Electronic Supplementary Material (ESI) for Green Chemistry.
This journal is © The Royal Society of Chemistry 2021

Electrochemical-Enabled Rhodium-Catalyzed [4+2] Annulations of Arenes with Alkynes

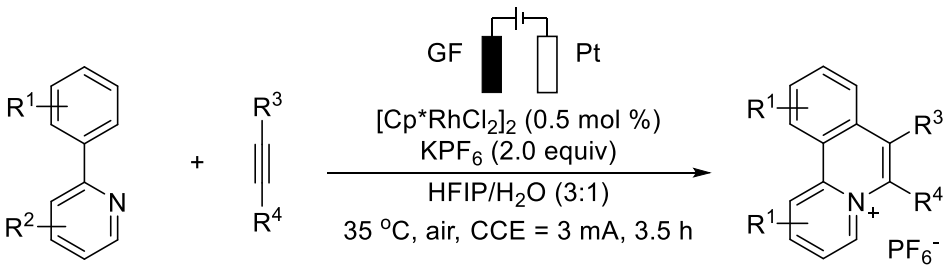
Contents

1. General Information 1
2. General procedure for oxidative annulation of 2-arylpyridines with alkynes. 1
3. General procedure for oxidative annulation of azobenzenes with alkynes. 2
4. Preparation of starting materials 2
    4.1 Synthesis of compounds **2n**, **1B** and **2o**. 2
    4.2 Synthesis of compounds **1D** 3
    4.3 Synthesis of compounds **1F** 3
    4.4 Synthesis of compounds **2p**, **2q**, **2r**, **2s**, **2t**, **2v** 4
    4.5 Synthesis of compounds **2u** 7
    4.6 Synthesis of compounds **2w** 8
    4.7 Synthesis of compounds **[D]$_5$-1a** 8
5. Mechanistic studies 9
    5.1 Reversible H/D exchange with D_2O. 9
    5.2 Reversible H/D exchange with H_2O. 10
    5.3 H/D exchange experiment with D_2O in presence of alkyne. 11
    5.4 Synthesis of Rh(III) Complex **6** 12
    5.5 Synthesis of Rh(I) Complex **7** 13
    5.6 Eletrolysis of complex **7** 16
    5.7 Reaction of complex **6** with **1a** and **2a** 16
    5.8 Reaction of complex **7** with **1a** and **2a** 17
    5.9 Competitive Experiments. 18
6. Cyclic Voltammetry Studies 20
7. Gram-scale reaction 22
8. Decagram-scale reaction 23
9. Synthesis of compounds **8aa-8ac** 24
10. Photoluminescence spectra of selected salts 24
11. Computational Details 25
12. Characterization data of compounds **3**, **5** and **8** 58
13. References 85
14 . ^{1}H NMR and ^{13}C NMR spectra of compounds **3**, **5** and **8** 86

1. General Information

All reagents and solvents were obtained from commercial suppliers and used without further purification. All reagents were weighed and handled in air at room temperature. Starting materials 2-arylpyridines[1], azobenzenes[2], *N*-Phenylpyrazole[3]were synthesized according to previously reported methods. $[Cp^*RhCl_2]_2$ was prepared from $RhCl_3.xH_2O$ following a literature procedure[4]. 1,2-Diphenylethyne, prop-1-ynylbenzene 1-(tert-butyl)-4-ethynylbenzene were used as purchased. The other alkynes used here are known compounds and synthesized according to the reported methods[5]. Other reagents were commercially available and used as purchased. NMR spectra were recorded in DMSO-d_6 or $CDCl_3$ on 400 MHz or 500 MHz spectrometers. Chemical shifts were reported in parts per million (δ) relative to tetramethylsilane (TMS). HRMS were performed on an Ultima Global spectrometer with an ESI source. DC power supply DPS-305CF was used for all experiments.

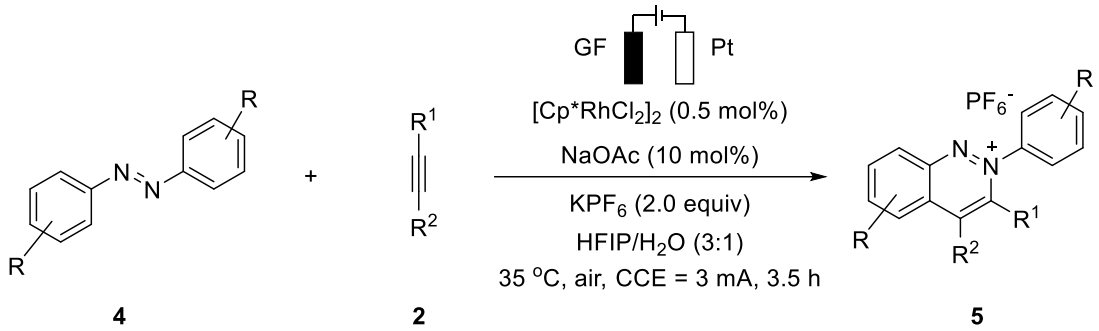
2. General procedure for oxidative annulation of 2-arylpyridines with alkynes.



1 **2** **3**

The electrocatalysis was carried out in an undivided cell under air, with a graphite felt (GF) anode (10 mm x 10 mm x 5 mm) and a platinum cathode (10 mm x 10 mm x 0.25 mm). To a 10-mL three-necked flask, 2-arylpyridines **1** (0.2 mmol), alkynes **2** (0.22 mmol), $[Cp^*RhCl_2]_2$ (0.5 mol %) and KPF_6 (0.4 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/H_2O (3:1, 5 mL). Electrocatalysis was performed at 35 ^oC with a constant current of 3.0 mA maintained for 3.5 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL). The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by silica gel column chromatography using DCM/MeOH (95:5) as eluent to give the desired product **3**.

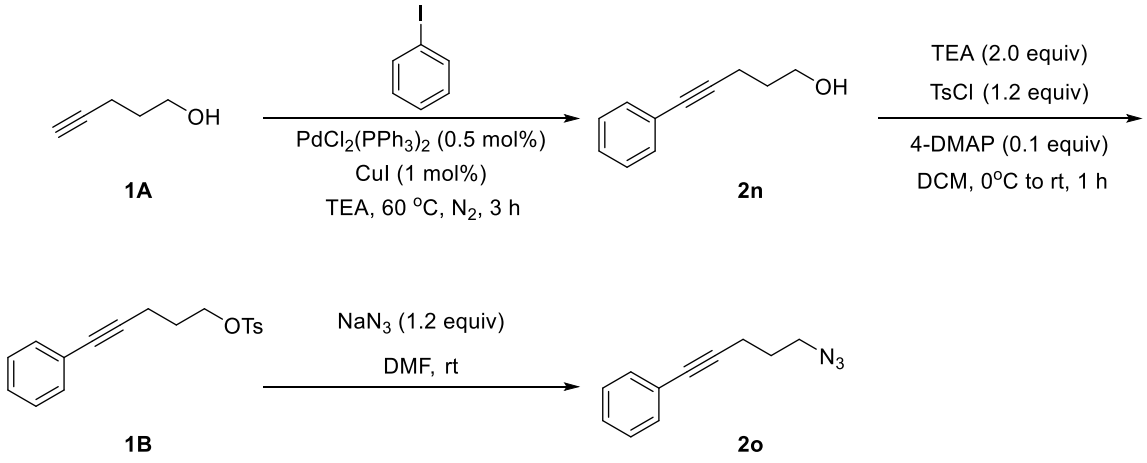
3. General procedure for oxidative annulation of azobenzenes with alkynes.



The electrocatalysis was carried out in an undivided cell under air, with a graphite felt (GF) anode (10 mm x 10 mm x 5 mm) and a platinum cathode (10 mm x 10 mm x 0.25 mm). To a 10-mL three-necked flask, azobenzenes **4** (0.2 mmol), alkynes **2** (0.22 mmol), $[Cp^*RhCl_2]_2$ (0.5 mol %), KPF_6 (0.4 mmol, 2.0 equiv), NaOAc (10 mol %) were dissolved in solvent mixture HFIP/H_2O (3:1, 5 mL). Electrocatalysis was performed at 35 °C with a constant current of 3.0 mA maintained for 3.5 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL).The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by silica gel column chromatography using DCM/MeOH (95:5) as eluent to give the desired product **5**.

4. Preparation of starting materials

4.1 Synthesis of compounds 2n, 1B and 2o.



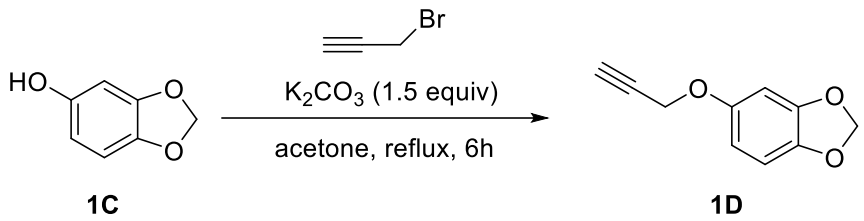
Step1: To a 50 mL Schlenk flask, under N_2, was added $PdCl_2$ $(PPh_3)_2$ (0.025 mmol, 0.5 mol%), CuI (0.05 mmol, 1.0 mol%), iodobenzene (6 mmol, 1.2 equiv.),

Compound **1A** (5 mmol, 1.0 equiv.) and anhydrous TEA (10 mL), then the tube was placed in a pre-heated oil bath (60 °C). The reaction was stirred 3 h and then cooled to room temperature and checked by TLC. The reaction is filtered over celite, washing with dichloromethane. The solvent was removed and the residue purified by flash column chromatography on silica gel (using 30% EtOAc/petroleum ether as eluent) to give compound **2n**[6] (orange oil, 84%)

Step2: To a stirred solution of Compound **2n** (5 mmol, 1.0 equiv) , 4-Dimethylaminopyridine (0.5 mmol, 0.1 equiv) and TEA (10 mmol, 2.0 equiv) in dry DCM (10 ml) at 0 °C was added *p*-toluenesulfonyl chloride (TsCl) (6 mmol, 1.2 equiv) portion wise.The reaction mixture was stirred for 1 h and then quenched with water, extracted with EtOAc, dried over anhydrous $MgSO_4$, concentrated and chromatographed (petroleum ether / EtOAc = 15/1) to afford compound **1B**[7] (white solid, 89%).

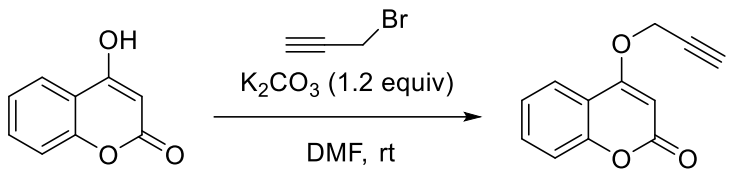
Step3: Sodium azide (6 mmol, 1.2 equiv) was added to a solution of **1B** in DMF (1.1 ml) and stirred at room temperature overnight. H_2O was added to the mixture and the aqueous phase was extracted with ethyl acetate. The combined organic extract was washed with saturated aqueous NaCl solution, dried over anhydrous $MgSO_4$. The solvent was removed and the residue purified by flash column chromatography on silica gel (using petroleum ether / EtOAc = 20/1 as eluent) to give compound **2o**[8] (yellow oil, 92%)

4.2 Synthesis of compounds 1D



Compound **1C** (5 mmol, 1.0 equiv) was dissolved in acetone (15 mL) and K_2CO_3 (7.5 mmol, 1.5 equiv) was added to the reaction mixture. After that, 80% propargyl bromide in toluene (0.96 mL, 6.5 mmol, 1.3 equiv) was added drop-wise and the reaction mixture was refluxed for 6 h. On completion of the reaction, the solvent was removed in vacuum and the residue was dissolved in ethyl acetate. The mixture was quenched by a saturated NH_4Cl solution, and was extracted with diethyl ether. The combined organic phase was washed with brine, dried over anhydrous $MgSO_4$. The solvent was evaporated in vacuum and purified by silica gel column chromatography to avail products **1D**[9] (white solid, 92%).

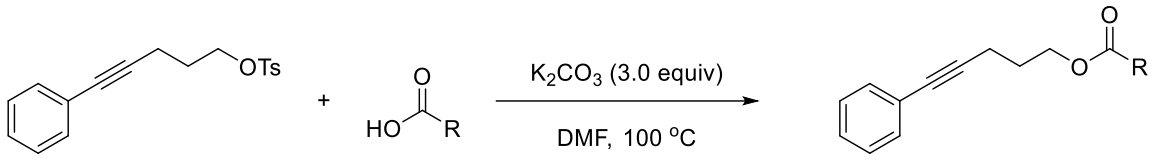
4.3 Synthesis of compounds 1F



1E **1F**

Compound **1E** (5 mmol, 1.0 equiv) were added to a stirring mixture of K_2CO_3 (6 mmol, 1.2 equiv) in DMF, followed by adding 80% propargyl bromide in toluene (0.96 mL, 6.5 mmol, 1.3 equiv). The reaction mixture was stirred at room temperature for 12 h. The combined organic phase was washed with brine, dried over anhydrous $MgSO_4$. The solvent was evaporated in vacuum and purified by silica gel column chromatography to avail products **1F**[9] (white solid, 80%).

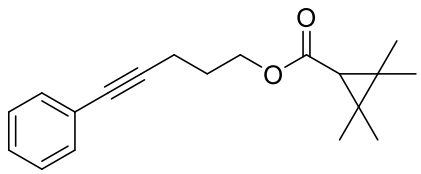
4.4 Synthesis of compounds 2p, 2q, 2r, 2s, 2t, 2v



1B **2p, 2q, 2r, 2s, 2t, 2v**

To a 50 mL Schlenk flask was added compound **1B** (2 mmol), carboxylic acid (3 mmol, 1.5 equiv), K_2CO_3 (6 mmol, 3.0 equiv) and DMF (15 mL), then the tube was placed in a pre-heated oil bath (100 °C) for 1 h. The mixture was allowed to cool to room temperature. H_2O was added to the mixture and the aqueous phase was extracted with ethyl acetate. The combined organic extract was washed with saturated aqueous NaCl solution, dried over anhydrous $MgSO_4$. The solvent was then removed in vacuo and the residue was further purified with flash column chromatography on silica gel to give products .

Characterization of compounds **2p, 2q, 2r, 2s, 2t, 2v**:
5-phenylpent-4-yn-1-yl 2,2,3,3-tetramethylcyclopropane-1-carboxylate (2p)

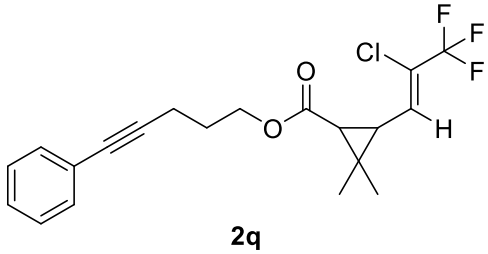


2p

Colorless oil; yield 96%
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.37 (m, 2H), 7.29 – 7.25 (m, 3H), 4.18 (t, *J* = 6.3 Hz, 2H), 2.52 (t, *J* = 7.1 Hz, 2H), 1.93 (p, *J* = 6.7 Hz, 2H), 1.25 (s, 6H), 1.20 (s, 1H), 1.18 (s, 6H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 172.14, 131.56, 128.19, 127.66, 123.74, 88.86, 81.15, 62.44, 35.73, 30.05, 28.07, 23.55, 16.61, 16.34.

HRMS (ESI) calcd for [$C_{19}H_{24}O_2$] $(M+Na)^+$:307.1674, found 307.1680

5-phenylpent-4-yn-1-yl (*Z*)-3-(2-chloro-3,3,3-trifluoroprop-1-en-1-yl)-2,2-dimethylcyclopropane-1-carboxylate (2q)



2q

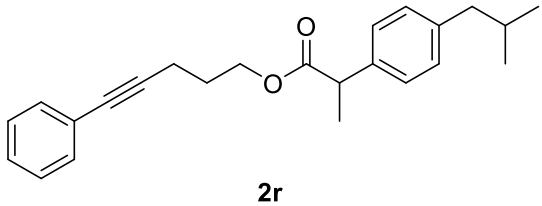
Colorless oil; yield 95%

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.37 (m, 2H), 7.31 – 7.27 (m, 3H), 6.94 (d, *J* = 9.4 Hz, 1H), 4.24 (t, *J* = 6.3 Hz, 2H), 2.53 (t, *J* = 7.0 Hz, 2H), 2.16 (t, *J* = 8.9 Hz, 1H), 2.01 – 1.92 (m, 3H), 1.30 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 168.40, 129.70, 128.27, 126.38, 125.90, 121.74, 119.90, 119.65, 117.50, 86.59, 79.49, 61.56, 31.07, 28.99, 26.77, 26.54, 25.96, 14.38, 13.09.

HRMS (ESI) calcd for [$C_{20}H_{20}ClF_3O_2$] $(M+H)^+$:385.1182, found 385.1192

5-phenylpent-4-yn-1-yl 2-(4-isobutylphenyl)propanoate (2r)



2r

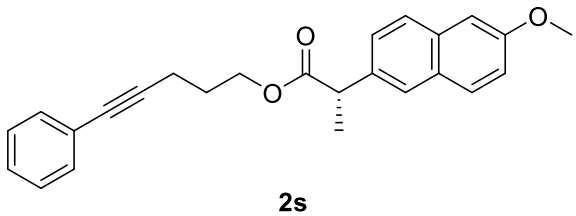
Colorless oil; yield 95%

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.31 – 7.27 (m, 3H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 4.24 (t, *J* = 5.7 Hz, 2H), 3.73 (q, *J* = 7.1 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 2.40 (t, *J* = 7.1 Hz, 2H), 1.93 – 1.83 (m, 3H), 1.52 (d, *J* = 7.2 Hz, 3H), 0.92 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 174.71, 140.54, 137.83, 131.58, 129.36, 128.22, 127.70, 127.15, 123.72, 88.61, 81.23, 63.36, 45.19, 45.06, 30.22, 27.80, 22.42, 18.47, 16.04.

HRMS (ESI) calcd for [$C_{24}H_{28}O_2$] $(M+Na)^+$:371.1987, found 371.1989

5-phenylpent-4-yn-1-yl (*S*)-2-(6-methoxynaphthalen-2-yl)propanoate (2s)



2s

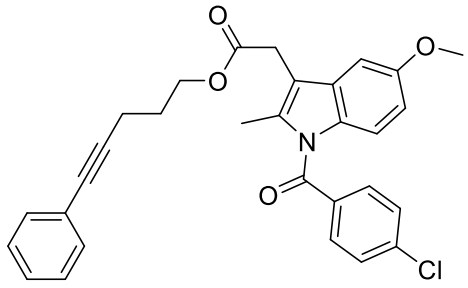
Colorless oil; yield 97%

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 – 7.59 (m, 3H), 7.38 – 7.33 (m, 1H), 7.32 – 7.27 (m, 2H), 7.23 – 7.19 (m, 3H), 7.10 – 7.03 (m, 2H), 4.18 (t, *J* = 6.3 Hz, 2H), 3.84 (s, 3H), 3.81 (q, 1H), 2.33 (t, *J* = 7.1 Hz, 2H), 1.82 (p, *J* = 6.7 Hz, 2H), 1.53 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 174.65, 157.63, 135.73, 133.69, 131.57, 129.30, 128.94, 128.21, 127.70, 127.16, 126.23, 125.91, 123.67, 118.99, 105.59, 88.56, 81.27, 63.48, 55.31, 45.50, 27.75, 18.55, 16.07.

HRMS (ESI) calcd for $[C_{25}H_{24}O_3]$ $(M+Na)^+$:395.1623, found 395.1627

5-phenylpent-4-yn-1-yl
2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetate (2t)



2t

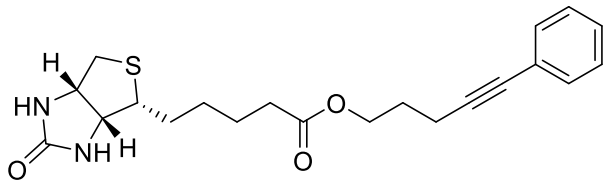
Colorless oil; yield 93%

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.33 (m, 2H), 7.29 – 7.24 (m, 3H), 6.98 (d, *J* = 2.1 Hz, 1H), 6.88 (d, *J* = 9.0 Hz, 1H), 6.68 (dd, *J* = 9.0, 2.3 Hz, 1H), 4.28 (t, *J* = 6.3 Hz, 2H), 3.83 (s, 3H), 3.68 (s, 2H), 2.45 (t, *J* = 7.0 Hz, 2H), 2.39 (s, 3H), 1.93 (p, *J* = 6.7 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.83, 168.28, 156.08, 139.23, 135.88, 133.91, 131.55, 131.18, 130.80, 130.62, 129.12, 128.25, 127.78, 123.55, 115.00, 112.61, 111.77, 101.20, 88.34, 81.42, 63.72, 55.70, 30.41, 27.74, 16.10, 13.39.

HRMS (ESI) calcd for $[C_{30}H_{26}ClNO_4]$ $(M+Na)^+$:522.1448, found 522.1447

5-phenylpent-4-yn-1-yl
5-((3a*R*,4*R*,6a*S*)-2-oxohexahydro-1H-thieno[3,4-*d*]imidazol-4-yl)pentanoate (2v)



2v

Colorless oil; yield 89%

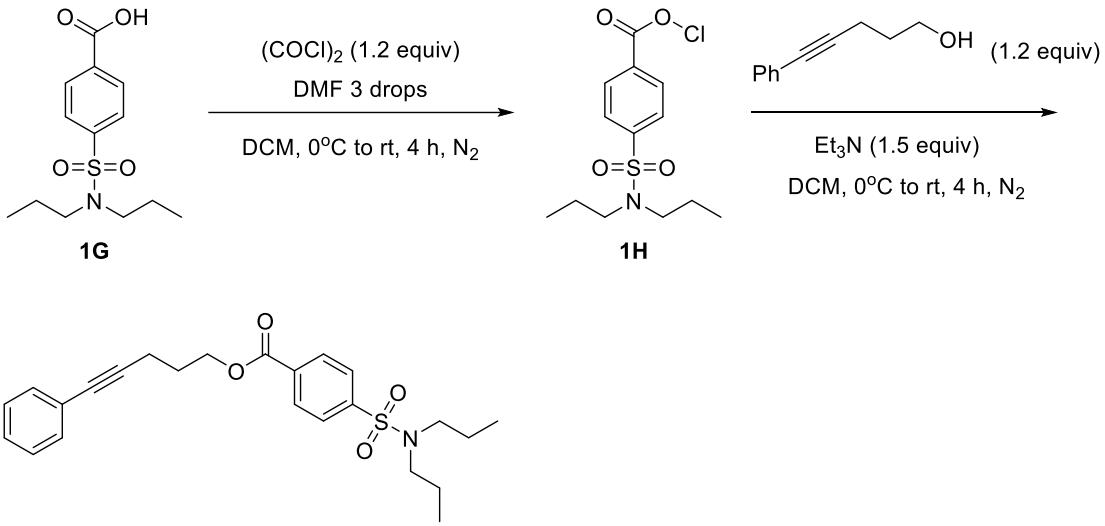
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 2H), 7.27 (d, *J* = 3.2 Hz, 3H), 6.12 (s, 1H), 5.69 (s, 1H), 4.49 – 4.42 (m, 1H), 4.27 (dd, *J* = 7.1, 4.8 Hz, 1H), 4.22 (t, *J* = 6.2 Hz, 2H), 3.12 (q, *J* = 7.1, 6.3 Hz, 1H), 2.87 (dd, *J* = 12.8, 4.9 Hz, 1H), 2.72 (d, *J* =

12.8 Hz, 1H), 2.51 (t, J = 7.0 Hz, 2H), 2.34 (t, J = 7.5 Hz, 2H), 1.96 – 1.88 (m, 2H), 1.67 (tt, J = 13.9, 6.7 Hz, 4H), 1.42 (dd, J = 13.6, 6.8 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 171.86, 161.99, 129.70, 126.39, 125.89, 121.76, 86.77, 79.43, 61.24, 60.10, 58.27, 53.64, 38.72, 32.08, 26.53, 26.39, 25.93, 22.98, 14.36.

HRMS (ESI) calcd for $[C_{21}H_{26}N_2O_3S]$ $(M+Na)^+$: 409.1562, found 409.1564

4.5 Synthesis of compounds 2u

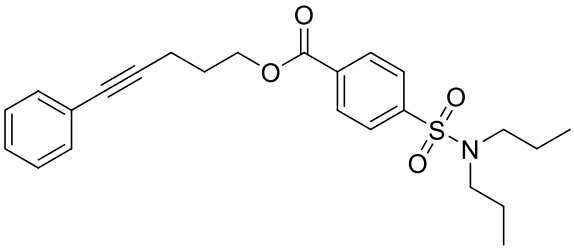


Step1: To a solution of Probenecid **1G** (5 mmol) and DMF (3 drops) in CH_2Cl_2 (15 mL) under N_2 atmosphere was dropwise added oxalyl chloride (0.5 mL, 6 mmol) at 0 °C. After 5 min, the mixture was stirred at room temperature for 4 h, then solvent was removed under reduced pressure to give the residue **1H**.

Step2: To a solution of 5-phenylpent-4-yn-1-ol (6 mmol), Et_3N (2.5 mL, 9 mmol) in CH_2Cl_2 (30 mL) under N_2 atmosphere was dropwise added **1H** (dissolved in 15 mL) at 0 °C. Then, the mixture was stirred at room temperature for 4 h. After 4 h, the reaction mixture was concentrated under reduced pressure and the residue was purified by flash chromatography to give the pure S6 as a colourless oil **2u**.

Characterization of compounds **2u**:

5-phenylpent-4-yn-1-yl 4-(*N*,*N*-dipropylsulfamoyl)benzoate (2u)

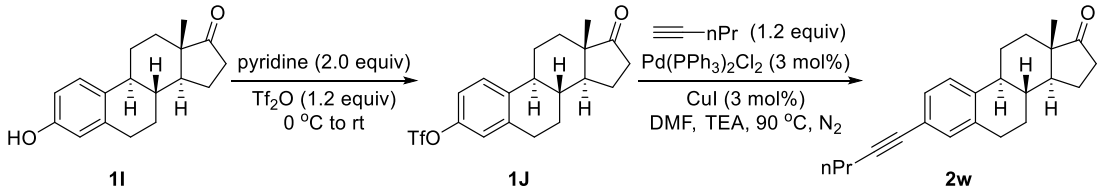


2u

Colorless oil; yield 90%

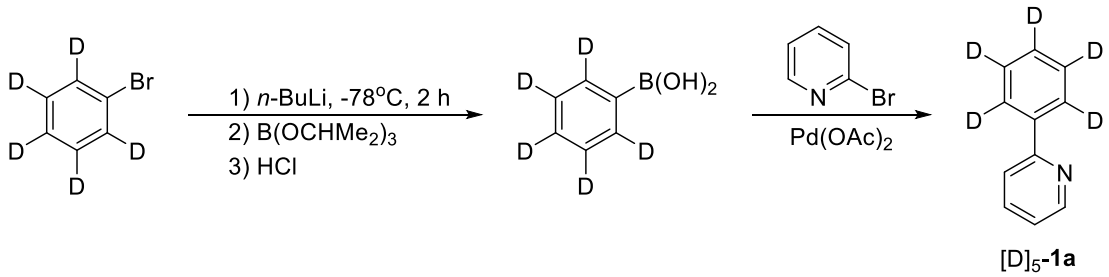
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.4 Hz, 2H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.40 – 7.34 (m, 2H), 7.28 – 7.23 (m, 3H), 4.51 (t, *J* = 6.2 Hz, 2H), 3.11 – 3.04 (m, 4H), 2.60 (t, *J* = 6.9 Hz, 2H), 2.13 – 2.04 (m, 2H), 1.57 – 1.48 (m, 4H), 0.85 (t, *J* = 7.4 Hz, 6H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 165.20, 144.23, 133.52, 131.54, 130.24, 128.24, 127.80, 126.98, 123.56, 88.44, 81.49, 64.46, 49.94, 27.85, 21.94, 16.43, 11.17.
HRMS (ESI) calcd for $[C_{24}H_{29}NO_4S]$ $(M+Na)^+$: 450.1715, found 450.1719

4.6 Synthesis of compounds 2w



Step1: To a solution of estrone **1I** (1.35 g, 5 mmol) and pyridine (0.81 g, 10 mmol) in dry CH_2Cl_2 (25 mL) was added Tf_2O (1 ml, 6 mmol) dropwise at 0 °C. After that, the mixture was warmed to rt, and stirred overnight. The mixture was then quenched with HCl (10%), extracted with CH_2Cl_2, washed twice with H_2O, dried over anhydrous $MgSO_4$ and concentrated by rotary evaporation.The residue was purified by flash column chromatography to afford **1J** (white solid, 1.77 g, 88 %).
Step2: To a solution of **1J** (1.77 g, 4.4 mmol), pent-1-yne (0.52 mL, 5.28 mmol) trimethylamine (3.0 mL), $Pd(PPh_3)_2Cl_2$ (92 mg, 0.132 mmol) CuI (25 mg, 0.132 mmol) in 15 mL DMF was stirred at 90 °C for 4 h under nitrogen. The mixture was quenched with water and extracted with EtOAc (50 mL x 3). The combined organic phases are washed with brine and dried over $MgSO_4$. The filtrate was concentrated in vacuo and the residue was purified by flash column chromatography to afford product **2w**[10] (white solid, 0.84g, 60%).

4.7 Synthesis of compounds $[D]_5$-1a



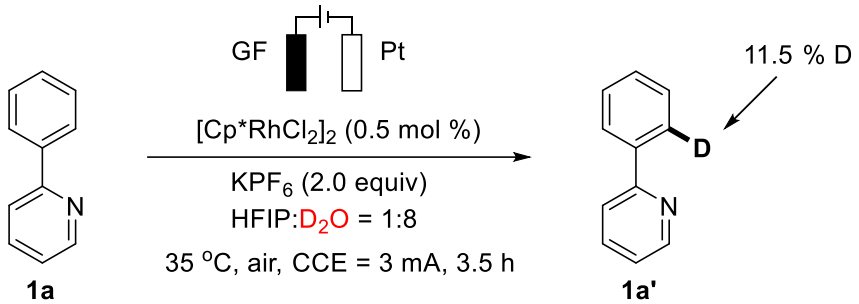
Step1: To a solution of the compound $[D]_5$-bromobenzene (8.1 mL, 40.0 mmol) in dried THF (100 mL), *n*-BuLi in *n*-hexane (25.0 mL, 1.6 M, 40.0 mmol) was added dropwise over 10 min at -78 °C under nitrogen atmosphere. The solution was stirred at -78°C for 2 h. And then triisopropyl borate (6.3 g, 60.0 mmol) dissolved in 10 mL of dry THF was added drop wise to the reaction system. After that, the reaction mixture was allowed to warm to room temperature and stirred overnight. The reaction

was quenched with dilute HCl (20%, 70 mL), and the reaction mixture was stirred for 3 h at room temperature. The resulted biphasic solution was extracted with Et_2O (2 x 50 mL),washed twice with H_2O and dried over anhydrous $MgSO_4$ and concentrated by rotary evaporation. To the crude product (viscous liquid), *n*-hexane 75 ml was added. The white ([D]$_5$-phenyl)boronic acid solid precipitated in *n*-hexane was filtered, dried and used without further purification (84% isolated yield).

Step2:A mixture of 2-bromopyridine (500 mg, 3.16 mmol), [D]$_5$-phenyl boronic acid (600 mg, 4.74 mmol), K_2CO_3 (873 mg, 6.32 mmol), $Pd(OAc)_2$ (10 mg, 0.04 mmol), water (12 mL) and ethanol (36 mL) was stirred at 80 °C in air for 1 h. The reaction mixture was added to brine (15 mL) and extracted with ethyl acetate (4 × 15 mL). The solvent was concentrated under vacuum, and the product was isolated by column chromatography on a short silica gel column to give **[D]$_5$-1a**[11] in 97% yield.

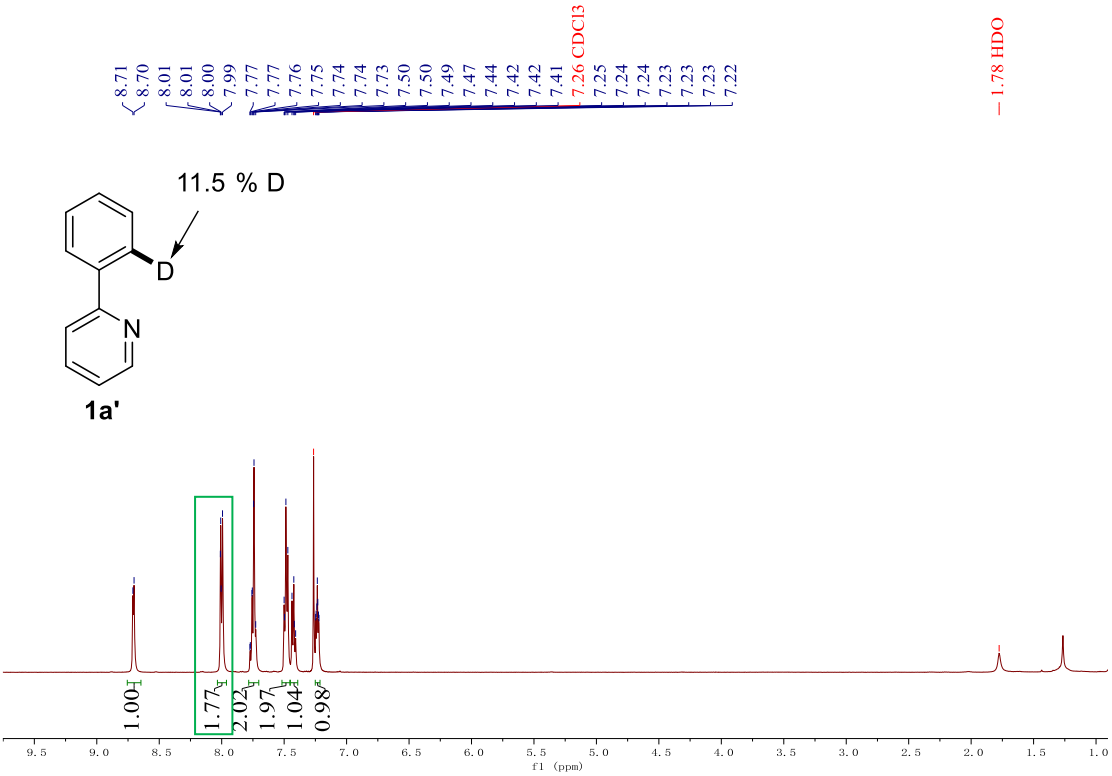
5. Mechanistic studies

5.1 Reversible H/D exchange with D_2O.

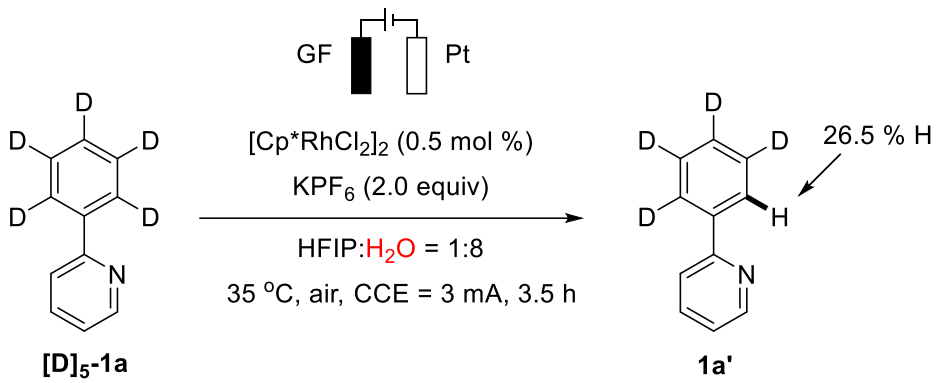


To a 10-mL three-necked flask, 2-phenylpyridine **1a** (0.2 mmol), $[Cp^*RhCl_2]_2$ (0.5 mol %) and KPF_6 (0.4 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/D_2O (1:8, 5 mL). Electrocatalysis was performed at 35 °C with a constant current of 3.0 mA maintained for 3.5 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL).The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by silica gel column chromatography using petroleum ether/ethyl acetate (20:1) as eluent to give the desired product **1a'**.The D/H-incorporation in **1a'** was determined by ^{1}H-NMR spectroscopy.

^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **1a'**.

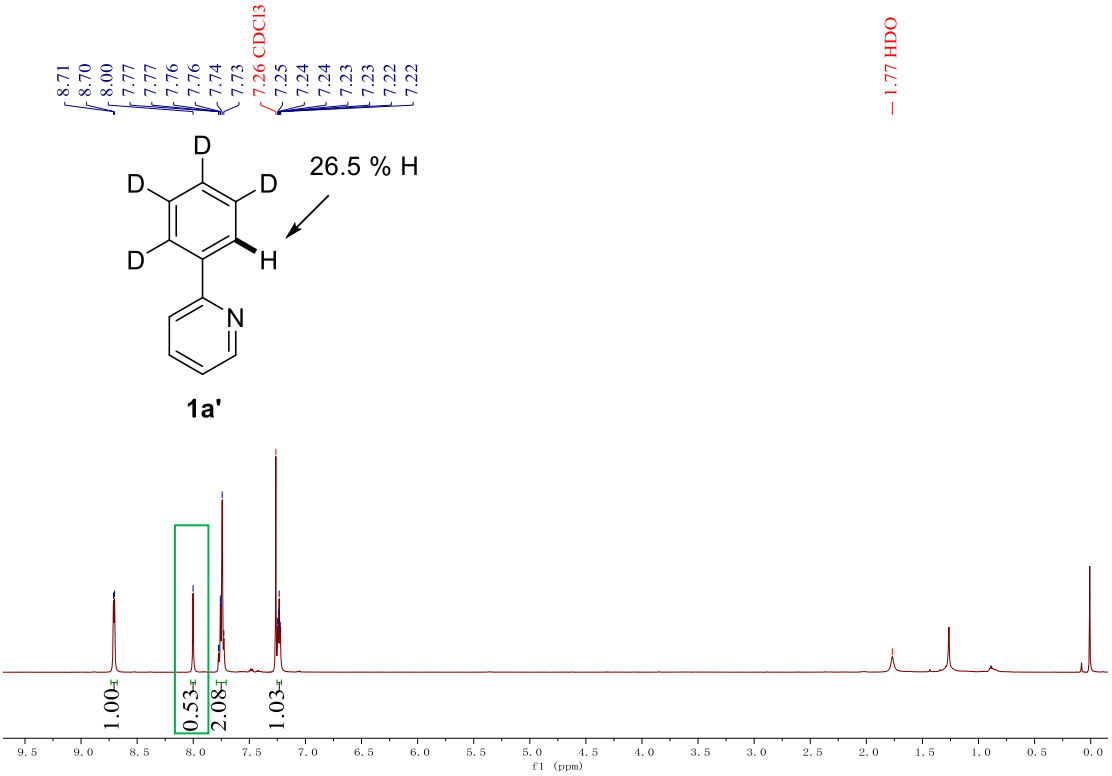


5.2 Reversible H/D exchange with H_2O.

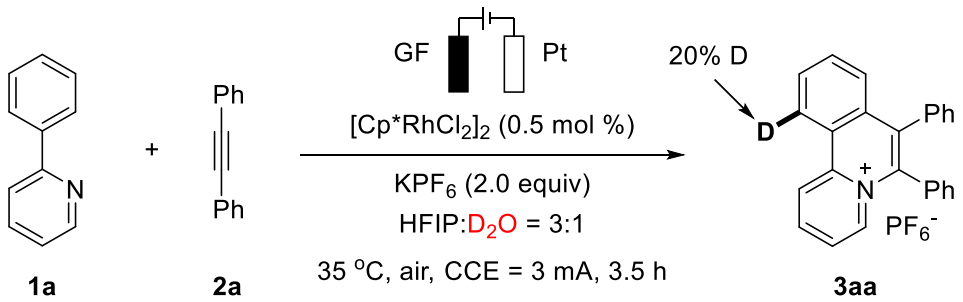


To a 10-mL three-necked flask, 2-phenylpyridine **[D]$_5$-1a** (0.2 mmol), [Cp*RhCl$_2$]$_2$ (0.5 mol %) and KPF_6 (0.4 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/H_2O (1:8, 5 mL). Electrocatalysis was performed at 35 °C with a constant current of 3.0 mA maintained for 3.5 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL). The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by silica gel column chromatography using petroleum ether/ethyl acetate (20:1) as eluent to give the desired product **1a'**. The D/H-incorporation in **1a'** was determined by ^{1}H-NMR spectroscopy.

^{1}H NMR (500 MHz, $CDCl_3$) spectra of compound **1a'**.

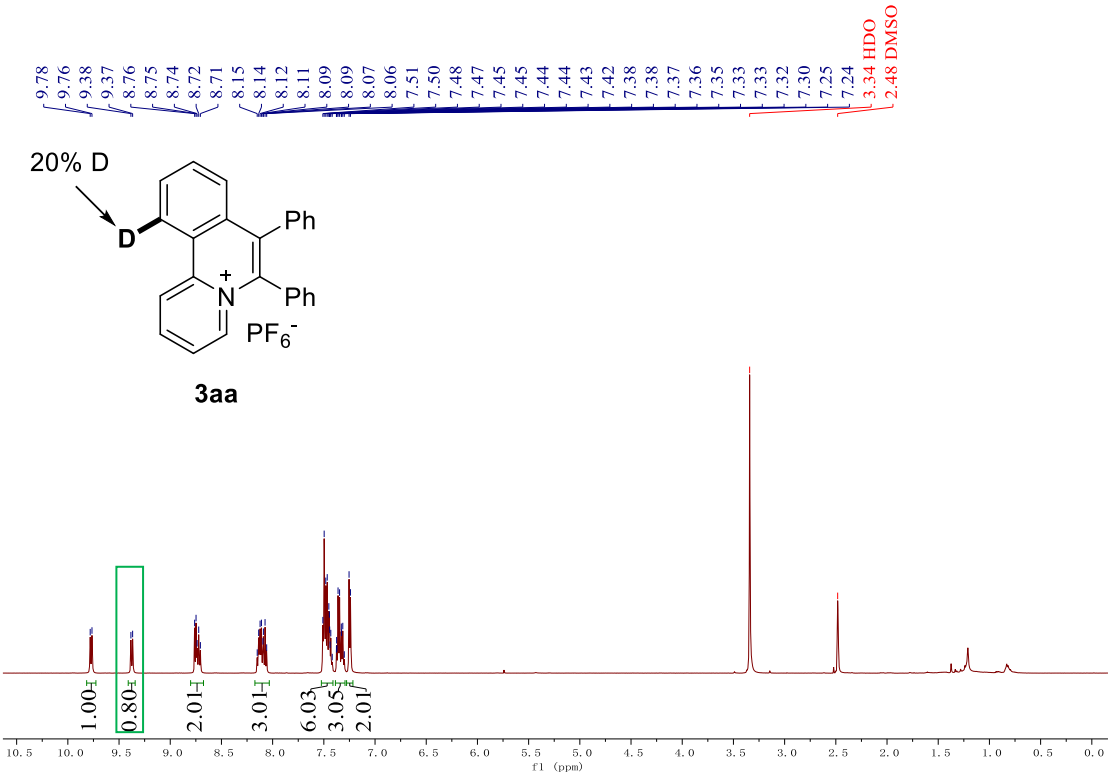


5.3 H/D exchange experiment with D_2O in presence of alkyne.

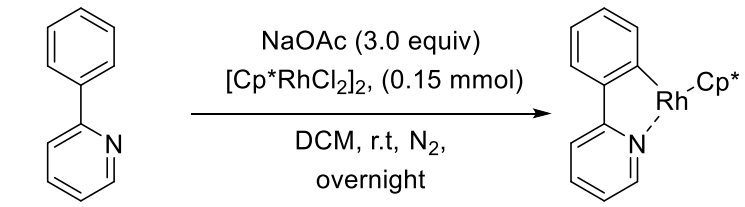


To a 10-mL three-necked flask, 2-phenylpyridine **1a** (0.2 mmol), Diphenylacetylene **2a** (0.22 mmol), $[Cp^*RhCl_2]_2$ (0.5 mol %) and KPF_6 (0.4 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/D_2O (3:1, 5 mL). Electrocatalysis was performed at 35 °C with a constant current of 3.0 mA maintained for 3.5 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL). The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by silica gel column chromatography using DCM/MeOH (95:5) as eluent to give the desired product **3aa**. The D/H-incorporation in **3aa** was determined by ^{1}H-NMR spectroscopy.

^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **3aa**.



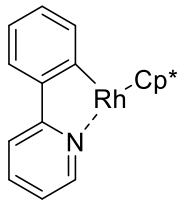
5.4 Synthesis of Rh(III) Complex 6



1a, (0.35 mmol) **6**, 80%

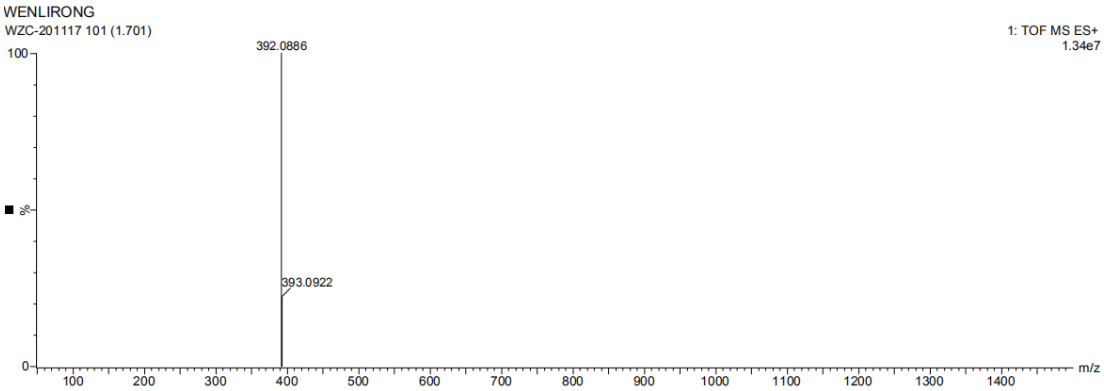
Rhodium(III) complex **6** is a known compound, and which was synthesized by following a literature report. $[Cp^*RhCl_2]_2$ (100.0 mg, 0.15 mmol), 2-phenylpyridine (0.35 mmol), sodium acetate (3.0 equiv.), and dichloromethane (DCM, 3 mL) were charged into a Schleck tube under N_2 atmosphere. Then, the mixture was stirred at room temperature for overnight. The resultant mixture was filtered through celite and evaporated to dryness. The product **6**[12] was purified via silica gel chromatography (eluent: petroleum ether/ethyl acetate = 1:1).

Rh(III) Complex 6[12]

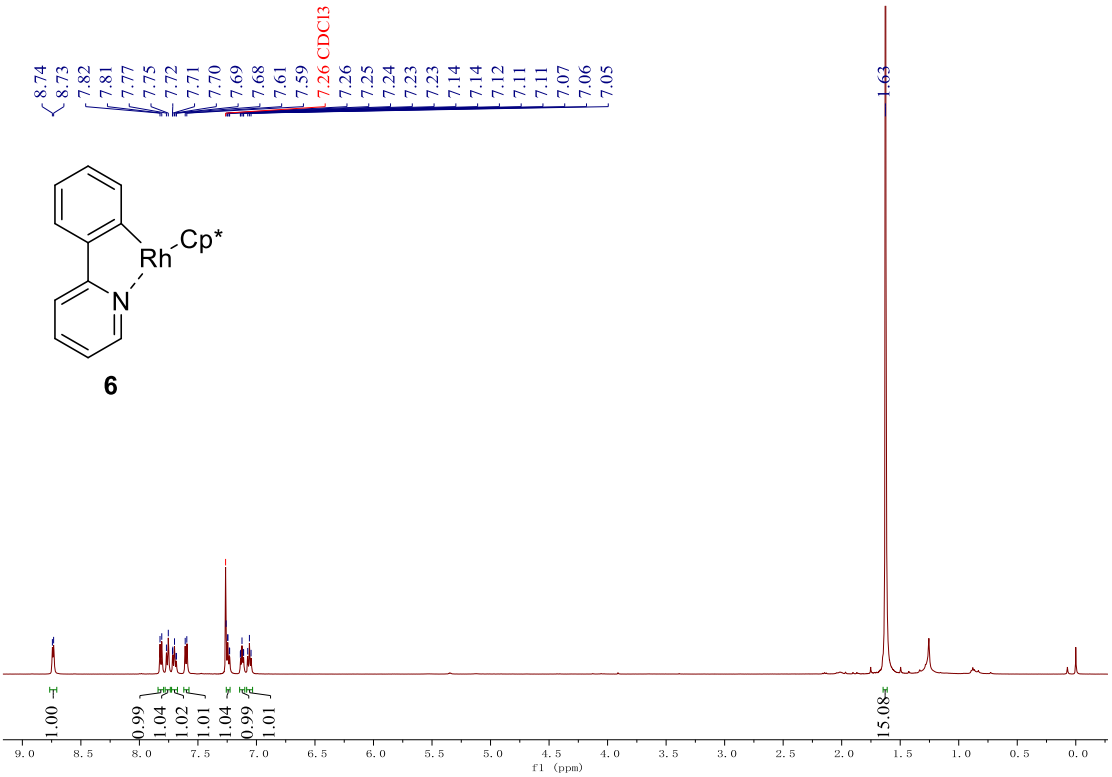


Orange solid; yield 80%

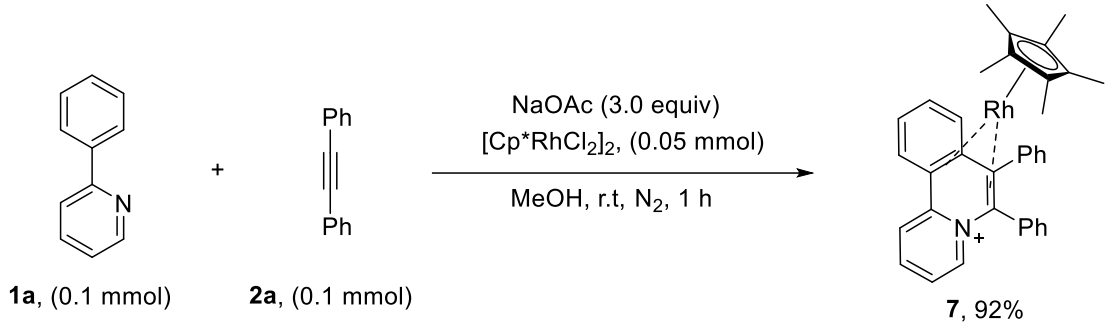
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 5.2 Hz, 1H), 7.82 (d, *J* = 7.5 Hz, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.60 (d, *J* = 6.8 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.14 – 7.10 (m, 1H), 7.06 (t, *J* = 7.1 Hz, 1H), 1.63 (s, 15H).
HRMS (ESI) calcd for [$C_{21}H_{23}NRh^+$] :392.0880, found 392.0886.



^{1}H NMR (500 MHz, $CDCl_3$) spectra of complex **6**.

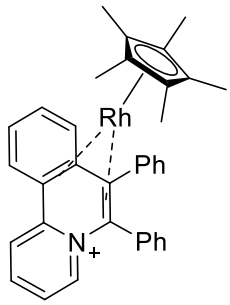


5.5 Synthesis of Rh(I) Complex 7



$[Cp^*RhCl_2]_2$ (100.0 mg, 0.05 mmol), 2-phenylpyridine (0.1 mmol), Diphenylacetylene (0.1 mmol), sodium acetate (0.30 mmol 3.0 equiv.), and methanol (MeOH, 3 mL) were charged into a Schleck tube under N_2 atmosphere. Then, the mixture was stirred at room temperature for 1 h, and then the corresponding solution was concentrated under vacuum to remove the solvent. The residue was carefully washed with anhydrous Et_2O (2.0 mL x 3) to give the **7** as a brown solid.

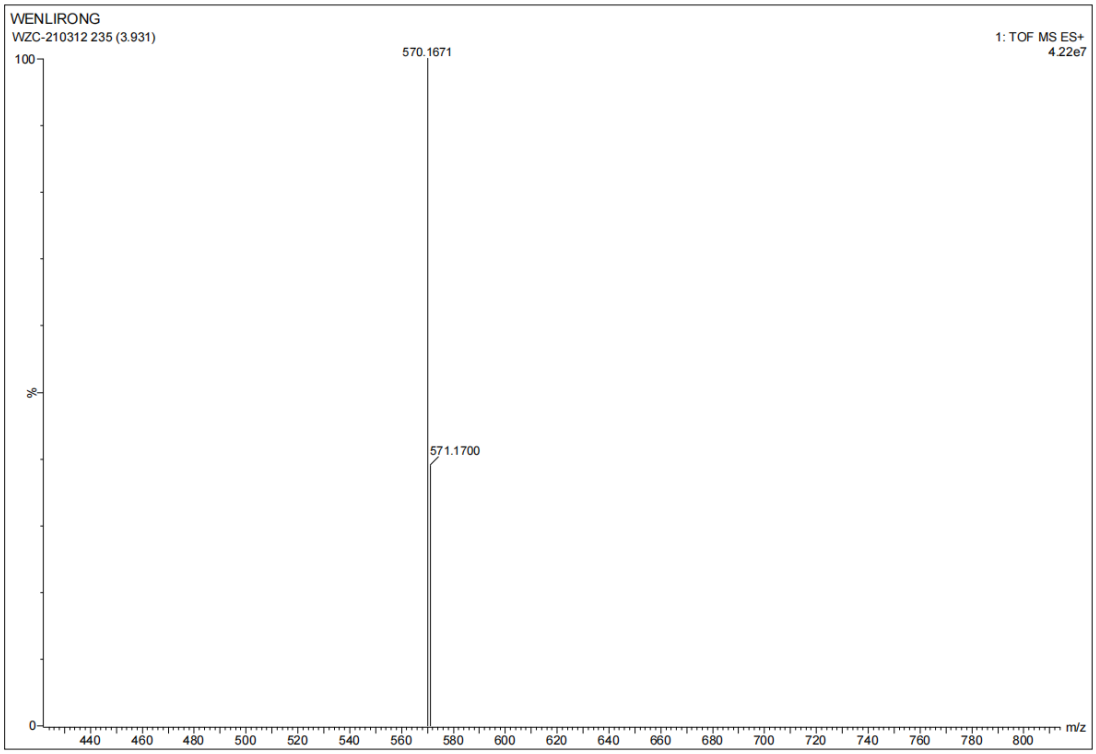
Rh(I) Complex 7[13]



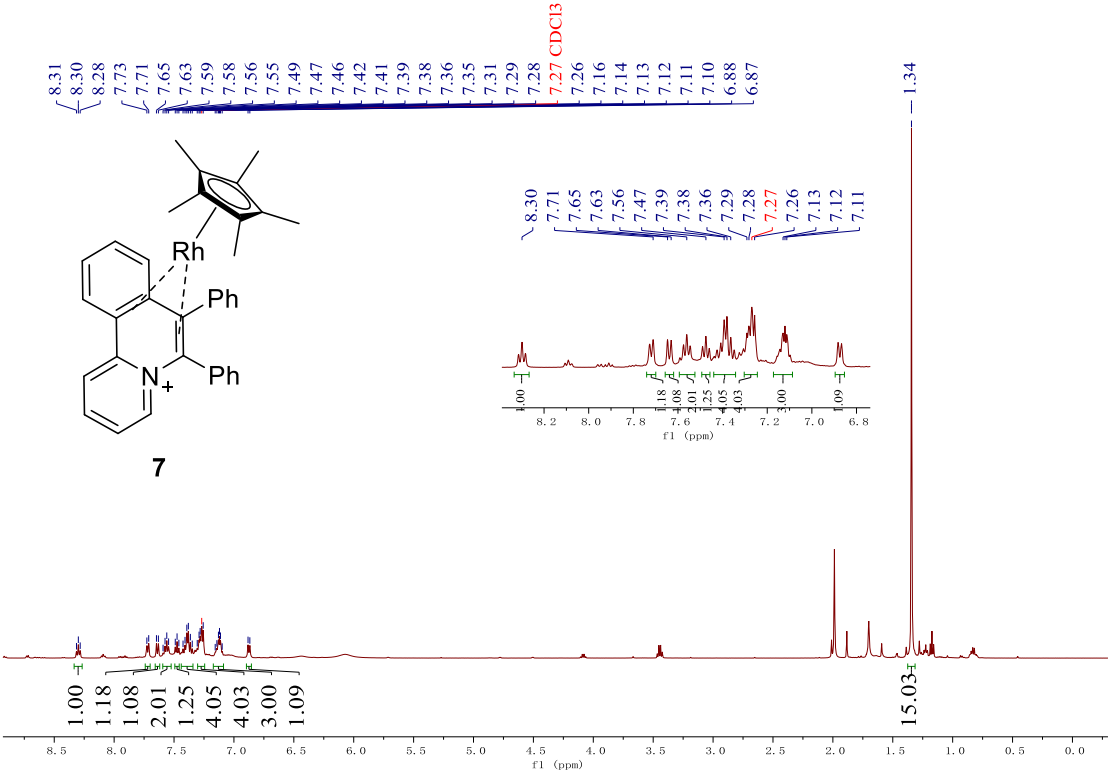
Brown solid; yield 92%

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (t, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.59 – 7.52 (m, 2H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.44 – 7.34 (m, 4H), 7.30 – 7.24 (m, 4H), 7.17 – 7.09 (m, 3H), 6.87 (d, *J* = 7.5 Hz, 1H), 1.34 (s, 15H).

HRMS (ESI) calcd for $[C_{35}H_{33}NRh^+]$:570.1663, found 570.1671.



^{1}H NMR (500 MHz, $CDCl_3$) spectra of complex **7**.



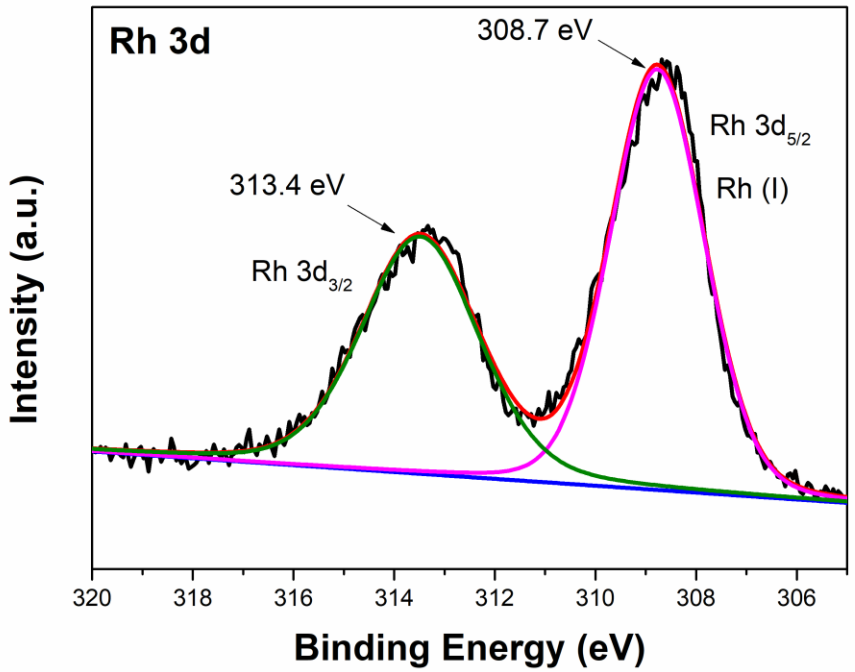
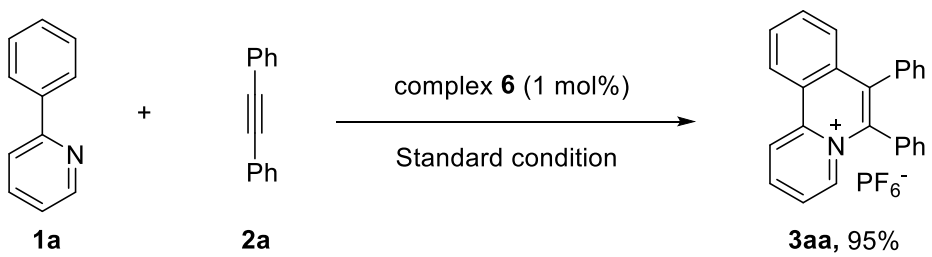


Figure S1. High resolution Rh3d XPS spectrum of complex **7**

5.6 Eletrolysis of complex 7

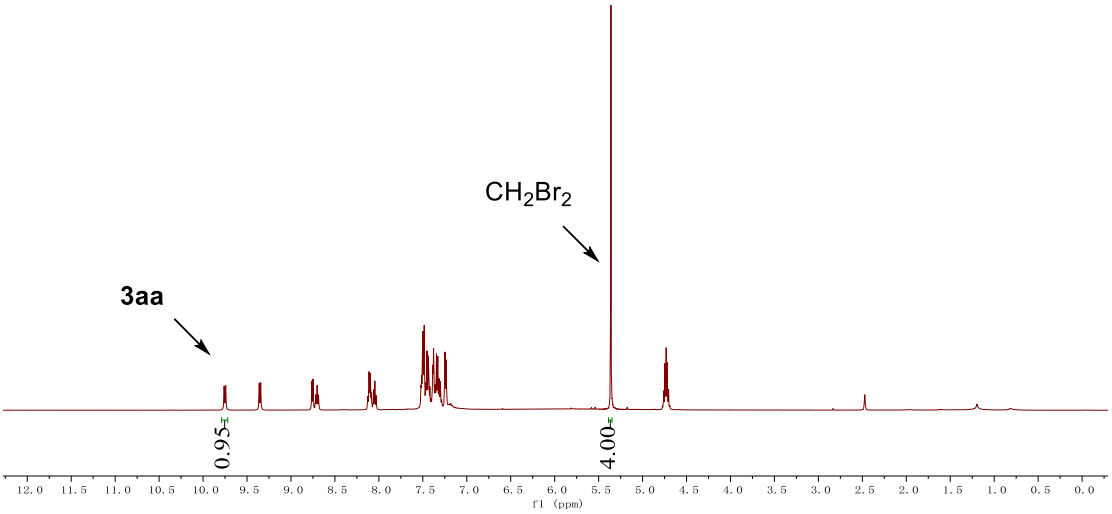
To a 10-mL three-necked flask, complex **7** (0.1 mmol), KPF_6 (0.2 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/H_2O (3:1, 5 mL). Electrocatalysis was performed at 35 ^oC with a constant current of 3.0 mA maintained for 1.5 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL). The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). After removal of the solvent in vacuum, **3aa** was isolated in 85% yield.

5.7 Reaction of complex 6 with 1a and 2a

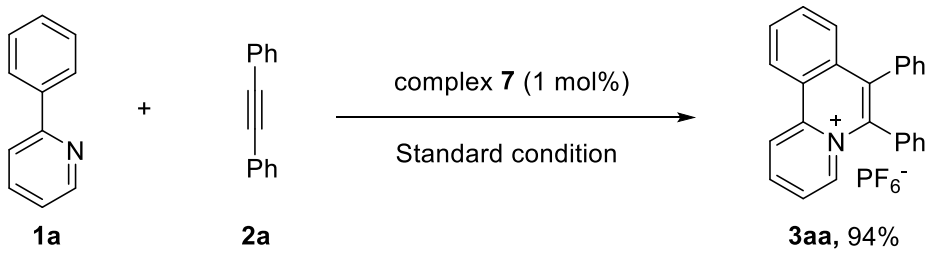


To a 10-mL three-necked flask, 2-phenylpyridine **1a** (0.1 mmol), Diphenylacetylene **2a** (0.12 mmol), complex **6** (1.0 mol %) and KPF_6 (0.2 mmol, 2.0 equiv) were

dissolved in solvent mixture HFIP/H_2O (3:1, 5 mL). Electrocatalysis was performed at 35 °C with a constant current of 3.0 mA maintained for 2 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL). The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). After removal of the solvent in vacuum, the residue was analyzed by ^{1}H NMR with CH_2Br_2 (0.2 mmol) as the internal standard.
^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **3aa**.

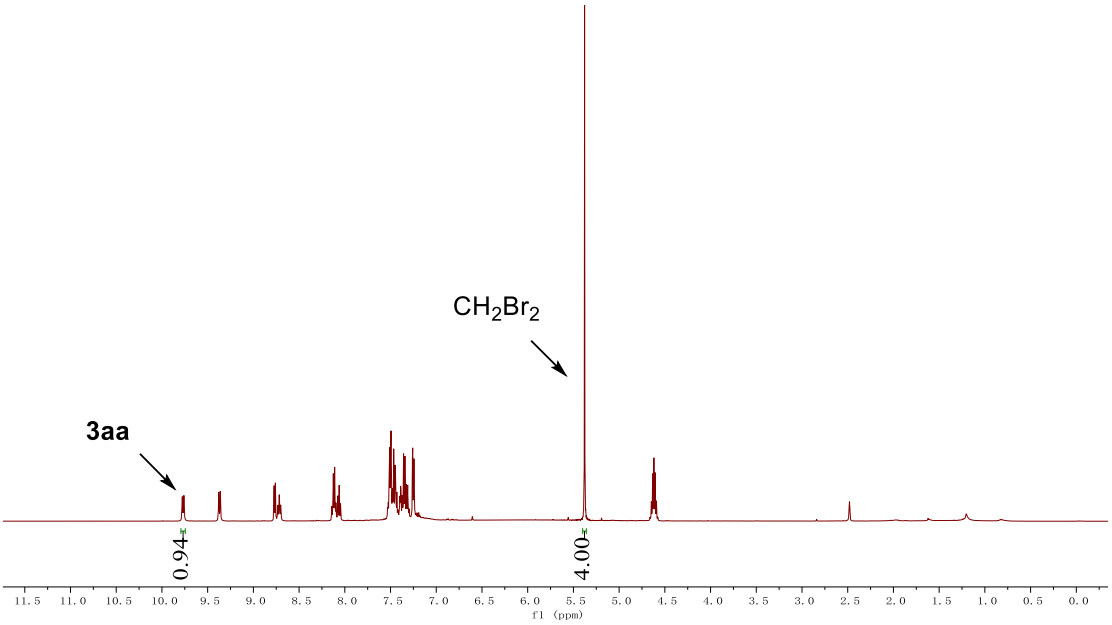


5.8 Reaction of complex 7 with 1a and 2a

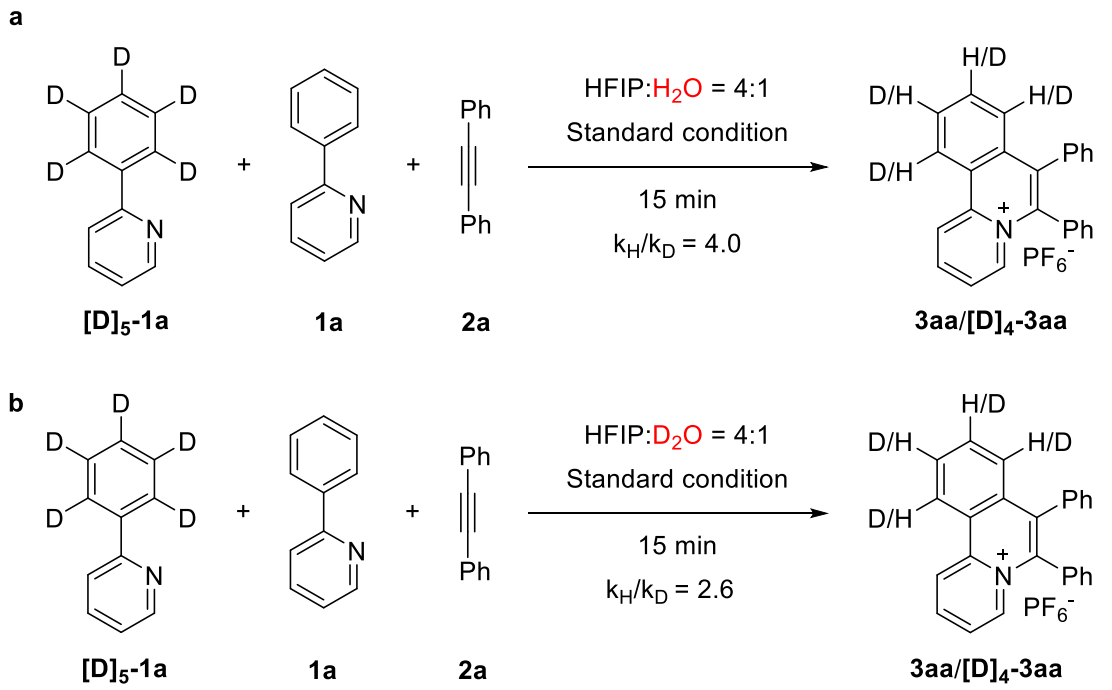


To a 10-mL three-necked flask, 2-phenylpyridine **1a** (0.1 mmol), Diphenylacetylene **2a** (0.12 mmol), complex **7** (1.0 mol %) and KPF_6 (0.2 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/H_2O (3:1, 5 mL). Electrocatalysis was performed at 35 °C with a constant current of 3.0 mA maintained for 2 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL). The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). After removal of the solvent in vacuum, the

residue was analyzed by ^{1}H NMR with CH_2Br_2 (0.2 mmol) as the internal standard. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **3aa**.



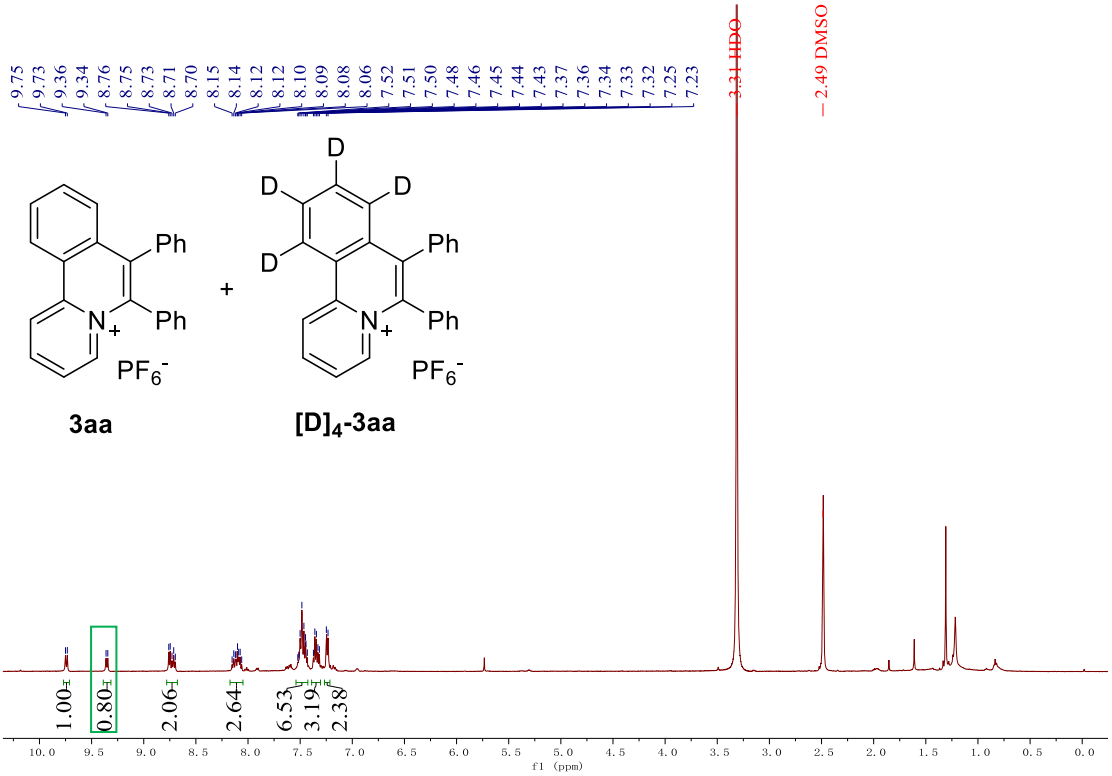
5.9 Competitive Experiments.

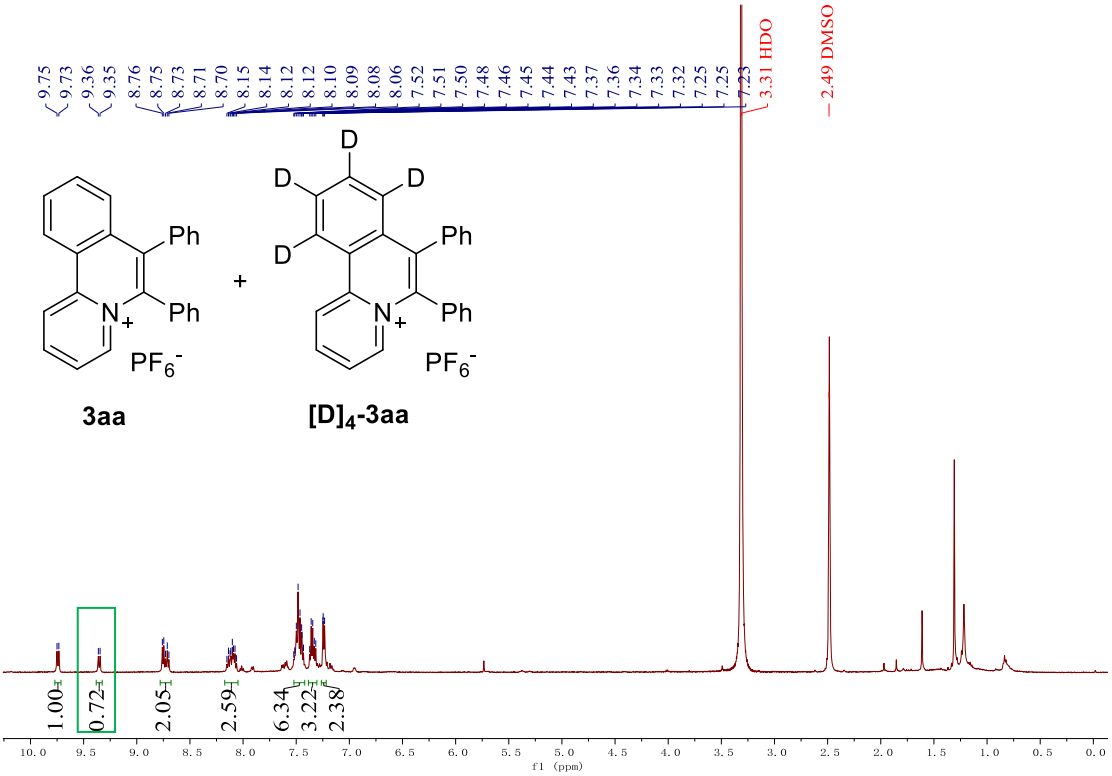


To a 10-mL three-necked flask, **[D]$_5$-1a**(0.20 mmol), **1a** (0.20 mmol), Diphenylacetylene **2a** (0.22 mmol), $[Cp^*RhCl_2]_2$ (0.5 mol %) and KPF_6 (0.4 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP:H_2O (or D_2O) (4:1, 5 mL).

Electrocatalysis was performed at 35 °C with a constant current of 3.0 mA maintained for 15 min. When the reaction was completed, the mixture was diluted with CH_2Cl_2 (10 mL). The GF anode was washed with CH_2Cl_2 (3 x 5 mL) in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2 (30 mL). The filtrate was concentrated and purified by silica gel column chromatography using DCM/MeOH (95:5) as eluent to give the desired product **3aa/[D]$_4$-3aa**. The D/H-incorporation in **3aa/[D]$_4$-3aa** was determined by ^{1}H-NMR spectroscopy. The kinetic isotopic effect of this reaction was determined to be $k_H/k_D \approx 4.0$ in H_2O and $k_H/k_D \approx 2.6$ in D_2O.

^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **3aa/[D]$_4$-3aa**.





6. Cyclic Voltammetry Studies

The voltammograms were recorded at room temperature in MeCN at a substrate concentration of 5 mmol/L and with 0.1 mol/L nBu$_4$NPF$_6$ as supporting electrolyte. Using glassy carbon electrode working electrode, Pt wire, and SCE as counter and reference electrodes at 100 mVs^{-1} scan rate.

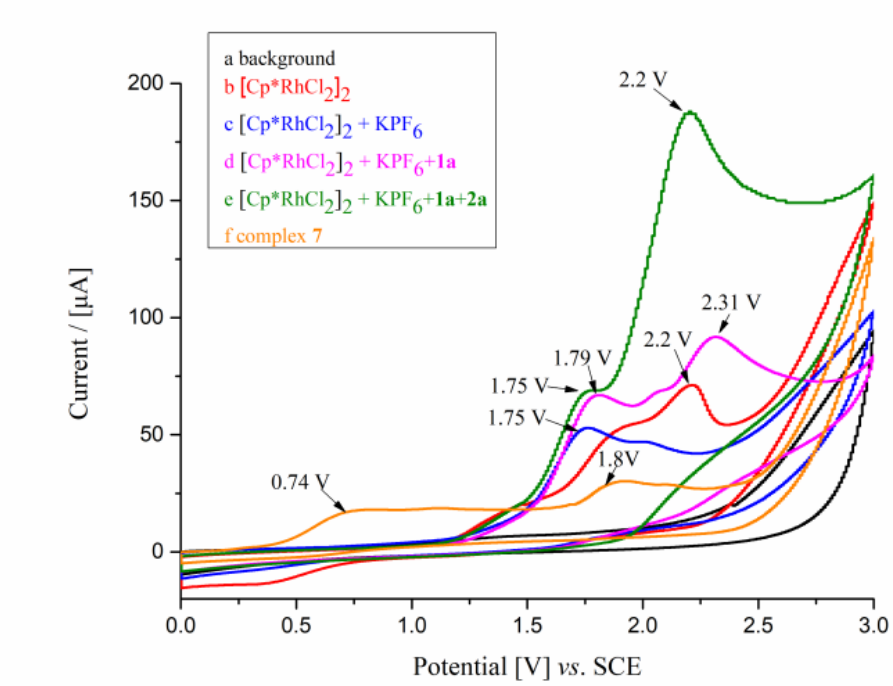


Figure S2. (a): nBu$_4$NPF$_6$ (0.1 M). (b): nBu$_4$NPF$_6$ (0.1 M) and[Cp*RhCl$_2$]$_2$ (2.0 mM).

(c): nBu$_4$NPF$_6$ (0.1 M), [Cp*RhCl$_2$]$_2$ (2.0 mM) and KPF$_6$ (4.0 mM). (d): nBu$_4$NPF$_6$ (0.1 M), [Cp*RhCl$_2$]$_2$ (2.0 mM), KPF$_6$ (4.0 mM), and **1a** (4.0 mM). (e): nBu$_4$NPF$_6$ (0.1 M), [Cp*RhCl$_2$]$_2$ (2.0 mM), KPF$_6$ (4.0 mM), **1a** (4.0 mM), and **2a** (4.0 mM) .(f): nBu$_4$NPF$_6$ (0.1 M) and complex **7** (2.0 mM).

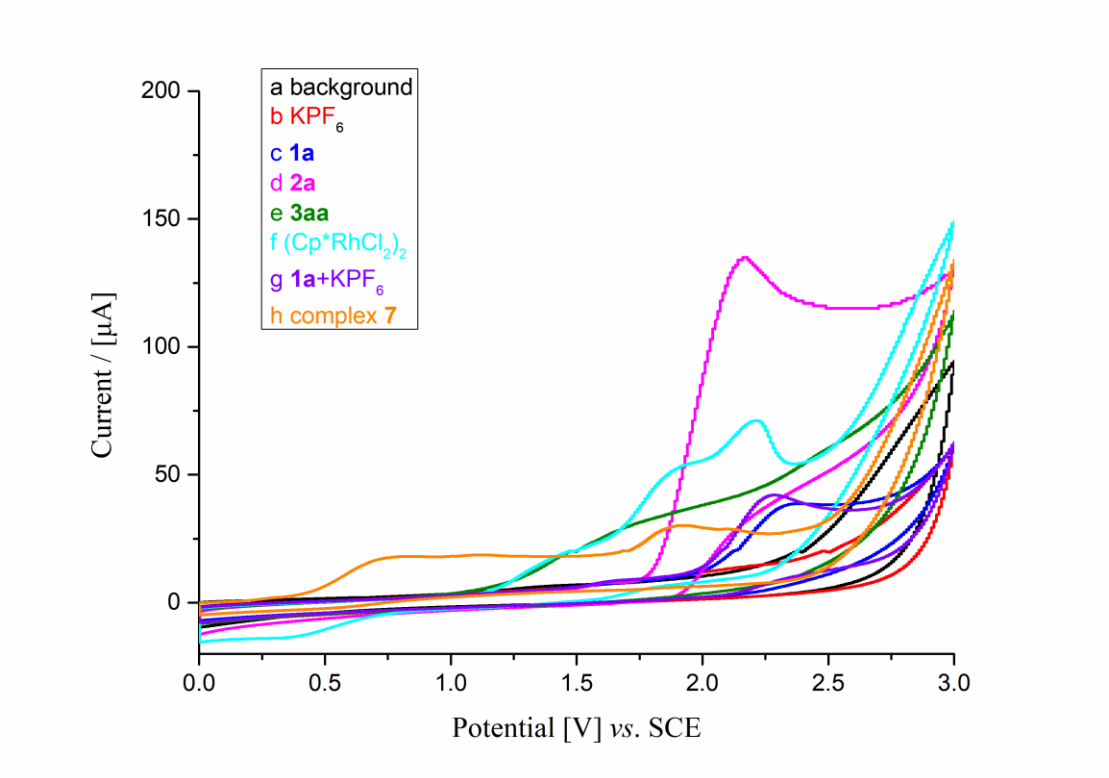


Figure S3. (a): nBu$_4$NPF$_6$ (0.1 M). (b): nBu$_4$NPF$_6$ (0.1 M) and KPF$_6$ (4.0 mM). (c): nBu$_4$NPF$_6$ (0.1 M) and **1a** (4.0 mM). (d): nBu$_4$NPF$_6$ (0.1 M) and **2a** (4.0 mM). (e): nBu$_4$NPF$_6$ (0.1 M) and **3aa** (4.0 mM).(f): nBu$_4$NPF$_6$ (0.1 M) and [Cp*RhCl$_2$]$_2$ (2.0 mM). (g): nBu$_4$NPF$_6$ (0.1 M), **1a** (4.0 mM) and KPF$_6$ (4.0 mM). (h) nBu$_4$NPF$_6$ (0.1 M) and complex **7** (4.0 mM).

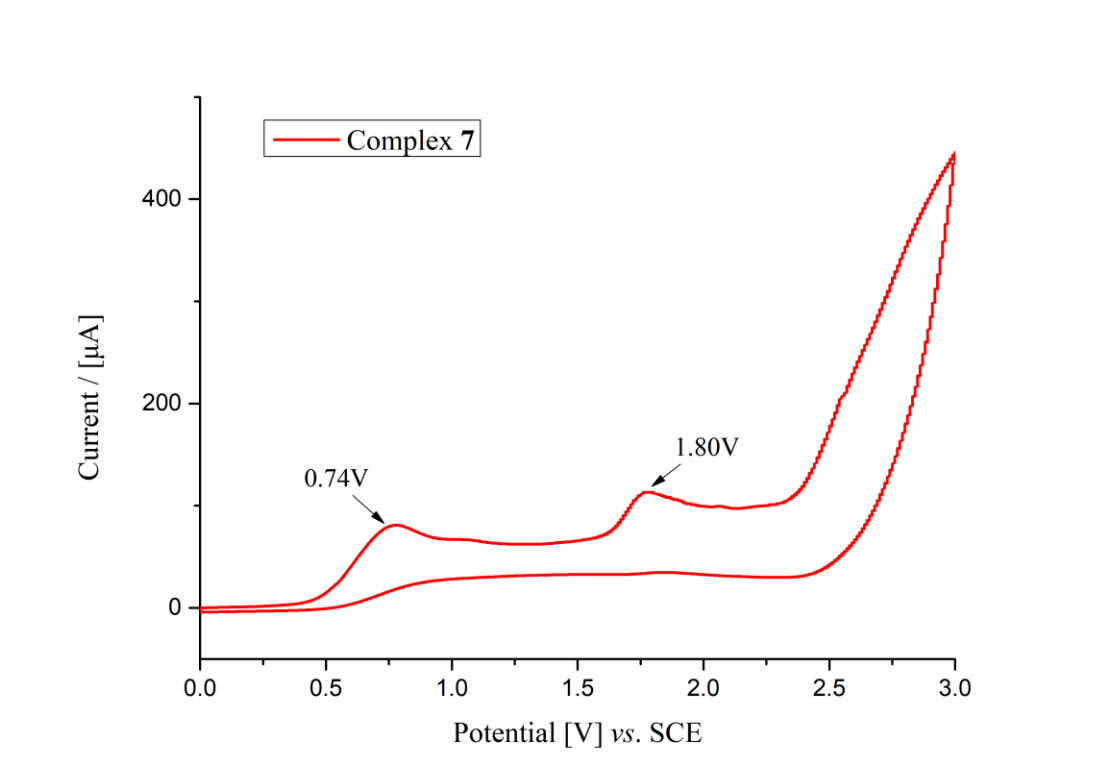
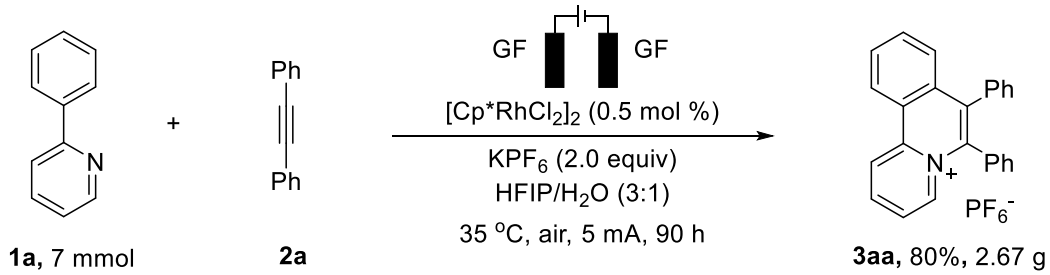


Figure S4. (a): nBu$_4$NPF$_6$ (0.1 M) and complex **7** (0.1 M).

7. Gram-scale reaction



The electrocatalysis was carried out in an undivided cell under air, with a graphite felt (GF) anode (4 cm x 2 cm x 0.5 cm) and a graphite felt (GF) anode (4 cm x 2 cm x 0.5 cm). To a 250 mL three-necked flask, 2-phenylpyridine **1a** (7 mmol, 1.0 equiv), diphenylacetylene **2a** (8.4 mmol, 1.2 equiv), [Cp*RhCl$_2$]$_2$ (0.5 mol %) and KPF$_6$ (14 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/H$_2$O (3:1, 52 mL). Electrocatalysis was performed at 35 ^{o}C with a constant current of 5.0 mA maintained for 90 h. When the reaction was completed, the mixture was diluted with CH$_2$Cl$_2$. The GF anode was washed with CH$_2$Cl$_2$ in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH$_2$Cl$_2$. The filtrate was concentrated and purified by silica gel column chromatography using DCM/MeOH (95:5) as eluent to give the desired product **3aa**.

8. Decagram-scale reaction

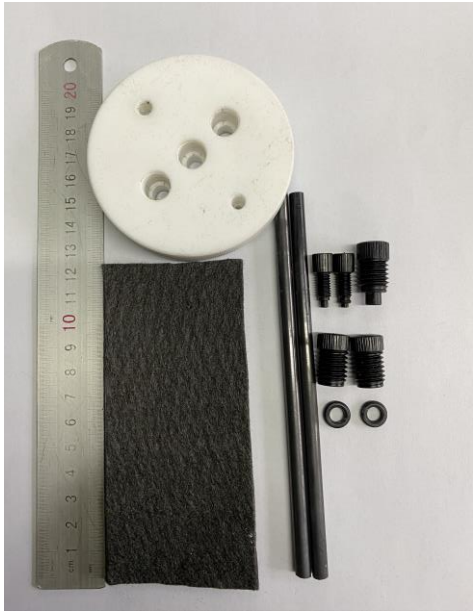


Figure S5. Components required for the decagram-scale reaction

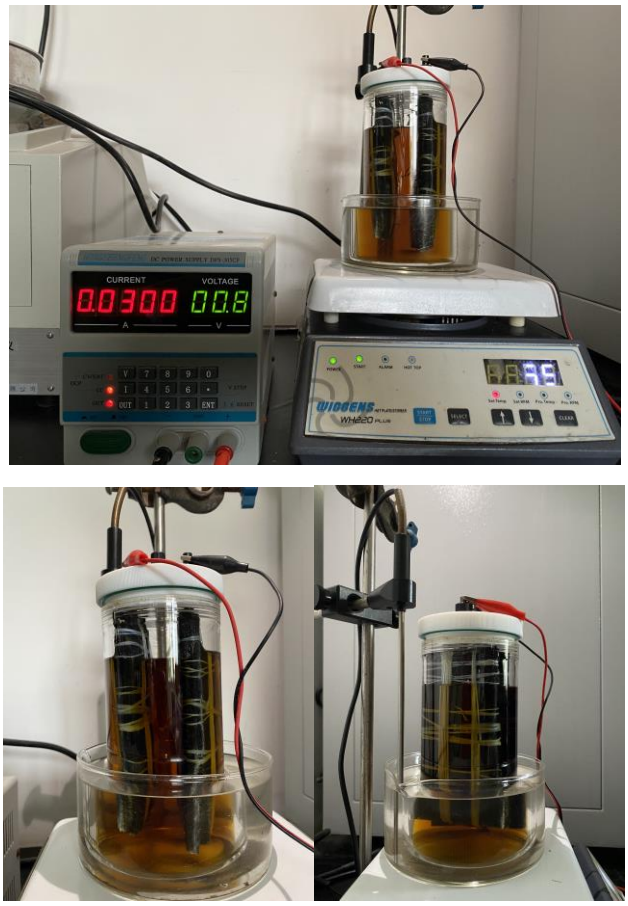
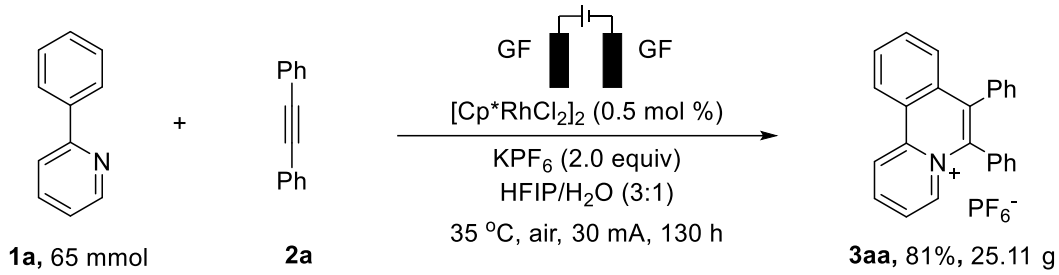
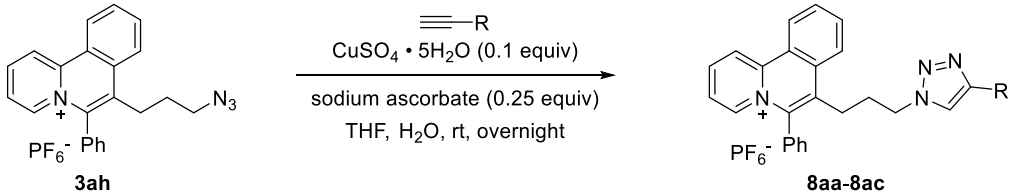


Figure S6. Typical reaction set up for the decagram-scale reaction



The electrocatalysis was carried out in an undivided cell under air, with a graphite felt (GF) anode (12.5 cm x 5.5 cm x 0.5 cm) and a graphite felt (GF) anode (12.5 cm x 5.5 cm x 0.5 cm). To a 500 mL beaker-type cell, 2-phenylpyridine **1a** (65 mmol, 1.0 equiv), diphenylacetylene **2a** (78 mmol, 1.2 equiv), $[Cp^*RhCl_2]_2$ (0.5 mol %) and KPF_6 (130 mmol, 2.0 equiv) were dissolved in solvent mixture HFIP/H_2O (3:1, 400 mL). Electrocatalysis was performed at 35 °C with a constant current of 30.0 mA maintained for 130 h. When the reaction was completed, the mixture was diluted with CH_2Cl_2. The GF anode was washed with CH_2Cl_2 in an ultrasonic bath, and all the solvent was transfered to a round bottom flask. The mixture was filtered through a Celite pad and the Celite pad was washed with CH_2Cl_2. The filtrate was concentrated and purified by silica gel column chromatography using DCM/MeOH (95:5) as eluent to give the desired product **3aa**.

9. Synthesis of compounds 8aa-8ac



To a solution of compound **3ah** (0.2 mmol) in a 1:1 mixture of THF:H_2O (5 mL) were added copper(II) sulfate (0.02 mmol, 0.1 equiv), sodium ascorbate (0.05 mmol, 0.25 equiv) and the corresponding alkynes (0.26 mmol, 1.3 equiv). The mixture was stirred at room temperature overnight. The combined organic phase was washed with brine, dried over anhydrous $MgSO_4$. The solvent was evaporated in vacuum and purified by silica gel column chromatography to avail products **8aa-8ac.**

10. Photoluminescence spectra of selected salts

We investigated the photophysical properties of **3aa**, **3ba**, **3na**, **3ha**, **3sa**, **3ra** and **3ua** as the representative examples. As shown in Figure S5, the synthesized polycyclic isoquinolinium salts showed deep-blue-to-orange fluorescence emission.

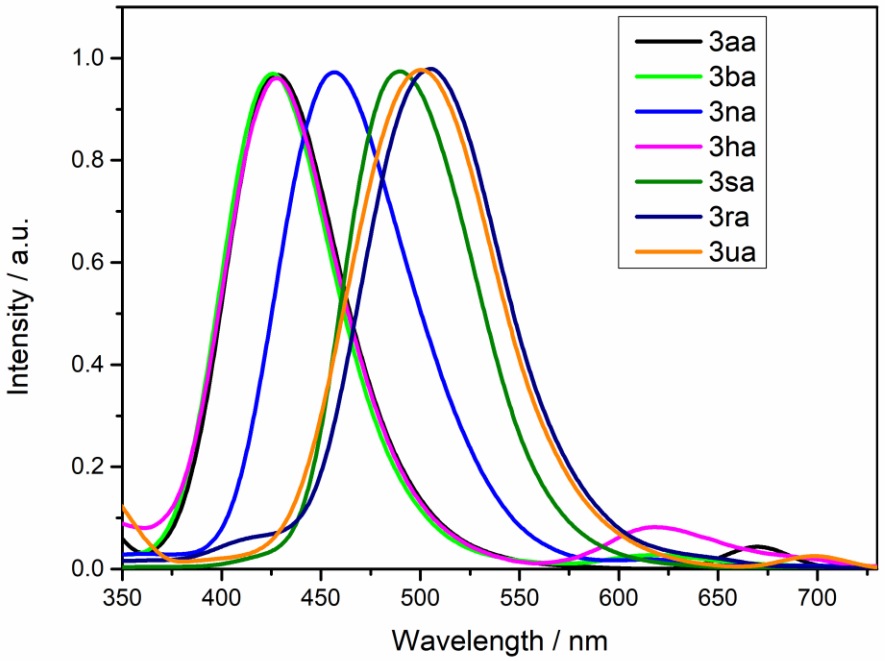


Figure S7. Photoluminescence spectra of selected salts in CH_2Cl_2 (1.0 X 10^{-5} M).

11. Computational Details

All calculations were performed using Gaussian 16, Revision A.03 package.[14]All of the reactants, intermediates, transition states, products were optimized by the DFT with the ωB97X-D functional. For geometry optimizations and frequency calculations, BS-I basis set system was employed. In BS-I, we employed LANL2DZ basis set for Rh with effective core potentials, 6-31G(d) basis sets for H, C, O, N, F, and P. All the stationary structures were characterized with no imaginary frequency and the transition state structures (TSs) were characterized with a single imaginary frequency. Intrinsic reaction coordinate (IRC) calculations4 were performed on all the TSs. The solvent effect was evaluated through the SMD[15] method, in which a better basis system BS-II was used. In BS-II, we employed LANL2DZ basis sets for Ni, 6-311++G** basis sets for the other atoms. All the 3D molecular structures of the species were generated by using the CYLview program.[16] The NCI polt was prepared by Multiwfn3.8.[17]

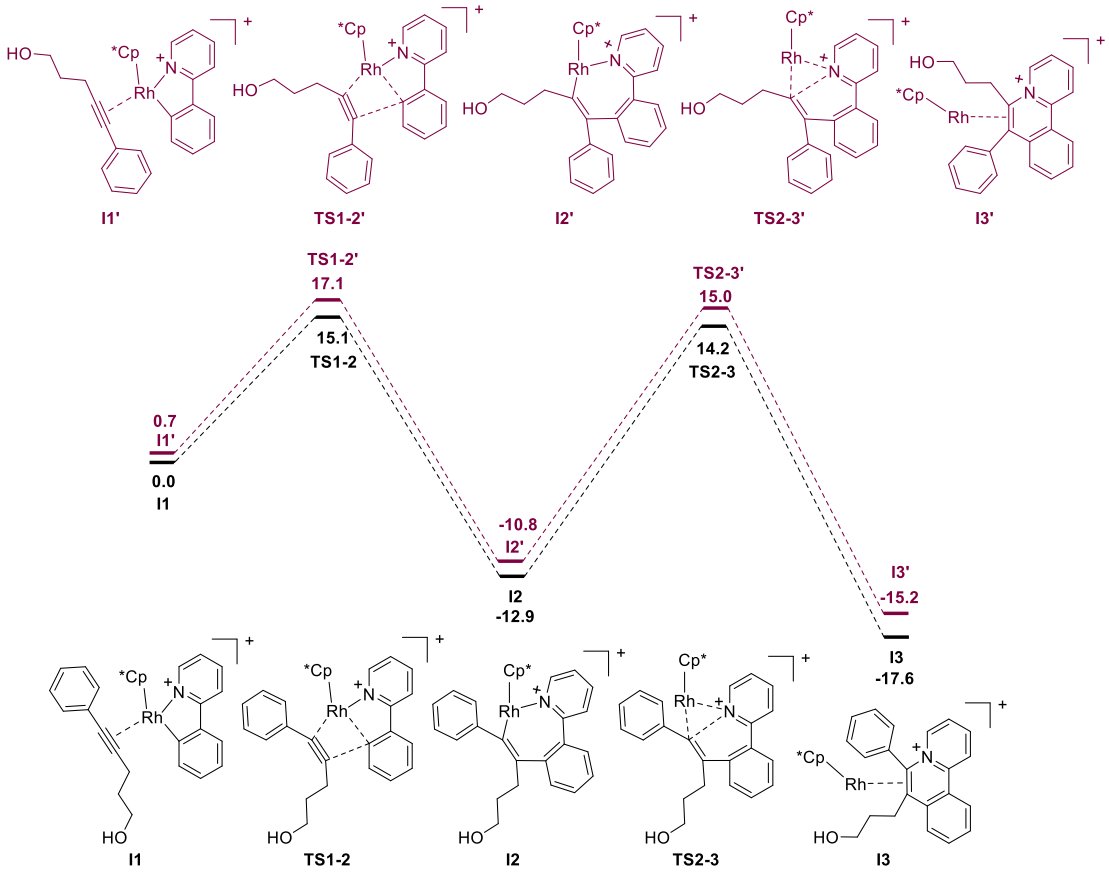


Figure S8. Gibbs free energy profile in kcal/mol for the migratory insertion and reductive elimination processes.

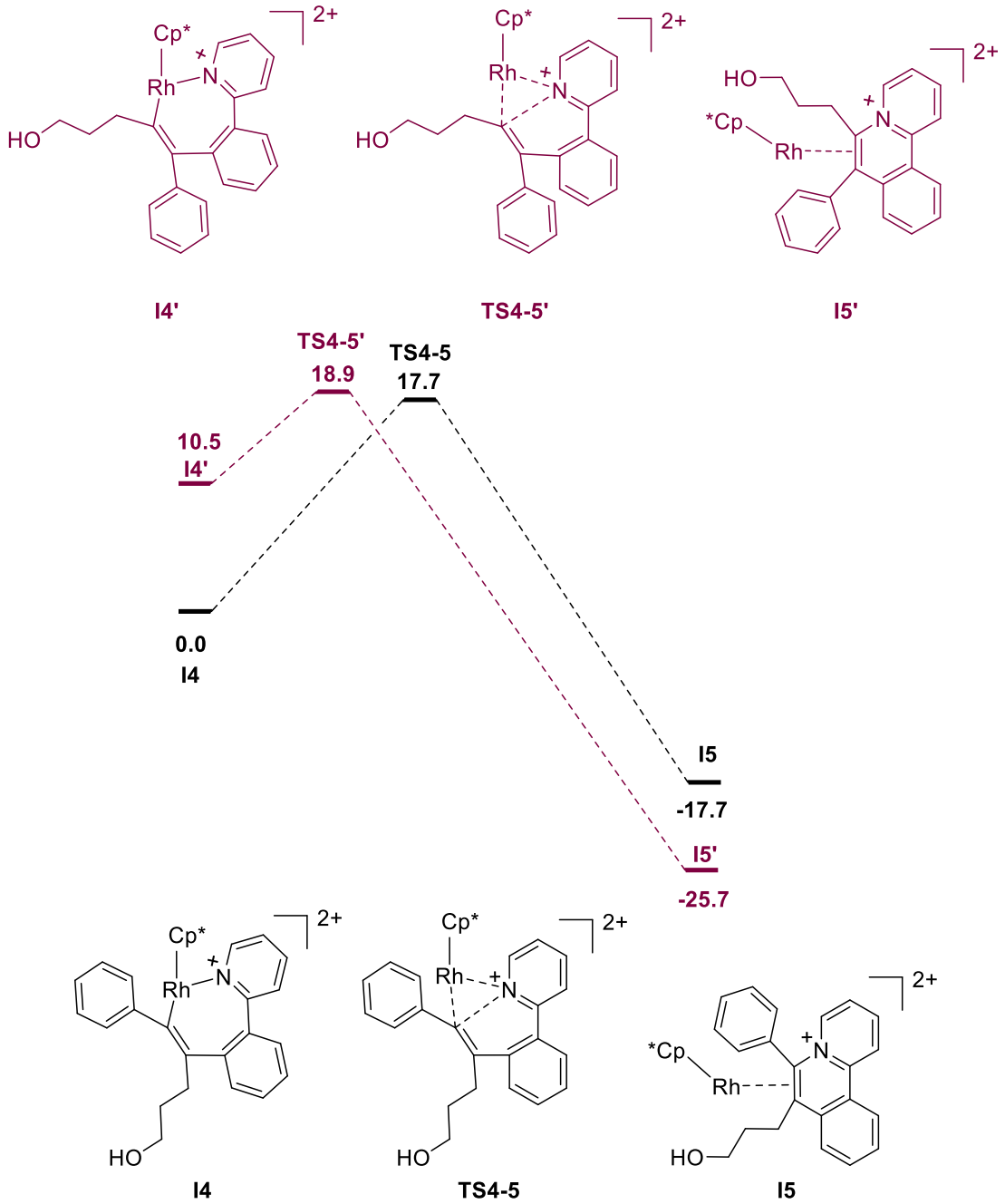


Figure S9. Gibbs free energy profile in kcal/mol for the oxidatively induced reductive elimination processes.

Cartesian coordinates of the optimized structures

I1

E = -1479.338168 a.u.

C	0.71919000	-2.03788100	0.79877800
C	1.38592300	-0.99386300	0.79716600
C	0.98334400	-0.59646600	-2.75648000
C	0.84846900	-1.97646700	-2.42345300

C	-0.33955700	-0.07646900	-2.92248700
C	-0.54982700	-2.33024200	-2.44376900
C	-1.29199500	-1.14020800	-2.74699100
C	1.97186800	-2.92952900	-2.16689200
H	2.38005800	-3.29128400	-3.11757900
H	2.78146100	-2.45566000	-1.60599200
H	1.63618300	-3.79840600	-1.59558100
C	-1.09230800	-3.72471300	-2.42002900
H	-0.90472200	-4.20672700	-3.38648000
H	-0.62057800	-4.34361900	-1.65171700
H	-2.17115900	-3.73294600	-2.25314400
C	-2.76810700	-1.04331900	-2.97264600
H	-3.00971600	-1.28424600	-4.01420100
H	-3.31558800	-1.73116300	-2.32384600
H	-3.13462100	-0.03495500	-2.76510200
C	-0.67759000	1.32550600	-3.31680500
H	0.14532700	2.01304400	-3.10723200
H	-0.87735200	1.36387200	-4.39396900
H	-1.56929500	1.68750200	-2.79854200
C	2.25762100	0.15201400	-3.00707100
H	2.37189200	1.02798100	-2.35965100
H	3.12792900	-0.48914600	-2.84892000
H	2.29384500	0.50149100	-4.04469100
Rh	-0.26249000	-0.86024000	-0.82770800
C	2.26495000	0.10478500	1.08908000
C	3.39746900	0.34564900	0.30093400
C	1.97884700	0.95013400	2.17000500
C	4.22544800	1.42521800	0.58360400
H	3.62743500	-0.32291100	-0.52160700
C	2.81326700	2.02508700	2.44929400
H	1.09802600	0.76036300	2.77549200
C	3.93227300	2.26786700	1.65465800
H	5.10564700	1.60443500	-0.02552900
H	2.59041700	2.67495200	3.28937000
H	4.58235700	3.10842500	1.87573200
C	-1.63146900	1.13027000	0.88538700
C	-1.91098600	2.34916500	1.50831400
C	-1.11093500	3.45173100	1.25423100
C	-0.02632200	3.32463700	0.38942600
C	0.21250000	2.08786100	-0.17966300
H	-1.32793900	4.40264600	1.72987200
H	0.63196100	4.15683400	0.17138000
H	1.06524100	1.92023900	-0.82670100
C	-2.39349100	-0.10993400	1.03384500

C	-3.54511100	-0.21789400	1.82210400
C	-4.22306300	-1.42515800	1.90411100
H	-3.92210100	0.63842000	2.37338200
C	-2.59660200	-2.42419600	0.41905100
C	-3.74561200	-2.52902200	1.20081500
H	-5.11722000	-1.50669900	2.51295800
H	-2.23953300	-3.30566300	-0.10229500
H	-4.26942400	-3.47858200	1.26211500
H	-2.75411100	2.43078400	2.18354900
N	-0.57082800	1.02539100	0.05279900
C	-1.90644600	-1.21801400	0.31678200
C	0.39849300	-3.41312300	1.22463500
H	0.01213200	-3.98648800	0.37475700
H	-0.41625300	-3.36825700	1.95670500
C	1.63138600	-4.10654800	1.81555200
H	2.42778800	-4.15580700	1.06463900
H	2.01995500	-3.52655700	2.65896100
C	1.31697100	-5.51830300	2.28800400
H	0.89848200	-6.10452300	1.45195400
H	0.54992100	-5.48119400	3.07853600
O	2.52206300	-6.07349600	2.75634600
H	2.34382300	-6.95351600	3.10663100

TS1-2

E = -1479.319845 a.u.

C	-0.58442400	-1.87979200	0.99928600
C	0.44460400	-1.11359100	1.06221300
C	0.99624200	0.33820100	-2.30888100
C	1.24187900	-1.05108100	-2.23012600
C	-0.40187600	0.52281900	-2.70583300
C	-0.00480300	-1.73229900	-2.48401800
C	-0.98797500	-0.74924900	-2.88303600
C	2.54109300	-1.74830900	-1.96792700
H	2.48217800	-2.39832700	-1.08917000
H	2.80547900	-2.37470900	-2.82730500
H	3.35742400	-1.03867200	-1.81553900
C	-0.14118700	-3.22165100	-2.55488600
H	0.25539100	-3.59227600	-3.50746000
H	0.41744700	-3.70669600	-1.74911400
H	-1.18364200	-3.54140400	-2.48891900
C	-2.37590200	-1.01689600	-3.37437900
H	-2.42141600	-0.87362600	-4.45966700
H	-2.68930000	-2.04090500	-3.16292100

H	-3.10515900	-0.34710400	-2.91049700
C	-1.04875400	1.84560900	-2.97209400
H	-0.75848500	2.59017700	-2.22515800
H	-0.75015000	2.22401800	-3.95649300
H	-2.13790700	1.76383500	-2.95654900
C	2.00730300	1.43930700	-2.21523800
H	2.76256900	1.24552700	-1.44860000
H	2.52738900	1.55410900	-3.17332300
H	1.53350300	2.39850200	-1.99039200
Rh	-0.36029300	-0.47829900	-0.73737800
C	1.55528400	-0.64940300	1.85642700
C	2.74546100	-0.19565300	1.27521500
C	1.41630000	-0.59434100	3.25249900
C	3.78628100	0.26933800	2.06875000
H	2.84653100	-0.22209000	0.19680800
C	2.45726400	-0.12258700	4.04230100
H	0.48164700	-0.91073900	3.70546900
C	3.64564000	0.30695000	3.45462000
H	4.70919200	0.60529100	1.60624400
H	2.33966700	-0.08646600	5.12075900
H	4.45729800	0.67437700	4.07421400
C	-1.88149300	1.06759800	1.30300500
C	-2.14464400	1.98082400	2.32689100
C	-1.23961400	2.99771700	2.58357400
C	-0.07310400	3.08004900	1.82480900
C	0.14036500	2.13161100	0.84147100
H	-1.43232800	3.71319200	3.37618000
H	0.66473600	3.85405500	1.99948000
H	1.04787200	2.12301200	0.24988000
C	-2.74983600	-0.04444900	0.91994100
C	-4.12290600	-0.04693500	1.18324900
C	-4.93142300	-1.06318000	0.69642600
H	-4.57147400	0.77374800	1.73511600
C	-3.00271400	-2.09919600	-0.31903300
C	-4.36720600	-2.08346500	-0.07004400
H	-5.99749400	-1.05339500	0.89622000
H	-2.58215000	-2.91817900	-0.89233500
H	-4.99500500	-2.87313900	-0.47091700
H	-3.04279600	1.87812300	2.92469600
N	-0.74477700	1.15901500	0.57934200
C	-2.15900000	-1.09554100	0.17955700
C	-0.96784000	-3.26899200	1.39231800
H	-1.10113400	-3.86766200	0.48186400
H	-1.93548400	-3.27155400	1.90295400

C	0.09461600	-3.92850900	2.27329100
H	1.05220000	-3.98092000	1.74051900
H	0.26831800	-3.31946000	3.16963500
C	-0.33638700	-5.33651500	2.68708500
H	0.45159700	-5.80232200	3.29516900
H	-0.46981200	-5.96021800	1.79664700
O	-1.58205400	-5.34855000	3.35235200
H	-1.44953900	-5.02693500	4.25176000

I2

E = -1479.370300 a.u.

C	-0.37992300	-2.57268600	0.19005100
C	0.52517700	-1.70505200	-0.23492800
C	1.24471300	1.42979900	-2.83293600
C	1.30891100	0.01068500	-3.20089700
C	-0.08812200	1.74563300	-2.57286400
C	-0.01790000	-0.50732700	-3.25648000
C	-0.88453200	0.52388600	-2.77110400
C	2.54755300	-0.65763700	-3.70117600
H	2.72024400	-0.36609100	-4.74414000
H	3.42463600	-0.36349200	-3.11977700
H	2.46708500	-1.74570800	-3.66318800
C	-0.42947900	-1.87632700	-3.69669900
H	-0.64915800	-1.88053200	-4.77046400
H	0.36179100	-2.60651300	-3.50985000
H	-1.32269200	-2.20998200	-3.16270900
C	-2.37695800	0.48378500	-2.75290900
H	-2.76170500	0.89832300	-3.69284100
H	-2.75382500	-0.53525300	-2.64796500
H	-2.78419800	1.08119900	-1.93347000
C	-0.66644500	3.06438500	-2.16697600
H	0.10581400	3.75652900	-1.82275000
H	-1.18115200	3.53119100	-3.01453900
H	-1.39896900	2.94641700	-1.36243400
C	2.44766200	2.31389100	-2.74399300
H	2.21930000	3.26360000	-2.25503300
H	3.25149800	1.82554500	-2.18267700
H	2.83140400	2.53466700	-3.74677300
Rh	0.47598400	0.05399700	-1.17821100
C	1.94862100	-1.48027900	-0.12288200
C	2.91479900	-2.23313800	-0.83821900
C	2.35815000	-0.28086400	0.51681300
C	4.21812300	-1.79879000	-0.91215300

H	2.60477600	-3.15817300	-1.31435400
C	3.68738400	0.16767300	0.38863000
H	1.70565200	0.18908600	1.24364800
C	4.60367000	-0.57507500	-0.32688700
H	4.95756000	-2.39773700	-1.43493100
H	3.99485700	1.07787100	0.89423300
H	5.63322900	-0.24150400	-0.40776400
C	-0.20784200	-4.78867500	3.37431100
C	-0.61862700	-3.62049600	2.47844100
H	-0.66655500	-4.67969200	4.36781500
H	-1.71451800	-3.56474400	2.44023900
H	-0.26833500	-2.67593200	2.91992200
C	-1.80792100	-0.00959400	0.97963400
C	-2.42758700	0.40371500	2.16535500
C	-1.96865000	1.51593600	2.85285300
C	-0.88843600	2.22115400	2.33327600
C	-0.30100700	1.75033800	1.17316700
H	-2.44903600	1.83079800	3.77344600
H	-0.49861800	3.10991600	2.81566800
H	0.55248300	2.25794900	0.73556200
C	-2.44781400	-1.12354400	0.21847400
C	-3.80997400	-0.96100100	-0.07036600
C	-4.52940800	-1.94515700	-0.73480000
H	-4.30625600	-0.03676400	0.21305000
C	-2.55211500	-3.31424500	-0.78956200
C	-3.89400300	-3.12863300	-1.10022200
H	-5.57910000	-1.79004000	-0.96134900
H	-2.06183900	-4.24533200	-1.05931000
H	-4.44389800	-3.90928800	-1.61618200
H	-3.27207500	-0.16614200	2.53555600
N	-0.72571600	0.65506200	0.51476500
C	-1.80800200	-2.32337200	-0.14107600
O	1.19443000	-4.93606100	3.46732600
H	1.53622000	-4.22017100	4.01564800
C	-0.04293200	-3.75824100	1.06397000
H	1.04217800	-3.87608800	1.13198300
H	-0.43411900	-4.67976400	0.61090100
H	-0.57576100	-5.72787000	2.94835900

TS2-3

E = -1479.323851 a.u.

C	-0.21832100	-1.08757500	0.43261100
C	0.25925500	0.23758100	0.64203000

C	1.27428700	1.08570200	-2.79075900
C	1.09611100	-0.35415600	-2.80189100
C	0.00652400	1.64995200	-3.03021400
C	-0.25634900	-0.65264200	-3.26325600
C	-0.93791300	0.56829100	-3.33331700
C	2.19793900	-1.35683900	-2.65617000
H	2.74633200	-1.45354800	-3.60075900
H	2.91023600	-1.06128400	-1.88091200
H	1.80787600	-2.34360100	-2.39566800
C	-0.79857800	-2.02606300	-3.51028100
H	-1.89019600	-2.03992100	-3.46605700
H	-0.49426800	-2.39229400	-4.49757600
H	-0.43285100	-2.73795000	-2.76374300
C	-2.37708100	0.79028200	-3.68514700
H	-2.47082300	1.14295000	-4.71879200
H	-2.96093000	-0.12780600	-3.58769200
H	-2.83323500	1.54528700	-3.03728800
C	-0.33396100	3.10667800	-3.09779000
H	0.39892000	3.71747700	-2.56332100
H	-0.35437600	3.44786400	-4.13971400
H	-1.32094900	3.30760000	-2.67011000
C	2.57307200	1.80295800	-2.59151500
H	3.24692500	1.23788700	-1.94133100
H	3.08465500	1.93909200	-3.55186100
H	2.42752900	2.79472900	-2.15356000
Rh	-0.15911700	0.30309800	-1.22941500
C	1.10832800	0.83501100	1.65664100
C	2.18089700	1.64929800	1.27373900
C	0.87172500	0.58937200	3.01849300
C	3.03105800	2.18098800	2.23528900
H	2.34657300	1.83017000	0.21608200
C	1.71034100	1.13797500	3.97930100
H	0.02024100	-0.01891600	3.30993100
C	2.79525400	1.92448000	3.58492100
H	3.87670400	2.79202600	1.93763700
H	1.52430100	0.95700700	5.03313700
H	3.45740800	2.34264900	4.33661400
C	2.36039700	-3.18669800	2.37208600
C	0.93013800	-2.82030100	1.97016400
H	2.35513000	-3.71234700	3.33733200
H	0.30539900	-3.72044400	1.96210400
H	0.50681500	-2.16593800	2.74291100
C	-2.52590800	0.69435100	1.00787200
C	-3.42399100	1.49705500	1.72982100

C	-3.22083300	2.86035200	1.81546800
C	-2.09939700	3.43492200	1.20461400
C	-1.21157200	2.59997000	0.57132900
H	-3.91815500	3.47882900	2.37115100
H	-1.90886900	4.50030200	1.25107200
H	-0.28470800	2.95687100	0.13634300
C	-2.71548000	-0.73379700	0.78815900
C	-4.01262700	-1.27005200	0.82554400
C	-4.24574300	-2.60596200	0.55749000
H	-4.85758200	-0.61895500	1.02448600
C	-1.87841900	-2.91884700	0.20625000
C	-3.16410800	-3.43039900	0.24425700
H	-5.25567100	-3.00022100	0.57725700
H	-1.06065800	-3.58590300	-0.03861100
H	-3.32653400	-4.48147000	0.02686100
H	-4.26606100	1.03843900	2.23298100
N	-1.42691600	1.26872600	0.46272200
C	-1.61138300	-1.56376300	0.47523500
O	3.21403800	-2.05950000	2.40364100
H	2.90631800	-1.46671200	3.10104200
C	0.90908200	-2.10192800	0.61322000
H	1.86133300	-1.57441300	0.50326400
H	0.88300400	-2.82774100	-0.20853800
H	2.79869800	-3.86463100	1.63289300

I3

E = -1479.383579 a.u.

C	-0.62324500	-1.21968400	0.38009300
C	-0.06619800	0.08574200	0.72869200
C	0.88448200	1.12931400	-2.71200300
C	1.46517300	-0.17445000	-2.44339400
C	-0.35830500	0.91008800	-3.35427500
C	0.61722200	-1.17644300	-3.03080000
C	-0.52708000	-0.51974400	-3.54956000
C	2.80966400	-0.42885400	-1.83682100
H	3.57067200	-0.49314100	-2.62336500
H	3.10030300	0.36635000	-1.14734500
H	2.82419400	-1.36904100	-1.27834700
C	0.87528000	-2.65076500	-3.04905700
H	1.39217500	-2.94177000	-3.97088700
H	1.50200900	-2.95822400	-2.20739100
H	-0.05901000	-3.21841100	-2.99931900
C	-1.67059400	-1.16975600	-4.26143500

H	-1.42223800	-1.32734100	-5.31752400
H	-1.91477100	-2.14215400	-3.82403700
H	-2.57074000	-0.55223900	-4.21701300
C	-1.31197100	1.95555700	-3.84069100
H	-1.14602800	2.91222200	-3.33905600
H	-1.18980500	2.11320800	-4.91870200
H	-2.34998100	1.65591700	-3.66548800
C	1.54439300	2.45378400	-2.48243200
H	0.82606600	3.21909000	-2.17408300
H	2.32075900	2.38698100	-1.71746900
H	2.02327900	2.79888400	-3.40636300
Rh	-0.42501900	-0.07891900	-1.36638400
C	1.32919400	0.36281000	1.19091800
C	1.85607000	1.62908000	0.88752000
C	2.12520000	-0.52575800	1.91756500
C	3.14008800	1.98767600	1.26923400
H	1.23953100	2.33120300	0.33270600
C	3.42807600	-0.17549900	2.27652100
H	1.76290600	-1.50426500	2.20778100
C	3.94132100	1.07438800	1.95608300
H	3.52265700	2.97279500	1.01982800
H	4.03740400	-0.89187000	2.81863200
H	4.95327100	1.34160300	2.24287800
C	0.52834900	-4.36809700	2.29467900
C	-0.37978300	-3.19646600	1.92985700
H	0.13001700	-4.90346100	3.16562300
H	-1.42260100	-3.53480800	1.87643100
H	-0.33603200	-2.44916200	2.73415000
C	-2.22800300	1.14841700	0.71617300
C	-3.18126700	2.02627000	1.22819600
C	-2.90952300	2.75082000	2.37712400
C	-1.70100900	2.54811300	3.04467700
C	-0.79279700	1.65654400	2.51918600
H	-3.64194300	3.44969200	2.76685300
H	-1.46067200	3.07222700	3.96130900
H	0.16294600	1.45127300	2.98097400
C	-2.41991000	0.24561100	-0.42052900
C	-3.56503600	0.42688700	-1.27873500
C	-4.19590300	-0.63609400	-1.84349800
H	-3.91582800	1.43739600	-1.47073100
C	-2.69650400	-2.21162600	-0.75218800
C	-3.78191900	-1.97147500	-1.53596600
H	-5.04351400	-0.48073900	-2.50268800
H	-2.40115100	-3.22930100	-0.52067000

H	-4.35117100	-2.80462600	-1.93597600
H	-4.13749600	2.11248300	0.72746400
N	-1.04470800	1.01131000	1.35947200
C	-1.92778500	-1.11712900	-0.22139500
O	1.86222500	-3.94030300	2.52106300
H	1.95989400	-3.73583400	3.45769600
C	0.03137400	-2.55648100	0.59514600
H	1.11750100	-2.45368900	0.55046300
H	-0.23635500	-3.22727600	-0.22889800
H	0.56881200	-5.08197700	1.46462900

I1’

E = -1479.337702 a.u.

C	1.29330900	-0.90717400	0.50667900
C	0.63942900	-1.90628100	0.83118700
C	0.47281800	0.07642000	-2.91358900
C	0.98737700	-1.20598900	-2.66779000
C	-0.98399900	-0.02568400	-2.91655800
C	-0.13133000	-2.13182100	-2.53372800
C	-1.33288900	-1.40720900	-2.80157400
C	2.42494200	-1.60611500	-2.56955200
H	2.70820300	-2.21103300	-3.43817500
H	3.08792200	-0.73832900	-2.53853500
H	2.60627600	-2.20624000	-1.67204700
C	-0.01097200	-3.62001800	-2.42492400
H	-0.20131000	-4.08707200	-3.39800500
H	0.99259400	-3.91169300	-2.10844300
H	-0.72018000	-4.03842400	-1.70503300
C	-2.69842700	-1.98306500	-2.99548800
H	-2.93259000	-1.99026200	-4.06639300
H	-2.75675300	-3.01192600	-2.63583800
H	-3.46697900	-1.40089000	-2.48204600
C	-1.93284400	1.09453900	-3.20572300
H	-1.60317300	2.02757000	-2.74018400
H	-2.00590700	1.26427600	-4.28615300
H	-2.93280700	0.86834400	-2.82810300
C	1.25240700	1.31921700	-3.21264600
H	0.67640900	2.22059300	-2.98824700
H	2.19219300	1.36249900	-2.65336900
H	1.50486800	1.35535500	-4.27856600
Rh	-0.38615500	-0.65668300	-0.92404000
C	0.15012300	-3.12186200	1.42025600
C	-0.76438300	-3.07762200	2.48099900

C	0.62003200	-4.35824700	0.95777700
C	-1.20527700	-4.25848400	3.06312000
H	-1.13336000	-2.11887800	2.83029000
C	0.17103700	-5.53561300	1.54321100
H	1.34872300	-4.38768100	0.15455200
C	-0.74361000	-5.48662100	2.59333300
H	-1.91406800	-4.22022400	3.88385900
H	0.54112600	-6.49109000	1.18586700
H	-1.09186300	-6.40735400	3.05065900
C	-1.77378100	1.20184300	0.92494700
C	-2.07447500	2.36729100	1.63640000
C	-1.27873800	3.49024800	1.48771300
C	-0.18027800	3.43899000	0.63041000
C	0.07049400	2.25554100	-0.03856200
H	-1.50952800	4.39884100	2.03411400
H	0.46870300	4.29426500	0.48366300
H	0.91683100	2.15565600	-0.70735900
C	-2.52904000	-0.05019800	0.97336900
C	-3.67561800	-0.23477200	1.75642200
C	-4.33608000	-1.45473500	1.74517500
H	-4.06099800	0.56975700	2.37566200
C	-2.69628000	-2.31945900	0.19436200
C	-3.84417000	-2.49713600	0.96137300
H	-5.22718500	-1.59512900	2.34794800
H	-2.30624900	-3.16167000	-0.36832800
H	-4.34761400	-3.45932000	0.95967900
H	-2.93056500	2.38952100	2.29970900
N	-0.70187700	1.16816800	0.10078100
C	-2.03079300	-1.09593400	0.17740500
C	2.44227600	0.01951500	0.56841900
H	2.17834000	0.86227600	1.21973000
H	2.63757400	0.44060800	-0.42538300
C	3.69745400	-0.68817900	1.09258900
H	3.49908500	-1.12104000	2.07825900
H	3.96377200	-1.51478400	0.42492800
C	4.88519900	0.25754000	1.19316200
H	4.65330700	1.06902600	1.90238800
H	5.07172400	0.72378500	0.21019100
O	5.98497300	-0.50863700	1.61890300
H	6.74374600	0.07337600	1.73910600

TS1-2’

E = -1479.315754 a.u.

C	0.41061300	-1.31857200	1.24236100
C	-0.63407100	-2.04661200	1.28258000
C	0.87243100	0.57717900	-1.89411500
C	1.36881600	-0.74579300	-1.82823500
C	-0.48994300	0.52193500	-2.42527900
C	0.30352600	-1.63558600	-2.22720900
C	-0.80683900	-0.82627600	-2.68968900
C	2.75881400	-1.15940900	-1.46127500
H	3.38262200	-1.19734200	-2.36192100
H	3.22313900	-0.45513500	-0.76608800
H	2.77588200	-2.15380600	-1.00811100
C	0.43502600	-3.12098400	-2.36094000
H	0.96055400	-3.37491400	-3.28871800
H	0.99975100	-3.54611700	-1.52696600
H	-0.53995900	-3.61256500	-2.38803400
C	-2.06419200	-1.31991300	-3.33215800
H	-2.00989700	-1.16306200	-4.41533200
H	-2.21813600	-2.38633300	-3.15888500
H	-2.94483500	-0.79368400	-2.95480300
C	-1.34408000	1.71588900	-2.71401400
H	-1.04527300	2.17943600	-3.66130100
H	-2.39854300	1.44061900	-2.78935200
H	-1.25023600	2.47122900	-1.92840800
C	1.65547600	1.83637600	-1.68901700
H	1.00983800	2.67302500	-1.40940800
H	2.43153800	1.72741200	-0.92647300
H	2.15295300	2.11490200	-2.62560800
Rh	-0.41222400	-0.55112600	-0.48440900
C	-1.11718300	-3.32100700	1.80898100
C	-2.30523000	-3.42361600	2.54119300
C	-0.31695100	-4.45412200	1.62431900
C	-2.68028100	-4.64358400	3.08596500
H	-2.93192400	-2.54716300	2.67343600
C	-0.70064900	-5.67650400	2.16717800
H	0.60481200	-4.36940900	1.05617200
C	-1.88151800	-5.77169700	2.89758400
H	-3.59897000	-4.71802200	3.65891200
H	-0.07714700	-6.55254200	2.01974100
H	-2.18156300	-6.72488000	3.32132600
C	-2.40351700	0.74704800	1.33207500
C	-2.96439100	1.62381100	2.26374200
C	-2.27240300	2.76660200	2.63061300
C	-1.02204300	3.01262300	2.06757500
C	-0.50877000	2.08643900	1.17655400

H	-2.70023400	3.45795900	3.34916400
H	-0.44929800	3.89786100	2.31809300
H	0.46986700	2.21779100	0.73262700
C	-3.05635100	-0.45990900	0.81821700
C	-4.43937500	-0.66573100	0.89277600
C	-5.01318300	-1.78263500	0.30273800
H	-5.07691700	0.06463900	1.38182000
C	-2.83333500	-2.51990200	-0.41968300
C	-4.20660200	-2.70676300	-0.36378200
H	-6.08650500	-1.93162900	0.35532500
H	-2.20815200	-3.27955600	-0.87824800
H	-4.65090300	-3.58338200	-0.82475700
H	-3.93184300	1.40405100	2.69960800
N	-1.17634100	0.98117600	0.81830500
C	-2.23709500	-1.39401900	0.15719700
C	1.73725100	-1.15900600	1.89301600
H	2.46079100	-1.74949000	1.31486300
H	1.69027100	-1.61650100	2.88917900
C	2.23279900	0.28342300	1.97781800
H	2.13240600	0.75385500	0.99413300
H	1.60461600	0.85607800	2.67190400
C	3.69818700	0.38644900	2.39206400
H	4.31551400	-0.19905400	1.70057400
H	3.84995300	-0.03902400	3.39509900
O	4.16916700	1.71325200	2.30814600
H	3.90075100	2.18550100	3.10425100

I2’

E = -1479.365583 a.u.

C	0.25359700	-1.13143200	0.57935200
C	-0.83859600	-1.73884500	1.05957500
C	1.41403100	0.82741800	-2.80799800
C	1.48773700	-0.62107300	-2.53013400
C	0.07754700	1.19073100	-2.95452100
C	0.17649800	-1.14419600	-2.56270700
C	-0.72094800	-0.00936400	-2.69506400
C	2.76614600	-1.38869400	-2.42037000
H	3.27434200	-1.40324800	-3.39191400
H	3.44115400	-0.94270700	-1.68387700
H	2.58042100	-2.42407600	-2.12549400
C	-0.23883400	-2.57519200	-2.45257100
H	-0.33004800	-3.01398500	-3.45282300
H	0.48946500	-3.15973700	-1.88641400

H	-1.20367900	-2.66713200	-1.94911800
C	-2.19999100	-0.08957000	-2.86527700
H	-2.42748900	-0.19384300	-3.93379600
H	-2.62533100	-0.94627000	-2.33939300
H	-2.69425400	0.81424000	-2.50281900
C	-0.49618300	2.54161800	-3.24676900
H	0.25913400	3.32637500	-3.16196700
H	-0.89983500	2.57505300	-4.26499300
H	-1.31279700	2.78316500	-2.55925700
C	2.62788200	1.69716200	-2.86614000
H	2.37715600	2.75762000	-2.79042000
H	3.32575900	1.44227600	-2.06164500
H	3.15348100	1.54115200	-3.81566800
Rh	0.33909800	0.23411400	-0.88777200
C	-0.78813800	-2.79227000	2.11498400
C	-1.63053000	-2.71549400	3.23063700
C	0.07890400	-3.88389400	2.00355600
C	-1.58683100	-3.69026900	4.22054900
H	-2.32296200	-1.88239500	3.32075700
C	0.12216300	-4.86260100	2.99277900
H	0.71378900	-3.97099700	1.12562300
C	-0.70825000	-4.76614500	4.10536400
H	-2.24111100	-3.61280900	5.08355100
H	0.79856700	-5.70560600	2.88898900
H	-0.67791200	-5.52967000	4.87633500
C	-1.97907500	1.09701700	0.96840600
C	-2.57822100	1.89779000	1.94604400
C	-1.97532700	3.07788400	2.35314600
C	-0.77398500	3.45469400	1.76141000
C	-0.22571100	2.61727100	0.80733300
H	-2.43631800	3.69577000	3.11674100
H	-0.26682100	4.37357700	2.03120400
H	0.71066600	2.86849800	0.31952000
C	-2.70822000	-0.10588400	0.48195500
C	-4.01567800	0.11000200	0.02428300
C	-4.81021800	-0.94253100	-0.40846100
H	-4.40677000	1.12368900	-0.00304300
C	-3.02471500	-2.46670400	0.12139100
C	-4.30851800	-2.24092200	-0.35882500
H	-5.81508500	-0.75200700	-0.77069500
H	-2.64661400	-3.48223700	0.19836600
H	-4.92124400	-3.07762200	-0.67926800
H	-3.51559600	1.57289900	2.38285900
N	-0.79925900	1.46175300	0.42368200

C	-2.19483600	-1.41498800	0.53188700
C	1.66485400	-1.25043500	1.10097300
H	2.28615600	-1.81426800	0.39361100
H	1.69844200	-1.78474000	2.05829700
C	2.27962400	0.15235600	1.28112500
H	2.10803600	0.78794000	0.38489500
H	1.79231100	0.66386900	2.11851900
C	3.78634500	0.14619500	1.47547300
H	4.12391400	1.13127500	1.82619000
H	4.05394400	-0.59772300	2.24015000
O	4.37511200	-0.16806500	0.22464000
H	5.32424200	-0.28596700	0.34632600

TS1-2’

E = -1479.315754 a.u.

C	0.41061300	-1.31857200	1.24236100
C	-0.63407100	-2.04661200	1.28258000
C	0.87243100	0.57717900	-1.89411500
C	1.36881600	-0.74579300	-1.82823500
C	-0.48994300	0.52193500	-2.42527900
C	0.30352600	-1.63558600	-2.22720900
C	-0.80683900	-0.82627600	-2.68968900
C	2.75881400	-1.15940900	-1.46127500
H	3.38262200	-1.19734200	-2.36192100
H	3.22313900	-0.45513500	-0.76608800
H	2.77588200	-2.15380600	-1.00811100
C	0.43502600	-3.12098400	-2.36094000
H	0.96055400	-3.37491400	-3.28871800
H	0.99975100	-3.54611700	-1.52696600
H	-0.53995900	-3.61256500	-2.38803400
C	-2.06419200	-1.31991300	-3.33215800
H	-2.00989700	-1.16306200	-4.41533200
H	-2.21813600	-2.38633300	-3.15888500
H	-2.94483500	-0.79368400	-2.95480300
C	-1.34408000	1.71588900	-2.71401400
H	-1.04527300	2.17943600	-3.66130100
H	-2.39854300	1.44061900	-2.78935200
H	-1.25023600	2.47122900	-1.92840800
C	1.65547600	1.83637600	-1.68901700
H	1.00983800	2.67302500	-1.40940800
H	2.43153800	1.72741200	-0.92647300
H	2.15295300	2.11490200	-2.62560800
Rh	-0.41222400	-0.55112600	-0.48440900

C	-1.11718300	-3.32100700	1.80898100
C	-2.30523000	-3.42361600	2.54119300
C	-0.31695100	-4.45412200	1.62431900
C	-2.68028100	-4.64358400	3.08596500
H	-2.93192400	-2.54716300	2.67343600
C	-0.70064900	-5.67650400	2.16717800
H	0.60481200	-4.36940900	1.05617200
C	-1.88151800	-5.77169700	2.89758400
H	-3.59897000	-4.71802200	3.65891200
H	-0.07714700	-6.55254200	2.01974100
H	-2.18156300	-6.72488000	3.32132600
C	-2.40351700	0.74704800	1.33207500
C	-2.96439100	1.62381100	2.26374200
C	-2.27240300	2.76660200	2.63061300
C	-1.02204300	3.01262300	2.06757500
C	-0.50877000	2.08643900	1.17655400
H	-2.70023400	3.45795900	3.34916400
H	-0.44929800	3.89786100	2.31809300
H	0.46986700	2.21779100	0.73262700
C	-3.05635100	-0.45990900	0.81821700
C	-4.43937500	-0.66573100	0.89277600
C	-5.01318300	-1.78263500	0.30273800
H	-5.07691700	0.06463900	1.38182000
C	-2.83333500	-2.51990200	-0.41968300
C	-4.20660200	-2.70676300	-0.36378200
H	-6.08650500	-1.93162900	0.35532500
H	-2.20815200	-3.27955600	-0.87824800
H	-4.65090300	-3.58338200	-0.82475700
H	-3.93184300	1.40405100	2.69960800
N	-1.17634100	0.98117600	0.81830500
C	-2.23709500	-1.39401900	0.15719700
C	1.73725100	-1.15900600	1.89301600
H	2.46079100	-1.74949000	1.31486300
H	1.69027100	-1.61650100	2.88917900
C	2.23279900	0.28342300	1.97781800
H	2.13240600	0.75385500	0.99413300
H	1.60461600	0.85607800	2.67190400
C	3.69818700	0.38644900	2.39206400
H	4.31551400	-0.19905400	1.70057400
H	3.84995300	-0.03902400	3.39509900
O	4.16916700	1.71325200	2.30814600
H	3.90075100	2.18550100	3.10425100

I3’

E = -1479.390604 a.u.

C	0.02005000	0.49666200	1.81915400
C	-0.13576400	-0.95409400	1.66136800
C	1.72445600	0.81224900	-1.83795800
C	1.74819200	-0.65140300	-1.95699700
C	0.38705200	1.22719700	-1.75188100
C	0.42718300	-1.12372700	-1.94629900
C	-0.42903300	0.02452100	-1.69835900
C	3.00695100	-1.44632200	-2.11548800
H	3.46109400	-1.26080100	-3.09583400
H	3.74117300	-1.17155300	-1.35139900
H	2.81888100	-2.51965700	-2.03166800
C	-0.05882100	-2.52685200	-2.13073400
H	-0.47421600	-2.66179700	-3.13671100
H	0.74796400	-3.25346900	-2.00422700
H	-0.84698700	-2.77212000	-1.41185900
C	-1.92094500	-0.00198800	-1.81247300
H	-2.20878400	0.10026600	-2.86604600
H	-2.33921700	-0.94009700	-1.44024600
H	-2.38899400	0.82215900	-1.26620200
C	-0.14036800	2.62682100	-1.71295300
H	0.60705900	3.33133800	-1.33637200
H	-0.43437000	2.95926000	-2.71587600
H	-1.02651400	2.70153200	-1.07443100
C	2.94936900	1.67233900	-1.88642300
H	2.75789300	2.67160000	-1.48532300
H	3.76471000	1.22552300	-1.30930400
H	3.30271200	1.78845500	-2.91799100
Rh	0.86267400	-0.09106600	0.02183900
C	0.68046900	-1.90424900	2.50660000
C	0.46599700	-1.97492100	3.88805500
C	1.59913700	-2.79307900	1.93355000
C	1.17625900	-2.87342000	4.67758800
H	-0.27122600	-1.31951300	4.34570300
C	2.30909900	-3.69940600	2.72181400
H	1.73223400	-2.78422000	0.85237100
C	2.10627900	-3.73428700	4.09780300
H	0.99822700	-2.90723700	5.74799500
H	3.01401500	-4.38127300	2.25602900
H	2.65933800	-4.43566700	4.71410700
C	-2.42908500	0.80130600	1.45449200
C	-3.50709100	1.70023500	1.35973600
C	-3.33520500	3.06207900	1.44856500

C	-2.04204100	3.56334100	1.61408700
C	-1.00737800	2.67405800	1.70933800
H	-4.18755300	3.72833600	1.37536400
H	-1.83573400	4.62564700	1.65643300
H	0.01311700	3.00875800	1.80005100
C	-2.59635600	-0.63833100	1.29456400
C	-3.86826100	-1.18775500	1.03327800
C	-4.03066400	-2.53960900	0.81623800
H	-4.74993700	-0.56089900	0.98874100
C	-1.66452200	-2.86249800	1.13848200
C	-2.91476700	-3.38170700	0.86441500
H	-5.01692400	-2.94212300	0.61312400
H	-0.80915800	-3.52601900	1.19199600
H	-3.02957400	-4.44759800	0.69447800
H	-4.50202900	1.30727700	1.21225500
N	-1.18376800	1.32229900	1.66393500
C	-1.47374700	-1.48544200	1.35120300
C	0.99121900	1.08345500	2.85416900
H	1.35940900	0.26669800	3.47992800
H	0.44122200	1.73594200	3.54239200
C	2.21309200	1.82658200	2.28335400
H	1.94245900	2.40425600	1.39124600
H	2.60735100	2.53231000	3.02422100
C	3.33142800	0.86453900	1.91318600
H	4.11525700	1.37299500	1.34632700
H	3.78282200	0.43834100	2.81559000
O	2.84594900	-0.21195500	1.09478800
H	2.81907200	-1.02806200	1.61851000

TS2-3’

E = -1479.323147 a.u.

C	0.83787400	0.94258900	0.88995500
C	0.49301100	-0.43421300	0.86895100
C	1.84917000	1.37140400	-2.58372300
C	1.39969100	-0.00826300	-2.66058200
C	0.70273200	2.17851700	-2.72479500
C	0.00024000	-0.03136500	-3.04128100
C	-0.44550500	1.29742200	-2.98938800
C	2.26712500	-1.22825400	-2.64106100
H	1.82719400	-2.02066600	-2.02803600
H	2.37649500	-1.61518000	-3.66100200
H	3.26663200	-1.01766200	-2.25580900
C	-0.78769400	-1.27460800	-3.31378300

H	-0.48717500	-1.72296100	-4.26788900
H	-0.63585700	-2.02442200	-2.52942000
H	-1.85908500	-1.06771500	-3.36479900
C	-1.84062500	1.79528400	-3.21055200
H	-2.57304700	0.99001200	-3.12191600
H	-2.10594200	2.56972900	-2.48390000
H	-1.93587100	2.23426600	-4.21023300
C	0.65095500	3.67474200	-2.75136600
H	-0.30619600	4.05076300	-2.37847300
H	1.45058400	4.11746100	-2.15010900
H	0.76663500	4.04372100	-3.77755100
C	3.26168300	1.82693400	-2.39039200
H	3.82260100	1.13849600	-1.75221000
H	3.78297300	1.88394500	-3.35315900
H	3.30435000	2.81664300	-1.92828200
Rh	0.38054800	0.81794200	-0.97324800
C	1.59248600	-1.35969200	1.29313500
C	1.37011800	-2.31866600	2.29180200
C	2.87982700	-1.23208100	0.76734100
C	2.41119600	-3.11871300	2.75072600
H	0.37601800	-2.43765200	2.71324100
C	3.92488900	-2.02638700	1.22934300
H	3.06217900	-0.49179800	-0.00613900
C	3.69453400	-2.97181200	2.22315200
H	2.22088000	-3.85841500	3.52239600
H	4.91940500	-1.90658100	0.81141200
H	4.50656500	-3.59469100	2.58393500
C	-1.92507000	1.18405000	1.24333000
C	-2.85048600	1.95027500	1.97238400
C	-2.74046300	3.32419400	2.00300900
C	-1.68780400	3.95127500	1.31770700
C	-0.76423300	3.16221000	0.68256100
H	-3.45688000	3.91577800	2.56336400
H	-1.58150100	5.02928000	1.30523900
H	0.10224800	3.57374600	0.17888600
C	-2.03064900	-0.24080100	1.03387000
C	-3.29195000	-0.86458200	1.02003000
C	-3.42356300	-2.19475000	0.68014300
H	-4.18098900	-0.27660100	1.22578200
C	-1.02933700	-2.34002000	0.36904400
C	-2.27823400	-2.92743200	0.34059200
H	-4.40304300	-2.65895500	0.65267700
H	-0.15294300	-2.92814800	0.11843900
H	-2.36948600	-3.97005000	0.05225600

H	-3.64261800	1.44837100	2.51480100
N	-0.87111800	1.80715400	0.64510700
C	-0.86279100	-0.98459800	0.72990500
C	1.70452600	1.75259800	1.78706500
C	1.17313700	1.95434900	3.21579000
H	1.81703100	2.69063100	3.70826500
H	0.15710800	2.36802500	3.20799500
C	1.19561500	0.66620100	4.02904600
H	0.85366400	0.87613500	5.05234500
H	0.49656200	-0.06175900	3.59270500
O	2.51850000	0.17748600	4.02990300
H	2.50173800	-0.78673200	4.03535900
H	2.65247200	1.20645600	1.86695600
H	1.93450200	2.70961200	1.30966000

Sub2

E = -977.910848 a.u.

C	1.14861600	0.06878200	-1.69830200
C	0.73719400	-1.33043500	-1.46754100
C	0.17614000	0.69473700	-2.47627500
C	-0.46616600	-1.56144600	-2.16613300
C	-0.90382700	-0.27056800	-2.67206000
C	1.56529400	-2.33337400	-0.73160800
H	2.38806500	-2.68063400	-1.36762200
H	2.00327700	-1.89996200	0.17172800
H	0.97506000	-3.20279300	-0.43466000
C	-1.16928100	-2.85816000	-2.40776300
H	-1.05540100	-3.13674500	-3.46148100
H	-0.74751900	-3.66596200	-1.80677800
H	-2.23727600	-2.78940100	-2.18721900
C	-2.13352800	-0.03840900	-3.48424900
H	-1.90434400	-0.18539500	-4.54707100
H	-2.92742800	-0.73524200	-3.20707300
H	-2.50998300	0.97960400	-3.35845700
C	0.17860500	2.08925200	-3.01654300
H	0.85999200	2.74136900	-2.46413400
H	0.50471400	2.08230700	-4.06276500
H	-0.82050000	2.53347200	-2.99133300
C	2.41146900	0.65469300	-1.15715200
H	2.44290400	1.73941900	-1.27650000
H	2.53039500	0.42474000	-0.09370200
H	3.27571200	0.23064600	-1.68157400
Rh	-0.83354300	-0.10615500	-0.58773300

C	-2.98347000	1.17415000	0.97360300
C	-3.79688000	2.16847900	1.51338100
C	-3.50753600	3.50358700	1.26752100
C	-2.40083700	3.83370700	0.48961400
C	-1.63577300	2.80213000	-0.02598700
H	-4.13814400	4.28182000	1.68481100
H	-2.13492200	4.86376600	0.28471500
H	-0.76199900	2.99729600	-0.63681200
C	-3.13351900	-0.27433000	1.18250100
C	-4.10304500	-0.83393600	2.01487300
C	-4.13637100	-2.21101500	2.21294500
H	-4.83164800	-0.21045000	2.52423800
C	-2.23291200	-2.46705500	0.74853800
C	-3.19564800	-3.02541700	1.59062300
H	-4.89059600	-2.64459600	2.86126800
H	-1.50724700	-3.12201300	0.27667000
H	-3.21113000	-4.09798200	1.75856800
H	-4.64983100	1.89974300	2.12459100
N	-1.92267200	1.51206100	0.19884800
C	-2.19076100	-1.09227400	0.52370000

I4

E = -1479.026663 a.u.

C	-0.16125200	-2.51434400	0.25364800
C	0.68961800	-1.58434900	-0.12202200
C	1.43924400	0.98267700	-2.94202200
C	0.88285300	-0.30354500	-3.24426600
C	0.35449900	1.89648800	-2.66037200
C	-0.54225700	-0.22305700	-3.06312500
C	-0.85759100	1.12957200	-2.65233300
C	1.60082900	-1.49973600	-3.77242800
H	1.40581900	-1.58581000	-4.84793900
H	2.68028900	-1.42479000	-3.63577900
H	1.24646000	-2.41968500	-3.29899700
C	-1.51650400	-1.29288200	-3.40623900
H	-1.75136900	-1.21884600	-4.47618600
H	-1.10581300	-2.28680500	-3.22099100
H	-2.44963500	-1.19547000	-2.84966300
C	-2.23411400	1.65719300	-2.41663200
H	-2.64982300	2.02110200	-3.36338900
H	-2.89549300	0.87569100	-2.03624400
H	-2.23529700	2.48767300	-1.70725700
C	0.48434600	3.35632600	-2.39643300

H	1.43563400	3.60092100	-1.91691100
H	0.44917000	3.90371200	-3.34740500
H	-0.33189600	3.73241400	-1.77518000
C	2.87651200	1.37022800	-3.03827100
H	3.15012100	2.09785400	-2.26982900
H	3.53439900	0.50584200	-2.93973100
H	3.06431000	1.82906500	-4.01618300
Rh	0.41291600	0.22001100	-1.13183700
C	2.01760700	-1.08020900	-0.04052200
C	3.08950500	-1.63497600	-0.80343500
C	2.26511000	0.08214300	0.74877200
C	4.33860700	-1.05919300	-0.75808400
H	2.90736200	-2.53725900	-1.37681100
C	3.52629500	0.67831900	0.74023900
H	1.50766400	0.41816800	1.44911100
C	4.55302400	0.11235300	-0.00697100
H	5.16514100	-1.50945200	-1.29824500
H	3.71792500	1.54814900	1.35952900
H	5.54185100	0.55968100	0.01232300
C	0.20538900	-4.25095400	3.67217700
C	-0.44520200	-3.40116300	2.58928000
H	-0.34417000	-4.11840400	4.61429000
H	-1.50665600	-3.65940100	2.50394900
H	-0.38045100	-2.34963000	2.89681900
C	-2.01539800	-0.17408700	0.80170000
C	-2.80730600	0.18703200	1.89715200
C	-2.54358300	1.34868400	2.60648500
C	-1.48258900	2.15456300	2.20209100
C	-0.72309900	1.73965200	1.12529500
H	-3.15663400	1.62395600	3.45822600
H	-1.24203600	3.08106300	2.71023000
H	0.11701500	2.33458600	0.77848800
C	-2.40816800	-1.37461400	0.01173600
C	-3.73838300	-1.42378600	-0.42990100
C	-4.23533700	-2.53999200	-1.09232500
H	-4.39203400	-0.57489200	-0.24786600
C	-2.09605000	-3.61452900	-0.84562500
C	-3.41074700	-3.64361300	-1.29544000
H	-5.26585300	-2.55411500	-1.43095600
H	-1.45975700	-4.48194800	-0.99513400
H	-3.79302800	-4.52837800	-1.79353900
H	-3.62566500	-0.46283900	2.18514400
N	-0.96632000	0.59897600	0.44693600
C	-1.57453800	-2.48498900	-0.20871900

O	1.54521500	-3.81740000	3.78719900
H	1.98892300	-4.35326300	4.45486100
C	0.26645400	-3.58244700	1.24001900
H	1.34635600	-3.53432700	1.39944300
H	0.03470200	-4.57212900	0.82687500
H	0.14843800	-5.31538200	3.39736600

TS4-5

E = -1478.996378 a.u.

C	-0.08585100	-1.52863100	0.86639100
C	0.32692000	-0.24707200	0.67583600
C	1.11950000	1.66313300	-2.88724600
C	1.02872900	0.21330500	-2.97117300
C	-0.19809100	2.21114800	-2.84240700
C	-0.34854700	-0.13905800	-2.89864200
C	-1.10221800	1.09921100	-2.75170300
C	2.16099700	-0.73844500	-3.17794000
H	2.23562900	-0.99183800	-4.24225800
H	3.12060400	-0.31000600	-2.88057900
H	2.01008700	-1.66971000	-2.62534700
C	-0.90821300	-1.51384100	-3.03460300
H	-0.99438600	-1.76373700	-4.09927000
H	-0.25807000	-2.25837000	-2.56902800
H	-1.90128700	-1.60021000	-2.59026000
C	-2.58941500	1.20971400	-2.68493700
H	-2.97732800	1.43121800	-3.68623900
H	-3.04925900	0.27983900	-2.34655500
H	-2.90313300	2.02128900	-2.02238100
C	-0.57193300	3.65742500	-2.86344600
H	0.21917500	4.28685700	-2.44942600
H	-0.74643500	3.98263300	-3.89598800
H	-1.48918400	3.84564900	-2.29969700
C	2.38286200	2.45722800	-2.94556600
H	3.24321700	1.88499500	-2.59327800
H	2.57908400	2.74681300	-3.98487700
H	2.31183700	3.37215100	-2.35258400
Rh	0.20205300	0.91524200	-1.04511400
C	1.45451400	0.51699400	1.20533200
C	2.57096400	0.74947800	0.37091200
C	1.42972200	1.07990100	2.49725600
C	3.60727100	1.58031000	0.80273600
H	2.67761500	0.19367600	-0.55618500
C	2.47414000	1.88089800	2.92147500

H	0.60142900	0.85577800	3.16149100
C	3.55217600	2.15072300	2.06679200
H	4.47065100	1.74378500	0.16648100
H	2.46560700	2.29180500	3.92547500
H	4.36470700	2.78252100	2.41060700
C	1.24810900	-2.95726000	4.10630400
C	0.17728500	-2.72000400	3.05183400
H	0.76581700	-3.20763900	5.06038100
H	-0.50059200	-3.57750400	2.99614400
H	-0.41764900	-1.85683500	3.37444600
C	-2.41151900	0.26033000	0.62477400
C	-3.55251700	0.91780200	1.10219200
C	-3.47940500	2.22184100	1.55823400
C	-2.24207500	2.87095700	1.57793500
C	-1.13399000	2.18150800	1.14388500
H	-4.36925400	2.72111800	1.92692500
H	-2.13407900	3.88442500	1.94583100
H	-0.14154900	2.61506400	1.18799800
C	-2.46035100	-1.12932200	0.16458400
C	-3.65564200	-1.62802500	-0.37576700
C	-3.78161700	-2.96483600	-0.72046000
H	-4.49385200	-0.96028200	-0.54805100
C	-1.53102800	-3.36460300	0.03702800
C	-2.71688900	-3.83953700	-0.49964900
H	-4.70947500	-3.32769300	-1.14929800
H	-0.71136100	-4.05640500	0.19369300
H	-2.81340100	-4.89056700	-0.75011800
H	-4.49085200	0.37927800	1.14842200
N	-1.21969500	0.91595600	0.65055900
C	-1.36331400	-2.00536800	0.34964900
O	1.99653900	-1.75901100	4.20372700
H	2.70684400	-1.89048200	4.84271600
C	0.81525200	-2.43244400	1.67248400
H	1.77484700	-1.93842300	1.83506900
H	1.01922100	-3.36731100	1.14139400
H	1.88625500	-3.80502000	3.81613200

I5

E = -1479.064330 a.u.

C	-0.77924000	-1.17484300	0.37492800
C	-0.31606400	0.08388500	0.84160400
C	1.01049600	1.05315400	-2.65815700
C	1.40145800	-0.30787800	-2.36616900

C	-0.21684200	1.00622400	-3.39196200
C	0.46371200	-1.19100900	-3.01065200
C	-0.56307500	-0.37579600	-3.59461600
C	2.64995400	-0.71711300	-1.65640500
H	3.48667500	-0.73105200	-2.36470500
H	2.90009400	-0.02252300	-0.85099900
H	2.56015600	-1.71659400	-1.22536300
C	0.53795400	-2.67905900	-3.08728400
H	0.88657600	-2.97973800	-4.08240800
H	1.23690800	-3.09031400	-2.35651400
H	-0.44276400	-3.13932100	-2.93221900
C	-1.73445000	-0.86953500	-4.37469800
H	-1.49542800	-0.85376800	-5.44472200
H	-1.99721300	-1.89453300	-4.10496200
H	-2.61363100	-0.23774100	-4.22330100
C	-0.96866300	2.18105100	-3.92610500
H	-0.80704800	3.07502600	-3.31916200
H	-0.62886500	2.40481600	-4.94465000
H	-2.04260300	1.98416400	-3.97438500
C	1.81244900	2.28185300	-2.38133900
H	1.18492700	3.12311100	-2.07369800
H	2.57092000	2.10854900	-1.61659300
H	2.33156200	2.58081400	-3.30013800
Rh	-0.53486400	0.04016300	-1.42151900
C	1.03853100	0.37094100	1.39433400
C	1.67329600	1.55498400	0.98383700
C	1.67816800	-0.45224300	2.32447500
C	2.93075500	1.89101300	1.46278000
H	1.16705000	2.21482300	0.28394800
C	2.94864800	-0.11859900	2.79282700
H	1.22047000	-1.36301400	2.69093000
C	3.57831800	1.04404500	2.36463200
H	3.40786300	2.80957300	1.13598600
H	3.43779600	-0.77617900	3.50334000
H	4.56478000	1.29930300	2.73737900
C	0.45814900	-4.34060700	2.17377600
C	-0.51769800	-3.24580000	1.76695400
H	0.04970100	-4.88213100	3.03663900
H	-1.49627600	-3.69093800	1.55420300
H	-0.65894100	-2.57169600	2.62045500
C	-2.50513500	1.12635600	0.51448400
C	-3.44480100	2.10278000	0.84032800
C	-3.20223900	2.99946000	1.86714500
C	-2.02061600	2.88881400	2.60057100

C	-1.11052900	1.91748600	2.25976900
H	-3.93848100	3.75632500	2.11550400
H	-1.80582500	3.54075000	3.43860000
H	-0.18315900	1.77853700	2.79556200
C	-2.73924900	0.07321000	-0.47834900
C	-3.85343700	0.14253500	-1.35931400
C	-4.32984800	-0.98892200	-1.97091100
H	-4.33577800	1.09592500	-1.54558900
C	-2.63349400	-2.34738800	-0.90068200
C	-3.73846200	-2.24646200	-1.70595000
H	-5.18277200	-0.92539600	-2.63801300
H	-2.18113700	-3.31563200	-0.72287300
H	-4.16010200	-3.13984500	-2.15488600
H	-4.38683600	2.12902100	0.30880400
N	-1.33387500	1.07368300	1.21679700
C	-2.07597200	-1.18756900	-0.28878400
O	1.68317500	-3.70847800	2.48928800
H	2.30258100	-4.36953800	2.82044000
C	-0.00491700	-2.45412400	0.54742200
H	1.05579800	-2.23701400	0.67967200
H	-0.08950700	-3.06831500	-0.35381700
H	0.58284100	-5.06129000	1.35123800

I4’

E = -1479.024449 a.u.

C	0.29229200	-0.95477200	0.67980400
C	-0.82842000	-1.63806300	1.18385400
C	1.38121500	0.78307300	-2.79575900
C	1.44991000	-0.65923900	-2.49102100
C	0.03971900	1.15208300	-2.95806000
C	0.13211200	-1.17191200	-2.51562100
C	-0.76187100	-0.03663800	-2.70400900
C	2.72224300	-1.42730800	-2.34371000
H	3.23816400	-1.47100700	-3.30997100
H	3.39350600	-0.95843000	-1.61772300
H	2.53284600	-2.45383000	-2.02247700
C	-0.29651700	-2.59593000	-2.38406700
H	-0.40588500	-3.03697400	-3.38138000
H	0.43643700	-3.18882100	-1.83291800
H	-1.25970700	-2.67615700	-1.87499300
C	-2.23875000	-0.11889900	-2.86513200
H	-2.46250300	-0.27948400	-3.92773200
H	-2.66721800	-0.94925900	-2.30078200

H	-2.72985200	0.80632300	-2.55738900
C	-0.51496300	2.50178900	-3.28878900
H	0.23243400	3.28767300	-3.16212000
H	-0.84850300	2.52634700	-4.33192900
H	-1.37516800	2.74607800	-2.65897200
C	2.59152500	1.65120200	-2.86484600
H	2.34682800	2.71128100	-2.77418100
H	3.31346100	1.38163600	-2.08735400
H	3.08720400	1.50410600	-3.83231900
Rh	0.30281500	0.26229200	-0.88686100
C	-0.73992700	-2.70633100	2.15702900
C	-1.79071800	-2.89581500	3.09378900
C	0.36282800	-3.59708300	2.19367400
C	-1.71674400	-3.89873900	4.04278500
H	-2.63635100	-2.21635400	3.09122400
C	0.41328900	-4.61681400	3.12359600
H	1.14813600	-3.51533100	1.45035800
C	-0.61935200	-4.76368100	4.05818700
H	-2.50950000	-4.01319800	4.77395500
H	1.24825800	-5.30902300	3.12597100
H	-0.56816700	-5.55766100	4.79631400
C	-1.94778900	1.26325500	0.96188300
C	-2.53259800	2.11775100	1.89741700
C	-1.94076900	3.33933300	2.19205200
C	-0.77139900	3.69590200	1.52875900
C	-0.23186800	2.80009300	0.62246300
H	-2.39036100	4.00536800	2.92099600
H	-0.28147700	4.64592100	1.70743800
H	0.68124600	3.03360000	0.08463100
C	-2.67240400	0.02258800	0.55671900
C	-3.98001000	0.21233800	0.10339000
C	-4.78626400	-0.85936300	-0.27372000
H	-4.37361800	1.22220900	0.03418700
C	-3.01279300	-2.36715800	0.31139000
C	-4.29621000	-2.15658600	-0.17801500
H	-5.79271000	-0.67609600	-0.63498300
H	-2.63582800	-3.38103300	0.40323300
H	-4.91202200	-3.00219500	-0.46517000
H	-3.45041900	1.81452600	2.38845000
N	-0.79341400	1.60685600	0.35117400
C	-2.17473200	-1.29707600	0.67508100
C	1.65054600	-0.95597300	1.31131600
H	2.30213700	-1.60590400	0.70608500
H	1.64930400	-1.34867400	2.33397300

C	2.28550300	0.45250700	1.29637100
H	2.11385400	0.95451000	0.32286700
H	1.82612400	1.08244800	2.06463800
C	3.79495000	0.41289300	1.47112600
H	4.17925100	1.43409300	1.58944600
H	4.05091900	-0.15450500	2.37720300
O	4.32121500	-0.20159000	0.30992400
H	5.27370800	-0.31780500	0.41418000

TS4-5’

E = -1478.987935 a.u.

C	0.79701900	0.72298300	0.81837100
C	0.53929500	-0.61104100	1.14843300
C	1.76261900	1.51710800	-2.65370700
C	1.10310300	0.25459400	-2.56838700
C	0.76955900	2.55183000	-2.99055000
C	-0.30904600	0.53429100	-2.65855200
C	-0.49134600	1.95428100	-2.98873000
C	1.71720900	-1.09508100	-2.39505100
H	1.12896200	-1.71573500	-1.71311000
H	1.76038300	-1.60838300	-3.36257200
H	2.73598600	-1.02995100	-2.00793300
C	-1.39169000	-0.48629300	-2.69378100
H	-1.52641100	-0.80896000	-3.73448200
H	-1.14387600	-1.36782000	-2.09917500
H	-2.34463700	-0.08185800	-2.34800100
C	-1.81753900	2.58905400	-3.25521100
H	-1.76439400	3.67814200	-3.20899800
H	-2.16898700	2.31177100	-4.25569800
H	-2.57190100	2.25321700	-2.53762900
C	1.10891000	3.98191400	-3.25292800
H	0.22797000	4.62500600	-3.21564800
H	1.84286100	4.36208000	-2.53633600
H	1.55267700	4.07684400	-4.25104100
C	3.23321100	1.75898400	-2.57314100
H	3.74360600	0.97436200	-2.01041400
H	3.65726100	1.77752200	-3.58454100
H	3.45867500	2.72227500	-2.10766400
Rh	0.45724100	1.56240300	-0.95409000
C	1.56981700	-1.41978900	1.82316500
C	1.19792200	-2.21909300	2.91887100
C	2.91365700	-1.38893200	1.42337700
C	2.16280000	-2.92566500	3.62478700

H	0.15961300	-2.25611000	3.23445500
C	3.87073600	-2.11090100	2.12202400
H	3.20795400	-0.81458100	0.54977000
C	3.49905900	-2.86971800	3.23047800
H	1.87250300	-3.52107700	4.48397900
H	4.90757200	-2.07982500	1.80607300
H	4.25018200	-3.42437000	3.78292600
C	-1.99870200	0.89836100	1.01914100
C	-3.15377200	1.44147500	1.59467800
C	-3.18968500	2.76786300	1.98661000
C	-2.04699000	3.55738800	1.83049800
C	-0.92296800	2.97884500	1.29158700
H	-4.08686300	3.18002900	2.43638900
H	-2.02434300	4.59649100	2.13676300
H	-0.00444200	3.54223400	1.18415600
C	-1.92346600	-0.51467300	0.63724900
C	-3.08895900	-1.17664500	0.23251800
C	-3.07640500	-2.53301400	-0.06293400
H	-4.01567600	-0.62364300	0.11781900
C	-0.72965400	-2.62175000	0.46990600
C	-1.89133200	-3.25829800	0.05981200
H	-3.98818000	-3.02313200	-0.38694500
H	0.19045200	-3.18863100	0.56001700
H	-1.87397100	-4.31932700	-0.16534700
H	-4.00895500	0.80046100	1.76951200
N	-0.89894100	1.68459800	0.87016900
C	-0.71317900	-1.24203200	0.75202200
C	1.81075600	1.65428700	1.41687800
C	1.68594900	2.00616100	2.91819200
H	1.90570400	3.07164500	3.04885000
H	0.66732000	1.83977500	3.28653300
C	2.67707300	1.18648600	3.76330700
H	2.66883700	1.56452100	4.79244600
H	2.37043600	0.13877100	3.79652900
O	3.97199800	1.20611200	3.20439900
H	4.45559500	1.96918500	3.54237700
H	2.79873800	1.20560900	1.26041900
H	1.85519500	2.58207100	0.81028600

I5’

E = -1479.083257 a.u.

C	-0.09986000	0.49920900	1.93805400
C	-0.13818900	-0.91058300	1.84721600
C	1.93288300	0.43784300	-1.85333100
C	1.44208800	-0.91613400	-1.93999200

C	0.81033700	1.33026100	-1.75456500
C	0.02686000	-0.87221400	-1.77071900
C	-0.36249100	0.51491700	-1.63267200
C	2.27963600	-2.13121100	-2.16578100
H	2.47253200	-2.25607800	-3.23825500
H	3.25038700	-2.04967600	-1.66902800
H	1.78318300	-3.03898400	-1.81405600
C	-0.90247400	-2.03581500	-1.86803500
H	-1.11856900	-2.23680500	-2.92409600
H	-0.46645300	-2.94128300	-1.43959900
H	-1.85212400	-1.84565400	-1.36404000
C	-1.76467800	1.02892500	-1.65083400
H	-2.04126000	1.27084600	-2.68379700
H	-2.47719400	0.28607500	-1.28891500
H	-1.87283500	1.94609300	-1.06474300
C	0.84598700	2.82285700	-1.77914800
H	1.79398500	3.21405300	-1.40153800
H	0.73032400	3.18484200	-2.80807900
H	0.03315100	3.25426400	-1.18765900
C	3.36699500	0.83691400	-1.98633300
H	3.54877900	1.83482200	-1.58121200
H	4.02574000	0.13542700	-1.46935400
H	3.64996200	0.84951300	-3.04505200
Rh	0.96868700	0.01609400	0.04650900
C	0.87345800	-1.76459500	2.56644800
C	0.81776400	-1.84385300	3.96189600
C	1.79889000	-2.56188800	1.87928200
C	1.69844800	-2.66751800	4.65766200
H	0.07445000	-1.26828100	4.50759400
C	2.68414300	-3.38181600	2.57809700
H	1.81249500	-2.55692000	0.79060600
C	2.63984700	-3.42938400	3.96947600
H	1.64308900	-2.71876100	5.74006700
H	3.39644300	-3.99318000	2.03338100
H	3.32514100	-4.07019100	4.51399900
C	-2.52190200	0.60067300	1.42554100
C	-3.67761400	1.39582000	1.31941600
C	-3.62573000	2.76717400	1.39059800
C	-2.37904000	3.38484100	1.55345000
C	-1.27152600	2.59881100	1.69521800
H	-4.53267500	3.35655300	1.31185100
H	-2.27285900	4.46250000	1.58674200
H	-0.29457600	3.03208800	1.83083700
C	-2.55208500	-0.84290100	1.26344900

C	-3.74072200	-1.50976500	0.90627500
C	-3.76698400	-2.88465900	0.77628900
H	-4.65794600	-0.96505800	0.72203300
C	-1.42944700	-2.99173200	1.35443900
C	-2.60732900	-3.62995000	1.01398800
H	-4.69081100	-3.38221600	0.50240900
H	-0.53959100	-3.57899300	1.54507500
H	-2.63102100	-4.71158300	0.93327300
H	-4.63381500	0.91184200	1.18372200
N	-1.32988700	1.22966700	1.67102100
C	-1.37535900	-1.59285900	1.46339100
C	0.87181600	1.23617200	2.86887500
H	1.35689100	0.48357900	3.49197800
H	0.27856400	1.83772300	3.56576600
C	1.97762700	2.09931100	2.22279600
H	1.63665300	2.56921400	1.29117900
H	2.25456900	2.91093900	2.90448100
C	3.22957200	1.28933000	1.92582500
H	3.94779500	1.86912300	1.34280500
H	3.71567300	0.96702500	2.85103900
O	2.90082800	0.11699100	1.14977200
H	2.99714100	-0.68126900	1.69394600

Sub2’

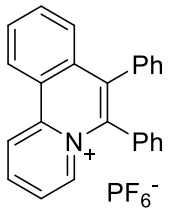
E = -977.520899 a.u.

C	1.12765100	-0.01656000	-1.59345700
C	0.75039900	-1.43964300	-1.43604700
C	0.13361700	0.62140500	-2.33422500
C	-0.43984000	-1.67129000	-2.15860200
C	-0.90827700	-0.37471400	-2.61674800
C	1.59603300	-2.45047600	-0.73929400
H	2.42797000	-2.73990300	-1.39349100
H	2.02867100	-2.04839500	0.18076400
H	1.03462100	-3.35323900	-0.49169600
C	-1.07192300	-2.98088200	-2.49887500
H	-0.82885100	-3.22494100	-3.53949100
H	-0.68964700	-3.79522500	-1.88036600
H	-2.16082300	-2.95014500	-2.41311200
C	-2.11482100	-0.13577600	-3.45312000
H	-1.83437500	-0.23067300	-4.51071900
H	-2.89999500	-0.86678500	-3.24953400
H	-2.51794700	0.86892800	-3.30757000
C	0.08658400	2.04048000	-2.79893000

H	0.80695000	2.66984000	-2.27189500
H	0.33588000	2.08243000	-3.86544600
H	-0.91119200	2.47332800	-2.68288300
C	2.36891300	0.57187100	-1.01387100
H	2.38870600	1.65967700	-1.09623500
H	2.48692800	0.30021800	0.04019900
H	3.24360400	0.17868700	-1.54604100
Rh	-0.87309800	-0.28784700	-0.50297600
C	-2.99074500	1.00433500	1.10158600
C	-3.74003400	1.99927100	1.73203000
C	-3.31070700	3.32145800	1.67402900
C	-2.13813800	3.62175900	0.99067100
C	-1.43585900	2.58756800	0.37433900
H	-3.88334900	4.10386400	2.16050900
H	-1.76176100	4.63664800	0.93190300
H	-0.51538000	2.77902700	-0.16510300
C	-3.30390100	-0.41542300	1.11657900
C	-4.40468600	-0.96082300	1.78443900
C	-4.55706400	-2.33432600	1.81550400
H	-5.13157500	-0.33538000	2.28983500
C	-2.53380600	-2.66566200	0.49540800
C	-3.60552300	-3.19108100	1.18446400
H	-5.40224200	-2.77449600	2.33504500
H	-1.82626500	-3.33705600	0.02418700
H	-3.74132200	-4.26603400	1.25362400
H	-4.64936000	1.75018600	2.26534400
N	-1.84614200	1.31881900	0.42293100
C	-2.34263900	-1.27349700	0.41774400

12. Characterization data of compounds 3, 5 and 8

6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3aa)



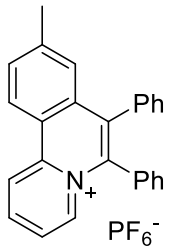
3aa

Yellow solid; yield 95%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.76 (d, *J* = 8.6 Hz, 1H), 9.36 (d, *J* = 8.3 Hz, 1H), 8.79 – 8.68 (m, 2H), 8.17 – 8.03 (m, 3H), 7.53 – 7.42 (m, 6H), 7.38 – 7.30 (m, 3H), 7.28 – 7.24 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 143.69, 140.44, 138.79, 137.33, 135.84, 134.84, 134.62, 132.52, 131.69, 131.44, 131.29, 130.55, 130.37, 129.80, 128.79, 128.72, 127.28, 126.44, 125.19, 125.09, 123.96.
HRMS (ESI) calcd for [$C_{25}H_{18}N^+$] (M-PF_6)$^+$:332.1434, found 332.1442

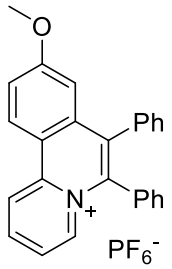
9-methyl-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ba)



3ba

Yellow solid; yield 83%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.67 (d, *J* = 8.6 Hz, 1H), 9.24 (d, *J* = 8.7 Hz, 1H), 8.80 – 8.52 (m, 2H), 8.03 (t, *J* = 7.0 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.50 – 7.38 (m, 5H), 7.35 – 7.27 (m, 3H), 7.24 – 7.20 (m, 3H), 2.47 (s, 3H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 145.59, 143.61, 140.13, 138.90, 137.01, 135.56, 134.85, 132.93, 132.74, 131.76, 131.44, 130.49, 130.38, 129.75, 128.78, 128.72, 126.49, 126.45, 124.66, 123.69, 123.07, 22.18.
HRMS (ESI) calcd for [$C_{26}H_{20}N^+$] (M-PF_6)$^+$:346.1590, found 346.1588

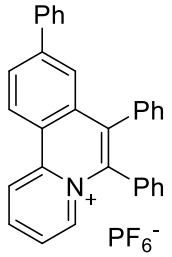
9-methoxy-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ca)



3ca

Yellow solid; yield 82%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.60 (d, *J* = 8.7 Hz, 1H), 9.30 (d, *J* = 9.3 Hz, 1H), 8.67 – 8.55 (m, 2H), 7.96 (t, *J* = 6.9 Hz, 1H), 7.77 (dd, *J* = 9.3, 2.5 Hz, 1H), 7.52 – 7.41 (m, 5H), 7.38 – 7.30 (m, 3H), 7.28 – 7.24 (m, 2H), 6.76 (d, *J* = 2.5 Hz, 1H), 3.78 (s, 3H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 163.73, 143.49, 139.75, 139.22, 136.62, 135.15, 135.11, 134.80, 131.77, 131.38, 130.51, 130.30, 129.75, 129.06, 128.85, 128.79, 123.72, 123.32, 120.67, 119.16, 108.50, 56.37.
HRMS (ESI) calcd for [$C_{26}H_{20}NO^+$] (M-PF_6)$^+$:362.1539, found 362.1537

6,7,9-triphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3da)



3da

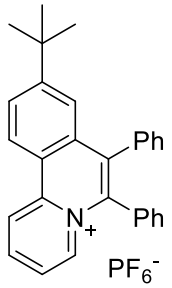
Yellow solid; yield 93%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.78 (d, *J* = 8.6 Hz, 1H), 9.43 (d, *J* = 8.8 Hz, 1H), 8.79 – 8.68 (m, 2H), 8.45 (d, *J* = 8.7 Hz, 1H), 8.10 (t, *J* = 6.9 Hz, 1H), 7.63 (d, *J* = 7.4 Hz, 3H), 7.53 – 7.44 (m, 8H), 7.39 – 7.34 (m, 3H), 7.32 – 7.30 (m, 2H).

^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 145.08, 143.00, 139.95, 138.69, 137.84, 136.80, 135.32, 134.16, 132.61, 131.15, 130.92, 130.08, 129.95, 129.42, 129.31, 129.23, 128.38, 128.35, 127.17, 126.94, 124.58, 123.72, 123.55.

HRMS (ESI) calcd for $[C_{31}H_{22}N^+]$ $(M\text{-}PF_6)^+$:408.1747, found 408.1749

9-(tert-butyl)-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ea)



3ea

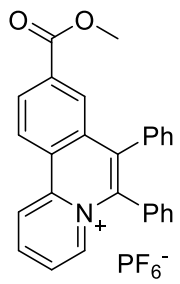
Yellow solid; yield 86%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.73 (d, *J* = 8.6 Hz, 1H), 9.30 (d, *J* = 8.9 Hz, 1H), 8.79 – 8.64 (m, 2H), 8.26 (d, *J* = 8.8 Hz, 1H), 8.08 (t, *J* = 6.9 Hz, 1H), 7.54 – 7.42 (m, 6H), 7.41 – 7.33 (m, 3H), 7.28 (d, *J* = 6.9 Hz, 2H), 1.26 (s, 9H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 157.19, 142.93, 139.63, 138.27, 136.50, 135.48, 134.33, 132.17, 131.26, 130.94, 130.03, 129.85, 129.29, 129.18, 128.25, 128.22, 125.93, 124.25, 123.31, 122.64, 122.03, 35.31, 30.30.

HRMS (ESI) calcd for $[C_{29}H_{26}N^+]$ $(M\text{-}PF_6)^+$:388.2060, found 388.2058

9-(methoxycarbonyl)-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3fa)



3fa

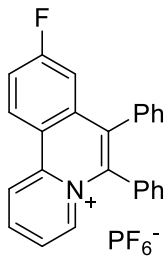
Yellow solid; yield 75%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.84 (d, *J* = 8.0 Hz, 1H), 9.51 (d, *J* = 8.5 Hz, 1H), 8.82 (dd, *J* = 18.4, 7.2 Hz, 2H), 8.52 (d, *J* = 8.5 Hz, 1H), 8.20 (t, *J* = 6.9 Hz, 1H), 8.05 – 8.01 (m, 1H), 7.52 – 7.44 (m, 5H), 7.41 – 7.34 (m, 3H), 7.30 – 7.26 (m, 2H), 3.86 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 164.83, 142.65, 140.74, 139.20, 137.43, 135.27, 133.88, 133.58, 131.91, 130.91, 130.86, 130.18, 129.94, 129.66, 129.34, 128.53, 128.42, 127.53, 127.39, 126.91, 125.76, 124.26, 52.96.

HRMS (ESI) calcd for [$C_{27}H_{20}NO_2^+$] (M-PF_6) $^+$:390.1489, found 390.1490

9-fluoro-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ga)



3ga

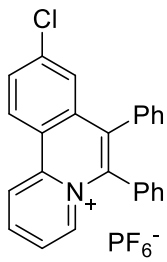
Yellow solid; yield 82%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.73 (d, *J* = 8.5 Hz, 1H), 9.49 (dd, *J* = 8.3, 5.0 Hz, 1H), 8.74 (dd, *J* = 18.4, 7.4 Hz, 2H), 8.16 – 7.99 (m, 2H), 7.53 – 7.42 (m, 5H), 7.40 – 7.32 (m, 3H), 7.25 (d, *J* = 7.2 Hz, 2H), 7.08 (d, *J* = 9.4 Hz, 1H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 165.60, 163.57, 142.87, 140.27, 139.36, 136.88, 134.67, 134.63, 134.60, 133.85, 130.96, 130.79, 130.16, 130.09, 130.01, 129.78, 129.31, 128.47, 128.45, 124.57, 123.47, 121.73, 120.05, 119.86, 111.58, 111.39.

HRMS (ESI) calcd for [$C_{25}H_{17}FN^+$] (M-PF_6) $^+$:350.1340, found 350.1339

9-chloro-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ha)



3ha

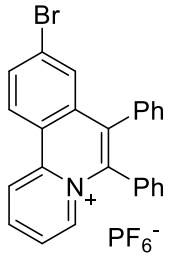
Yellow solid; yield 80%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.74 (d, *J* = 8.5 Hz, 1H), 9.39 (d, *J* = 9.0 Hz, 1H), 8.81 – 8.70 (m, 2H), 8.23 – 8.17 (m, 1H), 8.13 (t, *J* = 7.0 Hz, 1H), 7.51 – 7.43 (m, 5H), 7.39 – 7.32 (m, 4H), 7.26 (d, *J* = 6.7 Hz, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.86, 140.48, 139.53, 139.07, 137.09, 134.23, 133.71, 133.36, 130.97, 130.89, 130.78, 130.18, 129.84, 129.33, 128.53, 128.47, 128.42, 125.46, 125.02, 123.64, 123.43.

HRMS (ESI) calcd for [$C_{25}H_{17}ClN^+$] (M-PF_6) $^+$:366.1044, found 366.1048

9-bromo-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ia)



3ia

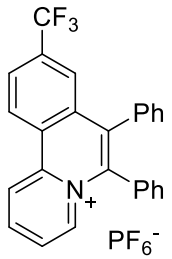
Yellow solid; yield 76%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.75 (d, *J* = 8.6 Hz, 1H), 9.31 (d, *J* = 9.0 Hz, 1H), 8.82 – 8.73 (m, 2H), 8.38 – 8.31 (m, 1H), 8.15 (t, *J* = 6.8 Hz, 1H), 7.54 (d, *J* = 1.6 Hz, 1H), 7.51 – 7.45 (m, 5H), 7.41 – 7.34 (m, 3H), 7.27 (d, *J* = 6.8 Hz, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 143.46, 140.98, 140.00, 137.64, 134.60, 134.18, 133.91, 131.38, 131.27, 130.68, 130.34, 129.83, 129.11, 129.04, 128.97, 128.76, 128.69, 125.58, 124.17, 124.04.

HRMS (ESI) calcd for [$C_{25}H_{17}BrN^+$] (M-PF_6) $^+$:410.0539, found 410.0539

6,7-diphenyl-9-(trifluoromethyl)pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ja)



3ja

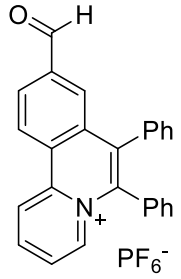
Yellow solid; yield 58%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.90 (d, *J* = 8.6 Hz, 1H), 9.62 (d, *J* = 8.8 Hz, 1H), 8.92 – 8.81 (m, 2H), 8.46 (d, *J* = 8.7 Hz, 1H), 8.24 (t, *J* = 7.0 Hz, 1H), 7.67 (s, 1H), 7.54 – 7.44 (m, 5H), 7.41 – 7.34 (m, 3H), 7.31 – 7.27 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.55, 141.04, 139.73, 137.60, 134.92, 133.53, 132.93, 132.67, 132.00, 130.78, 130.27, 129.88, 129.37, 128.65, 128.49, 128.00, 127.24, 126.31, 126.29, 126.01, 124.32, 124.22, 123.21, 123.18, 122.05.

HRMS (ESI) calcd for [$C_{26}H_{17}F_3N^+$] $(M\text{-}PF_6)^+$:400.1308, found 400.1306

9-formyl-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ka)



3ka

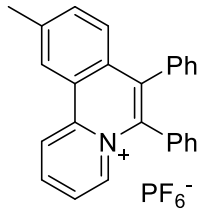
Brown solid; yield 55%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.18 (s, 1H), 9.88 (d, *J* = 8.6 Hz, 1H), 9.58 (d, *J* = 8.7 Hz, 1H), 8.90 – 8.79 (m, 2H), 8.57 – 8.49 (m, 1H), 8.23 (t, *J* = 7.0 Hz, 1H), 7.99 (s, 1H), 7.54 – 7.46 (m, 5H), 7.43 – 7.37 (m, 3H), 7.30 (d, *J* = 6.7 Hz, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 193.13, 143.23, 141.20, 139.74, 139.08, 137.98, 135.97, 134.36, 132.70, 131.43, 131.37, 130.68, 130.48, 129.84, 129.58, 129.01, 128.91, 128.77, 128.49, 127.66, 126.32, 124.91.

HRMS (ESI) calcd for [$C_{26}H_{18}NO^+$] $(M\text{-}PF_6)^+$:360.1383, found 360.1382

10-methyl-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3la)



3la

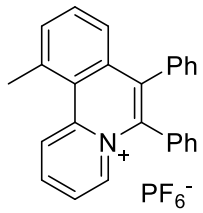
Yellow solid; yield 92%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.75 (d, *J* = 8.6 Hz, 1H), 9.23 (s, 1H), 8.78 – 8.68 (m, 2H), 8.11 (t, *J* = 7.5 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.54 – 7.44 (m, 5H), 7.42 – 7.32 (m, 4H), 7.27 – 7.24 (m, 2H), 2.71 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.87, 141.29, 139.54, 137.49, 136.67, 135.66, 135.27, 134.43, 131.24, 131.01, 130.03, 129.99, 129.83, 129.27, 128.25, 128.17, 126.62, 125.23, 124.66, 124.54, 123.42, 21.41.

HRMS (ESI) calcd for [$C_{26}H_{20}N^+$] $(M\text{-}PF_6)^+$:346.1590, found 346.1589

11-methyl-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ma)



3ma

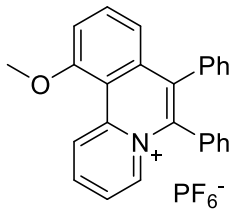
Yellow solid; yield 91%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.46 (d, *J* = 8.8 Hz, 1H), 8.84 (d, *J* = 6.7 Hz, 1H), 8.68 (t, *J* = 8.5 Hz, 1H), 8.13 (t, *J* = 6.5 Hz, 1H), 8.02 (d, *J* = 7.3 Hz, 1H), 7.94 (t, *J* = 7.8 Hz, 1H), 7.51 – 7.43 (m, 5H), 7.38 – 7.31 (m, 4H), 7.26 – 7.22 (m, 2H), 3.23 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 143.38, 138.93, 137.97, 137.67, 137.05, 135.48, 134.83, 134.81, 133.48, 132.86, 131.31, 130.87, 129.96, 129.89, 129.30, 128.25, 128.13, 127.21, 125.07, 124.67, 124.18, 25.78.

HRMS (ESI) calcd for [$C_{26}H_{20}N^+$] (M-PF_6)$^+$:346.1590, found 346.1588

11-methoxy-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3na)



3na

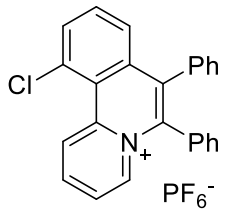
Yellow solid; yield 94%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.26 (d, *J* = 8.8 Hz, 1H), 8.81 (d, *J* = 6.8 Hz, 1H), 8.67 (t, *J* = 8.0 Hz, 1H), 8.11 – 7.98 (m, 2H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.51 – 7.41 (m, 5H), 7.37 – 7.29 (m, 3H), 7.25 – 7.21 (m, 2H), 7.06 (d, *J* = 8.0 Hz, 1H), 4.30 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 158.67, 142.42, 139.84, 138.55, 137.11, 135.22, 134.98, 134.70, 134.03, 131.53, 130.80, 129.94, 129.82, 129.29, 128.25, 128.11, 127.17, 123.82, 119.06, 114.40, 112.92, 57.29.

HRMS (ESI) calcd for [$C_{26}H_{20}NO^+$] (M-PF_6)$^+$:362.1539, found 362.1540

11-chloro-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3oa)



3oa

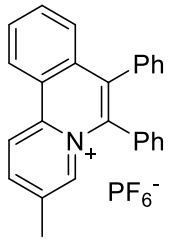
Yellow solid; yield 65%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.26 (d, *J* = 8.9 Hz, 1H), 8.89 (d, *J* = 6.8 Hz, 1H), 8.77 (t, *J* = 8.1 Hz, 1H), 8.29 (d, *J* = 7.8 Hz, 1H), 8.20 (t, *J* = 7.0 Hz, 1H), 8.00 (t, *J* = 8.0 Hz, 1H), 7.52 – 7.43 (m, 6H), 7.39 – 7.31 (m, 3H), 7.26 – 7.22 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 141.68, 139.64, 138.90, 137.71, 134.97, 134.91, 134.34, 134.29, 133.70, 131.75, 131.02, 130.76, 130.11, 129.88, 129.33, 128.38, 128.35, 126.50, 126.34, 125.30, 122.12, 99.49.

HRMS (ESI) calcd for [$C_{25}H_{17}ClN^+$] (M-PF_6)$^+$:366.1044, found 366.1040

3-methyl-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3pa)



3pa

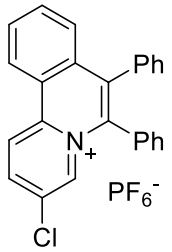
Yellow solid; yield 85%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.68 (d, *J* = 9.0 Hz, 1H), 9.33 (d, *J* = 8.4 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 8.46 (s, 1H), 8.11 (t, *J* = 7.6 Hz, 1H), 8.03 (t, *J* = 7.6 Hz, 1H), 7.51 – 7.42 (m, 6H), 7.37 – 7.29 (m, 3H), 7.27 – 7.22 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 141.68, 141.41, 137.94, 135.48, 135.17, 134.42, 133.76, 131.73, 131.06, 130.97, 130.76, 130.08, 129.86, 129.27, 128.25, 128.17, 126.73, 125.71, 124.57, 123.00, 18.23.

HRMS (ESI) calcd for $[C_{26}H_{20}N^+]$ $(M\text{-}PF_6)^+$:346.1590, found 346.1594

3-chloro-6,7-diphenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3qa)



3qa

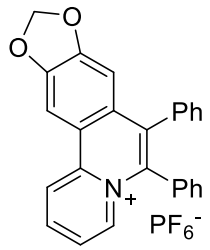
Yellow solid; yield 80%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.81 (d, *J* = 9.5 Hz, 1H), 9.40 (d, *J* = 8.4 Hz, 1H), 8.93 (dd, *J* = 9.4, 1.8 Hz, 1H), 8.55 (d, *J* = 1.8 Hz, 1H), 8.17 (t, *J* = 7.6 Hz, 1H), 8.11 (t, *J* = 7.6 Hz, 1H), 7.54 – 7.45 (m, 6H), 7.39 – 7.31 (m, 3H), 7.23 (d, *J* = 6.8 Hz, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.19, 139.77, 137.97, 136.38, 134.66, 134.01, 133.90, 132.10, 131.26, 130.97, 130.49, 129.74, 129.45, 128.39, 126.90, 126.21, 124.86, 124.40.

HRMS (ESI) calcd for $[C_{25}H_{17}ClN^+]$ $(M\text{-}PF_6)^+$:366.1044, found 366.1049

6,7-diphenyl-[1,3]dioxolo[4,5-*g*]pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ra)

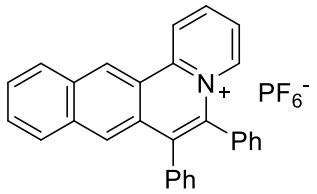


3ra

Yellow solid; yield 81%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.58 (d, *J* = 8.8 Hz, 1H), 8.99 (d, *J* = 9.0 Hz, 1H), 8.58 (t, *J* = 7.9 Hz, 1H), 8.54 (d, *J* = 6.9 Hz, 1H), 7.95 (t, *J* = 7.1 Hz, 1H), 7.83 (d, *J* = 8.9 Hz, 1H), 7.46 – 7.39 (m, 5H), 7.22 – 7.18 (m, 5H), 6.01 (s, 2H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 151.65, 143.70, 143.20, 139.98, 138.38, 136.66, 135.56, 131.19, 131.12, 130.84, 129.86, 129.48, 129.08, 127.74, 127.31, 123.57, 123.31, 122.37, 119.24, 116.39, 113.12, 103.07.
HRMS (ESI) calcd for [$C_{26}H_{18}NO_2^+$] (M-PF_6) $^+$:376.1332, found 376.1335

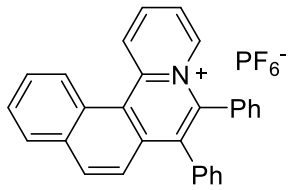
6,7-diphenylbenzo[g]pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3sa)



3sa

Yellow solid; yield 79%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.15 (s, 1H), 9.91 (d, *J* = 7.2 Hz, 1H), 8.82 (t, *J* = 6.6 Hz, 1H), 8.75 (d, *J* = 6.7 Hz, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 2H), 7.99 (s, 1H), 7.86 – 7.81 (m, 1H), 7.81 – 7.76 (m, 1H), 7.54 (d, *J* = 6.6 Hz, 2H), 7.50 – 7.45 (m, 3H), 7.43 – 7.37 (m, 3H), 7.33 (d, *J* = 7.9 Hz, 2H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 144.30, 141.20, 137.80, 136.71, 135.28, 134.55, 134.33, 132.54, 131.22, 129.96, 129.93, 129.84, 129.25, 129.05, 128.57, 128.38, 128.28, 127.92, 127.66, 126.13, 124.94, 123.72, 121.75.
HRMS (ESI) calcd for [$C_{29}H_{20}N^+$] (M-PF_6) $^+$:382.1590, found 382.1593

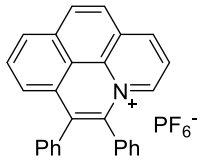
6,7-diphenylbenzo[h]pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ta)



3ta

Yellow solid; yield 64%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.63 (d, *J* = 8.7 Hz, 1H), 9.06 (d, *J* = 8.4 Hz, 1H), 8.87 (d, *J* = 6.9 Hz, 1H), 8.66 (t, *J* = 8.0 Hz, 1H), 8.48 (d, *J* = 8.8 Hz, 1H), 8.35 (d, *J* = 7.9 Hz, 1H), 8.14 (t, *J* = 7.0 Hz, 1H), 8.05 (t, *J* = 7.8 Hz, 1H), 7.98 (t, *J* = 7.4 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 2H), 7.53 – 7.46 (m, 3H), 7.42 – 7.34 (m, 4H), 7.31 (d, *J* = 7.1 Hz, 2H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.31, 139.77, 138.84, 136.26, 135.72, 135.51, 134.81, 134.01, 133.59, 131.61, 131.25, 130.60, 130.07, 129.99, 129.81, 129.63, 128.84, 128.32, 128.17, 127.83, 124.42, 123.05, 122.81.
HRMS (ESI) calcd for [$C_{29}H_{20}N^+$] (M-PF_6) $^+$:382.1590, found 382.1592

5,6-diphenylbenzo[de]pyrido[3,2,1-*ij*]quinolin-4-ium hexafluorophosphate (3ua)



3ua

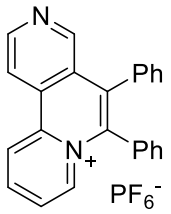
Yellow solid; yield 60%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.52 (d, *J* = 7.0 Hz, 1H), 9.19 (d, *J* = 4.7 Hz, 1H), 8.82 (d, *J* = 7.6 Hz, 1H), 8.76 (d, *J* = 6.9 Hz, 1H), 8.68 (d, *J* = 8.8 Hz, 1H), 8.53 (t, *J* = 5.7 Hz, 1H), 8.49 (t, *J* = 7.8 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.61 (d, *J* = 6.5 Hz, 2H), 7.56 – 7.47 (m, 3H), 7.44 – 7.39 (m, 2H), 7.36 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 140.07, 138.76, 136.35, 135.78, 134.36, 133.20, 132.68, 132.53, 131.11, 131.04, 130.58, 130.20, 130.14, 129.94, 129.52, 129.11, 128.78, 128.43, 128.35, 126.65, 125.19, 123.10, 118.33.

HRMS (ESI) calcd for $[C_{27}H_{18}N^+]$ $(M\text{-}PF_6)^+$:356.1434, found 356.1435

5,6-diphenylpyrido[2,1-*a*][2,6]naphthyridin-7-ium hexafluorophosphate (3va)



3va

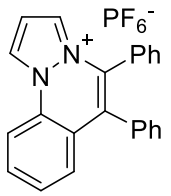
Yellow solid; yield 63%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.90 (d, *J* = 8.3 Hz, 1H), 9.24 (d, *J* = 5.6 Hz, 1H), 9.20 (d, *J* = 5.7 Hz, 1H), 8.93 – 8.85 (m, 2H), 8.79 (s, 1H), 8.29 (t, *J* = 6.9 Hz, 1H), 7.51 – 7.46 (m, 5H), 7.40 – 7.34 (m, 3H), 7.30 (d, *J* = 6.6 Hz, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 149.77, 148.82, 142.03, 141.32, 139.92, 137.92, 133.82, 132.77, 130.88, 130.48, 130.30, 129.95, 129.65, 129.39, 128.58, 128.39, 126.96, 125.43, 124.48, 117.51.

HRMS (ESI) calcd for $[C_{24}H_{17}N_2^+]$ $(M\text{-}PF_6)^+$:333.1386, found 333.1394

5,6-diphenylpyrazolo[1,2-*a*]cinnolin-4-ium hexafluorophosphate (3wa)



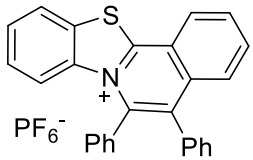
3wa

Yellow solid; yield 81%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.14 (d, *J* = 2.5 Hz, 1H), 8.79 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 3.0 Hz, 1H), 7.94 (t, *J* = 7.7 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.57 (t, *J* = 3.0 Hz, 1H), 7.50 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.47 – 7.43 (m, 3H), 7.38 – 7.32 (m, 3H), 7.29 – 7.24 (m, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 132.31, 131.71, 131.31, 130.46, 130.40, 130.26, 129.58, 129.42, 129.23, 128.48, 127.28, 125.51, 121.86, 116.03, 110.64.
HRMS (ESI) calcd for [$C_{23}H_{17}N_2^+$] (M-PF_6) $^+$:321.1386, found 321.1396

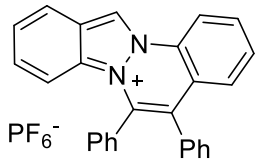
5,6-diphenylbenzo[4,5]thiazolo[2,3-*a*]isoquinolin-7-ium hexafluorophosphate (3xa)



3xa

Yellow solid; yield 83%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.95 (d, *J* = 7.7 Hz, 1H), 8.64 (d, *J* = 8.1 Hz, 1H), 8.22 – 8.09 (m, 2H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.58 – 7.47 (m, 6H), 7.44 – 7.34 (m, 4H), 7.28 – 7.24 (m, 2H), 6.31 (d, *J* = 9.0 Hz, 1H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 159.83, 139.97, 139.61, 136.48, 134.37, 133.33, 132.99, 132.13, 131.45, 130.69, 130.61, 130.29, 129.11, 129.06, 128.45, 128.32, 128.04, 127.29, 126.99, 125.14, 123.32, 119.52.
HRMS (ESI) calcd for [$C_{27}H_{18}NS^+$] (M-PF_6) $^+$:388.1154, found 388.1152

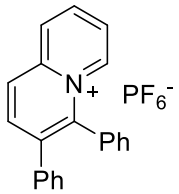
5,6-diphenylindazolo[2,1-a]cinnolin-7-ium hexafluorophosphate (3ya)



3ya

Yellow solid; yield 62%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.83 (s, 1H), 8.90 (d, *J* = 7.4 Hz, 1H), 8.36 (d, *J* = 7.5 Hz, 1H), 8.03 (t, *J* = 6.7 Hz, 1H), 7.82 (t, *J* = 7.1 Hz, 1H), 7.68 (t, 1H), 7.64 – 7.52 (m, 6H), 7.43 – 7.28 (m, 6H), 5.85 (d, *J* = 8.8 Hz, 1H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 134.84, 134.34, 132.89, 132.65, 131.69, 131.42, 131.32, 131.30, 131.10, 130.73, 129.87, 129.61, 128.97, 128.84, 127.60, 127.26, 124.37, 123.87, 123.66, 123.35, 121.22, 117.76, 114.02.
HRMS (ESI) calcd for [$C_{27}H_{19}N_2^+$] (M-PF_6) $^+$:371.1543, found 371.1544

3,4-diphenylquinolizin-5-ium hexafluorophosphate (3za)



3za

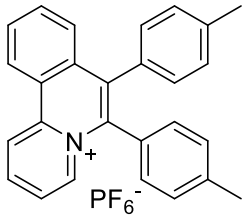
Yellow solid; yield 79%

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (d, *J* = 7.1 Hz, 1H), 8.47 – 8.40 (m, 2H), 8.18 (dd, *J* = 17.7, 8.4 Hz, 2H), 7.74 (t, *J* = 7.0 Hz, 1H), 7.47 (d, *J* = 3.7 Hz, 3H), 7.41 – 7.35 (m, 2H), 7.21 (d, *J* = 6.8 Hz, 3H), 7.17 – 7.11 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 143.67, 142.96, 138.91, 138.75, 136.41, 135.86, 132.98, 131.02, 130.56, 130.06, 129.66, 129.41, 128.62, 128.48, 128.40, 127.20, 124.27.

HRMS (ESI) calcd for $[C_{21}H_{16}N^+]$ $(M\text{-}PF_6)^+$:282.1277, found 282.1283

6,7-di-p-tolylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ab)



3ab

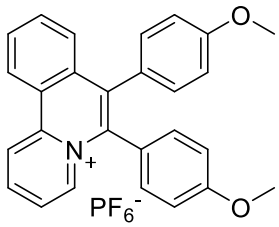
Yellow solid; yield 94%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.74 (d, *J* = 8.6 Hz, 1H), 9.34 (d, *J* = 8.3 Hz, 1H), 8.70 (dd, *J* = 13.2, 7.3 Hz, 2H), 8.14 – 8.02 (m, 3H), 7.47 (d, *J* = 7.9 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 2.31 (s, 3H), 2.28 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 143.18, 139.82, 139.54, 138.35, 137.45, 136.70, 135.34, 134.02, 132.26, 131.51, 130.75, 130.67, 130.00, 129.74, 128.94, 128.40, 126.81, 125.89, 124.61, 124.51, 123.44, 20.95, 20.77.

HRMS (ESI) calcd for $[C_{27}H_{22}N^+]$ $(M\text{-}PF_6)^+$:360.1747, found 360.1746

6,7-bis(4-methoxyphenyl)pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ac)



3ac

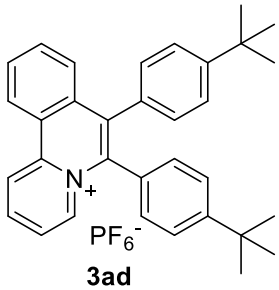
Yellow solid; yield 84%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.75 (d, *J* = 8.5 Hz, 1H), 9.34 (d, *J* = 8.2 Hz, 1H), 8.78 (d, *J* = 6.9 Hz, 1H), 8.69 (t, *J* = 7.7 Hz, 1H), 8.09 (t, *J* = 6.7 Hz, 2H), 8.04 (t, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.42 (d, *J* = 8.6 Hz, 2H), 7.17 (d, *J* = 8.6 Hz, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 3.76 (s, 3H), 3.73 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 160.41, 159.15, 143.60, 140.22, 139.01, 137.17, 135.89, 134.42, 132.93, 132.85, 131.61, 131.06, 127.28, 126.99, 126.35, 125.01, 124.94, 123.88, 123.77, 115.27, 114.23, 55.65, 55.50.

HRMS (ESI) calcd for [$C_{27}H_{22}NO_2^+$] (M-PF_6) $^+$:392.1645, found 392.1647

6,7-bis(4-(tert-butyl)phenyl)pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ad)



3ad

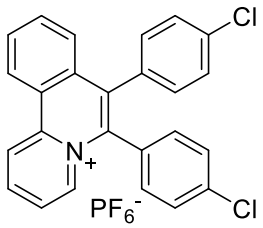
Yellow solid; yield 82%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.81 (d, *J* = 8.7 Hz, 1H), 9.40 (d, *J* = 8.3 Hz, 1H), 8.91 (d, *J* = 6.8 Hz, 1H), 8.74 (t, *J* = 7.9 Hz, 1H), 8.20 – 8.07 (m, 3H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.13 (d, *J* = 8.2 Hz, 2H), 1.24 (s, 9H), 1.23 (s, 9H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 152.29, 150.32, 143.03, 139.80, 138.68, 136.80, 135.67, 134.09, 131.94, 131.45, 130.77, 130.69, 129.65, 128.33, 126.81, 125.99, 125.71, 124.72, 124.68, 124.53, 123.52, 34.48, 34.26, 30.87, 30.77.

HRMS (ESI) calcd for [$C_{33}H_{34}N^+$] (M-PF_6) $^+$:444.2686, found 444.2682

6,7-bis(4-chlorophenyl)pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ag)



3ag

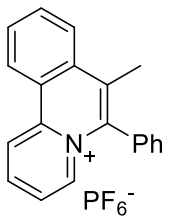
Yellow solid; yield 63%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.80 (d, *J* = 8.4 Hz, 1H), 9.40 (d, *J* = 8.3 Hz, 1H), 8.83 (d, *J* = 6.8 Hz, 1H), 8.75 (t, *J* = 7.7 Hz, 1H), 8.16 (t, *J* = 7.6 Hz, 1H), 8.10 (q, *J* = 7.4, 6.9 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.50 (dd, *J* = 7.8, 6.0 Hz, 3H), 7.30 (d, *J* = 8.3 Hz, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 143.73, 140.76, 137.78, 137.71, 135.59, 134.97, 134.77, 133.75, 133.61, 133.44, 132.27, 132.19, 131.51, 130.44, 130.10, 129.08, 127.22, 126.52, 125.32, 125.13, 123.98.

HRMS (ESI) calcd for [$C_{25}H_{16}Cl_2N^+$] (M-PF_6) $^+$:400.0654, found 400.0656

7-methyl-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ak)



3ak

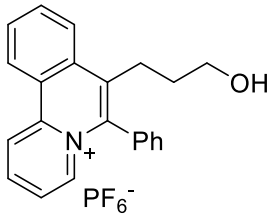
Yellow solid; yield 88%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.65 (d, *J* = 8.5 Hz, 1H), 9.27 (d, *J* = 8.3 Hz, 1H), 8.67 – 8.59 (m, 2H), 8.41 (d, *J* = 8.2 Hz, 1H), 8.21 (t, *J* = 7.6 Hz, 1H), 8.12 (t, *J* = 7.6 Hz, 1H), 8.04 (t, *J* = 6.9 Hz, 1H), 7.80 – 7.73 (m, 3H), 7.61 (d, *J* = 6.7 Hz, 2H), 2.43 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.66, 139.12, 137.36, 136.68, 134.11, 131.78, 131.57, 130.67, 130.35, 130.31, 129.97, 126.00, 125.36, 124.38, 124.17, 123.30, 16.82.

HRMS (ESI) calcd for [$C_{20}H_{16}N^+$] (M-PF_6) $^+$:270.1277, found 270.1279

7-(3-hydroxypropyl)-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3an)



3an

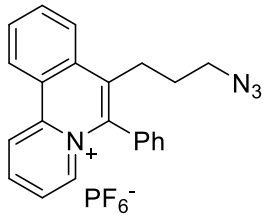
Yellow solid; yield 78%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.71 – 9.61 (m, 1H), 9.29 (d, *J* = 7.6 Hz, 1H), 8.64 – 8.54 (m, 2H), 8.47 (d, *J* = 8.2 Hz, 1H), 8.21 (t, *J* = 7.6 Hz, 1H), 8.11 (t, *J* = 7.5 Hz, 1H), 8.03 (t, *J* = 6.1 Hz, 1H), 7.79 – 7.72 (m, 3H), 7.64 – 7.60 (m, 2H), 3.32 (t, *J* = 6.1 Hz, 2H), 2.86 – 2.77 (m, 2H), 1.70 – 1.66 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.68, 139.10, 137.56, 136.68, 134.11, 133.97, 131.42, 130.80, 130.70, 130.59, 130.26, 130.17, 126.26, 125.23, 124.65, 124.35, 123.28, 60.26, 32.81, 26.65.

HRMS (ESI) calcd for [$C_{22}H_{20}NO^+$] (M-PF_6) $^+$:314.1539, found 314.1546

7-(3-azidopropyl)-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3ao)



3ao

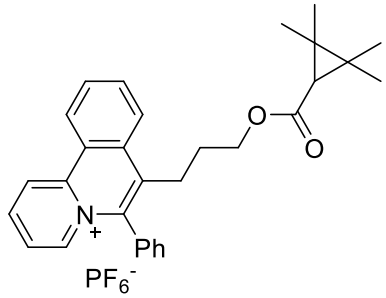
Yellow solid; yield 75%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.72 (d, *J* = 8.6 Hz, 1H), 9.34 (d, *J* = 8.4 Hz, 1H), 8.64 (dd, *J* = 16.2, 7.5 Hz, 2H), 8.50 (d, *J* = 8.3 Hz, 1H), 8.22 (t, *J* = 7.6 Hz, 1H), 8.16 – 8.05 (m, 2H), 7.84 – 7.77 (m, 3H), 7.71 – 7.67 (m, 2H), 3.35 (t, *J* = 6.4 Hz, 2H), 2.97 – 2.84 (m, 2H), 1.85 – 1.77 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.76, 139.28, 137.83, 136.72, 134.16, 133.07, 131.26, 130.78, 130.66, 130.62, 130.31, 130.14, 126.32, 125.18, 124.67, 124.42, 123.34, 50.28, 28.72, 26.90.

HRMS (ESI) calcd for [$C_{22}H_{19}N_4^+$] (M-PF_6) $^+$:339.1604, found 339.1607

6-phenyl-7-(3-((2,2,3,3-tetramethylcyclopropane-1-carbonyl)oxy)propyl)pyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate(3ap)



3ap

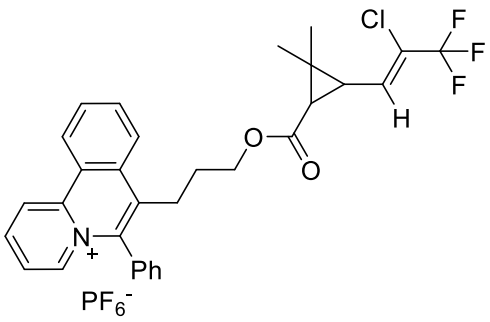
Yellow solid; yield 88%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.66 (d, *J* = 8.6 Hz, 1H), 9.30 (d, *J* = 8.4 Hz, 1H), 8.64 – 8.56 (m, 2H), 8.48 (d, *J* = 8.2 Hz, 1H), 8.21 (t, *J* = 7.6 Hz, 1H), 8.13 (t, *J* = 7.6 Hz, 1H), 8.03 (t, *J* = 7.0 Hz, 1H), 7.79 – 7.72 (m, 3H), 7.65 – 7.61 (m, 2H), 3.91 (t, *J* = 5.9 Hz, 2H), 2.92 – 2.84 (m, 2H), 1.87 – 1.79 (m, 2H), 1.14 (s, 6H), 1.10 (s, 6H), 0.98 (s, 1H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 170.94, 142.76, 139.26, 137.84, 136.76, 134.15, 133.21, 131.33, 130.75, 130.73, 130.67, 130.27, 130.20, 126.31, 125.23, 124.68, 124.40, 123.28, 62.58, 34.56, 29.26, 28.63, 26.39, 23.11, 23.05, 16.29, 16.21.

HRMS (ESI) calcd for [$C_{30}H_{32}NO_2^+$] (M-PF_6) $^+$:438.2428, found 438.2427

(*Z*)-7-(3-((3-(2-chloro-3,3,3-trifluoroprop-1-en-1-yl)-2,2-dimethylcyclopropane-1-carbonyl)oxy)propyl)-6-phenylpyrido[2,1-a]isoquinolin-5-ium hexafluorophosphate (3aq)



3aq

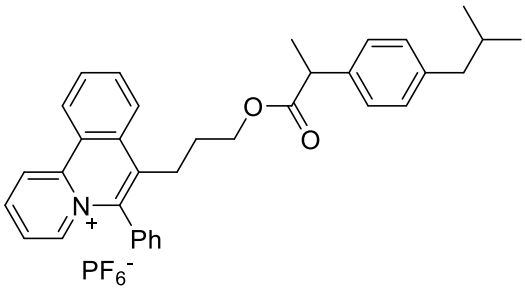
Yellow solid; yield 82%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.65 (d, *J* = 8.7 Hz, 1H), 9.30 (d, *J* = 8.4 Hz, 1H), 8.64 – 8.57 (m, 2H), 8.49 (d, *J* = 8.2 Hz, 1H), 8.21 (t, *J* = 7.6 Hz, 1H), 8.13 (t, *J* = 7.7 Hz, 1H), 8.03 (t, *J* = 7.0 Hz, 1H), 7.79 – 7.71 (m, 3H), 7.64 – 7.59 (m, 2H), 6.90 (d, *J* = 9.5 Hz, 1H), 4.05 – 3.99 (m, 1H), 3.98 – 3.93 (m, 1H), 2.88 (dd, *J* = 9.8, 6.0 Hz, 2H), 2.21 (t, *J* = 8.8 Hz, 1H), 1.92 (d, *J* = 8.3 Hz, 1H), 1.87 – 1.80 (m, 2H), 1.26 (s, 3H), 1.14 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 169.66, 142.77, 139.28, 137.88, 136.80, 134.15, 133.03, 131.82, 131.79, 131.32, 130.71, 130.66, 130.27, 130.17, 126.30, 125.23, 124.68, 124.40, 123.24, 63.58, 32.49, 29.91, 28.71, 28.46, 27.26, 26.16, 14.63.

HRMS (ESI) calcd for [$C_{31}H_{28}ClF_3NO_2^+$] (M-PF_6) $^+$:538.1755, found 538.1761

7-(3-((2-(4-isobutylphenyl)propanoyl)oxy)propyl)-6-phenylpyrido[2,1-a]isoquinolin-5-ium hexafluorophosphate(3ar)



3ar

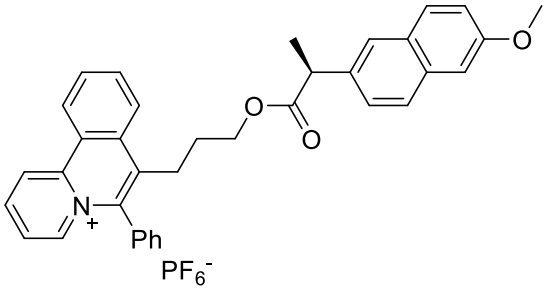
Yellow solid; yield 85%

^{1}H NMR (500 MHz, DMSO-*d6*) δ 9.66 (d, *J* = 8.6 Hz, 1H), 9.30 (d, *J* = 8.2 Hz, 1H), 8.65 – 8.53 (m, 2H), 8.30 (d, *J* = 8.1 Hz, 1H), 8.17 – 8.09 (m, 2H), 8.03 (t, *J* = 7.0 Hz, 1H), 7.80 – 7.74 (m, 3H), 7.63 – 7.58 (m, 2H), 7.10 – 7.06 (m, 4H), 4.02 – 3.96 (m, 1H), 3.96 – 3.91 (m, 1H), 3.55 (q, *J* = 7.1 Hz, 1H), 2.77 (t, *J* = 8.2 Hz, 2H), 2.36 (d, *J* = 7.1 Hz, 2H), 1.80 – 1.72 (m, 3H), 1.27 (d, *J* = 7.1 Hz, 3H), 0.78 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 174.17, 143.25, 140.28, 139.80, 138.32, 138.23, 137.24, 134.64, 133.44, 131.79, 131.30, 131.12, 130.81, 130.62, 129.55, 127.48, 126.82, 125.54, 125.16, 124.91, 123.79, 64.04, 44.62, 30.02, 28.99, 26.77, 22.57, 18.76.

HRMS (ESI) calcd for [$C_{35}H_{36}NO_2^+$] (M-PF_6) $^+$:502.2741, found 502.2738

(*S*)-7-(3-((2-(6-methoxynaphthalen-2-yl)propanoyl)oxy)propyl)-6-phenylpyrido[2,1-a]isoquinolin-5-ium hexafluorophosphate (3as)



3as

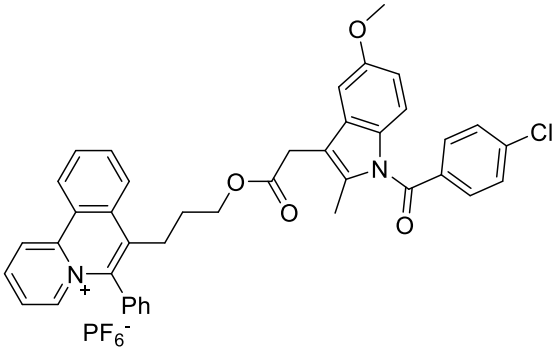
Yellow solid; yield 84%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.63 (d, *J* = 6.9 Hz, 1H), 9.27 (d, *J* = 7.7 Hz, 1H), 8.65 – 8.50 (m, 2H), 8.22 (d, *J* = 8.1 Hz, 1H), 8.07 (t, *J* = 7.4 Hz, 1H), 8.02 (t, *J* = 7.3 Hz, 2H), 7.79 – 7.73 (m, 5H), 7.66 (s, 1H), 7.62 – 7.58 (m, 2H), 7.30 – 7.27 (m, 1H), 7.24 (d, *J* = 2.1 Hz, 1H), 7.11 (dd, *J* = 8.9, 2.4 Hz, 1H), 4.03 – 3.94 (m, 2H), 3.81 (s, 3H), 3.73 (q, *J* = 7.0 Hz, 1H), 2.81 – 2.73 (m, 2H), 1.81 – 1.76 (m, 2H), 1.38 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 173.67, 157.15, 142.72, 139.25, 137.78, 136.68, 135.53, 134.04, 133.28, 132.90, 131.28, 130.80, 130.55, 130.31, 130.29, 130.11, 129.08, 128.33, 126.97, 126.29, 126.13, 125.53, 124.90, 124.63, 124.38, 123.25, 118.74, 105.68, 63.63, 55.12, 44.39, 28.51, 26.30, 18.21.

HRMS (ESI) calcd for [$C_{36}H_{32}NO_3^+$] (M-PF_6) $^+$:526.2377, found 526.2380

7-(3-(2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetoxy)propyl)-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3at)



3at

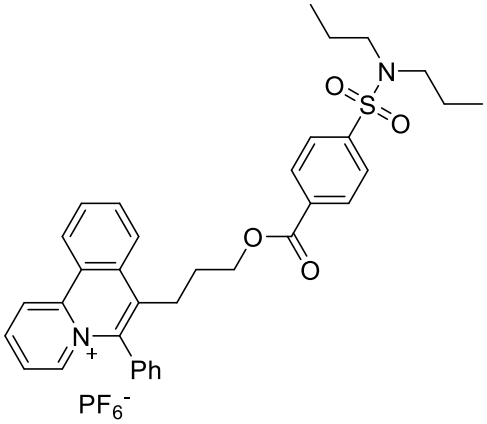
Yellow solid; yield 80%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.65 (d, *J* = 7.6 Hz, 1H), 9.29 (s, 1H), 8.65 – 8.54 (m, 2H), 8.38 – 8.31 (m, 1H), 8.12 (s, 2H), 8.06 – 7.99 (m, 1H), 7.76 (t, *J* = 7.1 Hz, 3H), 7.66 – 7.58 (m, 6H), 6.96 (s, 1H), 6.88 (d, *J* = 8.9 Hz, 1H), 6.71 – 6.65 (m, 1H), 3.99 (t, *J* = 4.5 Hz, 2H), 3.70 (s, 3H), 3.63 (s, 2H), 2.91 – 2.79 (m, 2H), 2.17 (s, 3H), 1.89 – 1.80 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 170.32, 167.80, 155.53, 142.77, 139.30, 137.86, 137.68, 136.78, 135.34, 134.11, 133.97, 132.98, 131.34, 131.11, 130.78, 130.65,

130.41, 130.32, 130.16, 129.04, 126.34, 125.02, 124.69, 124.42, 123.27, 114.59, 112.58, 111.34, 101.59, 63.74, 55.37, 29.25, 28.52, 26.23, 13.21.
HRMS (ESI) calcd for $[C_{41}H_{34}ClN_2O_4^+]$ $(M-PF_6)^+$:653.2202, found 653.2209

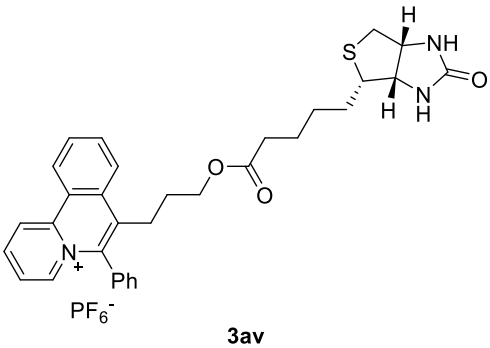
7-(3-((4-(*N*,*N*-dipropylsulfamoyl)benzoyl)oxy)propyl)-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3au)



3au

Yellow solid; yield 78%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.68 (d, *J* = 7.2 Hz, 1H), 9.31 (d, *J* = 7.8 Hz, 1H), 8.66 – 8.53 (m, 3H), 8.21 (t, *J* = 7.5 Hz, 1H), 8.12 (t, *J* = 7.5 Hz, 1H), 8.04 (t, *J* = 6.3 Hz, 1H), 7.95 – 7.84 (m, 4H), 7.70 – 7.61 (m, 4H), 7.52 (t, *J* = 7.3 Hz, 1H), 4.32 (t, *J* = 5.0 Hz, 2H), 3.12 – 3.06 (m, 4H), 3.04 – 2.98 (m, 2H), 2.06 – 1.94 (m, 2H), 1.51 – 1.44 (m, 4H), 0.82 (t, *J* = 7.3 Hz, 6H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 164.81, 144.12, 143.28, 139.82, 138.34, 137.23, 134.66, 133.52, 133.27, 131.84, 131.21, 131.17, 130.94, 130.71, 130.65, 130.52, 127.46, 126.84, 125.82, 125.19, 124.92, 123.83, 65.17, 50.02, 29.00, 26.99, 22.02, 11.42.

7-(3-((5-((3a*R*,4*R*,6a*S*)-2-oxohexahydro-1H-thieno[3,4-*d*]imidazol-4-yl)pentanoyl)oxy)propyl)-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (3av)



3av

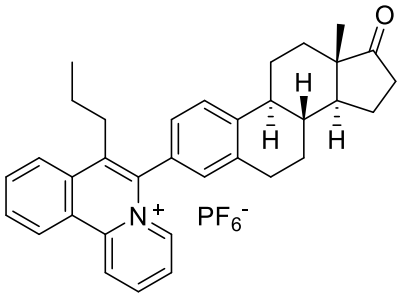
Yellow solid; yield 61%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.65 (d, *J* = 8.2 Hz, 1H), 9.29 (d, *J* = 8.0 Hz, 1H), 8.65 – 8.54 (m, 2H), 8.48 (d, *J* = 7.9 Hz, 1H), 8.20 (t, *J* = 7.1 Hz, 1H), 8.12 (t, *J* = 7.1 Hz, 1H), 8.03 (t, *J* = 6.3 Hz, 1H), 7.76 (s, 3H), 7.62 (d, *J* = 5.7 Hz, 2H), 6.44 (d, *J* =

36.5 Hz, 2H), 4.30 (s, 1H), 4.13 (s, 1H), 3.98 (s, 2H), 3.09 (s, 1H), 2.90 – 2.77 (m, 3H), 2.57 (d, *J* = 12.2 Hz, 1H), 2.09 (t, *J* = 6.7 Hz, 2H), 1.83 (s, 2H), 1.63 – 1.57 (m, 1H), 1.46 – 1.38 (m, 3H), 1.28 (s, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 172.58, 162.77, 142.78, 139.29, 137.84, 136.76, 134.20, 133.16, 131.33, 130.74, 130.69, 130.31, 130.19, 126.32, 125.25, 124.69, 124.42, 123.31, 62.99, 61.08, 59.23, 55.38, 54.89, 33.19, 28.63, 28.04, 28.01, 26.35, 24.36.

HRMS (ESI) calcd for [$C_{32}H_{34}N_3O_3S^+$] (M-PF_6) $^+$:540.2315, found 540.2317

6-((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl)-7-propylpyrido[2,1-a]isoquinolin-5-ium hexafluorophosphate (3aw)



3aw

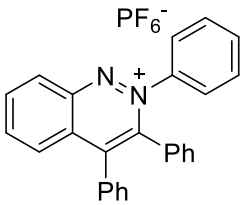
Yellow solid; yield 73%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.64 (d, 1H), 9.28 (d, *J* = 7.5 Hz, 1H), 8.74 – 8.52 (m, 2H), 8.42 (d, *J* = 8.1 Hz, 1H), 8.19 (t, *J* = 7.4 Hz, 1H), 8.13 – 8.03 (m, 2H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.40 – 7.29 (m, 2H), 2.96 (s, 2H), 2.88 – 2.68 (m, 2H), 2.46 – 2.39 (m, 2H), 2.13 – 1.93 (m, 4H), 1.82 (d, *J* = 11.8 Hz, 1H), 1.68 (s, 1H), 1.65 – 1.43 (m, 7H), 0.91 – 0.83 (m, 6H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 142.65, 142.62, 142.17, 142.12, 139.06, 138.40, 137.70, 137.64, 136.70, 134.04, 133.89, 130.79, 130.51, 130.14, 128.70, 128.67, 127.27, 127.03, 126.98, 126.23, 126.16, 125.33, 124.52, 124.38, 124.33, 123.31, 123.20, 94.71, 49.65, 49.61, 47.23, 47.20, 44.01, 43.81, 37.32, 37.28, 35.28, 31.58, 31.53, 31.30, 31.26, 28.85, 28.81, 25.74, 25.10, 25.00, 23.19, 23.16, 21.07, 14.14, 14.10, 13.51, 13.46.

HRMS (ESI) calcd for [$C_{34}H_{36}NO^+$] (M-PF_6) $^+$:474.2791, found 474.2787

2,3,4-triphenylcinnolin-2-ium hexafluorophosphate (5aa)

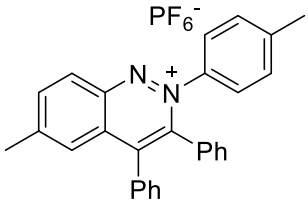


5aa

Brown solid; yield 88%

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.4 Hz, 1H), 8.03 – 7.92 (m, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 2H), 7.31 – 7.20 (m, 8H), 7.15 – 7.10 (m, 2H), 7.06 (t, *J* = 7.4 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 2H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 149.93, 136.76, 133.59, 129.13, 129.00, 128.81, 128.73, 128.18, 127.84, 127.40, 126.92, 126.78, 126.47, 124.53.
HRMS (ESI) calcd for $[C_{26}H_{19}N_2^+]$ $(M\text{-}PF_6)^+$:359.1543, found 359.1542

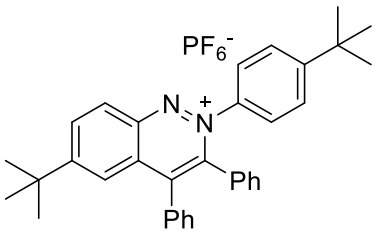
6-methyl-3,4-diphenyl-2-(*p*-tolyl)cinnolin-2-ium hexafluorophosphate (5ba)



5ba

Brown solid; yield 84%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.64 (d, *J* = 8.9 Hz, 1H), 8.24 (d, *J* = 8.9 Hz, 1H), 7.53 (s, 1H), 7.46 (d, *J* = 7.9 Hz, 2H), 7.36 (d, *J* = 5.5 Hz, 3H), 7.25 (dd, *J* = 12.3, 7.1 Hz, 4H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 6.6 Hz, 3H), 2.60 (s, 3H), 2.21 (s, 3H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 151.84, 151.73, 146.62, 145.79, 142.46, 140.49, 138.67, 131.38, 130.60, 130.47, 130.08, 129.71, 129.62, 129.52, 129.42, 129.33, 128.47, 127.73, 126.07, 123.54, 22.76, 20.63.
HRMS (ESI) calcd for $[C_{28}H_{23}N_2^+]$ $(M\text{-}PF_6)^+$:387.1856, found 387.1858

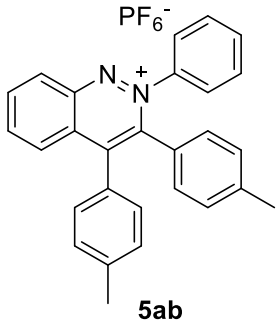
6-(tert-butyl)-2-(4-(tert-butyl)phenyl)-3,4-diphenylcinnolin-2-ium hexafluorophosphate (5ca)



5ca

Brown solid; yield 86%
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.76 (dd, *J* = 9.2, 1.9 Hz, 1H), 8.68 – 8.62 (m, 1H), 7.65 (s, 1H), 7.57 (dd, *J* = 8.7, 2.1 Hz, 2H), 7.52 – 7.49 (m, 2H), 7.48 – 7.44 (m, 3H), 7.37 – 7.33 (m, 4H), 7.21 – 7.15 (m, 3H), 1.35 (d, *J* = 2.0 Hz, 9H), 1.24 (d, *J* = 2.0 Hz, 9H).
^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 162.84, 153.40, 151.87, 146.67, 146.60, 142.37, 135.60, 131.27, 130.61, 130.38, 130.02, 129.71, 129.62, 129.54, 128.47, 127.73, 125.90, 125.74, 119.29, 36.47, 34.63, 30.76, 29.63.
HRMS (ESI) calcd for $[C_{34}H_{35}N_2^+]$ $(M\text{-}PF_6)^+$:471.2795, found 471.2796

2-phenyl-3,4-di-p-tolylcinnolin-2-ium hexafluorophosphate (5ab)



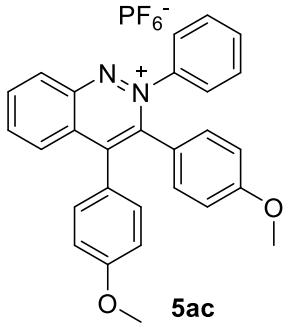
Yellow solid; yield 83%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.82 (d, *J* = 8.6 Hz, 1H), 8.49 – 8.43 (m, 1H), 8.38 (t, *J* = 7.6 Hz, 1H), 7.89 (d, *J* = 8.6 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.53 – 7.48 (m, 3H), 7.29 (d, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 7.3 Hz, 4H), 7.00 (d, *J* = 7.8 Hz, 2H), 2.33 (s, 3H), 2.14 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 152.28, 147.70, 147.55, 144.92, 139.42, 139.23, 139.05, 136.09, 130.60, 130.57, 130.22, 129.85, 129.56, 129.13, 129.03, 128.42, 127.43, 126.15, 125.79, 20.84, 20.75.

HRMS (ESI) calcd for [$C_{28}H_{23}N_2^+$] (M-PF_6) $^+$:387.1856, found 387.1855

3,4-bis(4-methoxyphenyl)-2-phenylcinnolin-2-ium hexafluorophosphate (5ac)



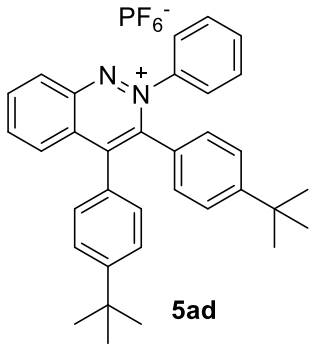
Yellow solid; yield 86%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.78 (d, *J* = 8.6 Hz, 1H), 8.43 (t, *J* = 7.6 Hz, 1H), 8.36 (t, *J* = 7.6 Hz, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.50 (s, 3H), 7.27 – 7.20 (m, 4H), 7.04 (d, *J* = 8.5 Hz, 2H), 6.75 (d, *J* = 8.6 Hz, 2H), 3.78 (s, 3H), 3.63 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 159.93, 159.74, 152.45, 147.82, 147.55, 145.08, 138.81, 135.96, 132.33, 131.33, 130.48, 130.29, 129.78, 129.06, 126.11, 125.85, 123.30, 122.36, 114.12, 113.37, 55.24, 55.09.

HRMS (ESI) calcd for [$C_{28}H_{23}N_2O_2^+$] (M-PF_6) $^+$:419.1754, found 419.1757

3,4-bis(4-(tert-butyl)phenyl)-2-phenylcinnolin-2-ium hexafluorophosphate (5ad)



5ad

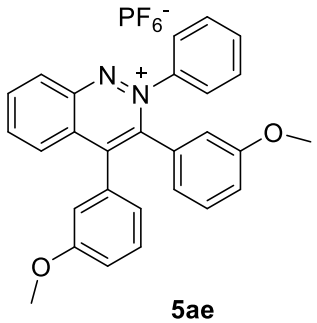
Yellow solid; yield 84%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.81 (d, *J* = 8.6 Hz, 1H), 8.45 (t, *J* = 7.6 Hz, 1H), 8.38 (t, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.68 (dd, *J* = 6.3, 2.9 Hz, 2H), 7.51 – 7.46 (m, 3H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 8.3 Hz, 4H), 7.15 (d, *J* = 8.4 Hz, 2H), 1.23 (s, 9H), 1.08 (s, 9H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 152.55, 152.33, 152.02, 147.98, 147.64, 144.89, 139.01, 136.10, 130.60, 130.49, 129.91, 129.82, 129.44, 129.01, 128.49, 127.51, 126.20, 125.80, 125.07, 124.39, 34.44, 34.34, 30.78, 30.59.

HRMS (ESI) calcd for [$C_{34}H_{35}N_2^+$] $(M\text{-}PF_6)^+$:471.2795, found 471.2793

3,4-bis(3-methoxyphenyl)-2-phenylcinnolin-2-ium hexafluorophosphate (5ae)



5ae

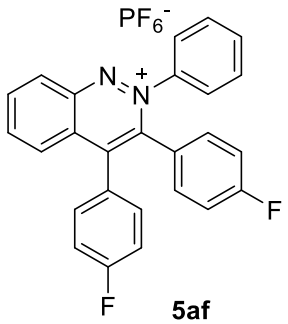
Yellow solid; yield 83%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.84 (d, *J* = 8.7 Hz, 1H), 8.47 (t, *J* = 7.6 Hz, 1H), 8.40 (t, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.73 – 7.67 (m, 2H), 7.55 – 7.48 (m, 3H), 7.41 (q, *J* = 8.3 Hz, 1H), 7.14 – 6.88 (m, 6H), 6.77 (d, *J* = 7.0 Hz, 1H), 3.68 (s, 3H), 3.54 (d, *J* = 7.7 Hz, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 159.31, 158.72, 158.69, 152.11, 148.22, 147.65, 145.26, 139.81, 136.78, 132.96, 131.76, 131.24, 130.56, 130.38, 130.35, 129.66, 129.60, 129.55, 126.66, 126.32, 123.61, 123.55, 122.41, 117.07, 117.06, 116.12, 116.01, 115.83, 115.76, 115.74, 115.65, 55.64, 55.59, 55.56.

HRMS (ESI) calcd for [$C_{28}H_{23}N_2O_2^+$] $(M\text{-}PF_6)^+$:419.1754, found 419.1755

3,4-bis(4-fluorophenyl)-2-phenylcinnolin-2-ium hexafluorophosphate (5af)



5af

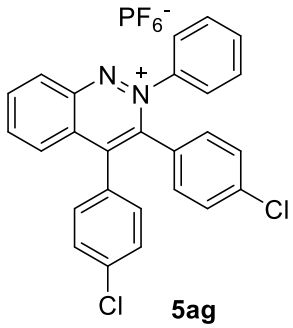
Yellow solid; yield 82%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.88 (d, *J* = 8.7 Hz, 1H), 8.55 – 8.40 (m, 2H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.66 (s, 2H), 7.54 (s, 3H), 7.45 – 7.34 (m, 6H), 7.10 (t, *J* = 8.5 Hz, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 163.50, 163.29, 161.53, 161.30, 151.45, 147.67, 146.89, 144.64, 139.56, 136.48, 133.26, 133.19, 132.05, 131.98, 130.83, 130.11, 129.99, 129.24, 127.49, 127.46, 126.65, 126.62, 126.13, 125.71, 116.02, 115.84, 115.37, 115.19.

HRMS (ESI) calcd for $[C_{26}H_{17}F_2N_2^+]$ $(M\text{-}PF_6)^+$:395.1354, found 395.1360

3,4-bis(4-chlorophenyl)-2-phenylcinnolin-2-ium hexafluorophosphate (3ag)



5ag

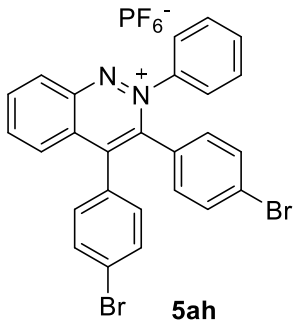
Yellow solid; yield 76%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.89 (d, *J* = 8.6 Hz, 1H), 8.51 (t, *J* = 7.5 Hz, 1H), 8.44 (t, *J* = 7.6 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.69 – 7.64 (m, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.57 – 7.53 (m, 3H), 7.40 – 7.33 (m, 6H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 150.95, 147.68, 146.45, 144.50, 139.73, 136.59, 134.99, 134.78, 132.46, 131.42, 130.96, 130.05, 129.93, 129.89, 129.30, 128.98, 128.92, 128.25, 126.13, 125.69.

HRMS (ESI) calcd for $[C_{26}H_{17}Cl_2N_2^+]$ $(M\text{-}PF_6)^+$:427.0763, found 427.0766

3,4-bis(4-bromophenyl)-2-phenylcinnolin-2-ium hexafluorophosphate (3ah)



5ah

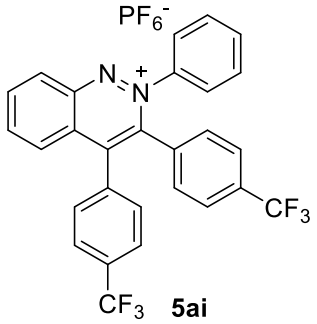
Yellow solid; yield 65%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.88 (d, *J* = 8.5 Hz, 1H), 8.49 (t, *J* = 7.7 Hz, 1H), 8.42 (t, *J* = 7.4 Hz, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.68 (d, *J* = 5.2 Hz, 2H), 7.54 (d, *J* = 5.1 Hz, 3H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.32 (dd, *J* = 10.8, 8.5 Hz, 4H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 151.35, 148.24, 146.90, 145.03, 140.21, 137.04, 133.13, 132.34, 132.12, 131.70, 131.46, 130.80, 130.58, 130.43, 129.86, 129.80, 126.66, 126.20, 124.48, 124.12.

HRMS (ESI) calcd for [$C_{26}H_{17}Br_2N_2^+$] (M-PF_6) $^+$:514.9753, found 514.9751

2-phenyl-3,4-bis(4-(trifluoromethyl)phenyl)cinnolin-2-ium hexafluorophosphate (5ai)



5ai

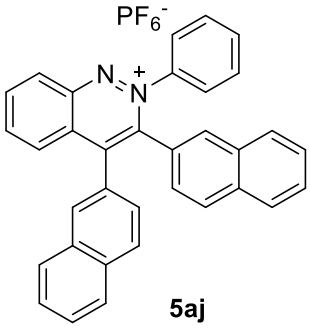
Yellow solid; yield 71%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.93 (d, *J* = 8.7 Hz, 1H), 8.54 (t, *J* = 7.7 Hz, 1H), 8.46 (t, *J* = 7.7 Hz, 1H), 7.93 (d, *J* = 8.6 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 2H), 7.70 – 7.65 (m, 2H), 7.62 (s, 4H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.55 – 7.51 (m, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 150.39, 147.81, 145.98, 144.27, 140.11, 136.82, 135.10, 134.05, 131.68, 131.11, 130.55, 130.27, 130.22, 130.19, 130.02, 129.96, 129.76, 129.33, 126.91, 126.57, 126.18, 125.68, 125.64, 124.98, 124.95, 124.75, 124.40, 122.58, 122.23, 120.41, 120.07.

HRMS (ESI) calcd for [$C_{28}H_{17}F_6N_2^+$] (M-PF_6) $^+$:495.1290, found 495.1288

3,4-di(naphthalen-2-yl)-2-phenylcinnolin-2-ium hexafluorophosphate (5aj)



5aj

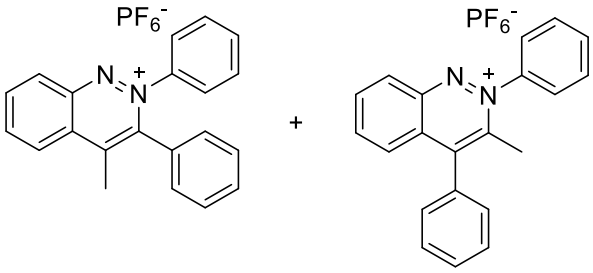
Yellow solid; yield 60%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.92 (d, *J* = 8.7 Hz, 1H), 8.55 – 8.48 (m, 1H), 8.44 – 8.37 (m, 1H), 8.04 – 7.87 (m, 6H), 7.77 (d, *J* = 7.9 Hz, 2H), 7.74 – 7.68 (m, 2H), 7.64 (t, *J* = 8.7 Hz, 1H), 7.59 – 7.50 (m, 3H), 7.48 – 7.39 (m, 6H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 152.05, 147.76, 147.61, 144.78, 139.45, 136.35, 132.57, 132.29, 131.83, 131.42, 131.25, 131.11, 130.69, 130.25, 130.01, 129.89, 129.59, 129.08, 128.75, 128.21, 128.13, 128.06, 127.88, 127.71, 127.64, 127.58, 127.47, 127.18, 127.09, 126.78, 126.33, 126.20, 126.03, 125.99.

HRMS (ESI) calcd for [$C_{34}H_{23}N_2^+$] (M-PF_6) $^+$:459.1856, found 459.1861

4-methyl-2,3-diphenylcinnolin-2-ium hexafluorophosphate and 3-methyl-2,4-diphenylcinnolin-2-ium hexafluorophosphate(5ak + 5ak' (1:0.18))



5ak (1:0.17) **5ak'**

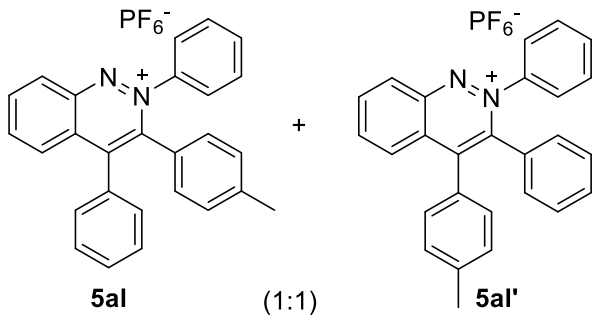
Yellow solid; yield 83%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.72 (dd, *J* = 8.1, 6.0 Hz, 2H), 8.48 (t, *J* = 7.3 Hz, 1H), 8.43 (t, 1H), 7.63 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.51 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.47 – 7.42 (m, 6H), 2.76 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 152.48, 151.44, 147.24, 146.62, 145.87, 144.79, 144.05, 138.73, 138.44, 136.05, 135.55, 131.50, 130.55, 130.35, 130.16, 130.11, 129.94, 129.36, 129.18, 128.92, 128.67, 126.13, 125.28, 125.12, 124.86, 20.50, 16.36.

HRMS (ESI) calcd for [$C_{21}H_{17}N_2^+$] (M-PF_6) $^+$:297.1386, found 297.1391

2,4-diphenyl-3-(p-tolyl)cinnolin-2-ium hexafluorophosphate and 2,3-diphenyl-4-(p-tolyl)cinnolin-2-ium hexafluorophosphate (5al + 5al' (1:1))



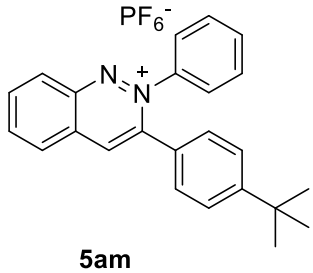
Yellow solid; yield 85%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.83 (d, *J* = 8.5 Hz, 2H), 8.46 (t, *J* = 7.6 Hz, 2H), 8.39 (t, *J* = 7.5 Hz, 2H), 7.90 (dd, *J* = 27.9, 8.6 Hz, 2H), 7.67 (dd, *J* = 6.3, 2.6 Hz, 4H), 7.54 – 7.43 (m, 10H), 7.34 (t, *J* = 8.0 Hz, 4H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.3 Hz, 4H), 7.18 (d, *J* = 6.2 Hz, 2H), 6.98 (d, *J* = 7.9 Hz, 2H), 2.30 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 152.25, 152.09, 147.75, 147.71, 147.63, 144.95, 144.87, 139.51, 139.31, 139.13, 139.08, 136.10, 131.42, 130.70, 130.62, 130.39, 130.33, 130.22, 129.93, 129.85, 129.64, 129.58, 129.12, 129.04, 128.52, 128.44, 128.38, 127.84, 127.42, 126.22, 125.84, 125.73, 20.84, 20.74.

HRMS (ESI) calcd for [$C_{27}H_{21}N_2^+$] (M-PF_6) $^+$:373.1699, found 373.1702

3-(4-(tert-butyl)phenyl)-2-phenylcinnolin-2-ium hexafluorophosphate (5am)



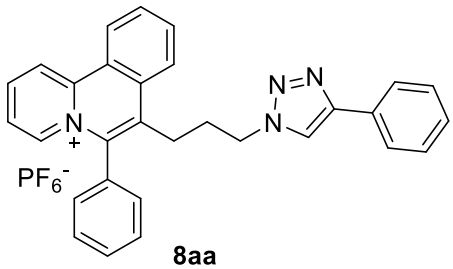
Yellow solid; yield 75%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.41 (s, 1H), 8.80 (d, *J* = 8.7 Hz, 1H), 8.49 – 8.39 (m, 3H), 8.37 – 8.31 (m, 2H), 7.91 (d, *J* = 7.9 Hz, 2H), 7.84 (s, 5H), 1.45 (s, 9H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 154.11, 148.97, 146.76, 144.44, 139.36, 138.79, 135.96, 132.24, 130.62, 130.31, 130.05, 128.41, 127.90, 126.31, 125.20, 124.67, 34.80, 30.93.

HRMS (ESI) calcd for [$C_{24}H_{23}N_2^+$] (M-PF_6) $^+$:339.1856, found 339.1859

6-phenyl-7-(3-(4-phenyl-1H-1,2,3-triazol-1-yl)propyl)pyrido[2,1-a]isoquinolin-5-ium hexafluorophosphate (8aa)



8aa

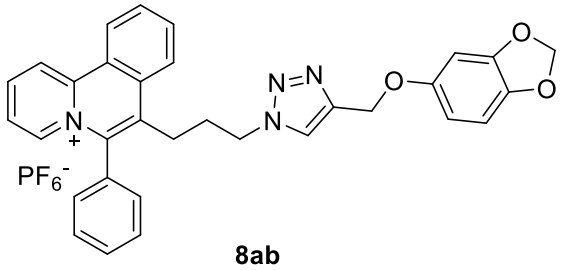
Yellow solid; yield 74%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.62 (d, *J* = 8.7 Hz, 1H), 9.28 (d, *J* = 8.4 Hz, 1H), 8.60 (t, *J* = 7.9 Hz, 1H), 8.49 (dd, *J* = 17.6, 7.6 Hz, 2H), 8.33 (s, 1H), 8.20 (t, *J* = 7.6 Hz, 1H), 8.12 (t, *J* = 7.7 Hz, 1H), 8.00 (t, *J* = 7.0 Hz, 1H), 7.79 (d, *J* = 7.3 Hz, 2H), 7.56 (t, *J* = 7.7 Hz, 2H), 7.52 – 7.45 (m, 4H), 7.37 – 7.30 (m, 2H), 4.42 (t, *J* = 6.3 Hz, 2H), 2.85 – 2.70 (m, 2H), 2.19 – 2.05 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 146.34, 142.77, 139.31, 137.89, 136.75, 134.19, 132.65, 130.92, 130.84, 130.70, 130.45, 130.14, 129.82, 128.82, 127.76, 126.33, 125.23, 125.15, 124.68, 124.40, 123.29, 121.05, 49.14, 29.86, 26.82.

HRMS (ESI) calcd for [$C_{30}H_{25}N_4^+$] (M-PF_6) $^+$:441.2074, found 441.2065

7-(3-(4-((benzo[d][1,3]dioxol-5-yloxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (8ab)



8ab

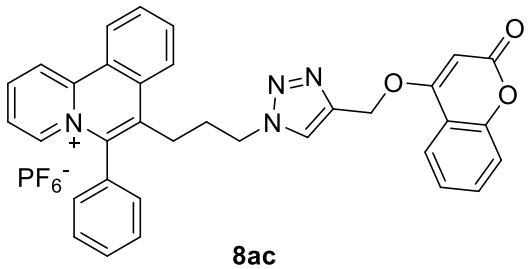
Yellow solid; yield 68%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.66 – 9.59 (m, 1H), 9.28 (d, *J* = 8.3 Hz, 1H), 8.64 – 8.50 (m, 2H), 8.39 (d, *J* = 8.2 Hz, 1H), 8.22 – 8.07 (m, 2H), 8.01 (t, *J* = 7.0 Hz, 1H), 7.98 (s, 1H), 7.73 – 7.64 (m, 3H), 7.52 (dd, *J* = 6.3, 2.7 Hz, 2H), 6.80 (d, *J* = 8.5 Hz, 1H), 6.72 (d, *J* = 2.4 Hz, 1H), 6.47 (dd, *J* = 8.5, 2.5 Hz, 1H), 5.94 (s, 2H), 5.00 (s, 2H), 4.38 (t, *J* = 6.3 Hz, 2H), 2.80 – 2.69 (m, 2H), 2.11 – 2.02 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 153.39, 147.86, 142.77, 142.66, 141.27, 139.29, 137.87, 136.72, 134.15, 132.62, 130.98, 130.67, 130.64, 130.30, 129.86, 126.29, 125.08, 124.65, 124.39, 124.07, 123.26, 107.98, 106.06, 101.00, 97.93, 61.82, 48.96, 29.82, 26.75.

HRMS (ESI) calcd for [$C_{32}H_{27}N_4O_3^+$] (M-PF_6) $^+$:515.2078, found 515.2076

7-(3-(4-(((2-oxo-2H-chromen-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)propyl)-6-phenylpyrido[2,1-*a*]isoquinolin-5-ium hexafluorophosphate (8ac)



8ac

Yellow solid; yield 65%

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.62 (d, *J* = 8.5 Hz, 1H), 9.28 (d, *J* = 8.3 Hz, 1H), 8.61 (t, *J* = 7.8 Hz, 1H), 8.53 (d, *J* = 6.7 Hz, 1H), 8.42 (d, *J* = 8.1 Hz, 1H), 8.21 – 8.15 (m, 2H), 8.11 (t, *J* = 7.6 Hz, 1H), 8.01 (t, *J* = 6.8 Hz, 1H), 7.74 – 7.70 (m, 1H), 7.69 – 7.65 (m, 3H), 7.64 – 7.61 (m, 1H), 7.53 (dd, *J* = 6.1, 2.8 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H), 6.20 (s, 1H), 5.38 (s, 2H), 4.43 (t, *J* = 6.2 Hz, 2H), 2.82 – 2.72 (m, 2H), 2.14 – 2.05 (m, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 164.27, 161.52, 152.74, 142.77, 140.89, 139.32, 137.91, 136.77, 134.18, 132.81, 132.58, 131.00, 130.67, 130.29, 129.86, 126.30, 125.10, 124.83, 124.67, 124.41, 124.16, 123.23, 122.77, 116.47, 115.05, 99.51, 91.38, 62.78, 49.11, 29.82, 26.77.

HRMS (ESI) calcd for [$C_{34}H_{27}N_4O_3^+$] $(M-PF_6)^+$:539.2078, found 539.2081

13. References

[1] Zhang, S.-S.; Jiang, C.-Y.; W, J.-Q.; Liu, X.-G.; Li, Q.-j.; Huang, Z.-S.; D. Li, Wang, H.-g. Cp*Rh(III) and Cp*Ir(III)-Catalysed Redox-Neutral C–H Arylation with Quinone Diazides: Quick and Facile Synthesis of Arylated Phenols. *Chem. Commun*. **2015**, *51*, 10240-10243.

[2] Zhang, C.; Jiao, N. Copper-Catalyzed Aerobic Oxidative Dehydrogenative Coupling of Anilines Leading to Aromatic Azo Compounds using Dioxygen as an Oxidant. *Angew. Chem. Int. Ed*. **2010**, *49*, 6174-6177.

[3] Verma, A. K.; Singh, J.; Sankar, V. K.; Chaudhary, R.; Chandra, R. Benzotriazole: an Excellent Ligand for Cu-Catalyzed N-arylation of Imidazoles with Aryl and Heteroaryl halides. *Tetrahedron Lett*. **2007**, *48*, 4207-4210.

[4] Fujita, K.; Takahashi, Y.; Owaki, M.; Yamamoto, K.; Yamaguchi, R. Synthesis of Five-, Six-, and Seven-Membered Ring Lactams by Cp*Rh Complex-Catalyzed Oxidative N-Heterocyclization of Amino Alcohols. *Org. Lett*. **2004**, *6*, *16*, 2785-2788.

[5] Chuentragool, P.; Vongnamb, K.; Rashatasakhon, P.; Sukwattanasinitt, M.; Wacharasindhu, S. Calcium Carbide as a Cost-Effective Starting Material for Symmetrical Diarylethynes via Pd-Catalyzed Coupling Reaction. *Tetrahedron*. **2011**, *67*, 8177-8182.

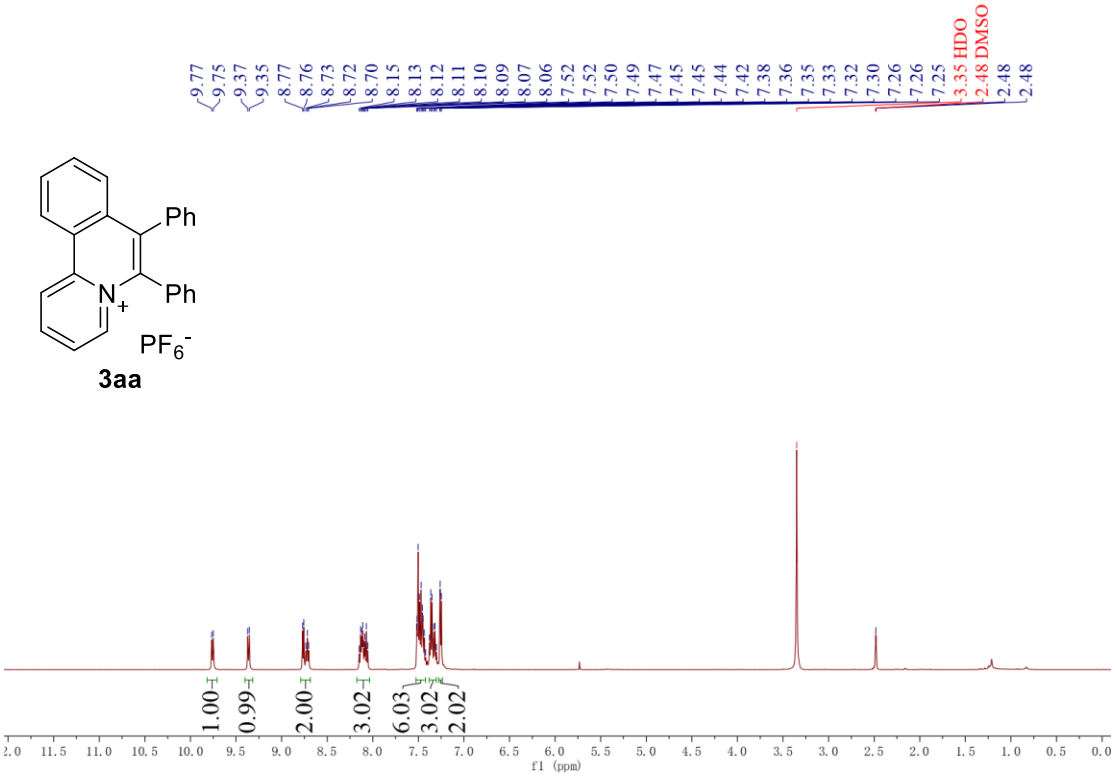
[6] Zhang,L.-B.; Geng, R.-S.; Wang, Z.-C.; Ren, G.-Y.; Wen, L.-R.; Li, M. Electrochemical intramolecular C–H/N–H functionalization for the synthesis of isoxazolidine-fused isoquinolin-1(2H)-ones. *Green Chem*. **2020**, *22*, 16-21.

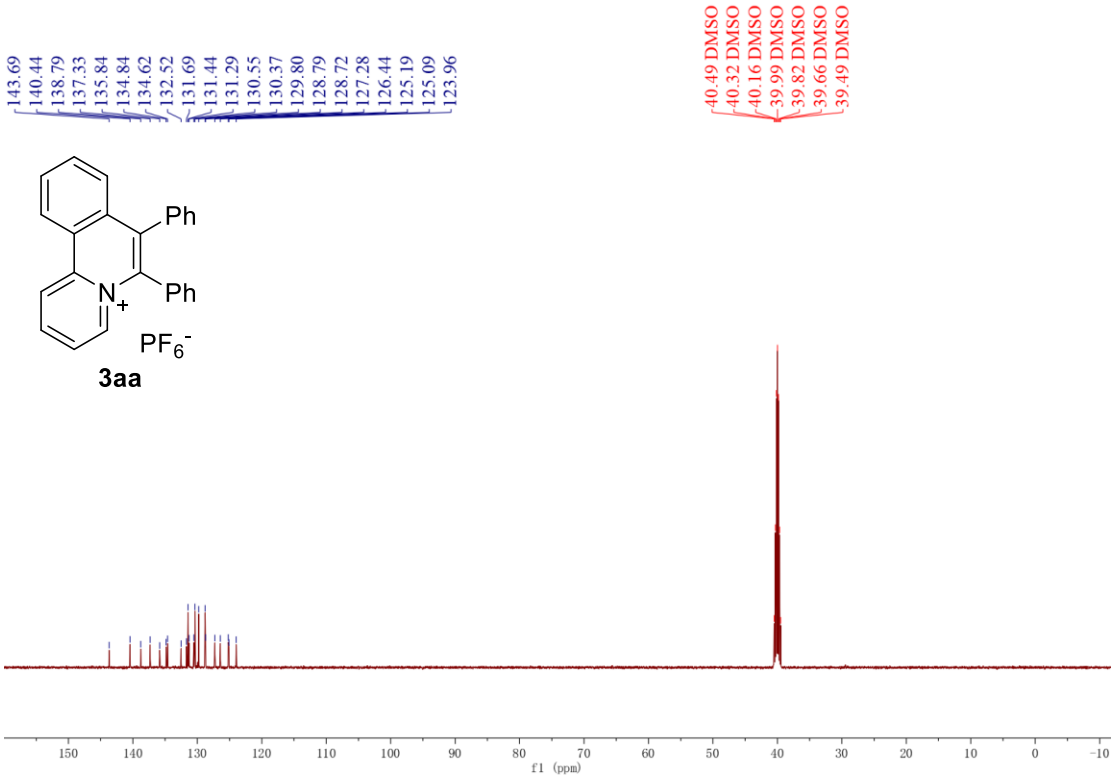
[7] Su, X.; Sun, Y.; Yao,J.; Chen, H.; Chen, C. Acid-Promoted Bicyclization of Arylacetylenes to Benzobicyclo[3.2.1]octanes through Cationic Rearrangements. *Chem. Commun*. **2016**, *52*, 4537-4540.

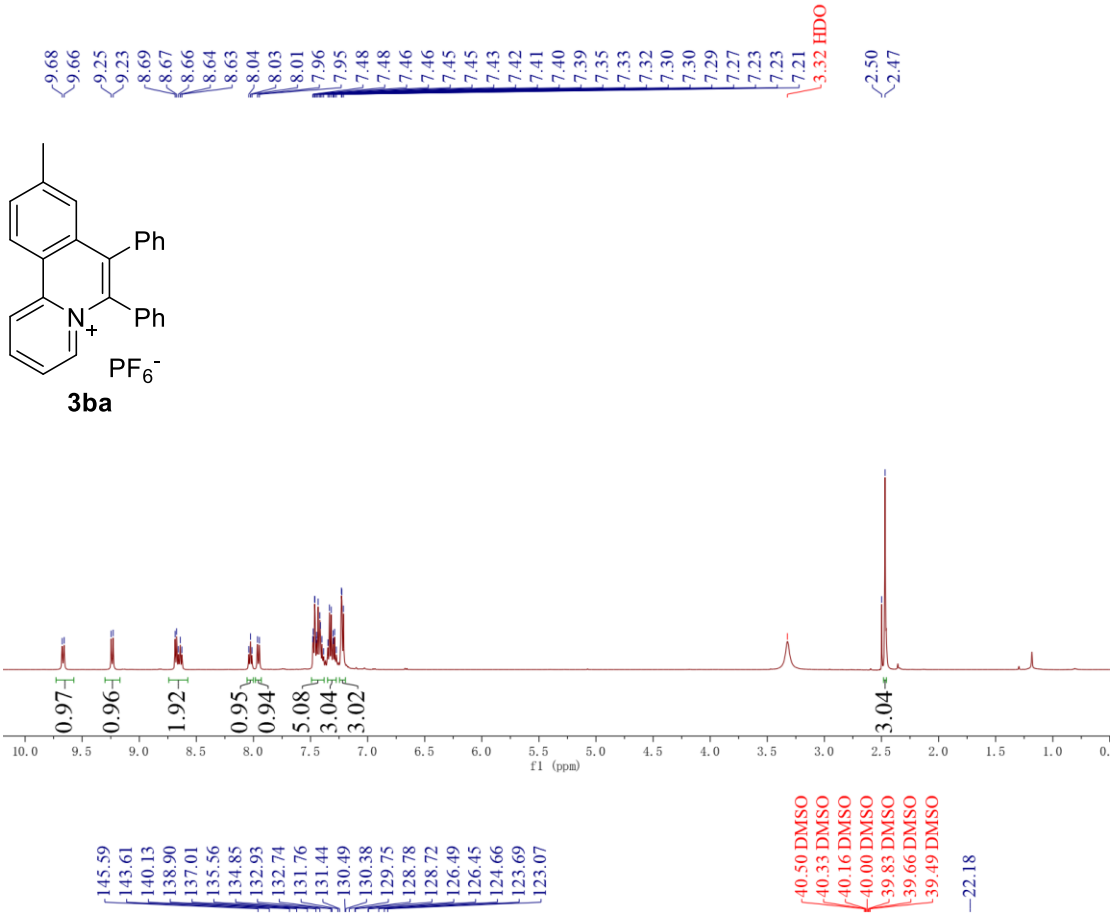
[8] Hiroya, K.; Matsumoto, S.; Ashikawa, M.; Ogiwara, K.; Sakamoto, T. Cyclization Reactions of

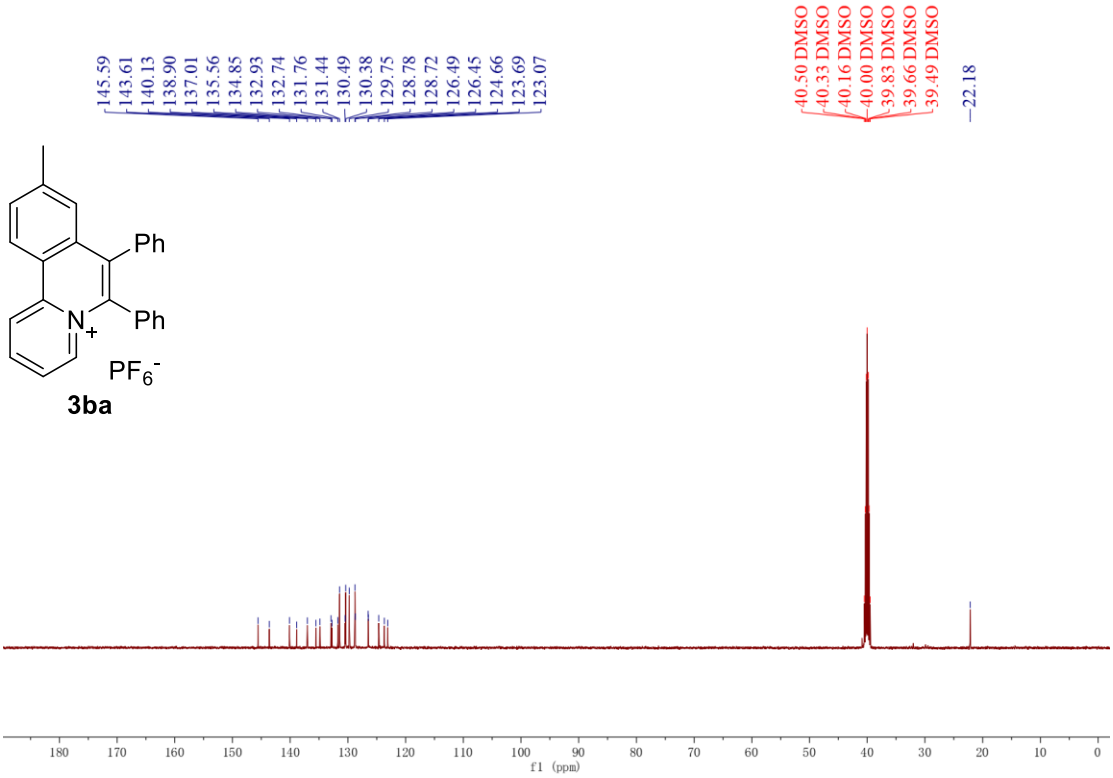
Homopropargyl Azide Derivatives Catalyzed by PtCl4 in Ethanol Solution: Synthesis of Functionalized Pyrrole Derivatives. *Org. Lett.* **2006**, 8, 5349–5352.
[9] Ashooriha, M.; Khoshneviszadeh, M.; Khoshneviszadeh, M.; Rafiei, A.; Kardan, M.; Yazdian-Robati, R.; Emami, Saeed. Kojic Acid–Natural Product Conjugates as Mushroom Tyrosinase Inhibitors. *European Journal of Medicinal Chemistry*, Volume 201, **2020**, 112480.
[10] Zhang, Z.; Luo, Y.; Du, H.; Xu, J.; Li, P. Synthesis of α-Heterosubstituted Ketones through Sulfur Mediated Difunctionalization of Internal Alkynes. *Chem. Sci.* **2019**, *10*, 5156-5161.
[11] Luo, C.-Z.; Gandeepan, P.; Jayakumar, J.; Parthasarathy, K.; Chang, Y.-W.; Cheng, C.-H. RhIII-Catalyzed C-H Activation: A Versatile Route towards Various Polycyclic Pyridinium Salts. Cheng, *Chem. - Eur. J.* **2013**, *19*, 14181-14186.
[12] Li, H.; Zhang, S.; Yu, X.; Feng,X.; Yamamoto, Y.; Bao, M. Rhodium(III)-Catalyzed Aromatic C–H Cyanation with Dimethylmalononitrile as a Cyanating Agent. *Chem. Commun.* **2019**, *55*, 1209-1212.
[13] Zhang, G.; Yang, L.; Wang, Y.; Xie, Y.; Huang, H. An Efficient Rh/O_2 Catalytic System for Oxidative C–H Activation/Annulation: Evidence for Rh(I) to Rh(III) Oxidation by Molecular Oxygen. *J. Am. Chem. Soc.* **2013**, *135*, 8850-8853.
[14] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.
[15] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B.* **2009**, *113*, 6378-6396.
[16] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, **2009** (http://www.cylview.org)
[17] T. Lu, F. W. Chen, *J. Comput. Chem.*, **2012**, *33*, 580-592.

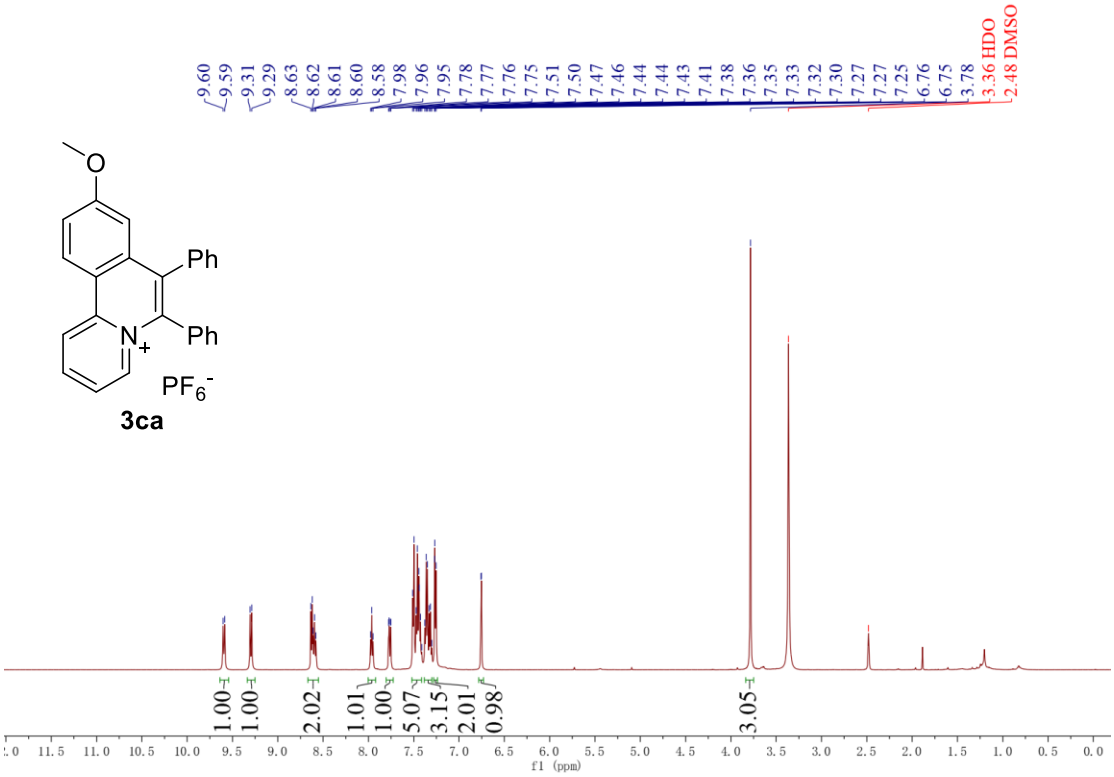
14 . ^{1}H NMR and ^{13}C NMR spectra of compounds 3, 5 and 8

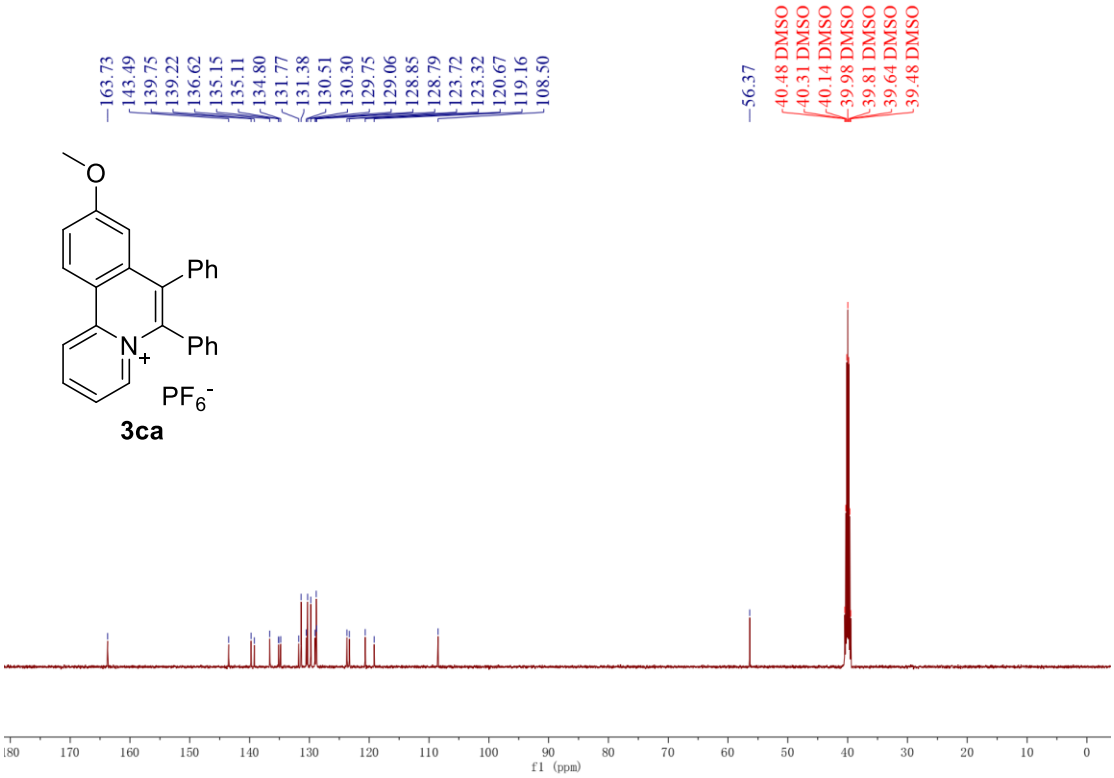

9.77
9.75
9.37
9.35
8.77
8.76
8.73
8.72
8.70
8.15
8.13
8.12
8.11
8.10
8.09
8.07
8.06
7.52
7.52
7.50
7.49
7.47
7.45
7.45
7.44
7.42
7.38
7.36
7.35
7.33
7.32
7.30
7.26
7.26
7.25
3.35 HDO
2.48 DMSO
2.48
2.48
Ph
Ph
N+
PF6-
3aa
1.00
0.99
2.00
3.02
6.03
3.02
2.02
f1 (ppm)

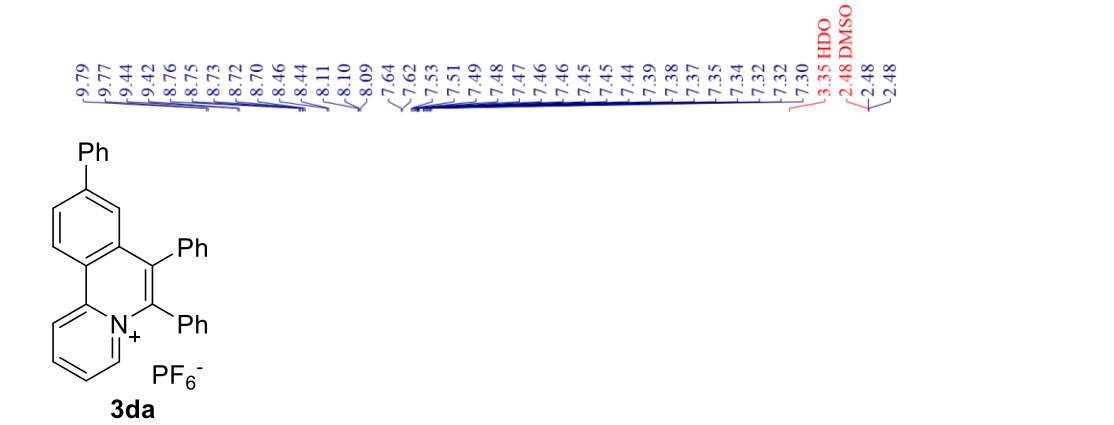

143.69
140.44
138.79
137.33
135.84
134.84
134.62
132.52
131.69
131.44
131.29
130.55
130.37
129.80
128.79
128.72
127.28
126.44
125.19
125.09
123.96
40.49 DMSO
40.32 DMSO
40.16 DMSO
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
Ph
Ph
N+
PF6-
3aa
f1 (ppm)

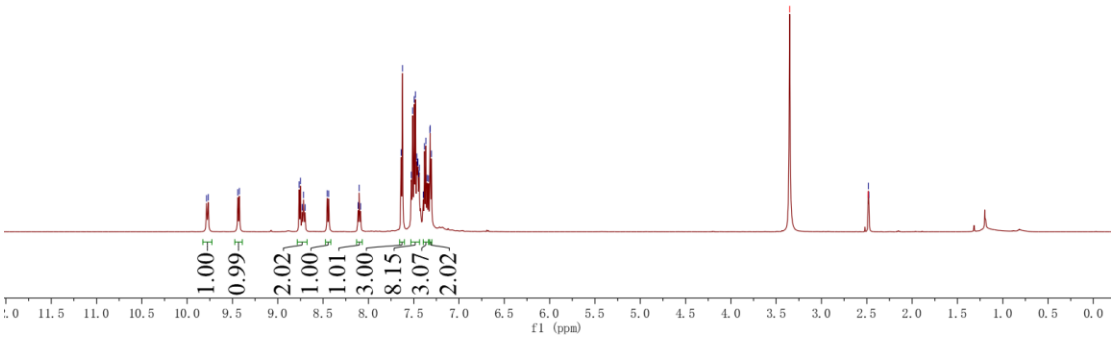

9.68
9.66
9.25
9.23
8.69
8.67
8.66
8.64
8.63
8.04
8.03
8.01
7.96
7.95
7.48
7.48
7.46
7.46
7.45
7.45
7.43
7.42
7.41
7.40
7.39
7.35
7.33
7.32
7.30
7.30
7.29
7.27
7.23
7.23
7.21
3.32 HDO
2.50
2.47
Ph
Ph
N+
PF6-
3ba
0.97
0.96
1.92
0.95
0.94
5.08
3.04
3.02
3.04
f1 (ppm)

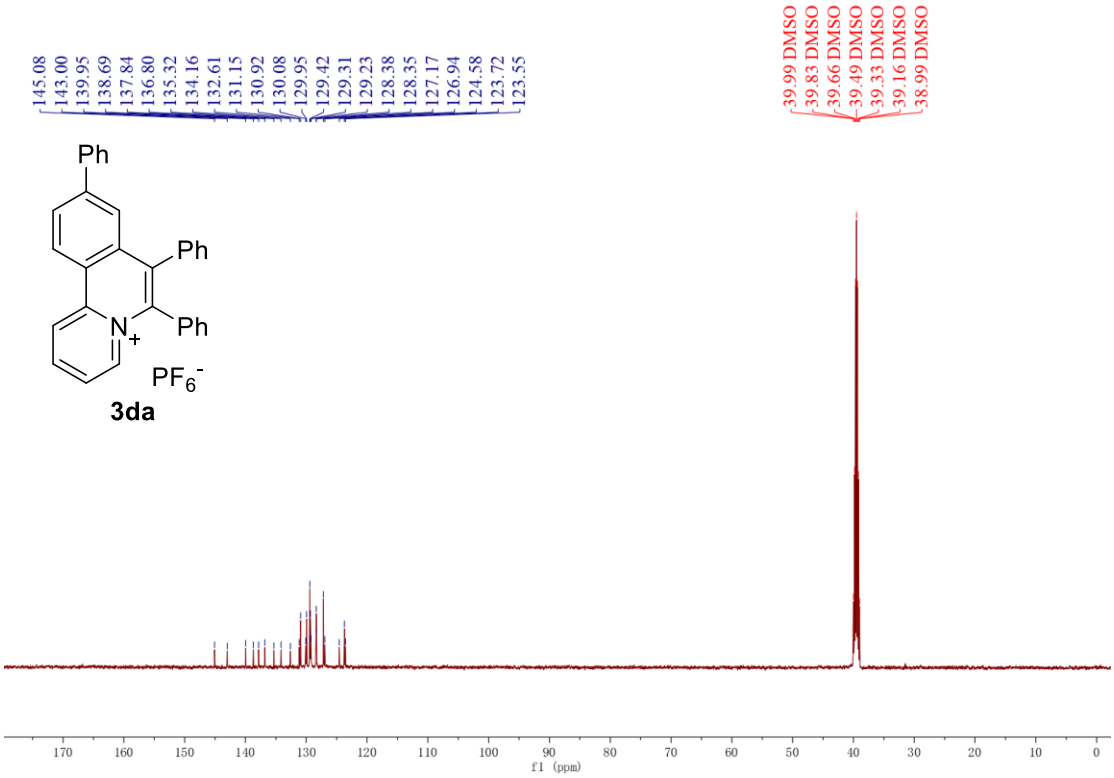

145.59
143.61
140.13
138.90
137.01
135.56
134.85
132.93
132.74
131.76
131.44
130.49
130.38
129.75
128.78
128.72
126.49
126.45
124.66
123.69
123.07
40.50 DMSO
40.33 DMSO
40.16 DMSO
40.00 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
22.18
Ph
Ph
N+
PF6-
3ba
f1 (ppm)

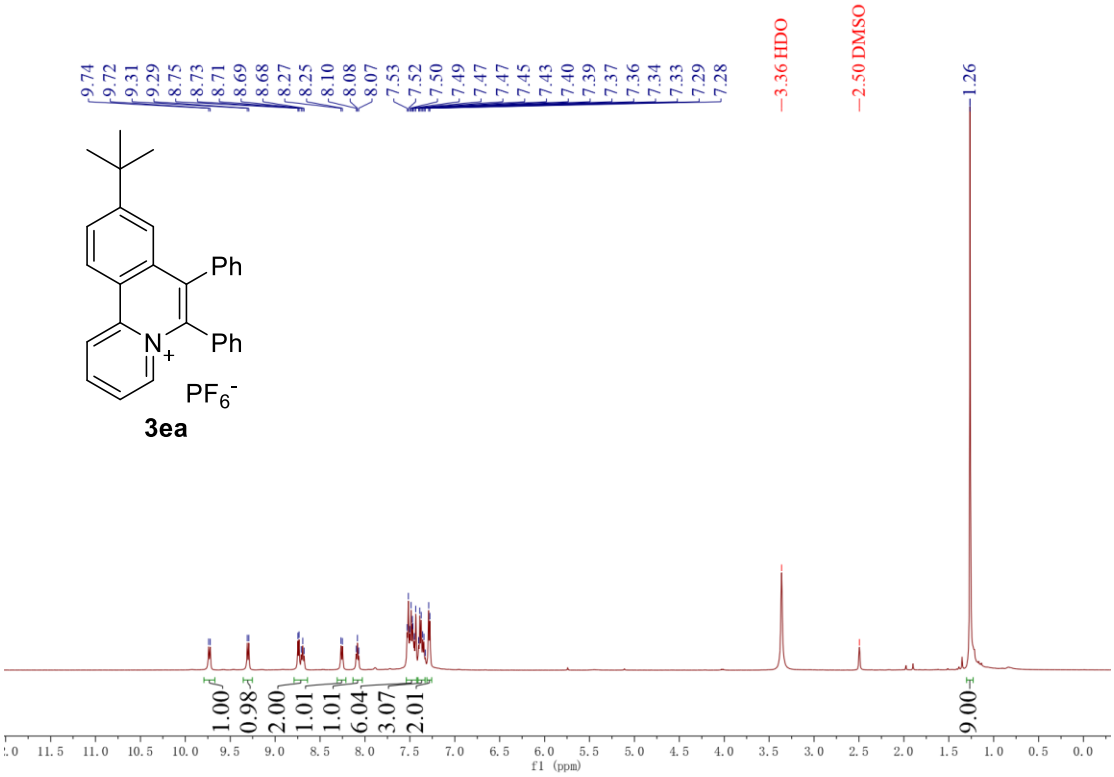

9.60
9.59
9.31
9.29
8.63
8.62
8.61
8.60
8.58
7.98
7.96
7.95
7.78
7.77
7.76
7.75
7.51
7.50
7.47
7.46
7.44
7.44
7.43
7.41
7.38
7.36
7.35
7.33
7.32
7.30
7.27
7.27
7.25
6.76
6.75
3.78
3.36 HDO
2.48 DMSO
O
Ph
Ph
N+
PF6-
3ca
1.00
1.00
2.02
1.01
1.00
5.07
3.15
2.01
0.98
3.05
f1 (ppm)

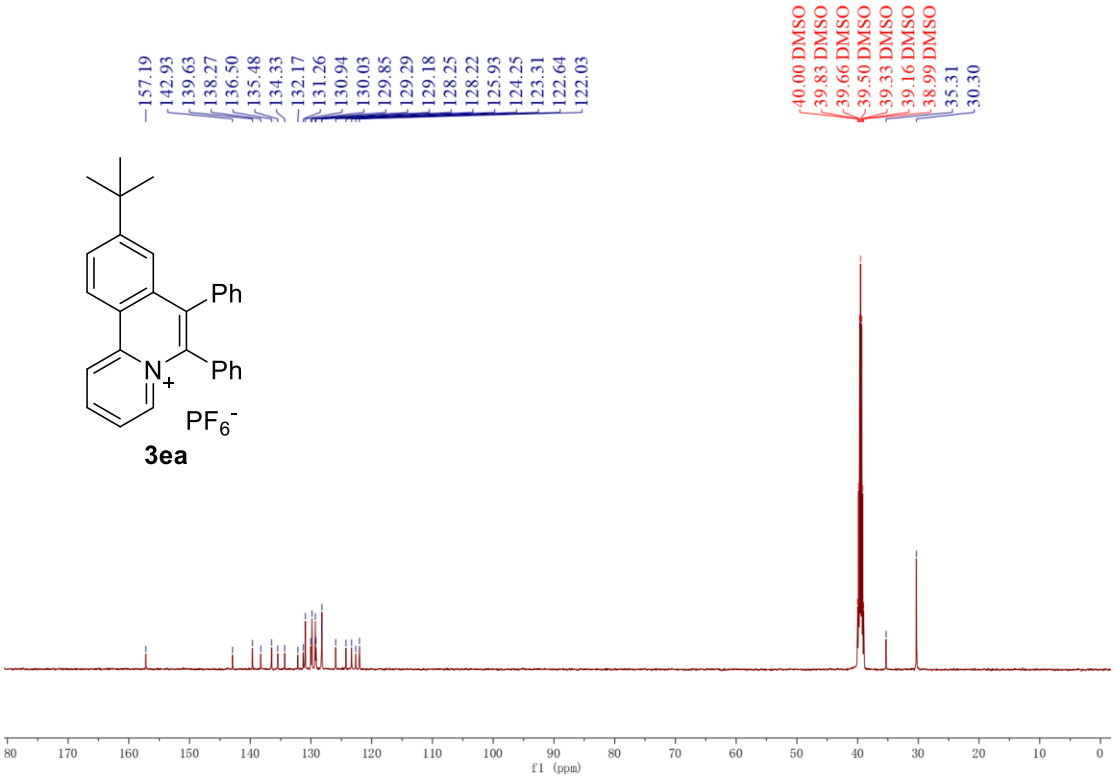

163.73
143.49
139.75
139.22
136.62
135.15
135.11
134.80
131.77
131.38
130.51
130.30
129.75
129.06
128.85
128.79
123.72
123.32
120.67
119.16
108.50
56.37
40.48 DMSO
40.31 DMSO
40.14 DMSO
39.98 DMSO
39.81 DMSO
39.64 DMSO
39.48 DMSO
O
Ph
Ph
N+
PF6-
3ca
f1 (ppm)

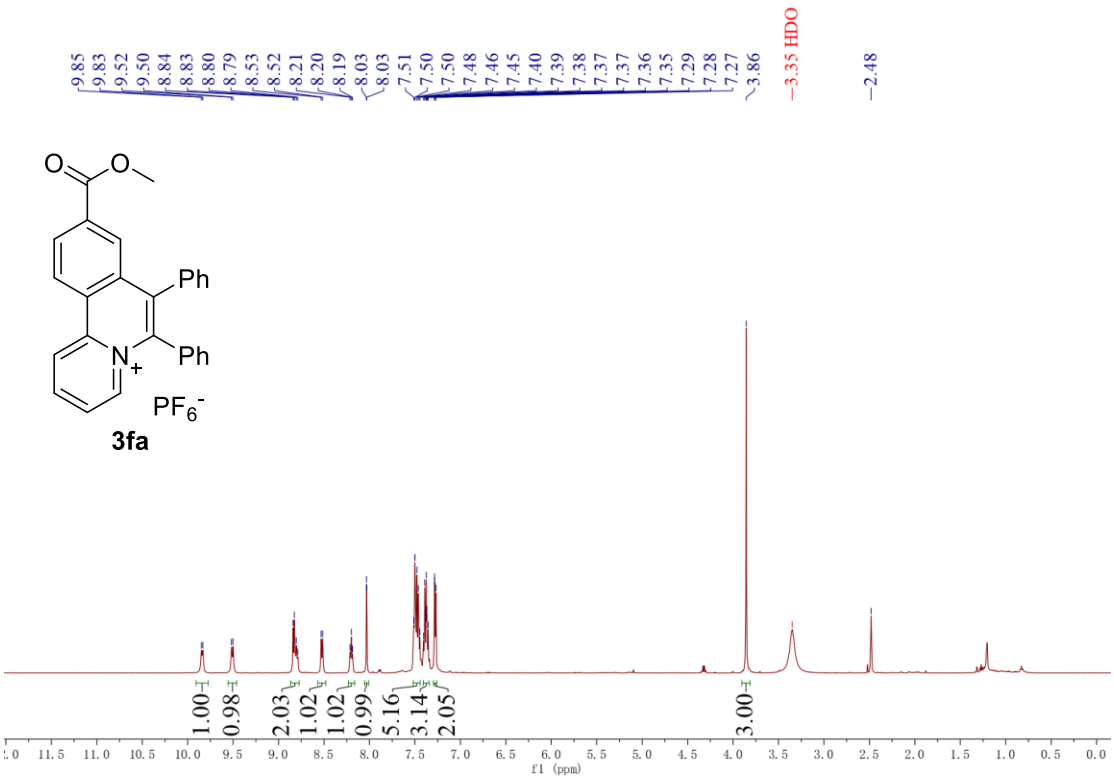

9.79
9.77
9.44
9.42
8.76
8.75
8.73
8.72
8.70
8.46
8.44
8.11
8.10
8.09
7.64
7.62
7.53
7.51
7.49
7.48
7.47
7.46
7.46
7.45
7.45
7.44
7.39
7.38
7.37
7.35
7.34
7.32
7.32
7.30
3.35 HDO
2.48 DMSO
2.48
2.48
Ph
Ph
Ph
N+
PF6-
3da

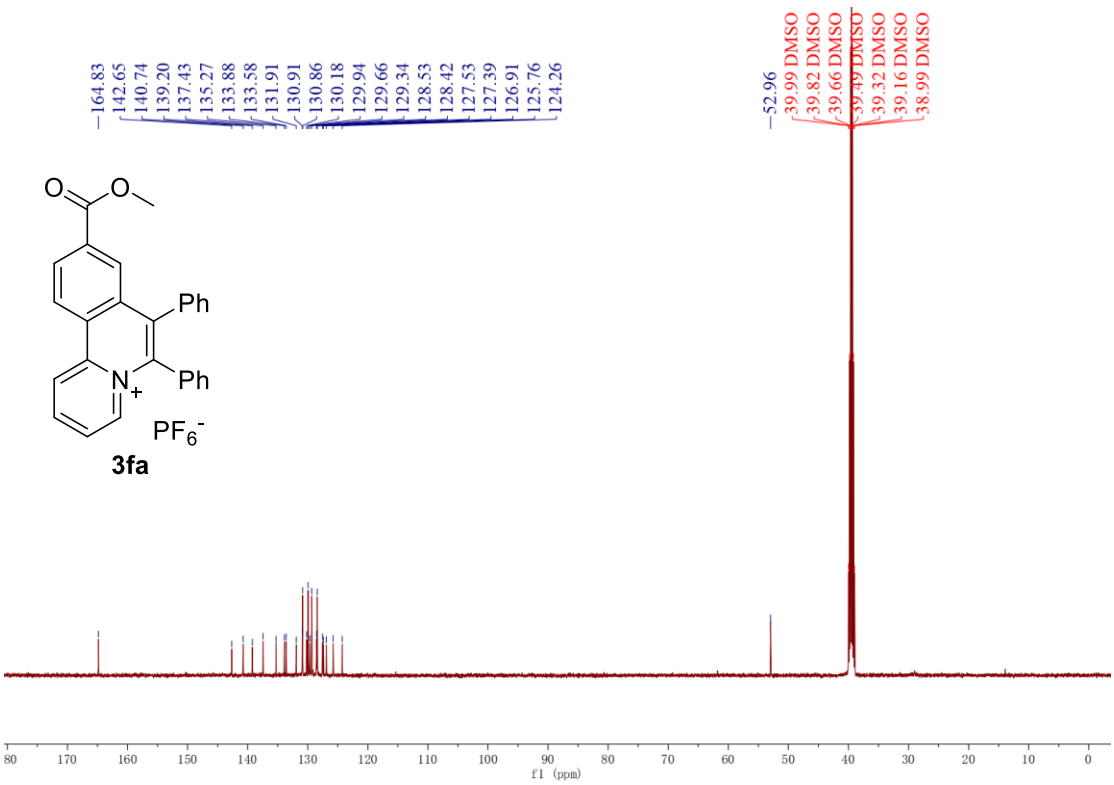

1.00
0.99
2.02
1.00
1.01
3.00
8.15
3.07
2.02
f1 (ppm)

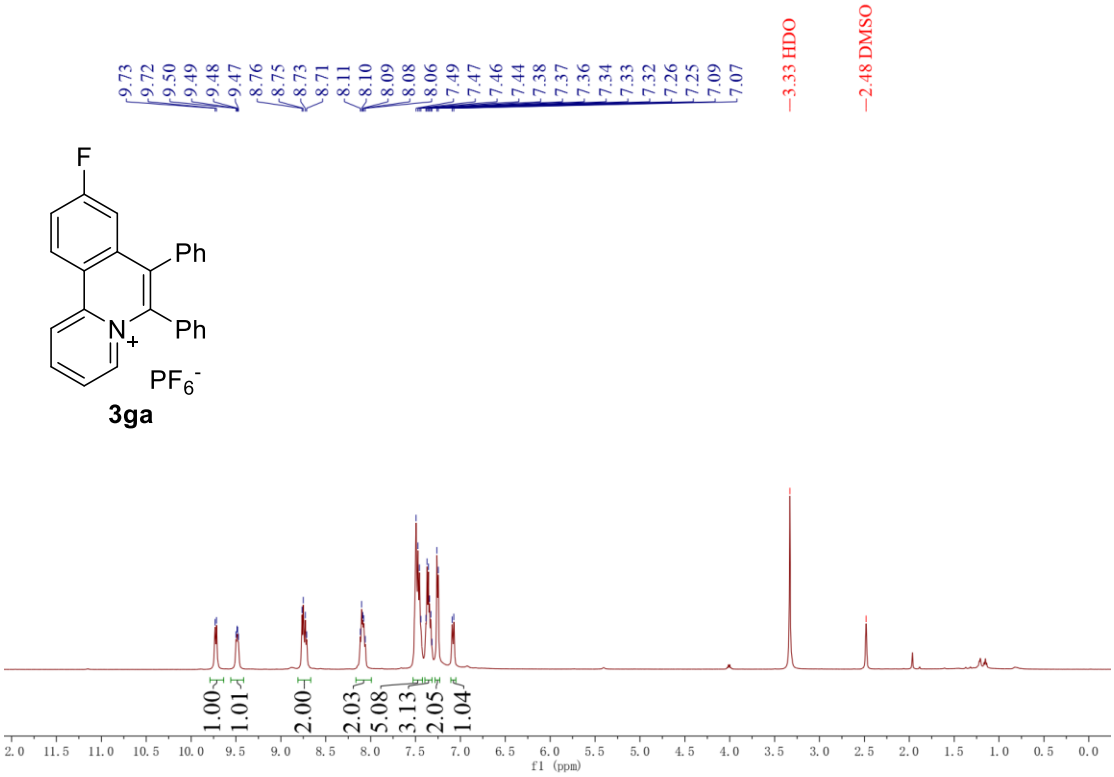

145.08
143.00
139.95
138.69
137.84
136.80
135.32
134.16
132.61
131.15
130.92
130.08
129.95
129.42
129.31
129.23
128.38
128.35
127.17
126.94
124.58
123.72
123.55
39.99 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
39.33 DMSO
39.16 DMSO
38.99 DMSO
Ph
Ph
Ph
N+
PF6-
3da
f1 (ppm)

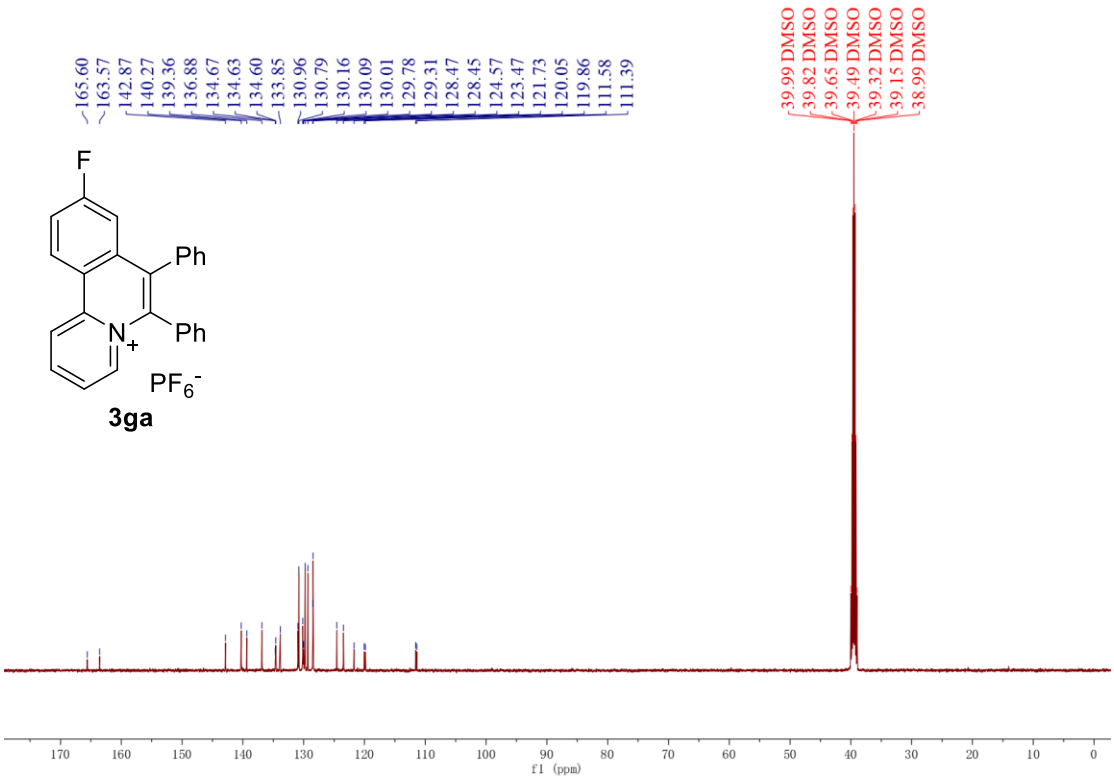

9.74
9.72
9.31
9.29
8.75
8.73
8.71
8.69
8.68
8.27
8.25
8.10
8.08
8.07
7.53
7.52
7.50
7.49
7.47
7.47
7.45
7.43
7.40
7.39
7.37
7.36
7.34
7.33
7.29
7.28
3.36 HDO
2.50 DMSO
1.26
Ph
Ph
N+
PF6-
3ea
1.00
0.98
2.00
1.01
1.01
6.04
3.07
2.01
9.00
f1 (ppm)

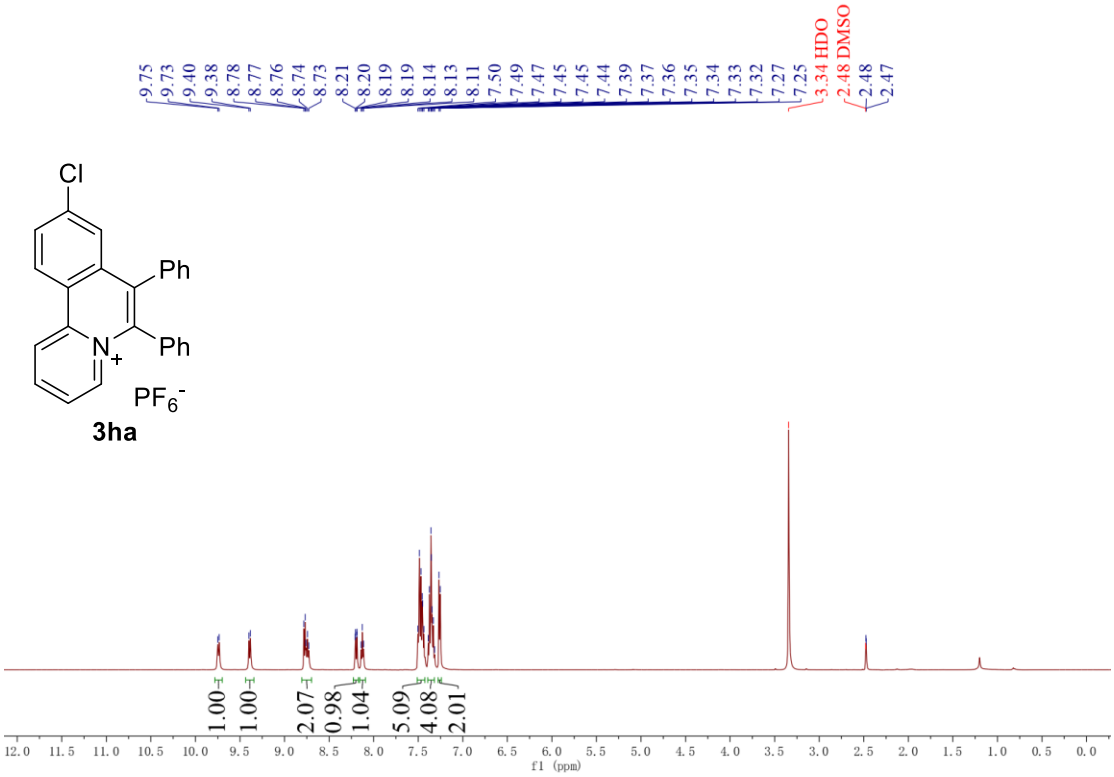

157.19
142.93
139.63
138.27
136.50
135.48
134.33
132.17
131.26
130.94
130.03
129.85
129.29
129.18
128.25
128.22
125.93
124.25
123.31
122.64
122.03
40.00 DMSO
39.83 DMSO
39.66 DMSO
39.50 DMSO
39.33 DMSO
39.16 DMSO
38.99 DMSO
35.31
30.30
Ph
Ph
N+
PF6-
3ea
f1 (ppm)

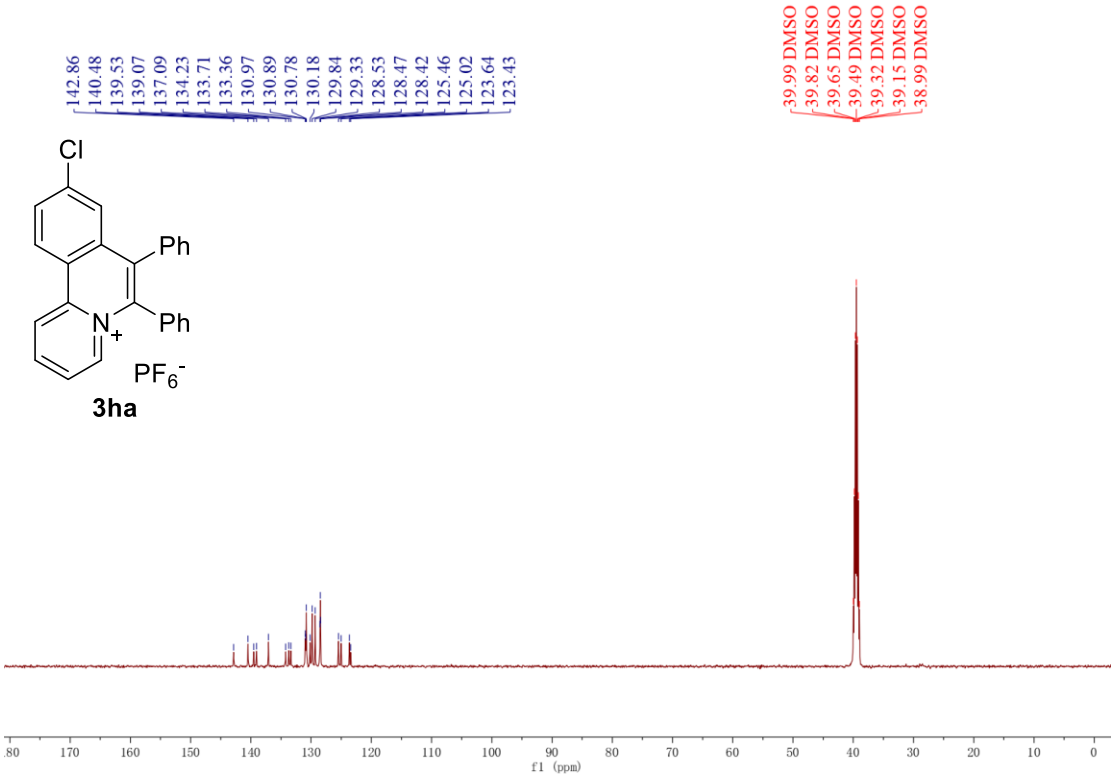

9.85
9.83
9.52
9.50
8.84
8.83
8.80
8.79
8.53
8.52
8.21
8.20
8.19
8.03
8.03
7.51
7.50
7.50
7.48
7.46
7.45
7.40
7.39
7.38
7.37
7.37
7.36
7.35
7.29
7.28
7.27
3.86
3.35 HDO
2.48
O
O
Ph
Ph
N+
PF6-
3fa
1.00
0.98
2.03
1.02
1.02
0.99
5.16
3.14
2.05
3.00
f1 (ppm)

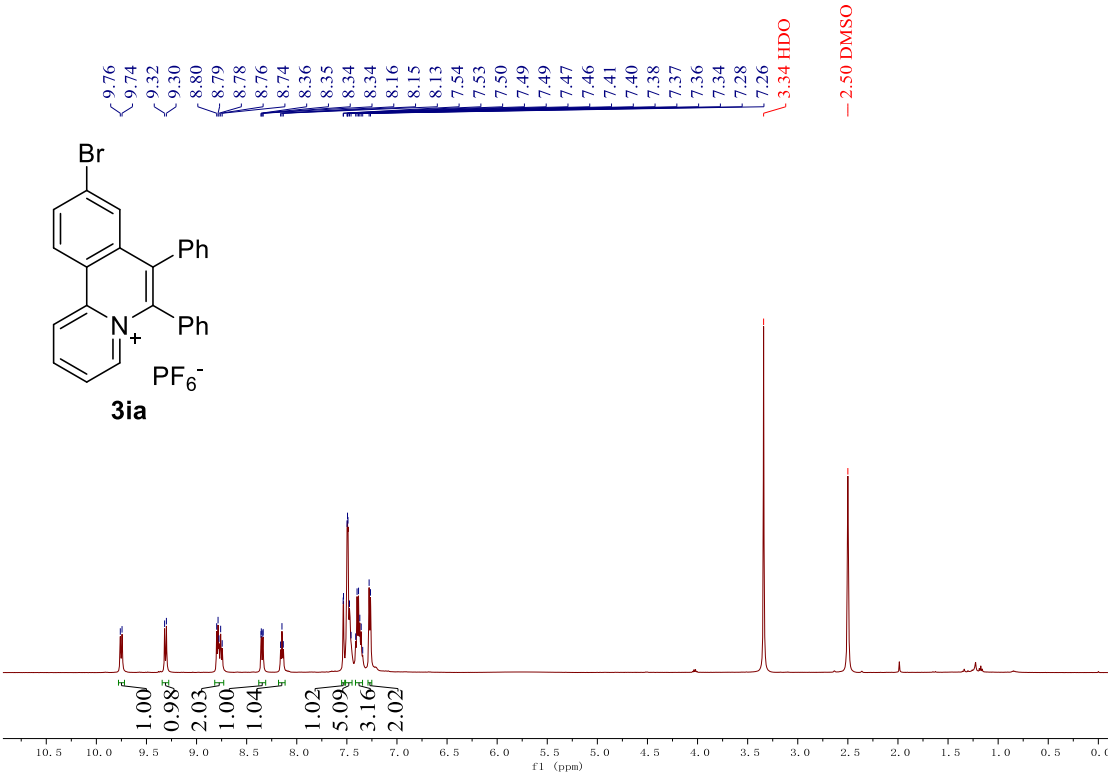

164.83
142.65
140.74
139.20
137.43
135.27
133.88
133.58
131.91
130.91
130.86
130.18
129.94
129.66
129.34
128.53
128.42
127.53
127.39
126.91
125.76
124.26
52.96
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
O
O
Ph
Ph
N+
PF6-
3fa
f1 (ppm)

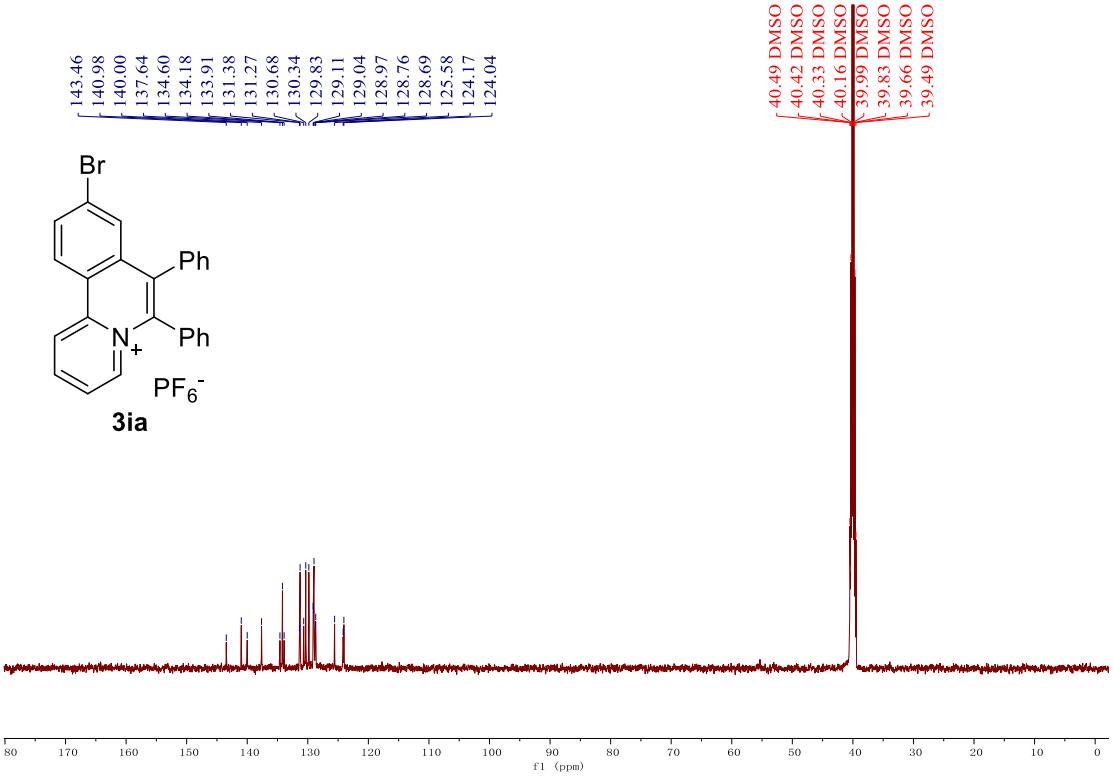

9.73
9.72
9.50
9.49
9.48
9.47
8.76
8.75
8.73
8.71
8.11
8.10
8.09
8.08
8.06
7.49
7.47
7.46
7.44
7.38
7.37
7.36
7.34
7.33
7.32
7.26
7.25
7.09
7.07
3.33 HDO
2.48 DMSO
F
Ph
Ph
N+
PF6-
3ga
1.00
1.01
2.00
2.03
5.08
3.13
2.05
1.04
f1 (ppm)

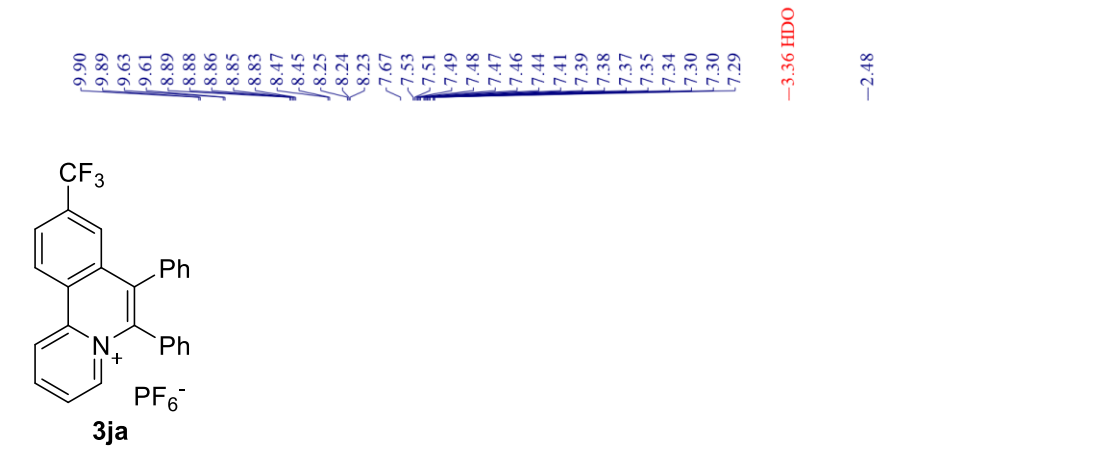

165.60
163.57
142.87
140.27
139.36
136.88
134.67
134.63
134.60
133.85
130.96
130.79
130.16
130.09
130.01
129.78
129.31
128.47
128.45
124.57
123.47
121.73
120.05
119.86
111.58
111.39
39.99 DMSO
39.82 DMSO
39.65 DMSO
39.49 DMSO
39.32 DMSO
39.15 DMSO
38.99 DMSO
F
Ph
Ph
N+
PF6-
3ga
f1 (ppm)

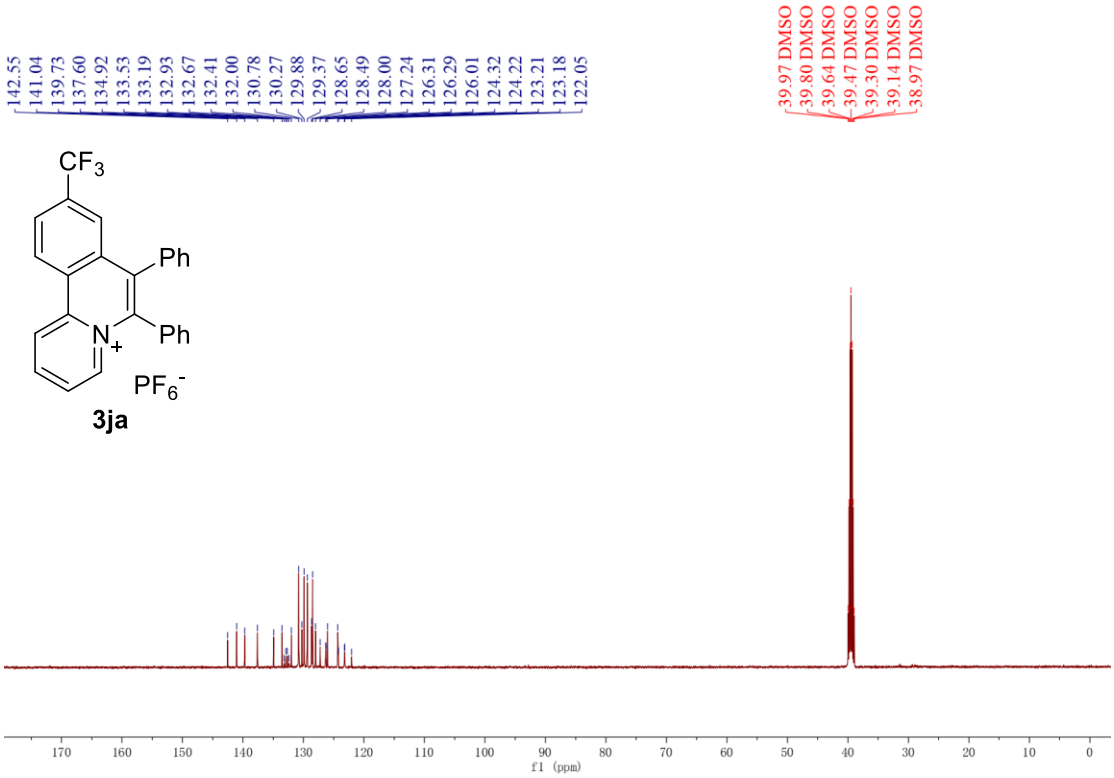

9.75
9.73
9.40
9.38
8.78
8.77
8.76
8.74
8.73
8.21
8.20
8.19
8.19
8.14
8.13
8.11
7.50
7.49
7.47
7.45
7.45
7.44
7.39
7.37
7.36
7.35
7.34
7.33
7.32
7.27
7.25
3.34 HDO
2.48 DMSO
2.48
2.47
Cl
Ph
Ph
N+
PF6-
3ha
1.00
1.00
2.07
0.98
1.04
5.09
4.08
2.01
f1 (ppm)

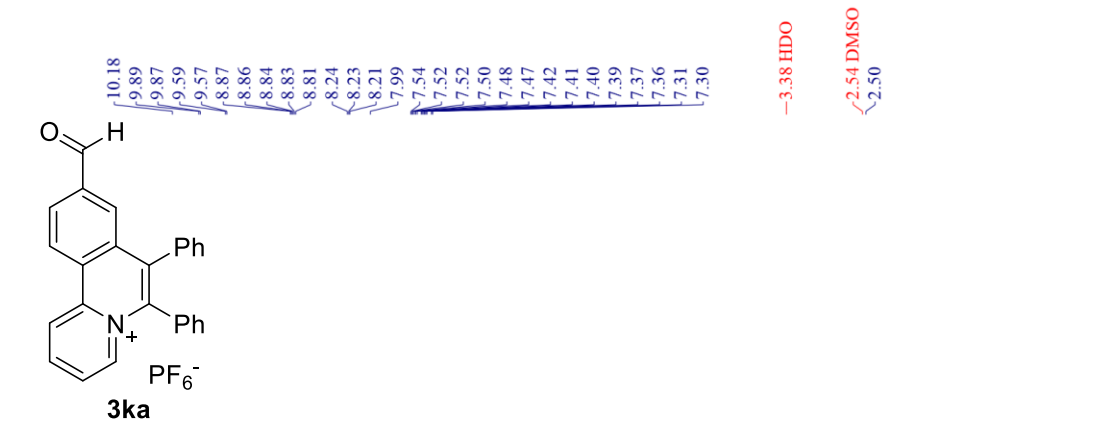

142.86
140.48
139.53
139.07
137.09
134.23
133.71
133.36
130.97
130.89
130.78
130.18
129.84
129.33
128.53
128.47
128.42
125.46
125.02
123.64
123.43
39.99 DMSO
39.82 DMSO
39.65 DMSO
39.49 DMSO
39.32 DMSO
39.15 DMSO
38.99 DMSO
Cl
Ph
Ph
N+
PF6-
3ha
f1 (ppm)

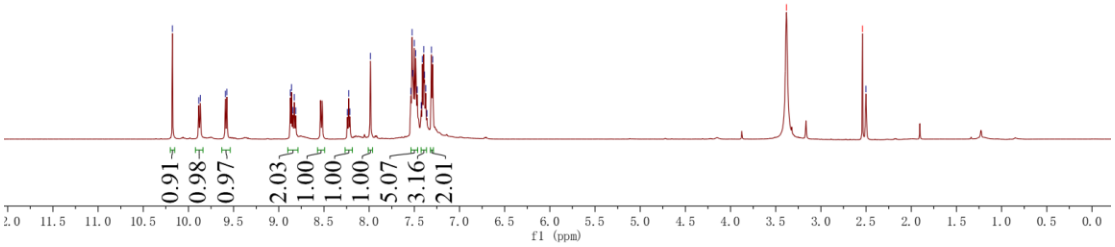

9.76
9.74
9.32
9.30
8.80
8.79
8.78
8.76
8.74
8.36
8.35
8.34
8.34
8.16
8.15
8.13
7.54
7.53
7.50
7.49
7.49
7.47
7.46
7.41
7.40
7.38
7.37
7.36
7.34
7.28
7.26
3.34 HDO
2.50 DMSO
Br
Ph
Ph
N+
PF6-
3ia
1.00
0.98
2.03
1.00
1.04
1.02
5.09
3.16
2.02
f1 (ppm)

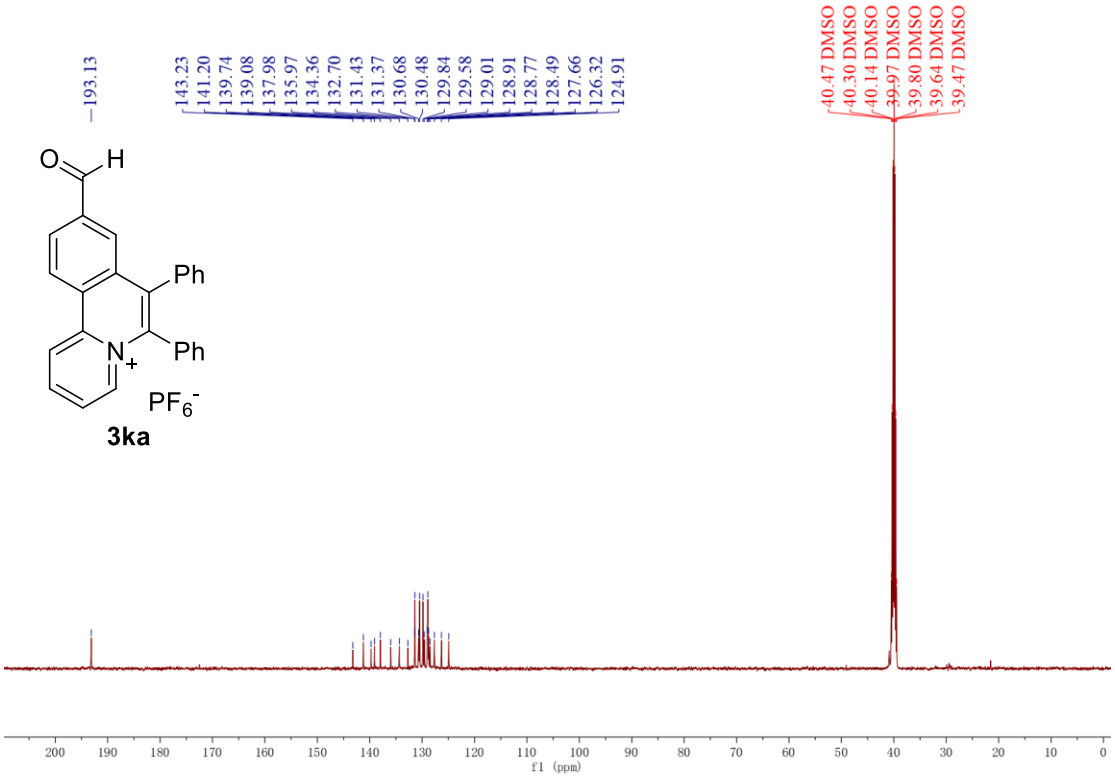

143.46
140.98
140.00
137.64
134.60
134.18
133.91
131.38
131.27
130.68
130.34
129.83
129.11
129.04
128.97
128.76
128.69
125.58
124.17
124.04
40.49 DMSO
40.42 DMSO
40.33 DMSO
40.16 DMSO
39.99 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
Br
Ph
Ph
N+
PF6-
3ia
f1 (ppm)

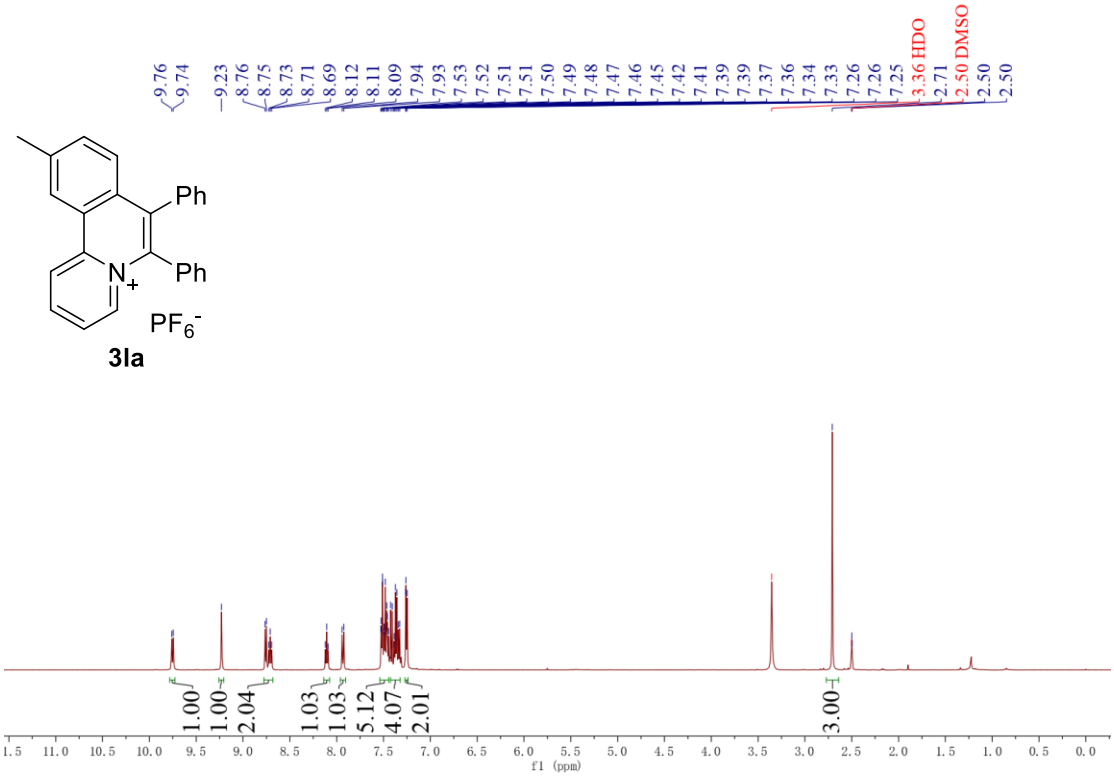

9.90
9.89
9.63
9.61
8.89
8.88
8.86
8.85
8.83
8.47
8.45
8.25
8.24
8.23
7.67
7.53
7.51
7.49
7.48
7.47
7.46
7.44
7.41
7.39
7.38
7.37
7.35
7.34
7.30
7.30
7.29
3.36 HDO
2.48
CF3
Ph
Ph
N+
PF6-
3ja
1.00
1.00
2.02
0.98
1.00
1.00
5.04
3.09
2.02
f1 (ppm)

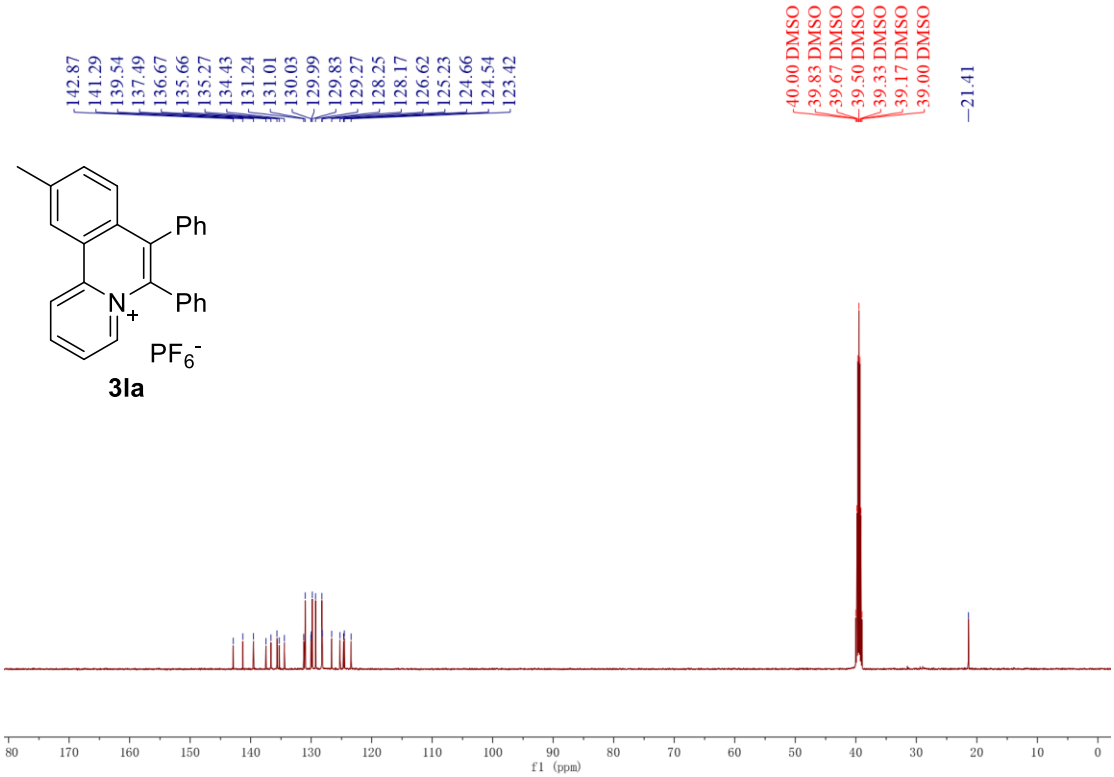

142.55
141.04
139.73
137.60
134.92
133.53
133.19
132.93
132.67
132.41
132.00
130.78
130.27
129.88
129.37
128.65
128.49
128.00
127.24
126.31
126.29
126.01
124.32
124.22
123.21
123.18
122.05
39.97 DMSO
39.80 DMSO
39.64 DMSO
39.47 DMSO
39.30 DMSO
39.14 DMSO
38.97 DMSO
CF3
Ph
Ph
N+
PF6-
3ja
f1 (ppm)

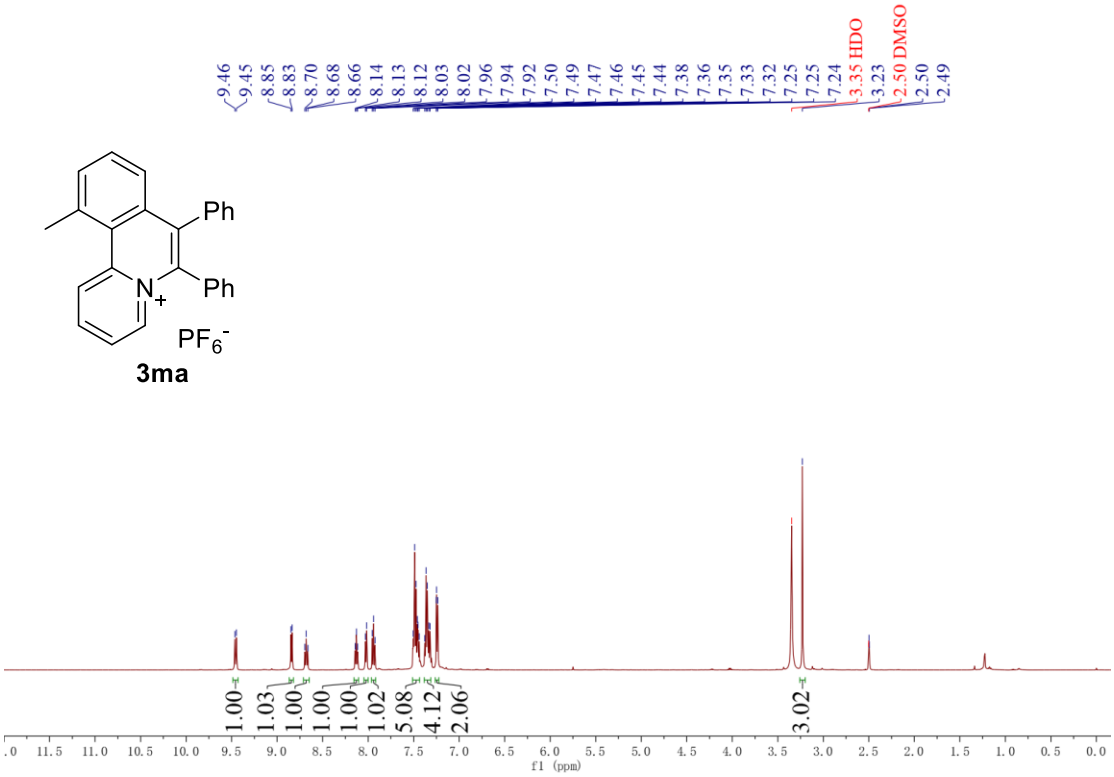

10.18
9.89
9.87
9.59
9.57
8.87
8.86
8.84
8.83
8.81
8.24
8.23
8.21
7.99
7.54
7.52
7.52
7.50
7.48
7.47
7.42
7.41
7.40
7.39
7.37
7.36
7.31
7.30
3.38 HDO
2.54 DMSO
2.50
O
H
Ph
Ph
N+
PF6-
3ka

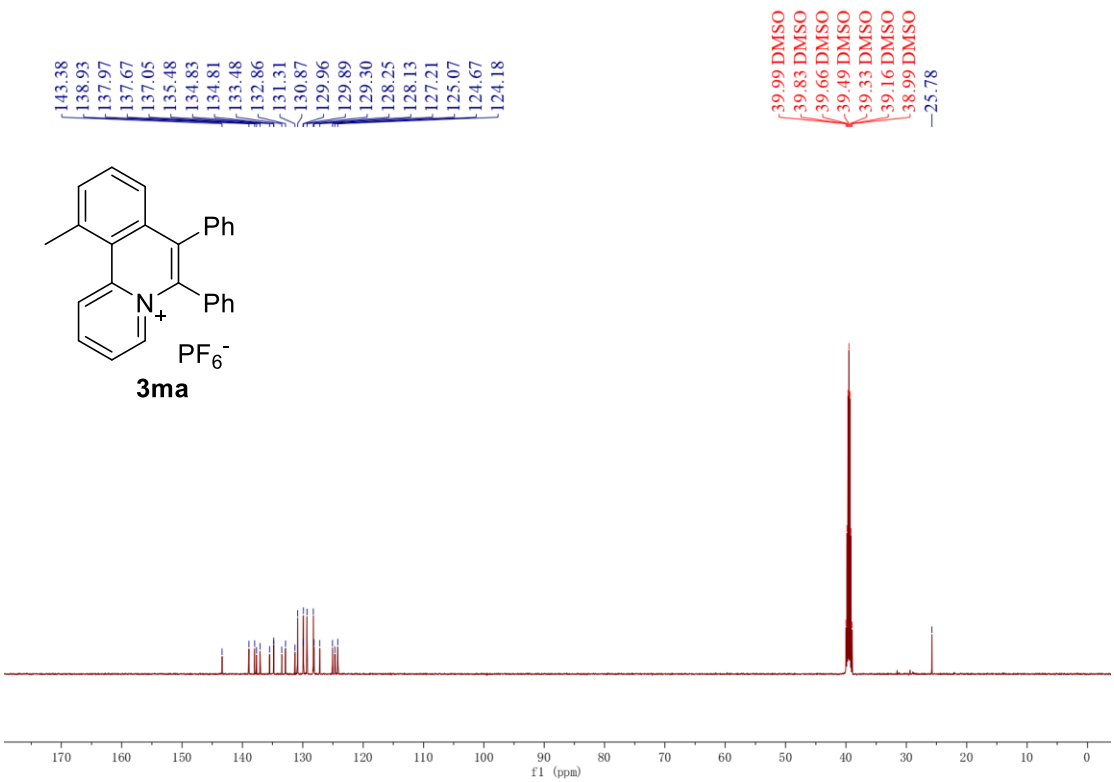

0.91
0.98
0.97
2.03
1.00
1.00
1.00
5.07
3.16
2.01
f1 (ppm)

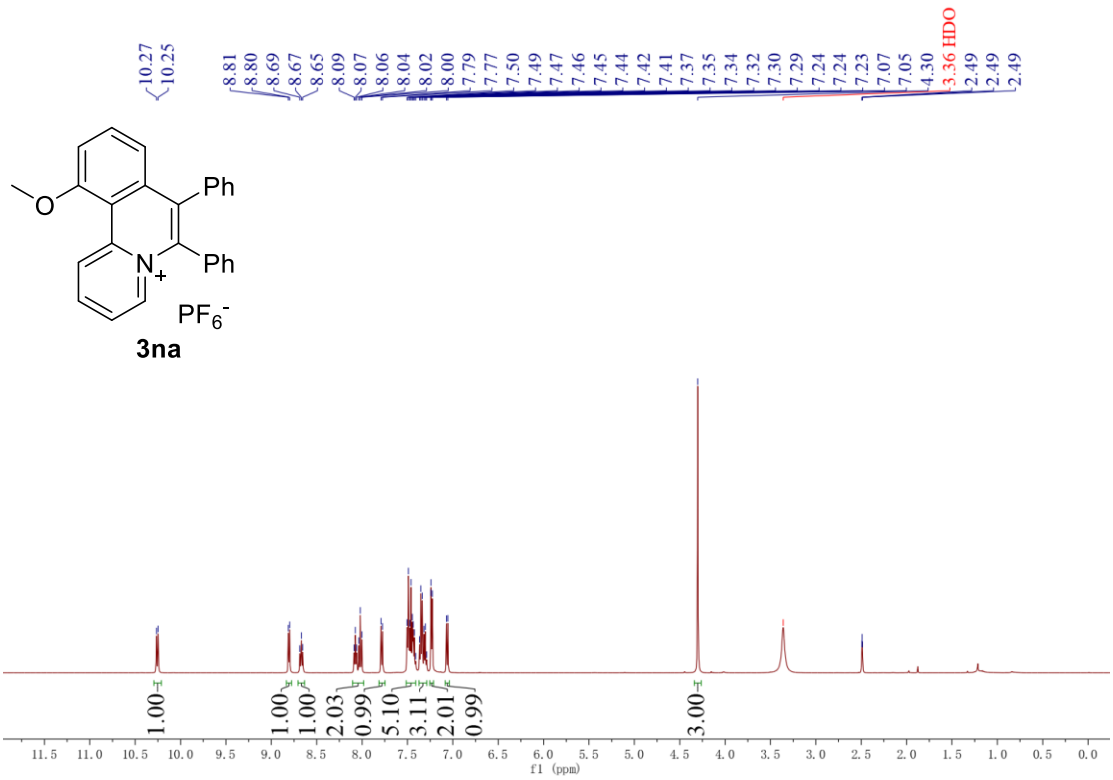

193.13
143.23
141.20
139.74
139.08
137.98
135.97
134.36
132.70
131.43
131.37
130.68
130.48
129.84
129.58
129.01
128.91
128.77
128.49
127.66
126.32
124.91
40.47 DMSO
40.30 DMSO
40.14 DMSO
39.97 DMSO
39.80 DMSO
39.64 DMSO
39.47 DMSO
O
H
Ph
Ph
N+
PF6-
3ka
f1 (ppm)

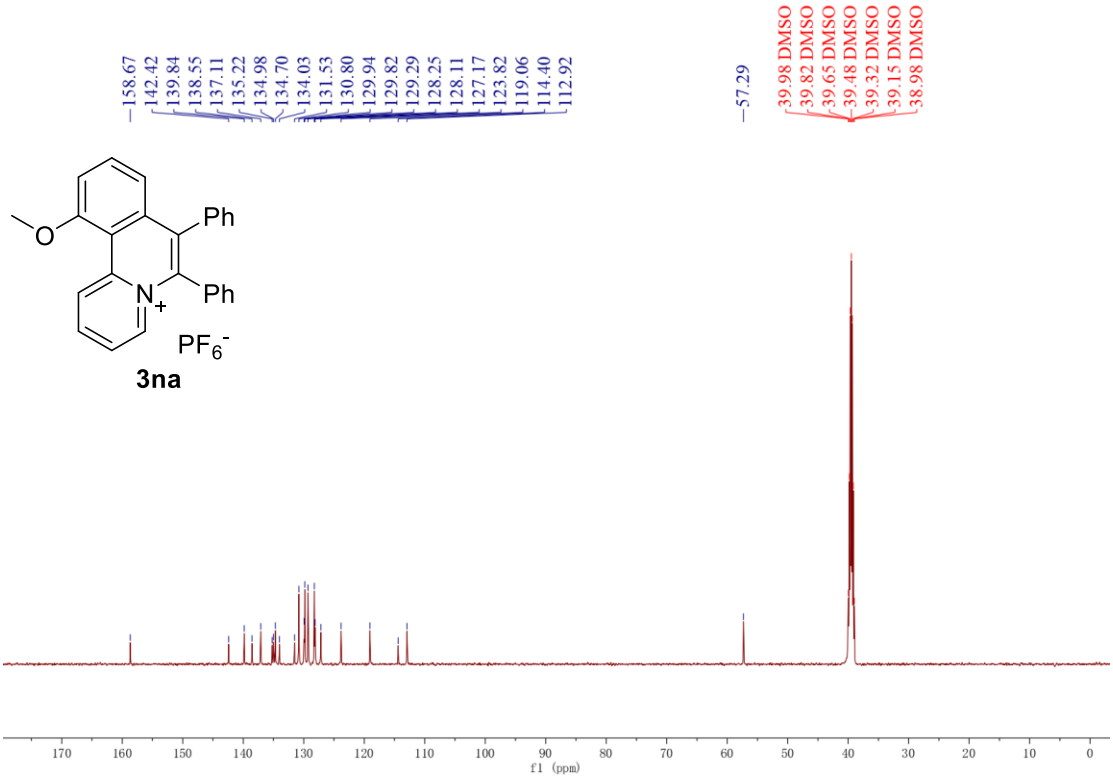

9.76
9.74
9.23
8.76
8.75
8.73
8.71
8.69
8.12
8.11
8.09
7.94
7.93
7.53
7.52
7.51
7.51
7.50
7.49
7.48
7.47
7.46
7.45
7.42
7.41
7.39
7.39
7.37
7.36
7.34
7.33
7.26
7.26
7.25
3.36 HDO
2.71
2.50 DMSO
2.50
2.50
Ph
Ph
N+
PF6-
3Ia
1.00
1.00
2.04
1.03
1.03
5.12
4.07
2.01
3.00
f1 (ppm)

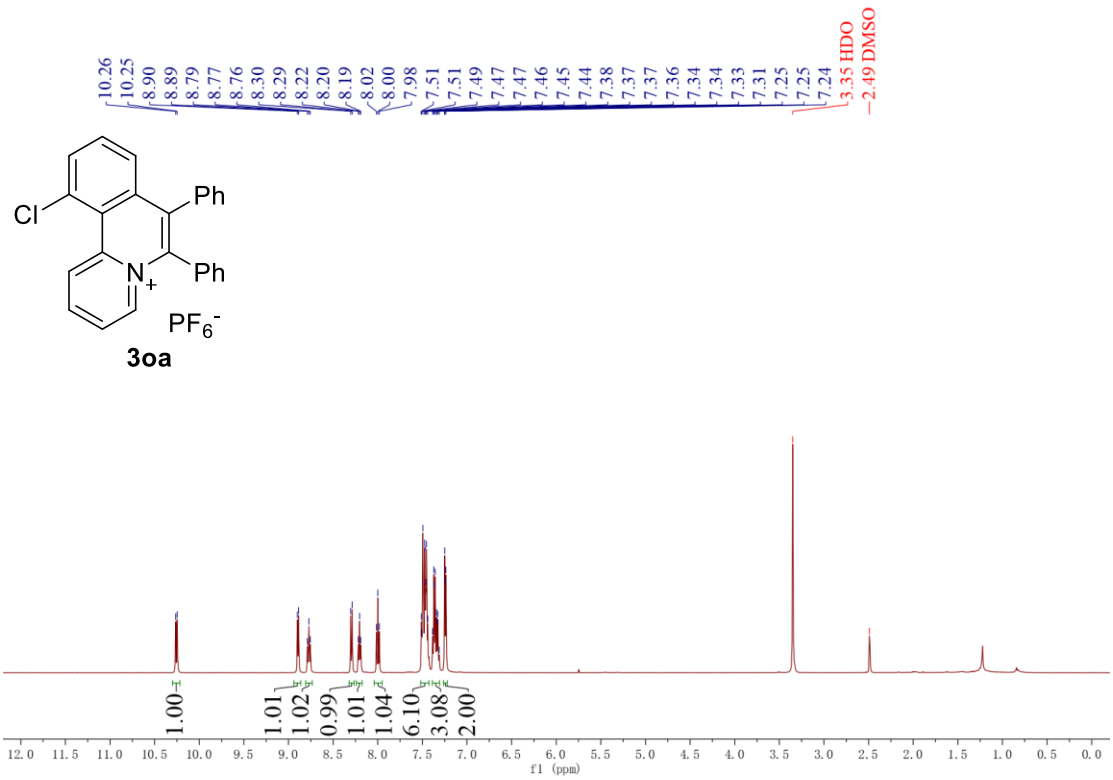

142.87
141.29
139.54
137.49
136.67
135.66
135.27
134.43
131.24
131.01
130.03
129.99
129.83
129.27
128.25
128.17
126.62
125.23
124.66
124.54
123.42
40.00 DMSO
39.83 DMSO
39.67 DMSO
39.50 DMSO
39.33 DMSO
39.17 DMSO
39.00 DMSO
21.41
Ph
Ph
N+
PF6-
3Ia
f1 (ppm)

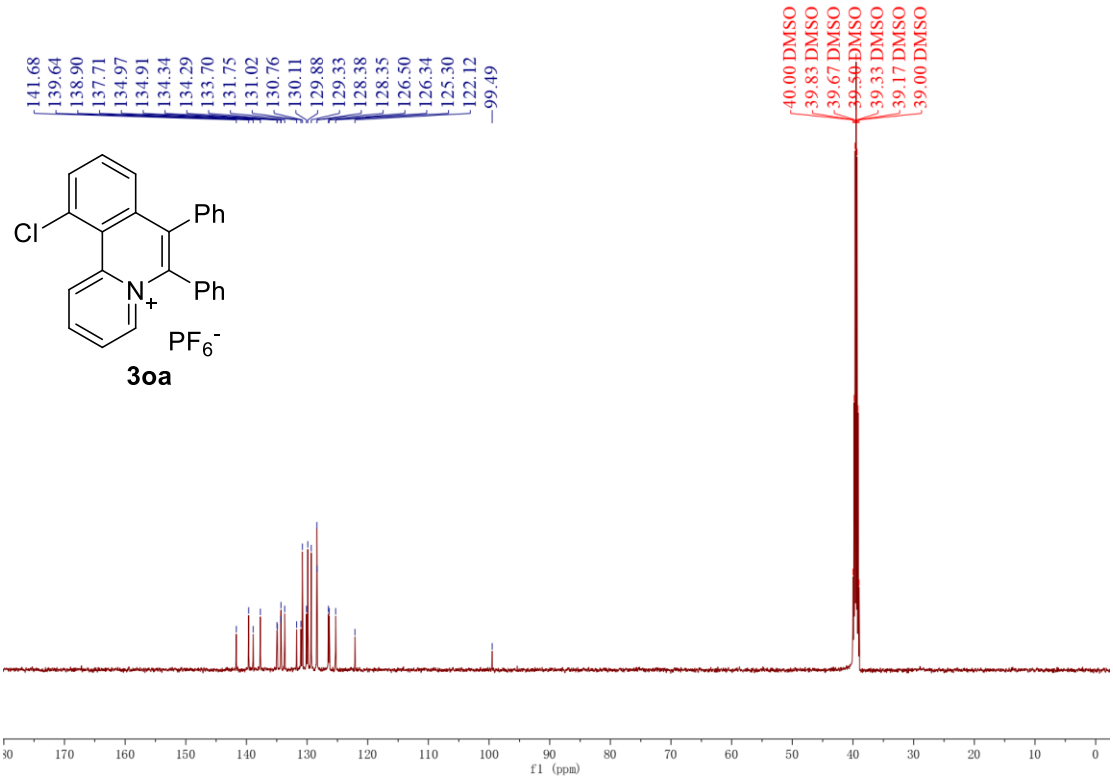

9.46
9.45
8.85
8.83
8.70
8.68
8.66
8.14
8.13
8.12
8.03
8.02
7.96
7.94
7.92
7.50
7.49
7.47
7.46
7.45
7.44
7.38
7.36
7.35
7.33
7.32
7.25
7.25
7.24
3.35 HDO
3.23
2.50 DMSO
2.50
2.49
Ph
Ph
N+
PF6-
3ma
1.00
1.03
1.00
1.00
1.00
1.02
5.08
4.12
2.06
3.02
f1 (ppm)

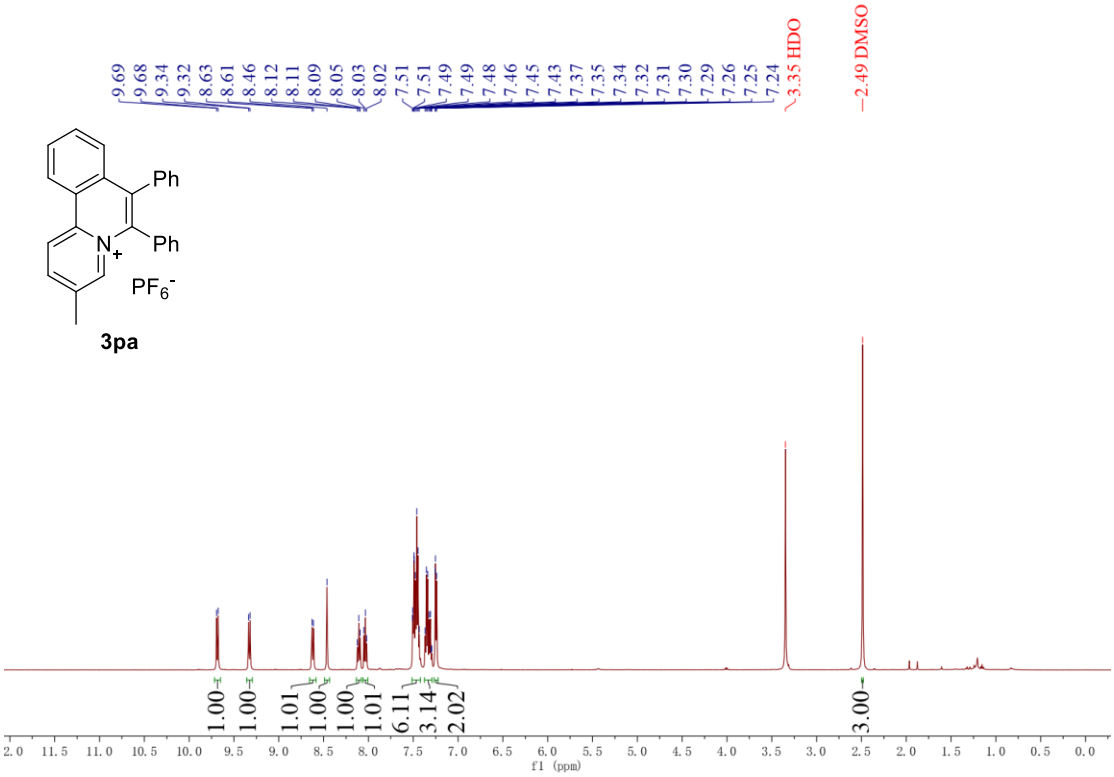

143.38
138.93
137.97
137.67
137.05
135.48
134.83
134.81
133.48
132.86
131.31
130.87
129.96
129.89
129.30
128.25
128.13
127.21
125.07
124.67
124.18
39.99 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
39.33 DMSO
39.16 DMSO
38.99 DMSO
25.78
Ph
Ph
N+
PF6-
3ma
f1 (ppm)

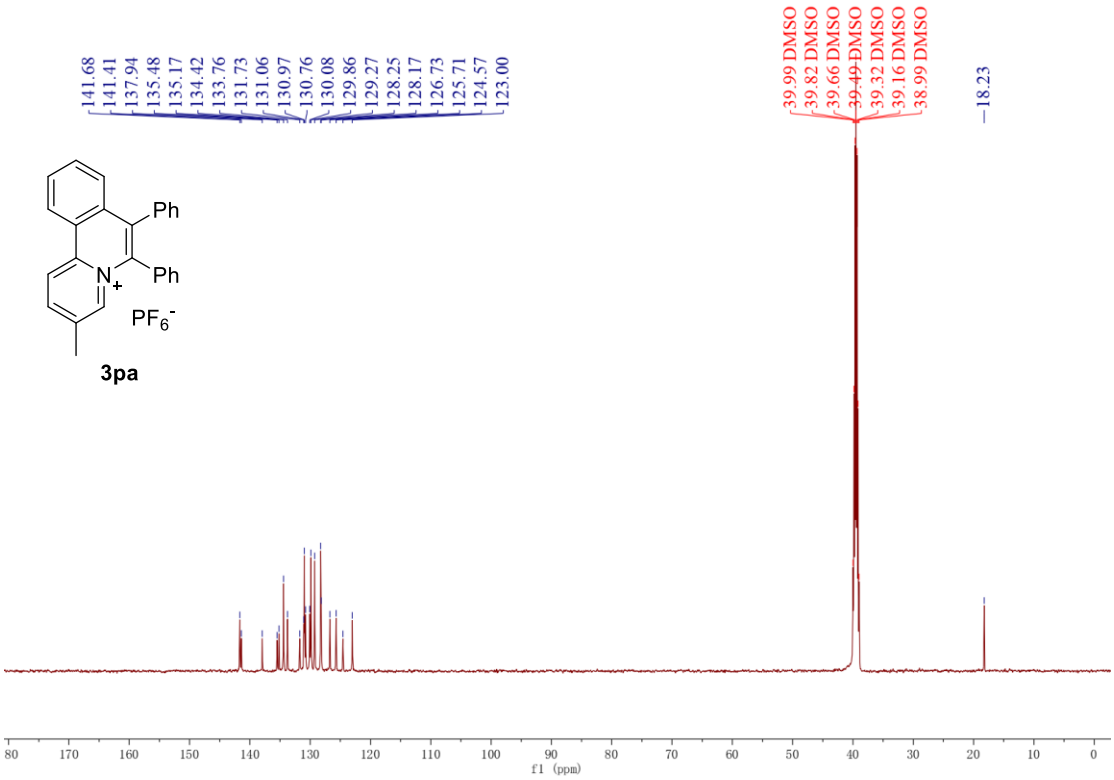

10.27
10.25
8.81
8.80
8.69
8.67
8.65
8.09
8.07
8.06
8.04
8.02
8.00
7.79
7.77
7.50
7.49
7.47
7.46
7.45
7.44
7.42
7.41
7.37
7.35
7.34
7.32
7.30
7.29
7.24
7.24
7.23
7.07
7.05
4.30
3.36 HDO
2.49
2.49
2.49
O
Ph
Ph
N+
PF6-
3na
1.00
1.00
1.00
2.03
0.99
5.10
3.11
2.01
0.99
3.00
f1 (ppm)

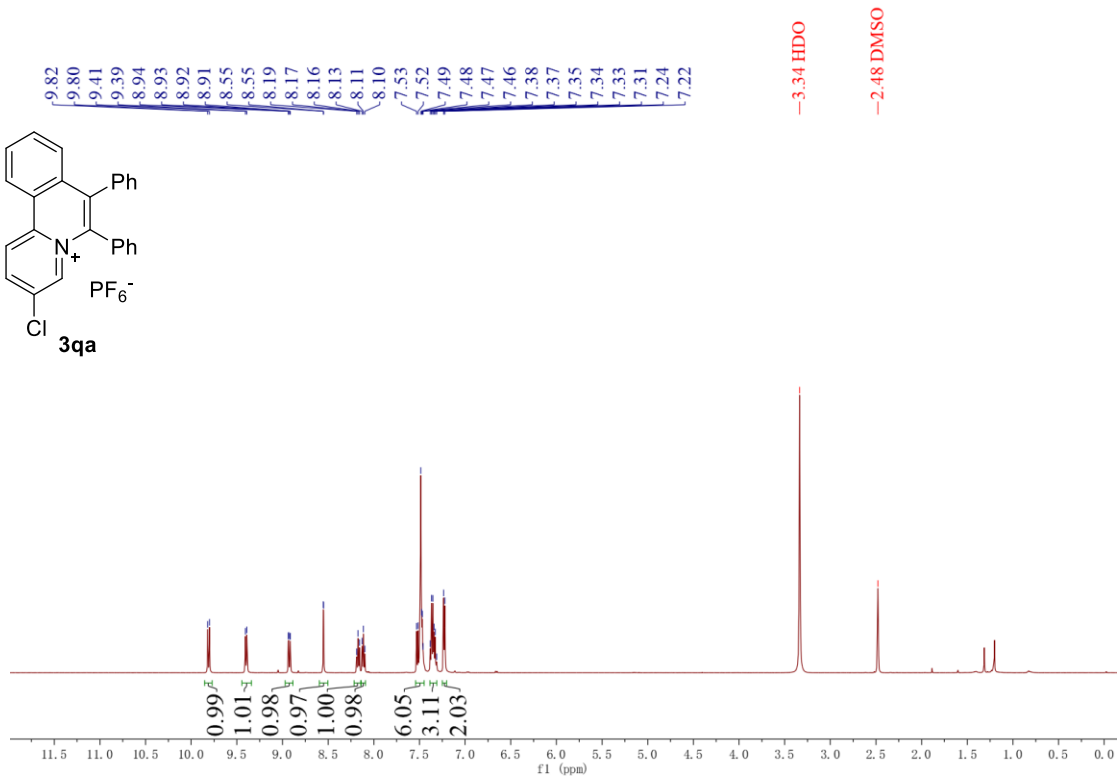

158.67
142.42
139.84
138.55
137.11
135.22
134.98
134.70
134.03
131.53
130.80
129.94
129.82
129.29
128.25
128.11
127.17
123.82
119.06
114.40
112.92
57.29
39.98 DMSO
39.82 DMSO
39.65 DMSO
39.48 DMSO
39.32 DMSO
39.15 DMSO
38.98 DMSO
O
Ph
Ph
N+
PF6-
3na
f1 (ppm)

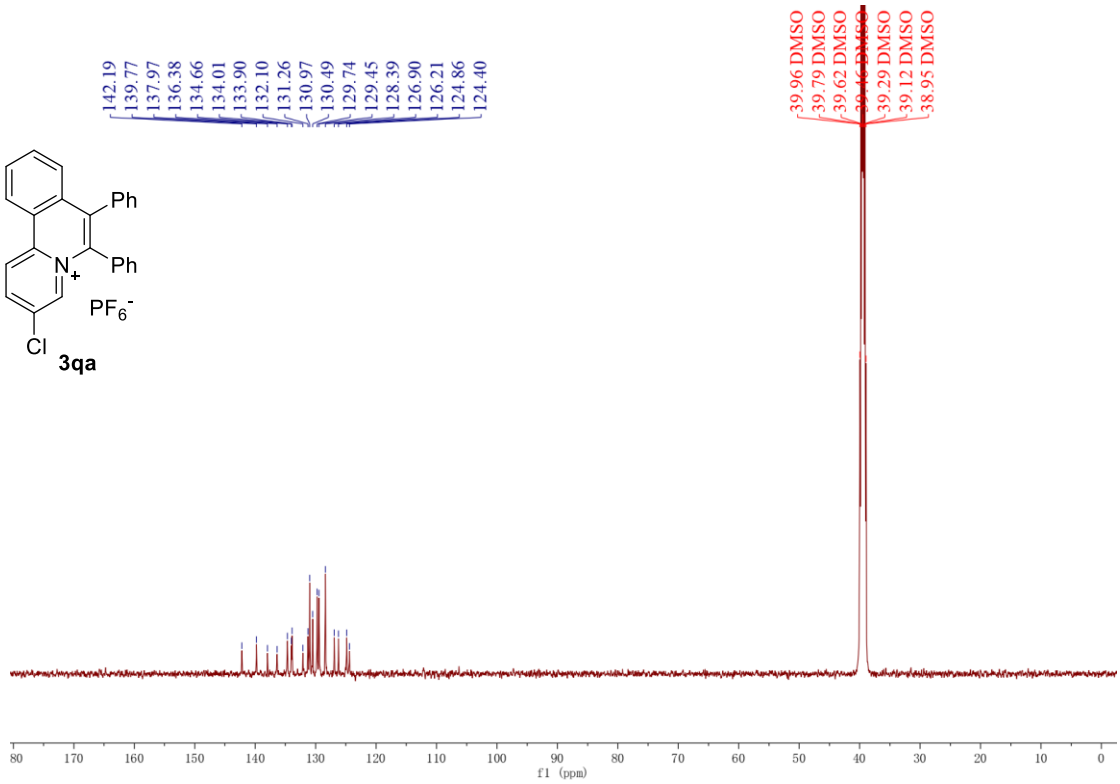

10.26
10.25
8.90
8.89
8.79
8.77
8.76
8.30
8.29
8.22
8.20
8.19
8.02
8.00
7.98
7.51
7.51
7.49
7.47
7.47
7.46
7.45
7.44
7.38
7.37
7.37
7.36
7.34
7.34
7.33
7.31
7.25
7.25
7.24
3.35 HDO
2.49 DMSO
Cl
Ph
Ph
N+
PF6-
3oa
1.00
1.01
1.02
0.99
1.01
1.04
6.10
3.08
2.00
f1 (ppm)

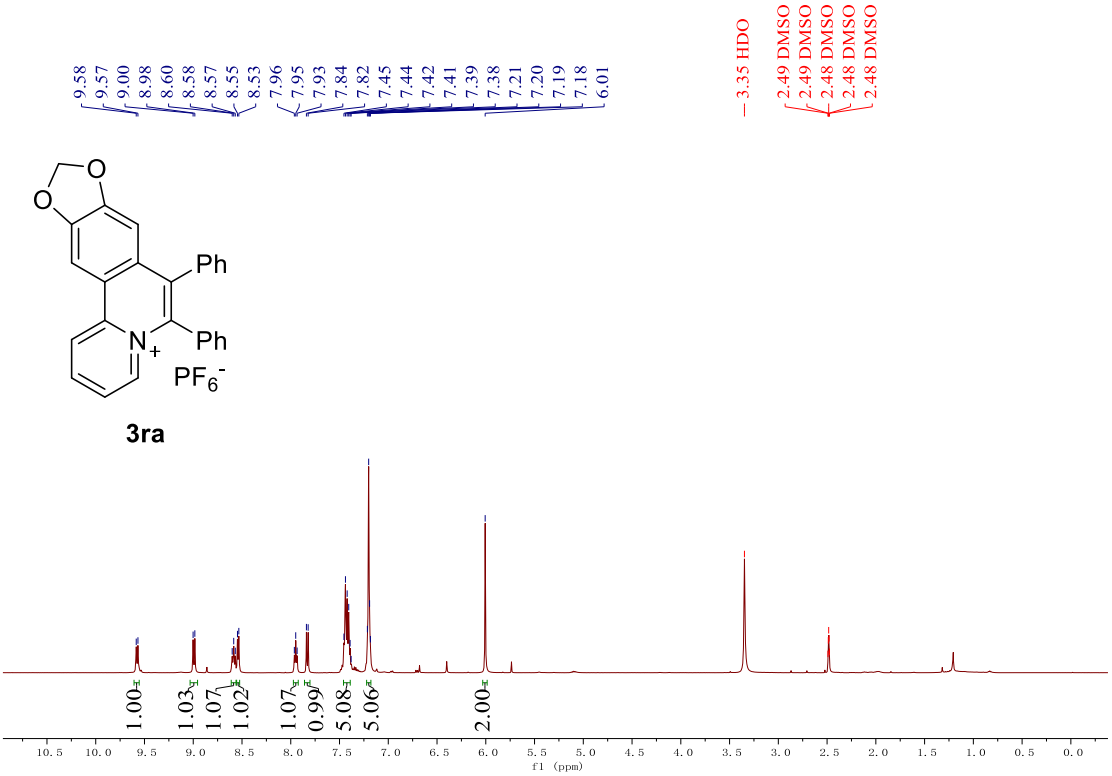

141.68
139.64
138.90
137.71
134.97
134.91
134.34
134.29
133.70
131.75
131.02
130.76
130.11
129.88
129.33
128.38
128.35
126.50
126.34
125.30
122.12
99.49
40.00 DMSO
39.83 DMSO
39.67 DMSO
39.50 DMSO
39.33 DMSO
39.17 DMSO
39.00 DMSO
Cl
Ph
Ph
N+
PF6-
3oa
f1 (ppm)

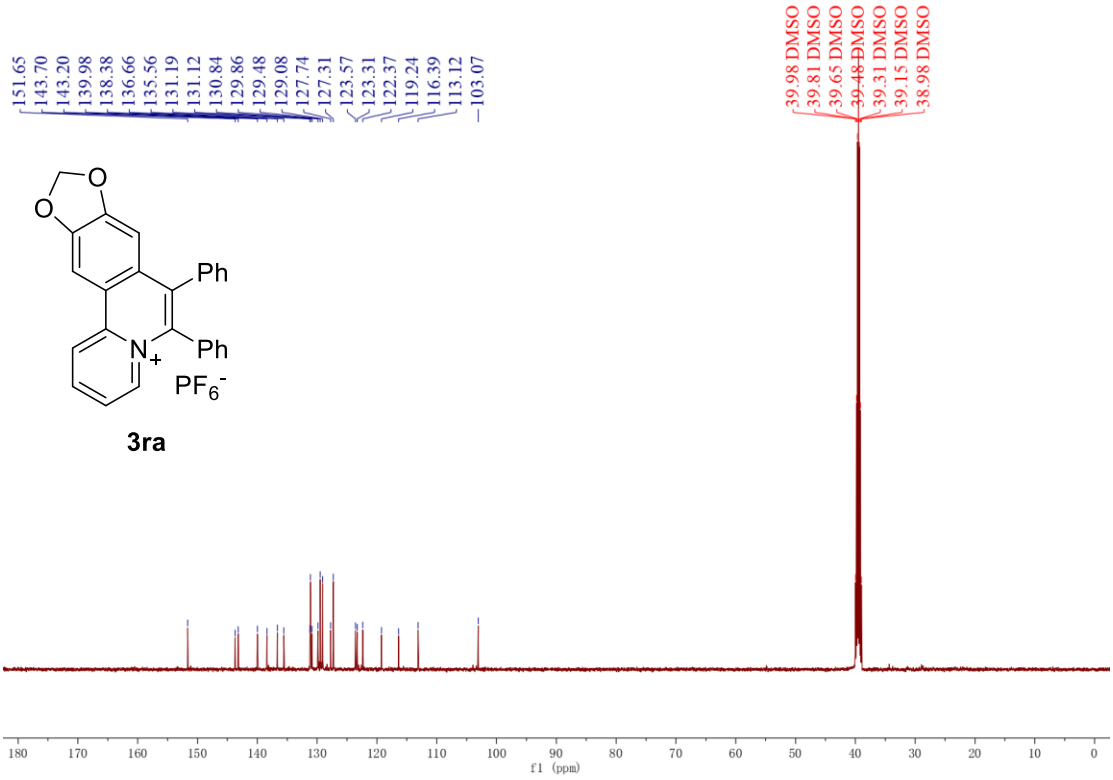

9.69
9.68
9.34
9.32
8.63
8.61
8.46
8.12
8.11
8.09
8.05
8.03
8.02
7.51
7.51
7.49
7.49
7.48
7.46
7.45
7.43
7.37
7.35
7.34
7.32
7.31
7.30
7.29
7.26
7.25
7.24
3.35 HDO
2.49 DMSO
Ph
Ph
N+
PF6-
3pa
1.00
1.00
1.01
1.00
1.00
1.01
6.11
3.14
2.02
3.00
f1 (ppm)

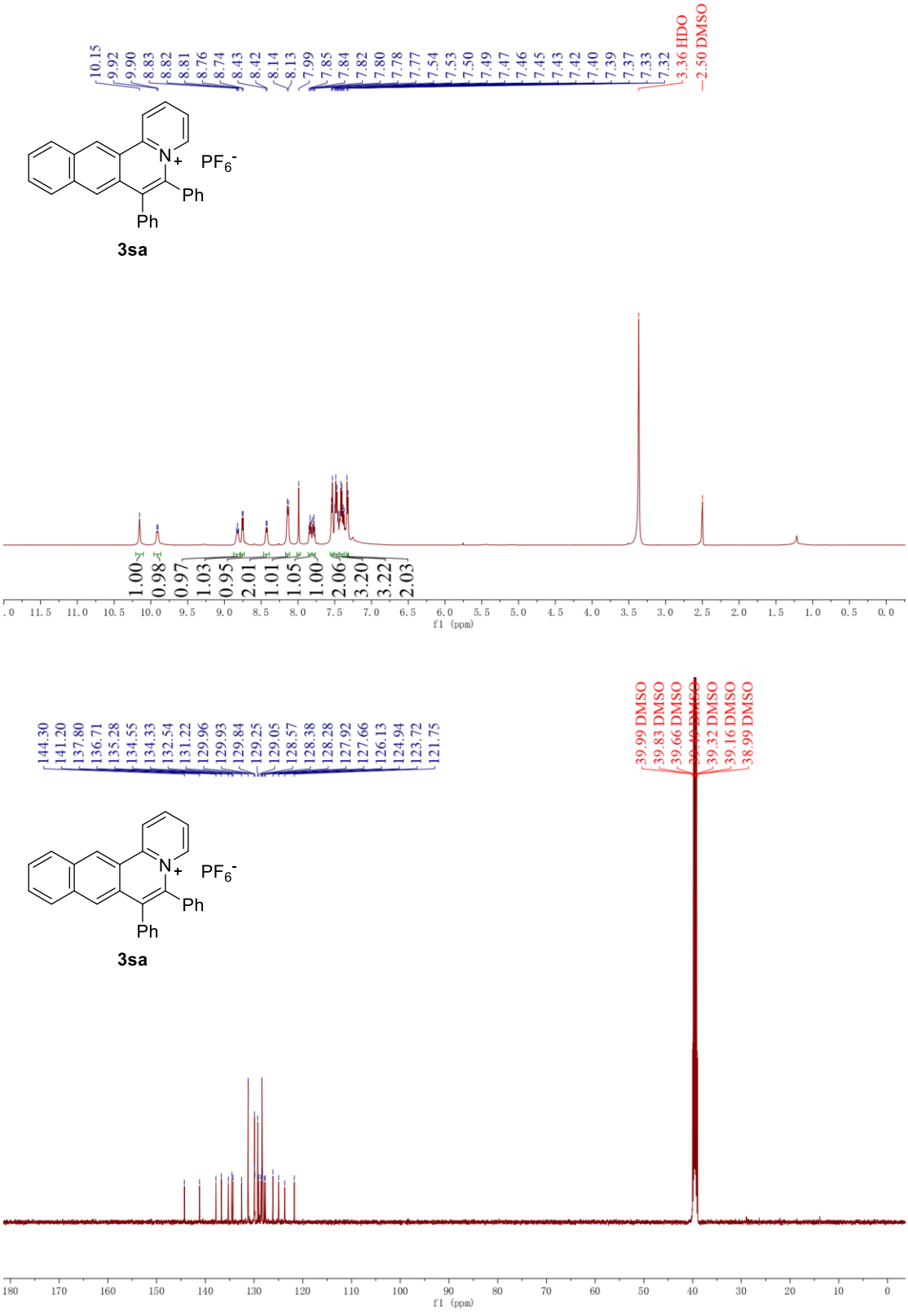

141.68
141.41
137.94
135.48
135.17
134.42
133.76
131.73
131.06
130.97
130.76
130.08
129.86
129.27
128.25
128.17
126.73
125.71
124.57
123.00
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
18.23
Ph
Ph
N+
PF6-
3pa
f1 (ppm)

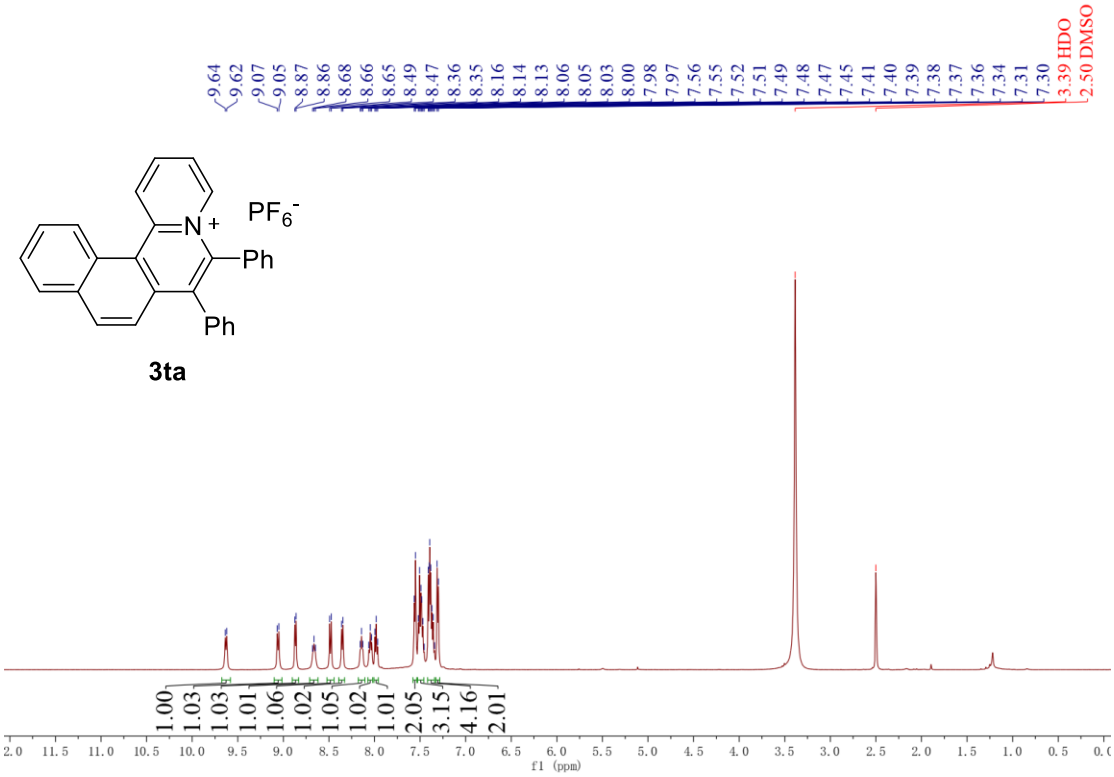

9.82
9.80
9.41
9.39
8.94
8.93
8.92
8.91
8.55
8.55
8.19
8.17
8.16
8.13
8.11
8.10
7.53
7.52
7.49
7.48
7.47
7.46
7.38
7.37
7.35
7.34
7.33
7.31
7.24
7.22
3.34 HDO
2.48 DMSO
Ph
Ph
N+
PF6-
Cl
3qa
0.99
1.01
0.98
0.97
1.00
0.98
6.05
3.11
2.03
f1 (ppm)

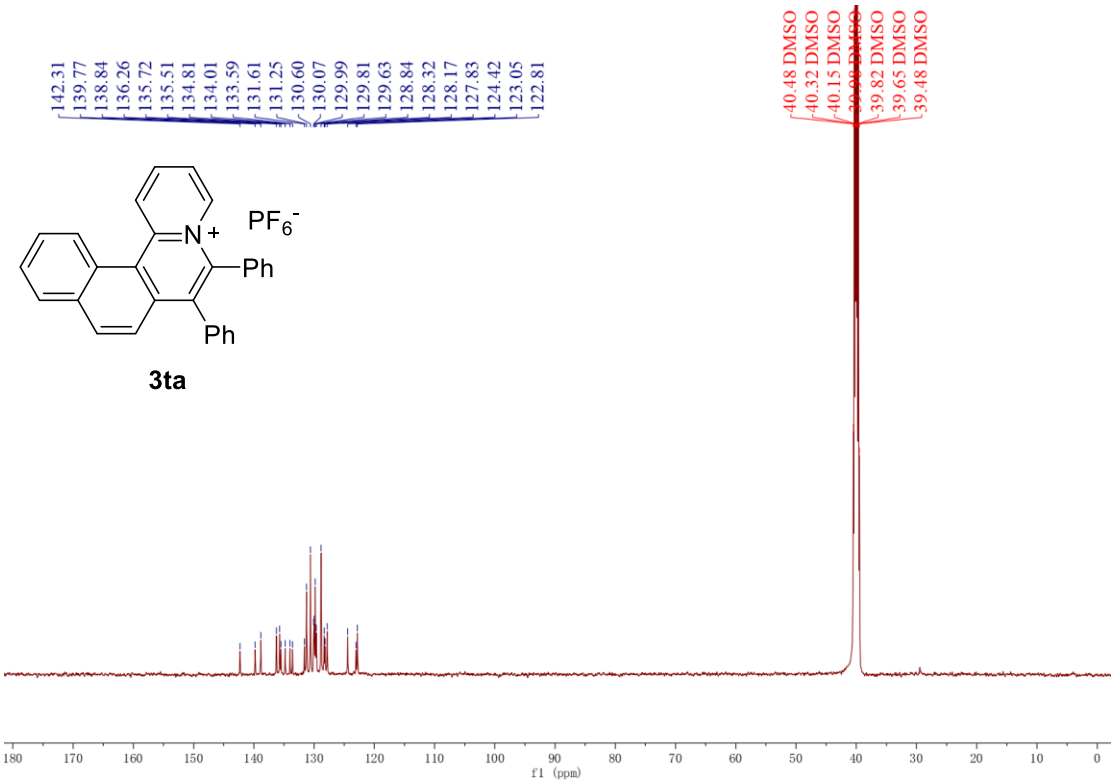

142.19
139.77
137.97
136.38
134.66
134.01
133.90
132.10
131.26
130.97
130.49
129.74
129.45
128.39
126.90
126.21
124.86
124.40
39.96 DMSO
39.79 DMSO
39.62 DMSO
39.29 DMSO
39.12 DMSO
38.95 DMSO
Ph
Ph
N+
PF6-
Cl
3qa
f1 (ppm)

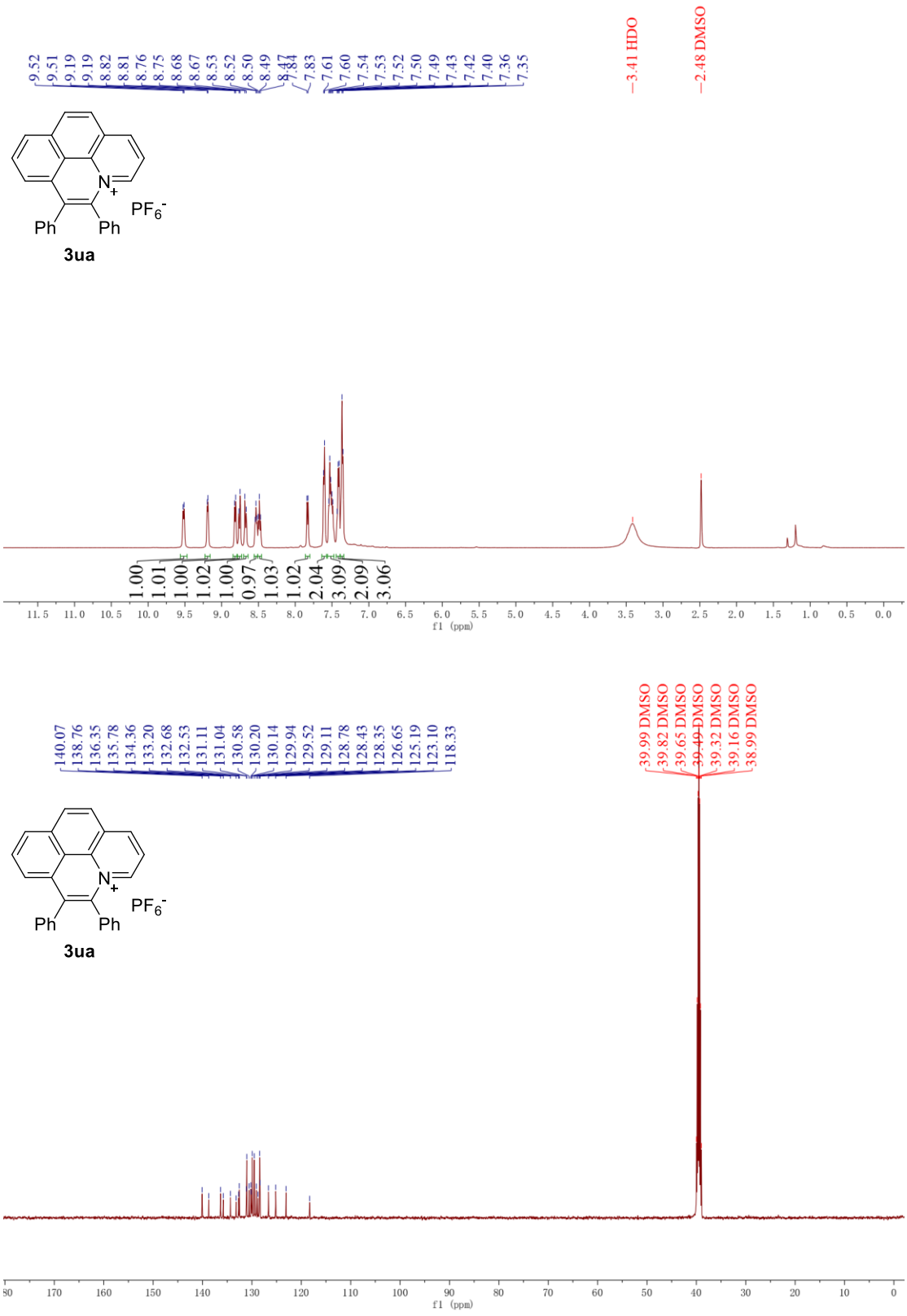

9.58
9.57
9.00
8.98
8.60
8.58
8.57
8.55
8.53
7.96
7.95
7.93
7.84
7.82
7.45
7.44
7.42
7.41
7.39
7.38
7.21
7.20
7.19
7.18
6.01
3.35 HDO
2.49 DMSO
2.49 DMSO
2.48 DMSO
2.48 DMSO
2.48 DMSO
O
O
Ph
Ph
N+
PF6-
3ra
1.00
1.03
1.07
1.02
1.07
0.99
5.08
5.06
2.00
f1 (ppm)


151.65
143.70
143.20
139.98
138.38
136.66
135.56
131.19
131.12
130.84
129.86
129.48
129.08
127.74
127.31
123.57
123.31
122.37
119.24
116.39
113.12
103.07
39.98 DMSO
39.81 DMSO
39.65 DMSO
39.48 DMSO
39.31 DMSO
39.15 DMSO
38.98 DMSO
O
O
Ph
Ph
N+
PF6-
3ra
f1 (ppm)

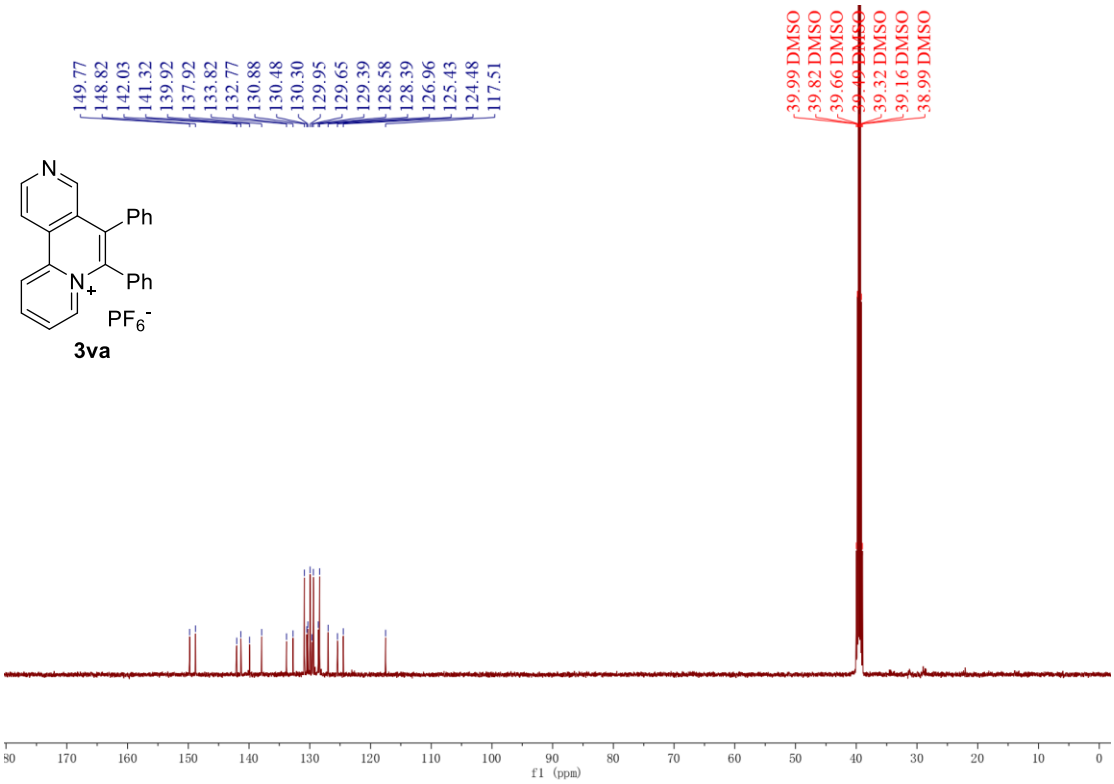

10.15
9.92
9.90
8.83
8.82
8.81
8.76
8.74
8.43
8.42
8.14
8.13
7.99
7.85
7.84
7.82
7.80
7.78
7.77
7.54
7.53
7.50
7.49
7.47
7.46
7.45
7.43
7.42
7.40
7.39
7.37
7.33
7.32
3.36 HDO
2.50 DMSO
N+
PF6-
Ph
Ph
3sa
1.00
0.98
0.97
1.03
0.95
2.01
1.01
1.05
1.00
2.06
3.20
3.22
2.03
f1 (ppm)
144.30
141.20
137.80
136.71
135.28
134.55
134.33
132.54
131.22
129.96
129.93
129.84
129.25
129.05
128.57
128.38
128.28
127.92
127.66
126.13
124.94
123.72
121.75
39.99 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
N+
PF6-
Ph
Ph
3sa
f1 (ppm)

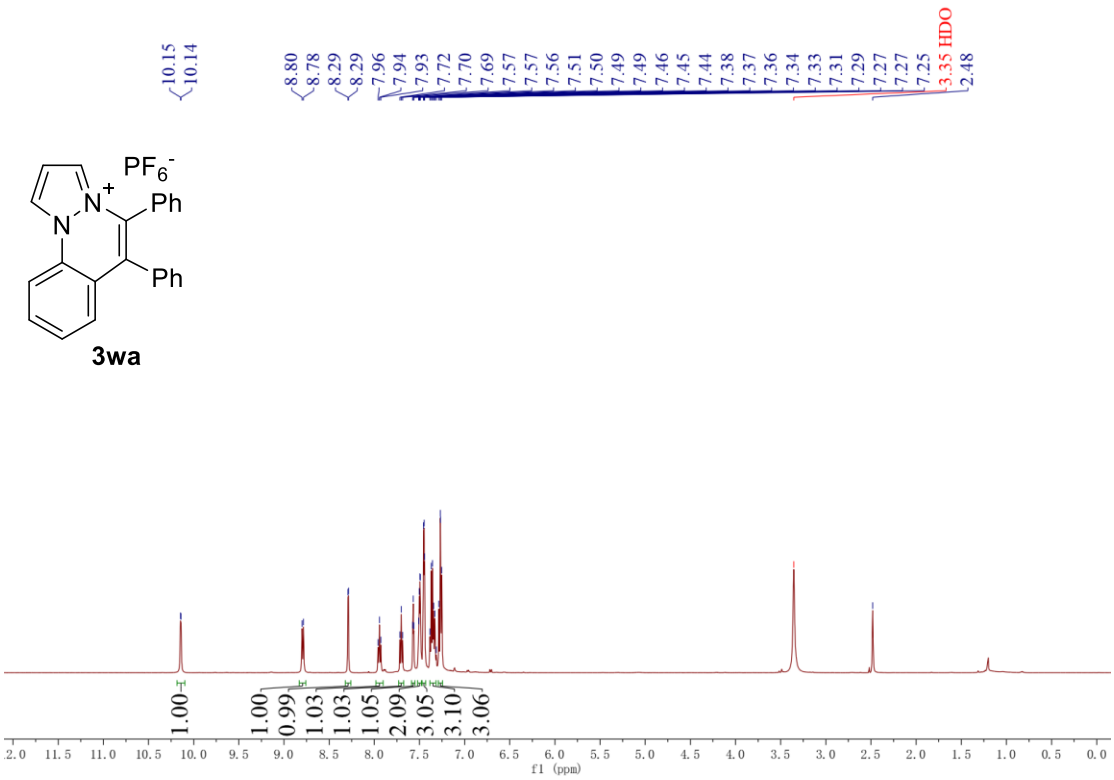

9.64
9.62
9.07
9.05
8.87
8.86
8.68
8.66
8.65
8.49
8.47
8.36
8.35
8.16
8.14
8.13
8.06
8.05
8.03
8.00
7.98
7.97
7.56
7.55
7.52
7.51
7.49
7.48
7.47
7.45
7.41
7.40
7.39
7.38
7.37
7.36
7.34
7.31
7.30
3.39 HDO
2.50 DMSO
N+
PF6-
Ph
Ph
3ta
1.00
1.03
1.03
1.01
1.06
1.02
1.05
1.02
1.01
2.05
3.15
4.16
2.01
f1 (ppm)

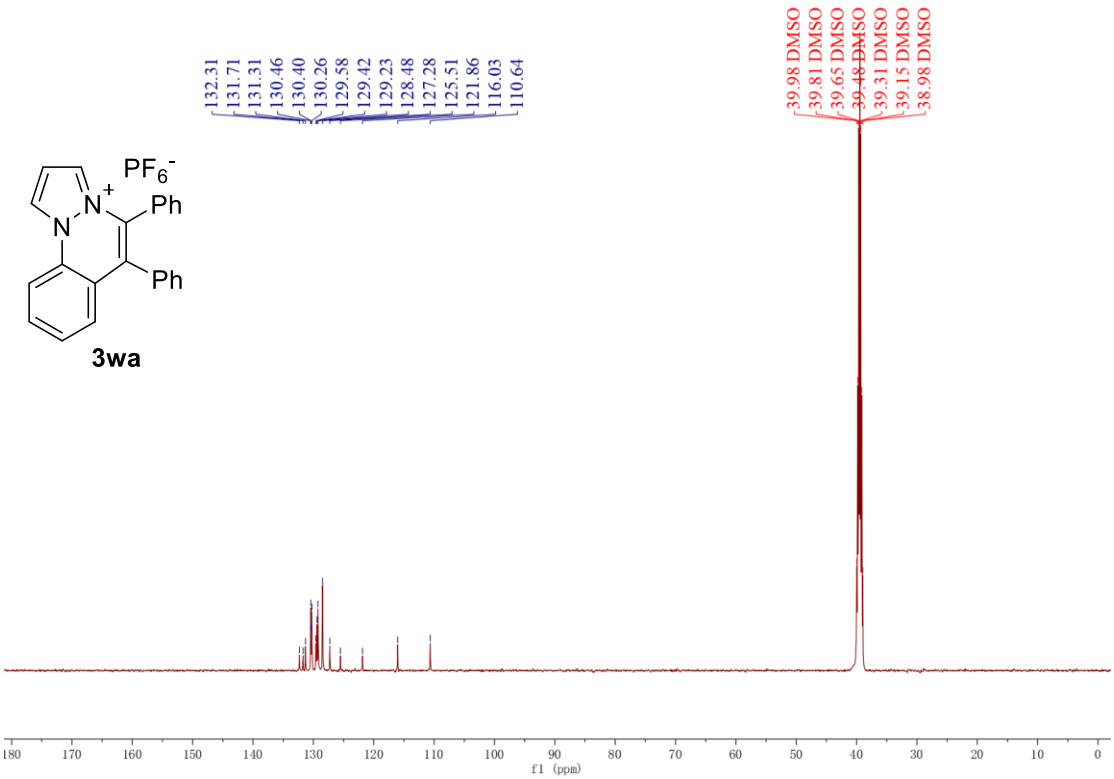

142.31
139.77
138.84
136.26
135.72
135.51
134.81
134.01
133.59
131.61
131.25
130.60
130.07
129.99
129.81
129.63
128.84
128.32
128.17
127.83
124.42
123.05
122.81
40.48 DMSO
40.32 DMSO
40.15 DMSO
39.82 DMSO
39.65 DMSO
39.48 DMSO
N+
PF6-
Ph
Ph
3ta
f1 (ppm)

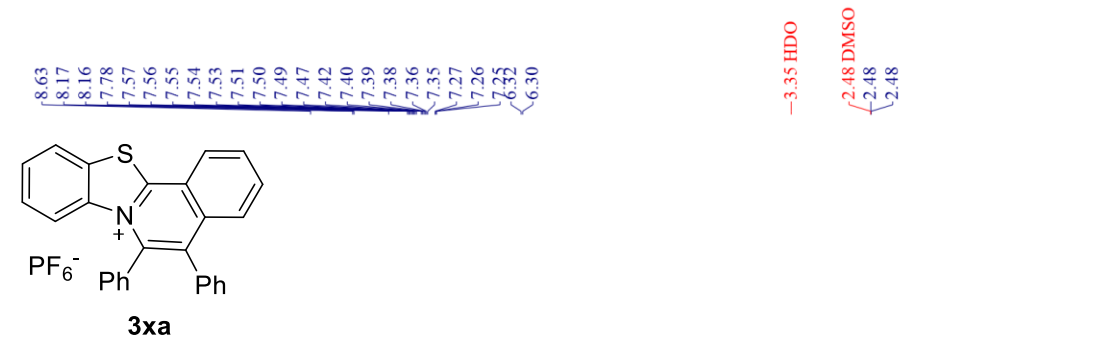

9.52
9.51
9.19
9.19
8.82
8.81
8.76
8.75
8.68
8.67
8.53
8.52
8.50
8.49
8.47
8.84
7.83
7.61
7.60
7.54
7.53
7.52
7.50
7.49
7.43
7.42
7.40
7.36
7.35
3.41 HDO
2.48 DMSO
N+
PF6-
Ph
Ph
3ua
1.00
1.01
1.00
1.02
1.00
0.97
1.03
1.02
2.04
3.09
2.09
3.06
f1 (ppm)
140.07
138.76
136.35
135.78
134.36
133.20
132.68
132.53
131.11
131.04
130.58
130.20
130.14
129.94
129.52
129.11
128.78
128.43
128.35
126.65
125.19
123.10
118.33
39.99 DMSO
39.82 DMSO
39.65 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
N+
PF6-
Ph
Ph
3ua
f1 (ppm)

9.91
9.89
9.24
9.23
9.20
9.19
8.92
8.91
8.90
8.88
8.86
8.79
8.30
8.29
8.28
7.50
7.49
7.49
7.48
7.47
7.46
7.40
7.39
7.37
7.36
7.35
7.30
7.29
3.37 HDO
2.48 DMSO
N
Ph
Ph
N+
PF6-
3va
1.00
0.95
1.00
2.01
1.01
0.99
5.07
3.18
2.03
f1 (ppm)

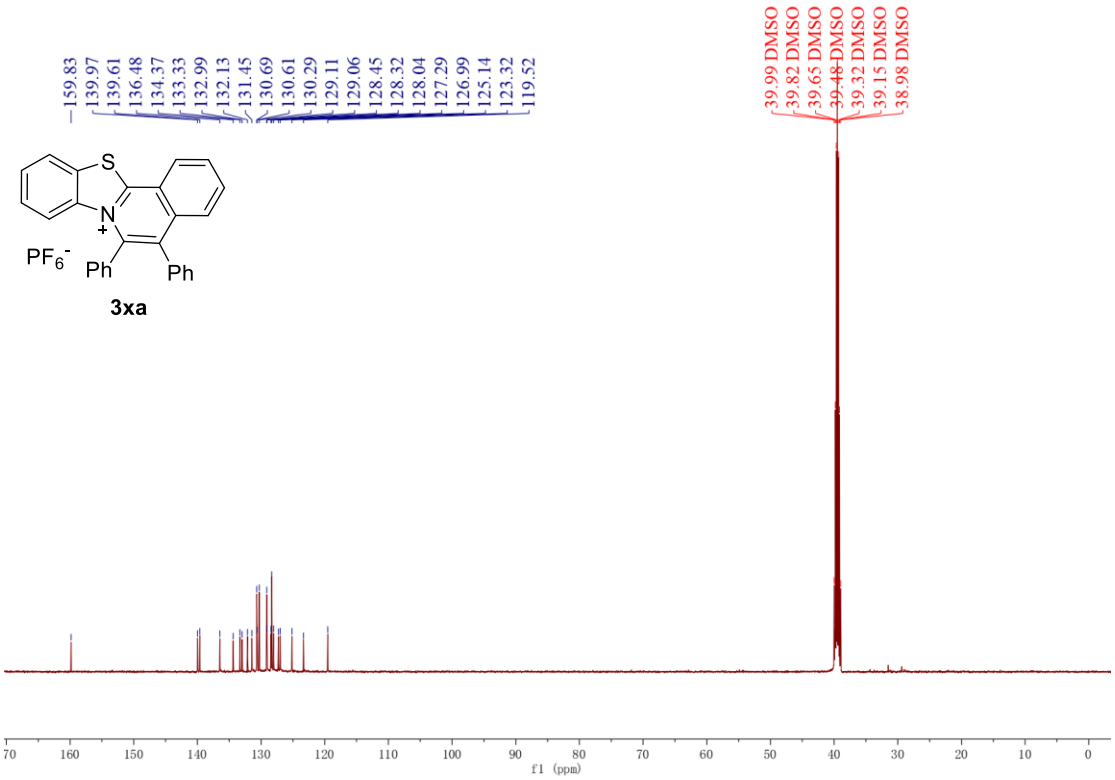

149.77
148.82
142.03
141.32
139.92
137.92
133.82
132.77
130.88
130.48
130.30
129.95
129.65
129.39
128.58
128.39
126.96
125.43
124.48
117.51
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
N
Ph
Ph
N+
PF6-
3va
f1 (ppm)


10.15
10.14
8.80
8.78
8.29
8.29
7.96
7.94
7.93
7.72
7.70
7.69
7.57
7.57
7.56
7.51
7.50
7.49
7.49
7.46
7.45
7.44
7.38
7.37
7.36
7.34
7.33
7.31
7.29
7.27
7.27
7.25
3.35 HDO
2.48
PF6-
N+
N
Ph
Ph
3wa
1.00
1.00
0.99
1.03
1.03
1.05
2.09
3.05
3.10
3.06
f1 (ppm)

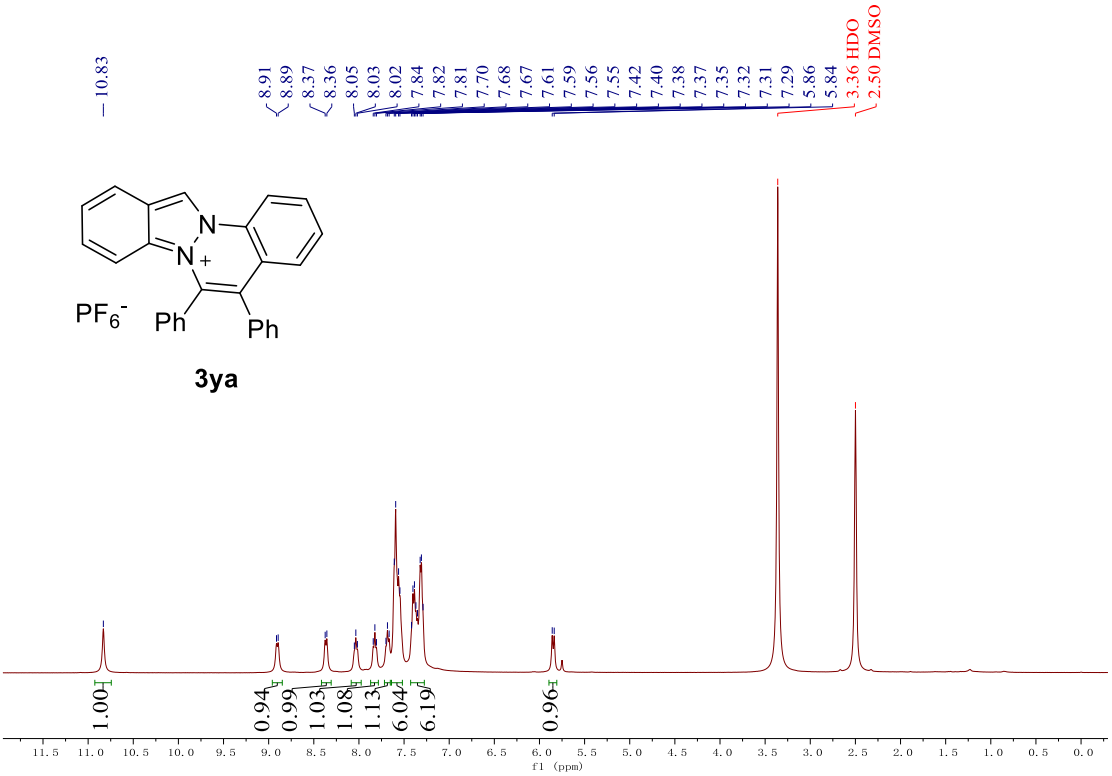

132.31
131.71
131.31
130.46
130.40
130.26
129.58
129.42
129.23
128.48
127.28
125.51
121.86
116.03
110.64
39.98 DMSO
39.81 DMSO
39.65 DMSO
39.48 DMSO
39.31 DMSO
39.15 DMSO
38.98 DMSO
PF6-
N+
N
Ph
Ph
3wa
f1 (ppm)

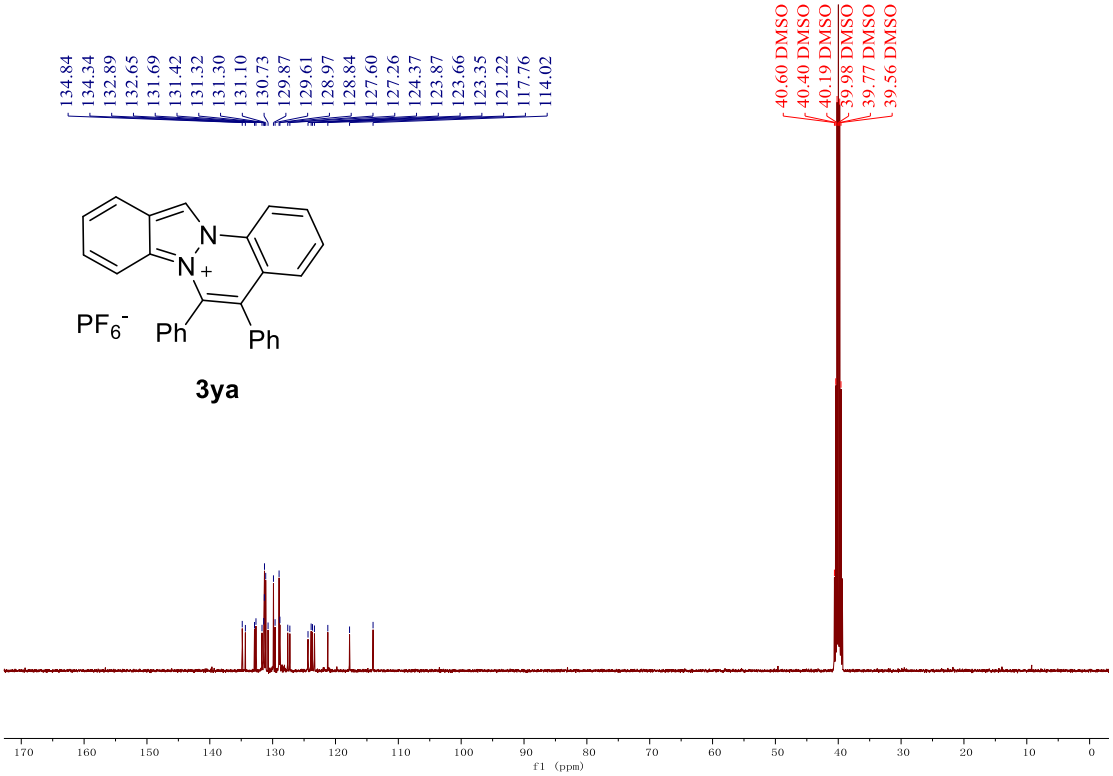

8.63
8.17
8.16
7.78
7.57
7.56
7.55
7.54
7.53
7.51
7.50
7.49
7.47
7.42
7.40
7.39
7.38
7.36
7.35
7.27
7.26
7.25
6.32
6.30
3.35 HDO
2.48 DMSO
2.48
2.48
S
N
+
PF6-
Ph
Ph
0.96
0.97
2.03
1.05
6.14
4.21
2.06
0.98
f1 (ppm)

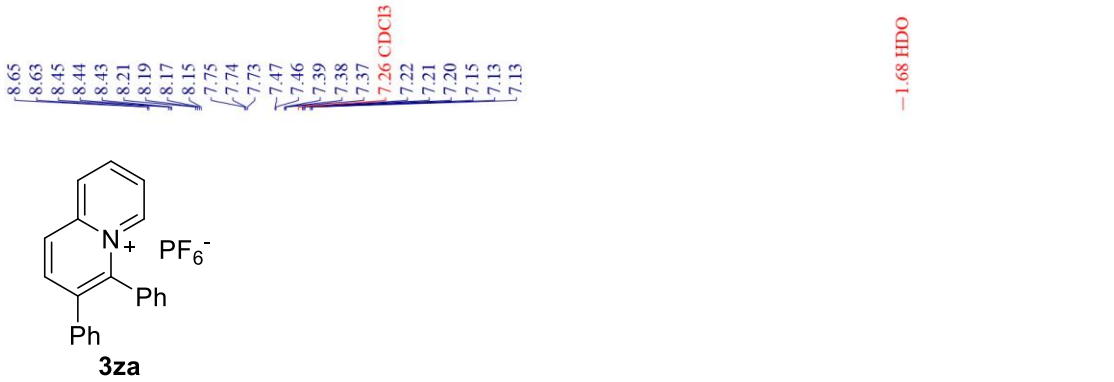
3xa

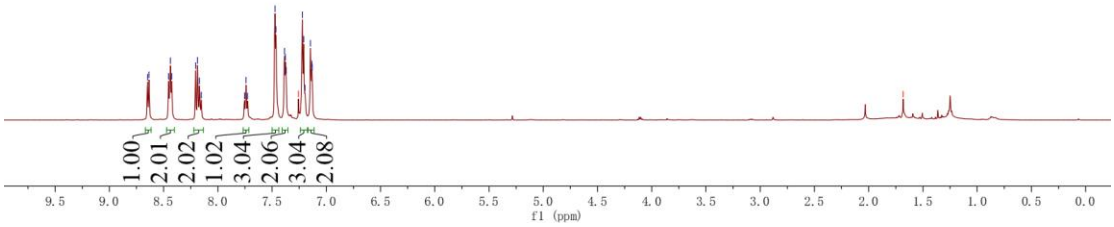

159.83
139.97
139.61
136.48
134.37
133.33
132.99
132.13
131.45
130.69
130.61
130.29
129.11
129.06
128.45
128.32
128.04
127.29
126.99
125.14
123.32
119.52
39.99 DMSO
39.82 DMSO
39.65 DMSO
39.48 DMSO
39.32 DMSO
39.15 DMSO
38.98 DMSO
S
N
+
PF6-
Ph
Ph
f1 (ppm)

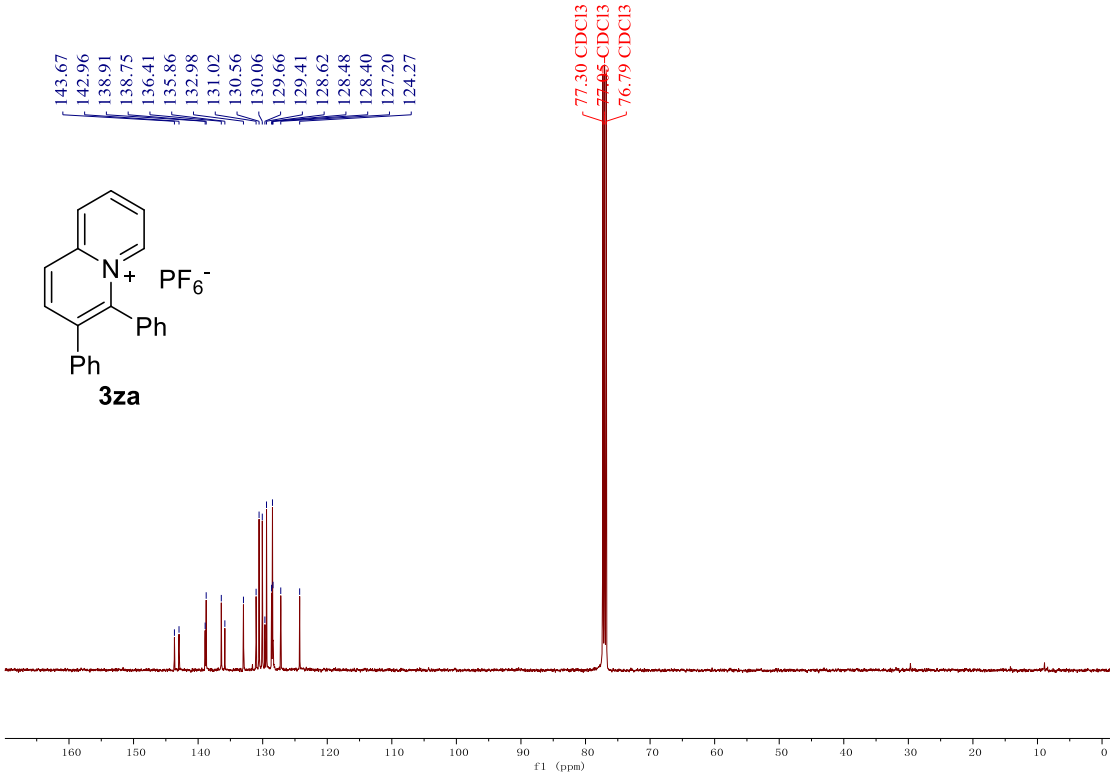
3xa

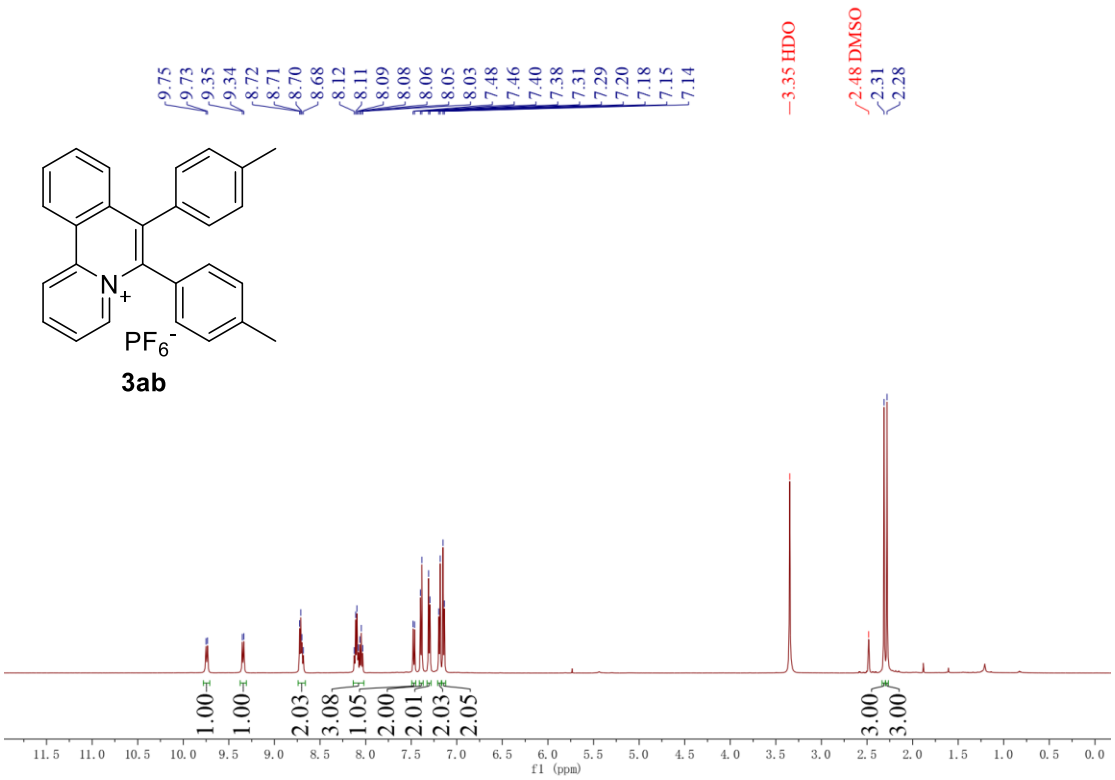

10.83
8.91
8.89
8.37
8.36
8.05
8.03
8.02
7.84
7.82
7.81
7.70
7.68
7.67
7.61
7.59
7.56
7.55
7.42
7.40
7.38
7.37
7.35
7.32
7.31
7.29
5.86
5.84
3.36 HDO
2.50 DMSO
N
N+
PF6-
Ph
Ph
3ya
1.00
0.94
0.99
1.03
1.08
1.13
6.04
6.19
0.96
f1 (ppm)

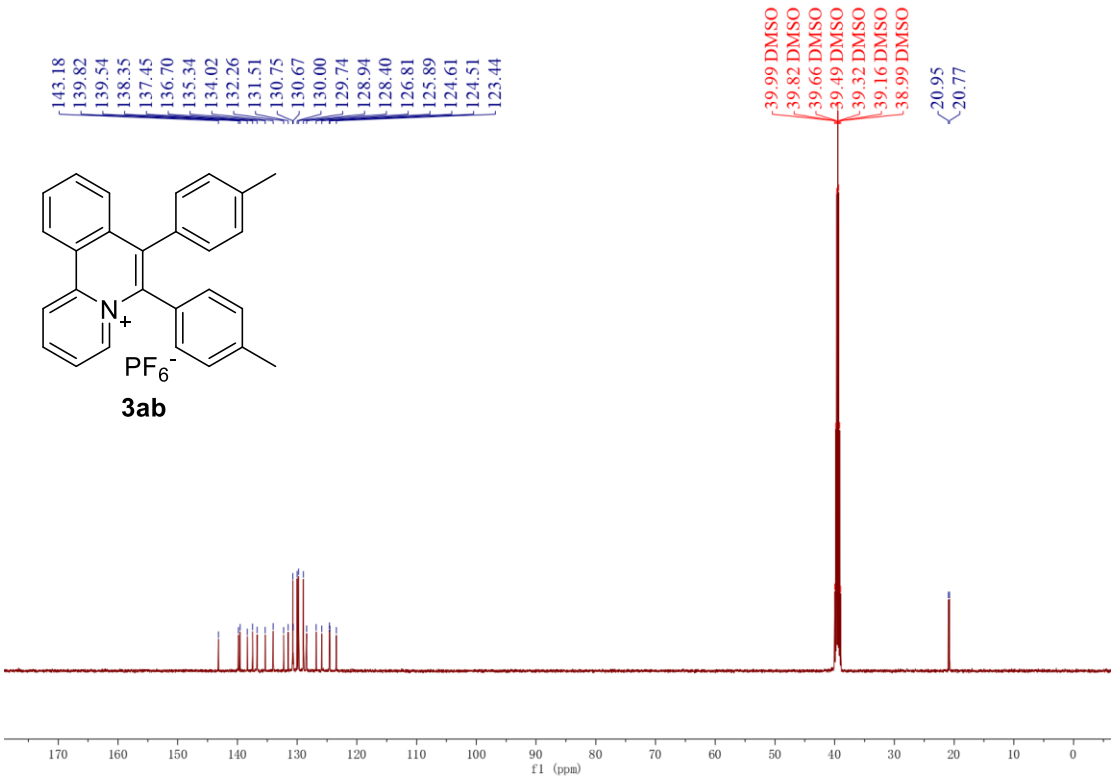

134.84
134.34
132.89
132.65
131.69
131.42
131.32
131.30
131.10
130.73
129.87
129.61
128.97
128.84
127.60
127.26
124.37
123.87
123.66
123.35
121.22
117.76
114.02
40.60 DMSO
40.40 DMSO
40.19 DMSO
39.98 DMSO
39.77 DMSO
39.56 DMSO
N
N+
PF6-
Ph
Ph
3ya
f1 (ppm)

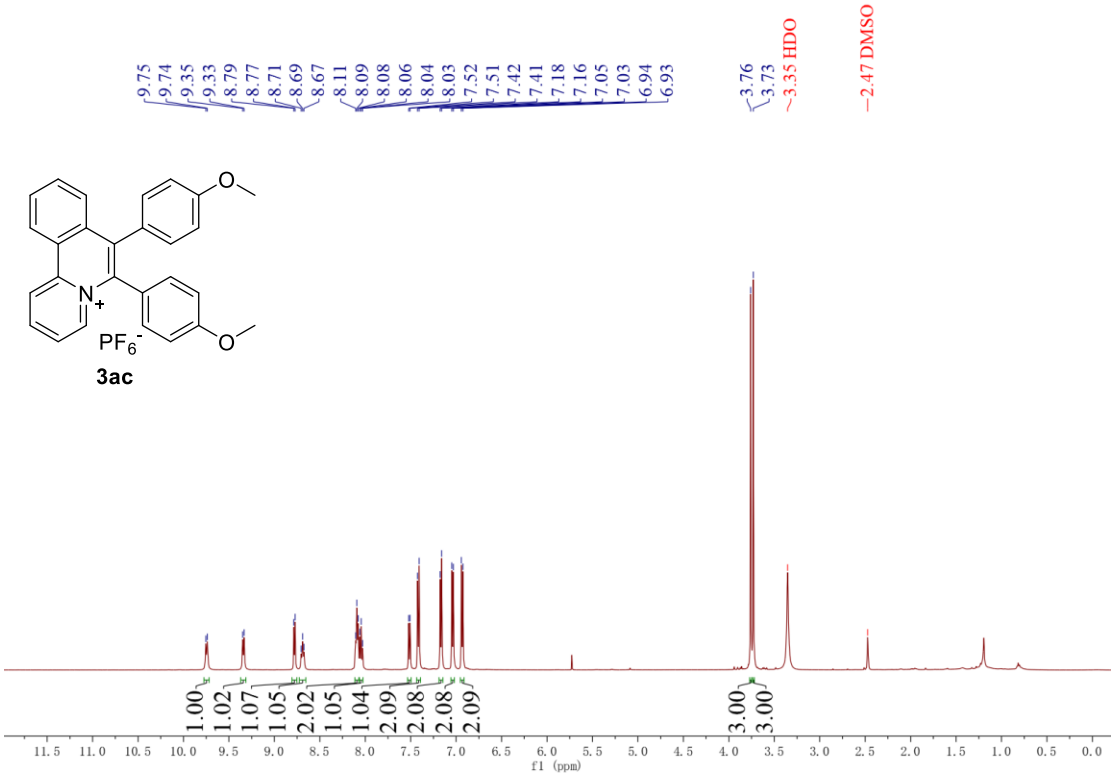

8.65
8.63
8.45
8.44
8.43
8.21
8.19
8.17
8.15
7.75
7.74
7.73
7.47
7.46
7.39
7.38
7.37
7.26 CDCl3
7.22
7.21
7.20
7.15
7.13
7.13
1.68 HDO
N+
PF6-
Ph
Ph
3za

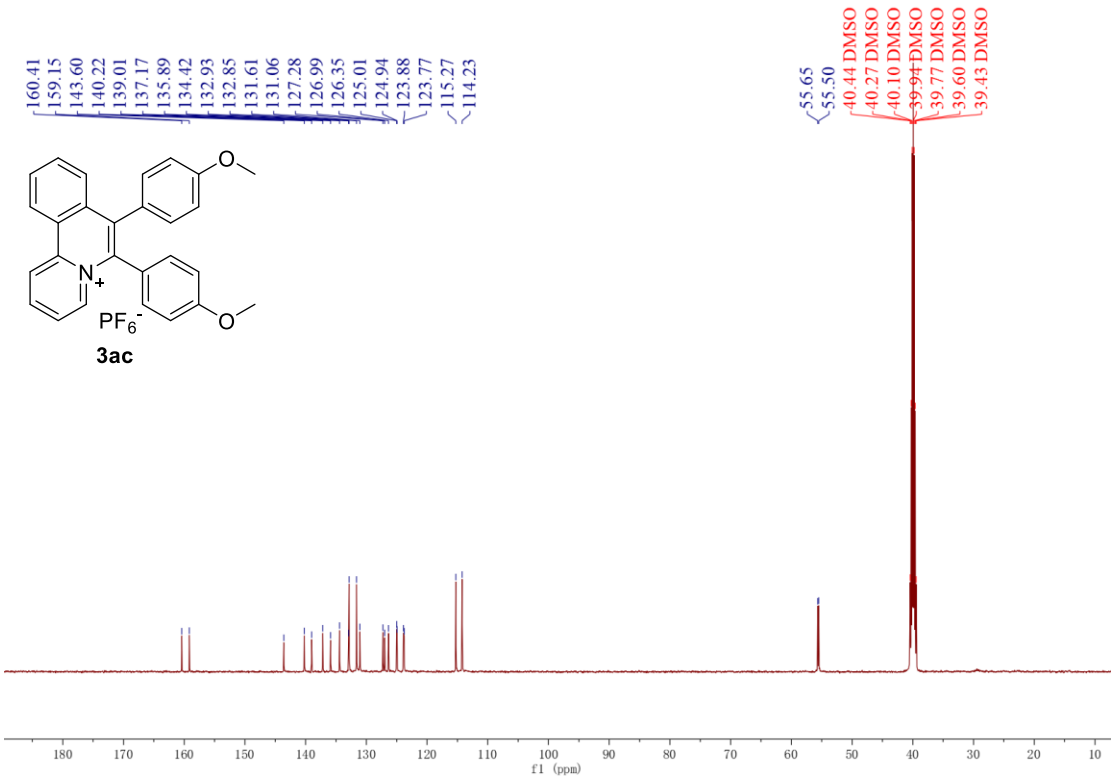

1.00
2.01
2.02
1.02
3.04
2.06
3.04
2.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

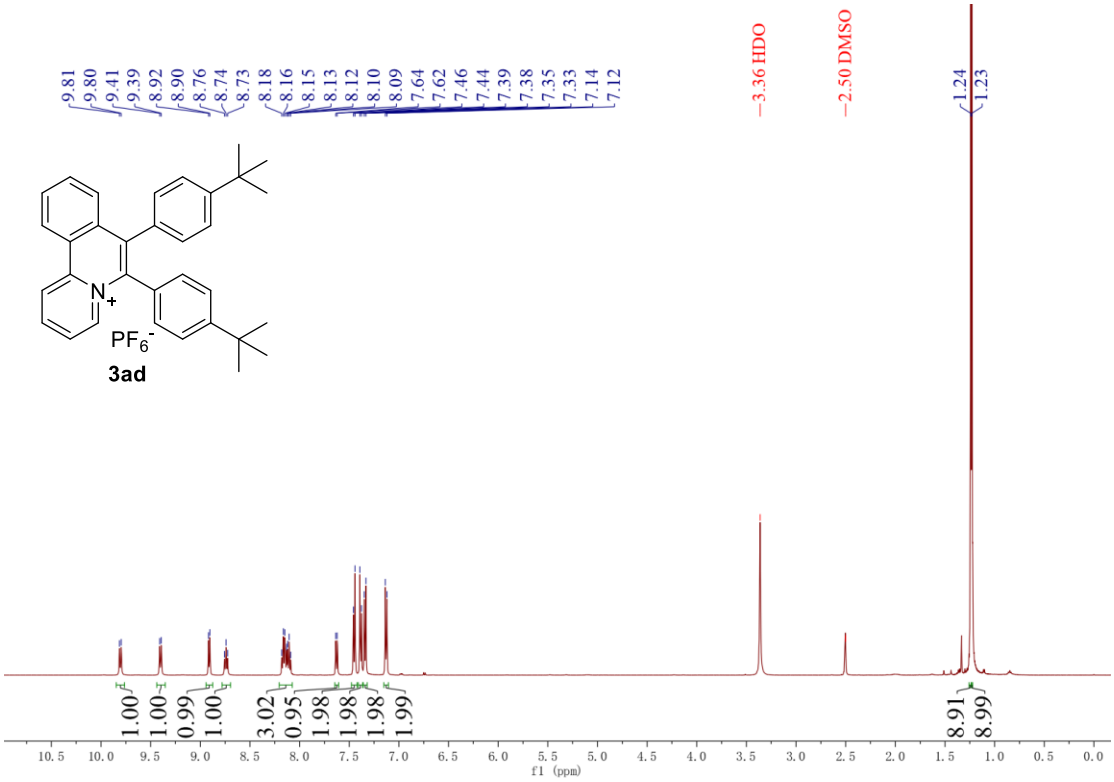

143.67
142.96
138.91
138.75
136.41
135.86
132.98
131.02
130.56
130.06
129.66
129.41
128.62
128.48
128.40
127.20
124.27
77.30 CDCl3
77.05 CDCl3
76.79 CDCl3
N+
PF6-
Ph
Ph
3za
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

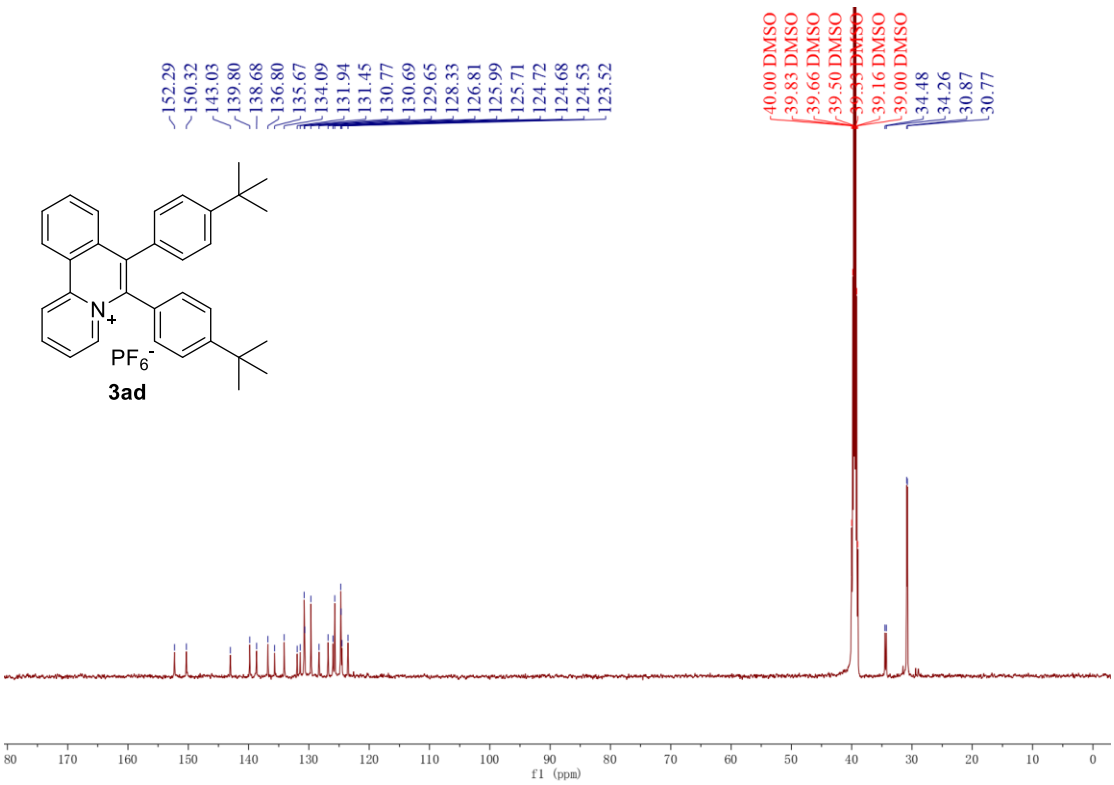

9.75
9.73
9.35
9.34
8.72
8.71
8.70
8.68
8.12
8.11
8.09
8.08
8.06
8.05
8.03
7.48
7.46
7.40
7.38
7.31
7.29
7.20
7.18
7.15
7.14
3.35 HDO
2.48 DMSO
2.31
2.28
N+
PF6-
3ab
1.00
1.00
2.03
3.08
1.05
2.00
2.01
2.03
2.05
3.00
3.00
f1 (ppm)

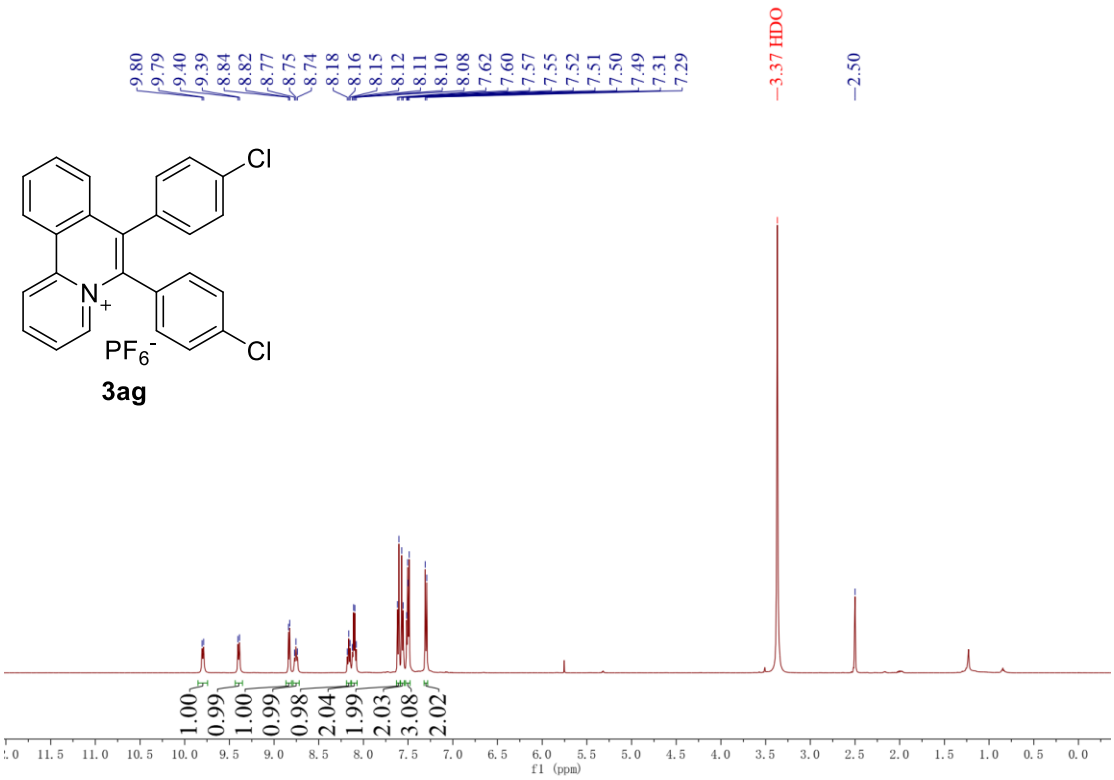

143.18
139.82
139.54
138.35
137.45
136.70
135.34
134.02
132.26
131.51
130.75
130.67
130.00
129.74
128.94
128.40
126.81
125.89
124.61
124.51
123.44
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
20.95
20.77
N+
PF6-
3ab
f1 (ppm)

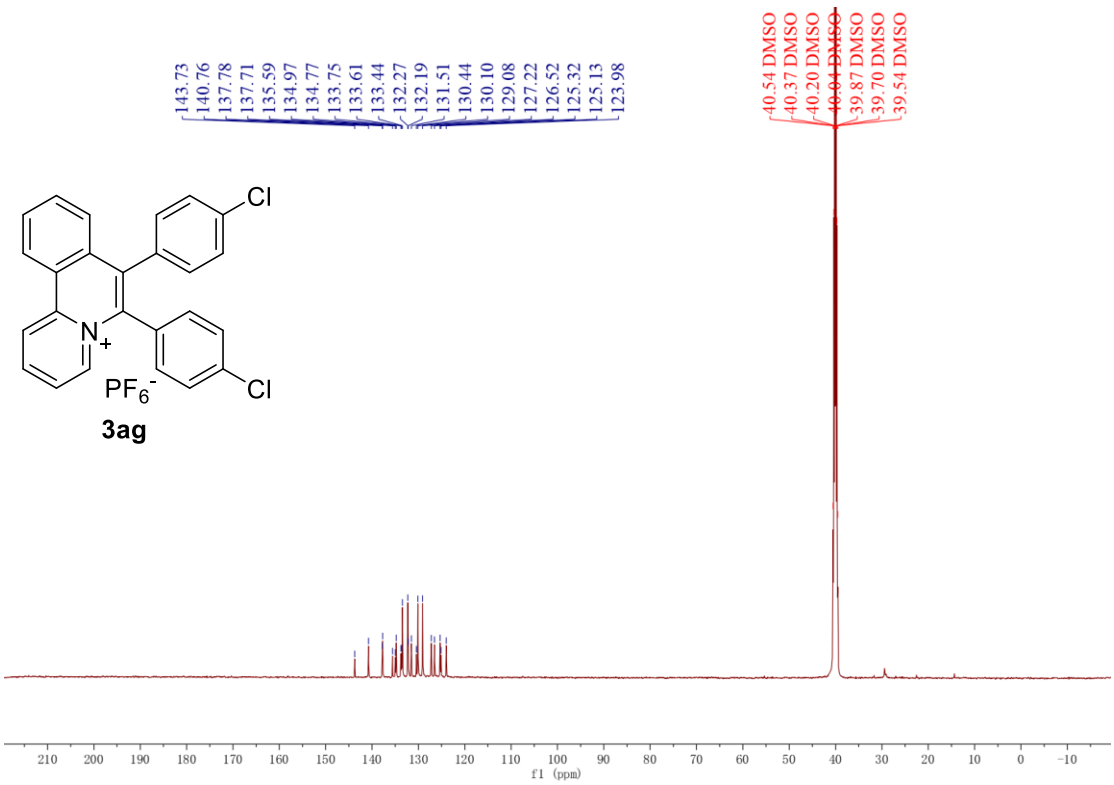

9.75
9.74
9.35
9.33
8.79
8.77
8.71
8.69
8.67
8.11
8.09
8.08
8.06
8.04
8.03
7.52
7.51
7.42
7.41
7.18
7.16
7.05
7.03
6.94
6.93
3.76
3.73
3.35 HDO
2.47 DMSO
O
N+
PF6-
O
3ac
1.00
1.02
1.07
1.05
2.02
1.05
1.04
2.09
2.08
2.08
2.09
3.00
3.00
f1 (ppm)

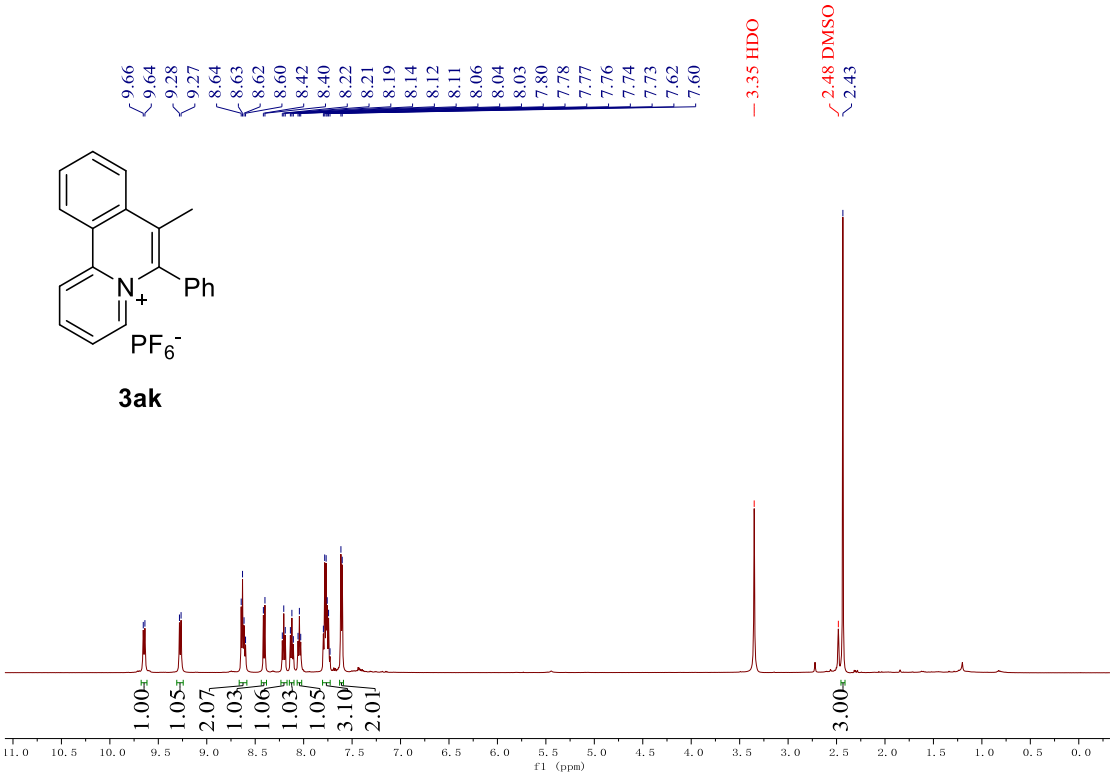

160.41
159.15
143.60
140.22
139.01
137.17
135.89
134.42
132.93
132.85
131.61
131.06
127.28
126.99
126.35
125.01
124.94
123.88
123.77
115.27
114.23
55.65
55.50
40.44 DMSO
40.27 DMSO
40.10 DMSO
39.94 DMSO
39.77 DMSO
39.60 DMSO
39.43 DMSO
O
N+
PF6-
O
3ac
f1 (ppm)

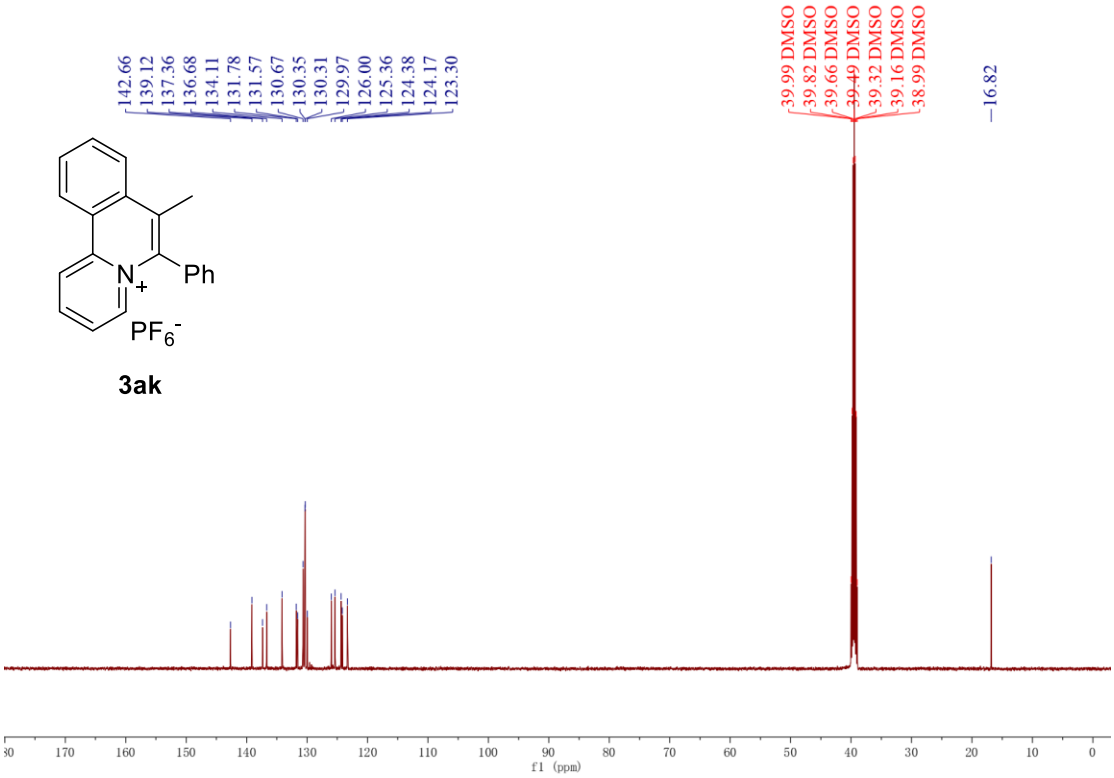

9.81
9.80
9.41
9.39
8.92
8.90
8.76
8.74
8.73
8.18
8.16
8.15
8.13
8.12
8.10
8.09
7.64
7.62
7.46
7.44
7.39
7.38
7.35
7.33
7.14
7.12
3.36 HDO
2.50 DMSO
1.24
1.23
N+
PF6-
3ad
1.00
1.00
0.99
1.00
3.02
0.95
1.98
1.98
1.98
1.99
8.91
8.99
f1 (ppm)

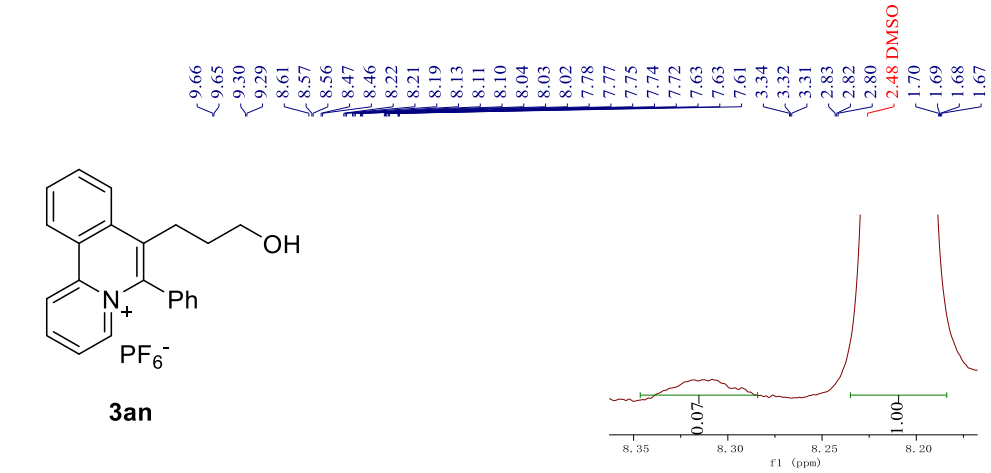

152.29
150.32
143.03
139.80
138.68
136.80
135.67
134.09
131.94
131.45
130.77
130.69
129.65
128.33
126.81
125.99
125.71
124.72
124.68
124.53
123.52
40.00 DMSO
39.83 DMSO
39.66 DMSO
39.50 DMSO
39.33 DMSO
39.16 DMSO
39.00 DMSO
34.48
34.26
30.87
30.77
N+
PF6-
3ad
f1 (ppm)

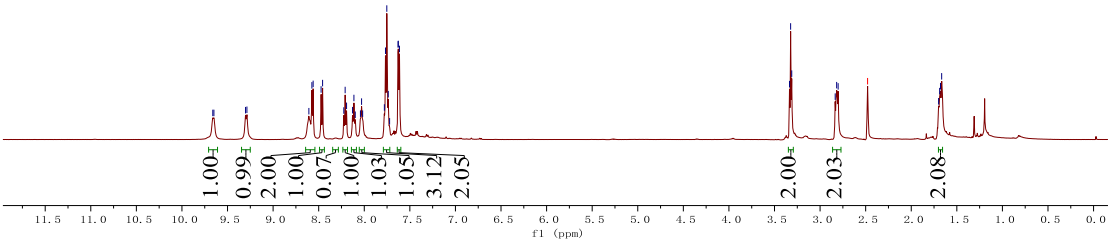

9.80
9.79
9.40
9.39
8.84
8.82
8.77
8.75
8.74
8.18
8.16
8.15
8.12
8.11
8.10
8.08
7.62
7.60
7.57
7.55
7.52
7.51
7.50
7.49
7.31
7.29
3.37 HDO
2.50
Cl
N+
PF6-
Cl
3ag
1.00
0.99
1.00
0.99
0.98
2.04
1.99
2.03
3.08
2.02
f1 (ppm)

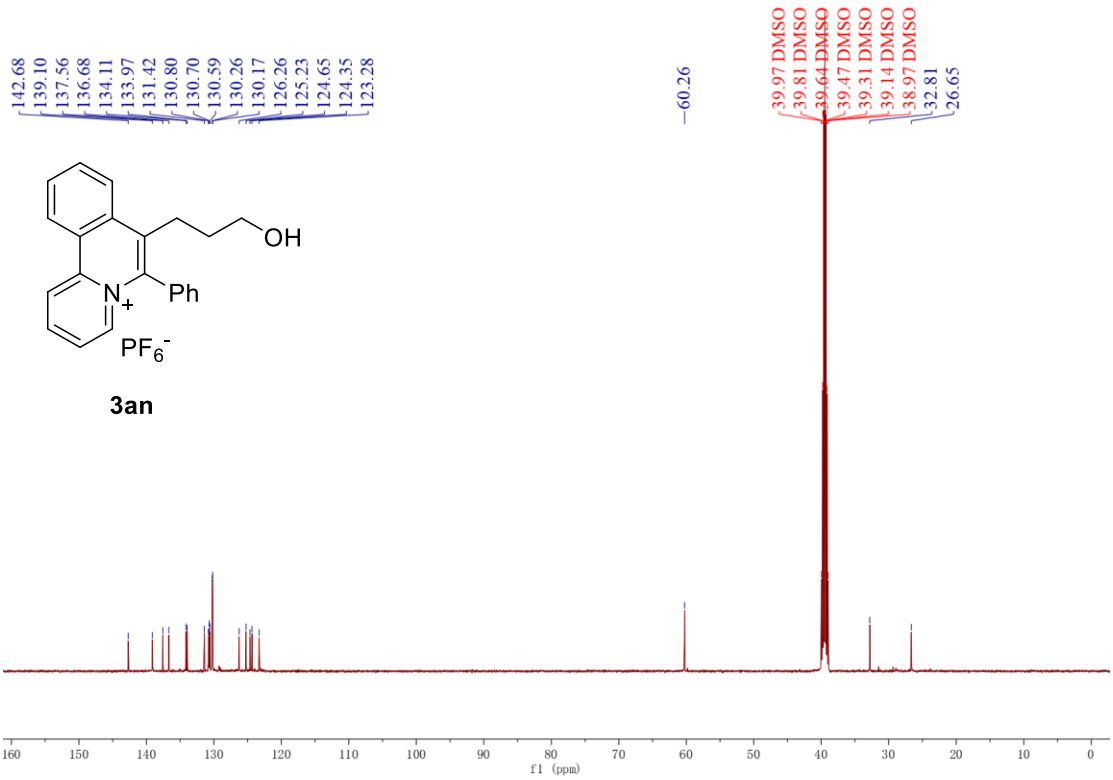

143.73
140.76
137.78
137.71
135.59
134.97
134.77
133.75
133.61
133.44
132.27
132.19
131.51
130.44
130.10
129.08
127.22
126.52
125.32
125.13
123.98
40.54 DMSO
40.37 DMSO
40.20 DMSO
40.04 DMSO
39.87 DMSO
39.70 DMSO
39.54 DMSO
Cl
N+
PF6-
Cl
3ag
f1 (ppm)

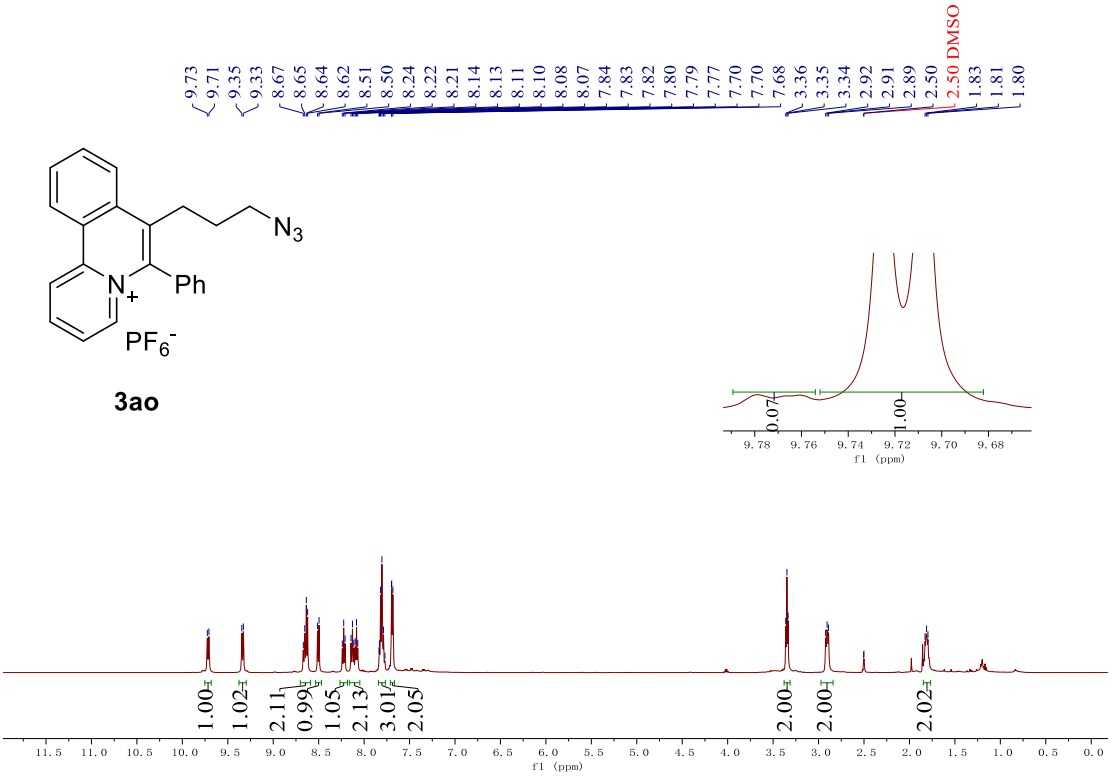

9.66
9.64
9.28
9.27
8.64
8.63
8.62
8.60
8.42
8.40
8.22
8.21
8.19
8.14
8.12
8.11
8.06
8.04
8.03
7.80
7.78
7.77
7.76
7.74
7.73
7.62
7.60
3.35 HDO
2.48 DMSO
2.43
N+
Ph
PF6-
3ak
1.00
1.05
2.07
1.03
1.06
1.03
1.05
3.10
2.01
3.00
f1 (ppm)

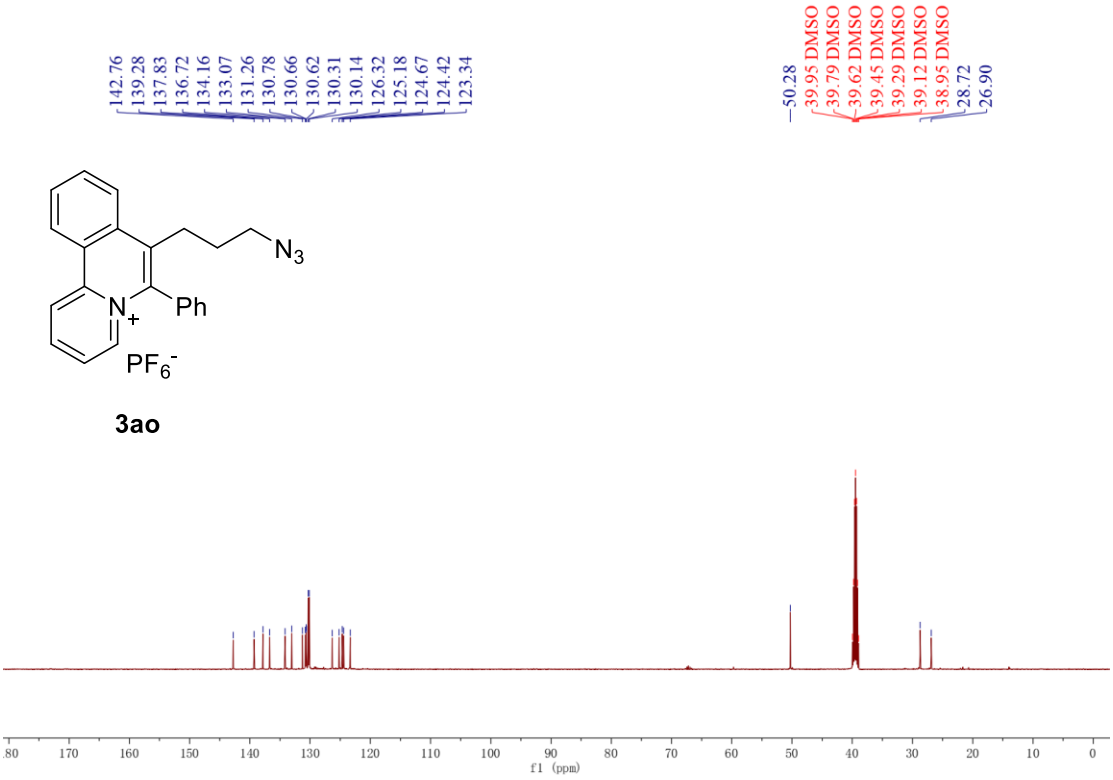

142.66
139.12
137.36
136.68
134.11
131.78
131.57
130.67
130.35
130.31
129.97
126.00
125.36
124.38
124.17
123.30
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
16.82
N+
Ph
PF6-
3ak
f1 (ppm)

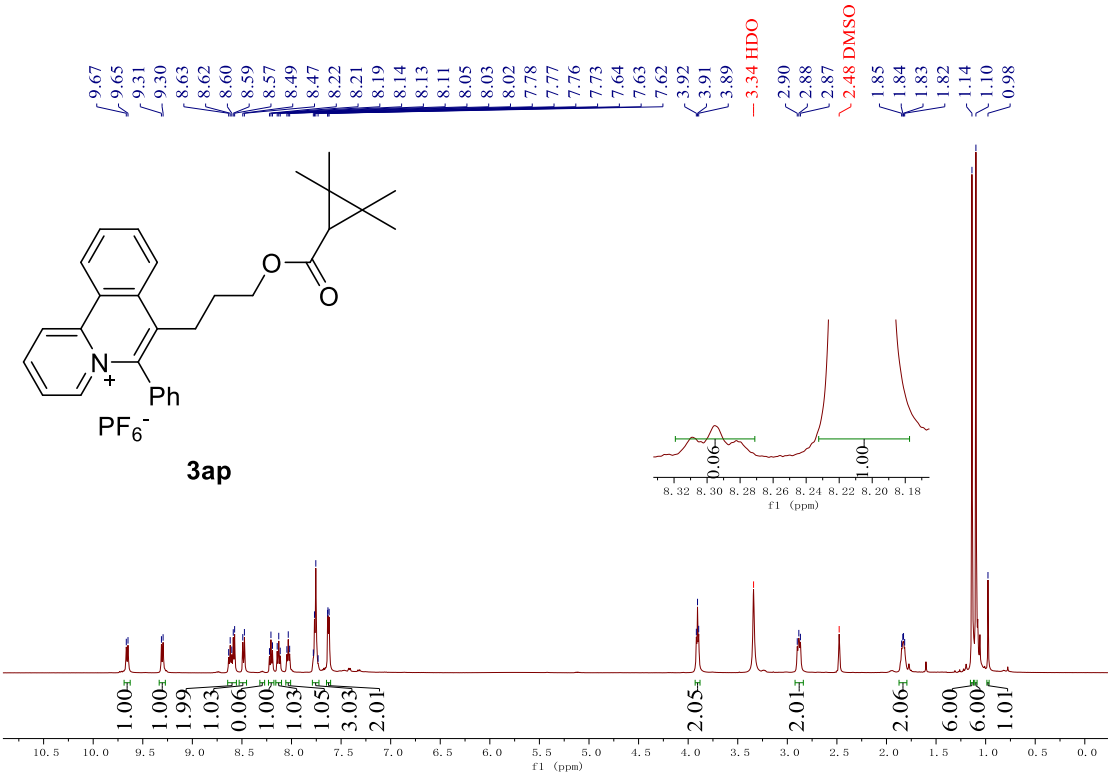

9.66
9.65
9.30
9.29
8.61
8.57
8.56
8.47
8.46
8.22
8.21
8.19
8.13
8.11
8.10
8.04
8.03
8.02
7.78
7.77
7.75
7.74
7.72
7.63
7.63
7.61
3.34
3.32
3.31
2.83
2.82
2.80
2.48 DMSO
1.70
1.69
1.68
1.67
OH
Ph
N+
PF6-
3an
0.07
1.00
8.35
8.30
8.25
8.20
f1 (ppm)

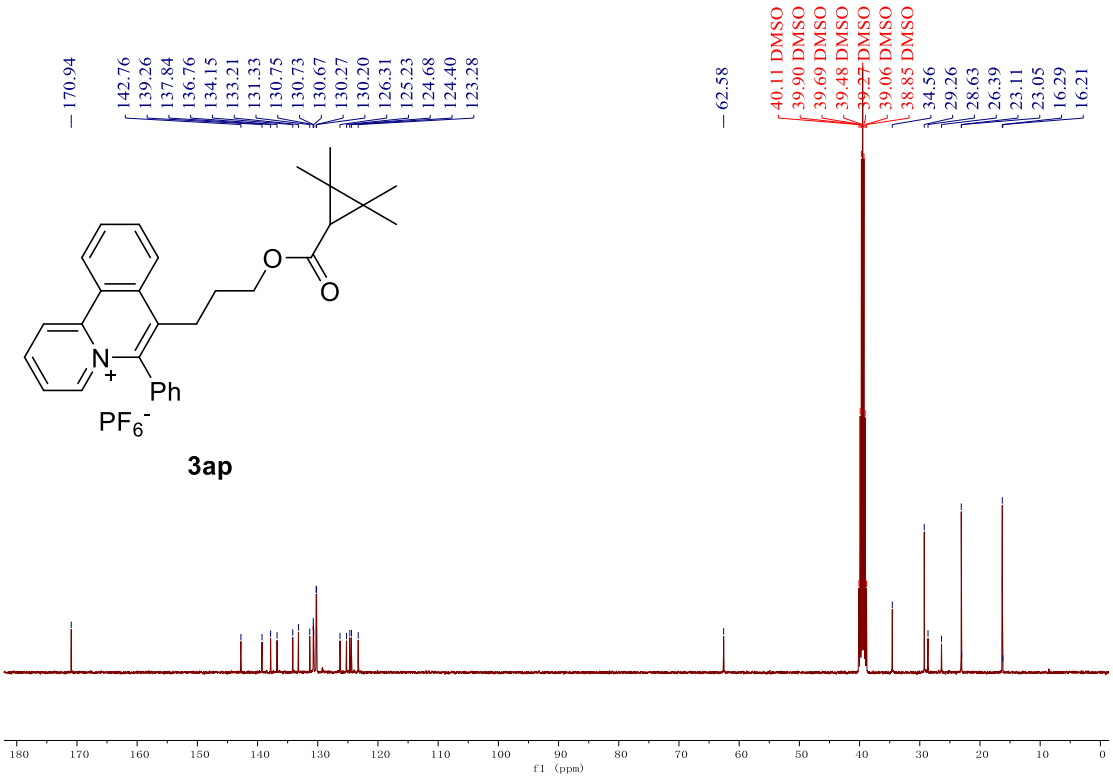

1.00
0.99
2.00
1.00
0.07
1.00
1.03
1.05
3.12
2.05
2.00
2.03
2.08
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

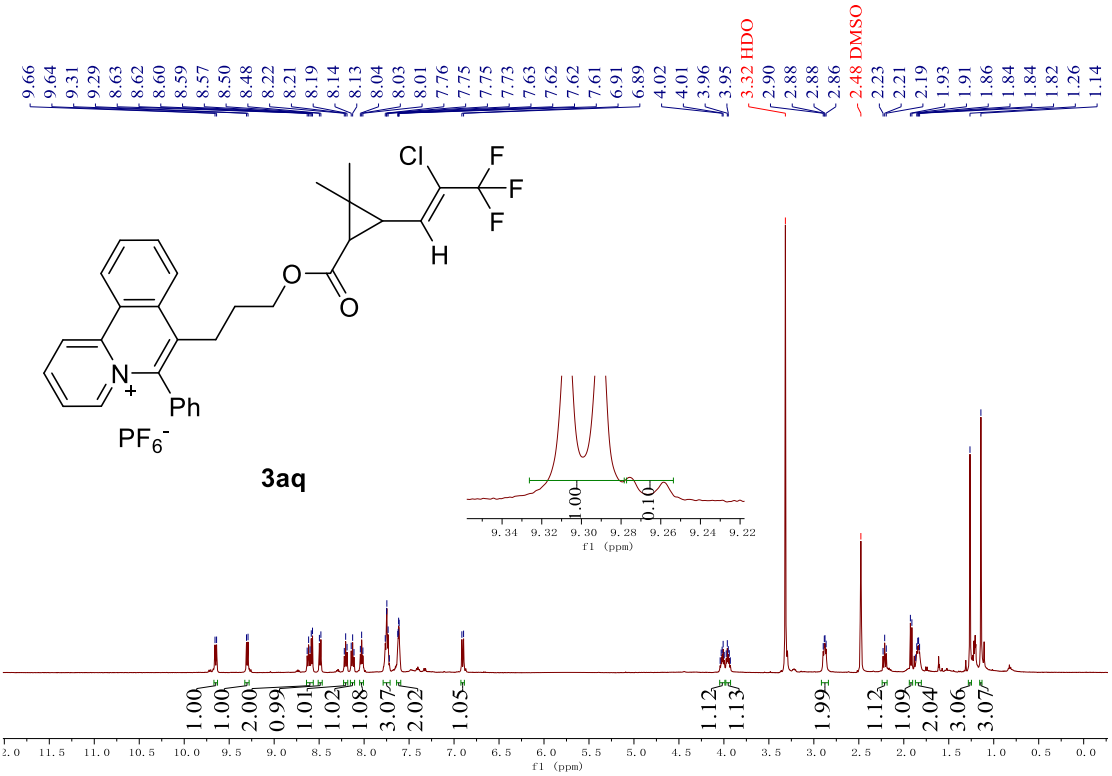

142.68
139.10
137.56
136.68
134.11
133.97
131.42
130.80
130.70
130.59
130.26
130.17
126.26
125.23
124.65
124.35
123.28
60.26
39.97 DMSO
39.81 DMSO
39.64 DMSO
39.47 DMSO
39.31 DMSO
39.14 DMSO
38.97 DMSO
32.81
26.65
OH
Ph
N+
PF6-
3an
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

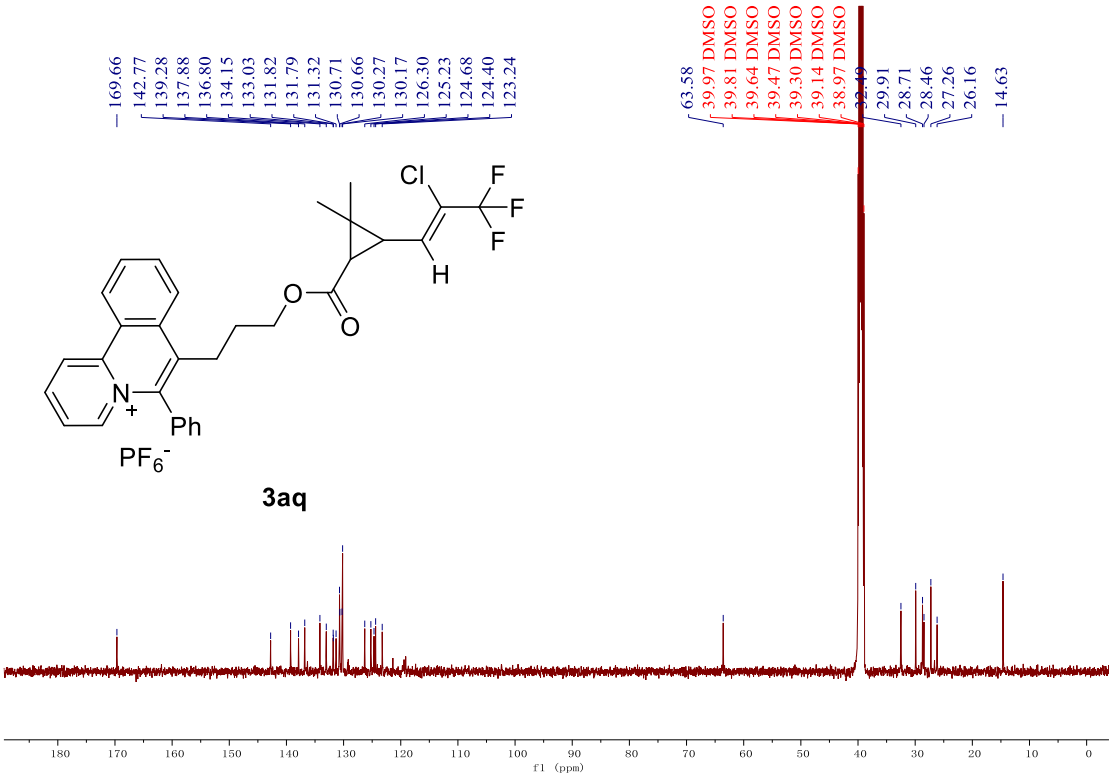

9.73
9.71
9.35
9.33
8.67
8.65
8.64
8.62
8.51
8.50
8.24
8.22
8.21
8.14
8.13
8.11
8.10
8.08
8.07
7.84
7.83
7.82
7.80
7.79
7.77
7.70
7.70
7.68
3.36
3.35
3.34
2.92
2.91
2.89
2.50
2.50 DMSO
1.83
1.81
1.80
N3
Ph
N+
PF6-
3ao
0.07
1.00
9.78
9.76
9.74
9.72
9.70
9.68
f1 (ppm)
1.00
1.02
2.11
0.99
1.05
2.13
3.01
2.05
2.00
2.00
2.02
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
f1 (ppm)

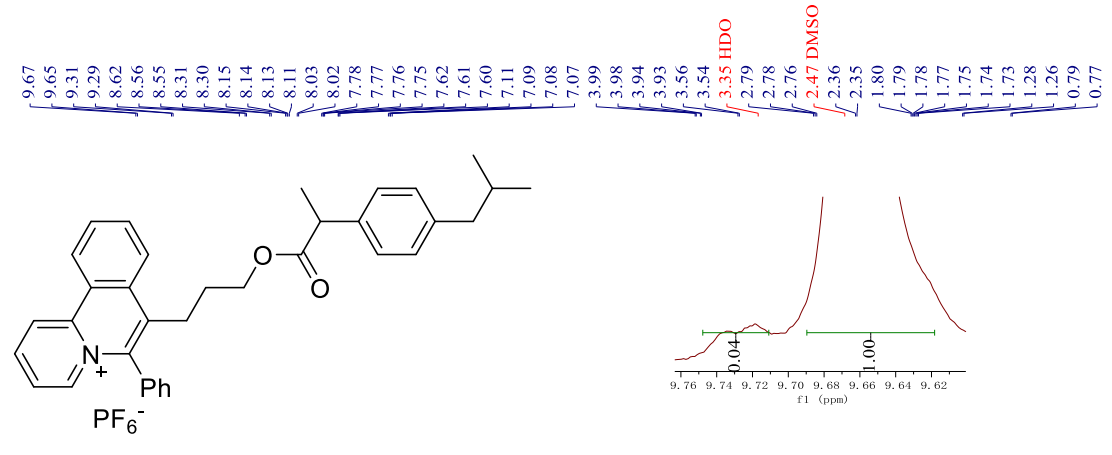

142.76
139.28
137.83
136.72
134.16
133.07
131.26
130.78
130.66
130.62
130.31
130.14
126.32
125.18
124.67
124.42
123.34
50.28
39.95 DMSO
39.79 DMSO
39.62 DMSO
39.45 DMSO
39.29 DMSO
39.12 DMSO
38.95 DMSO
28.72
26.90
N3
Ph
N+
PF6-
3ao
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.67
9.65
9.31
9.30
8.63
8.62
8.60
8.59
8.57
8.49
8.47
8.22
8.21
8.19
8.14
8.13
8.11
8.05
8.03
8.02
7.78
7.77
7.76
7.73
7.64
7.63
7.62
3.92
3.91
3.89
3.34 HDO
2.90
2.88
2.87
2.48 DMSO
1.85
1.84
1.83
1.82
1.14
1.10
0.98
O
O
N
+
Ph
PF6-
3ap
0.06
1.00
8.32 8.30 8.28 8.26 8.24 8.22 8.20 8.18
f1 (ppm)
1.00
1.00
1.99
1.03
0.06
1.00
1.03
1.05
3.03
2.01
2.05
2.01
2.06
6.00
6.00
1.01
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
f1 (ppm)

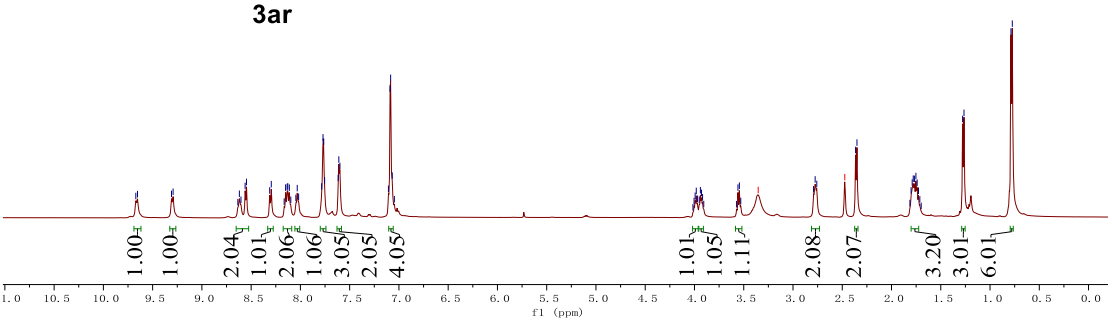

170.94
142.76
139.26
137.84
136.76
134.15
133.21
131.33
130.75
130.73
130.67
130.27
130.20
126.31
125.23
124.68
124.40
123.28
62.58
40.11 DMSO
39.90 DMSO
39.69 DMSO
39.48 DMSO
39.27 DMSO
39.06 DMSO
38.85 DMSO
34.56
29.26
28.63
26.39
23.11
23.05
16.29
16.21
O
O
N
+
Ph
PF6-
3ap
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

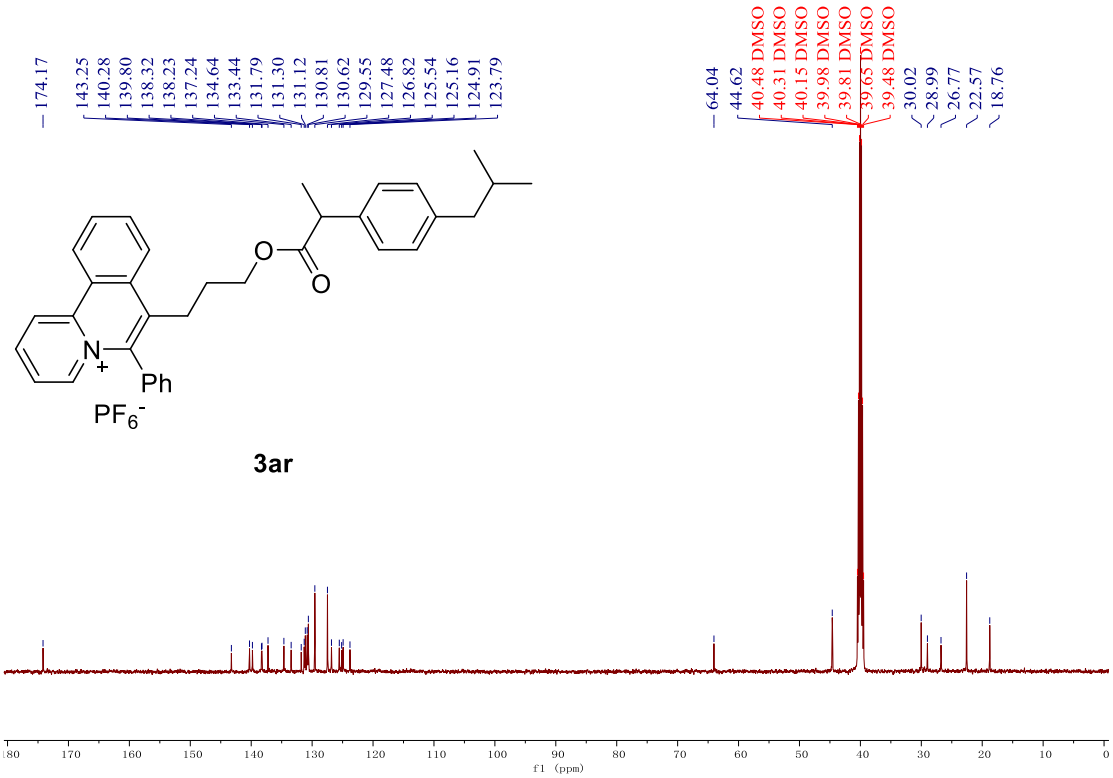

9.66 9.64 9.31 9.29 8.63 8.62 8.60 8.59 8.57 8.50 8.48 8.22 8.21 8.19 8.14 8.13 8.04 8.03 8.01 7.76 7.75 7.75 7.73 7.63 7.62 7.62 7.61 6.91 6.89 4.02 4.01 3.96 3.95 3.32 HDO 2.90 2.88 2.88 2.86 2.48 DMSO 2.23 2.21 2.19 1.93 1.91 1.86 1.84 1.84 1.82 1.26 1.14
Cl
F
F
F
H
O
O
N+
Ph
PF6-
3aq
1.00
0.10
9.34 9.32 9.30 9.28 9.26 9.24 9.22
f1 (ppm)
1.00 1.00 2.00 0.99 1.01 1.02 1.08 3.07 2.02 1.05 1.12 1.13 1.99 1.12 1.09 2.04 3.06 3.07
f1 (ppm)

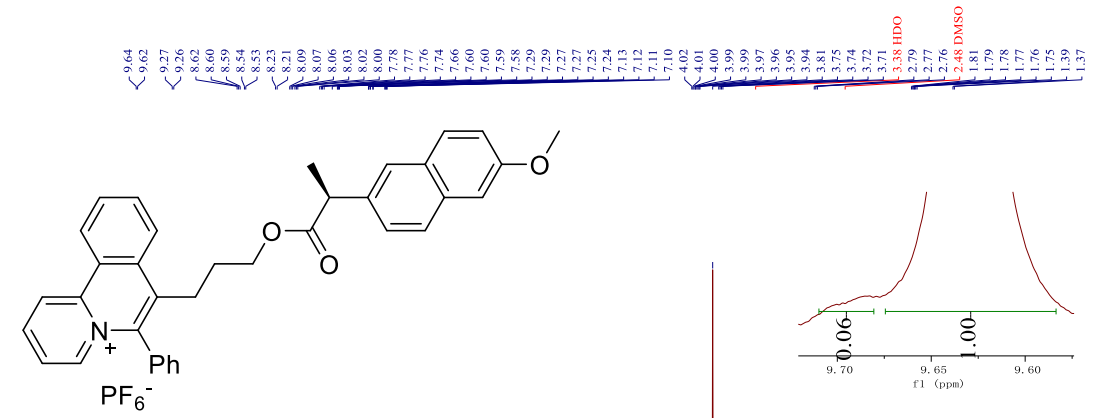

169.66 142.77 139.28 137.88 136.80 134.15 133.03 131.82 131.79 131.32 130.71 130.66 130.27 130.17 126.30 125.23 124.68 124.40 123.24
63.58 39.97 DMSO 39.81 DMSO 39.64 DMSO 39.47 DMSO 39.30 DMSO 39.14 DMSO 38.97 DMSO 32.49 29.91 28.71 28.46 27.26 26.16 14.63
Cl
F
F
F
H
O
O
N+
Ph
PF6-
3aq
f1 (ppm)


9.67 9.65 9.31 9.29 8.62 8.56 8.55 8.31 8.30 8.15 8.14 8.13 8.11 8.03 8.02 7.78 7.77 7.76 7.75 7.62 7.61 7.60 7.11 7.09 7.08 7.07 3.99 3.98 3.94 3.93 3.56 3.54 3.35 HDO 2.79 2.78 2.76 2.47 DMSO 2.36 2.35 1.80 1.79 1.78 1.77 1.75 1.74 1.73 1.28 1.26 0.79 0.77
O
O
N
+
Ph
PF6-
0.04
1.00
9.76 9.74 9.72 9.70 9.68 9.66 9.64 9.62
f1 (ppm)

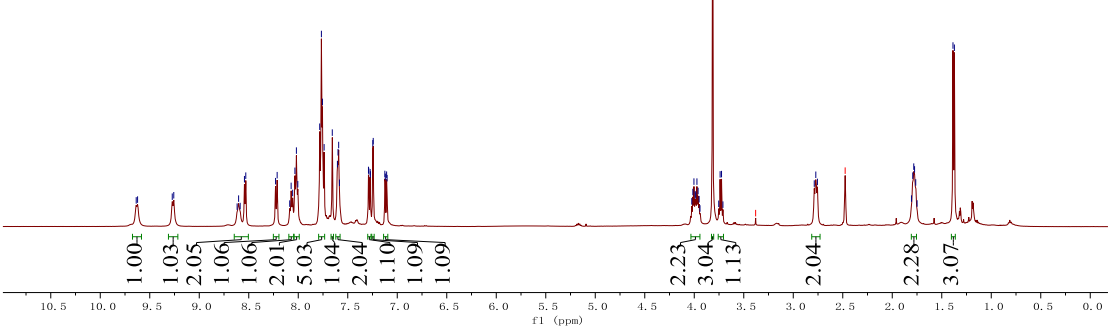
3ar

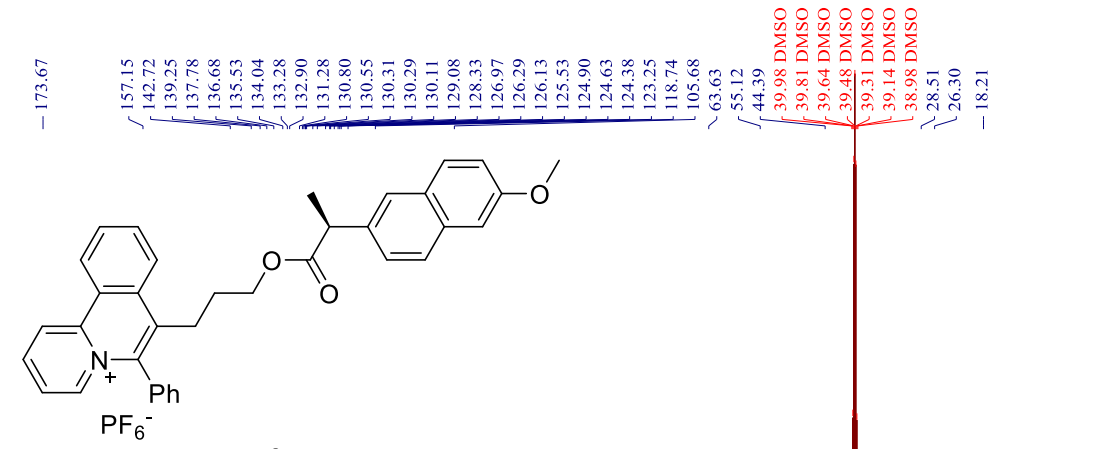

1.00 1.00 2.04 1.01 2.06 1.06 3.05 2.05 4.05 1.01 1.05 1.11 2.08 2.07 3.20 3.01 6.01
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


174.17
143.25 140.28 139.80 138.32 138.23 137.24 134.64 133.44 131.79 131.30 131.12 130.81 130.62 129.55 127.48 126.82 125.54 125.16 124.91 123.79
64.04
44.62
40.48 DMSO 40.31 DMSO 40.15 DMSO 39.98 DMSO 39.81 DMSO 39.65 DMSO 39.48 DMSO
30.02 28.99 26.77 22.57 18.76
O
O
N
+
Ph
PF6-
3ar
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

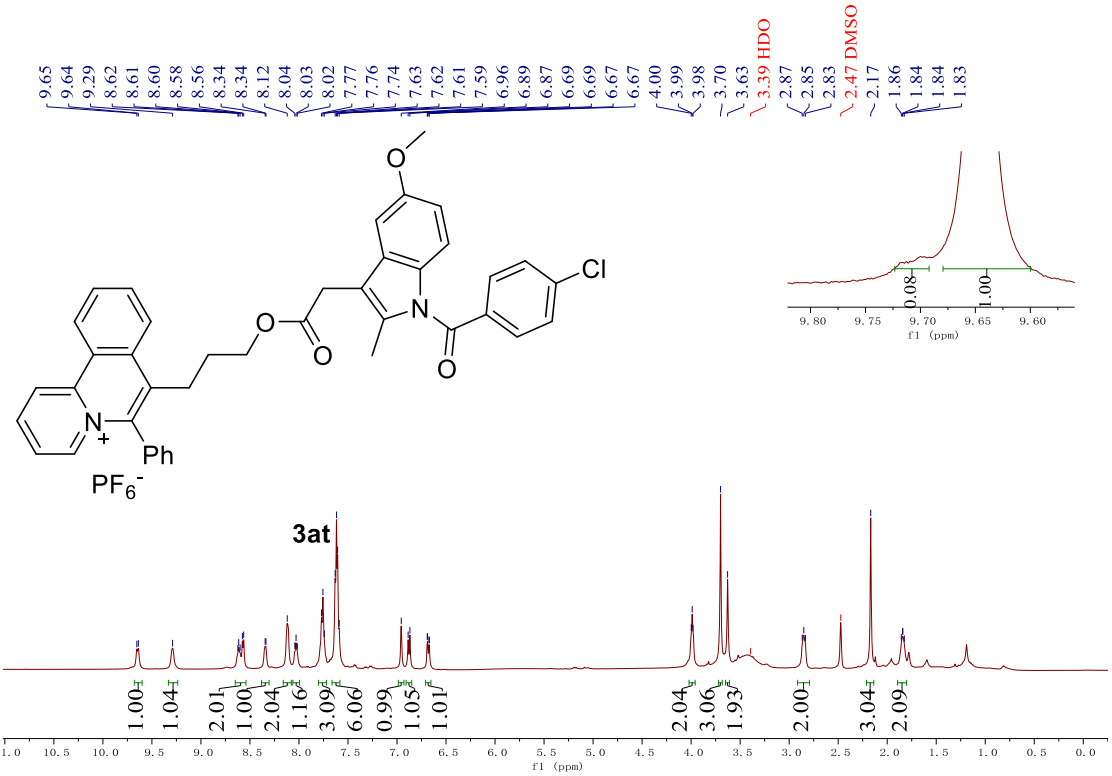

9.64 9.62 9.27 9.26 8.62 8.60 8.59 8.54 8.53 8.23 8.21 8.09 8.07 8.06 8.03 8.02 8.00 7.78 7.77 7.76 7.74 7.66 7.60 7.60 7.59 7.58 7.29 7.29 7.27 7.27 7.25 7.24 7.13 7.12 7.11 7.10 4.02 4.01 4.00 3.99 3.99 3.97 3.96 3.95 3.94 3.81 3.75 3.74 3.72 3.71 3.38 HDO 2.79 2.77 2.76 2.48 DMSO 1.81 1.79 1.78 1.77 1.76 1.75 1.39 1.37
O
O
O
N+
Ph
PF6-
0.06
1.00
9.70
9.65
9.60
f1 (ppm)

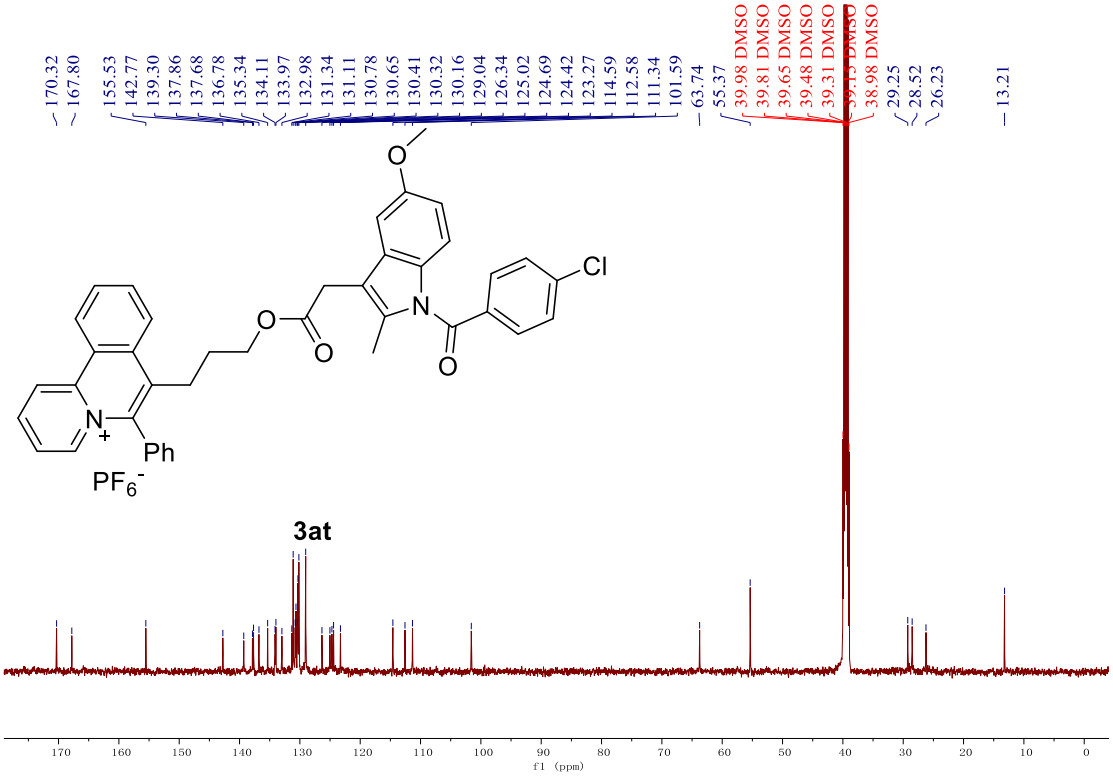
3as

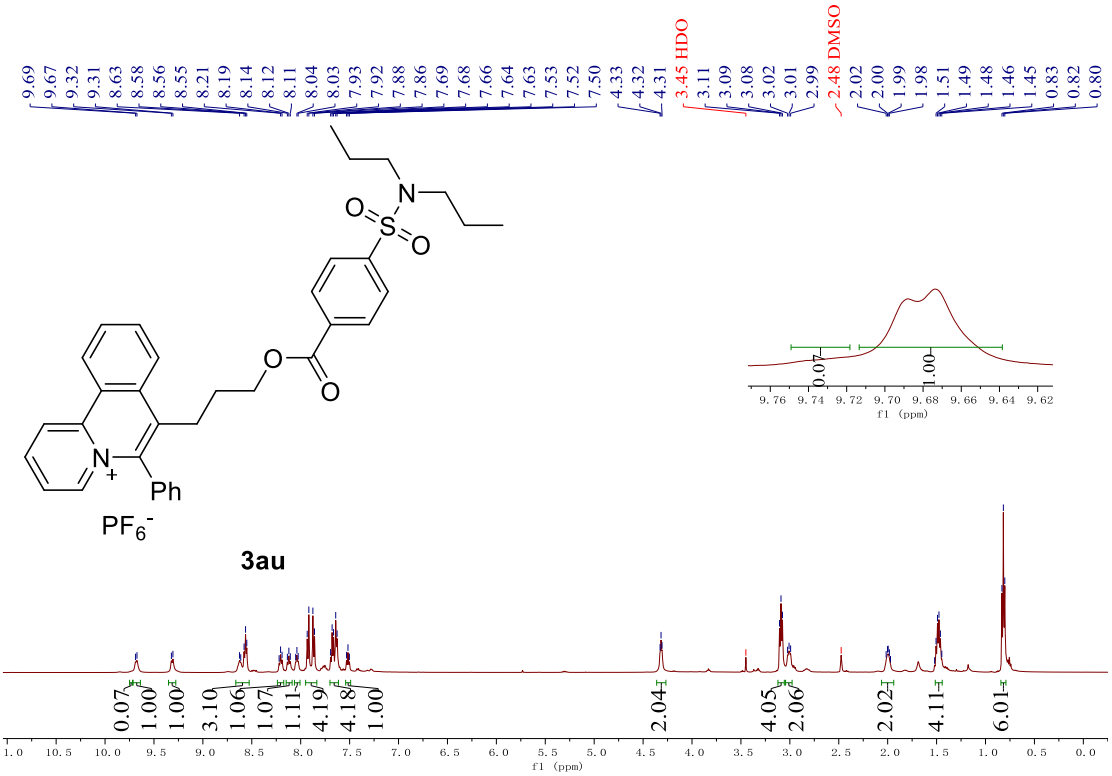

1.00 1.03 2.05 1.06 1.06 2.01 5.03 1.04 2.04 1.10 1.09 1.09 2.23 3.04 1.13 2.04 2.28 3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

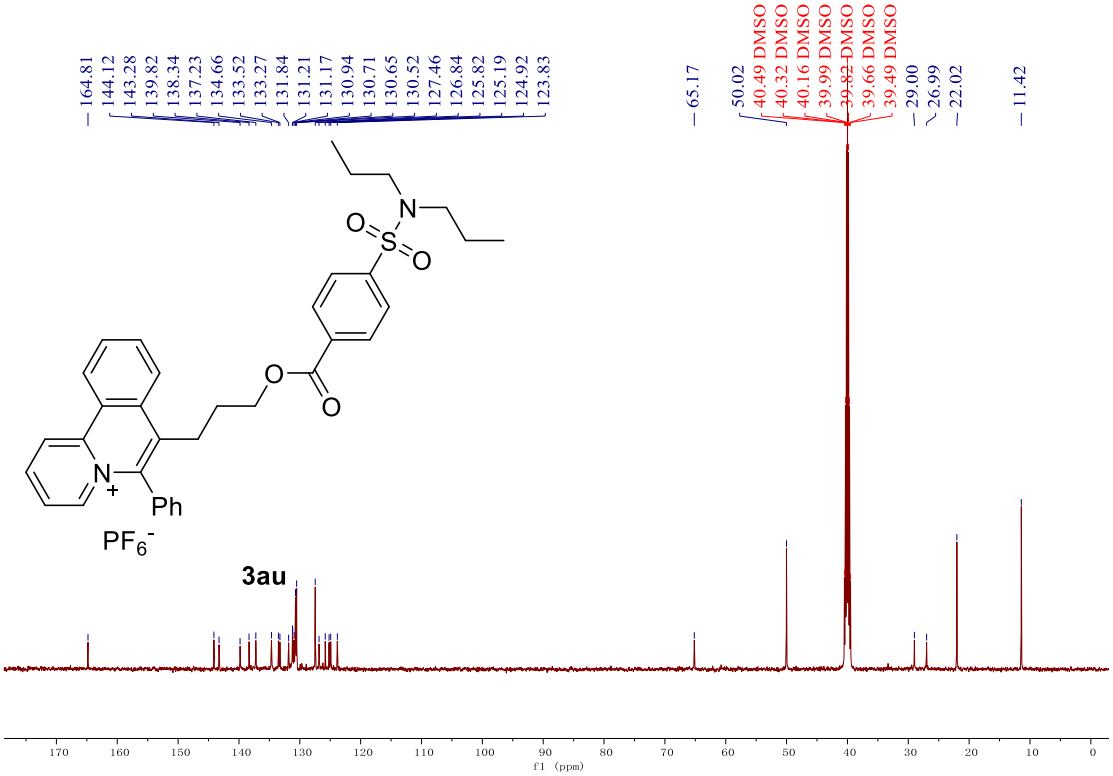

173.67
157.15 142.72 139.25 137.78 136.68 135.53 134.04 133.28 132.90 131.28 130.80 130.55 130.31 130.29 130.11 129.08 128.33 126.97 126.29 126.13 125.53 124.90 124.63 124.38 123.25 118.74 105.68 63.63 55.12 44.39
39.98 DMSO 39.81 DMSO 39.64 DMSO 39.48 DMSO 39.31 DMSO 39.14 DMSO 38.98 DMSO
28.51 26.30 18.21
O
O
O
N+
Ph
PF6-

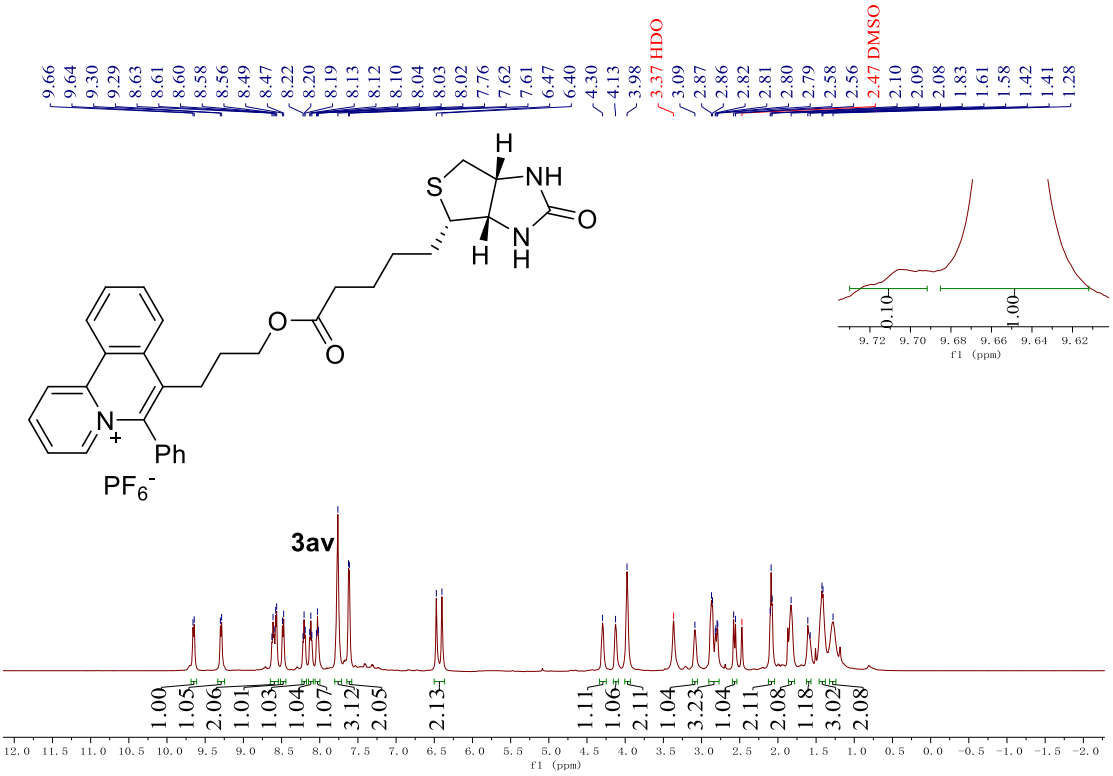
3as

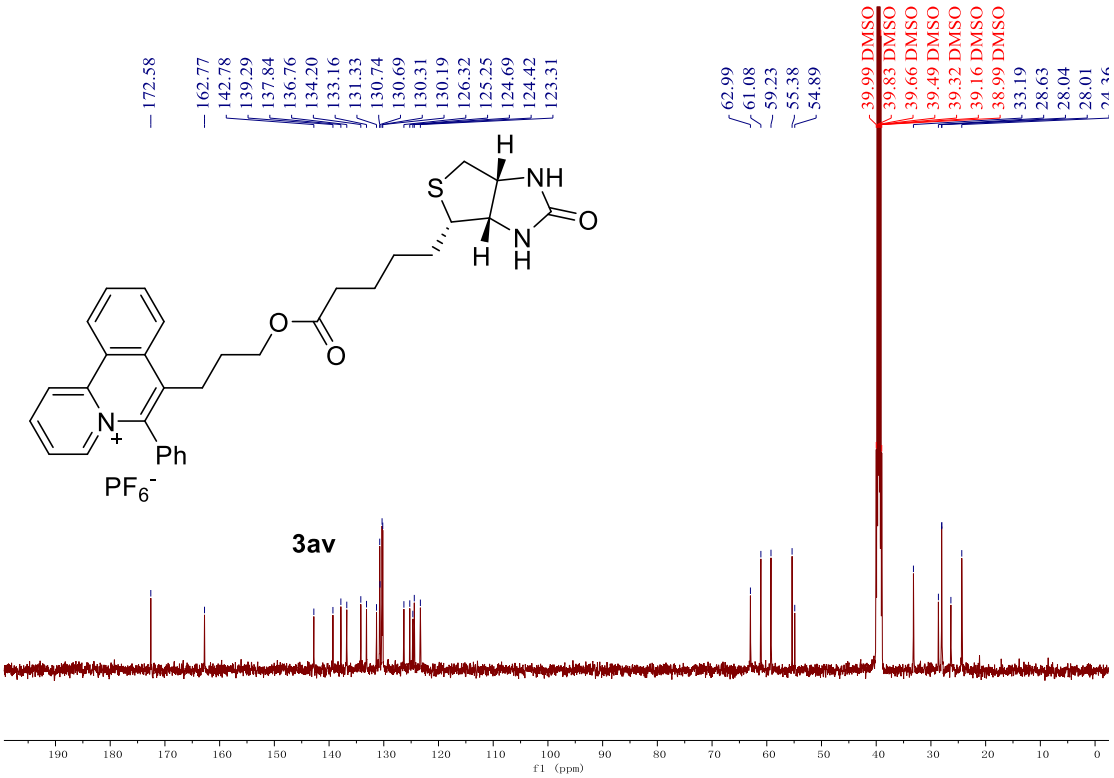

9.65 9.64 9.29 8.62 8.61 8.60 8.58 8.56 8.34 8.34 8.12 8.04 8.03 8.02 7.77 7.76 7.74 7.63 7.62 7.61 7.59 6.96 6.89 6.87 6.69 6.69 6.67 6.67 4.00 3.99 3.98 3.70 3.63 3.39 HDO 2.87 2.85 2.83 2.47 DMSO 2.17 1.86 1.84 1.84 1.83
O
Cl
N
O
O
O
N
+
Ph
PF6-
3at
0.08
1.00
f1 (ppm)
1.00 1.04 2.01 1.00 2.04 1.16 3.09 6.06 0.99 1.05 1.01 2.04 3.06 1.93 2.00 3.04 2.09
f1 (ppm)

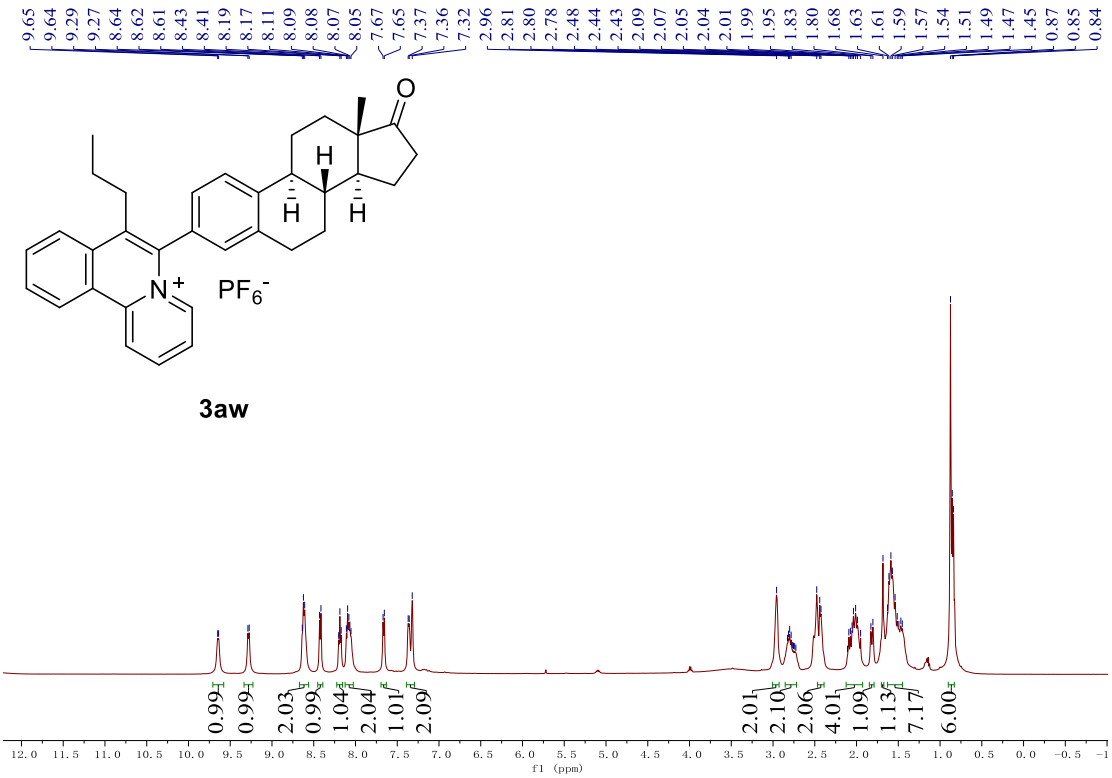

170.32 167.80 155.53 142.77 139.30 137.86 137.68 136.78 135.34 134.11 133.97 132.98 131.34 131.11 130.78 130.65 130.41 130.32 130.16 129.04 126.34 125.02 124.69 124.42 123.27 114.59 112.58 111.34 101.59 63.74 55.37 39.98 DMSO 39.81 DMSO 39.65 DMSO 39.48 DMSO 39.31 DMSO 39.15 DMSO 38.98 DMSO 29.25 28.52 26.23 13.21
O
Cl
N
O
O
O
N
+
Ph
PF6-
3at
f1 (ppm)


9.69 9.67 9.32 9.31 8.63 8.58 8.56 8.55 8.21 8.19 8.14 8.12 8.11 8.04 8.03 7.93 7.92 7.88 7.86 7.69 7.68 7.66 7.64 7.63 7.53 7.52 7.50 4.33 4.32 4.31 3.45 HDO 3.11 3.09 3.08 3.02 3.01 2.99 2.48 DMSO 2.02 2.00 1.99 1.98 1.51 1.49 1.48 1.46 1.45 0.83 0.82 0.80
N
O
S
O
O
O
N
+
Ph
PF6-
3au
0.07
1.00
f1 (ppm)
0.07 1.00 1.00 3.10 1.06 1.07 1.11 4.19 4.18 1.00 2.04 4.05 2.06 2.02 4.11 6.01
f1 (ppm)

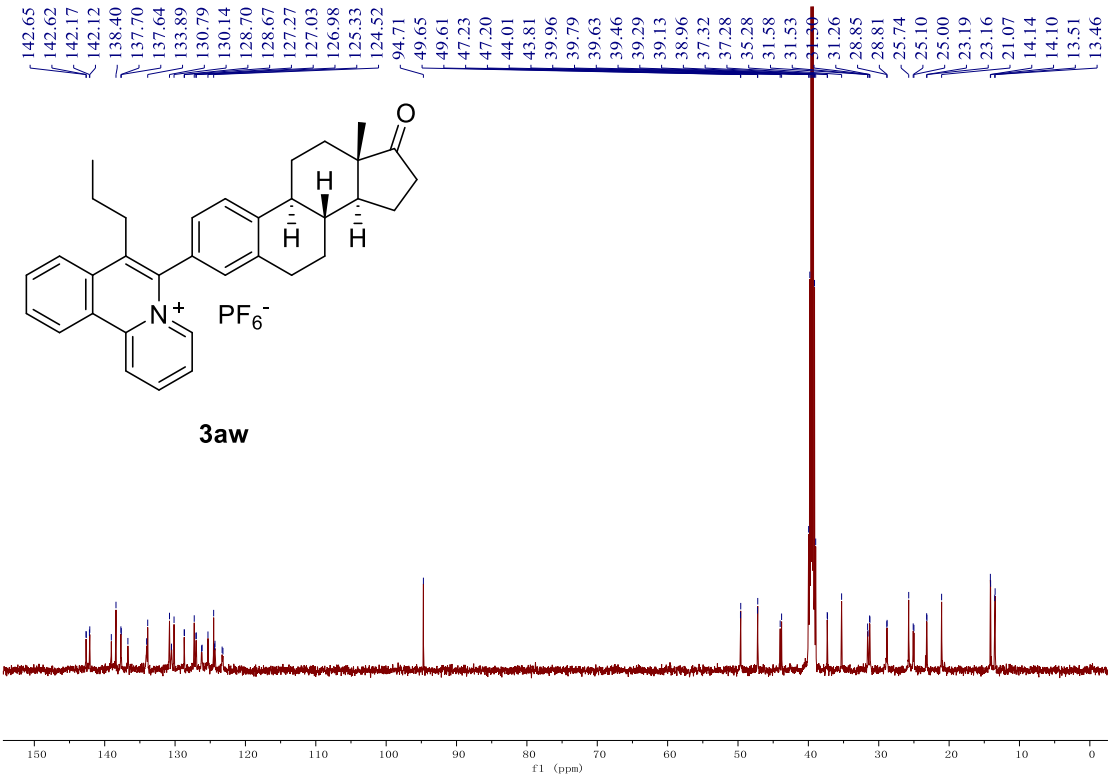

164.81 144.12 143.28 139.82 138.34 137.23 134.66 133.52 133.27 131.84 131.21 131.17 130.94 130.71 130.65 130.52 127.46 126.84 125.82 125.19 124.92 123.83 65.17 50.02 40.49 DMSO 40.32 DMSO 40.16 DMSO 39.99 DMSO 39.82 DMSO 39.66 DMSO 39.49 DMSO 29.00 26.99 22.02 11.42
N
O
S
O
O
O
N
+
Ph
PF6-
3au
f1 (ppm)


3av
PF6-
Ph
f1 (ppm)

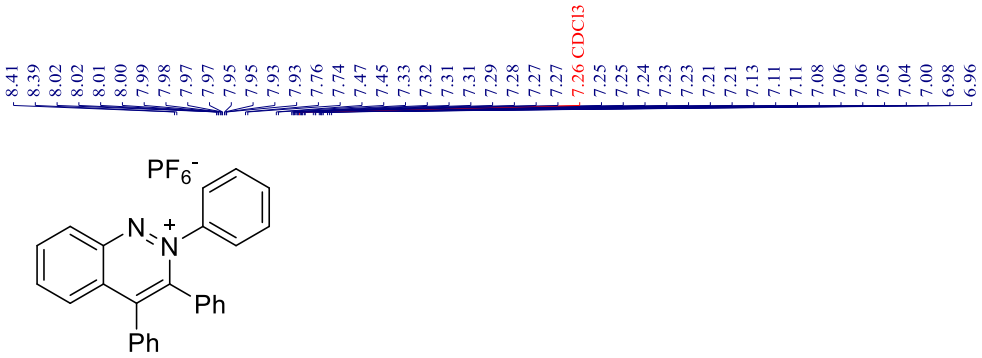

3av
PF6-
Ph
f1 (ppm)


9.65 9.64 9.29 9.27 8.64 8.62 8.61 8.43 8.41 8.19 8.17 8.11 8.09 8.08 8.07 8.05 7.67 7.65 7.37 7.36 7.32 2.96 2.81 2.80 2.78 2.48 2.44 2.43 2.09 2.07 2.05 2.04 2.01 1.99 1.95 1.83 1.80 1.68 1.63 1.61 1.59 1.57 1.54 1.51 1.49 1.47 1.45 0.87 0.85 0.84
O
H
H
H
N+
PF6-
0.99 0.99 2.03 0.99 1.04 2.04 1.01 2.09 2.01 2.10 2.06 4.01 1.09 1.13 7.17 6.00
f1 (ppm)

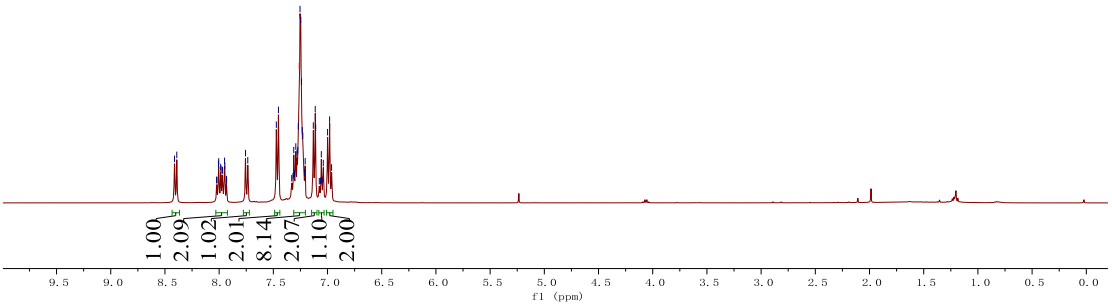
3aw

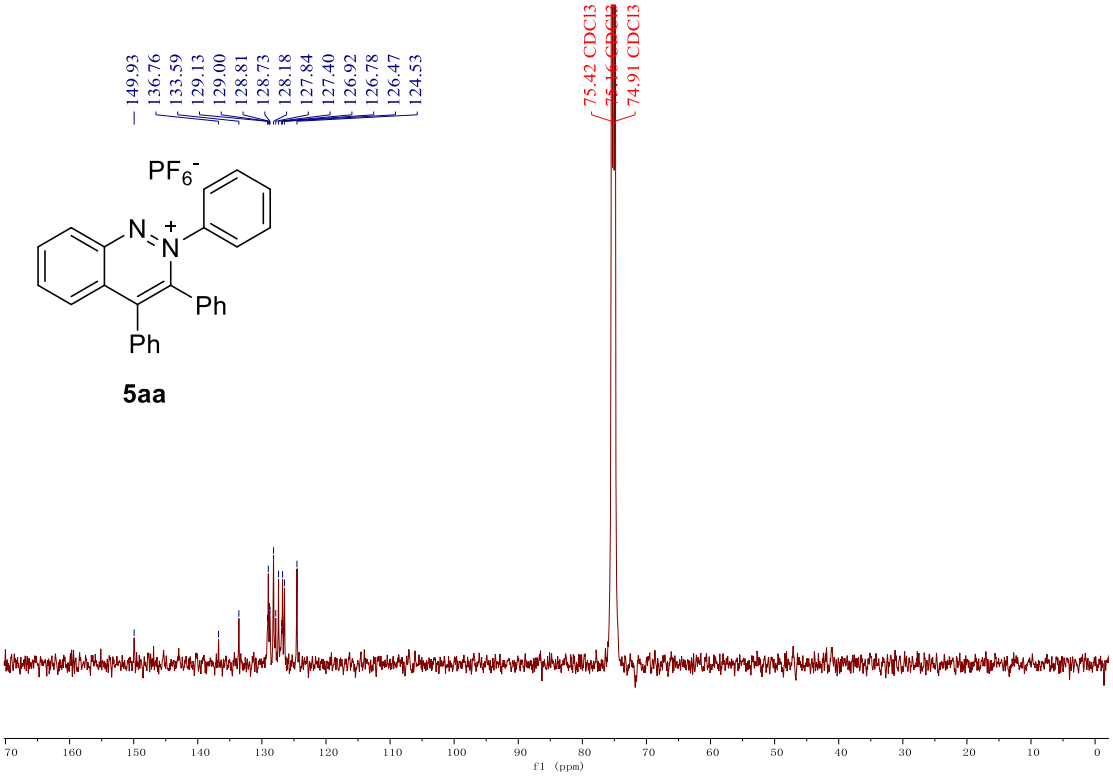

142.65 142.62 142.17 142.12 138.40 137.70 137.64 133.89 130.79 130.14 128.70 128.67 127.27 127.03 126.98 125.33 124.52 94.71 49.65 49.61 47.23 47.20 44.01 43.81 39.96 39.79 39.63 39.46 39.29 39.13 38.96 37.32 37.28 35.28 31.58 31.53 31.30 31.26 28.85 28.81 25.74 25.10 25.00 23.19 23.16 21.07 14.14 14.10 13.51 13.46
O
H
H
H
N+
PF6-
f1 (ppm)

3aw


8.41
8.39
8.02
8.02
8.01
8.00
7.99
7.98
7.97
7.97
7.95
7.95
7.93
7.93
7.76
7.74
7.47
7.45
7.33
7.32
7.31
7.31
7.29
7.28
7.27
7.27
7.26 CDCl3
7.25
7.25
7.24
7.23
7.23
7.21
7.21
7.13
7.11
7.11
7.08
7.06
7.06
7.05
7.04
7.00
6.98
6.96
PF6-
N
N
+
Ph
Ph

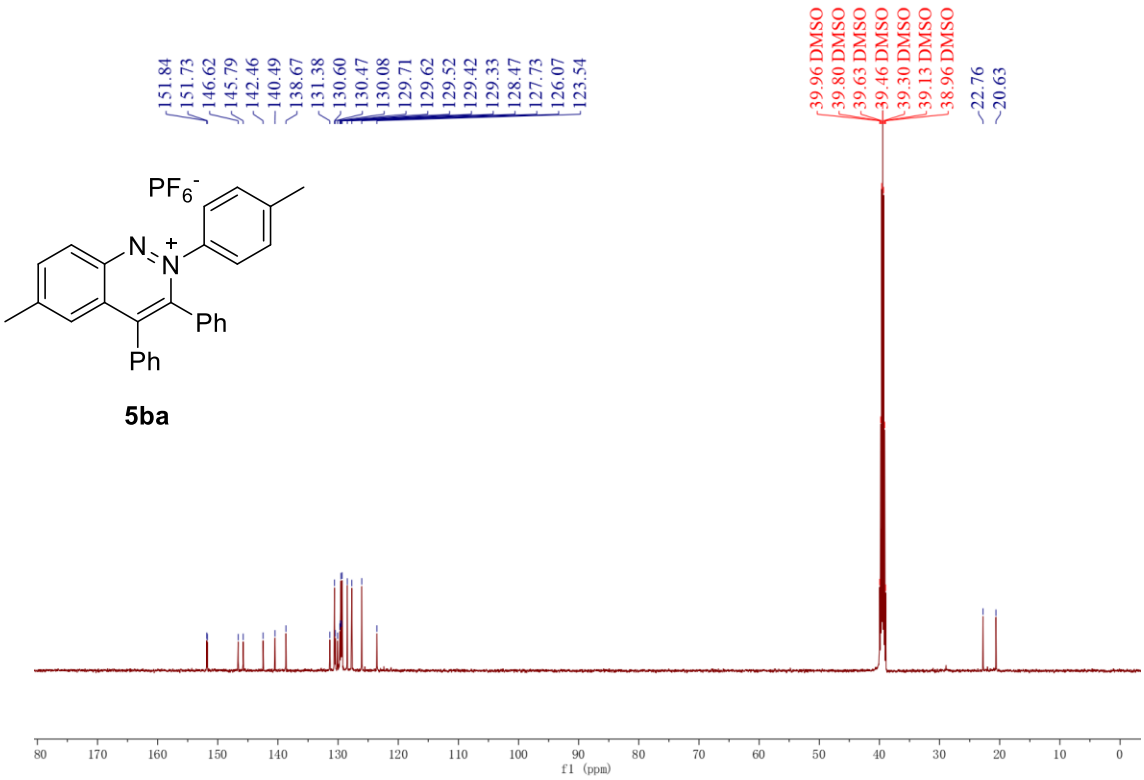
5aa


1.00
2.09
1.02
2.01
8.14
2.07
1.10
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

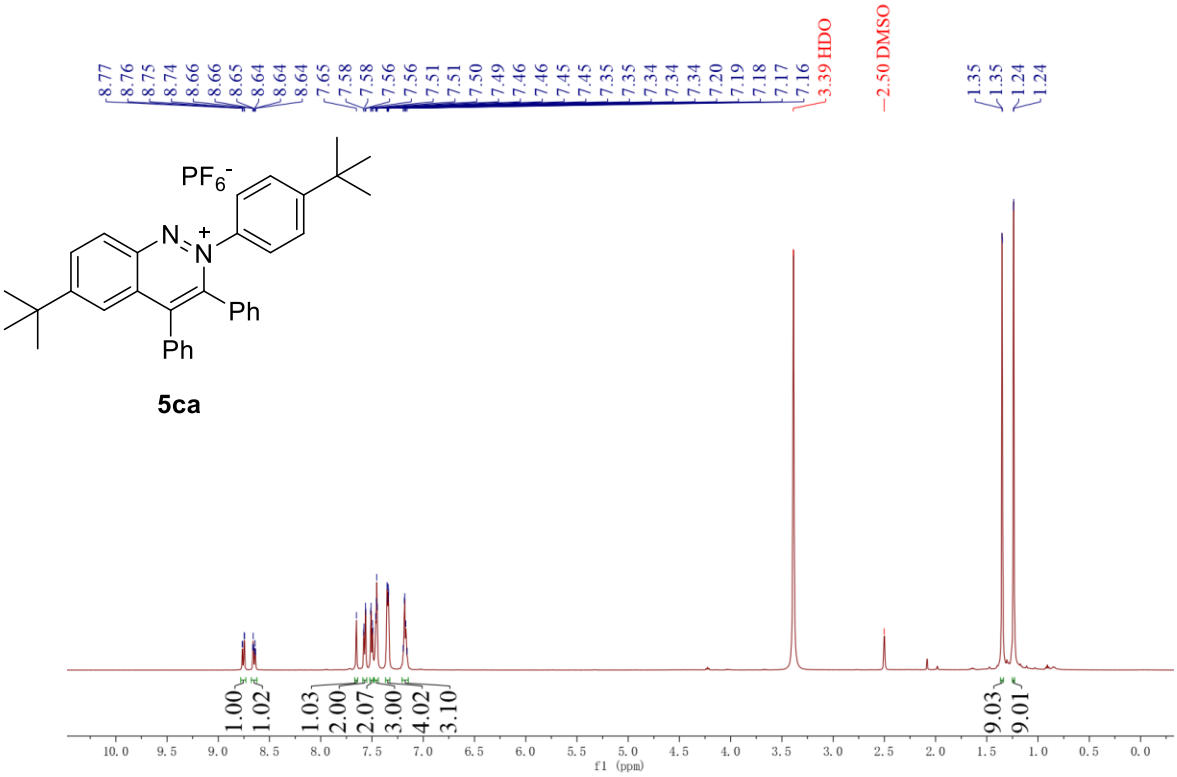

149.93
136.76
133.59
129.13
129.00
128.81
128.73
128.18
127.84
127.40
126.92
126.78
126.47
124.53
75.42 CDCl3
75.16 CDCl3
74.91 CDCl3
PF6-
N
N
+
Ph
Ph
5aa
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

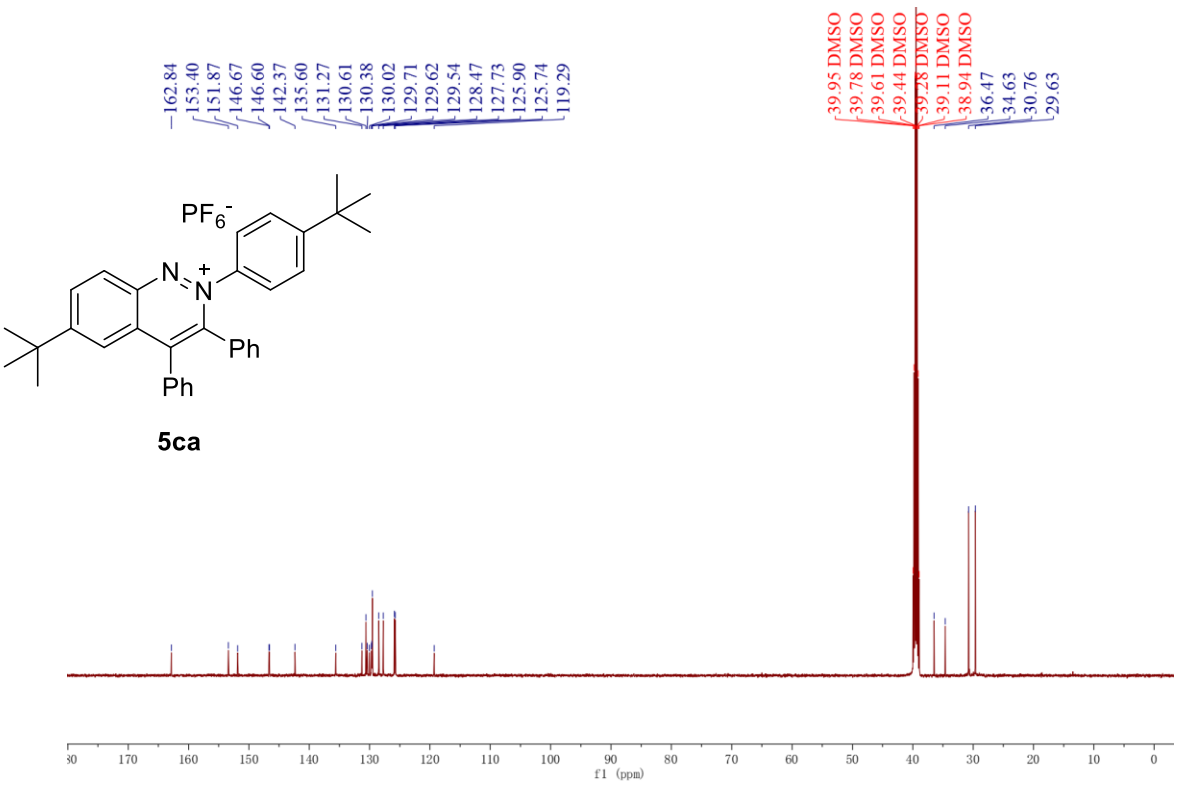
8.65
8.64
8.25
8.23
7.53
7.47
7.46
7.36
7.35
7.27
7.26
7.25
7.23
7.20
7.19
7.09
7.08
3.27
2.60
2.41
2.21
PF6-
N
N
+
Ph
Ph
1.01
1.00
1.05
2.06
3.12
4.06
2.01
3.01
3.00
3.00
f1 (ppm)

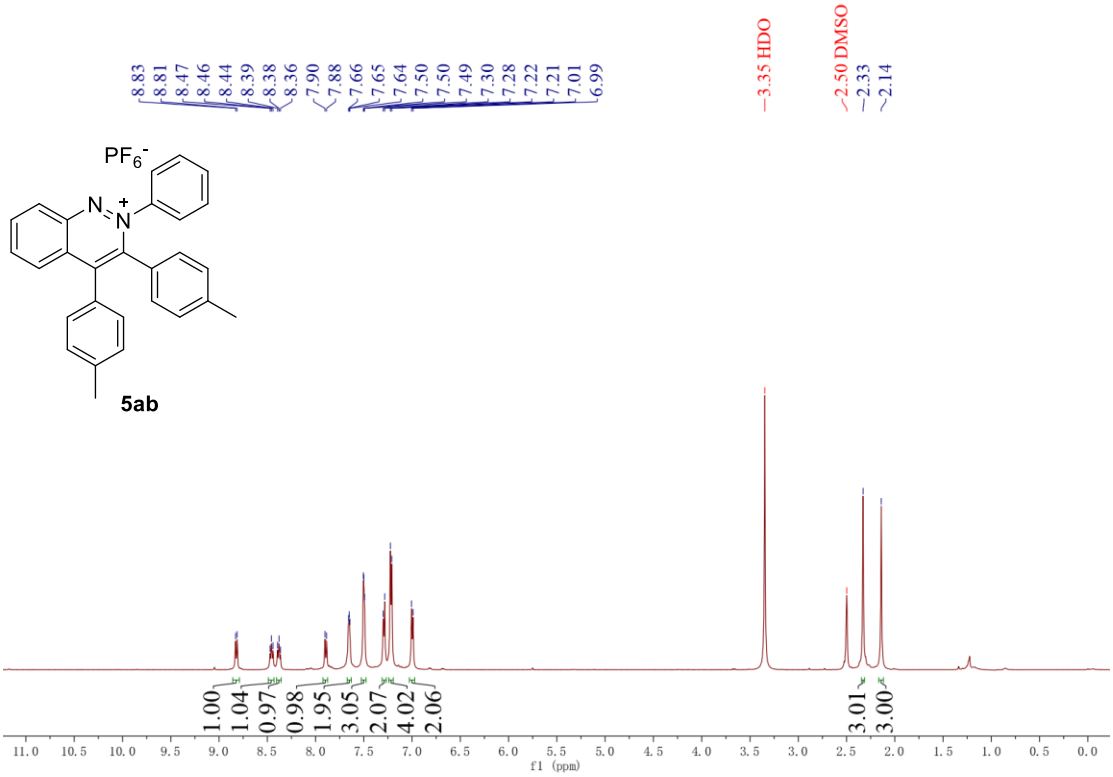
5ba

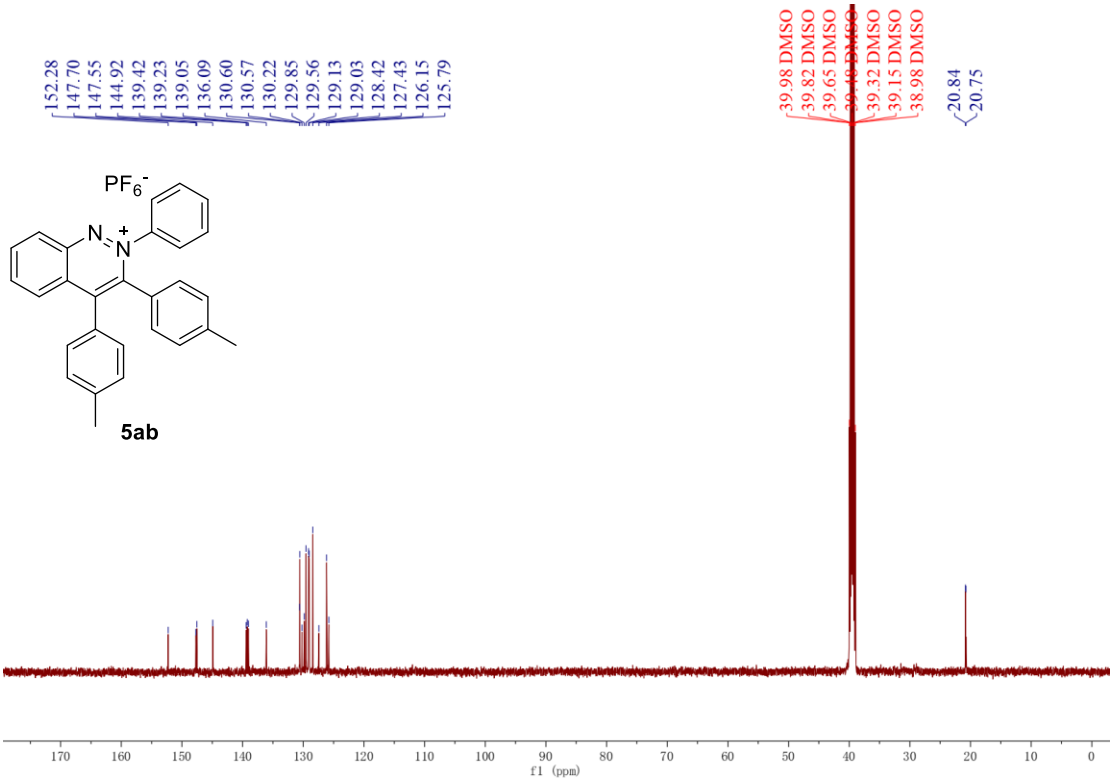

151.84
151.73
146.62
145.79
142.46
140.49
138.67
131.38
130.60
130.47
130.08
129.71
129.62
129.52
129.42
129.33
128.47
127.73
126.07
123.54
39.96 DMSO
39.80 DMSO
39.63 DMSO
39.46 DMSO
39.30 DMSO
39.13 DMSO
38.96 DMSO
22.76
20.63
PF6-
N
N
+
Ph
Ph
f1 (ppm)

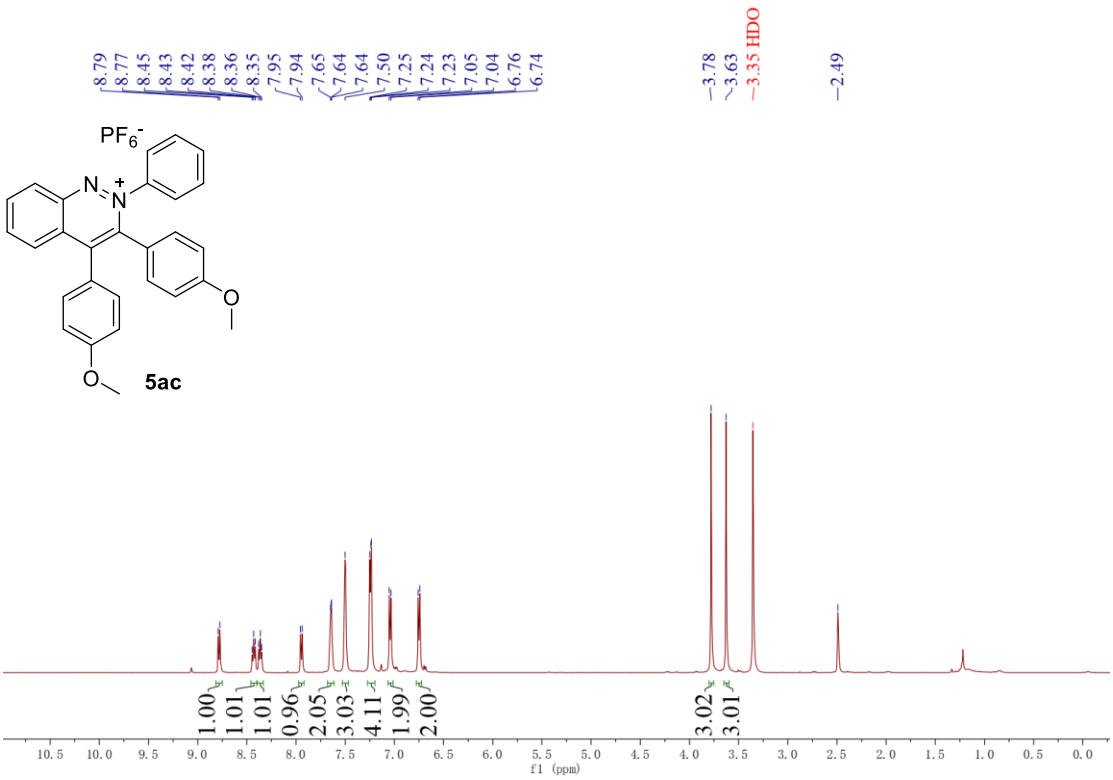
5ba

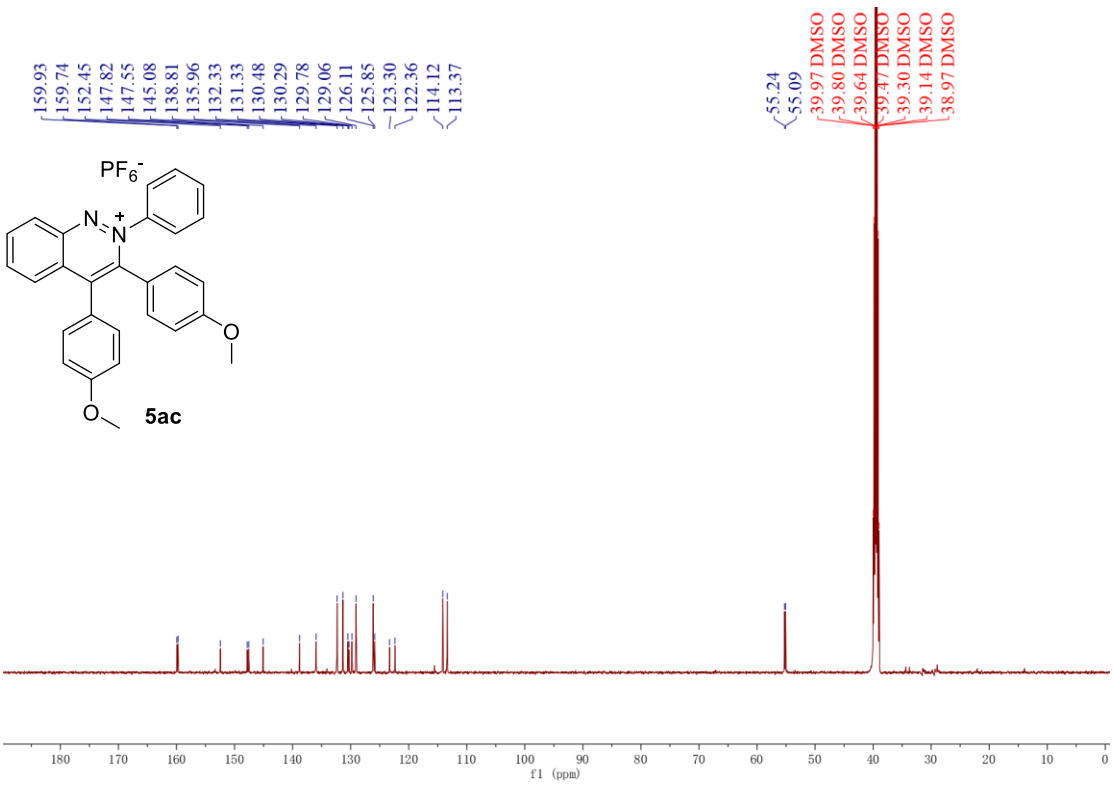

8.77
8.76
8.75
8.74
8.66
8.66
8.65
8.64
8.64
8.64
7.65
7.58
7.58
7.56
7.56
7.51
7.51
7.50
7.49
7.46
7.46
7.45
7.45
7.35
7.35
7.34
7.34
7.34
7.20
7.19
7.18
7.17
7.16
3.39 HDO
2.50 DMSO
1.35
1.35
1.24
1.24
PF6-
N
N
+
Ph
Ph
5ca
1.00
1.02
1.03
2.00
2.07
3.00
4.02
3.10
9.03
9.01
f1 (ppm)

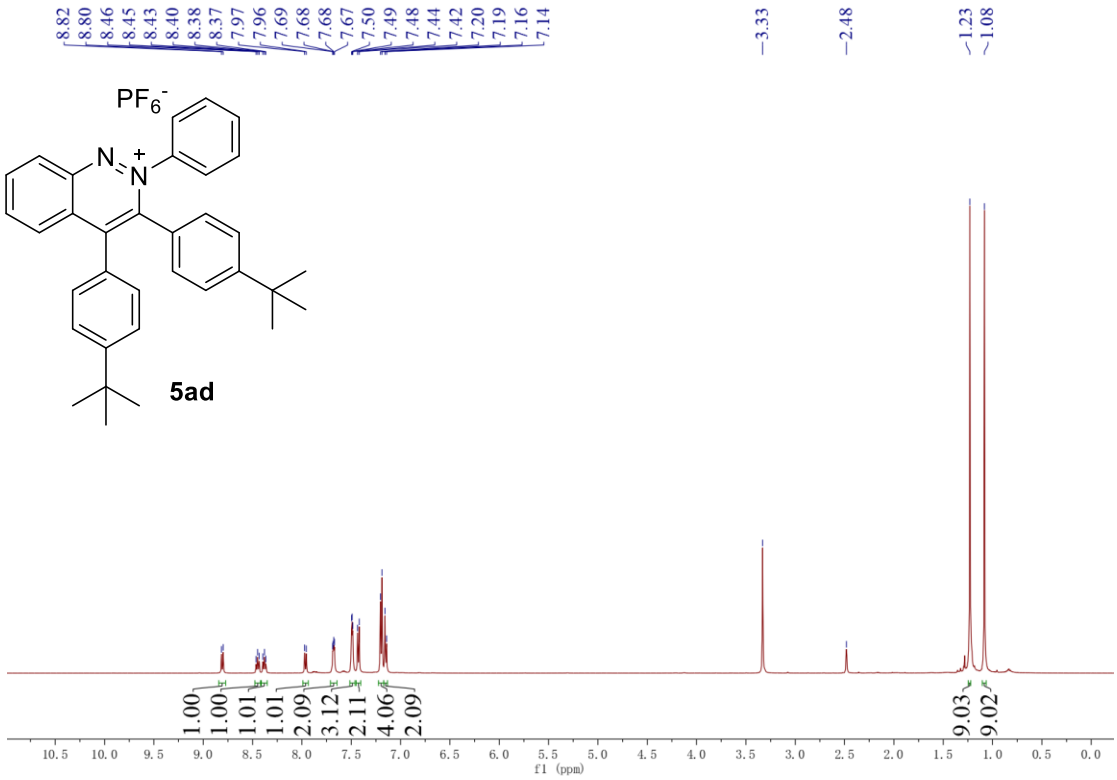

162.84
153.40
151.87
146.67
146.60
142.37
135.60
131.27
130.61
130.38
130.02
129.71
129.62
129.54
128.47
127.73
125.90
125.74
119.29
39.95 DMSO
39.78 DMSO
39.61 DMSO
39.44 DMSO
39.28 DMSO
39.11 DMSO
38.94 DMSO
36.47
34.63
30.76
29.63
PF6-
N
N
+
Ph
Ph
5ca
f1 (ppm)

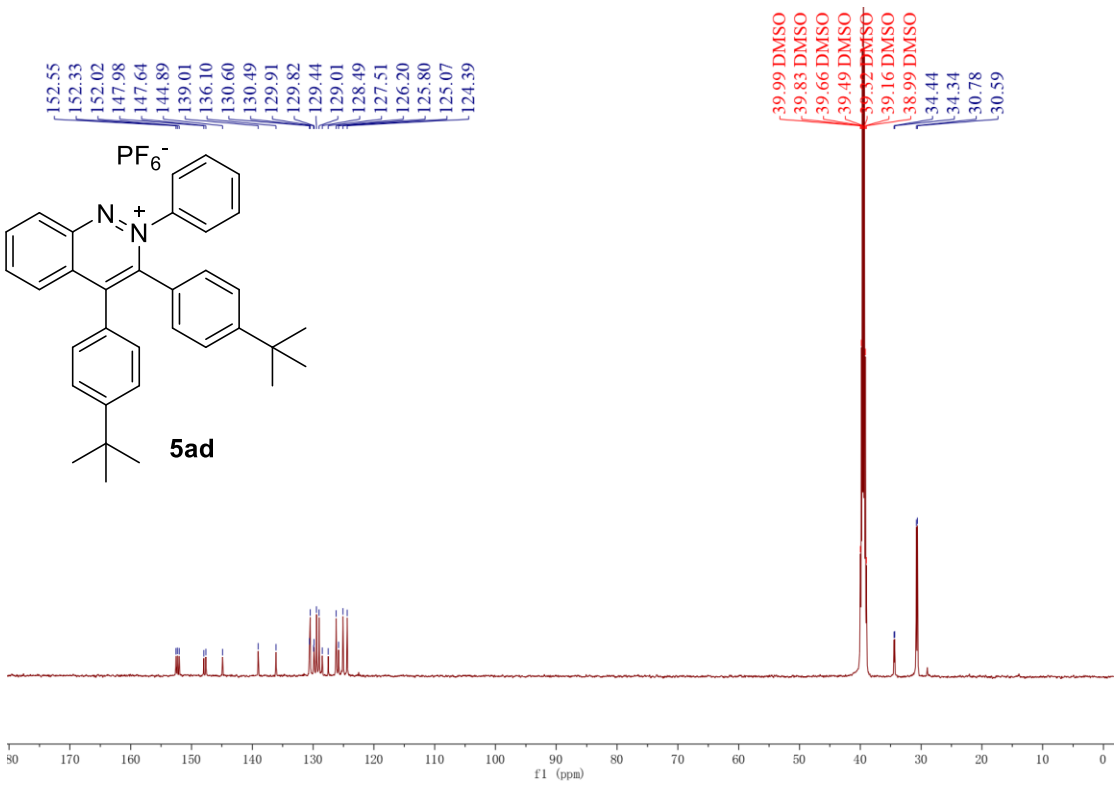

8.83
8.81
8.47
8.46
8.44
8.39
8.38
8.36
7.90
7.88
7.66
7.65
7.64
7.50
7.50
7.49
7.30
7.28
7.22
7.21
7.01
6.99
3.35 HDO
2.50 DMSO
2.33
2.14
PF6-
N
N
+
5ab
1.00
1.04
0.97
0.98
1.95
3.05
2.07
4.02
2.06
3.01
3.00
f1 (ppm)

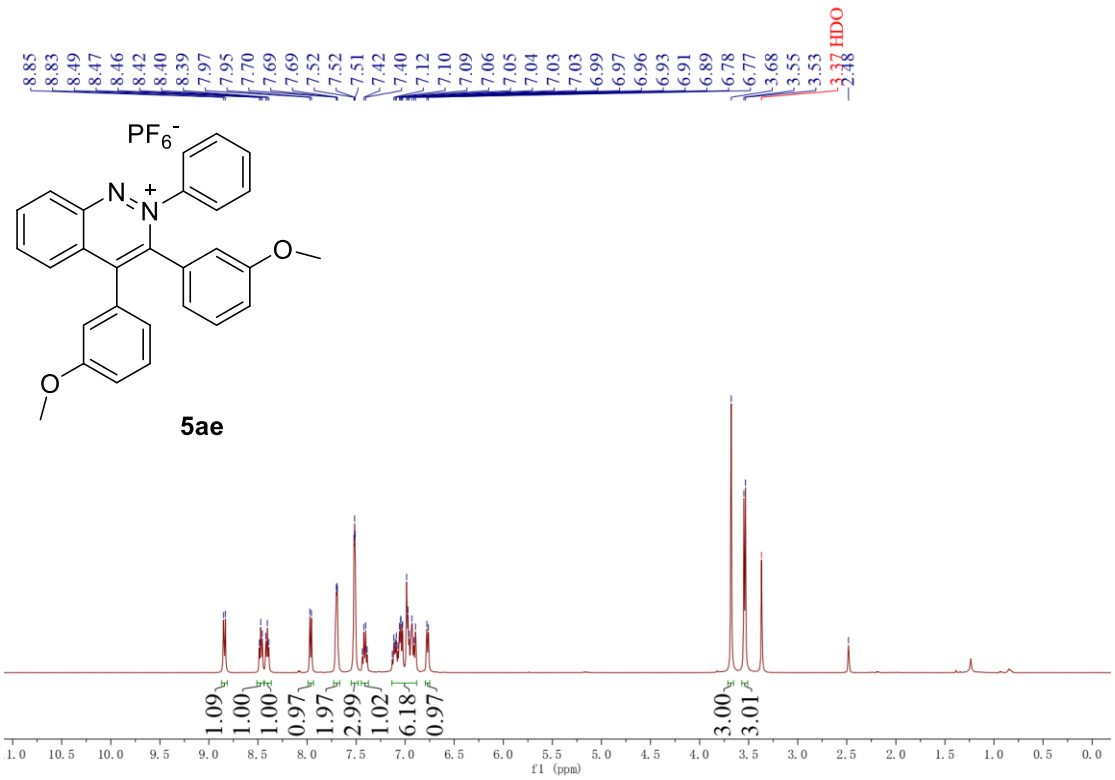

152.28
147.70
147.55
144.92
139.42
139.23
139.05
136.09
130.60
130.57
130.22
129.85
129.56
129.13
129.03
128.42
127.43
126.15
125.79
39.98 DMSO
39.82 DMSO
39.65 DMSO
39.48 DMSO
39.32 DMSO
39.15 DMSO
38.98 DMSO
20.84
20.75
PF6-
N
N
+
5ab
f1 (ppm)

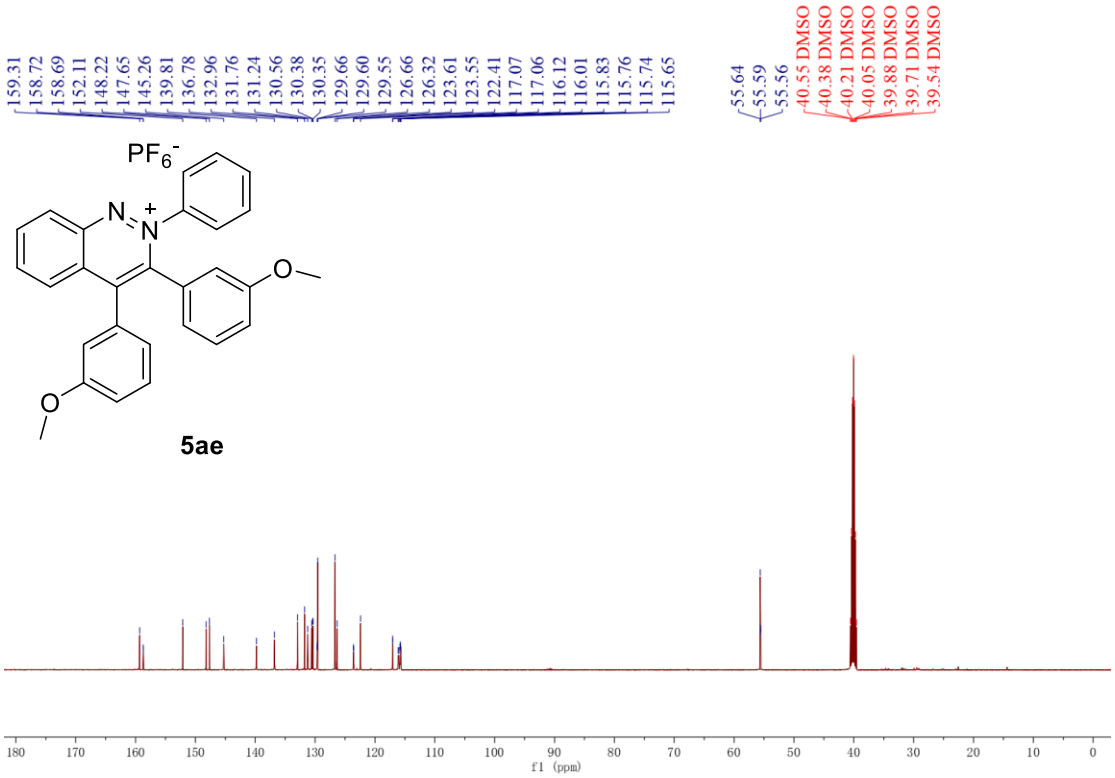

8.79
8.77
8.45
8.43
8.42
8.38
8.36
8.35
7.95
7.94
7.65
7.64
7.64
7.50
7.25
7.24
7.23
7.05
7.04
6.76
6.74
3.78
3.63
3.35 HDO
2.49
PF6-
5ac
1.00
1.01
1.01
0.96
2.05
3.03
4.11
1.99
2.00
3.02
3.01
f1 (ppm)

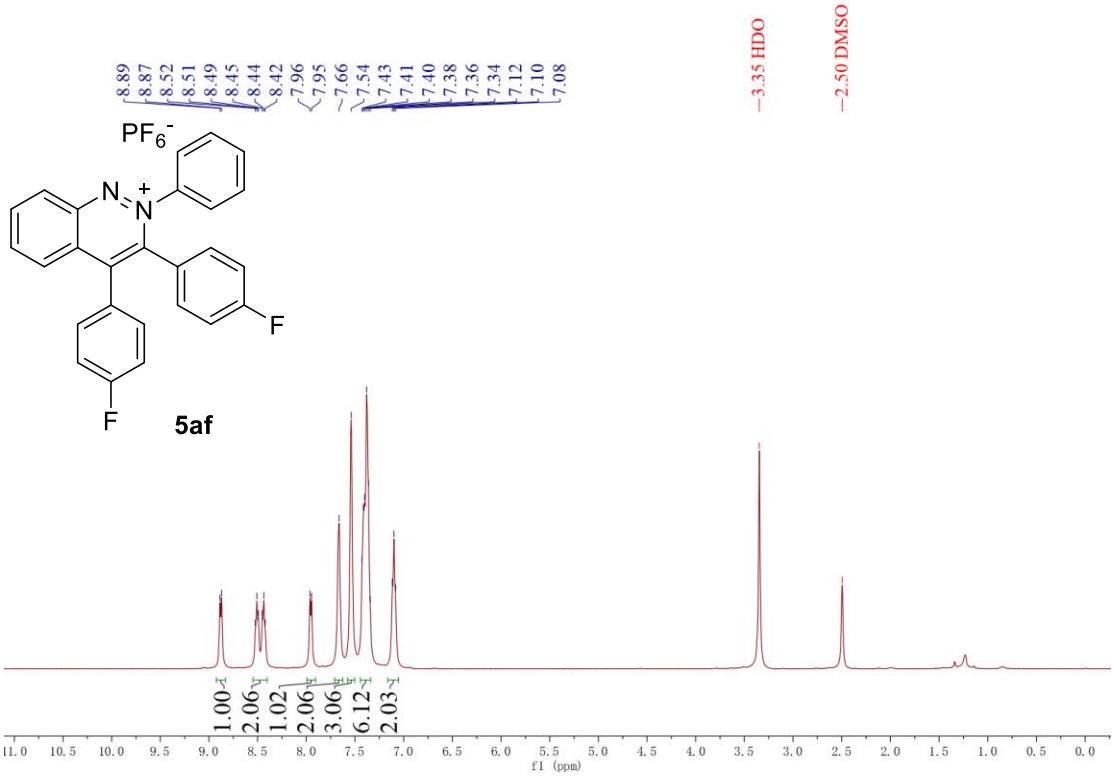

159.93
159.74
152.45
147.82
147.55
145.08
138.81
135.96
132.33
131.33
130.48
130.29
129.78
129.06
126.11
125.85
123.30
122.36
114.12
113.37
55.24
55.09
39.97 DMSO
39.80 DMSO
39.64 DMSO
39.47 DMSO
39.30 DMSO
39.14 DMSO
38.97 DMSO
PF6-
5ac
f1 (ppm)

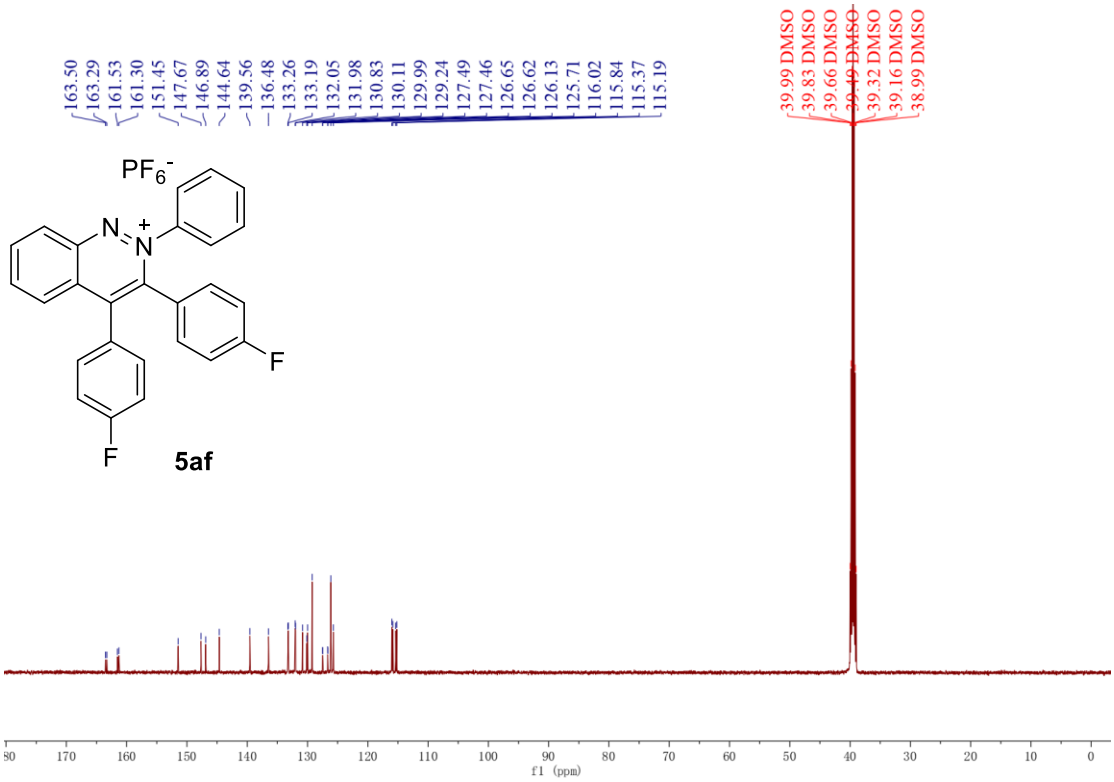

8.82
8.80
8.46
8.45
8.43
8.40
8.38
8.37
7.97
7.96
7.69
7.68
7.68
7.67
7.50
7.49
7.48
7.44
7.42
7.20
7.19
7.16
7.14
3.33
2.48
1.23
1.08
PF6-
N
N
5ad
1.00
1.00
1.01
1.01
2.09
3.12
2.11
4.06
2.09
9.03
9.02
f1 (ppm)

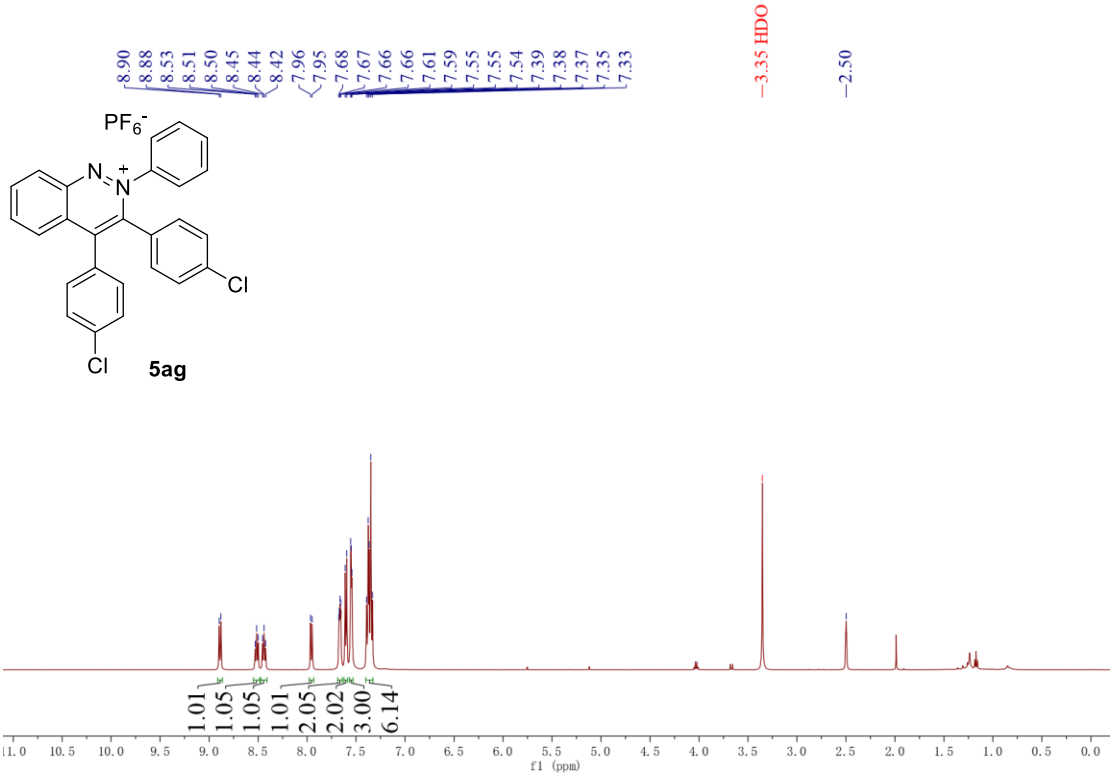

152.55
152.33
152.02
147.98
147.64
144.89
139.01
136.10
130.60
130.49
129.91
129.82
129.44
129.01
128.49
127.51
126.20
125.80
125.07
124.39
39.99 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
34.44
34.34
30.78
30.59
PF6-
N
N
5ad
f1 (ppm)

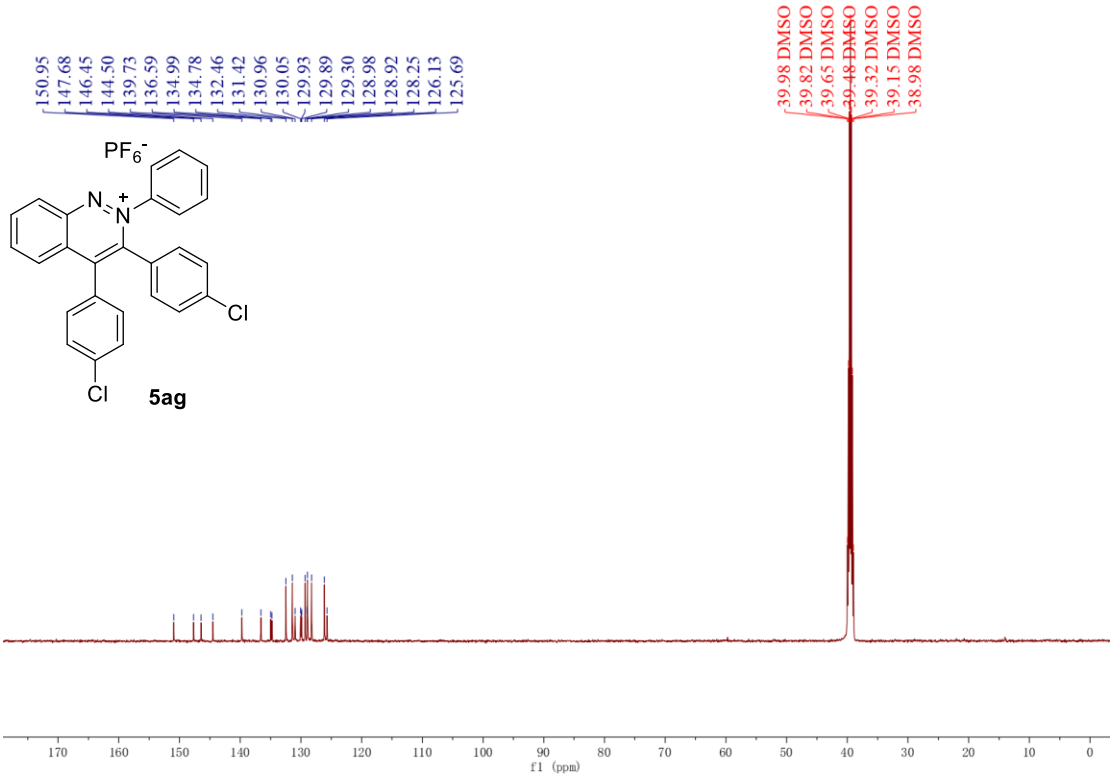

8.85
8.83
8.49
8.47
8.46
8.42
8.40
8.39
7.97
7.95
7.70
7.69
7.69
7.52
7.52
7.51
7.42
7.40
7.12
7.10
7.09
7.06
7.05
7.04
7.03
7.03
6.99
6.97
6.96
6.93
6.91
6.89
6.78
6.77
3.68
3.55
3.53
3.37 HDO
2.48
PF6-
N
N
O
O
5ae
1.09
1.00
1.00
0.97
1.97
2.99
1.02
6.18
0.97
3.00
3.01
f1 (ppm)

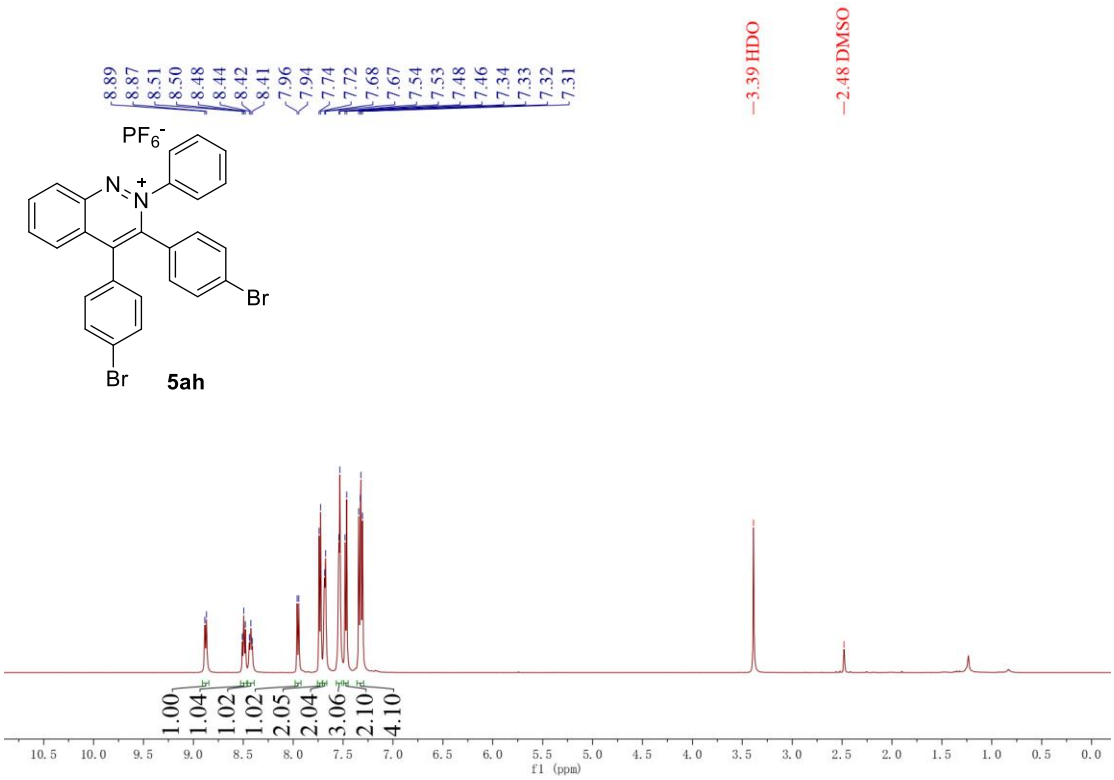

159.31
158.72
158.69
152.11
148.22
147.65
145.26
139.81
136.78
132.96
131.76
131.24
130.56
130.38
130.35
129.66
129.60
129.55
126.66
126.32
123.61
123.55
122.41
117.07
117.06
116.12
116.01
115.83
115.76
115.74
115.65
55.64
55.59
55.56
40.55 DMSO
40.38 DMSO
40.21 DMSO
40.05 DMSO
39.88 DMSO
39.71 DMSO
39.54 DMSO
PF6-
N
N
O
O
5ae
f1 (ppm)

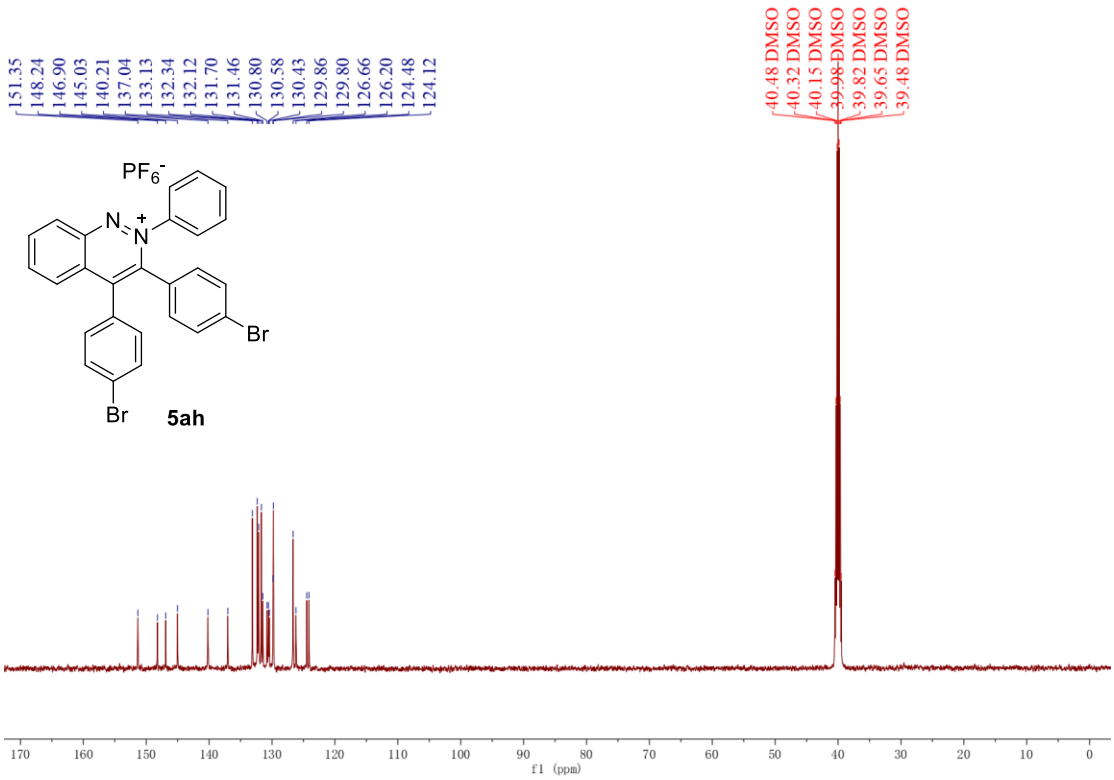

8.89
8.87
8.52
8.51
8.49
8.45
8.44
8.42
7.96
7.95
7.66
7.54
7.43
7.41
7.40
7.38
7.36
7.34
7.12
7.10
7.08
3.35 HDO
2.50 DMSO
PF6-
N
N
+
F
F
5af
1.00
2.06
1.02
2.06
3.06
6.12
2.03
f1 (ppm)

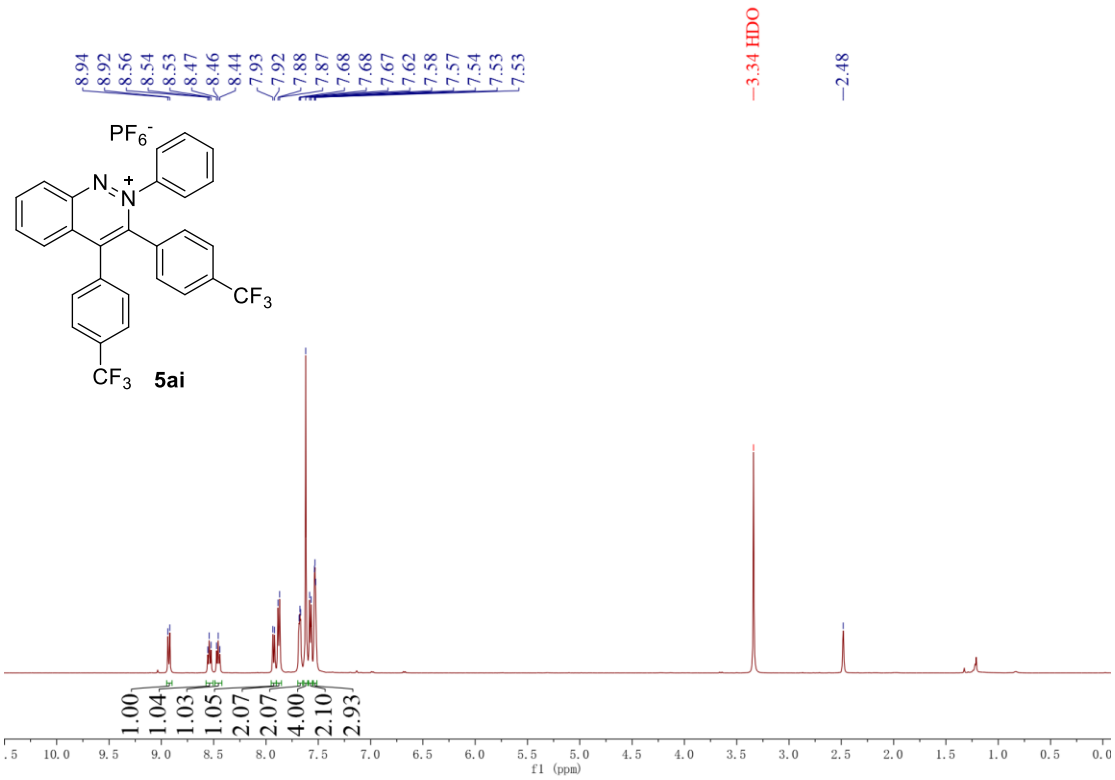

163.50
163.29
161.53
161.30
151.45
147.67
146.89
144.64
139.56
136.48
133.26
133.19
132.05
131.98
130.83
130.11
129.99
129.24
127.49
127.46
126.65
126.62
126.13
125.71
116.02
115.84
115.37
115.19
39.99 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
PF6-
N
N
+
F
F
5af
f1 (ppm)

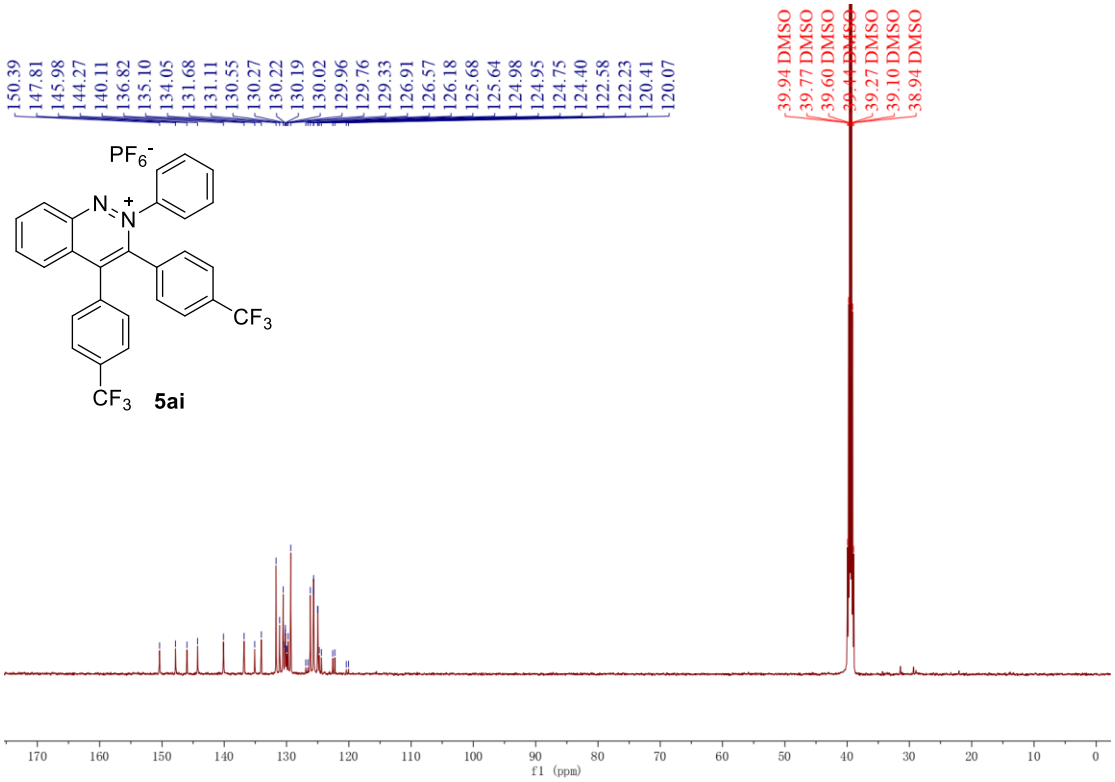

8.90
8.88
8.53
8.51
8.50
8.45
8.44
8.42
7.96
7.95
7.68
7.67
7.66
7.66
7.61
7.59
7.55
7.55
7.54
7.39
7.38
7.37
7.35
7.33
3.35 HDO
2.50
PF6-
N
N+
Cl
Cl
5ag
1.01
1.05
1.05
1.01
2.05
2.02
3.00
6.14
f1 (ppm)

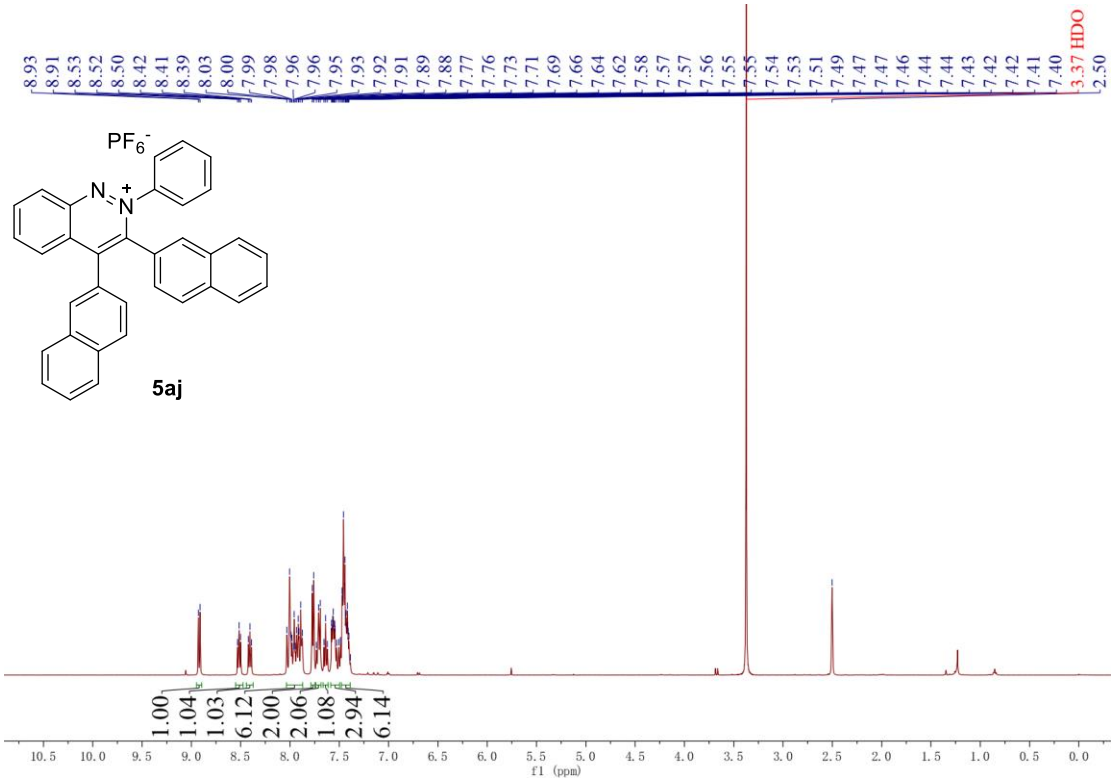

150.95
147.68
146.45
144.50
139.73
136.59
134.99
134.78
132.46
131.42
130.96
130.05
129.93
129.89
129.30
128.98
128.92
128.25
126.13
125.69
39.98 DMSO
39.82 DMSO
39.65 DMSO
39.48 DMSO
39.32 DMSO
39.15 DMSO
38.98 DMSO
PF6-
N
N+
Cl
Cl
5ag
f1 (ppm)

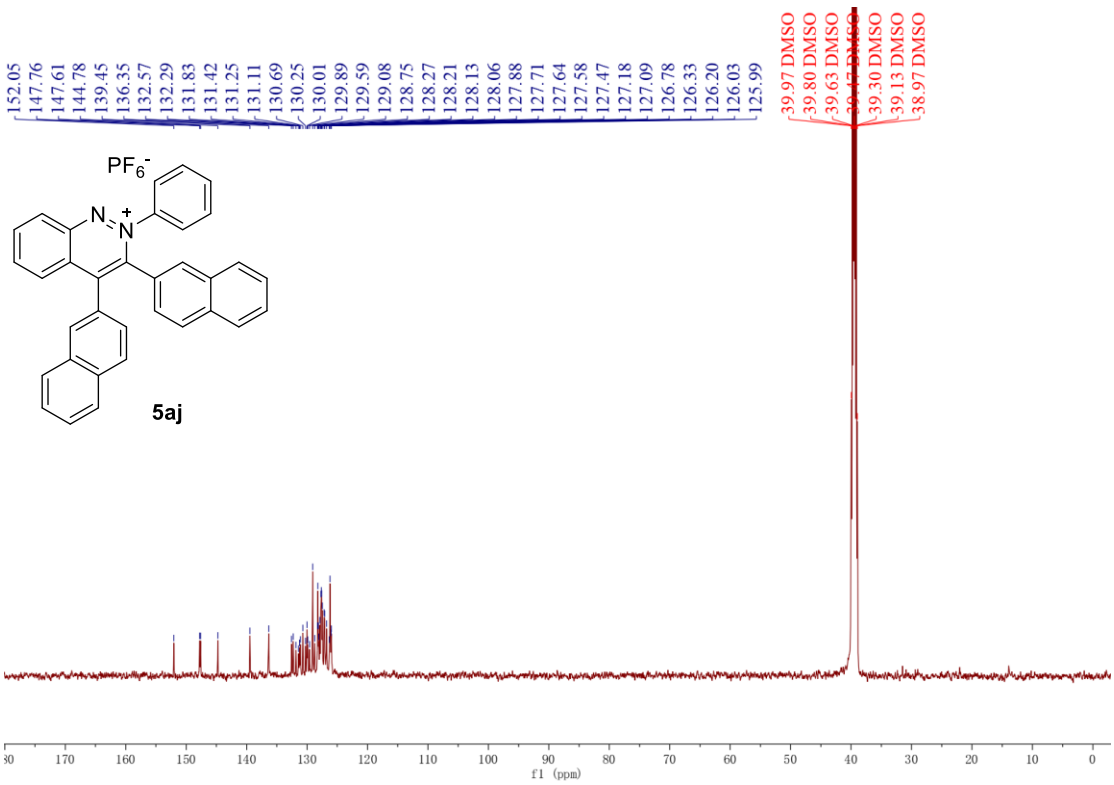

8.89
8.87
8.51
8.50
8.48
8.44
8.42
8.41
7.96
7.94
7.74
7.72
7.68
7.67
7.54
7.53
7.48
7.46
7.34
7.33
7.32
7.31
3.39 HDO
2.48 DMSO
PF6-
N
N
+
Br
Br
5ah
1.00
1.04
1.02
1.02
2.05
2.04
3.06
2.10
4.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

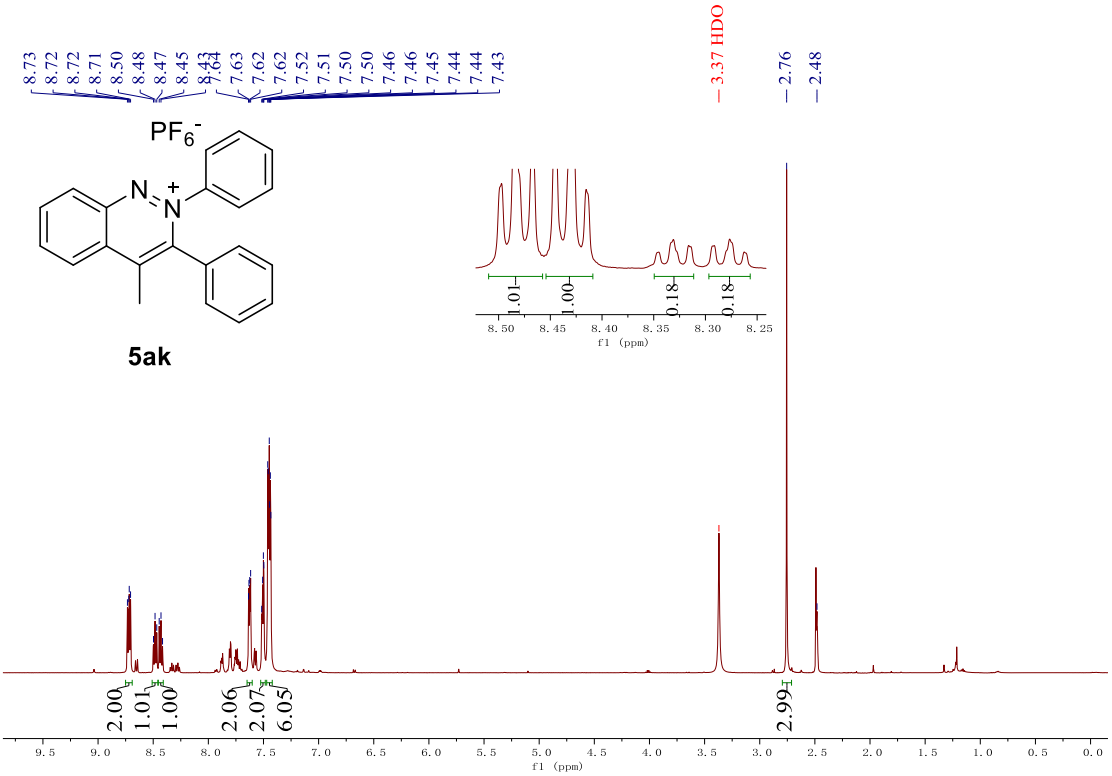

151.35
148.24
146.90
145.03
140.21
137.04
133.13
132.34
132.12
131.70
131.46
130.80
130.58
130.43
129.86
129.80
126.66
126.20
124.48
124.12
40.48 DMSO
40.32 DMSO
40.15 DMSO
39.98 DMSO
39.82 DMSO
39.65 DMSO
39.48 DMSO
PF6-
N
N
+
Br
Br
5ah
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

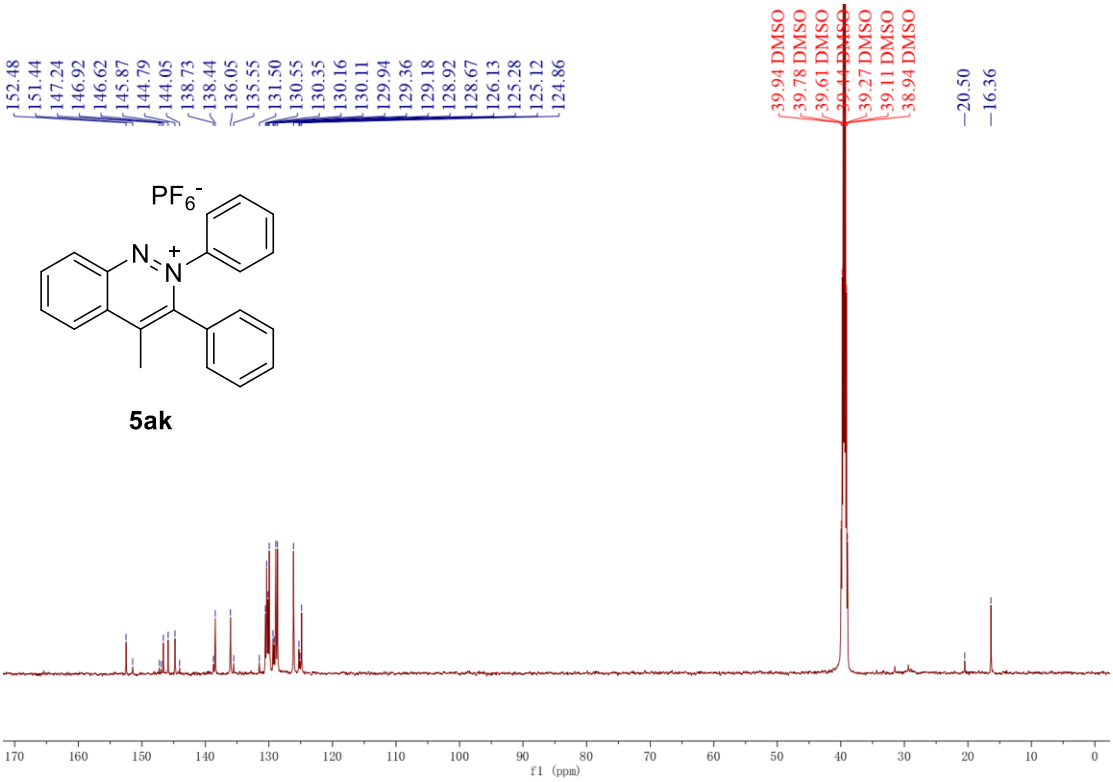

8.94
8.92
8.56
8.54
8.53
8.47
8.46
8.44
7.93
7.92
7.88
7.87
7.68
7.68
7.67
7.62
7.58
7.57
7.54
7.53
7.53
3.34 HDO
2.48
PF6-
N
N
+
CF3
CF3
5ai
1.00
1.04
1.03
1.05
2.07
2.07
4.00
2.10
2.93
f1 (ppm)

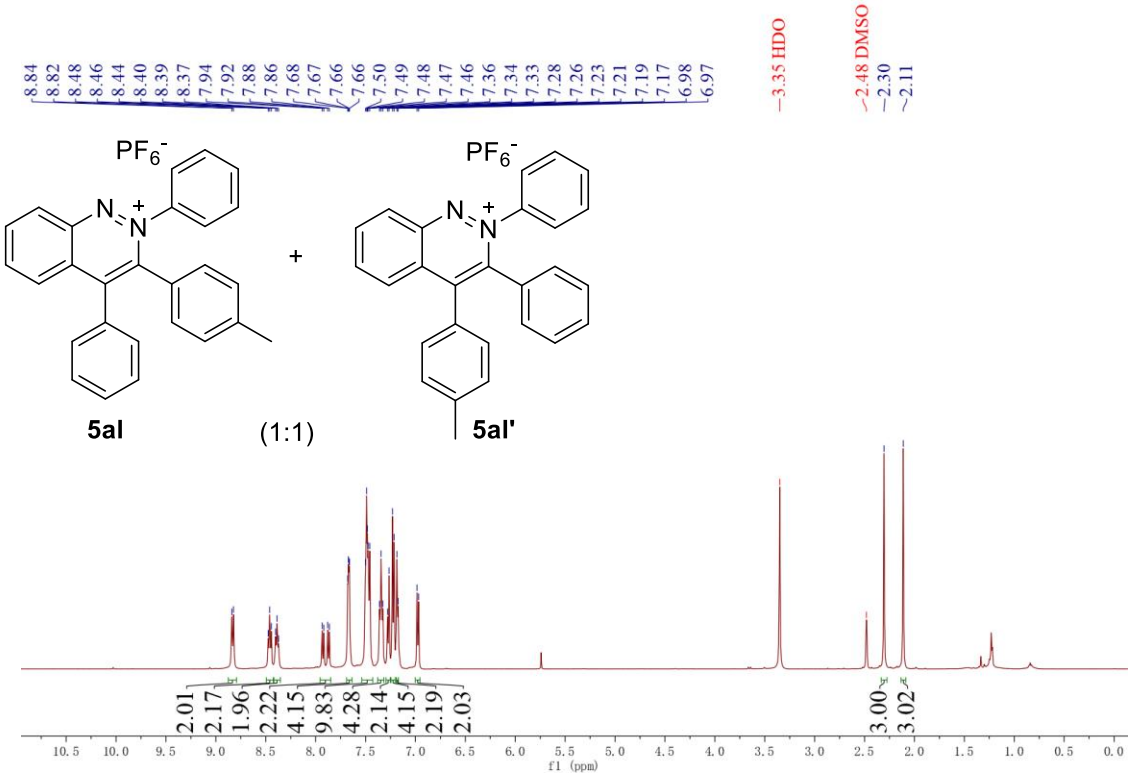

150.39
147.81
145.98
144.27
140.11
136.82
135.10
134.05
131.68
131.11
130.55
130.27
130.22
130.19
130.02
129.96
129.76
129.33
126.91
126.57
126.18
125.68
125.64
124.98
124.95
124.75
124.40
122.58
122.23
120.41
120.07
39.94 DMSO
39.77 DMSO
39.60 DMSO
39.44 DMSO
39.27 DMSO
39.10 DMSO
38.94 DMSO
PF6-
N
N
+
CF3
CF3
5ai
f1 (ppm)

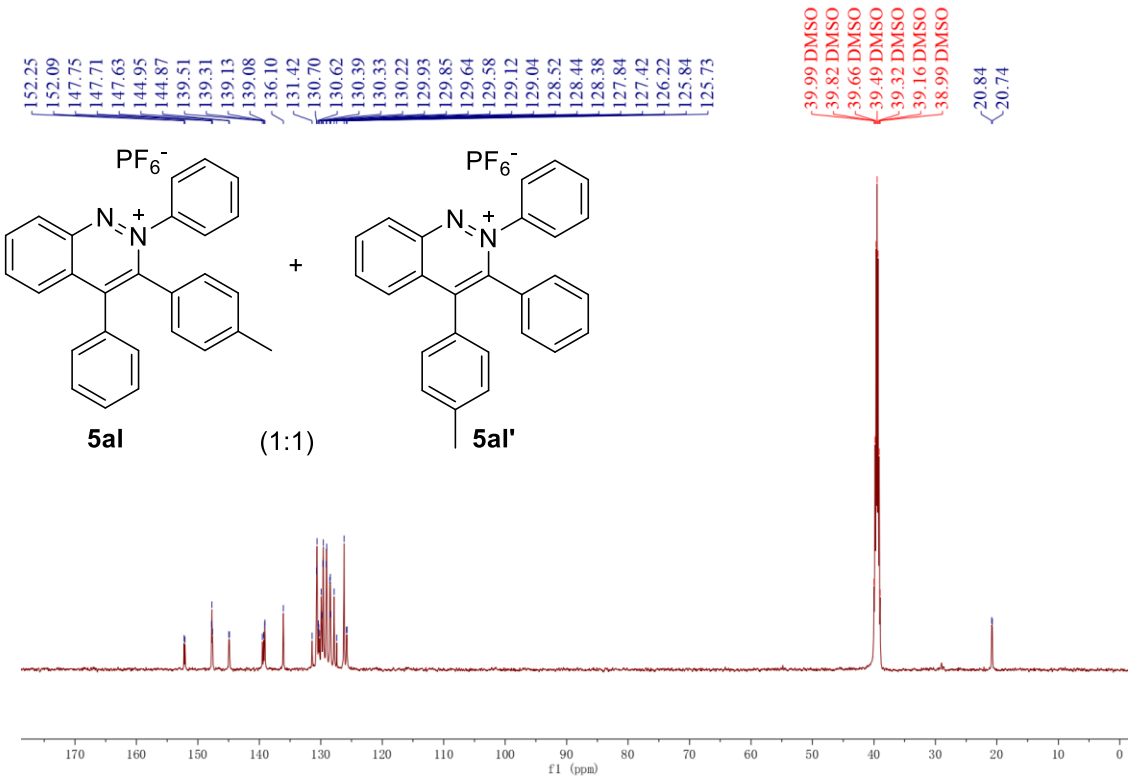

8.93
8.91
8.53
8.52
8.50
8.42
8.41
8.39
8.03
8.00
7.99
7.98
7.96
7.96
7.95
7.93
7.92
7.91
7.89
7.88
7.77
7.76
7.73
7.71
7.69
7.66
7.64
7.62
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.51
7.49
7.47
7.47
7.46
7.44
7.44
7.43
7.42
7.42
7.41
7.40
3.37 HDO
2.50
PF6-
N
N
+
5aj
1.00
1.04
1.03
6.12
2.00
2.06
1.08
2.94
6.14
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
f1 (ppm)

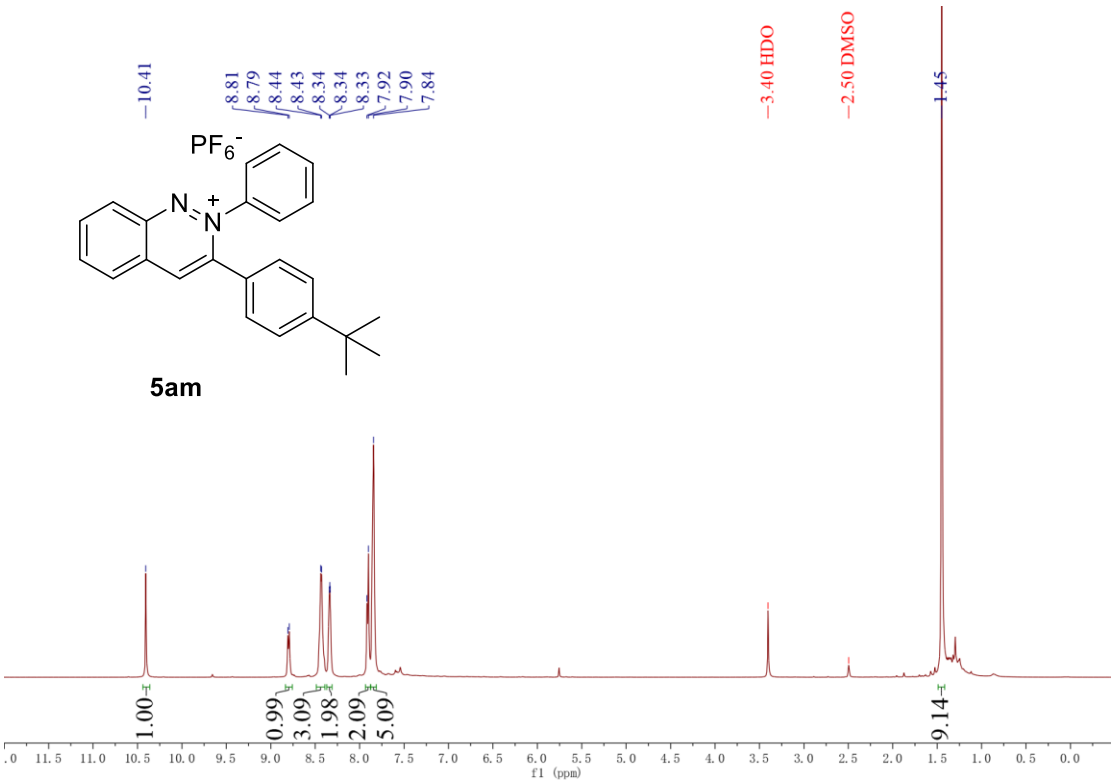

152.05
147.76
147.61
144.78
139.45
136.35
132.57
132.29
131.83
131.42
131.25
131.11
130.69
130.25
130.01
129.89
129.59
129.08
128.75
128.27
128.21
128.13
128.06
127.88
127.71
127.64
127.58
127.47
127.18
127.09
126.78
126.33
126.20
126.03
125.99
39.97 DMSO
39.80 DMSO
39.63 DMSO
39.30 DMSO
39.13 DMSO
38.97 DMSO
PF6-
N
N
+
5aj
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

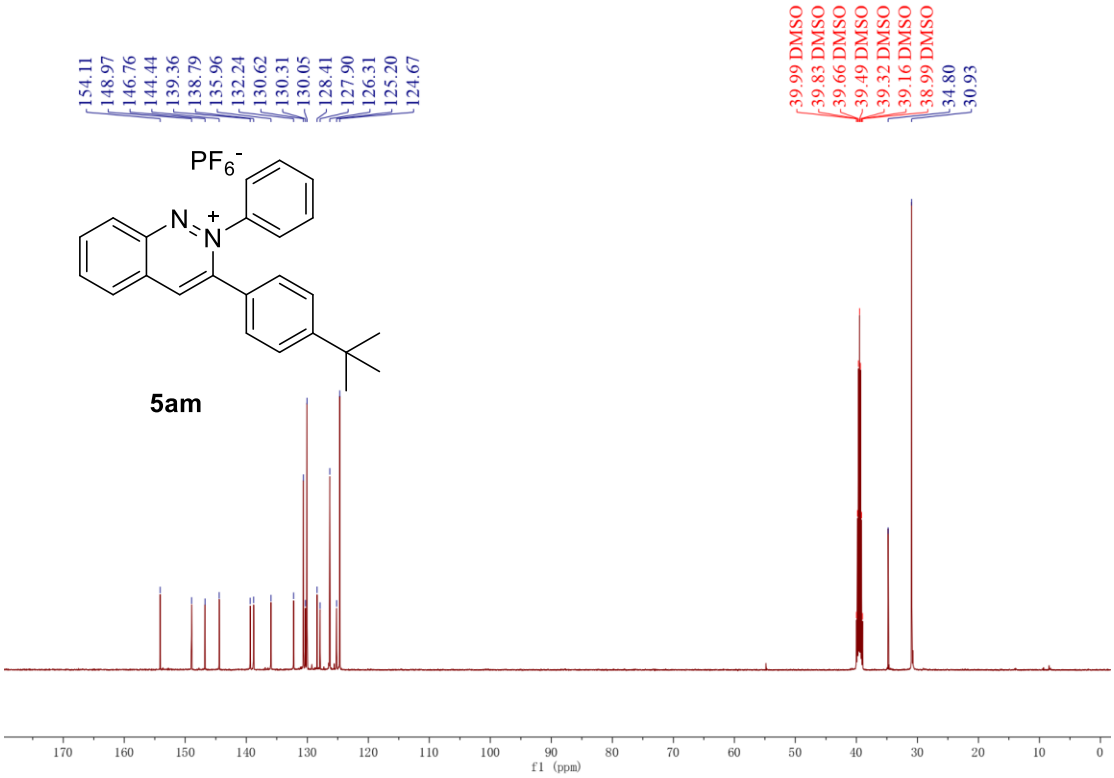

8.73
8.72
8.72
8.71
8.50
8.48
8.47
8.45
8.43
8.64
7.63
7.62
7.62
7.52
7.51
7.50
7.50
7.46
7.46
7.45
7.44
7.44
7.43
3.37 HDO
2.76
2.48
PF6-
N
N
+
5ak
1.01
1.00
0.18
0.18
8.50
8.45
8.40
8.35
8.30
8.25
f1 (ppm)
2.00
1.01
1.00
2.06
2.07
6.05
2.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

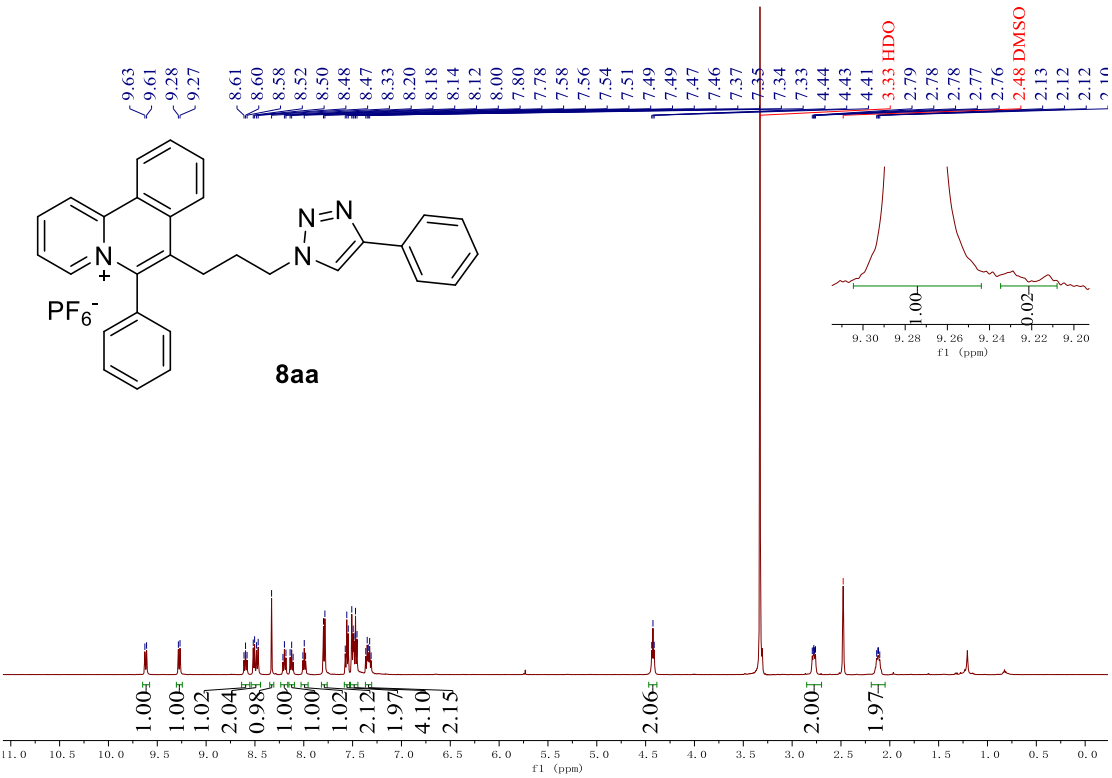

152.48
151.44
147.24
146.92
146.62
145.87
144.79
144.05
138.73
138.44
136.05
135.55
131.50
130.55
130.35
130.16
130.11
129.94
129.36
129.18
128.92
128.67
126.13
125.28
125.12
124.86
39.94 DMSO
39.78 DMSO
39.61 DMSO
39.44 DMSO
39.27 DMSO
39.11 DMSO
38.94 DMSO
20.50
16.36
PF6-
N
N
+
5ak
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

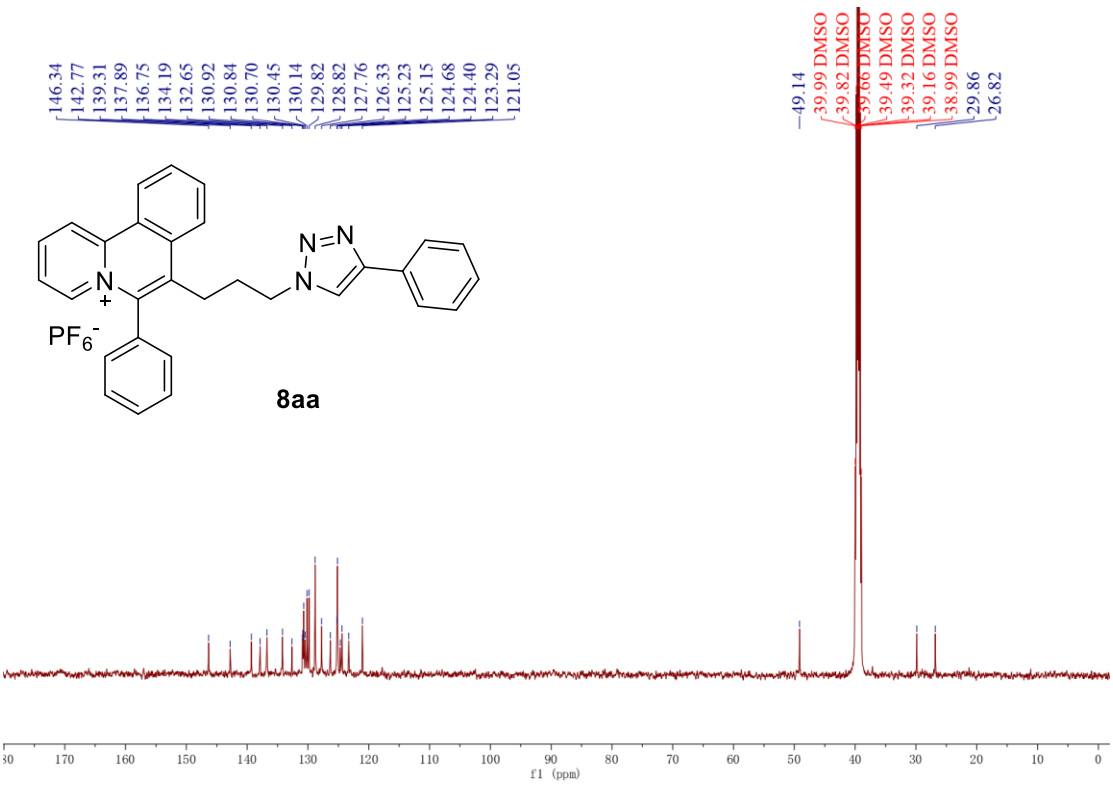

8.84
8.82
8.48
8.46
8.44
8.40
8.39
8.37
7.94
7.92
7.88
7.86
7.68
7.67
7.66
7.66
7.50
7.49
7.48
7.47
7.46
7.36
7.34
7.33
7.28
7.26
7.23
7.21
7.19
7.17
6.98
6.97
3.35 HDO
2.48 DMSO
2.30
2.11
PF6-
N
N
+
5al
(1:1)
5al'
2.01
2.17
1.96
2.22
4.15
9.83
4.28
2.14
4.15
2.19
2.03
3.00
3.02
f1 (ppm)

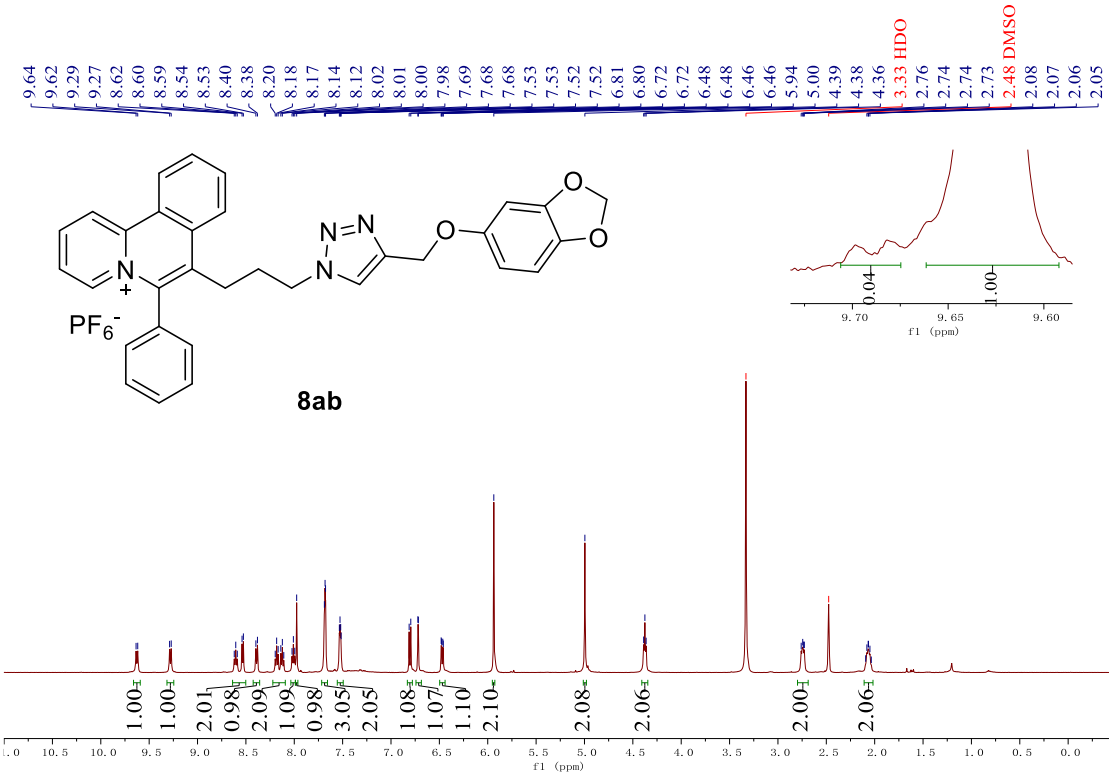

152.25
152.09
147.75
147.71
147.63
144.95
144.87
139.51
139.31
139.13
139.08
136.10
131.42
130.70
130.62
130.39
130.33
130.22
129.93
129.85
129.64
129.58
129.12
129.04
128.52
128.44
128.38
127.84
127.42
126.22
125.84
125.73
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
20.84
20.74
PF6-
N
N
+
5al
(1:1)
5al'
f1 (ppm)

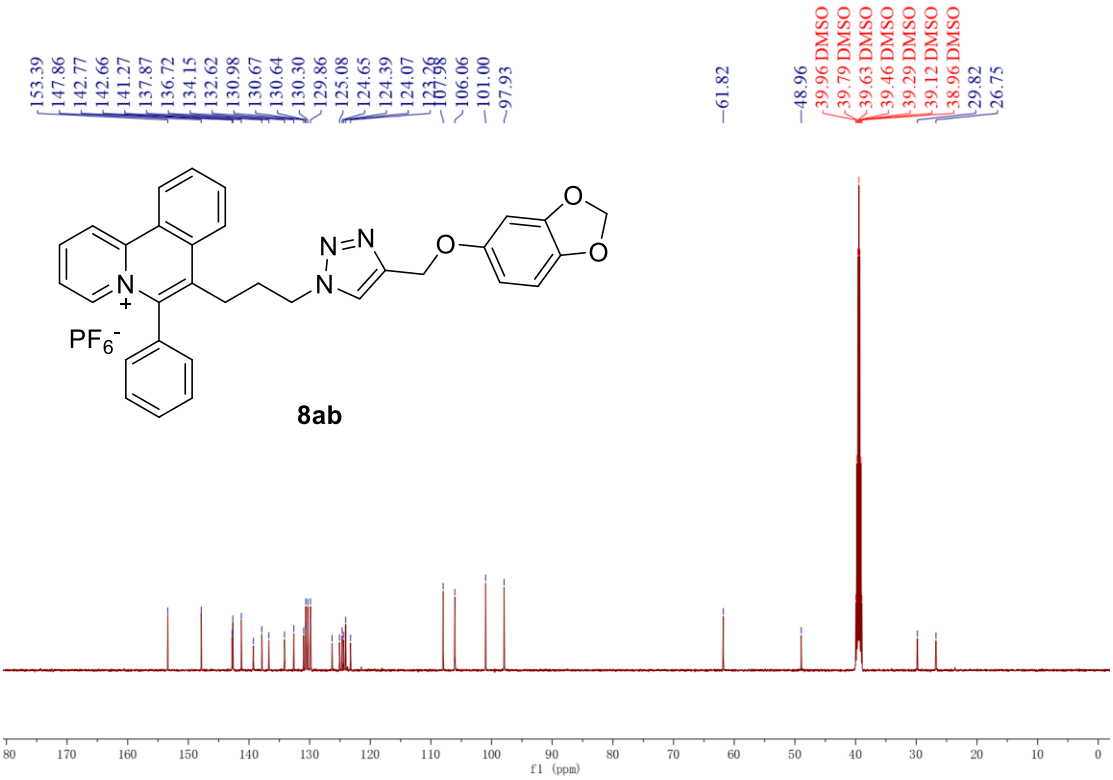

10.41
8.81
8.79
8.44
8.43
8.34
8.34
8.33
7.92
7.90
7.84
3.40 HDO
2.50 DMSO
1.45
PF6-
N
N
+
5am
1.00
0.99
3.09
1.98
2.09
5.09
9.14
f1 (ppm)

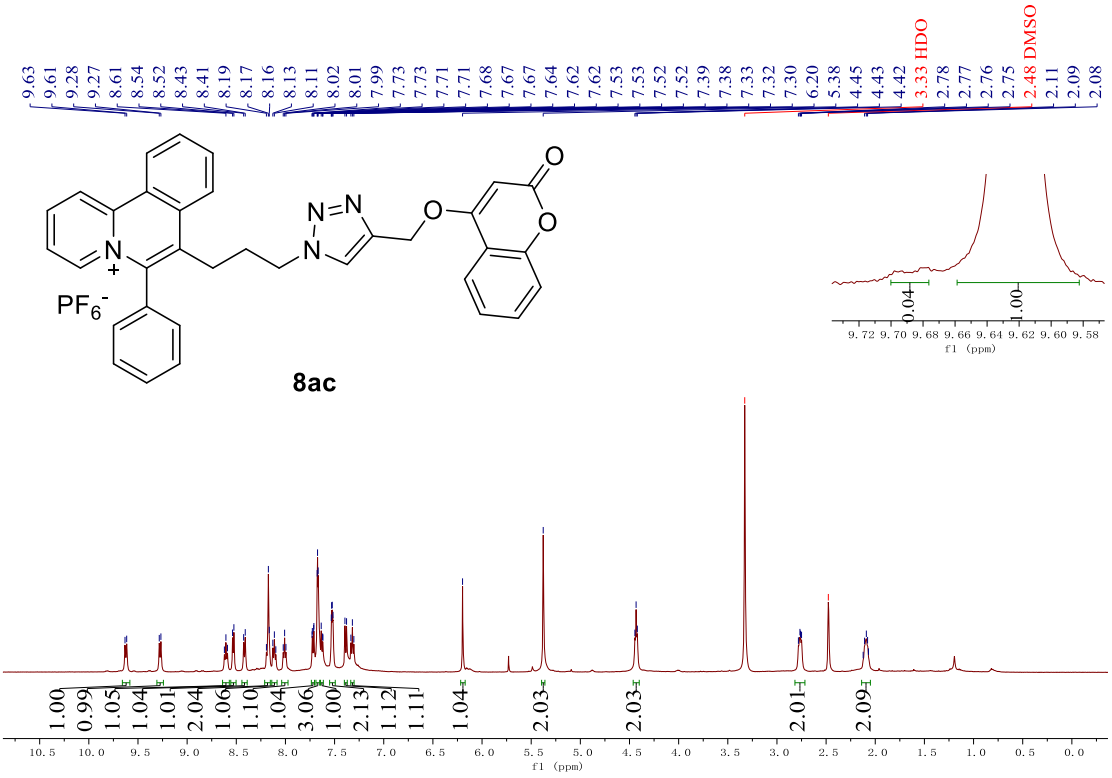

154.11
148.97
146.76
144.44
139.36
138.79
135.96
132.24
130.62
130.31
130.05
128.41
127.90
126.31
125.20
124.67
39.99 DMSO
39.83 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
34.80
30.93
PF6-
N
N
+
5am
f1 (ppm)

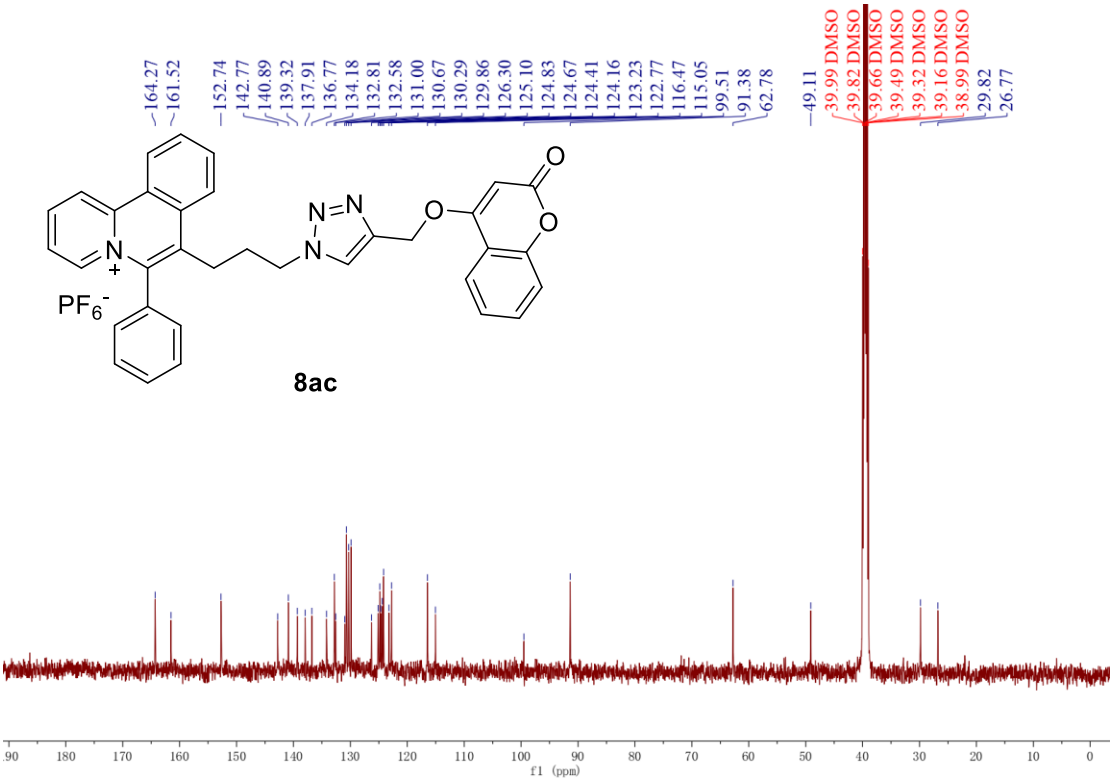

8aa
PF6-
3.33 HDO
2.48 DMSO
f1 (ppm)

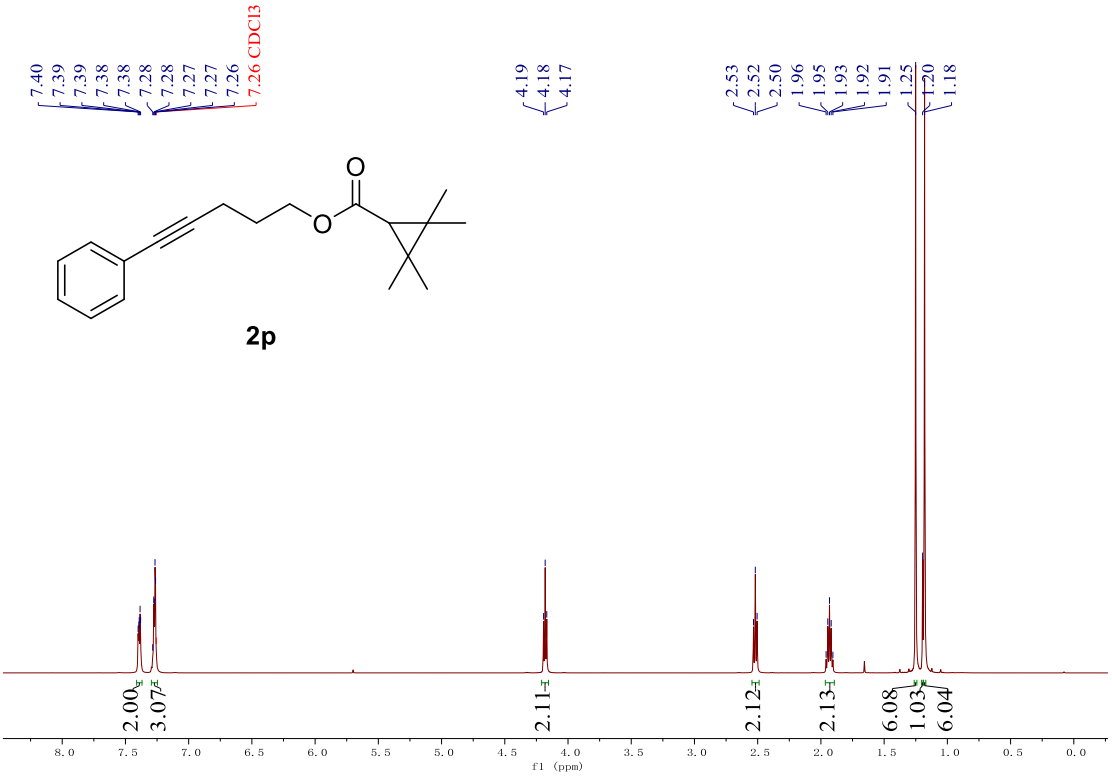

8aa
PF6-
39.99 DMSO
39.82 DMSO
39.66 DMSO
39.49 DMSO
39.32 DMSO
39.16 DMSO
38.99 DMSO
f1 (ppm)

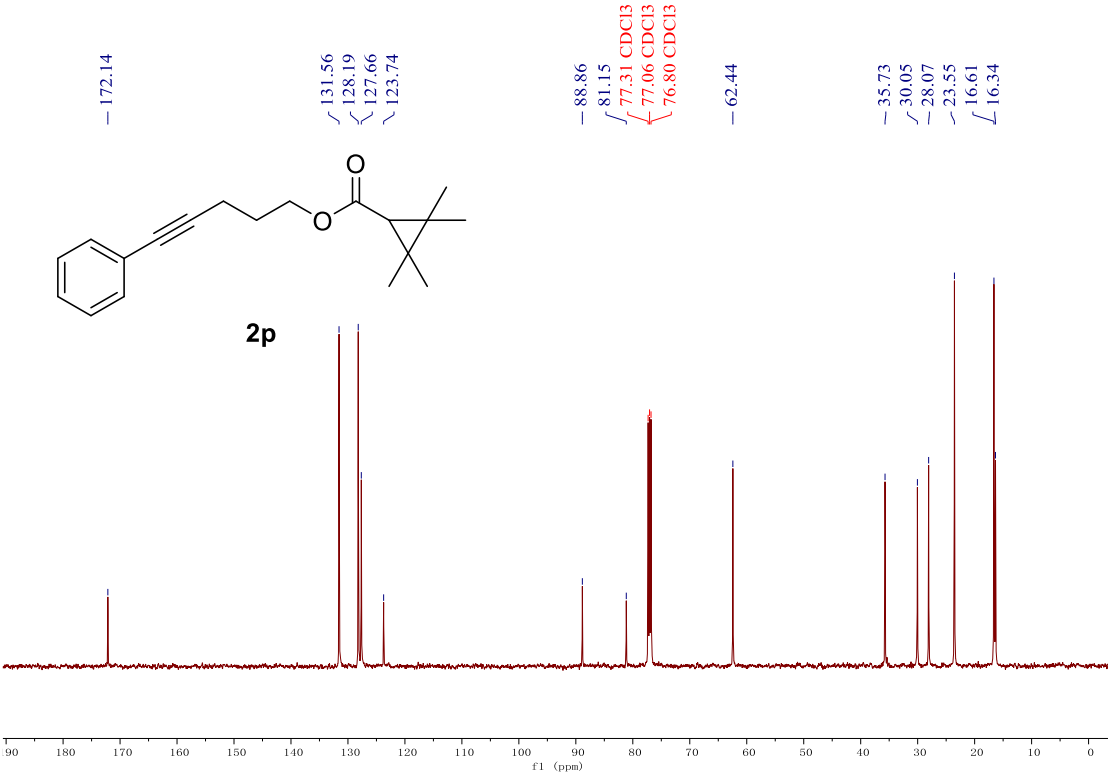

9.64 9.62 9.29 9.27 8.62 8.60 8.59 8.54 8.53 8.40 8.38 8.20 8.18 8.17 8.14 8.12 8.02 8.01 8.00 7.98 7.69 7.68 7.68 7.53 7.53 7.52 7.52 6.81 6.80 6.72 6.72 6.48 6.48 6.46 6.46 5.94 5.00 4.39 4.38 4.36 3.33 HDO 2.76 2.74 2.74 2.73 2.48 DMSO 2.08 2.07 2.06 2.05
N=N
N
O
O
O
N
+
PF6-
8ab
0.04
1.00
9.70
9.65
9.60
f1 (ppm)
1.00 1.00 2.01 0.98 2.09 1.09 0.98 3.05 2.05 1.08 1.07 1.10 2.10 2.08 2.06 2.00 2.06
f1 (ppm)

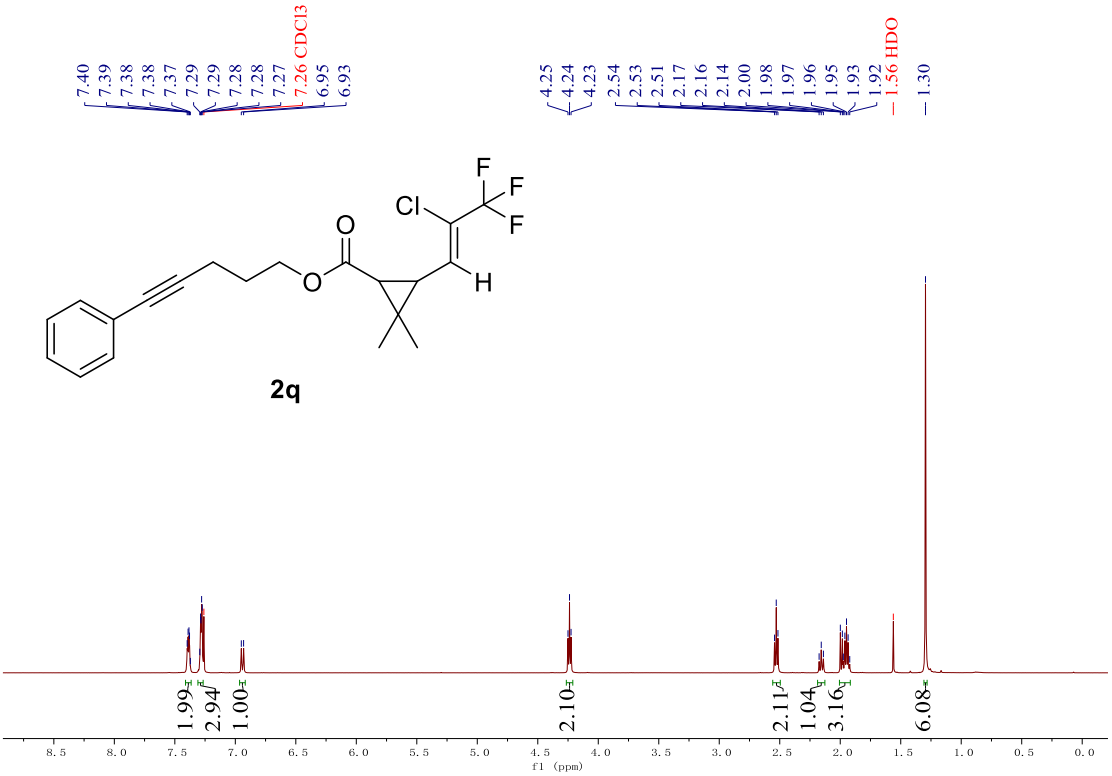

153.39 147.86 142.77 142.66 141.27 137.87 136.72 134.15 132.62 130.98 130.67 130.64 130.30 129.86 125.08 124.65 124.39 124.07 123.26 107.98 106.06 101.00 97.93
61.82
48.96
39.96 DMSO 39.79 DMSO 39.63 DMSO 39.46 DMSO 39.29 DMSO 39.12 DMSO 38.96 DMSO
29.82
26.75
N=N
N
O
O
O
N
+
PF6-
8ab
f1 (ppm)

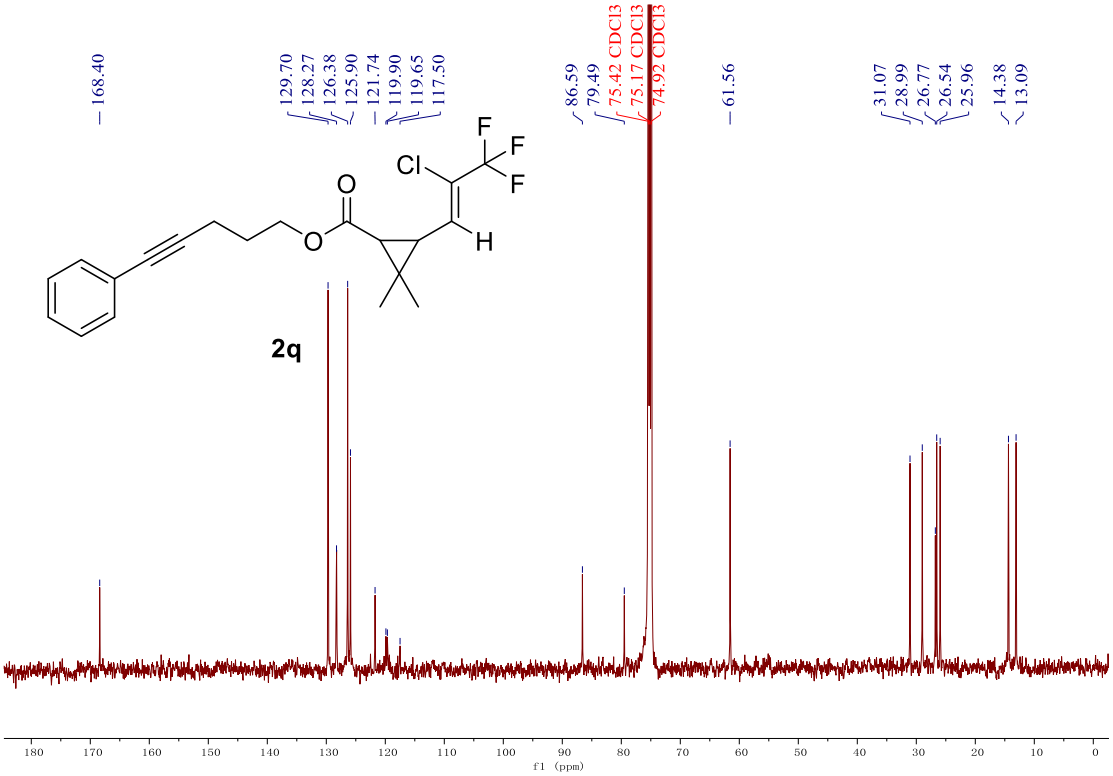

9.63 9.61 9.28 9.27 8.61 8.54 8.52 8.43 8.41 8.19 8.17 8.16 8.13 8.11 8.02 8.01 7.99 7.73 7.73 7.71 7.71 7.68 7.67 7.67 7.64 7.62 7.62 7.53 7.53 7.52 7.52 7.39 7.38 7.33 7.32 7.30 6.20 5.38 4.45 4.43 4.42 3.33 HDO 2.78 2.77 2.76 2.75 2.48 DMSO 2.11 2.09 2.08
PF6-
8ac
0.04
1.00
9.72 9.70 9.68 9.66 9.64 9.62 9.60 9.58
f1 (ppm)
1.00 0.99 1.05 1.04 1.01 2.04 1.06 1.10 1.04 3.06 1.00 2.13 1.12 1.11 1.04 2.03 2.03 2.01 2.09
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
f1 (ppm)

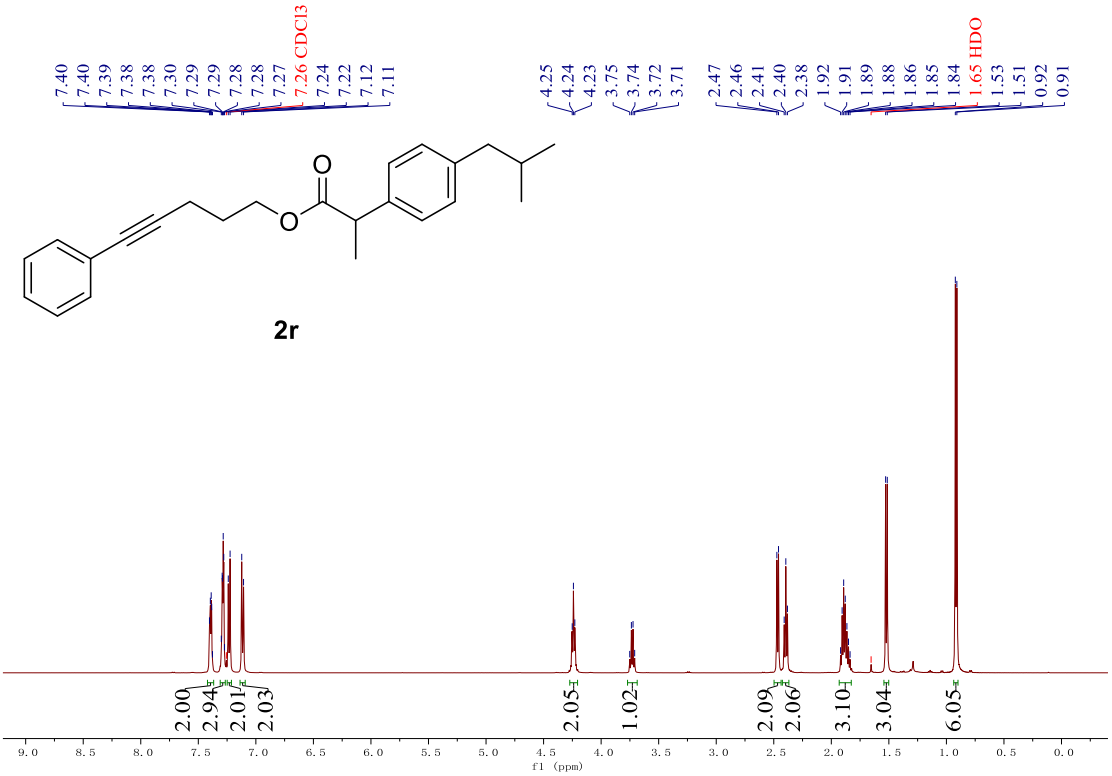

164.27 161.52 152.74 142.77 140.89 139.32 137.91 136.77 134.18 132.81 132.58 131.00 130.67 130.29 129.86 126.30 125.10 124.83 124.67 124.41 124.16 123.23 122.77 116.47 115.05 99.51 91.38 62.78 49.11 39.99 DMSO 39.82 DMSO 39.66 DMSO 39.49 DMSO 39.32 DMSO 39.16 DMSO 38.99 DMSO 29.82 26.77
PF6-
8ac
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

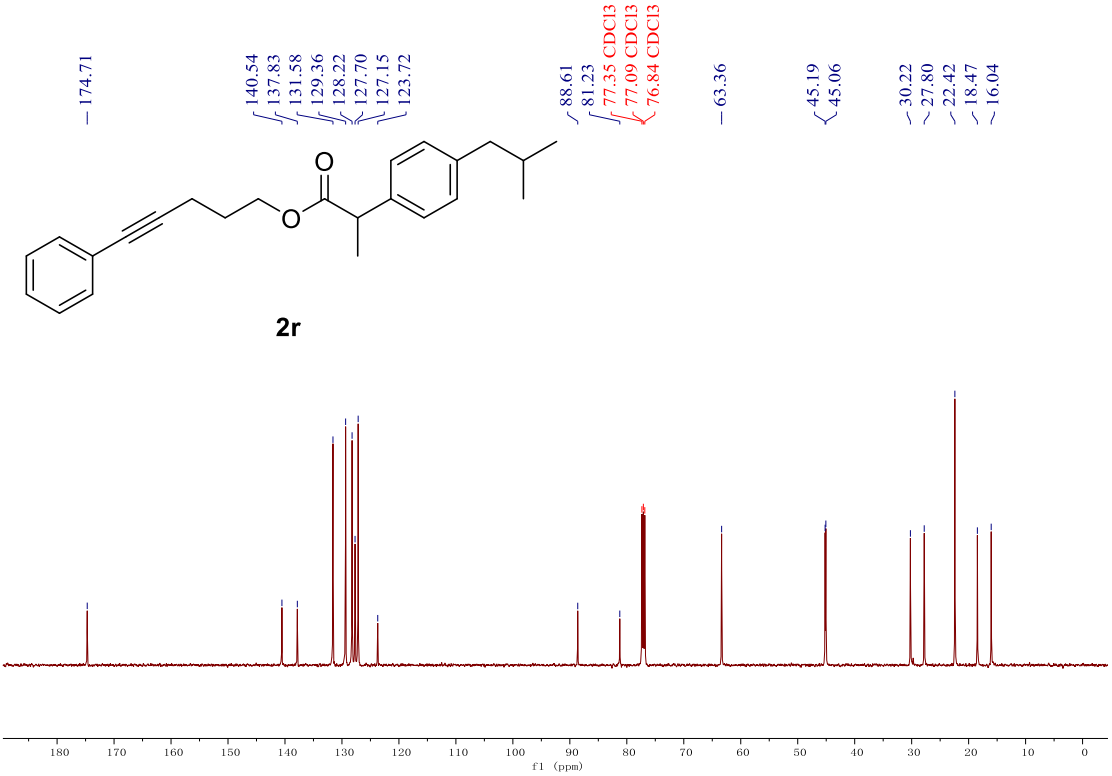

7.40
7.39
7.39
7.38
7.38
7.28
7.28
7.27
7.27
7.26
7.26 CDCl3
4.19
4.18
4.17
2.53
2.52
2.50
1.96
1.95
1.93
1.92
1.91
1.25
1.20
1.18
O
O
2p
2.00
3.07
2.11
2.12
2.13
6.08
1.03
6.04
f1 (ppm)

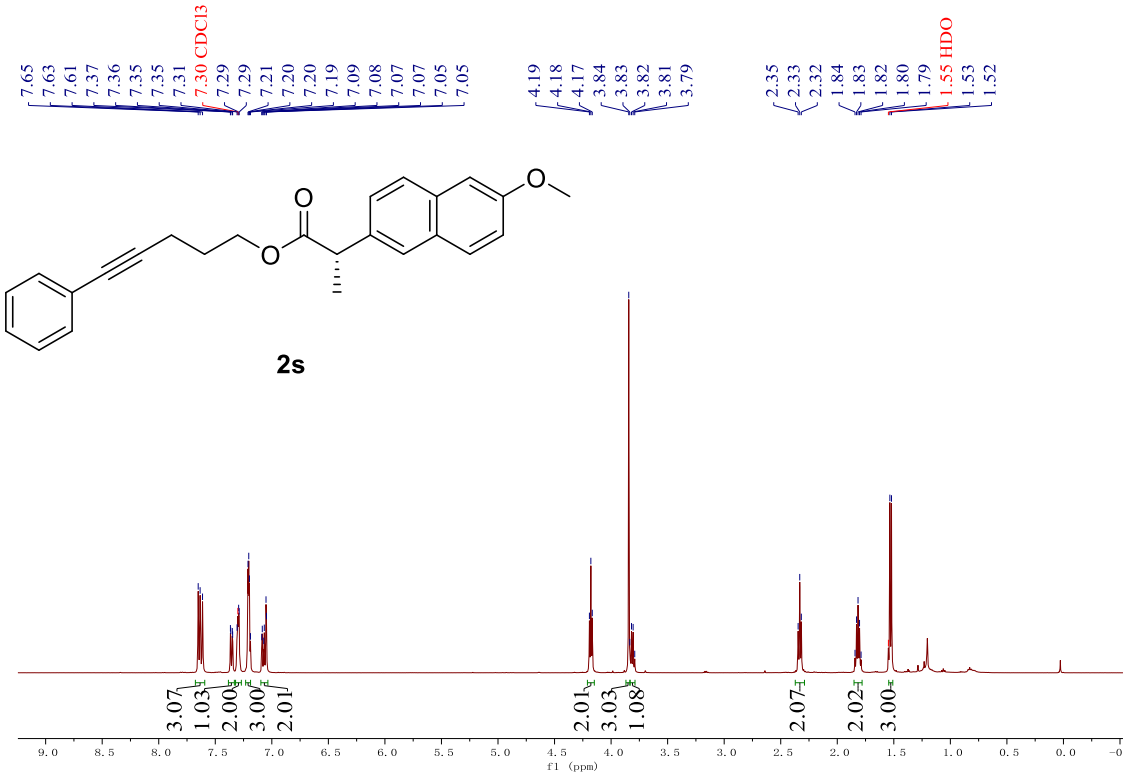

172.14
131.56
128.19
127.66
123.74
88.86
81.15
77.31 CDCl3
77.06 CDCl3
76.80 CDCl3
62.44
35.73
30.05
28.07
23.55
16.61
16.34
O
O
2p
f1 (ppm)

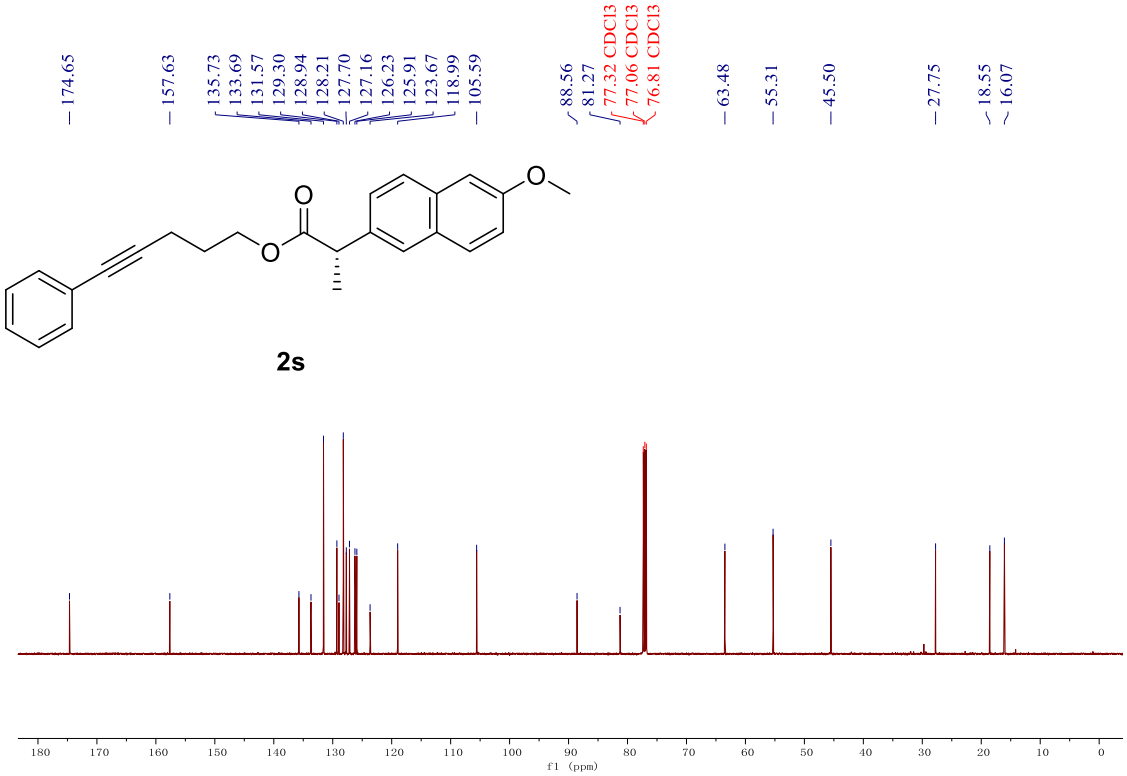

7.40
7.39
7.38
7.38
7.37
7.29
7.29
7.28
7.28
7.27
7.26 CDCl3
6.95
6.93
4.25
4.24
4.23
2.54
2.53
2.51
2.17
2.16
2.14
2.00
1.98
1.97
1.96
1.95
1.93
1.92
1.56 HDO
1.30
F
F
F
Cl
O
O
H
2q
1.99
2.94
1.00
2.10
2.11
1.04
3.16
6.08
f1 (ppm)

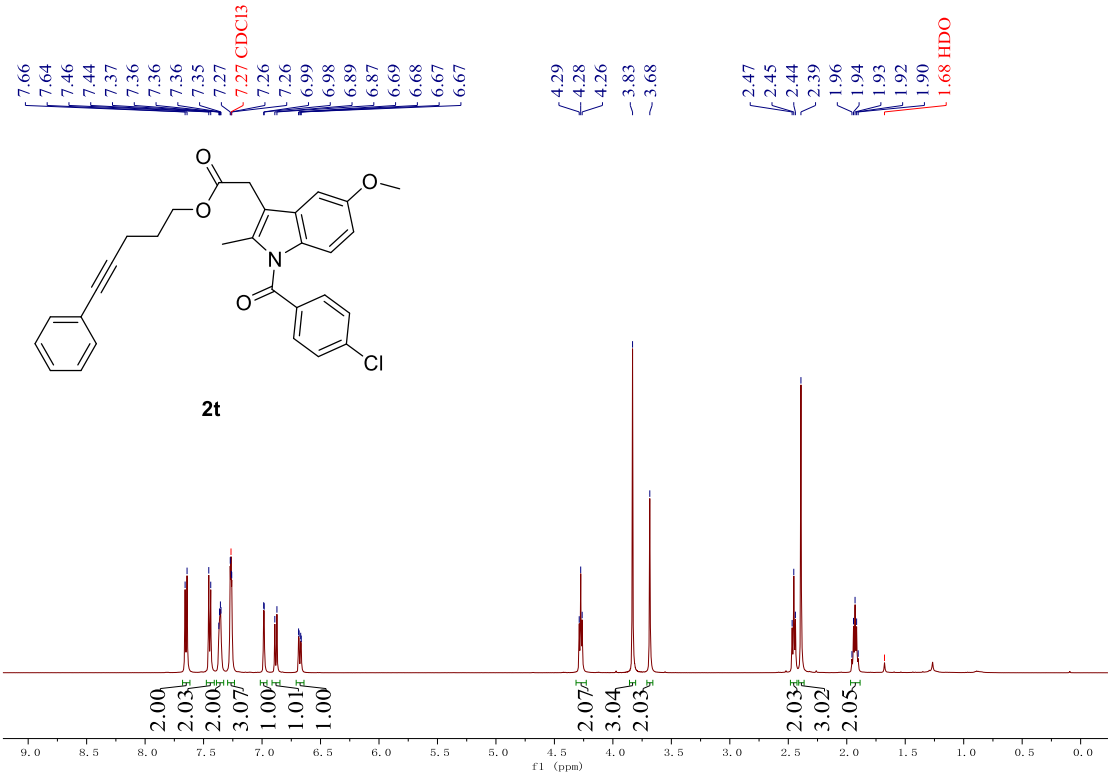

168.40
129.70
128.27
126.38
125.90
121.74
119.90
119.65
117.50
86.59
79.49
75.42 CDCl3
75.17 CDCl3
74.92 CDCl3
61.56
31.07
28.99
26.77
26.54
25.96
14.38
13.09
F
F
F
Cl
O
O
H
2q
f1 (ppm)


7.40
7.40
7.39
7.38
7.38
7.30
7.29
7.29
7.28
7.28
7.27
7.26 CDCl3
7.24
7.22
7.12
7.11
4.25
4.24
4.23
3.75
3.74
3.72
3.71
2.47
2.46
2.41
2.40
2.38
1.92
1.91
1.89
1.88
1.86
1.85
1.84
1.65 HDO
1.53
1.51
0.92
0.91
O
O
2r
2.00
2.94
2.01
2.03
2.05
1.02
2.09
2.06
3.10
3.04
6.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

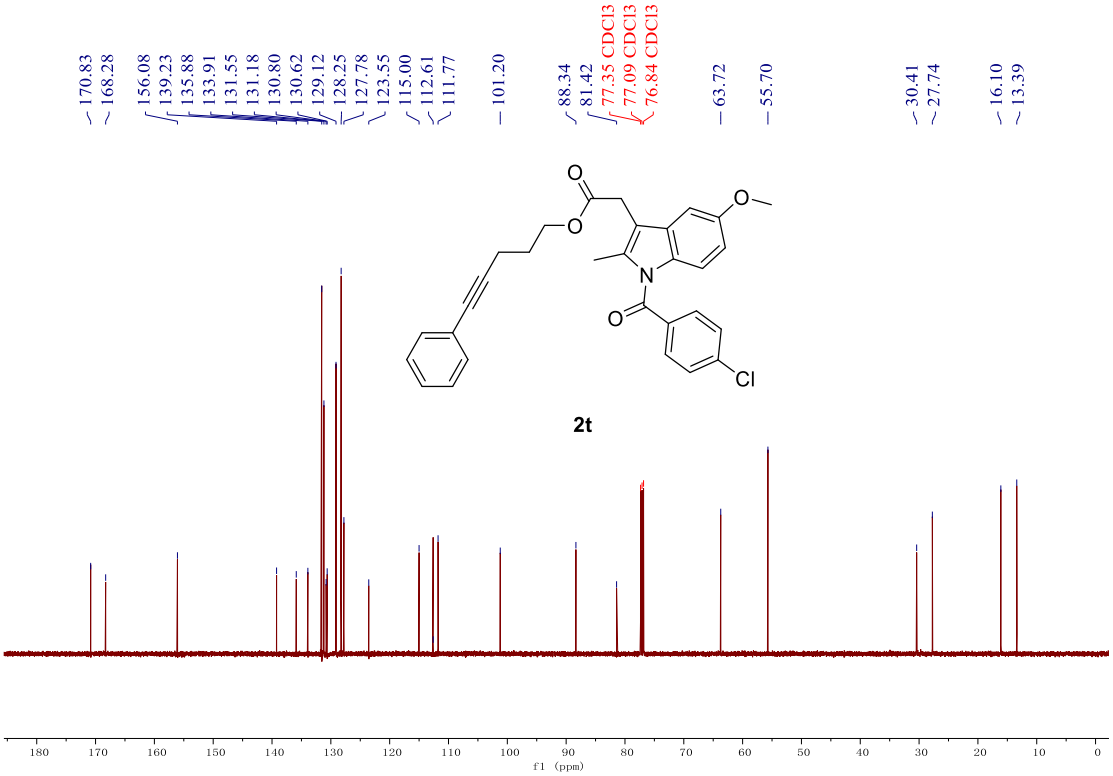

174.71
140.54
137.83
131.58
129.36
128.22
127.70
127.15
123.72
88.61
81.23
77.35 CDCl3
77.09 CDCl3
76.84 CDCl3
63.36
45.19
45.06
30.22
27.80
22.42
18.47
16.04
O
O
2r
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.65
7.63
7.61
7.37
7.36
7.35
7.35
7.31
7.30 CDCl3
7.29
7.29
7.21
7.20
7.20
7.19
7.09
7.08
7.07
7.07
7.05
7.05
4.19
4.18
4.17
3.84
3.83
3.82
3.81
3.79
2.35
2.33
2.32
1.84
1.83
1.82
1.80
1.79
1.55 HDO
1.53
1.52
2s
3.07
1.03
2.00
3.00
2.01
2.01
3.03
1.08
2.07
2.02
3.00
f1 (ppm)

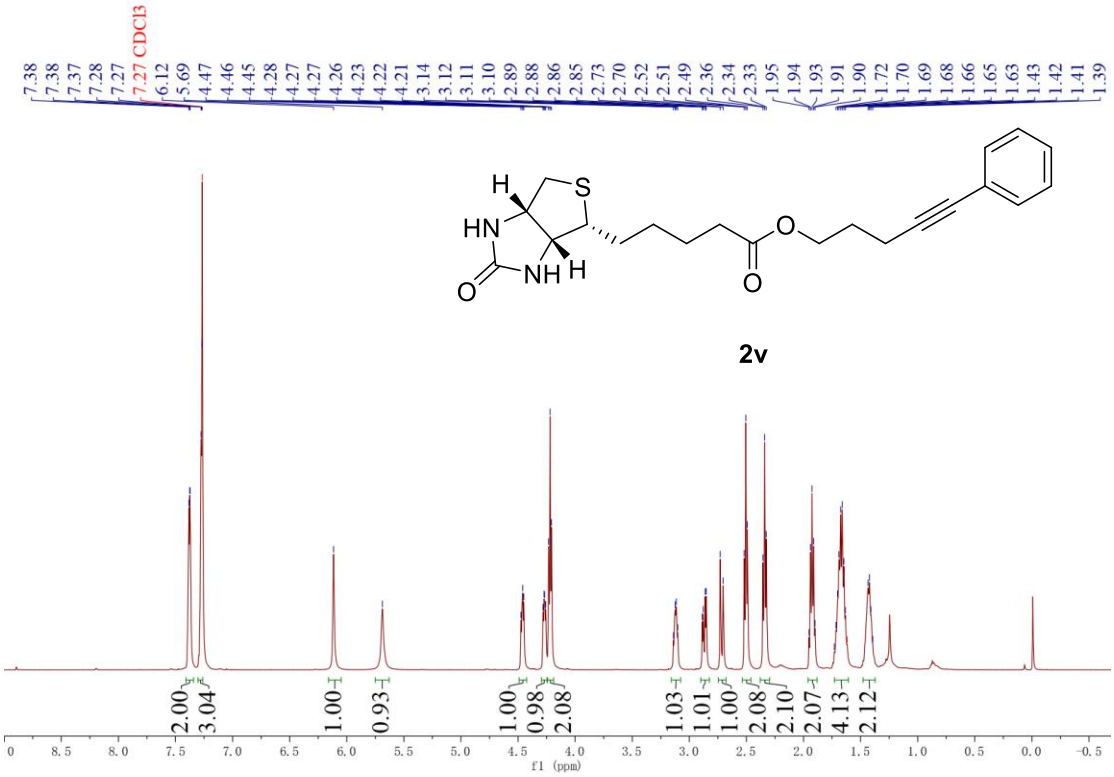

174.65
157.63
135.73
133.69
131.57
129.30
128.94
128.21
127.70
127.16
126.23
125.91
123.67
118.99
105.59
88.56
81.27
77.32 CDCl3
77.06 CDCl3
76.81 CDCl3
63.48
55.31
45.50
27.75
18.55
16.07
2s
f1 (ppm)


7.66
7.64
7.46
7.44
7.37
7.36
7.36
7.35
7.27
7.27 CDCl3
7.26
7.26
6.99
6.98
6.89
6.87
6.69
6.68
6.67
6.67
4.29
4.28
4.26
3.83
3.68
2.47
2.45
2.44
2.39
1.96
1.94
1.93
1.92
1.90
1.68 HDO
2.00
2.03
2.00
3.07
1.00
1.01
1.00
2.07
3.04
2.03
2.03
3.02
2.05
f1 (ppm)

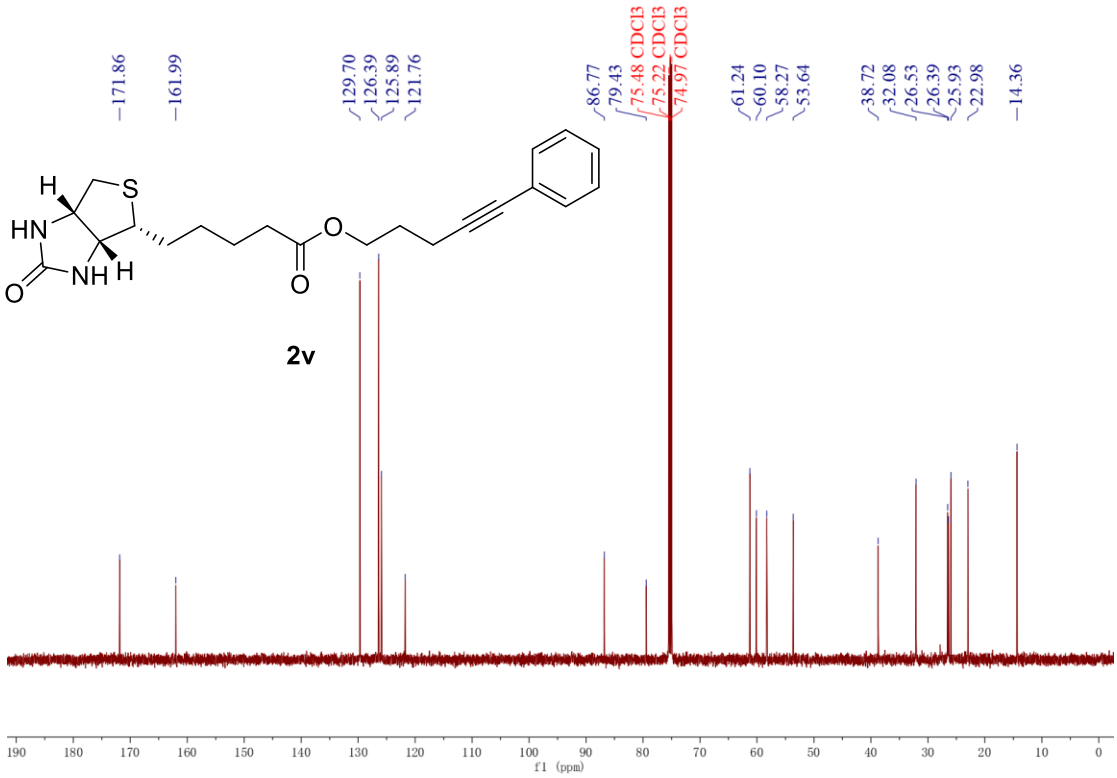
2t


170.83
168.28
156.08
139.23
135.88
133.91
131.55
131.18
130.80
130.62
129.12
128.25
127.78
123.55
115.00
112.61
111.77
101.20
88.34
81.42
77.35 CDCl3
77.09 CDCl3
76.84 CDCl3
63.72
55.70
30.41
27.74
16.10
13.39
f1 (ppm)

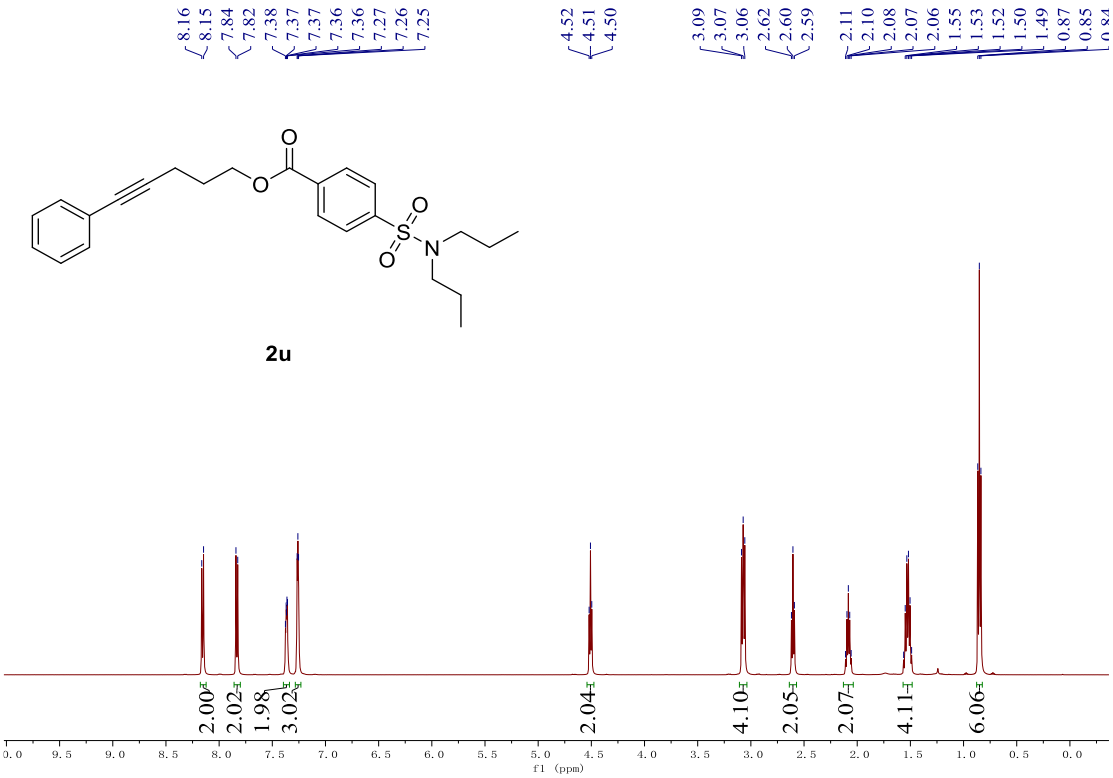
2t

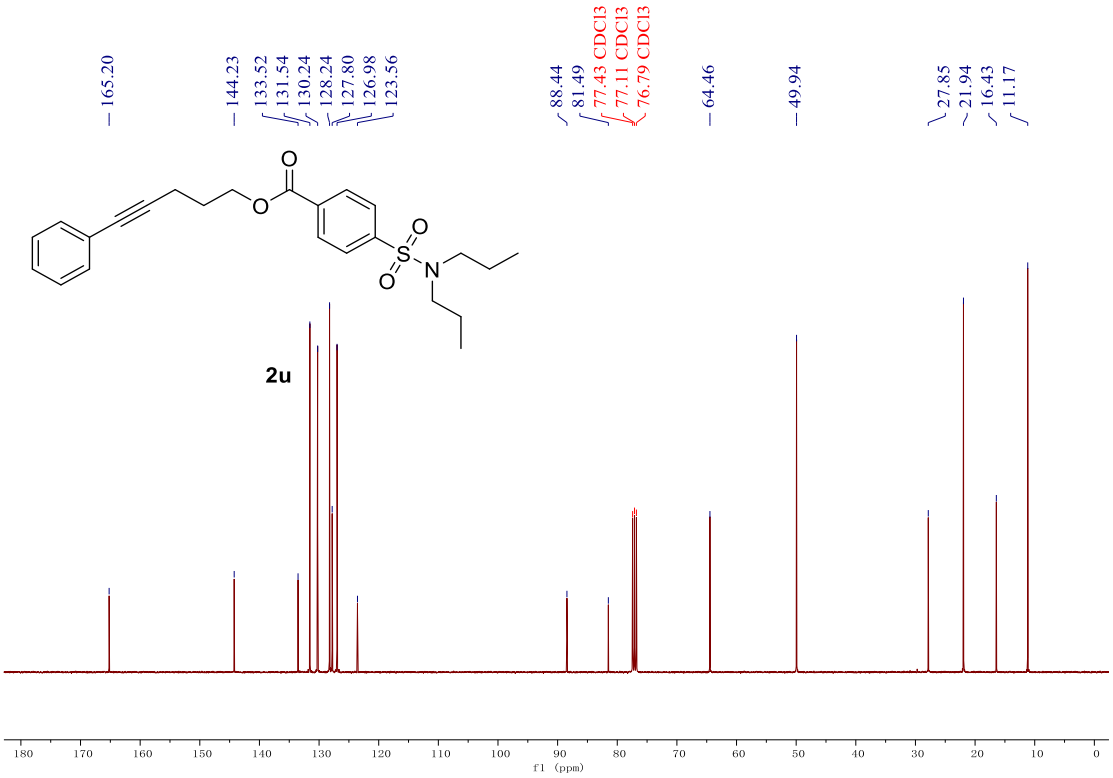

7.38
7.38
7.37
7.28
7.27
7.27 CDCl3
6.12
5.69
4.47
4.46
4.45
4.28
4.27
4.27
4.26
4.23
4.22
4.21
3.14
3.12
3.11
3.10
2.89
2.88
2.86
2.85
2.73
2.70
2.52
2.51
2.49
2.36
2.34
2.33
1.95
1.94
1.93
1.91
1.90
1.72
1.70
1.69
1.68
1.66
1.65
1.63
1.43
1.42
1.41
1.39
H
S
HN
O
NH H
O
O
2.00
3.04
1.00
0.93
1.00
0.98
2.08
1.03
1.01
1.00
2.08
2.10
2.07
4.13
2.12
f1 (ppm)

2v


171.86
161.99
129.70
126.39
125.89
121.76
86.77
79.43
75.48 CDCl3
75.22 CDCl3
74.97 CDCl3
61.24
60.10
58.27
53.64
38.72
32.08
26.53
26.39
25.93
22.98
14.36
H
S
HN
O
NH H
O
O
f1 (ppm)

2v


8.16
8.15
7.84
7.82
7.38
7.37
7.37
7.36
7.36
7.27
7.26
7.25
4.52
4.51
4.50
3.09
3.07
3.06
2.62
2.60
2.59
2.11
2.10
2.08
2.07
2.06
1.55
1.53
1.52
1.50
1.49
0.87
0.85
2u
2.00
2.02
1.98
3.02
2.04
4.10
2.05
2.07
4.11
6.06
f1 (ppm)


165.20
144.23
133.52
131.54
130.24
128.24
127.80
126.98
123.56
88.44
81.49
77.43 CDCl3
77.11 CDCl3
76.79 CDCl3
64.46
49.94
27.85
21.94
16.43
11.17
2u
f1 (ppm)