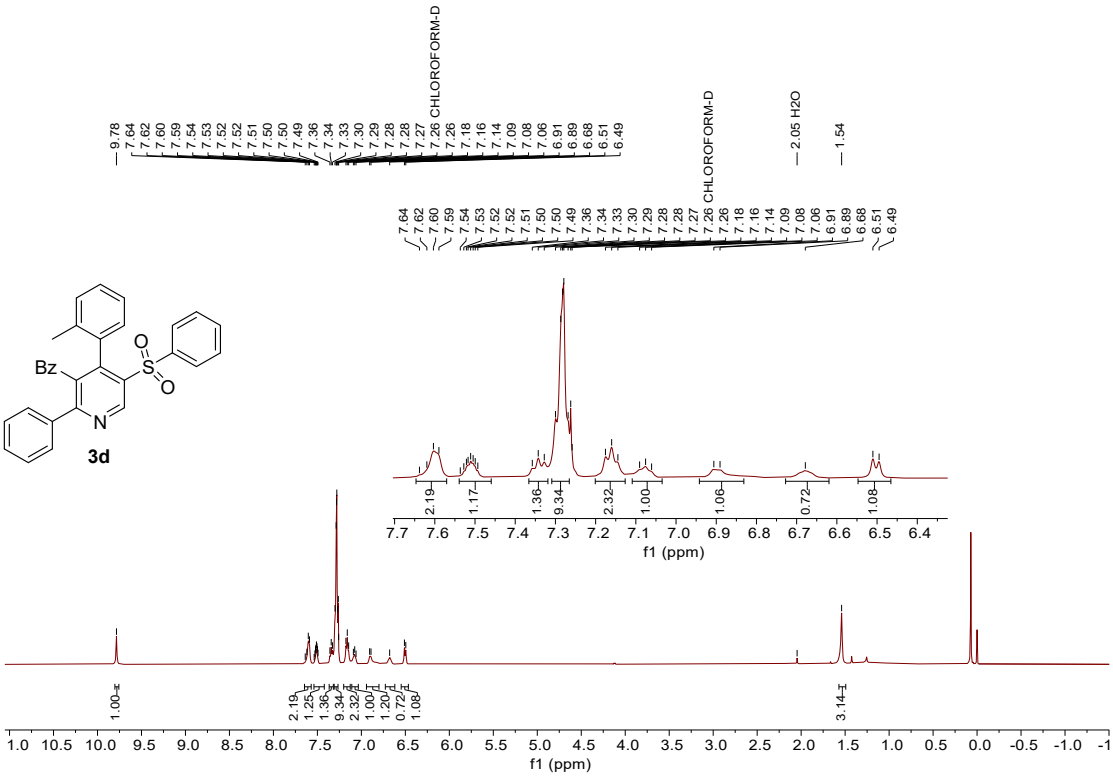
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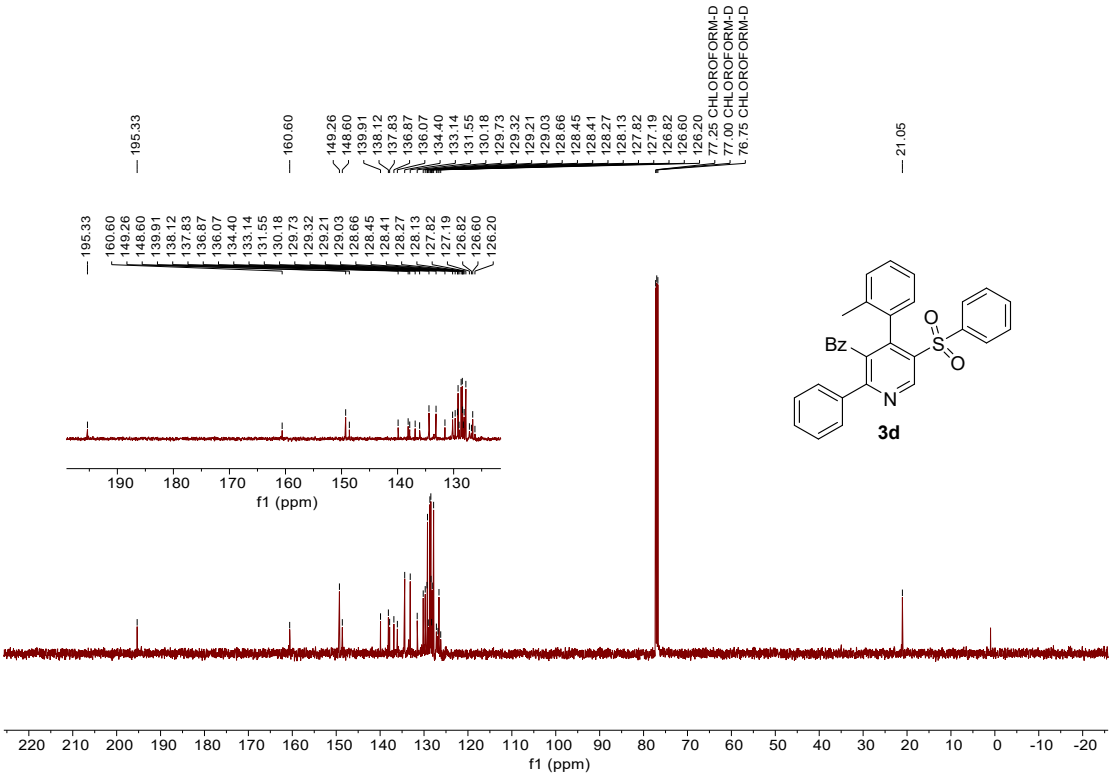
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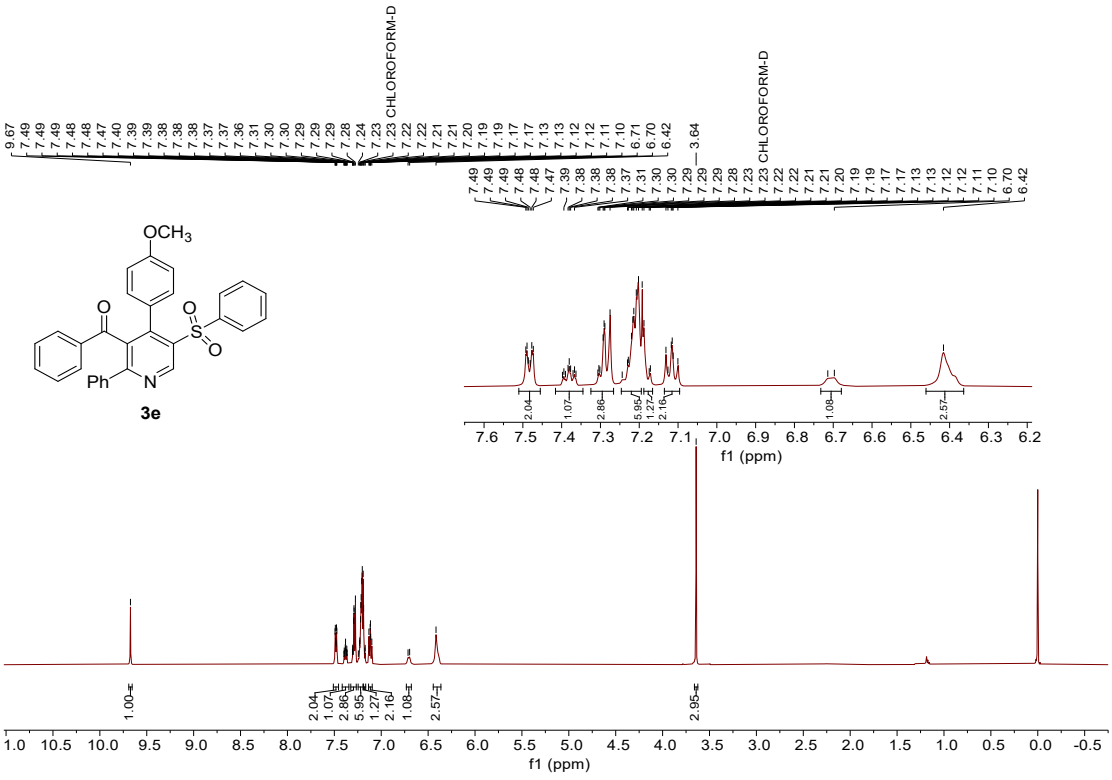
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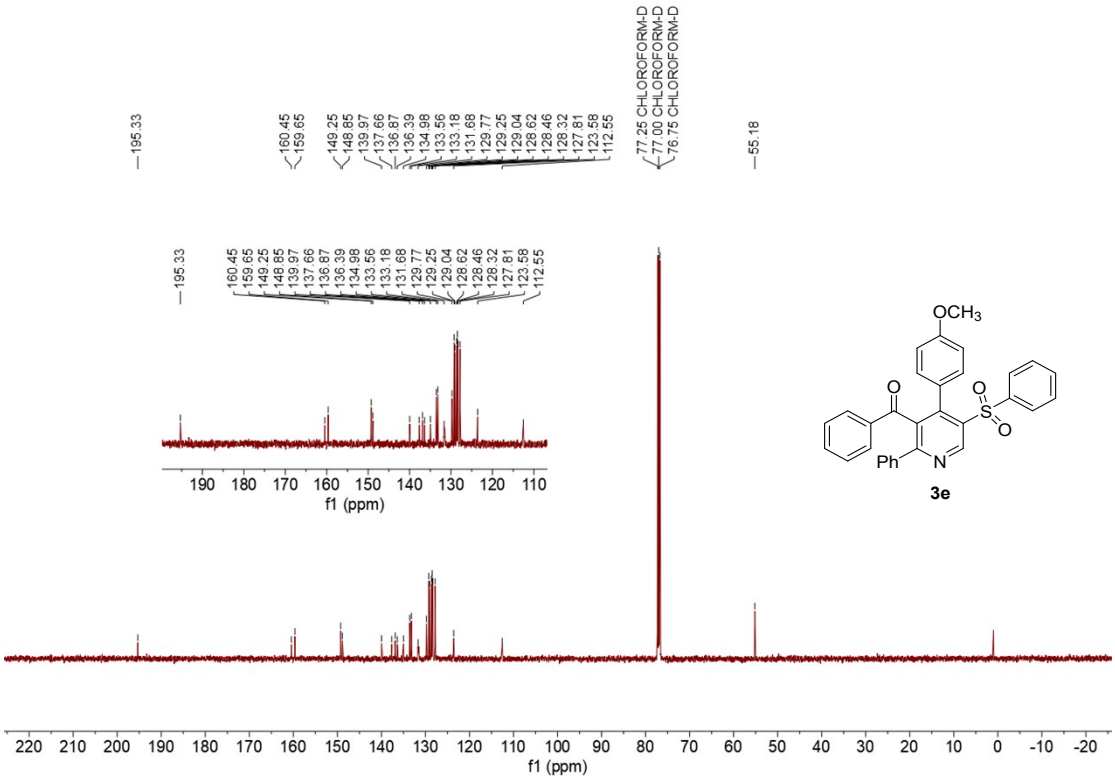
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N
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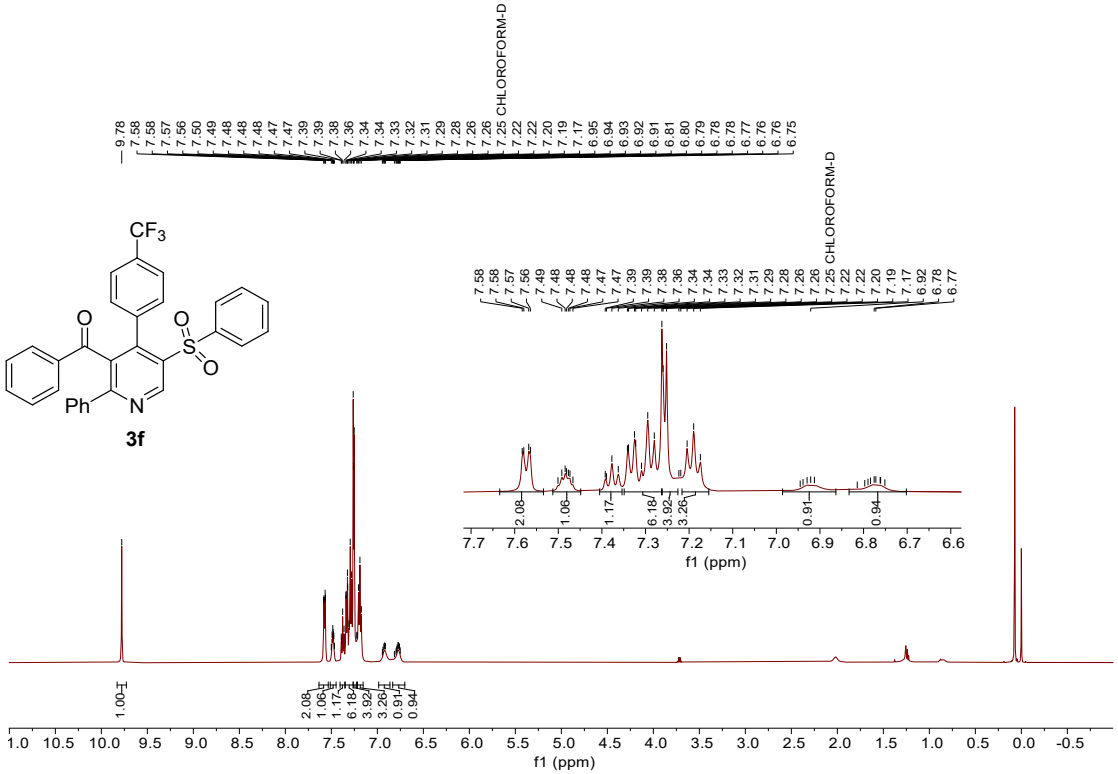
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S
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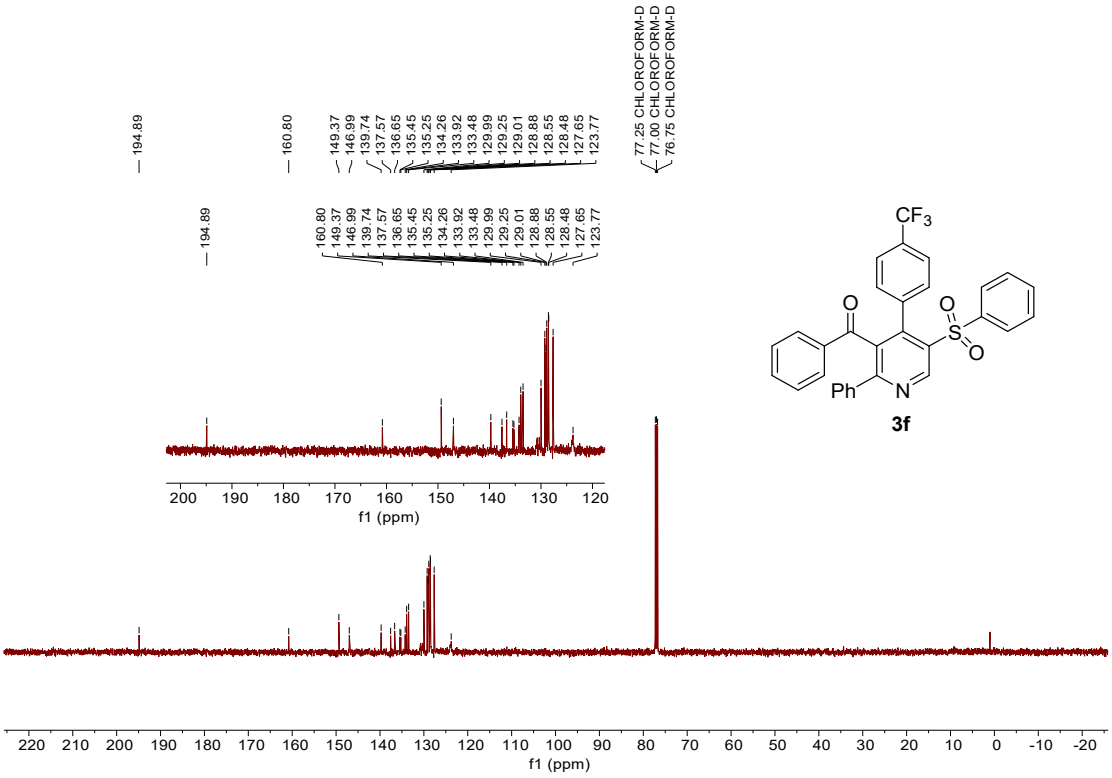
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f1 (ppm)
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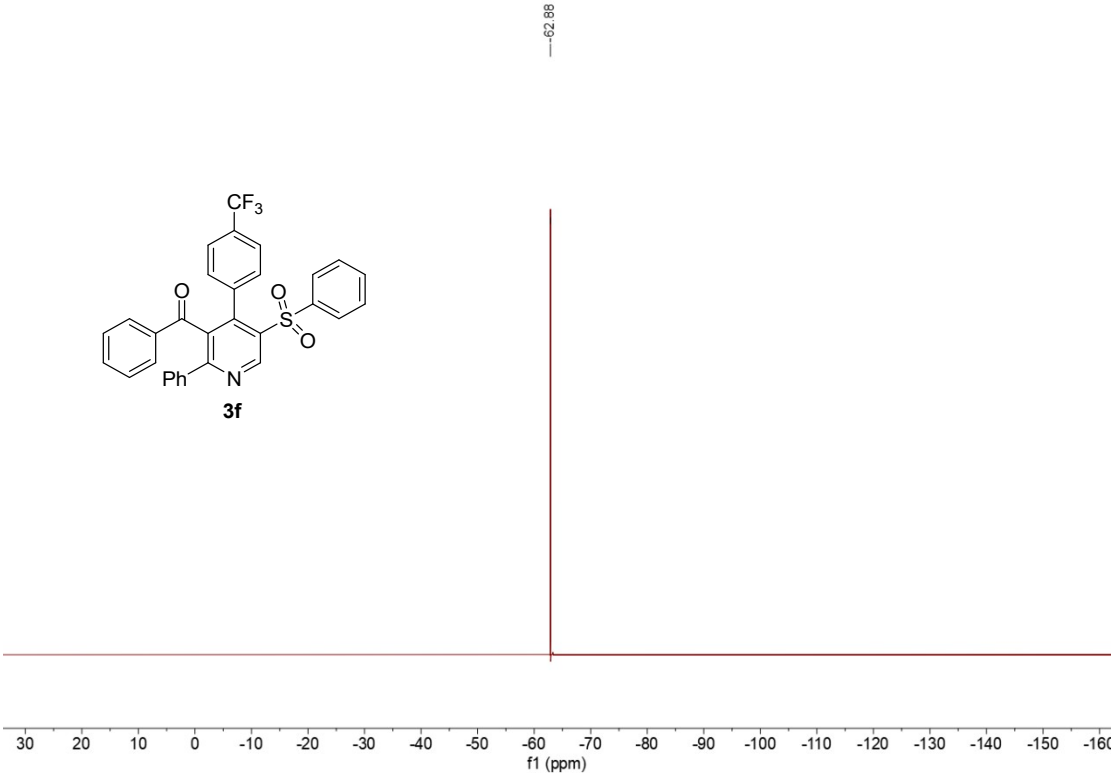
f1 (ppm)

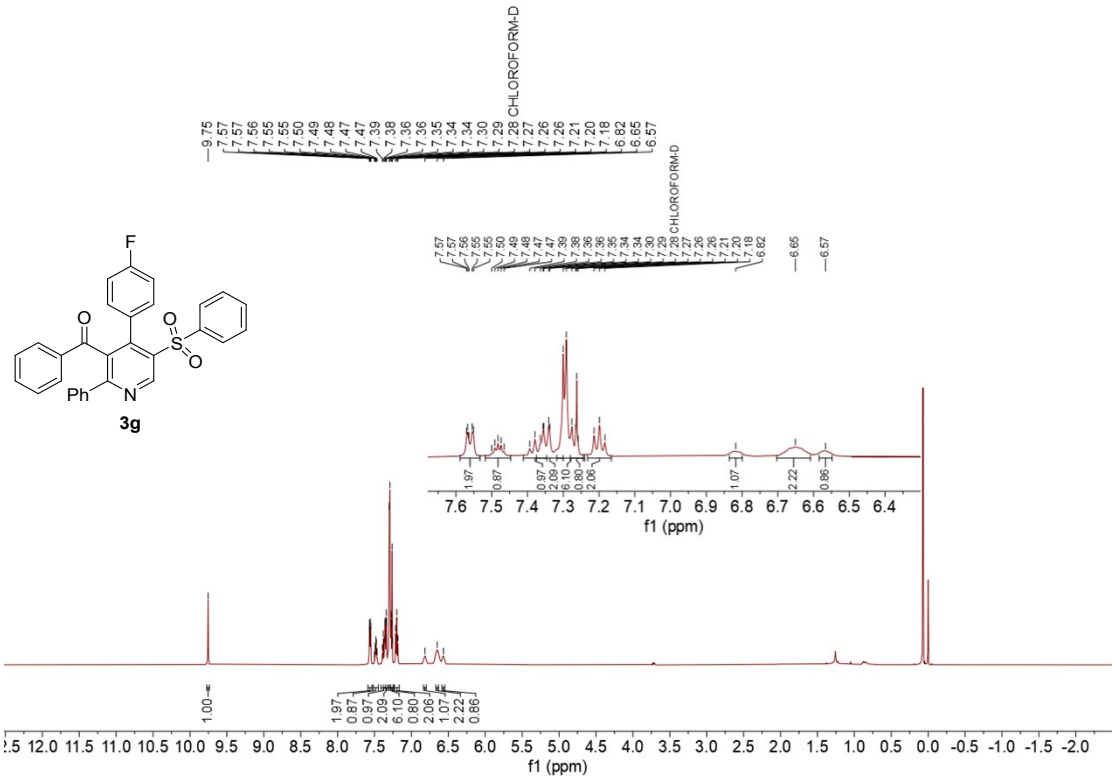
CF3
O
O
S
O
Ph
N

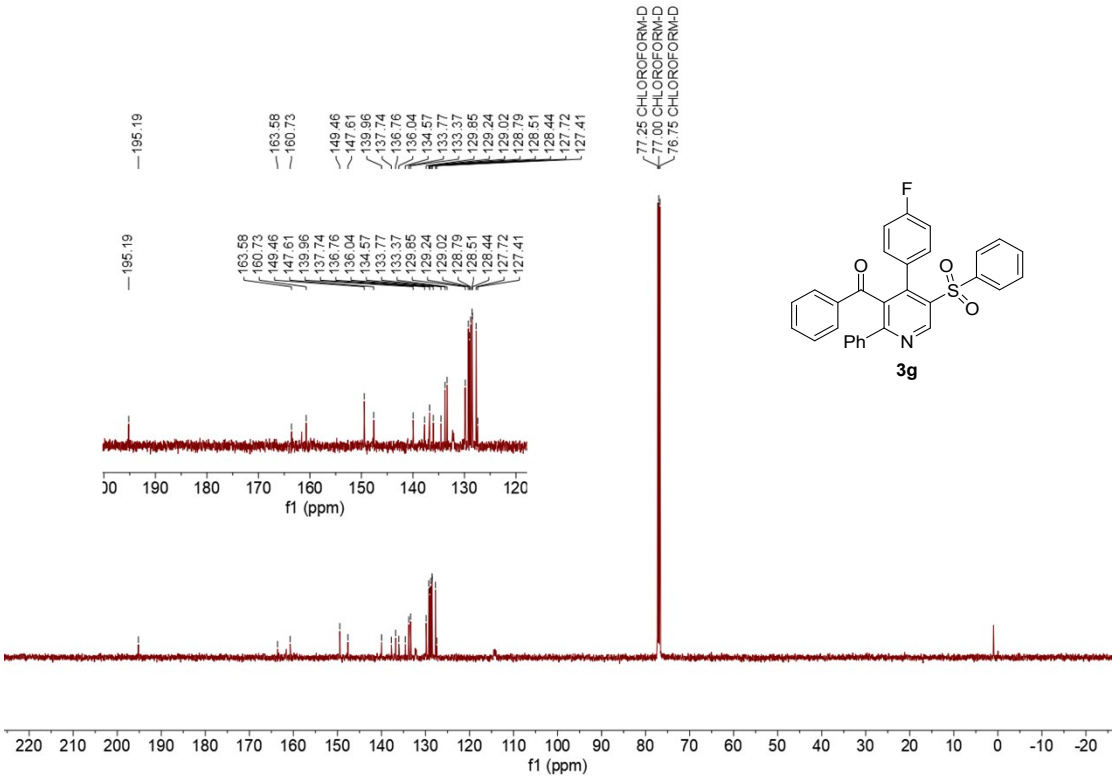
3f

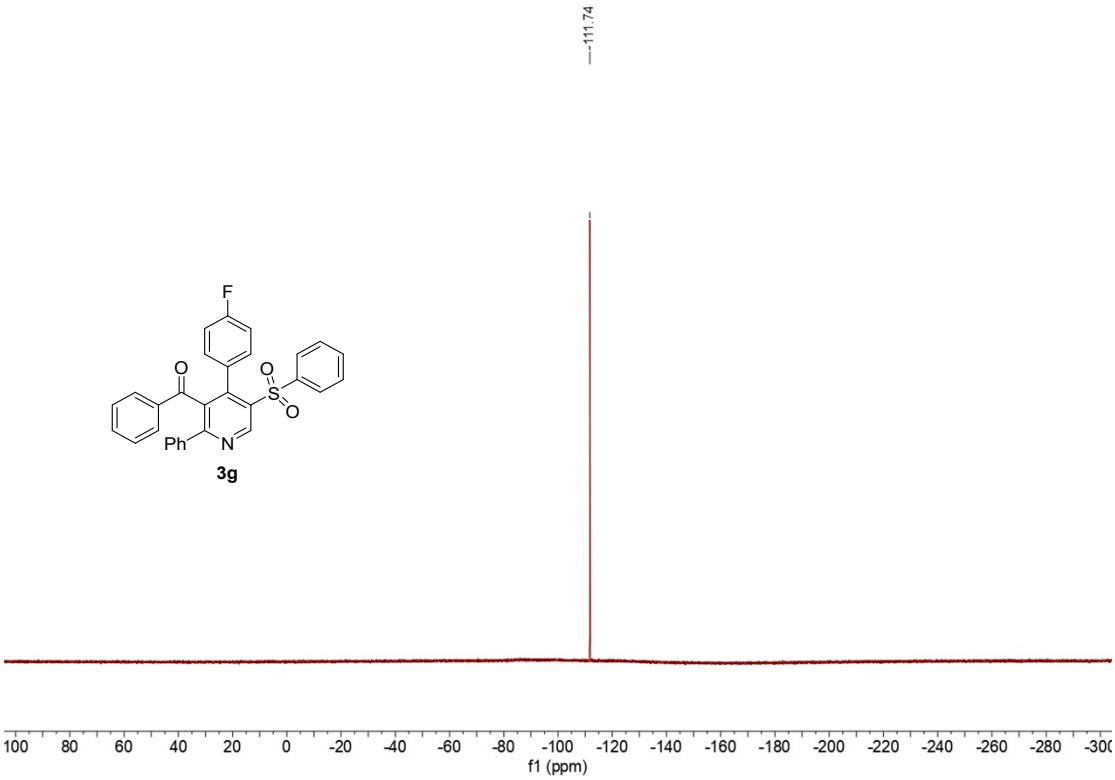

62.88
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160
f1 (ppm)

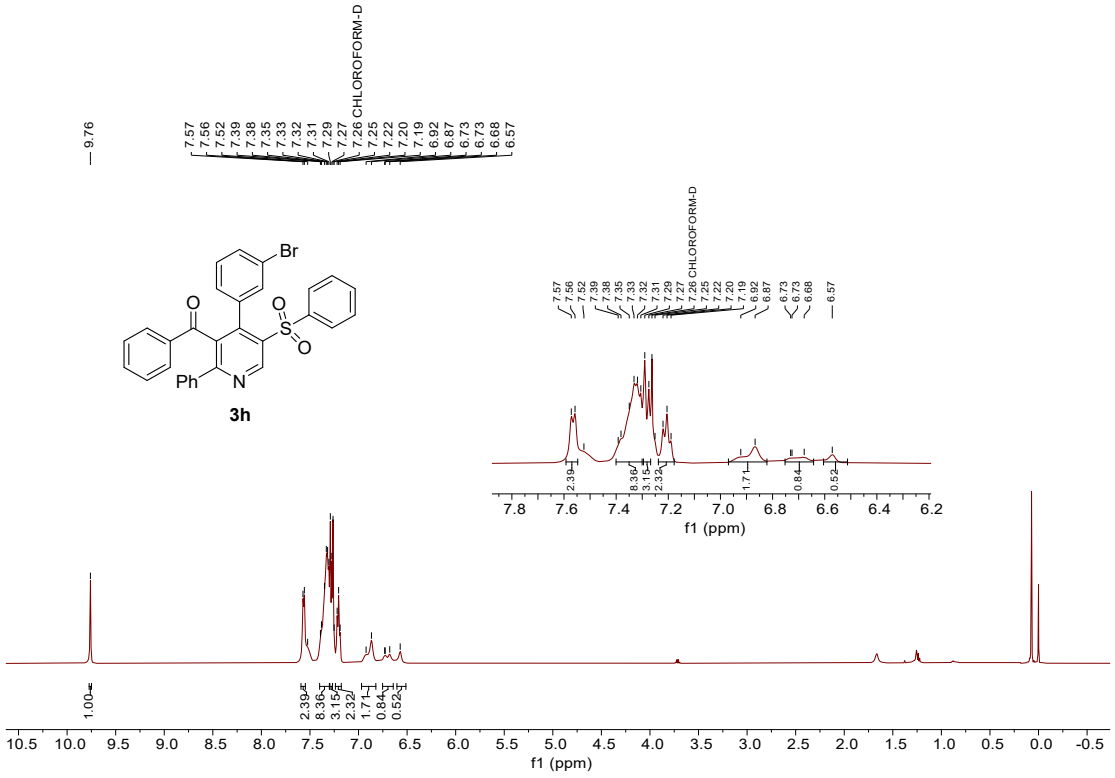
CF3
O
O
S
O
Ph
N

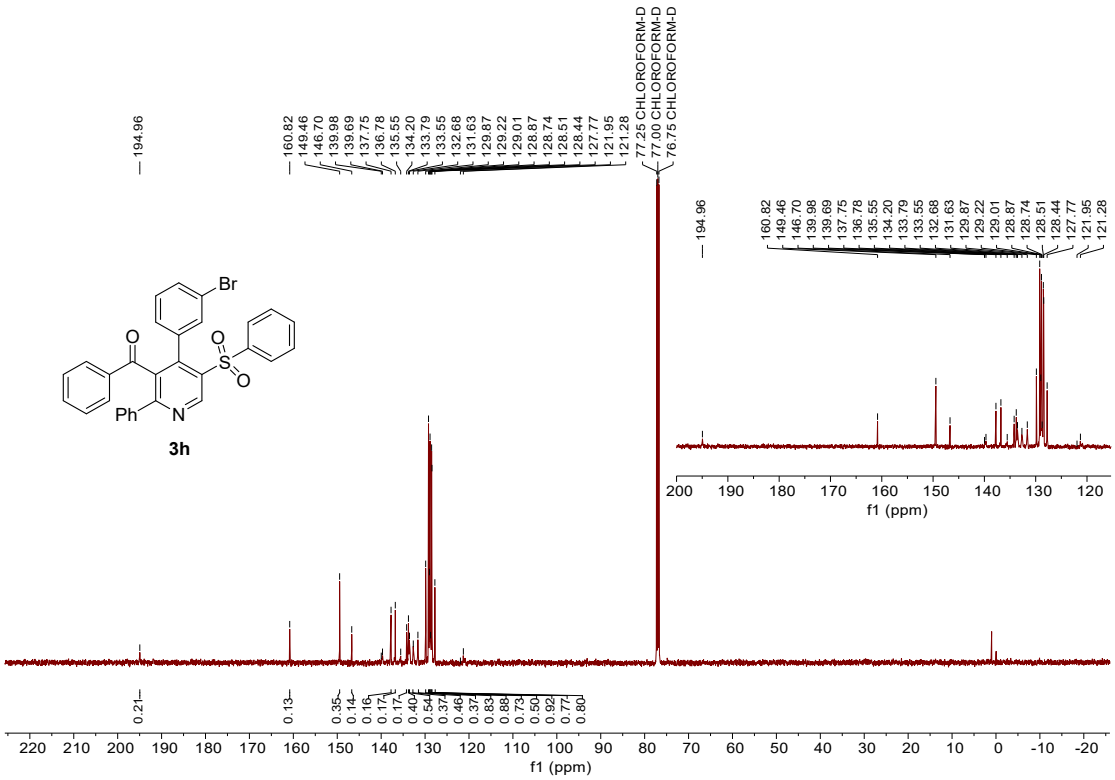
3f


F
O
O
S
O
Ph
N
3g
f1 (ppm)


F
O
O
S
O
Ph
N
3g
f1 (ppm)


111.74
F
O
O
S
O
Ph
N
3g
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)


9.76
7.57 7.56 7.52 7.39 7.38 7.35 7.33 7.32 7.31 7.29 7.27 7.26 CHLOROFORM-D 7.25 7.22 7.20 7.19 6.92 6.87 6.73 6.73 6.68 6.57
Br
O
O
S
O
Ph
N
3h
2.39 8.36 3.15 2.32 1.71 0.84 0.52
1.00
10.5 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 -0.5
f1 (ppm)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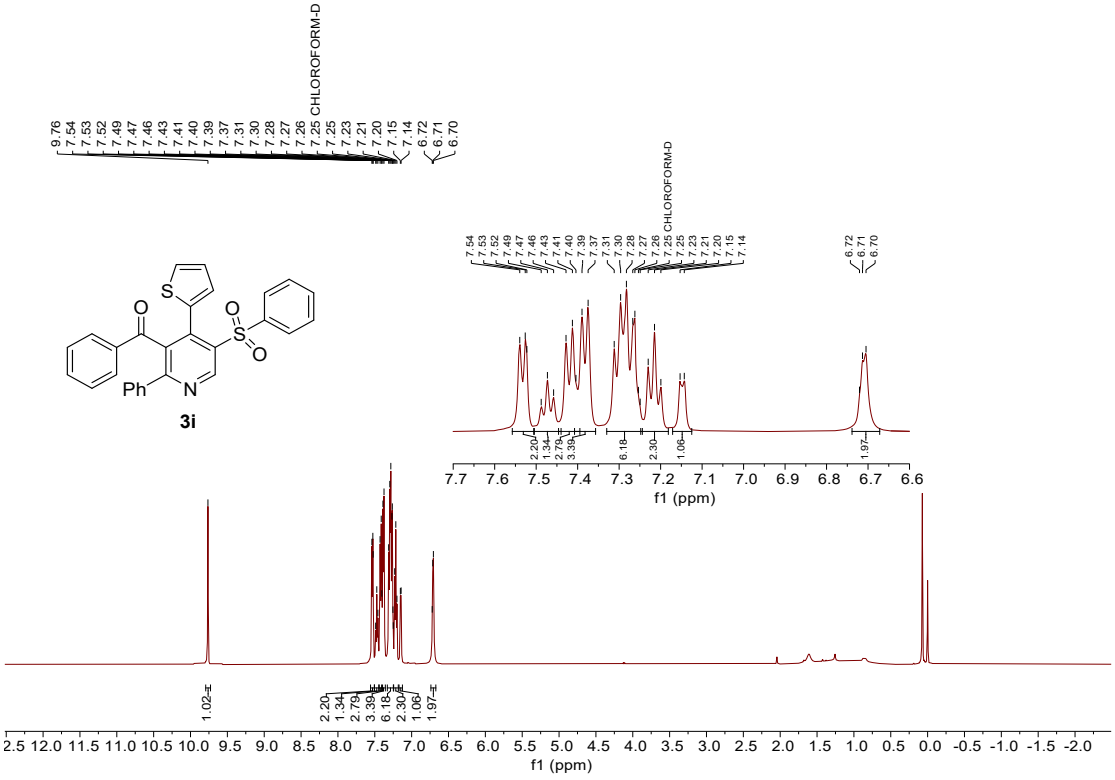
134.20
133.79
133.55
132.68
131.63
129.87
129.22
129.01
128.87
128.74
128.51
128.44
127.77
121.95
121.28
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
Br
O
O
S
O
Ph
N
3h
f1 (ppm)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7.54
7.53
7.52
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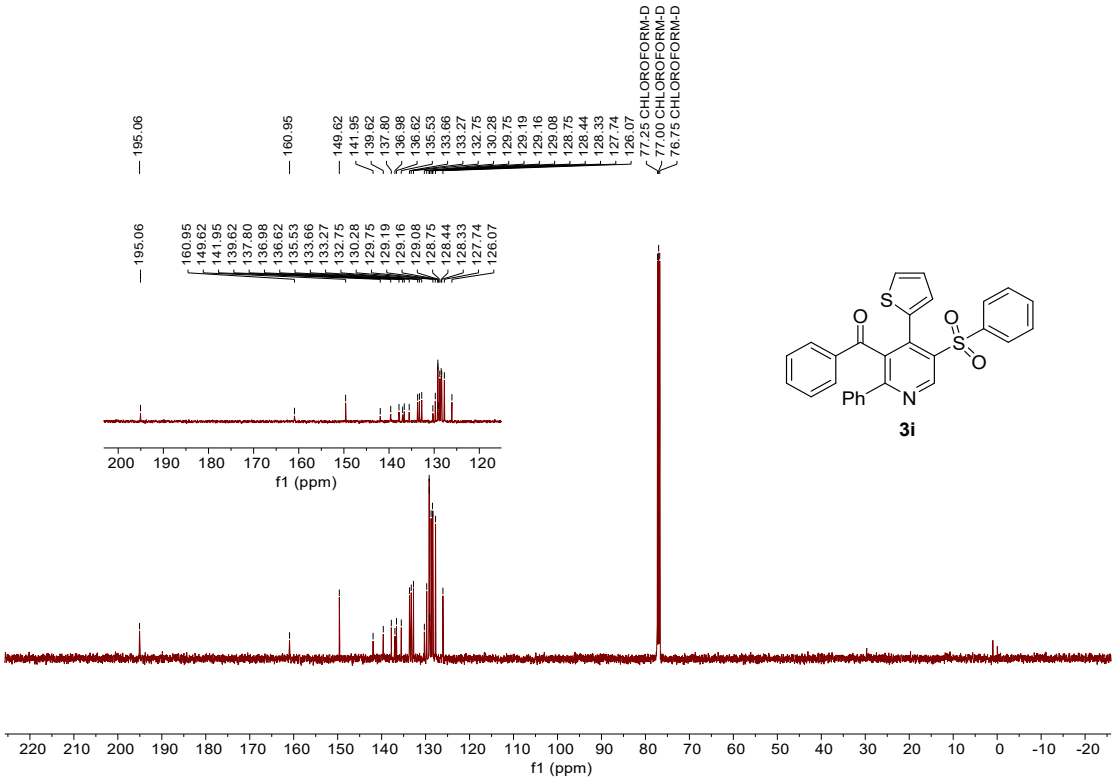
7.47
7.46
7.43
7.41
7.40
7.39
7.37
7.31
7.30
7.28
7.27
7.26
7.25 CHLOROFORM-D
7.25
7.23
7.21
7.20
7.15
7.14
6.72
6.71
6.70
S
O
O
S
O
Ph
N
3i
f1 (ppm)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160.95
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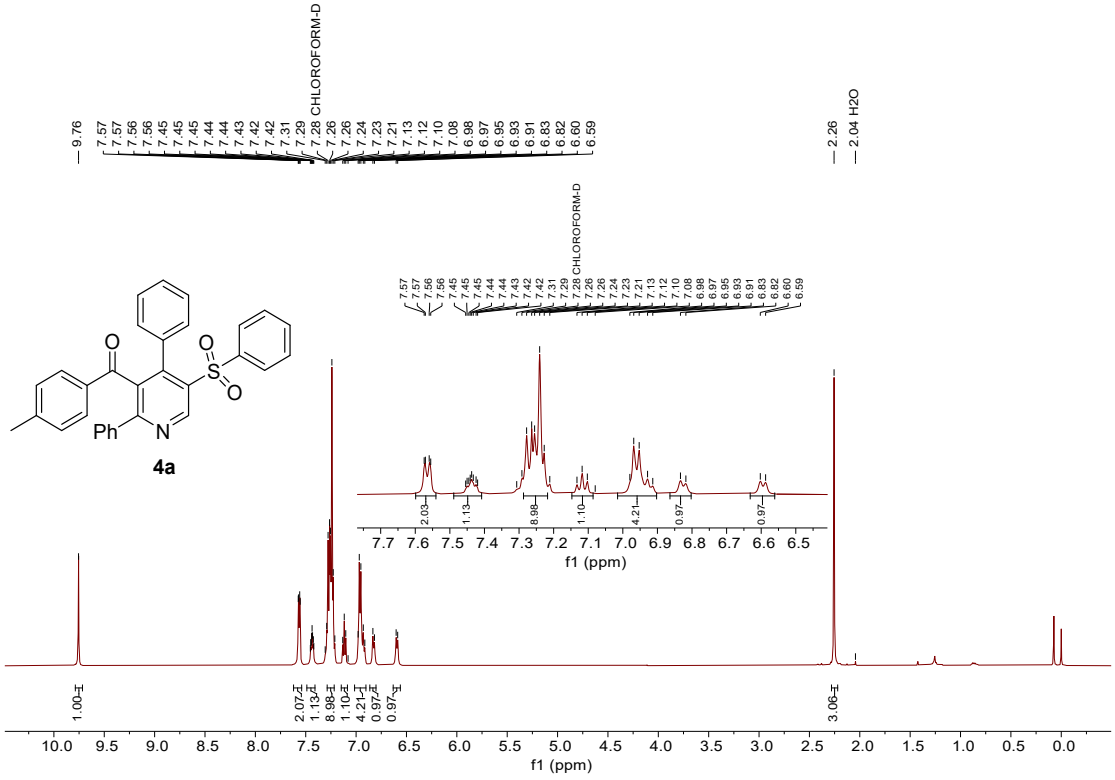
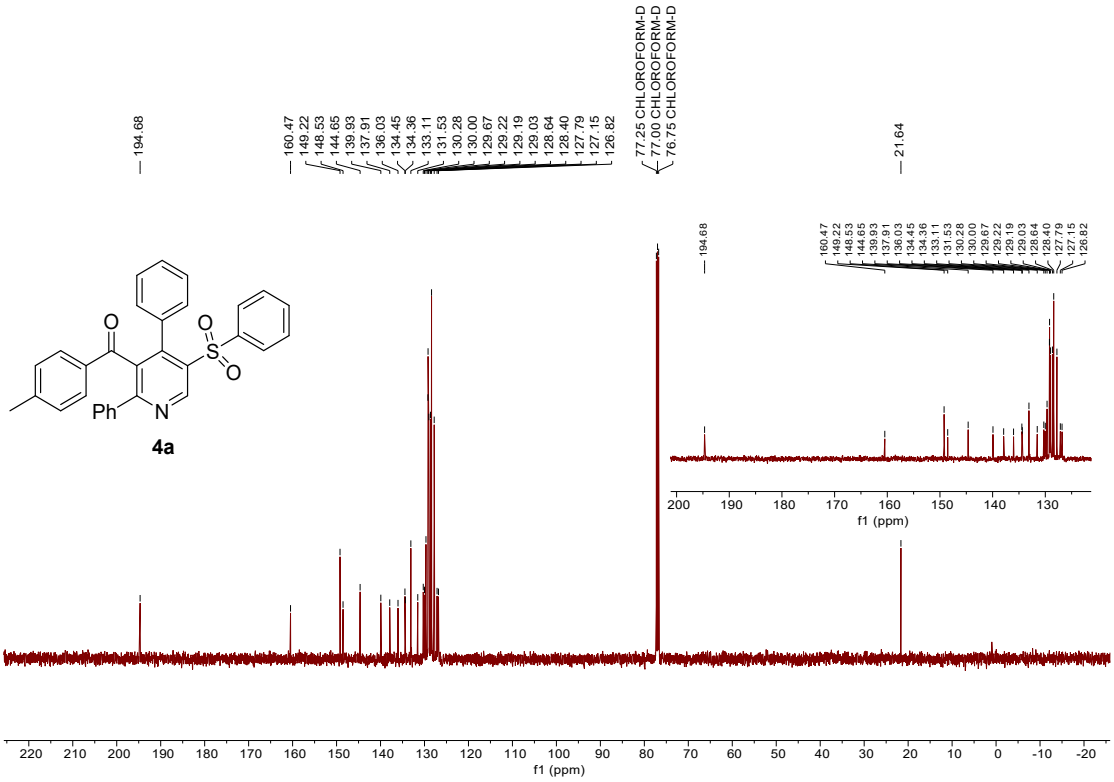
133.66
133.27
132.75
130.28
129.75
129.19
129.16
129.08
128.75
128.44
128.33
127.74
126.07
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
f1 (ppm)
S
O
O
S
O
Ph
N
3i


9.76
7.57
7.56
7.45
7.44
7.43
7.42
7.31
7.29
7.28 CHLOROFORM-D
7.26
7.24
7.23
7.21
7.13
7.12
7.10
7.08
6.98
6.97
6.95
6.93
6.91
6.83
6.82
6.60
6.59
2.26
2.04 H2O
1.00
2.07
1.13
8.98
1.10
4.21
0.97
0.97
3.06
f1 (ppm)
O
O
S
O
Ph
N
4a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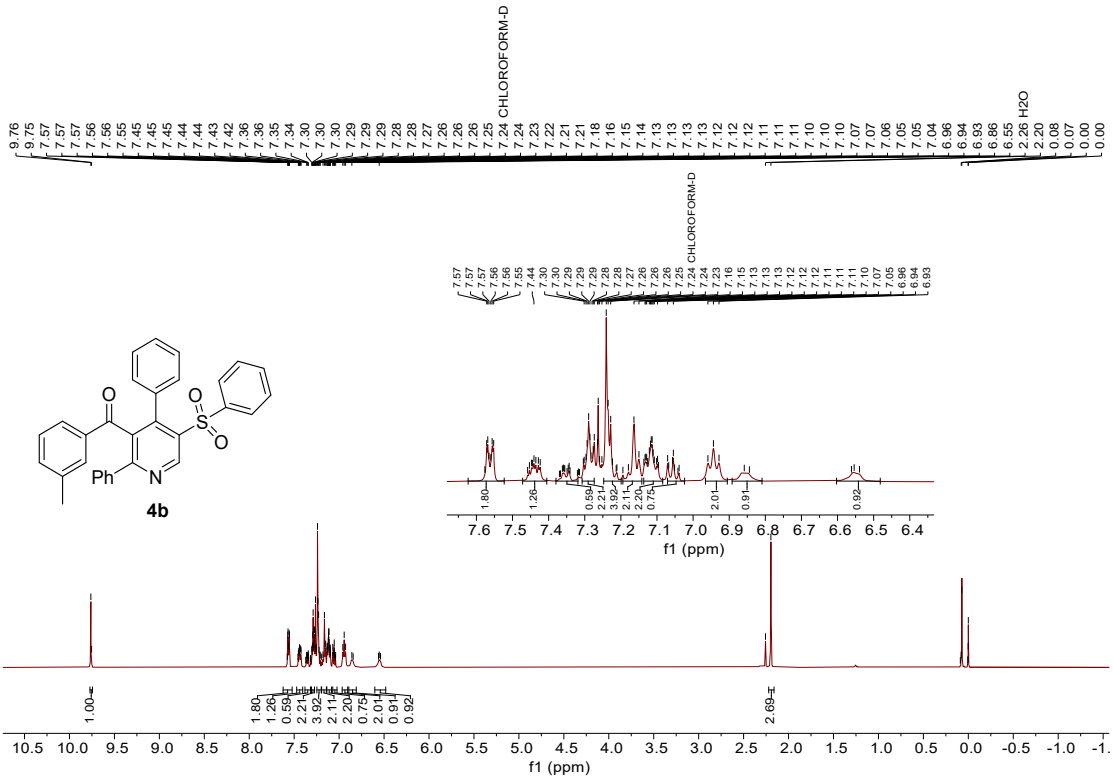
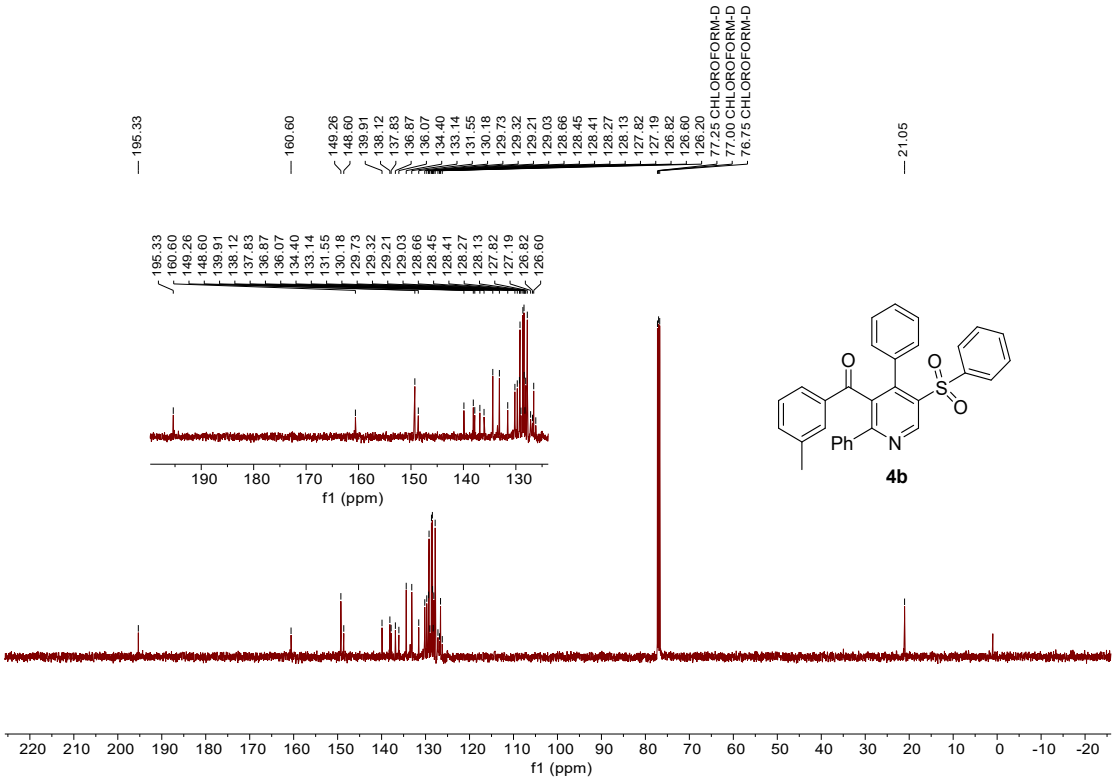
144.65
139.93
137.91
136.03
134.45
134.36
133.11
131.53
130.28
130.00
129.67
129.22
129.19
129.03
128.64
128.40
127.79
127.15
126.82
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.64
O
O
S
O
Ph
N
4a
f1 (ppm)


9.76
7.57
7.56
7.55
7.45
7.44
7.43
7.42
7.36
7.35
7.34
7.30
7.29
7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.18
7.16
7.15
7.14
7.13
7.12
7.11
7.10
7.07
7.06
7.05
7.04
6.96
6.94
6.93
6.86
6.55
CHLOROFORM-D
2.26
H2O
2.20
0.08
0.07
0.00
1.80
1.26
0.59
2.21
3.92
2.11
2.20
0.75
2.01
0.91
0.92
1.00
2.69
O
O
S
O
Ph
N
4b
f1 (ppm)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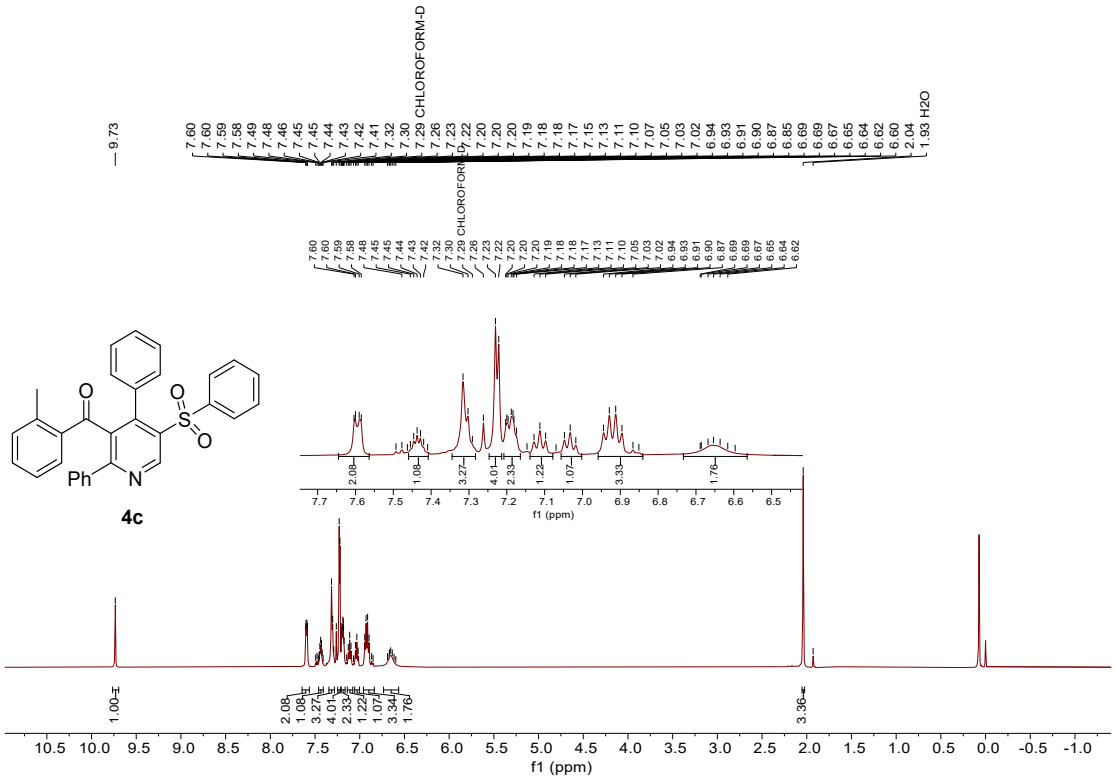
148.60
139.91
138.12
137.83
136.87
136.07
134.40
133.14
131.55
130.18
129.73
129.32
129.21
129.03
128.66
128.45
128.41
128.27
128.13
127.82
127.19
126.82
126.60
126.20
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.05
f1 (ppm)
Ph
N
O
S
4b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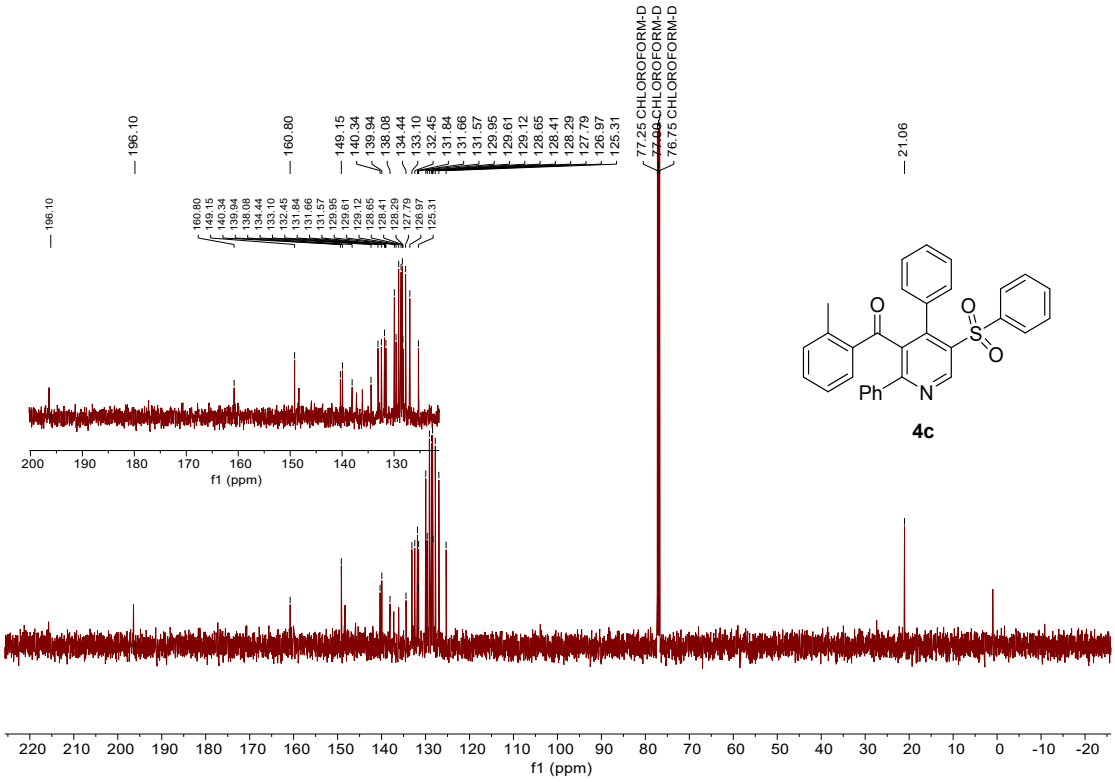
7.58
7.49
7.48
7.46
7.45
7.44
7.43
7.42
7.41
7.32
7.30
7.29 CHLOROFORM-D
7.26
7.23
7.22
7.20
7.19
7.18
7.17
7.15
7.13
7.11
7.10
7.07
7.05
7.03
7.02
6.94
6.93
6.91
6.90
6.89
6.87
6.69
6.67
6.65
6.64
6.62
6.60
2.04
1.93 H2O
2.08
1.08
3.27
4.01
2.33
1.22
1.07
3.33
1.76
3.36
f1 (ppm)
Ph
N
O
S
4c


196.10
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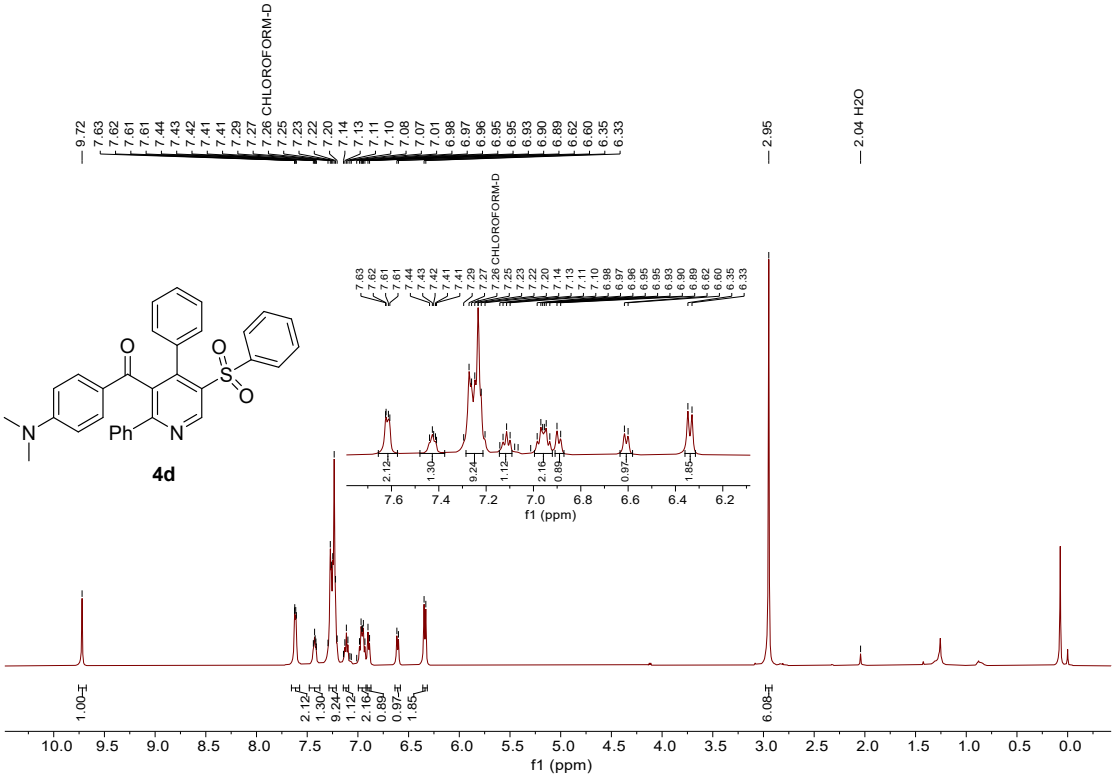
131.84
131.66
131.57
129.95
129.61
129.12
128.65
128.41
128.29
127.79
126.97
125.31
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.06
f1 (ppm)
4c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7.62
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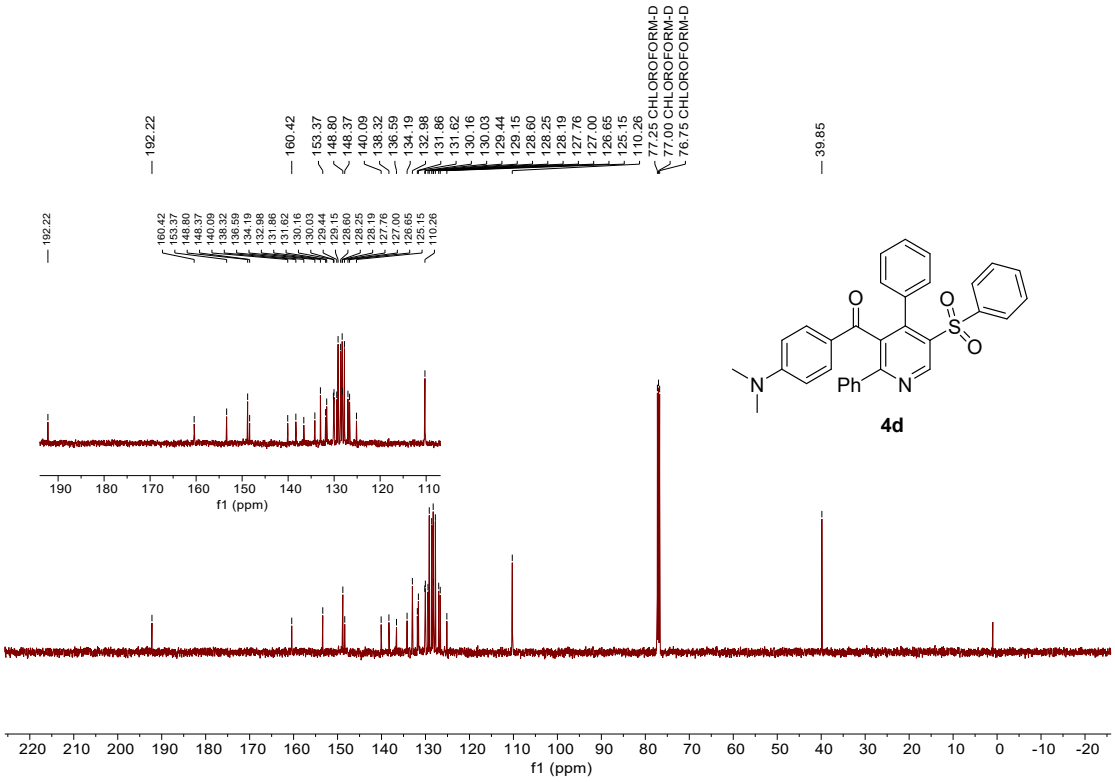
7.61
7.44
7.43
7.42
7.41
7.41
7.29
7.27
7.26 CHLOROFORM-D
7.25
7.23
7.22
7.20
7.14
7.13
7.11
7.10
7.08
7.07
7.01
6.98
6.97
6.96
6.95
6.95
6.93
6.90
6.89
6.62
6.60
6.35
6.33
2.95
2.04 H2O
1.00
2.12
1.30
9.24
1.12
2.16
0.89
0.97
1.85
6.08
f1 (ppm)
4d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138.32
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132.98
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131.62
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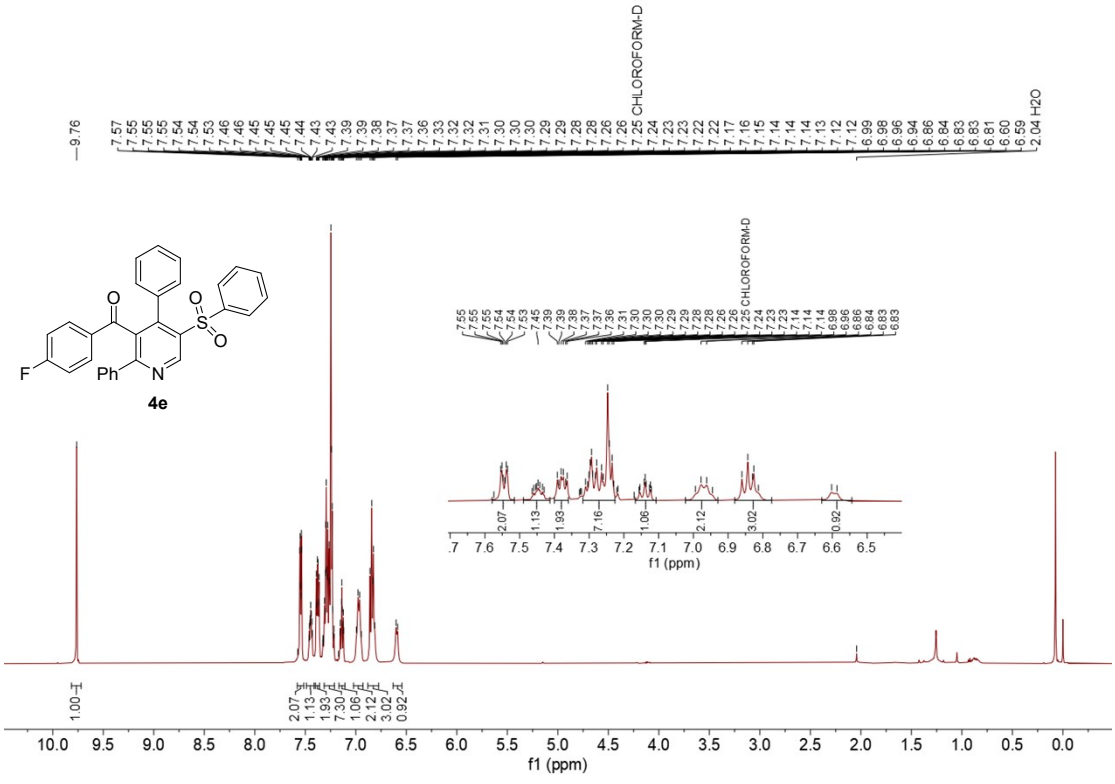
130.03
129.44
129.15
128.60
128.25
128.19
127.76
127.00
126.65
125.15
110.26
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
39.85
f1 (ppm)

4d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7.46
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7.45
7.45
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7.43
7.43
7.39
7.39
7.38
7.37
7.37
7.36
7.33
7.32
7.32
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.28
7.26
7.26
CHLOROFORM-D
7.25
7.24
7.23
7.23
7.22
7.22
7.17
7.16
7.15
7.14
7.14
7.14
7.13
7.12
7.12
6.99
6.98
6.96
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6.86
6.84
6.83
6.83
6.81
6.60
6.59
2.04 H2O
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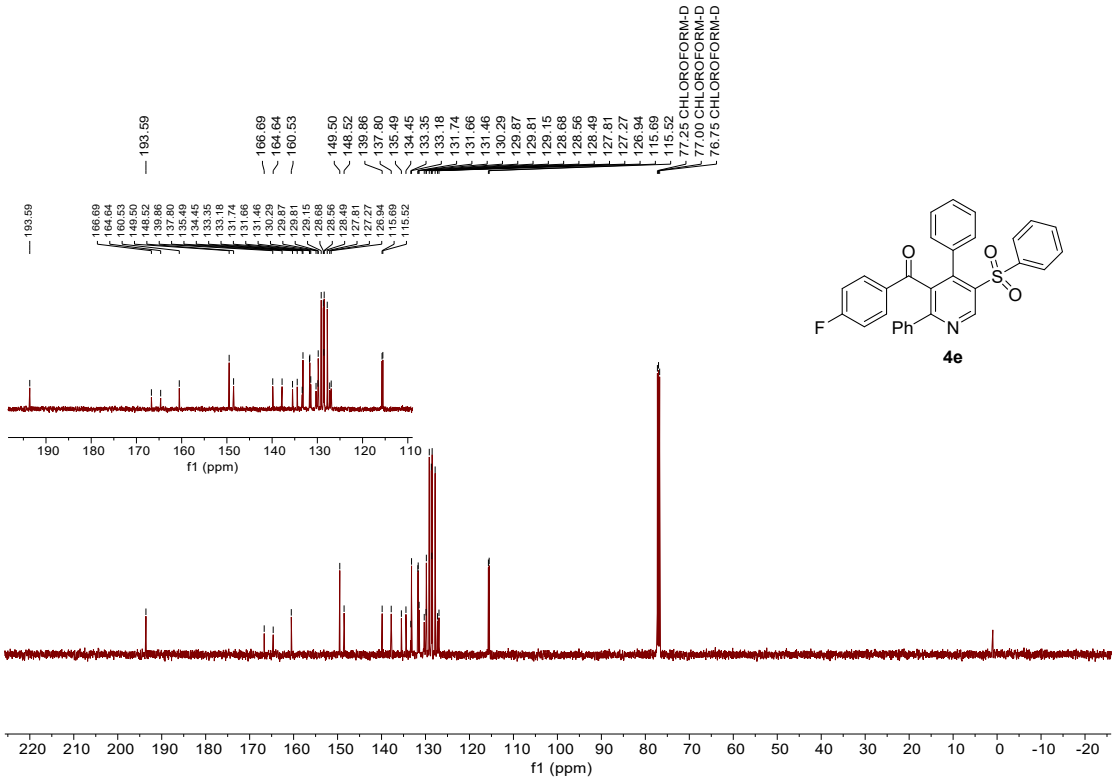
1.13
1.93
7.30
1.06
2.12
3.02
0.92
f1 (ppm)

4e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137.80
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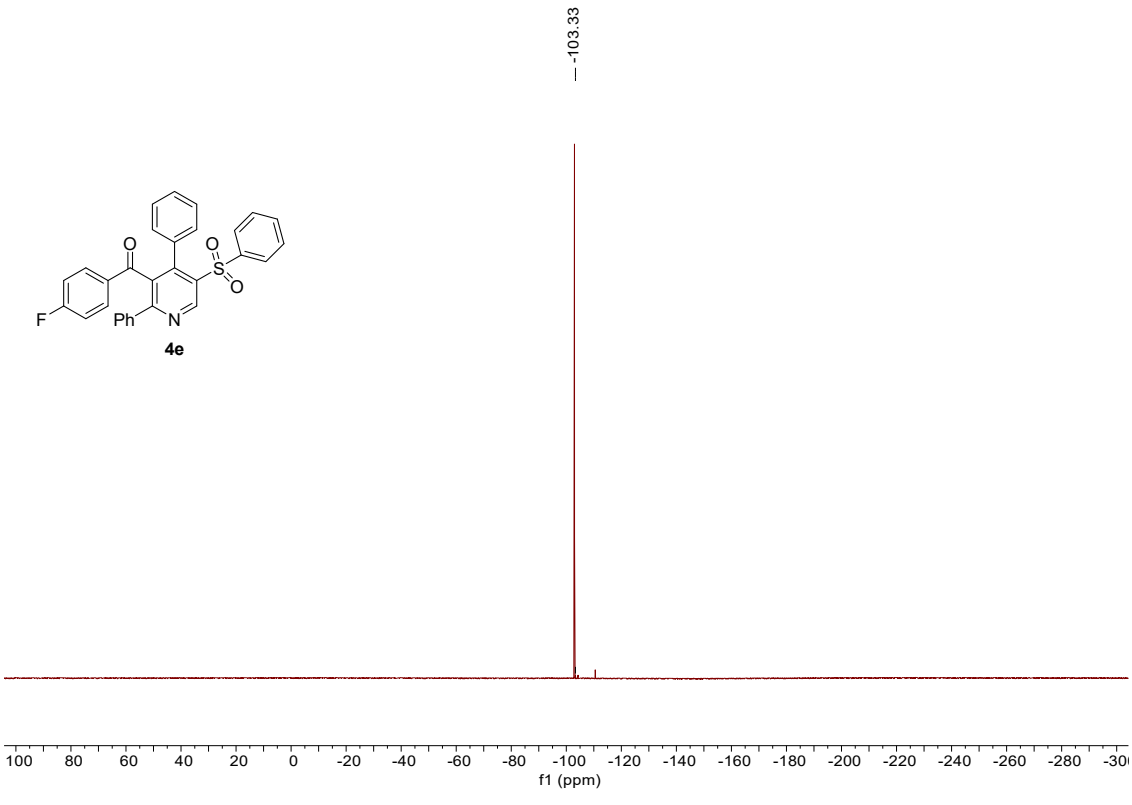
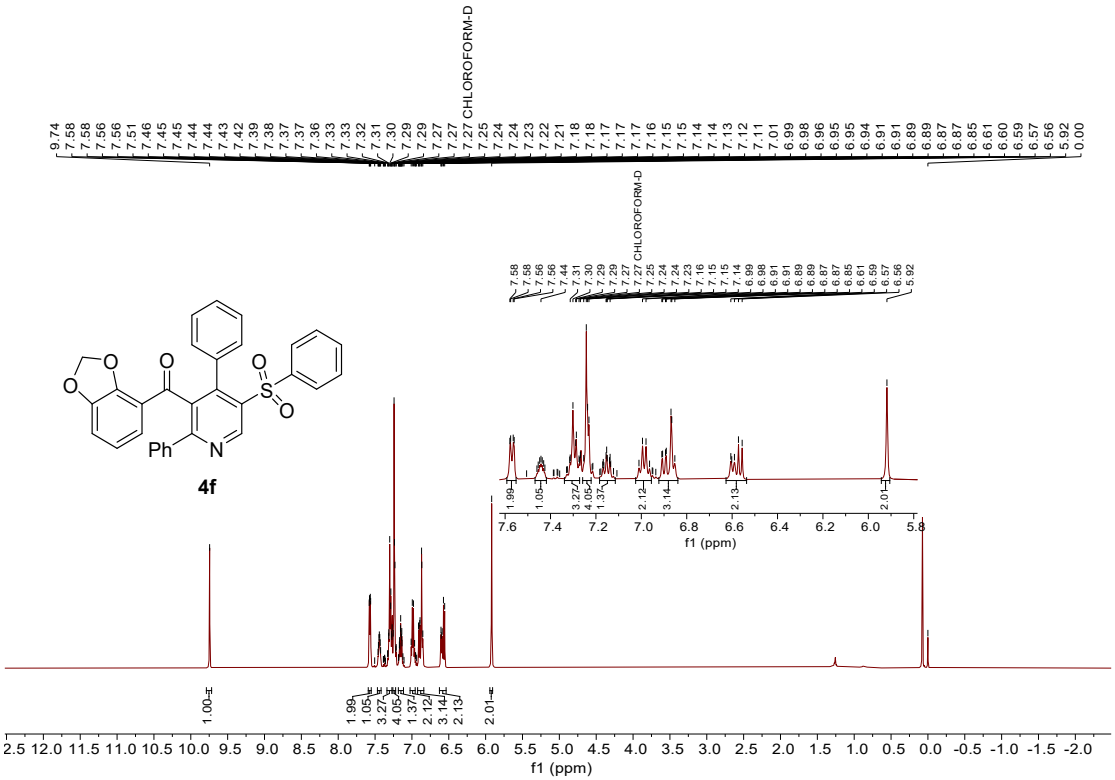
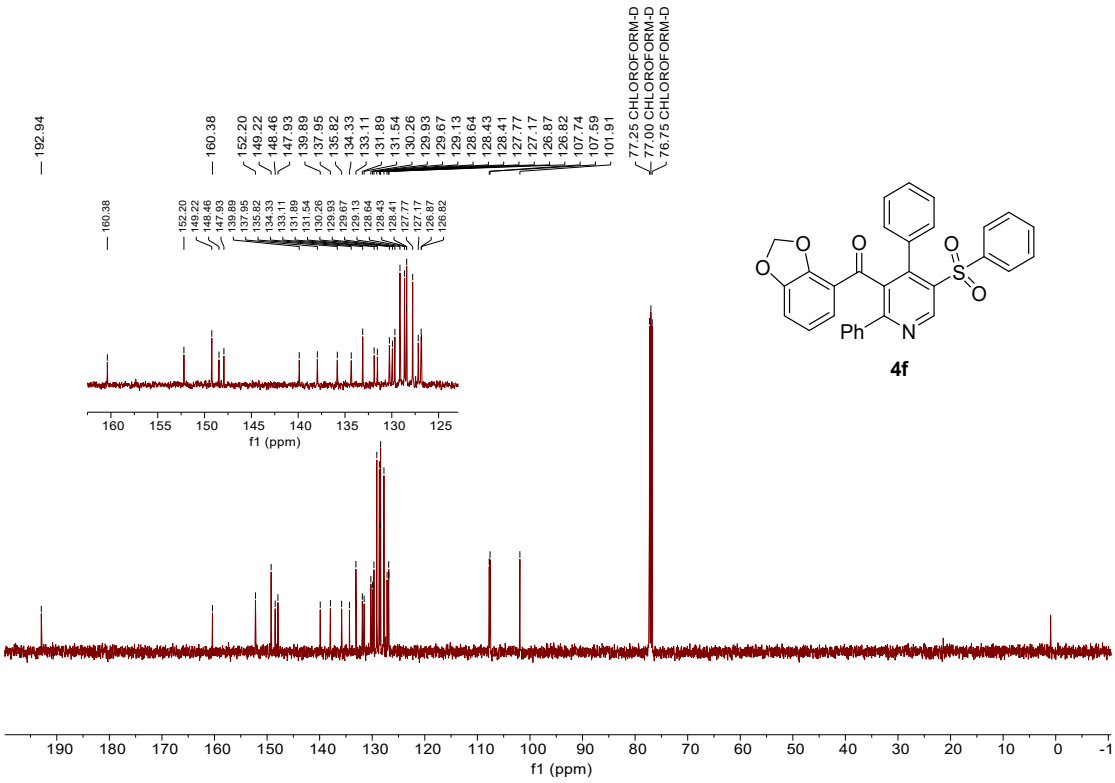
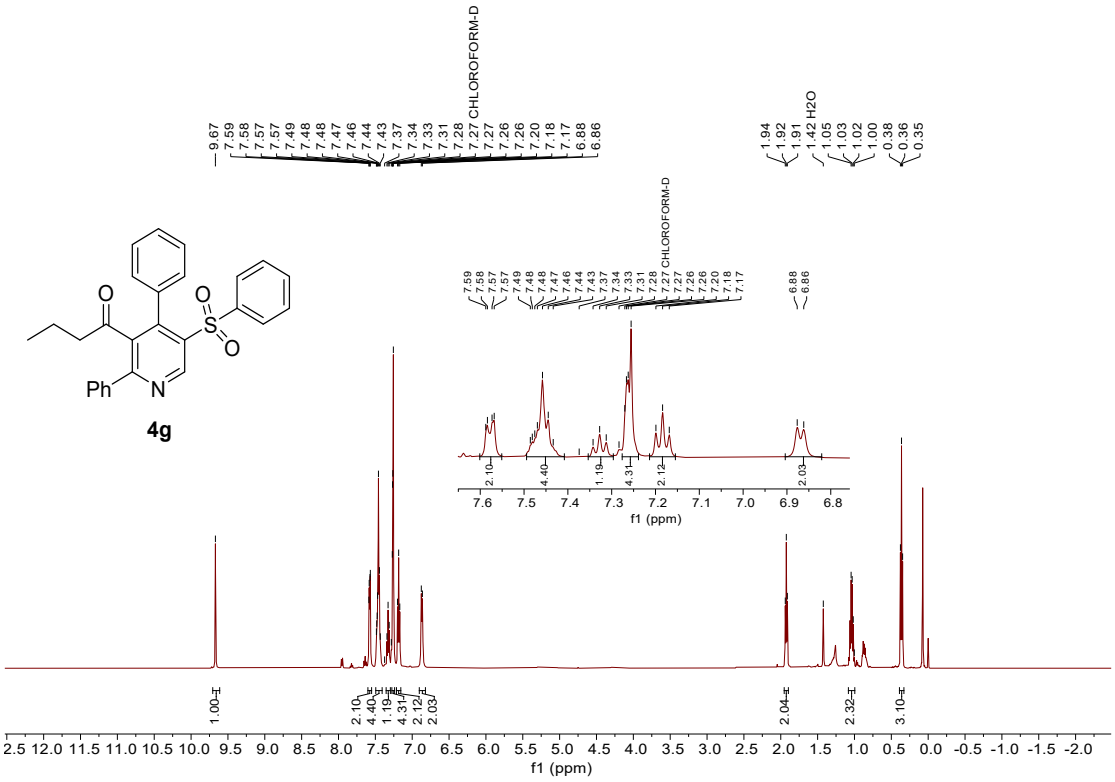
134.45
133.35
133.18
131.74
131.66
131.46
130.29
129.87
129.81
129.15
128.68
128.56
128.49
127.81
127.27
126.94
115.69
115.52
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
f1 (ppm)
4e


-103.33
f1 (ppm)
4e


4f
f1 (ppm)


4f
f1 (ppm)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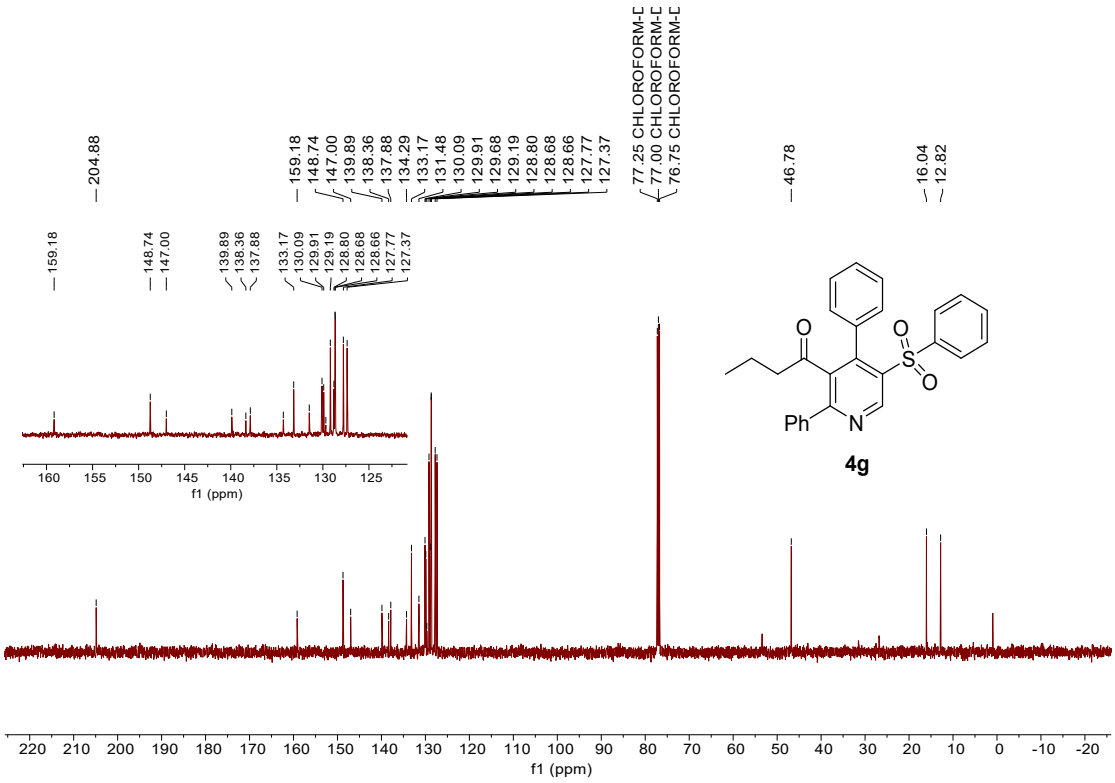
7.43
7.37
7.34
7.33
7.31
7.28
7.27 CHLOROFORM-D
7.27
7.26
7.26
7.20
7.18
7.17
6.88
6.86
1.94
1.92
1.91
1.42 H2O
1.05
1.03
1.02
1.00
0.38
0.36
0.35
O
O
S
O
Ph
N
4g
1.00
2.10
4.40
1.19
4.31
2.12
2.03
2.04
2.32
3.10
f1 (ppm)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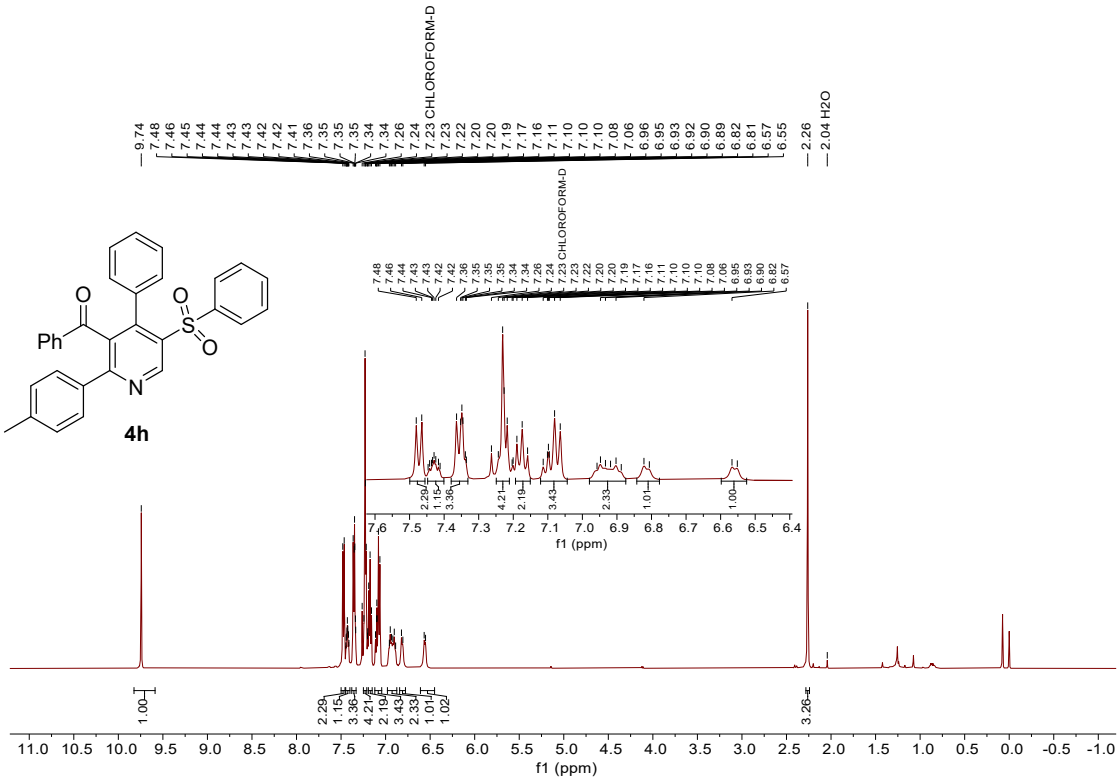
130.09
129.91
129.68
129.19
128.80
128.68
128.66
127.77
127.37
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
46.78
16.04
12.82
O
O
S
O
Ph
N
4g
f1 (ppm)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7.48
7.46
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7.44
7.43
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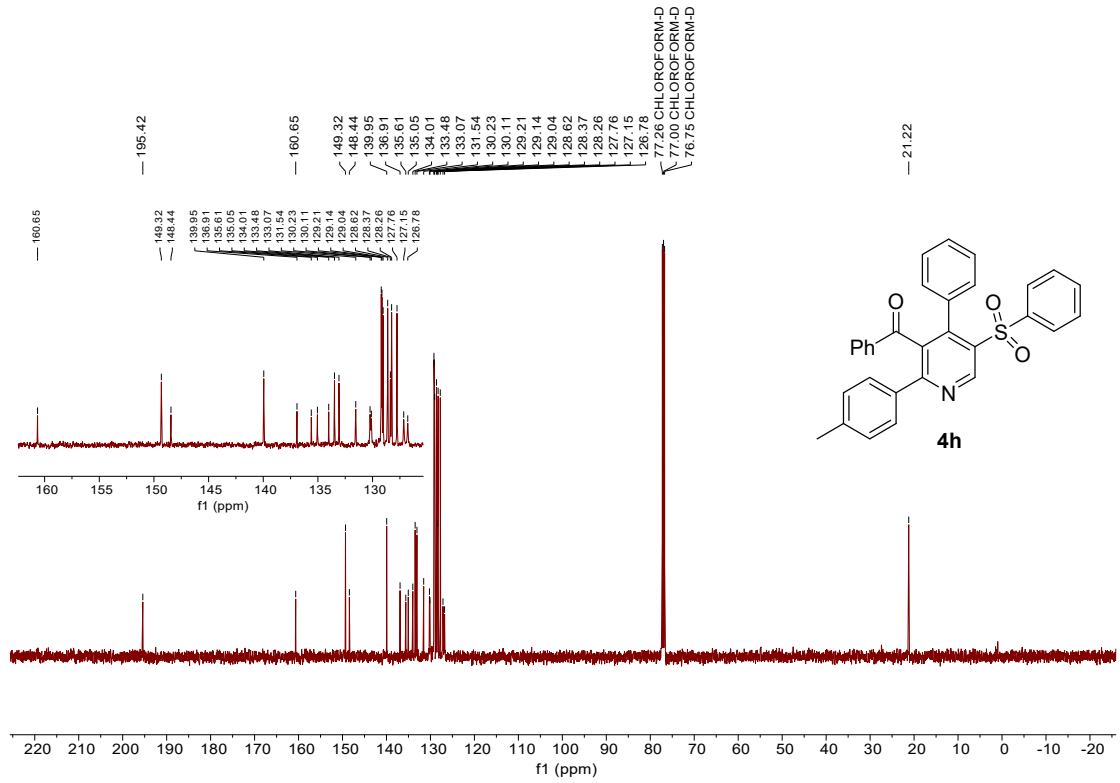
7.42
7.42
7.41
7.36
7.35
7.35
7.35
7.34
7.34
7.26
7.24
7.23 CHLOROFORM-D
7.23
7.22
7.20
7.20
7.19
7.17
7.16
7.11
7.10
7.10
7.10
7.08
7.06
6.96
6.95
6.93
6.92
6.90
6.89
6.82
6.81
6.57
6.55
2.26
2.04 H2O
Ph
O
O
S
O
N
4h
1.00
2.29
1.15
3.36
4.21
2.19
3.43
2.33
1.01
1.02
3.26
f1 (ppm)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139.95
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133.07
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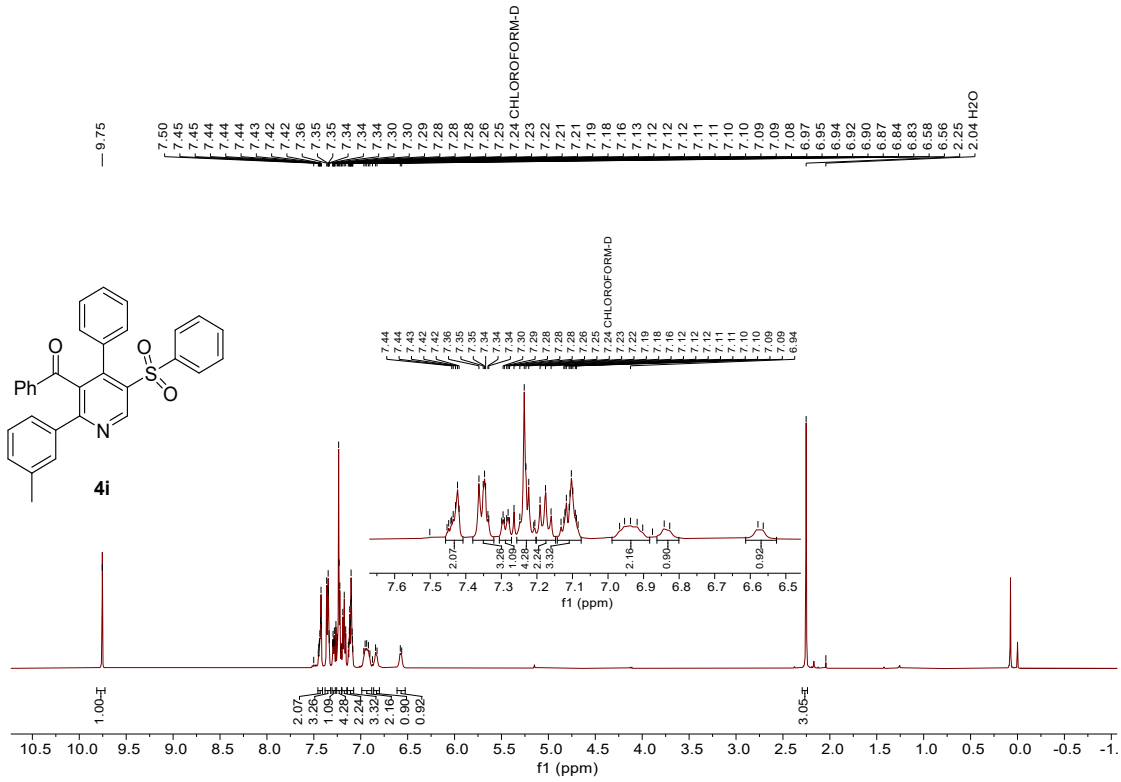
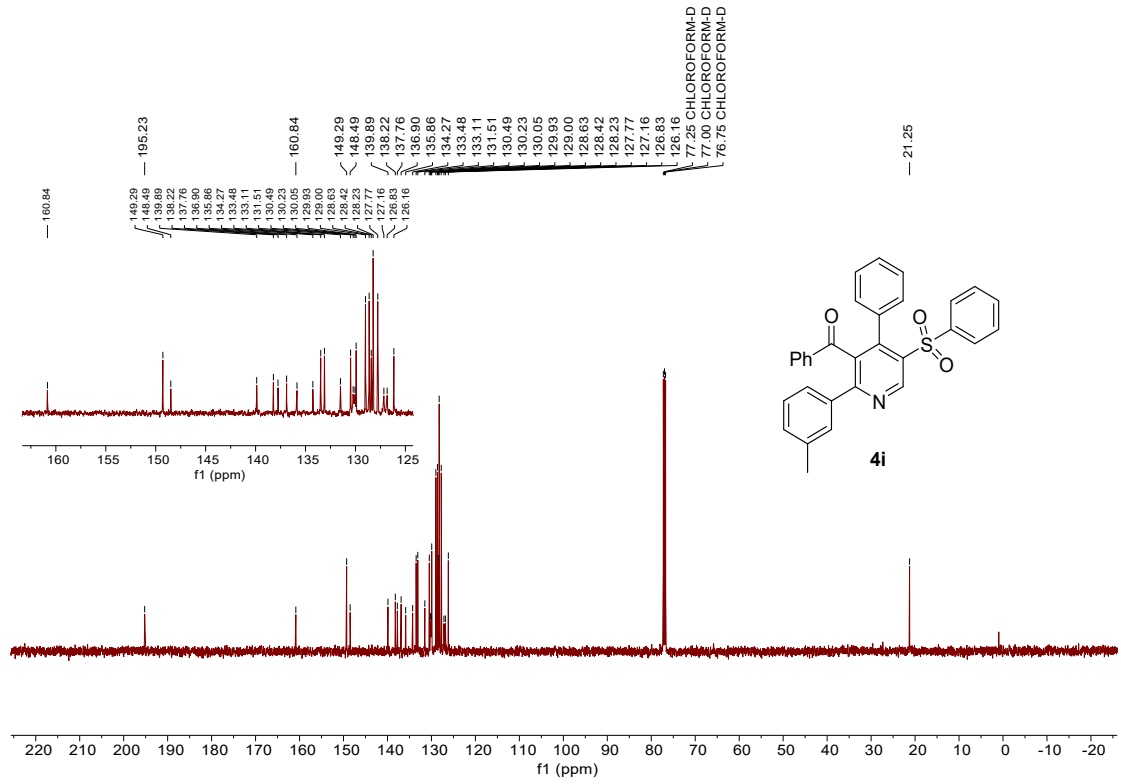
130.23
130.11
129.21
129.14
129.04
128.62
128.37
128.26
127.76
127.15
126.78
77.26 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.22
Ph
O
O
S
O
N
4h
f1 (ppm)


9.75
7.50 7.45 7.45 7.44 7.44 7.44 7.43 7.42 7.42 7.36 7.35 7.35 7.34 7.34 7.34 7.30 7.30 7.29 7.28 7.28 7.28 7.26 7.25 7.24 CHLOROFORM-D 7.23 7.22 7.21 7.21 7.19 7.18 7.16 7.13 7.12 7.12 7.12 7.11 7.11 7.10 7.10 7.09 7.09 7.08 6.97 6.95 6.94 6.92 6.90 6.87 6.84 6.83 6.58 6.56 2.25 2.04 H2O
Ph
O
O
S
O
N
4i
1.00
2.07
3.26
1.09
4.28
2.24
3.32
2.16
0.90
0.92
3.05
f1 (ppm)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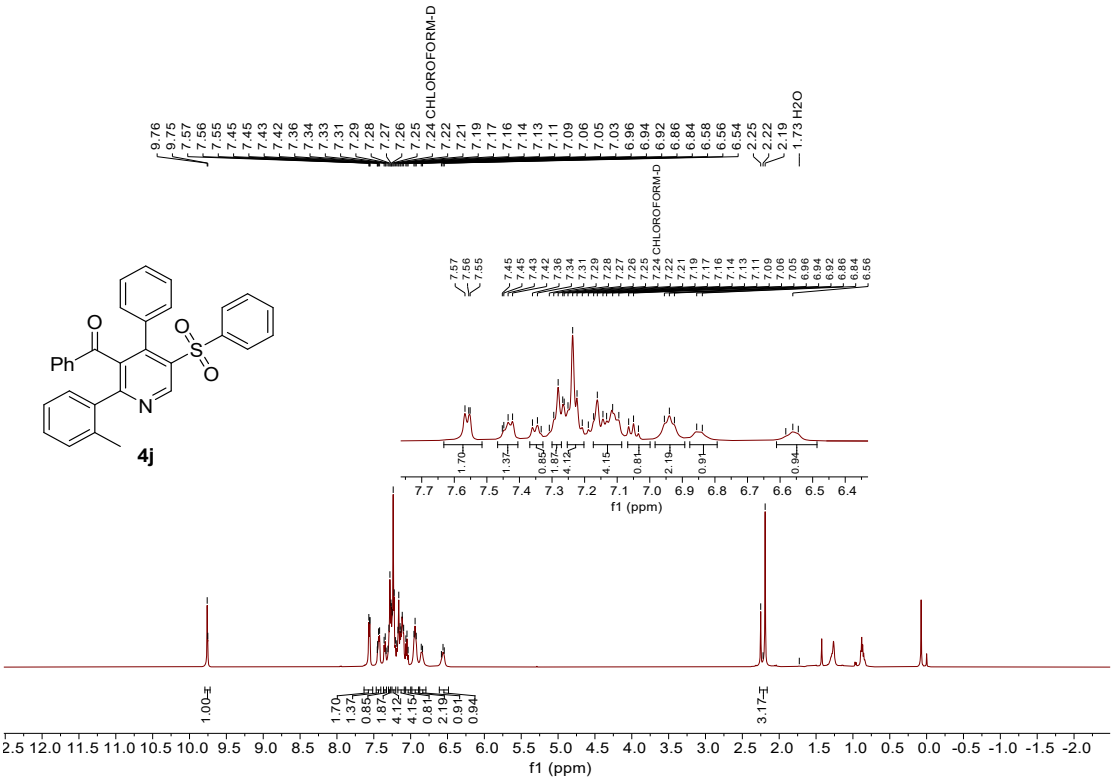
195.23
149.29 148.49 139.89 138.22 137.76 136.90 135.86 134.27 133.48 133.11 131.51 130.49 130.23 130.05 129.93 129.00 128.63 128.42 128.23 127.77 127.16 126.83 126.16
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.25
Ph
O
O
S
O
N
4i
f1 (ppm)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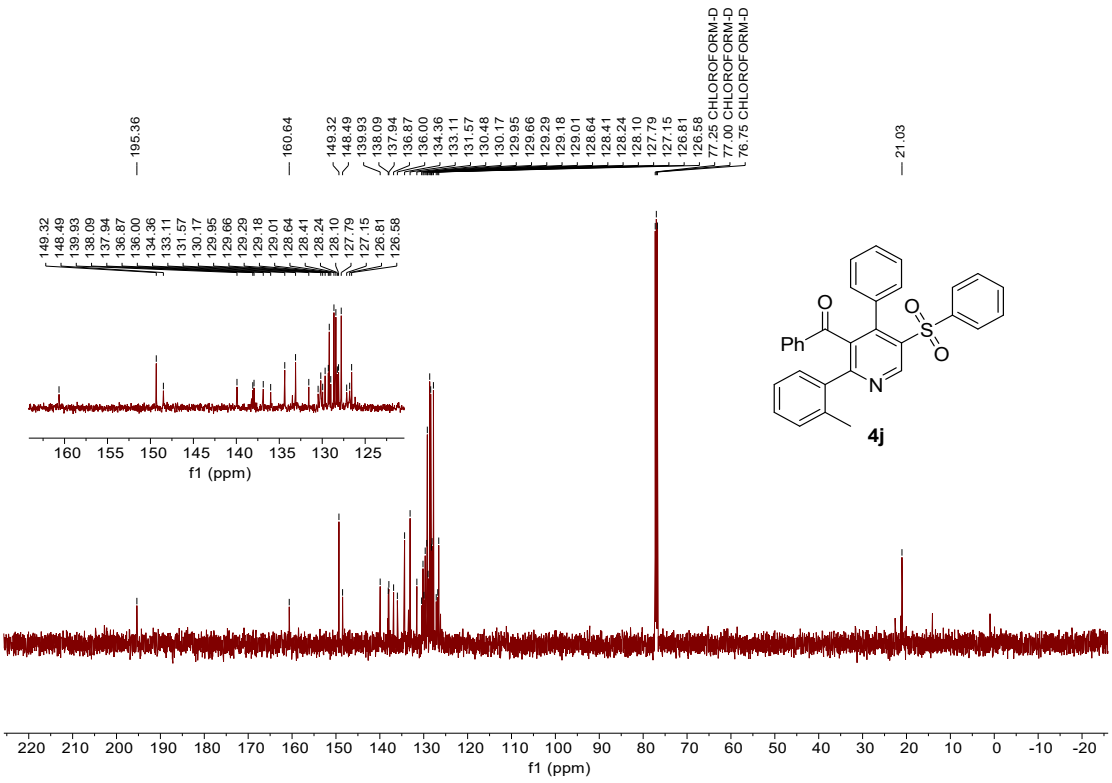
7.29
7.28
7.27
7.26
7.25
7.24 CHLOROFORM-D
7.22
7.21
7.19
7.17
7.16
7.14
7.13
7.11
7.09
7.06
7.05
6.96
6.94
6.92
6.86
6.84
6.58
6.56
6.54
2.25
2.22
2.19
1.73 H2O
Ph
O
S
N
4j
1.00
1.70
1.37
0.85
1.87
4.12
4.15
0.81
2.19
0.91
0.94
3.17
f1 (ppm)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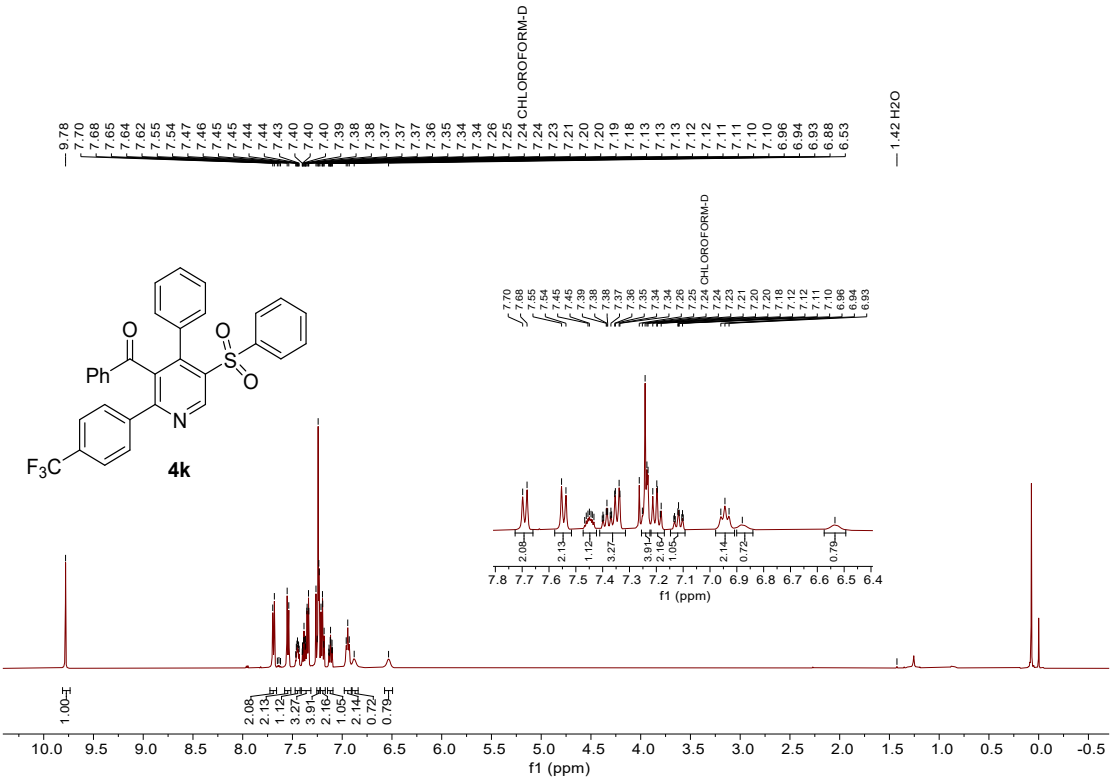
129.95
129.66
129.29
129.18
129.01
128.64
128.41
128.24
128.10
127.79
127.15
126.81
126.58
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.03
Ph
O
S
N
4j
f1 (ppm)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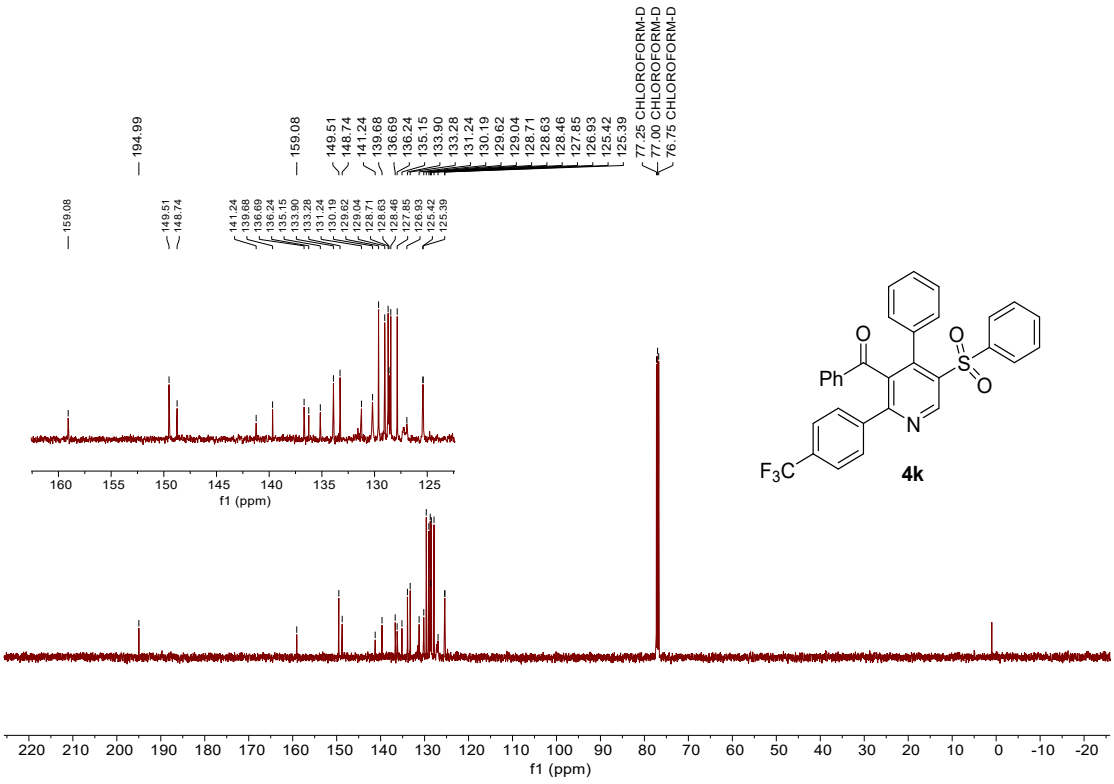
1.42 H2O
4k
1.00 2.08 2.13 1.12 3.27 3.91 2.16 1.05 2.14 0.72 0.79
f1 (ppm)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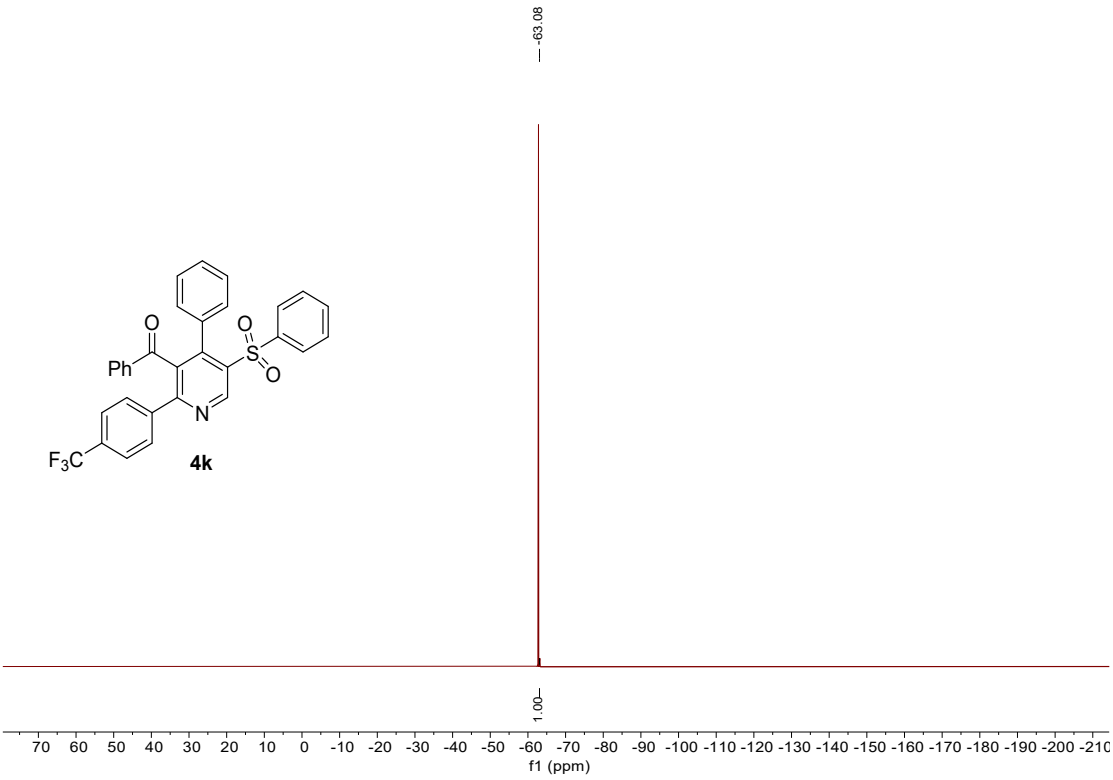
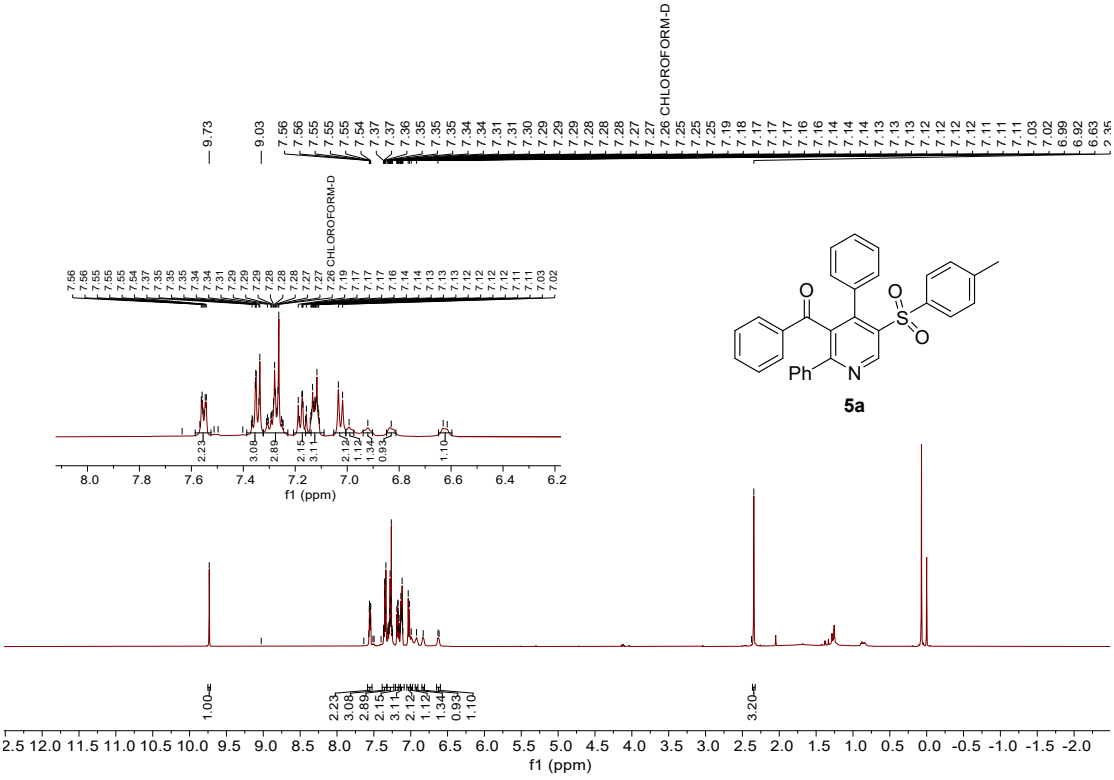
159.08
149.51 148.74 141.24 139.68 136.69 136.24 135.15 133.90 133.28 131.24 130.19 129.62 129.04 128.71 128.63 128.46 127.85 126.93 125.42 125.39
77.25 CHLOROFORM-D 77.00 CHLOROFORM-D 76.75 CHLOROFORM-D
4k
f1 (ppm)


-63.08
1.00
f1 (ppm)

O
Ph
O
S
O
N
F3C

4k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7.56
7.55
7.54
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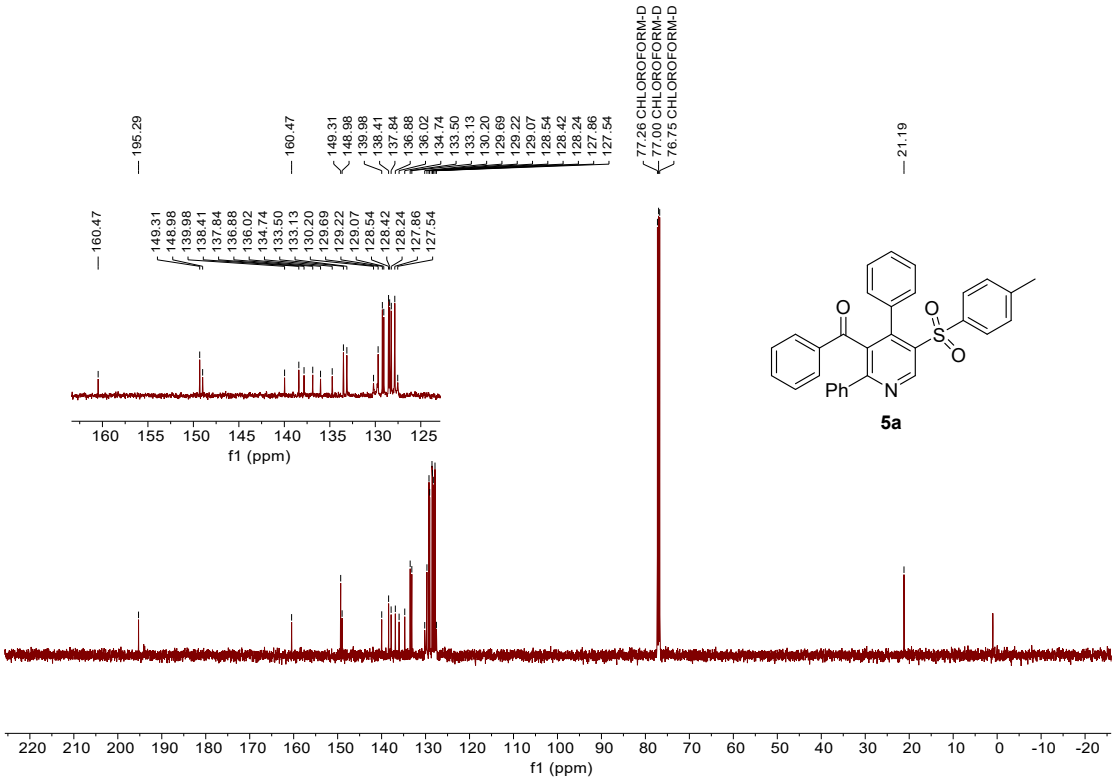
7.35
7.34
7.31
7.30
7.29
7.28
7.27
7.26 CHLOROFORM-D
7.25
7.19
7.18
7.17
7.16
7.14
7.13
7.12
7.11
7.03
7.02
6.99
6.92
6.83
2.23
3.08
2.89
2.15
3.11
2.12
1.12
1.34
0.93
1.10
3.20
f1 (ppm)

O
O
S
O
Ph
N

5a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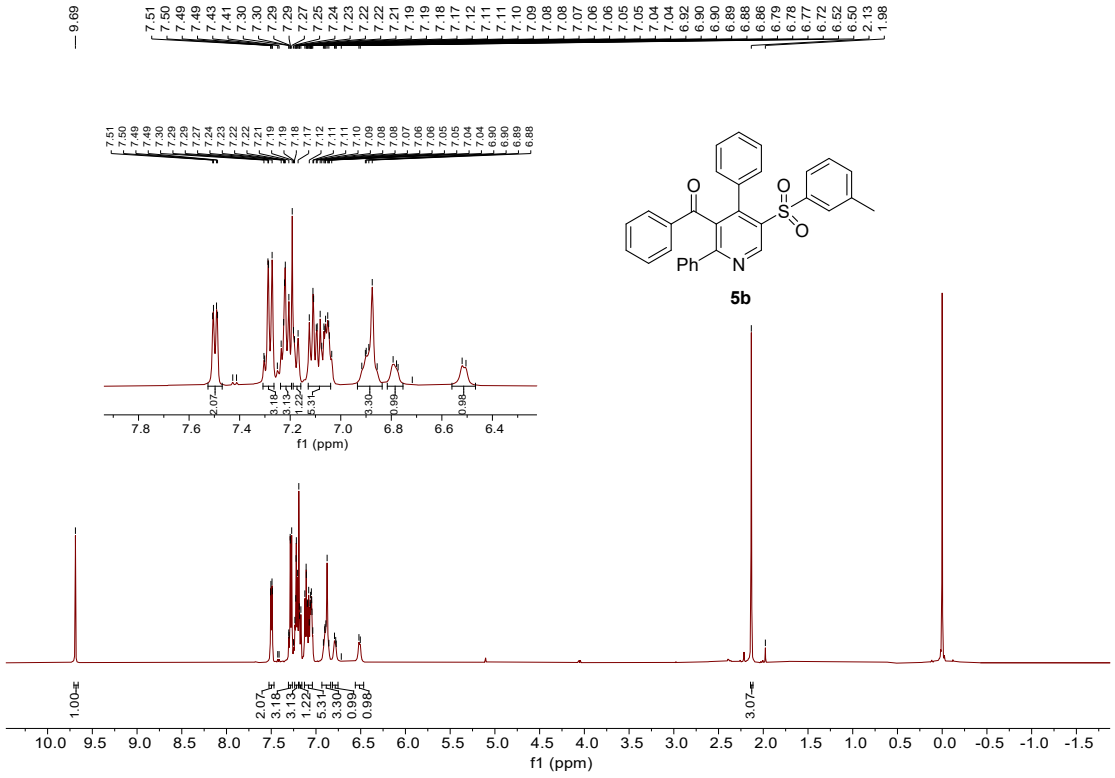
136.88
136.02
134.74
133.50
133.13
130.20
129.69
129.22
129.07
128.54
128.42
128.24
127.86
127.54
77.26 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.19
f1 (ppm)
5a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7.30
7.29
7.29
7.27
7.25
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7.23
7.22
7.22
7.21
7.19
7.19
7.18
7.17
7.12
7.11
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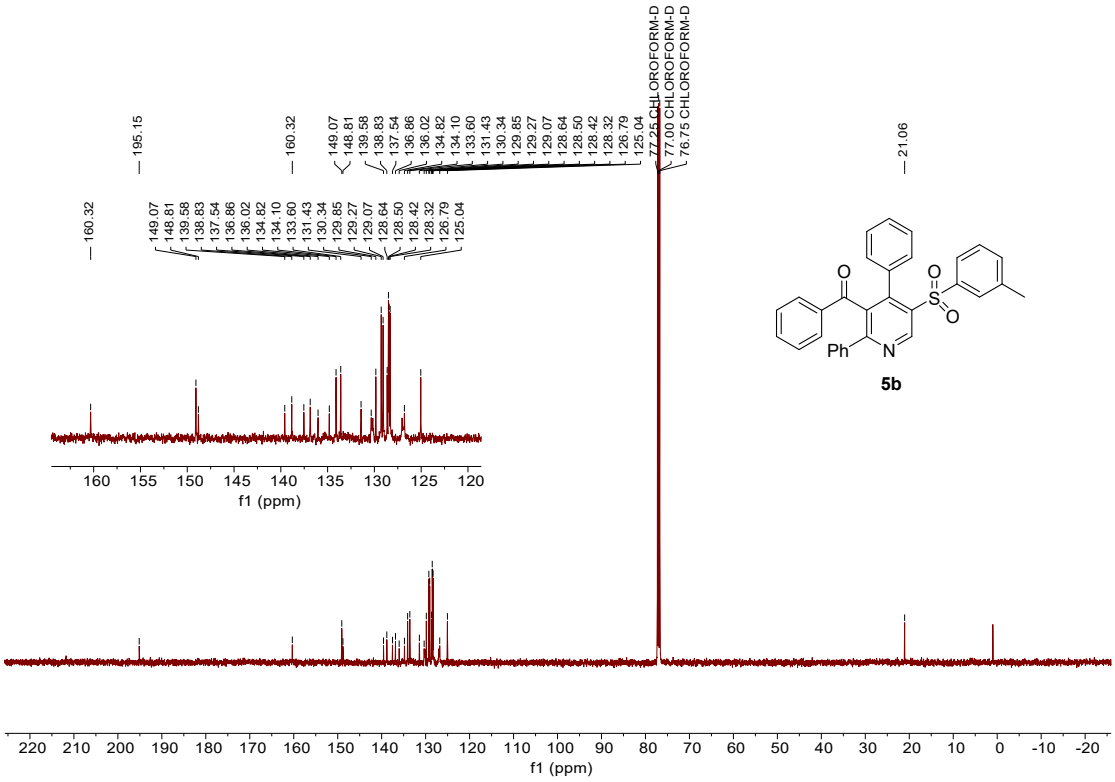
7.10
7.09
7.08
7.08
7.07
7.06
7.06
7.05
7.05
7.04
7.04
6.92
6.90
6.90
6.89
6.88
6.86
6.79
6.78
6.77
6.72
6.52
6.50
2.13
1.98
1.00
2.07
3.18
3.13
1.22
5.31
3.30
0.99
0.98
3.07
f1 (ppm)
5b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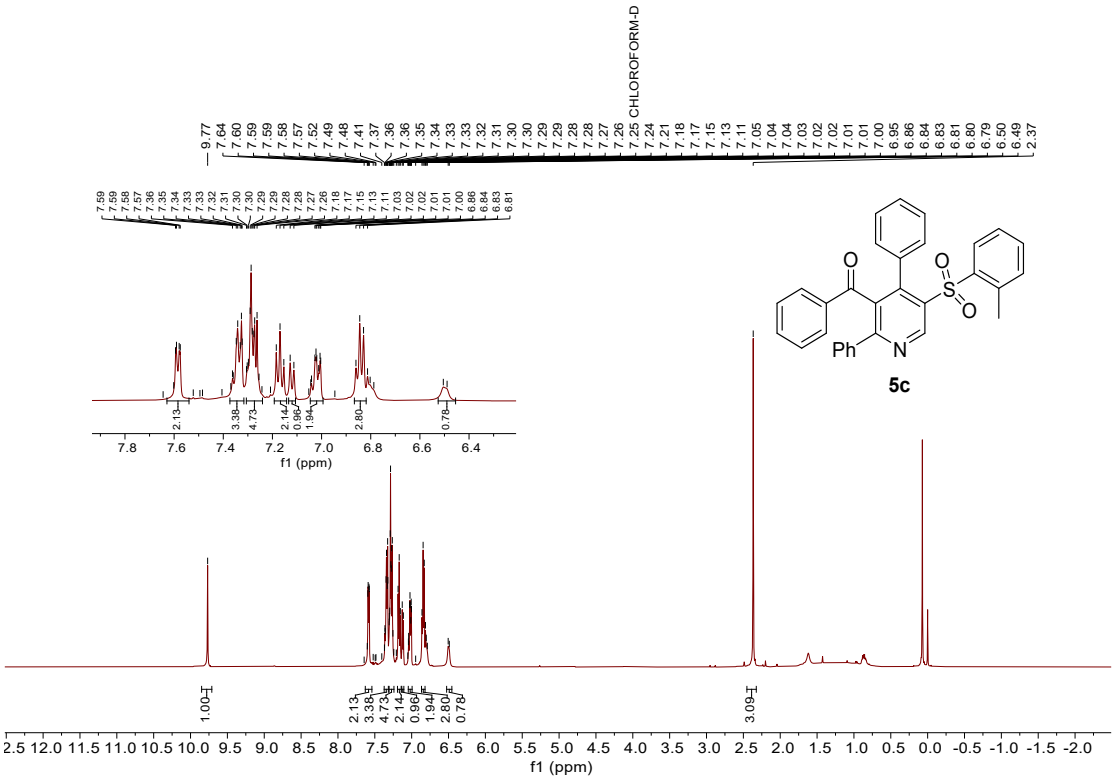
136.86
136.02
134.82
134.10
133.60
131.43
130.34
129.85
129.27
129.07
128.64
128.50
128.42
128.32
126.79
125.04
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
21.06
f1 (ppm)
Ph
N
O
S
5b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7.36
7.35
7.34
7.33
7.33
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.26
7.25 CHLOROFORM-D
7.24
7.21
7.18
7.17
7.15
7.13
7.11
7.05
7.04
7.04
7.03
7.02
7.02
7.01
7.01
7.00
6.95
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6.83
6.81
6.80
6.79
6.50
6.49
2.37
1.00
2.13
3.38
4.73
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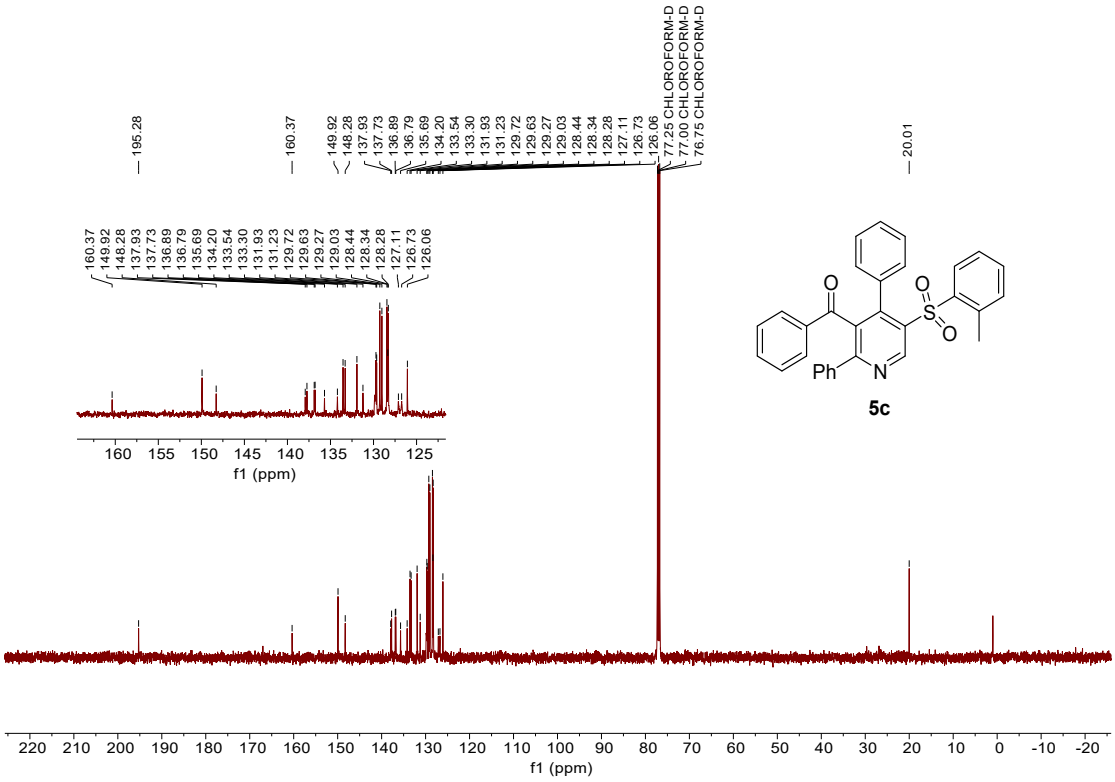
0.96
1.94
2.80
0.78
3.09
f1 (ppm)
Ph
N
O
S
5c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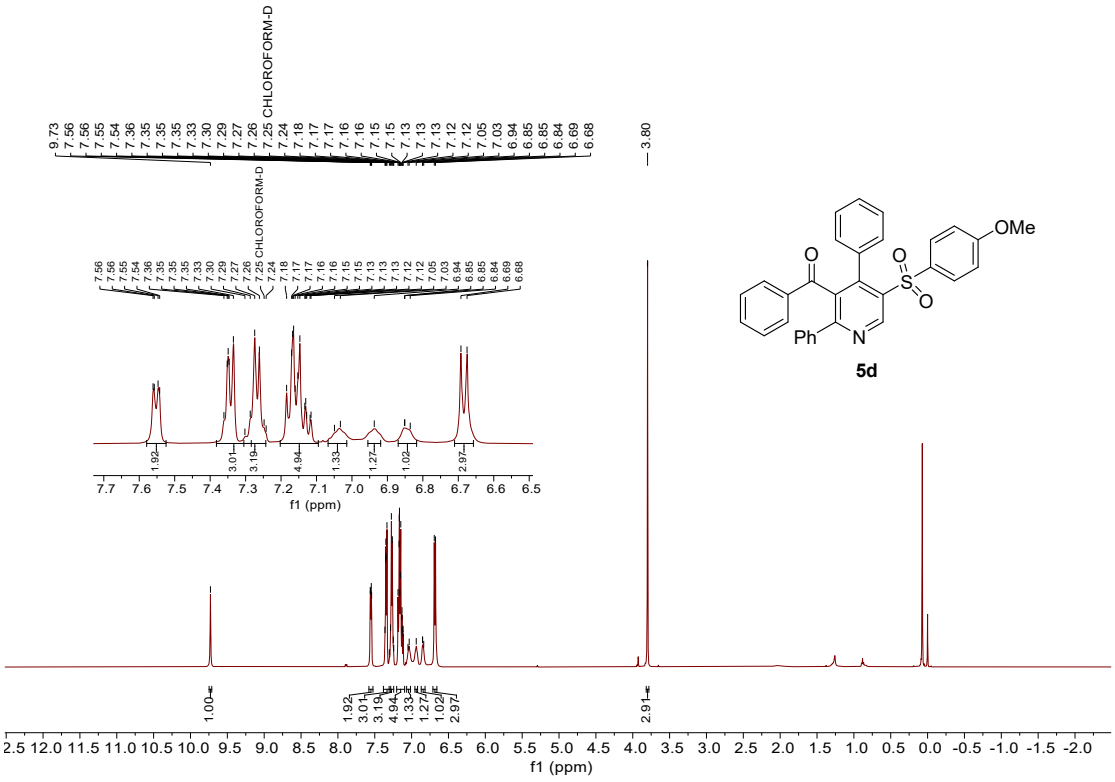
133.30
131.93
131.23
129.72
129.63
129.27
129.03
128.44
128.34
128.28
127.11
126.73
126.06
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
20.01
f1 (ppm)
f1 (ppm)
O
O
S
O
Ph
N

5c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7.56
7.55
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7.35
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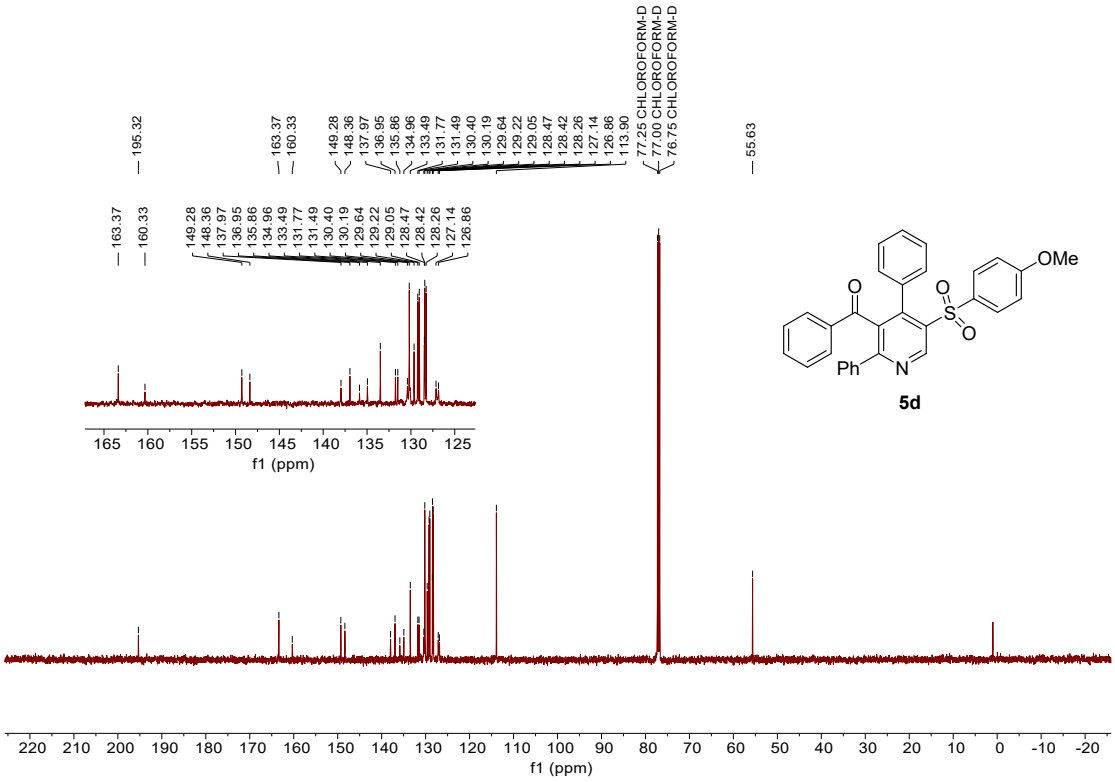
7.33
7.30
7.29
7.27
7.26
7.25 CHLOROFORM-D
7.24
7.18
7.17
7.17
7.16
7.16
7.15
7.15
7.13
7.13
7.13
7.12
7.12
7.05
7.03
6.94
6.85
6.85
6.84
6.69
6.68
3.80
1.92
3.01
3.19
4.94
1.33
1.27
1.02
2.97
f1 (ppm)
1.00
1.92
3.01
3.19
4.94
1.33
1.27
1.02
2.97
2.91
f1 (ppm)
O
O
S
O
Ph
N
OMe

5d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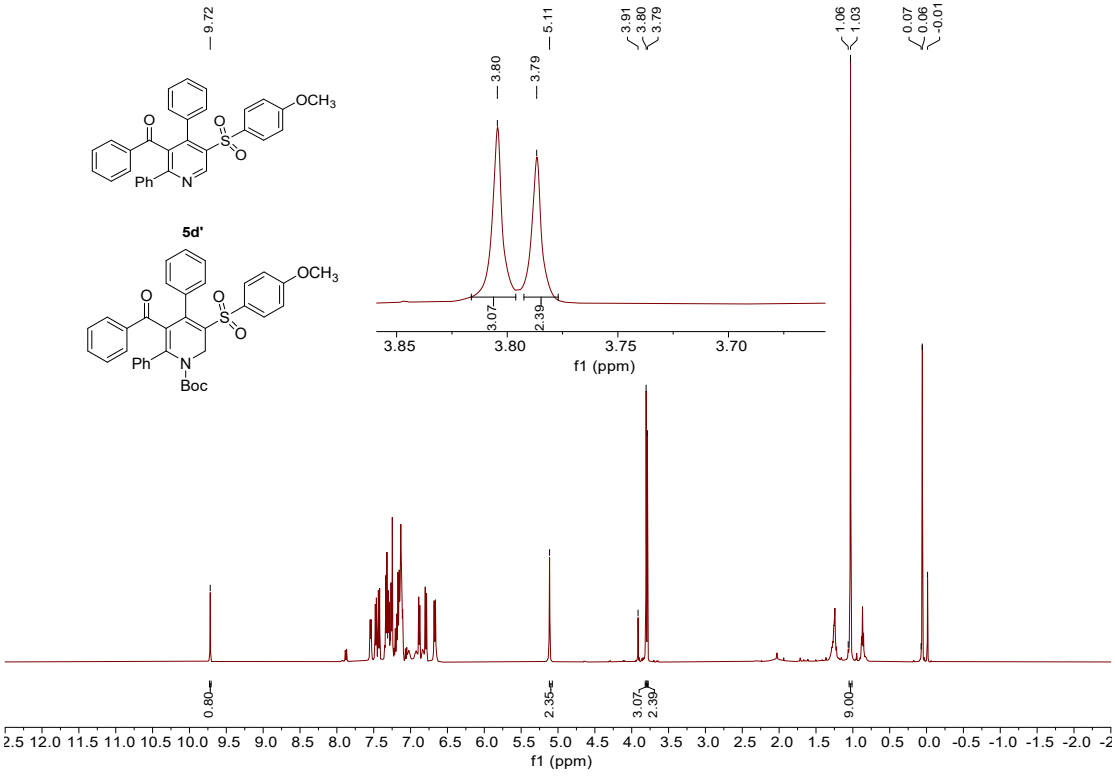
133.49
131.77
131.49
130.40
130.19
129.64
129.22
129.05
128.47
128.42
128.26
127.14
126.86
113.90
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
55.63
OMe
O
S
Ph
N
5d
f1 (ppm)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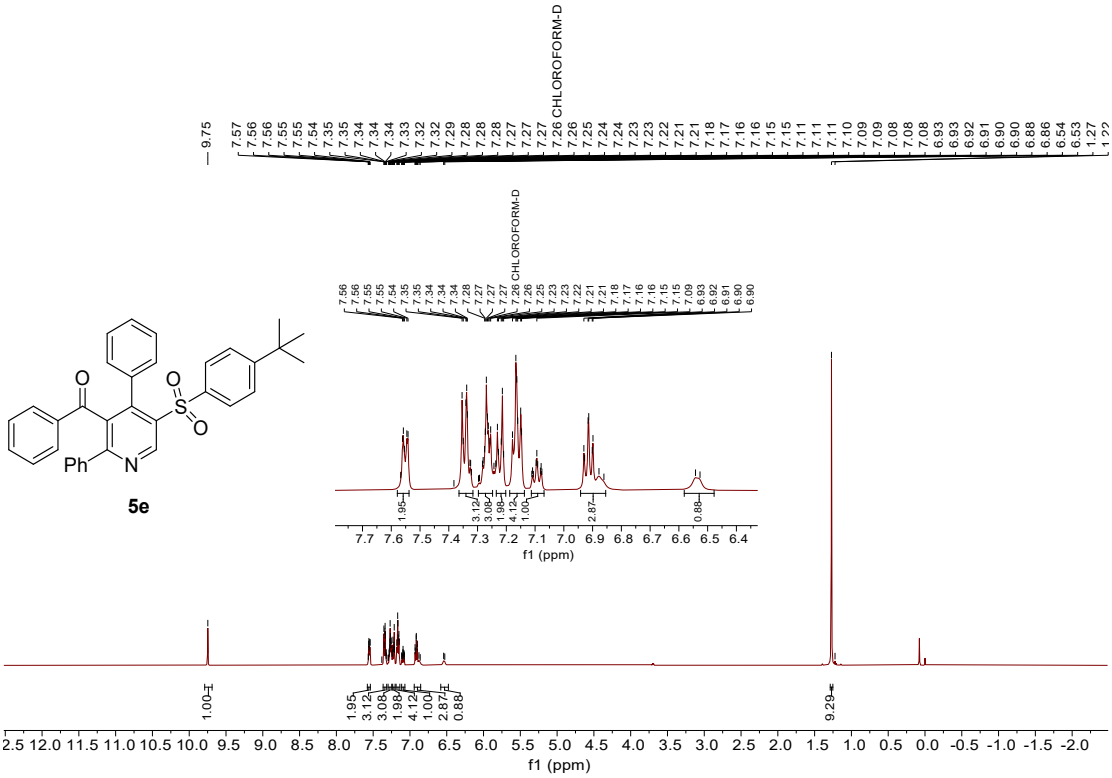
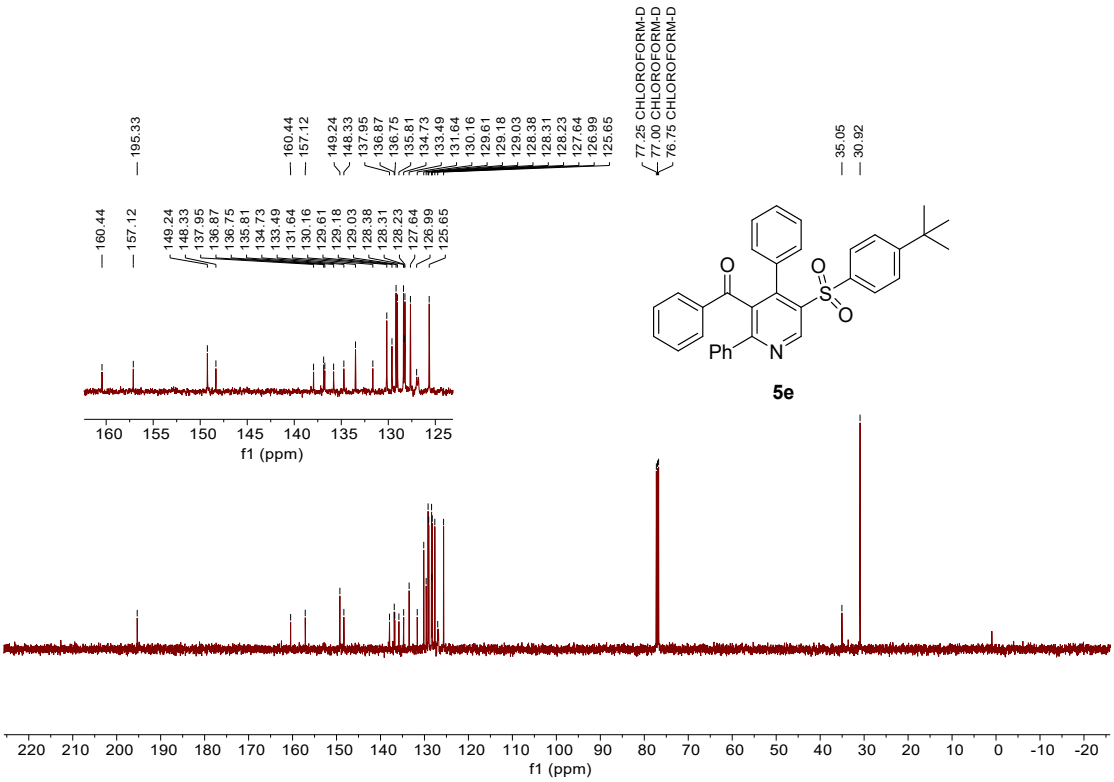
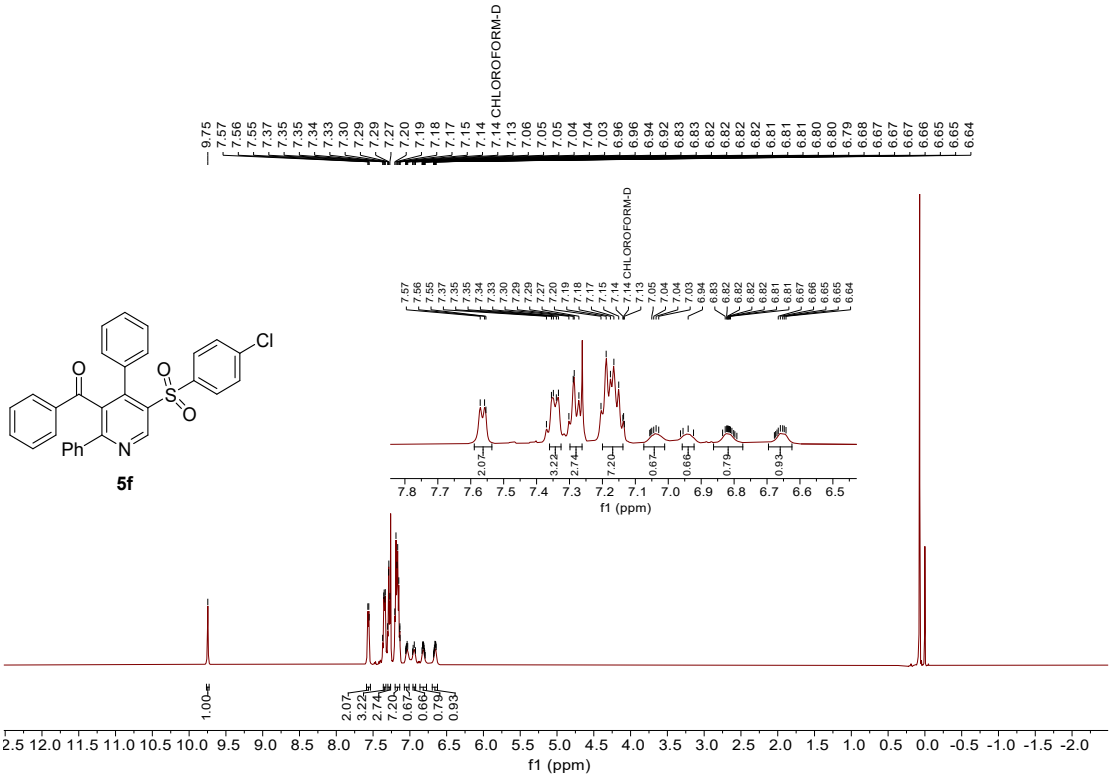
5.11
3.91
3.80
3.79
1.06
1.03
0.07
0.06
-0.01
OCH3
Ph
N
Boc
5d'
3.07
2.39
0.80
2.35
9.00
f1 (ppm)


CHLOROFORM-D
5e
f1 (ppm)


CHLOROFORM-D
5e
f1 (ppm)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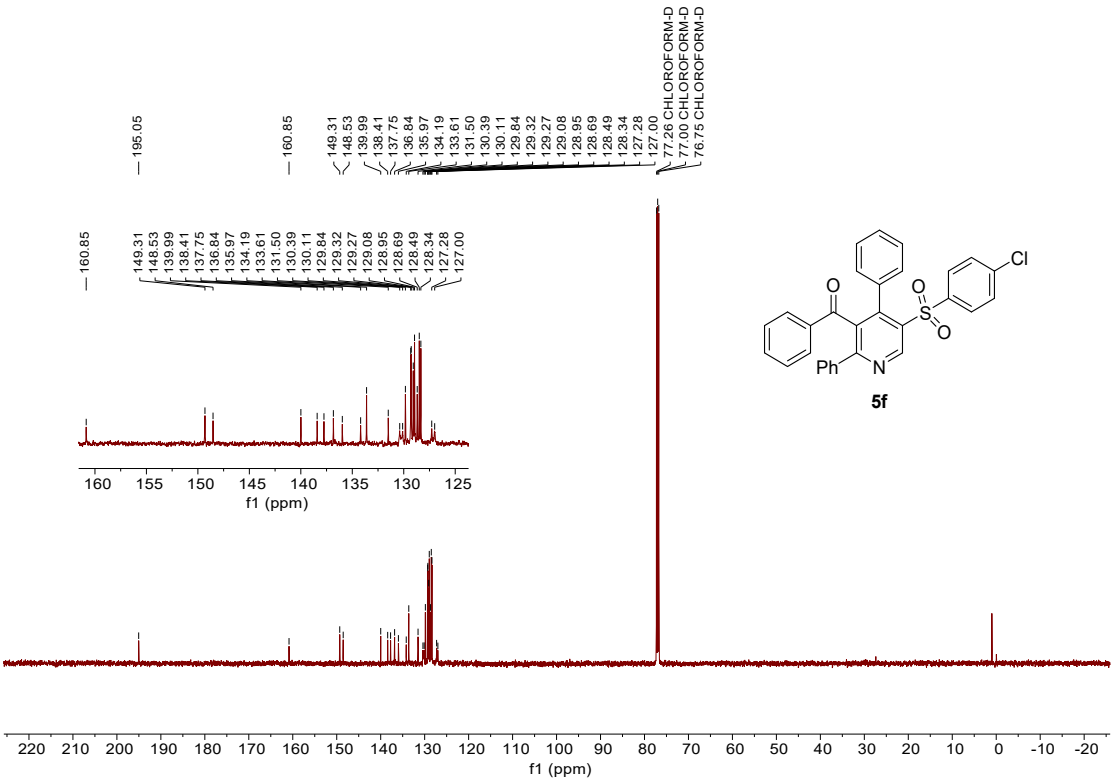
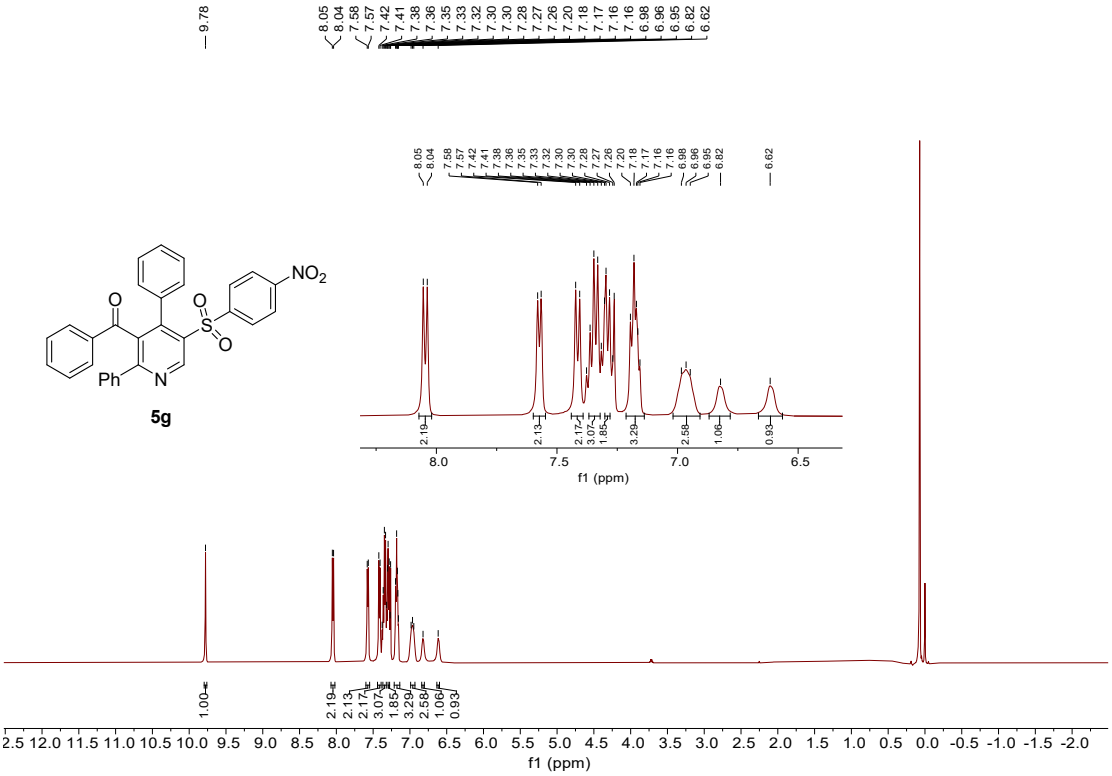
1.00 2.07 3.22 2.74 7.20 0.67 0.66 0.79 0.93
f1 (ppm)
5f


195.05 160.85 149.31 148.53 139.99 138.41 137.75 136.84 135.97 134.19 133.61 131.50 130.39 130.11 129.84 129.32 129.27 129.08 128.95 128.69 128.49 128.34 127.28 127.00 77.26 CHLOROFORM-D 77.00 CHLOROFORM-D 76.75 CHLOROFORM-D
f1 (ppm)
5f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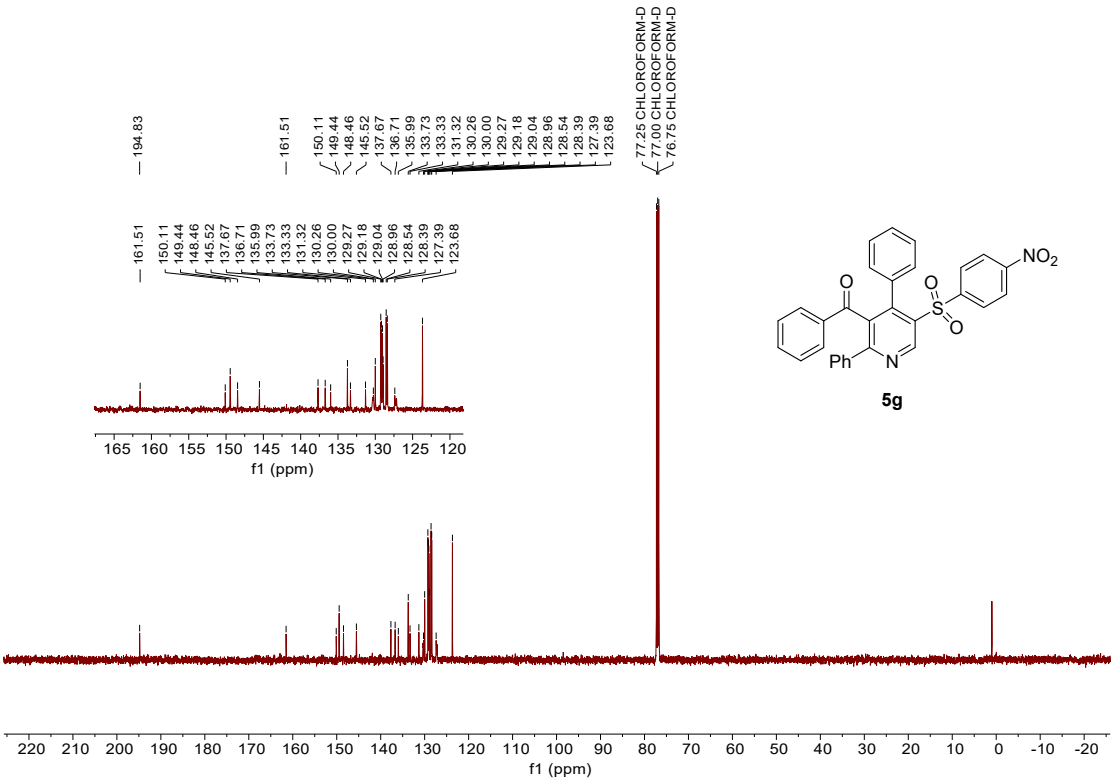
7.32
7.30
7.30
7.28
7.27
7.26
7.20
7.18
7.17
7.16
7.16
6.98
6.96
6.95
6.82
6.62
NO2
O
O
S
O
Ph
N
5g
2.19
2.13
2.17
3.07
1.85
3.29
2.58
1.06
0.93
8.0
7.5
7.0
6.5
f1 (ppm)
1.00
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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145.52
137.67
136.71
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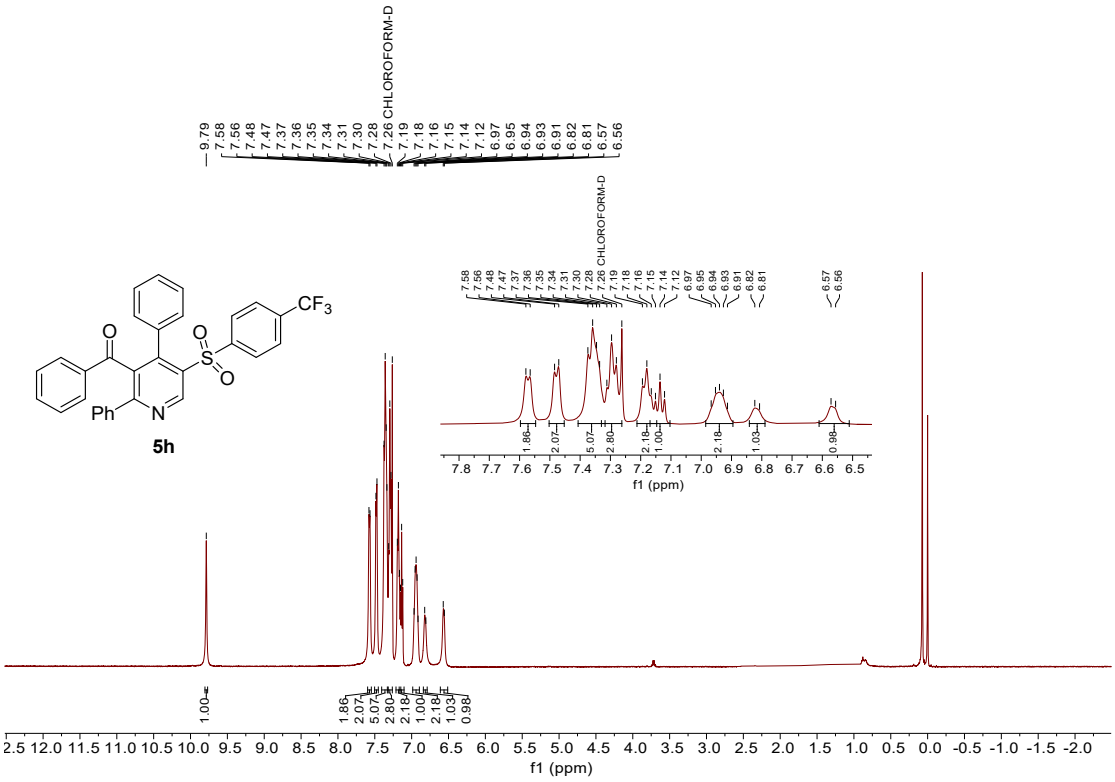
133.73
133.33
131.32
130.26
130.00
129.27
129.18
129.04
128.96
128.54
128.39
127.39
123.68
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
NO2
O
O
S
O
Ph
N
5g
165 160 155 150 145 140 135 130 125 120
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.37
7.36
7.35
7.34
7.31
7.30
7.28
7.26 CHLOROFORM-D
7.19
7.18
7.16
7.15
7.14
7.12
6.97
6.95
6.94
6.93
6.91
6.82
6.81
6.57
6.56
CF3
O
S
O
O
Ph
N
5h
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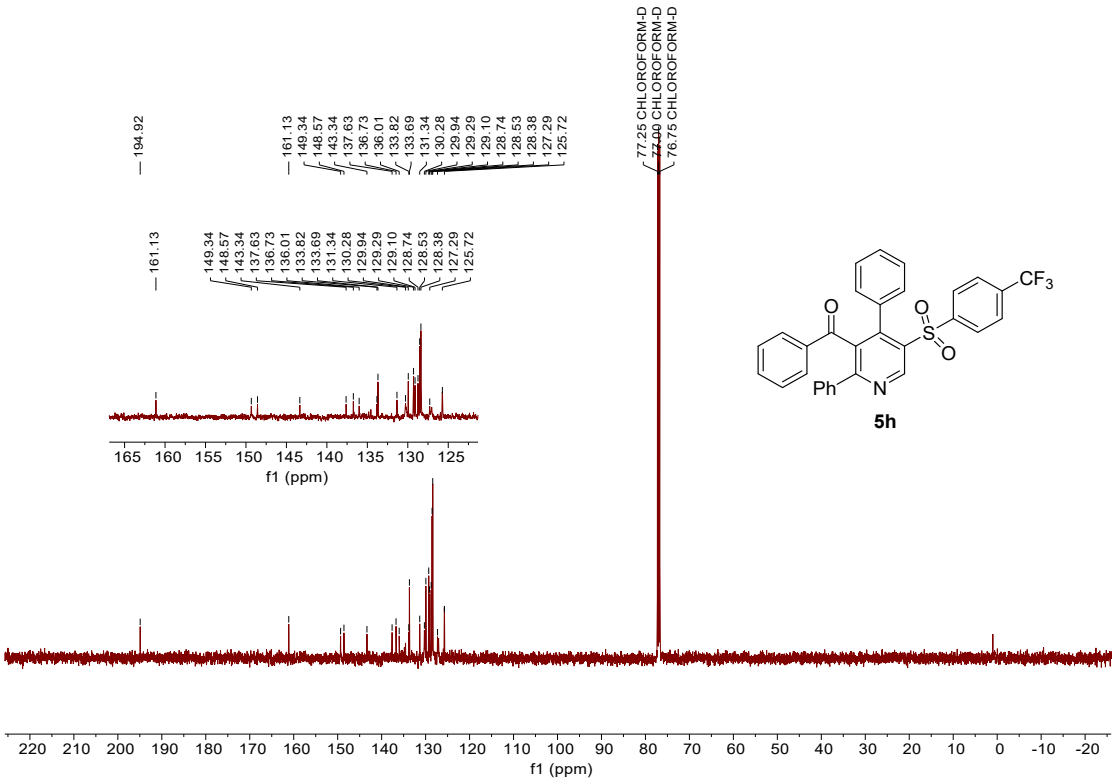
2.07
5.07
2.80
2.18
1.00
2.18
1.03
0.98
f1 (ppm)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133.69
131.34
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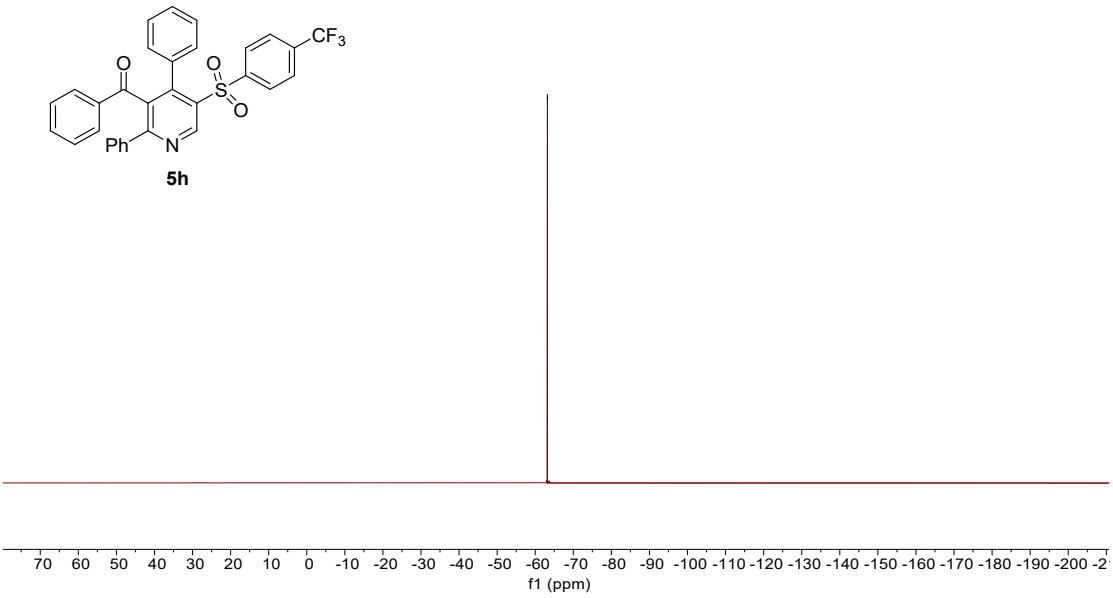
129.94
129.29
129.10
128.74
128.53
128.38
127.29
125.72
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
CF3
O
S
O
O
Ph
N
5h
f1 (ppm)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CF3
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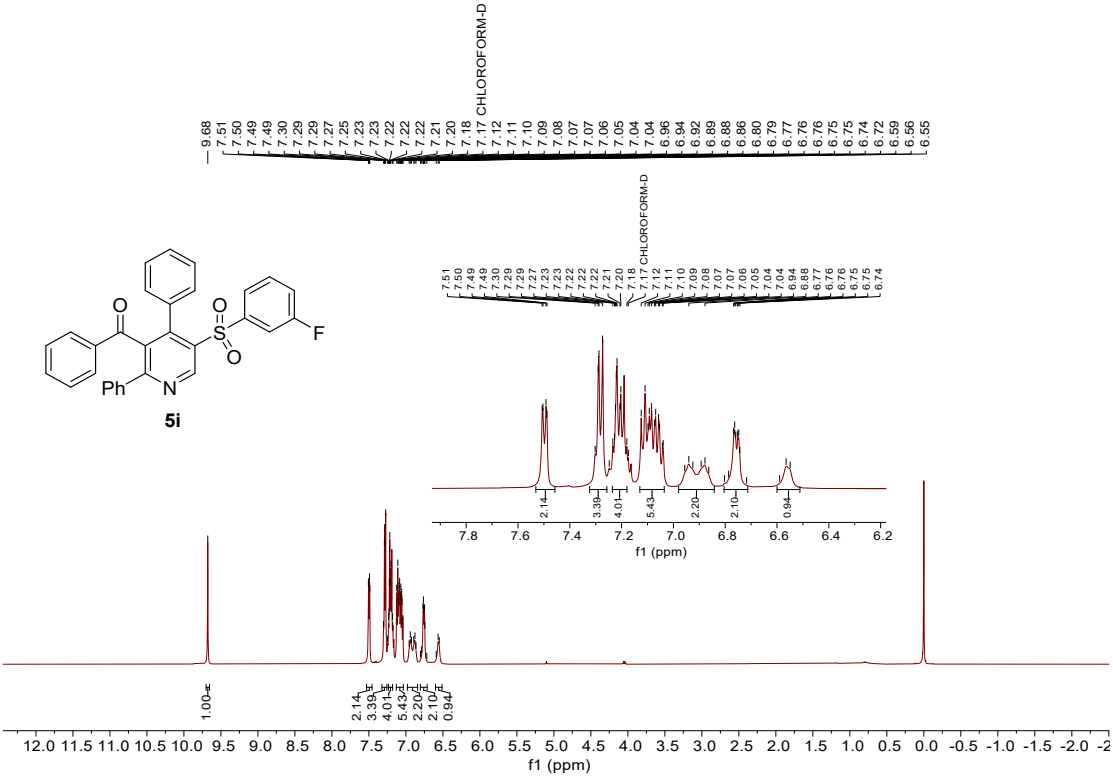
Ph
N
5h
f1 (ppm)


CHLOROFORM-D
CHLOROFORM-D
F
O
O
S
O
Ph
N
5i
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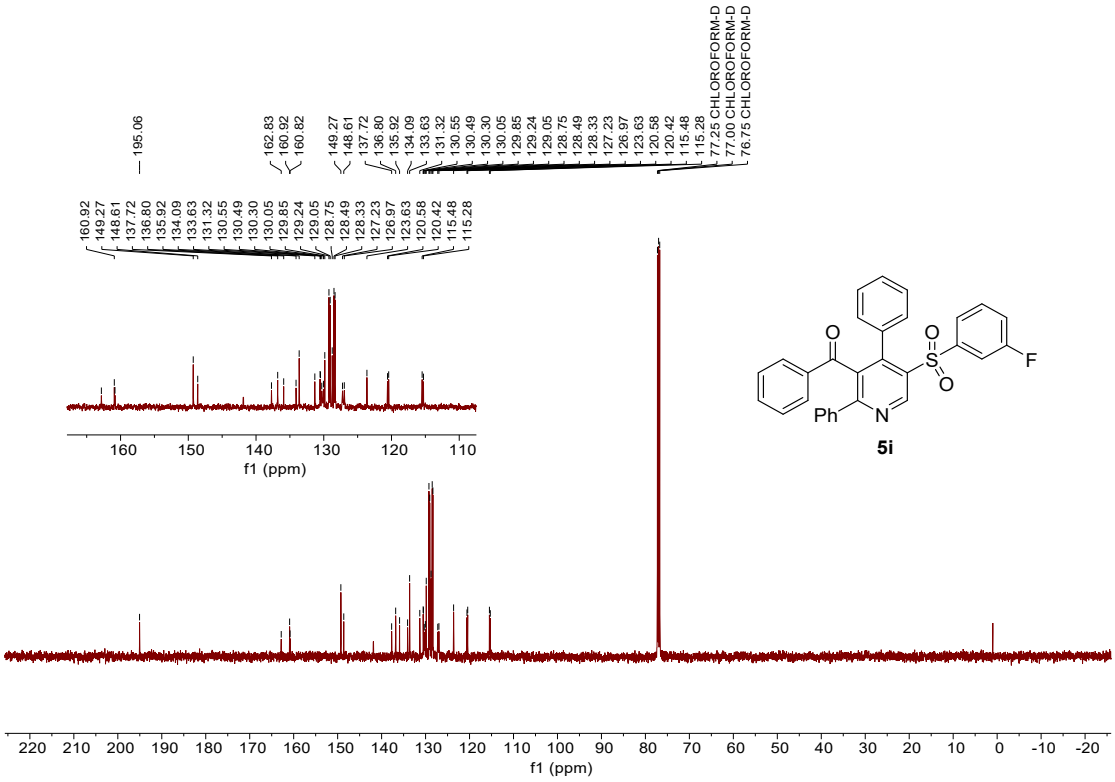
3.39
4.01
5.43
2.20
2.10
0.94
1.00
f1 (ppm)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136.80
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133.63
131.32
130.55
130.49
130.30
130.05
129.85
129.24
129.05
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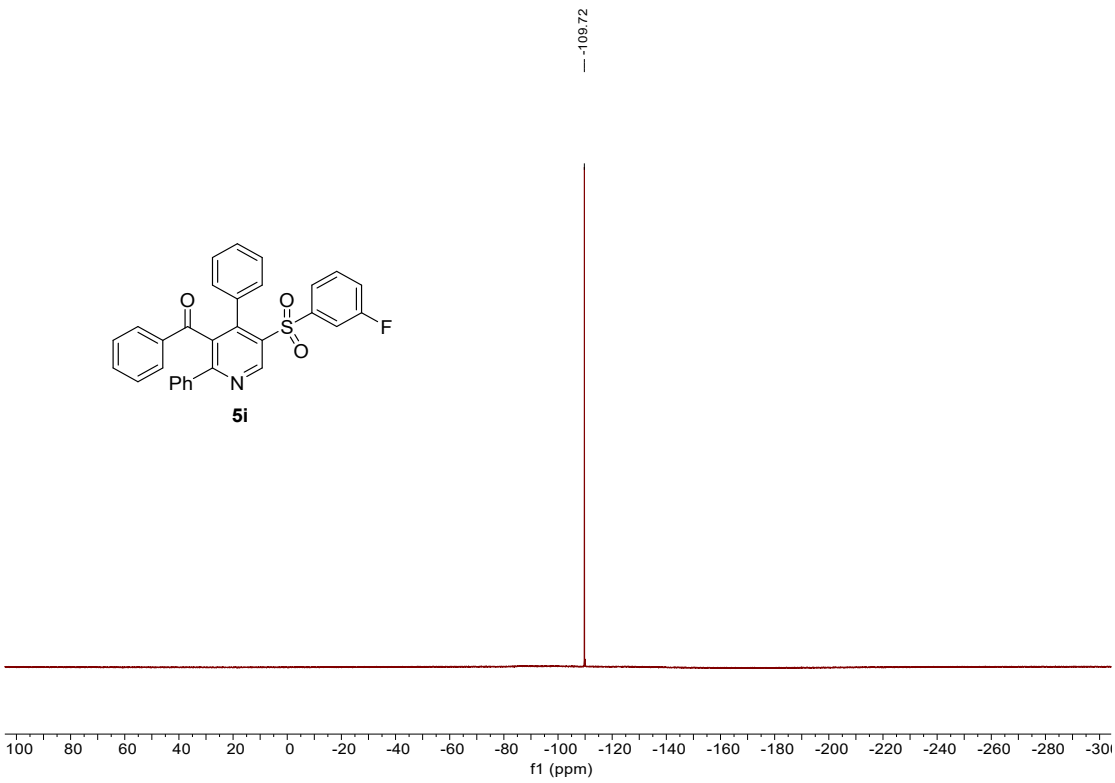
128.49
128.33
127.23
126.97
123.63
120.58
120.42
115.48
115.28
77.25 CHLOROFORM-D
77.00 CHLOROFORM-D
76.75 CHLOROFORM-D
f1 (ppm)
O
O
S
O
F
Ph
N
5i


-109.72
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f1 (ppm)