Supporting Information

Synthesis of cationic π-extended imidazolium salts by sequential Cu-catalyzed arylation/annulation and photocyclization

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Table of Contents

I. General Remarks

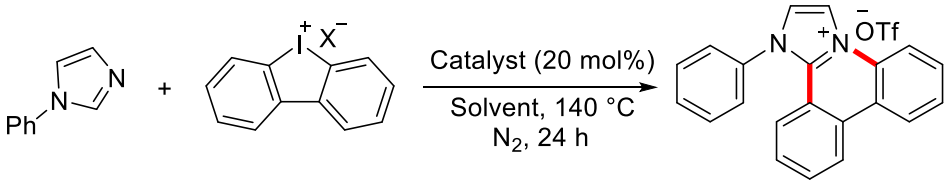
All commercially available reagents were used without further purification unless otherwise noted. DMF was dried through a solvent purification system from Innovative Technology. Cu_2O (99% purity) was purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. MeOH (AR) and MeCN (AR) were purchased from Chengdu Kelong Chemical Engineering Reagent (China) CO., Ltd. Analytical thin layer chromatography was performed on HG/T2354-92 GF254 plates (Qingdao Haiyang Chemical Co., Ltd.). The 1-arylimidazoles[1], 1,2,3-triaryl imidazolium salts[2] and cyclic diaryliodonium salts[3] were prepared according to the literature procedures.

NMR spectroscopy were obtained on a Agilent 400-MR DD2 spectrometer. The ^{1}H NMR (400 MHz) chemical shifts were recorded relative to $CDCl_3$ or DMSO-d_6 as the internal reference ($CDCl_3$: δ = 7.26 ppm; DMSO-d_6: δ = 2.50 ppm). The ^{13}C NMR (100 MHz) chemical shifts were given using $CDCl_3$ or DMSO-d_6 as the internal standard ($CDCl_3$: δ = 77.16 ppm; DMSO-d_6: δ = 39.52 ppm). High resolution mass spectra (HR-MS) were obtained with a Shimadzu LCMS-ITTOF (ESI). Single crystal X-Ray diffraction data were collected on an Agilent Technologies Gemini single-crystal diffractometer. Absorption spectra were obtained on a HITACHI U-2910 spectrometer. Fluorescence spectra and absolute quantum yields were collected on a Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer with a calibrated integrating sphere system. Photocyclization reactions were performed with a Rayonet reactor (RPR-200) with 254 nm (168 W) lamps in quartz flasks.

II. Optimization of Reaction Conditions and General Procedures

a) Screening of reaction conditions

Table S1 Optimization for the arylation/annulation of 1a.[a]



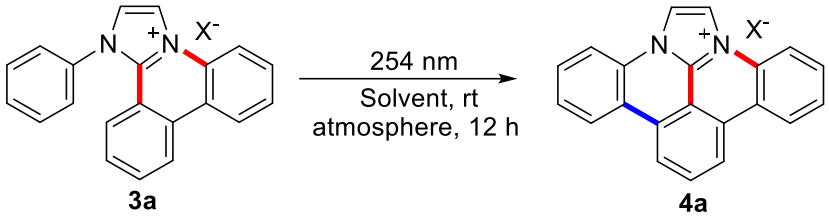
1a **2a** **3a**

Entry	Catalyst	Solvent	Base	X^-	Yield (%)[b]
1	Cu_2O	DMF	--	OTf^-	95
2	$Cu(OAc)_2 \cdot H_2O$	DMF	--	OTf^-	91
3	Cu_2O	DMF	NaOAc	OTf^-	53
4	Cu_2O	DMF	--	BF_4^-	94

5	Cu_2O	DMF	--	Cl^-	trace
6	Cu_2O	Dioxane	--	OTf^-	94
7	Cu_2O	1,2-Dichlorobenzene	--	OTf^-	75

[a]**1a** (0.2 mmol), **2a** (0.4 mmol), a catalyst (20 mol%), and a solvent (1 mL) at 140 °C, N_2, 24 h; [b]Isolated yield.

Table S2 Optimization for the photocyclization of 3a.[a]

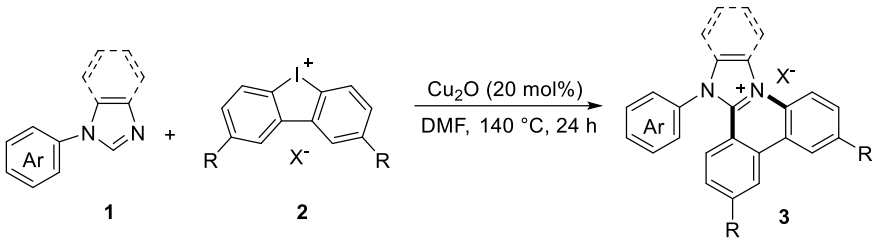


3a **4a**

Entry	Solvent	X^-	Atmosphere	Yield (%)[b]
1	MeOH	OTf^-	air	70
2	MeOH	BF_4^-	air	67
3	DMF	OTf^-	air	trace
4	MeCN	OTf^-	air	trace
5	DCM	OTf^-	air	13
6	MeOH	OTf^-	N_2	trace

[a]**3a** (30 mg) in a solvent (30 mL) under 254 nm UV-light (168 W), rt, 12 h; [b]Isolated yield.

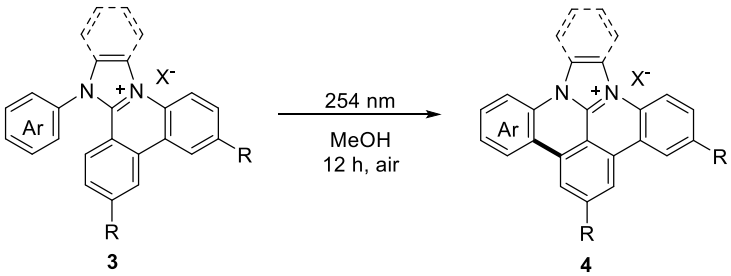
b) General procedure for the synthesis of 3



1 **2** **3**

A flame-dried Schlenk tube with a magnetic stirring bar was charged with 1-arylimidazole **1** (0.2 mmol), cyclic diaryliodonium salt **2** (0.4 mmol), Cu_2O (5.7 mg, 20 mol%), and DMF (1 mL) under N_2. The reaction mixture was heated at 140 ℃ for 24 h. After reaction was complete, the reaction mixture was concentrated and the residue was purified by column chromatography on silica gel with CH_2Cl_2/MeOH (v/v, 40/1−25/1) to provide product **3**.

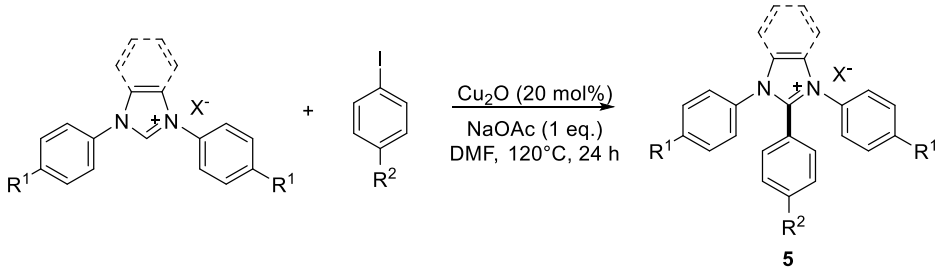
c) General procedure for the intramolecular photocyclization reaction of 3



3 **4**

A quartz tube was charged with **3** (30 mg) and MeOH (30 mL) in air. The reaction mixture reacted at room temperature for 12 hours under the irradiation of 254 nm ultraviolet light. Then the reaction mixture was concentrated and the residue was purified by column chromatography on silica gel with CH_2Cl_2/MeOH (v/v, 40/1−10/1) to provide product **4**.

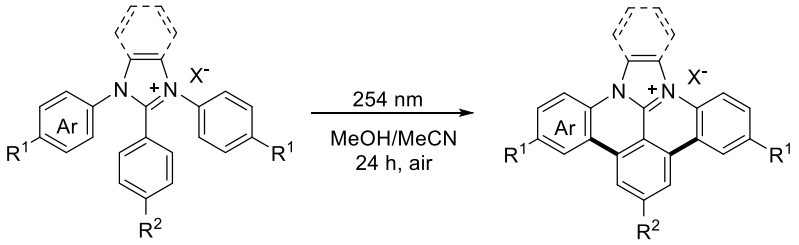
d) General procedure for the synthesis of 5



5

A flame-dried Schlenk tube with a magnetic stirring bar was charged with 1,3-diaryl imidazolium salt (0.2 mmol), an iodoaromatic compounds (0.4 mmol), Cu_2O (5.7 mg, 20 mol%), NaOAc (16.4 mg, 0.2 mmol) and DMF (1 mL) under N_2. The reaction mixture was heated at 120 ℃ for 24 h. After reaction was complete, the reaction mixture was concentrated and the residue was purified by column chromatography on silica gel with CH_2Cl_2/MeOH (v/v, 50/1−30/1) to provide product **5**.

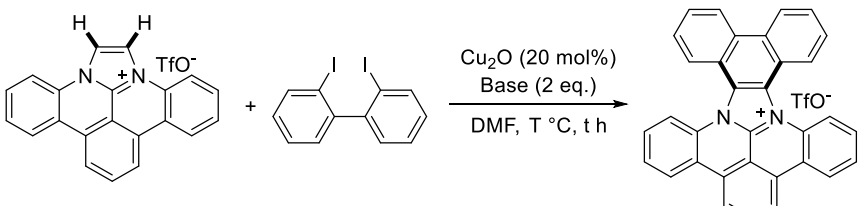
e) General procedure for the intramolecular photocybisclization reaction of 5



5 **6**

A quartz tube was charged with **5** (30 mg) and MeOH/MeCN (26 mL/4 mL) in air. The reaction mixture reacted at room temperature for 24 hours under the irradiation of 254 nm ultraviolet light. Then the reaction mixture was concentrated and the residue was purified by column chromatography on silica gel with CH_2Cl_2/MeOH (v/v, 40/1−10/1) to provide product **6**.

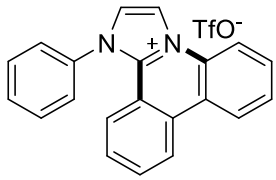
f) Synthesis of 4x



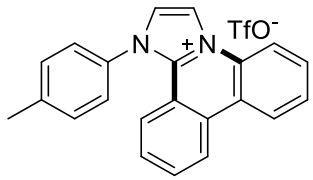
4a **4x**

A flame-dried Schlenk tube with a magnetic stirring bar was charged with **4a** (44.2 mg, 0.1 mmol), 2,2'-diiodo-1,1'-biphenyl (81.2 mg, 0.2 mmol), Cu_2O (2.8 mg, 20 mol%), KOAc (39.2 mg, 0.2 mmol) and DMF (1 mL) under N_2. The reaction mixture was heated at 120 ℃ for 24 h. After reaction was complete, the reaction mixture was concentrated and the residue was purified by column chromatography on silica gel with CH_2Cl_2/MeOH (v/v, 50/1−25/1) to provide product **4x** as a light yellow solid (30.8 mg, 52% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.94-8.04 (m, 8H), 8.52 (t, J = 8.0 Hz, 1H), 8.64 (d, J = 7.6 Hz, 4H), 9.11-9.18 (m, 6H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 112.1, 120.0, 120.9, 122.5, 123.0, 123.8, 125.2, 126.1, 126.3, 127.7, 128.6, 128.9, 129.98, 130.03, 130.1, 131.1, 134.5, 138.9 ppm. HRMS (ESI$^+$): calcd for $C_{28}H_{12}N_5^+$ [M−$CF_3SO_3^-$]$^+$ 443.1543, found 443.1590.

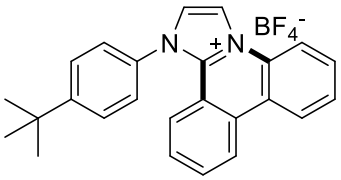
III. Characterization of 3, 4, 5 and 6



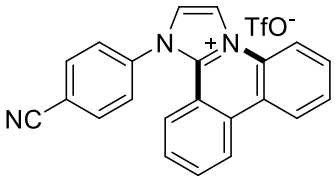
1-phenyl-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3a): A white solid (84.4 mg, 95% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.26 (d, J = 8.4 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H), 7.82-8.00 (m, 7H), 8.03-8.07 (m, 1H), 8.59 (d, J = 2.0 Hz, 1H), 8.76 (d, J = 8.0 Hz, 1H), 9.00 (d, J = 8.4 Hz, 2H), 9.42 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 115.2, 116.7, 117.4, 121.8, 123.7, 124.4, 125.0, 127.1, 127.4, 128.6, 129.1, 129.2, 130.3, 130.9, 131.1, 131.7, 132.6, 136.5, 136.7 ppm. HRMS (ESI$^+$): calcd for $C_{21}H_{15}N_2$ [M−$CF_3SO_3^-$]$^+$ 295.1230, found 295.1225.



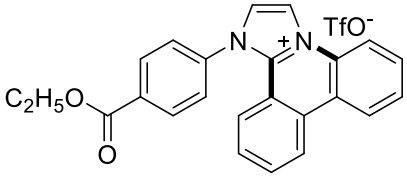
1-(*p*-tolyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3b): A white solid (86 mg, 94% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.40 (d, J = 2.0 Hz, 1H), 8.99 (d, J = 7.6 Hz, 2H), 8.75 (d, J = 8.4 Hz, 1H), 8.53 (d, J = 1.6 Hz, 1H), 7.90-8.06 (m, 3H), 7.73 (d, J = 8 Hz, 2H), 7.63 (d, J = 7.2 Hz, 3H), 7.34 (d, J = 8.4 Hz, 1H), 2.54 (s, 3H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 21.0, 115.1, 116.8, 117.4, 121.8, 123.8, 124.4, 125.0, 126.8, 127.6, 128.6, 129.1, 129.3, 130.2, 131.1, 131.3, 132.5, 134.1, 136.7, 141.6 ppm. HRMS (ESI$^+$): calcd for $C_{22}H_{17}N_2$ [M−$CF_3SO_3^-$]$^+$ 309.1386, found 309.1357.



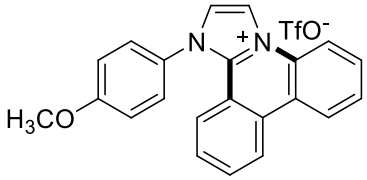
1-(4-(*tert*-butyl)phenyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium tetrafluoroborate (3c): A white solid (73.6 mg, 84% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.43 (s, 9H), 7.29 (d, J = 8.0 Hz, 1H), 7.60 (t, J = 8.0 Hz, 1H), 7.77 (d, J = 8.8 Hz, 2H), 7.85 (d, J = 8.4 Hz, 2H), 7.93 (t, J = 8.0 Hz, 1H), 7.98 (t, J = 7.2 Hz, 1H), 8.04 (t, J = 8.0 Hz, 1H), 8.57 (d, J = 2.4 Hz, 1H), 8.75 (d, J = 8.0 Hz, 1H), 8.99 (d, J = 8.4 Hz, 2H), 9.40 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 31.0, 35.0, 115.1, 116.7, 117.3, 121.8, 123.7, 124.4, 124.9, 126.5, 127.5, 127.6, 128.6, 129.1, 129.2, 130.2, 131.0, 132.5, 134.0, 136.7, 154.5 ppm. HRMS (ESI$^+$): calcd for $C_{25}H_{23}N_2$ [M−BF_4^-]$^+$ 351.1856, found 351.1852.



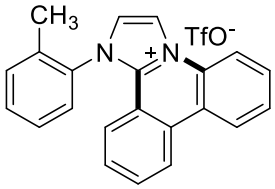
1-(4-cyanophenyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3d): A white solid (88.5 mg, 94% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.31 (d, J = 8.0 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.95 (t, J = 7.6 Hz, 1H), 8.00-8.11 (m, 4H), 8.34-8.38 (m, 2H), 8.61 (d, J = 2.4 Hz, 1H), 8.77 (d, J = 8.0 Hz, 1H), 9.02 (dd, J = 3.6 Hz, J = 8.4 Hz, 2H), 9.46 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 114.5, 115.5, 116.4, 117.4, 117.9, 121.9, 124.1, 124.5, 125.0, 127.2, 128.4, 128.8, 129.1, 129.5, 130.3, 131.2, 132.8, 135.1, 136.9, 140.1 ppm. HRMS (ESI$^+$): calcd for $C_{22}H_{14}N_3$ [M−$CF_3SO_3^-$]$^+$ 320.1182, found 320.1178.



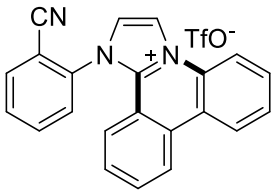
1-(4-(ethoxycarbonyl)phenyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3e): A white solid (92.5 mg, 90% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.40 (t, J = 6.8 Hz, 3H), 4.44 (q, J = 6.8 Hz, 2H), 7.30 (d, J = 8.4 Hz, 1H), 7.63 (t, J = 7.6 Hz, 1H), 7.91-8.07 (m, 5H), 8.39 (d, J = 8.0 Hz, 2H), 8.61 (d, J = 2.4 Hz, 1H), 8.75 (d, J = 8.4 Hz, 1H), 8.99 (dd, 2H, J = 3.6 Hz, J = 8.4 Hz), 9.44 (d, J = 2.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 14.1, 61.5, 115.4, 116.5, 117.4, 121.8, 123.9, 124.4, 124.9, 127.1, 127.7, 128.6, 129.1, 129.3, 130.2, 131.1, 131.6, 132.6, 132.6, 136.8, 140.1, 164.7 ppm. HRMS (ESI$^+$): calcd for $C_{24}H_{19}N_2O_2$ [M−$CF_3SO_3^-$]$^+$ 367.1441, found 367.1440.



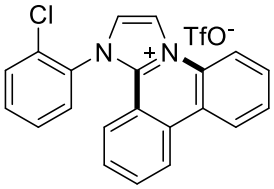
1-(4-methoxyphenyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3f): A white solid (87.2 mg, 92% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.94 (s, 3H), 7.34-7.38 (m, 3H), 7.65 (t, J = 7.6 Hz, 1H), 7.76-7.78 (m, 2H), 7.92 (t, J = 7.6 Hz, 1H), 7.96-8.06 (m, 2H), 8.51 (d, J = 2.0 Hz, 1H), 8.75 (d, J = 8.8 Hz, 1H), 8.98-9.00 (m, 2H), 9.38 (d, J = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 55.9, 115.0, 115.9, 116.8, 117.3, 119.1, 121.8, 122.3, 123.8, 124.4, 124.9, 127.8, 128.4, 128.6, 129.0, 129.2, 129.2, 130.2, 131.1, 132.5, 136.9, 161.1 ppm. HRMS (ESI$^+$): calcd for $C_{22}H_{17}N_2O$ [M−$CF_3SO_3^-$]$^+$ 325.1335, found 325.1334.



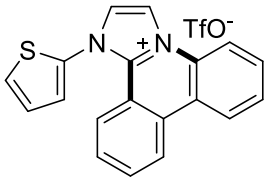
1-(*o*-tolyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3g): A white solid (89.8 mg, 98% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.17 (s, 3H), 7.16 (d, J = 8.4 Hz, 1H), 7.59-7.65 (m, 2H), 7.72-7.79 (m, 3H), 7.92-8.08 (m, 3H), 8.56 (d, J = 2.0 Hz, 1H), 8.78 (d, J = 8.8 Hz, 1H), 9.01 (d, J = 8.4 Hz, 2H), 9.48 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 16.8, 115.8, 116.7, 117.4, 121.9, 122.9, 124.5, 124.9, 126.7, 127.6, 128.4, 128.6, 129.45, 129.48, 130.4, 131.0, 131.9, 132.2, 132.7, 135.1, 135.4, 136.3 ppm. HRMS (ESI$^+$): calcd for $C_{22}H_{17}N_2$ [M−$CF_3SO_3^-$]$^+$ 309.1386, found 309.1386.



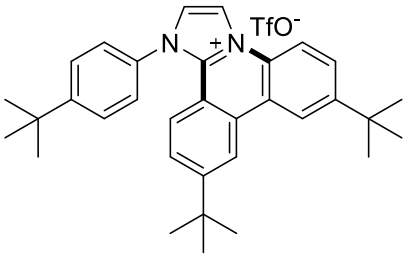
1-(3-cyanophenyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3h): A white solid (91.0 mg, 97% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.30 (d, J = 8.4 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.95 (t, J = 7.6 Hz, 1H), 8.00-8.08 (m, 3H), 8.21-8.24 (m, 1H), 8.37 (d, J = 7.6 Hz, 1H), 8.46 (s, 1H), 8.60 (d, J = 2.0 Hz, 1H), 8.76 (d, J = 8.4 Hz, 1H), 9.02 (d, J = 8.4 Hz, 2H), 9.45 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.6, 115.4, 116.4, 117.4, 117.5, 121.9, 124.1, 124.5, 125.0, 127.4, 128.8, 129.0, 129.5, 130.3, 131.0, 131.2, 132.3, 132.8, 135.5, 137.0, 137.1 ppm. HRMS (ESI$^+$): calcd for $C_{22}H_{14}N_3$ [M−$CF_3SO_3^-$]$^+$ 320.1182, found 320.1182.



1-(2-chlorophenyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3i): A white solid (92.7 mg, 97% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.20 (d, J = 8.4 Hz, 1H), 7.69 (t, J = 7.6 Hz, 1H), 7.84 (t, J = 7.6 Hz, 1H), 7.91-7.98 (m, 2H), 8.01-8.09 (m, 4H), 8.68 (d, J = 2.0 Hz, 1H), 8.79 (d, J = 8.4 Hz, 1H), 9.02-9.05 (m, 2H), 9.54 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 116.1, 116.2, 117.6, 121.9, 122.8, 124.7, 125.0, 127.1, 128.9, 129.2, 129.7, 129.9, 130.0, 130.5, 130.6, 131.3, 131.4, 133.2, 133.6, 133.8, 136.6 ppm. HRMS (ESI$^+$): calcd for $C_{21}H_{14}ClN_2$ [M−$CF_3SO_3^-$]$^+$ 329.0840, found 329.0840.

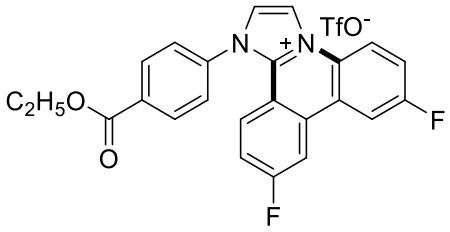


1-(thiophen-2-yl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3j): A white solid (89.3 mg, 99% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.39-7.43 (m, 2H), 7.70-7.74 (m, 2H), 7.93 (t, J = 7.6 Hz, 1H), 8.01-8.06 (m, 3H), 8.64 (d, J = 2.4 Hz, 1H), 8.74 (d, J = 8.4 Hz, 1H), 9.00 (dd, J = 3.2 Hz, J = 8.4 Hz, 2H), 9.40 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 115.2, 116.5, 117.4, 121.9, 123.7, 124.4, 124.9, 127.1, 128.6, 128.7, 129.0, 129.1, 129.3, 129.9, 130.5, 131.1, 132.9, 135.3, 138.0 ppm. HRMS (ESI$^+$): calcd for $C_{19}H_{13}N_2S$ [M−$CF_3SO_3^-$]$^+$ 301.0794, found 301.0790.

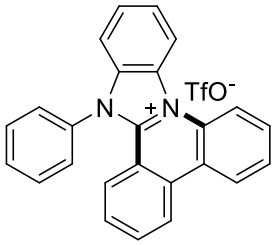


7,10-di-*tert*-butyl-1-(4-(*tert*-butyl)phenyl)-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3k): A white solid (67.7 mg, 55% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.429-1.433 (m, 18H), 1.52 (s, 9H), 7.26 (d, J = 8.8 Hz, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.76 (d, J = 8.8 Hz, 2H), 7.84 (d, J = 8.4 Hz, 2H), 8.09 (d, J = 9.2 Hz, 1H), 8.51 (d, J = 2.0 Hz, 1H), 8.66 (d, J = 8.8 Hz, 1H), 8.80 (s, 2H), 9.36 (d, J = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 30.7, 31.1, 31.1, 35.0, 35.3, 35.6, 114.5, 114.8, 117.2, 120.0, 120.5, 121.4, 123.7, 126.6, 127.1, 127.3, 127.4, 127.6, 128.7, 130.2, 134.0, 136.5, 151.2, 154.4, 155.7 ppm. HRMS (ESI$^+$): calcd for $C_{33}H_{39}N_2$

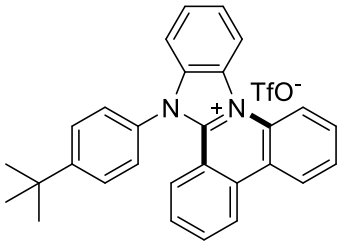
$[M-CF_3SO_3^-]^+$ 463.3108, found 463.3109.



1-(4-(ethoxycarbonyl)phenyl)-7,10-difluoro-1*H*-imidazo[1,2-*f*]phenanthridin-4-ium trifluoromethanesulfonate (3l): A white solid (59.0 mg, 53% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.40 (t, J = 7.2 Hz, 3H), 4.43 (q, J = 7.2 Hz, 2H), 7.34-7.38 (m, 1H), 7.59-7.64 (m, 1H), 7.99-8.07 (m, 3H), 8.37-8.40 (m, 2H), 8.60 (d, J = 2.4 Hz, 1H), 8.83-8.87 (m, 1H), 8.88-8.94 (m, 2H), 9.42 (d, J = 2.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 14.1, 61.5, 111.3 (d, J_{CF} = 24.8 Hz), 111.5 (d, J_{CF} = 25.2 Hz), 113.9, 115.5, 118.6 (d, J_{CF} = 23.7 Hz), 119.9 (d, J_{CF} = 24.9 Hz), 120.2 (d, J_{CF} = 9.4 Hz), 123.6, 126.2, 127.1, 127.3 (d, J_{CF} = 9.5 Hz), 127.6, 131.7, 132.66, 132.74 (d, J_{CF} = 3.2 Hz), 132.8 (d, J_{CF} = 2.5 Hz), 136.4, 139.8, 161.3 (d, J_{CF} = 244.7 Hz), 163.9 (d, J_{CF} = 251.8 Hz), 164.7 ppm. HRMS (ESI$^+$): calcd for $C_{24}H_{17}F_2N_2O_2$ $[M-CF_3SO_3^-]^+$ 403.1253, found 403.1250.

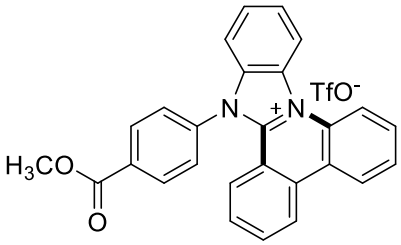


9-phenyl-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium trifluoromethanesulfonate (3m): A yellow solid (69.1 mg, 70% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.45 (dd, J = 8.8 Hz, J = 3.2 Hz, 2H), 7.65 (t, J = 8.0 Hz, 1H), 7.85-8.01 (m, 8H), 8.08-8.15 (m, 2H), 9.06-9.12 (m, 2H), 9.24-9.29 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.3, 116.2, 117.0, 118.3, 119.1, 122.1, 122.3, 124.4, 125.3, 125.7, 127.3, 127.9, 128.1, 128.5, 129.2, 131.2, 131.65, 131.67, 132.1, 132.3, 134.2, 134.3, 134.8, 142.2 ppm. HRMS (ESI$^+$): calcd for $C_{25}H_{17}N_2$ $[M-CF_3SO_3^-]^+$ 345.1386, found 345.1386.

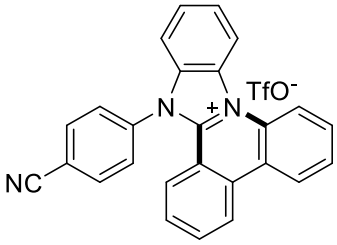


9-(4-(*tert*-butyl)phenyl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium trifluoromethanesulfonate (3n): A yellow solid (110.6 mg, 83% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.48 (s, 9H), 7.43-7.46 (m, 2H), 7.64 (t, J = 7.6 Hz, 1H), 7.82-7.88 (m, 3H), 7.93-8.01 (m, 4H), 8.07-8.14 (m, 2H), 9.07 (d, J = 8.4 Hz, 1H), 9.11 (d, J = 8.0 Hz, 1H), 9.23 (d, J = 8.8 Hz,1H), 9.27 (d, J = 8.4 Hz,1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 31.1, 35.1, 113.4, 116.4, 117.0,

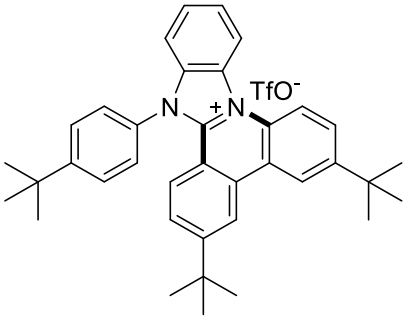
118.3, 122.1, 124.4, 125.3, 125.6, 127.3, 127.4, 127.8, 128.1, 128.4, 128.5, 129.2, 131.2, 131.6, 131.7, 132.3, 134.3, 134.9, 142.3, 154.9 ppm. HRMS (ESI$^+$): calcd for $C_{29}H_{25}N_2$ [M−$CF_3SO_3^-$]$^+$ 401.2012, found 401.2012.



9-(4-(methoxycarbonyl)phenyl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium trifluoromethanesulfonate (3o): A white solid (66.3 mg, 60% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 4.01 (s, 3H), 7.47-7.50 (m, 2H), 7.66-7.71 (m, 1H), 7.87 (t, J = 8.0 Hz, 1H), 7.94-8.03 (m, 2H), 8.07-8.16 (m, 4H), 8.49-8.51 (m, 2H), 9.09 (d, J = 8.4 Hz, 1H), 9.13 (d, J = 8.0 Hz, 1H), 9.26 (d, J = 8.8 Hz, 1H), 9.29 (d, J = 8.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 52.8, 113.3, 116.1, 117.1, 118.4, 122.2, 124.4, 125.3, 125.9, 127.4, 128.0, 128.2, 128.6, 129.5, 131.1, 131.8, 132.3, 132.5, 132.8, 134.5, 134.5, 138.1, 142.3, 165.3 ppm. HRMS (ESI$^+$): calcd for $C_{27}H_{19}N_2O_2$ [M−$CF_3SO_3^-$]$^+$ 403.1441, found 403.1437.

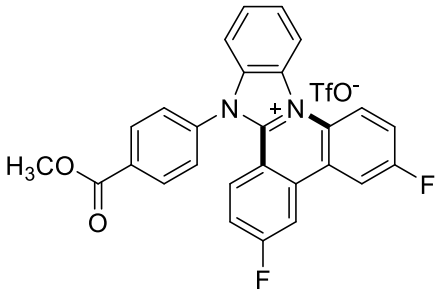


9-(4-cyanophenyl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium trifluoromethanesulfonate (3p): A yellow solid (56.1 mg, 54% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.48 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.72 (t, J = 7.6 Hz, 1H), 7.88 (t, J = 7.6 Hz, 1H), 7.95-8.03 (m, 2H), 8.12-8.16 (m, 4H), 8.46 (d, J = 8.0 Hz, 2H), 9.09-9.15 (m, 2H), 9.25-9.31 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.3, 115.0, 116.0, 117.1, 117.9, 118.4, 122.2, 124.5, 125.3, 126.0, 127.5, 127.9, 128.3, 128.7, 129.3, 129.7, 131.0, 131.8, 132.3, 134.4, 134.6, 135.9, 138.1, 142.3 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{16}N_3$ [M−$CF_3SO_3^-$]$^+$ 370.1339, found 370.1334.

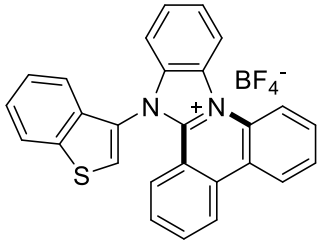


3,6-di-*tert*-butyl-9-(4-(*tert*-butyl)phenyl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium

trifluoromethanesulfonate (3q): A yellow solid (110.0 mg, 83% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.45 (s, 9H), 1.48 (s, 9H), 1.55 (s, 9H), 7.40 (t, J = 7.2 Hz, 2H), 7.72 (d, J = 8.0 Hz, 1H), 7.80-7.85 (m, 3H), 7.89-7.96 (m, 3H), 8.12 (d, J = 8.4 Hz, 1H), 8.87 (s, 1H), 8.91 (s, 1H), 9.16 (d, J = 7.2 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 30.4, 30.8, 30.9, 34.85, 34.87, 35.6, 113.0, 113.9, 116.6, 117.9, 119.9, 120.8, 121.7, 123.3, 125.4, 126.7, 126.8, 127.0, 127.2, 127.5, 128.1, 128.2, 128.6, 129.1, 131.4, 132.0, 134.7, 141.7, 150.3, 154.6, 157.5 ppm. HRMS (ESI$^+$): calcd for $C_{37}H_{41}N_2$ [M−$CF_3SO_3^-$]$^+$ 513.3264, found 513.3260.

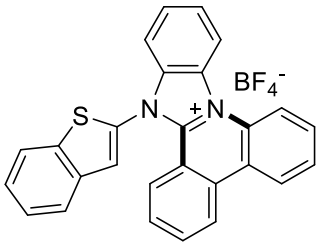


9-(4-(ethoxycarbonyl)phenyl)-3,6-difluoro-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium trifluoromethanesulfonate (3r): A pale yellow solid (62.6 mg, 52% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 4.01 (s, 3H), 7.49-7.55 (m, 2H), 7.67 (t, J = 8.0 Hz, 1H), 7.89 (t, J = 7.6 Hz, 1H), 7.95-8.07 (m, 4H), 8.50 (d, J = 8.0 Hz, 2H), 9.01 (t, J = 12.0 Hz, 2H), 9.21 (d, J = 8.4 Hz, 1H), 9.33-9.36 (m, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 53.8, 111.5 (d, J_{CF} = 24.6 Hz), 112.0 (d, J_{CF} = 25.0 Hz), 113.4, 113.5, 116.8, 119.0 (d, J_{CF} = 23.8 Hz), 120.0 (d, J_{CF} = 23.7 Hz), 121.1 (d, J_{CF} = 9.0 Hz), 124.05 (d, J_{CF} = 2.8 Hz), 124.14 (d, J_{CF} = 3.3 Hz), 127.6, 127.8, 128.0, 128.6, 128.8, 129.4 (d, J_{CF} = 10.2 Hz), 132.6, 132.9, 134.4, 134.9 (d, J_{CF} = 12.7 Hz), 137.8, 141.7, 160.7 (d, J_{CF} = 245.3 Hz), 165.1 (d, J_{CF} = 254.1 Hz), 165.3 ppm. HRMS (ESI$^+$): calcd for $C_{28}H_{19}F_2N_2O_2$ [M−$CF_3SO_3^-$]$^+$ 439.1253, found 439.1258.

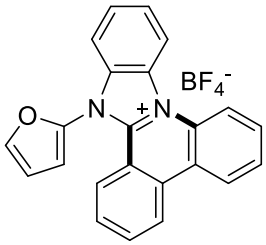


9-(benzo[*b*]thiophen-3-yl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium tetrafluoroborate (3s): A white solid (72.2 mg, 74% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.42-7.47 (m, 2H), 7.54 (d, J = 8.4 Hz, 1H), 7.62 (q, J = 7.6 Hz, 2H), 7.75 (d, J = 8.0 Hz, 1H), 7.83 (t, J = 7.6 Hz, 1H), 7.96 (t, J = 8.4 Hz, 1H), 8.03 (t, J = 7.2 Hz, 1H), 8.08 (t, J = 8.0 Hz, 1H), 8.17 (t, J = 8.4 Hz, 1H), 8.40 (d, J = 8.4 Hz, 1H), 8.63 (s, 1H), 9.09-9.16 (m, 2H), 9.28-9.34 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.2, 116.1, 117.2, 118.5, 121.3, 122.3, 124.3, 124.4, 125.05, 125.12, 125.3, 126.0,

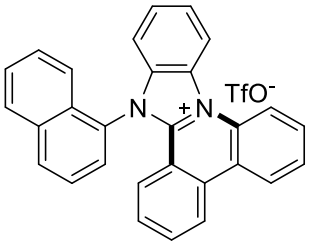
126.5, 127.5, 128.2, 128.3, 128.7, 129.6, 130.4, 131.5, 131.8, 132.5, 133.3, 134.6, 134.6, 139.0, 142.7 ppm. HRMS (ESI^+): calcd for $C_{27}H_{17}N_2S$ $[M-BF_4^-]^+$ 401.1107, found 401.1103.



9-(benzo[*b*]thiophen-2-yl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium tetrafluoroborate (3t): A light yellow solid (52.0 mg, 53% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 7.64-7.79 (m, 4H), 7.90 (t, J = 7.6 Hz, 1H), 7.96-8.05 (m, 3H), 8.13-8.22 (m, 4H), 8.30 (d, J = 7.6 Hz, 1H), 9.10-9.16 (m, 2H), 9.24-9.30 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.4, 116.1, 117.1, 118.4, 122.3, 123.6, 124.3, 125.3, 125.8, 127.1, 127.6, 127.9, 128.4, 128.9, 129.7, 131.1, 131.8, 132.5, 133.0, 134.7, 135.3, 137.0, 139.5, 143.3 ppm. HRMS (ESI^+): calcd for $C_{27}H_{17}N_2S$ $[M-BF_4^-]^+$ 401.1107, found 401.1108.

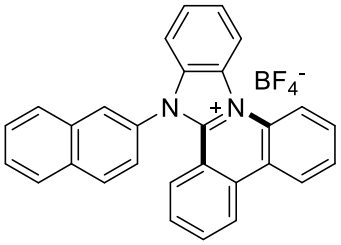


9-(furan-2-yl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium tetrafluoroborate (3u): A light yellow solid (33.8 mg, 47% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 7.14 (s, 1H), 7.22-7.25 (m, 2H), 7.75 (d, J = 6.8 Hz, 1H), 7.87 (t, J = 6.8 Hz, 1H), 7.96-8.03 (m, 3H), 8.13 (t, J = 7.6 Hz, 1H), 8.20 (t, J = 6.8 Hz, 1H), 8.30 (s, 1H), 9.11-9.14 (m, 2H), 9.22-9.27 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 110.7, 113.0, 113.6, 115.5, 117.5, 118.7, 122.5, 124.5, 124.8, 125.3, 127.8, 128.1, 128.6, 129.2, 130.0, 131.1, 131.9, 132.8, 134.3, 135.1, 137.1, 143.5, 144.9 ppm. HRMS (ESI^+): calcd for $C_{23}H_{15}N_2O$ $[M-BF_4^-]^+$ 335.1179, found 335.1172.

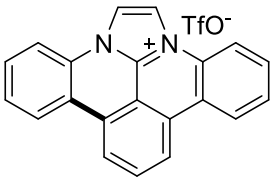


9-(naphthalen-1-yl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium trifluoromethanesulfonate (3v): A white solid (42.4 mg, 39% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 7.20 (d, J = 8.4 Hz, 1H), 7.25 (d, J = 8.4 Hz, 1H), 7.48 (t, J = 7.6 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.75-7.82 (m, 3H), 7.94-8.05 (m, 4H), 8.12-8.20 (m, 2H), 8.36 (d, J = 8.4 Hz, 1H), 8.57 (d, J = 8.4 Hz, 1H), 9.09 (d, J = 8.0 Hz, 1H), 9.15 (d, J = 8.4 Hz, 1H), 9.31-9.38 (m, 2H) ppm. ^{13}C NMR (100

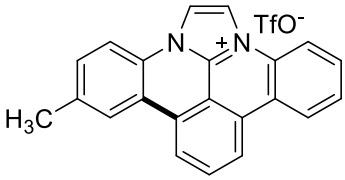
MHz, DMSO-d_6): δ = 113.3, 116.1, 117.3, 118.5, 122.1, 122.3, 124.4, 125.2, 125.3, 126.8, 127.3, 127.4, 128.09, 128.13, 128.4, 128.6, 128.7, 128.898, 128.904, 129.1, 129.4, 130.3, 131.65, 131.71, 132.49, 132.52, 134.4, 134.5, 134.9, 142.6 ppm. HRMS (ESI$^+$): calcd for $C_{29}H_{19}N_2$ [M−TfO$^-$]$^+$ 395.1543, found 395.1543.



9-(naphthalen-2-yl)-9*H*-benzo[4,5]imidazo[1,2-*f*]phenanthridin-14-ium tetrafluoroborate (3w): A white solid (66.5 mg, 69% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.52-7.58 (m, 3H), 7.81-7.86 (m, 3H), 7.93-8.08 (m, 4H), 8.15 (t, J = 7.6 Hz, 1H), 8.22 (d, J = 7.2 Hz, 1H), 8.30 (m, J = 7.6 Hz, 1H), 8.51 (d, J = 8.0 Hz, 1H), 8.58 (s, 1H), 9.07-9.13 (m, 2H), 9.26-9.31 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.6, 116.3, 117.0, 118.4, 122.2, 124.3, 124.4, 125.3, 125.8, 127.4, 127.5, 127.9, 128.1, 128.2, 128.4, 128.6, 128.7, 128.8, 129.4, 131.3, 131.6, 131.7, 132.0, 132.3, 133.3, 133.9, 134.4, 135.0, 142.4 ppm. HRMS (ESI$^+$): calcd for $C_{29}H_{19}N_2$ [M−BF_4^-]$^+$ 395.1543, found 395.1543.

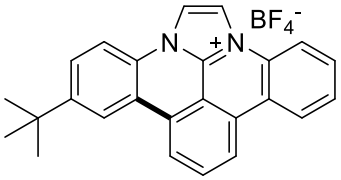


tribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (4a): A yellow solid (21.2 mg, 70% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.86 (t, J = 7.2 Hz, 2H), 8.00 (t, J = 7.6 Hz, 2H), 8.29 (t, J = 7.6 Hz, 1H), 8.61 (d, J = 8.0 Hz, 2H), 8.88 (d, J = 7.6 Hz, 4H), 9.53 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.6, 117.0, 117.4, 121.9, 122.1, 125.6, 128.2, 128.3, 129.6, 131.2, 133.1, 133.3 ppm. HRMS (ESI$^+$): calcd for $C_{21}H_{13}N_2^+$ [M−$CF_3SO_3^-$]$^+$ 293.1073, found 293.1075.

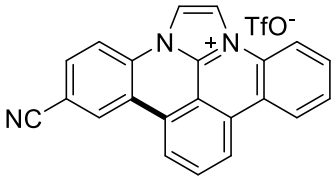


12-methyltribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (4b): A light yellow solid (24.6 mg, 82% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.53 (s, 3H), 7.70 (d, J = 8.4 Hz, 1H), 7.84 (t, J = 7.6 Hz, 1H), 7.99 (t, J = 7.6 Hz, 1H), 8.21 (t, J = 8.0 Hz, 1H), 8.36 (d, J = 8.4 Hz, 1H), 8.52 (s, 1H), 8.57 (d, J = 8.4 Hz, 1H), 8.71 (d, J = 7.6 Hz, 1H), 8.78-8.83 (m, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 20.9, 111.2, 116.75, 116.80, 116.9, 117.2, 121.4, 121.7,

121.77, 121.83, 125.0, 125.5, 127.2, 127.8, 128.0, 128.2, 129.4, 131.1, 132.0, 132.4, 133.0, 138.2. ppm. HRMS (ESI^+): calcd for $C_{22}H_{15}N_2^+$ $[M-CF_3SO_3^-]^+$ 307.1230, found 307.1226.

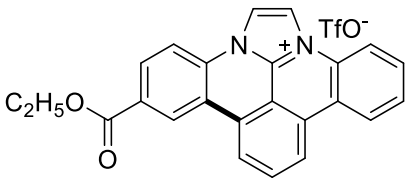


12-(*tert*-butyl)tribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium tetrafluoroborate (4c): A white solid (18.6 mg, 62% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 1.53 (s, 9H), 7.87 (t, J = 7.2 Hz, 1H), 8.01 (t, J = 8.0 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 8.30 (t, J = 8.0 Hz, 1H), 8.55 (d, J = 8.8 Hz, 1H), 8.61 (d, J = 8.4 Hz, 1H), 8.80 (s, 1H), 8.89 (t, J = 8.0 Hz, 2H), 9.04 (d, J = 8.4 Hz, 1H), 9.52 (d, J = 5.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 31.2, 35.3, 111.8, 116.9, 117.0, 117.2, 117.4, 121.6, 121.7, 122.0, 122.4, 125.6, 127.7, 128.2, 128.3, 128.4, 128.9, 129.7, 131.2, 133.0, 133.1, 151.3 ppm. HRMS (ESI^+): calcd for $C_{25}H_{21}N_2^+$ $[M-BF_4^-]^+$ 349.1699, found 349.1693.



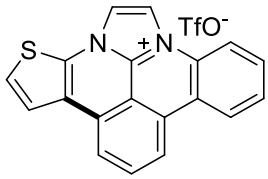
12-cyanotribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (4d):

A yellow solid (18.9 mg, 63% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 7.93 (t, J = 7.6 Hz, 1H), 8.07 (t, J = 8.0 Hz, 1H), 8.45 (t, J = 8.0 Hz, 1H), 8.52 (t, J = 8.8 Hz, 1H), 8.70 (d, J = 8.4 Hz, 1H), 8.87 (d, J = 8.4 Hz, 1H), 9.0 (d, J = 8.0 Hz, 1H), 9.06-9.12 (m, 2H), 9.59 (s, 1H), 9.65 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.2, 112.3, 117.57, 117.63, 117.7, 118.0, 118.9, 121.9, 122.0, 122.9, 123.3, 125.9, 127.4, 128.5, 128.7, 129.7, 130.9, 131.6, 132.4, 133.8, 134.0, 134.2, 135.1 ppm. HRMS (ESI^+): calcd for $C_{22}H_{12}N_3^+$ $[M- CF_3SO_3^-]^+$ 318.1026, found 318.1024.

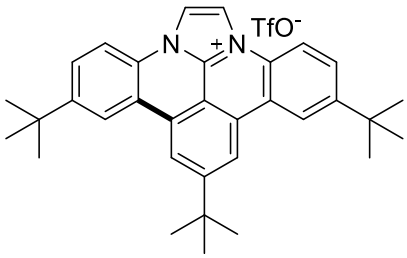


12-(ethoxycarbonyl)tribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (4e): A light yellow solid (24.6 mg, 82% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 1.46 (t, J = 7.2 Hz, 3H), 4.46 (q, J = 7.2 Hz, 2H), 7.87 (t, J = 7.2 Hz, 1H), 8.03 (t, J = 7.2 Hz, 1H), 8.33 (t, J = 8.0 Hz, 1H), 8.39 (dd, J = 1.2 Hz, J = 8.8 Hz, 1H), 8.63-8.69 (m, 2H), 8.88-8.95 (m, 3H), 9.15 (s, 1H), 9.59 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 14.2, 61.7, 111.7, 117.47, 117.54, 118.1, 119.1, 121.87, 121.93, 122.3, 122.5, 122.8, 125.7, 126.3, 127.6, 128.4, 128.6,

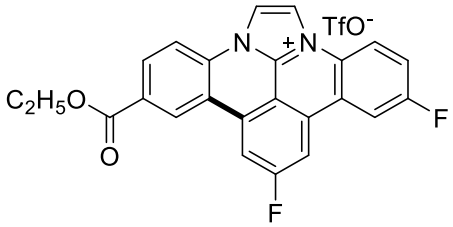
129.4, 129.5, 131.0, 131.5, 132.3, 133.6, 133.7, 164.5 ppm. HRMS (ESI$^+$): calcd for $C_{24}H_{17}N_2O_2^+$ [M−$CF_3SO_3^-$]$^+$ 365.1285, found 365.1280.



dibenzo[*b*,*de*]imidazo[1,2,3-*ij*]thieno[3,2-*g*][1,8]naphthyridin-14-ium trifluoromethanesulfonate (4j): A yellow solid (24.0 mg, 80% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.87 (t, J = 7.2 Hz, 1H), 8.00-8.05 (m, 2H), 8.30-8.36 (m, 2H), 8.66 (t, J = 9.6 Hz, 2H), 8.87 (d, J = 8.0 Hz, 1H), 8.92 (d, J = 8.8 Hz, 1H), 9.39 (d, J = 2.4 Hz, 1H), 9.59 (d, J = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.3, 117.3, 117.5, 117.6, 120.7, 122.0, 122.1, 122.3, 122.7, 124.7, 125.7, 126.9, 127.2, 128.35, 128.39, 130.0, 131.3, 133.0, 133.3, 133.6 ppm. HRMS (ESI$^+$): calcd for $C_{19}H_{11}N_2S^+$ [M−$CF_3SO_3^-$]$^+$ 299.0637, found 299.0634.

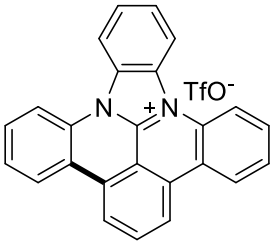


6,9,12-tri-*tert*-butyltribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (4k): A yellow solid (21.0 mg, 70% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.54 (s, 18H), 1.68 (s, 9H), 8.08 (d, J = 8.8 Hz, 2H), 8.59 (d, J = 8.8 Hz, 2H), 8.92 (s, 2H), 9.00 (s, 2H), 9.53 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 31.2, 31.4, 35.3, 36.8, 110.4, 116.7, 117.1, 119.3, 121.8, 121.1, 128.0, 128.45, 128.52, 133.1, 151.1, 157.2 ppm. HRMS (ESI$^+$): calcd for $C_{33}H_{37}N_2^+$ [M−$CF_3SO_3^-$]$^+$ 461.2951, found 461.2946.

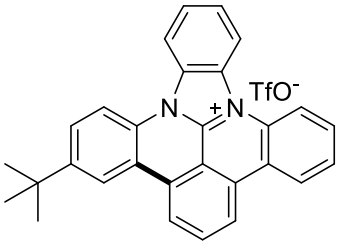


12-(ethoxycarbonyl)-6,9-difluorotribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (4l): A yellow solid (15.9 mg, 53% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.46 (t, J = 7.2 Hz, 3H), 4.47 (q, J = 7.2 Hz, 2H), 8.04-8.09 (m, 1H), 8.50 (d, J = 8.8 Hz, 1H), 8.76-8.81 (m, 2H), 8.90 (dd, J = 2.8 Hz, J = 10.0 Hz, 1H), 9.00 (d, J = 10.0 Hz, 1H), 9.13 (d, J = 10.0 Hz, 1H), 9.32 (s, 1H), 9.64 (d, J = 5.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 14.2, 61.7, 108.7, 111.1 (d, J_{CF} = 10.7 Hz), 111.4 (d, J_{CF} = 11.0 Hz), 112.3 (d, J_{CF} = 25.2 Hz), 117.6 (d, J_{CF} = 26.0

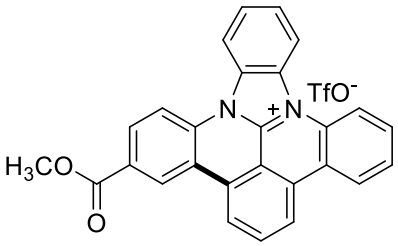
Hz), 118.1, 119.1, 120.1 (d, J_{CF} = 14.3 Hz), 120.3, 121.2 (d, J_{CF} = 3.6 Hz), 122.3, 123.4 (dd, J_{CF} = 3.5 Hz, J_{CF} = 9.6 Hz), 126.4, 127.0, 130.0, 130.5 (d, J_{CF} = 11.2 Hz), 130.6 (dd, J_{CF} = 3.0 Hz, J_{CF} = 11.1 Hz), 131.8, 132.3, 132.7, 161.1 (d, J_{CF} = 245.7 Hz), 164.2, 165.3 (d, J_{CF} = 250.3 Hz) ppm. HRMS (ESI^+): calcd for $C_{24}H_{15}F_2N_2O_2^+$ $[M-CF_3SO_3^-]^+$ 401.1096, found 401.1089.



tribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (4m): A white solid (17.1 mg, 57% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 7.91 (t, J = 7.6 Hz, 2H), 8.03-8.10 (m, 4H), 8.40 (t, J = 8.0 Hz, 1H), 8.97 (t, J = 8.0 Hz, 4H), 9.13 (d, J = 8.4 Hz, 2H), 9.27-9.29 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.9, 116.8, 118.4, 122.0, 122.1, 125.8, 128.1, 129.1, 130.0, 131.3, 132.0, 135.2, 138.8 ppm. HRMS (ESI^+): calcd for $C_{25}H_{15}N_2^+$ $[M-CF_3SO_3^-]^+$ 343.1230, found 343.1228.

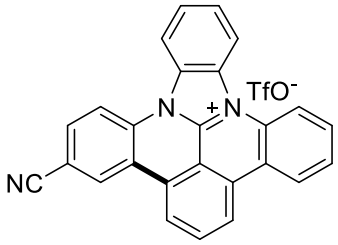


14-(*tert*-butyl)tribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (4n): A light yellow solid (24.1 mg, 80% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 1.56 (s, 9H), 7.91 (t, J = 7.6 Hz, 1H), 8.03-8.12 (m, 4H), 8.41 (t, J = 8.0 Hz, 1H), 8.89 (s, 1H), 8.97 (t, J = 8.8 Hz, 2H), 9.06 (d, J = 8.8 Hz, 1H), 9.11-9.14 (m, 2H), 9.26 (q, J = 4.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 31.1, 35.1, 111.9, 116.7, 116.8, 118.1, 118.3, 119.1, 121.86, 121.94, 121.97, 122.01, 122.04, 122.3, 122.4, 125.8, 127.99, 128.02, 129.08, 129.11, 129.16, 129.23, 130.0, 130.2, 131.3, 131.9, 135.1, 138.5, 150.8 ppm. HRMS (ESI^+): calcd for $C_{29}H_{23}N_2^+$ $[M-CF_3SO_3^-]^+$ 399.1856, found 399.1852.

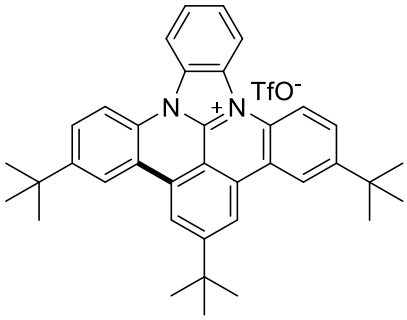


14-(methoxycarbonyl)tribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (4o): A white solid (18.9 mg, 63% yield). ^1H NMR (400 MHz, DMSO-d_6): δ = 4.04 (s, 3H), 7.95 (t, J = 7.6 Hz, 1H), 8.06-8.13 (m, 3H), 8.36-8.40 (m, 2H), 8.99-9.02 (m,

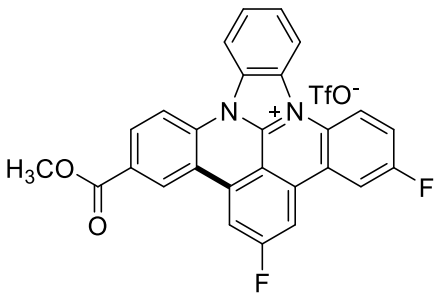
3H), 9.16-9.26 (m, 4H), 9.31-9.34 (m, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 52.9, 111.9, 116.7, 117.1, 118.5, 119.0, 122.0, 122.2, 122.6, 122.8, 125.9, 126.4, 128.4, 128.5, 128.7, 129.0, 129.2, 129.3, 130.2, 131.1, 131.6, 132.2, 133.8, 135.5, 139.1, 164.9 ppm. HRMS (ESI$^+$): calcd for $C_{27}H_{17}N_2O_2^+$ [M−$CF_3SO_3^-$]$^+$ 401.1285, found 401.1288.



14-cyanotribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (4p): A light yellow solid (14.1 mg, 47% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.00 (t, J = 7.6 Hz, 1H), 8.11-8.16 (m, 3H), 8.48 (dd, J = 2.0 Hz, J = 8.6 Hz, 1H), 8.57 (t, J = 8.0 Hz, 1H), 9.12-9.27 (m, 4H), 9.35-9.41 (m, 3H), 9.69 (d, J = 2.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 110.9, 112.6, 116.9, 117.1, 117.8, 118.6, 119.7, 122.2, 123.0, 123.1, 123.3, 126.1, 128.45, 128.48, 129.1, 129.2, 129.4, 130.3, 130.9, 131.3, 132.3, 133.9, 134.5, 135.6, 139.8 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{14}N_3^+$ [M−$CF_3SO_3^-$]$^+$ 368.1182, found 368.1181.

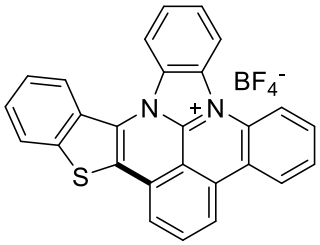


8,11,14-tri-*tert*-butyltribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (4q): A white solid (18.8 mg, 63% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.57 (s, 18H), 1.71 (s, 9H), 8.08-8.11 (m, 4H), 9.02 (d, J = 2.0 Hz, 2H), 9.07 (s, 2H), 9.14 (t, J = 8.8 Hz, 2H), 9.30-9.32 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 31.2, 31.3, 35.2, 36.9, 39.5, 110.7, 116.6, 118.1, 119.2, 122.2, 127.7, 128.9, 129.3, 129.6, 130.3, 138.7, 150.6, 159.2 ppm. HRMS (ESI$^+$): calcd for $C_{37}H_{39}N_2^+$ [M−$CF_3SO_3^-$]$^+$ 511.3108, found 511.3103.

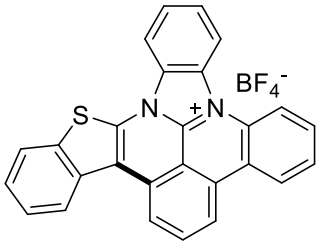


8,11-difluoro-14-(methoxycarbonyl)tribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-

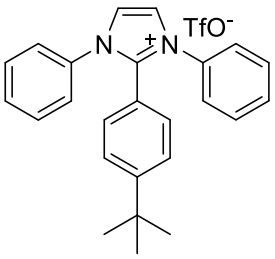
***ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (4r):** A light yellow solid (26.1 mg, 87% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 4.02 (s, 3H), 7.98 (t, J = 8.4 Hz, 1H), 8.11-8.13 (m, 2H), 8.43 (d, J = 8.8 Hz, 1H), 8.95-9.01 (m, 2H), 9.10 (d, J = 10.0 Hz, 1H), 9.21-9.31 (m, 5H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 52.9, 109.3, 111.3 (d, J_{CF} = 26.7 Hz), 111.5 (d, J_{CF} = 26.7 Hz), 112.8 (d, J_{CF} = 25.3 Hz), 116.7, 116.8, 119.0, 119.1, 120.4 (d, J_{CF} = 23.7 Hz), 121.3 (d, J_{CF} = 9.3 Hz), 121.6 (d, J_{CF} = 3.5 Hz), 122.3, 127.2, 128.02, 128.04, 128.6 (d, J_{CF} = 3.0 Hz), 128.8, 129.0 (d, J_{CF} = 12.5 Hz), 132.4, 132.8 (d, J_{CF} = 11.7 Hz), 134.0, 138.5, 160.7 (d, J_{CF} = 246.2 Hz), 164.8, 166.5 (d, J_{CF} = 252.8 Hz) ppm. HRMS (ESI$^+$): calcd for $C_{25}H_{17}F_2N_2O_2^+$ [M−$CF_3SO_3^-$]$^+$ 437.1096, found 437.1089.



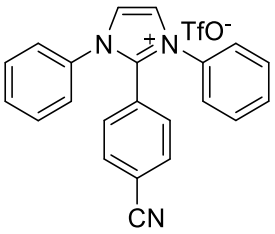
dibenzo[*b*,*de*]benzo[4,5]imidazo[1,2,3-*ij*]benzo[4,5]thieno[2,3-*g*][1,8]naphthyridin-5-ium tetrafluoroborate (4s): A yellow solid (16.8 mg, 56% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.78-7.84 (m, 2H), 7.92 (t, J = 7.6 Hz, 1H), 8.07-8.15 (m, 3H), 8.40-8.45 (m, 3H), 8.80 (d, J = 8.0 Hz, 1H), 8.96-9.00 (m, 3H), 9.16 (d, J = 8.4 Hz, 1H), 9.28 (d, J = 8.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.8, 116.5, 116.9, 118.6, 121.9, 122.0, 122.0, 123.8, 124.7, 125.9, 126.0, 126.8, 126.8, 127.96, 128.04, 128.09, 128.13, 128.6, 128.9, 129.1, 129.2, 130.3, 131.4, 132.2, 135.7, 138.1, 139.3 ppm. HRMS (ESI$^+$): calcd for $C_{27}H_{15}N_2S^+$ [M−BF_4^-]$^+$ 399.0950, found 399.0948.



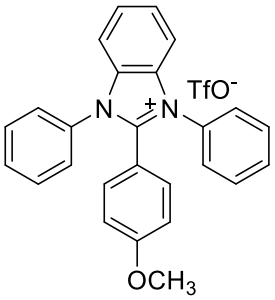
dibenzo[*b*,*de*]benzo[4,5]imidazo[1,2,3-*ij*]benzo[4,5]thieno[3,2-*g*][1,8]naphthyridin-5-ium tetrafluoroborate (4t): A light yellow solid (18.0 mg, 60% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.65-7.72 (m, 2H), 7.91 (t, J = 7.6 Hz, 1H), 8.05 (t, J = 8.0 Hz, 1H), 8.16-8.21 (m, 2H), 8.30-8.36 (m, 2H), 8.68-8.71 (m, 1H), 8.77 (d, J = 6.8 Hz, 1H), 8.90 (d, J = 8.0 Hz, 1H), 8.96 (d, J = 8.0 Hz, 2H), 9.09 (d, J = 8.4 Hz, 1H), 9.29-9.32 (m, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.3, 114.4, 117.0, 118.2, 119.1, 120.6, 121.4, 122.0, 124.0, 124.2, 126.0, 127.0, 127.2, 127.3, 128.15, 128.19, 128.5, 128.6, 129.0, 130.6, 131.2, 131.9, 132.3, 134.1, 134.7, 135.7, 137.2 ppm. HRMS (ESI$^+$): calcd for $C_{27}H_{15}N_2S^+$ [M−BF_4^-]$^+$ 399.0950, found 399.0946.



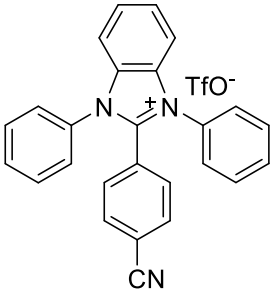
2-(4-(*tert*-butyl)phenyl)-1,3-diphenyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (5b): A light yellow solid (87.4 mg, 87% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.16 (s, 9H), 7.32 (q, J = 10.4 Hz, 4H), 7.48-7.55 (m, 10H), 8.39 (d, J = 0.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 30.6, 34.7, 118.6, 124.0, 125.4, 126.4, 129.7, 130.3, 131.0, 135.1, 144.6, 154.5 ppm. HRMS (ESI$^+$): calcd for $C_{25}H_{25}N_2$ [M−$CF_3SO_3^-$]$^+$ 353.2012, found 353.2010.



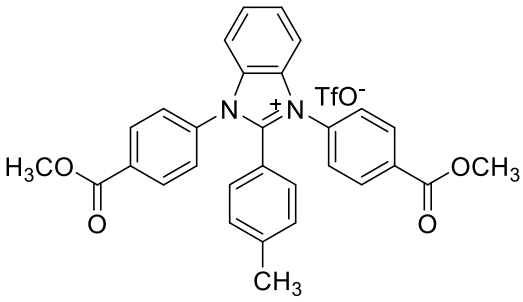
2-(4-cyanophenyl)-1,3-diphenyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (5c): A yellow solid (87.6 mg, 93% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.48-7.55 (m, 10H), 7.63 (d, J = 8.4 Hz, 2H), 7.87 (s, J = 8.0 Hz, 2H), 8.49 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 114.4, 117.6, 124.5, 126.2, 126.4, 129.9, 130.6, 132.40, 132.44, 134.6, 142.7 ppm. HRMS (ESI$^+$): calcd for $C_{22}H_{16}N_3$ [M−$CF_3SO_3^-$]$^+$ 322.1339, found 322.1340.



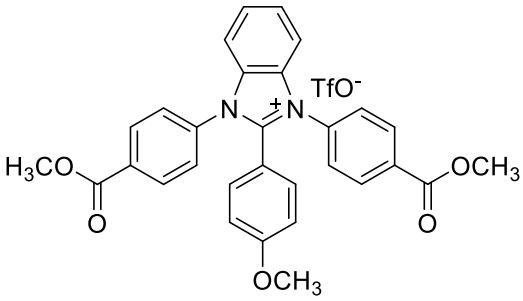
2-(4-methoxyphenyl)-1,3-diphenyl-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (5d): A white solid (97.9 mg, 93% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.70 (s, 3H), 6.91 (d, J = 8.8 Hz, 2H), 7.41 (q, J = 8.8 Hz, 2H), 7.62-7.69 (m, 12H), 7.74-7.79 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 55.4, 112.8, 113.2, 114.1, 127.5, 127.6, 130.3, 130.8, 132.4, 132.7, 133.1, 150.9, 161.8 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{21}N_2O$ [M−$CF_3SO_3^-$]$^+$ 377.1648, found 377.1644.



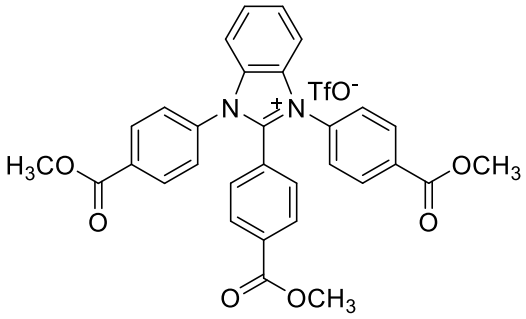
2-(4-cyanophenyl)-1,3-diphenyl-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (5e): A light yellow solid (99.0 mg, 95% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.66 (br, 10H), 7.70-7.73 (m, 2H), 7.77 (d, J = 8.4 Hz, 2H), 7.81-7.85 (m, 2H), 7.92 (d, J = 8.4 Hz, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.6, 114.9, 117.4, 126.0, 127.4, 128.2, 130.5, 131.2, 132.0, 132.2, 132.5, 148.8 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{18}N_3$ [M−$CF_3SO_3^-$]$^+$ 372.1495, found 372.1496.



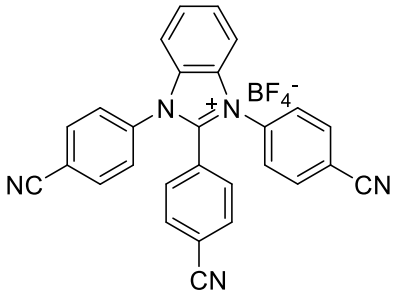
1,3-bis(4-(methoxycarbonyl)phenyl)-2-(*p*-tolyl)-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (5f): A light yellow solid (110.2 mg, 88% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.23 (s, 3H), 3.90 (s, 6H), 7.18 (d, J = 7.6 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.71-7.75 (m, 2H), 7.78-7.83 (m, 6H), 8.20-8.22 (m, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 21.0, 52.6, 113.4, 117.8, 127.9, 128.1, 129.3, 131.1, 131.2, 131.7, 132.3, 136.2, 143.0, 150.8, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{30}H_{25}N_2O_4$ [M−$CF_3SO_3^-$]$^+$ 477.1809, found 477.1813.



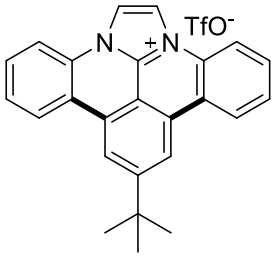
1,3-bis(4-(methoxycarbonyl)phenyl)-2-(4-methoxyphenyl)-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (5g): A light yellow solid (105.3 mg, 82% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.70 (s, 3H), 3.90 (s, 6H), 6.92 (d, J = 8.8 Hz, 2H), 7.38 (d, J = 8.8 Hz, 2H), 7.70-7.73 (m, 2H), 7.77-7.80 (m, 6H), 8.23 (d, J = 8.4 Hz, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 52.6, 55.4, 112.2, 113.3, 114.4, 127.8, 128.1, 131.2, 131.6, 132.2, 133.2, 136.4, 150.8, 162.0, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{30}H_{25}N_2O_5$ [M−$CF_3SO_3^-$]$^+$ 493.1758, found 493.1755.



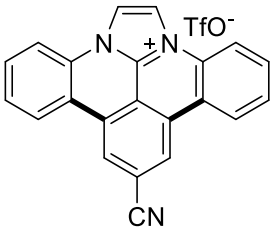
1,2,3-tris(4-(methoxycarbonyl)phenyl)-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (5h): A light yellow solid (122.0 mg, 91% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 3.79 (s, 3H), 3.89 (s, 6H), 7.66 (d, J = 8.0 Hz, 2H), 7.76-7.86 (m, 8H), 7.92 (d, J = 8.4 Hz, 2H), 8.20 (d, J = 8.8 Hz, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 52.6, 52.7, 128.0, 128.1, 128.3, 129.3, 129.6, 131.3, 131.8, 131.87, 131.90, 132.3, 133.0, 135.8, 165.0, 165.1 ppm. HRMS (ESI$^+$): calcd for $C_{31}H_{25}N_2O_6$ $[M-CF_3SO_3^-]^+$ 521.1707, found 521.1705.



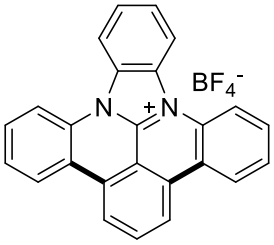
1,2,3-tris(4-cyanophenyl)-1*H*-benzo[*d*]imidazol-3-ium tetrafluoroborate (5i): A light yellow solid (97.7 mg, 96% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.71 (d, J = 8.0 Hz, 2H), 7.81-7.88 (m, 8H), 7.95 (d, J = 8.4 Hz, 2H), 8.18 (d, J = 8.4 Hz, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 113.7, 114.1, 115.4, 117.4, 117.5, 124.9, 128.6, 128.7, 132.1, 132.3, 132.9, 134.8, 135.5, 148.8 ppm. HRMS (ESI$^+$): calcd for $C_{28}H_{16}N_5$ $[M-BF_4^-]^+$ 422.1400, found 422.1397.



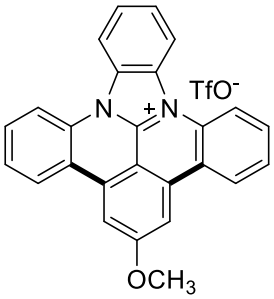
9-(*tert*-butyl)tribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (6b): A yellow solid (15.9 mg, 53% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.64 (s, 9H), 7.91 (t, J = 7.2 Hz, 2H), 8.04 (t, J = 7.6 Hz, 2H), 8.68 (d, J = 8.4 Hz, 2H), 9.02 (s, 2H), 9.19 (d, J = 8.0 Hz, 2H), 9.56 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 31.4, 36.7, 110.0, 116.9, 117.3, 119.4, 122.1, 125.9, 128.1, 128.2, 129.8, 131.0, 133.3, 157.5 ppm. HRMS (ESI$^+$): calcd for $C_{25}H_{21}N_2^+$ $[M-CF_3SO_3^-]^+$ 349.1699, found 349.1699.



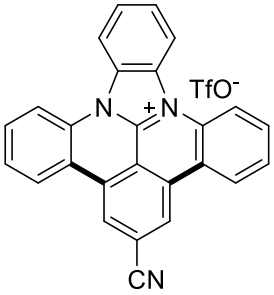
9-cyanotribenzo[*b*,*de*,*g*]imidazo[1,2,3-*ij*][1,8]naphthyridin-3-ium trifluoromethanesulfonate (6c): A light yellow solid (11.1 mg, 37% yield)**.** ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.98 (t, J = 8.0 Hz, 2H), 8.14 (t, J = 8.0 Hz, 2H), 8.77 (d, J = 8.4 Hz, 2H), 9.11 (d, J = 8.4 Hz, 2H), 9.57 (s, 2H), 9.74 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 114.1, 115.5, 117.7, 118.0, 118.4, 121.3, 125.8, 126.3, 128.8, 129.1, 130.1, 132.3, 132.7 ppm. HRMS (ESI$^+$): calcd for $C_{22}H_{12}N_3^+$ [M−$CF_3SO_3^-$]$^+$ 318.1026, found 318.1023.



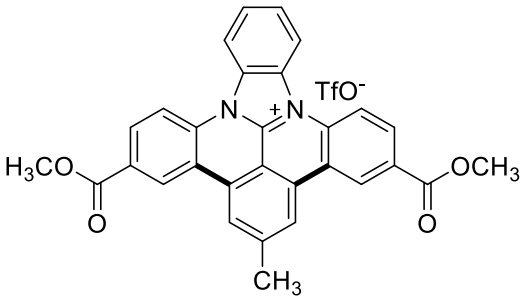
tribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium tetrafluoroborate (4m'): A light yellow solid (15.1 mg, 50% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 7.95 (t, J = 7.2 Hz, 2H), 8.06-8.12 (m, 4H), 8.48 (t, J = 8.0 Hz, 1H), 9.04-9.07 (m, 4H), 9.20 (d, J = 8.4 Hz, 2H), 9.32-9.35 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.6, 116.7, 118.3, 121.9, 122.0, 125.7, 128.1, 129.0, 129.9, 131.1, 132.0, 135.2, 138.5 ppm. HRMS (ESI$^+$): calcd for $C_{25}H_{15}N_2^+$ [M− BF_4^-]$^+$ 343.1230, found 343.1226.



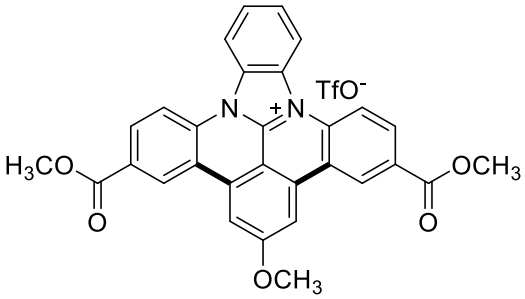
11-methoxytribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (6d): A red solid (14.1 mg, 47% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 4.09 (s, 3H), 7.75 (t, J = 7.6 Hz, 2H), 7.94 (t, J = 8.0 Hz, 2H), 7.99-8.01 (m, 2H), 8.16 (s, 2H), 8.79 (d, J = 8.0 Hz, 2H), 8.92 (s, J = 8.4 Hz, 2H), 9.08-9.10 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 56.9, 105.4, 107.9, 116.5, 118.1, 121.2, 126.0, 127.65, 127.74, 128.8, 131.1, 132.06, 132.11, 137.9, 165.0 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{17}N_2O^+$ [M−$CF_3SO_3^-$]$^+$373.1335, found 373.1325.



11-cyanotribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (6e): A yellow solid (18.9 mg, 63% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.00 (t, J = 7.6 Hz, 2H), 8.14-8.18 (m, 4H), 9.17 (d, J = 8.0 Hz, 2H), 9.27 (d, J = 8.8 Hz, 2H), 9.39-9.42 (m, 2H), 9.60 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 114.1, 117.1, 117.2, 118.1, 118.6, 121.3, 125.5, 126.4, 128.5, 128.7, 129.3, 130.8, 131.6, 133.0, 138.2 ppm. HRMS (ESI$^+$): calcd for $C_{26}H_{14}N_3^+$ [M−$CF_3SO_3^-$]$^+$ 368.1182, found 368.1185.

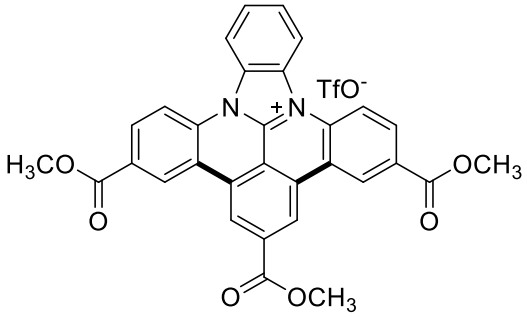


8,14-bis(methoxycarbonyl)-11-methyltribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (6f): A light yellow solid (15.9 mg, 53% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.46 (s, 3H), 4.03 (s, 6H), 8.11-8.13 (m, 2H), 8.30 (d, J = 8.8 Hz, 2H), 8.59 (s, 2H), 8.93 (s, 2H), 9.08 (d, J = 9.2 Hz, 2H), 9.16-9.18 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 22.2, 52.9, 116.8, 119.0, 121.8, 123.6, 123.7, 126.2, 126.3, 128.6, 128.8, 128.9, 129.0, 131.7, 133.6, 148.0, 164.8 ppm. HRMS (ESI$^+$): calcd for $C_{30}H_{21}N_2O_4^+$ [M−$CF_3SO_3^-$]$^+$ 473.1496, found 473.1493.

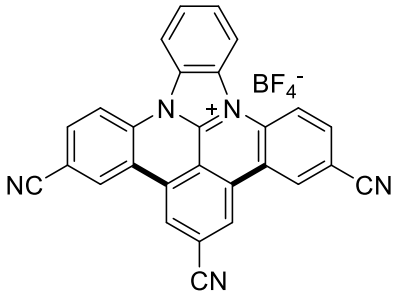


11-methoxy-8,14-bis(methoxycarbonyl)tribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (6g): A light yellow solid (12.0 mg, 40% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 4.02-4.03 (m, 9H), 8.04-8.06 (m, 2H), 8.13 (s, 2H), 8.29 (d, J = 9.2 Hz, 2H), 9.00-9.02 (m, 4H), 9.06-9.09 (m, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ =

52.8, 57.1, 105.3, 108.9, 116.5, 118.7, 121.2, 126.6, 128.3, 128.5, 128.7, 131.4, 131.9, 133.5, 138.4, 164.7, 165.3 ppm. HRMS (ESI^+): calcd for $C_{30}H_{21}N_2O_5^+$ $[M-CF_3SO_3^-]^+$ 489.1445, found 489.1442.

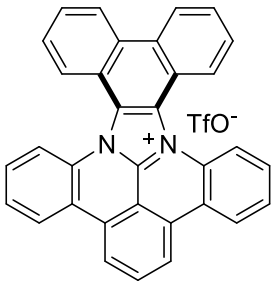


8,11,14-tris(methoxycarbonyl)tribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium trifluoromethanesulfonate (6h): A yellow solid (15.3 mg, 51% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 4.07 (s, 6H), 4.10 (s, 3H), 8.21-8.23 (m, 2H), 8.52 (dd, J = 2.0 Hz, J = 8.8 Hz, 2H), 9.33-9.38 (m, 8H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 52.9, 53.0, 114.9, 117.0, 119.3, 122.1, 122.9, 126.8, 128.9, 129.2, 129.3, 130.0, 132.3, 134.1, 135.7, 139.6, 164.9, 165.3 ppm. HRMS (ESI^+): calcd for $C_{31}H_{21}N_2O_6^+$ $[M-CF_3SO_3^-]^+$ 517.1394, found 517.1393.



8,11,14-tricyanotribenzo[*b*,*de*,*g*]benzo[4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-5-ium tetrafluoroborate (6i):

Filtration with a funnel and washing with dichloromethane and methanol to provide **6i** as a yellow solid (24.3 mg, 81% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.24 (d, J = 6.4 Hz, 2H), 8.61 (d, J = 8.8 Hz, 2H), 9.47-9.51 (m, 4H), 9.82 (d, J = 5.2 Hz, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 111.5, 115.0, 117.3, 117.4, 117.6, 117.7, 120.1, 122.2, 127.2, 129.3, 129.7, 131.5, 133.9, 135.4, 139.7 ppm. HRMS (ESI^+): calcd for $C_{28}H_{12}N_5^+$ $[M-BF_4^-]^+$ 418.1087, found 418.1089.



tribenzo[*b*,*de*,*g*]phenanthro[9',10':4,5]imidazo[1,2,3-*ij*][1,8]naphthyridin-17-ium trifluoromethanesulfonate (4x): A light yellow solid (30.8 mg, 52% yield). ^{1}H NMR (400 MHz,

DMSO-d_6): δ = 7.94-8.04 (m, 8H), 8.52 (t, J = 8.0 Hz, 1H), 8.64 (d, J = 7.6 Hz, 4H), 9.11-9.18 (m, 6H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 112.1, 120.0, 120.9, 122.5, 123.0, 123.8, 125.2, 126.1, 126.3, 127.7, 128.6, 128.9, 129.98, 130.03, 130.1, 131.1, 134.5, 138.9 ppm. HRMS (ESI$^+$): calcd for $C_{28}H_{12}N_5^+$ [M−$CF_3SO_3^-$]$^+$ 443.1543, found 443.1590.

IV. DFT Calculations

Density functional theory (DFT) calculations were performed using the Gaussian 09 program. The configuration optimizations were finished using B3LYP level of density functional theory with the 6-31G(d) basis. The counter anion was deleted. Electron-density difference maps of the lowest lying relaxed singlet excited state (S1) as compared to the ground state (S0) at the same geometry for **5a** (a), **3f** (b) and **5x** (c); isocontour value = 0.001 au. The green (red) color indicates an increase (decrease) of electron density in a given molecular region upon excitation.

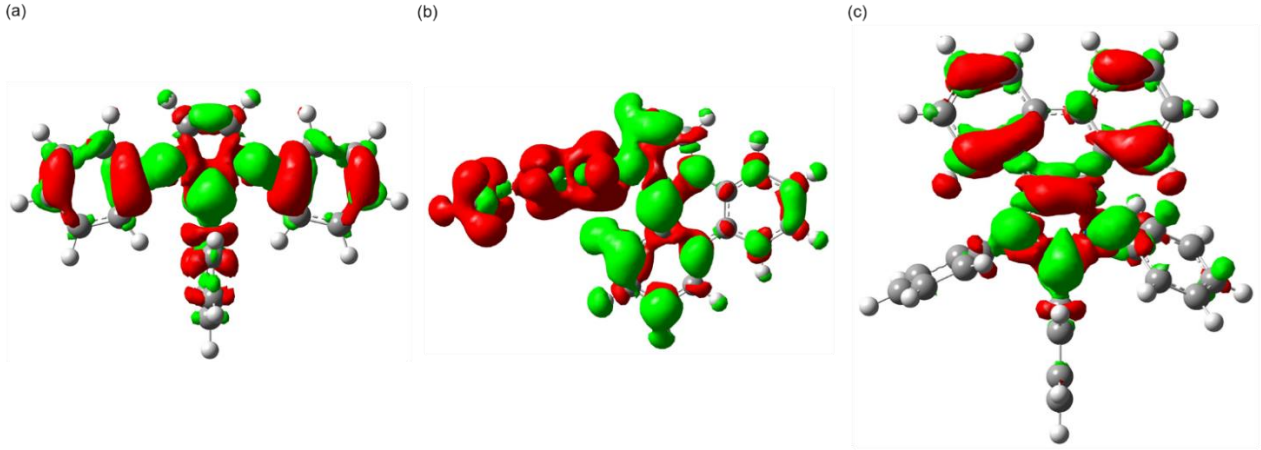
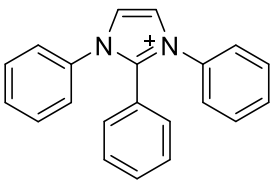


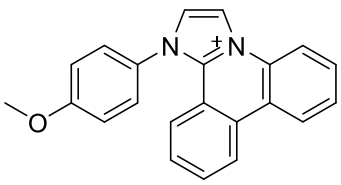
Fig. S1 Electron-density difference maps of **5a** (a), **3f** (b) and **5x** (c).

Table S3 Cartesian coordinates of optimized species



Symbolic	Z-matrix		
Charge = 1	Multiplicity = 1		
C	-4.57772	1.77229	-0.47557
C	-3.44963	2.50897	-0.67039
N	-2.34822	1.6903	-0.45041
C	-2.84132	0.46412	-0.12428
N	-4.20242	0.47931	-0.13033
C	-5.17652	-0.62273	0.16198

C	-1.97389	-0.77652	0.20783
C	-0.92688	2.15268	-0.57145
C	0.1696	1.32472	-0.35001
C	1.47706	1.81583	-0.47886
C	1.70218	3.14039	-0.83066
C	0.61869	3.9784	-1.05479
C	-0.68718	3.48879	-0.92627
C	-1.58192	-1.02643	1.53303
C	-0.80218	-2.14431	1.8275
C	-0.41275	-3.01204	0.80625
C	-0.79909	-2.76854	-0.51247
C	-1.57883	-1.65304	-0.81584
C	-4.79085	-1.91461	0.50703
C	-5.74987	-2.90386	0.76918
C	-7.1053	-2.61169	0.68909
C	-7.5055	-1.3279	0.34623
C	-6.54846	-0.33946	0.08427
H	-5.60911	2.06541	-0.55522
H	-3.34639	3.54314	-0.94611
H	0.10885	0.28768	-0.07457
H	2.32387	1.15418	-0.30192
H	2.71837	3.51645	-0.92934
H	0.78885	5.01742	-1.33076
H	-1.47457	4.20468	-1.11743
H	-1.88164	-0.35472	2.33514
H	-0.49526	-2.34367	2.85277
H	0.1961	-3.88418	1.03971
H	-0.48976	-3.45187	-1.30145
H	-1.87613	-1.4703	-1.84668
H	-3.77274	-2.24684	0.59731
H	-5.4306	-3.90985	1.03787
H	-7.84536	-3.38278	0.89345
H	-8.56642	-1.09293	0.2819
H	-6.94188	0.63348	-0.17574



Symbolic Z-matrix

Charge = 1 Multiplicity = 1

C	-16.72662	-0.06214	0.01059
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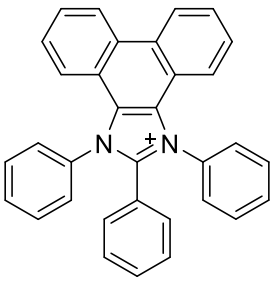
N	-15.38258	-1.79333	0.08476
C	-14.60091	-0.70706	0.11265
N	-15.40701	0.36999	0.06257
C	-15.01684	1.7527	0.05622

C	-13.04662	-0.84143	0.18596
C	-14.8076	-3.16734	0.11482
C	-15.66819	-4.27645	0.08037
C	-15.15256	-5.56756	0.09951
C	-13.78088	-5.75044	0.15245
C	-12.92577	-4.64277	0.18944
C	-13.39778	-3.30525	0.17389
C	-12.52308	-2.16069	0.21344
C	-11.11021	-2.2717	0.28125
C	-10.26455	-1.1613	0.31994
C	-10.80228	0.11082	0.29116
C	-12.18308	0.2689	0.22393
C	-14.88529	2.40634	1.27176
C	-14.4962	3.74422	1.25079
C	-14.25148	4.40072	0.03502
C	-14.42678	3.71673	-1.17388
C	-14.818	2.37612	-1.16878
O	-13.8559	5.70157	0.16642
C	-13.3924	6.36195	-1.00653
H	-17.51593	0.67013	-0.03074
H	-17.49419	-2.16026	-0.00318
H	-16.74507	-4.16955	0.03724
H	-15.81652	-6.42944	0.07199
H	-13.36478	-6.75711	0.16531
H	-11.86242	-4.86896	0.22923
H	-10.61611	-3.24055	0.30871
H	-9.18617	-1.29858	0.37352
H	-10.14869	0.98031	0.32216
H	-12.54599	1.28772	0.20474
H	-15.06419	1.90101	2.21436
H	-14.37056	4.28841	2.18584
H	-14.26794	4.20576	-2.13082
H	-14.95111	1.84188	-2.10367
H	-13.02432	7.34927	-0.71165
H	-12.55895	5.81786	-1.46366
H	-14.2082	6.50773	-1.7217



Symbolic Z-matrix

Charge = 1 Multiplicity = 1

C	-3.05049	1.77632	-3.89376
C	-2.4412	0.63616	-4.52797
N	-1.69667	-0.08299	-3.52596

C	-1.80916	0.6092	-2.37535
N	-2.595	1.81749	-2.58245
C	-2.474	2.93542	-1.73319
C	-1.04293	0.23698	-1.07382
C	-0.84468	-1.23934	-3.6565
C	-1.32039	-2.46227	-3.20197
C	-0.48847	-3.57364	-3.31147
C	0.7903	-3.43704	-3.86361
C	1.24534	-2.18989	-4.30758
C	0.42183	-1.07139	-4.20278
C	0.21715	0.79388	-0.82642
C	0.91778	0.45613	0.33062
C	0.36498	-0.44338	1.24088
C	-0.88856	-1.00466	0.99737
C	-1.5931	-0.66567	-0.15815
C	-2.04112	4.16662	-2.24133
C	-1.90964	5.25925	-1.38365
C	-2.20252	5.12376	-0.02699
C	-2.6263	3.89515	0.47809
C	-2.7601	2.79647	-0.37162
C	-3.95245	2.62442	-4.5514
C	-4.10173	2.42876	-5.95092
C	-3.44103	1.33123	-6.62274
C	-2.6478	0.39051	-5.90348
C	-4.71054	3.59235	-3.86874
C	-5.55334	4.45699	-4.56073
C	-5.6639	4.3469	-5.93537
C	-4.95978	3.34586	-6.61147
C	-3.57007	1.09262	-8.01505
C	-2.99155	-0.00837	-8.65213
C	-2.26711	-0.92695	-7.91476
C	-2.09898	-0.73188	-6.54597
H	-2.31452	-2.5529	-2.78017
H	-0.82917	-4.54746	-2.96687
H	1.43841	-4.30827	-3.94433
H	2.24324	-2.09651	-4.73014
H	0.76169	-0.09758	-4.53624
H	0.65274	1.49784	-1.53147
H	1.89382	0.89472	0.52412
H	0.91305	-0.70737	2.14257
H	-1.31384	-1.70711	1.71035
H	-2.56845	-1.10857	-0.3417
H	-1.78872	4.29374	-3.29149
H	-1.5757	6.21863	-1.77218
H	-2.09967	5.97755	0.63895
H	-2.85712	3.79502	1.53603
H	-3.11745	1.85911	0.04559
H	-4.68733	3.69411	-2.78822
H	-6.12294	5.21168	-4.02382

H	-6.3159	5.02065	-6.48651
H	-5.12145	3.29355	-7.68476
H	-4.14256	1.76301	-8.65067
H	-3.12595	-0.1499	-9.72211
H	-1.83279	-1.79734	-8.40104
H	-1.54156	-1.49462	-6.02125

V. Single Crystal X-ray Crystallographic Data

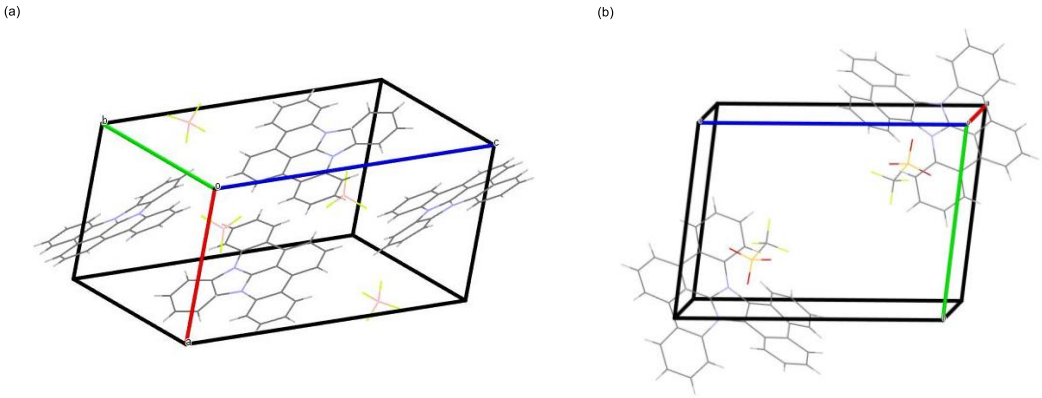
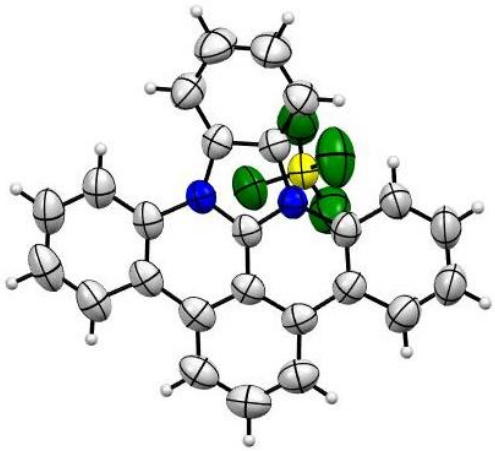


Fig. S2 Wireframe model of the packing structures of **4m′** (a) and **4x** (b)

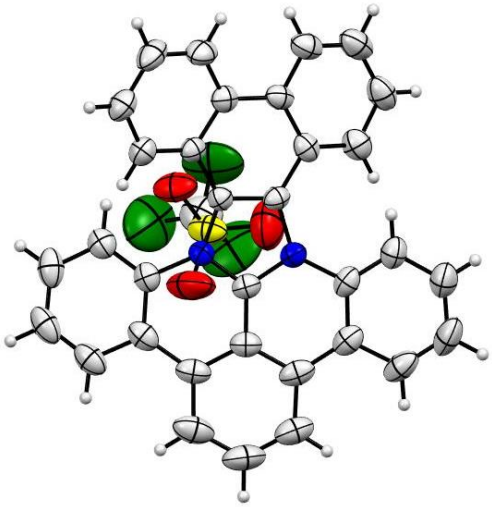
Table S4. Crystal data and structure refinement for **4m′**



Identification code	2114143
Empirical formula	$C_{25}H_{15}BF_4N_2$
Formula weight	430.20
Temperature/K	301.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.4814(4)

b/Å	14.5840(9)
c/Å	16.2845(10)
α/°	90
β/°	103.547(2)
γ/°	90
Volume/Å^3	1958.23(19)
Z	4
ρ_{calc}g/cm^3	1.459
μ/mm^{-1}	0.112
F(000)	880.0
Crystal size/mm^3	0.38 × 0.34 × 0.29
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.008 to 55.074
Index ranges	-10 ≤ h ≤ 11, -18 ≤ k ≤ 18, -21 ≤ l ≤ 21
Reflections collected	90776
Independent reflections	4495 [R_{int} = 0.0999, R_{sigma} = 0.0298]
Data/restraints/parameters	4495/4/289
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0718, wR_2 = 0.2064
Final R indexes [all data]	R_1 = 0.1228, wR_2 = 0.2533
Largest diff. peak/hole/eÅ^{-3}	0.72/-0.31

Table S5. Crystal data and structure refinement for **4x**



Identification code	2114141
Empirical formula	$C_{34}H_{19}F_3N_2O_3S$
Formula weight	592.57
Temperature/K	293.15
Crystal system	triclinic
Space group	P-1
a/Å	9.3567(6)
b/Å	10.7079(6)
c/Å	14.3234(8)
α/°	81.633(5)
β/°	87.519(5)
γ/°	83.289(5)
Volume/Å^3	1409.56(14)
Z	2
ρ_{calc}g/cm^3	1.396
μ/mm^{-1}	0.174
F(000)	608.0
Crystal size/mm^3	0.35 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.904 to 52.742
Index ranges	-8 ≤ h ≤ 11, -13 ≤ k ≤ 13, -17 ≤ l ≤ 16
Reflections collected	11362
Independent reflections	5757 [R_{int} = 0.0249, R_{sigma} = 0.0506]
Data/restraints/parameters	5757/0/388
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0749, wR_2 = 0.2067
Final R indexes [all data]	R_1 = 0.1117, wR_2 = 0.2298
Largest diff. peak/hole/eÅ^{-3}	0.99/-0.35

VI. Optical Properties of Selected Compounds

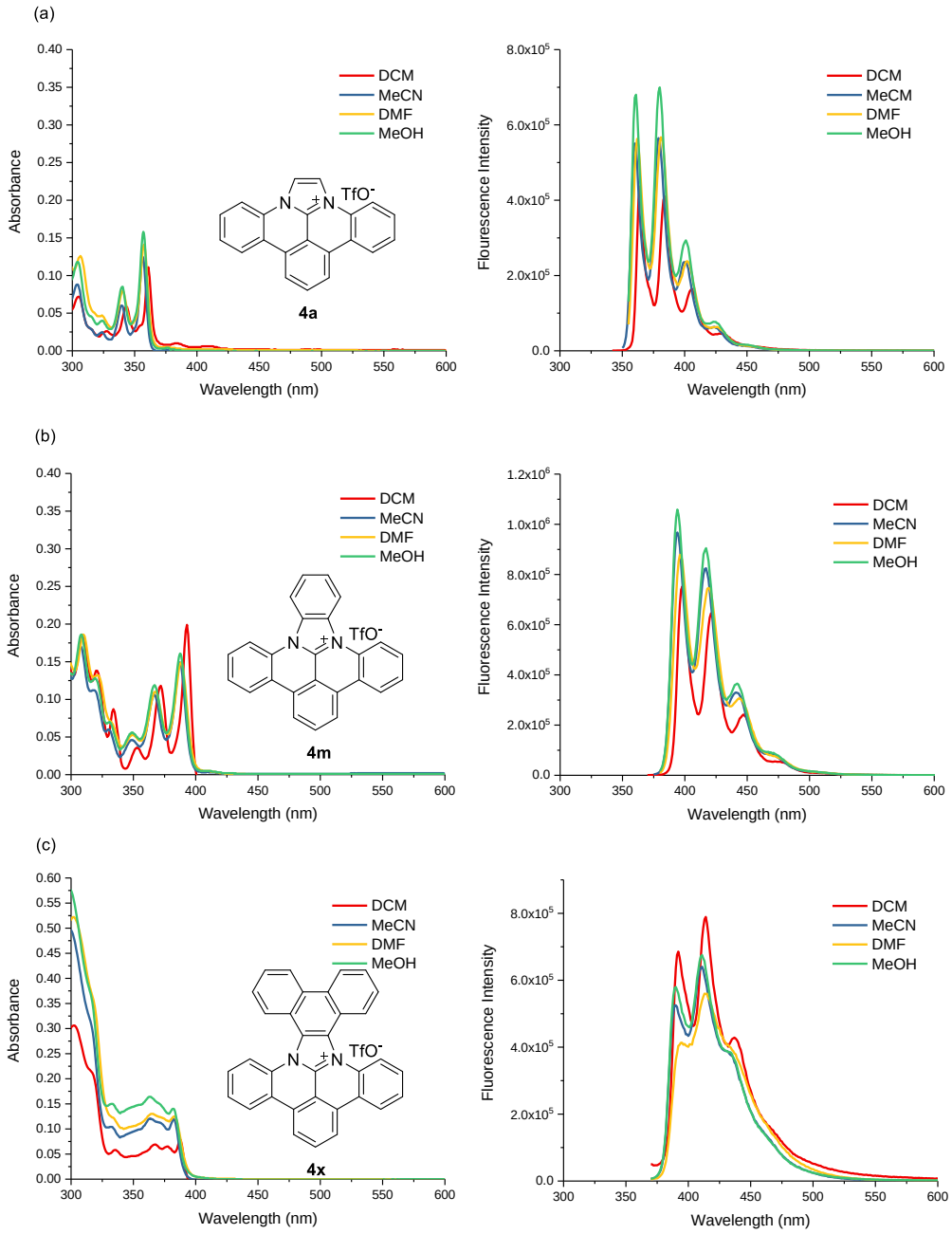


Fig. S3 UV-visible absorption and emission spectra of **4a** (a), **4m** (b) and **4x** (c) in different solvents.

Table S6 UV-visible absorption and emission data of some selected compounds

Compd.	$\lambda_{abs}{}^{a}$ (nm)	ε (M^{-1} cm^{-1})	$\lambda_{em}{}^{b}$ (nm)	$\Phi_F{}^{c}$
4a	361	11100	364, 384, 406, 430	0.29
4c	362	22900	366, 386, 408, 433	0.34
4d	393	11200	398, 422, 447, 477	0.27
4j	368	17400	373, 394, 416, 443	0.14
4m	393	19900	398, 422, 447, 477	0.29
4n	396	25800	401, 425, 451, 483	0.30
4p	363	10200	368, 387, 409, 433	0.29
4q	393	24200	398, 422, 448, 480	0.46

4s	306	30300	434, 459, 489	0.34
4t	418	26100	430, 454, 485	0.12
4x	302	30600	392, 414, 437	0.30
6c	376	12800	379, 401, 424, 451	0.18
6d	310	35400	379, 401, 425, 451	0.21
6e	312	20800	415, 441, 470, 504	0.18
6h	408	11400	413, 438, 467, 501	0.22

[a]The maximum absorption band over 300 nm. [b]Emission bands excited at the longest maximum absorption band. [c]Absolute quantum yield. Concentration: 1.0×10^{-5} M in CH_2Cl_2.

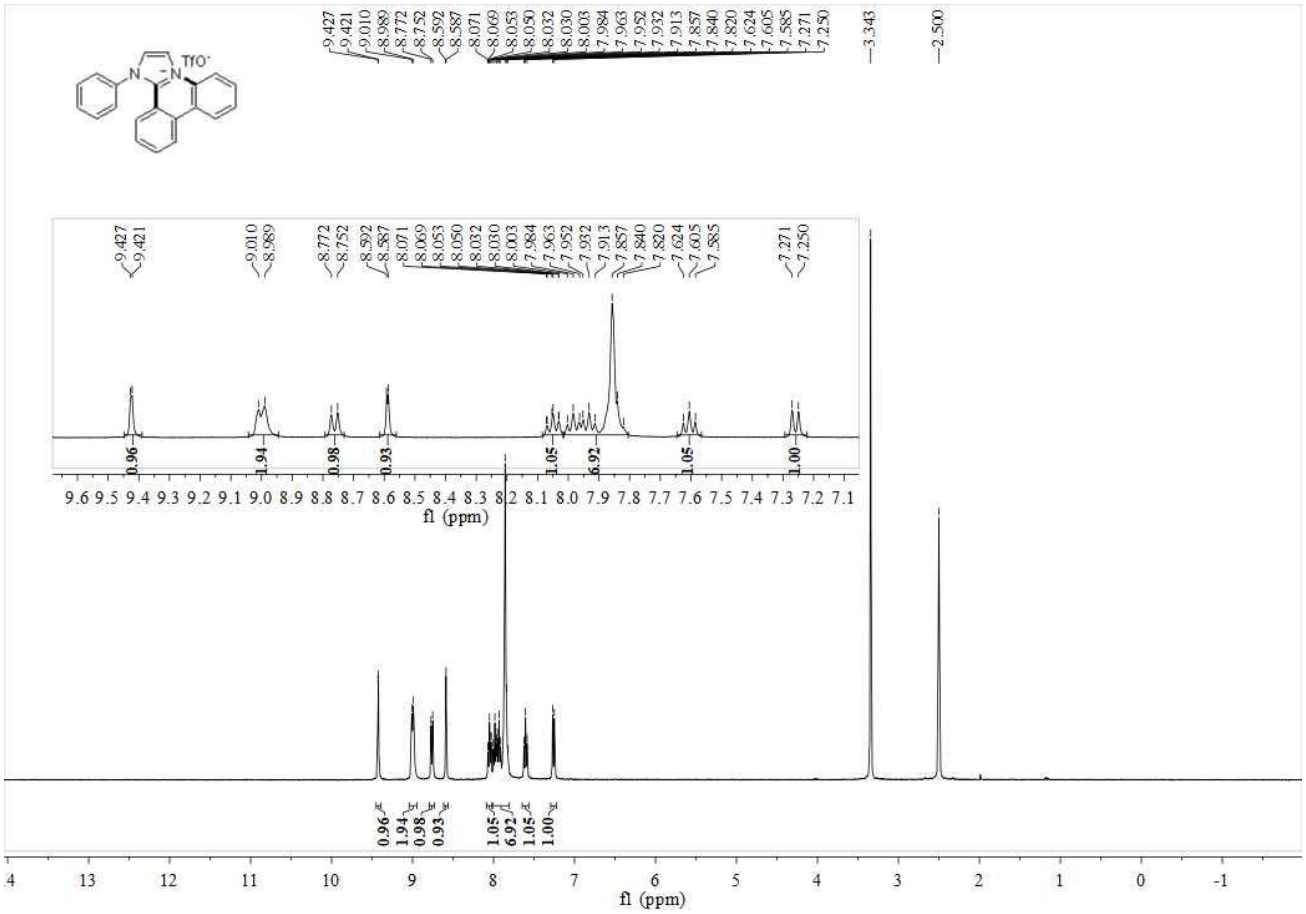
VII. References

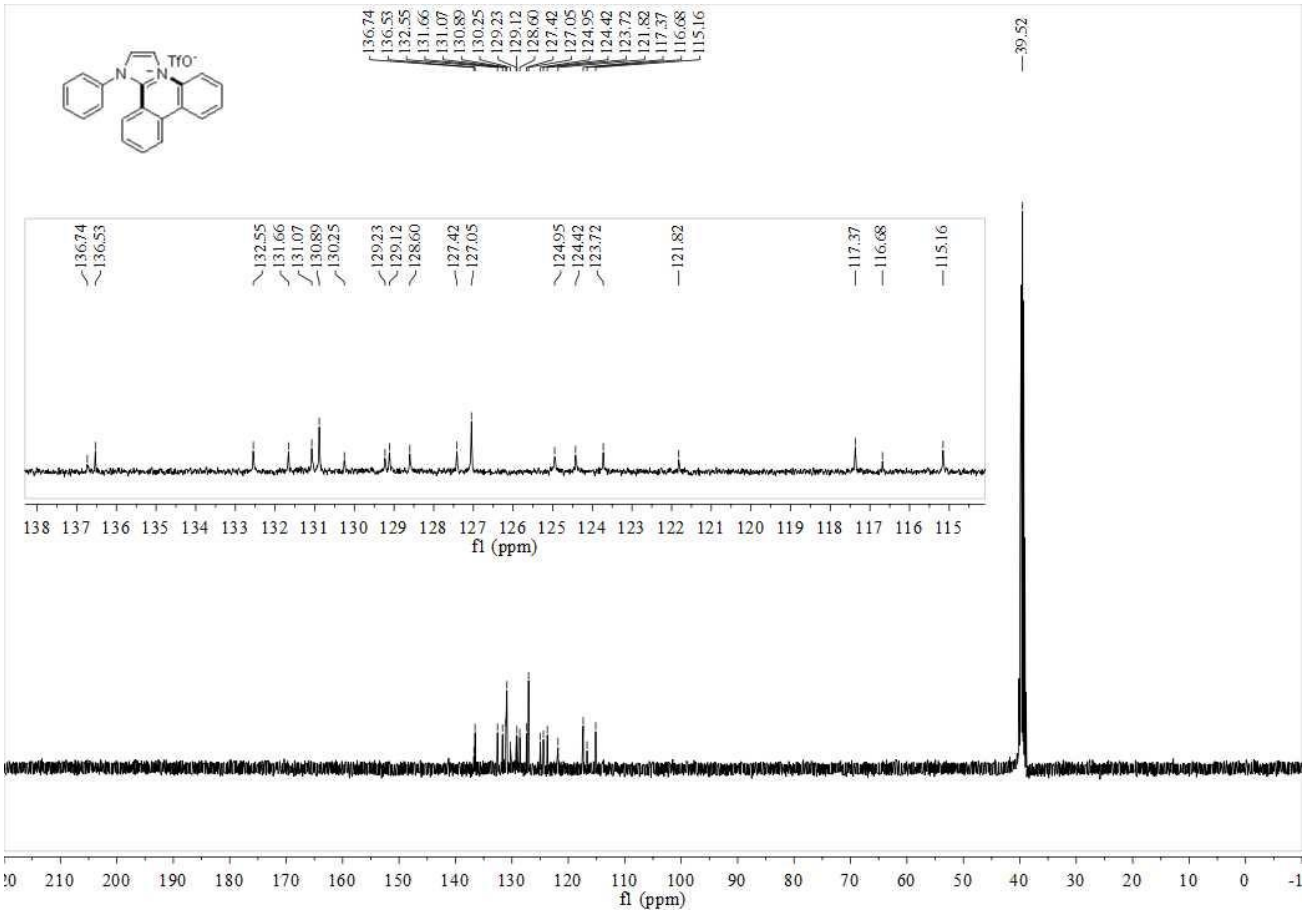
[1] (a) H. Zhang, Q. Cai, D. Ma, *J. Org. Chem*., 2005, **70**, 5164. (b) L. Zhu, L. Cheng, Y. Zhang, R. Xie, J. You, *J. Org. Chem*., 2007, **72**, 2737. (c) L. Zhu, P. Guo, G. Li, J. Lan, R. Xie, J. You, *J. Org. Chem*., 2007, **72**, 8535.

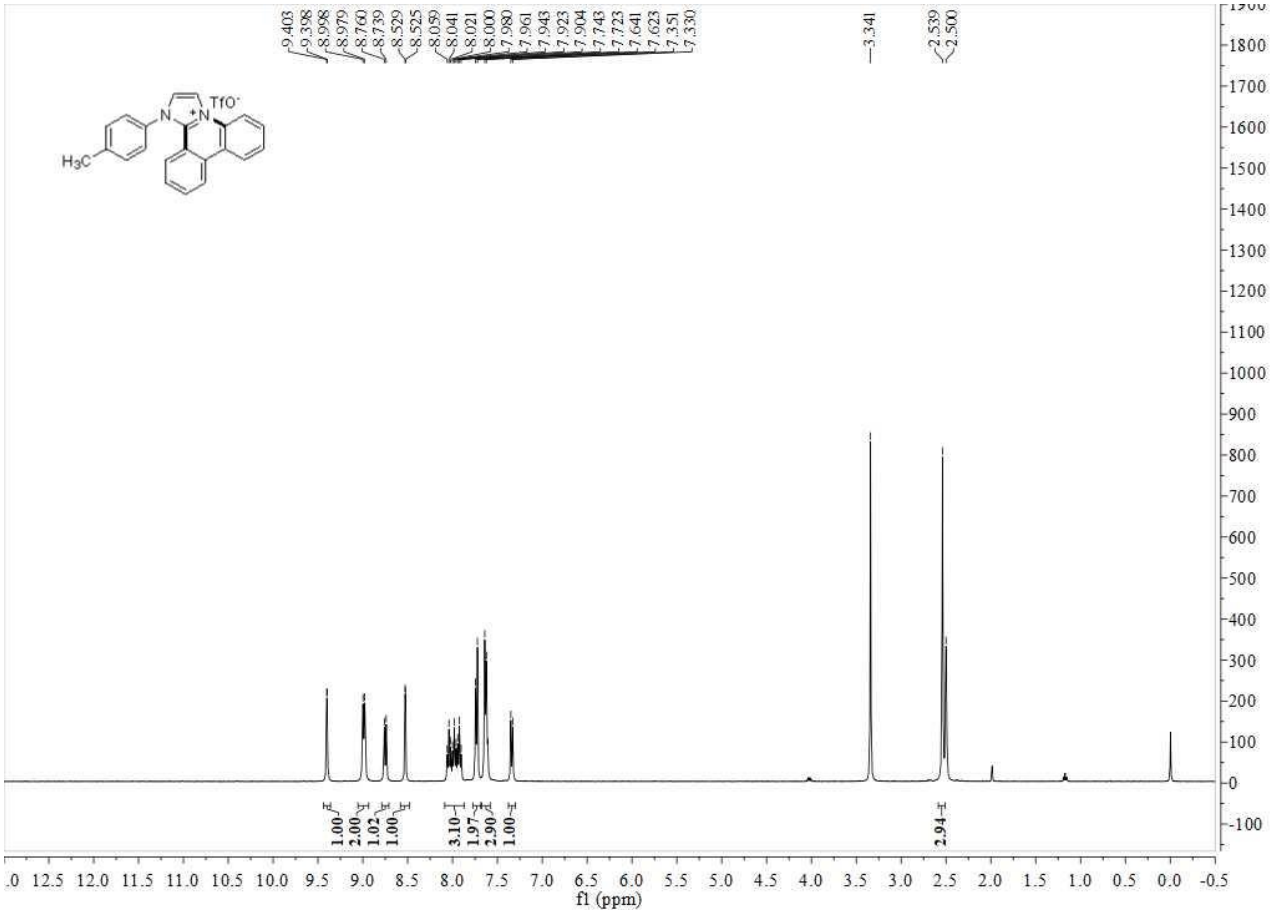
[2] (a) T. Lv, Z. Wang, J. You, J. Lan, G. Gao, *J. Org. Chem*., 2013, **78**, 5723. (b) T.-Y. Lv, L. Yang, Y.-S. Zhao, F.-J. Song, J.-B. Lan, J.-S. You, G. Gao, *Chin. Chem. Lett.*, 2013, **24**, 773; (c) S. Li, J. Tang, Y. Zhao, R. Jiang, T. Wang, G. Gao, J. You, *Chem. Commun*., 2017, **53**, 3489. (d) S. Li, H. Lv, Y. Yu, X. Ye, B. Li, S. Yang, Y. Mo, X. Kong, *Chem. Commun*., 2019, **55**, 11267.

[3] (a) D. Zhu, Q. Liu, B. Luo, M. Chen, P. Huang, R. Pi, S. Wen, *Adv. Synth. Catal*., 2013, **355**, 2172. (b) G. Akimoto, M. Otsuka, K. Miyamoto, A. Muranaka, D. Hashizume, R. Takita, M. Uchiyama, *Chem. Asian J*., 2018, **13**, 913. (c) W. Liang, Y. Yang, M. Yang, M. Zhang, C. Li, Y. Ran, J. Lan, Z. Bin, J. You, *Angew. Chem. Int. Ed*., 2021, **60**, 3493.

VIII. Copies of ^{1}H and ^{13}C NMR Spectra



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8.998
8.979
8.760
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7.961
7.943
7.923
7.904
7.743
7.723
7.641
7.623
7.351
7.330
3.341
2.539
2.500
TfO⁻
H3C
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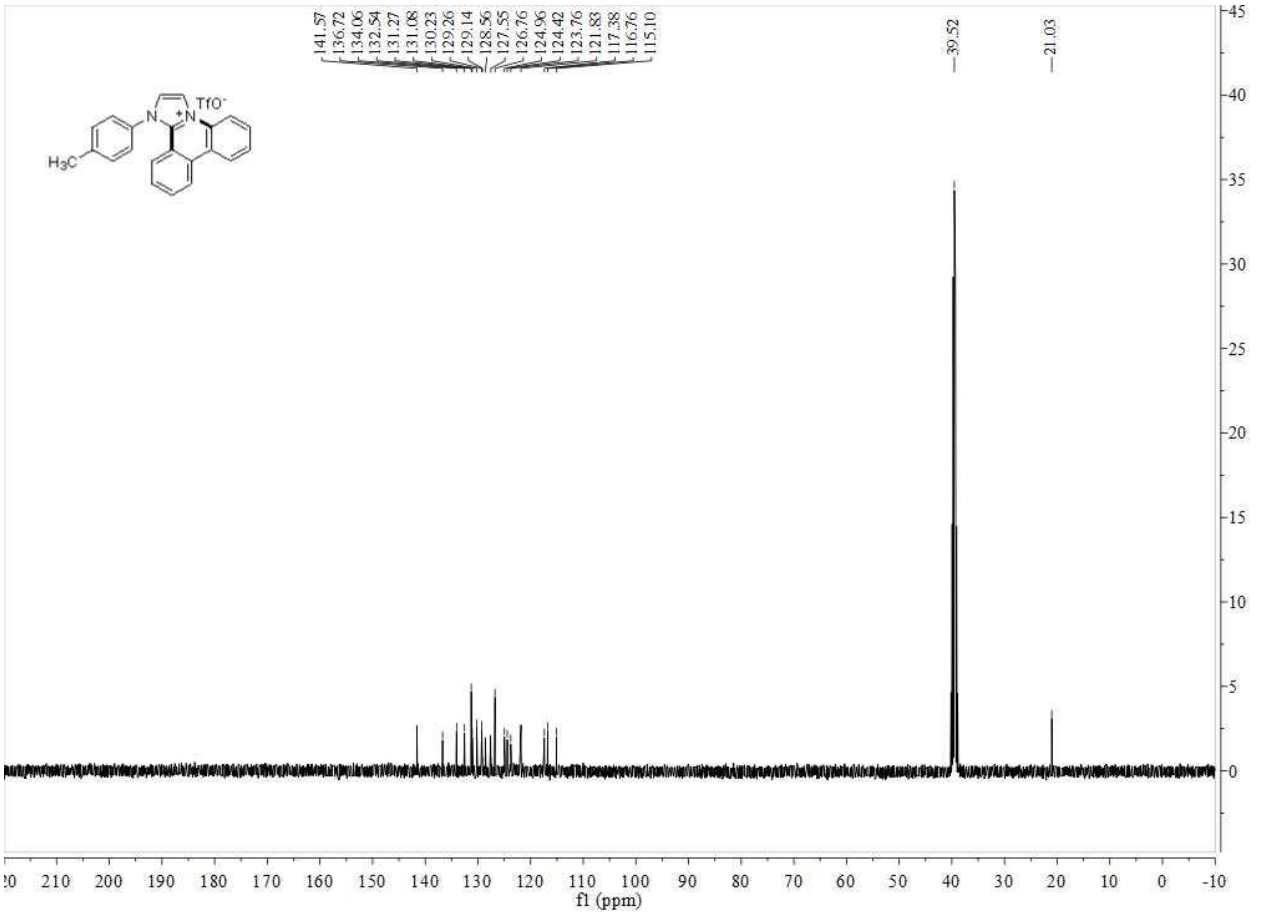
2.00
1.02
1.00
3.10
1.97
2.90
1.00
2.94
f1 (ppm)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136.72
134.06
132.54
131.27
131.08
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129.26
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127.55
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124.96
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115.10
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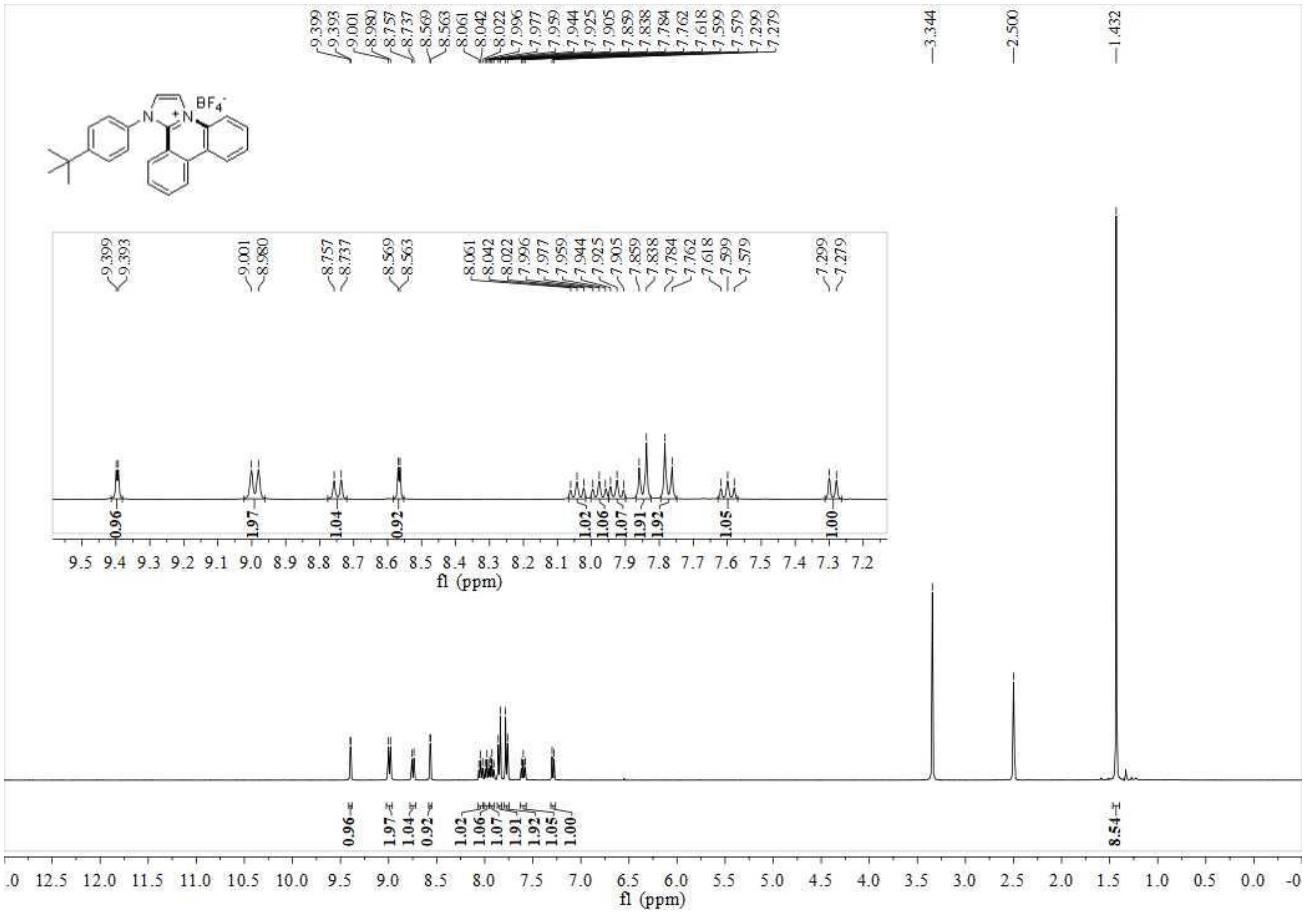
21.03
TfO⁻
H3C
f1 (ppm)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7.959
7.944
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7.599
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3.344
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1.432
BF4-
0.96
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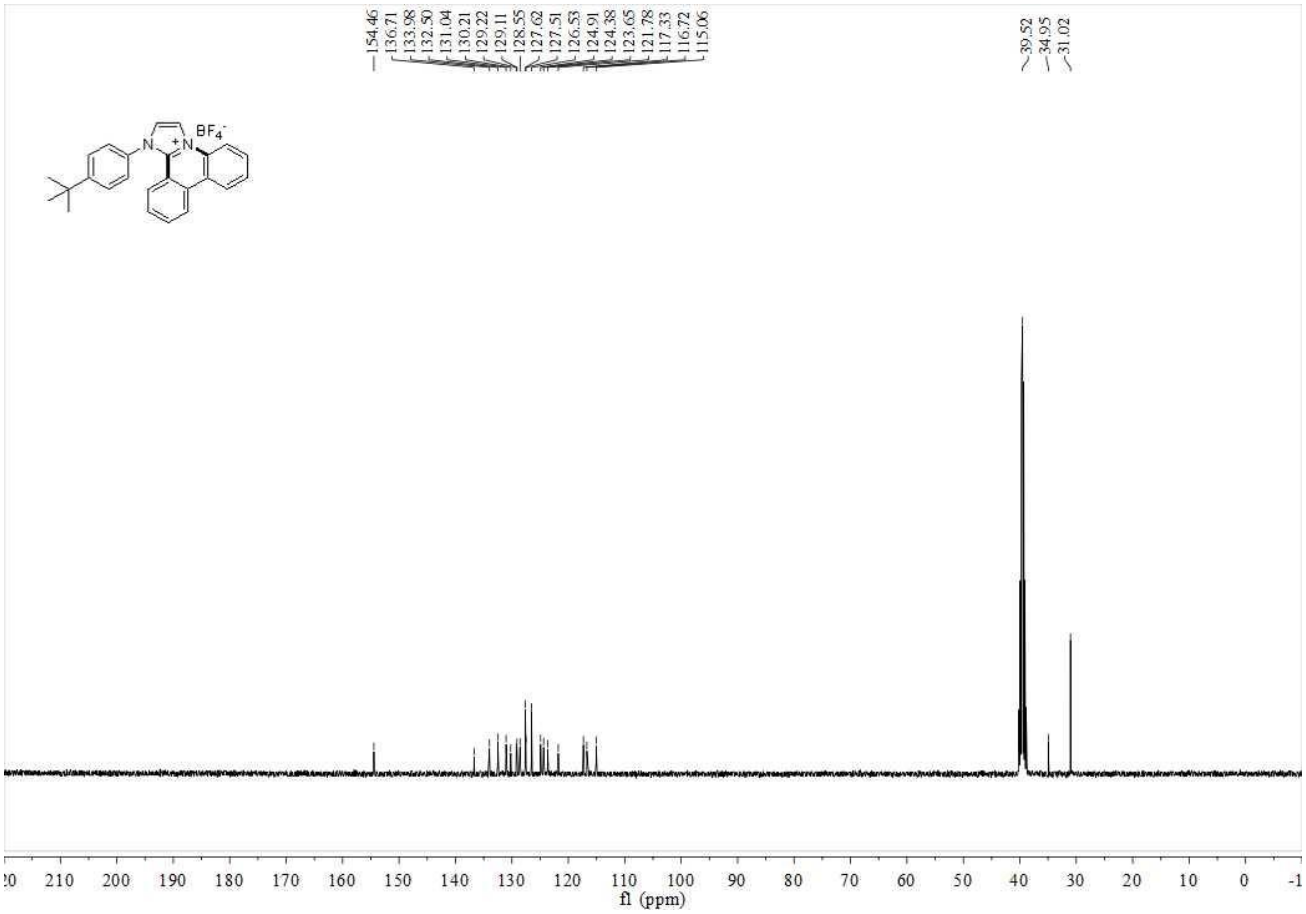
1.00
8.54
fl (ppm)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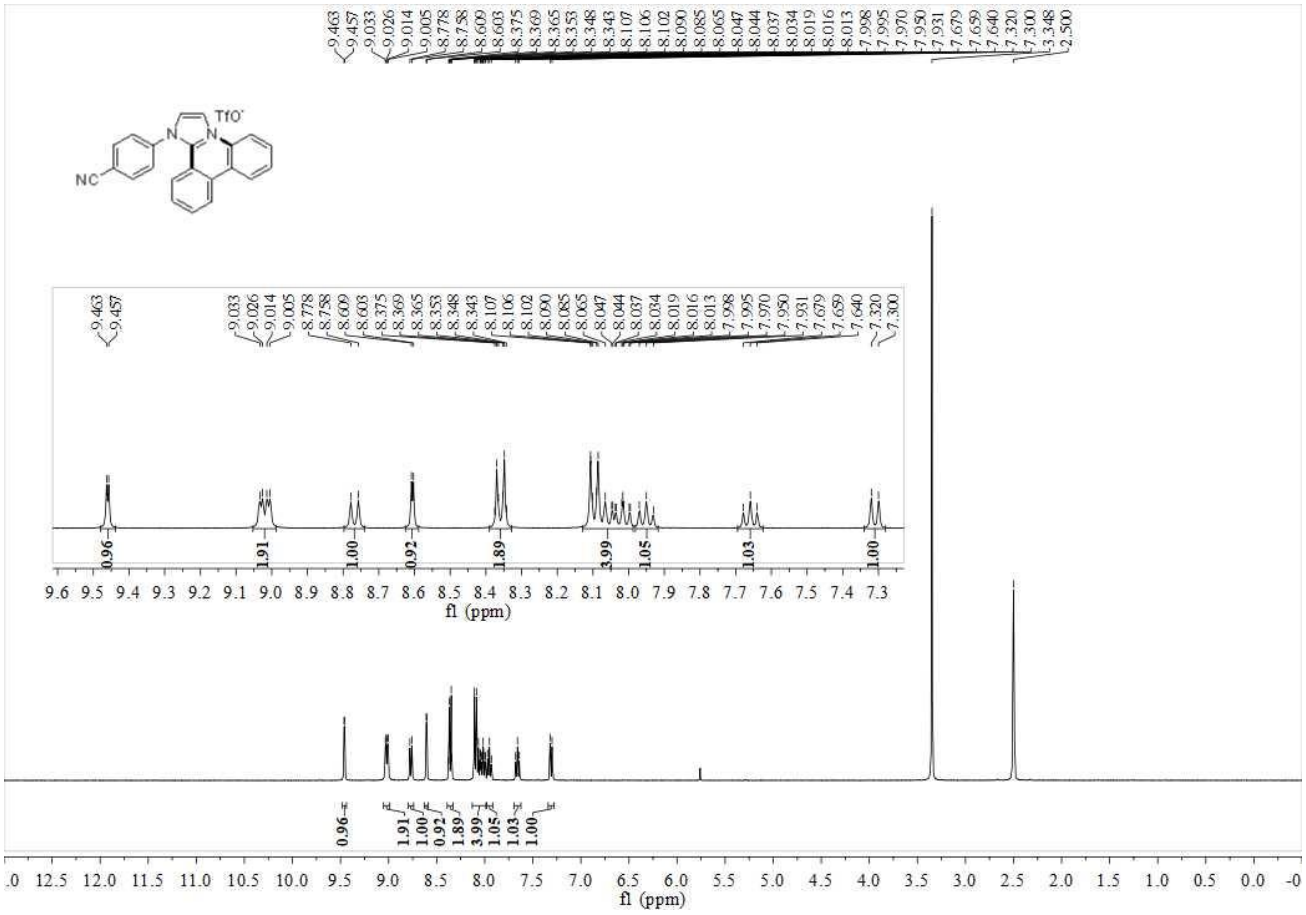
31.02
BF4-
fl (ppm)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7.300
3.348
2.500
TfO-
NC
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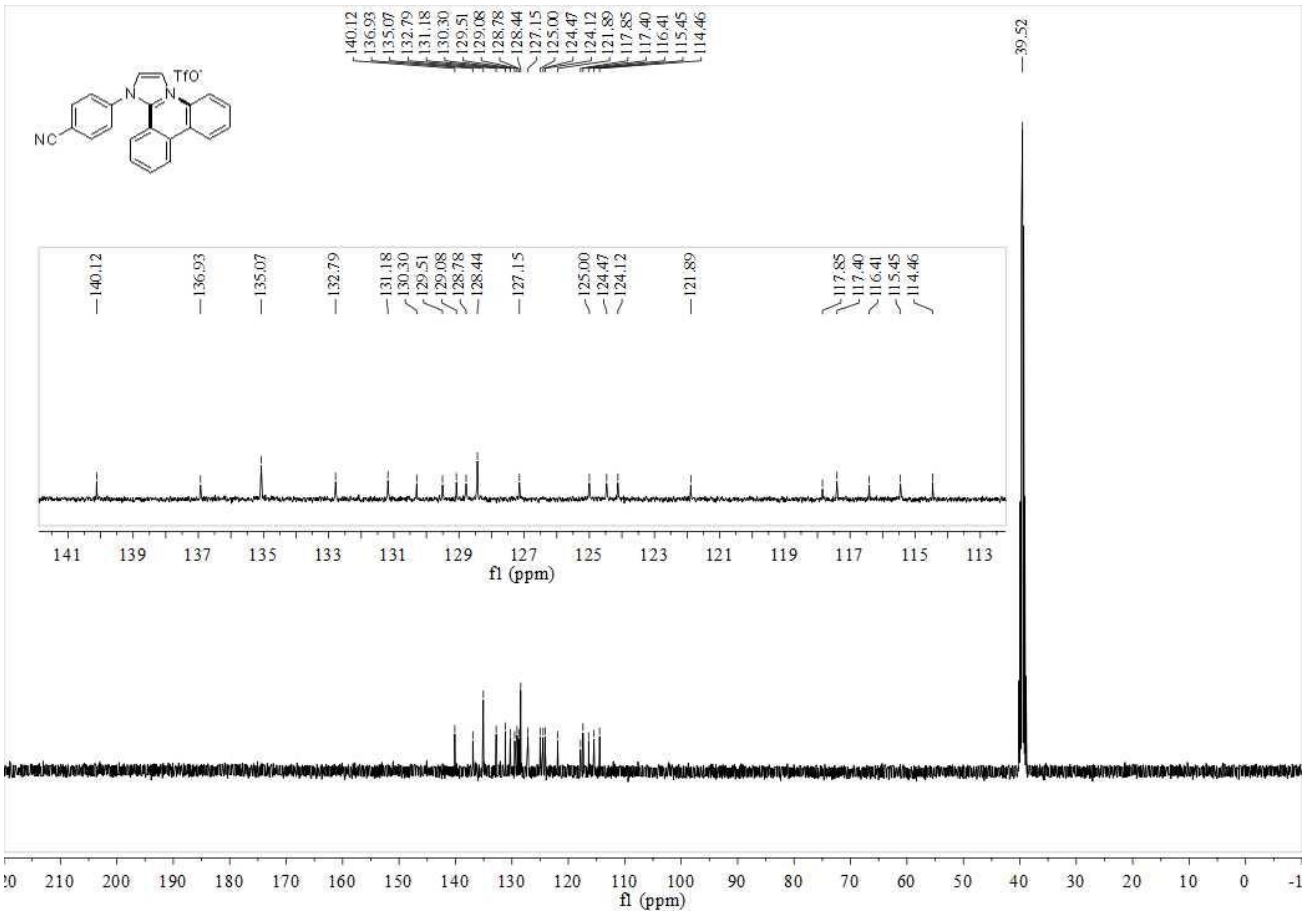
1.00
0.92
1.89
3.99
1.05
1.03
1.00
fl (ppm)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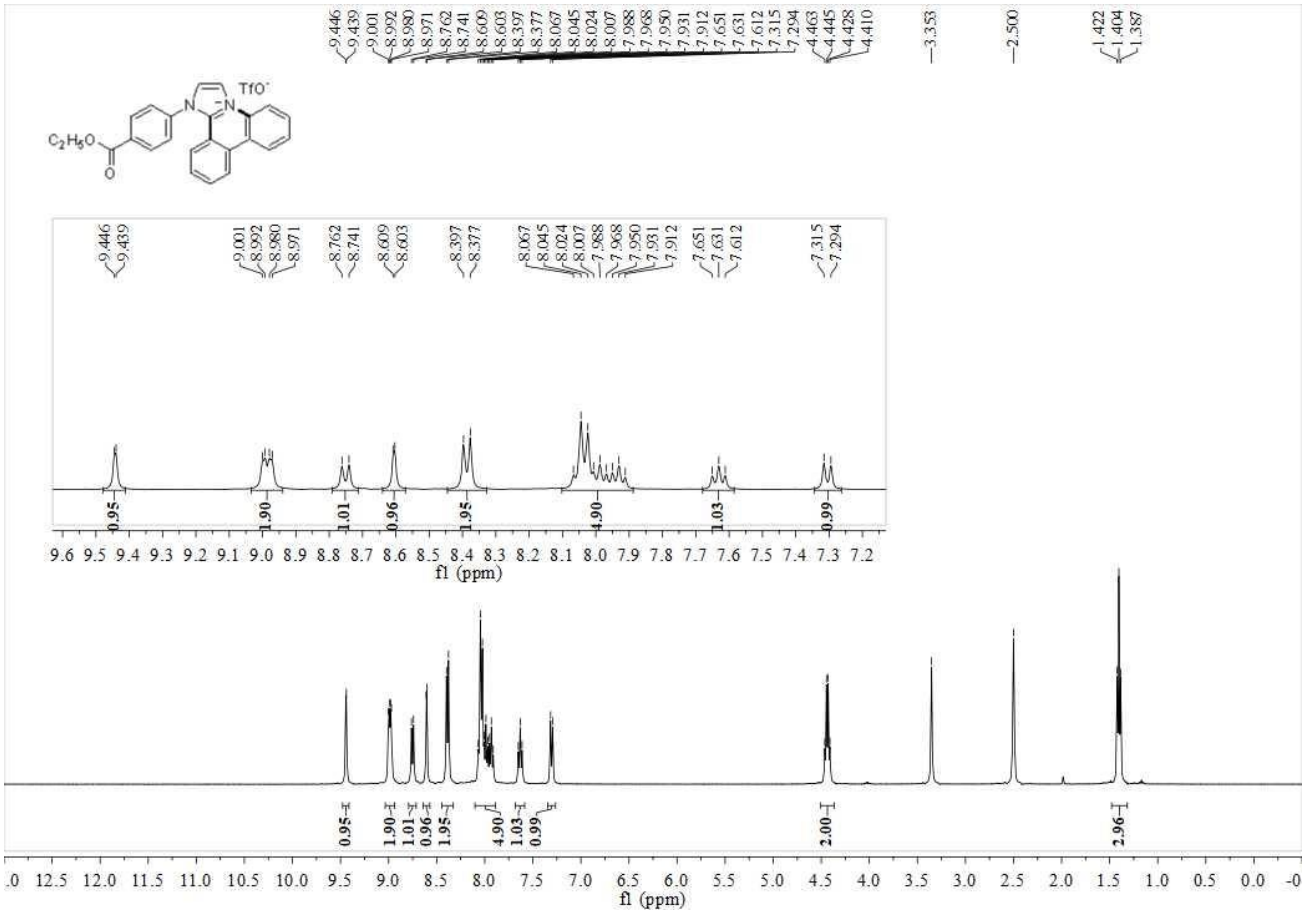
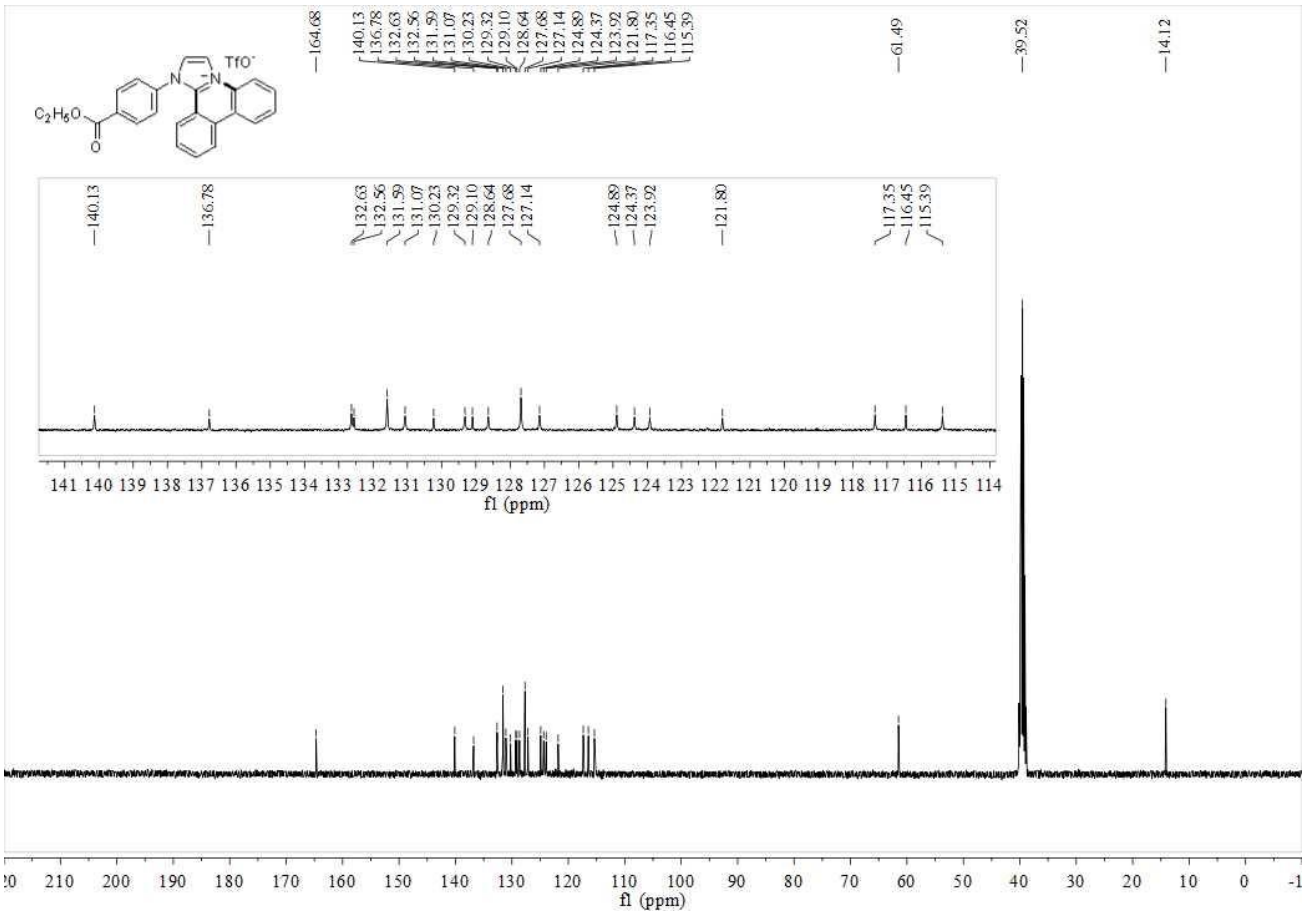
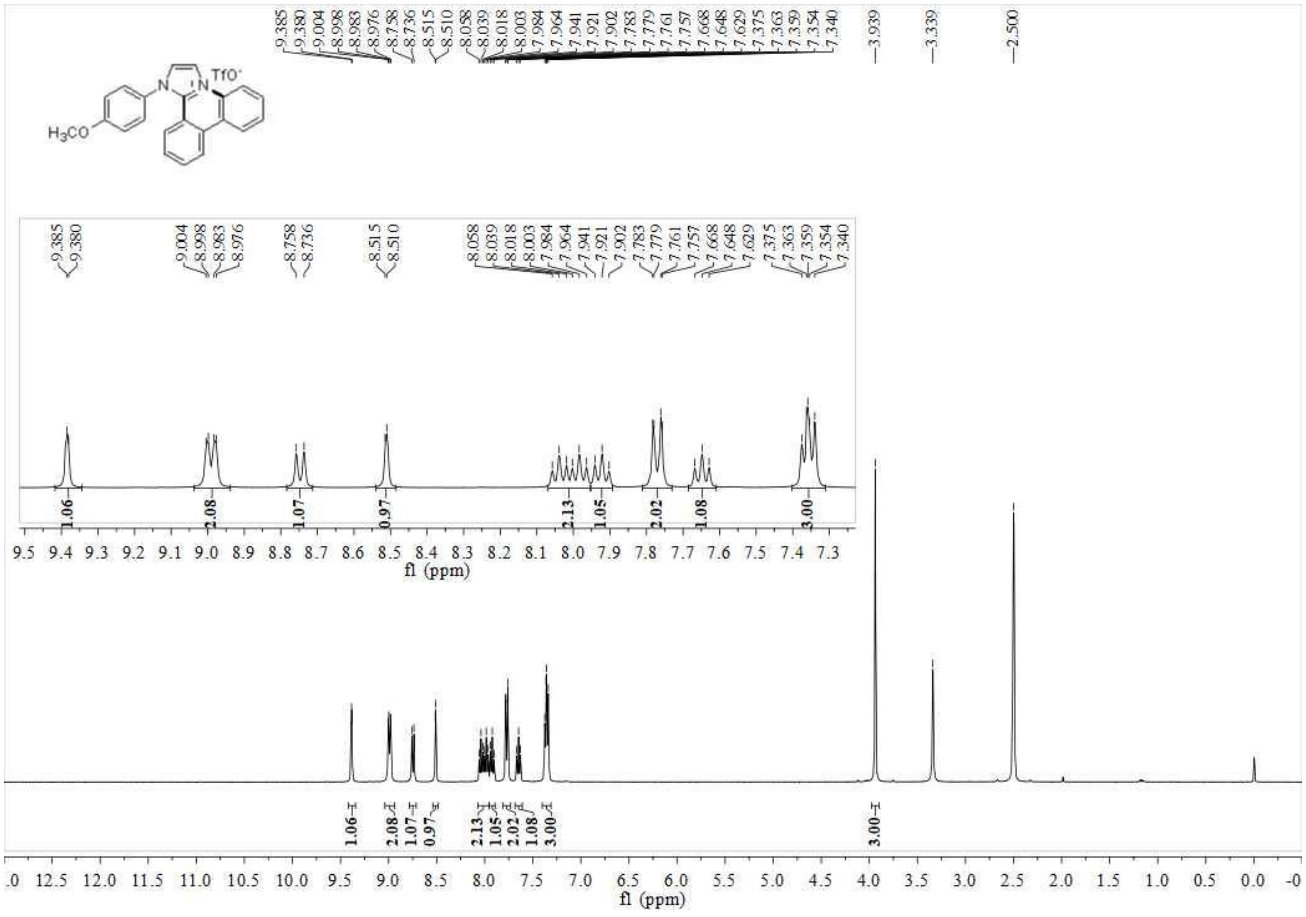
136.93
135.07
132.79
131.18
130.30
129.51
129.08
128.78
128.44
127.15
125.00
124.47
124.12
121.89
117.85
117.40
116.41
115.45
114.46
39.52
TfO-
NC
fl (ppm)


TfO⁻
C2H5O
O
9.446
9.439
9.001
8.992
8.980
8.971
8.762
8.741
8.609
8.603
8.397
8.377
8.067
8.045
8.024
8.007
7.988
7.968
7.950
7.931
7.912
7.651
7.631
7.612
7.315
7.294
4.463
4.445
4.428
4.410
3.353
2.500
1.422
1.404
1.387
0.95
1.90
1.01
0.96
1.95
4.90
1.03
0.99
2.00
2.96
fl (ppm)


TfO⁻
C2H5O
O
164.68
140.13
136.78
132.63
132.56
131.59
131.07
130.23
129.32
129.10
128.64
127.68
127.14
124.89
124.37
123.92
121.80
117.35
116.45
115.39
61.49
39.52
14.12
fl (ppm)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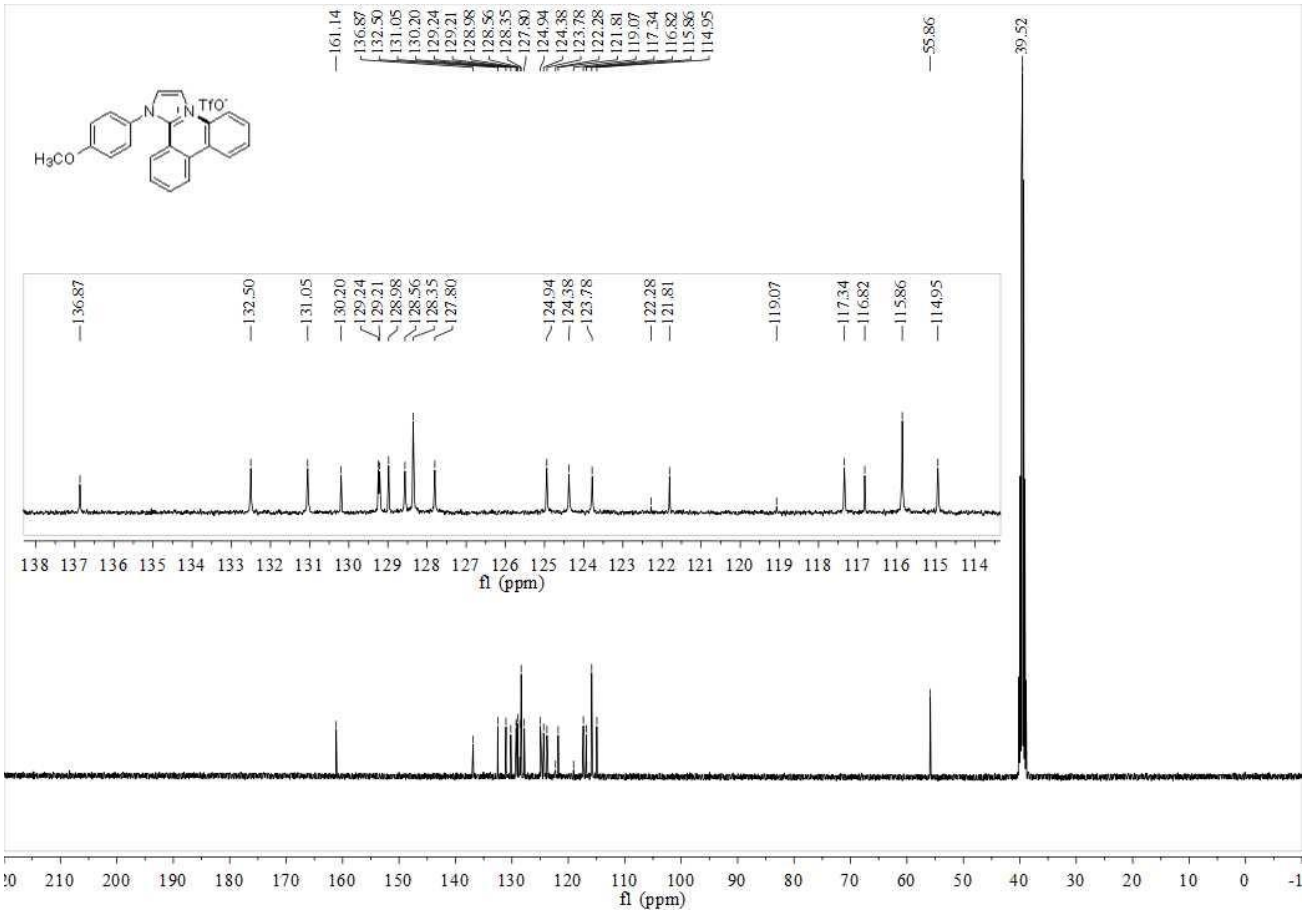
8.976
8.758
8.736
8.515
8.510
8.058
8.039
8.018
8.003
7.984
7.964
7.941
7.921
7.902
7.783
7.779
7.761
7.757
7.668
7.648
7.629
7.375
7.363
7.359
7.354
7.340
3.939
3.339
2.500
TfO⁻
H3CO
1.06
2.08
1.07
0.97
2.13
1.05
2.02
1.08
3.00
fl (ppm)


161.14
136.87
132.50
131.05
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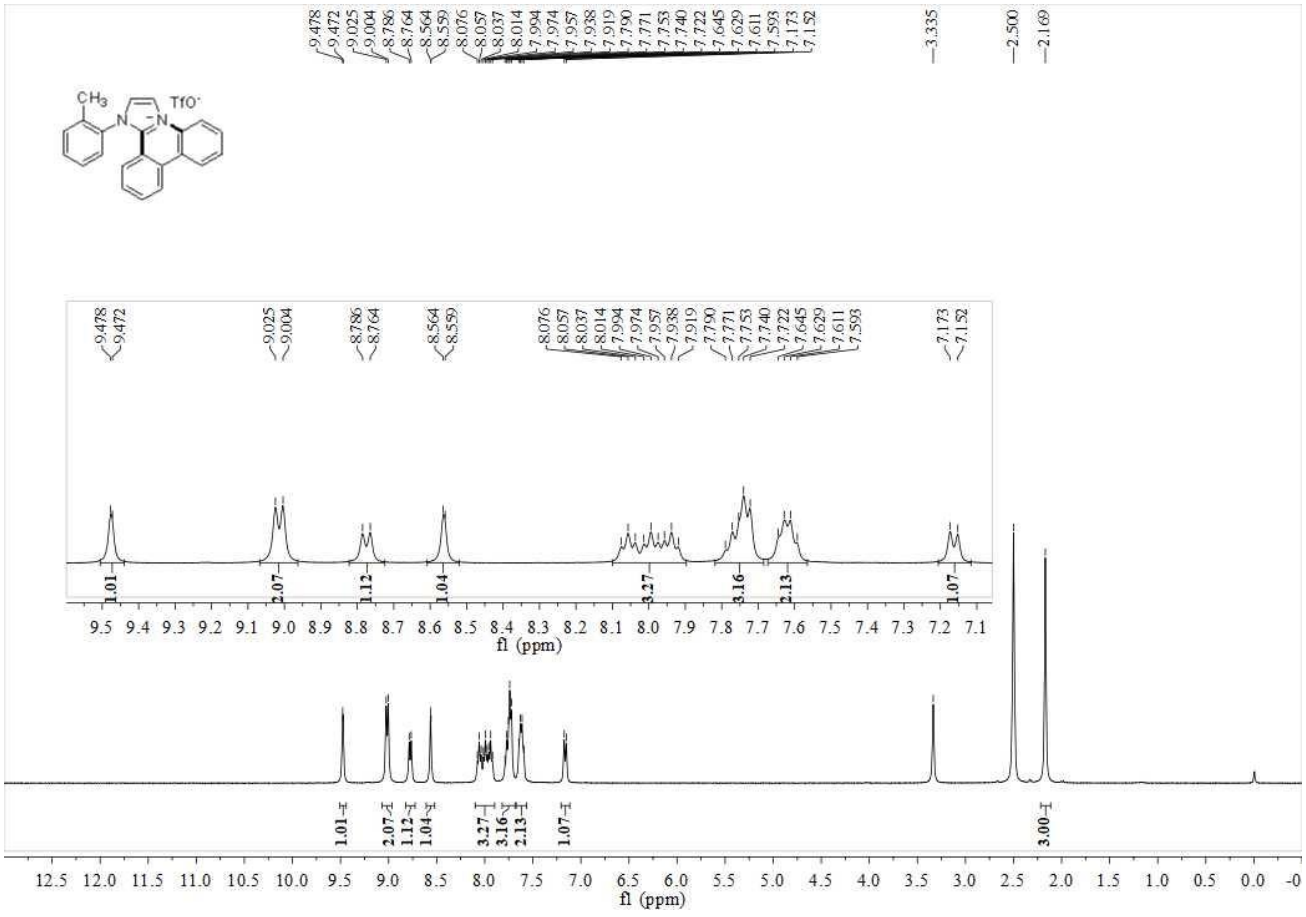
129.24
129.21
128.98
128.56
128.35
127.80
124.94
124.38
123.78
122.28
121.81
119.07
117.34
116.82
115.86
114.95
55.86
39.52
TfO⁻
H3CO
fl (ppm)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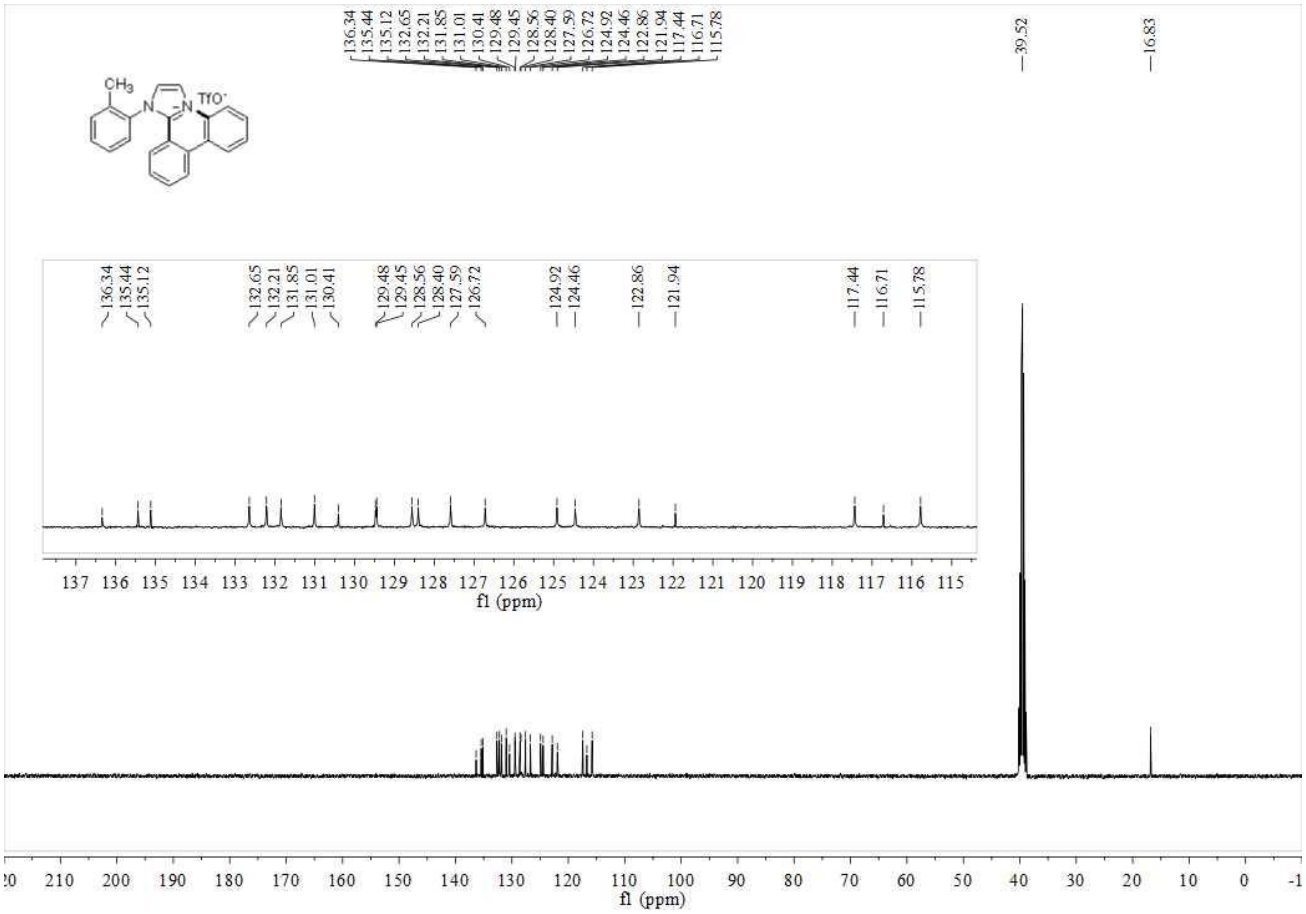
9.472
9.025
9.004
8.786
8.764
8.564
8.559
8.076
8.057
8.037
8.014
7.994
7.974
7.957
7.938
7.919
7.790
7.771
7.753
7.740
7.722
7.645
7.629
7.611
7.593
7.173
7.152
3.335
2.500
2.169
TfO-
1.01
2.07
1.12
1.04
3.27
3.16
2.13
1.07
3.00
fl (ppm)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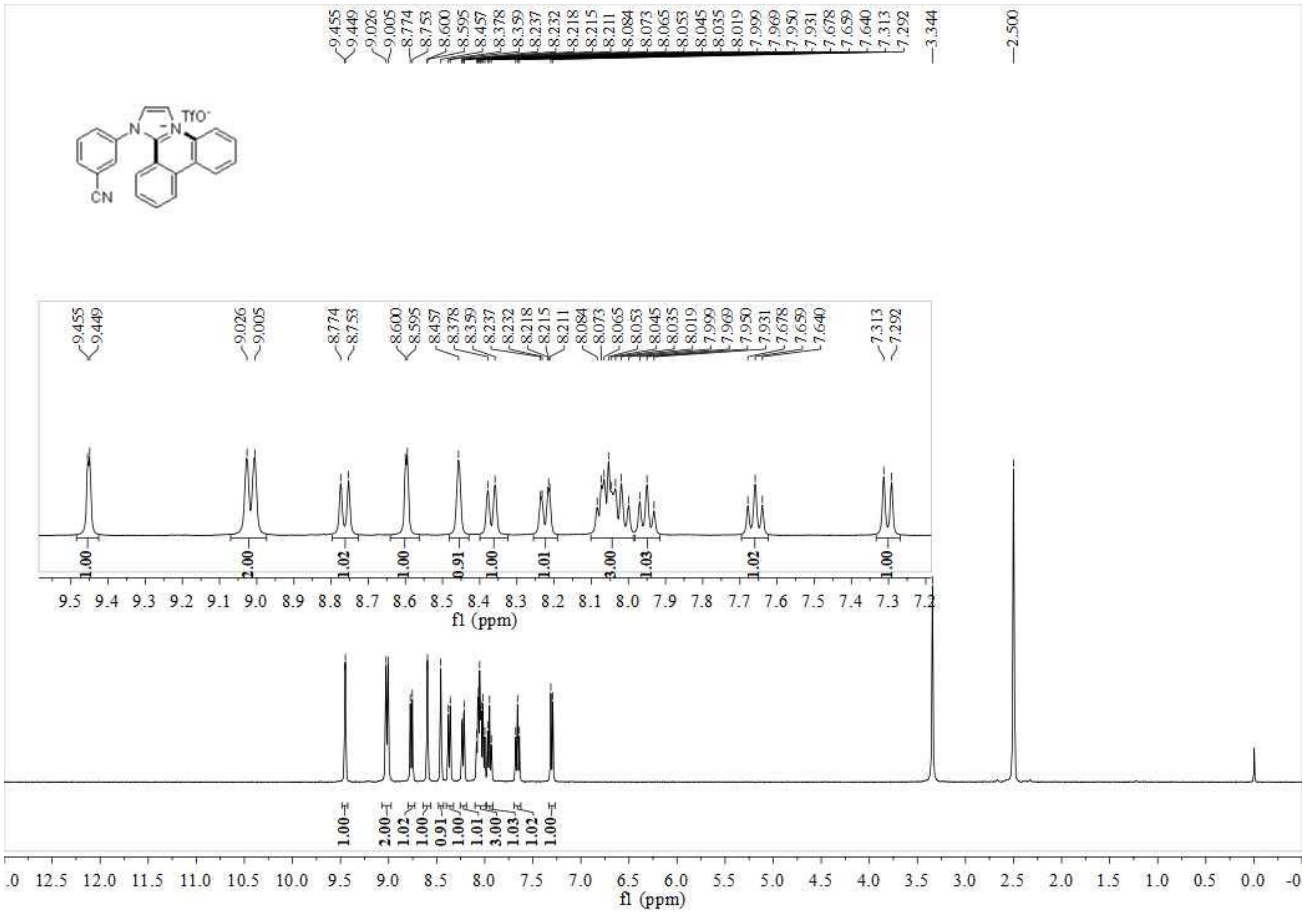
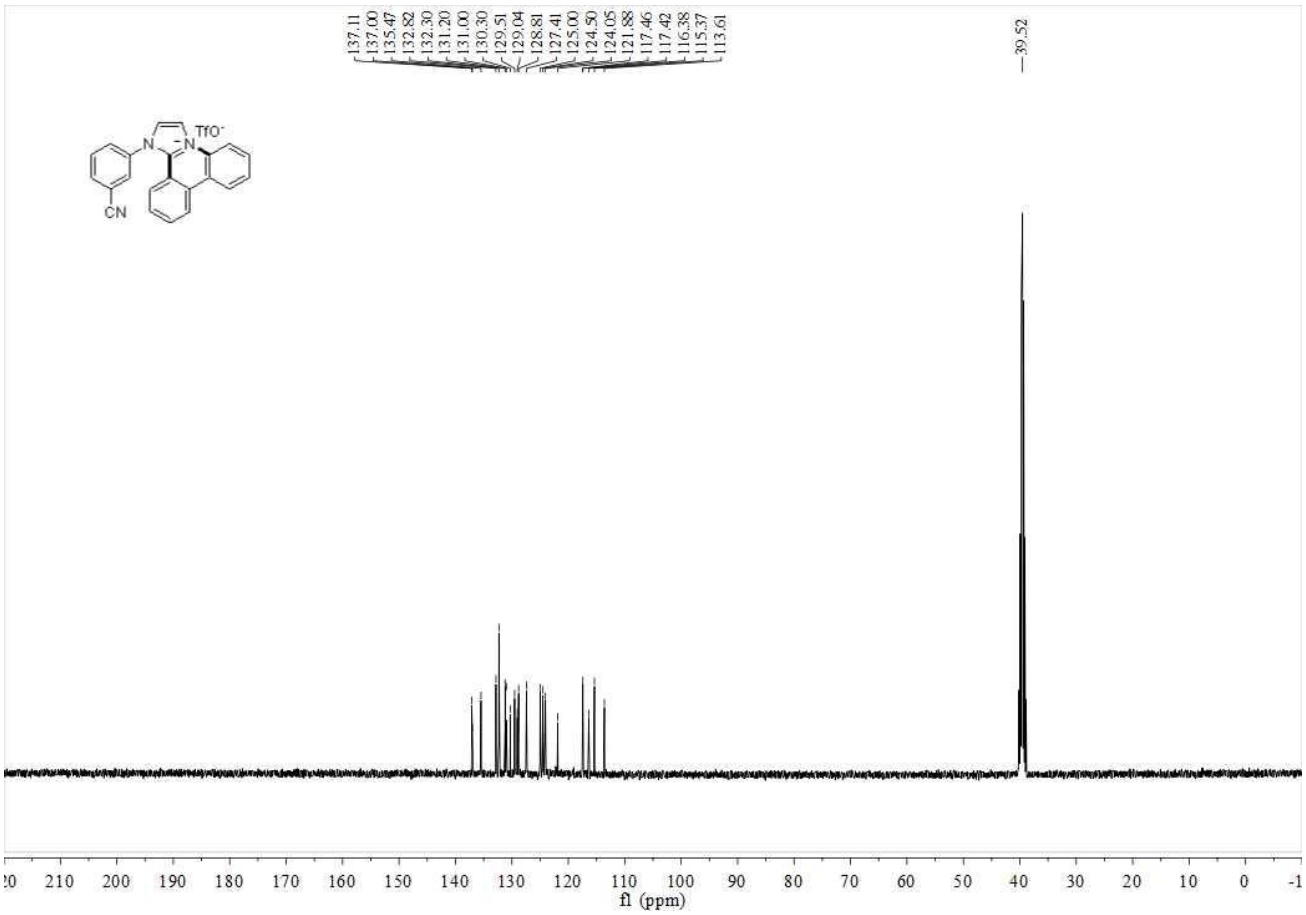
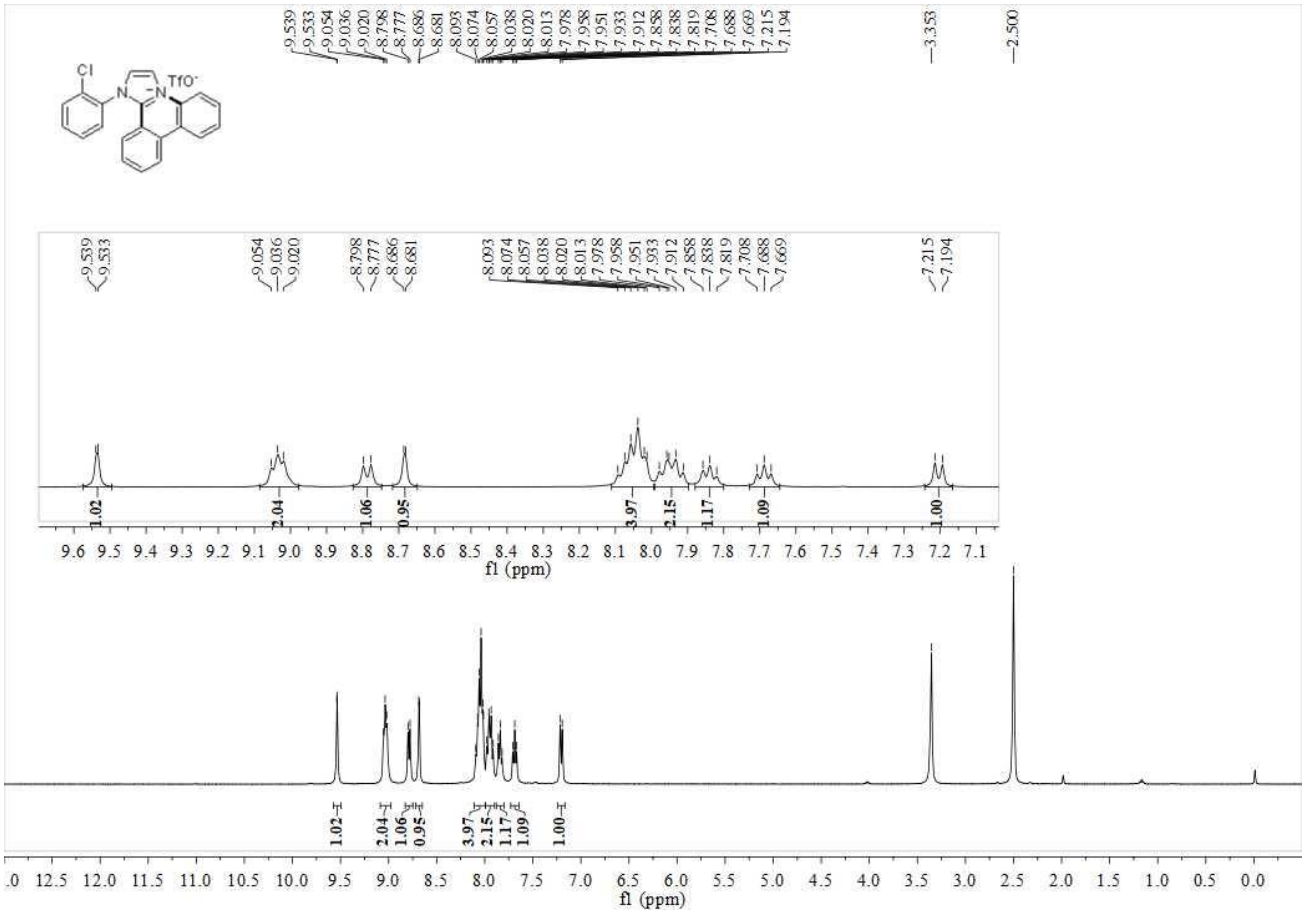
135.44
135.12
132.65
132.21
131.85
131.01
130.41
129.48
129.45
128.56
128.40
127.59
126.72
124.92
124.46
122.86
121.94
117.44
116.71
115.78
39.52
16.83
TfO-
fl (ppm)


9.455
9.449
9.026
9.005
8.774
8.753
8.600
8.595
8.457
8.378
8.359
8.237
8.232
8.218
8.215
8.211
8.084
8.073
8.065
8.053
8.045
8.035
8.019
7.999
7.969
7.950
7.931
7.678
7.659
7.640
7.313
7.292
3.344
2.500
TfO⁻
CN
1.00
2.00
1.02
1.00
0.91
1.00
1.01
3.00
1.03
1.02
1.00
fl (ppm)


137.11
137.00
135.47
132.82
132.30
131.20
131.00
130.30
129.51
129.04
128.81
127.41
125.00
124.50
124.05
121.88
117.46
117.42
116.38
115.37
113.61
39.52
TfO⁻
CN
fl (ppm)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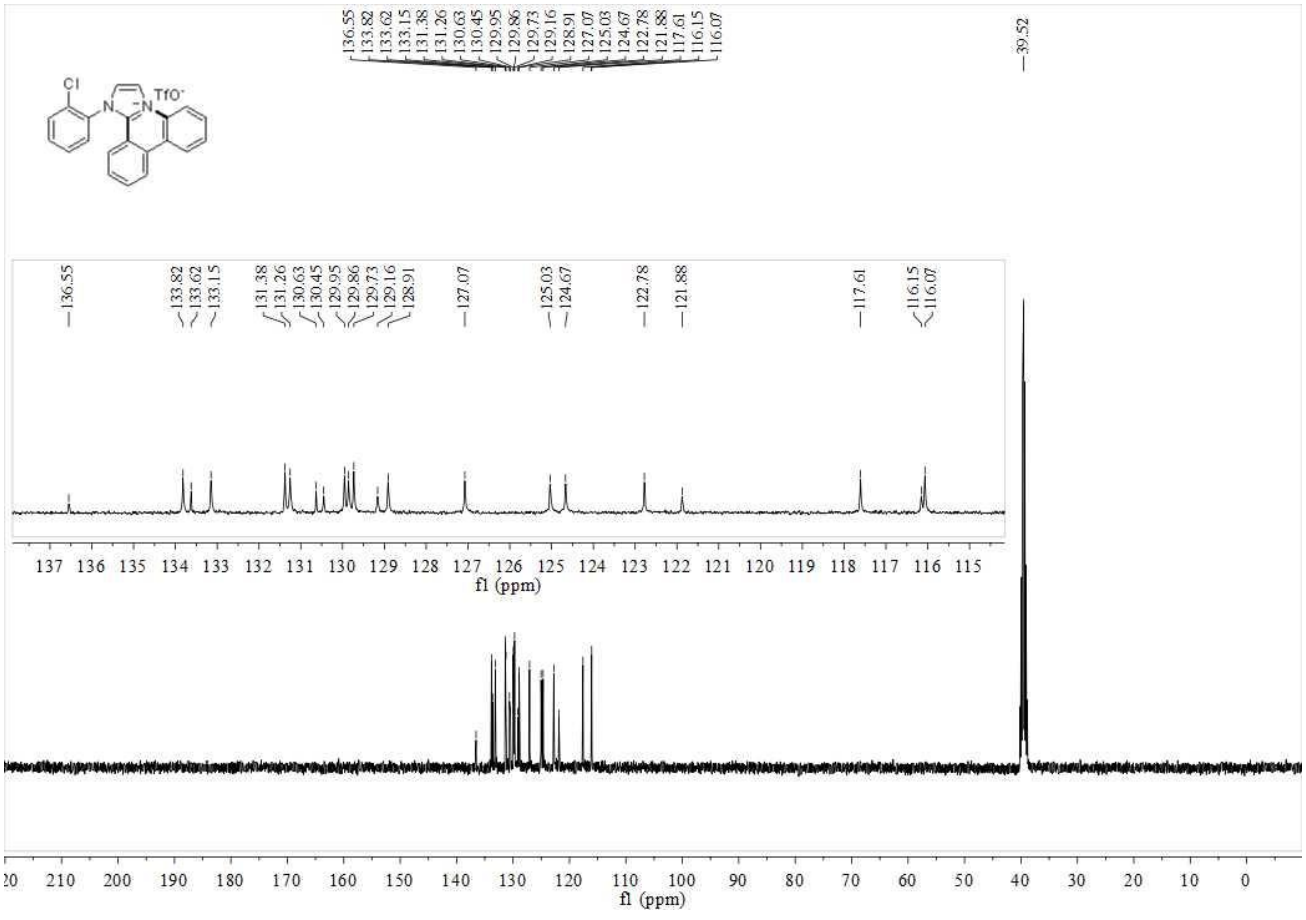
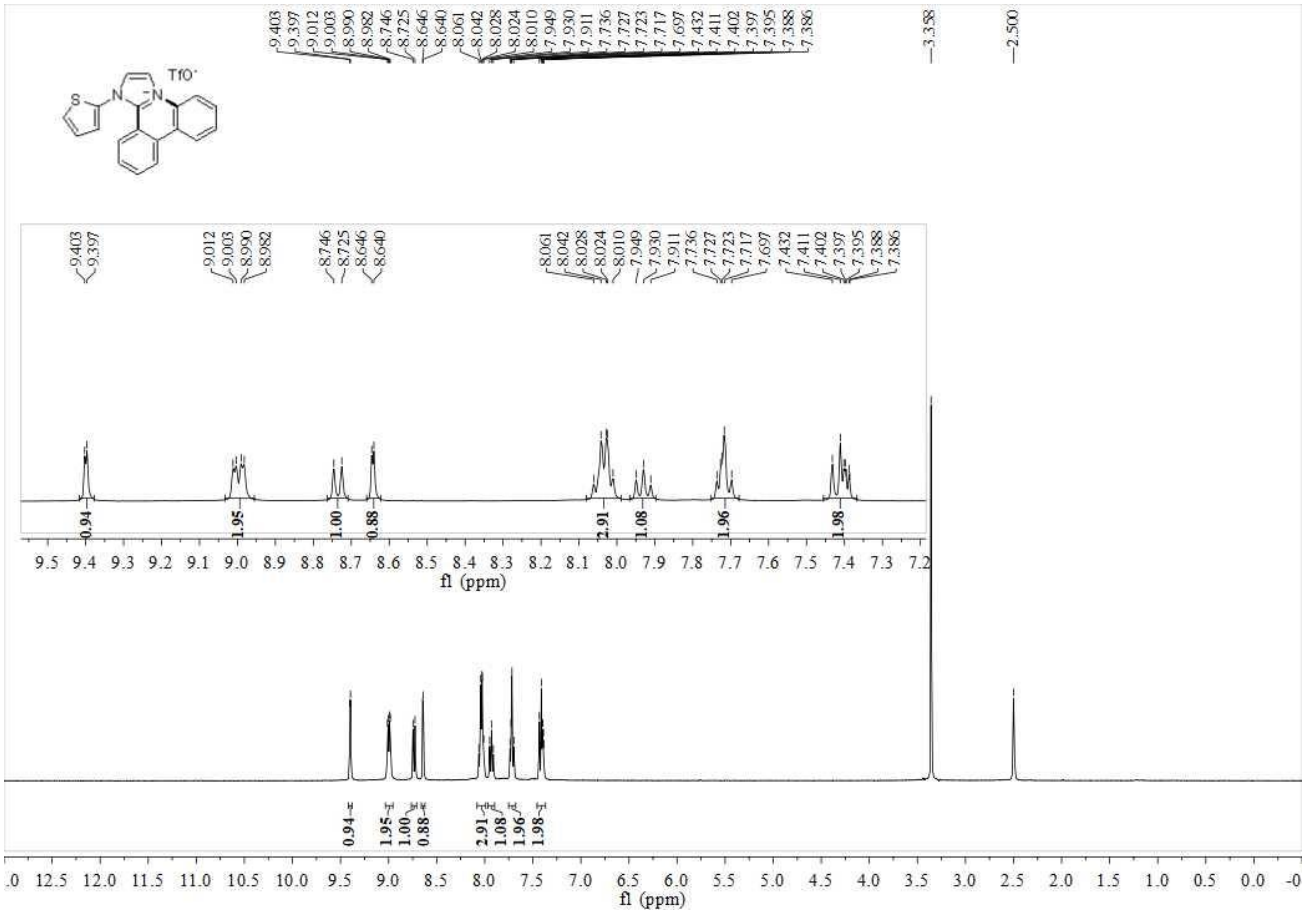
9.533
9.054
9.036
9.020
8.798
8.777
8.686
8.681
8.093
8.074
8.057
8.038
8.020
8.013
7.978
7.958
7.951
7.933
7.912
7.858
7.838
7.819
7.708
7.688
7.669
7.215
7.194
3.353
2.500
Cl
TfO⁻
1.02
2.04
1.06
0.95
3.97
2.15
1.17
1.09
1.00
f1 (ppm)


136.55
133.82
133.62
133.15
131.38
131.26
130.63
130.45
129.95
129.86
129.73
129.16
128.91
127.07
125.03
124.67
122.78
121.88
117.61
116.15
116.07
39.52
Cl
TfO⁻
f1 (ppm)


TfO⁻
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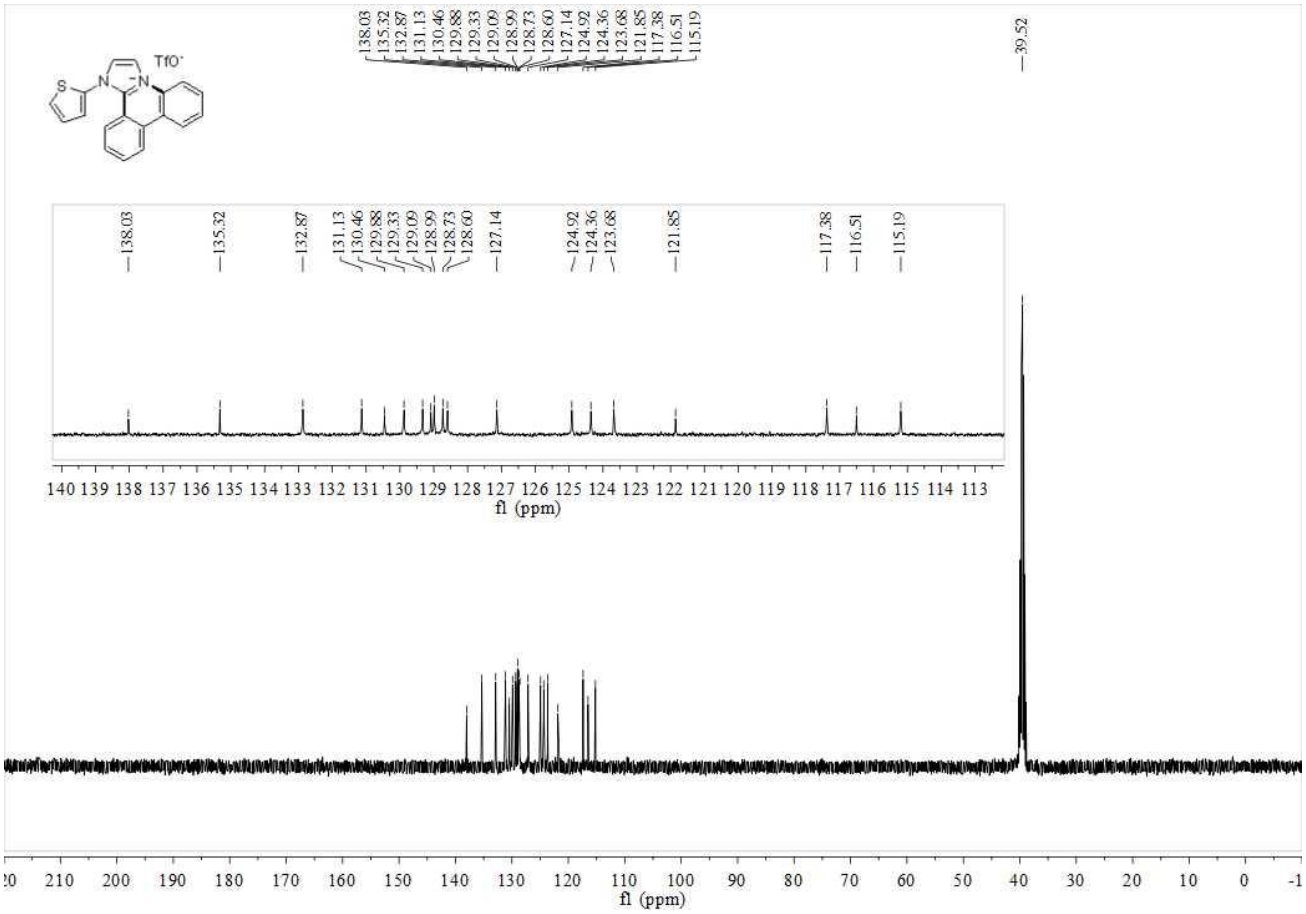
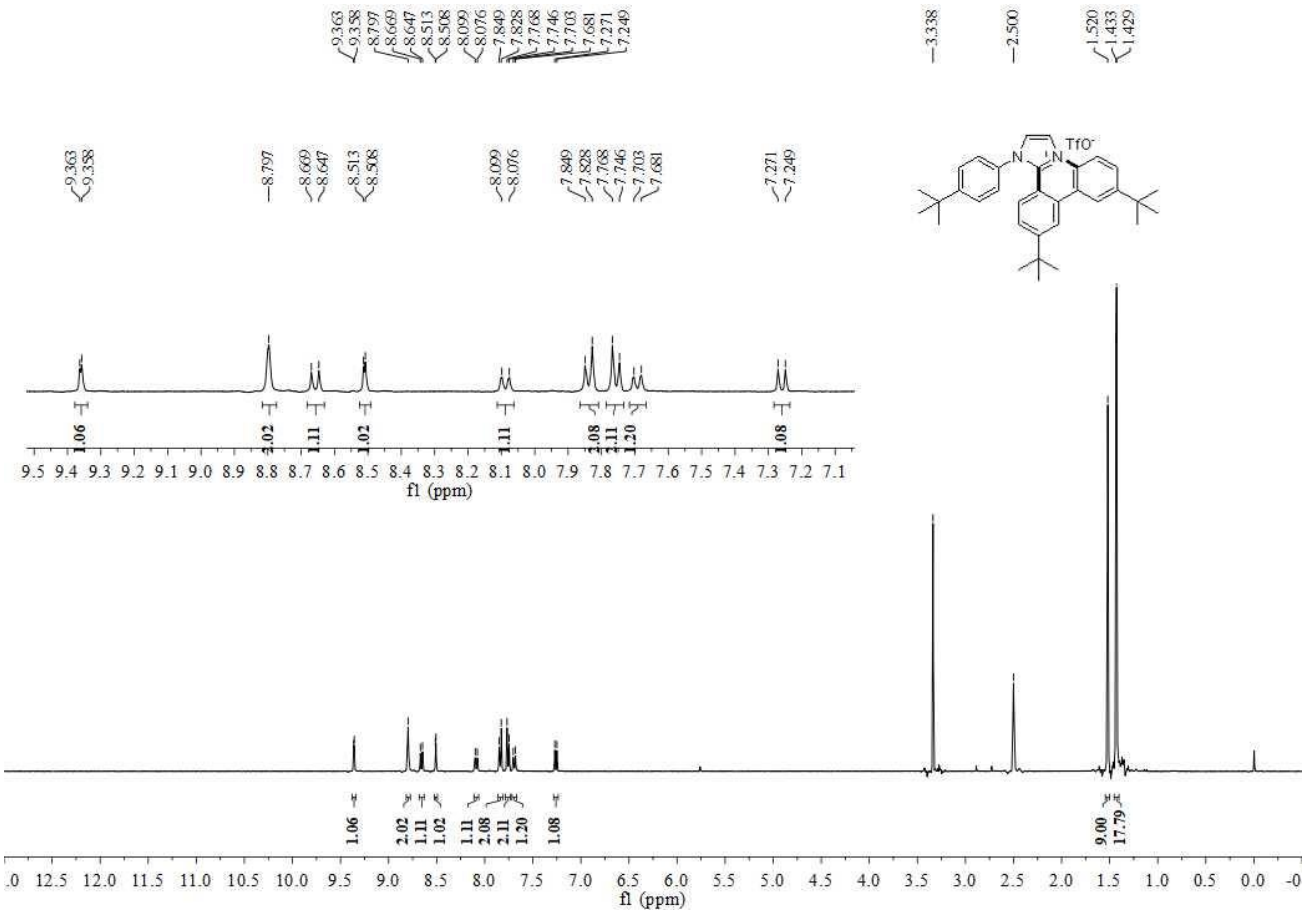
9.397
9.012
9.003
8.990
8.982
8.746
8.725
8.646
8.640
8.061
8.042
8.028
8.024
8.010
7.949
7.930
7.911
7.736
7.727
7.723
7.717
7.697
7.432
7.411
7.402
7.397
7.395
7.388
7.386
3.358
2.500
0.94
1.95
1.00
0.88
2.91
1.08
1.96
1.98
fl (ppm)


TfO⁻
138.03
135.32
132.87
131.13
130.46
129.88
129.33
129.09
128.99
128.73
128.60
127.14
124.92
124.36
123.68
121.85
117.38
116.51
115.19
39.52
fl (ppm)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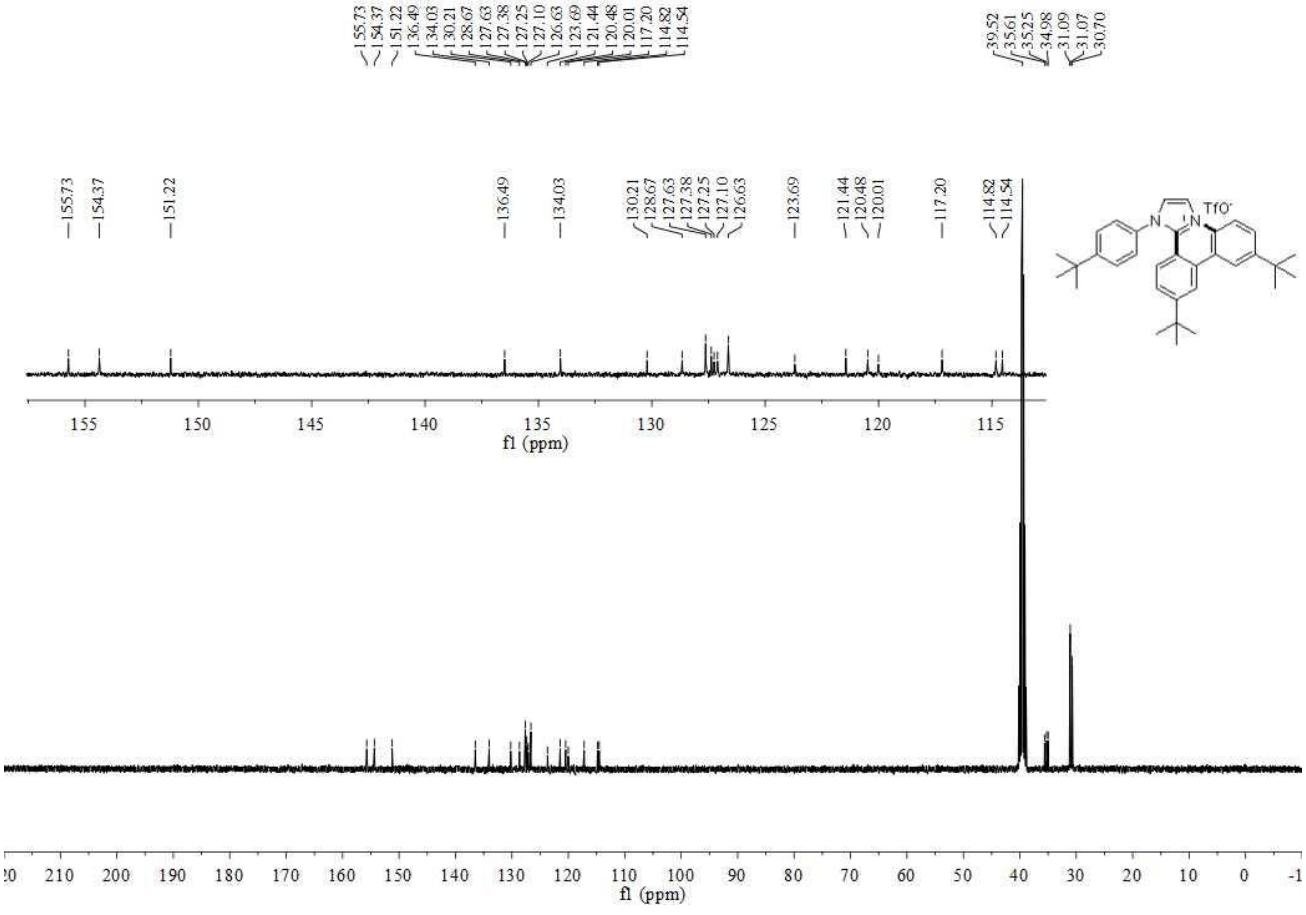
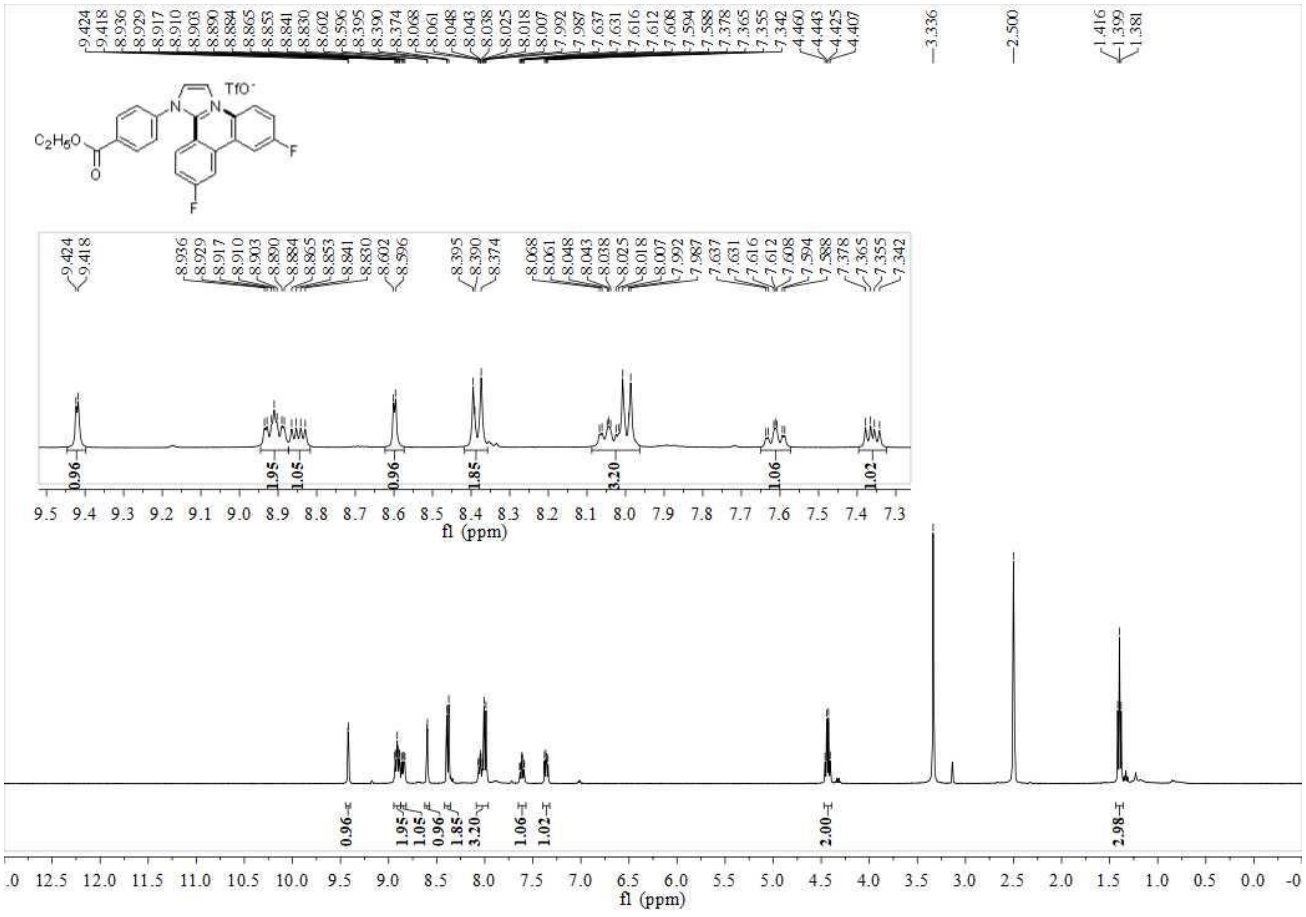
8.647
8.513
8.508
8.099
8.076
7.849
7.828
7.768
7.746
7.703
7.681
7.271
7.249
3.338
2.500
1.520
1.433
1.429
TfO-
1.06
2.02
1.11
1.02
1.11
2.08
2.11
1.20
1.08
9.00
17.79
fl (ppm)


155.73
154.37
151.22
136.49
134.03
130.21
128.67
127.63
127.38
127.25
127.10
126.63
123.69
121.44
120.48
120.01
117.20
114.82
114.54
39.52
35.61
35.25
34.98
31.09
31.07
30.70
TfO-
fl (ppm)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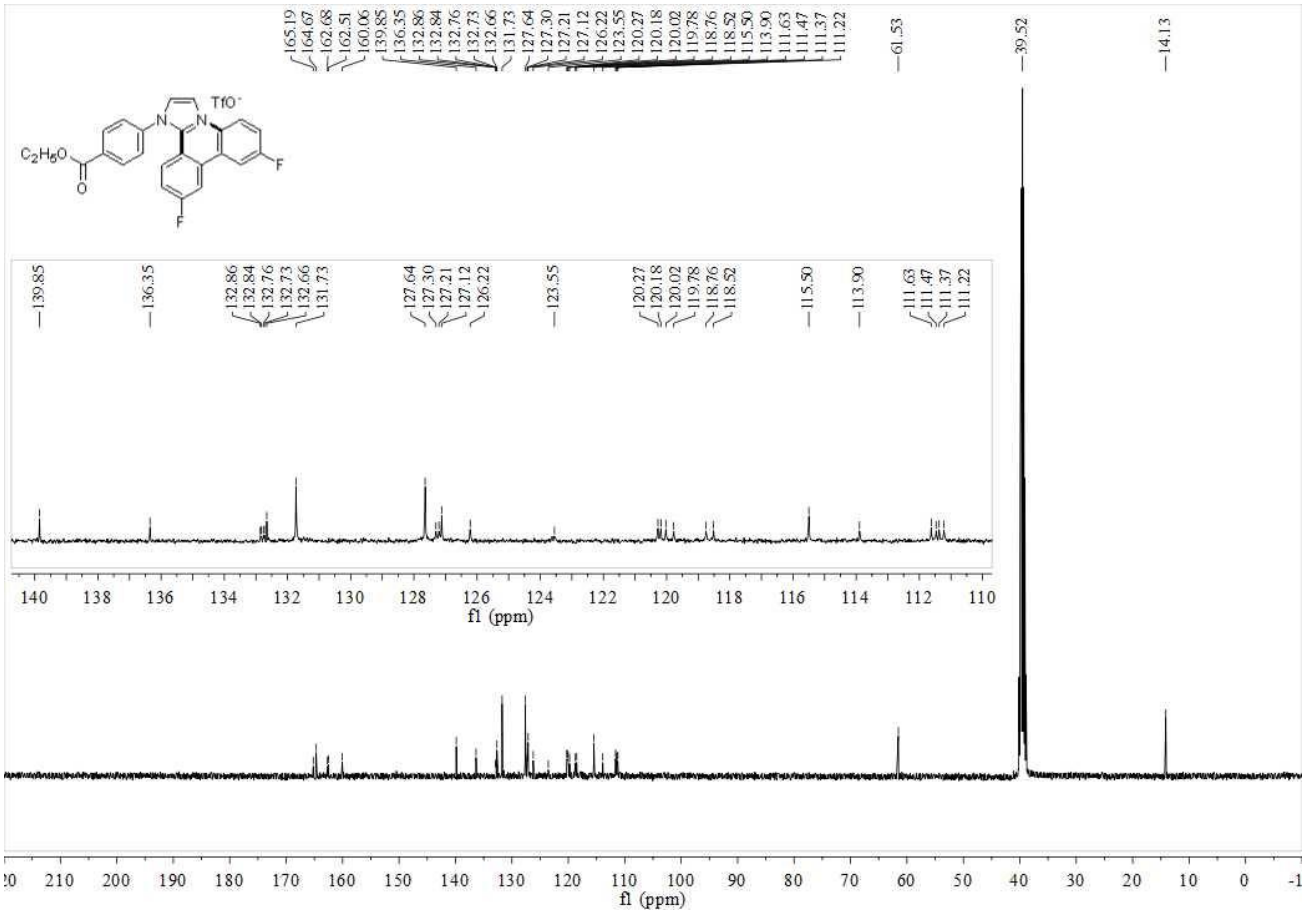
8.903
8.890
8.884
8.865
8.853
8.841
8.830
8.602
8.596
8.395
8.390
8.374
8.068
8.061
8.048
8.043
8.038
8.025
8.018
8.007
7.992
7.987
7.637
7.631
7.616
7.612
7.608
7.594
7.588
7.378
7.365
7.355
7.342
4.460
4.443
4.425
4.407
3.336
2.500
1.416
1.399
1.381
TfO⁻
C2H5O
O
F
F
0.96
1.95
1.05
0.96
1.85
3.20
1.06
1.02
2.00
2.98
fl (ppm)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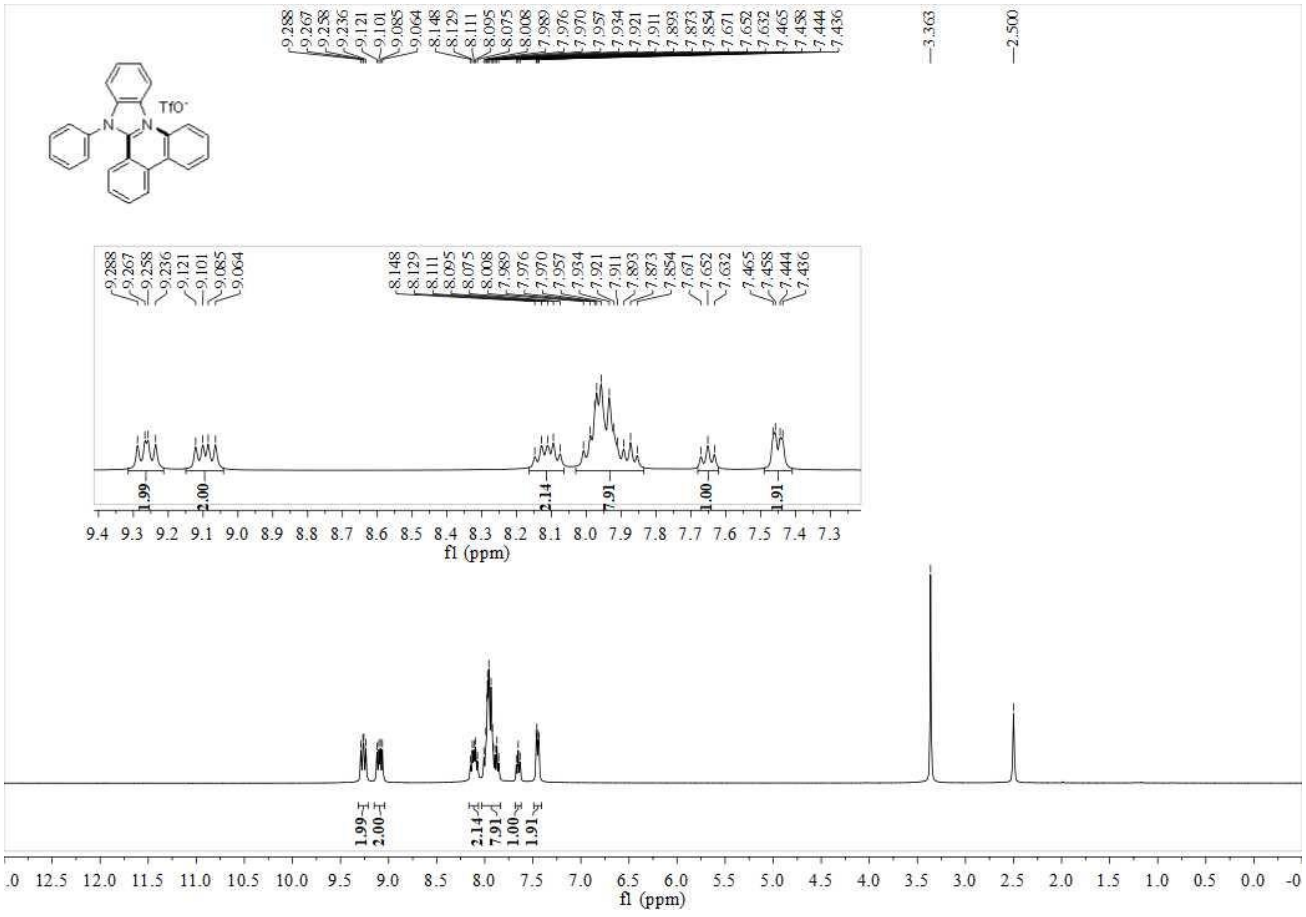
164.67
162.68
162.51
160.06
139.85
136.35
132.86
132.84
132.76
132.73
132.66
131.73
127.64
127.30
127.21
127.12
126.22
123.55
120.27
120.18
120.02
119.78
118.76
118.52
115.50
113.90
111.63
111.47
111.37
111.22
61.53
39.52
14.13
TfO⁻
C2H5O
O
F
F
fl (ppm)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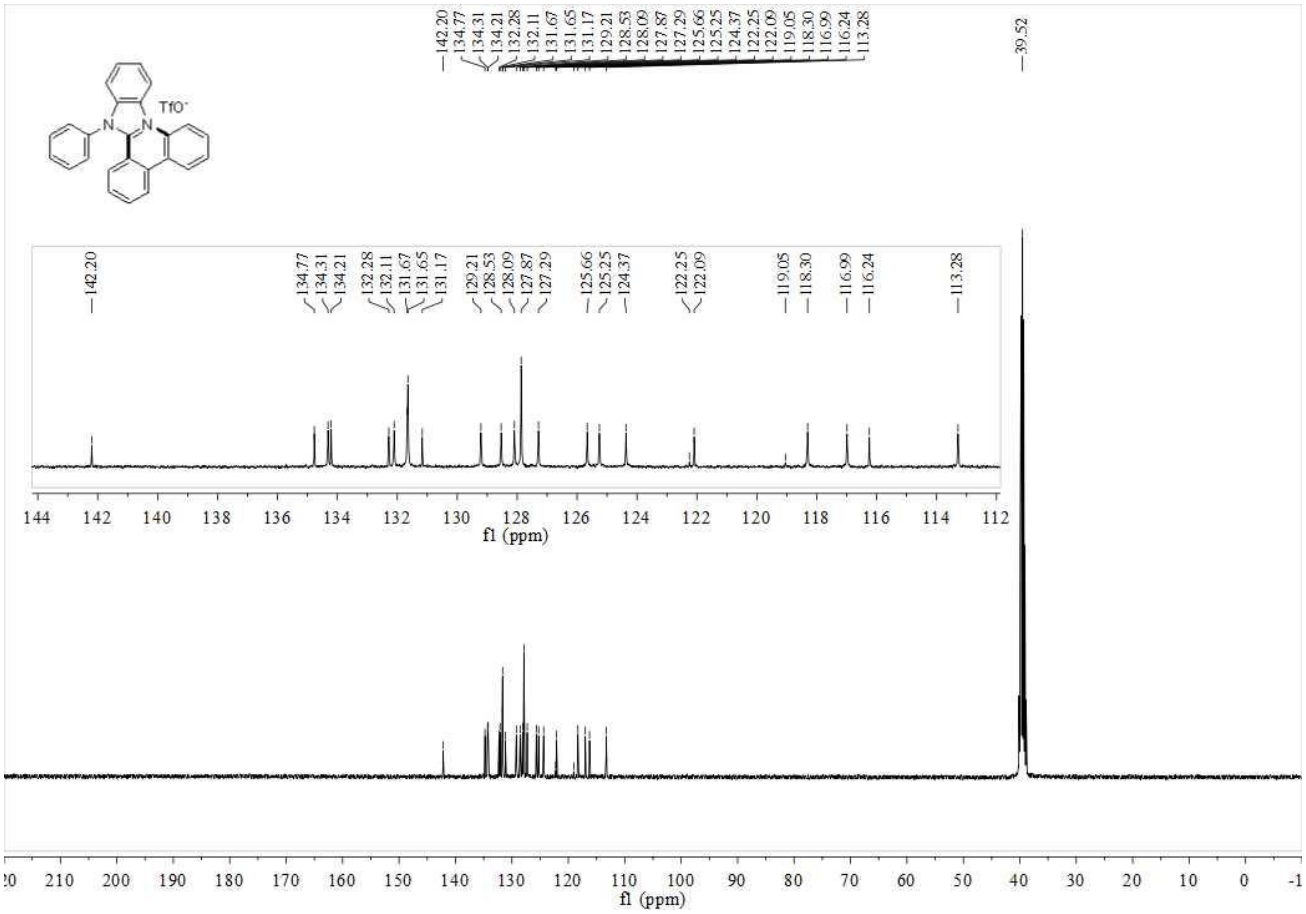
9.064
8.148
8.129
8.111
8.095
8.075
8.008
7.989
7.976
7.970
7.957
7.934
7.921
7.911
7.893
7.873
7.854
7.671
7.652
7.632
7.465
7.458
7.444
7.436
3.363
2.500
TfO⁻
1.99
2.00
2.14
7.91
1.00
1.91
fl (ppm)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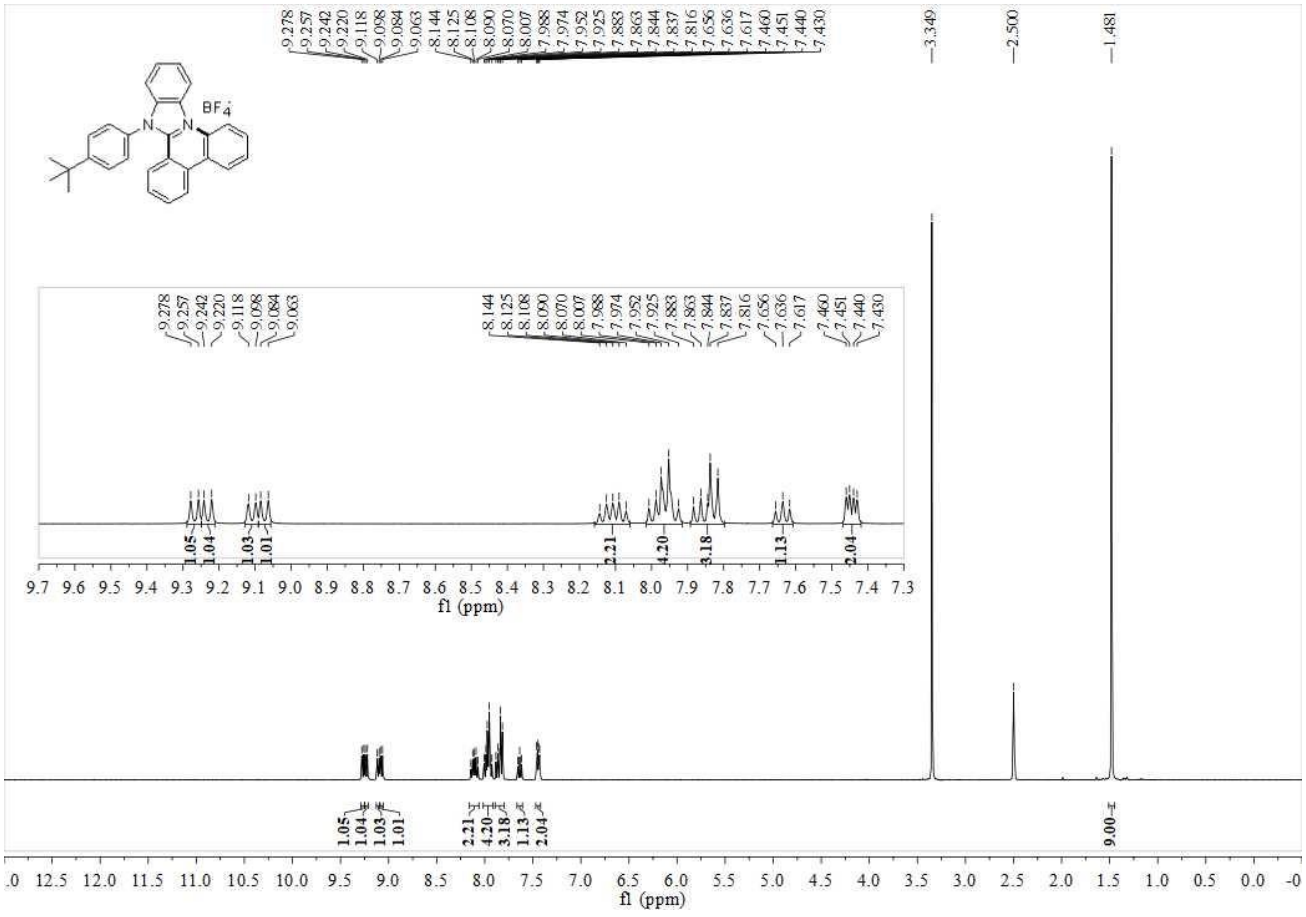
134.31
134.21
132.28
132.11
131.67
131.65
131.17
129.21
128.53
128.09
127.87
127.29
125.66
125.25
124.37
122.25
122.09
119.05
118.30
116.99
116.24
113.28
39.52
TfO⁻
fl (ppm)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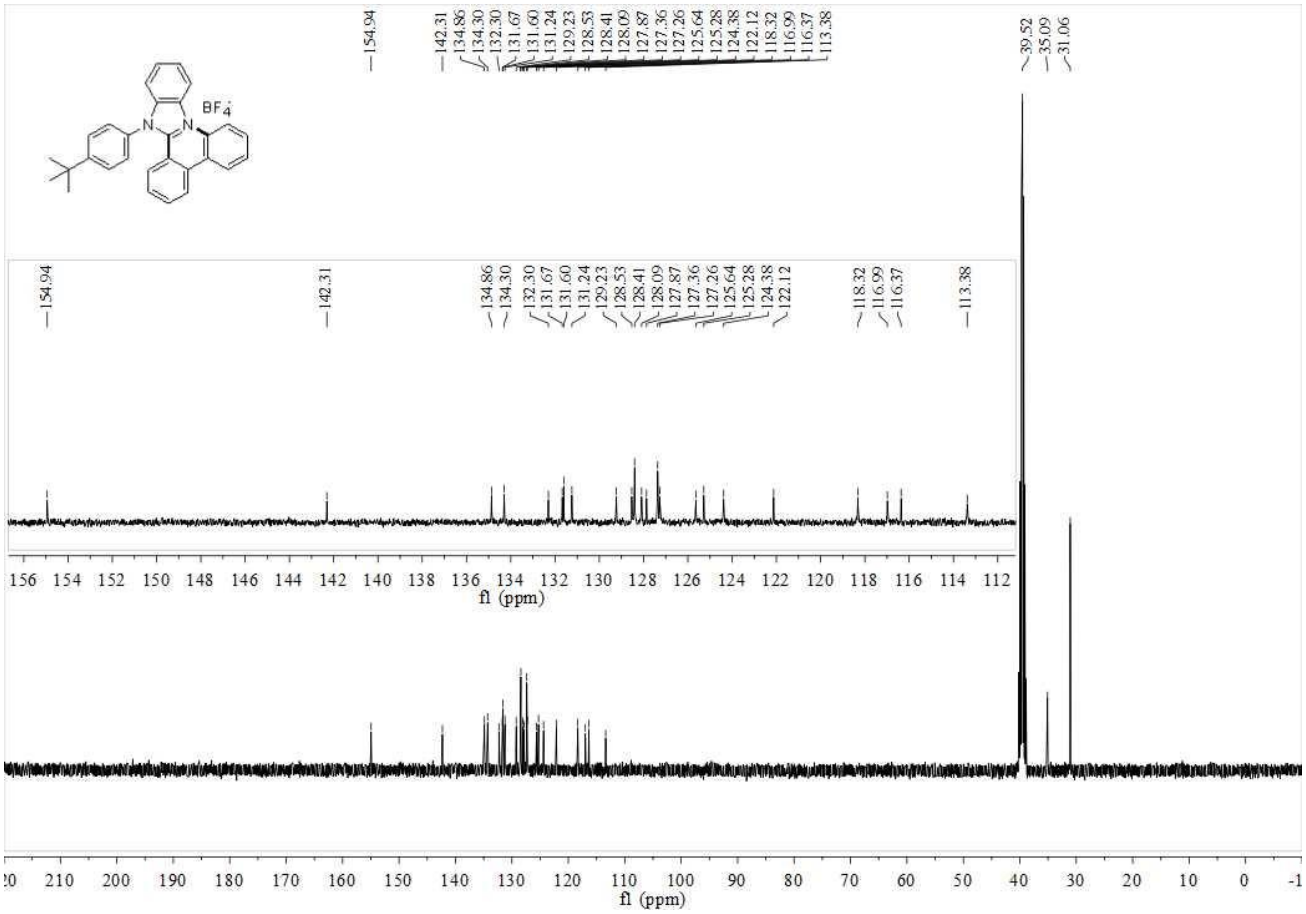
9.242
9.220
9.118
9.098
9.084
9.063
8.144
8.125
8.108
8.090
8.070
8.007
7.988
7.974
7.952
7.925
7.883
7.863
7.844
7.837
7.816
7.656
7.636
7.617
7.460
7.451
7.440
7.430
3.349
2.500
1.481
BF4-
1.05
1.04
1.03
1.01
2.21
4.20
3.18
1.13
2.04
9.00
fl (ppm)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142.31
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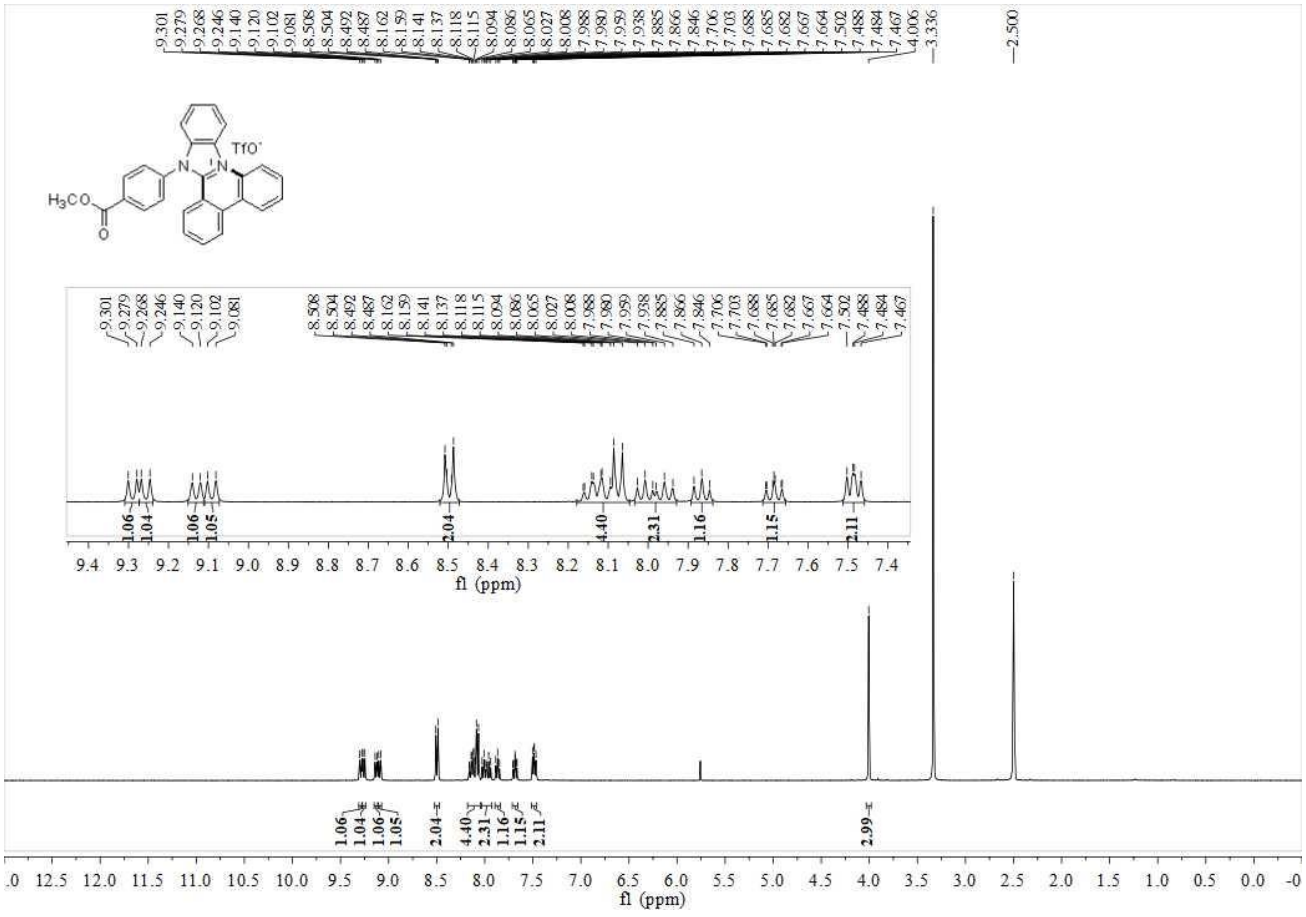
132.30
131.67
131.60
131.24
129.23
128.53
128.41
128.09
127.87
127.36
127.26
125.64
125.28
124.38
122.12
118.32
116.99
116.37
113.38
39.52
35.09
31.06
BF4-
fl (ppm)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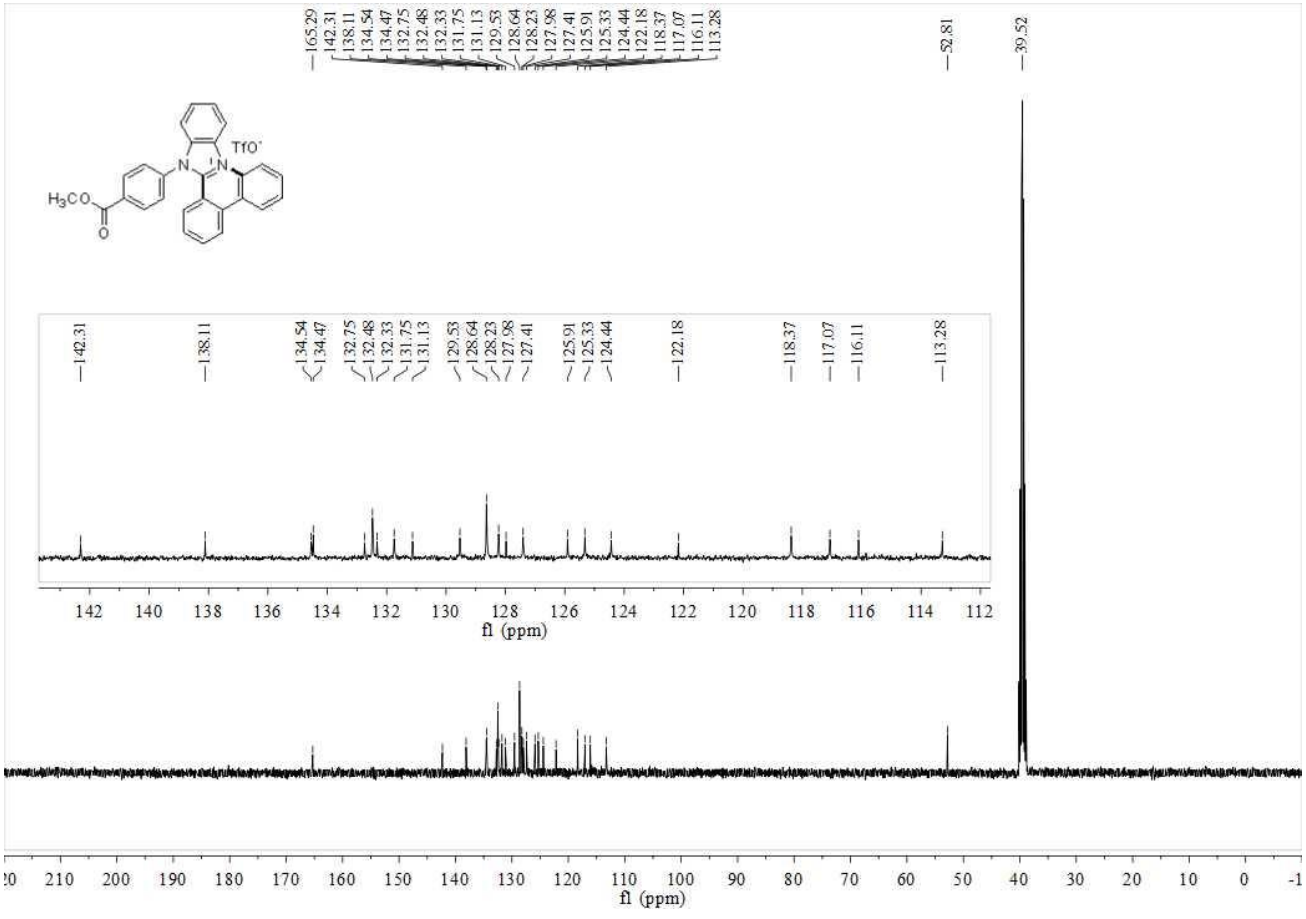
9.120
9.102
9.081
8.508
8.504
8.492
8.487
8.162
8.159
8.141
8.137
8.118
8.115
8.094
8.086
8.065
8.027
8.008
7.988
7.980
7.959
7.938
7.885
7.866
7.846
7.706
7.703
7.688
7.685
7.682
7.667
7.664
7.502
7.488
7.484
7.467
4.006
3.336
2.500
TfO⁻
H3CO
1.06
1.04
1.06
1.05
2.04
4.40
2.31
1.16
1.15
2.11
2.99
fl (ppm)


165.29
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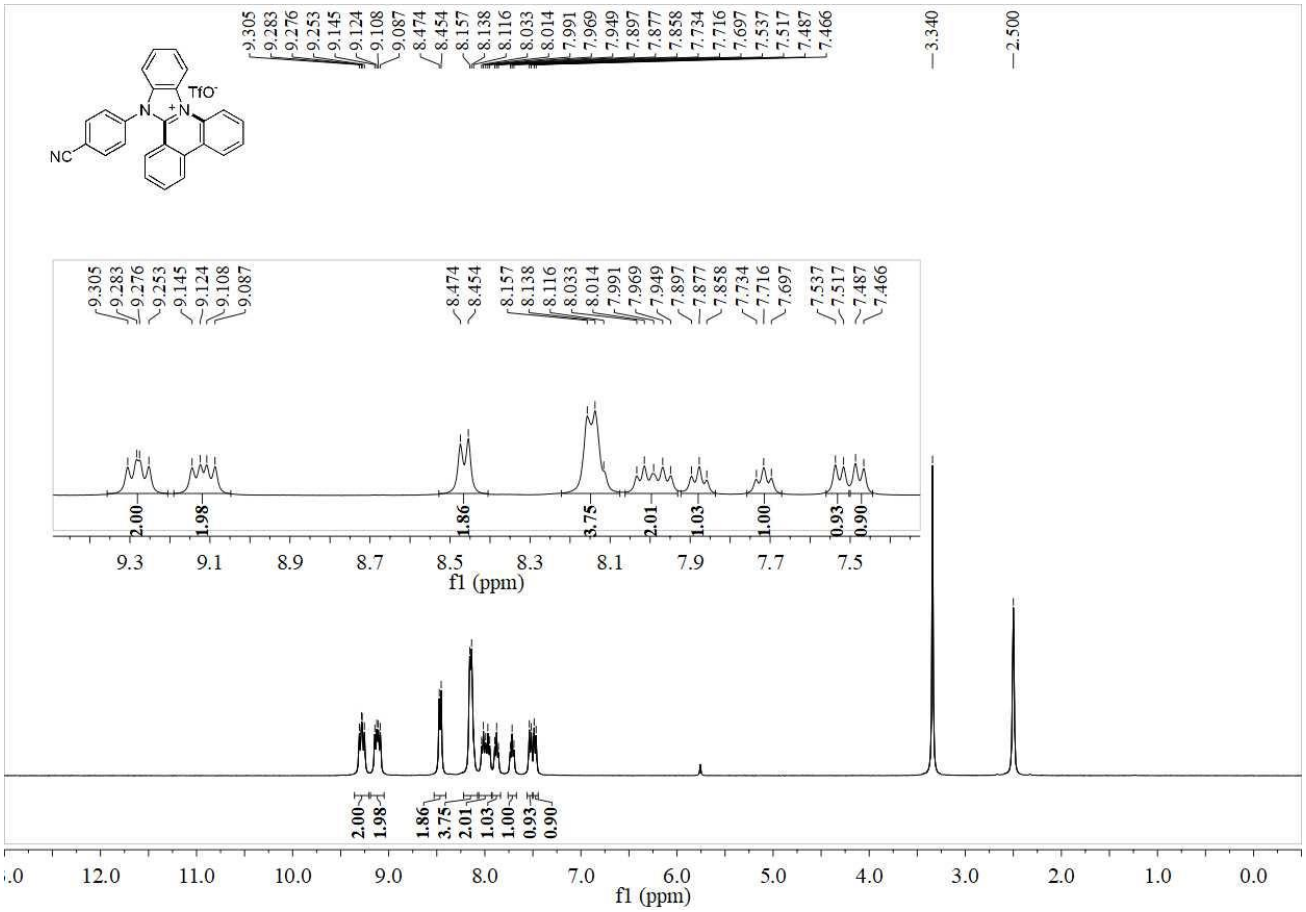
138.11
134.54
134.47
132.75
132.48
132.33
131.75
131.13
129.53
128.64
128.23
127.98
127.41
125.91
125.33
124.44
122.18
118.37
117.07
116.11
113.28
52.81
39.52
TfO⁻
H3CO
fl (ppm)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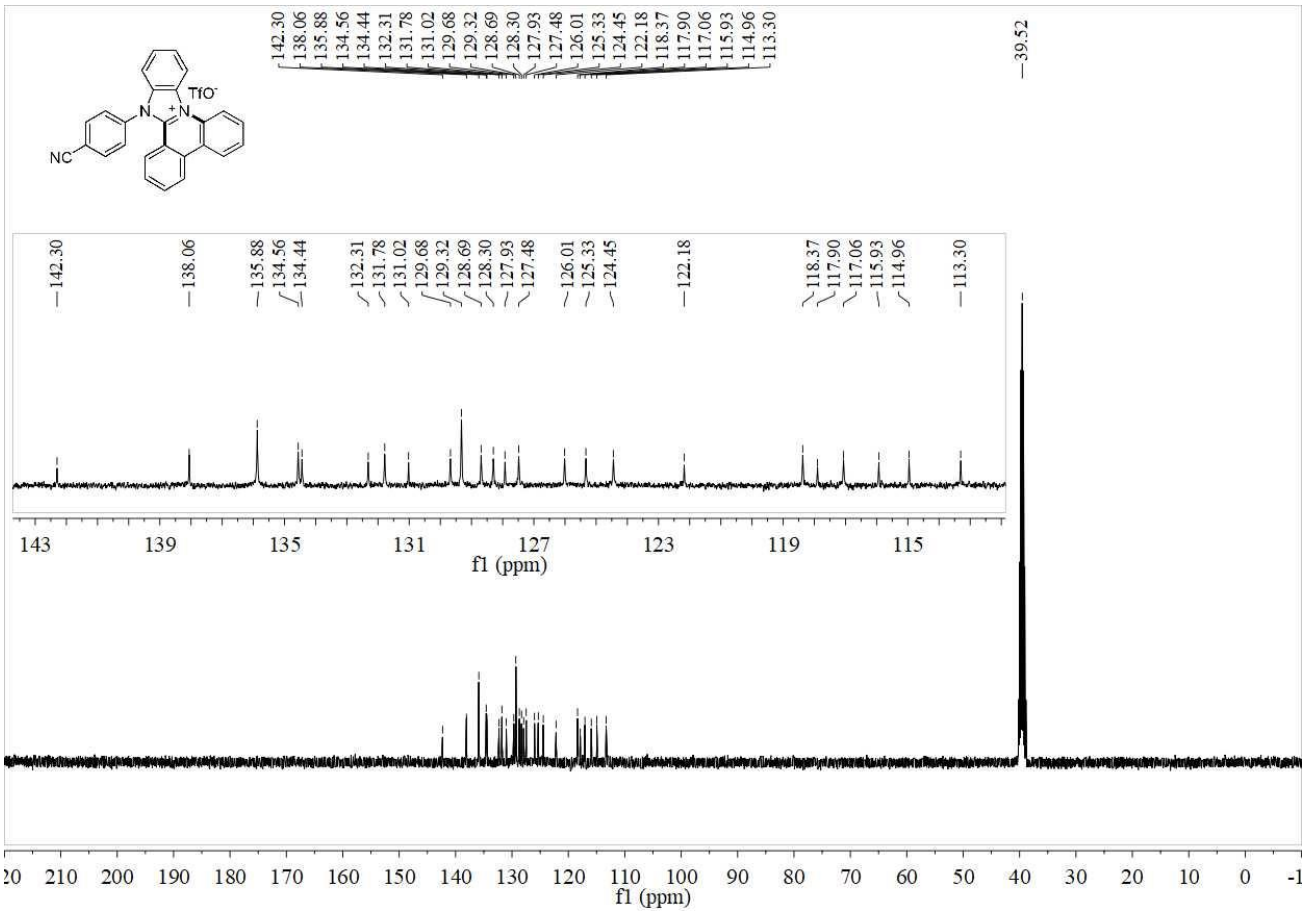
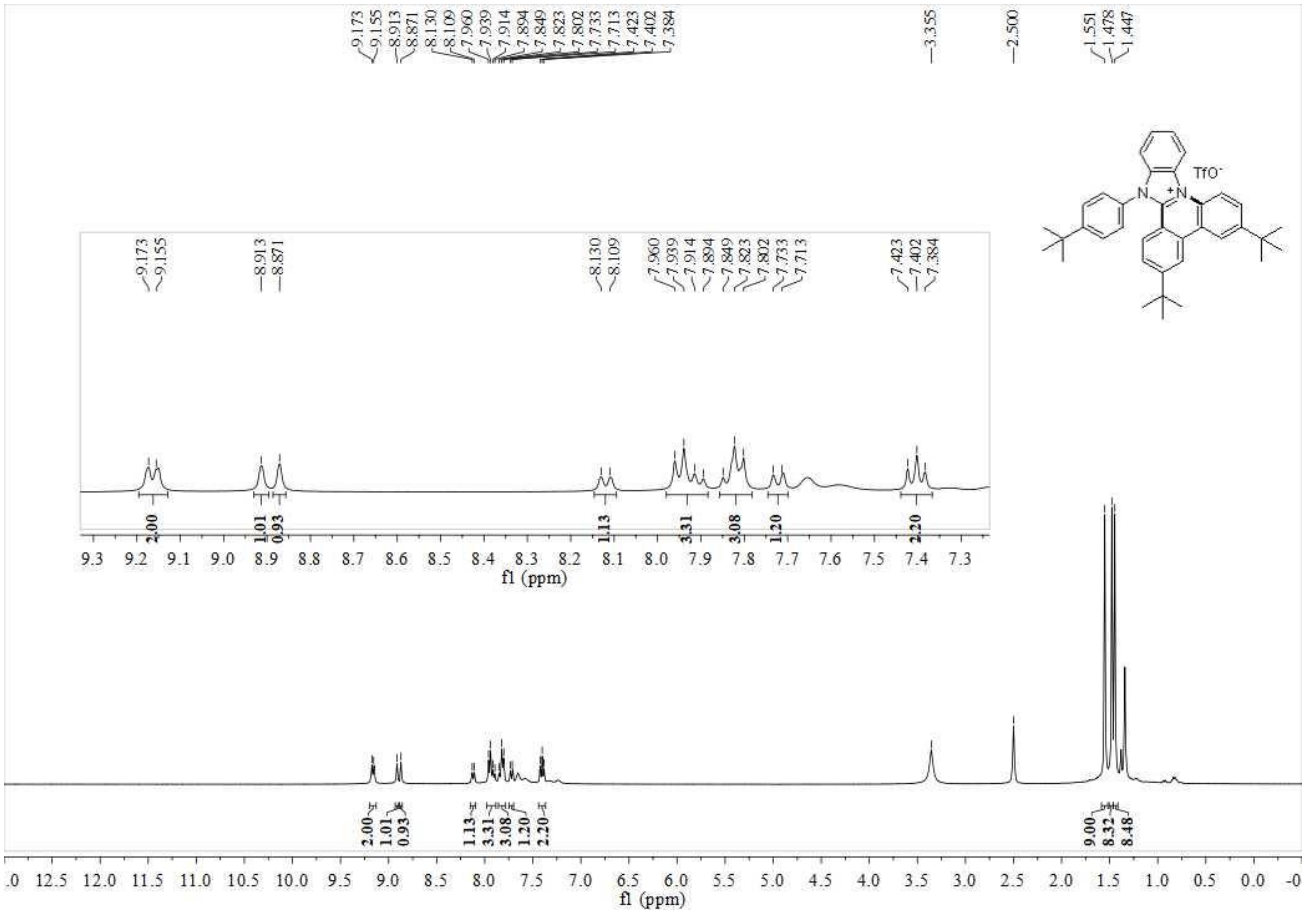
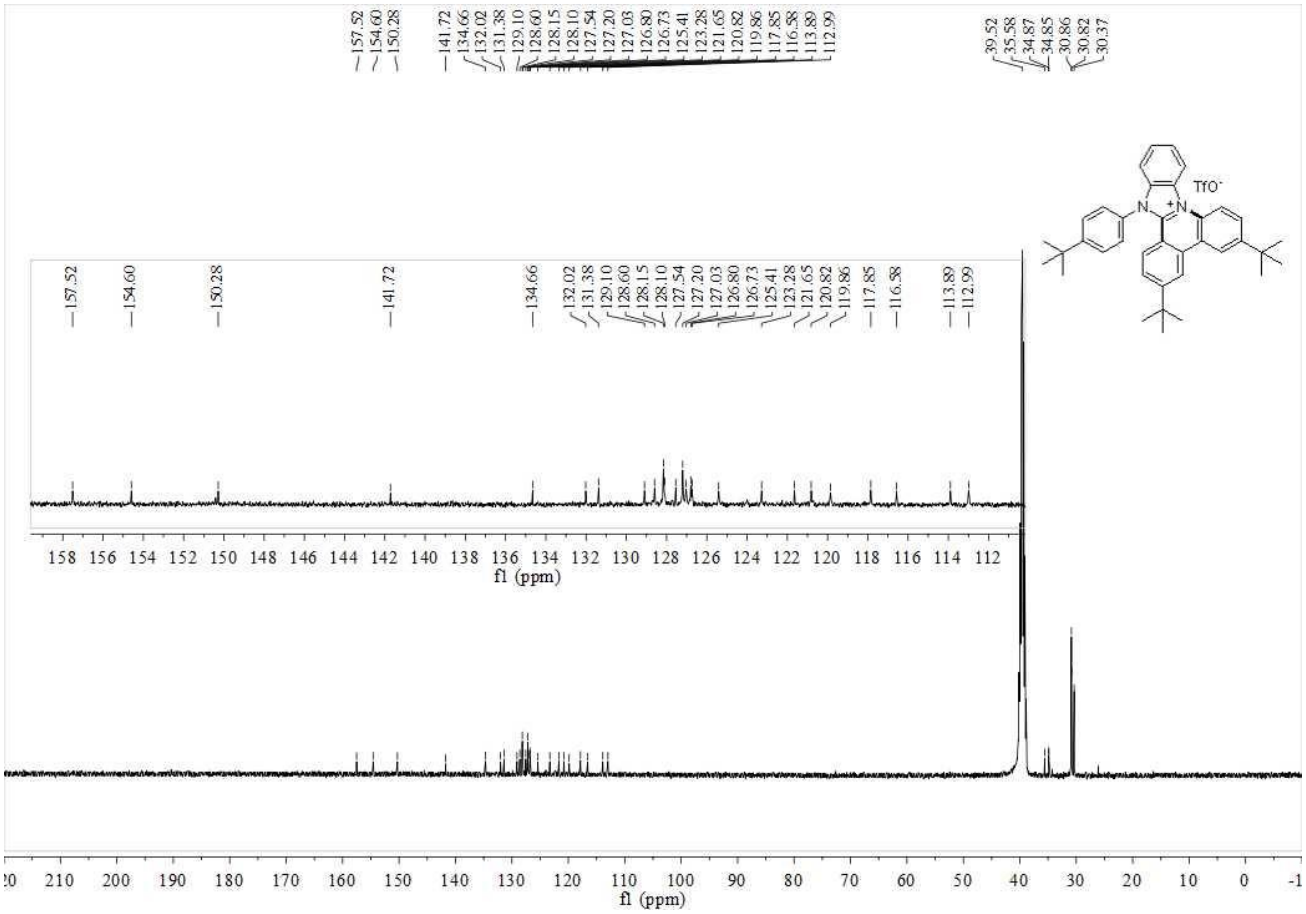
9.124
9.108
9.087
8.474
8.454
8.157
8.138
8.116
8.033
8.014
7.991
7.969
7.949
7.897
7.877
7.858
7.734
7.716
7.697
7.537
7.517
7.487
7.466
3.340
2.500
TfO⁻
NC
2.00
1.98
1.86
3.75
2.01
1.03
1.00
0.93
0.90
f1 (ppm)


142.30
138.06
135.88
134.56
134.44
132.31
131.78
131.02
129.68
129.32
128.69
128.30
127.93
127.48
126.01
125.33
124.45
122.18
118.37
117.90
117.06
115.93
114.96
113.30
39.52
TfO⁻
NC
f1 (ppm)


9.173
9.155
8.913
8.871
8.130
8.109
7.960
7.939
7.914
7.894
7.849
7.823
7.802
7.733
7.713
7.423
7.402
7.384
3.355
2.500
1.551
1.478
1.447
TfO⁻
2.00
1.01
0.93
1.13
3.31
3.08
1.20
2.20
9.00
8.32
8.48
fl (ppm)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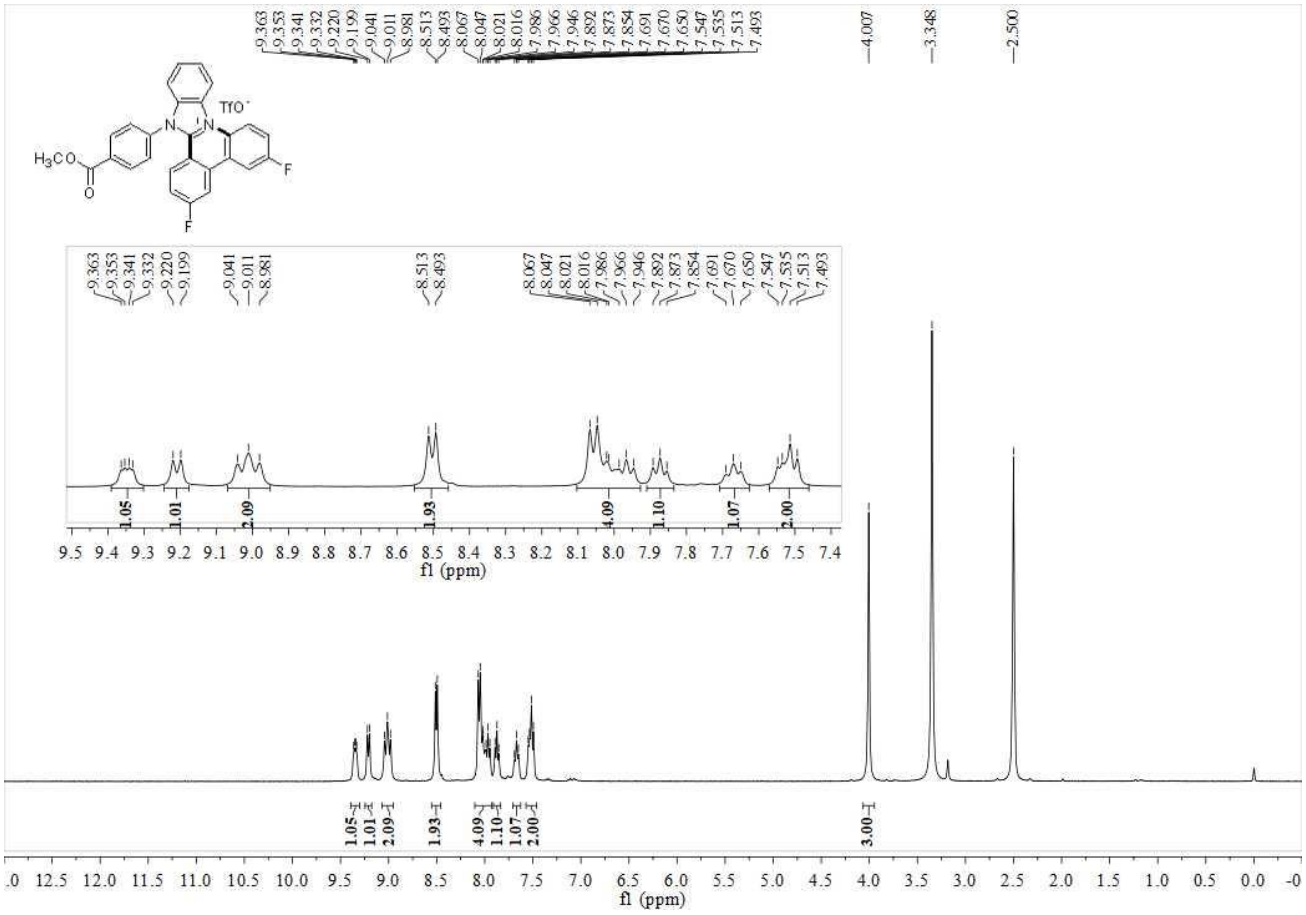
154.60
150.28
141.72
134.66
132.02
131.38
129.10
128.60
128.15
128.10
127.54
127.20
127.03
126.80
126.73
125.41
123.28
121.65
120.82
119.86
117.85
116.38
113.89
112.99
39.52
35.58
34.87
34.85
30.86
30.82
30.37
TfO⁻
fl (ppm)


TfO⁻
H3CO
O
F
F
9.363
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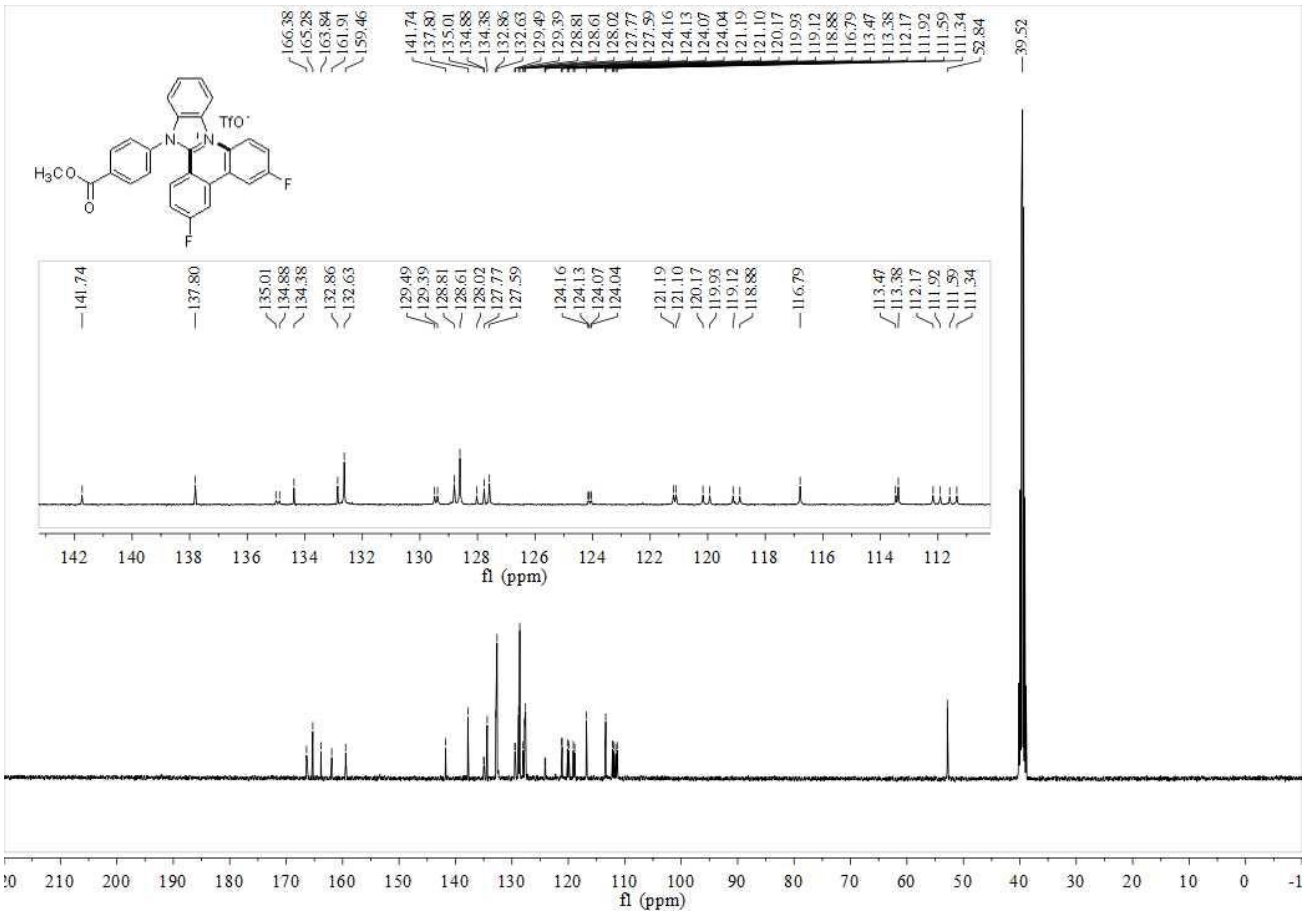
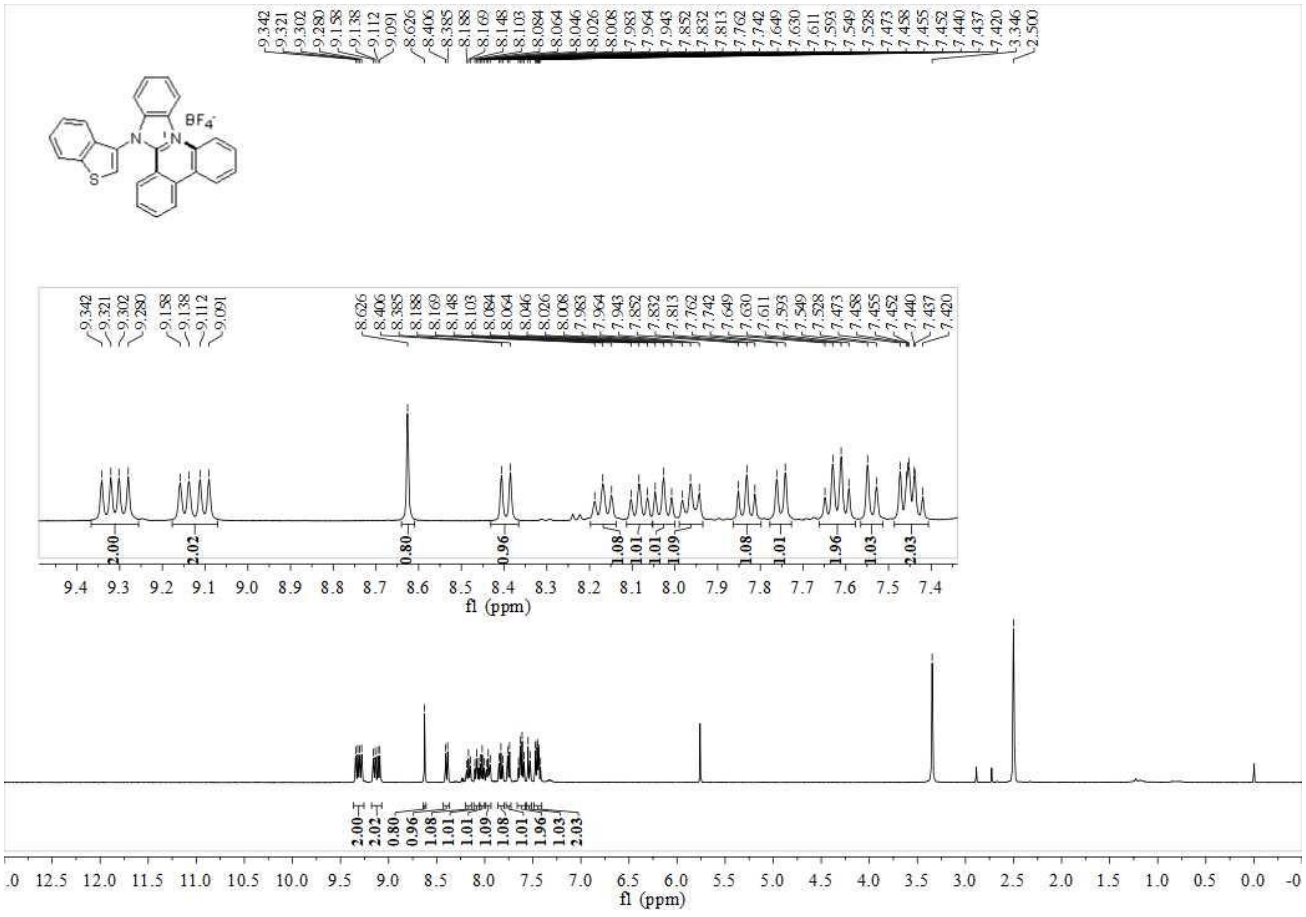
9.341
9.332
9.220
9.199
9.041
9.011
8.981
8.513
8.493
8.067
8.047
8.021
8.016
7.986
7.966
7.946
7.892
7.873
7.854
7.691
7.670
7.650
7.547
7.535
7.513
7.493
4.007
3.348
2.500
1.05
1.01
2.09
1.93
4.09
1.10
1.07
2.00
3.00
fl (ppm)


TfO⁻
H3CO
O
F
F
166.38
165.28
163.84
161.91
159.46
141.74
137.80
135.01
134.88
134.38
132.86
132.63
129.49
129.39
128.81
128.61
128.02
127.77
127.59
124.16
124.13
124.07
124.04
121.19
121.10
120.17
119.93
119.12
118.88
116.79
113.47
113.38
112.17
111.92
111.59
111.34
52.84
39.52
fl (ppm)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9.112
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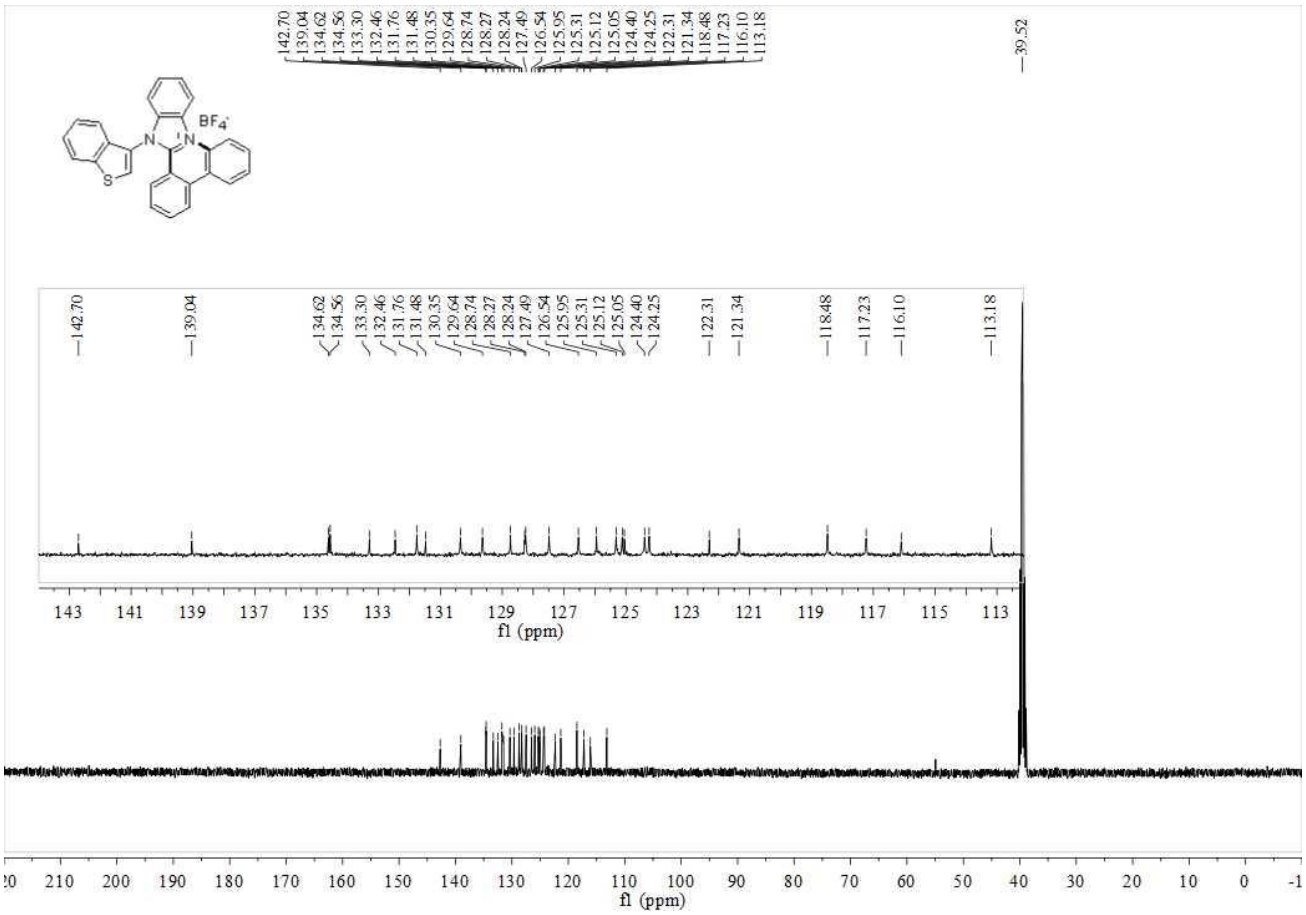
8.385
8.188
8.169
8.148
8.103
8.084
8.064
8.046
8.026
8.008
7.983
7.964
7.943
7.852
7.832
7.813
7.762
7.742
7.649
7.630
7.611
7.593
7.549
7.528
7.473
7.458
7.455
7.452
7.440
7.437
7.420
3.346
2.500
BF4-
2.00
2.02
0.80
0.96
1.08
1.01
1.01
1.09
1.08
1.01
1.96
1.03
2.03
fl (ppm)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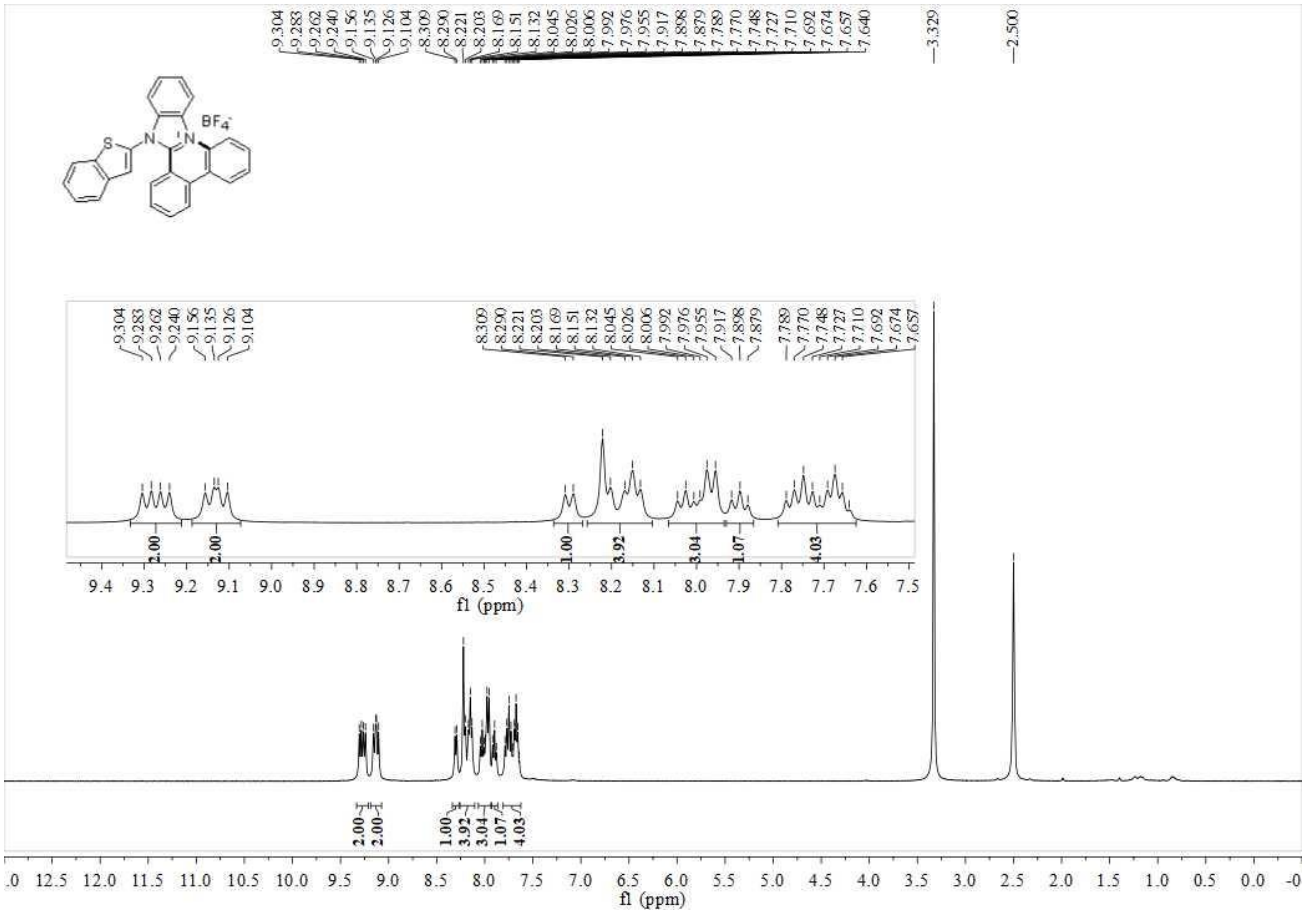
134.62
134.56
133.30
132.46
131.76
131.48
130.35
129.64
128.74
128.27
128.24
127.49
126.54
125.95
125.31
125.12
125.05
124.40
124.25
122.31
121.34
118.48
117.23
116.10
113.18
39.52
BF4-
fl (ppm)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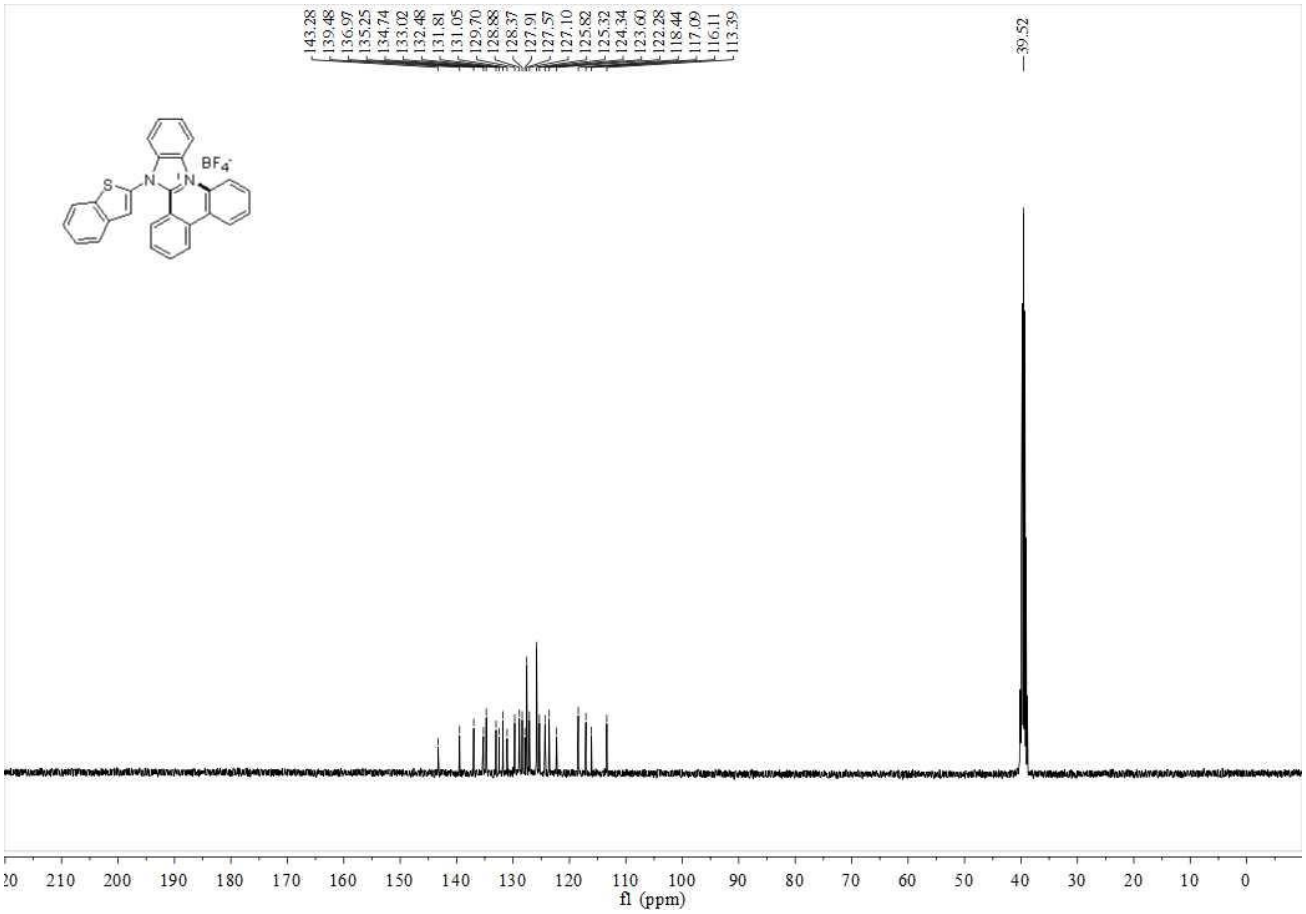
9.283
9.262
9.240
9.156
9.135
9.126
9.104
8.309
8.290
8.221
8.203
8.169
8.151
8.132
8.045
8.026
8.006
7.992
7.976
7.955
7.917
7.898
7.879
7.789
7.770
7.748
7.727
7.710
7.692
7.674
7.657
7.640
3.329
2.500
BF4-
2.00
2.00
1.00
3.92
3.04
1.07
4.03
fl (ppm)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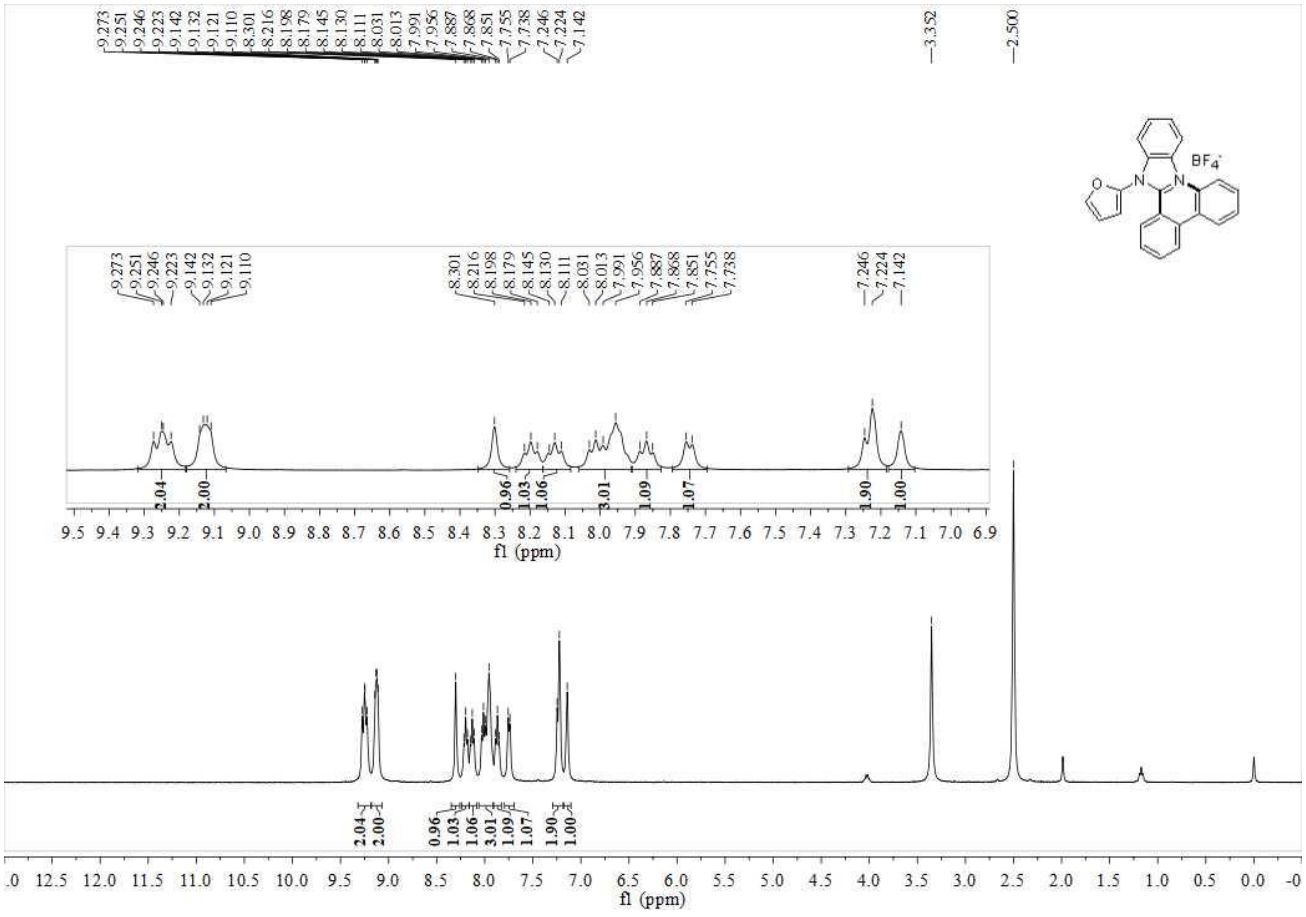
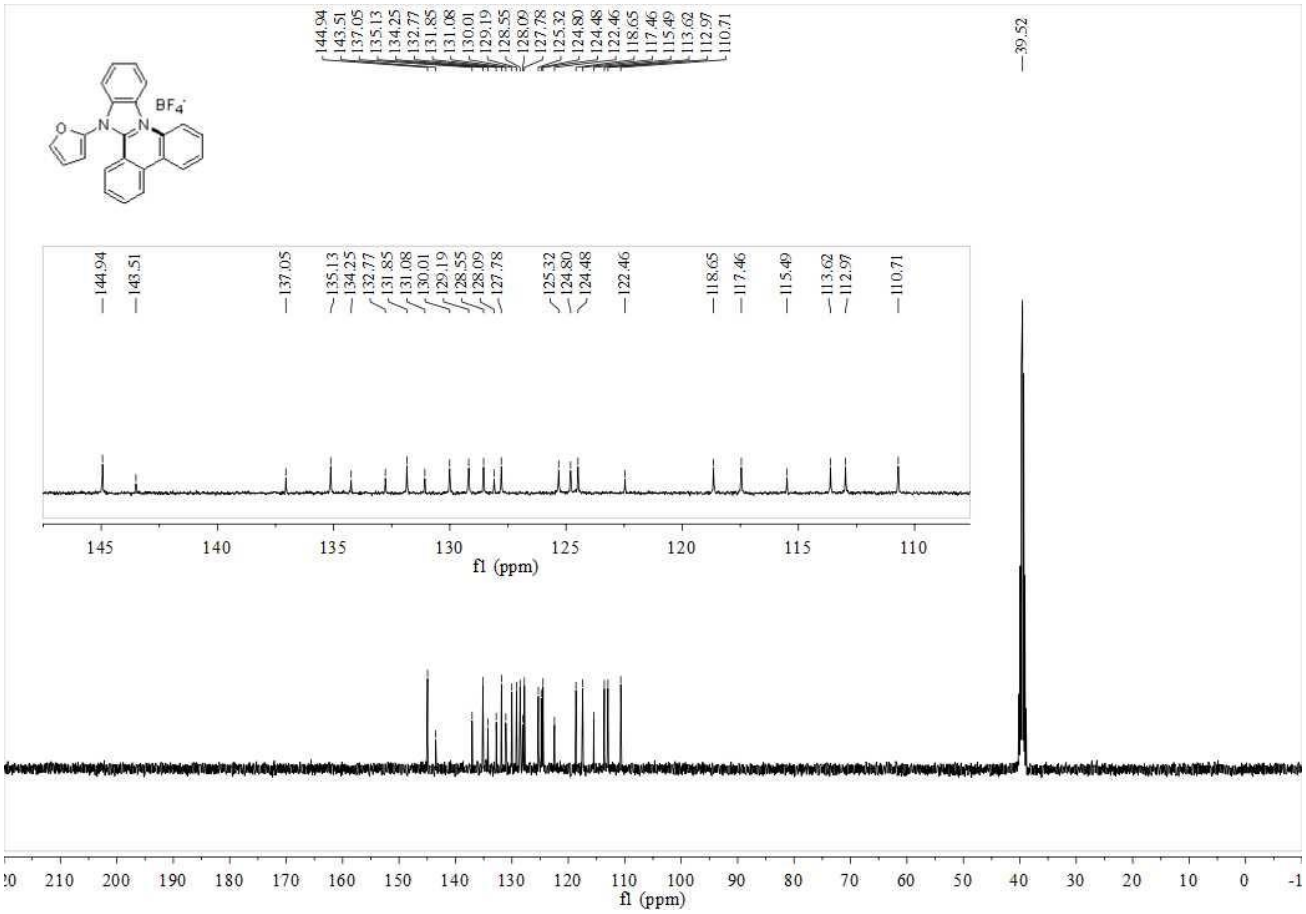
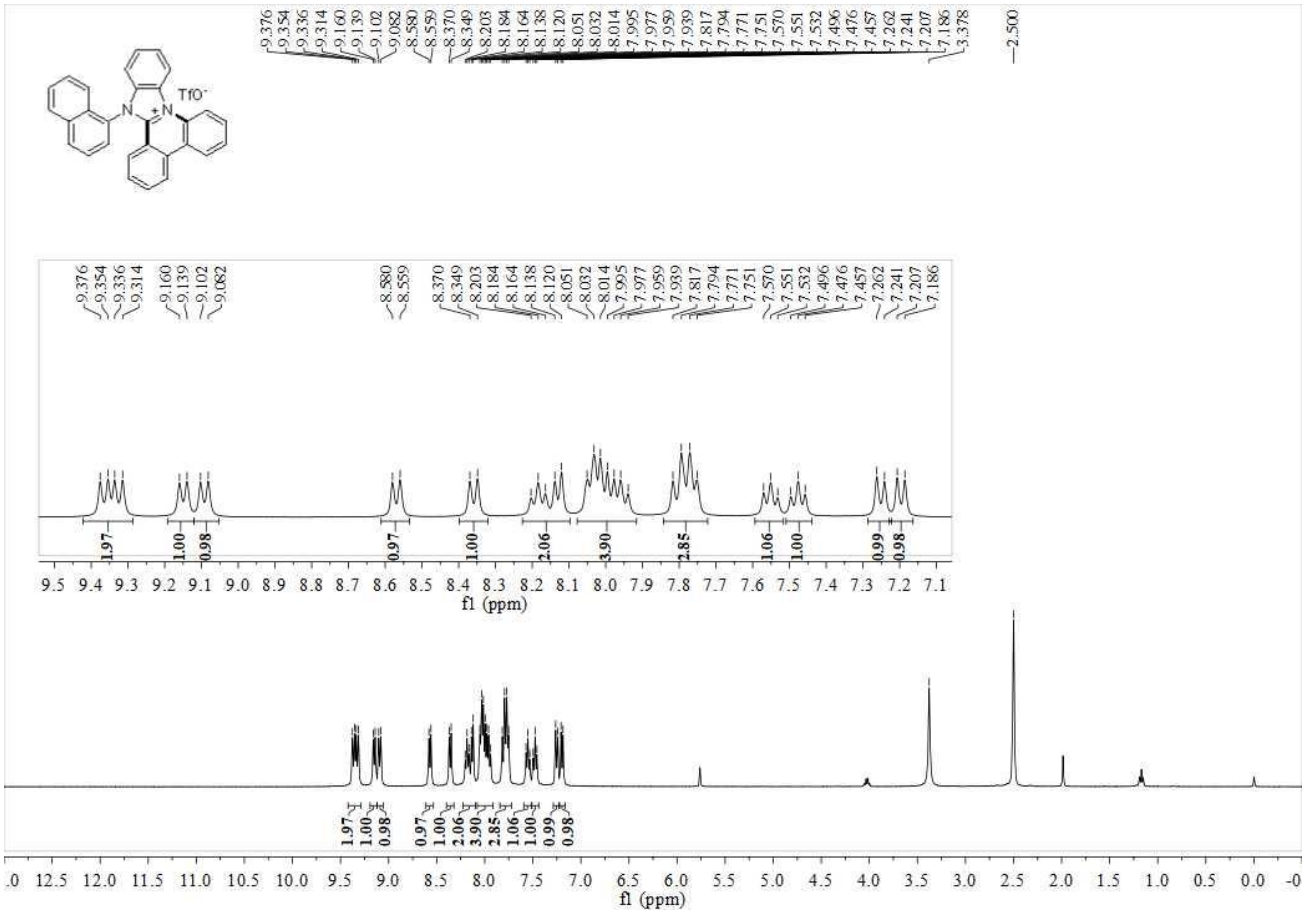
133.02
132.48
131.81
131.05
129.70
128.88
128.37
127.91
127.57
127.10
125.82
125.32
124.34
123.60
122.28
118.44
117.09
116.11
113.39
39.52
BF4-
fl (ppm)


9.273
9.251
9.246
9.223
9.142
9.132
9.121
9.110
8.301
8.216
8.198
8.179
8.145
8.130
8.111
8.031
8.013
7.991
7.956
7.887
7.868
7.851
7.755
7.738
7.246
7.224
7.142
3.352
2.500
BF4-
2.04
2.00
0.96
1.03
1.06
3.01
1.09
1.07
1.90
1.00
fl (ppm)


144.94
143.51
137.05
135.13
134.25
132.77
131.85
131.08
130.01
129.19
128.55
128.09
127.78
125.32
124.80
124.48
122.46
118.65
117.46
115.49
113.62
112.97
110.71
39.52
BF4-
fl (ppm)


TfO-
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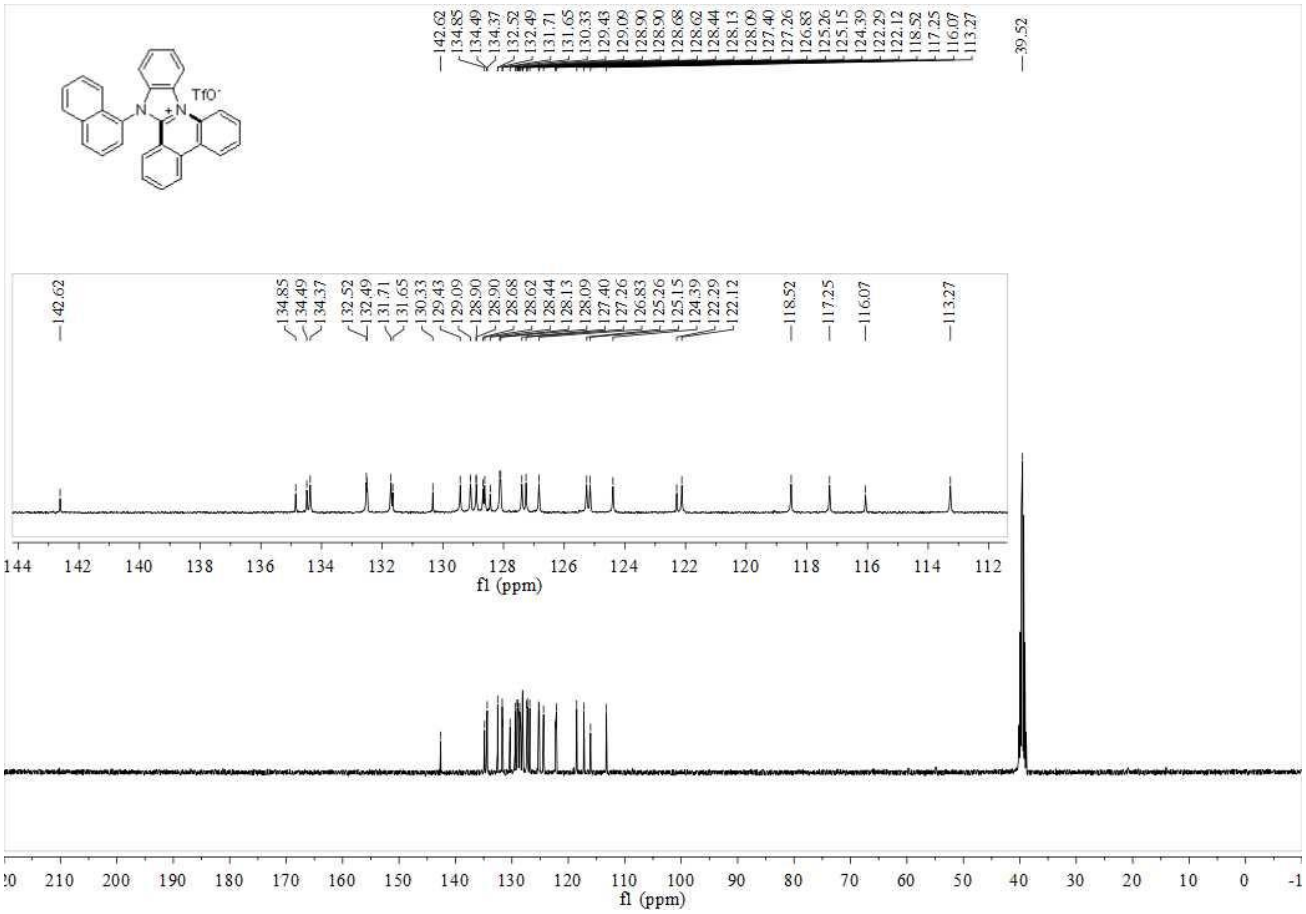
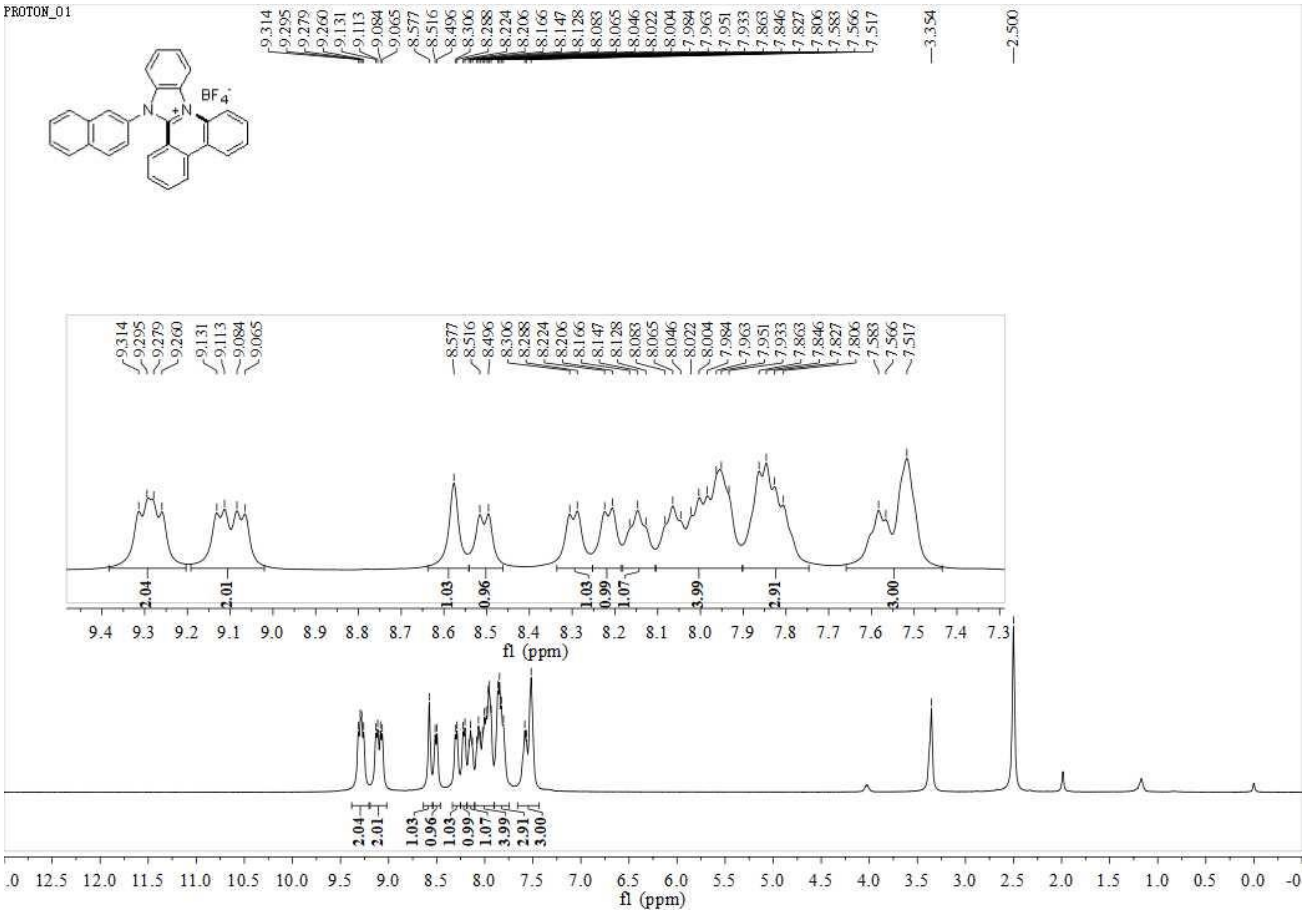
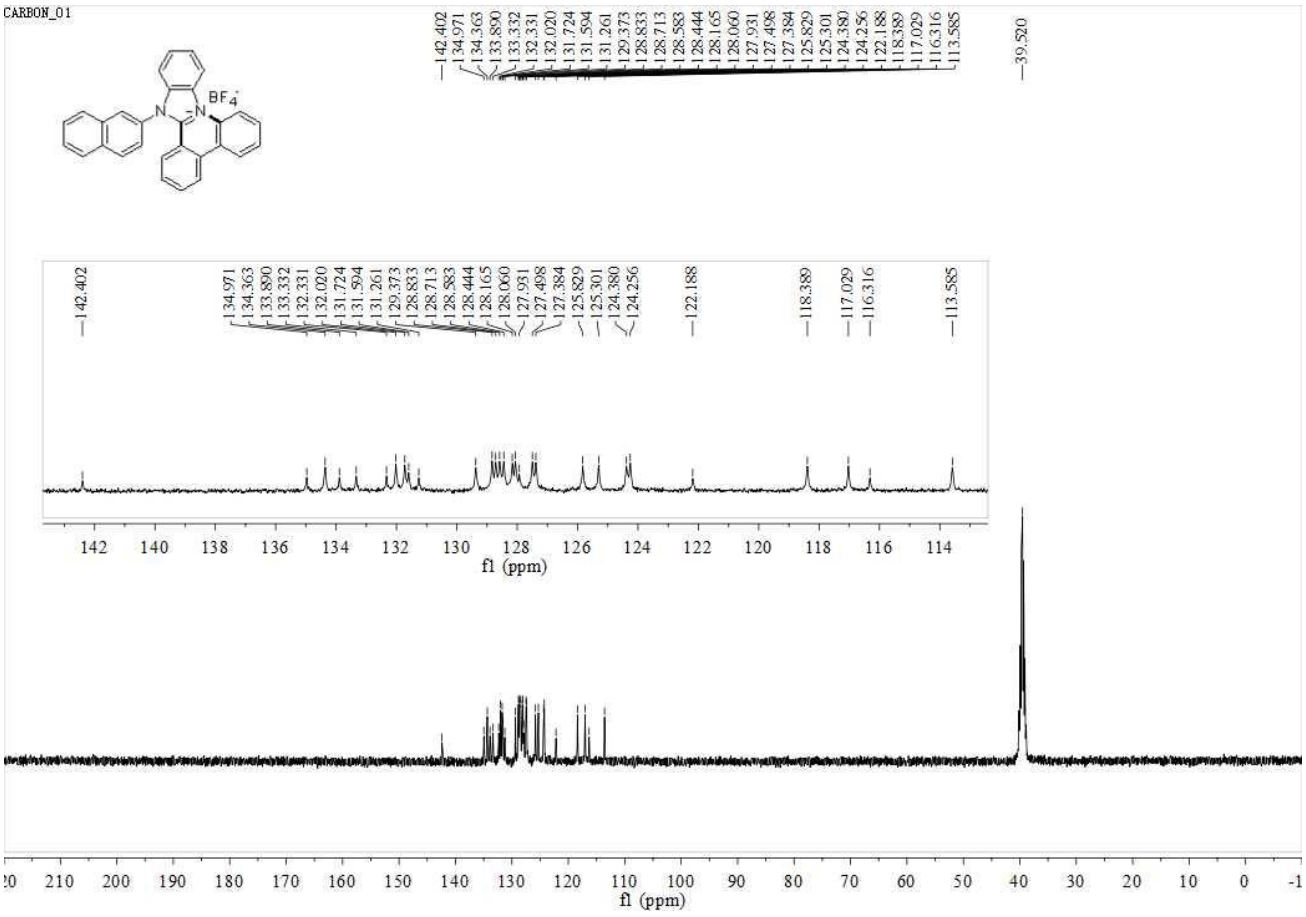
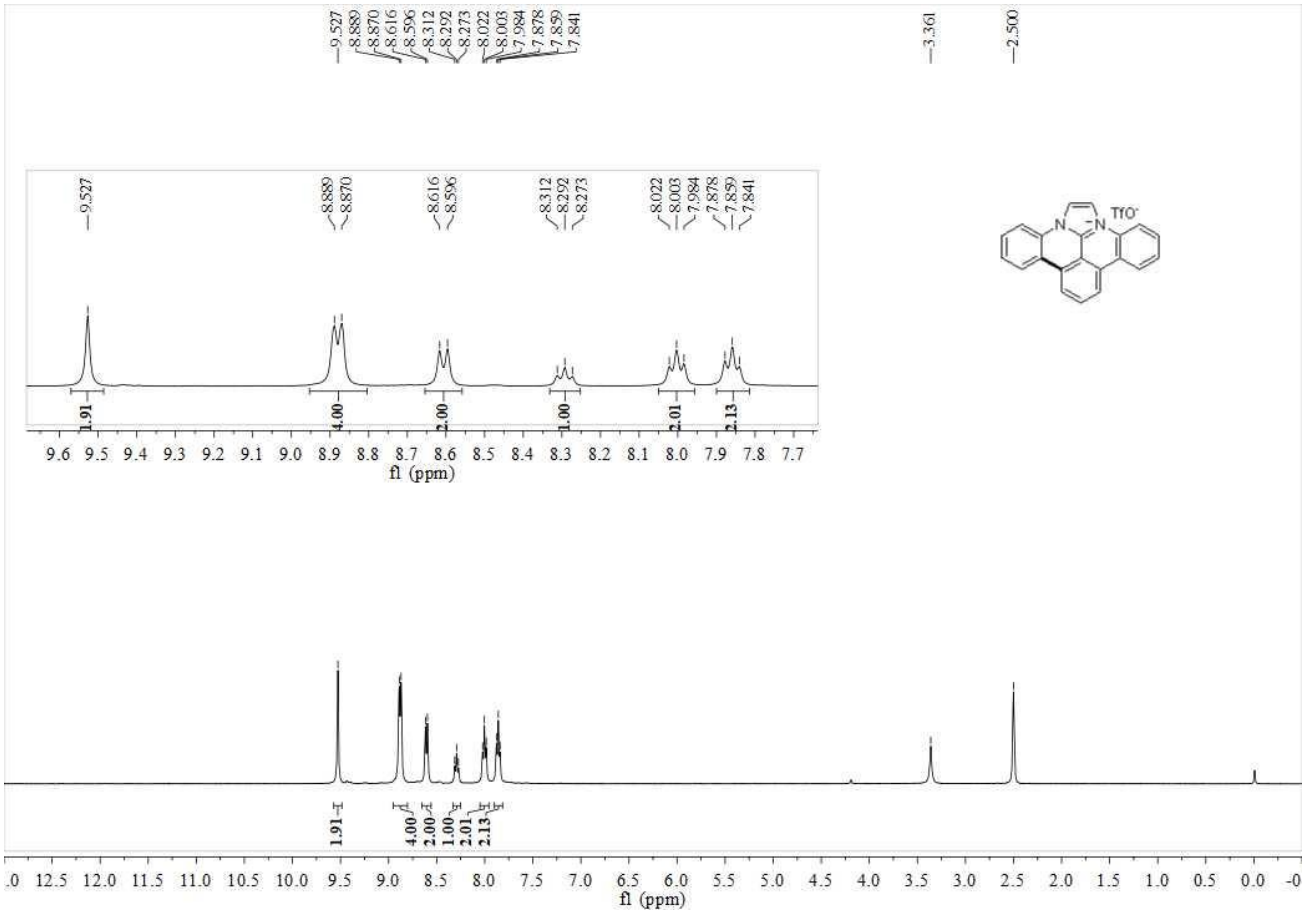
9.354
9.336
9.314
9.160
9.139
9.102
9.082
8.580
8.559
8.370
8.349
8.203
8.184
8.164
8.138
8.120
8.051
8.032
8.014
7.995
7.977
7.959
7.939
7.817
7.794
7.771
7.751
7.570
7.551
7.532
7.496
7.476
7.457
7.262
7.241
7.207
7.186
3.378
2.500
1.97
1.00
0.98
0.97
1.00
2.06
3.90
2.85
1.06
1.00
0.99
0.98
fl (ppm)


TfO-
142.62
134.85
134.49
134.37
132.52
132.49
131.71
131.65
130.33
129.43
129.09
128.90
128.68
128.62
128.44
128.13
128.09
127.40
127.26
126.83
125.26
125.15
124.39
122.29
122.12
118.52
117.25
116.07
113.27
39.52
fl (ppm)


PROTON_01
BF4-
9.314
9.295
9.279
9.260
9.131
9.113
9.084
9.065
8.577
8.516
8.496
8.306
8.288
8.224
8.206
8.166
8.147
8.128
8.083
8.065
8.046
8.022
8.004
7.984
7.963
7.951
7.933
7.863
7.846
7.827
7.806
7.583
7.566
7.517
3.354
2.500
2.04
2.01
1.03
0.96
1.03
0.99
1.07
3.99
2.91
3.00
fl (ppm)


CARBON_01
BF4-
142.402
134.971
134.363
133.890
133.332
132.331
132.020
131.724
131.594
131.261
129.373
128.833
128.713
128.583
128.444
128.165
128.060
127.931
127.498
127.384
125.829
125.301
124.380
124.256
122.188
118.389
117.029
116.316
113.585
39.520
fl (ppm)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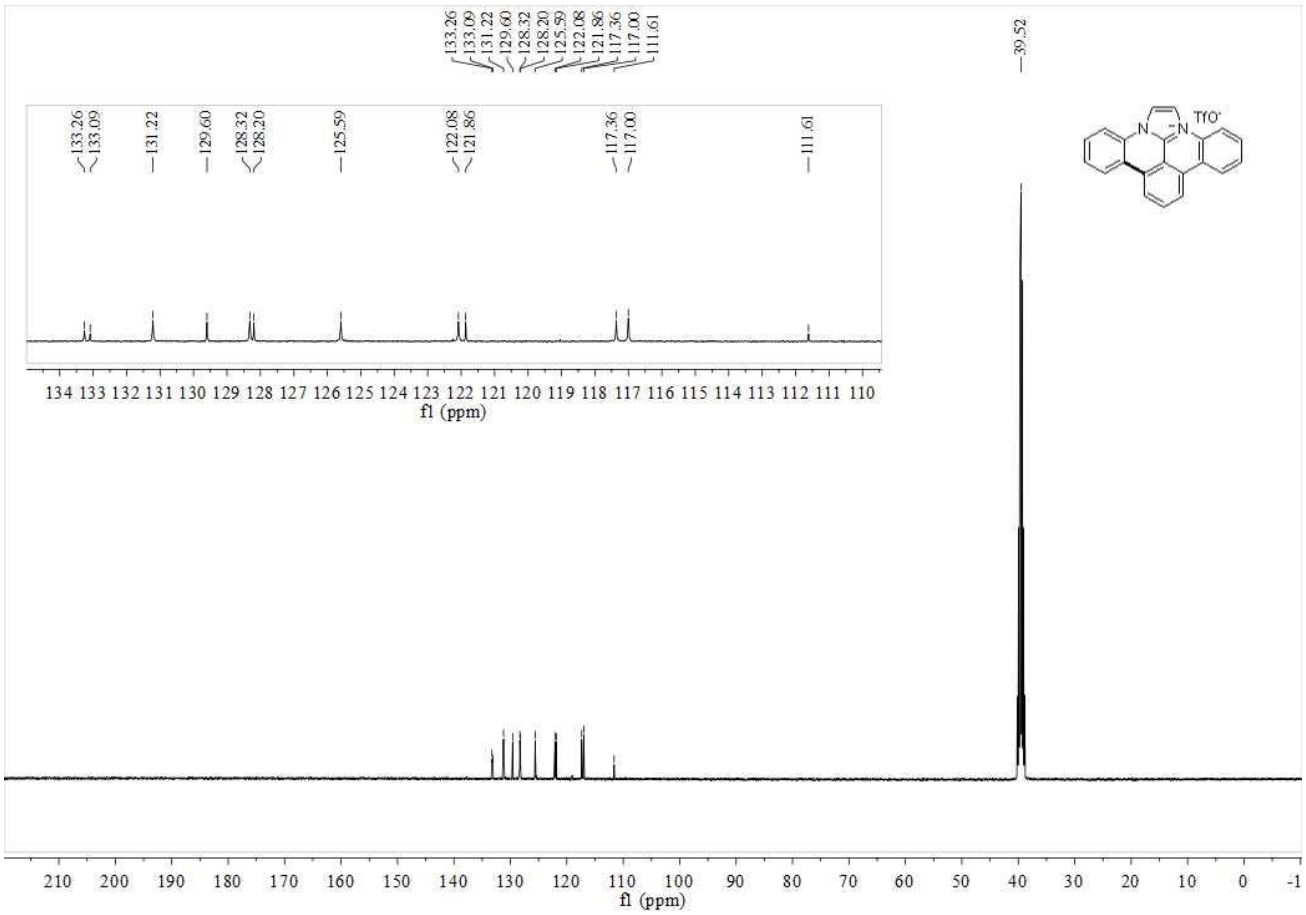
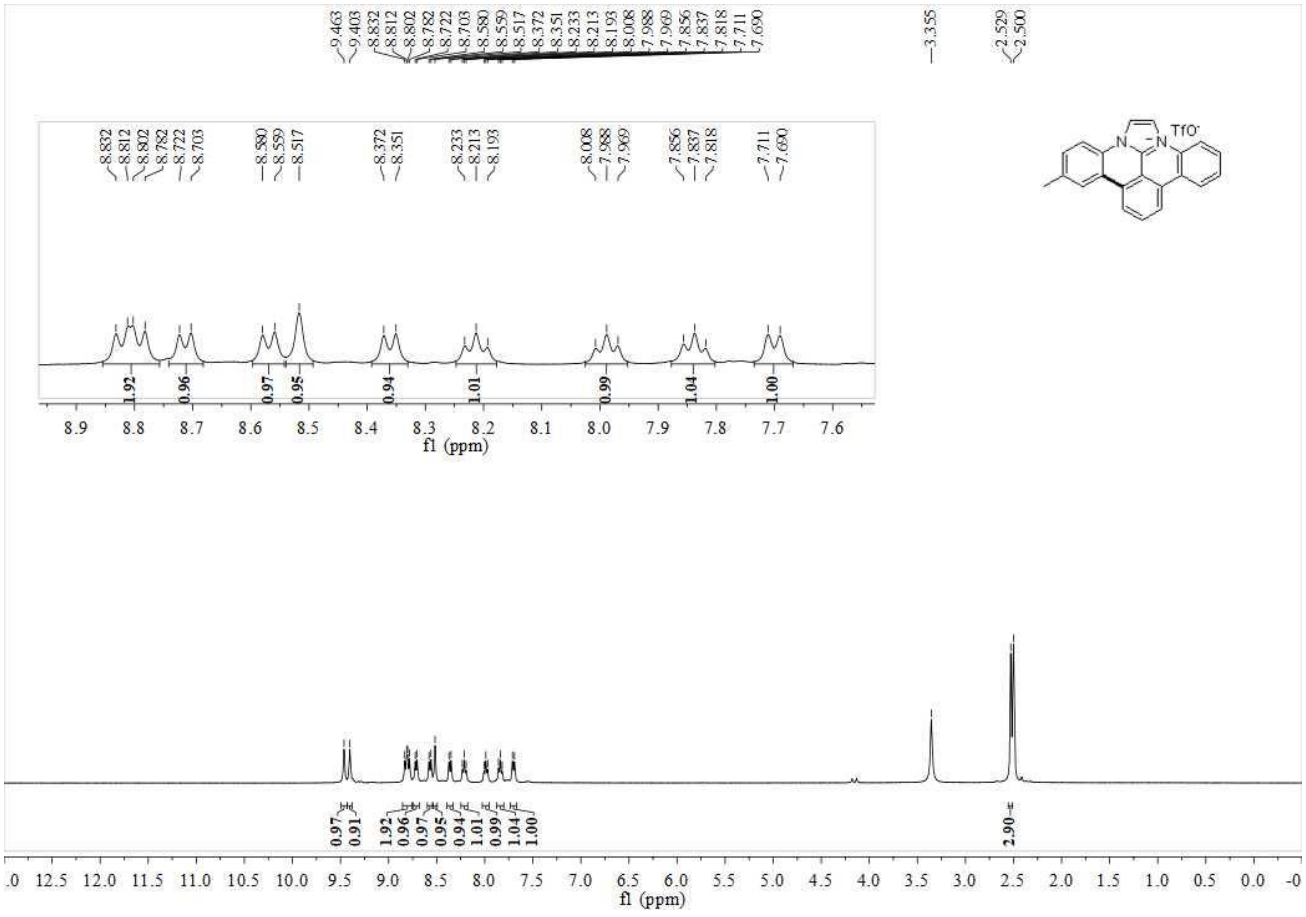
8.889
8.870
8.616
8.596
8.312
8.292
8.273
8.022
8.003
7.984
7.878
7.859
7.841
3.361
2.500
TfO-
1.91
4.00
2.00
1.00
2.01
2.13
fl (ppm)


133.26
133.09
131.22
129.60
128.32
128.20
125.59
122.08
121.86
117.36
117.00
111.61
39.52
TfO-
fl (ppm)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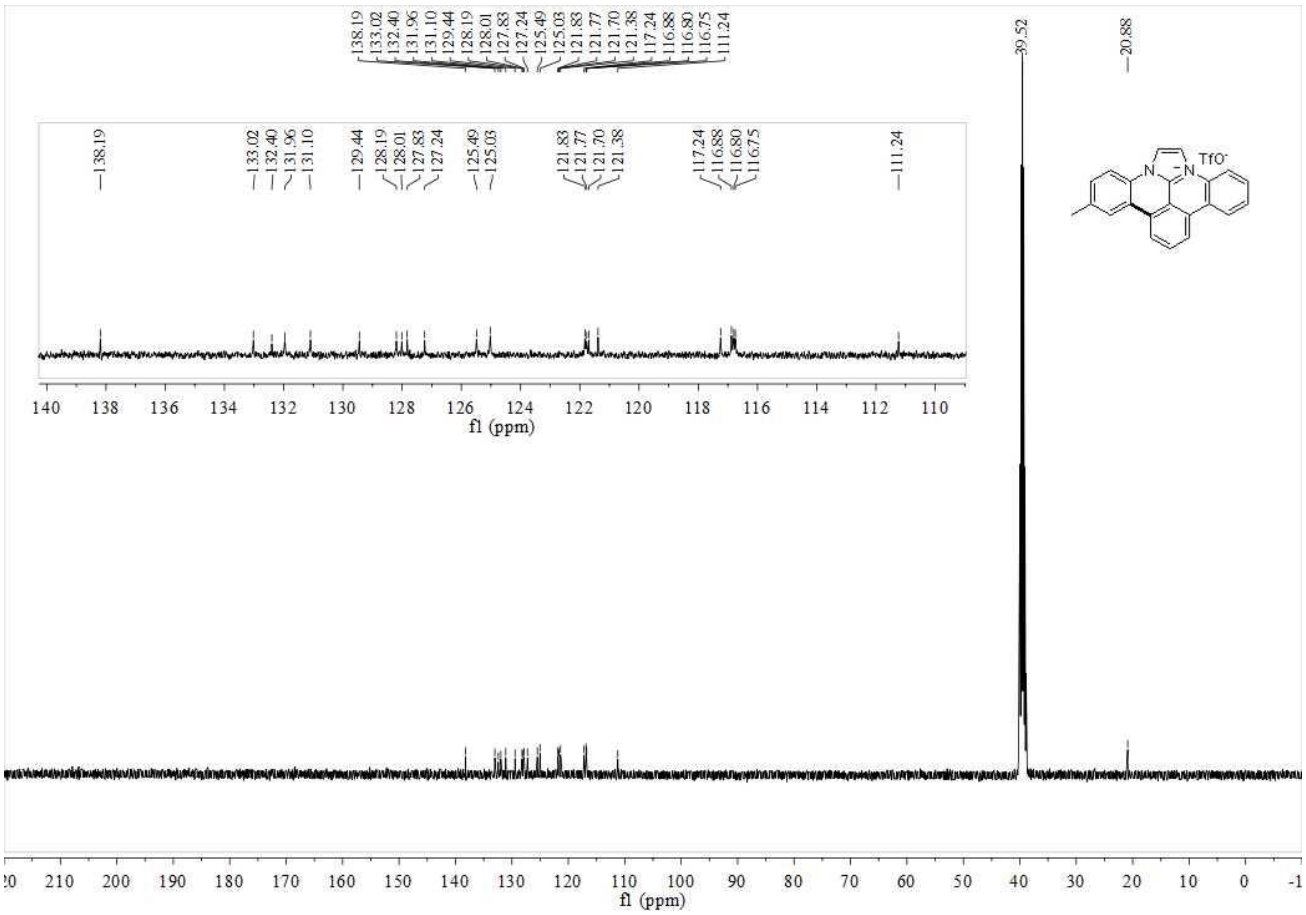
8.812
8.802
8.782
8.722
8.703
8.580
8.559
8.517
8.372
8.351
8.233
8.213
8.193
8.008
7.988
7.969
7.856
7.837
7.818
7.711
7.690
3.355
2.529
2.500
TfO-
0.97
0.91
1.92
0.96
0.97
0.95
0.94
1.01
0.99
1.04
1.00
2.90
fl (ppm)


138.19
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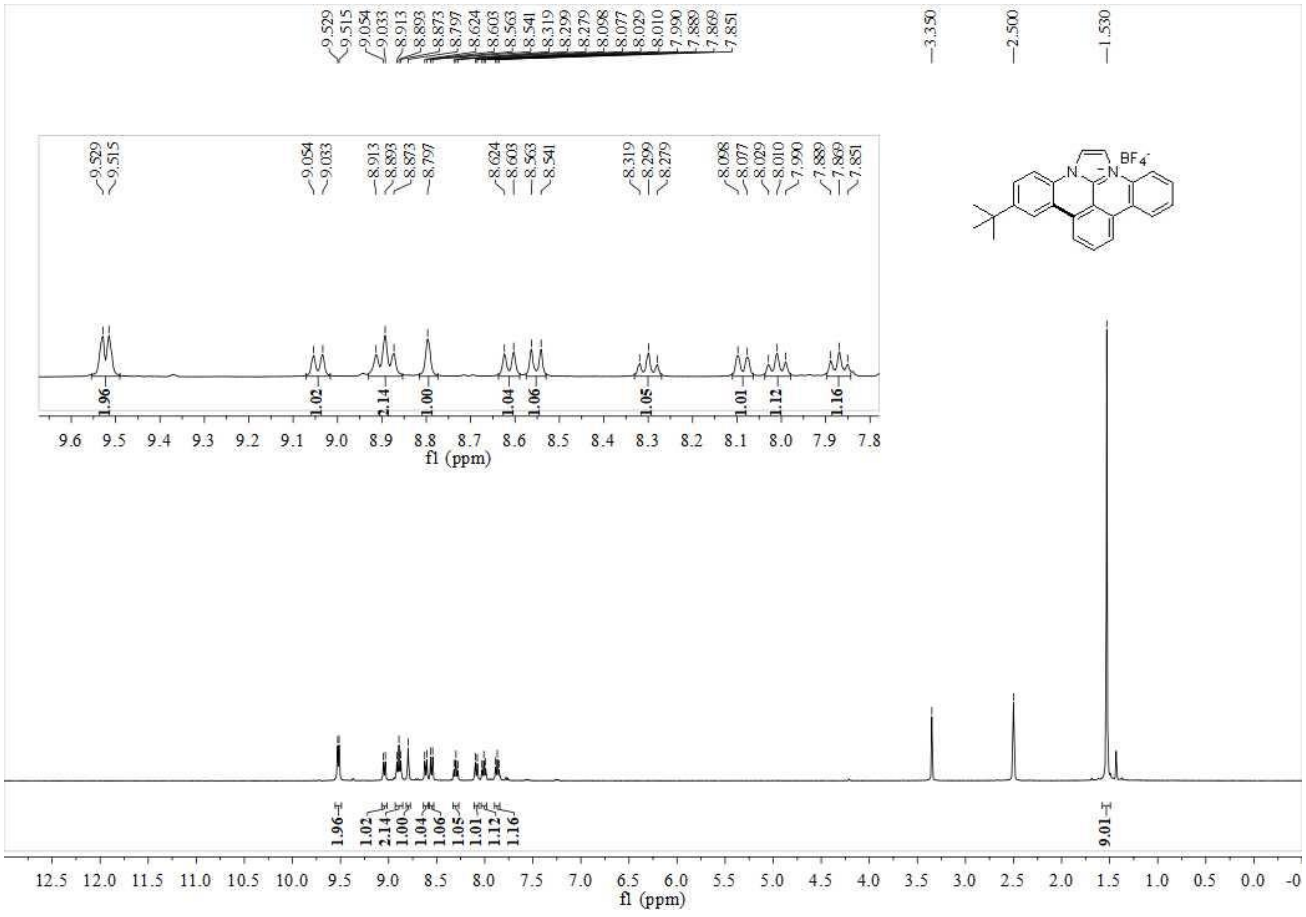
131.96
131.10
129.44
128.19
128.01
127.83
127.24
125.49
125.03
121.83
121.77
121.70
121.38
117.24
116.88
116.80
116.75
111.24
39.52
20.88
TfO-
fl (ppm)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9.054
9.033
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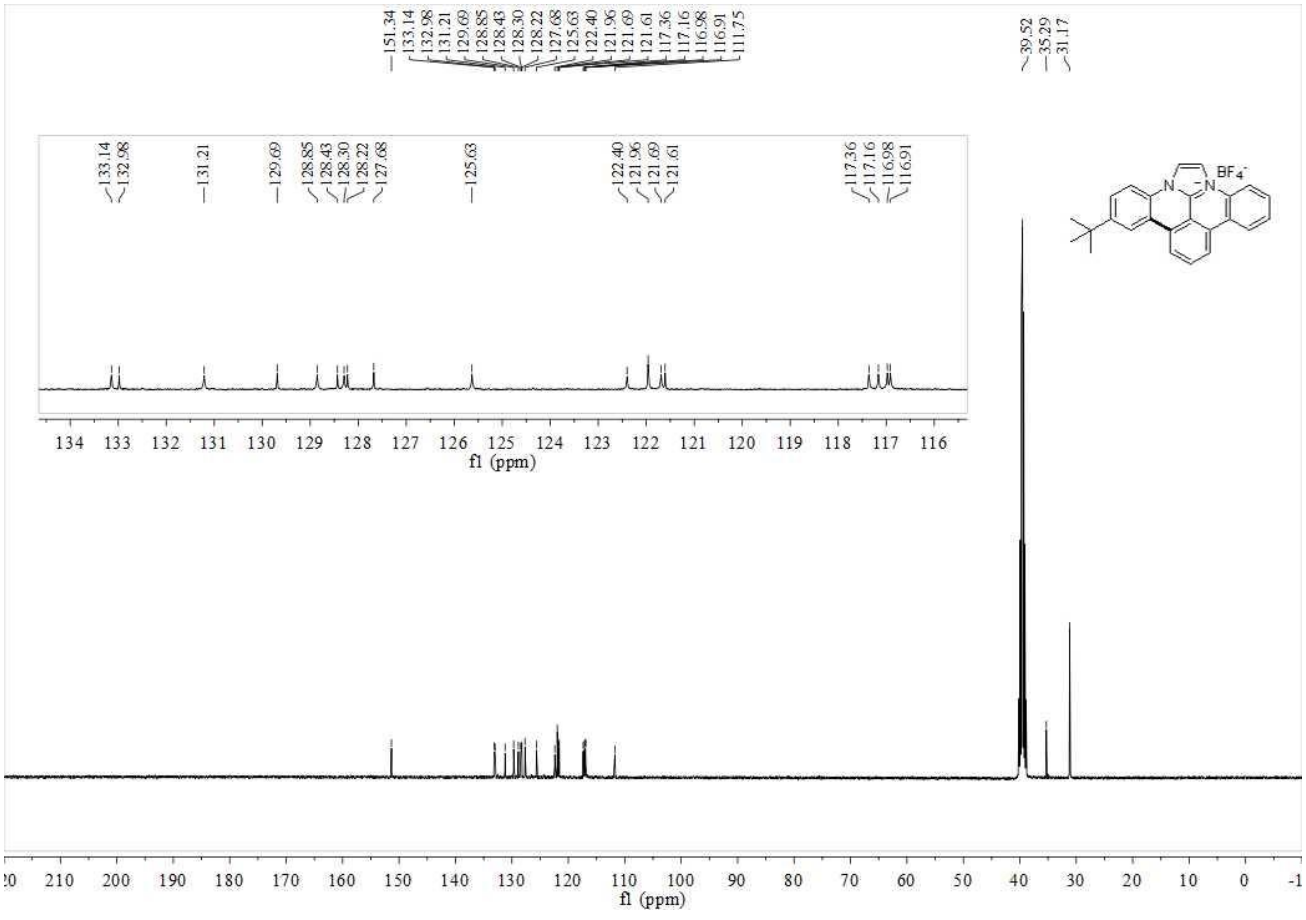
8.893
8.873
8.797
8.624
8.603
8.563
8.541
8.319
8.299
8.279
8.098
8.077
8.029
8.010
7.990
7.889
7.869
7.851
3.350
2.500
1.530
BF4-
1.96
1.02
2.14
1.00
1.04
1.06
1.05
1.01
1.12
1.16
9.01
fl (ppm)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132.98
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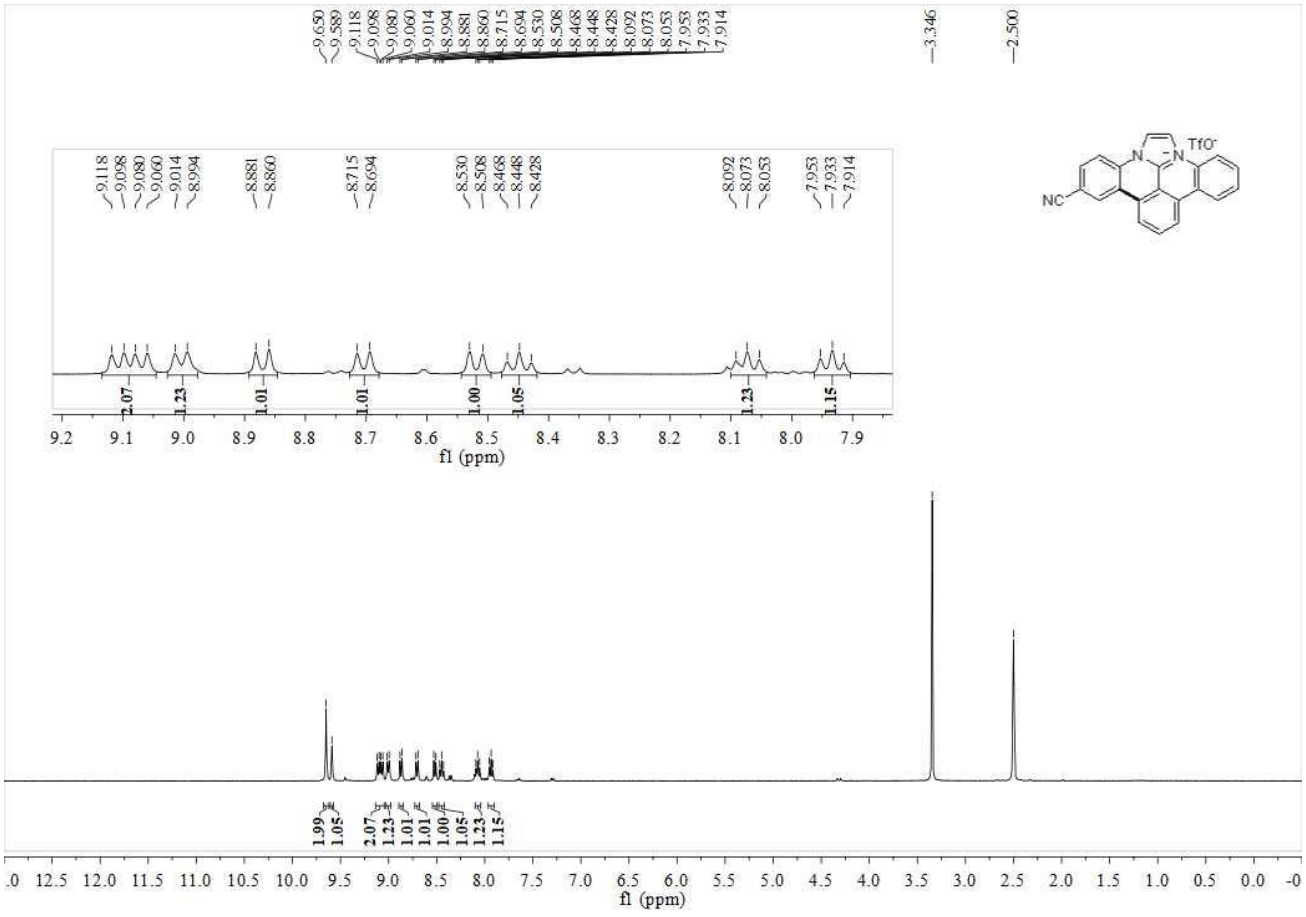
129.69
128.85
128.43
128.30
128.22
127.68
125.63
122.40
121.96
121.69
121.61
117.36
117.16
116.98
116.91
111.75
39.52
35.29
31.17
BF4-
fl (ppm)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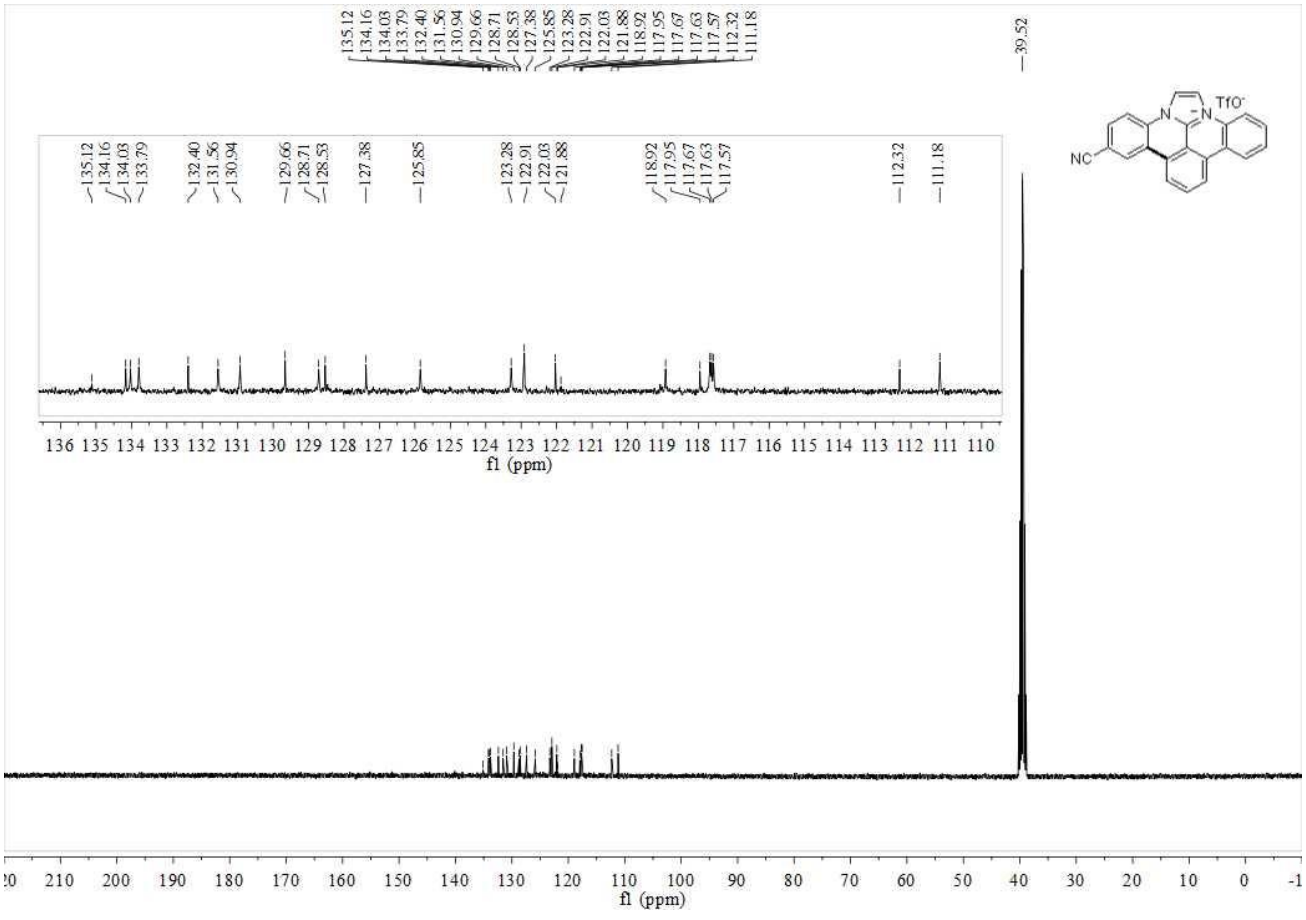
9.589
9.118
9.098
9.080
9.060
9.014
8.994
8.881
8.860
8.715
8.694
8.530
8.508
8.468
8.448
8.428
8.092
8.073
8.053
7.953
7.933
7.914
3.346
2.500
TfO⁻
NC
1.99
1.05
2.07
1.23
1.01
1.01
1.00
1.05
1.23
1.15
f1 (ppm)


135.12
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131.56
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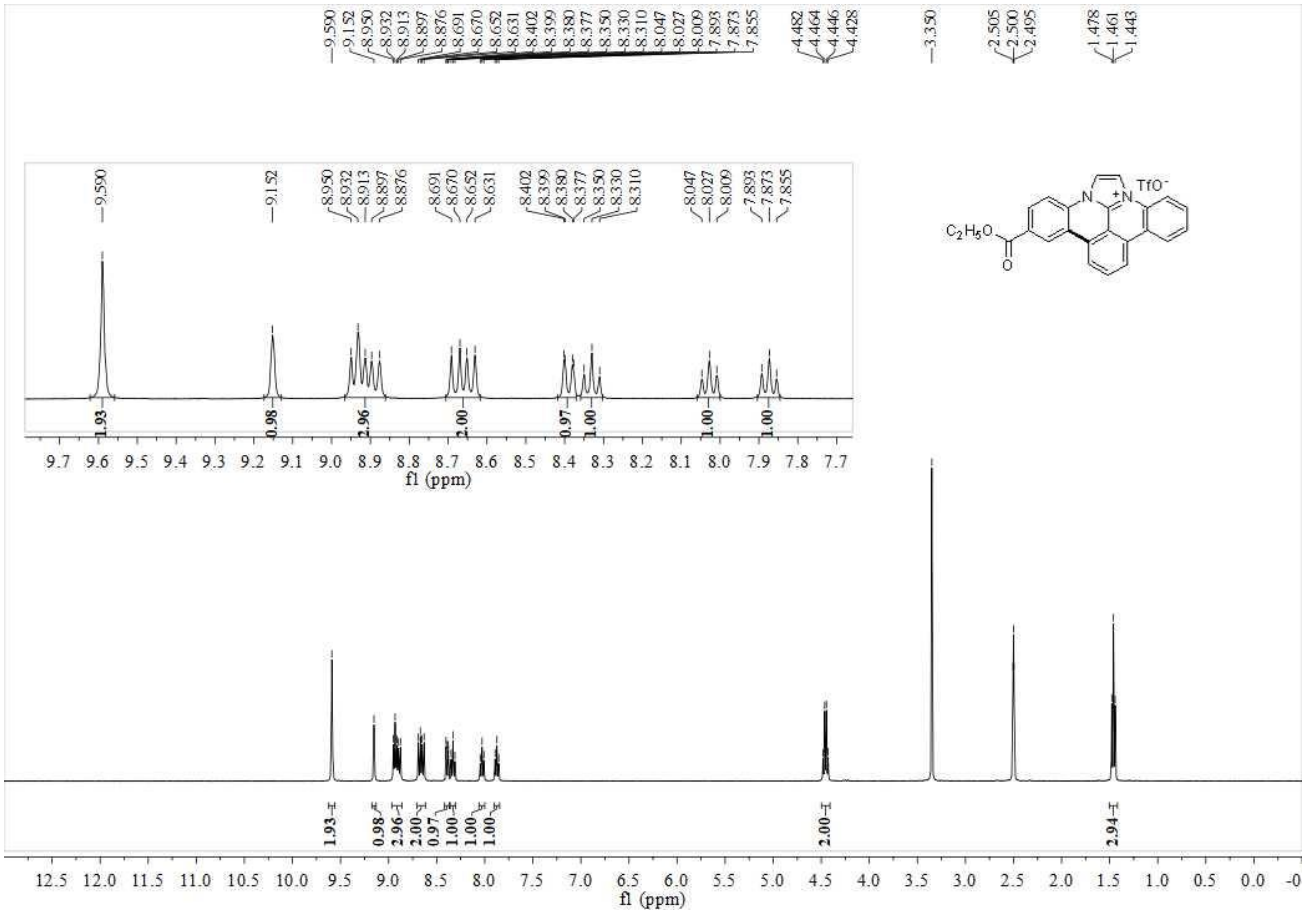
129.66
128.71
128.53
127.38
125.85
123.28
122.91
122.03
121.88
118.92
117.95
117.67
117.63
117.57
112.32
111.18
39.52
TfO⁻
NC
f1 (ppm)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8.932
8.913
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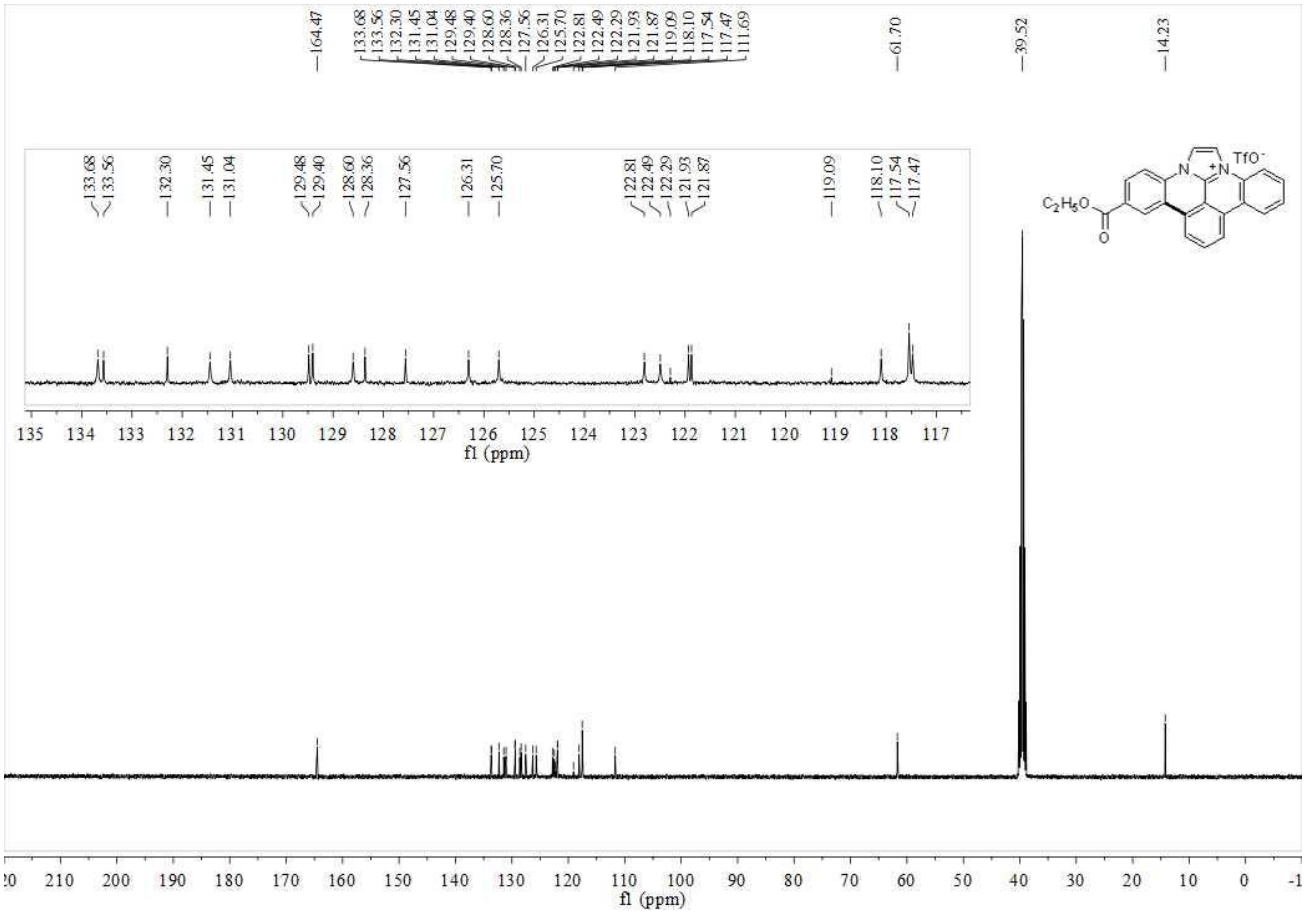
8.876
8.691
8.670
8.652
8.631
8.402
8.399
8.380
8.377
8.350
8.330
8.310
8.047
8.027
8.009
7.893
7.873
7.855
4.482
4.464
4.446
4.428
3.350
2.505
2.500
2.495
1.478
1.461
1.443
TfO⁻
C2H5O
O
1.93
0.98
2.96
2.00
0.97
1.00
1.00
1.00
2.00
2.94
fl (ppm)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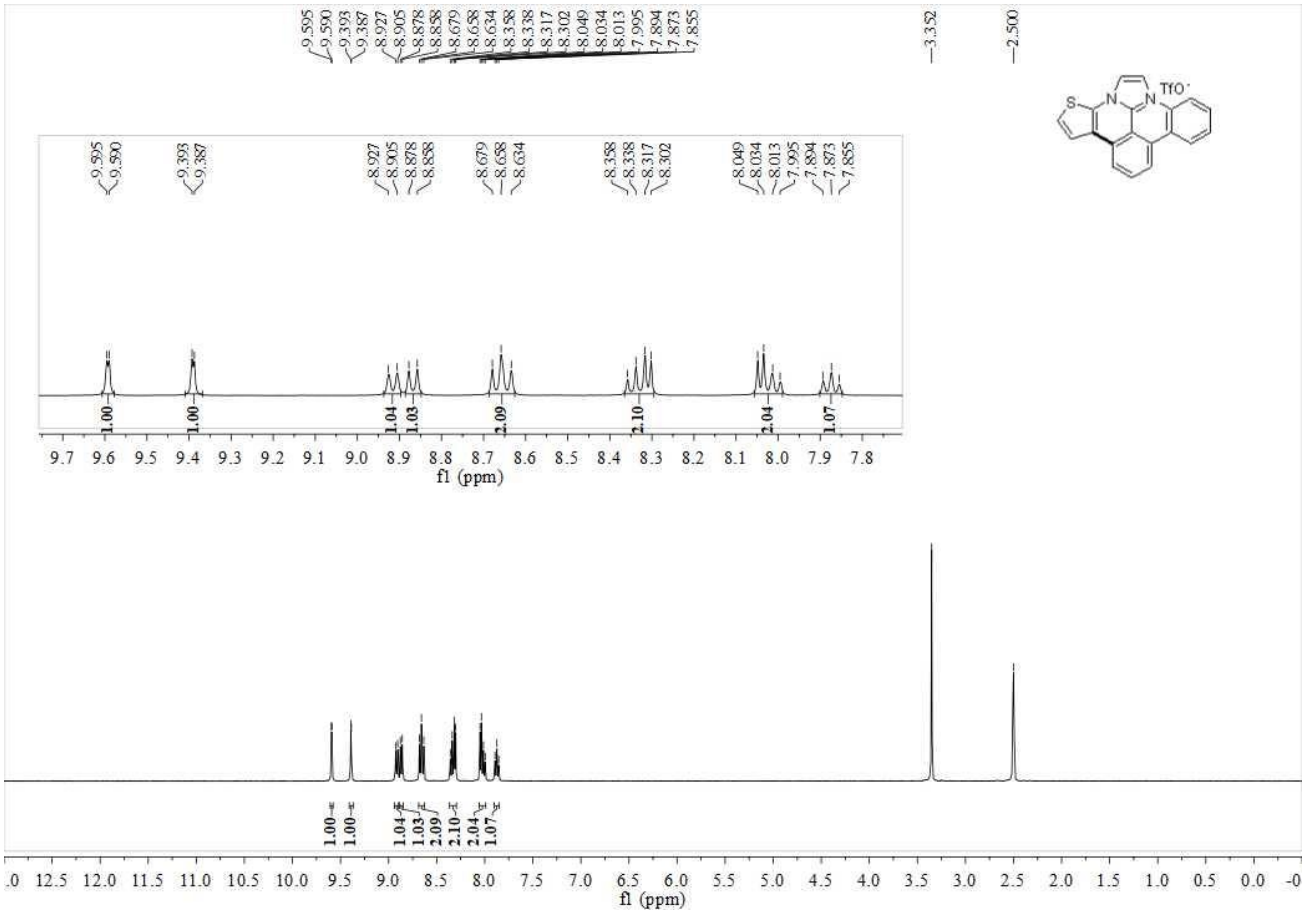
129.48
129.40
128.60
128.36
127.56
126.31
125.70
122.81
122.49
122.29
121.93
121.87
119.09
118.10
117.54
117.47
111.69
61.70
39.52
14.23
TfO⁻
C2H5O
O
fl (ppm)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8.858
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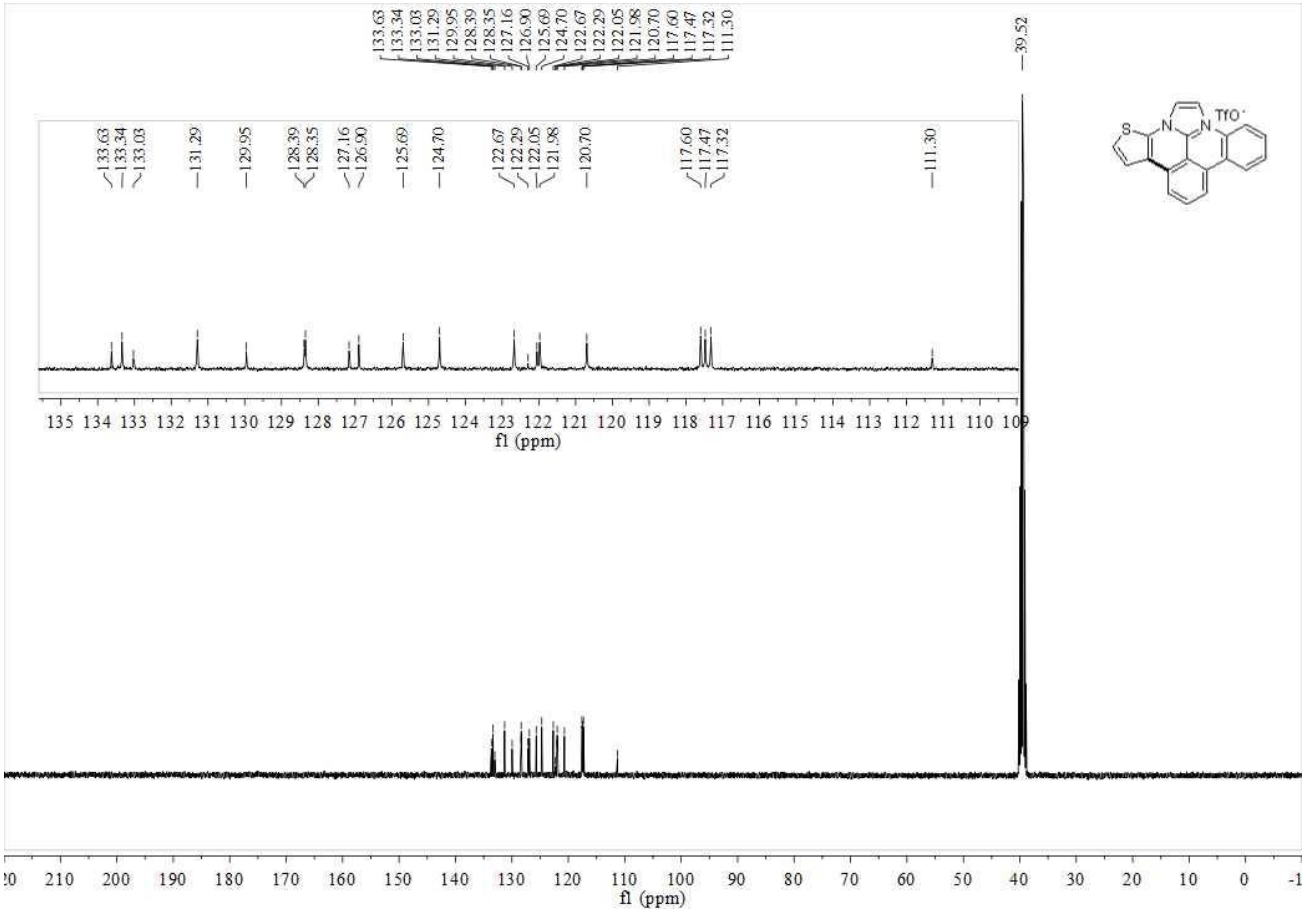
8.634
8.358
8.338
8.317
8.302
8.049
8.034
8.013
7.995
7.894
7.873
7.855
3.352
2.500
TfO
1.00
1.00
1.04
1.03
2.09
2.10
2.04
1.07
fl (ppm)


133.63
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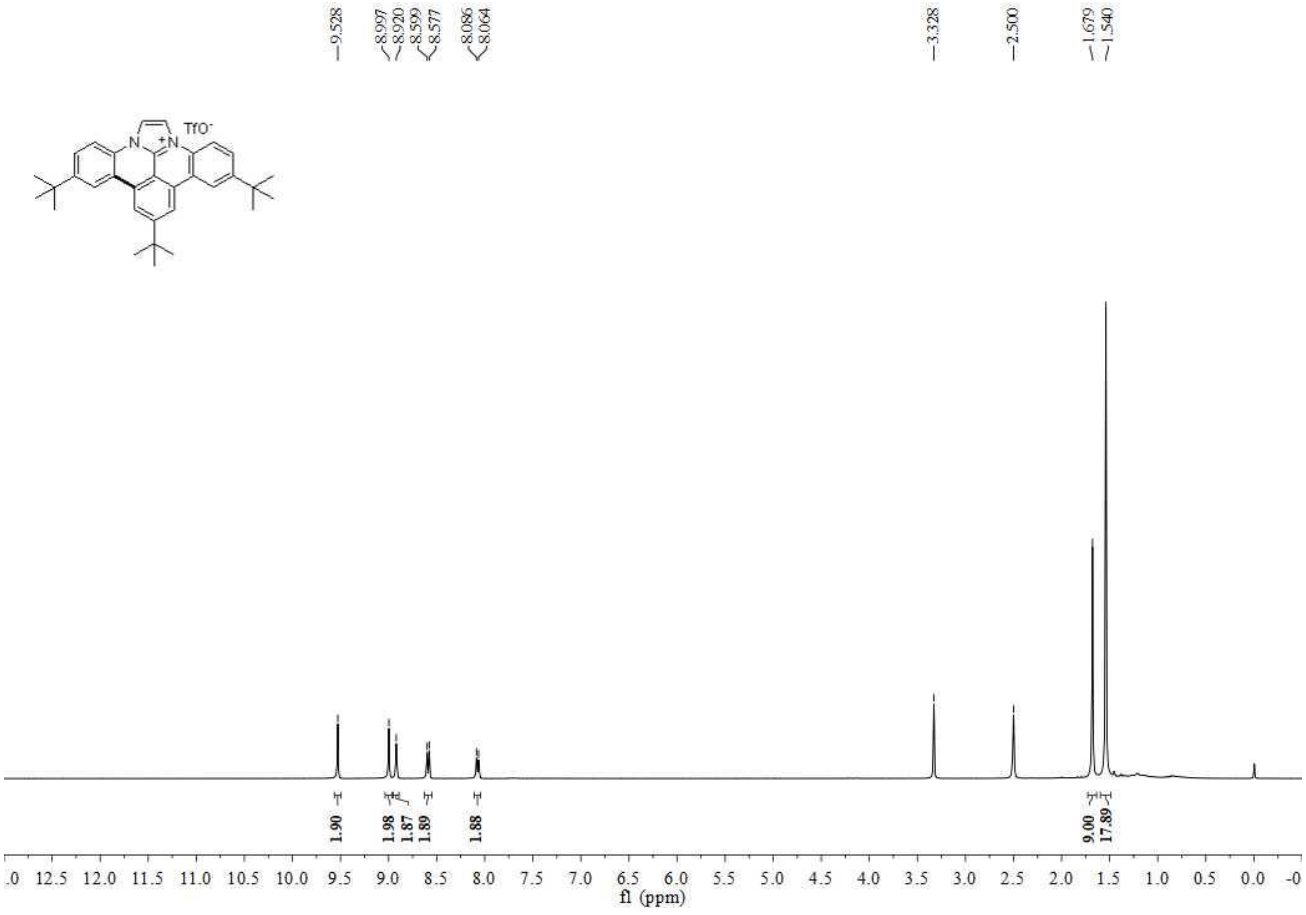
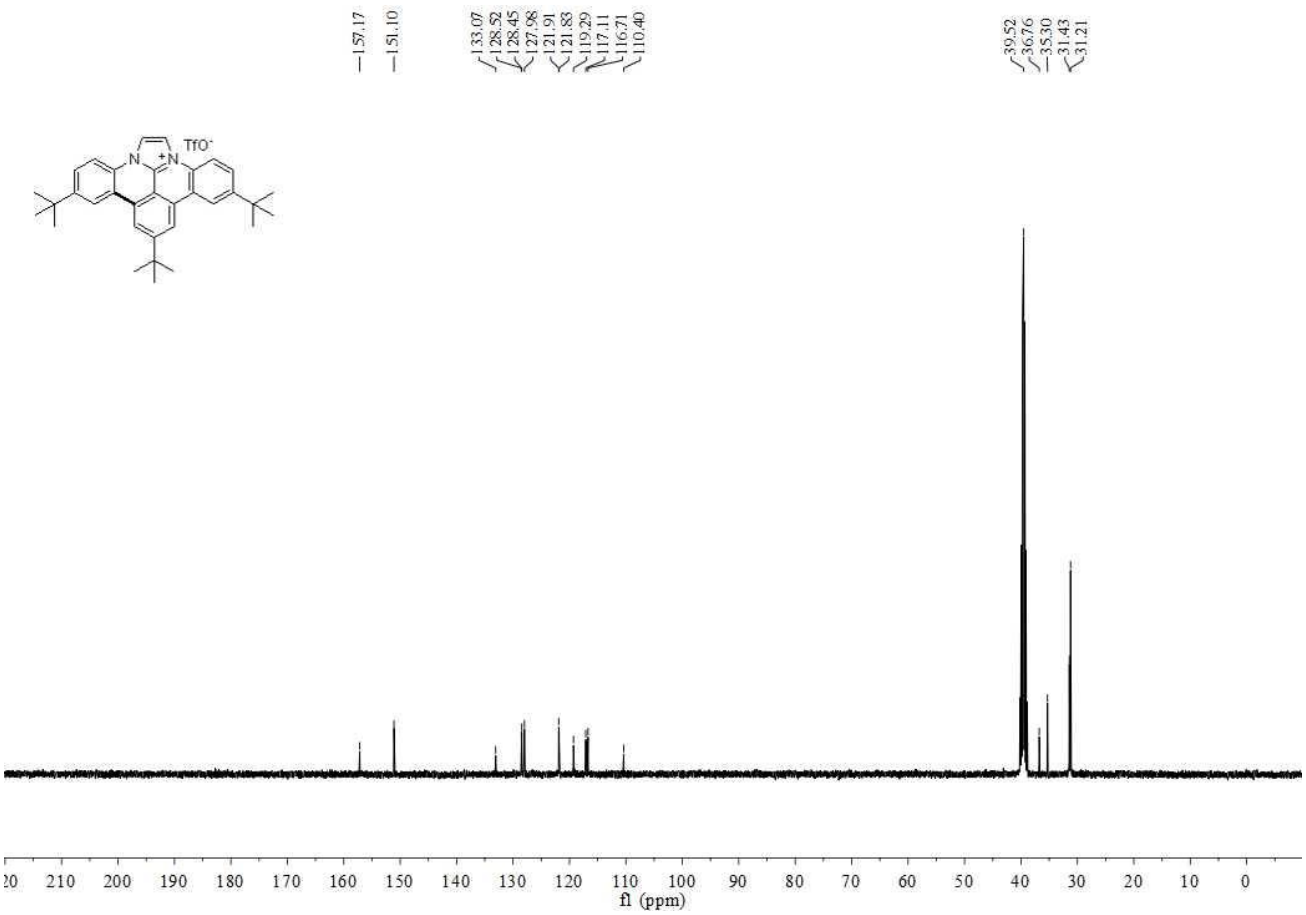
133.03
131.29
129.95
128.39
128.35
127.16
126.90
125.69
124.70
122.67
122.29
122.05
121.98
120.70
117.60
117.47
117.32
111.30
39.52
TfO
fl (ppm)


9.528
8.997
8.920
8.599
8.577
8.086
8.064
3.328
2.500
1.679
1.540
TfO⁻
1.90
1.98
1.87
1.89
1.88
9.00
17.89
f1 (ppm)


157.17
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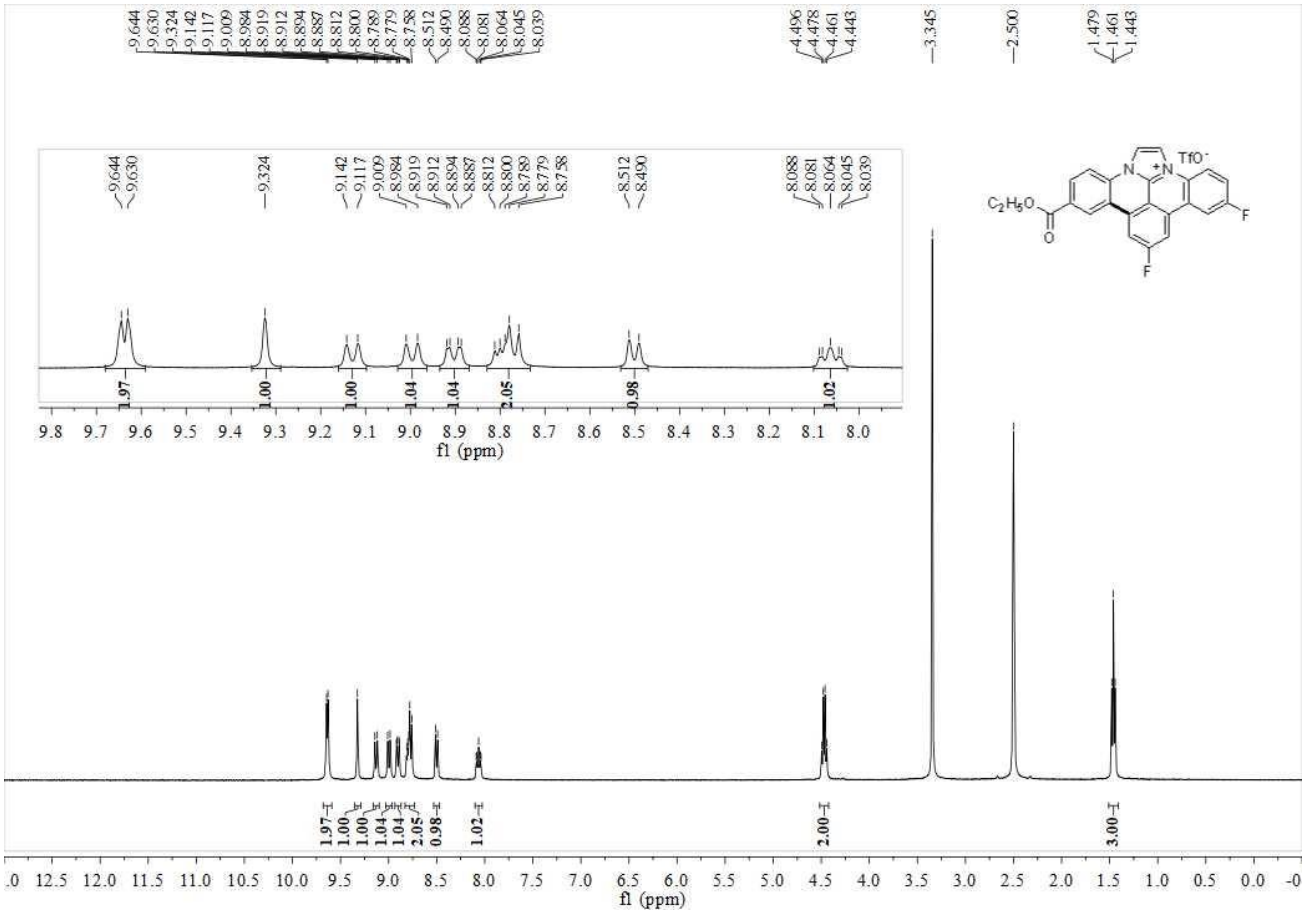
133.07
128.52
128.45
127.98
121.91
121.83
119.29
117.11
116.71
110.40
39.52
36.76
35.30
31.43
31.21
TfO⁻
f1 (ppm)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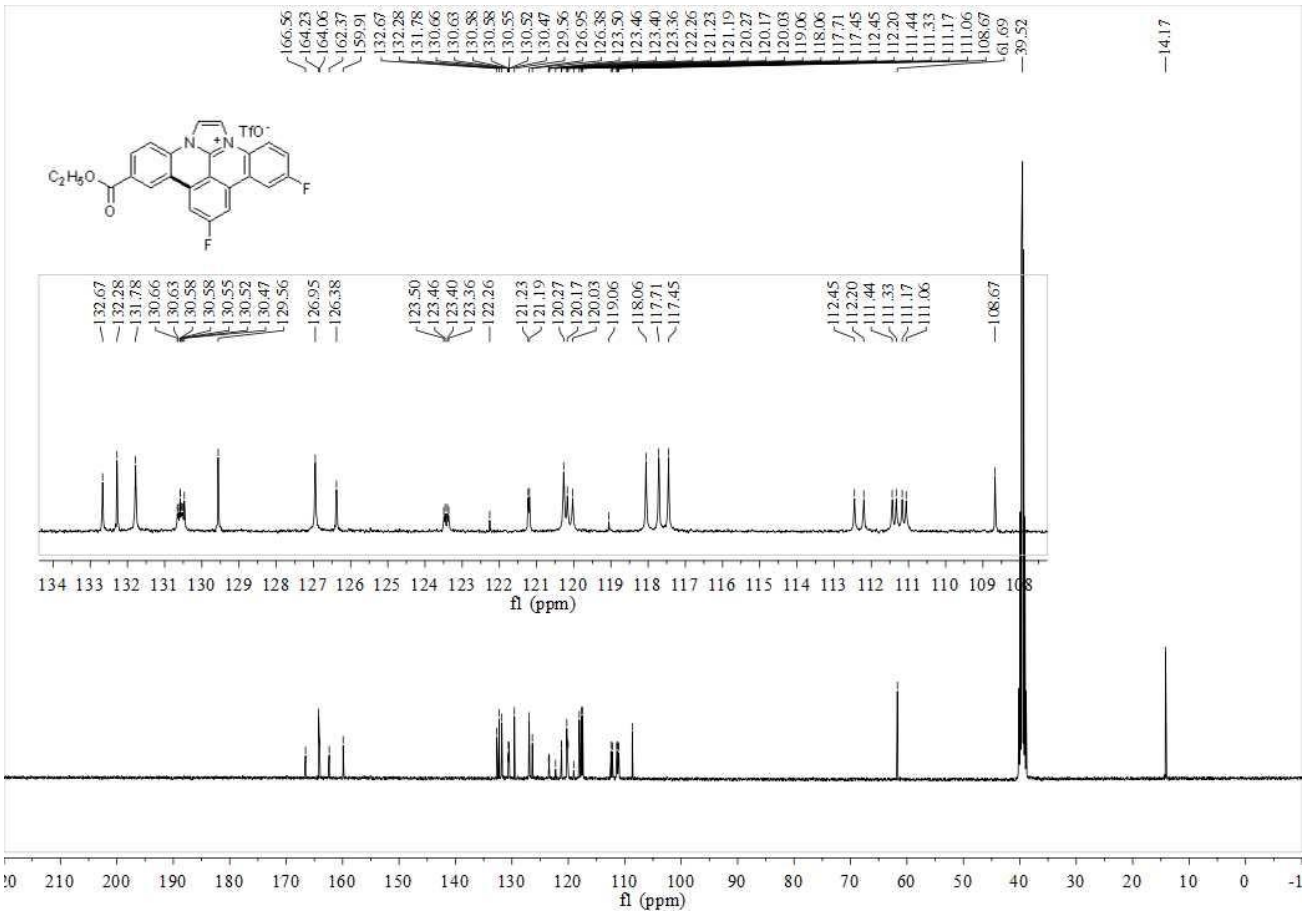
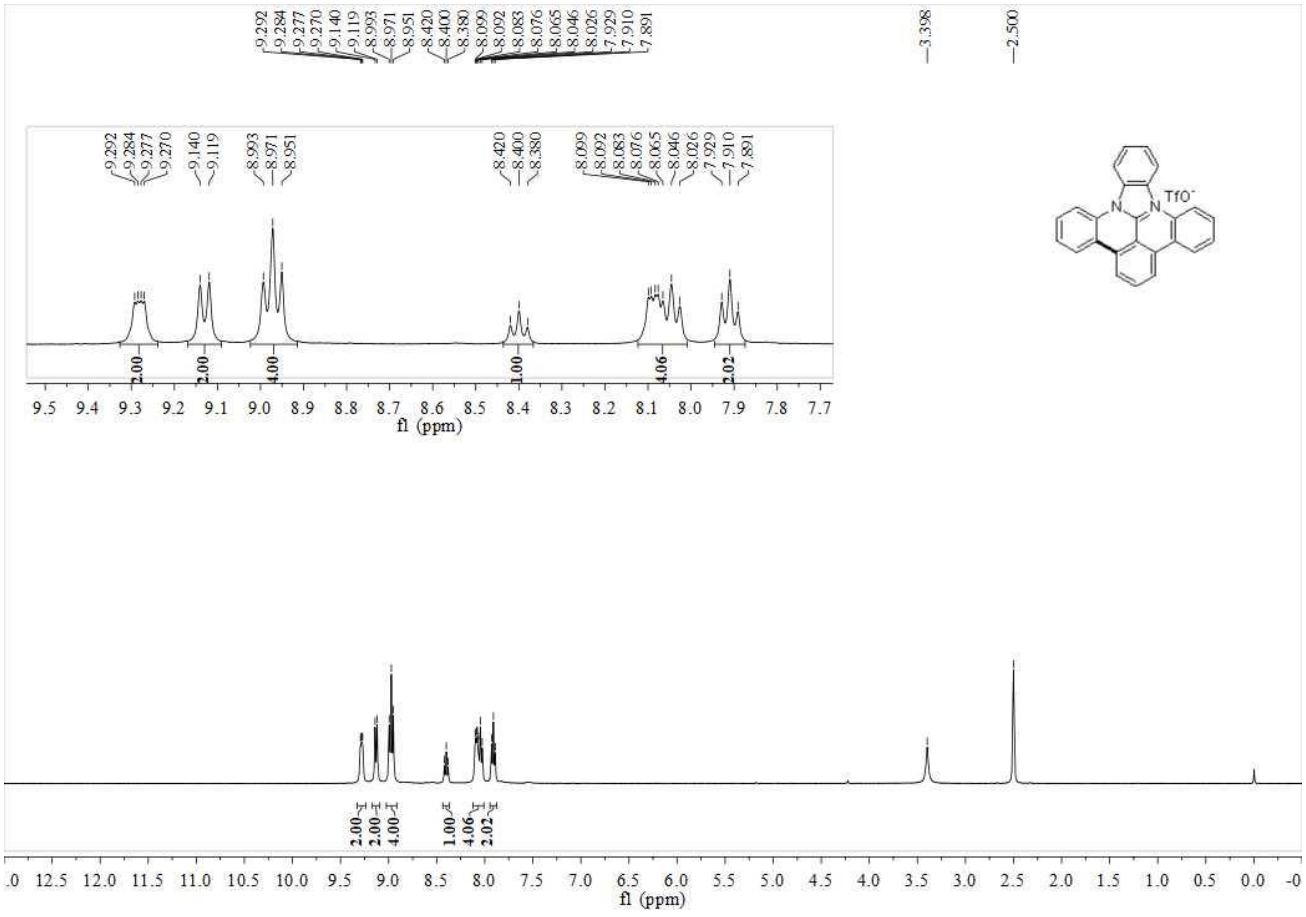
9.630
9.324
9.142
9.117
9.009
8.984
8.919
8.912
8.894
8.887
8.812
8.800
8.789
8.779
8.758
8.512
8.490
8.088
8.081
8.064
8.045
8.039
4.496
4.478
4.461
4.443
3.345
2.500
1.479
1.461
1.443
TfO⁻
C2H5O
O
F
F
1.97
1.00
1.00
1.04
1.04
2.05
0.98
1.02
2.00
3.00
fl (ppm)


166.56
164.23
164.06
162.37
159.91
132.67
132.28
131.78
130.66
130.63
130.58
130.55
130.52
130.47
129.56
126.95
126.38
123.50
123.46
123.40
123.36
122.26
121.23
121.19
120.27
120.17
120.03
119.06
118.06
117.71
117.45
112.45
112.20
111.44
111.33
111.17
111.06
108.67
61.69
39.52
14.17
TfO⁻
C2H5O
O
F
F
fl (ppm)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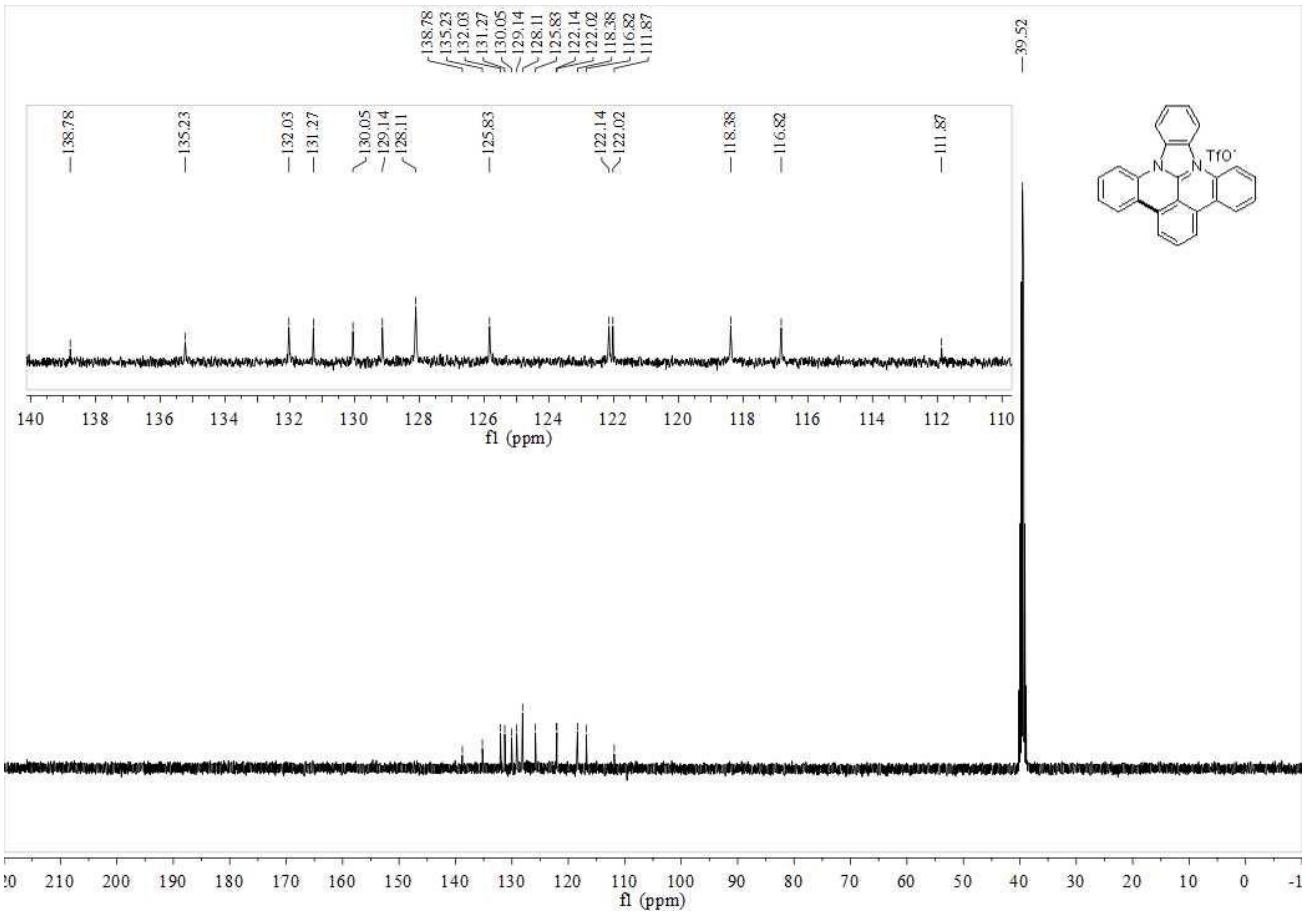
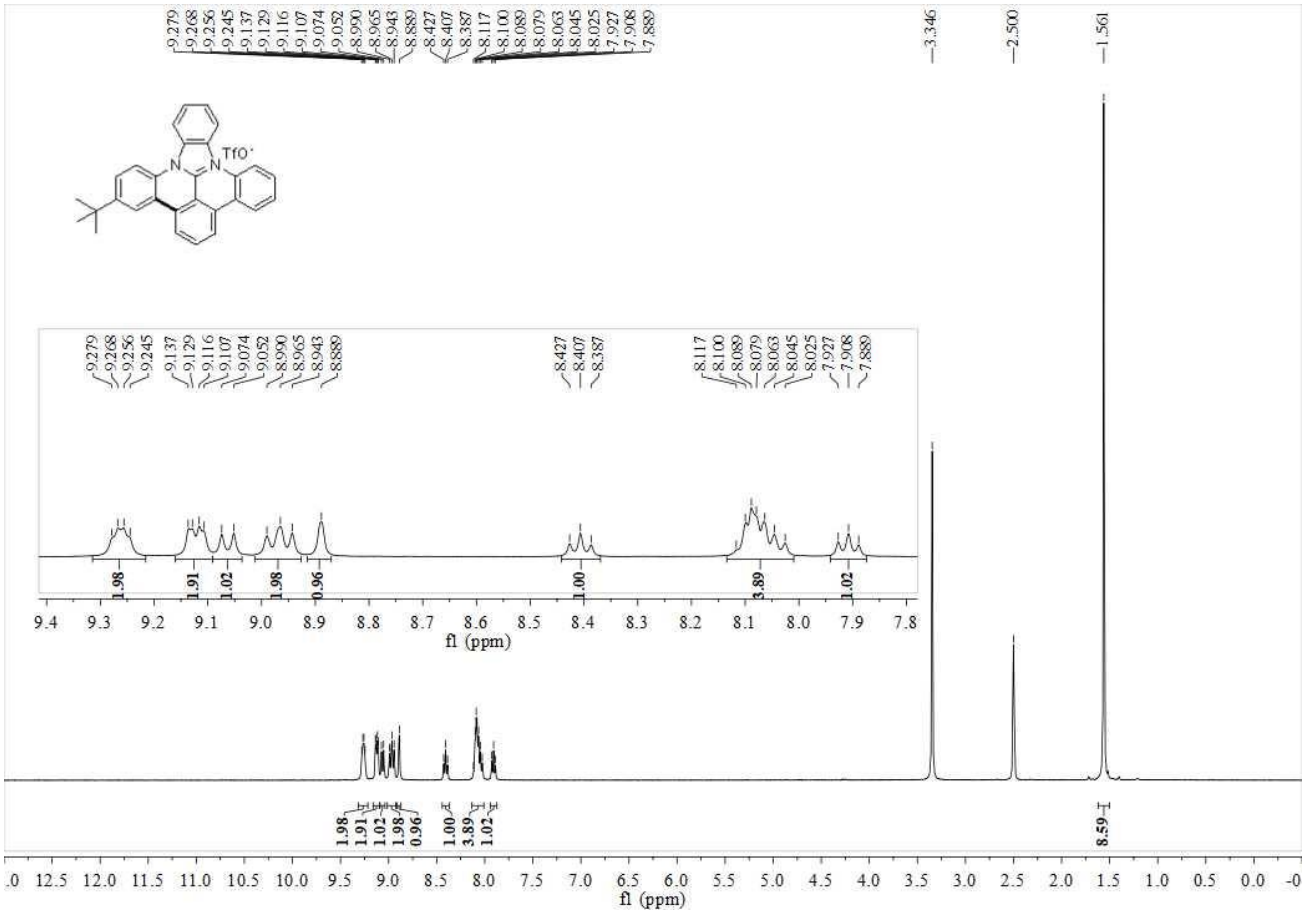
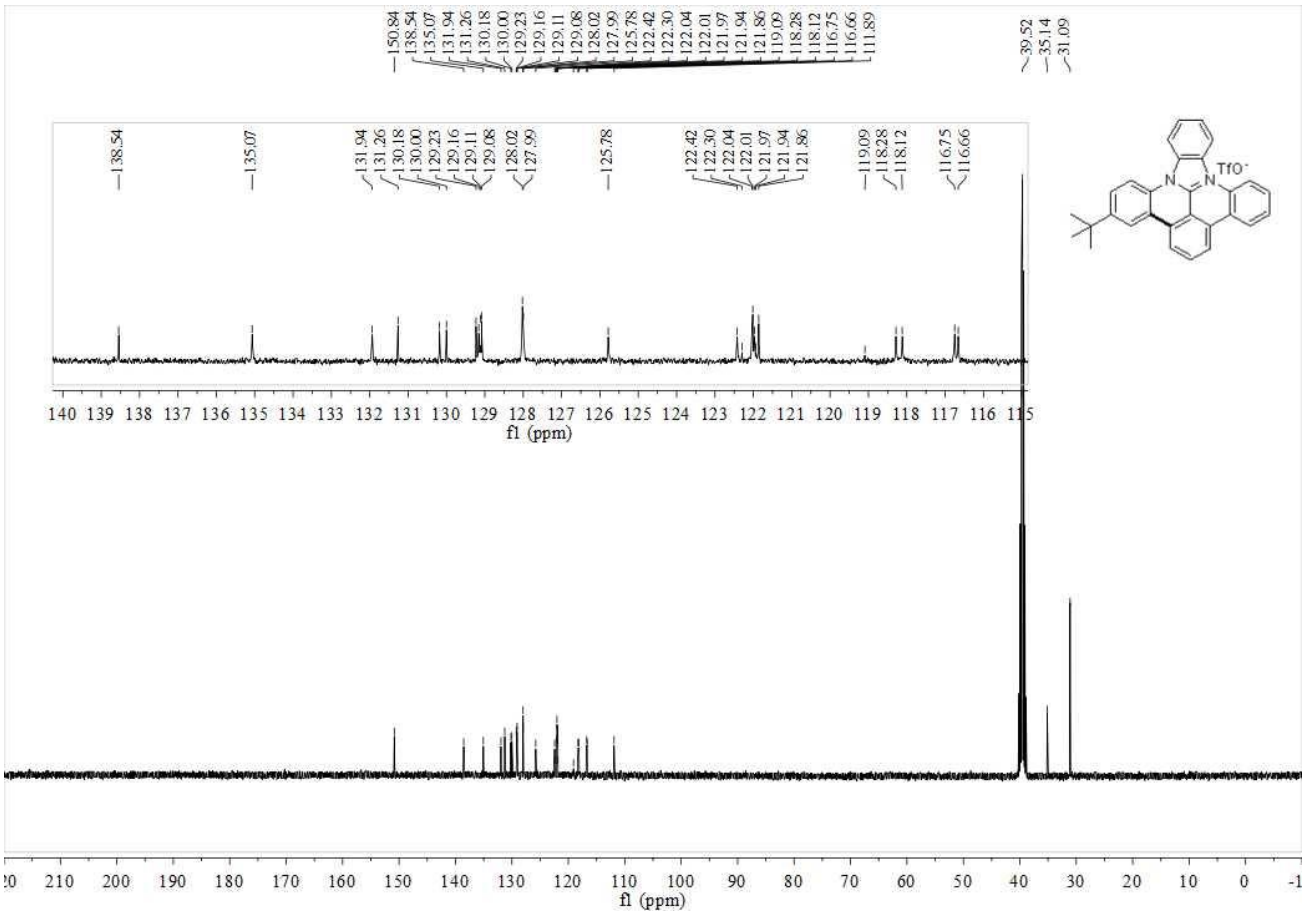
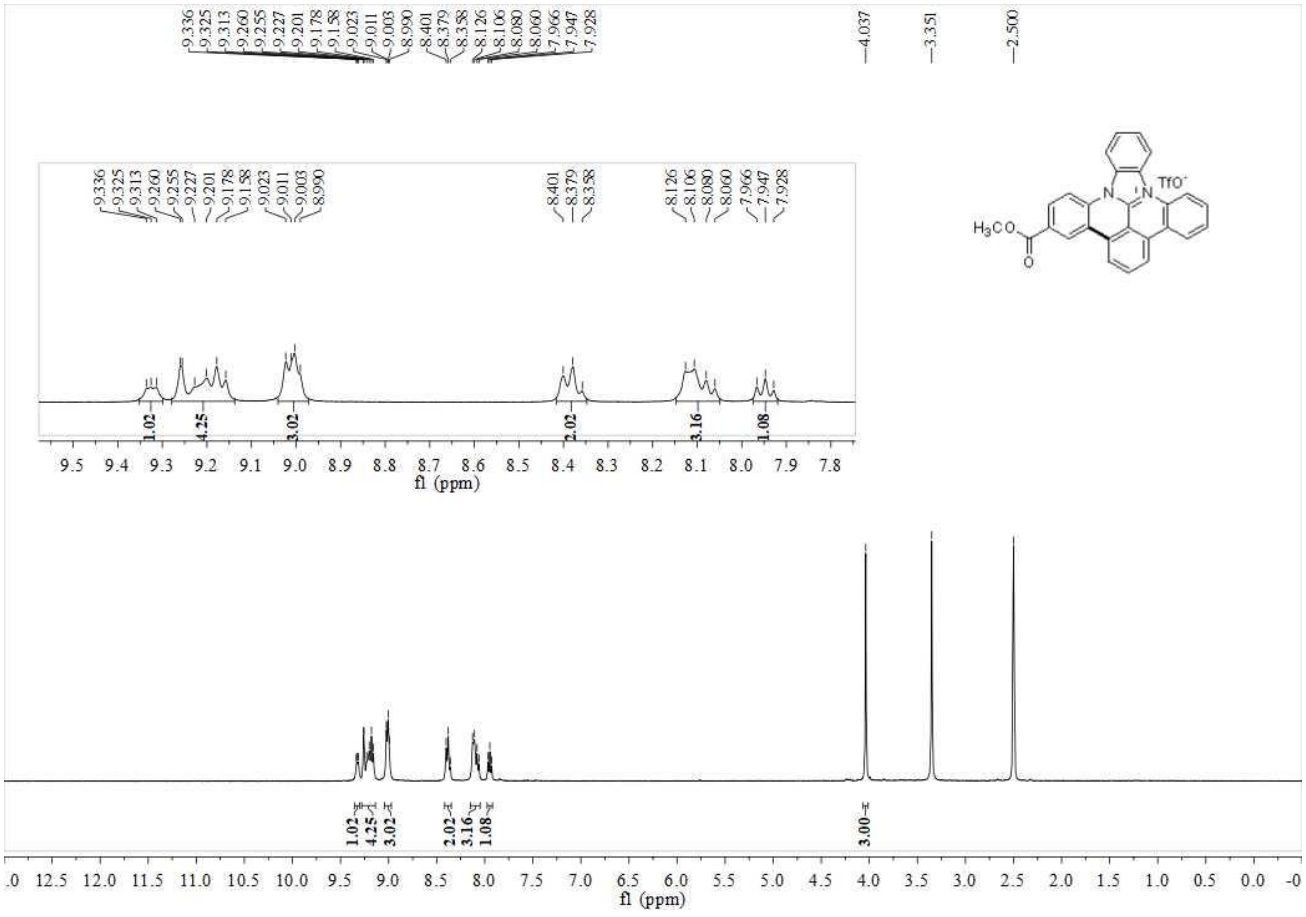
9.284
9.277
9.270
9.140
9.119
8.993
8.971
8.951
8.420
8.400
8.380
8.099
8.092
8.083
8.076
8.065
8.046
8.026
7.929
7.910
7.891
3.398
2.500
TfO⁻
2.00
2.00
4.00
1.00
4.06
2.02
f1 (ppm)


138.78
135.23
132.03
131.27
130.05
129.14
128.11
125.83
122.14
122.02
118.38
116.82
111.87
39.52
TfO⁻
f1 (ppm)


9.279
9.268
9.256
9.245
9.137
9.129
9.116
9.107
9.074
9.052
8.990
8.965
8.943
8.889
8.427
8.407
8.387
8.117
8.100
8.089
8.079
8.063
8.045
8.025
7.927
7.908
7.889
3.346
2.500
1.561
TfO⁻
1.98
1.91
1.02
1.98
0.96
1.00
3.89
1.02
8.59
fl (ppm)


150.84
138.54
135.07
131.94
131.26
130.18
130.00
129.23
129.16
129.11
129.08
128.02
127.99
125.78
122.42
122.30
122.04
122.01
121.97
121.94
121.86
119.09
118.28
118.12
116.75
116.66
111.89
39.52
35.14
31.09
TfO⁻
fl (ppm)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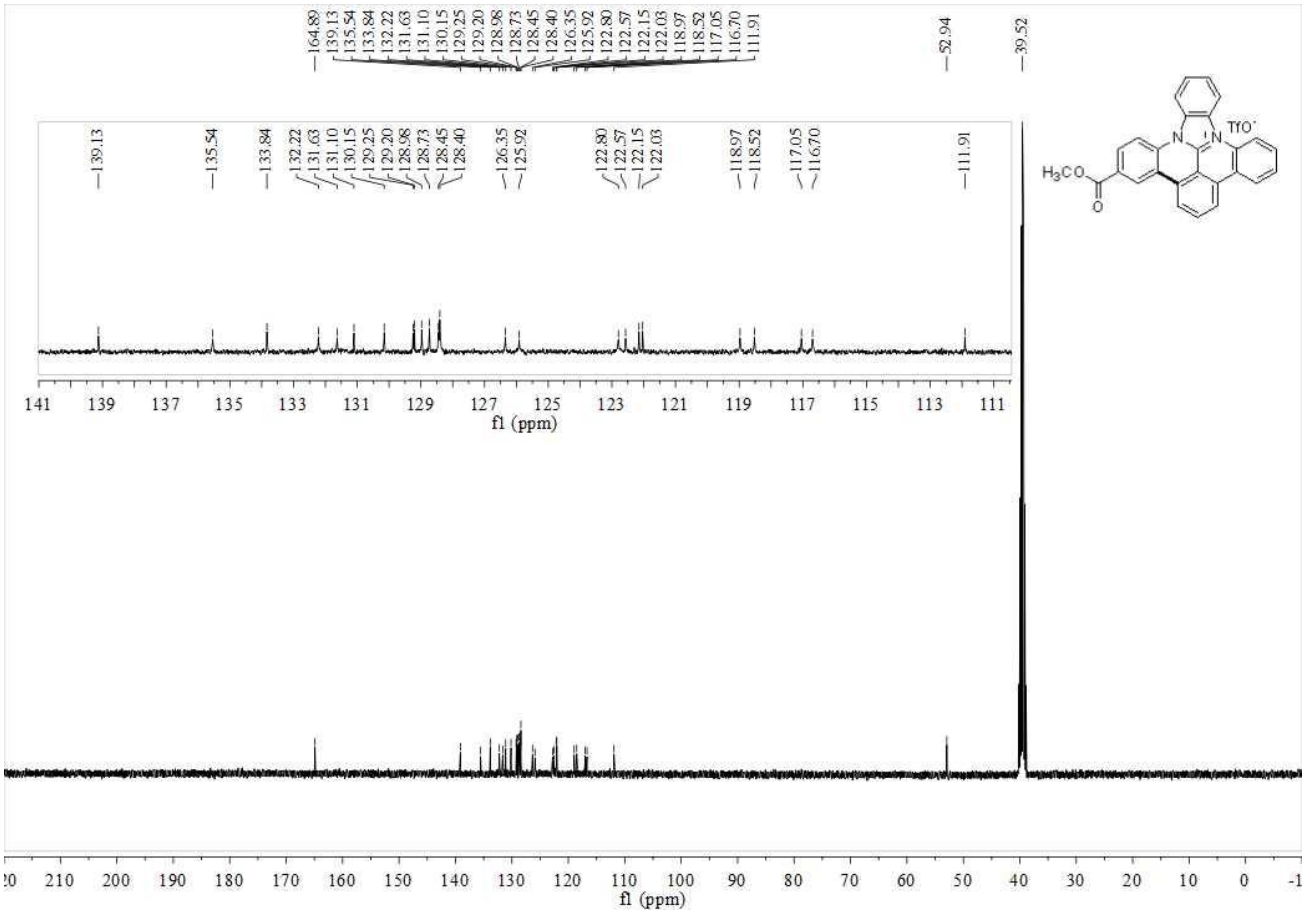
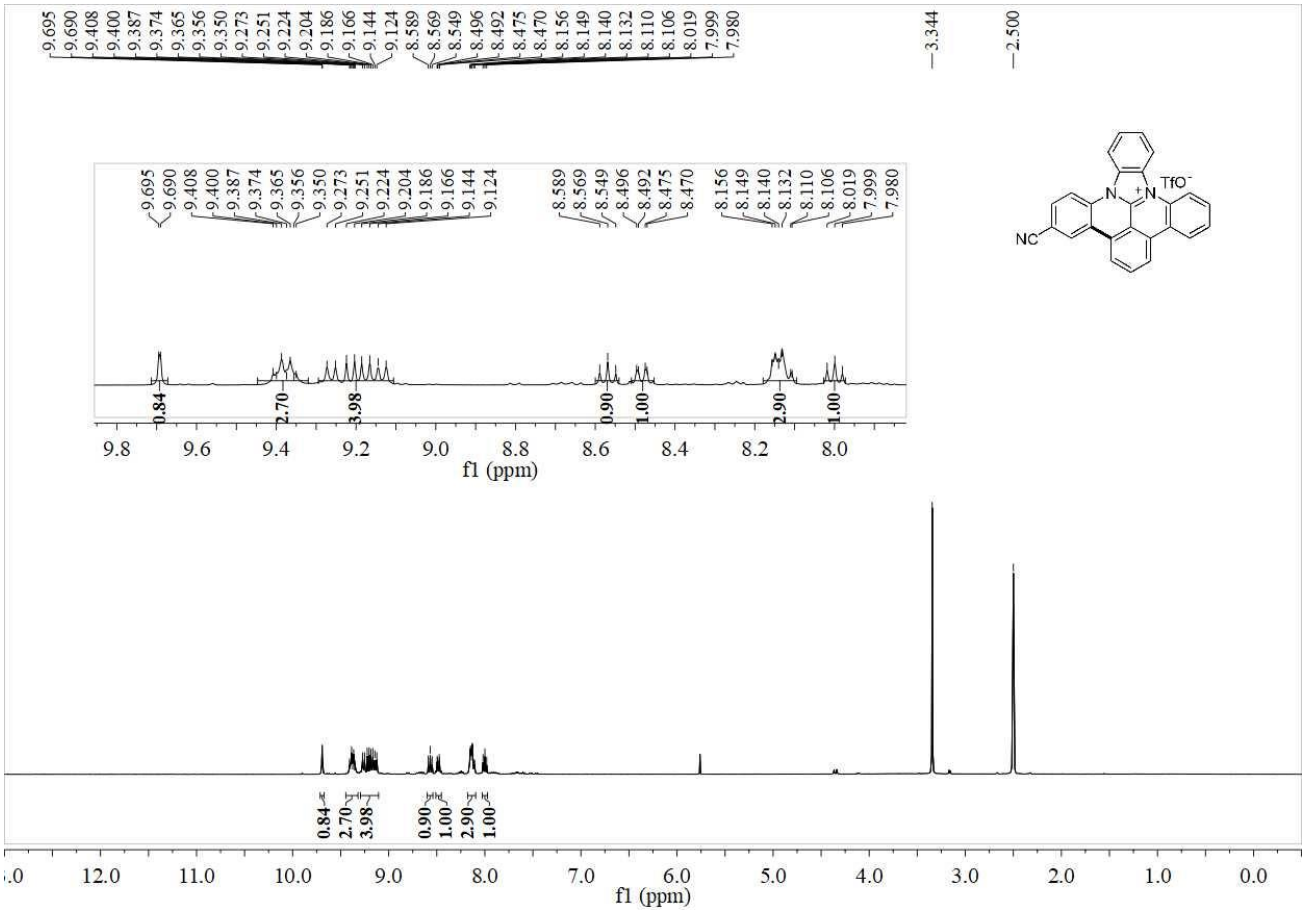
9.325
9.313
9.260
9.255
9.227
9.201
9.178
9.158
9.023
9.011
9.003
8.990
8.401
8.379
8.358
8.126
8.106
8.080
8.060
7.966
7.947
7.928
4.037
3.351
2.500
TfO⁻
H3CO
O
1.02
4.25
3.02
2.02
3.16
1.08
3.00
fl (ppm)


164.89
139.13
135.54
133.84
132.22
131.63
131.10
130.15
129.25
129.20
128.98
128.73
128.45
128.40
126.35
125.92
122.80
122.57
122.15
122.03
118.97
118.52
117.05
116.70
111.91
52.94
39.52
TfO⁻
H3CO
O
fl (ppm)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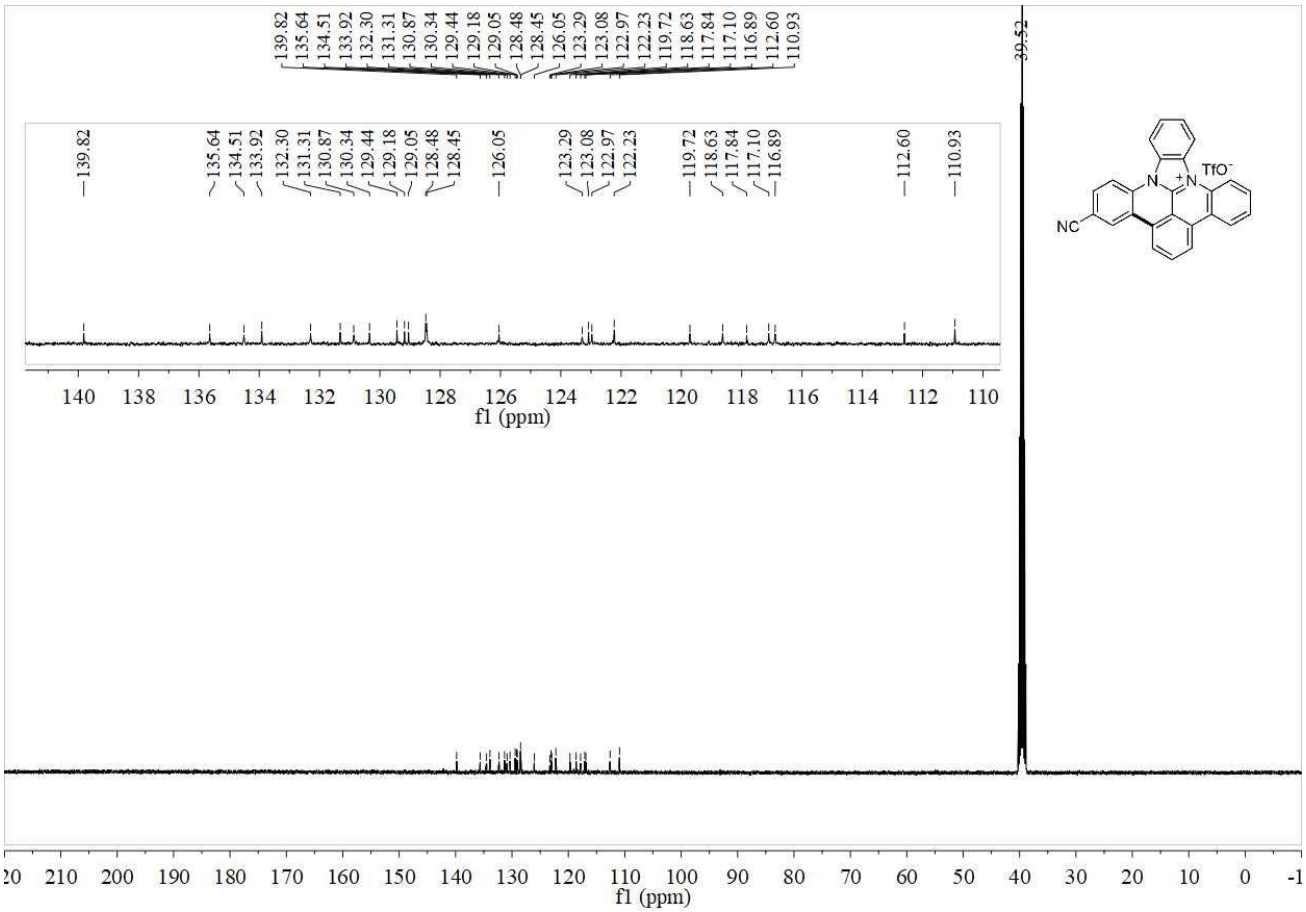
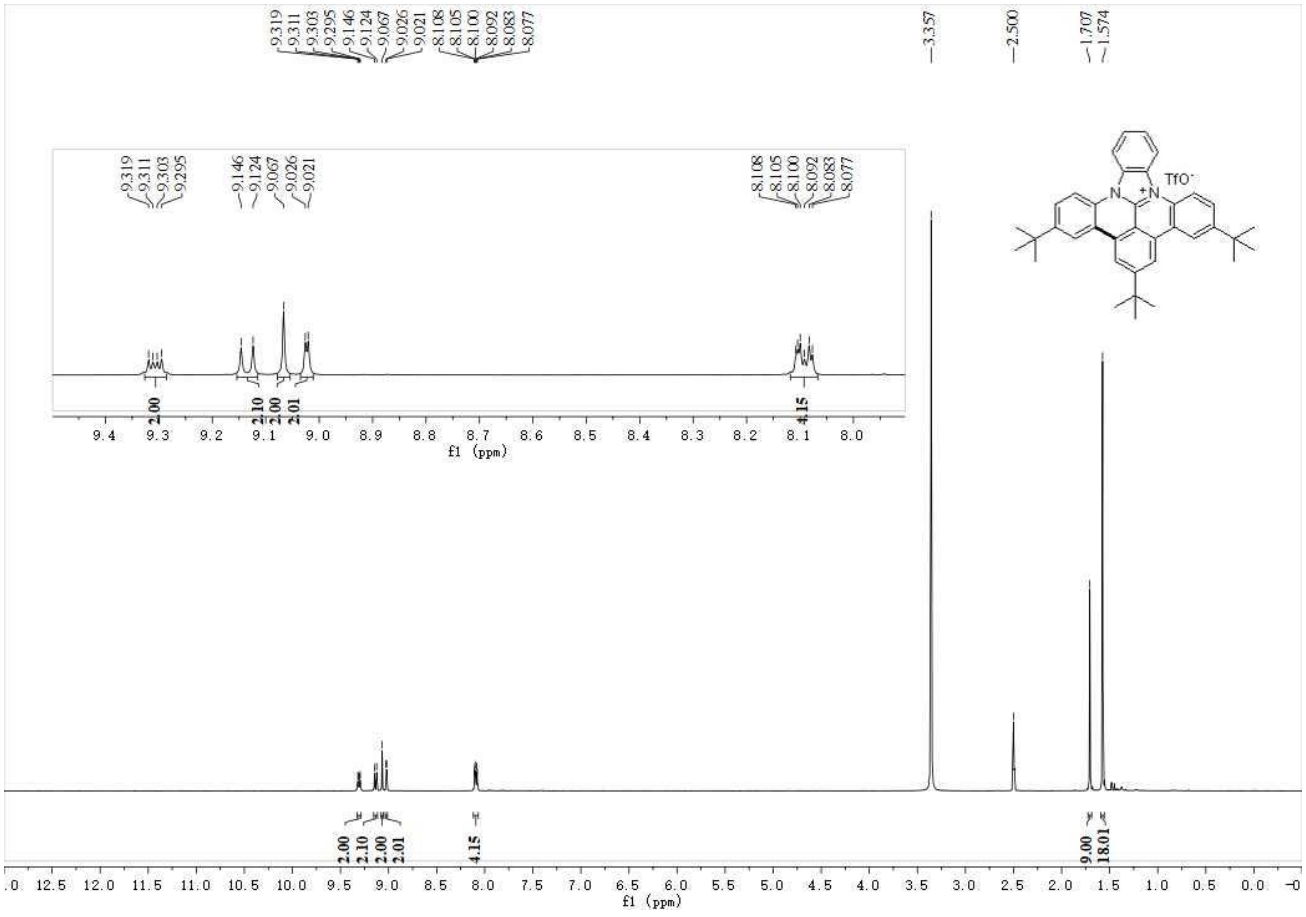
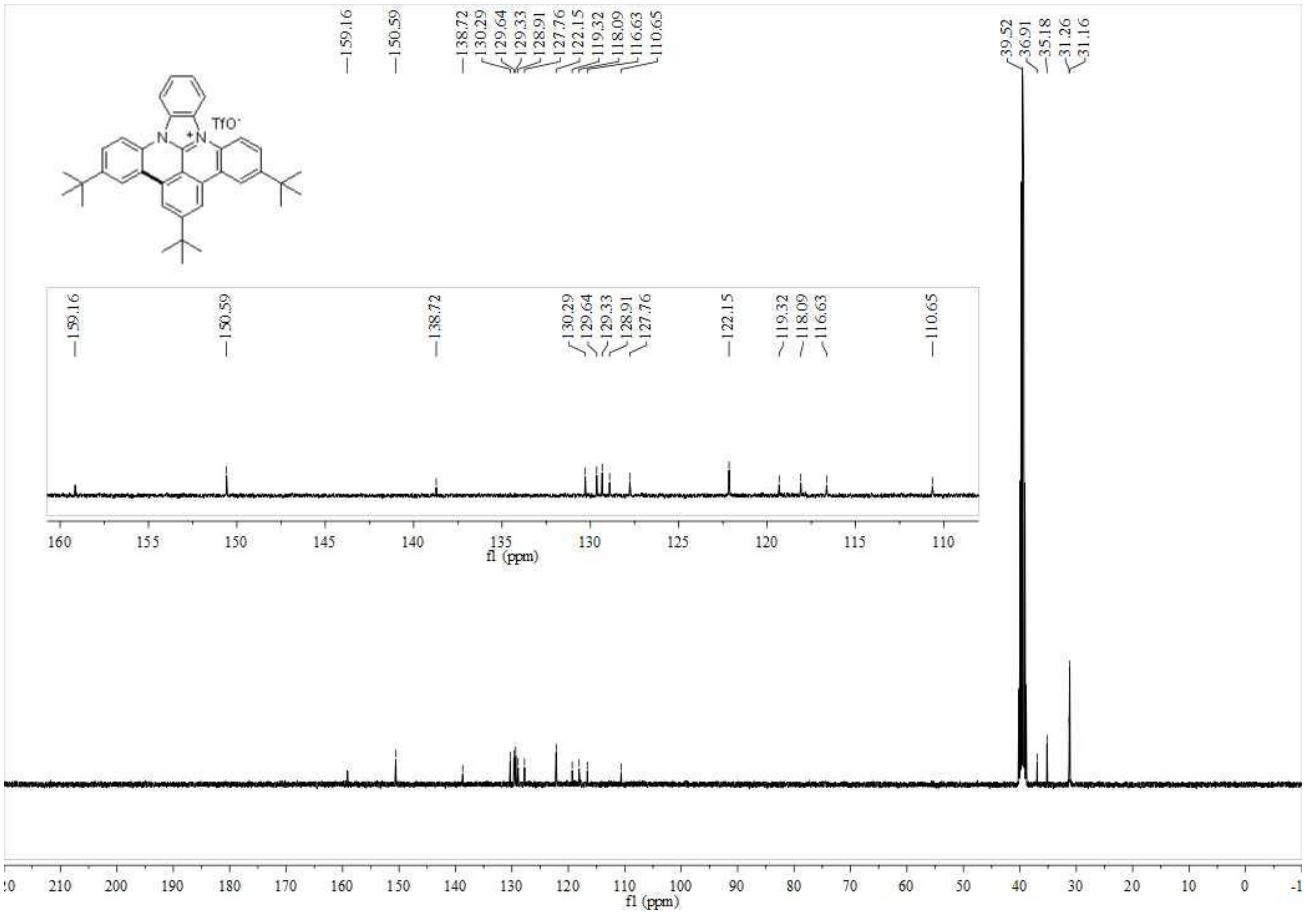
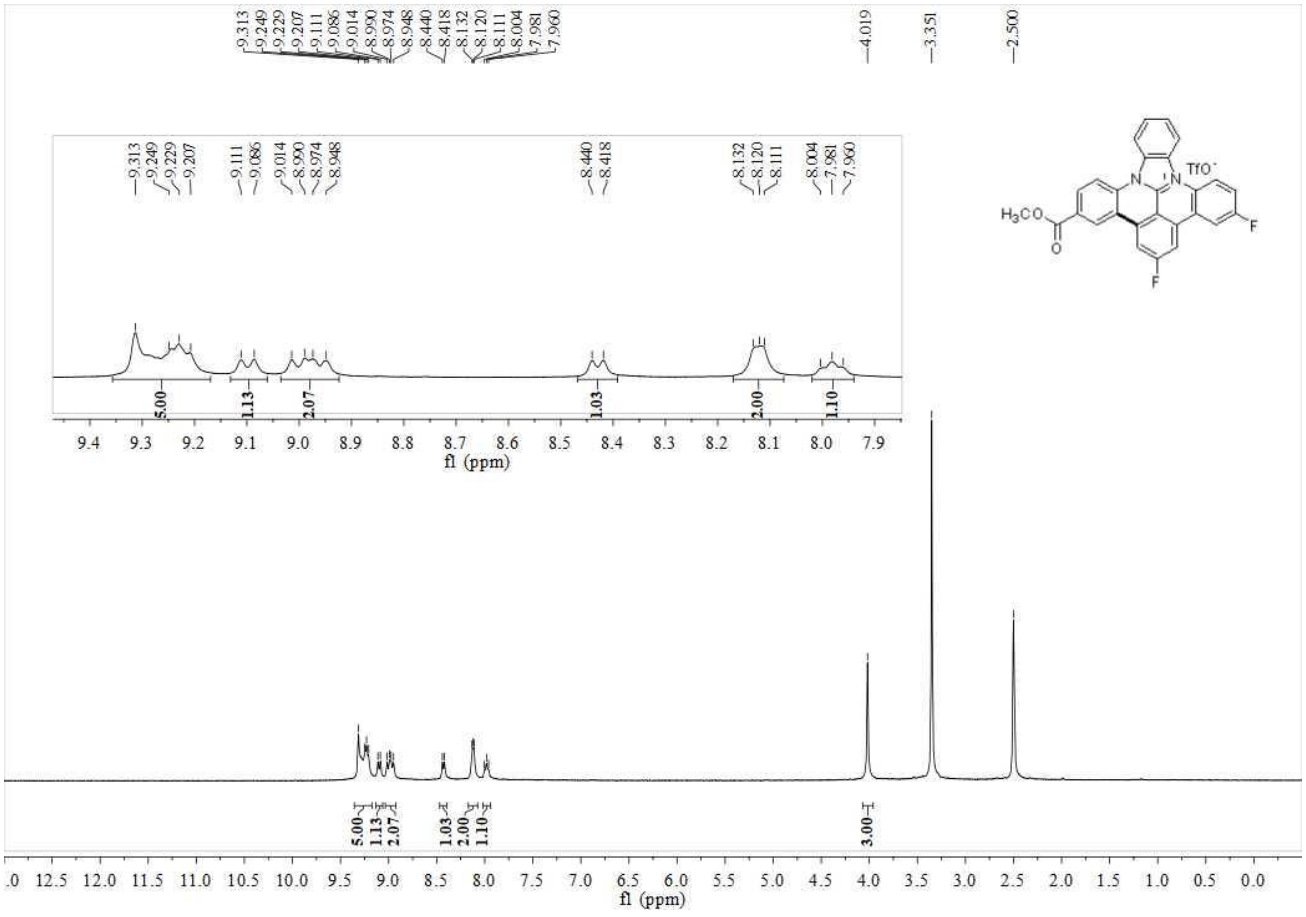
9.690
9.408
9.400
9.387
9.374
9.365
9.356
9.350
9.273
9.251
9.224
9.204
9.186
9.166
9.144
9.124
8.589
8.569
8.549
8.496
8.492
8.475
8.470
8.156
8.149
8.140
8.132
8.110
8.106
8.019
7.999
7.980
3.344
2.500
0.84
2.70
3.98
0.90
1.00
2.90
1.00
f1 (ppm)
TfO⁻
NC


139.82
135.64
134.51
133.92
132.30
131.31
130.87
130.34
129.44
129.18
129.05
128.48
128.45
126.05
123.29
123.08
122.97
122.23
119.72
118.63
117.84
117.10
116.89
112.60
110.93
39.52
f1 (ppm)
TfO⁻
NC


9.319
9.311
9.303
9.295
9.146
9.124
9.067
9.026
9.021
8.108
8.105
8.100
8.092
8.083
8.077
3.357
2.500
1.707
1.574
TfO⁻
2.00
2.10
2.00
2.01
4.15
9.00
18.01
f1 (ppm)


159.16
150.59
138.72
130.29
129.64
129.33
128.91
127.76
122.15
119.32
118.09
116.63
110.65
39.52
36.91
35.18
31.26
31.16
TfO⁻
f1 (ppm)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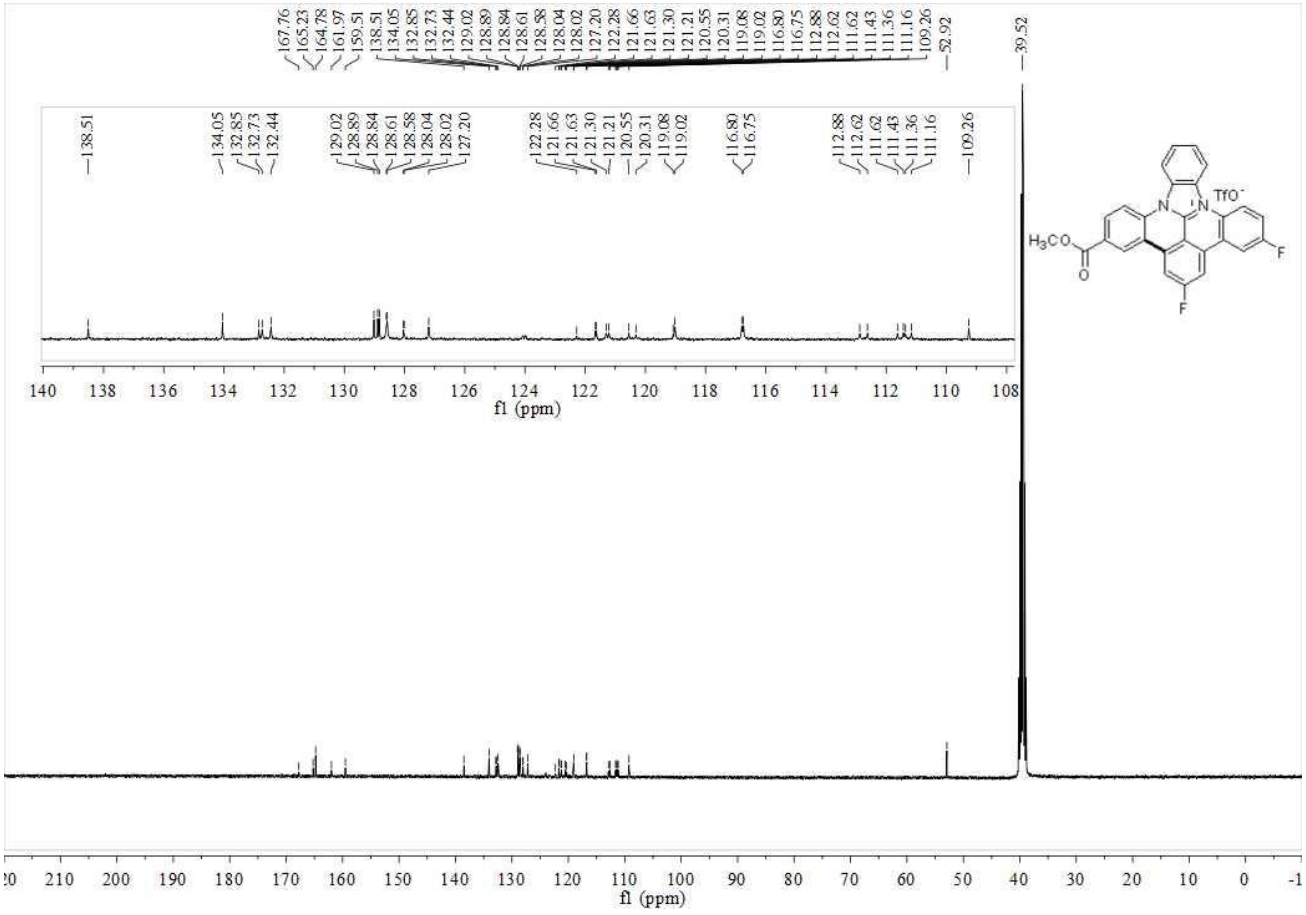
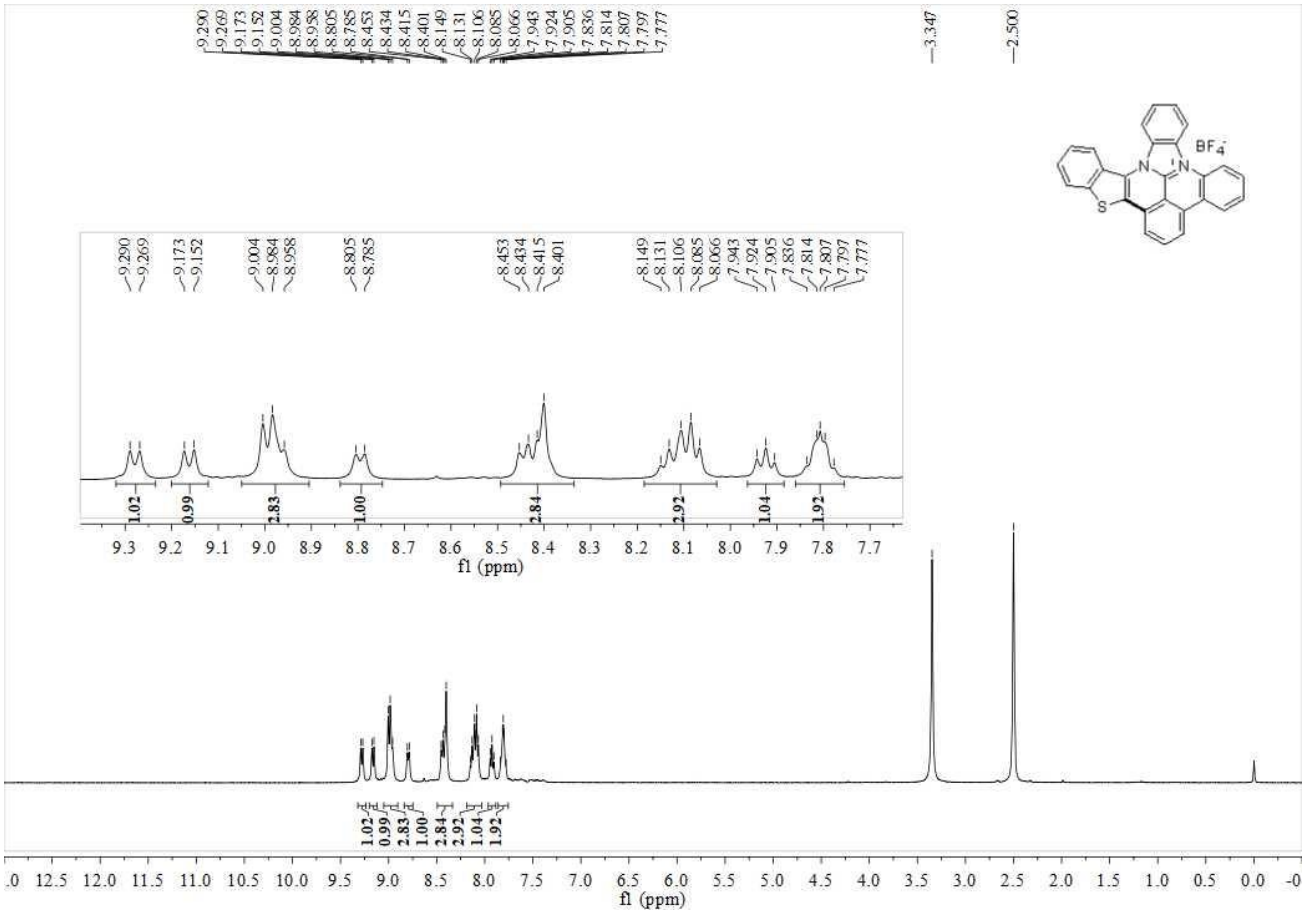
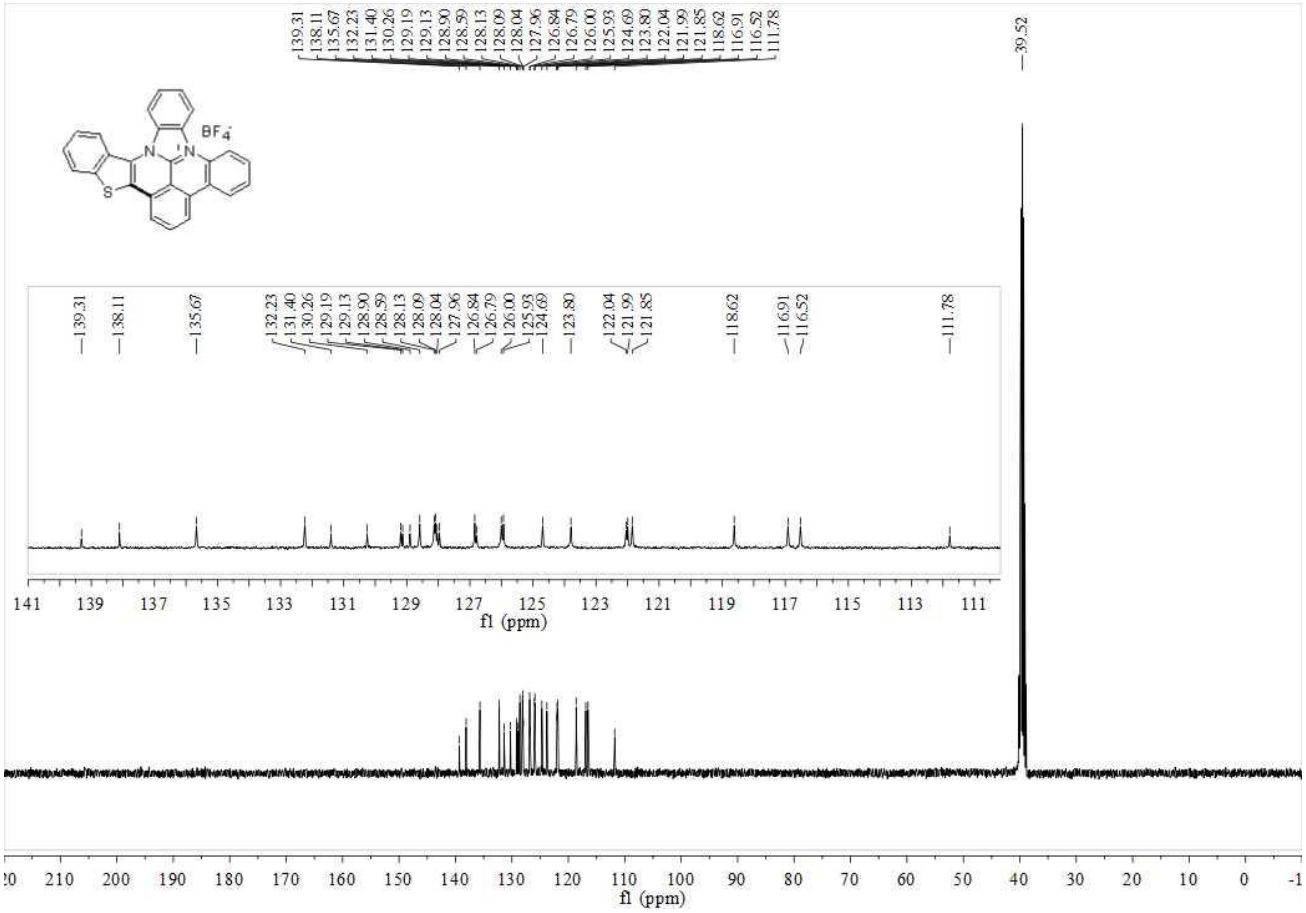
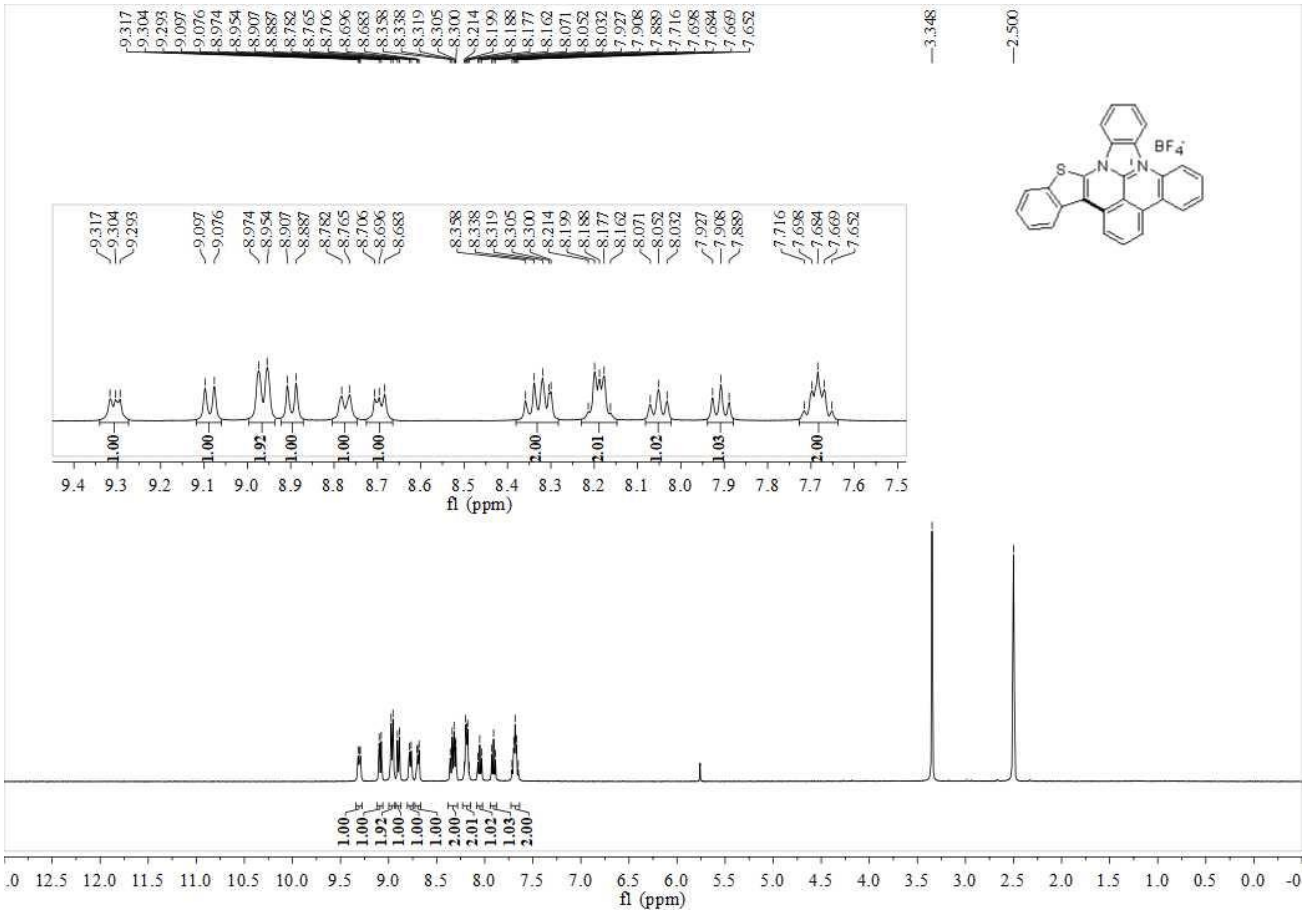
9.249
9.229
9.207
9.111
9.086
9.014
8.990
8.974
8.948
8.440
8.418
8.132
8.120
8.111
8.004
7.981
7.960
4.019
3.351
2.500
5.00
1.13
2.07
1.03
2.00
1.10
3.00
fl (ppm)
TfO⁻
H3CO
O
F
F


167.76
165.23
164.78
161.97
159.51
138.51
134.05
132.85
132.73
132.44
129.02
128.89
128.84
128.61
128.58
128.04
128.02
127.20
122.28
121.66
121.63
121.30
121.21
120.55
120.31
119.08
119.02
116.80
116.75
112.88
112.62
111.62
111.43
111.36
111.16
109.26
52.92
39.52
fl (ppm)
TfO⁻
H3CO
O
F
F


9.290
9.269
9.173
9.152
9.004
8.984
8.958
8.805
8.785
8.453
8.434
8.415
8.401
8.149
8.131
8.106
8.085
8.066
7.943
7.924
7.905
7.836
7.814
7.807
7.799
7.777
3.347
2.500
BF4-
1.02
0.99
2.83
1.00
2.84
2.92
1.04
1.92
fl (ppm)


139.31
138.11
135.67
132.23
131.40
130.26
129.19
129.13
128.90
128.59
128.13
128.09
128.04
127.96
126.84
126.79
126.00
125.93
124.69
123.80
122.04
121.99
121.85
118.62
116.91
116.52
111.78
39.52
BF4-
fl (ppm)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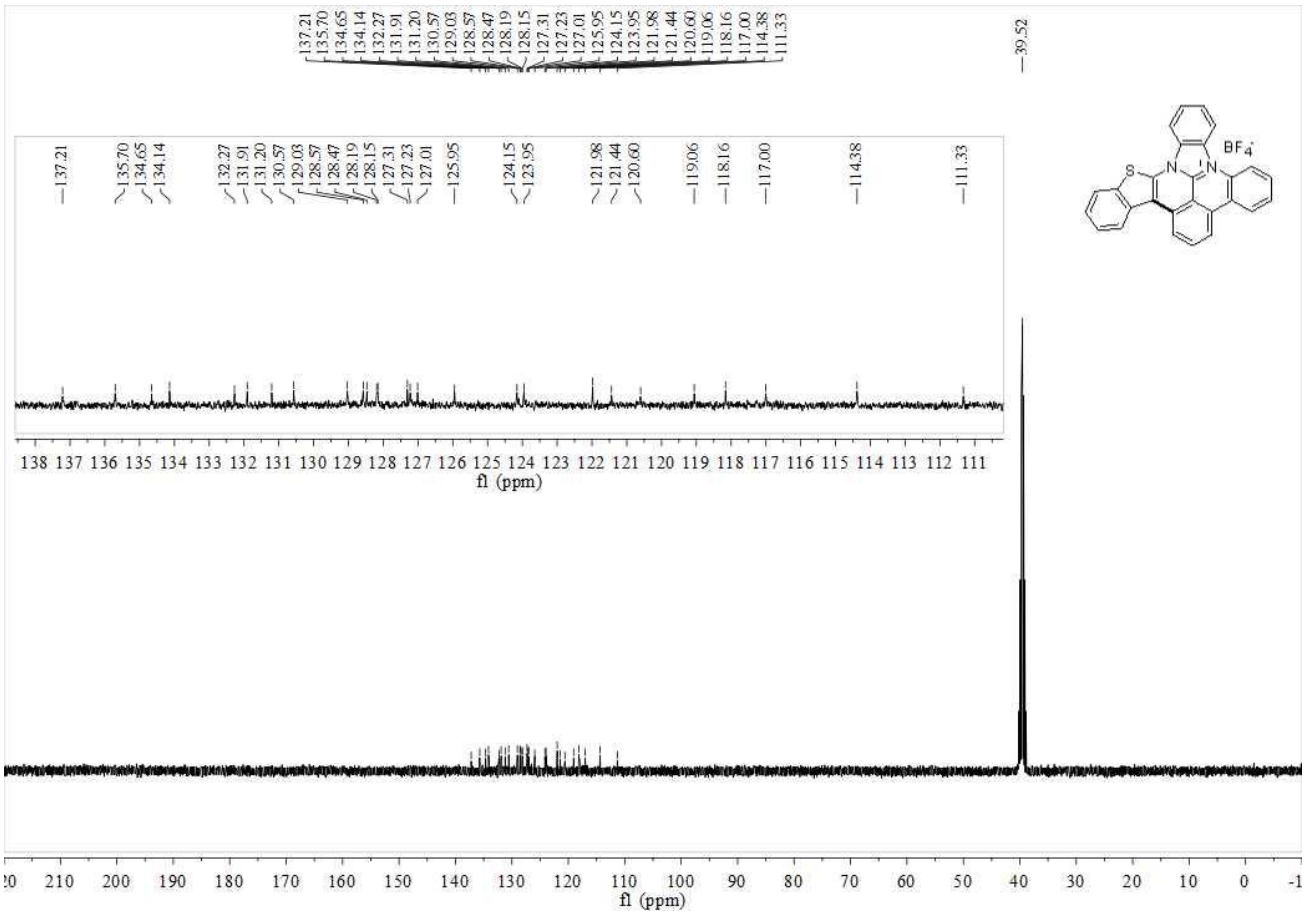
9.293
9.097
9.076
8.974
8.954
8.907
8.887
8.782
8.765
8.706
8.696
8.683
8.358
8.338
8.319
8.305
8.300
8.214
8.199
8.188
8.177
8.162
8.071
8.052
8.032
7.927
7.908
7.889
7.716
7.698
7.684
7.669
7.652
3.348
2.500
BF4-
1.00
1.00
1.92
1.00
1.00
1.00
2.00
2.01
1.02
1.03
2.00
fl (ppm)


137.21
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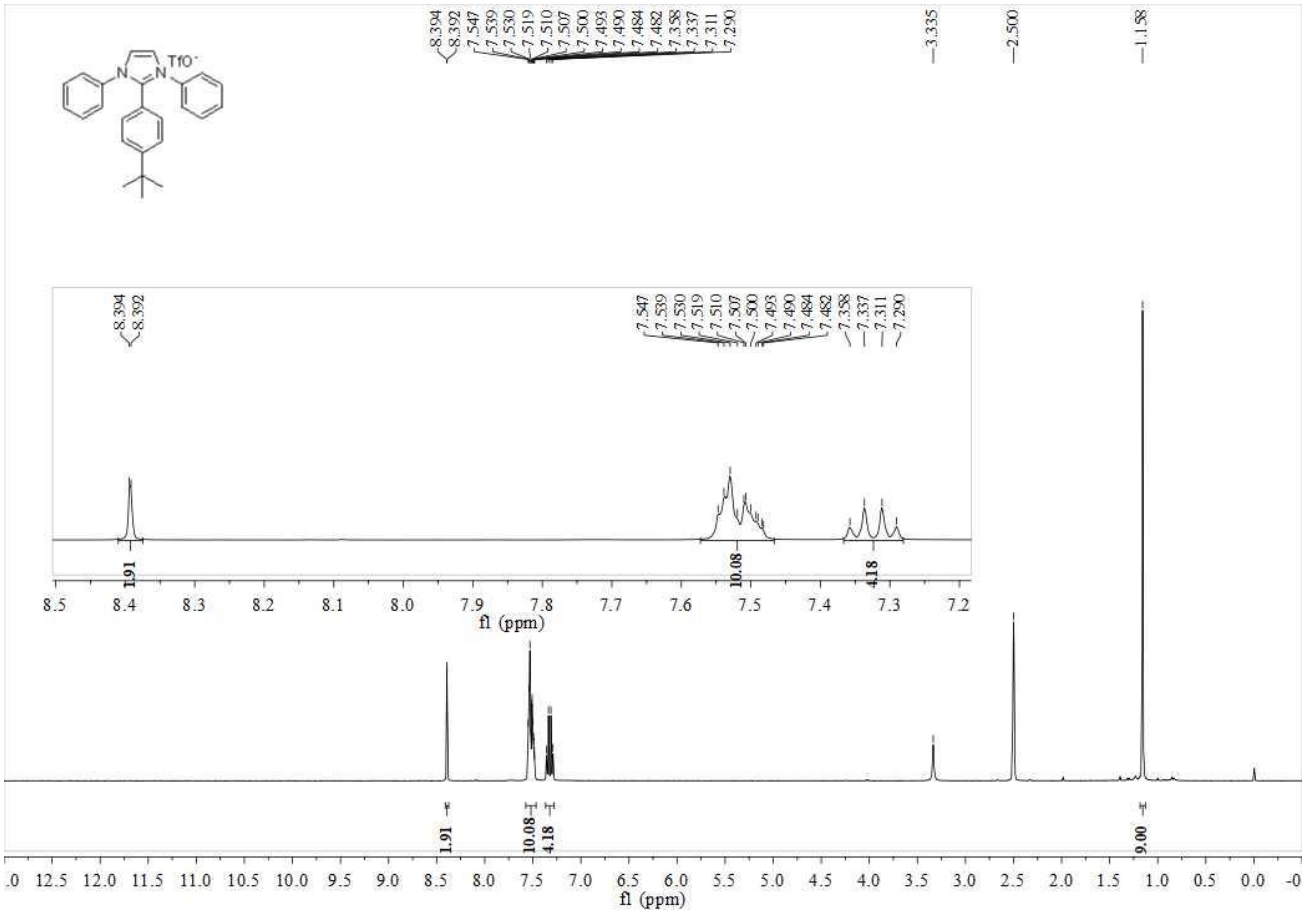
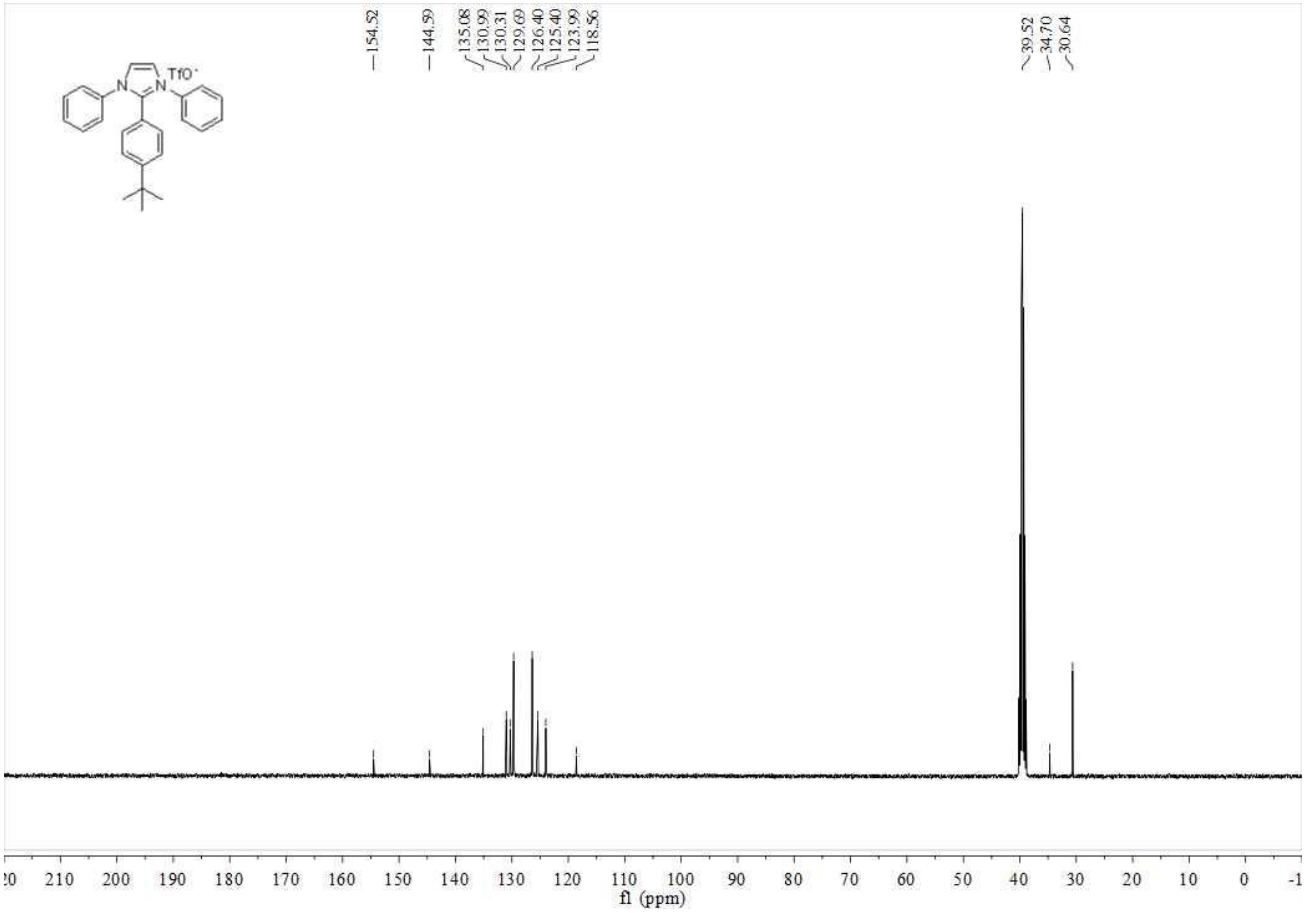
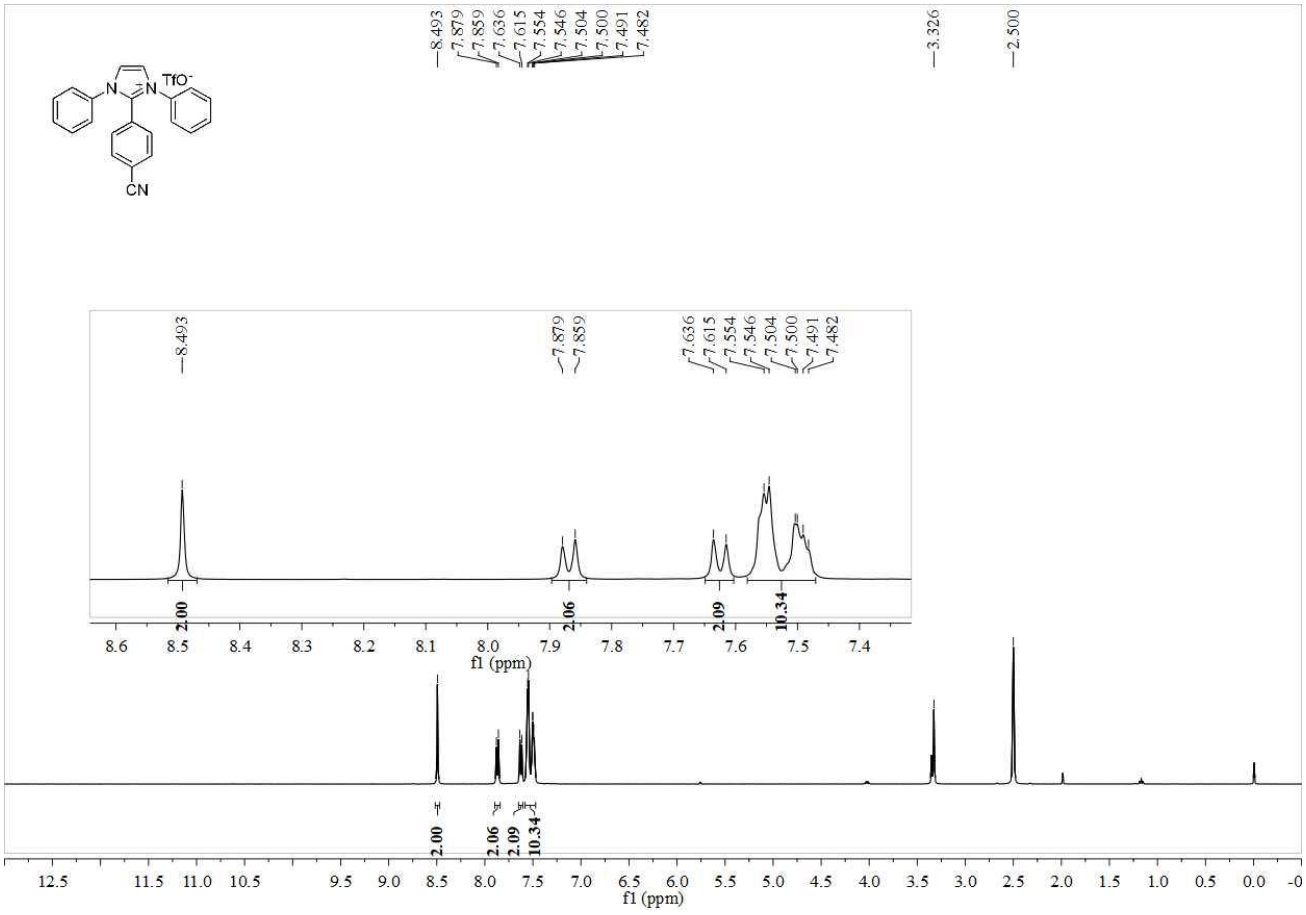
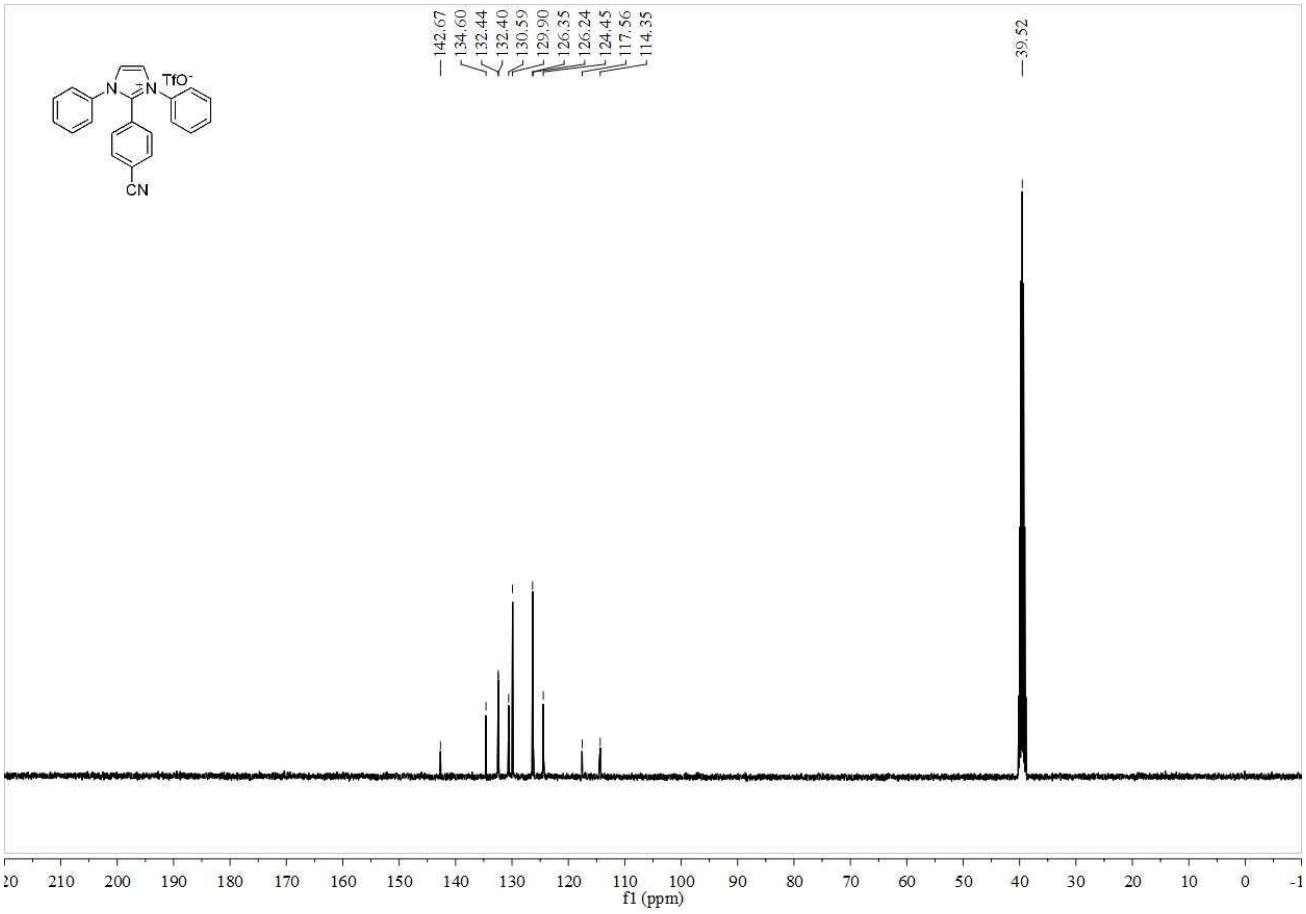
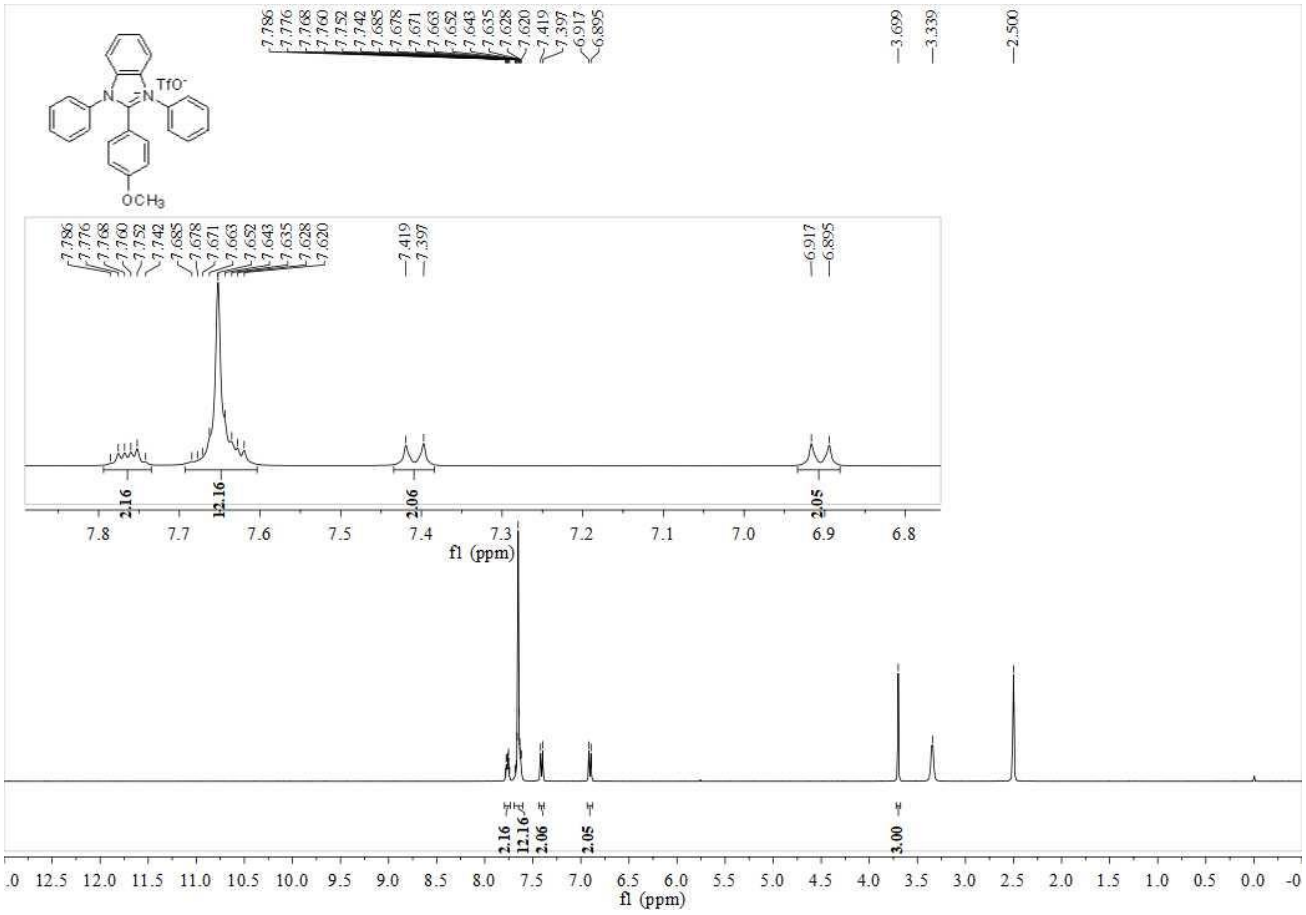
134.65
134.14
132.27
131.91
131.20
130.57
129.03
128.57
128.47
128.19
128.15
127.31
127.23
127.01
125.95
124.15
123.95
121.98
121.44
120.60
119.06
118.16
117.00
114.38
111.33
39.52
BF4-
fl (ppm)

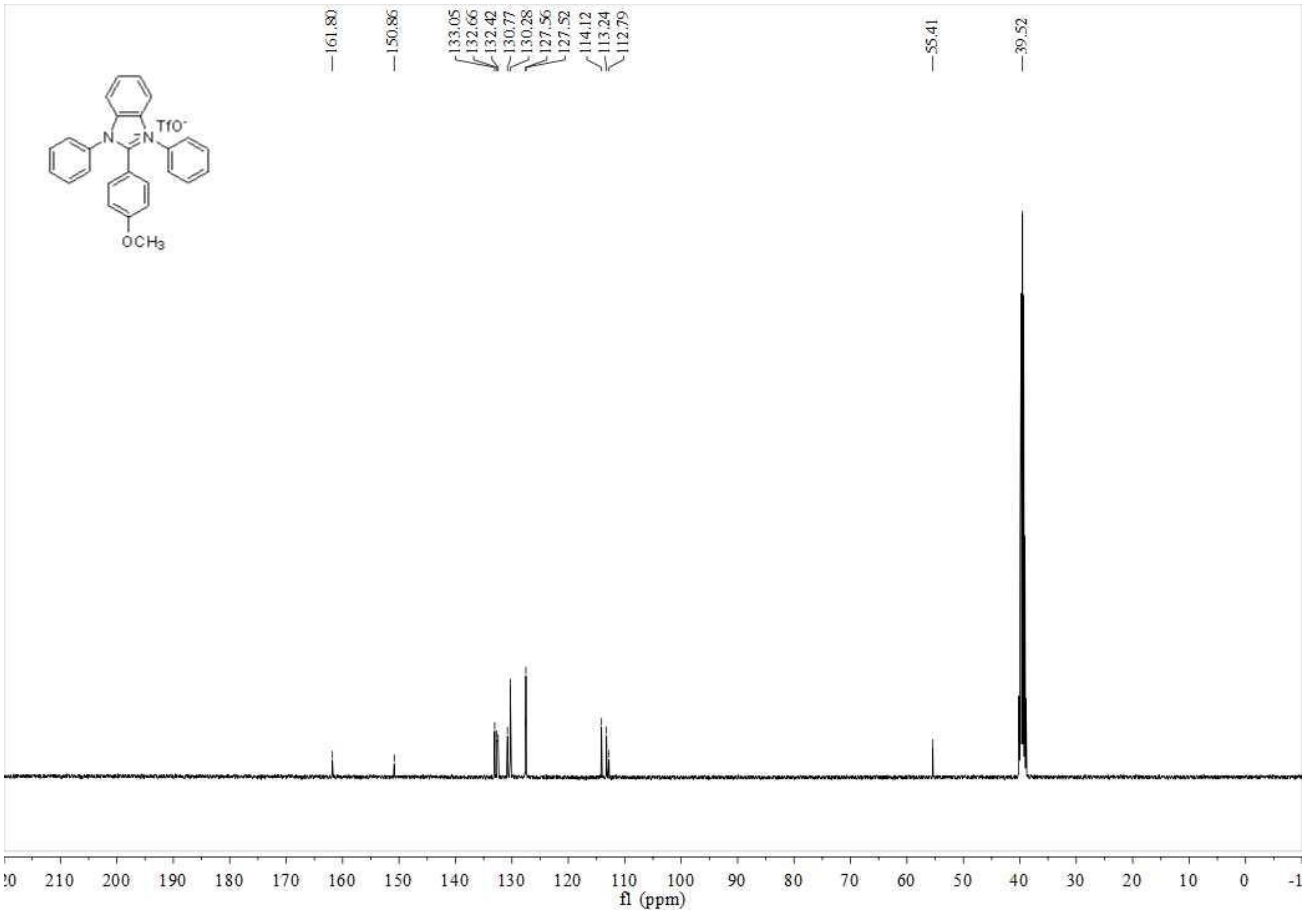

TfO⁻
8.394
8.392
7.547
7.539
7.530
7.519
7.510
7.507
7.500
7.493
7.490
7.484
7.482
7.358
7.337
7.311
7.290
3.335
2.500
1.588
1.91
10.08
4.18
9.00
fl (ppm)

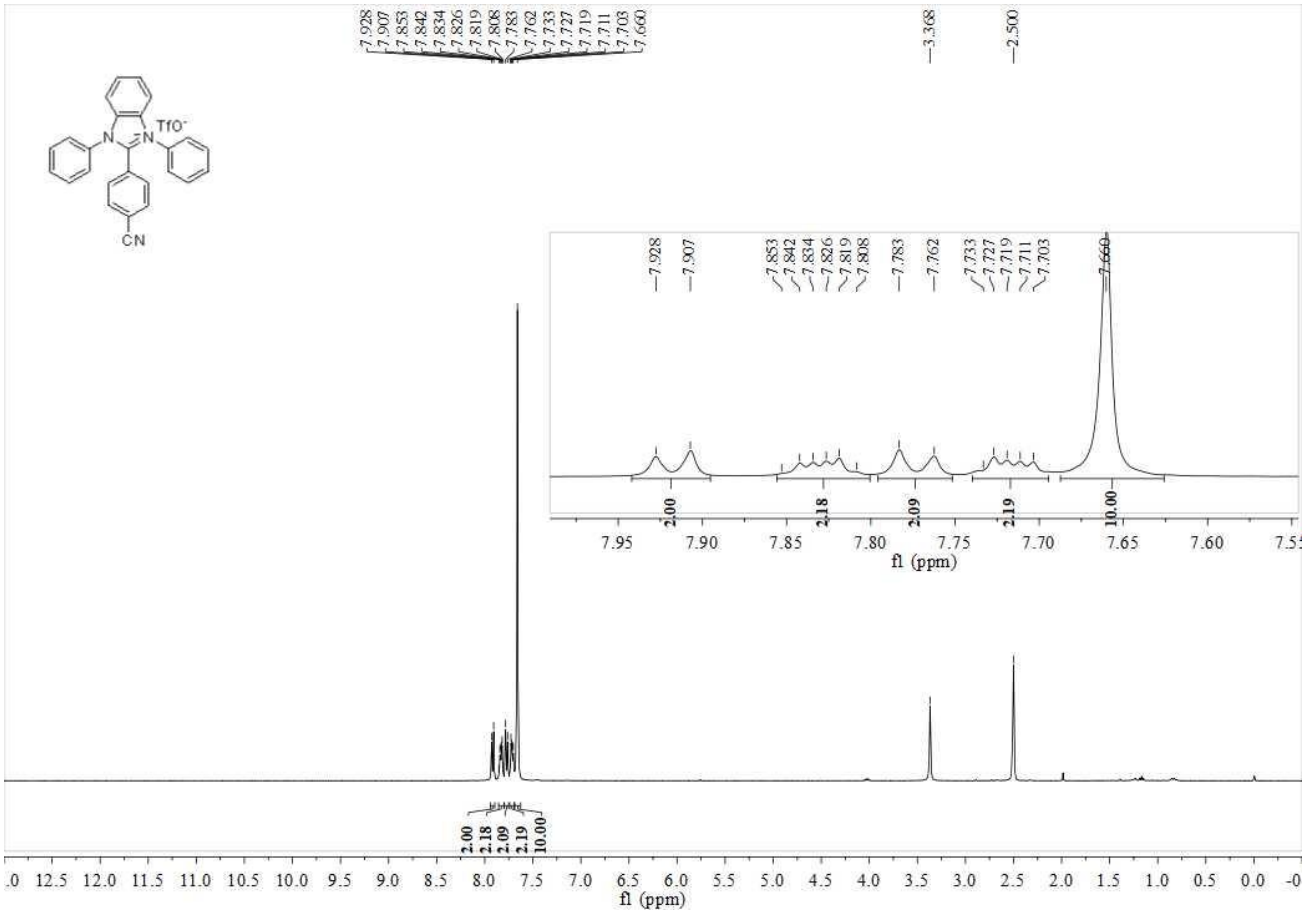

TfO⁻
154.52
144.59
135.08
130.99
130.31
129.69
126.40
125.40
123.99
118.56
39.52
34.70
30.64
fl (ppm)

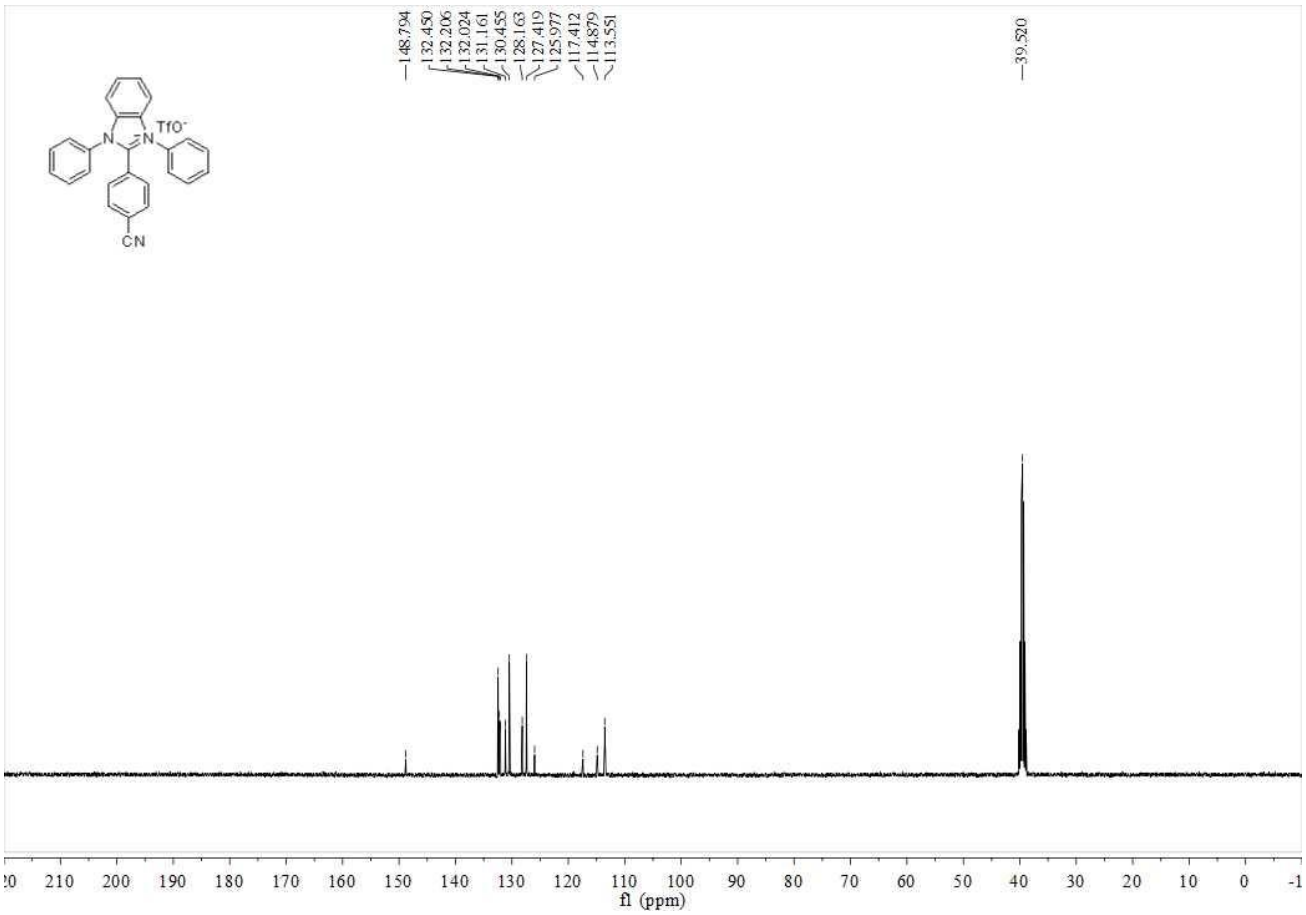

8.493
7.879
7.859
7.636
7.615
7.554
7.546
7.504
7.500
7.491
7.482
3.326
2.500
TfO-
CN
2.00
2.06
2.09
10.34
f1 (ppm)

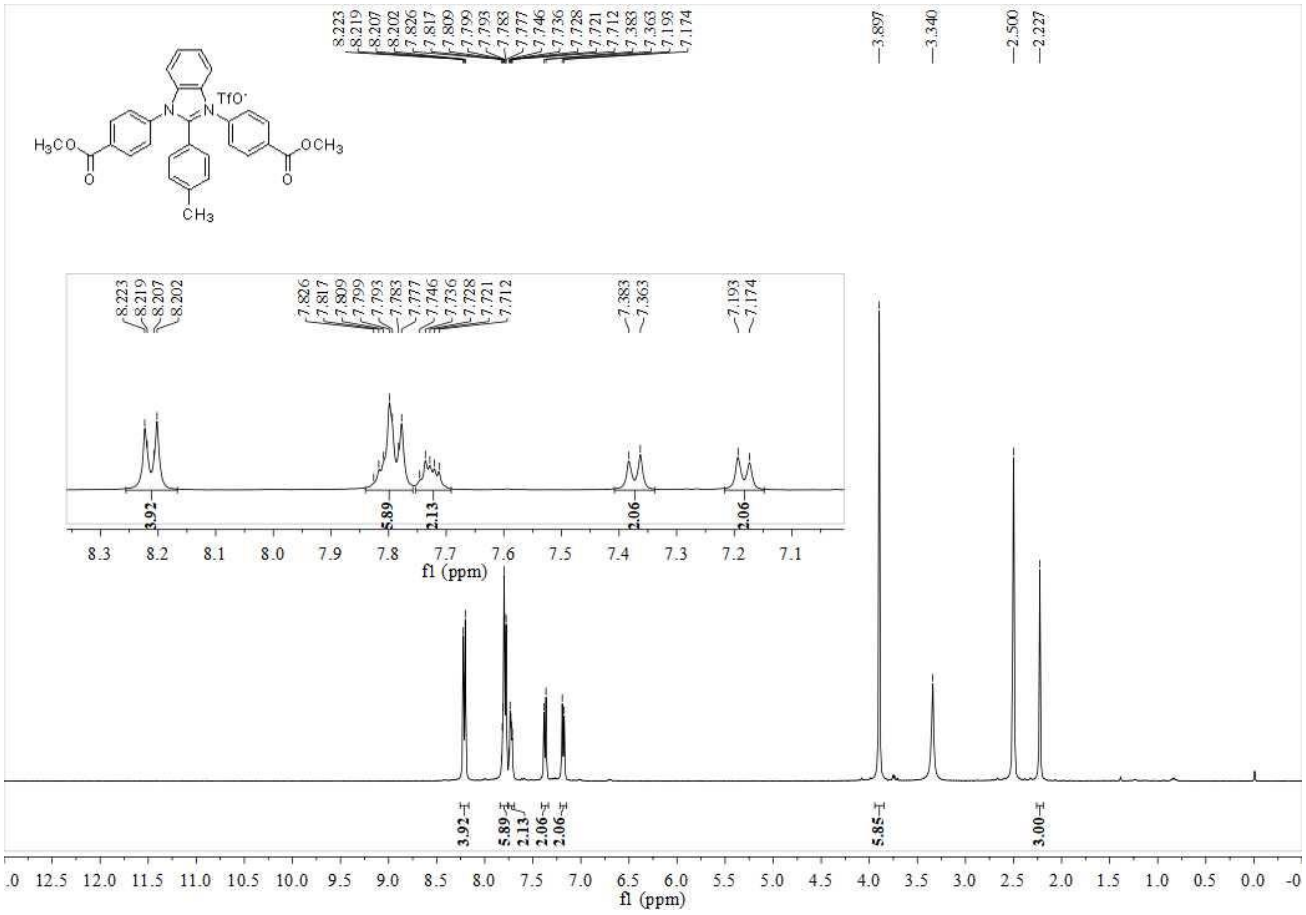

142.67
134.60
132.44
132.40
130.59
129.90
126.35
126.24
124.45
117.56
114.35
39.52
TfO-
CN
f1 (ppm)

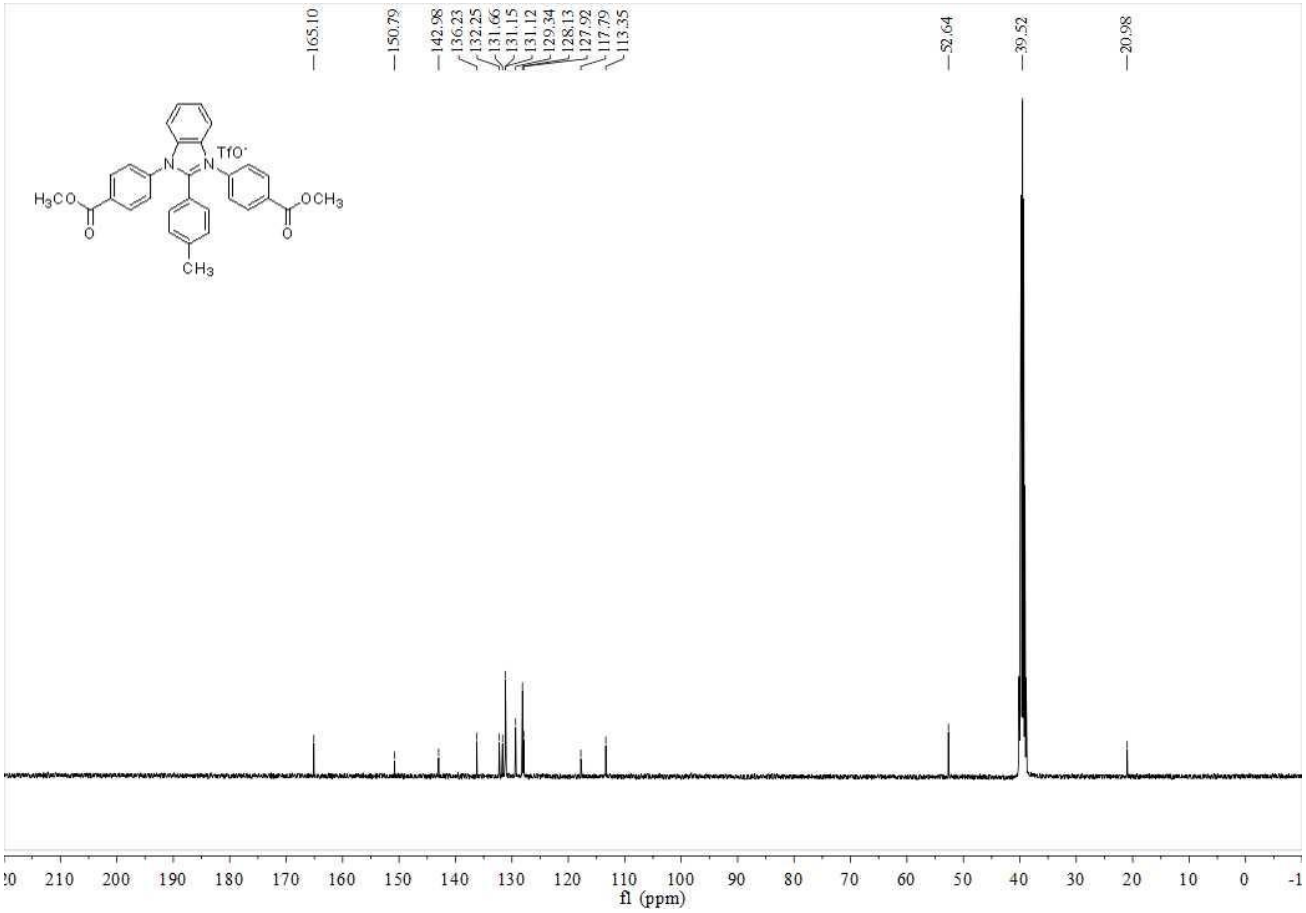

7.786
7.776
7.768
7.760
7.752
7.742
7.685
7.678
7.671
7.663
7.652
7.643
7.635
7.628
7.620
7.419
7.397
6.917
6.895
3.699
3.339
2.500
TfO⁻
OCH3
2.16
12.16
2.06
2.05
3.00
f1 (ppm)

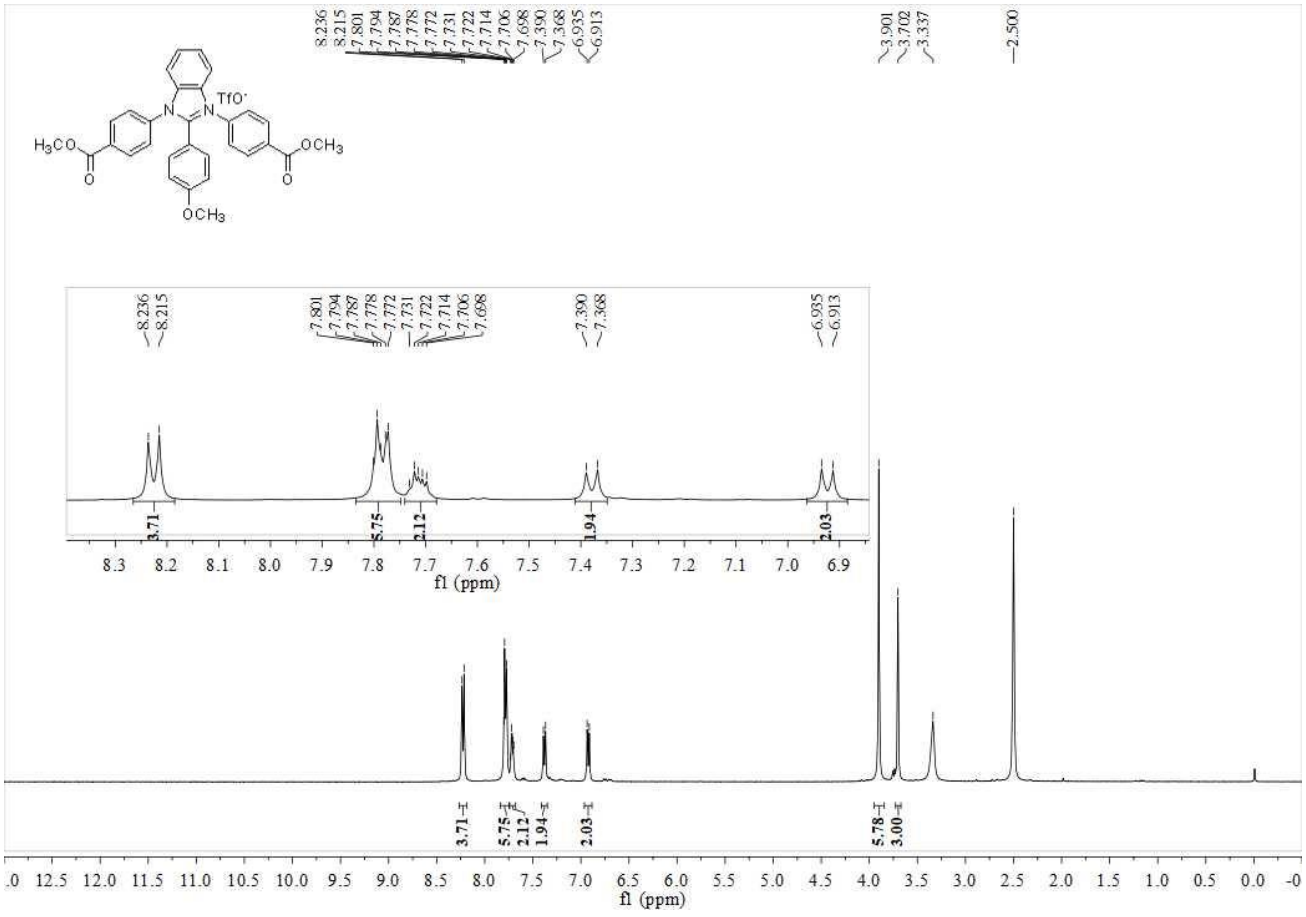

161.80
150.86
133.05
132.66
132.42
130.77
130.28
127.56
127.52
114.12
113.24
112.79
55.41
39.52
TfO⁻
OCH3
f1 (ppm)


7.928
7.907
7.853
7.842
7.834
7.826
7.819
7.808
7.783
7.762
7.733
7.727
7.719
7.711
7.703
7.660
3.368
2.500
TfO⁻
N
N
CN
2.00
2.18
2.09
2.19
10.00
fl (ppm)


148.794
132.450
132.206
132.024
131.161
130.455
128.163
127.419
125.977
117.412
114.879
113.551
39.520
TfO⁻
N
N
CN
fl (ppm)


8.223
8.219
8.207
8.202
7.826
7.817
7.809
7.799
7.793
7.783
7.777
7.746
7.736
7.728
7.721
7.712
7.383
7.363
7.193
7.174
3.897
3.340
2.500
2.227
TfO⁻
H3CO
OCH3
CH3
3.92
5.89
2.13
2.06
2.06
5.85
3.00
fl (ppm)


165.10
150.79
142.98
136.23
132.25
131.66
131.15
131.12
129.34
128.13
127.92
117.79
113.35
52.64
39.52
20.98
TfO⁻
H3CO
OCH3
CH3
fl (ppm)


8.236
8.215
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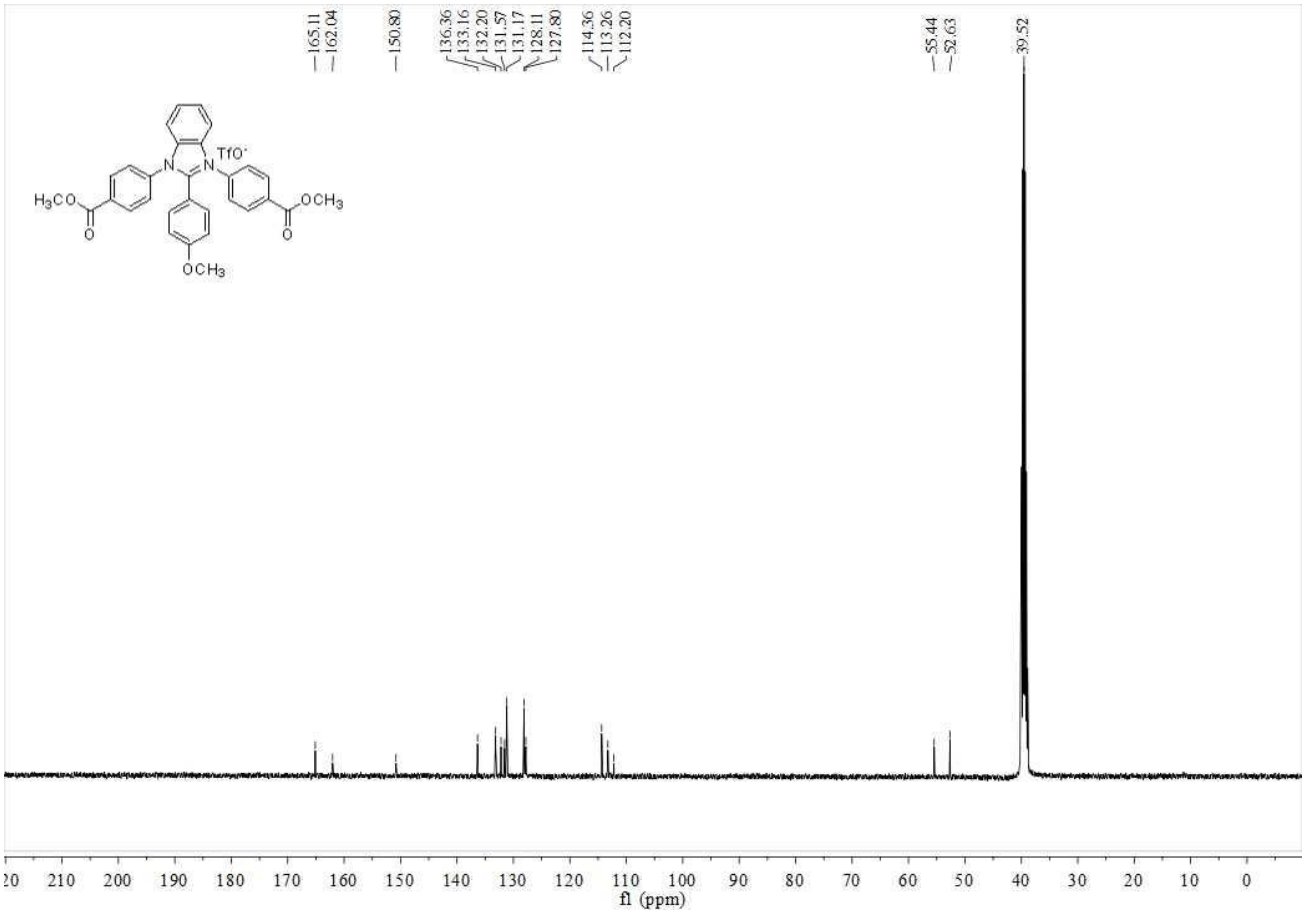
7.794
7.787
7.778
7.772
7.731
7.722
7.714
7.706
7.698
7.390
7.368
6.935
6.913
3.901
3.702
3.337
2.500
TfO⁻
H3CO
OCH3
OCH3
3.71
5.75
2.12
1.94
2.03
5.78
3.00
f1 (ppm)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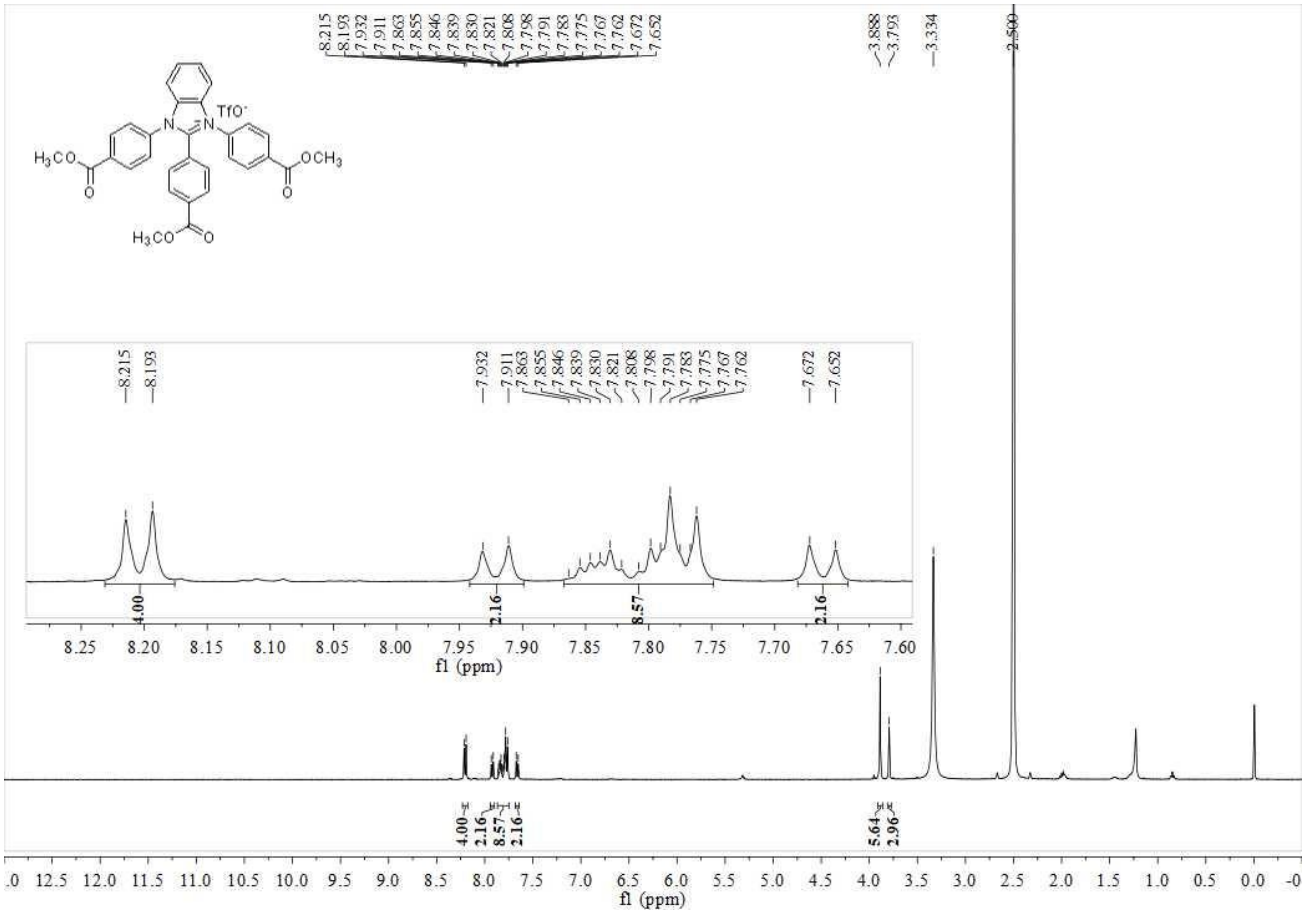
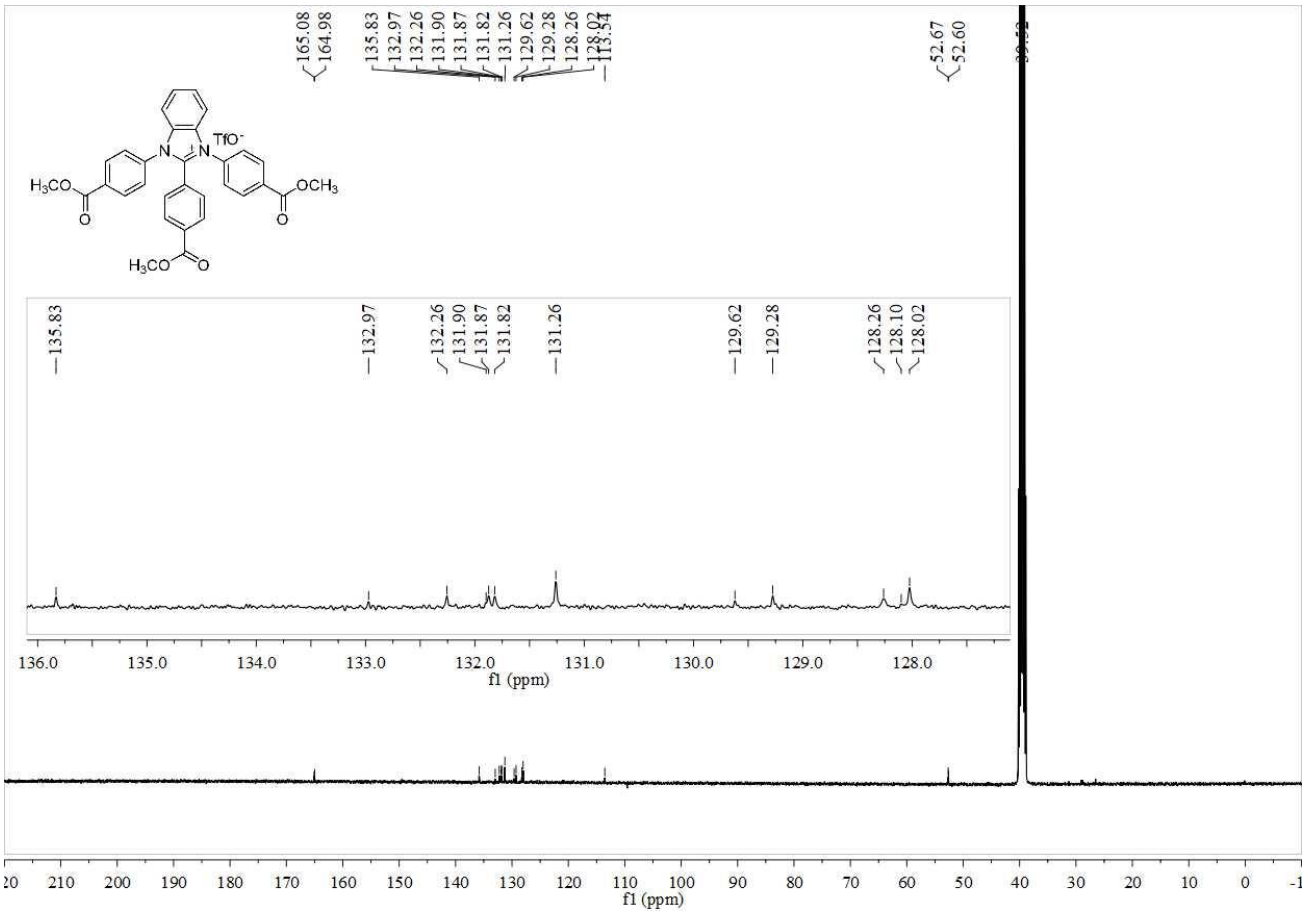
162.04
150.80
136.36
133.16
132.20
131.57
131.17
128.11
127.80
114.36
113.26
112.20
55.44
52.63
39.52
TfO⁻
H3CO
OCH3
OCH3
f1 (ppm)


8.215
8.193
7.932
7.911
7.863
7.855
7.846
7.839
7.830
7.821
7.808
7.798
7.791
7.783
7.775
7.767
7.762
7.672
7.652
3.888
3.793
3.334
2.500
Tf0-
H3CO
OCH3
H3CO
4.00
2.16
8.57
2.16
fl (ppm)
5.64
2.96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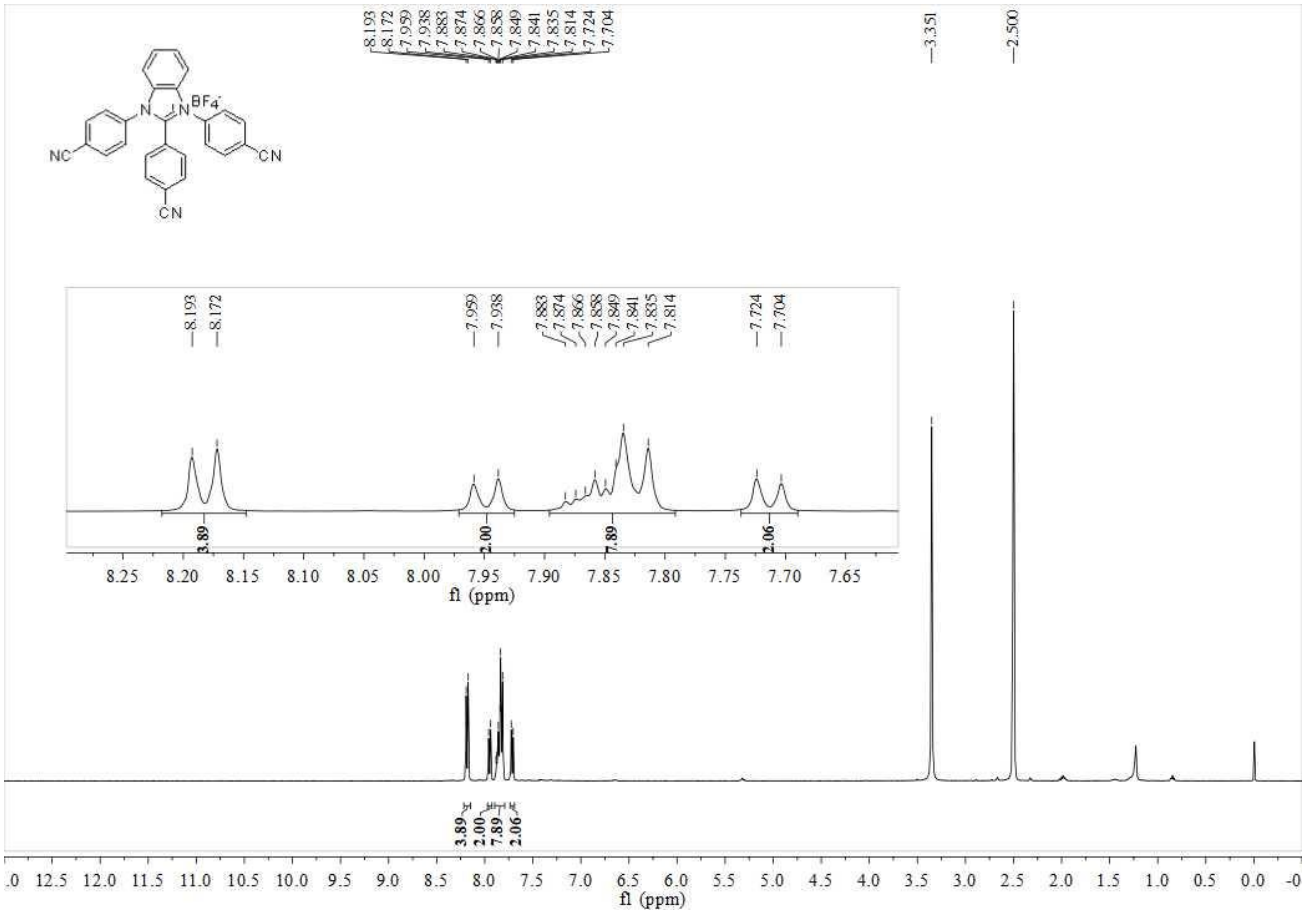
164.98
135.83
132.97
132.26
131.90
131.87
131.82
131.26
129.62
129.28
128.26
128.10
128.02
52.67
52.60
39.52
Tf0-
H3CO
OCH3
H3CO
fl (ppm)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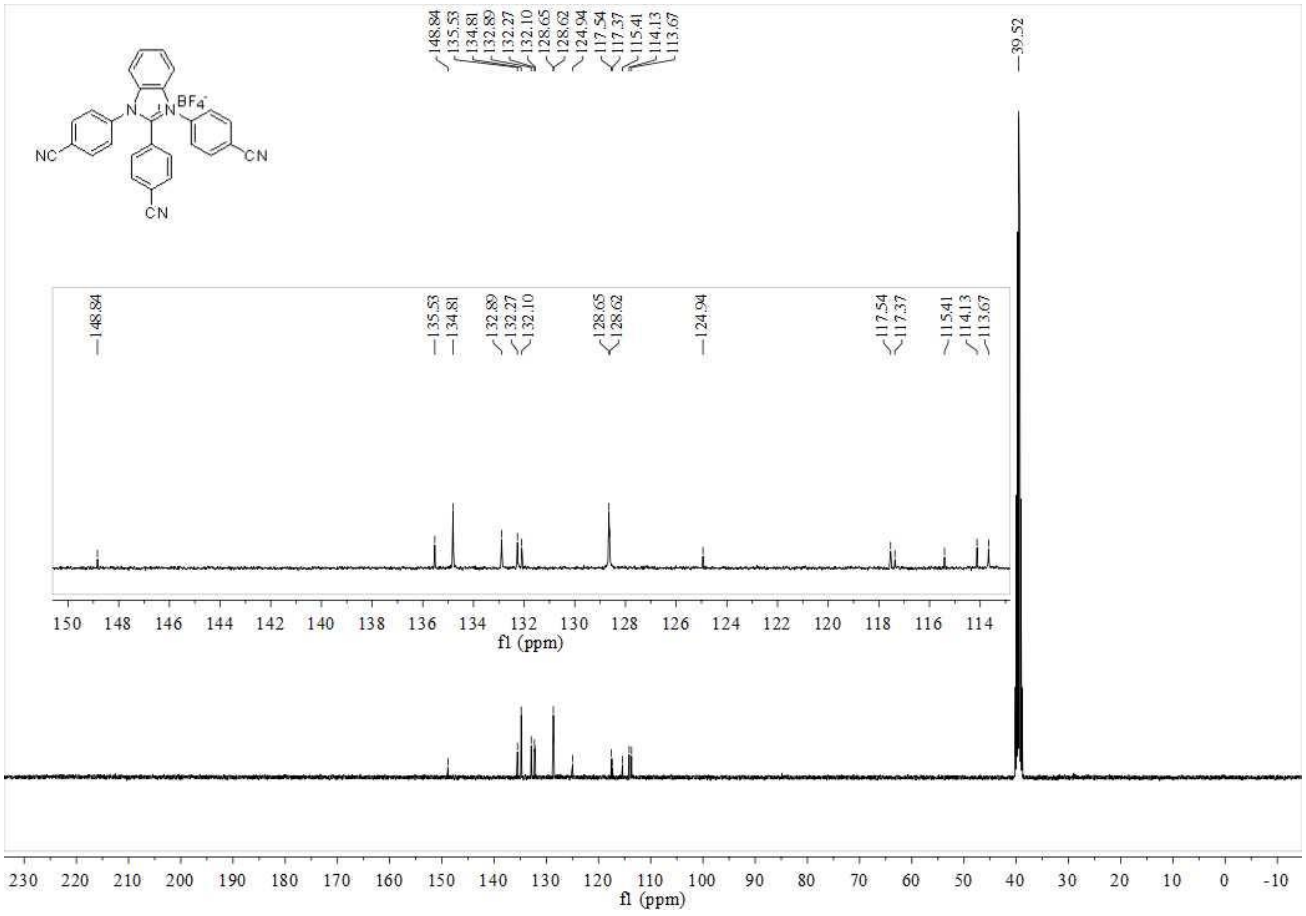
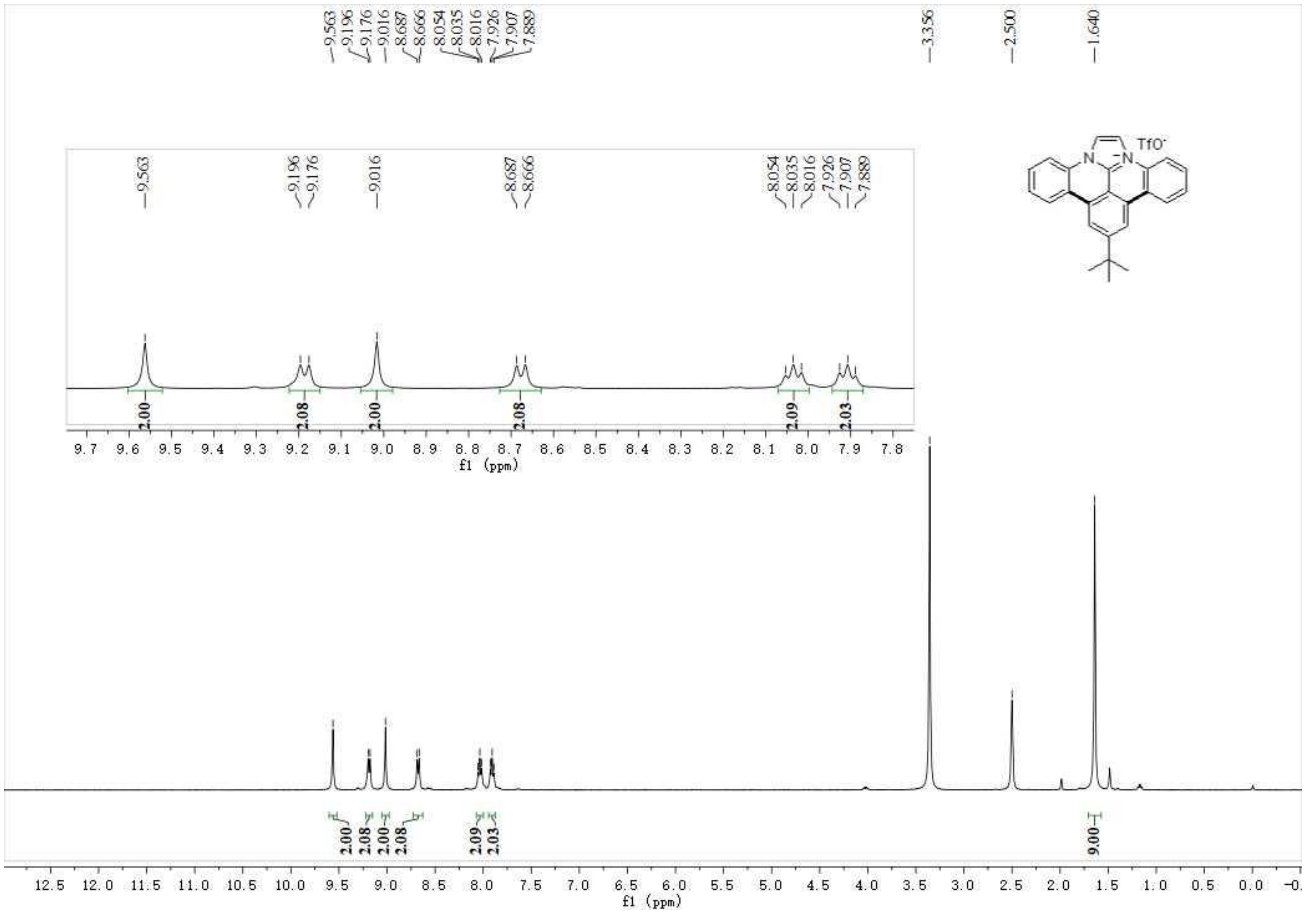
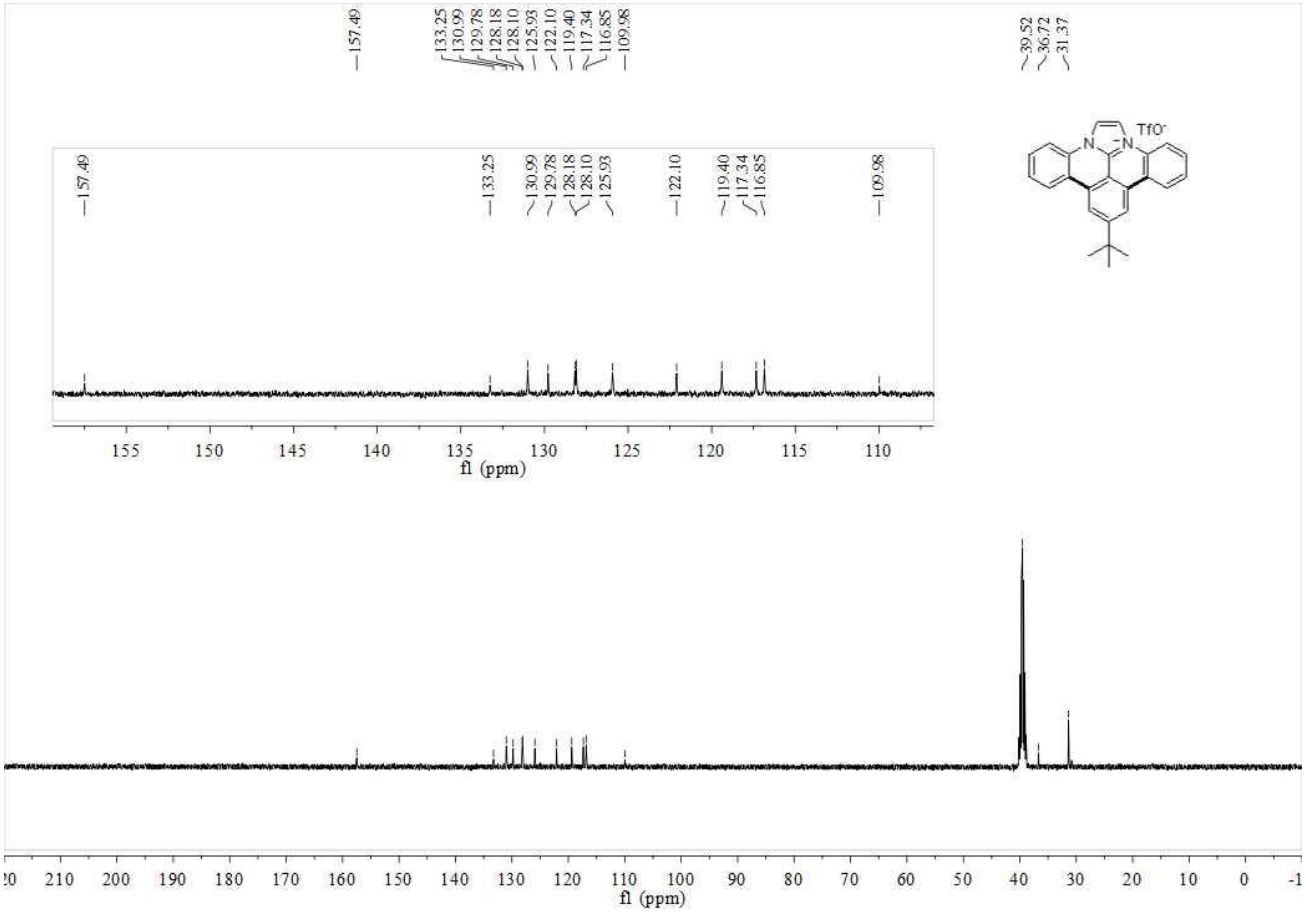
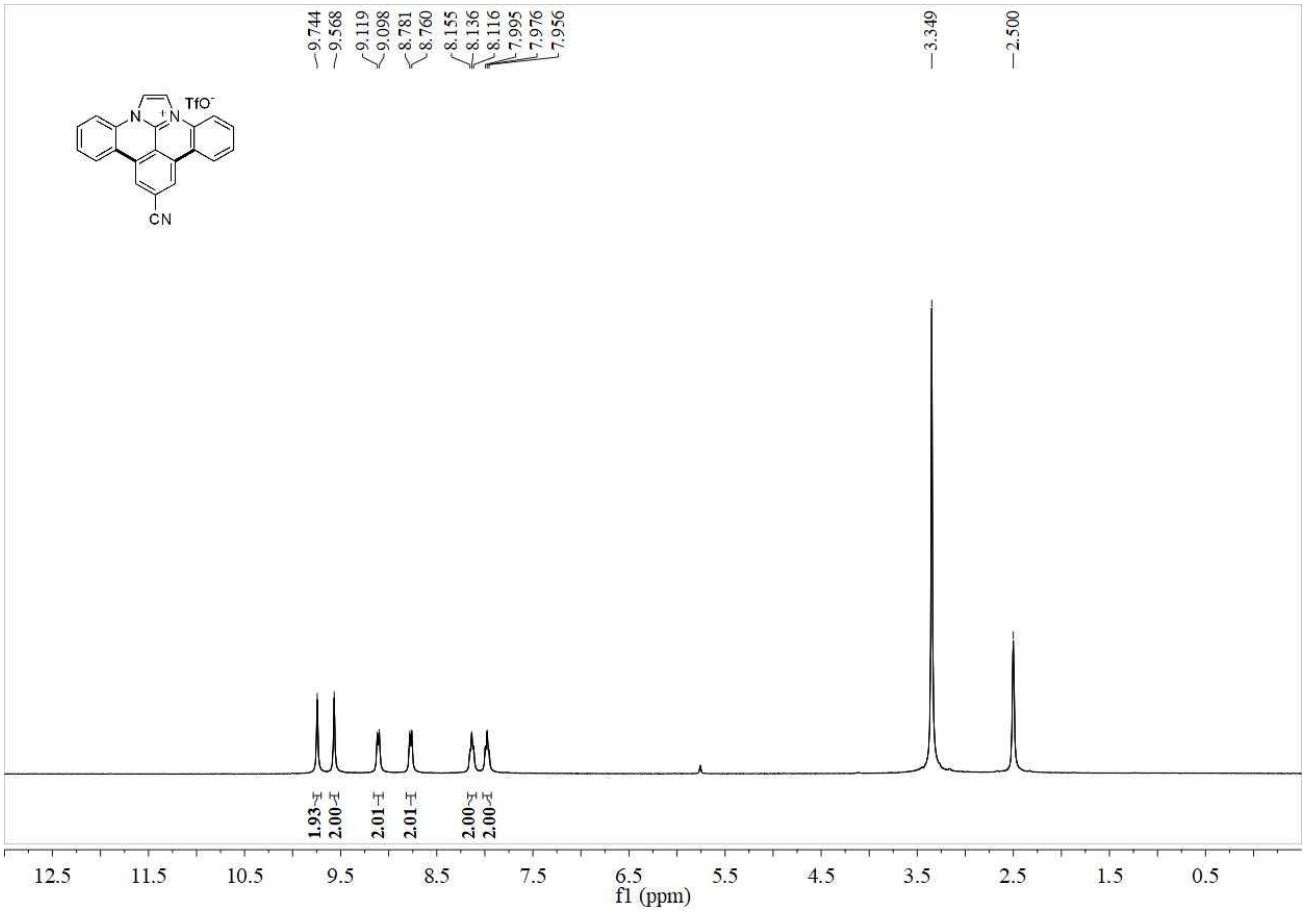
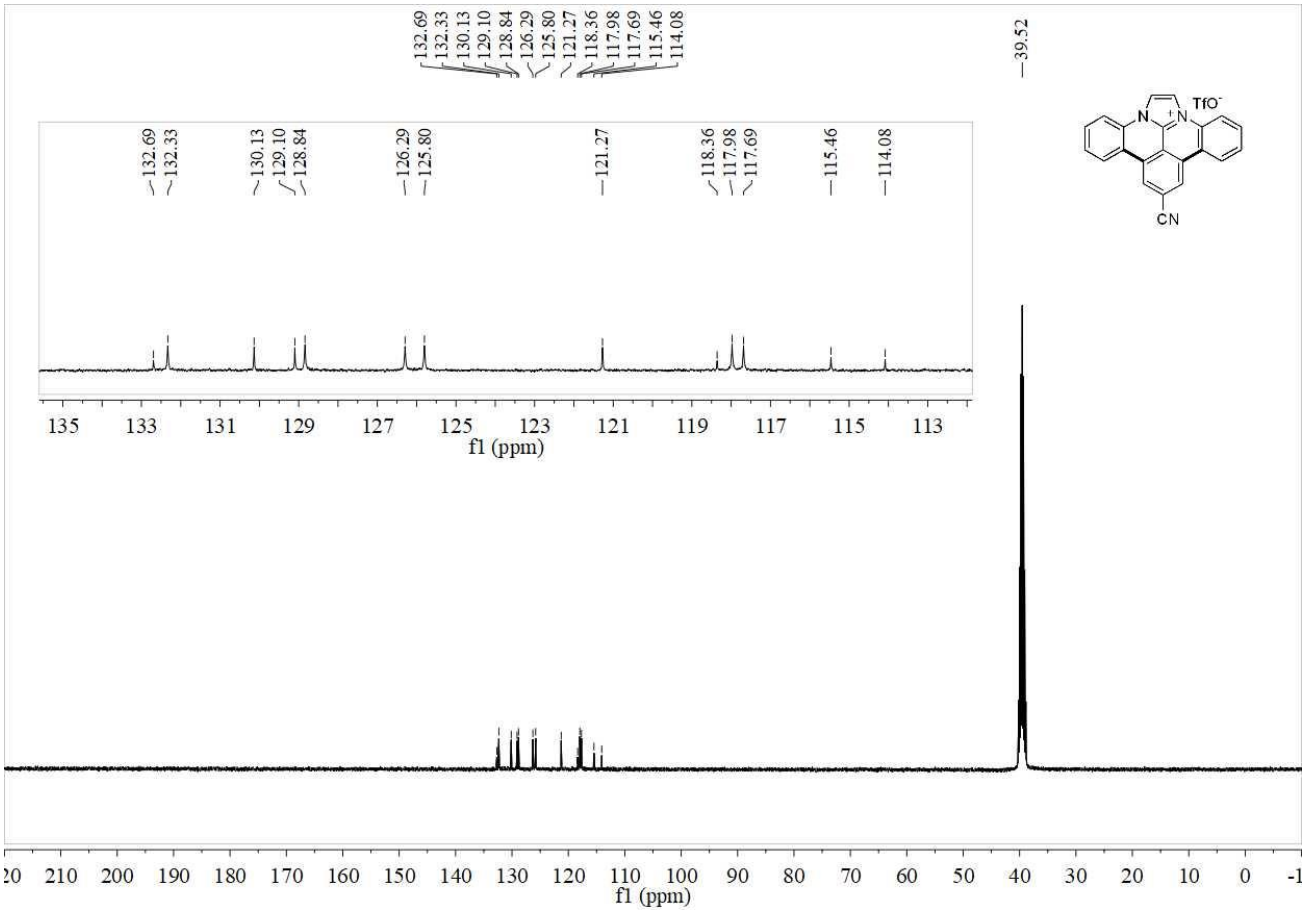
8.172
7.959
7.938
7.883
7.874
7.866
7.858
7.849
7.841
7.835
7.814
7.724
7.704
3.351
2.500
BF4-
NC
CN
CN
CN
3.89
2.00
7.89
2.06
fl (ppm)

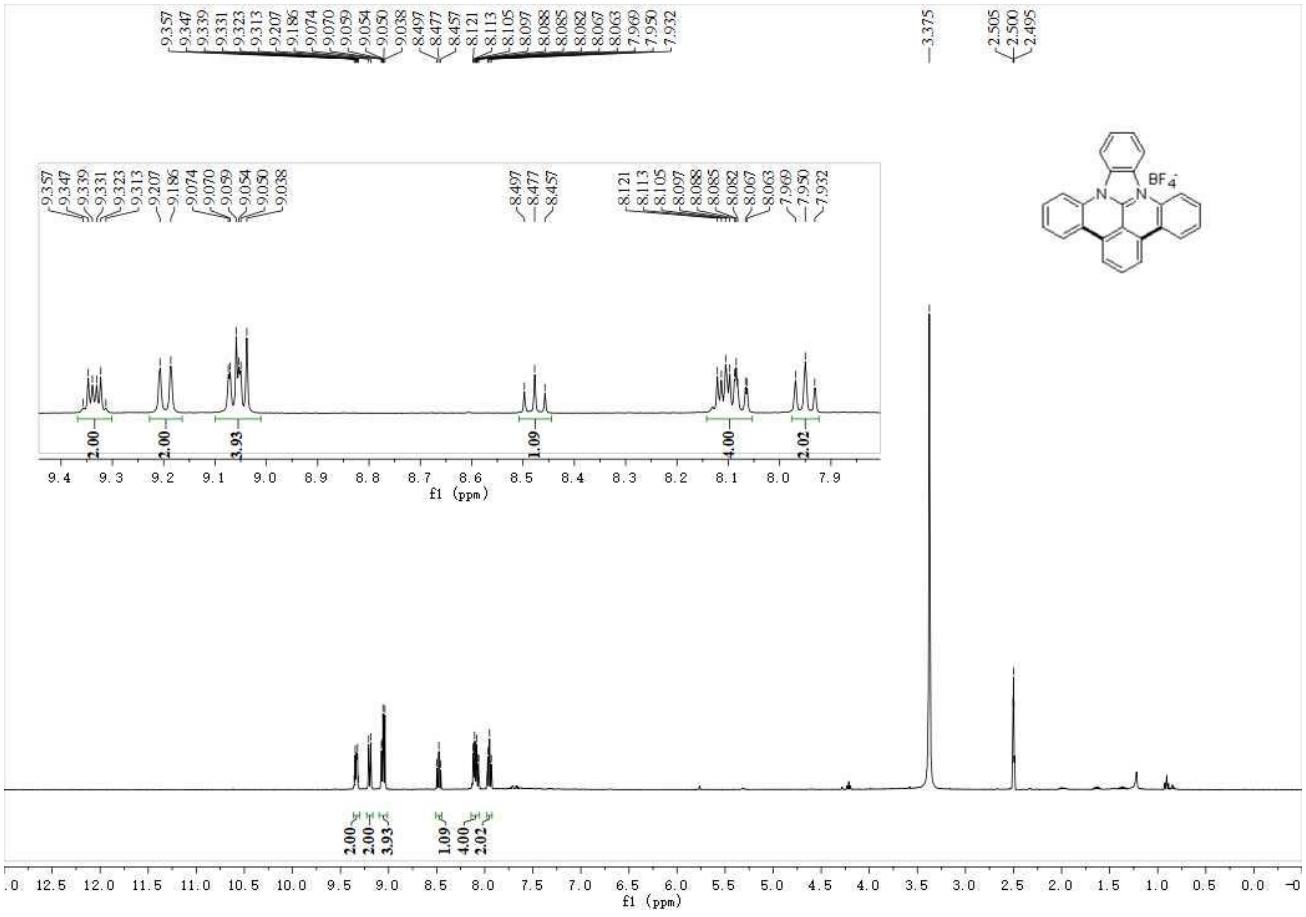

148.84
135.53
134.81
132.89
132.27
132.10
128.65
128.62
124.94
117.54
117.37
115.41
114.13
113.67
39.52
BF4-
NC
CN
CN
fl (ppm)

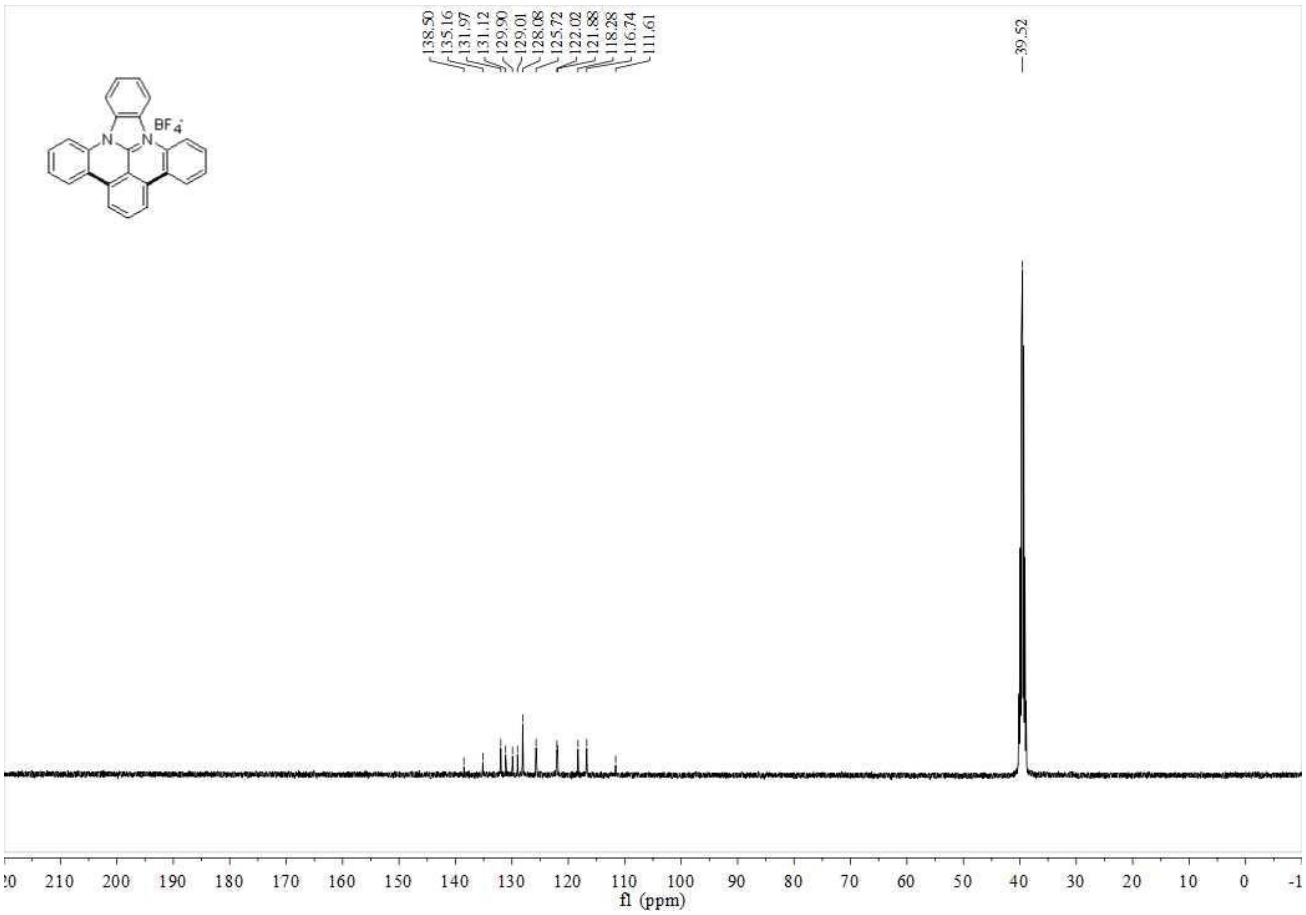

9.563
9.196
9.176
9.016
8.687
8.666
8.054
8.035
8.016
7.926
7.907
7.889
3.356
2.500
1.640
TfO-
2.00
2.08
2.00
2.08
2.09
2.03
9.00
f1 (ppm)

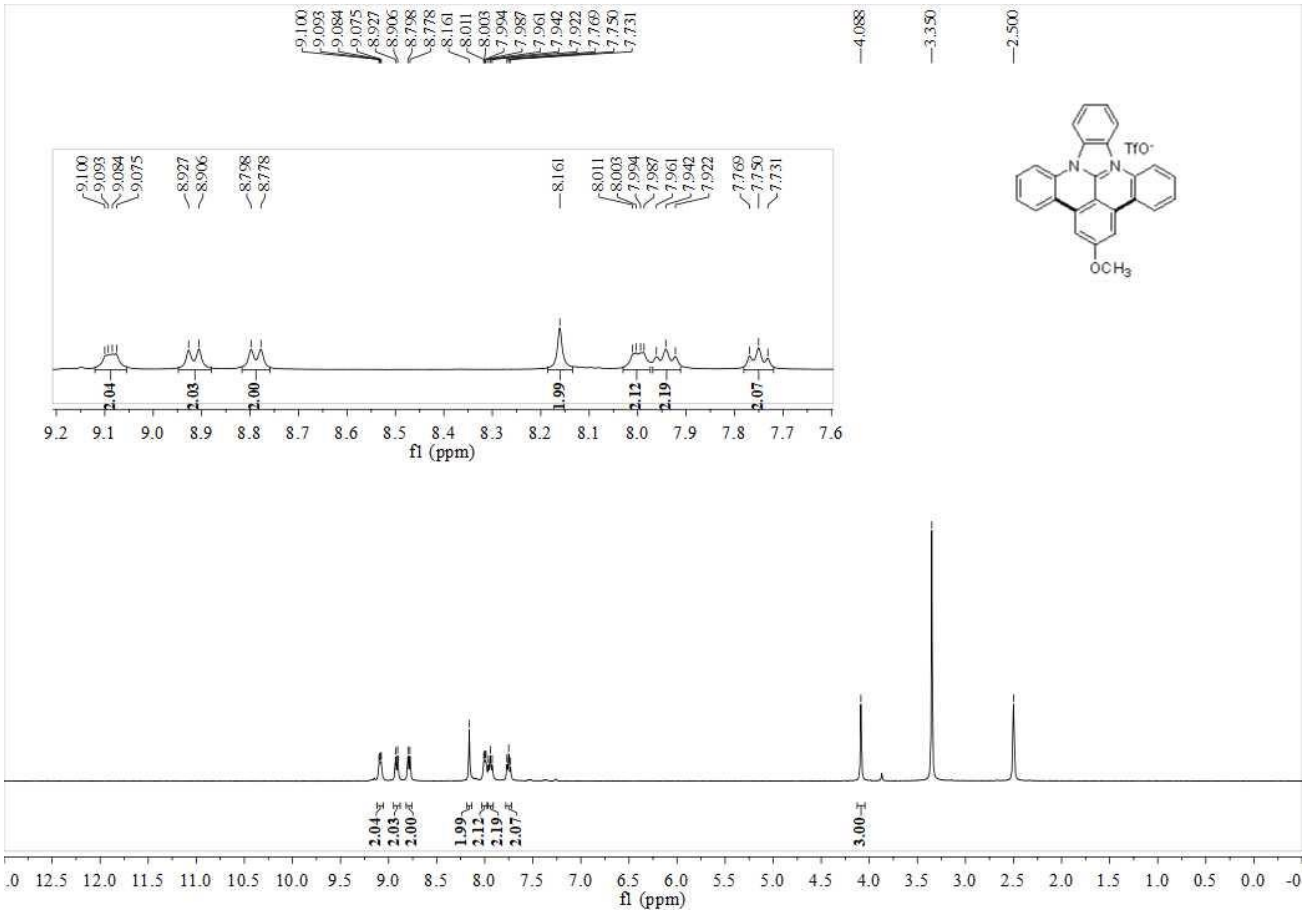

157.49
133.25
130.99
129.78
128.18
128.10
125.93
122.10
119.40
117.34
116.85
109.98
39.52
36.72
31.37
TfO-
f1 (ppm)

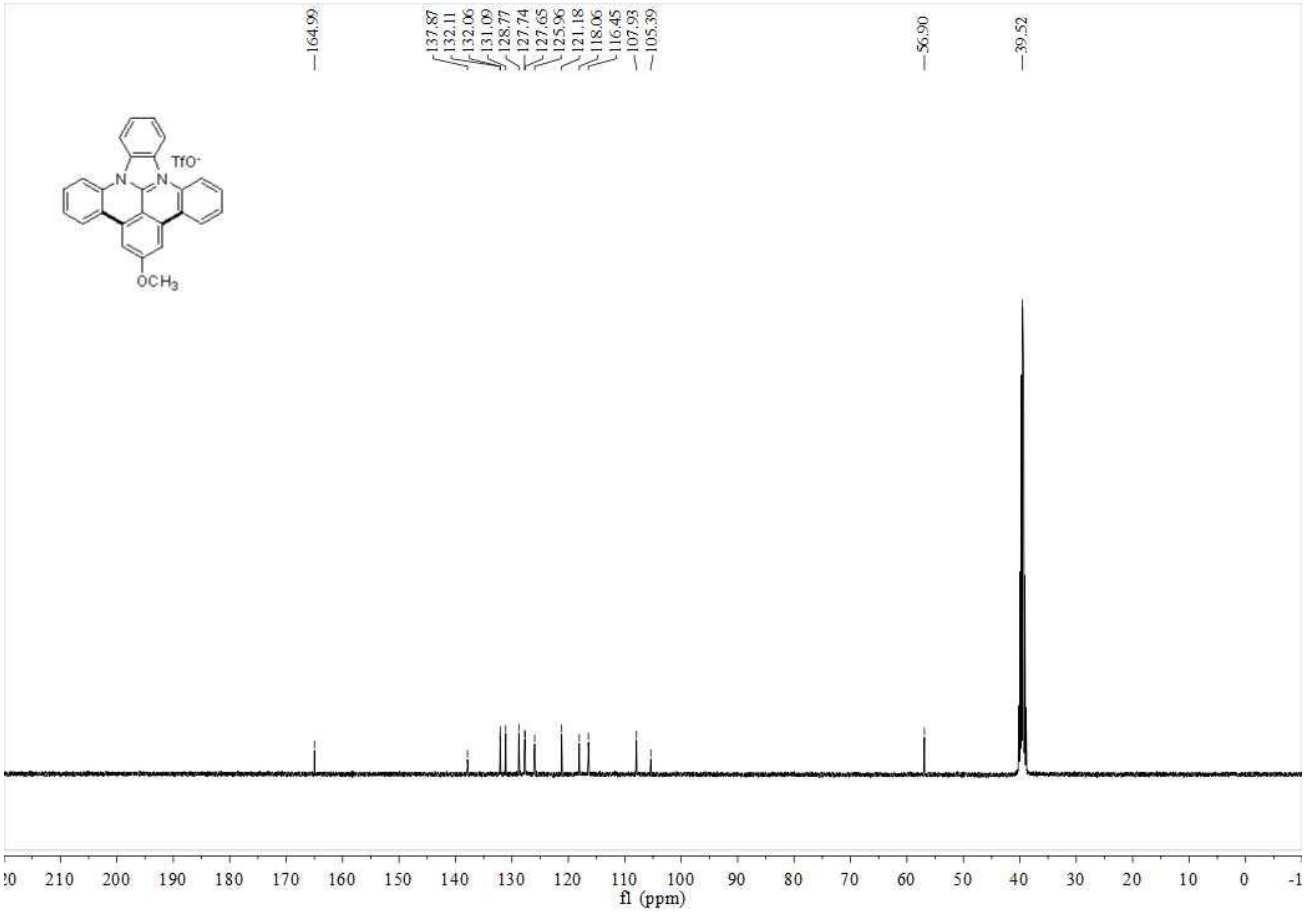

9.744
9.568
9.119
9.098
8.781
8.760
8.155
8.136
8.116
7.995
7.976
7.956
3.349
2.500
TfO⁻
N
N
CN
1.93
2.00
2.01
2.01
2.00
2.00
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

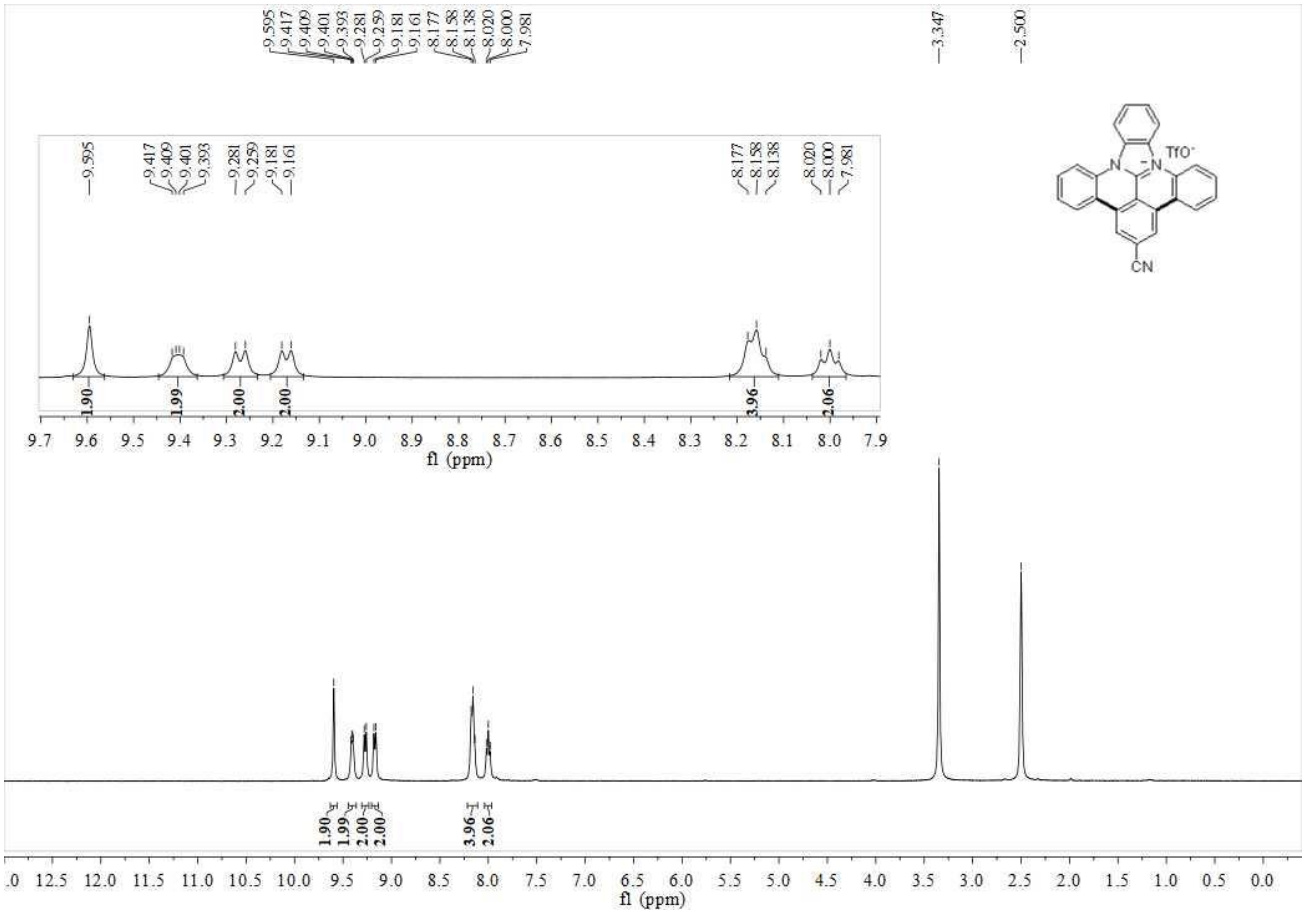

132.69
132.33
130.13
129.10
128.84
126.29
125.80
121.27
118.36
117.98
117.69
115.46
114.08
39.52
TfO⁻
N
N
CN
135
133
131
129
127
125
123
121
119
117
115
113
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

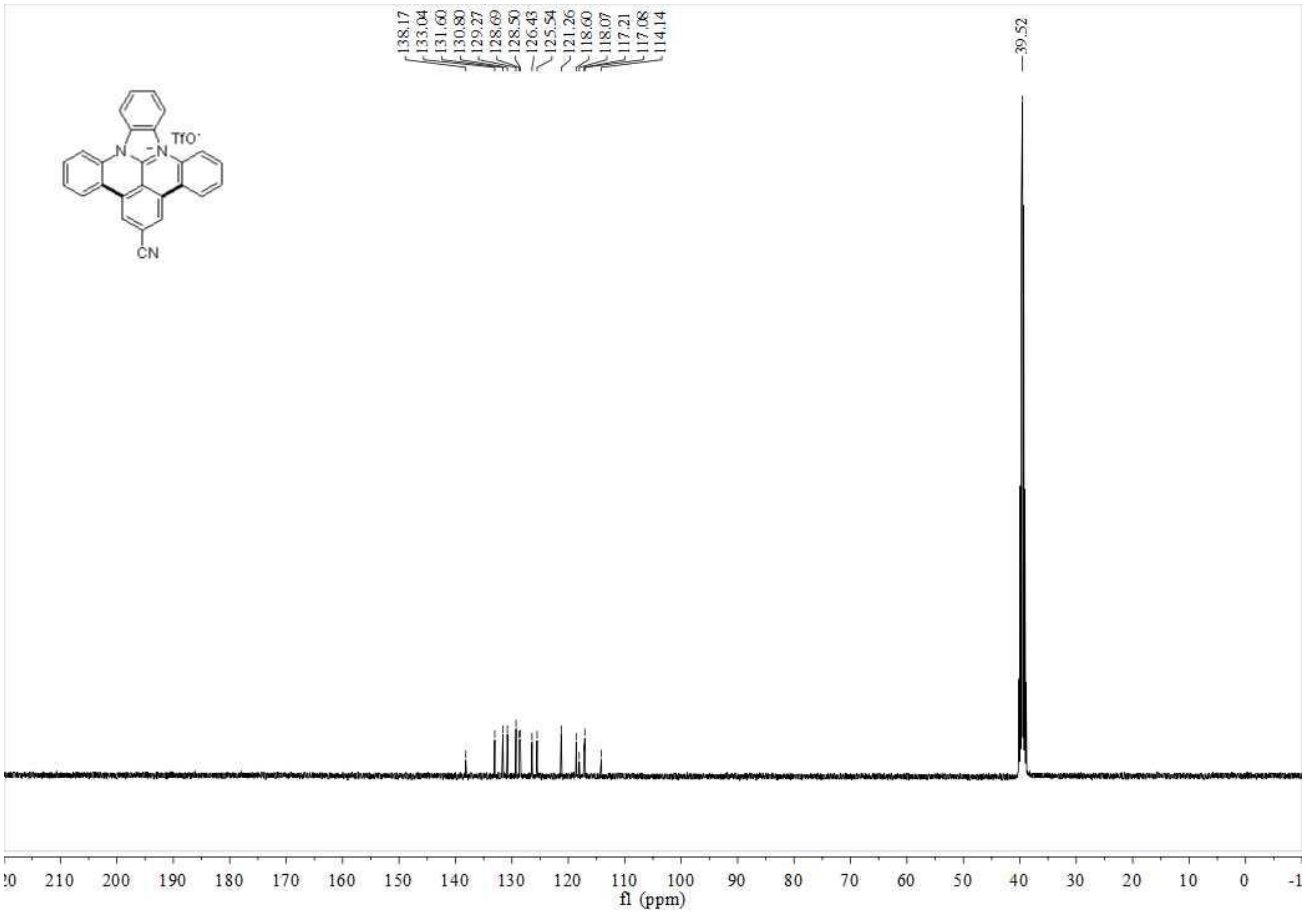

9.357
9.347
9.339
9.331
9.323
9.313
9.207
9.186
9.074
9.070
9.059
9.054
9.050
9.038
8.497
8.477
8.457
8.121
8.113
8.105
8.097
8.088
8.085
8.082
8.067
8.063
7.969
7.950
7.932
3.375
2.505
2.500
2.495
BF4-
2.00
2.00
3.93
1.09
4.00
2.02
f1 (ppm)

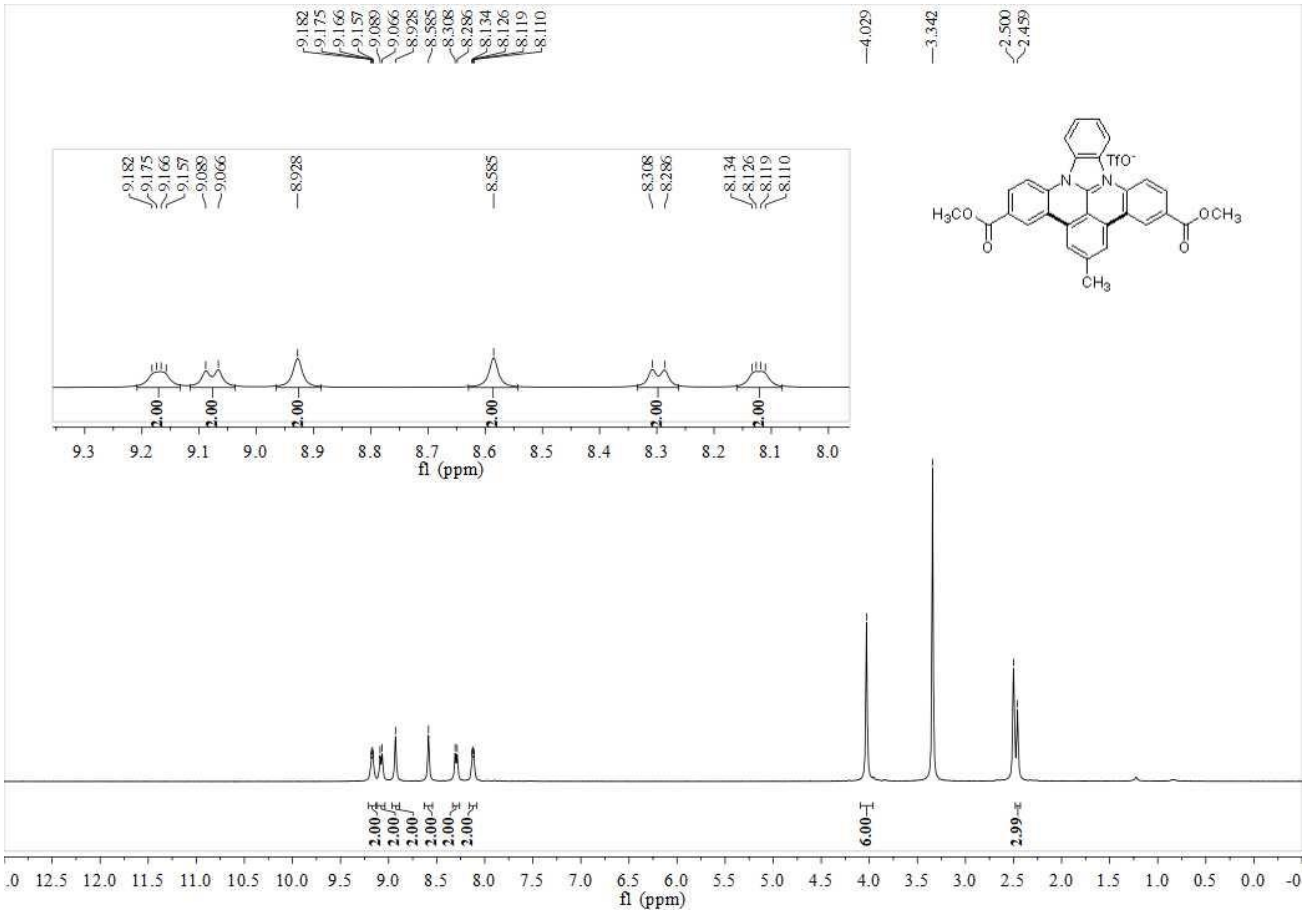

138.50
135.16
131.97
131.12
129.90
129.01
128.08
125.72
122.02
121.88
118.28
116.74
111.61
39.52
BF4-
f1 (ppm)


9.100
9.093
9.084
9.075
8.927
8.906
8.798
8.778
8.161
8.011
8.003
7.994
7.987
7.961
7.942
7.922
7.769
7.750
7.731
4.088
3.350
2.500
TfO⁻
OCH3
2.04
2.03
2.00
1.99
2.12
2.19
2.07
3.00
fl (ppm)


164.99
137.87
132.11
132.06
131.09
128.77
127.74
127.65
125.96
121.18
118.06
116.45
107.93
105.39
56.90
39.52
TfO⁻
OCH3
fl (ppm)


9.595
9.417
9.409
9.401
9.393
9.281
9.259
9.181
9.161
8.177
8.158
8.138
8.020
8.000
7.981
3.347
2.500
TfO⁻
CN
1.90
1.99
2.00
2.00
3.96
2.06
fl (ppm)


138.17
133.04
131.60
130.80
129.27
128.69
128.50
126.43
125.54
121.26
118.60
118.07
117.21
117.08
114.14
39.52
TfO⁻
CN
fl (ppm)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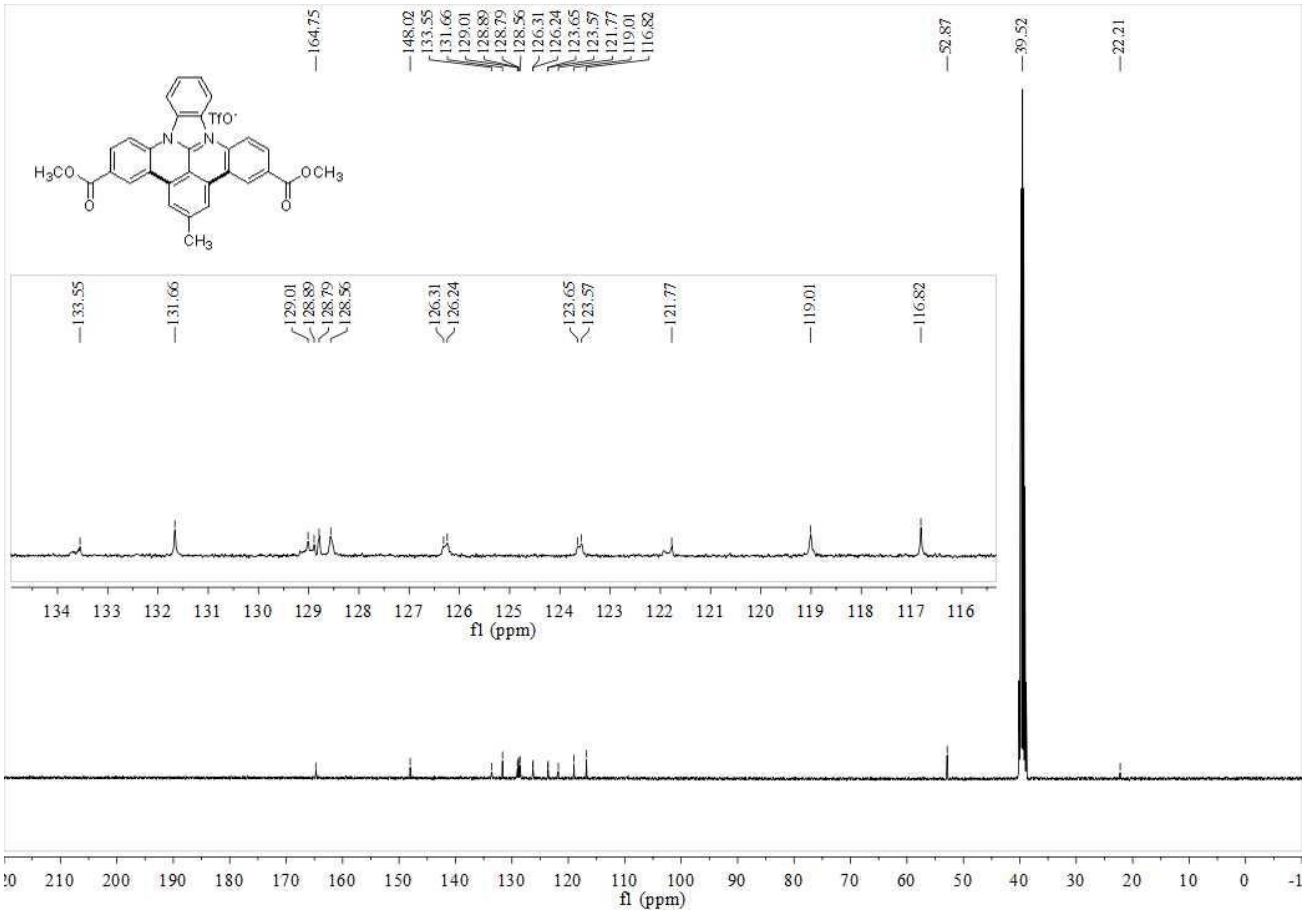
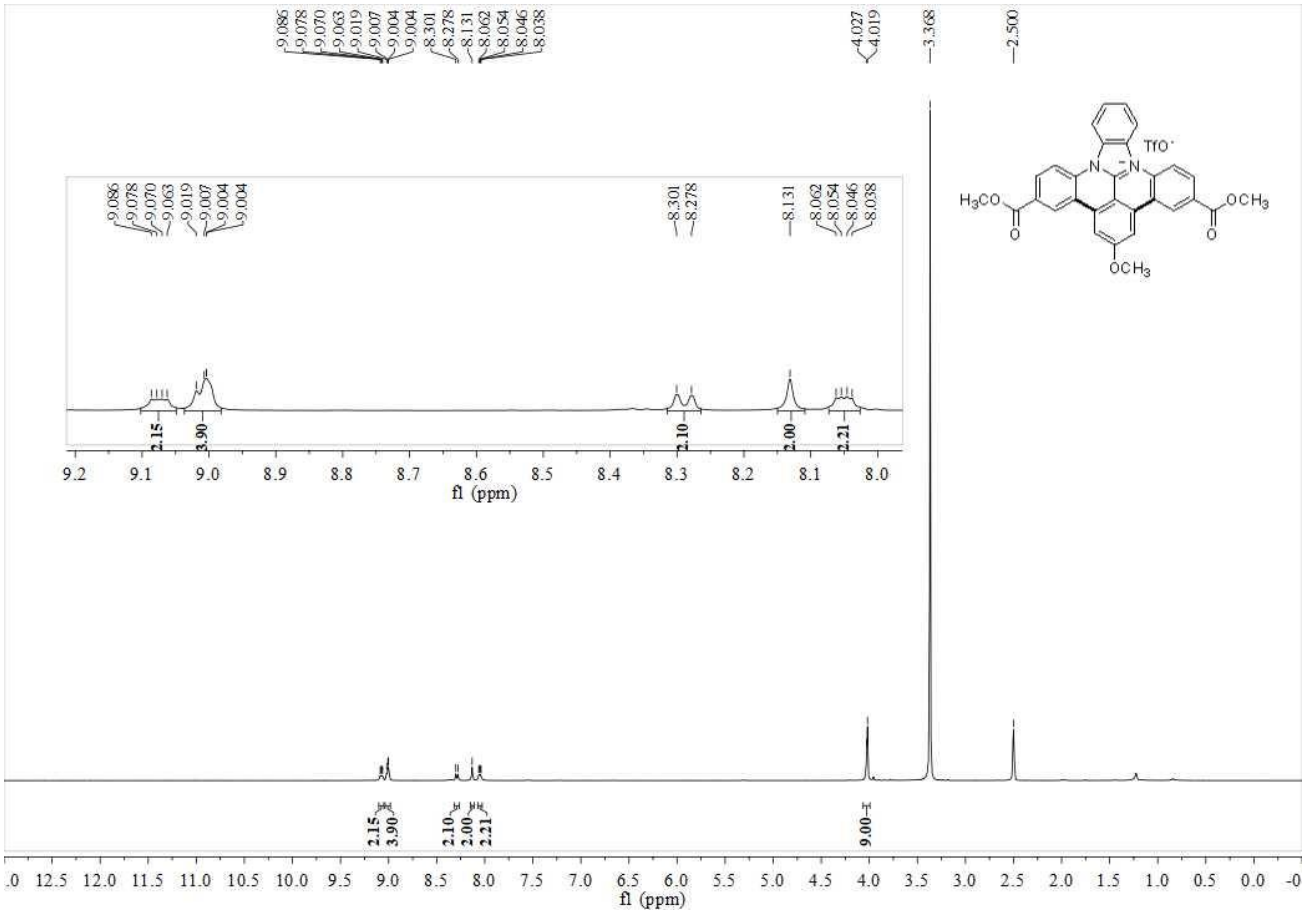
9.166
9.157
9.089
9.066
8.928
8.585
8.308
8.286
8.134
8.126
8.119
8.110
4.029
3.342
2.500
2.459
TfO⁻
H3CO
OCH3
CH3
2.00
6.00
2.99
fl (ppm)


164.75
148.02
133.55
131.66
129.01
128.89
128.79
128.56
126.31
126.24
123.65
123.57
121.77
119.01
116.82
52.87
39.52
22.21
TfO⁻
H3CO
OCH3
CH3
fl (ppm)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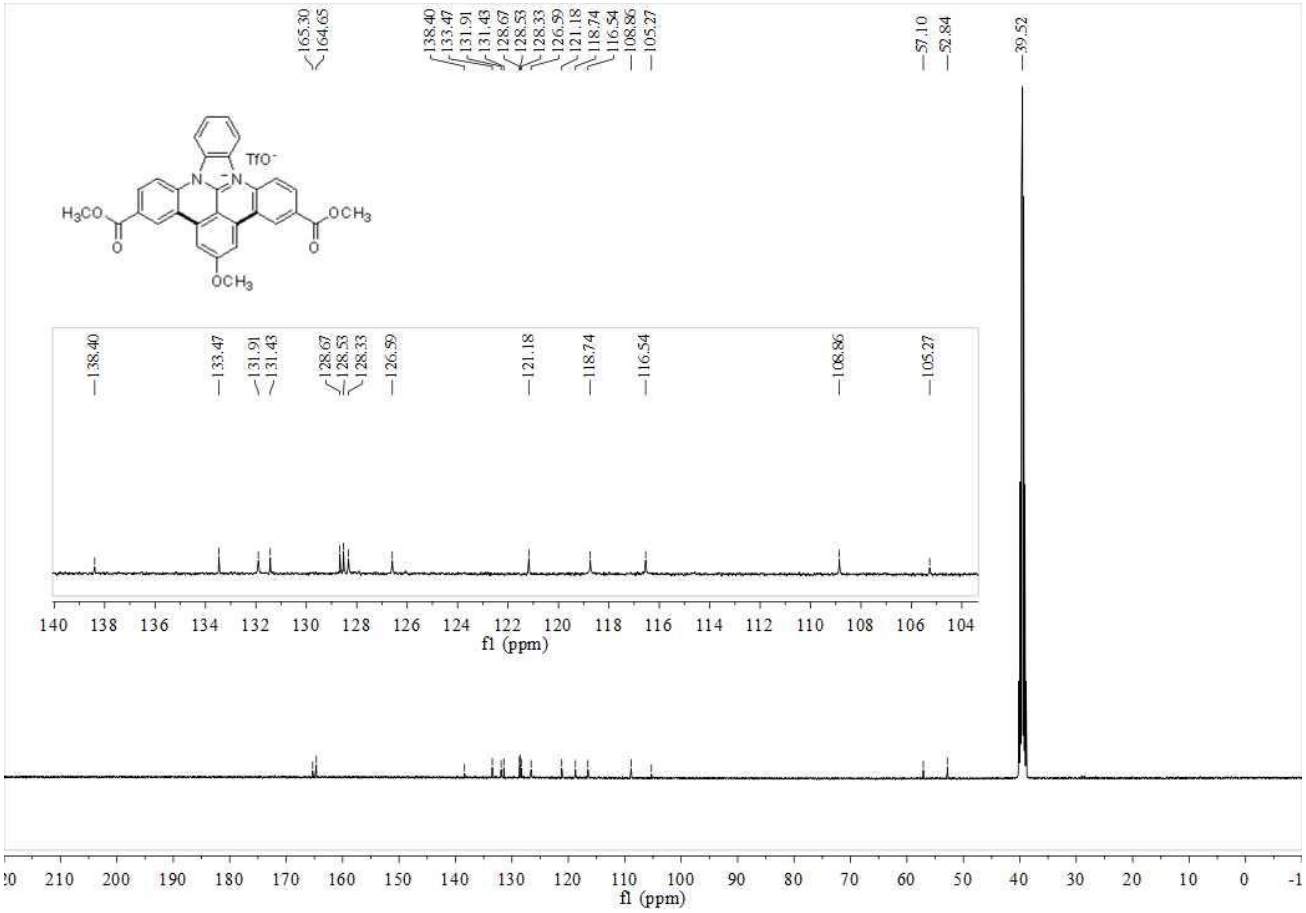
9.070
9.063
9.019
9.007
9.004
9.004
8.301
8.278
8.131
8.062
8.054
8.046
8.038
4.027
4.019
3.368
2.500
TfO⁻
H3CO
OCH3
OCH3
2.15
3.90
2.10
2.00
2.21
9.00
fl (ppm)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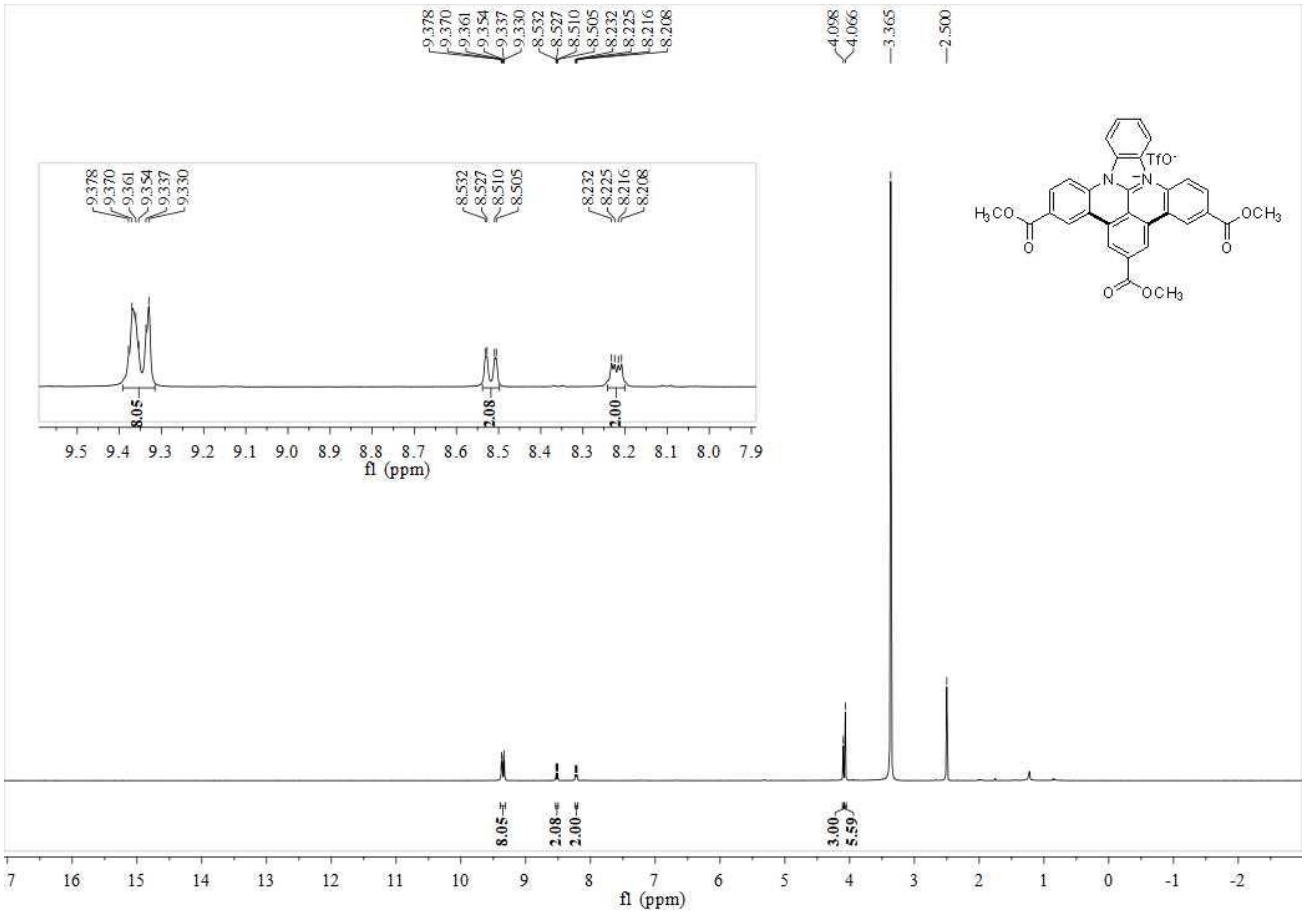
164.65
138.40
133.47
131.91
131.43
128.67
128.53
128.33
126.99
121.18
118.74
116.54
108.86
105.27
57.10
52.84
39.52
TfO⁻
H3CO
OCH3
OCH3
fl (ppm)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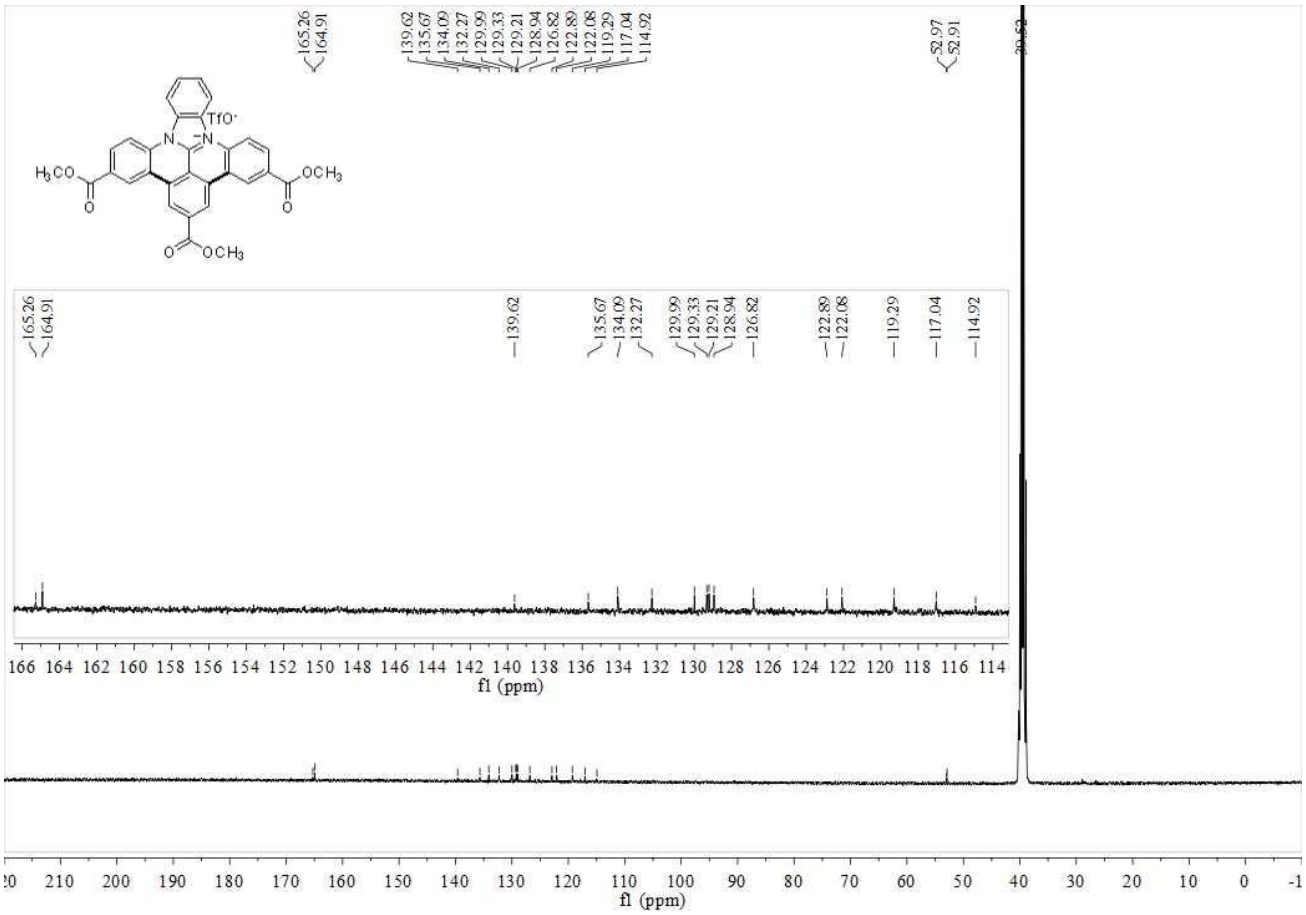
9.370
9.361
9.354
9.337
9.330
8.532
8.527
8.510
8.505
8.232
8.225
8.216
8.208
4.098
4.066
3.365
2.500
TfO⁻
H3CO
OCH3
8.05
2.08
2.00
3.00
5.59
fl (ppm)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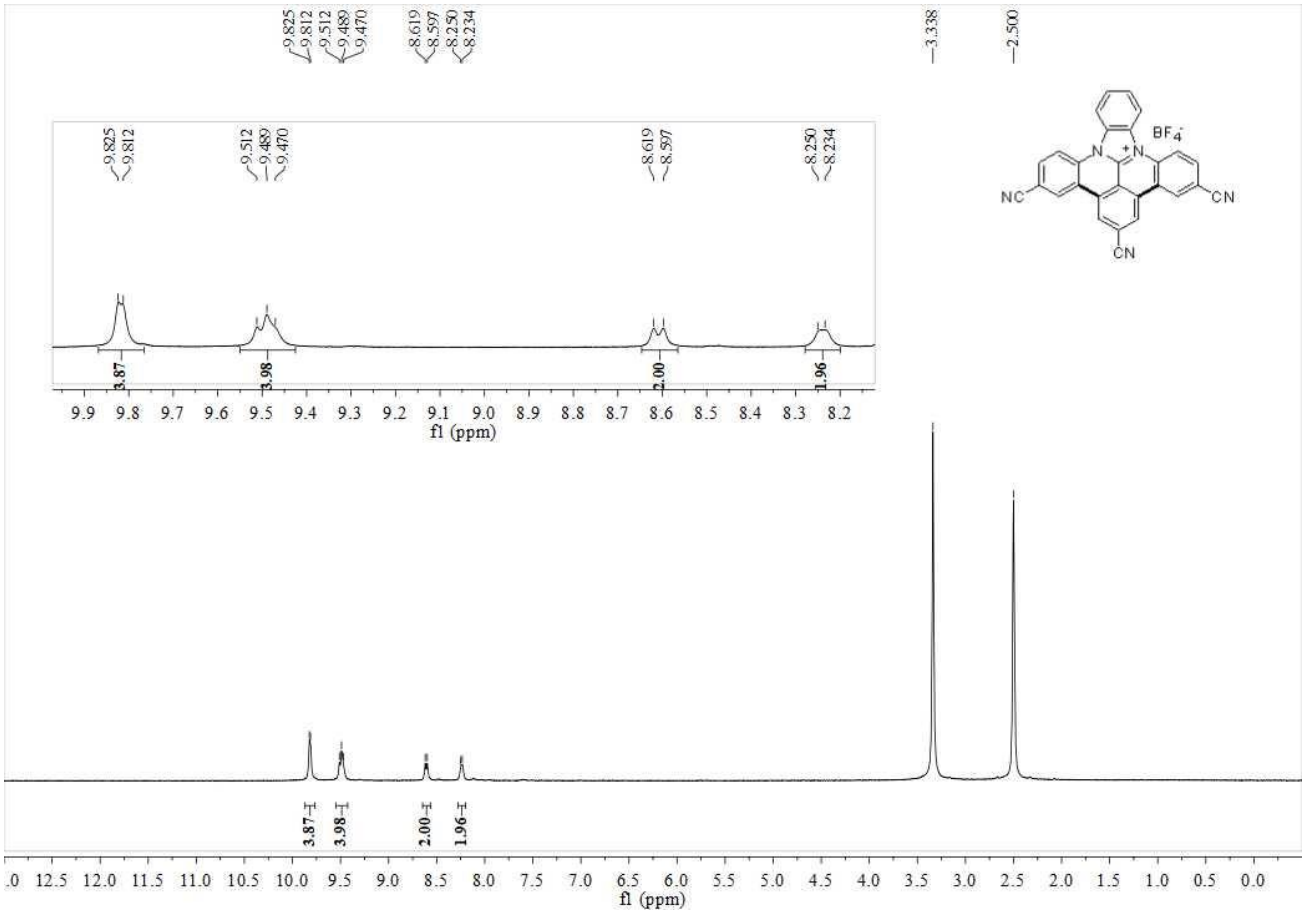
164.91
139.62
135.67
134.09
132.27
129.99
129.33
129.21
128.94
126.82
122.89
122.08
119.29
117.04
114.92
52.97
52.91
39.53
TfO⁻
H3CO
OCH3
fl (ppm)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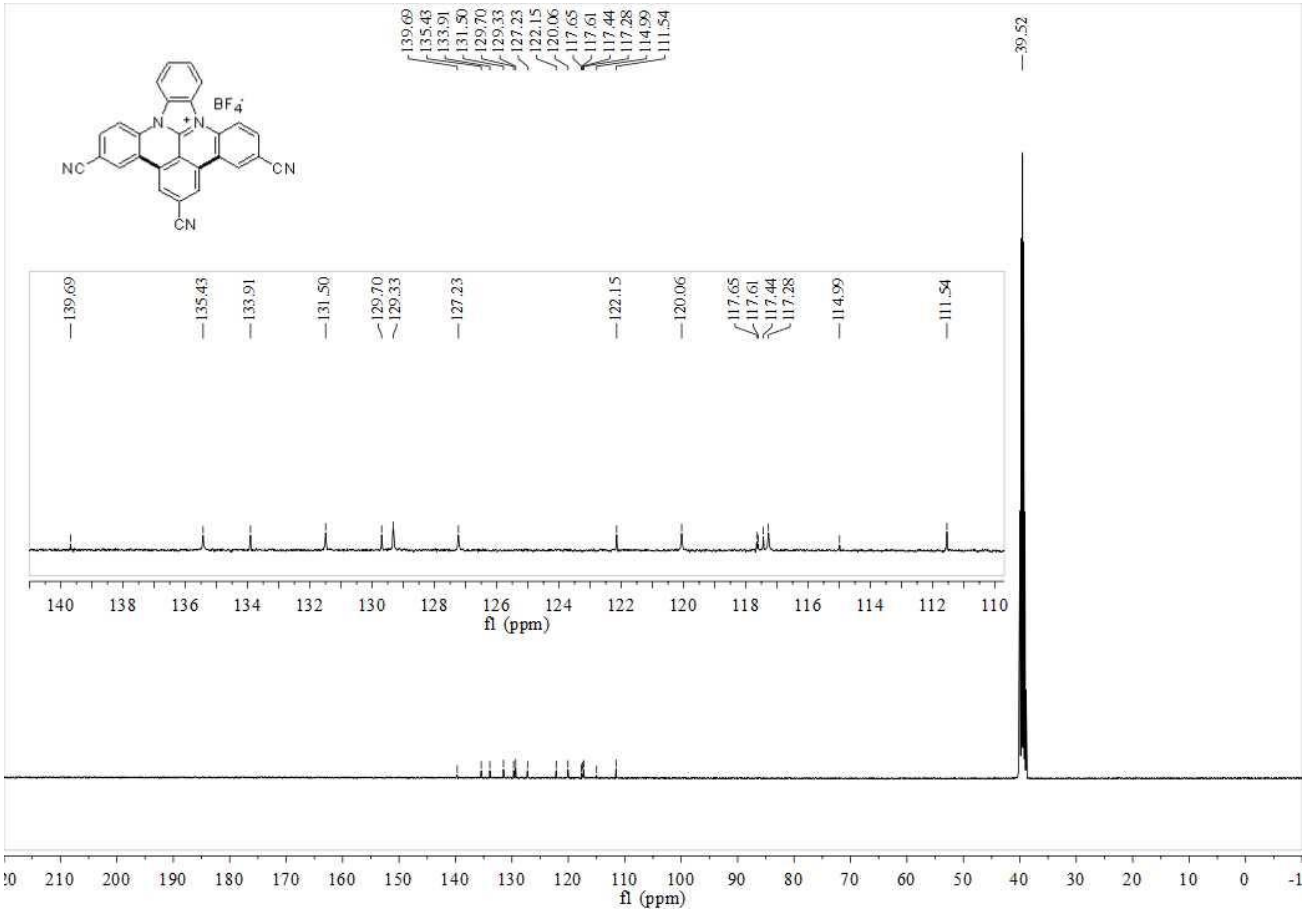
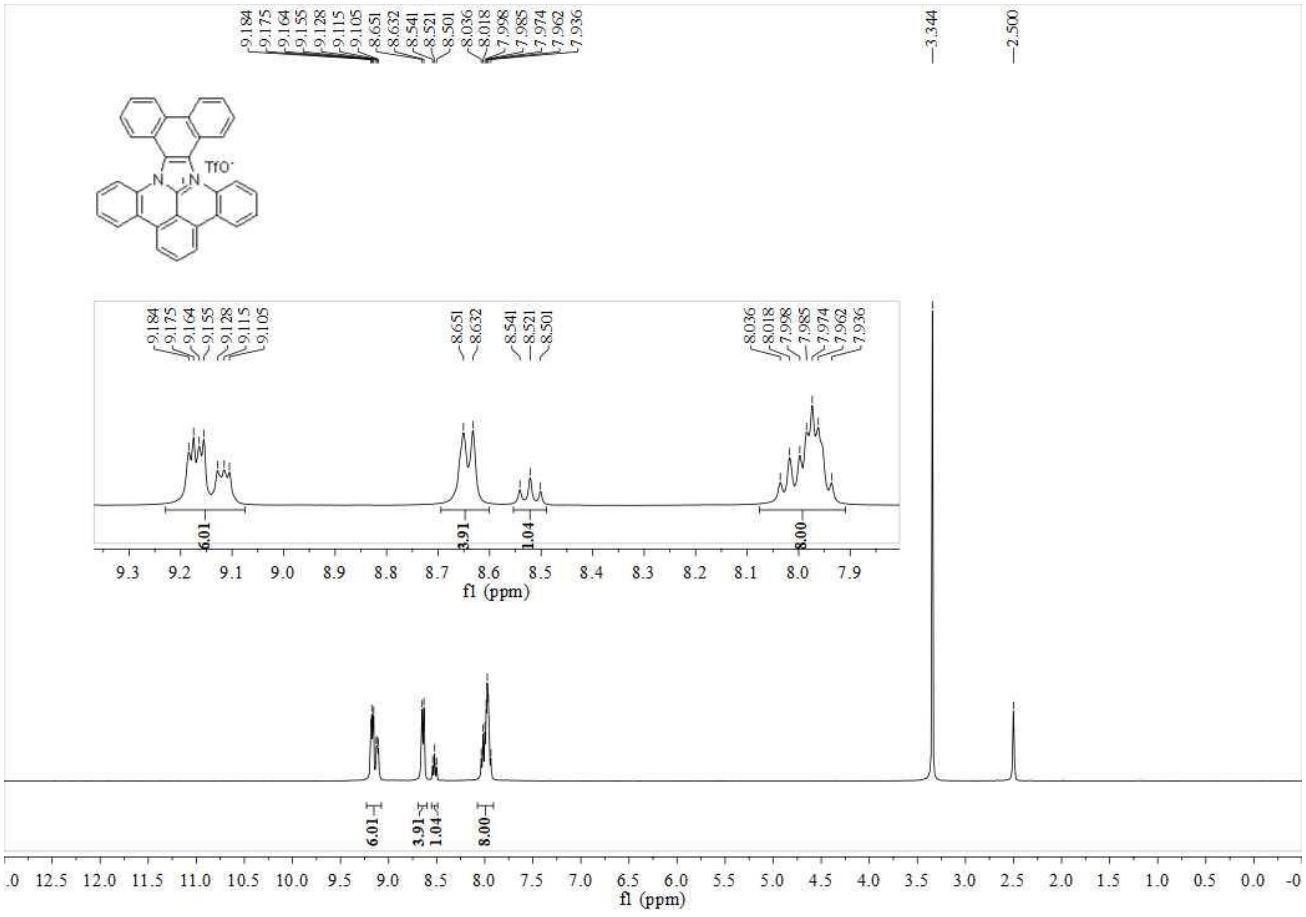
9.812
9.512
9.489
9.470
8.619
8.597
8.250
8.234
3.338
2.500
BF4-
NC
CN
CN
3.87
3.98
2.00
1.96
fl (ppm)


139.69
135.43
133.91
131.50
129.70
129.33
127.23
122.15
120.06
117.65
117.61
117.44
117.28
114.99
111.54
39.52
BF4-
NC
CN
CN
fl (ppm)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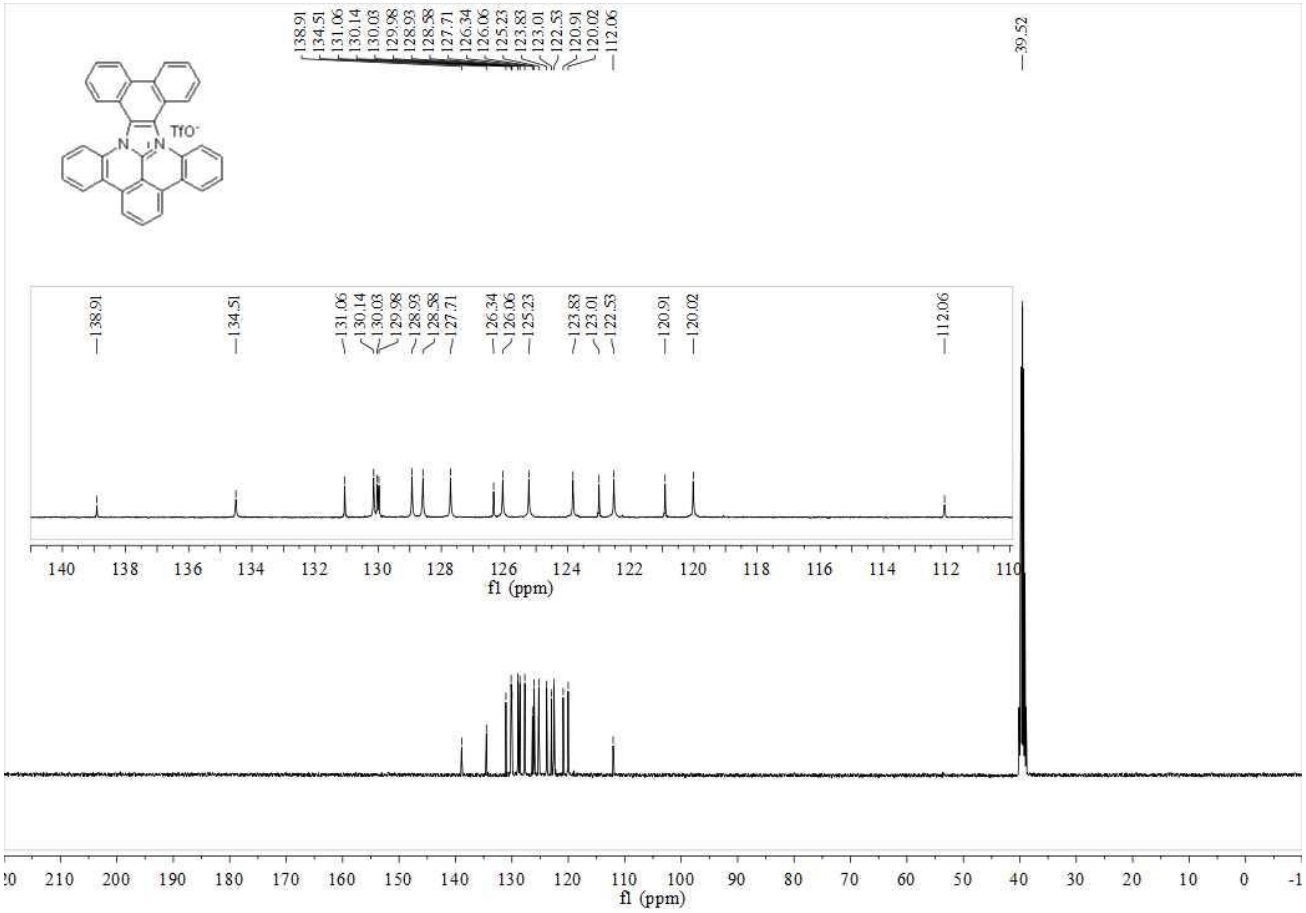
9.175
9.164
9.155
9.128
9.115
9.105
8.651
8.632
8.541
8.521
8.501
8.036
8.018
7.998
7.985
7.974
7.962
7.936
3.344
2.500
TfO⁻
6.01
3.91
1.04
8.00
f1 (ppm)


138.91
134.51
131.06
130.14
130.03
129.98
128.93
128.58
127.71
126.34
126.06
125.23
123.83
123.01
122.53
120.91
120.02
112.06
39.52
TfO⁻
f1 (ppm)