Supporting Information

Palladium-catalyzed radical cascade cyanoalkylsulfonylation/-cyclization of 3-arylethynyl-[1,1'-biphenyl]-2-carbonitriles with cyclobutanone oxime esters and DABSO

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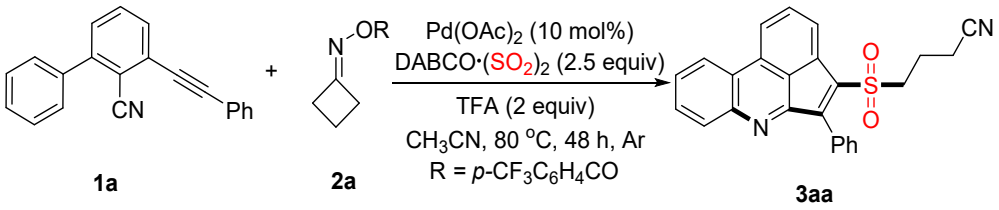
General Information:

All reactions were carried out under Ar atmosphere unless otherwise noted. All catalysts and solvents were obtained from commercial suppliers. Reactions were monitored by TLC on silica gel plates (GF254), and the analytical thin-layer chromatography (TLC) was performed on precoated, glass-backed silica gel plates. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker Ascend 400 MHz NMR spectrometer at room temperature. Chemical shifts (δ) are reported in ppm downfield fromtetramethylsilane. Chemical shifts (δ) are given in ppm relative to $CDCl_3$ (7.26 ppm for ^{1}H and 77 ppm for ^{13}C) to internal TMS (δ = 0 ppm) as internal standard. High-resolution mass spectra (HRMS) were obtained using ESI-TOF, APCI-TOF in positive mode. All substrates **1** and cycloketone oxime esters **2** were synthesized according to the literature.[1,2]

Table 1 Optimization of reaction conditions [a]



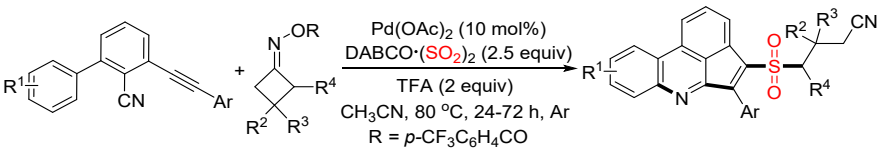
1a **2a** **3aa**

entry	Variation from the standard conditions	yield(%)[b]
1	None	73
2	$Pd(PPh_3)_2Cl_2$ instead of $Pd(OAc)_2$	57
3	$Pd(PPh_3)_4$ instead of $Pd(OAc)_2$	9
4	$Pd(TFA)_2$ instead of $Pd(OAc)_2$	53
5	CuCl/CuI/$Cu(OAc)_2$ instead of $Pd(OAc)_2$	0/0/0
6	$FeCl_2$/$FeCl_3$ instead of $Pd(OAc)_2$	33/trace
7	$NiCl_2$•glyme instead of $Pd(OAc)_2$	43%
8	$Na_2S_2O_5$ instead of DABCO·$(SO_2)_2$	trace
9	$K_2S_2O_5$ instead of DABCO·$(SO_2)_2$	trace
10	DCM instead of CH_3CN	40
11	CH_3NO_2 instead of CH_3CN	trace
12	Toluene instead of CH_3CN	0
13	1,4-dioxane instead of CH_3CN	0
14	DMF instead of CH_3CN	0
15	DMSO instead of CH_3CN	0
16	at 60 °C	0
17	at 100 °C	40
18	**2a** (2.0 equiv)	53
19	**2a** (3.0 equiv)	57
20	DABCO·$(SO_2)_2$ (2.0 equiv)	59
21	DABCO·$(SO_2)_2$ (3.0 equiv)	62

22	$Pd(OAc)_2$ (5 mol%)	58
23	$Pd(OAc)_2$ (20 mol%)	61
24	TFA (1.0 equiv)	55
25	TFA (3.0 equiv)	51
26	$H^+P^tBu_3 \cdot {}^-BF_4$ was used as a ligand	43
27	BINAP was used as a ligand	57
28	Xantphos was used as a ligand	13
29	DPPF was used as a ligand	18
30	PPh_3 was used as a ligand	16
31	PCy_3 was used as a ligand	54
32	DPPE was used as a ligand	62
33	K_2CO_3 instead of TFA	trace
34	Cs_2CO_3 instead of TFA	trace
35	AcONa instead of TFA	trace
36	HAc instead of TFA	51
37	H_2SO_4 instead of TFA	57
38	Without TFA	45
39	24 h	49
40	72 h	65

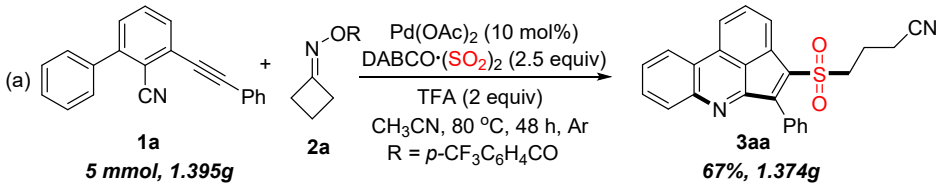
[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.25 mmol, 2.5 equiv.), DABCO·$(SO_2)_2$ (0.25 mmol, 2.5 equiv.), TFA (2.0 equiv), $Pd(OAc)_2$ (10 mol%) and CH_3CN (1 mL) at 80 °C under an argon atmosphere for 48 h. [b] Yield of the isolated product.

General procedures for synthesis of cyanoalkylsulfonylated cyclopenta[*gh*]phenanthridines 3



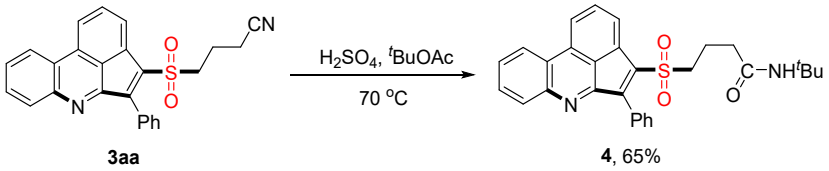
An oven-dried Schlenk tube (10 mL) was equipped with a magnetic stir bar, **1** (0.1 mmol), cyclobutanone *O*-acyl oximes **2** (1.5 equiv, 0.15 mmol), DABCO·$(SO_2)_2$ (0.25 mmol, 2.5 equiv.), TFA (2.0 equiv), $Pd(OAc)_2$ (10 mol%). The flask was evacuated and backfilled with Ar for 3 times. 1 mL CH_3CN was added with syringe under Ar. The tube was then sealed and the mixture was stirred at 80 °C for 24-72 h. After the reaction was finished, the organic solvent was removed under the reduced pressure. The residue was purified by column chromatography (DCM) to afford the desired products **3**.

Experimental procedure for gram-up reaction



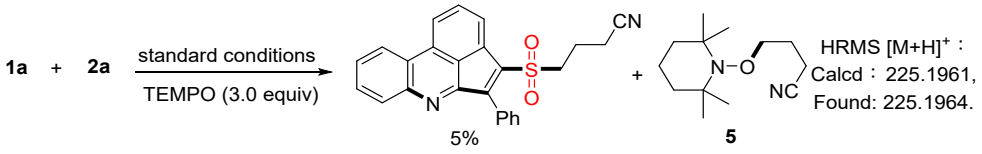
An oven-dried Schlenk tube (100 mL) was equipped with a magnetic stir bar, **1a** (5 mmol), cyclobutanone O-acyl oximes **2a** (7.5 mmol. 1.5 equiv.), DABCO•$(SO_2)_2$ (12.5 mmol, 2.5 equiv.), TFA (2.0 equiv), $Pd(OAc)_2$ (10 mol%). The flask was evacuated and backfilled with Ar for 3 times. 50 mL CH_3CN was added with syringe under Ar. The tube was then sealed and the mixture was stirred at 80 °C for 48 h. After the reaction was finished, the organic solvent was removed under the reduced pressure. The residue was purified by column chromatography to afford the desired product **3aa** in 67%.

General Procedure for the Synthesis of 4

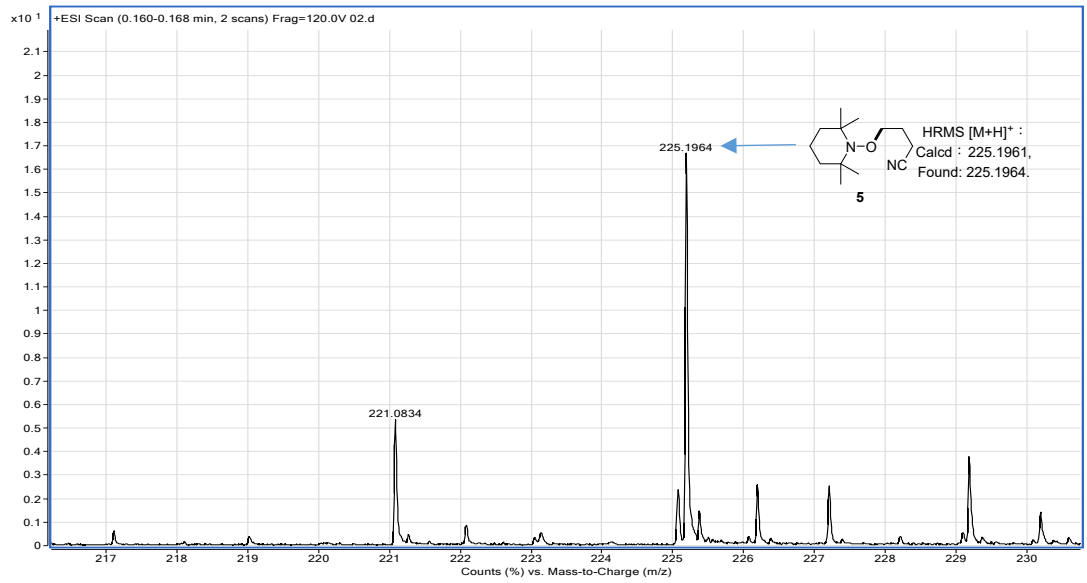


To a 10 mL Schlenk were sequentially added **3aa** (82.0 mg, 0.2 mmol, 1.0 equiv.), tert-butyl acetate (2 mL) and conc. H_2SO_4 (4 drops). The reaction mixture was stirred at 70 °C overnight. After cooling to room temperature, the reaction mixture was quenched with $NaHCO_3$ aq. and extracted with DCM (15 mL × 3). The combined organic layer was washed with brine (20 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuum. The residue was purified by silica gel chromatography (DCM/MeOH=20:1, v/v) to afford the desired product **4** in 65% yield (62.9 mg) as a yellow solid. ^1H NMR (400 MHz, $CDCl_3$): δ = 8.61-8.58 (m, 1H), 8.43-8.37 (m, 2H), 8.25 (d, *J* = 7.2 Hz, 1H), 7.94-7.90 (m, 2H), 7.89-7.85 (m, 1H), 7.83-7.79 (m, 2H), 7.61-7.55 (m, 3H), 5.29 (s, 1H), 3.10 (t, *J* = 7.2 Hz, 2H), 2.15 (t, *J* = 7.2 Hz, 2H), 2.06-2.00 (m, 2H), 1.26 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.3, 160.9, 148.4, 148.3, 139.8, 135.3, 133.0, 132.5, 131.3, 130.1, 129.7, 129.2, 129.042, 128.964, 128.1, 125.3, 124.6, 123.5, 123.0, 119.6, 54.6, 51.3, 35.0, 28.7, 18.8 ppm. ESI-HRMS: m/z Calcd for $C_{36}H_{34}N_2O_3S+H^+$: 485.1893, found 485.1896.

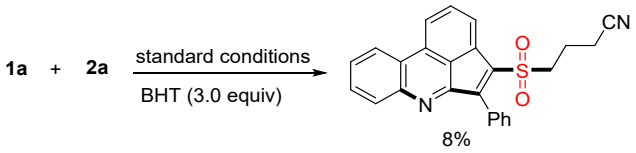
Trapping experiment with TEMPO



An oven-dried Schlenk tube (10 mL) was equipped with a magnetic stir bar, **1** (0.1 mmol), cyclobutanone *O*-acyl oximes **2** (1.5 equiv, 0.15 mmol), DABCO·$(SO_2)_2$ (0.25 mmol, 2.5 equiv.), TFA (2.0 equiv), $Pd(OAc)_2$ (10 mol%). The flask was evacuated and backfilled with Ar for 3 times. 1 mL CH_3CN was added with syringe under Ar. The tube was then sealed and the mixture was stirred at 80 °C for 48 h. However, product **3aa** was obtained in 5% yield, the intermediate **6** was formed, suggesting that this transformation proceeds through a radical pathway.

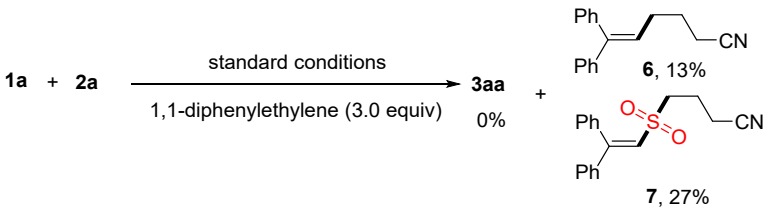


Trapping experiment with BHT



An oven-dried Schlenk tube (10 mL) was equipped with a magnetic stir bar, **1** (0.1 mmol), cyclobutanone *O*-acyl oximes **2** (1.5 equiv, 0.15 mmol), DABCO·$(SO_2)_2$ (0.25 mmol, 2.5 equiv.), TFA (2.0 equiv), $Pd(OAc)_2$ (10 mol%). The flask was evacuated and backfilled with Ar for 3 times. 1 mL CH_3CN was added with syringe under Ar. The tube was then sealed and the mixture was stirred at 80 °C for 48 h. However, product **3aa** was obtained in 8% yield

Trapping experiment with 1,1-diphenylethene



An oven-dried Schlenk tube (10 mL) was equipped with a magnetic stir bar, **1** (0.2 mmol), cyclobutanone *O*-acyl oximes **2** (1.5 equiv, 0.30 mmol), DABCO·$(SO_2)_2$ (0.50 mmol, 2.5 equiv.), TFA (2.0 equiv), $Pd(OAc)_2$ (10 mol%). The flask was evacuated and backfilled with Ar for 3 times. 1 mL MeCN was added with syringe under Ar. The tube was then sealed and the mixture was stirred at 80 °C for 48 h. After the reaction finished, the residue was concentrated in vacuo, then purified by column chromatography to afford **6** (6.4 mg, 13%) and **7** (16.8 mg, 27%). *6,6-diphenylhex-5-enenitrile (**6**).* Yellow oil; (7.4 mg, 15%); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.40-7.36 (m, 2H), , 7.33 (d, *J* = 6.8 Hz, 1H), 7.27-7.20 (m, 5H), 7.17-7.14 (m, 2H), 6.01 (t, *J* = 7.2 Hz, 2H), 2.32-2.23 (m, 4H), 1.83-1.76 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.8, 142.1, 139.6, 129.6, 128.3, 128.1, 127.2, 127.2, 127.1, 126.6, 119.5, 28.7, 25.7, 16.6 ppm. 4-((2,2-diphenylvinyl)sulfonyl)butanenitrile (***7***). Yellow oil; (19.9 mg, 32%); ^{1}H NMR (400 MHz, $CDCl_3$):

δ = 7.49-7.42 (m, 4H), 7.39-7.36 (m, 4H), 7.29-7.27 (m, 2H), 6.79 (s, 1H), 2.86 (t, *J* = 7.2 Hz, 2H), 2.47 (t, *J* = 7.2 Hz, 2H), 2.12-2.05 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 156.7, 138.7, 135.3, 130.7, 129.7, 129.6, 128.7, 128.324, 128.304, 125.6, 118.1, 52.7, 18.7, 16.1 ppm.

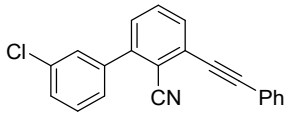
Reference：

[1] (a) N. Zhou, M. Wu, K. Kuang, S. Wu, M. Zhang, *Adv. Synth. Catal.* 2020, **362**, 5391-5397. (b) N. Zhou, M. Wu, M. Zhang, X. Zhou, W. Zhou, *Org. Biomol. Chem.,* 2020, **18**, 1733-1737.

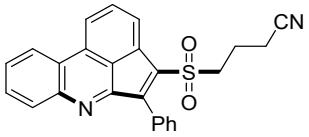
[2] (a) T. Nishimura, Y. Nishiguchi, Y. Maeda, S. Uemura, *J. Org. Chem.* 2004, **69**, 5342. (b) Y.-R. Gu, X.-H. Duan, L. Yang, L.-N. Guo, *Org. Lett.* 2017, **19**, 5908.

B. Zhao, H. Tan, C. Chen, N. Jiao, N. and Z. Shi, *Chin. J. Chem.* 2018, **36**, 995.

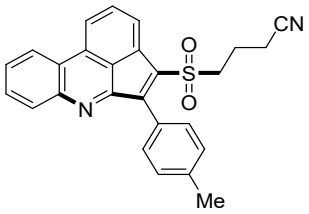
Characterization data of compounds



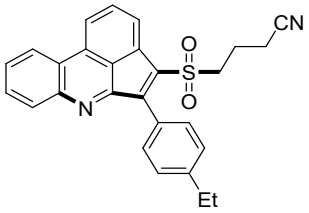
4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(1s)***. White solid; melting point: 110-111 °C; R_f = 0.5 (ethyl acetate / hexane = 1:20); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.66-7.64 (m, 1H), 7.64-7.62 (m, 2H), 7.61-7.58 (m, 1H), 7.53-7.52 (m, 1H), 7.49-7.47 (m, 1H), 7.46-7.41 (m, 3H), 7.40-7.38 (m, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.6, 139.6, 134.6, 132.2, 132.1, 131.1, 130.0, 129.3, 129.2, 129.0, 128.8, 128.6, 128.4, 127.0, 122.0, 116.8, 114.1, 96.3, 85.9 ppm. ESI-HRMS: m/z Calcd for $C_{21}H_{12}ClN+NH_4^+$: 331.0997, found 331.0997.



4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3aa)***. Yellow solid; (29.9 mg, 73%); melting point: 188-189 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.57-8.54 (m, 1H), 8.40-8.35 (m, 2H), 8.23 (d, *J* = 7.2 Hz, 1H), 7.94-7.91 (m, 2H), 7.87-7.83 (m, 1H), 7.82-7.77 (m, 2H), 7.63-7.58 (m, 3H), 3.13 (t, *J* = 7.2 Hz, 2H), 2.42 (t, *J* = 7.2 Hz, 2H), 2.10-2.03 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.5, 148.5, 148.3, 139.3, 134.9, 133.0, 132.5, 131.2, 130.4, 129.4, 129.2, 129.106, 129.078, 128.3, 125.3, 124.5, 123.6, 123.0, 119.4, 118.0, 53.6, 18.9, 16.0 ppm. ESI-HRMS: m/z Calcd for $C_{25}H_{18}N_2O_2S+H^+$: 411.1162, found 411.1170.

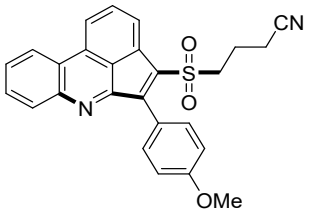


4-((5-(p-tolyl)cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ba)***. Yellow solid; (25.9 mg, 61%); melting point: 219-220 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59-8.56 (m, 1H), 8.41-8.38 (m, 2H), 8.23 (d, *J* = 7.2 Hz, 1H), 7.88-7.78 (m, 5H), 7.41 (d, *J* = 7.6 Hz, 2H), 3.15 (t, *J* = 7.2 Hz, 2H), 2.49 (s, 3H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.11-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.7, 148.7, 148.3, 140.9, 138.6, 135.1, 133.0, 132.5, 131.3, 129.239, 129.163, 129.1, 129.0, 126.5, 125.2, 124.6, 123.5, 123.0, 119.6, 118.0, 53.5, 21.6, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{26}H_{20}N_2O_2S+H^+$: 425.1318, found 425.1317.

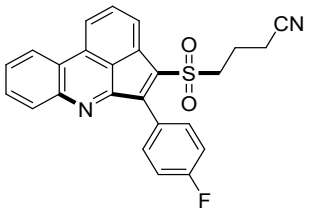


4-((5-(4-ethylphenyl)cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ca)***. Yellow solid; (37.7 mg, 86%); melting point: 228-229 °C; R_f = 0.6 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.57-8.54 (m, 1H), 8.38 (d, *J* = 7.6 Hz, 2H), 8.22 (d, *J* = 7.2 Hz, 1H), 7.90-7.77 (m, 5H), 7.44 (d, *J* = 8.0 Hz, 2H), 3.14 (t, *J* = 7.2 Hz, 2H), 2.79 (q, *J* = 15.2 Hz, *J* = 7.6 Hz, 2H), 2.42 (t, *J* = 7.2 Hz, 2H),

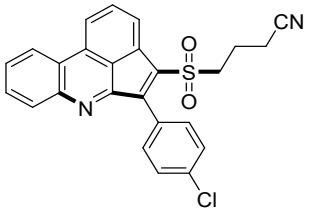
2.11-2.03 (m, 2H), 1.34 (t, J = 7.6 Hz, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.7, 148.7, 148.3, 147.0, 138.6, 135.1, 133.0, 132.5, 131.4, 129.2, 129.1, 129.0, 128.0, 126.7, 125.2, 124.5, 123.4, 123.0, 119.5, 118.0, 53.5, 28.9, 19.0, 16.1, 15.1 ppm. ESI-HRMS: m/z Calcd for $C_{27}H_{22}N_2O_2S+H^+$: 439.1475, found 439.1473.



4-((5-(4-methoxyphenyl)cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3da)***. Yellow solid; (28.2 mg, 64%); melting point: 209-210 °C; R_f = 0.3 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.57-8.55 (m, 1H), 8.38 (m, 2H), 8.21 (d, J = 7.2 Hz, 1H), 7.99 (d, J = 7.6 Hz, 2H), 7.86-7.79 (m, 3H), 7.13 (d, J = 8.4 Hz, 2H), 3.93 (s, 3H), 3.17 (t, J = 7.2 Hz, 2H), 2.45 (t, J = 7.2 Hz, 2H), 2.11-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.6, 160.7, 148.246, 148.211, 137.6, 135.3, 133.3, 133.0, 132.4, 129.2, 129.1, 129.0, 125.0, 124.5, 123.2, 123.0, 121.6, 120.0, 118.0, 114.0, 55.4, 53.3, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{26}H20N_2O_3S+H^+$: 441.1267, found 441.1264.

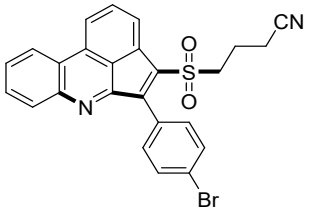


4-((5-(4-fluorophenyl)cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ea)***. Yellow solid; (23.1 mg, 54%); melting point: 205-206 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.60-8.58 (m, 1H), 8.43 (d, J = 8.8 Hz, 1H), 8.40-8.38 (m, 1H), 8.23 (d, J = 7.2 Hz, 1H), 8.00-7.96 (m, 2H), 7.90-7.86 (m, 1H), 7.85-7.80 (m, 2H), 7.32-7.26 (m, 2H), 3.19 (t, J = 7.2 Hz, 2H), 2.48 (t, J = 7.2 Hz, 2H), 2.14-2.07 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$):δ 164.1 (d, J = 252.8 Hz), 160.3, 148.3, 147.7, 139.0, 134.8, 133.7, 133.6, 133.1, 132.5, 129.3, 129.2, 125.312, 125.264, 124.6, 123.8, 123.1, 119.4, 117.9, 115.6 (d, J = 21.8 Hz), 53.8, 18.9, 16.1 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ -109.4 ppm. ESI-HRMS: m/z Calcd for $C_{25}H_{17}FN_2O_2S+H^+$: 429.1068, found 429.1066.

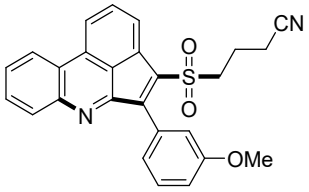


4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3fa)***. Yellow solid; (19.1 mg, 43%); melting point: 215-216 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.62-8.58 (m, 1H), 8.45 (d, J = 8.4 Hz, 1H), 8.41-8.37 (m, 1H), 8.24 (d, J = 7.2 Hz, 1H), 7.93-7.81 (m, 5H), 7.60-7.57 (m, 2H), 3.20 (t, J = 7.2 Hz, 2H), 2.49 (t, J = 7.2 Hz, 2H), 2.16-2.08 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.2, 148.4, 147.6, 139.4, 136.9, 134.8, 133.2, 132.9, 132.6, 129.4, 129.3, 128.7, 127.7, 125.4, 124.6, 124.0, 119.5, 117.9, 53.9, 18.9, 16.2 ppm. ESI-HRMS: m/z Calcd

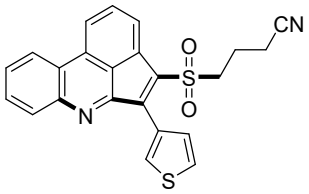
for $C_{25}H_{17}ClN_2O_2S+H^+$: 445.0772, found 445.0775.



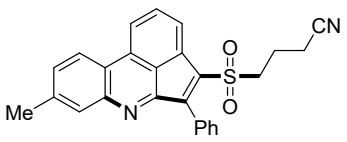
4-((5-(4-bromophenyl)cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ga)***. Yellow solid; (22.4 mg, 46%); melting point: 237-238 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.62-8.59 (m, 1H), 8.45 (d, *J* = 8.0 Hz, 1H), 8.40-8.38 (m, 1H), 8.24 (d, *J* = 7.2 Hz, 1H), 7.91-7.81 (m, 5H), 7.76-7.73 (m, 2H), 3.21 (t, *J* = 7.2 Hz, 2H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.16-2.09 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.1, 148.4, 147.6, 139.3, 134.8, 133.1, 133.0, 132.5, 131.6, 129.4, 129.3, 128.2, 125.4, 125.3, 124.6, 123.9, 123.1, 119.5, 117.9, 53.9, 18.9, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{25}H_{17}BrN_2O_2S+H^+$: 489.0267, found 489.0260.



4-((5-(3-methoxyphenyl)cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ha)***. Yellow solid; (34.8 mg, 79%); melting point: 70-71 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.58-8.56 (m, 1H), 8.42-8.38 (m, 2H), 8.26 (d, *J* = 7.2 Hz, 1H), 7.88-7.80 (m, 3H), 7.53-7.51 (m, 3H), 7.15-7.12 (m, 1H), 3.92 (s, 3H), 3.15 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.12-2.05 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 159.3, 148.3, 148.1, 139.4, 134.9, 133.0, 132.5, 130.6, 129.5, 129.2, 129.1, 125.5, 124.5, 123.7, 123.6, 123.0, 119.4, 117.9, 116.6, 116.5, 55.4, 53.4, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{26}H_{20}N_2O_3S+H^+$: 441.1267, found 441.1272.

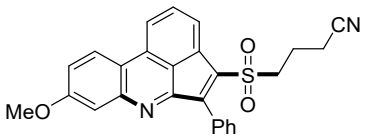


4-((5-(thiophen-3-yl)cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ia)***. Yellow solid; (21.2 mg, 51%); melting point: 75-76 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59-8.56 (m, 2H), 8.43-8.37 (m, 2H), 8.26 (d, *J* = 6.8 Hz, 1H), 8.08 (d, *J* = 4.8 Hz, 1H), 7.86-7.79 (m, 3H), 7.57-7.55 (m, 1H), 3.26 (t, *J* = 7.2 Hz, 2H), 2.50 (t, *J* = 7.2 Hz, 2H), 2.17-2.10 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 148.1, 142.3, 136.8, 135.5, 133.1, 132.4, 132.1, 130.4, 129.9, 129.2, 129.146, 129.098, 125.9, 125.4, 124.5, 123.3, 123.0, 119.5, 117.9, 52.9, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{23}H_{16}N_2O_2S_2+H^+$: 417.0726, found 417.0726.

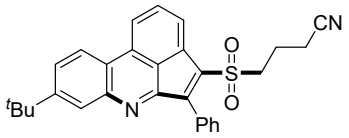


4-((8-methyl-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3la)***. Yellow solid; (28.8 mg, 68%); melting point: 178-179 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.43

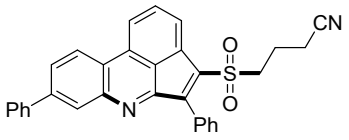
(d, *J* = 8.4 Hz, 1H), 8.35 (d, *J* = 8.4 Hz,1H), 8.19 (t, *J* = 7.2 Hz, 2H), 7.93-7.90 (m, 2H), 7.83 (t, *J* = 7.6 Hz,1H), 7.63-7.58 (m, 4H), 3.13 (t, *J* = 7.2 Hz, 2H), 2.61 (s, 3H), 2.42 (t, *J* = 7.2 Hz, 2H), 2.10-2.03 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 148.6, 148.5, 139.5, 139.0, 134.9, 132.9, 132.0, 131.2, 130.9, 130.3, 129.5, 129.2, 128.3, 124.9, 123.5, 122.7, 122.2, 119.1, 117.9, 53.6, 21.5, 18.9, 16.0 ppm. ESI-HRMS: m/z Calcd for $C_{26}H_{20}N_2O_2S+H^+$: 425.1318, found 425.1313.



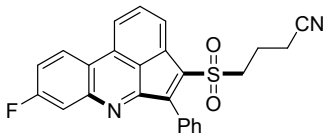
4-((8-methoxy-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ma)***. Yellow solid; (30.4 mg, 69%); melting point: 201-202 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.46 (d, *J* = 9.2 Hz, 1H), 8.34 (d, *J* = 8.4 Hz, 1H), 8.19 (d, *J* = 7.2 Hz, 1H), 7.94-7.91 (m, 2H), 7.86-7.82 (m, 1H), 7.78 (d, *J* = 2.8 Hz, 1H), 7.64-7.58 (m, 3H),7.45-7.42 (m, 1H), 3.99 (s, 3H), 3.13 (t, *J* = 7.2 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.11-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.8, 160.3, 150.2, 148.6, 139.0, 134.9, 133.0, 131.2, 130.4, 129.5, 129.3, 128.3, 124.7, 123.7, 123.5, 120.5, 118.7, 118.6, 117.9, 112.0, 55.7, 53.7, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{26}H_{20}N_2O_3S+H^+$: 441.1267, found 441.1274.



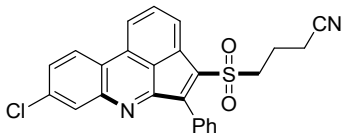
4-((8-(tert-butyl)-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3na)***. Yellow solid; (28.9 mg, 62%); melting point: 190-192 °C; R_f = 0.6 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.52 (d, *J* = 8.8 Hz, 1H), 8.41-8.37 (m, 2H), 8.23 (d, *J* = 7.2 Hz, 1H), 7.96-7.93 (m, 2H), 7.91-7.83 (m, 2H), 7.63-7.59 (m, 3H), 3.14 (t, *J* = 7.2 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.11-2.04 (m, 2H),1.47 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 152.7, 148.7, 148.6, 139.0, 134.9, 132.9, 131.3, 130.4, 129.5, 129.1, 128.6, 128.3, 127.6, 125.0, 123.6, 122.6, 122.2, 119.3, 117.9, 53.6, 35.2, 31.3, 18.9, 16.0 ppm. ESI-HRMS: m/z Calcd for $C_{29}H_{26}N_2O_2S+H^+$: 467.1788, found 467.1789.



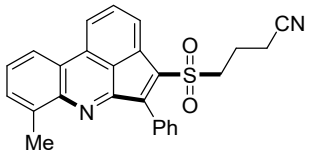
4-((5,8-diphenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile (3oa). Yellow solid; (19.4 mg, 40%); melting point: 212-213 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.65-8.63 (m, 2H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.26 (d, *J* = 6.8 Hz, 1H), 8.09-8.06 (m, 1H), 7.97-7.94 (m, 2H), 7.91-7.87 (m, 1H), 7.81-7.79 (m, 2H), 7.65-7.59 (m, 2H), 7.53-7.50 (m, 2H), 7.45-7.41 (m, 1H), 3.15 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.13-2.06 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.0, 148.8, 148.5, 142.0, 139.7, 139.4, 135.0, 133.2, 131.3, 130.5, 130.3, 129.4, 129.1, 129.0, 128.4, 128.3, 128.0, 127.4, 125.4, 123.7, 123.5, 119.5, 117.9, 53.6, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{31}H_{22}N_2O_2S+H^+$: 487.1475, found 487.1467.



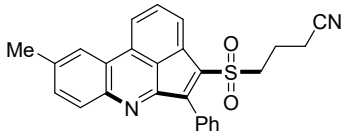
4-((8-fluoro-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3pa)***. Yellow solid; (32.1 mg, 75%); melting point: 160-161 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56-8.52 (m, 1H), 8.35 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 7.2 Hz, 1H), 8.04-8.01 (m, 2H), 7.93-7.90 (m, 2H), 7.89-7.85 (m, 1H), 7.64-7.56 (m, 4H), 3.14 (t, *J* = 7.2 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.11-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.6 (d, *J* = 250.6 Hz), 161.7, 161.4, 149.5 (d, *J* = 11.9 Hz), 148.3, 139.8, 135.0, 133.4, 131.2, 130.5, 129.2, 129.1, 128.4, 125.4, 124.6 (d, *J* = 9.5 Hz), 123.5, 121.1 (d, *J* = 2.1 Hz), 119.1, 118.1 (d, *J* = 36.4 Hz), 118.0, 117.0 (d, *J* = 21.1 Hz), 53.6, 18.9, 16.1 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ -110.3 ppm. ESI-HRMS: m/z Calcd for $C_{25}H_{17}FN_2O_2S+H^+$:429.1068, found 429.1076.



4-((8-chloro-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3qa)***. Yellow solid; (28.9 mg, 65%); melting point: 223-224 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.47 (d, *J* = 8.8 Hz, 1H), 8.37-8.33 (m, 2H), 8.24 (d, *J* = 7.2 Hz, 1H), 7.92-7.85 (m, 3H), 7.75-7.72 (m, 1H), 7.62-7.59 (m, 3H), 3.14 (t, *J* = 7.2 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.11-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 161.6, 148.8, 148.3, 139.9, 135.0, 134.9, 133.5, 131.5, 131.2, 130.5, 129.5, 129.2, 128.9, 128.4, 125.8, 124.1, 123.6, 122.9, 119.4, 117.9, 53.5, 18.9, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{25}H_{17}ClN_2O_2S+H^+$: 445.0772, found 445.0770.

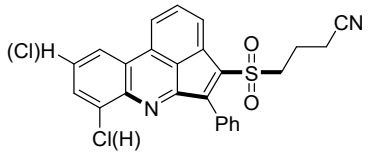


4-((7-methyl-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ra)***. Yellow solid; (8.5 mg, 20%); melting point: 171-172 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.57-8.54 (m, 1H), 8.43-8.38 (m, 2H), 8.23 (d, *J* = 7.2 Hz, 1H), 8.03-8.01 (m, 2H), 7.84 (t, *J* = 7.6 Hz, 1H), 7.70-7.66 (m, 2H), 7.62-7.59 (m, 3H), 3.16 (t, *J* = 7.2 Hz, 2H), 2.85 (s, 3H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.11-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.9, 148.5, 147.1, 140.7, 138.5, 135.0, 132.7, 131.6, 130.3, 130.0, 129.7, 129.5, 128.8, 128.1, 125.1, 124.4, 123.8, 120.8, 119.2, 118.0, 53.6, 19.0, 18.7, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{26}H_{20}N_2O_2S+H^+$: 425.1318, found 425.1327.

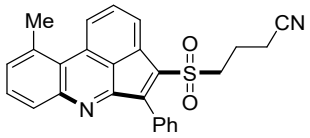


4-((9-methyl-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ra')***. Yellow solid; (25.0 mg, 59%); melting point: 165-167 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.42 (d, *J* = 8.4 Hz, 1H), 8.37 (s, 1H), 8.28-8.24 (m, 2H), 7.95-7.92 (m, 2H), 7.88-7.85 (m, 1H), 7.66-7.58 (m, 4H), 3.14 (t, *J* = 7.2 Hz, 2H), 2.68 (s, 3H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.12-2.04 (m, 2H)

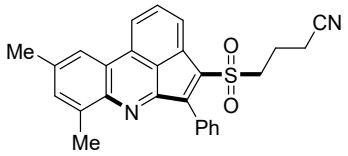
ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.5, 148.7, 146.9, 139.8, 138.7, 134.9, 132.8, 132.2, 131.3, 130.9, 130.3, 129.6, 129.0, 128.3, 125.3, 124.5, 123.6, 122.7, 119.6, 117.9, 53.6, 22.1, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{26}H_{20}N_2O_2S+H^+$: 425.1318, found 425.1317.



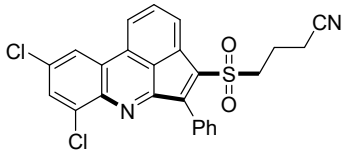
4-((7-chloro-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3sa)*** *and 4-((9-chloro-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile* ***(3sa')***. Yellow solid; (27.5 mg, 62%); melting point: 86-87 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$):8.50-8.46 (m, 1H), 8.38-8.36 (m,1H), 8.34-8.26 (m, 2H), 8.07-8.05 (m, 2H), 7.94-7.85 (m, 3H), 7.76-7.68 (m, 1H), 7.64-7.59 (m, 4H), 3.18-3.11 (m, 3H), 2.43 (t, *J* = 7.2 Hz), 2.13-2.04 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ160.7, 148.3, 148.1, 146.6, 144.4, 139.5, 139.4, 137.0, 135.3, 135.2, 135.0, 133.7, 133.5, 133.3, 131.7, 131.2, 130.6, 130.5, 129.8, 129.7, 129.2, 129.1, 128.9, 128.4, 128.3, 126.2, 126.1, 126.0, 125.5, 123.7, 123.5, 122.7, 121.8, 119.6, 117.9, 53.6, 53.4, 18.907, 18.884, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{25}H_{17}ClN_2O_2S+H^+$: 445.0772, found 445.0762.



4-((10-methyl-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ta)***. Yellow solid; (25.0 mg, 59%); melting point: 186-187 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.71 (d, *J* = 8.8 Hz, 1H), 8.30 (d, *J* = 7.2 Hz, 1H), 7.95-7.92 (m, 1H), 7.90-7.86 (m, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.65-7.59 (m, 4H), 3.15 (t, *J* = 7.6 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.12-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.0, 149.6, 148.0, 138.9, 136.4, 135.0, 132.9, 132.5, 131.8, 131.4, 130.5, 130.3, 129.5, 128.4, 128.349, 128.275, 128.2, 124.7, 123.9, 119.9, 117.9, 53.7, 25.5, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{26}H_{20}N_2O_2S+H^+$: 425.1318, found 425.1308.

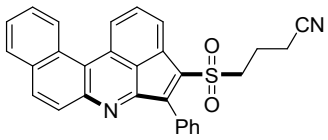


4-((7,9-dimethyl-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ua)***. Yellow solid; (27.2 mg, 62%); melting point: 199-200 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.37 (d, *J* = 8.0 Hz, 1H), 8.20 (t, *J* = 7.2 Hz, 2H), 8.03-8.00 (m, 2H), 7.82 (t, *J* = 8.0 Hz, 1H), 7.62-7.57 (m, 3H), 7.50 (s, 1H), 3.16 (t, *J* = 7.2 Hz, 2H), 2.80 (s, 3H), 2.61 (s, 3H), 2.42 (t, *J* = 7.2 Hz, 2H), 2.11-2.04 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.8, 148.6, 145.6, 140.2, 139.3, 137.8, 134.9, 132.4, 131.8, 131.7, 130.2, 129.8, 129.1, 128.1, 125.0, 124.4, 123.7, 120.5, 119.3, 118.0, 53.6, 22.1, 19.0, 18.5, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{27}H_{22}N_2O_2S+H^+$: 439.1475, found 439.1476.

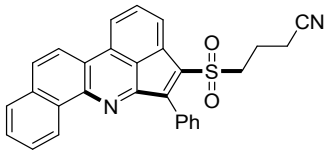


4-((7,9-dichloro-5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3va)***. Yellow

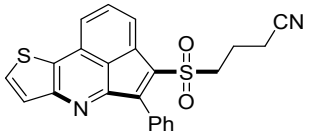
solid; (19.6 mg, 41%); melting point: 215-216 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.44 (d, *J* = 2.4 Hz, 1H), 8.34-8.30 (m, 2H), 8.07-8.04 (m, 2H), 7.92-7.89 (m, 2H), 7.63-7.61 (m, 3H), 3.16 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.12-2.05 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.9, 148.0, 143.0, 139.7, 137.9, 135.4, 134.7, 133.8, 131.7, 130.8, 130.1, 129.0, 128.4, 128.3, 126.7, 123.6, 121.6, 119.9, 117.9, 53.4, 18.9, 16.1 ppm. APCI-HRMS: m/z Calcd for $C_{25}H_{16}Cl_2N_2O_2S+H^+$: 479.0382, found 479.0373.



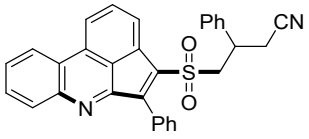
4-((5-phenylbenzo[a]cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3wa)***. Yellow solid; (23.9 mg, 52%); melting point: 207-208 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.16 (d, *J* = 8.4 Hz, 1H), 8.98 (d, *J* = 8.8 Hz, 1H), 8.34-8.25 (m, 2H), 8.06 (t, *J* = 8.4 Hz, 2H), 7.99-7.90 (m, 3H), 7.81-7.72 (m, 2H), 7.65-7.61 (m, 3H), 3.17 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.13-2.06 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.7, 148.7, 148.5, 137.9, 135.4, 134.1, 133.1, 131.4, 130.5, 130.4, 130.2, 130.1, 129.7, 129.5, 129.0, 128.745, 128.689, 128.3, 127.6, 127.3, 125.6, 122.4, 120.2, 118.0, 53.8, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{29}H_{20}N_2O_2S+H^+$: 461.1318, found 461.1324.



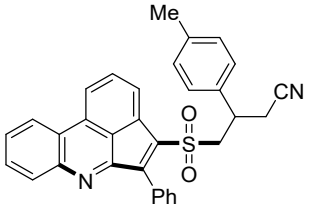
4-((5-phenylbenzo[c]cyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3xa)***. Yellow solid; (29.0 mg, 63%); melting point: 177-178 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.34-9.32 (m, 2H), 8.51-8.45 (m, 2H), 8.29 (d, *J* = 6.8 Hz, 1H), 8.13-8.06 (m, 3H), 8.01-7.98 (m, 1H), 7.90-7.86 (m, 1H), 7.77-7.64 (m, 5H), 3.18 (t, *J* = 7.2 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.13-2.06 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.3, 148.9, 145.7, 137.5, 135.1, 133.3, 132.9, 132.8, 131.6, 130.3, 129.8, 129.2, 128.3, 127.943, 127.871, 127.6, 126.1, 125.2, 124.4, 122.5, 120.3, 119.6, 118.0, 53.7, 19.0, 16.1 ppm. ESI-HRMS: m/z Calcd for $C_{29}H_{20}N_2O_2S+H^+$: 461.1318, found 461.1319.



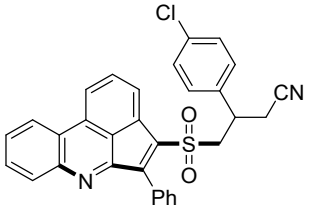
4-((5-phenylcyclopenta[ij]thieno[3,2-c]isoquinolin-4-yl)sulfonyl)butanenitrile ***(3ya)***. Yellow solid; (22.0 mg, 53%); melting point: 76-77 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.28 (d, *J* = 6.8 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.92-7.90 (m, 2H), 7.87-7.80 (m, 3H), 7.63-7.57 (m, 3H), 3.12 (t, *J* = 7.2 Hz, 2H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.10-2.03 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 158.4, 155.8, 149.8, 136.3, 135.3, 133.1, 131.136, 131.092, 130.4, 129.6, 128.4, 127.9, 127.7, 127.1, 126.4, 124.6, 118.4, 117.9, 53.8, 19.0, 16.0 ppm. ESI-HRMS: m/z Calcd for $C_{23}H_{16}N_2O_2S_2+H^+$: 417.0726, found 417.0723.



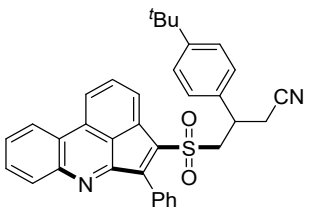
3-phenyl-4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ab)***. Yellow solid; (29.2 mg, 60%); melting point: 98-99 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59-8.56 (m, 1H), 8.40-8.35 (m, 2H), 8.21 (d, *J* = 7.2 Hz, 1H), 7.94-7.91 (m, 2H), 7.86-7.80 (m, 3H), 7.60-7.56 (m, 3H), 7.03 (t, *J* = 7.6 Hz, 2H), 6.95-6.91 (m, 3H), 3.63-3.56 (m, 1H), 3.49-3.37 (m, 2H), 2.81-2.74 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 148.4, 148.2, 139.5, 138.3, 135.1, 132.9, 132.5, 131.6, 130.4, 129.3, 129.094, 129.068, 128.7, 128.3, 127.9, 126.9, 125.3, 124.5, 123.5, 123.0, 119.5, 117.0, 58.8, 36.7, 24.3 ppm. ESI-HRMS: m/z Calcd for $C_{31}H_{22}N_2O_2S+H^+$: 487.1475, found 487.1477.



4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)-3-(p-tolyl)butanenitrile ***(3ac)***. Yellow solid; (28.0 mg, 56%); melting point: 100-101 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.58-8.56 (m, 1H), 8.40-8.35 (m, 2H), 8.18 (d, *J* = 7.2 Hz, 1H), 7.97-7.94 (m, 2H), 7.85-7.78 (m, 3H), 7.62-7.58 (m, 3H), 6.78-6.69 (m, 4H), 3.59-3.52 (m, 1H), 3.42-3.39 (m, 2H), 2.70 (d, *J* = 6.8 Hz, 2H), 1.80 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 148.3, 148.2, 139.5, 137.8, 135.2, 134.7, 132.8, 132.4, 131.7, 130.4, 129.3, 129.2, 129.0, 128.9, 128.2, 126.8, 125.3, 124.5, 123.3, 122.9, 119.5, 117.1, 58.9, 36.6, 24.5, 20.5 ppm. ESI-HRMS: m/z Calcd for $C_{32}H_{24}N_2O_2S+H^+$: 501.1631, found 501.1640.

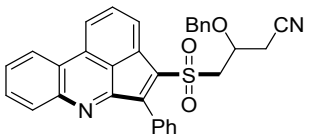


3-(4-chlorophenyl)-4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ad)***. Yellow solid; (25.5 mg, 49%); melting point: 102-103 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.61-8.59 (m, 1H), 8.45-8.37 (m, 2H), 8.19 (d, *J* = 7.2 Hz, 1H), 7.97-7.94 (m, 2H), 7.87-7.80 (m, 3H), 7.62-7.58 (m, 3H), 6.96-6.84 (m, 4H), 3.61-3.55 (m, 1H), 3.43-3.33 (m, 2H), 2.78-2.67 (m, 2H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.2, 148.3, 139.4, 136.4, 135.0, 134.0, 132.8, 132.5, 131.6, 130.6, 129.3, 129.2, 129.1, 128.8, 128.4, 125.3, 124.6, 123.6, 123.0, 119.4, 116.7, 58.5, 36.4, 24.3 ppm. ESI-HRMS: m/z Calcd for $C_{31}H_{21}ClN_2O_2S+H^+$: 521.1085, found 521.1078.

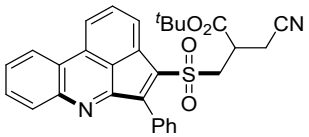


3-(4-(tert-butyl)phenyl)-4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3ae)***. Yellow solid; (37.4 mg, 69%); melting point: 102-103 °C; R_f = 0.5 (DCM); ^{1}H NMR (400

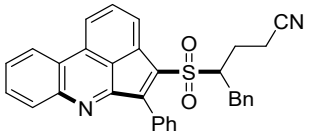
MHz, $CDCl_3$): δ = 8.57-8.55 (m, 1H), 8.39-8.33 (m, 2H), 8.23 (d, *J* = 6.8 Hz, 1H), 7.90-7.77 (m, 5H), 7.60-7.56 (m, 3H), 6.97-6.80 (m, 4H), 3.63-3.56 (m, 1H), 3.48-3.39 (m, 2H), 2.78-2.67 (m, 2H), 0.94 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 151.1, 148.3, 148.2, 139.5, 135.2, 135.0, 132.9, 132.5, 131.7, 130.4, 129.3, 129.044, 129.028, 128.2, 126.6, 125.5, 125.3, 124.6, 123.4, 122.9, 119.5, 117.2, 59.0, 36.5, 34.1, 30.8, 24.5 ppm. ESI-HRMS: m/z Calcd for $C_{35}H_{30}N_2O_2S+H^+$: 543.2101, found 543.2110.



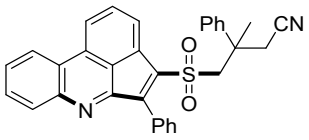
3-(benzyloxy)-4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3af)***. Yellow solid; (20.1 mg, 39%); melting point: 67-68 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59-8.56 (m, 1H), 8.40-8.35 (m, 2H), 8.23 (d, *J* = 6.8 Hz, 1H), 7.89-7.81 (m, 5H), 7.62-7.58 (m, 3H), 6.92-6.83 (m, 5H), 4.36 (d, *J* = 11.2 Hz, 1H), 4.21-4.14 (m, 2H), 3.45 (dd, *J* = 14.8 Hz, *J* = 6.0 Hz, 1H), 3.19 (dd, *J* = 14.8 Hz, *J* = 6.0 Hz, 1H), 2.69 (dd, *J* = 16.8 Hz, *J* = 4.8 Hz, 1H), 2.53 (dd, *J* = 16.8 Hz, *J* = 5.6 Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.5, 148.4, 148.3, 140.1, 135.7, 135.0, 132.9, 132.5, 131.4, 130.4, 129.5, 129.2, 129.1, 129.0, 128.4, 128.0, 127.7, 127.3, 125.1, 124.7, 123.5, 123.0, 119.5, 116.0, 72.0, 69.2, 58.2, 23.3 ppm. ESI-HRMS: m/z Calcd for $C_{32}H_{24}N_2O_3S+H^+$: 517.1580, found 517.1577.



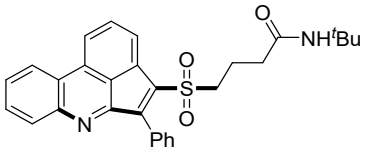
tert-butyl 3-cyano-2-(((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)methyl)propanoate ***(3ag)***. Yellow solid; (17.3 mg, 34%); melting point: 117-119 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.62-8.60 (m, 1H), 8.47-8.39 (m, 2H), 8.25 (d, *J* = 6.8 Hz, 1H), 7.96-7.82 (m, 5H), 7.63-7.60 (m, 3H), 3.65 (dd, *J* = 14.4 Hz, *J* = 4.0 Hz, 1H), 3.30-3.25 (m, 1H), 3.20-3.14 (m, 1H), 2.83 (d, *J* = 5.6 Hz, 2H), 1.37 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.2, 160.5, 149.2, 148.4, 139.2, 134.8, 133.1, 132.6, 131.4, 130.5, 129.342, 129.296, 129.2, 128.3, 125.3, 124.6, 123.7, 123.1, 119.6, 116.4, 83.8, 54.9, 37.0, 27.7, 19.4 ppm. ESI-HRMS: m/z Calcd for $C_{30}H_{26}N_2O_4S+H^+$: 511.1686, found 511.1678.



(S)-5-phenyl-4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)pentanenitrile ***(3ai)***. Yellow solid; (13 mg, 26%); melting point: 108-109 °C; R_f = 0.5 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.61-8.59 (m, 1H), 8.45-8.38 (m, 2H), 8.32 (d, *J* = 7.2 Hz, 1H), 8.05-8.02 (m, 2H), 7.91-7.87 (m, 1H), 7.85-7.80 (m, 2H), 7.69-7.63 (m, 3H), 7.10-7.00 (m, 3H), 6.80-6.78 (m, 2H), 3.31-3.20 (m, 2H), 2.68-2.62 (m, 1H), 2.40-2.36 (m, 2H), 2.28-2.19 (m, 1H), 1.90-1.81 (m, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 148.6, 148.4, 138.7, 135.5, 133.1, 132.6, 131.6, 130.6, 129.6, 129.2, 129.1, 128.729, 128.709, 128.4, 127.1, 125.6, 124.6, 123.7, 123.0, 119.6, 118.3, 62.9, 35.0, 23.0, 15.4 ppm. ESI-HRMS: m/z Calcd for $C_{32}H_{24}N_2O_2S+Na^+$: 523.1451, found 523.1447.

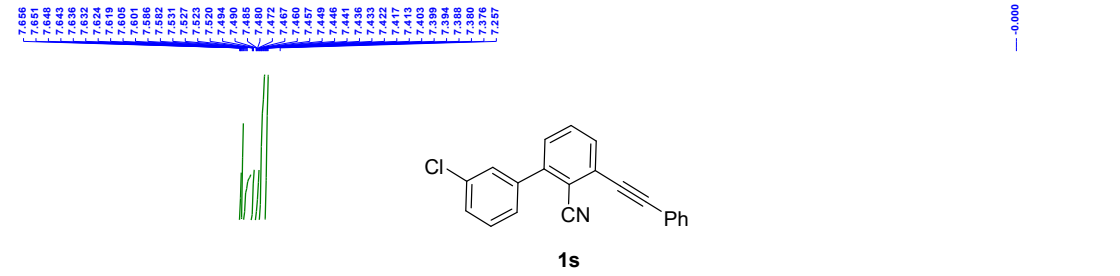


3-methyl-3-phenyl-4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanenitrile ***(3aj)***. Yellow solid; (29.5 mg, 59%); melting point: 95-96 °C; R_f = 0.4 (DCM); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59-8.56 (m, 1H), 8.38-8.35 (m, 2H), 8.14 (d, *J* = 6.8 Hz, 1H), 8.00-7.96 (m, 2H), 7.83-7.79 (m, 3H), 7.65-7.61 (m, 3H), 7.03-6.92 (m, 4H), 6.74 (t, *J* = 7.2 Hz, 1H), 3.41 (q, *J* = 26.8 Hz, *J* = 14.8 Hz, 2H), 3.11 (dd, *J* = 62.4 Hz, *J* = 16.8 Hz, 2H), 1.65 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.5, 148.2, 147.6, 140.8, 140.7, 135.0, 132.8, 132.5, 131.6, 130.4, 129.6, 129.020, 128.981, 128.4, 128.3, 127.2, 125.5, 125.4, 124.5, 123.3, 123.0, 119.5, 117.3, 64.0, 40.1, 29.1, 26.1 ppm. ESI-HRMS: m/z Calcd for $C_{32}H_{24}N_2O_2S+H^+$: 501.1631, found 501.1637.



N-(tert-butyl)-4-((5-phenylcyclopenta[gh]phenanthridin-4-yl)sulfonyl)butanamide ***(4)***. Yellow solid; melting point: 178-179 °C; R_f = 0.6 (DCM/MeOH=20:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.61-8.58 (m, 1H), 8.43-8.37 (m, 2H), 8.25 (d, *J* = 7.2 Hz, 1H), 7.94-7.90 (m, 2H), 7.89-7.85 (m, 1H), 7.83-7.79 (m, 2H), 7.61-7.55 (m, 3H), 5.29 (s, 1H), 3.10 (t, *J* = 7.2 Hz, 2H), 2.15 (t, *J* = 7.2 Hz, 2H), 2.06-2.00 (m, 2H), 1.26 (s, 9H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ 170.3, 160.9, 148.4, 148.3, 139.8, 135.3, 133.0, 132.5, 131.3, 130.1, 129.7, 129.2, 129.042, 128.964, 128.1, 125.3, 124.6, 123.5, 123.0, 119.6, 54.6, 51.3, 35.0, 28.7, 18.8 ppm. ESI-HRMS: m/z Calcd for $C_{36}H_{34}N_2O_3S+H^+$: 485.1893, found 485.1896.

Copies of ^{1}H NMR, ^{13}C NMR, ^{19}F NMR



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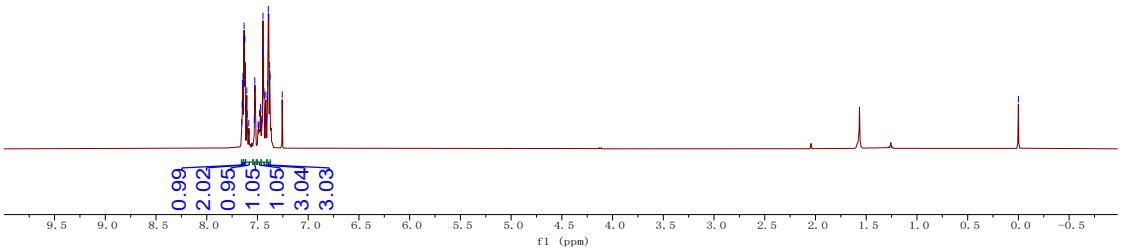

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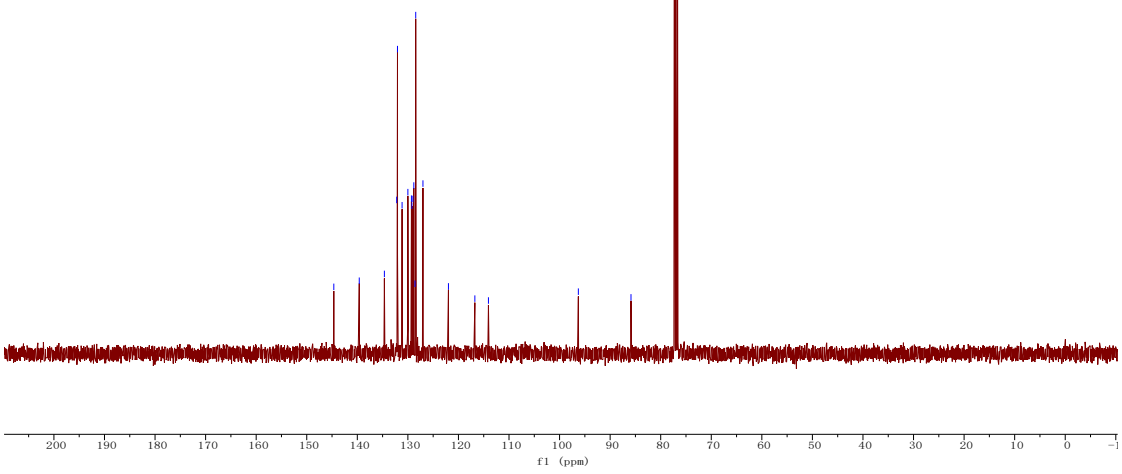

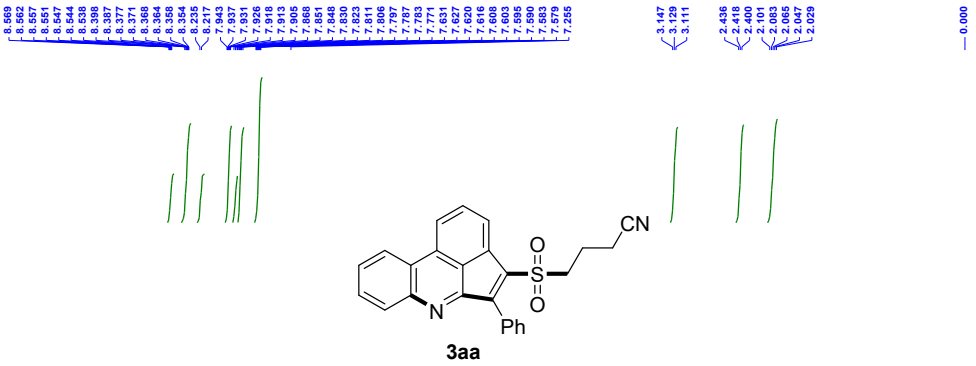
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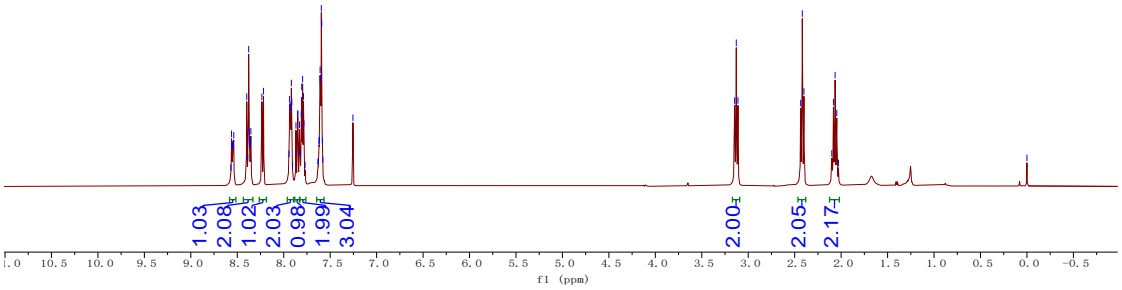
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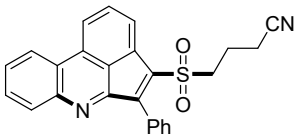
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S
O
N
Ph

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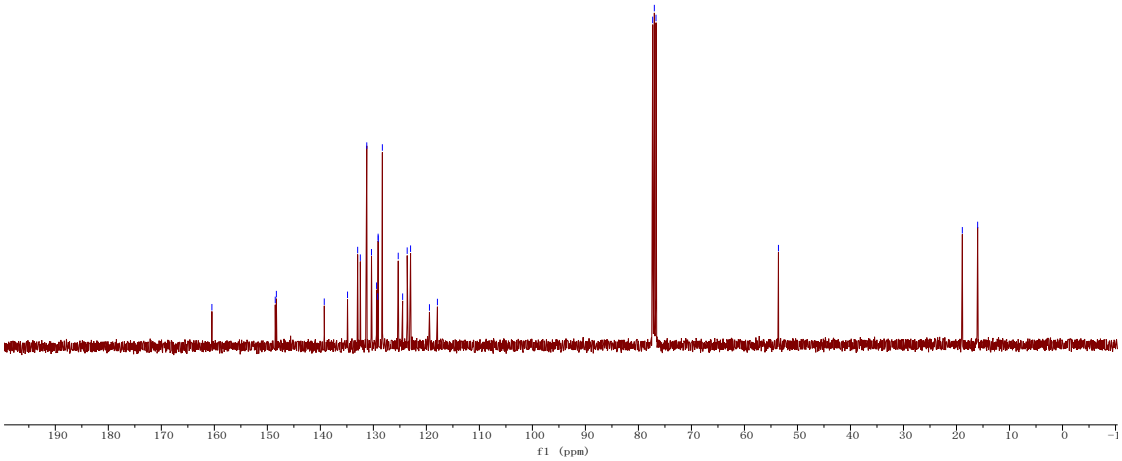
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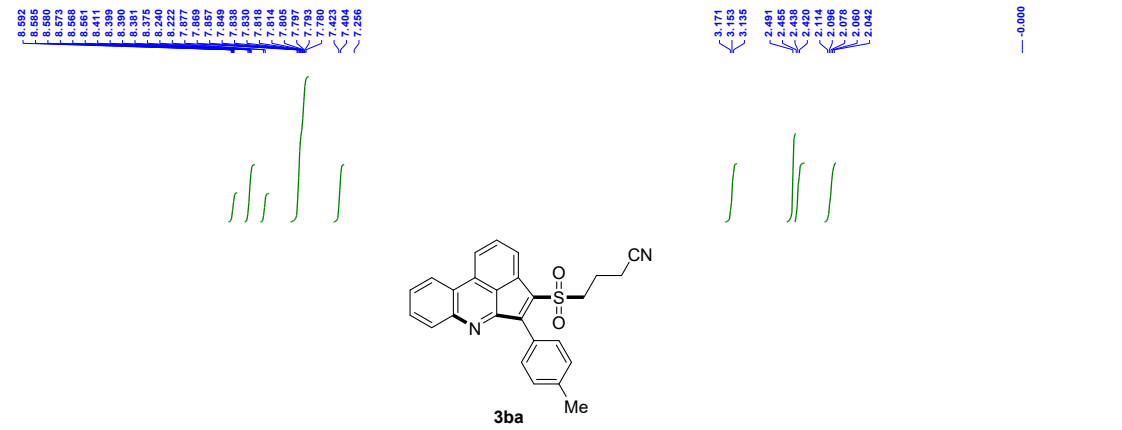
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8.222
7.877
7.869
7.857
7.849
7.838
7.830
7.818
7.814
7.805
7.797
7.793
7.780
7.423
7.404
7.266
3.171
3.153
3.135
2.491
2.455
2.438
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2.078
2.060
2.042
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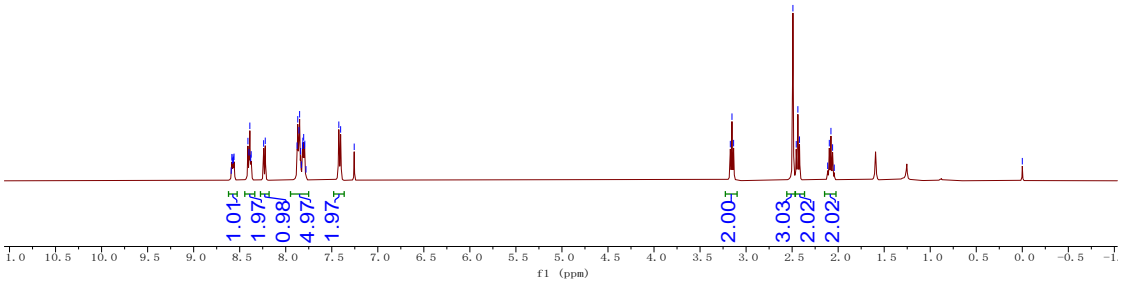
CN
O
S
O
N
Me

3ba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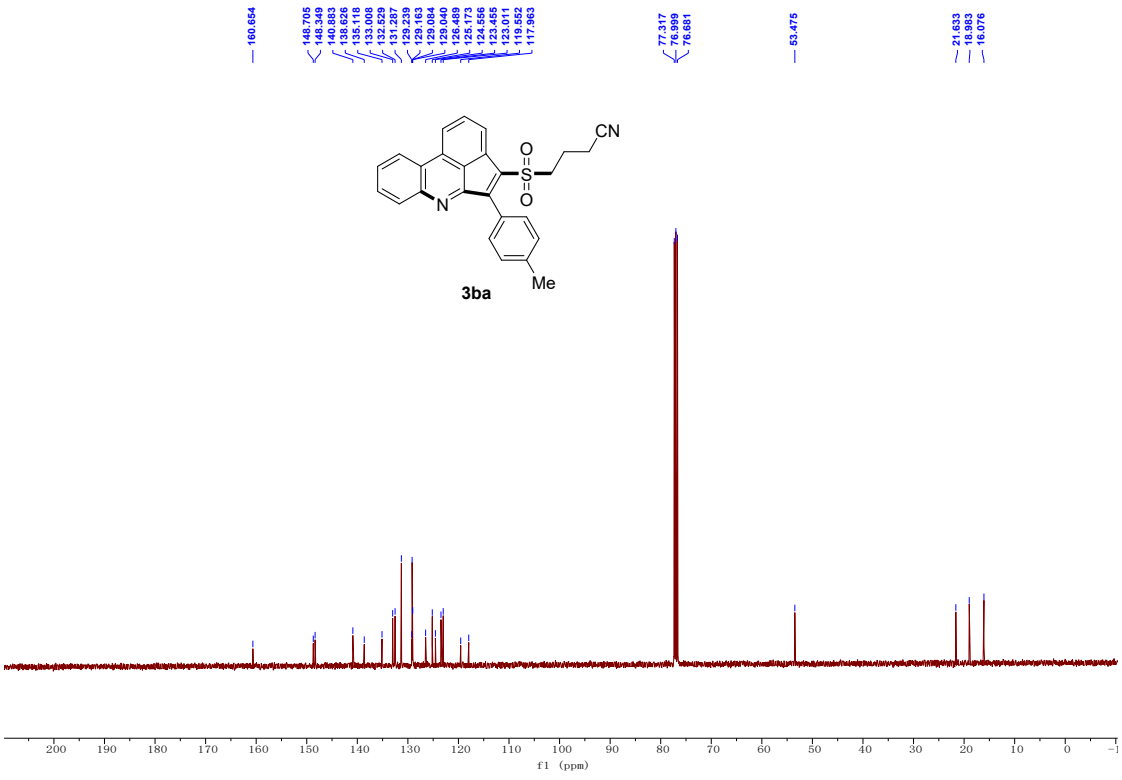
2.02
2.02
f1 (ppm)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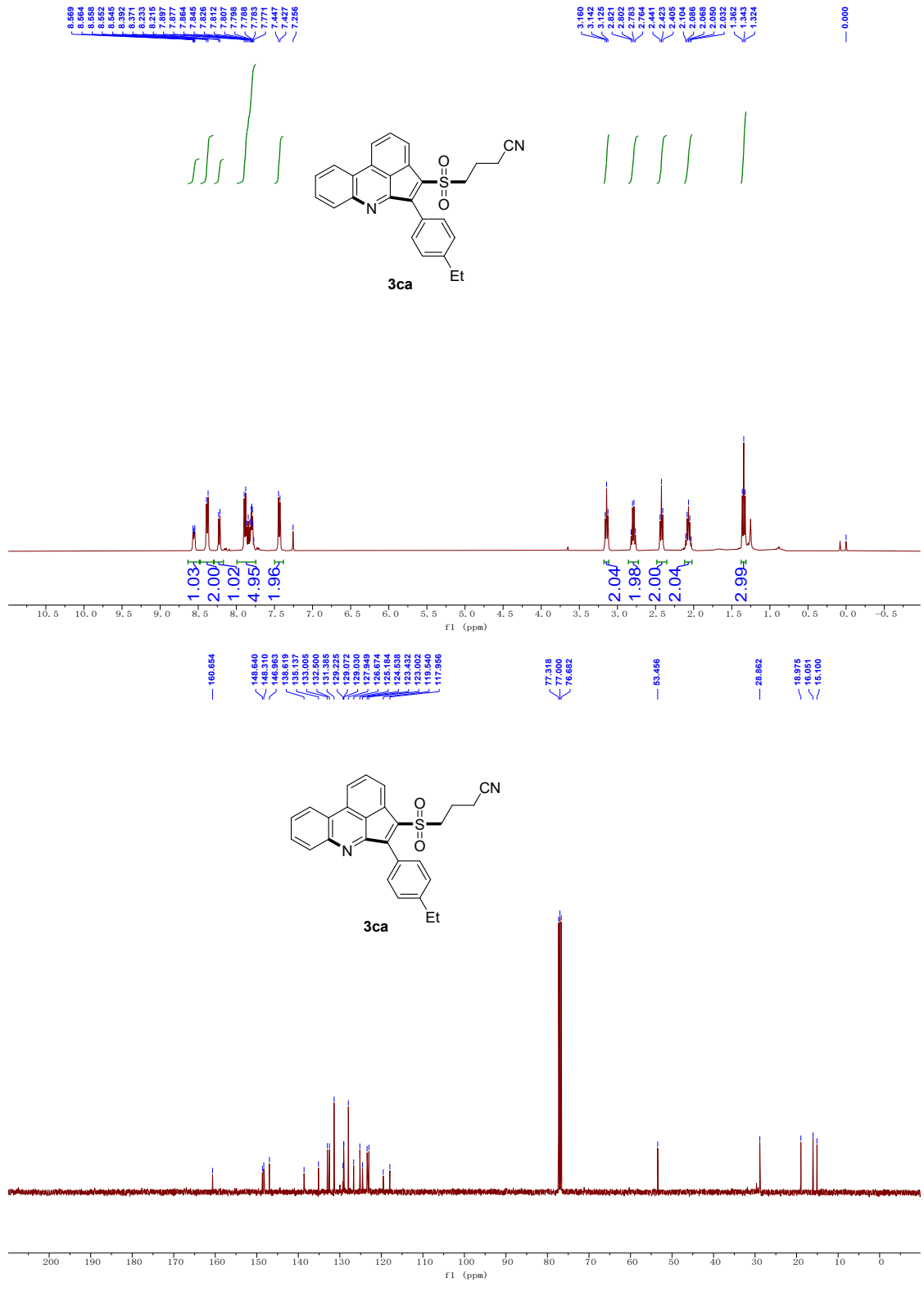
132.529
131.237
129.239
129.163
129.084
129.040
126.489
125.173
124.556
123.455
123.011
120.041
119.552
117.963
77.317
76.999
76.681
53.475
21.633
18.983
16.076
CN
O
S
O
N
Me
f1 (ppm)

3ba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8.233
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7.877
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7.845
7.826
7.812
7.807
7.798
7.788
7.783
7.771
7.447
7.427
7.256
3.160
3.142
3.125
2.821
2.802
2.783
2.764
2.441
2.423
2.405
2.104
2.086
2.068
2.050
2.032
1.362
1.343
1.324
0.000
CN
O
S
O
N
Et
3ca
1.03
2.00
1.02
4.95
1.96
2.04
1.98
2.00
2.04
2.99
f1 (ppm)
160.654
148.640
148.310
146.963
138.619
135.137
133.005
131.500
131.385
129.225
129.072
129.030
127.949
126.674
125.184
124.538
123.472
123.002
119.540
117.956
77.318
77.000
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53.456
28.862
18.975
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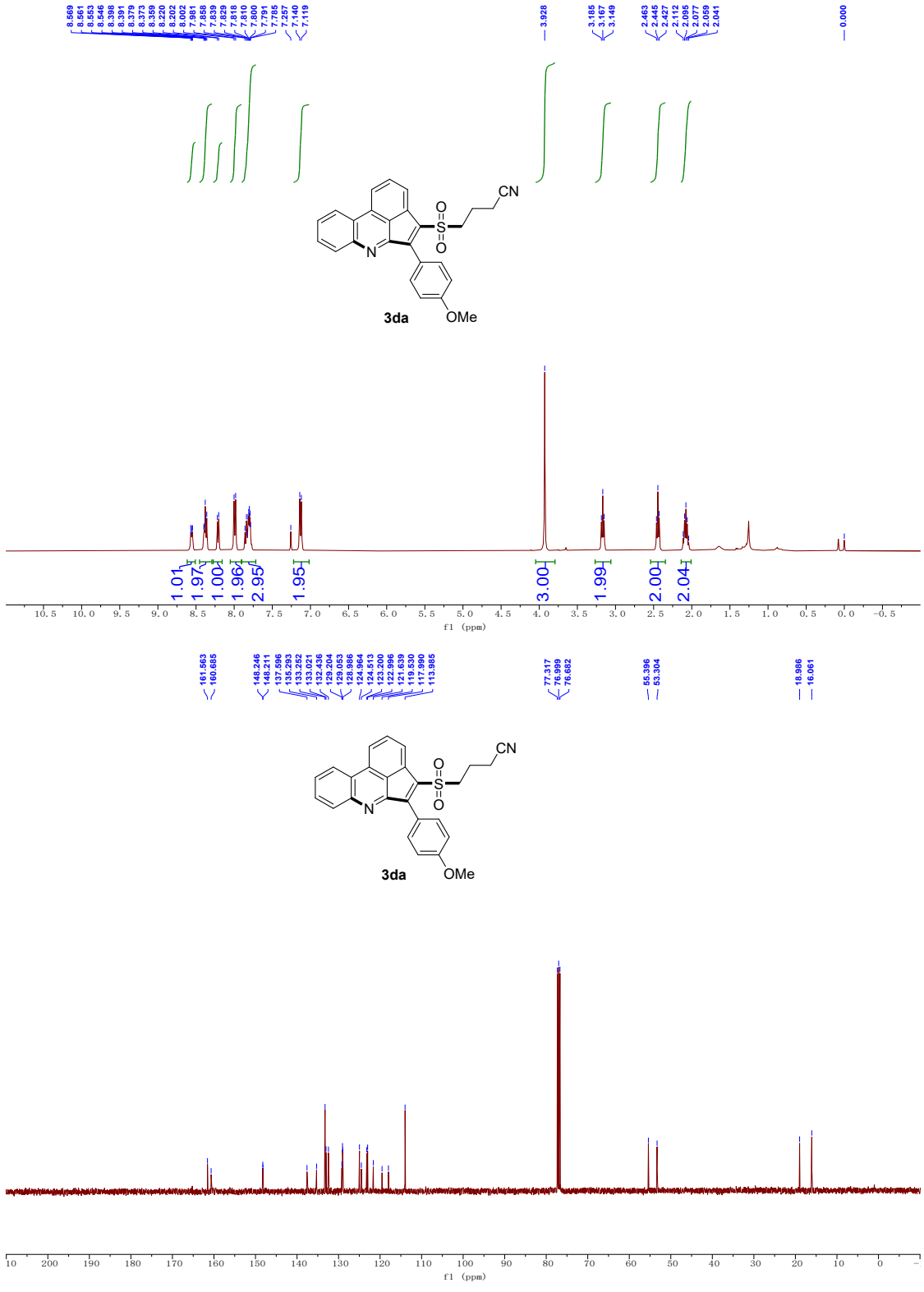
CN
O
S
O
N
Et
3ca
f1 (ppm)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8.220
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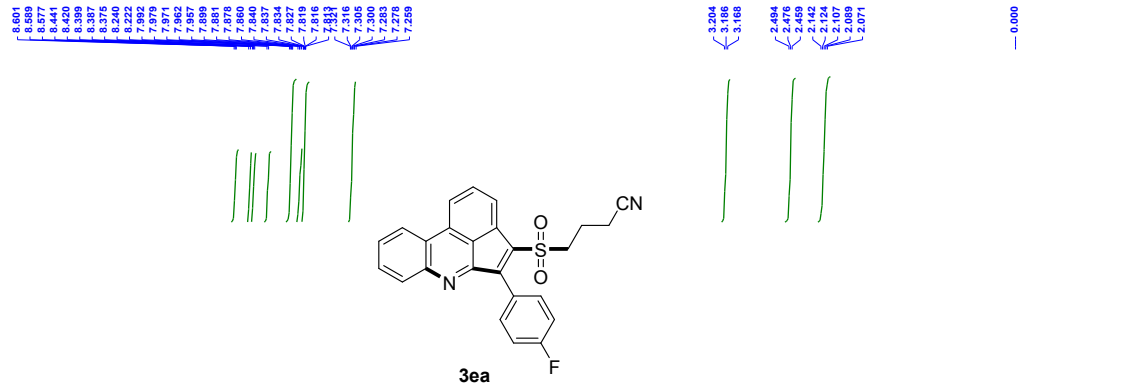
7.981
7.858
7.839
7.829
7.816
7.810
7.800
7.791
7.785
7.257
7.140
7.119
3.928
3.185
3.167
3.149
2.463
2.445
2.427
2.112
2.095
2.077
2.059
2.041
0.000
CN
O
S
O
N
OMe
3da
1.01
1.97
1.00
1.96
2.95
1.95
3.00
1.99
2.00
2.04
f1 (ppm)
161.563
160.685
148.246
148.211
137.596
135.293
133.252
133.021
132.436
129.204
129.053
128.986
124.964
124.513
123.200
122.996
121.639
119.530
117.990
113.985
77.317
76.999
76.682
55.396
53.304
18.986
16.061
CN
O
S
O
N
OMe
3da
f1 (ppm)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8.577
8.441
8.420
8.399
8.387
8.375
8.240
8.222
7.992
7.979
7.971
7.962
7.957
7.899
7.881
7.878
7.860
7.840
7.837
7.834
7.827
7.819
7.816
7.316
7.305
7.300
7.283
7.278
7.259
3.204
3.186
3.168
2.494
2.476
2.458
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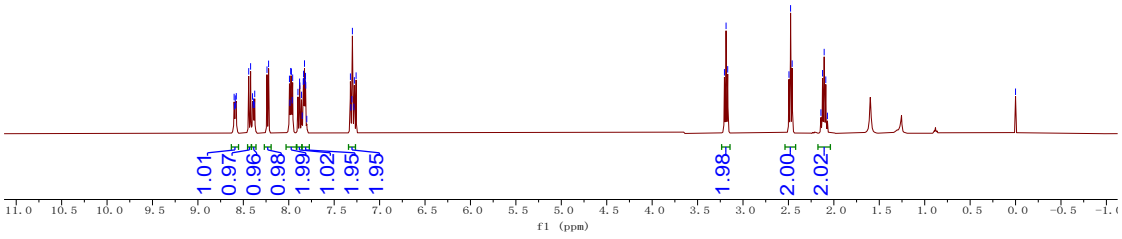
2.124
2.107
2.089
2.071
0.000
CN
O
S
O
N
F
3ea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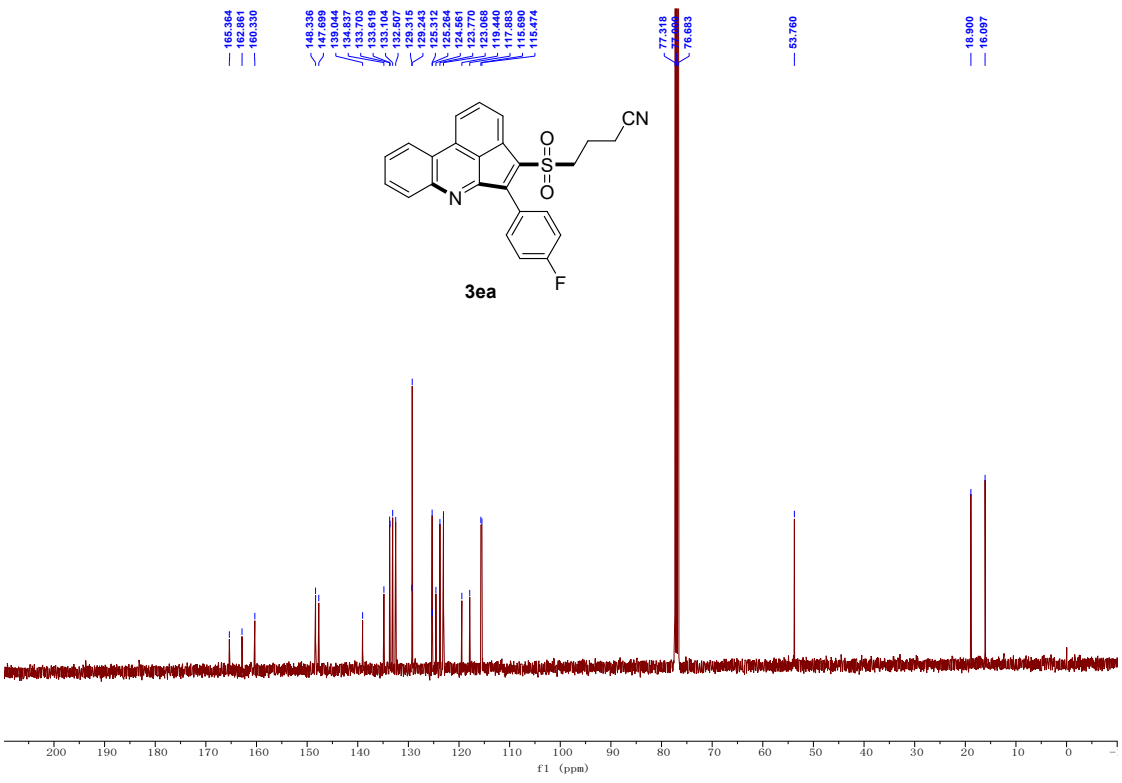
0.98
1.99
1.02
1.95
1.95
1.98
2.00
2.02
f1 (ppm)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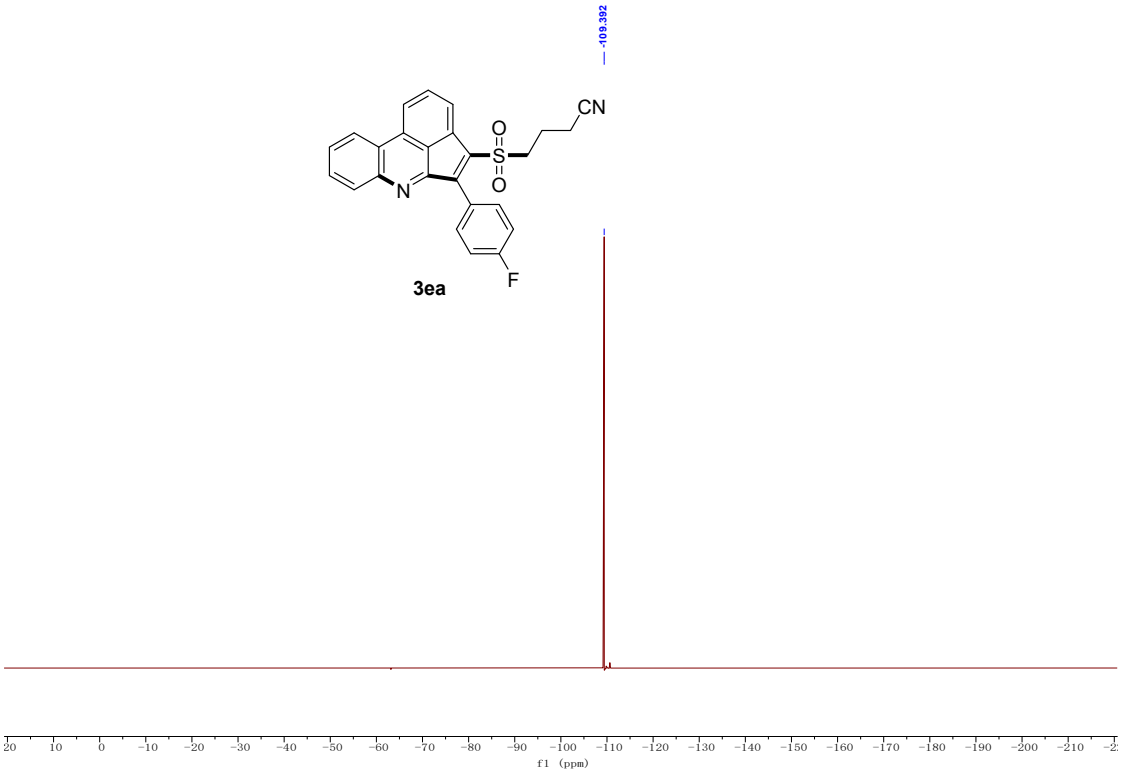
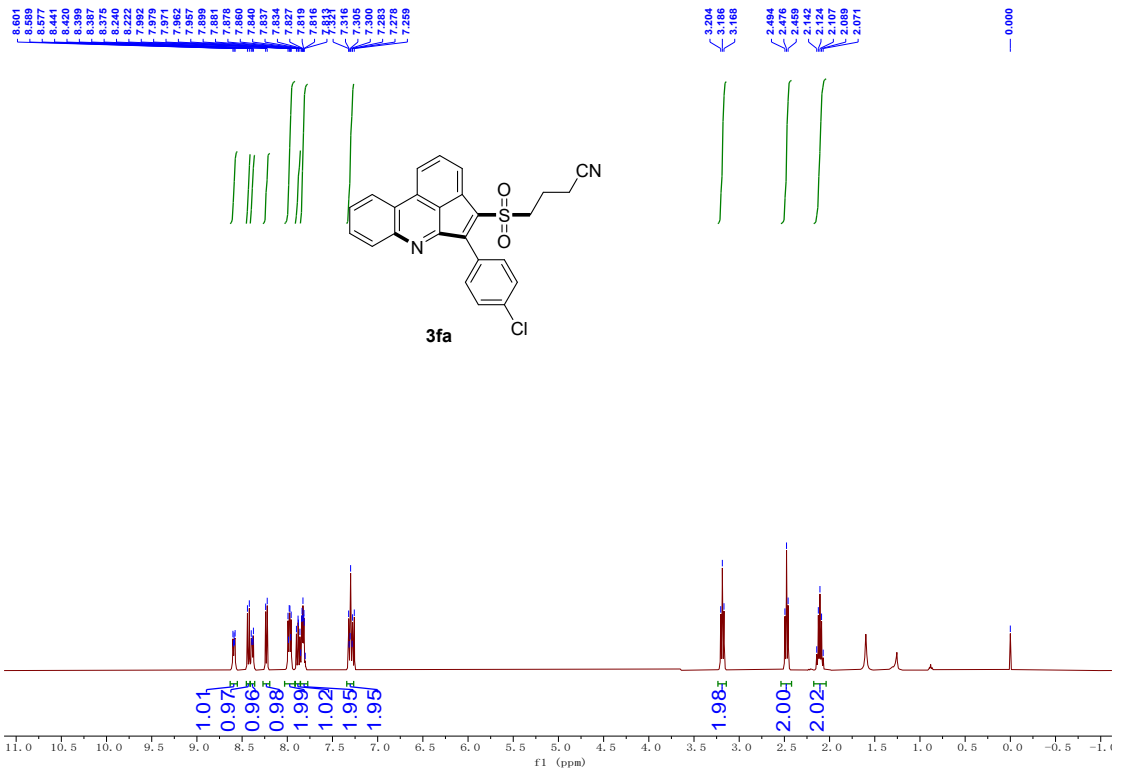
160.330
148.336
147.699
139.044
134.837
133.703
133.619
133.104
132.507
129.315
129.245
125.312
125.264
124.561
123.770
123.068
119.440
117.883
115.690
115.474
77.318
77.000
76.683
53.760
18.900
16.097
CN
O
S
O
N
F
3ea
f1 (ppm)


-109.392
CN
O
S
O
N
F
3ea
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)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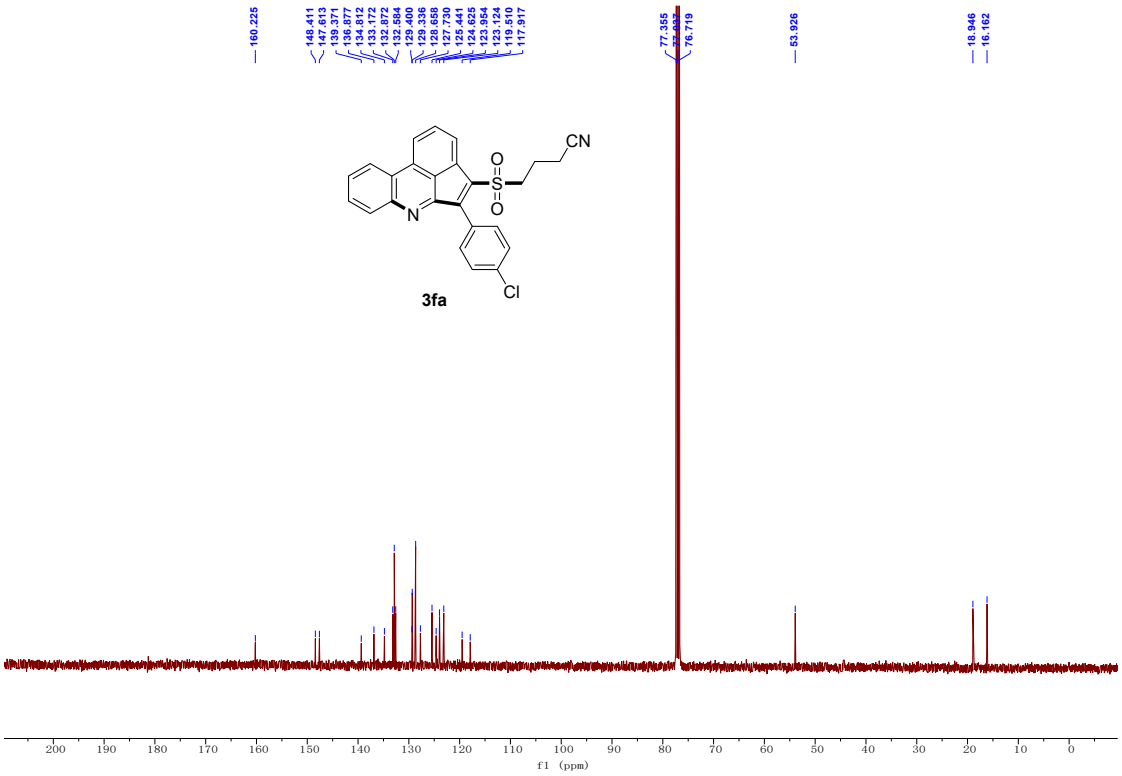
8.589
8.577
8.441
8.420
8.399
8.387
8.375
8.240
8.223
7.992
7.979
7.971
7.962
7.957
7.899
7.881
7.878
7.860
7.840
7.837
7.834
7.827
7.819
7.816
7.321
7.316
7.305
7.300
7.283
7.278
7.259
3.204
3.186
3.168
2.494
2.476
2.459
2.142
2.124
2.107
2.089
2.071
0.000
CN
O
S
O
N
Cl
3fa
1.01
0.97
0.96
0.98
1.99
1.02
1.95
1.95
1.98
2.00
2.02
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
f1 (ppm)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134.812
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132.872
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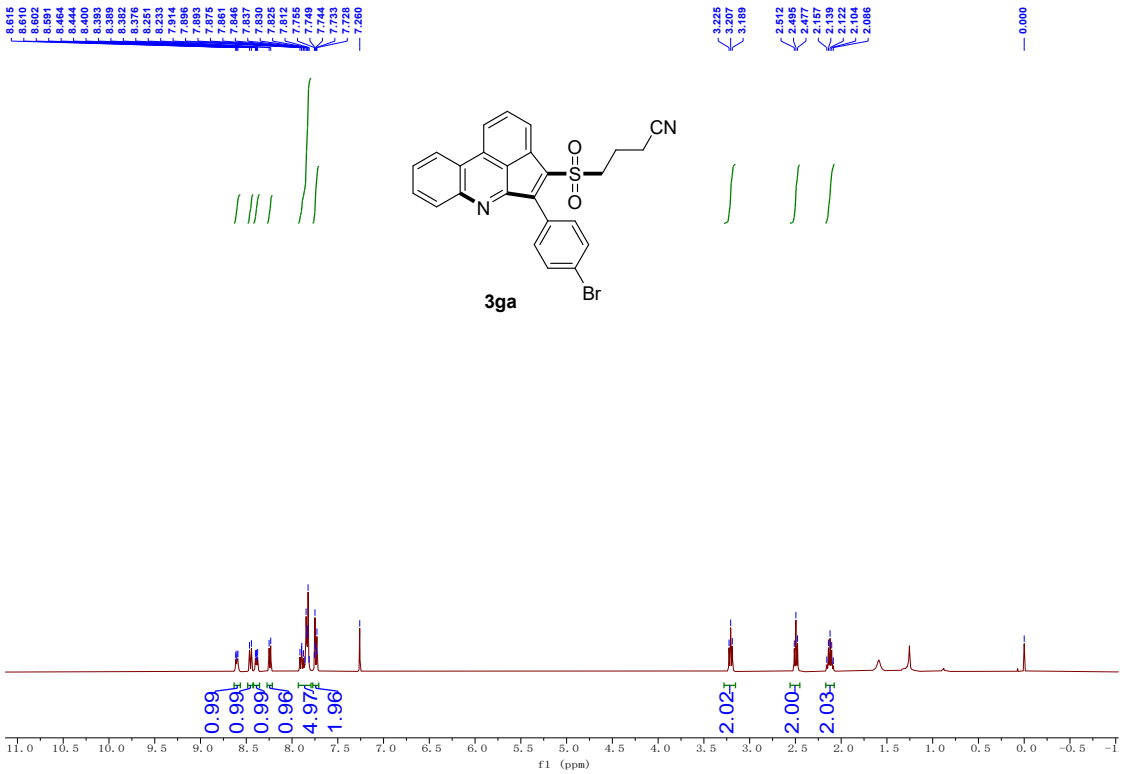
129.400
129.236
128.656
127.730
125.441
124.625
123.954
123.124
119.510
117.917
77.355
77.033
76.719
53.926
18.946
16.162
CN
O
S
O
N
Cl
3fa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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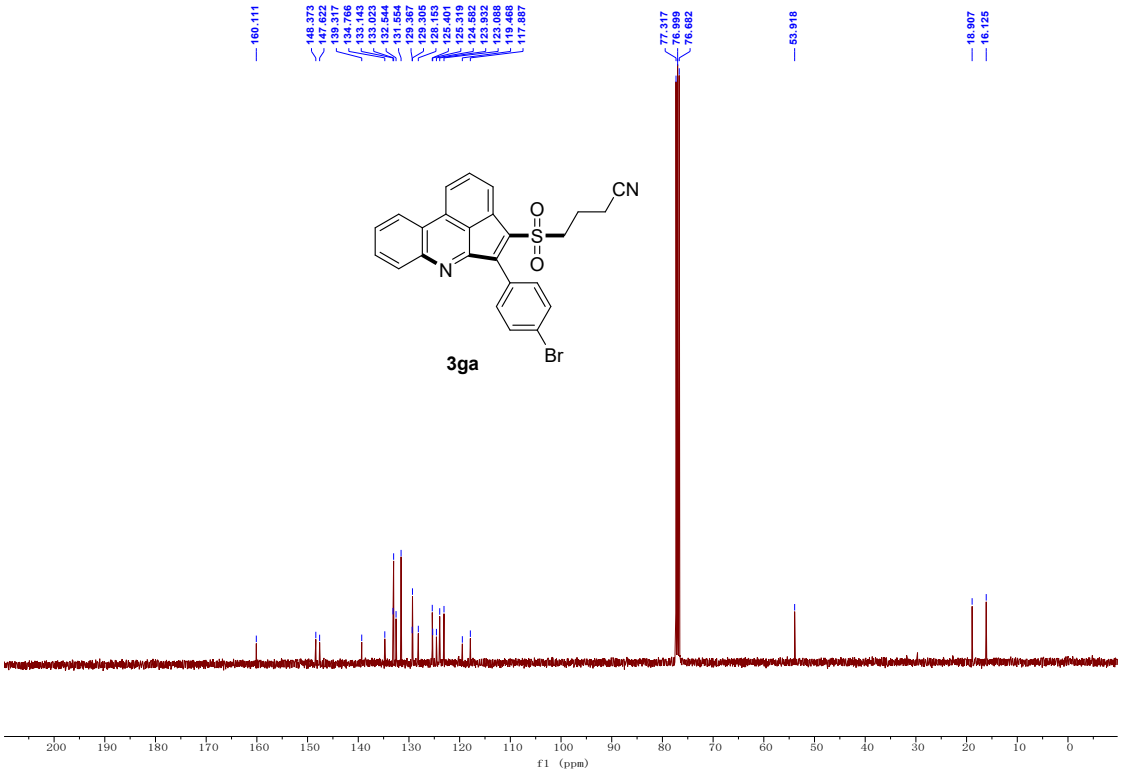
8.444
8.400
8.393
8.389
8.382
8.376
8.251
8.233
7.914
7.896
7.893
7.875
7.861
7.846
7.837
7.830
7.825
7.812
7.755
7.749
7.744
7.733
7.728
7.260
3.225
3.207
3.189
2.512
2.495
2.477
2.157
2.139
2.122
2.104
2.086
0.000
CN
O
S
O
N
Br
3ga
0.99
0.99
0.99
0.96
4.97
1.96
2.02
2.00
2.03
11.0 10.5 10.0 9.5 9.0 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
f1 (ppm)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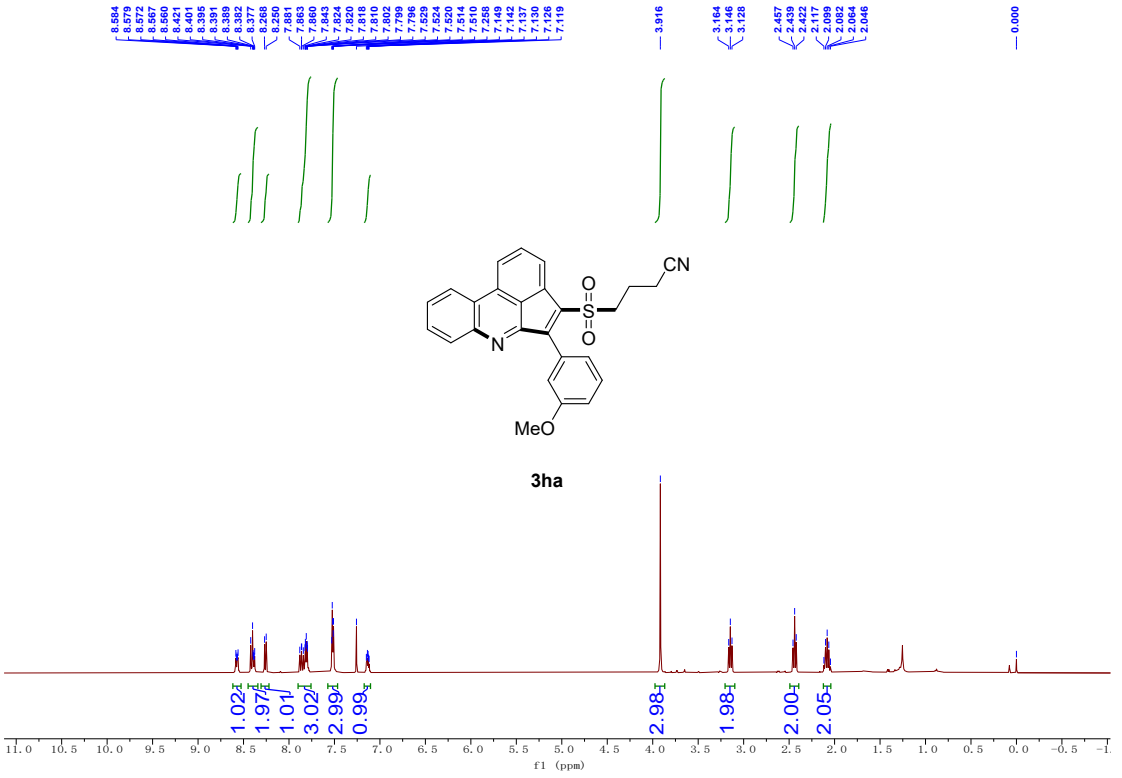
125.401
125.319
124.582
123.932
123.088
119.468
117.887
77.317
76.999
76.682
53.918
18.907
16.125
CN
O
S
O
N
Br
3ga
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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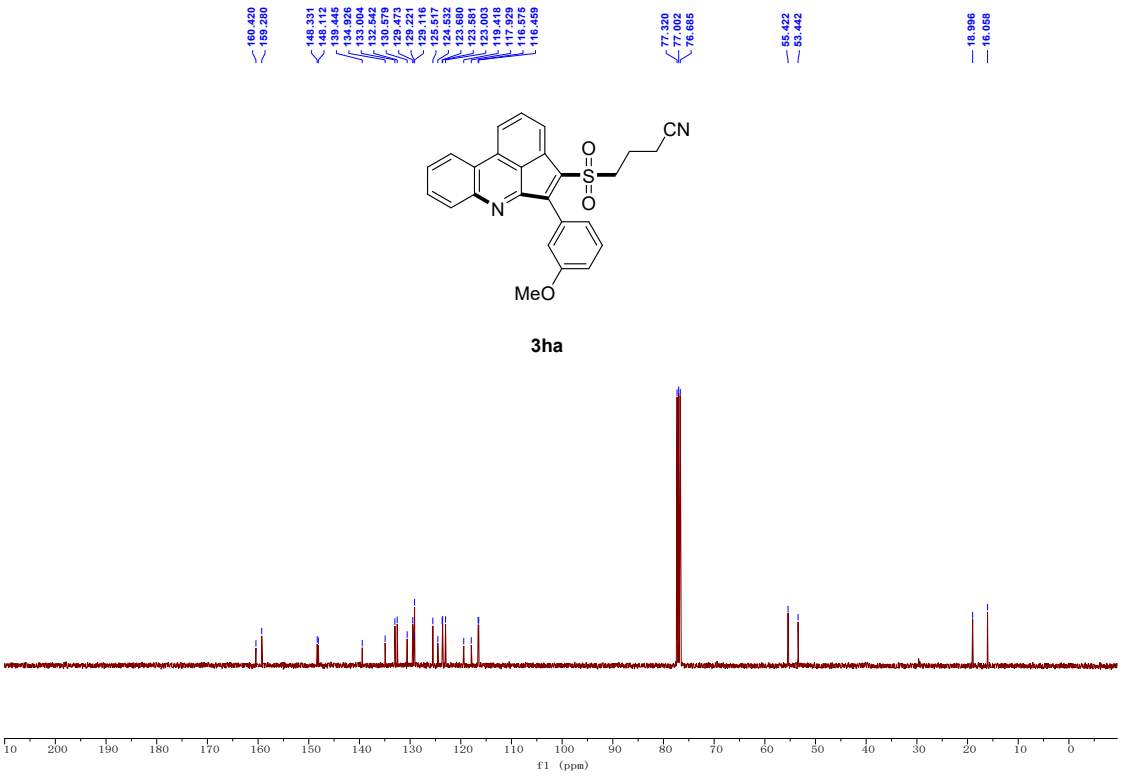
8.268
8.250
7.881
7.865
7.860
7.843
7.834
7.820
7.818
7.810
7.802
7.799
7.796
7.529
7.524
7.520
7.514
7.510
7.258
7.149
7.142
7.137
7.130
7.126
7.119
3.916
3.164
3.146
3.128
2.457
2.439
2.422
2.117
2.099
2.082
2.064
2.046
0.000
CN
O
S
O
N
MeO
3ha
1.02
1.97
1.01
3.02
2.99
0.99
2.98
1.98
2.00
2.05
11.0 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
f1 (ppm)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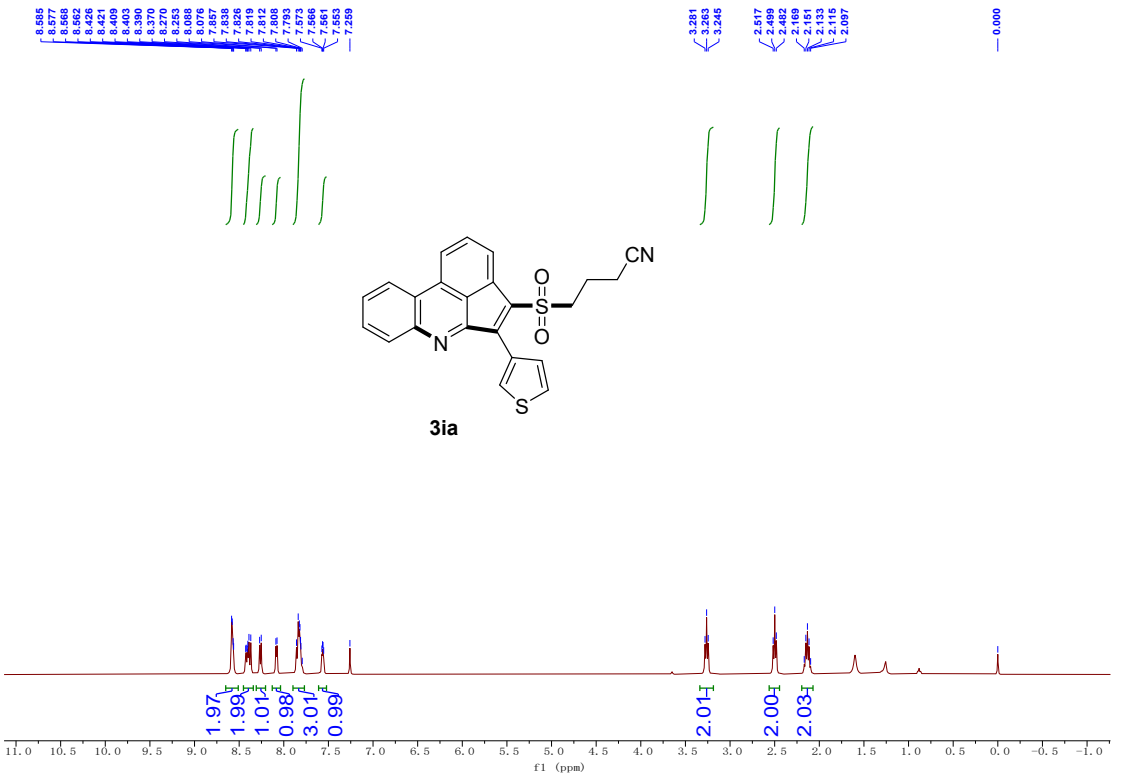
134.926
133.004
132.542
130.579
129.473
129.221
129.116
125.517
124.532
123.680
123.581
123.003
119.418
117.929
116.575
116.459
77.320
77.002
76.685
55.422
53.442
18.996
16.058
CN
O
S
O
N
MeO
f1 (ppm)

3ha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8.370
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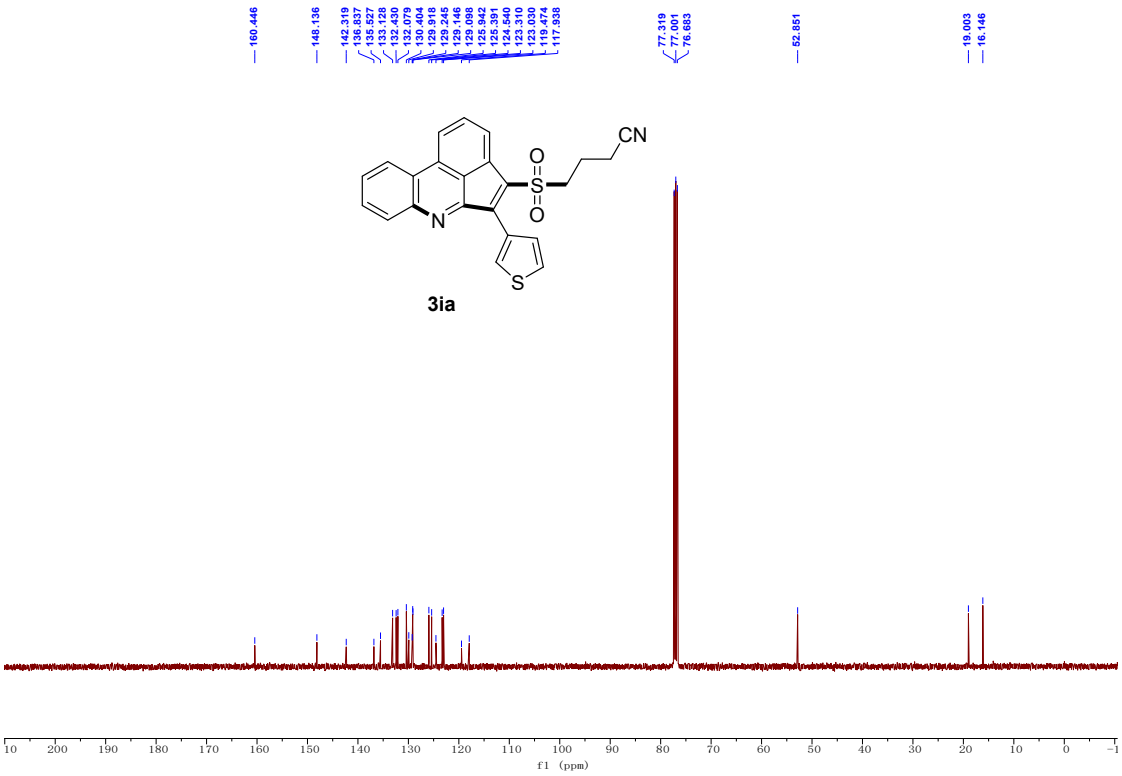
8.253
8.088
8.076
7.857
7.838
7.826
7.819
7.812
7.808
7.793
7.573
7.566
7.561
7.553
7.259
3.281
3.263
3.245
2.517
2.499
2.482
2.169
2.151
2.133
2.115
2.097
0.000
CN
O
S
O
N
S
1.97
1.99
1.01
0.98
3.01
0.99
2.01
2.00
2.03
f1 (ppm)

3ia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132.430
132.070
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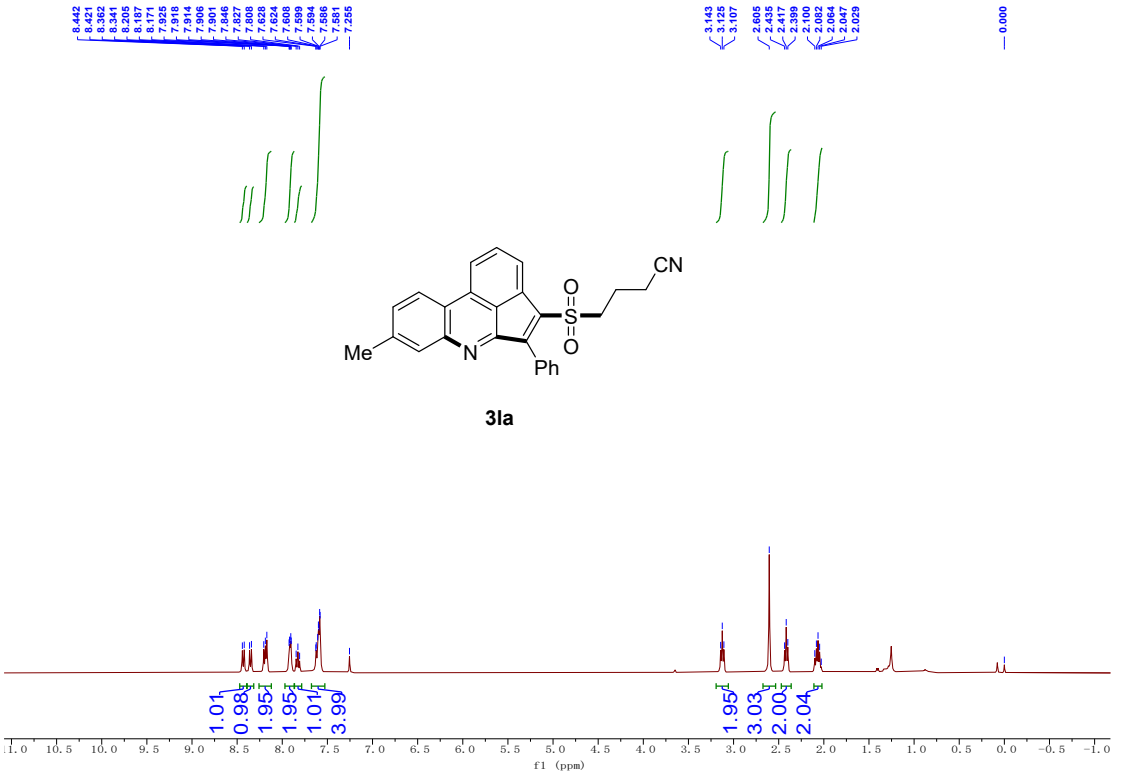
129.918
129.245
129.146
129.098
125.942
125.391
124.440
124.310
123.030
119.474
117.938
77.319
77.001
76.683
52.851
19.003
16.146
CN
O
S
O
N
S
f1 (ppm)

3ia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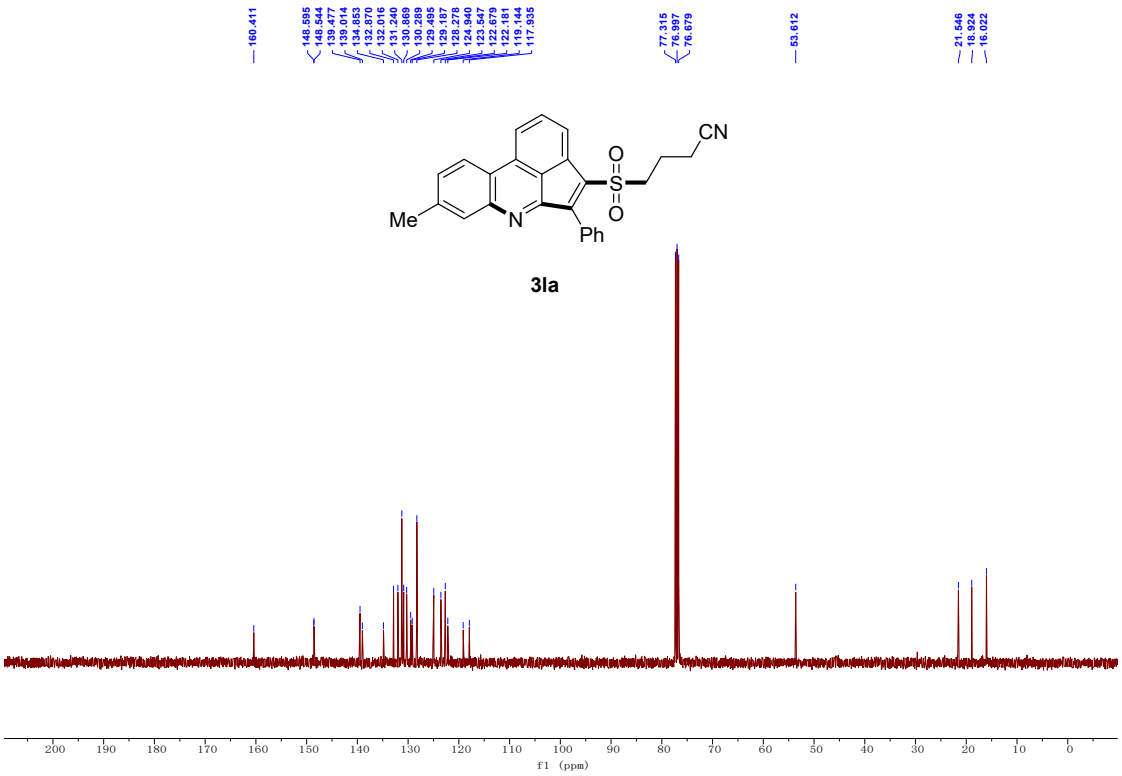
7.918
7.914
7.906
7.901
7.846
7.827
7.808
7.628
7.624
7.608
7.599
7.594
7.586
7.581
7.255
3.143
3.125
3.107
2.605
2.435
2.417
2.399
2.100
2.082
2.064
2.047
2.029
0.000
CN
O
S
O
Me
N
Ph
1.01
0.98
1.95
1.95
1.01
3.99
1.95
3.03
2.00
2.04
f1 (ppm)

3la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132.016
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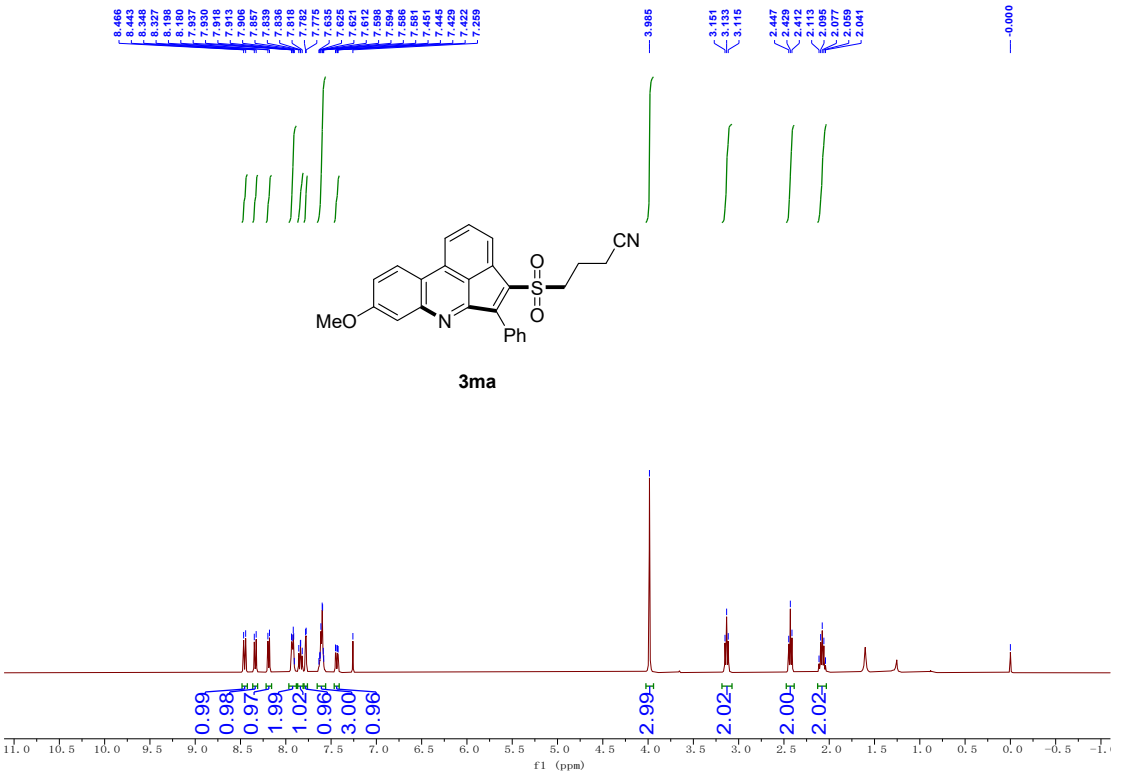
130.869
130.289
129.495
129.187
128.278
124.940
123.547
122.679
122.151
119.144
117.935
77.315
76.997
76.679
53.612
21.546
18.924
16.022
CN
O
S
O
Me
N
Ph
f1 (ppm)

3la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8.327
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8.180
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7.930
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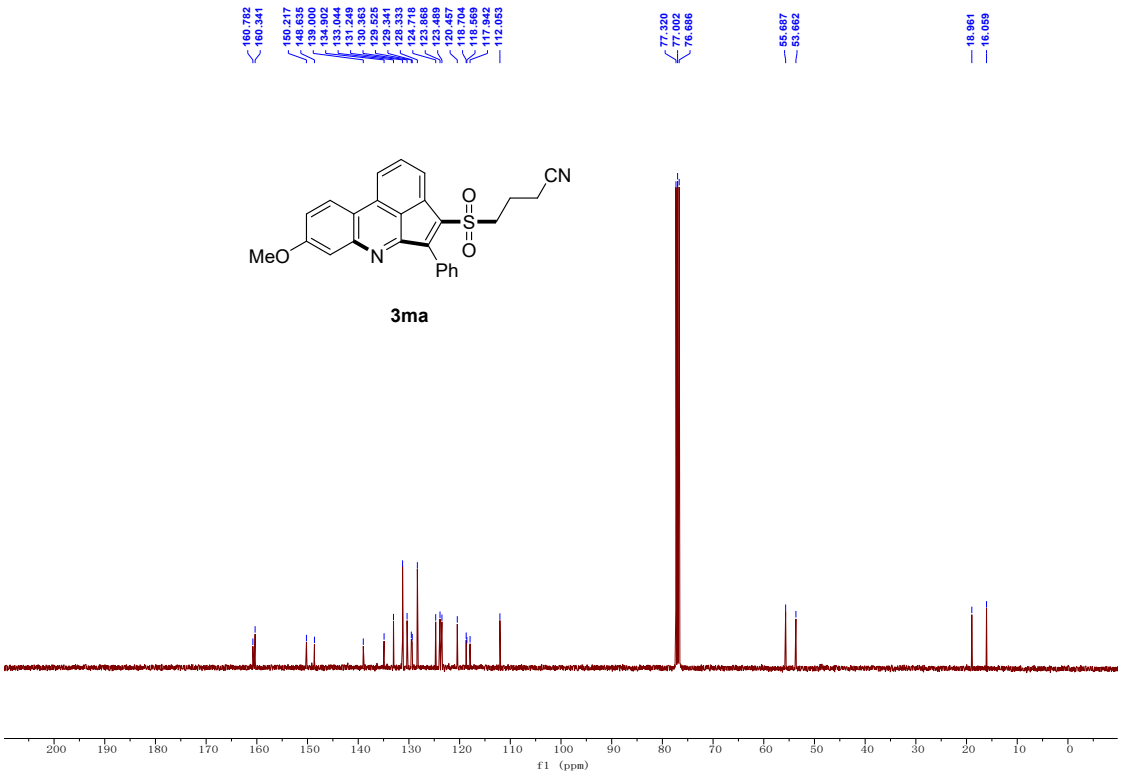
7.857
7.839
7.836
7.818
7.782
7.775
7.635
7.625
7.621
7.612
7.598
7.594
7.586
7.581
7.451
7.445
7.429
7.422
7.259
3.985
3.151
3.133
3.115
2.447
2.429
2.412
2.113
2.095
2.077
2.069
2.041
0.000
CN
O
S
O
MeO
N
Ph
0.99
0.98
0.97
1.99
1.02
0.96
3.00
0.96
2.99
2.02
2.00
2.02
f1 (ppm)

3ma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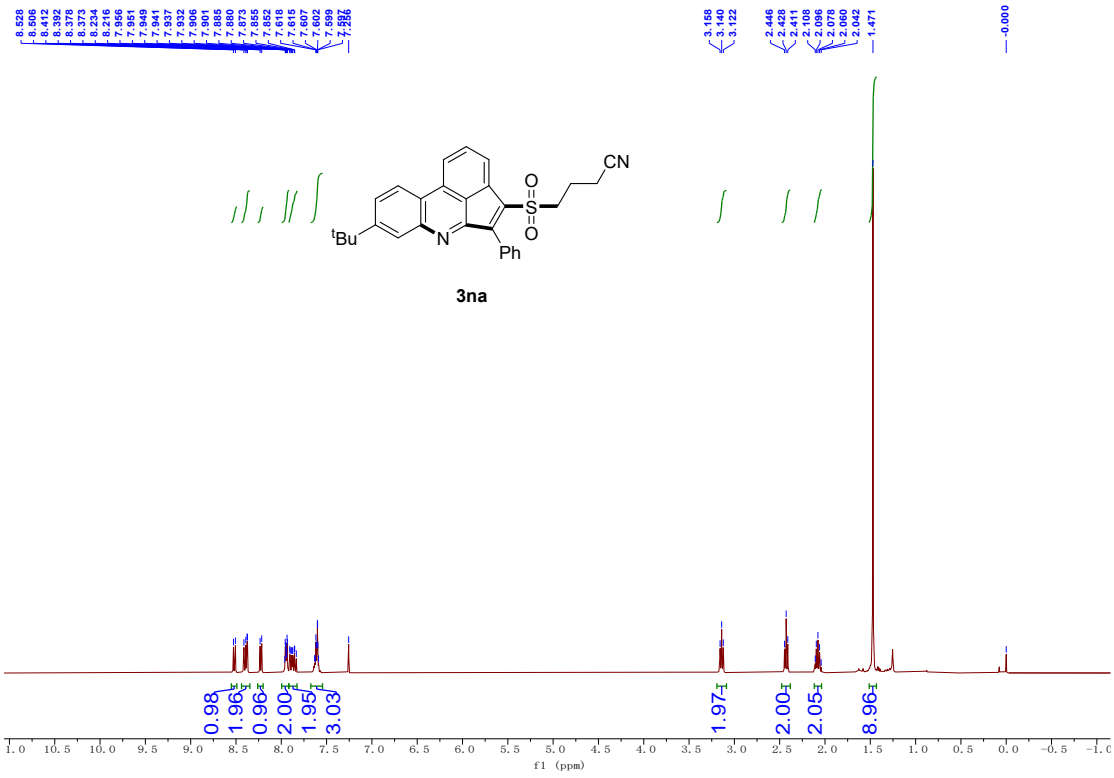
134.992
134.044
131.249
130.363
129.525
129.341
128.333
124.718
123.868
123.459
120.457
118.704
118.569
117.942
112.053
77.320
77.002
76.686
55.687
53.662
18.961
16.059
CN
O
S
O
MeO
N
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3ma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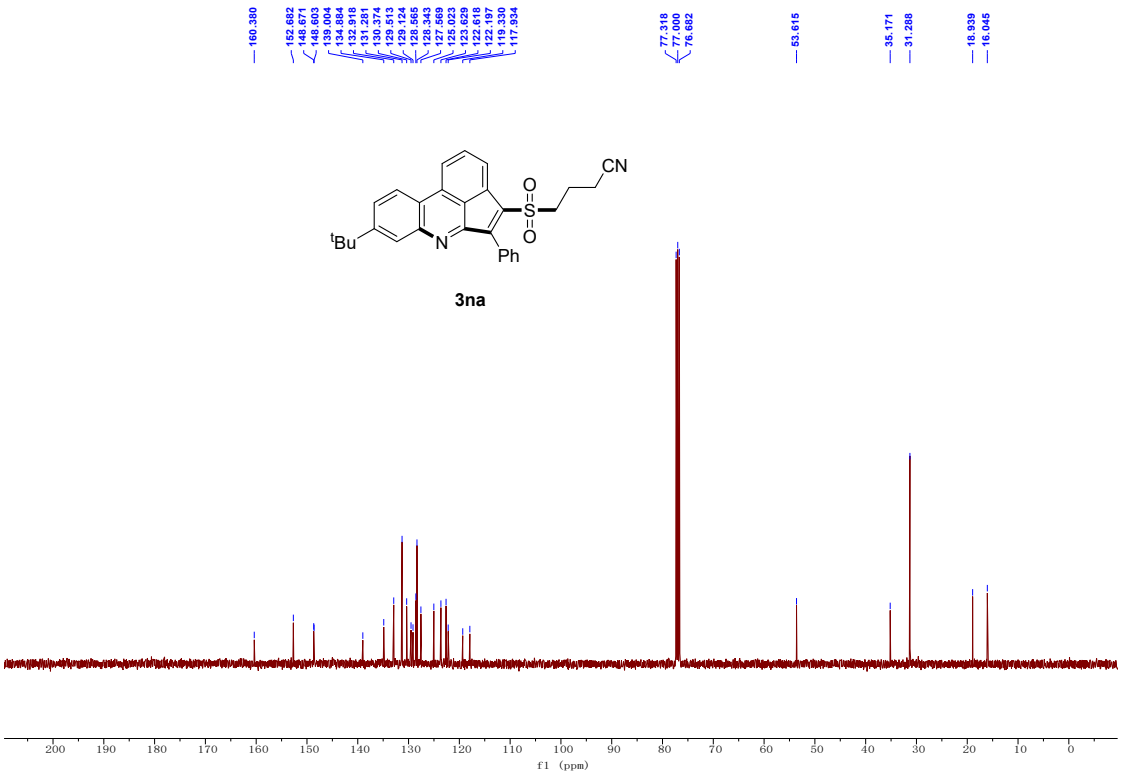
8.412
8.392
8.378
8.373
8.234
8.216
7.956
7.951
7.949
7.941
7.937
7.932
7.906
7.901
7.885
7.880
7.873
7.855
7.852
7.618
7.615
7.607
7.602
7.599
7.587
7.584
3.158
3.140
3.122
2.446
2.428
2.411
2.108
2.096
2.078
2.060
2.042
1.471
-0.000
CN
O
S
O
tBu
N
Ph
0.98
1.96
0.96
2.00
1.95
3.03
1.97
2.00
2.05
8.96
f1 (ppm)

3na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131.281
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129.513
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128.565
128.343
127.569
126.023
123.678
122.615
122.197
119.330
117.934
77.318
77.000
76.682
53.615
35.171
31.288
18.939
16.045
CN
O
S
O
tBu
N
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
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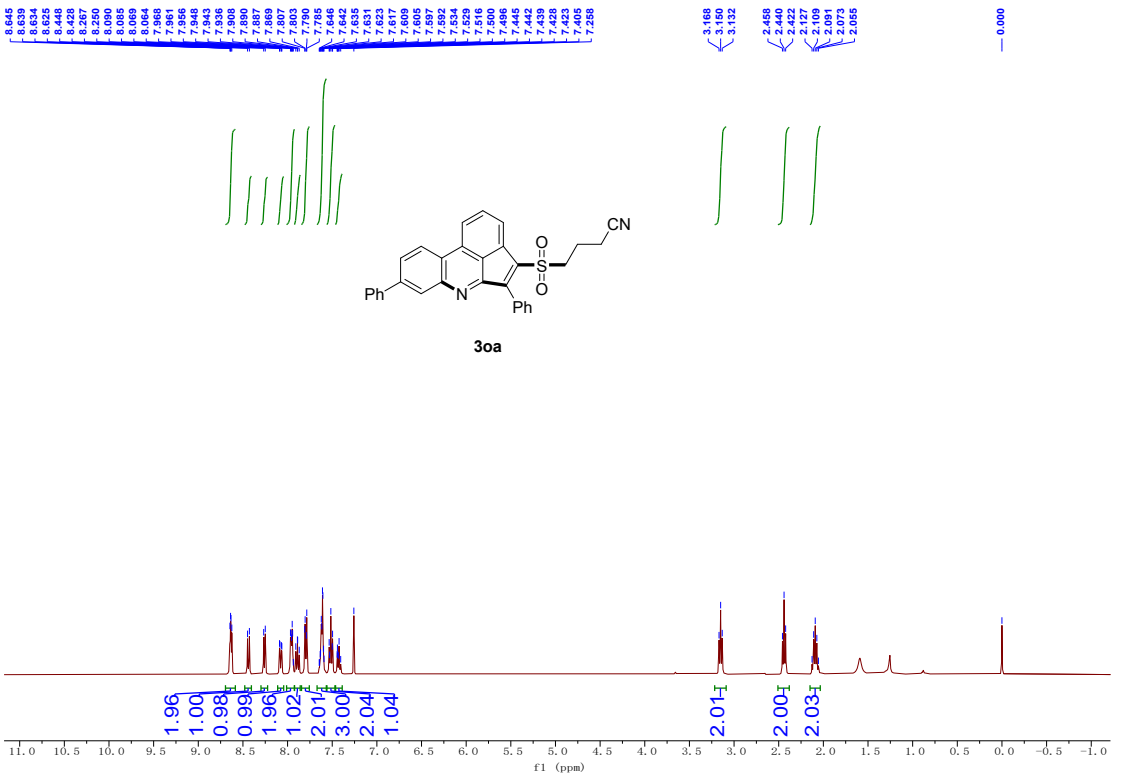
30
20
10
0
f1 (ppm)

3na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8.625
8.446
8.439
8.267
8.250
8.090
8.085
8.069
8.064
7.968
7.961
7.956
7.948
7.943
7.936
7.908
7.890
7.887
7.869
7.807
7.803
7.790
7.785
7.646
7.642
7.635
7.631
7.623
7.617
7.609
7.605
7.597
7.592
7.534
7.529
7.516
7.500
7.496
7.445
7.442
7.439
7.428
7.423
7.405
7.258
3.168
3.150
3.132
2.458
2.440
2.422
2.127
2.109
2.091
2.073
2.055
0.000
CN
O
S
O
Ph
N
Ph
1.96
1.00
0.98
0.99
1.96
1.02
2.01
3.00
2.04
1.04
2.01
2.00
2.03
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
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2.0
1.5
1.0
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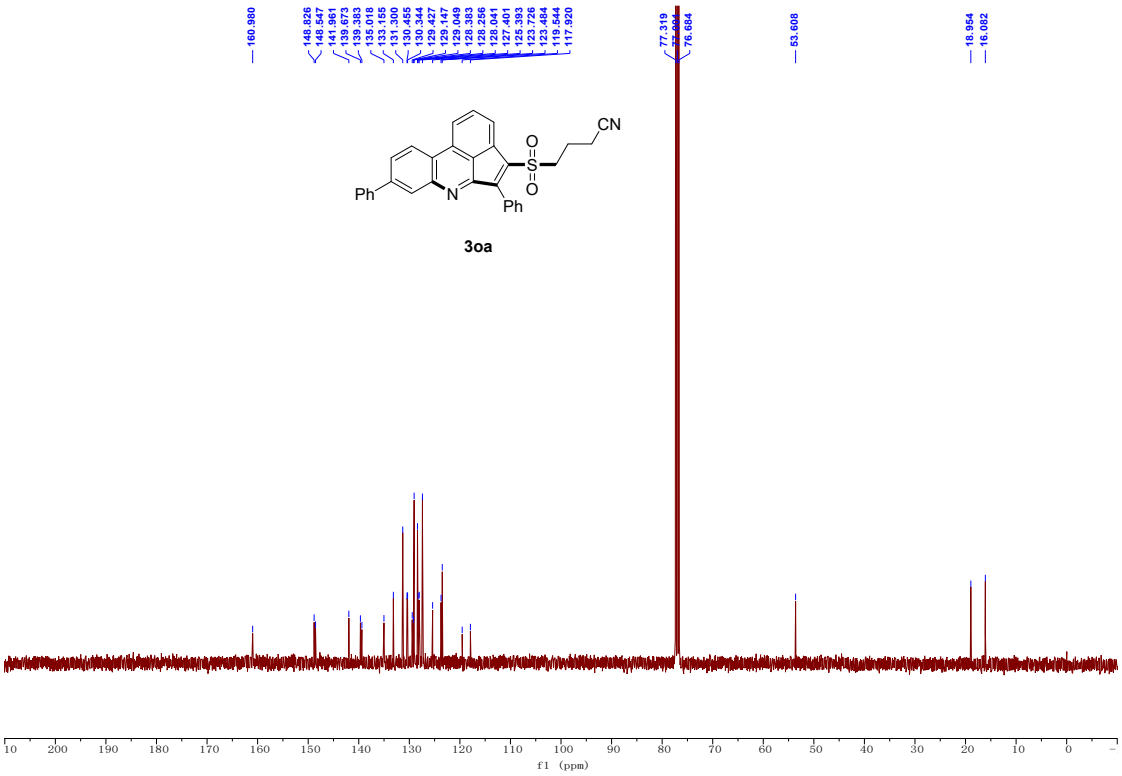
−1.0
f1 (ppm)

3oa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135.018
133.155
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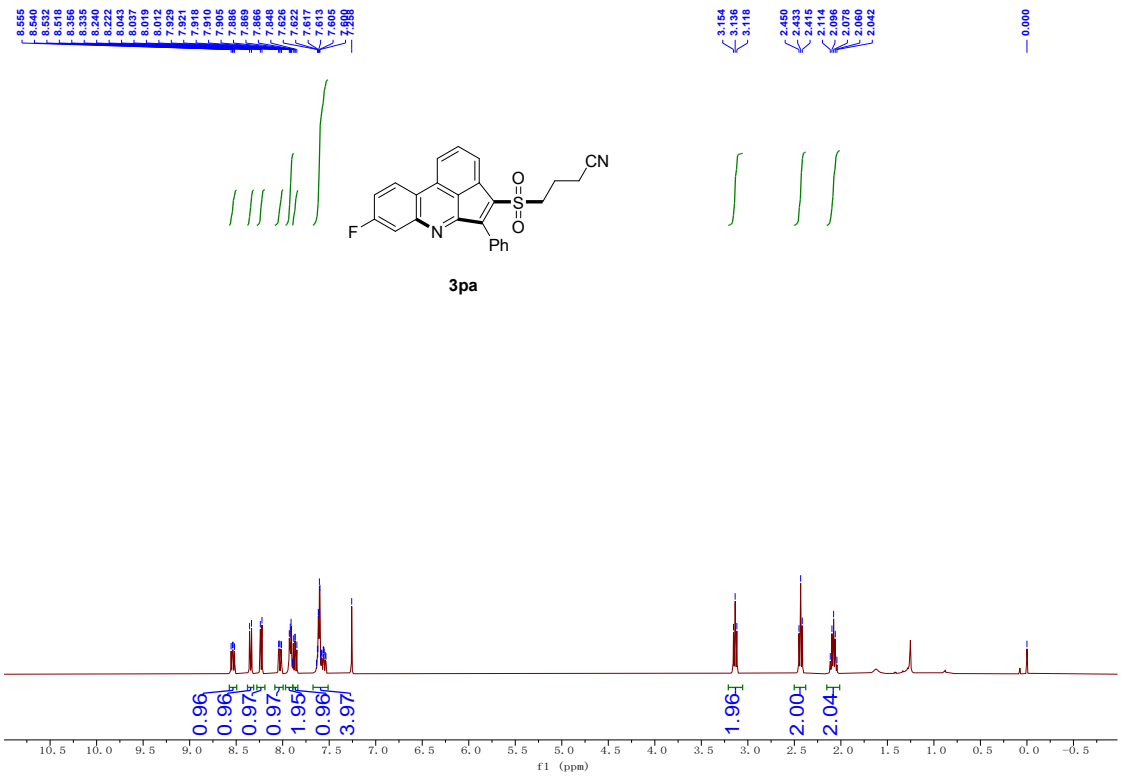
130.455
130.344
129.427
129.147
129.049
128.383
128.256
128.041
127.401
125.393
123.726
123.484
119.544
117.920
77.319
77.004
76.684
53.608
18.954
16.082
CN
O
S
O
Ph
N
Ph
f1 (ppm)

3oa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8.540
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8.335
8.240
8.222
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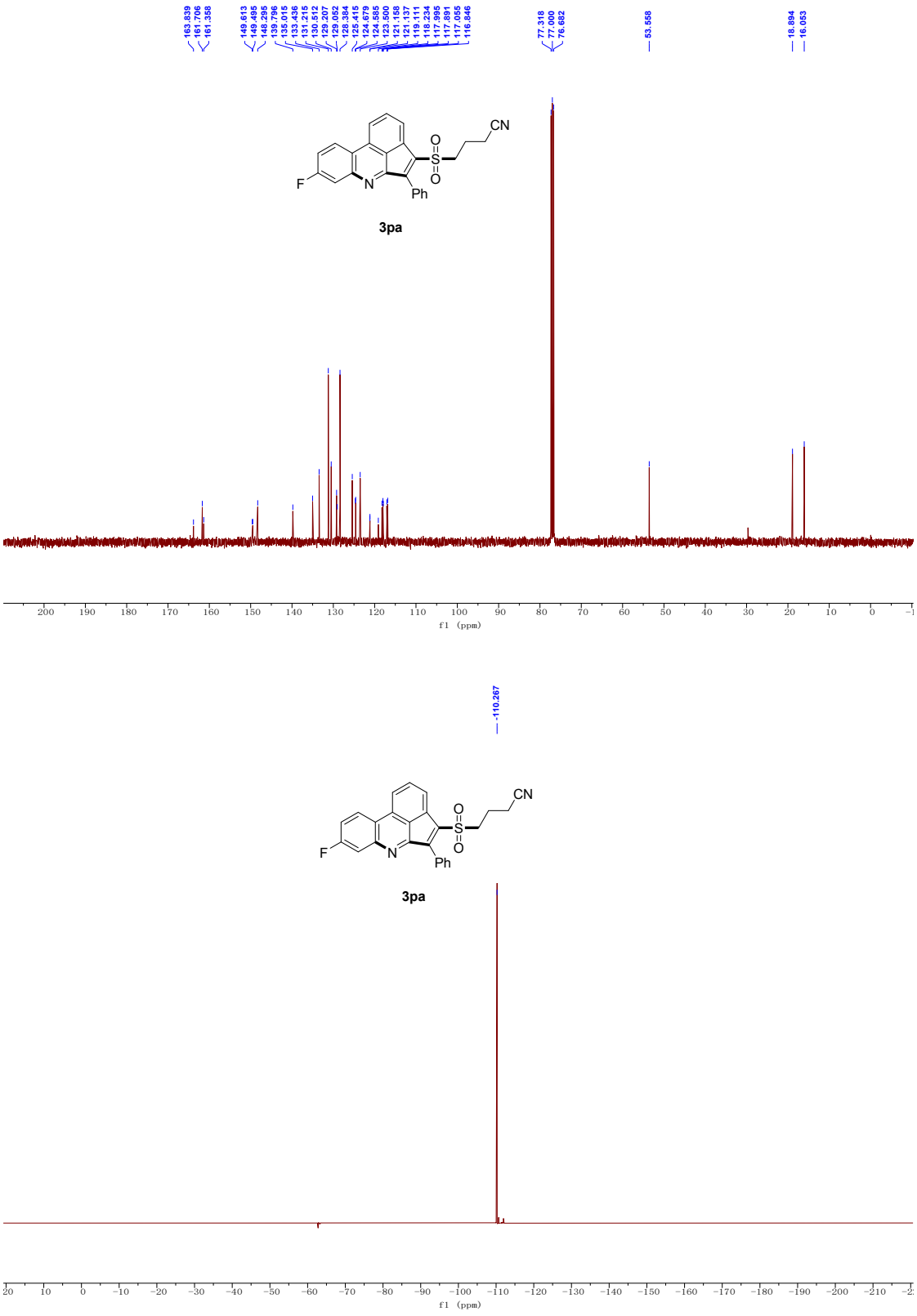
8.037
8.019
8.012
7.939
7.921
7.918
7.910
7.905
7.886
7.869
7.866
7.848
7.626
7.622
7.617
7.613
7.605
7.288
3.154
3.136
3.118
2.450
2.433
2.415
2.114
2.096
2.078
2.060
2.042
0.000
CN
O
S
O
F
N
Ph
0.96
0.96
0.97
0.97
1.95
0.96
3.97
1.96
2.00
2.04
f1 (ppm)

3pa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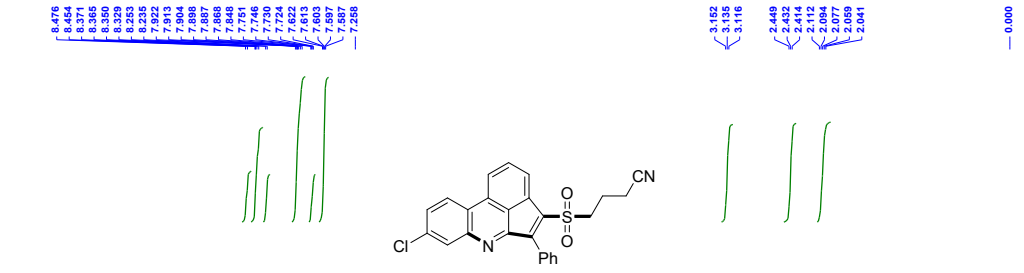
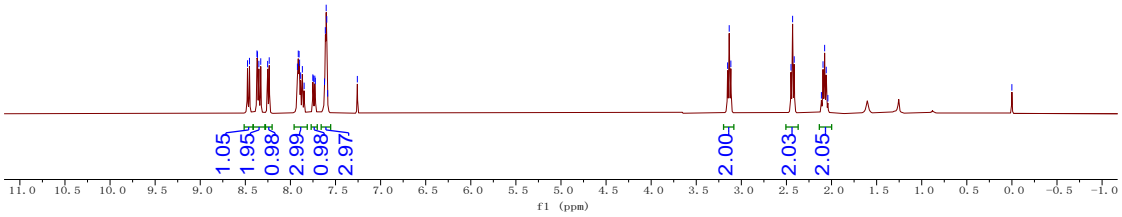
161.706
161.358
149.613
149.495
149.295
139.796
135.015
133.436
131.215
130.512
129.207
129.052
128.304
125.415
124.679
124.585
123.500
121.158
121.137
119.111
118.234
117.895
117.391
117.055
116.846
77.318
77.000
76.682
53.558
18.894
16.053
CN
O
S
O
F
N
Ph
3pa
f1 (ppm)
-110.267
CN
O
S
O
F
N
Ph
3pa
f1 (ppm)


8.476
8.454
8.371
8.365
8.350
8.329
8.253
8.235
7.922
7.913
7.904
7.898
7.887
7.868
7.848
7.751
7.746
7.730
7.722
7.622
7.613
7.603
7.597
7.587
7.258
3.152
3.135
3.116
2.449
2.432
2.414
2.112
2.094
2.077
2.059
2.041
0.000
CN
O
S
O
Cl
N
Ph

3qa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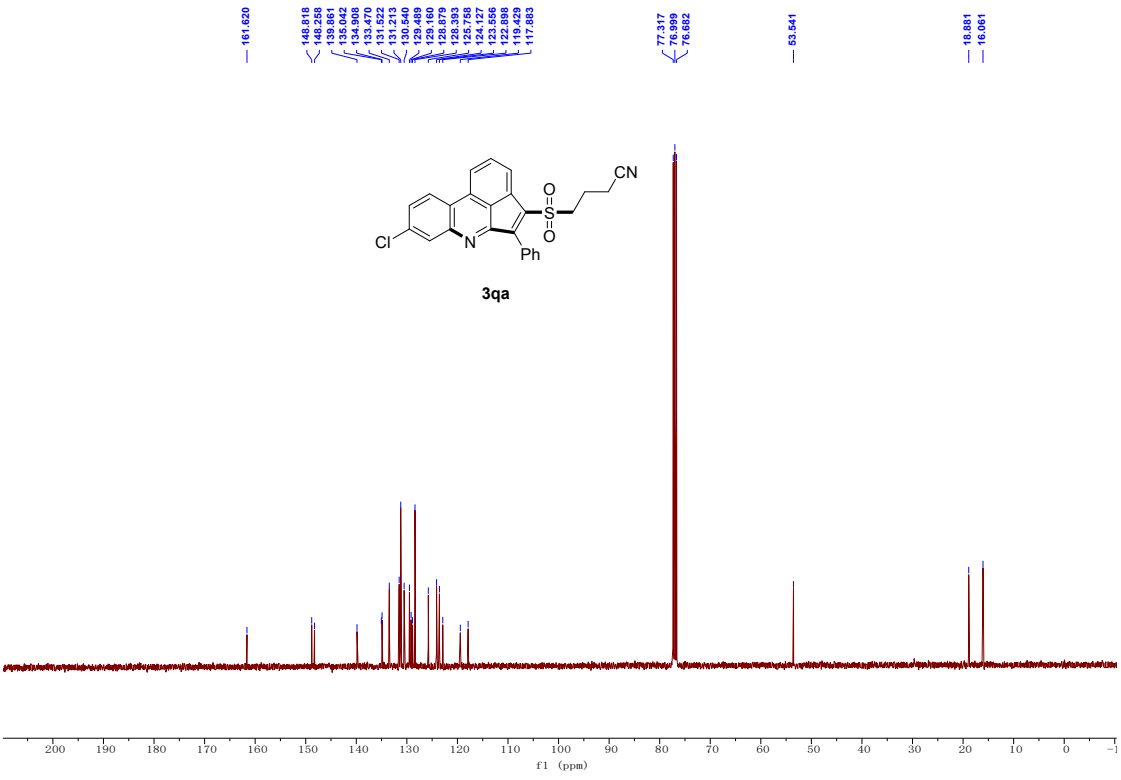
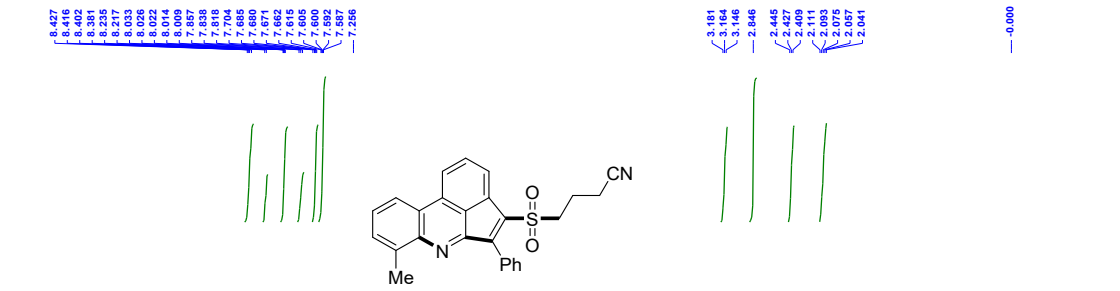
1.95
0.98
2.99
0.98
2.97
2.00
2.03
2.05
f1 (ppm)


161.620
148.818
148.258
139.861
135.042
134.908
133.470
131.622
131.213
130.540
129.489
129.160
128.879
128.393
125.758
124.127
123.566
120.988
119.429
117.883
77.317
76.999
76.682
53.541
18.881
16.061
CN
O
S
O
Cl
N
Ph
f1 (ppm)

3qa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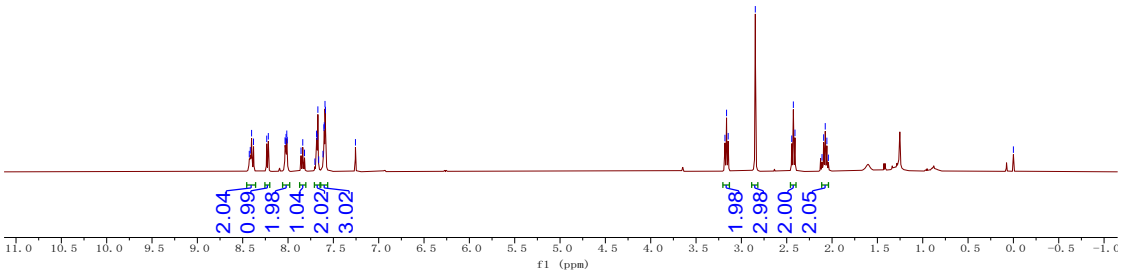
8.235
8.217
8.033
8.026
8.022
8.014
8.009
7.857
7.838
7.818
7.704
7.685
7.680
7.671
7.662
7.615
7.605
7.600
7.592
7.587
7.256
3.181
3.164
3.146
2.846
2.445
2.427
2.409
2.111
2.093
2.075
2.057
2.041
-0.000
CN
O
S
O
N
Ph
Me

3ra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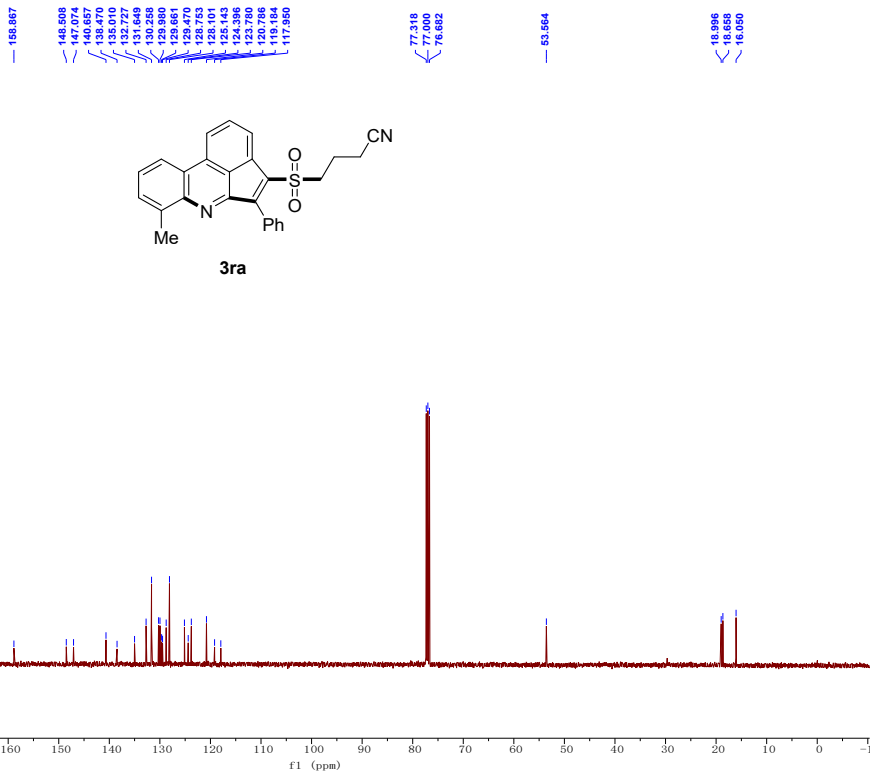
0.99
1.98
1.04
2.02
3.02
1.98
2.98
2.00
2.05
f1 (ppm)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147.074
140.657
138.470
135.010
132.727
131.649
130.258
129.980
129.661
129.470
128.753
128.101
125.143
124.396
123.780
120.786
119.184
117.950
77.318
77.000
76.682
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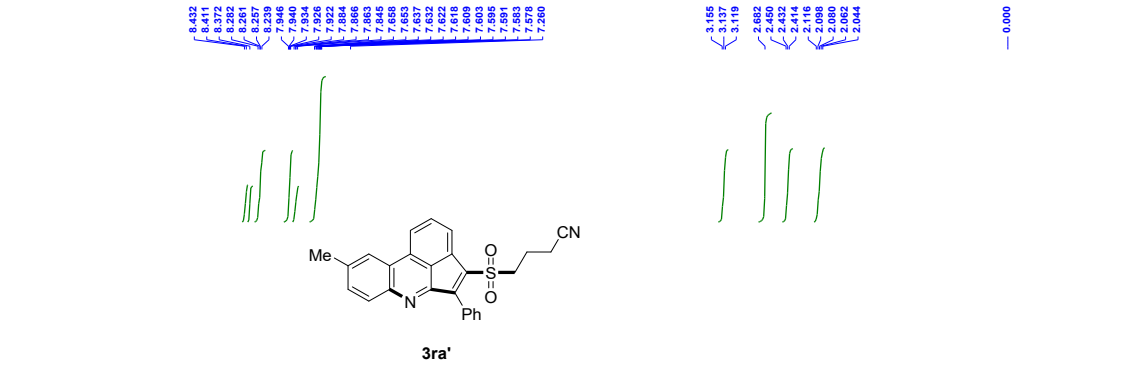
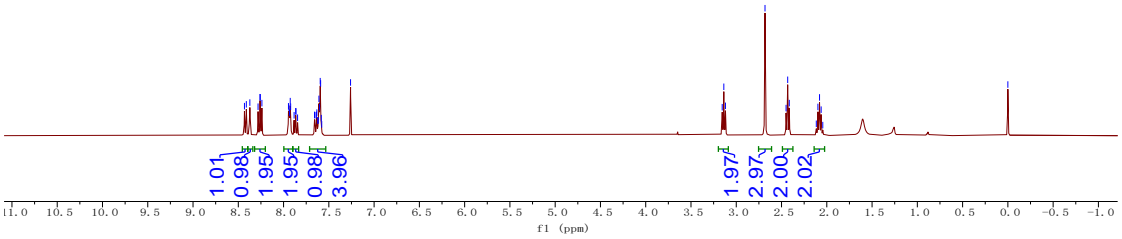
18.996
18.658
16.050
CN
O
S
O
N
Ph
Me
f1 (ppm)

3ra


8.432
8.411
8.372
8.282
8.261
8.257
8.238
7.948
7.940
7.934
7.926
7.922
7.884
7.866
7.863
7.844
7.655
7.653
7.637
7.632
7.622
7.618
7.609
7.603
7.595
7.591
7.583
7.578
7.260
3.155
3.137
3.119
2.682
2.450
2.432
2.414
2.116
2.098
2.080
2.062
2.044
0.000
Me
N
O
S
O
CN
Ph

3ra'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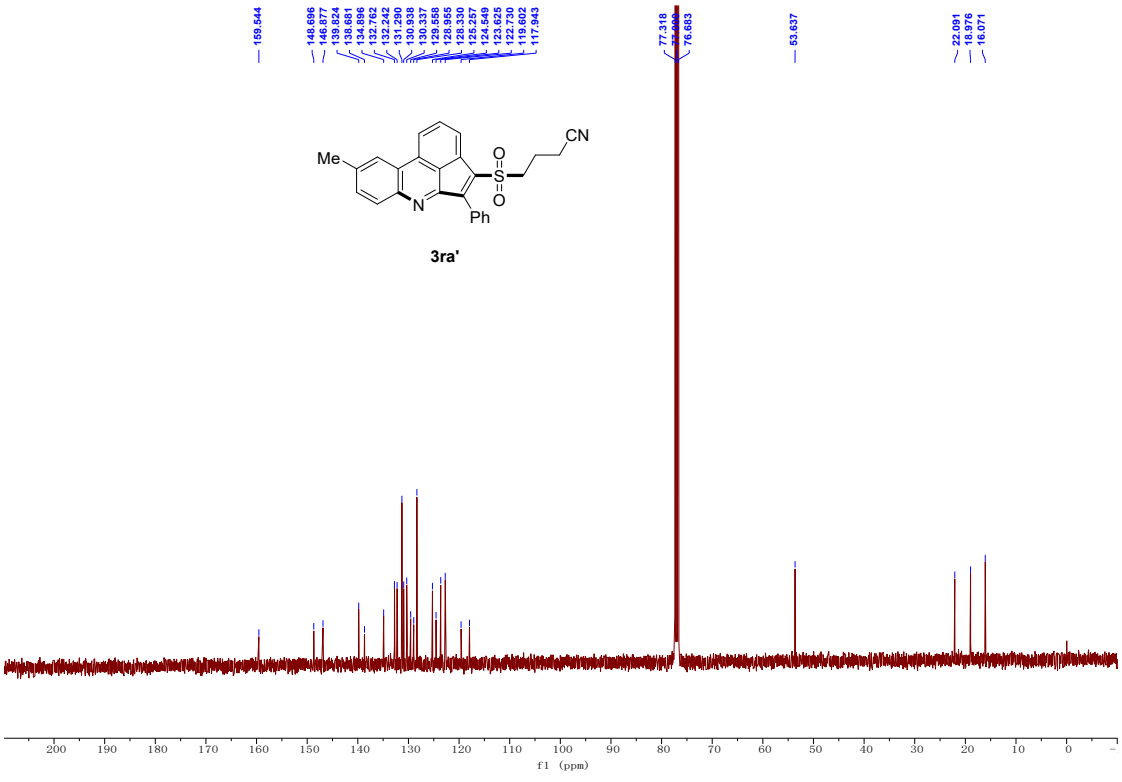
0.98
1.95
1.95
0.98
3.96
1.97
2.97
2.00
2.02
f1 (ppm)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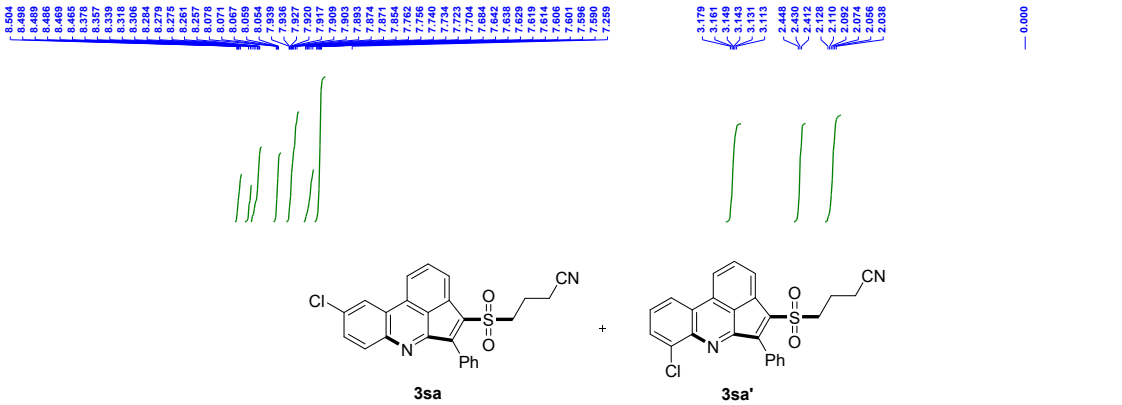
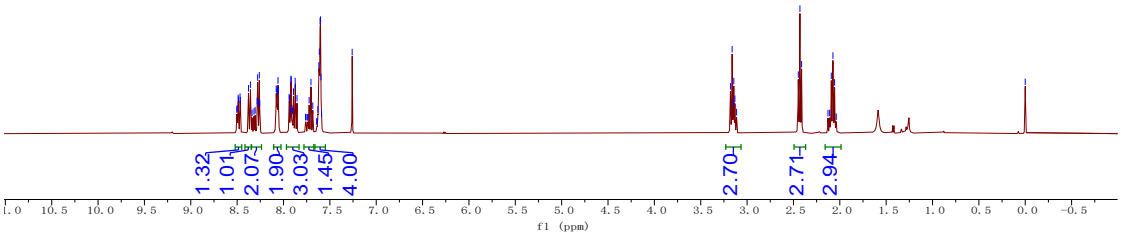
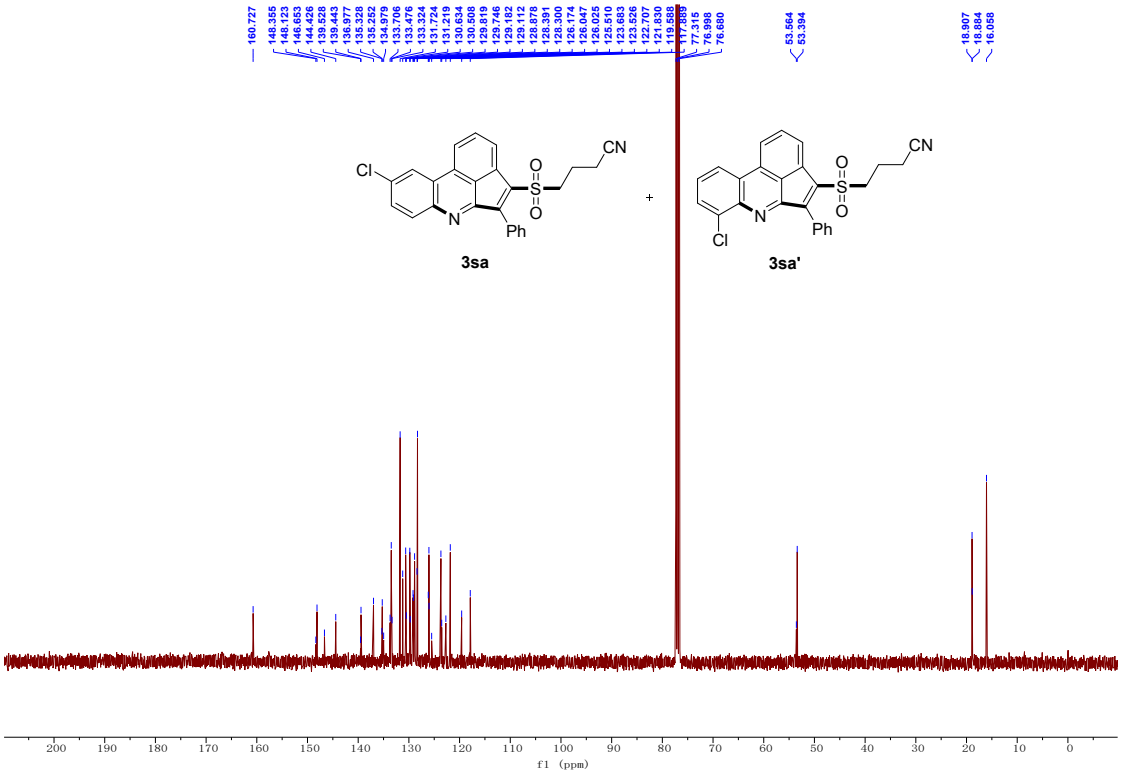
138.681
134.896
132.762
132.242
131.290
130.338
130.337
129.155
128.955
128.330
125.257
124.549
123.625
122.730
119.602
117.943
77.318
77.000
76.683
53.637
22.091
18.976
16.071
Me
N
O
S
O
CN
Ph
f1 (ppm)

3ra'

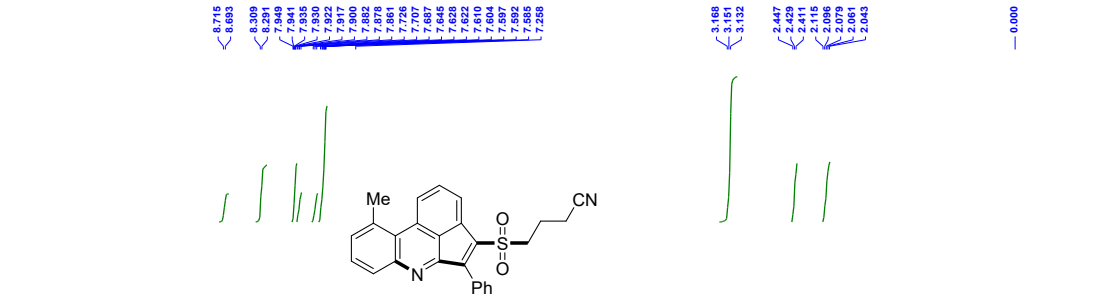


3sa **3sa'**

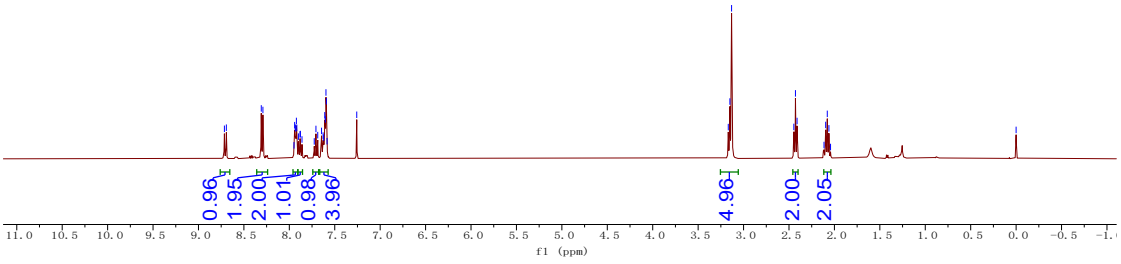




3sa **3sa'**


Me
CN
O
S
O
N
Ph

3ta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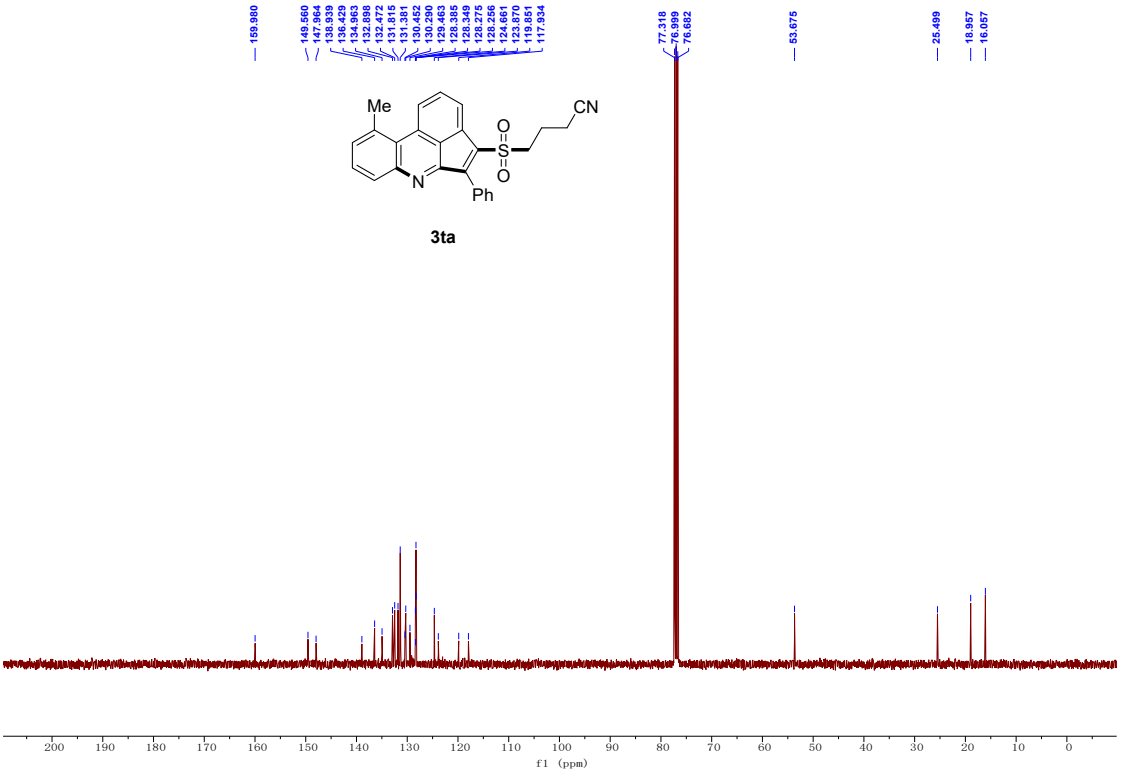
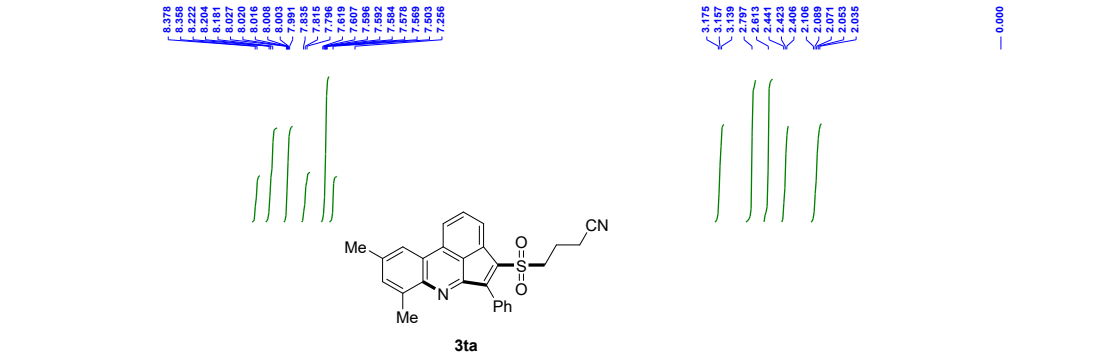
1.01
0.98
3.96
4.96
2.00
2.05
f1 (ppm)


Me
CN
O
S
O
N
Ph
f1 (ppm)

3ta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8.020
8.016
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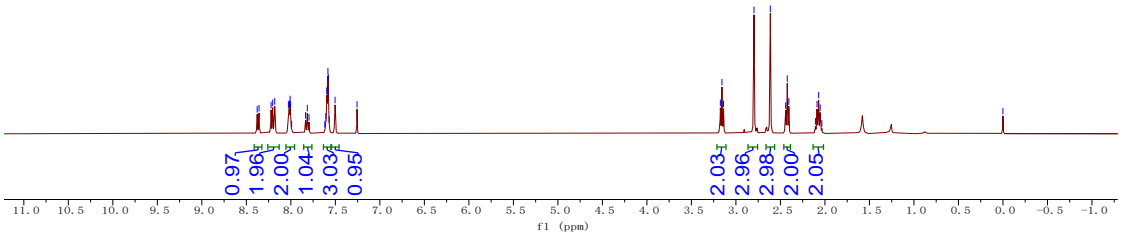
8.003
7.991
7.835
7.815
7.796
7.619
7.607
7.596
7.592
7.584
7.578
7.569
7.503
7.256
3.175
3.157
3.139
2.797
2.551
2.441
2.423
2.406
2.106
2.089
2.071
2.053
2.035
0.000
Me
Me
N
O
S
O
CN
Ph

3ta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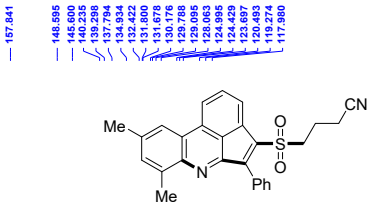
0.95
2.03
2.96
2.98
2.00
2.05
f1 (ppm)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148.595
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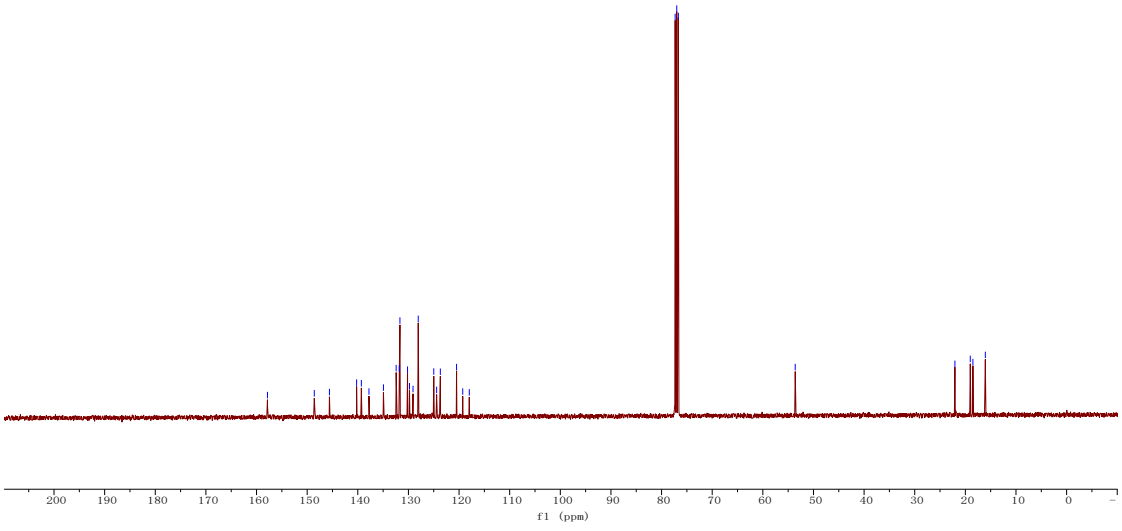
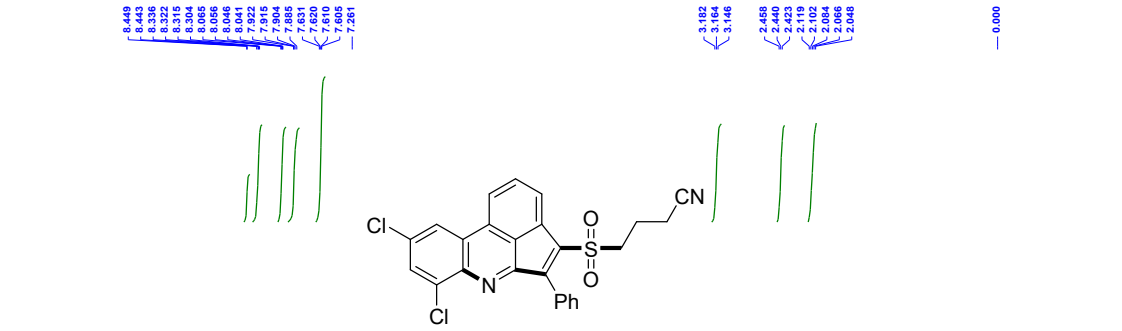
140.235
139.288
137.794
134.934
132.422
131.800
131.678
130.176
129.788
129.085
124.995
124.429
123.697
120.493
119.274
117.980
77.318
77.000
76.683
53.602
22.064
19.026
18.508
16.054
Me
Me
N
O
S
O
CN
Ph

3ta


f1 (ppm)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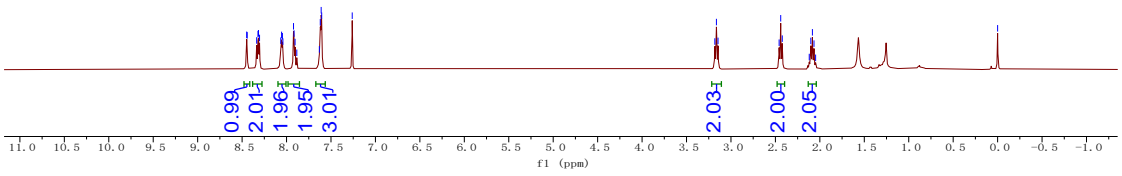
8.322
8.315
8.304
8.065
8.056
8.046
8.041
7.922
7.915
7.904
7.885
7.631
7.620
7.610
7.605
7.261
3.182
3.164
3.146
2.458
2.440
2.423
2.419
2.102
2.084
2.066
2.048
0.000
Cl
N
Cl
O
S
O
CN
Ph

3va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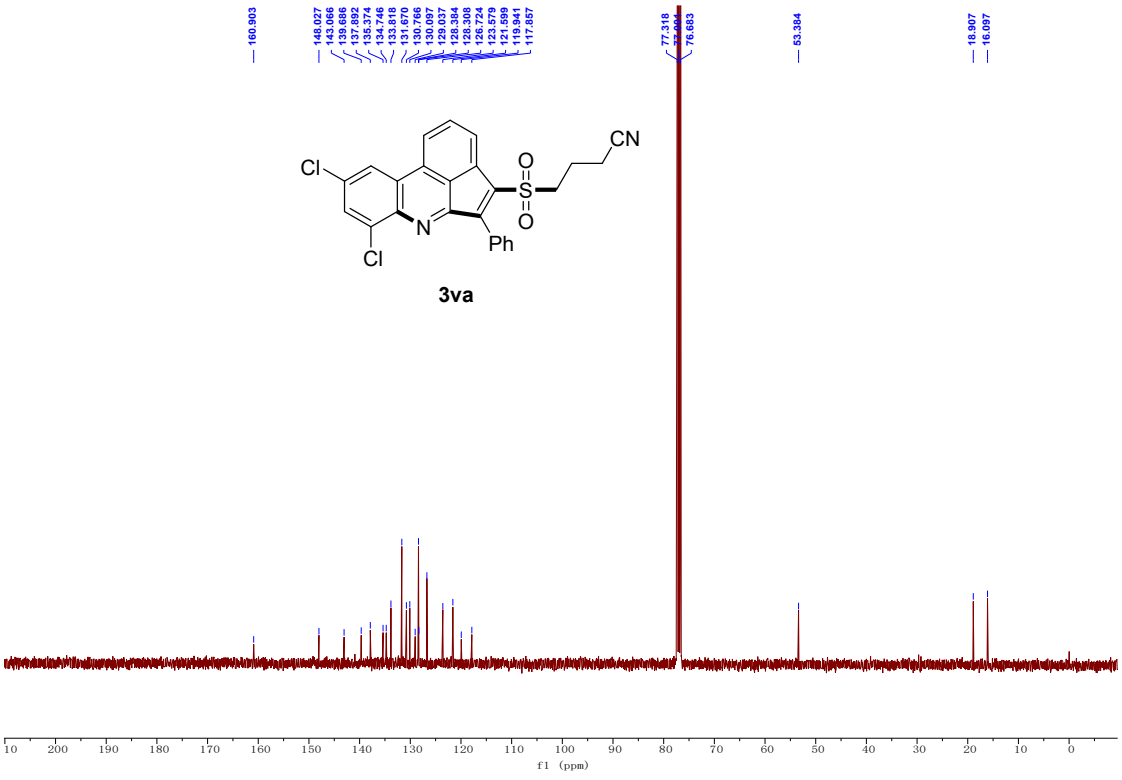
1.96
1.95
3.01
2.03
2.00
2.05
f1 (ppm)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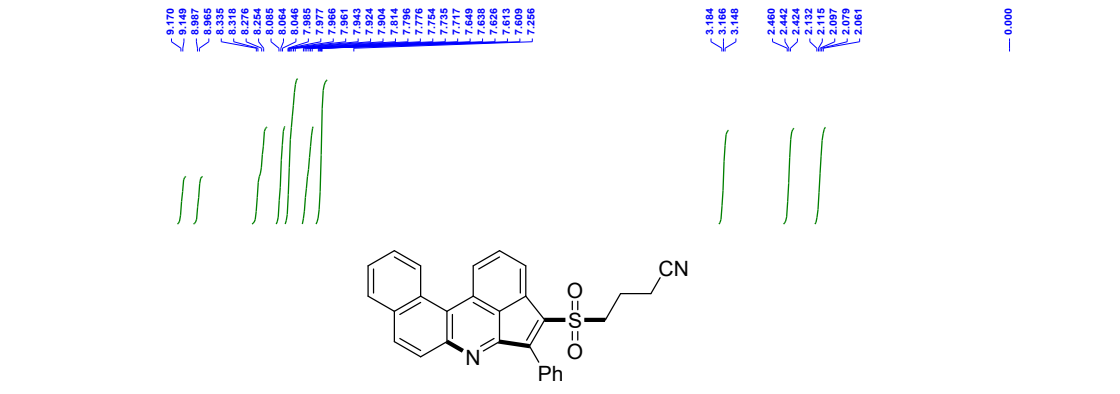
137.882
135.374
134.746
133.818
131.670
130.766
130.097
129.037
128.384
128.308
126.724
125.579
121.599
119.941
117.857
77.318
77.064
76.683
53.384
18.907
16.097
Cl
N
Cl
O
S
O
CN
Ph
f1 (ppm)

3va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8.254
8.085
8.064
8.046
8.025
7.977
7.966
7.961
7.943
7.924
7.904
7.814
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7.638
7.626
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7.599
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3.166
3.148
2.460
2.442
2.424
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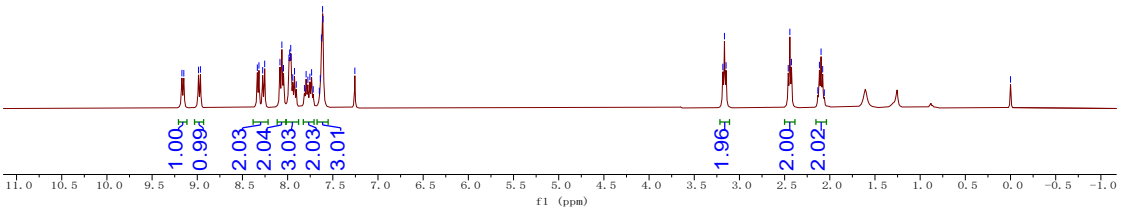
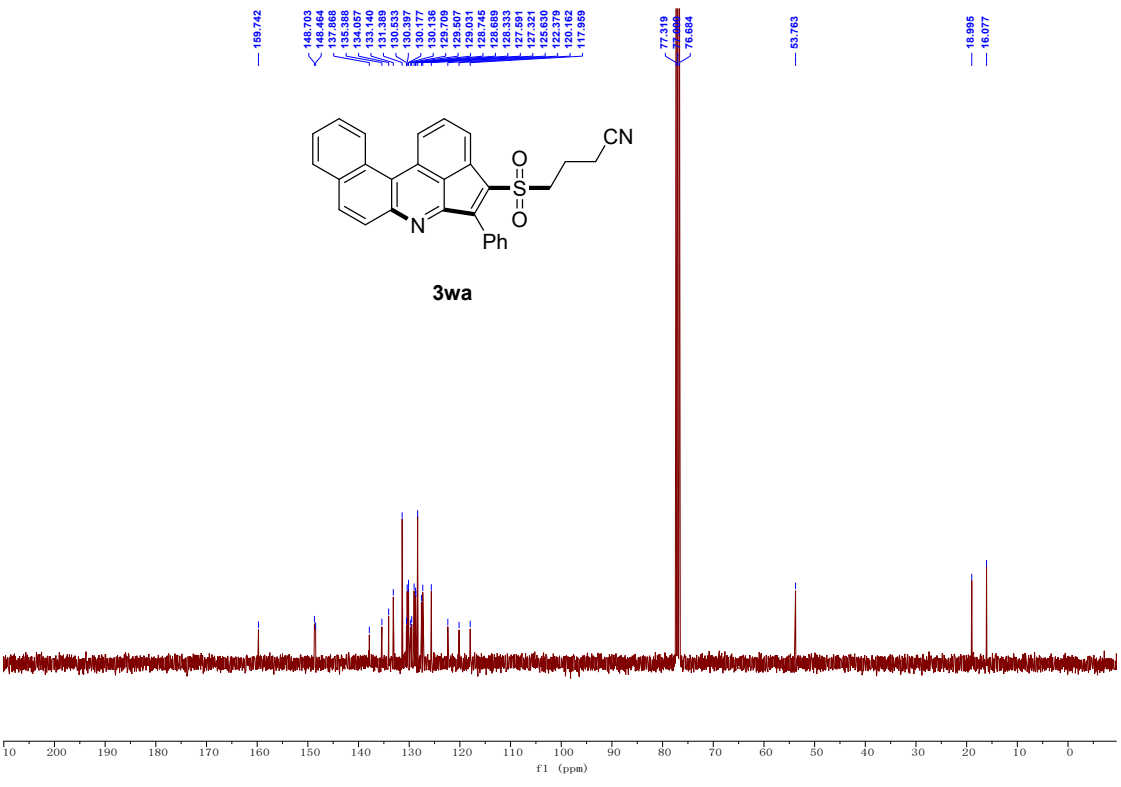
2.115
2.097
2.079
2.061
0.000
CN
O
S
O
N
Ph

3wa


1.00
0.99
2.03
2.04
3.03
2.03
3.01
1.96
2.00
2.02
f1 (ppm)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148.464
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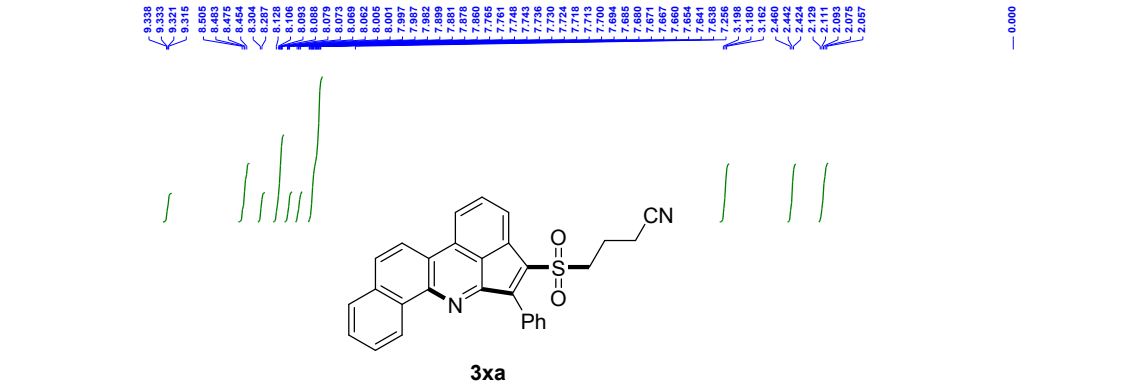
135.388
134.057
133.140
131.389
130.533
130.337
130.177
130.136
129.709
129.507
129.031
128.745
128.689
128.333
127.594
127.321
125.630
122.379
120.162
117.959
77.319
77.000
76.684
53.763
18.995
16.077
CN
O
S
O
N
Ph
f1 (ppm)

3wa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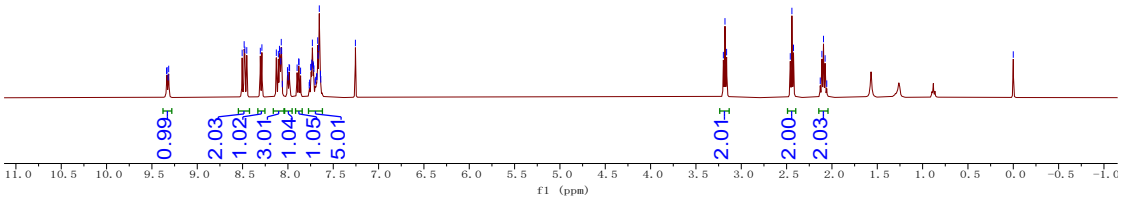
9.333
9.321
9.315
8.505
8.483
8.475
8.454
8.304
8.287
8.128
8.106
8.093
8.088
8.079
8.073
8.069
8.062
8.005
8.001
7.997
7.987
7.982
7.899
7.891
7.878
7.860
7.765
7.761
7.748
7.743
7.736
7.730
7.724
7.715
7.711
7.700
7.694
7.685
7.680
7.671
7.667
7.660
7.654
7.641
7.638
7.256
3.198
3.180
3.162
2.460
2.442
2.424
2.129
2.111
2.093
2.075
2.057
0.000
CN
O
S
O
N
Ph

3xa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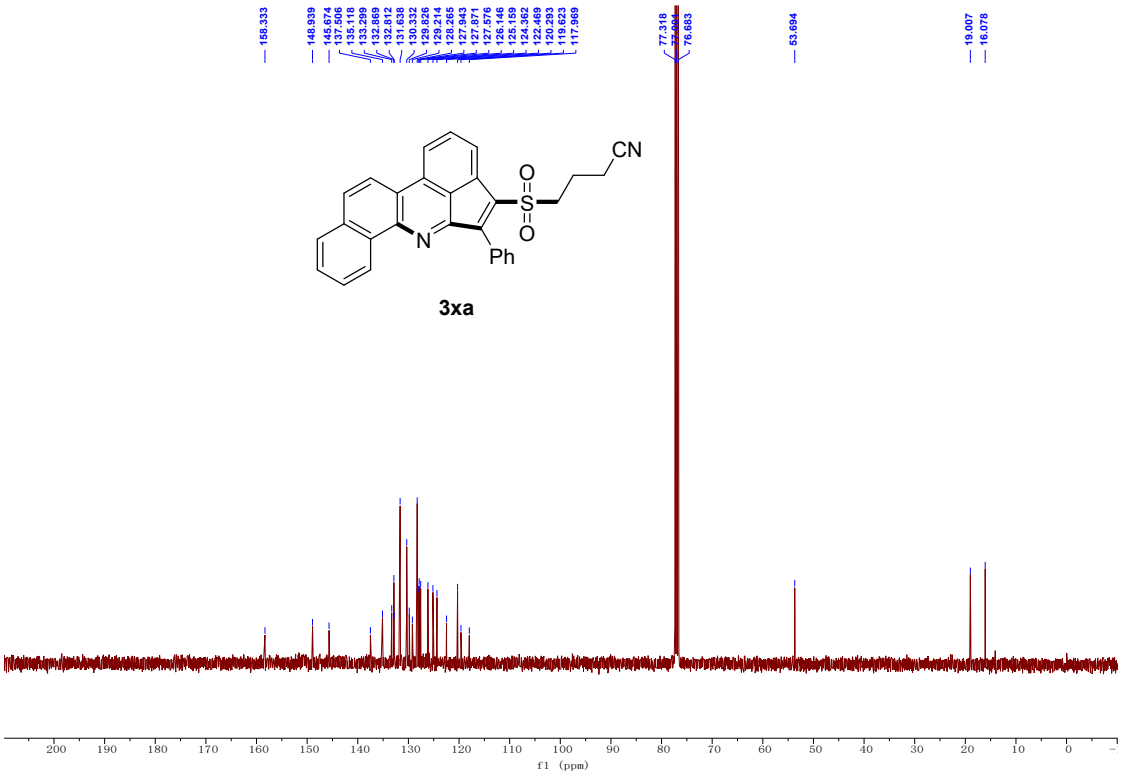
2.03
1.02
3.01
1.04
1.05
5.01
2.01
2.00
2.03
f1 (ppm)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145.674
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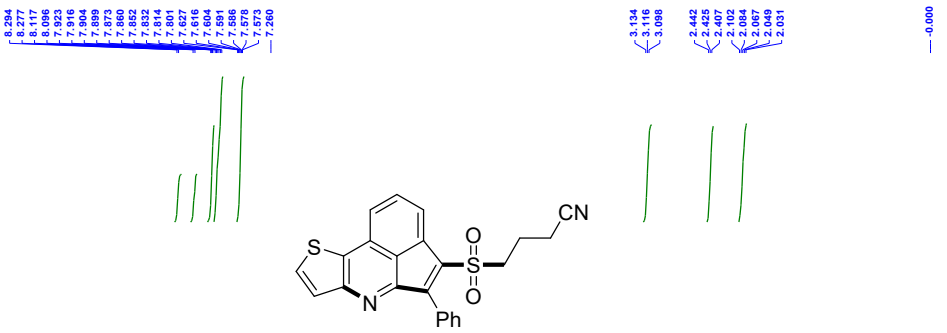
133.299
132.869
132.812
131.638
130.332
129.826
129.214
128.955
127.943
127.871
127.576
126.146
125.159
124.362
122.469
120.293
119.623
117.969
77.318
77.064
76.683
53.694
19.007
16.078
CN
O
S
O
N
Ph
f1 (ppm)

3xa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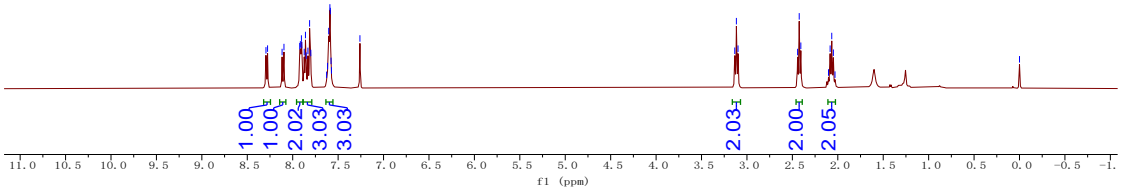
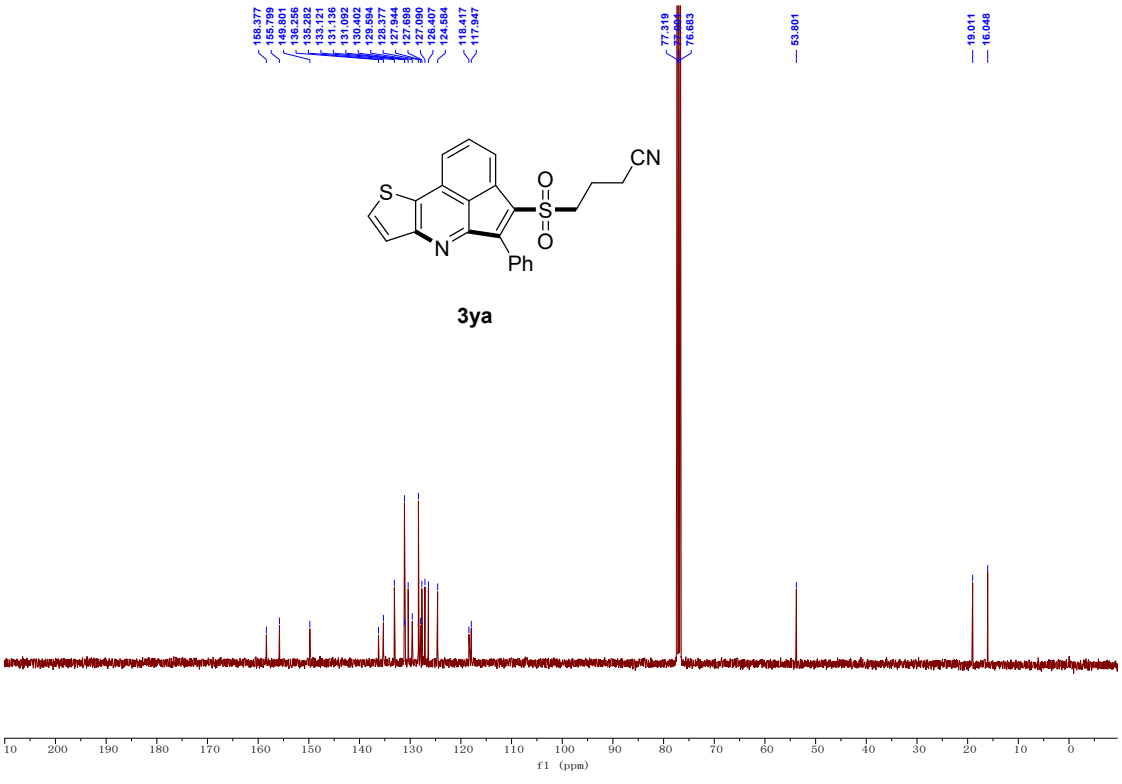
8.277
8.117
8.096
7.923
7.916
7.904
7.899
7.873
7.860
7.852
7.832
7.814
7.801
7.627
7.616
7.604
7.591
7.586
7.578
7.573
7.260
3.134
3.116
3.098
2.442
2.425
2.407
2.102
2.084
2.067
2.049
2.031
-0.000
CN
O
S
O
S
N
Ph

3ya


1.00
1.00
2.02
3.03
3.03
2.03
2.00
2.05
f1 (ppm)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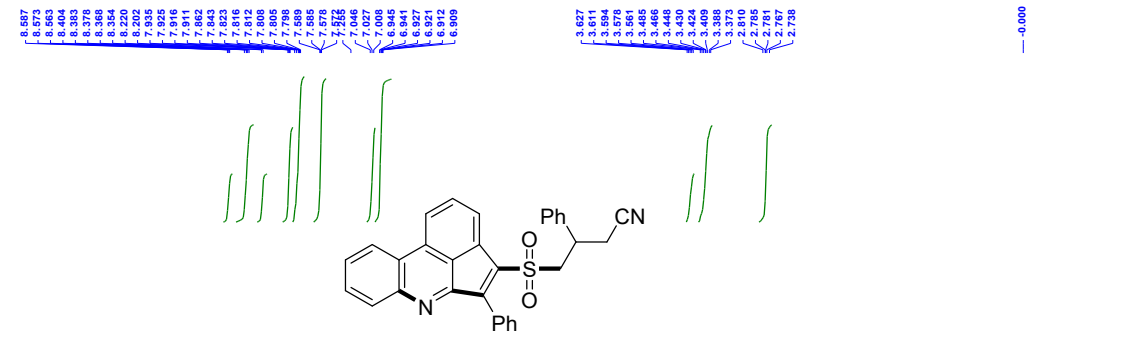
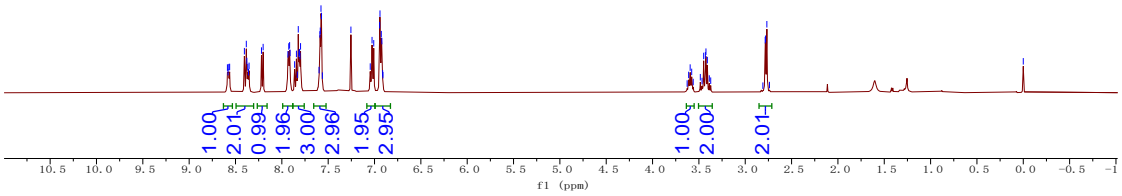
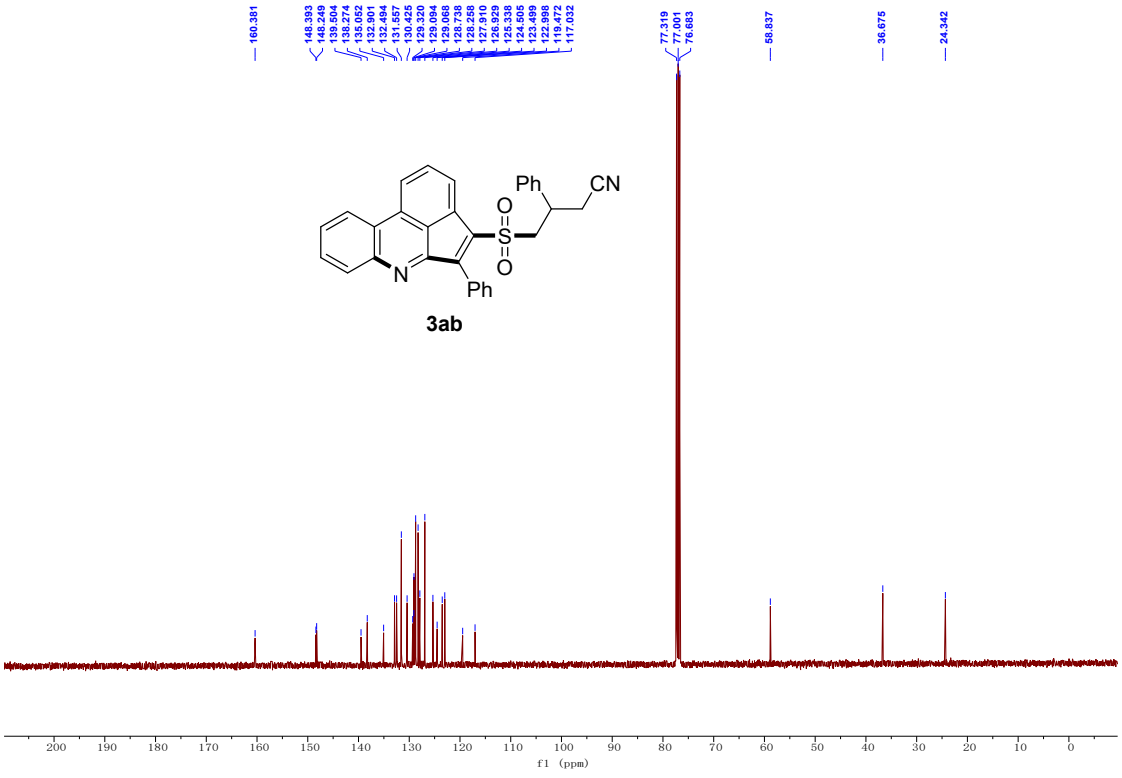
155.799
148.091
138.356
135.282
133.121
131.136
131.092
130.402
129.594
128.377
127.744
127.698
127.090
126.407
124.584
118.417
117.947
77.319
77.064
76.683
53.801
19.011
16.048
CN
O
S
O
S
N
Ph
f1 (ppm)

3ya

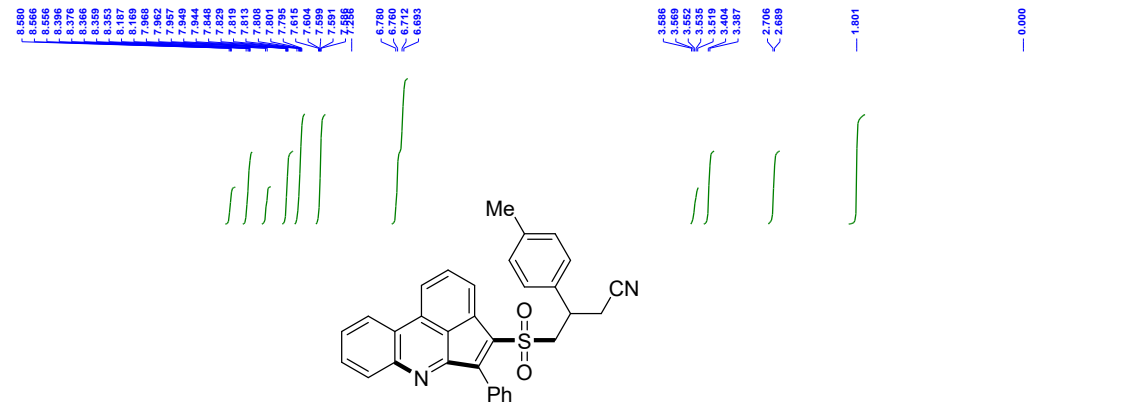

Ph
CN
O
S
O
N
Ph

3ab

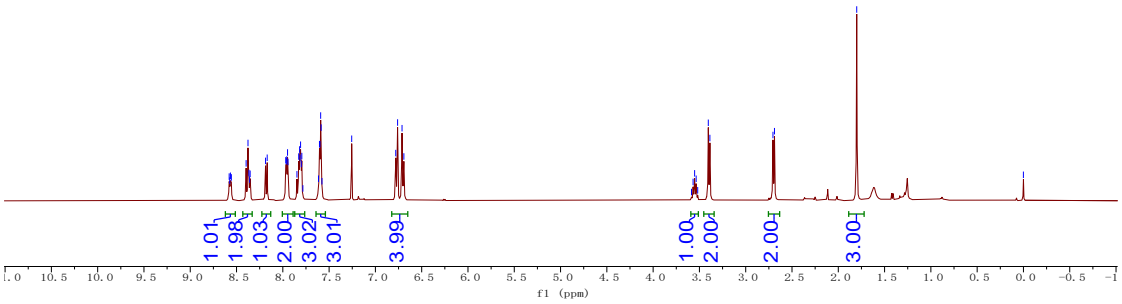

1.00
2.01
0.99
1.96
3.00
2.96
1.95
2.95
1.00
2.00
2.01
f1 (ppm)

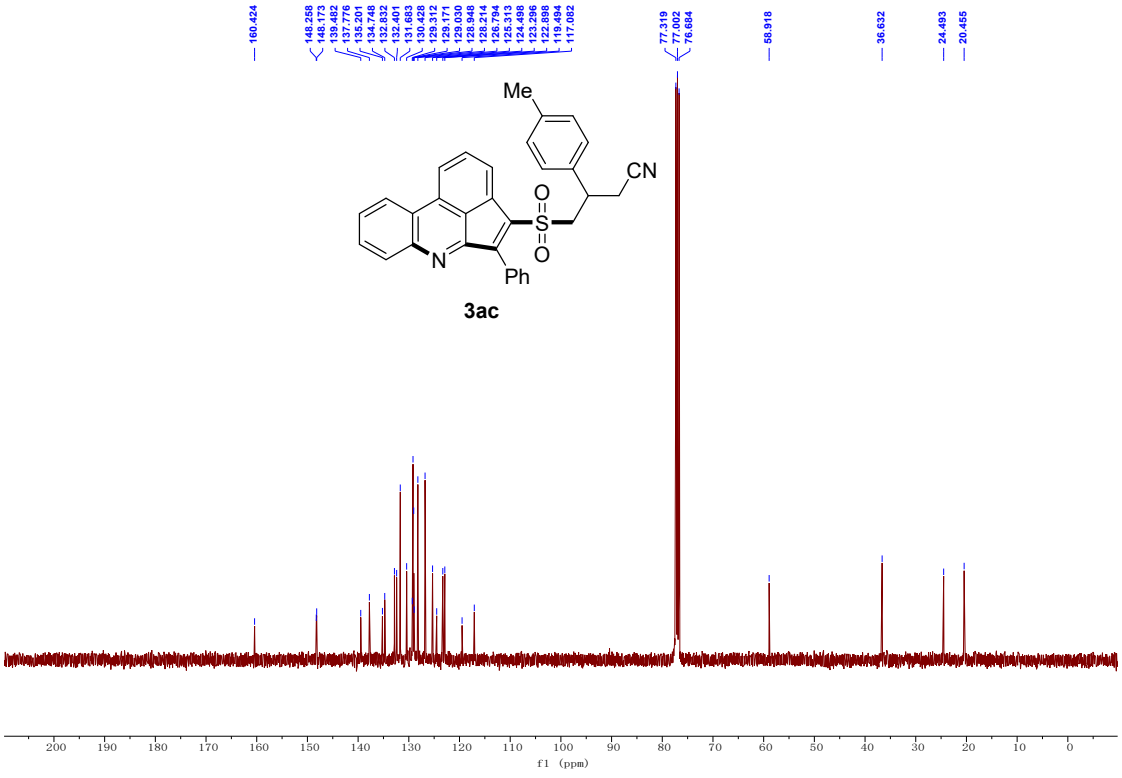

Ph
CN
O
S
O
N
Ph
f1 (ppm)

3ab

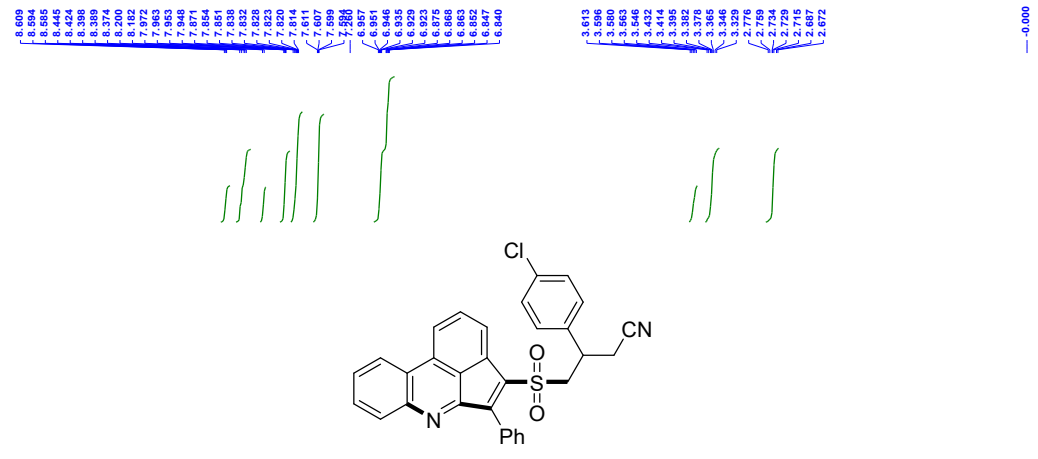

Me
CN
O
S
O
N
Ph

3ac


1.01
1.98
1.03
2.00
3.02
3.01
3.99
1.00
2.00
2.00
3.00
f1 (ppm)


Me
CN
O
S
O
N
Ph
f1 (ppm)

3ac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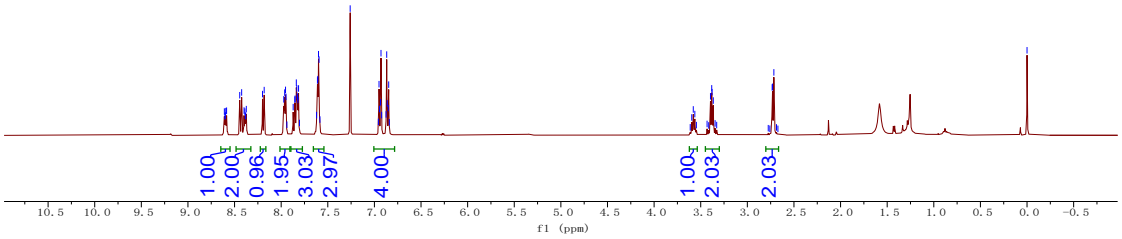
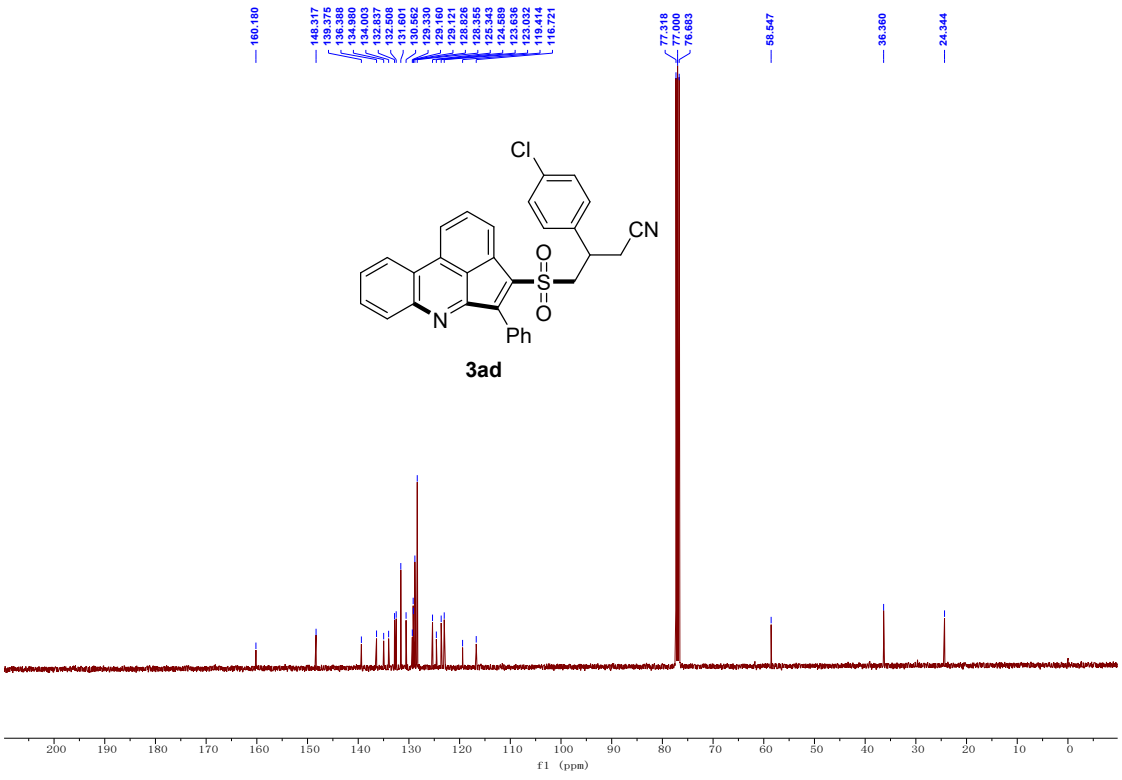
8.594
8.445
8.424
8.398
8.389
8.374
8.200
8.182
7.972
7.965
7.953
7.948
7.871
7.854
7.851
7.838
7.832
7.828
7.823
7.820
7.814
7.611
7.607
7.599
6.957
6.951
6.946
6.935
6.929
6.923
6.875
6.868
6.865
6.852
6.847
6.840
3.613
3.596
3.580
3.563
3.546
3.432
3.414
3.395
3.382
3.376
3.365
3.346
3.329
2.776
2.759
2.734
2.720
2.715
2.687
2.672
-0.000
Cl
CN
O
S
O
N
Ph

3ad


1.00
2.00
0.96
1.95
3.03
2.97
4.00
1.00
2.03
2.03
f1 (ppm)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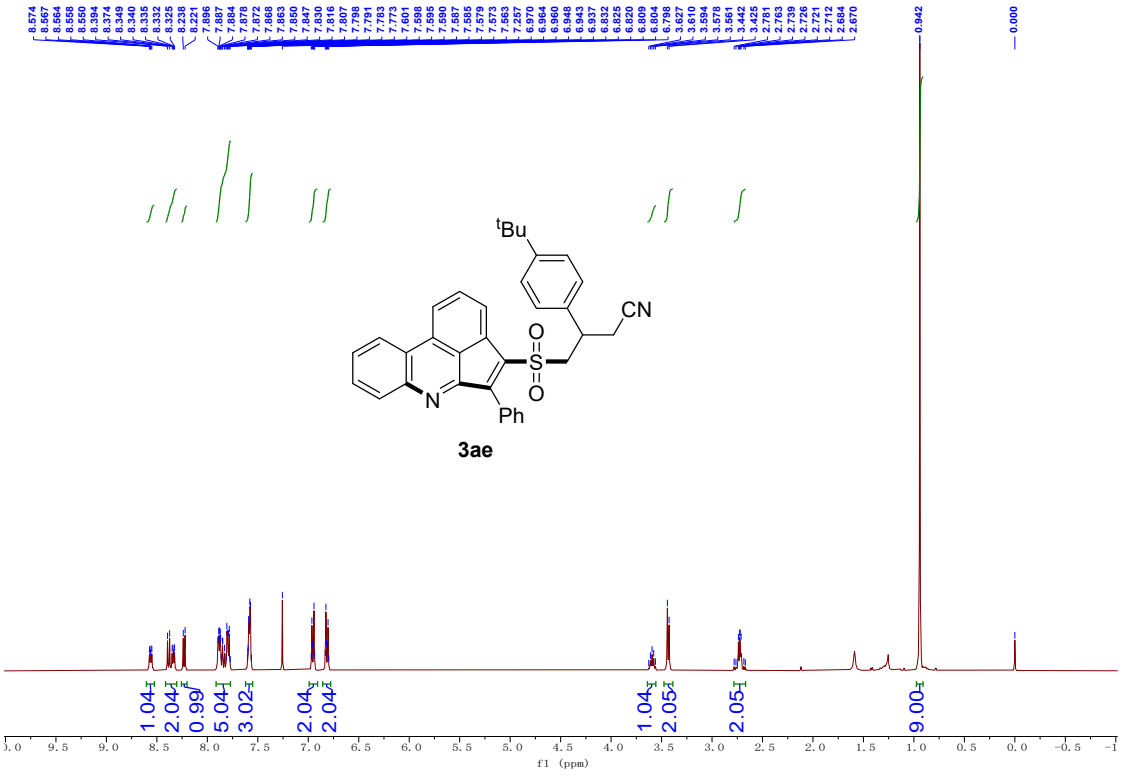
148.317
139.375
136.388
134.600
134.003
132.837
132.508
131.601
130.562
129.330
129.160
129.121
128.436
128.355
125.343
124.589
123.636
123.032
119.414
116.721
77.318
77.000
76.683
58.547
36.360
24.344
Cl
CN
O
S
O
N
Ph
f1 (ppm)

3ad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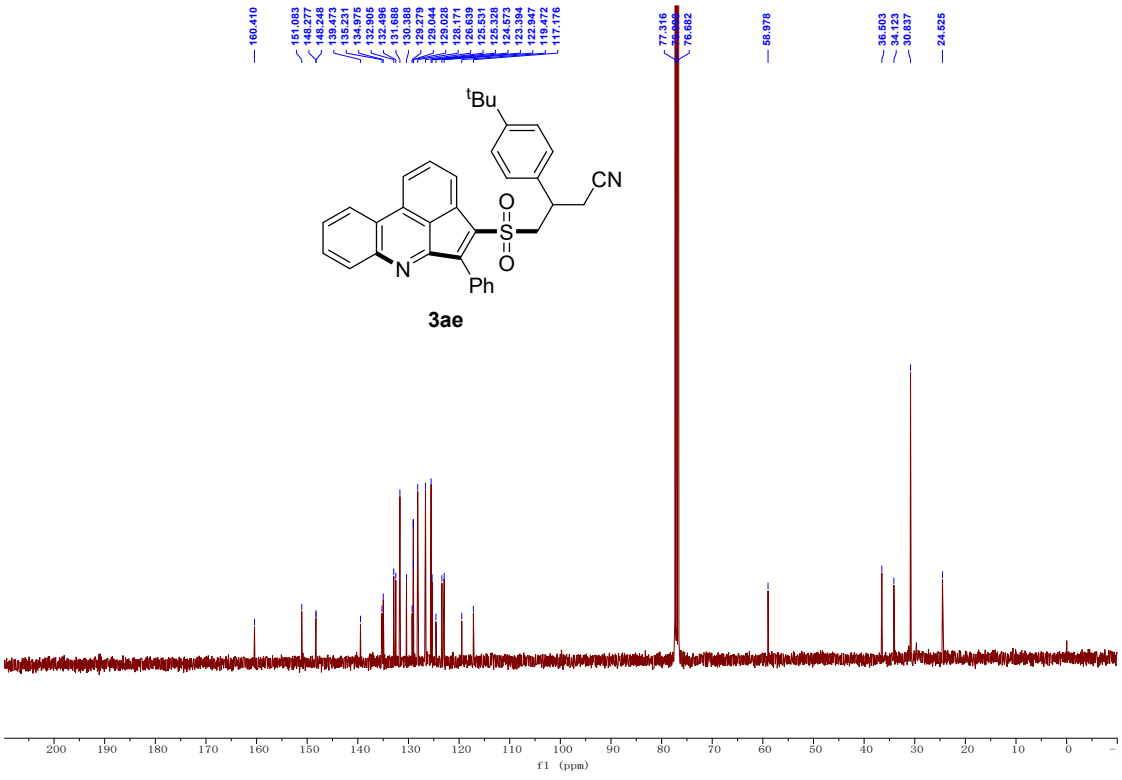
8.567
8.564
8.558
8.550
8.394
8.374
8.349
8.340
8.335
8.332
8.235
8.238
8.221
7.896
7.887
7.884
7.878
7.872
7.868
7.865
7.850
7.847
7.830
7.816
7.807
7.798
7.791
7.783
7.773
7.601
7.598
7.595
7.590
7.587
7.585
7.579
7.573
7.563
7.257
6.970
6.964
6.960
6.948
6.943
6.937
6.832
6.825
6.820
6.809
6.804
6.798
3.627
3.610
3.594
3.578
3.561
3.442
3.425
2.781
2.763
2.739
2.726
2.721
2.712
2.684
2.670
0.942
0.000
tBu
CN
O
S
O
N
Ph
3ae
1.04
2.04
0.99
5.04
3.02
2.04
2.04
1.04
2.05
2.05
9.00
f1 (ppm)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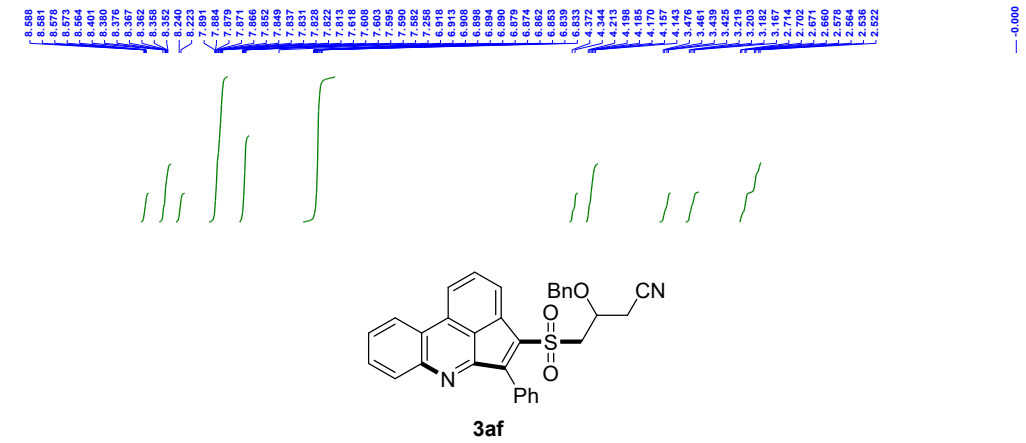
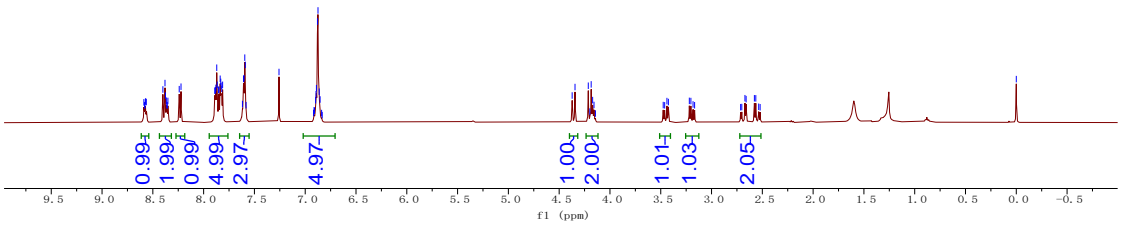
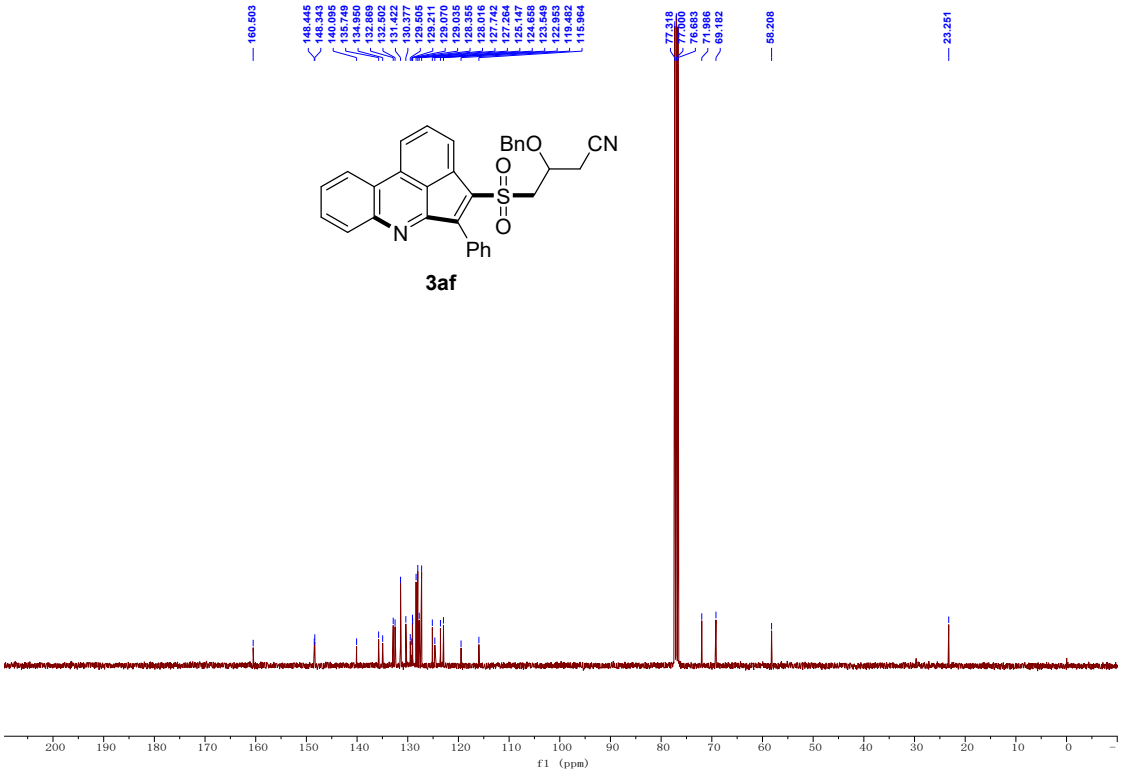
148.248
139.473
135.231
134.975
132.905
132.496
131.688
130.588
129.279
129.044
129.028
128.171
126.639
125.531
125.328
124.573
122.394
122.947
119.472
117.176
77.316
77.000
76.682
58.978
36.503
34.123
30.837
24.525
tBu
CN
O
S
O
N
Ph
3ae
f1 (ppm)

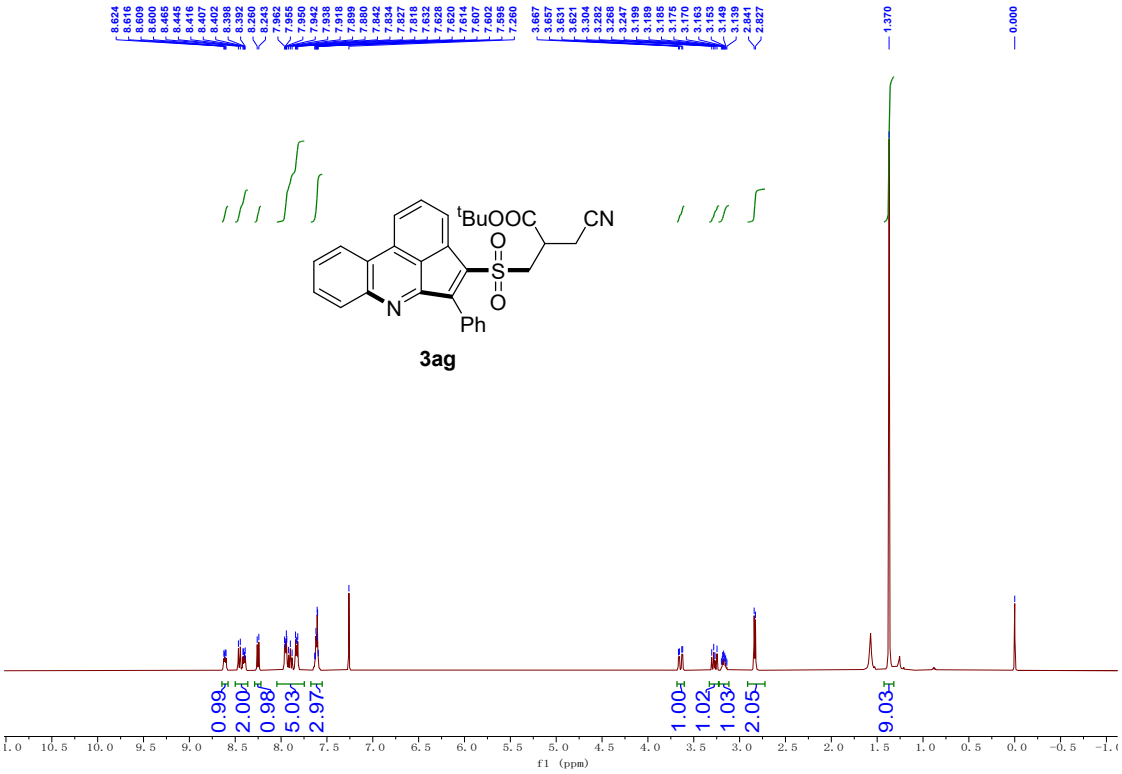

BnO
CN
O
S
O
N
Ph

3af


0.99
1.99
0.99
4.99
2.97
4.97
1.00
2.00
1.01
1.03
2.05
f1 (ppm)


BnO
CN
O
S
O
N
Ph
f1 (ppm)

3af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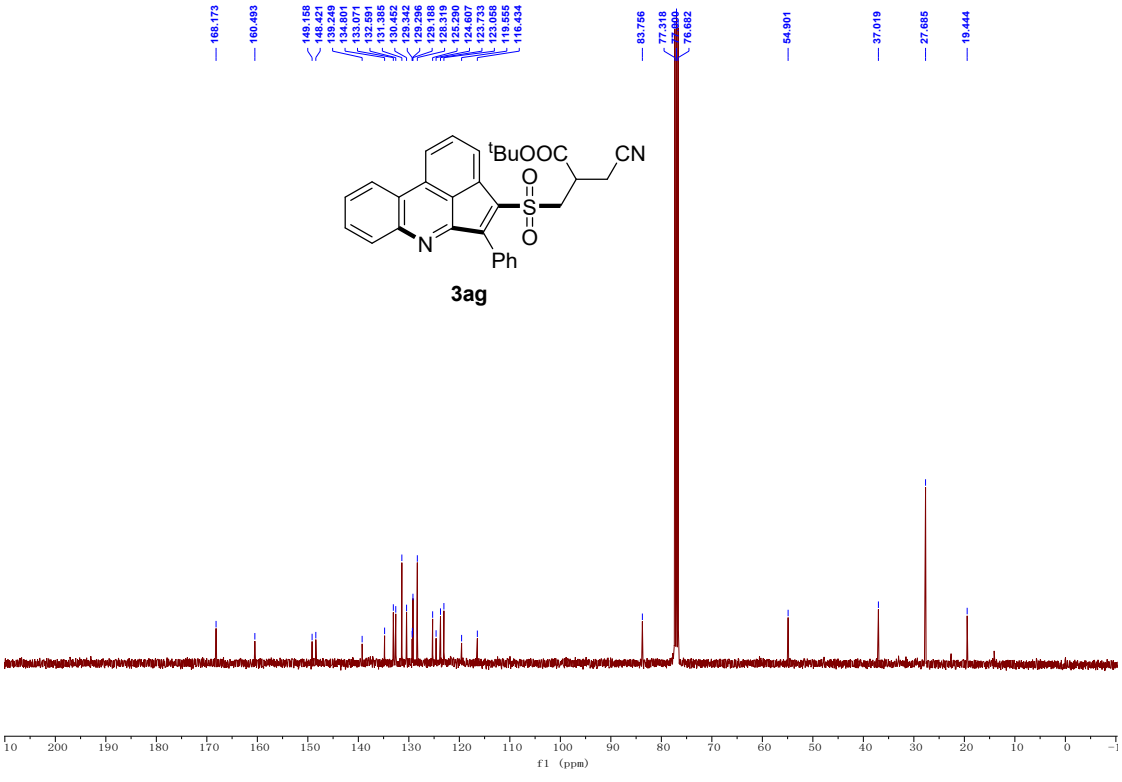
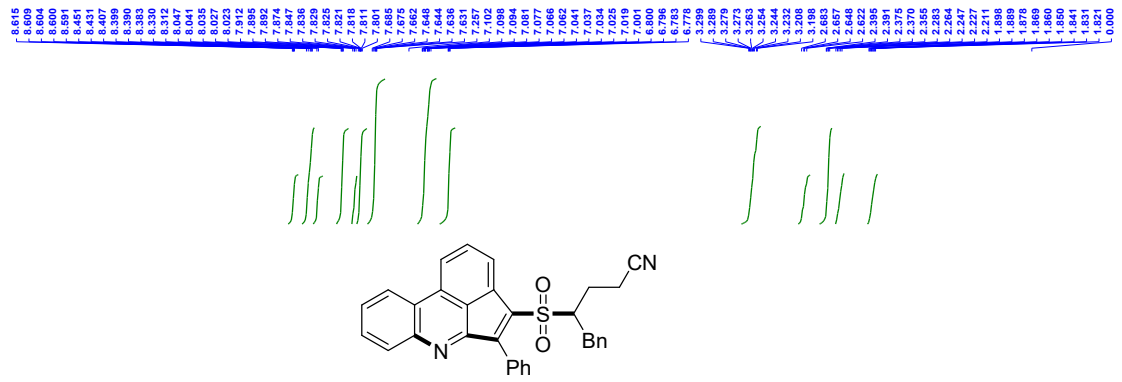
8.445
8.416
8.407
8.402
8.398
8.393
8.262
8.243
7.962
7.955
7.950
7.942
7.938
7.916
7.899
7.880
7.842
7.834
7.827
7.818
7.632
7.628
7.620
7.614
7.607
7.602
7.595
7.260
3.667
3.657
3.651
3.621
3.304
3.282
3.268
3.247
3.199
3.189
3.185
3.175
3.170
3.163
3.153
3.149
3.139
2.841
2.827
1.370
0.000
tBuOOC
CN
O
S
O
N
Ph
0.99
2.00
0.98
5.03
2.97
1.00
1.02
1.03
2.05
9.03
f1 (ppm)

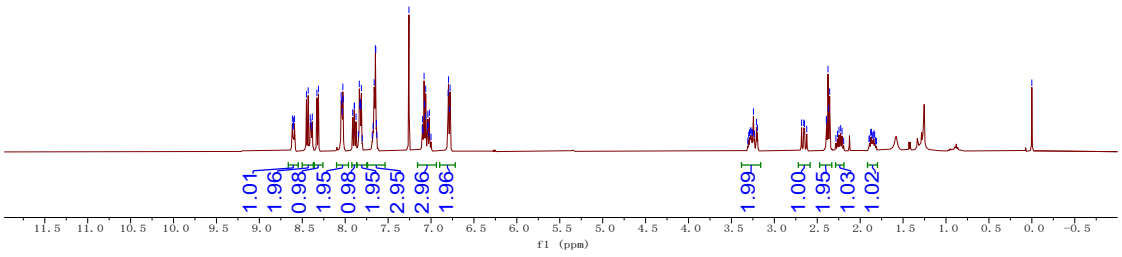
3ag


168.173
160.493
149.158
148.421
139.249
134.801
133.071
132.591
131.385
130.457
129.342
129.296
129.188
128.319
125.290
124.607
123.733
123.068
116.555
116.434
83.756
77.318
77.000
76.682
54.901
37.019
27.685
19.444
tBuOOC
CN
O
S
O
N
Ph
f1 (ppm)

3ag


CN
O
S
O
Bn
N
Ph

3ai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1.96
0.98
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0.98
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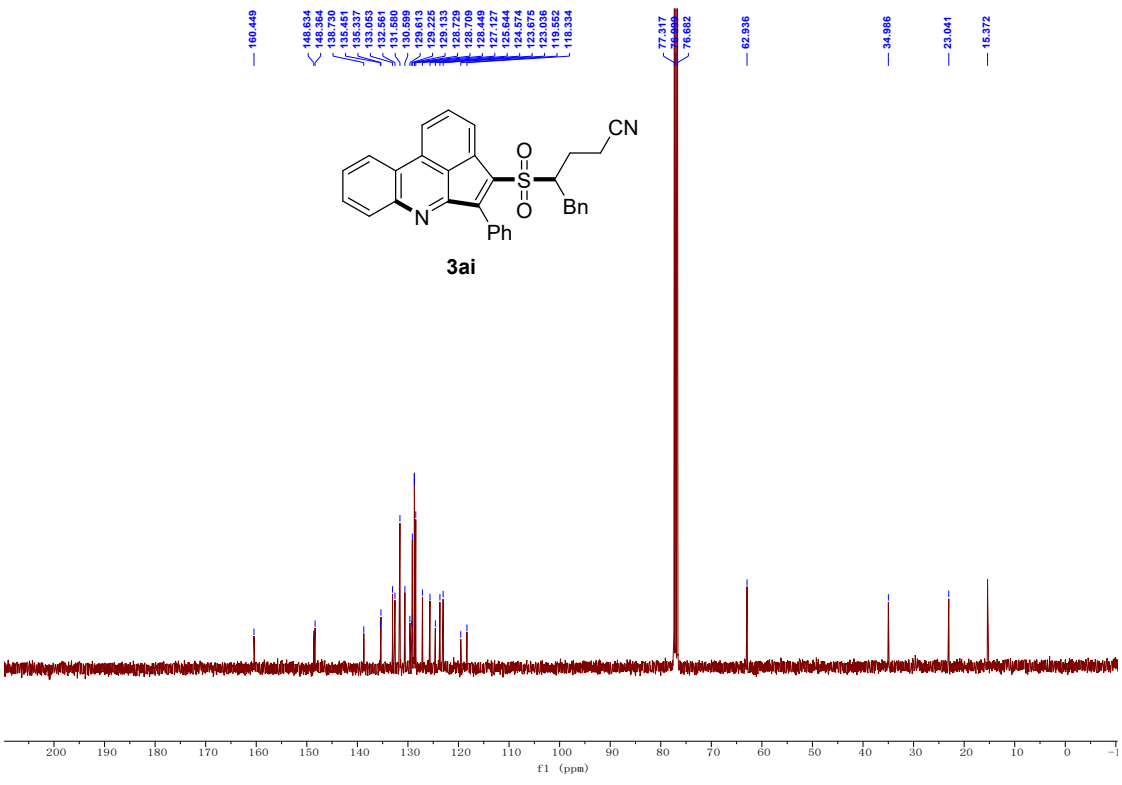
2.95
2.96
1.96
1.99
1.00
1.95
1.03
1.02
f1 (ppm)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138.730
135.451
135.337
133.053
132.861
131.580
130.599
129.613
129.225
129.133
128.729
128.709
128.449
127.127
125.444
124.574
123.675
123.036
119.552
118.334
77.317
77.000
76.682
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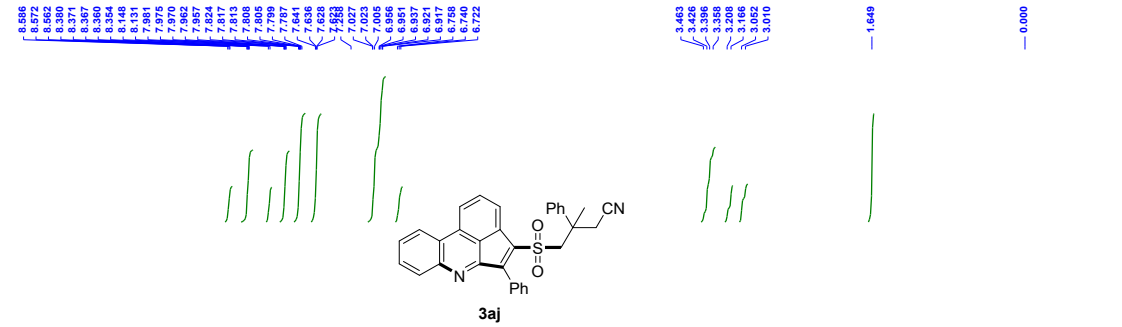
34.986
23.041
15.372
CN
O
S
O
Bn
N
Ph
f1 (ppm)

3ai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8.367
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8.354
8.148
8.131
7.981
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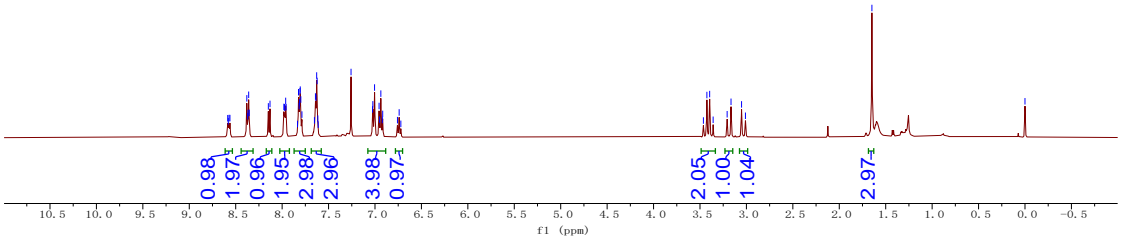
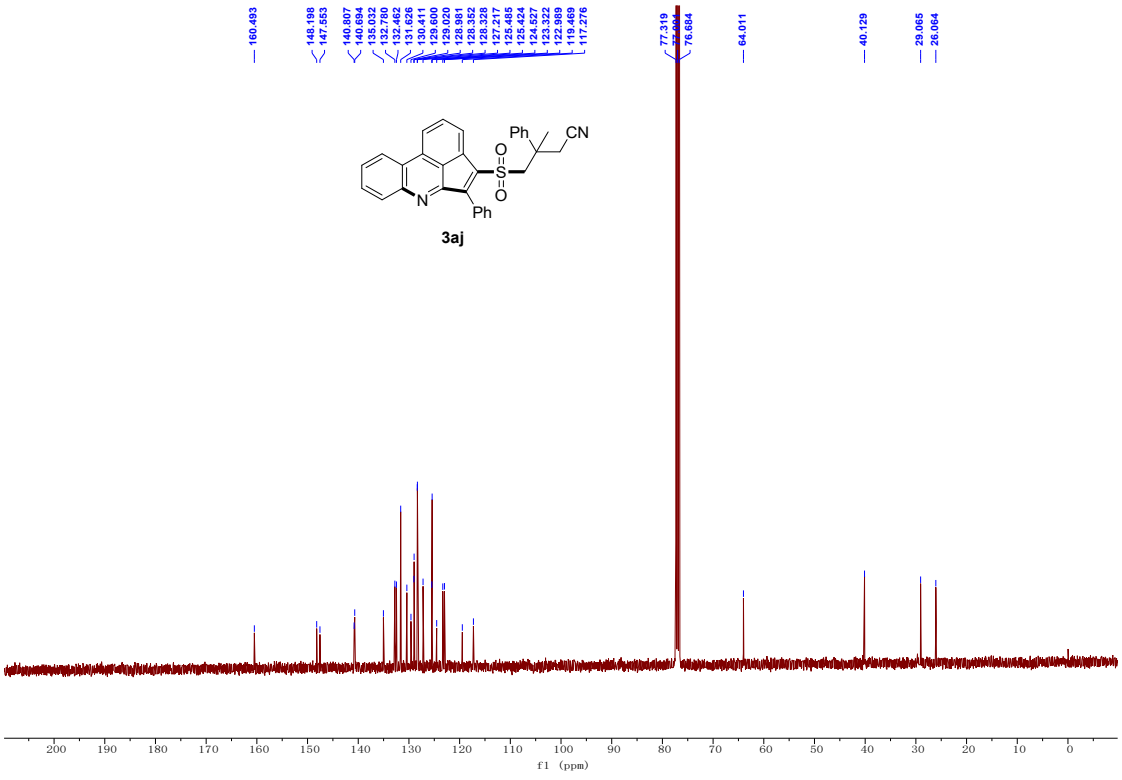
7.970
7.962
7.957
7.824
7.817
7.813
7.808
7.805
7.799
7.787
7.644
7.636
7.628
7.623
7.258
7.027
7.023
7.005
6.956
6.951
6.937
6.921
6.917
6.758
6.750
6.722
3.463
3.426
3.396
3.358
3.008
3.166
3.052
3.010
1.649
0.000
Ph
CN
O
S
O
N
Ph

3aj


0.98
1.97
0.96
1.95
2.98
2.96
3.98
0.97
2.05
1.00
1.04
2.97
f1 (ppm)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140.684
135.032
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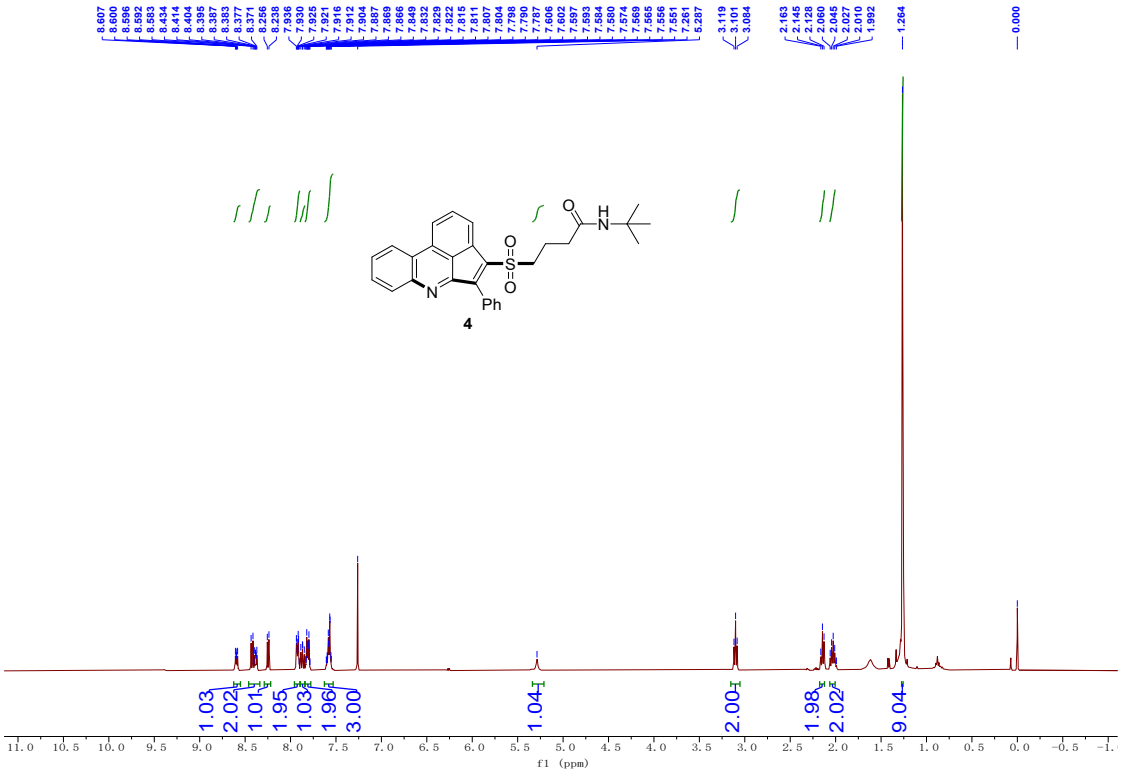
132.462
131.626
131.411
130.600
129.020
128.981
128.352
128.328
127.217
125.486
125.424
124.477
123.322
122.989
119.469
117.276
77.319
77.004
76.684
64.011
40.129
29.065
26.064
Ph
CN
O
S
O
N
Ph
f1 (ppm)

3aj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8.592
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8.414
8.404
8.395
8.387
8.383
8.377
8.371
8.256
8.238
7.936
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7.916
7.912
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7.887
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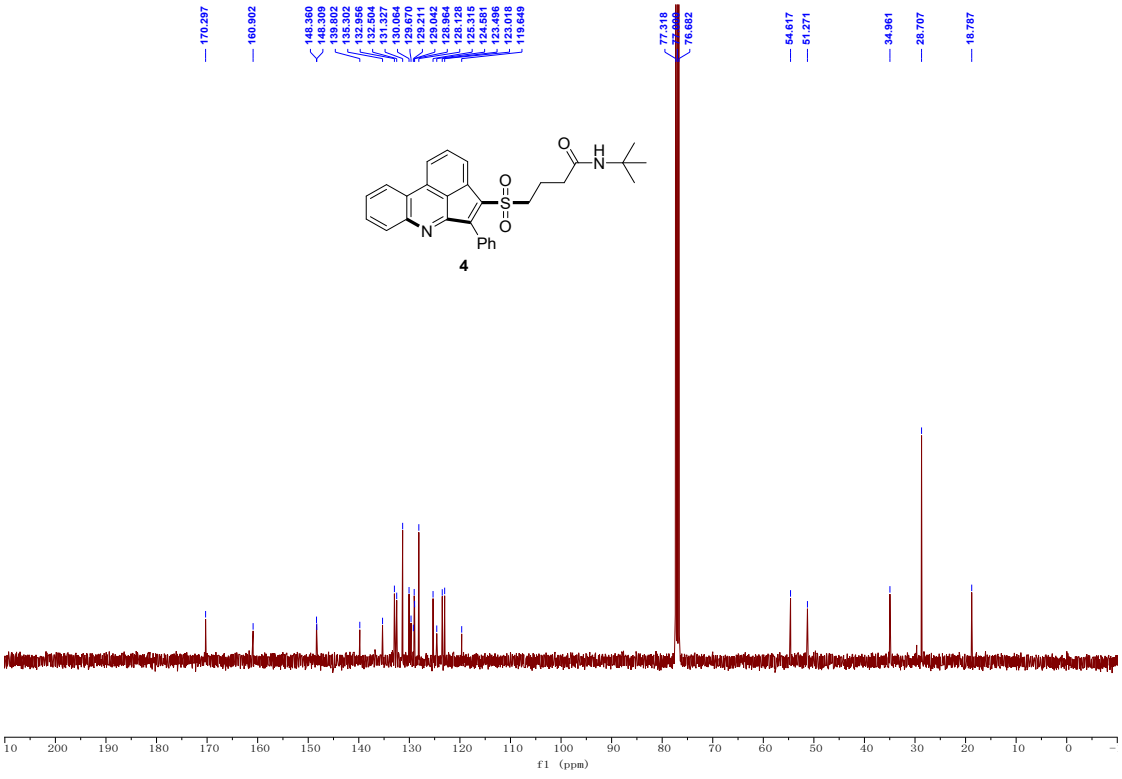
7.565
7.556
7.551
7.261
5.287
3.119
3.101
3.084
2.163
2.145
2.128
2.060
2.045
2.027
2.010
1.992
1.264
0.000
O
H
N
O
S
O
N
Ph
4
1.03
2.02
1.01
1.95
1.03
1.96
3.00
1.04
2.00
1.98
2.02
9.04
f1 (ppm)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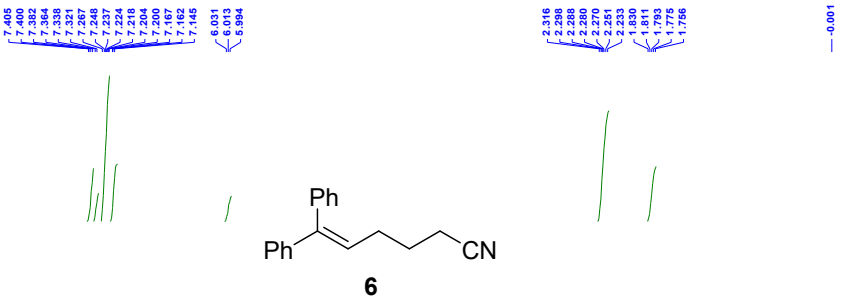
160.902
148.360
148.309
139.802
135.302
132.956
132.504
131.327
130.064
129.670
129.271
129.042
128.964
128.128
125.315
124.581
123.496
123.018
119.649
77.318
77.000
76.682
54.617
51.271
34.961
28.707
18.787
O
H
N
O
S
O
N
Ph
4
f1 (ppm)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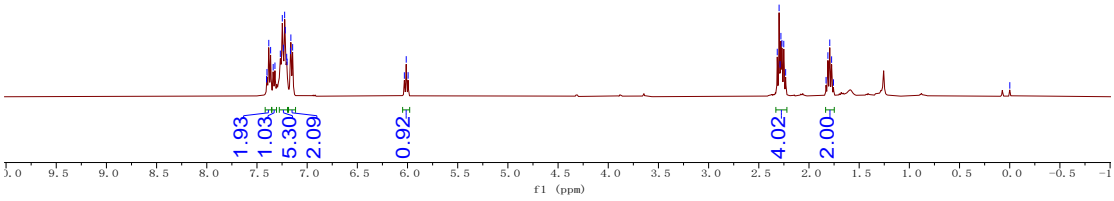
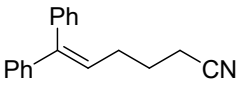
7.400
7.392
7.364
7.338
7.321
7.267
7.248
7.237
7.224
7.214
7.204
7.200
7.167
7.162
7.145
6.031
6.013
5.994
2.316
2.298
2.288
2.280
2.270
2.251
2.233
1.830
1.811
1.793
1.775
1.756
-0.001

Ph
Ph
CN

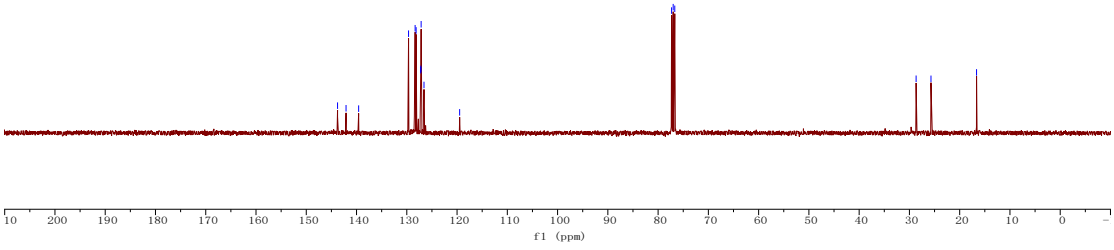
6

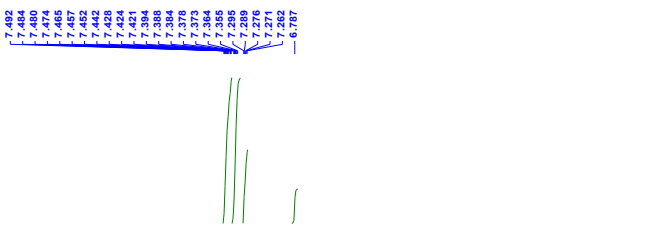

1.93
1.03
5.30
2.09
0.92
4.02
2.00
f1 (ppm)

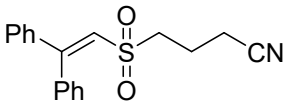

143.776
142.086
139.579
129.649
128.342
128.142
127.226
127.208
127.147
126.577
119.485
77.319
77.000
76.684
28.668
25.710
16.643


Ph
Ph
CN

6


f1 (ppm)





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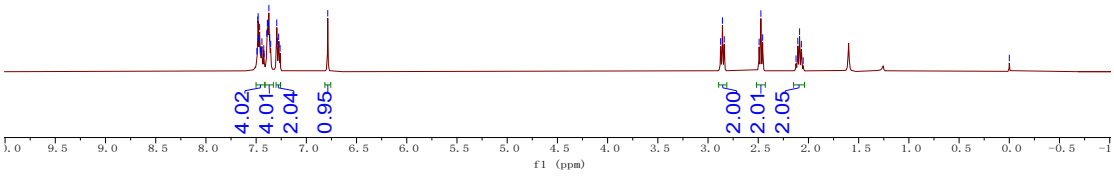

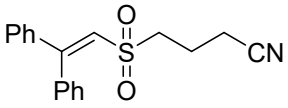

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