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Ruthenium-Catalyzed *meta*-Selective C-H Sulfonation of Azoarenes with Arylsulfonyl Chlorides

Gang Li,* Xulu Lv,† Kexiao Guo,† Ya Wang, Suling Yang, Liuyang Yu, Yantang Yu, and Junjie Wang*

College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang 455002, P. R. China

Henan Province Key Laboratory of New Optoelectronic Functional Materials, Anyang Normal University, Anyang 455002, P. R. China

ligang@aynu.edu.cn; wjjaysy@163.com.

Supporting information

1. General Information

All commercial reagents and solvents were used directly without additional purification. Column chromatography were performed on silica gel 200-300 mesh. ^{1}H

NMR and ^{13}C NMR spectra were registered on a Bruker Ascend^{TM} 400 spectrometer (Germany). Chemical shifts were reported in units (ppm) referenced to 0.0 ppm of TMS in the ^{1}H spectrum and 77.0 ppm of $CDCl_3$ in the ^{13}C spectrum. All coupling constants were reported in Hertz (Hz). HRMS data were obtained on a Waters LCT Premierxe^{TM} (USA), Single-crystal X-ray crystallography was carried out on a Bruker Smart Apex II diffractometer system.

CCDC 1501752 and CCDC 1501755 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from Cambridge Crystallographic Data Centre via: https://summary.ccdc.cam.ac.uk/structure-summary-form

2. Experimental Section

2.1. General Procedure for the Synthesis of symmetrical Azobenzenes.[1]

A mixture of CuBr (4.2 mg, 0.03 mmol), pyridine (8.7 mg, 0.09 mmol), and arylamine (1 mmol) in toluene (4 mL) was stirred at 60 °C under air (1 atm) for 20 h and then cooled to room temperature and concentrated under vacuum. The residue was purified by flash chromatography on a short silica gel column, eluting with petroleum ether, to afford the desired products.

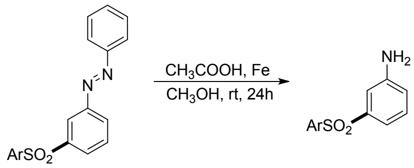
2.2. General Procedure for the Synthesis of Dissymmetric Azobenzenes.[2]

Nitrosobenzene derivative (0.80 mmol) was dissolved in glacial acetic acid (2 mL), and the amine (0.80 mmol) in EtOH (0.5 mL) was added to the solution. After being stirred for 6 h at 40 °C, the mixture was poured onto ice and filtered. The crude brown product was then purified by column chromatography with silica and ethyl acetate/etroleum ether.

2.3. Typical Experimental Procedure of the *meta*-Selective C-H Sulfonation of Azoarenes

Azobenzenes (0.2 mmol), Aryl sulfonyl chloride (0.6 mmol, 3.0 equiv.), [Ru(*p*-Cymene)Cl_2]$_2$, (0.01 mmol, 5 mol %), Cs_2CO_3 (0.4 mmol, 2.0 equiv), dry Acetonitrile (1.5 mL) were charged into a pre-dried 30-mL pressure tube sealed with rubber plugs under N_2 atmosphere. The reaction mixture was stirred at 110 °C for 24 h. The reaction was cooled down to room temperature. The mixture was passed through a short pad of celite, washing with a mixture of EtOAc. The organic layer was concentrated under reduced pressure to give a crude oil, which was purified by column chromatography (ethyl acetate/etroleum ether as eluent) on silica gel to afford the desired products.

2.4. Experimental Procedure for the Reduction of Azobenzenes Product.



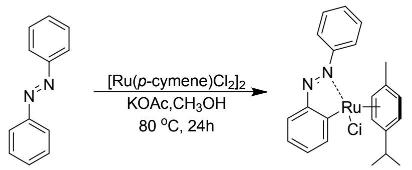
Azobenzenes, Fe powder (3.0 equiv.), CH_3COOH, (6.0 equiv.), CH_3OH (3 mL) were charged into a one-neck flask under N_2 atmosphere. The reaction mixture was stirred at room temperature for 24 h. The reaction was cooled down to room temperature. An aqueous solution of saturated Na_2CO_3 was added to the mixture, and then stirred for additional 5 min. The aqueous layer was extracted with EtOAc (3 x 20 mL). The organic phase were combined and dried over anhydrous Na_2SO_4, filtered and evaporated under reduced pressure to give crude product, which was purified by column chromatography (ethyl acetate/etroleum ether). The products were identified by NMR and MS spectra.

3. Mechanistic Studies

3.1 Isotope Labelling Studies in the Ruthenium-Catalyzed *Meta*-Selective C-H Functionalization of Azoarenes

Under standard conditions, the ruthenium-catalyzed *meta*-selective C-H alkylation and sulfonation of isotope labelling azobenzene were characterized by ^1H NMR spectra respectively.

3.2. Preparation of Azoarene-Ruthenium Complex[3]



$[RuCl_2(p\text{-cymene})]_2$ (0.5 mmol, 306 mg), KOAc (2 mmol, 196 mg), azobenzene (1 mmol, 182mg) and dry CH_3OH (10 mL) were charged into a pre-dried 50-mL pressure tube sealed with rubber plugs under N_2 atmosphere. The reaction was stirred at 80 °C for 48 h. The reaction was then concentrated to dryness, dissolved in a minimal amount of ethyl acetate and then purified through neutral alumina with EtOAc as the solvent to yield the complex as a dark red solid. And the structure was definitely confirmed by single-crystal X-ray diffraction (Figure 2).

4. References

1. D. Zhang, X.-L Cui, Q.-Q Zhang, Y.-J. Wu, *J. Org. Chem*. **2015**, *80*, 1517-1522.
2. T.H.L. Nguyen, N. Gigant, S. Delarue-Cochin, D. Joseph, *J. Org. Chem*. **2016**, *81*, 1850-1857.
3. A.J. Paterson, S.S. John-Campbell, M.F. Mahon, N.J. Pressc, C.G. Frost, *Chem. Commun*. **2015**, *51*, 12807-12810.

5. Data and Spectra of ^{1}H NMR and ^{13}C NMR

(E)-1-phenyl-2-(3-tosylphenyl)diazene (**3aa,** orange red solid, M.p. 166-169 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (t, *J* = 1.8 Hz, 1H), 8.10 (m, 1H), 8.06-8.02 (m, 1H), 7.97-7.93 (m, 2H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.66 (t, *J* = 7.9 Hz, 1H), 7.57-7.52 (m, 3H), 7.33 (d, *J* = 8.1 Hz, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.76, 152.27, 144.46, 143.35, 138.31, 131.89, 130.10, 130.05, 129.22, 129.20, 127.88, 127.39, 123.18, 121.58, 21.59.HRMS (ESI) Calcd. For $C_{19}H_{17}N_2O_2S$: $[M+H]^+$, 337.1011, Found: *m/z* 337.1017.

(E)-1-(2-methyl-5-tosylphenyl)-2-(o-tolyl)diazene (**3ba,** orange red solid, M.p. 132-134 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.8 Hz, 1H), 7.82 (t, *J* = 7.0 Hz, 3H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.9 Hz, 1H), 7.40 -7.30 (m, 4H), 7.25 (s, 1H), 2.84 (s, 3H), 2.74 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.28, 150.75, 144.14, 141.04, 138.66, 138.28, 137.57, 131.55, 131.44, 131.23, 129.72, 127.84, 126.43, 126.39, 121.13, 115.82, 21.56, 17.57, 13.50. HRMS (ESI) Calcd. For $C_{21}H_{21}N_2O_2S$: $[M+H]^+$, 365.1324, Found: *m/z* 365.1324.

(E)-1-(3-methyl-5-tosylphenyl)-2-(*m*-tolyl)diazene (**3ca,** orange red solid, M.p. 137-138 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.90 (d, *J* = 8.2 Hz, 3H), 7.85 (s, 1H), 7.74 (s, 2H), 7.43 (t, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 3H), 2.51 (s, 3H), 2.48 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.86, 152.41, 144.32, 143.04, 140.66, 139.14, 138.46, 132.57, 130.00, 129.51, 129.01, 127.85, 127.65, 123.21, 120.77, 119.28, 21.59, 21.37, 21.35.HRMS (ESI) Calcd. For $C_{21}H_{21}N_2O_2S$: $[M+H]^+$, 365.1324, Found: *m/z* 365.1326.

(E)-1-(4-methyl-3-tosylphenyl)-2-(*p*-tolyl)diazene (**3da,** orange red solid, M.p. 176-179 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.78 (s, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.85 (m, 4H), 7.39-7.30 (m, 5H), 2.53 (s, 3H), 2.46 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.96, 150.52, 144.21, 142.30, 140.27, 140.10, 137.99, 133.46, 129.86, 129.75, 127.92, 126.86, 124.01, 123.13, 21.60, 21.58, 20.23. HRMS (ESI) Calcd. For $C_{21}H_{21}N_2O_2S$: $[M+H]^+$, 365.1324, Found: *m/z* 365.1325.

(E)-1-([1,1'-biphenyl]-4-yl)-2-(2-tosyl-[1,1'-biphenyl]-4-yl)diazene (**3ea,** orange red solid, M.p. 186-188 ^oC): ^1HNMR (400 MHz, $CDCl_3$) δ 9.01 (s, 1H), 8.10 (d, *J* = 8.2 Hz, 2H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 3H), 7.71 (d, *J* = 6.8 Hz, 3H), 7.51 (d, *J* = 6.1 Hz, 2H), 7.43 (s, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 8.2 Hz, 2H), 7.05 (dd, *J* = 16.2, 7.5 Hz, 3H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.57, 144.57, 144.08, 143.57, 141.29, 140.06, 137.71, 133.65, 129.94, 129.00, 128.95, 128.89, 128.07, 127.94, 127.90, 127.78, 127.33, 127.23, 127.19, 126.32, 123.77, 123.39, 21.49. HRMS (ESI) Calcd. For $C_{31}H_{25}N_2O_2S$: $[M+H]^+$, 489.1637, Found: *m/z* 489.1631.

(E)-1-(4-methoxy-3-tosylphenyl)-2-(4-methoxyphenyl)diazene (**3fa,** orange red solid, M.p. 113-116 ^oC): ^1H NMR(400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 2.3 Hz, 1H), 8.10 (m, 1H), 7.93 (m, 4H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.03 (dd, *J* = 8.7, 6.7 Hz, 3H), 3.92 (s, 3H), 3.87 (s, 3H), 2.43 (s, 3H). ^{13}C NMR(101 MHz, $CDCl_3$) δ 162.21, 158.18, 146.76, 146.15, 144.02, 138.21, 130.13, 129.80, 129.22, 128.63, 124.83, 123.96, 114.29, 112.58, 56.31, 55.62, 21.63. HRMS (ESI) Calcd. For $C_{21}H_{21}N_2O_4S$: $[M+H]^+$, 397.1222, Found: *m/z* 397.1220.

(E)-1-(3-tosyl-4-(trifluoromethoxy)phenyl)-2-(4-(trifluoromethoxy)phenyl)diazene (**3ga,** orange red solid, M.p. 129-133 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.70 (s, 1H), 7.94 (s, 1H), 7.87 (d, *J* = 8.9 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.45 (d, *J* = 8.8 Hz, 2H), 7.40 (s, 1H), 7.17 (d, *J* = 7.8 Hz, 3H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.54, 151.30, 150.42, 149.96, 149.91, 148.24, 147.52, 146.68, 145.18, 143.58, 137.56, 137.23, 134.48, 129.78, 128.68, 124.84, 124.55, 123.18, 122.73, 122.16, 121.08, 118.14, 117.64, 21.66. HRMS (ESI) Calcd. For $C_{21}H_{15}F_6N_2O_4S$: $[M+H]^+$, 505.0657, Found: *m/z* 505.0650.

(E)-1-(4-fluoro-3-tosylphenyl)-2-(4-fluorophenyl)diazene (**3ha,** orange red solid, M.p. 180-183 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.67 (m, 1H), 8.13 (m, 1H), 8.01-7.94 (m, 4H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.26-7.21 (m, 3H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.15, 163.62, 161.44, 158.84, 148.71, 148.51, 145.03, 137.65, 136.48, 131.00, 130.84, 130.00, 129.91, 129.86, 129.34, 128.39, 128.37, 127.61, 125.32, 125.23, 123.85, 118.16, 117.93, 116.38, 116.15, 21.64.HRMS (ESI) Calcd. For $C_{19}H_{15}F_2N_2O_2S$: $[M+H]^+$, 373.0822, Found: *m/z* 373.0822.

(E)-1-(4-bromo-3-tosylphenyl)-2-(4-bromophenyl)diazene (**3ia,** orange red solid, M.p. 164-166 ^oC): ^1H NMR (400 MHz, CDCl3) δ 8.94 (d, *J* = 2.3 Hz, 1H), 7.95 (m, 1H), 7.89 (m, 3H), 7.86 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.73-7.68 (m, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 2.45 (s, 3H).^{13}C NMR (101 MHz, CDCl3) δ 136.53, 132.60, 129.61 (d), 128.92, 124.73. HRMS (ESI) Calcd. For $C_{19}H_{15}Br_2N_2O_2S$: $[M+H]^+$, 492.9221, Found: *m/z* 492.9229.

(E)-1-(*p*-tolyl)-2-(3-tosylphenyl)diazene (**3ja,** orange red solid, M.p. 143-144 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 2.0 Hz, 1H), 8.03 (m, 1H), 7.97 (m, 2H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 7.5 Hz, 3H), 7.39 (d, *J* = 8.1 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 2.54 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.36, 150.86, 144.26, 140.46, 140.34, 137.92, 133.49, 131.59, 129.76, 129.20, 127.94, 126.98, 124.12, 123.10, 21.61, 20.26. HRMS (ESI) Calcd. For $C_{20}H_{19}N_2O_2S$: $[M+H]^+$, 351.1167, Found: *m/z* 351.1163.

(E)-1-(4-(tert-butyl)phenyl)-2-(3-tosylphenyl)diazene (**3ka,** orange red solid, M.p. 124-126 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.10 -8.07 (m, 1H), 8.02 (d, *J* = 7.9 Hz, 1H), 7.92 -7.88 (m, 4H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.55 (s, 2H), 7.33 (d, *J* = 8.2 Hz, 2H), 2.42 (s, 3H), 1.39 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.66, 152.95, 150.27, 144.43, 143.26, 138.37, 130.02, 128.90, 127.88, 127.22, 126.15, 125.75, 122.95, 121.54, 35.05, 31.22, 21.36. HRMS (ESI) Calcd. For $C_{23}H_{25}N_2O_2S$: $[M+H]^+$, 393.1637, Found: *m/z* 393.1639.

(E)-1-(naphthalen-2-yl)-2-(4-tosylnaphthalen-2-yl)diazene (**3la,** orange red solid, M.p. 115-117 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.72 (s, 2H), 8.63 (s, 1H), 8.15 (s, 1H), 8.10 (d, J = 6.1 Hz, 2H), 7.94 (d, J = 8.2 Hz, 4H), 7.64 (d, J = 7.6 Hz, 4H), 7.30 (d, J = 8.1 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.08, 148.56, 144.18, 138.62, 137.98, 135.18, 134.67, 133.55, 132.63, 130.45, 129.83, 129.61, 129.49, 129.30, 129.24, 127.99, 127.65, 127.62, 124.87, 121.88, 116.75, 21.54. HRMS (ESI) Calcd. For $C_{27}H_{21}N_2O_2S$ $[M+H]^+$, 437.1324, Found: *m/z* 437.1327.

(E)-1-phenyl-2-(3-(phenylsulfonyl)phenyl)diazene (**3ab,** orange red solid, M.p. 103-106 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 8.12 (d, J = 7.9 Hz, 1H), 8.08 -8.01 (m, 3H), 7.97 - 7.93 (m, 2H), 7.67 (t, J = 7.9 Hz, 1H), 7.62 -7.50 (m, 7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.78, 152.24, 142.96, 141.26, 133.45, 131.95, 130.21, 129.43, 129.34, 129.24, 127.82, 127.61, 123.21, 121.69.HRMS (ESI) Calcd. For $C_{18}H_{15}N_2O_2S$: $[M+H]^+$, 323.0854, Found: *m/z* 323.0851.

(E)-1-phenyl-2-(3-(*o*-tolylsulfonyl)phenyl)diazene (**3ac,** orange red solid, M.p. 166-169 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (t, J = 1.7 Hz, 1H), 8.32- 8.27 (m, 1H), 8.15- 8.10 (m, 1H), 8.00 - 7.92 (m, 3H), 7.67 (t, J = 7.9 Hz, 1H), 7.54 (d, J = 2.7 Hz, 4H), 7.44 (t, J = 7.6 Hz, 1H), 7.27 (d, J = 6.9 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.60, 152.26, 142.68, 138.53, 138.10, 133.85, 132.79, 131.91, 129.91, 129.62, 129.27 (d), 127.14, 126.64, 123.20, 121.97, 20.32. HRMS (ESI) Calcd. For $C_{19}H_{17}N_2O_2S$: $[M+H]^+$, 337.1011, Found: *m/z* 337.1016.

(E)-1-(3-([1,1'-biphenyl]-4-ylsulfonyl)phenyl)-2-phenyldiazene (**3ad,** orange red solid, M.p. 110-112 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1H), 8.15-8.07 (m, 4H), 7.99-7.95 (m, 2H), 7.75-7.68 (m, 3H), 7.59-7.54 (m, 5H), 7.50-7.41 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 131.90, 130.18, 129.40-128.95 (m), 128.62, 128.36, 128.05, 127.45 (d), 123.20, 121.71. HRMS (ESI) Calcd. For $C_{24}H_{19}N_2O_2S$: $[M+H]^+$, 399.1167, Found: *m/z*399.1171.

(E)-1-(3-((4-fluorophenyl)sulfonyl)phenyl)-2-phenyldiazene (**3ae,** orange red solid, M.p. 155-156 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.13 (d, J = 7.9 Hz, 1H), 8.07-8.02 (m, 3H), 7.96 (m, 2H), 7.69 (t, J = 7.9 Hz, 1H), 7.57-7.53 (m, 3H), 7.22 (t, J = 8.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.88, 164.33, 152.84, 152.24, 142.83, 137.37, 137.34, 131.99, 130.73, 130.63, 130.28, 129.24, 129.18, 127.76, 123.21, 121.55, 116.86, 116.64.HRMS (ESI) Calcd. For $C_{18}H_{14}FN_2O_2S$ $[M+H]^+$, 341.0760, Found: *m/z* 341.0762.

(E)-1-(3-((4-chlorophenyl)sulfonyl)phenyl)-2-phenyldiazene (**3af,** orange red solid, M.p. 144-146 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.48 (t, *J* = 1.6 Hz, 1H), 8.14 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 4H), 7.69 (t, *J* = 7.9 Hz, 1H), 7.56-7.49 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.85, 152.23, 142.57, 140.20, 139.81, 132.01, 130.32, 129.76, 129.29, 129.24, 127.89, 123.23, 121.60.HRMS (ESI) Calcd. For $C_{18}H_{14}ClN_2O_2S$: $[M+H]^+$, 357.0465, Found: m/z 357.0460.

(E)-1-(3-((4-bromophenyl)sulfonyl)phenyl)-2-phenyldiazene (**3ag,** orange red solid, M.p. 116-118 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.14 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.96 (m, 2H), 7.88 (d, *J* = 8.5 Hz, 2H), 7.69 (t, *J* = 8.0 Hz, 3H), 7.58 - 7.53 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.86, 152.24, 142.52, 140.35, 132.74, 132.00, 130.31, 129.35, 129.24, 128.77, 127.91, 123.22, 121.60. HRMS (ESI) Calcd. For $C_{18}H_{14}BrN_2O_2S$: $[M+H]^+$, 400.9959, Found: *m/z* 400.9950.

(E)-1-(3-((4-iodophenyl)sulfonyl)phenyl)-2-phenyldiazene (**3ah,** orange red solid, M.p. 137-140 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.14 (d, *J* = 7.9 Hz, 1H), 8.03 (d, *J* = 7.8 Hz, 1H), 7.98 -7.94 (m, 2H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.70 (m, 3H), 7.58-7.53 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.85, 152.22, 142.48, 141.00, 138.71, 132.01, 130.32, 129.24, 129.16, 127.93, 123.23, 121.59, 101.36. HRMS (ESI) Calcd. For $C_{18}H_{14}IN_2O_2S$: $[M+H]^+$, 448.9821, Found: *m/z* 448.9826.

(E)-1-(3-((4-methoxyphenyl)sulfonyl)phenyl)-2-phenyldiazene (**3ai,** orange red solid, M.p. 105-108 ^oC): ^1H NMR (400 MHz, $CDCl_3$) δ 8.45 (t, *J* = 1.8 Hz, 1H), 8.09-8.05 (m, 1H), 8.03 -7.99 (m, 1H), 7.96 -7.91 (m, 4H), 7.64 (t, *J* = 7.9 Hz, 1H), 7.55-7.50 (m, 3H), 6.98 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.58, 152.76, 152.28, 143.73, 132.75, 131.86, 130.06, 129.21, 129.02, 127.22, 123.18, 121.40, 114.65, 55.66. HRMS (ESI) Calcd. For $C_{19}H_{17}N_2O_3S$: $[M+H]^+$, 353.0960, Found: *m/z* 353.0959.

(E)-1-(3-((4-nitrophenyl)sulfonyl)phenyl)-2-phenyldiazene (**3aj,** orange red solid, M.p. 155-157 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (t, *J* = 1.7 Hz, 1H), 8.38 (d, *J* = 8.9 Hz, 2H), 8.23-8.17 (m, 3H), 8.08 (m, 1H), 7.98 -7.94 (m, 2H), 7.73 (t, *J* = 7.9 Hz, 1H), 7.56 (dd, *J* = 5.1, 1.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.98, 152.17, 150.52, 147.02, 141.40, 132.19, 130.60, 129.48, 129.28, 129.17, 128.63, 124.64, 123.27, 121.82. HRMS (ESI) Calcd. For $C_{18}H_{14}N_3O_4S$: $[M+H]^+$, 368.0705, Found: *m/z* 368.0703.

(E)-1-phenyl-2-(3-((4-(trifluoromethyl)phenyl)sulfonyl)phenyl)diazene (**3ak,** orange red solid, M.p. 116-118 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 1.7 Hz, 1H), 8.14 (d, *J* = 8.2 Hz, 3H), 8.07-8.04 (m, 1H), 7.94 (d, *J* = 1.8 Hz, 2H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.70 (t, *J* = 7.9 Hz, 1H), 7.55-7.50 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.91, 152.20, 144.88, 141.92, 135.26, 134.93, 132.09, 130.45, 129.58, 129.43, 129.26, 128.90, 128.83, 128.38, 128.27, 128.19, 126.60, 126.56, 124.43, 123.25, 122.91, 121.78, 121.71, 115.58, 115.24. HRMS (ESI) Calcd. For $C_{19}H_{14}F_3N_2O_2S$: $[M+H]^+$, 391.0728, Found: *m/z* 391.0724.

(E)-4-((3-(phenyldiazenyl)phenyl)sulfonyl)benzonitrile (**3al,** orange red solid, M.p. 141-143 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.18 (d, *J* = 7.3 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 2H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.96 (m, 2H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.73 (t, *J* = 7.9 Hz, 1H), 7.56 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.76-158.53 (m), 153.00, 159.76-129.45(m), 132.13, 132.13, 130.52, 130.52, 129.34(d), 128.44, 123.25, 121.83, 117.12 (d). HRMS (ESI) Calcd. For $C_{19}H_{14}N_3O_2S$: $[M+H]^+$, 348.0807, Found: *m/z* 348.0804.

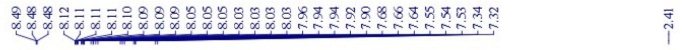
(E)-1-(4-((3-(phenyldiazenyl)phenyl)sulfonyl)phenyl)ethanone (**3am,** orange red solid, M.p. 160-162 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.17- 8.05 (m, 6H), 7.95 (d, *J* = 5.2 Hz, 2H), 7.70 (t, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 5.3 Hz, 3H), 2.63 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.53, 152.87, 152.19, 145.07, 142.22, 140.51, 132.03, 130.35, 129.39, 129.24, 129.15, 128.16, 128.06, 123.22, 121.79, 26.83. HRMS (ESI) Calcd. For $C_{20}H_{17}N_2O_3S$: $[M+H]^+$, 365.0960, Found: *m/z* 365.0959.

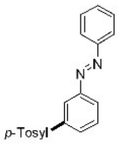
(E)-1-(3-(naphthalen-2-ylsulfonyl)phenyl)-2-phenyldiazene (**3an,** orange red solid, M.p. 157-158 °C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (s, 1H), 8.56 (d, *J* = 1.3 Hz, 1H), 8.11 (m, 2H), 8.02 (d, J = 8.2 Hz, 1H), 7.96 (m, 4H), 7.89 (d, J = 7.8 Hz, 1H), 7.70-7.62 (m, 3H), 7.55 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.81, 152.27, 143.02, 138.07, 135.13, 132.26, 131.90, 130.17, 129.80, 129.47, 129.39, 129.36, 129.27, 129.21, 127.95, 127.70, 127.52, 123.19, 122.70, 121.81. HRMS (ESI) Calcd. For $C_{22}H_{17}N_2O_2S$: $[M+H]^+$, 373.1011, Found: *m/z* 373.1016.

(E)-1-phenyl-2-(3-(thiophen-2-ylsulfonyl)phenyl)diazene (**3ao,** orange red solid, M.p. 120-122 ^{o}C): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (t, J = 1.7 Hz, 1H), 8.12 (m, 2H), 7.98-7.94 (m, 2H), 7.79 (m, 1H), 7.69 (m, 2H), 7.57-7.53 (m, 3H), 7.14-7.10 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ152.82, 152.26, 143.42, 142.61, 134.27, 133.78, 131.95, 130.21, 129.23, 128.96, 128.01, 127.71, 123.22, 121.34. HRMS (ESI) Calcd. For $C_{16}H_{13}N_2O_2S_2$: $[M+H]^+$, 329.0418, Found: *m/z* 329.0417.

3-tosylaniline (**4,** white solid): ^{1}H NMR (400 MHz, $CDCl_3$) δ7.80 (d, J = 8.2 Hz, 2H), 7.29-7.18 (m, 5H), 6.83-6.71 (m, 1H), 3.67 (2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ147.20, 143.96, 142.70, 138.82, 130.13, 129.80, 127.64, 119.18, 117.18, 113.09, 21.53. HRMS (ESI) Calcd. For $C_{13}H_{14}NO_2S$: $[M+H]^+$, 248.0745, Found: *m/z* 248.0738

Complex **I** (brown black solid)**:** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 - 8.27 (m, 1H), 8.22-8.18 (m, 2H), 7.51 (d, J = 6.8 Hz, 4H), 7.24-7.15 (m, 2H), 5.70 (d, J = 6.2 Hz, 1H), 5.55 (d, J = 6.0 Hz, 1H), 5.18 (d, J = 6.2 Hz, 1H), 5.07 (d, J = 6.0 Hz, 1H), 2.29 (m, 1H), 2.12 (s, 3H), 0.91 (d, J = 6.9 Hz, 3H), 0.74 (d, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.33, 130.64, 129.89, 128.37, 123.71, 123.08, 92.62, 86.59, 86.17, 30.90, 22.82, 21.27.





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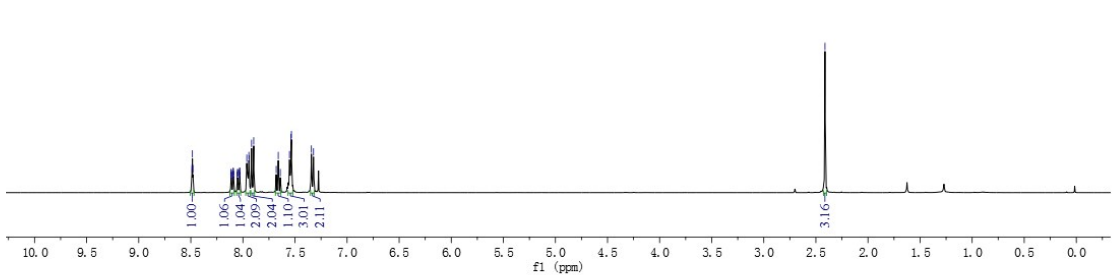

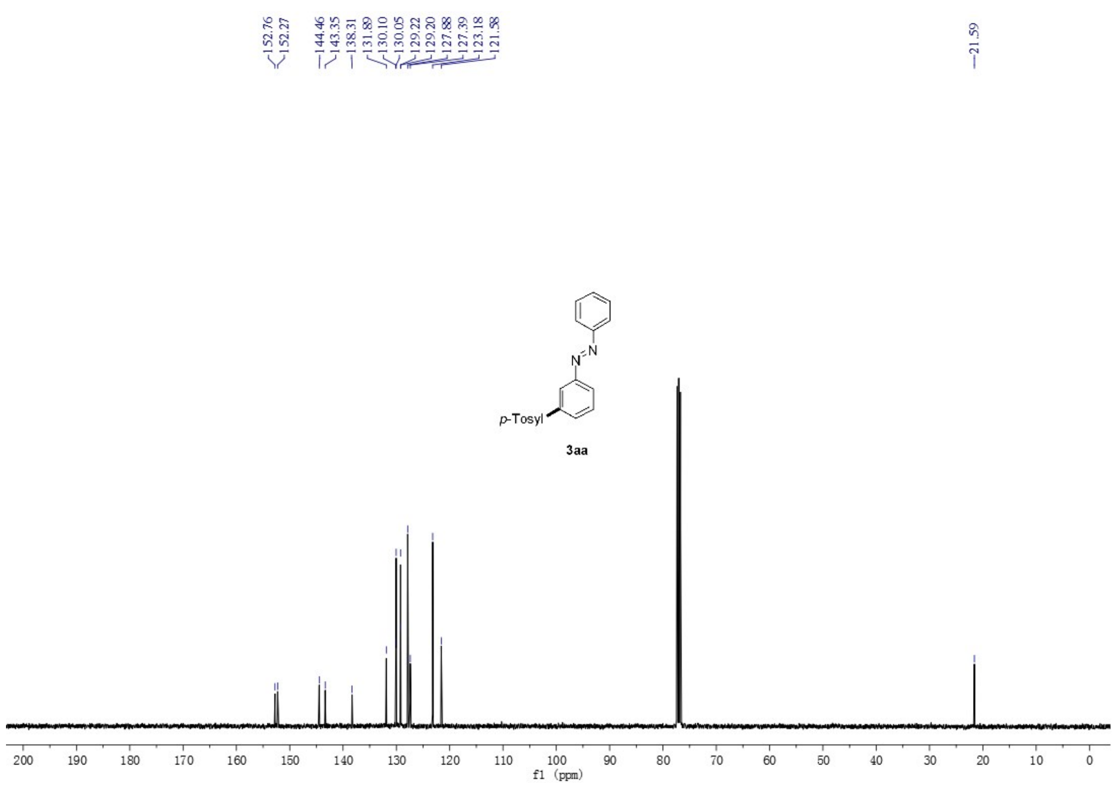
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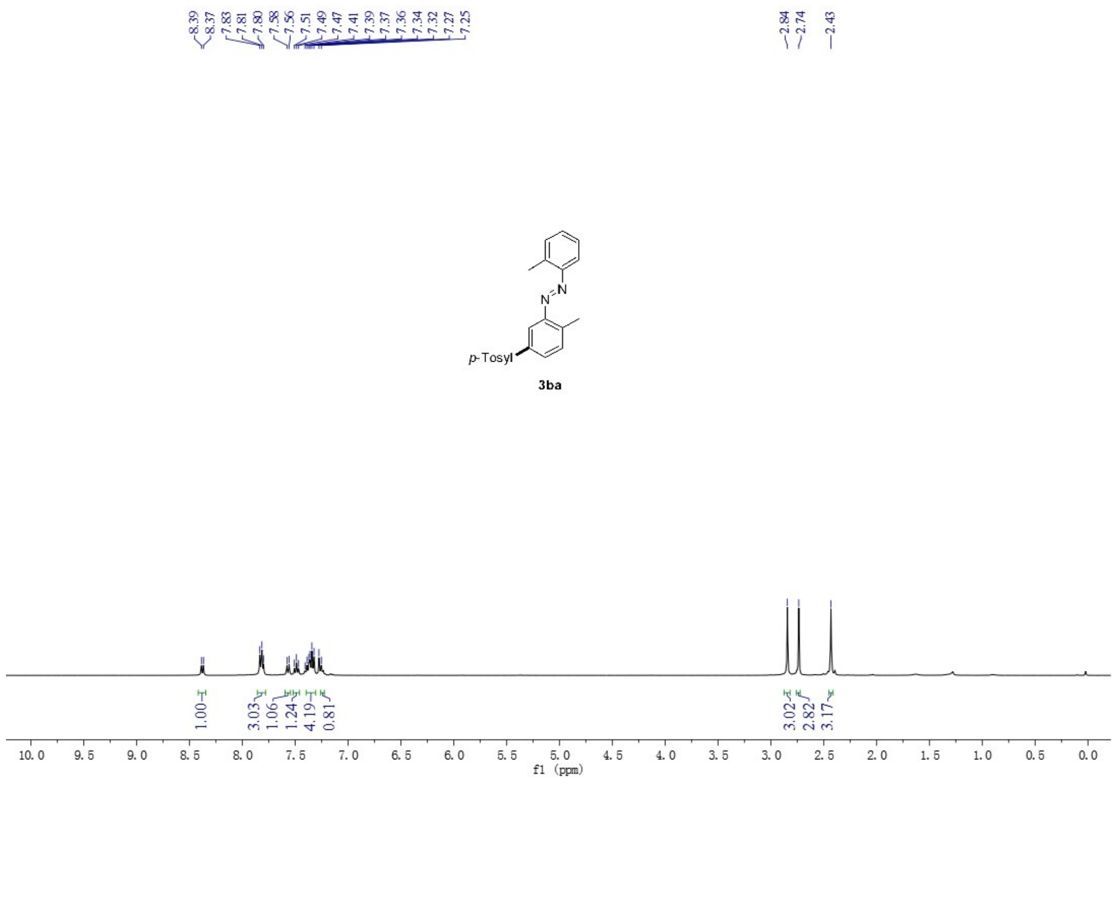
f1 (ppm)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7.27
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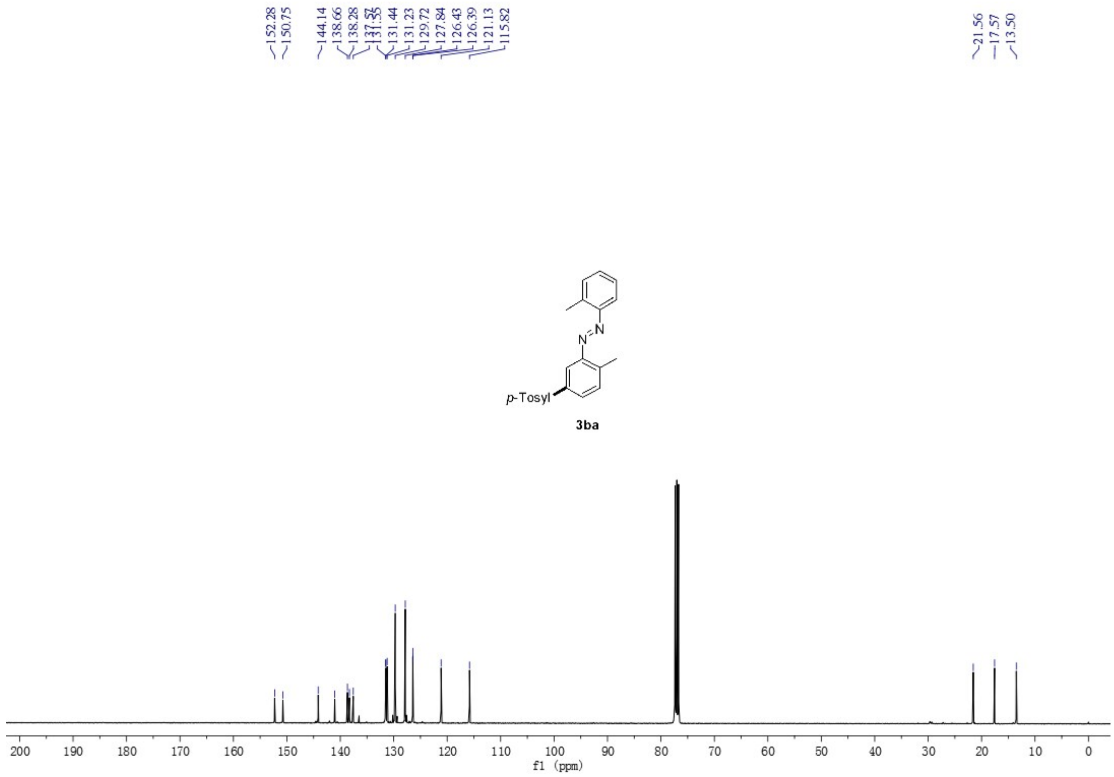
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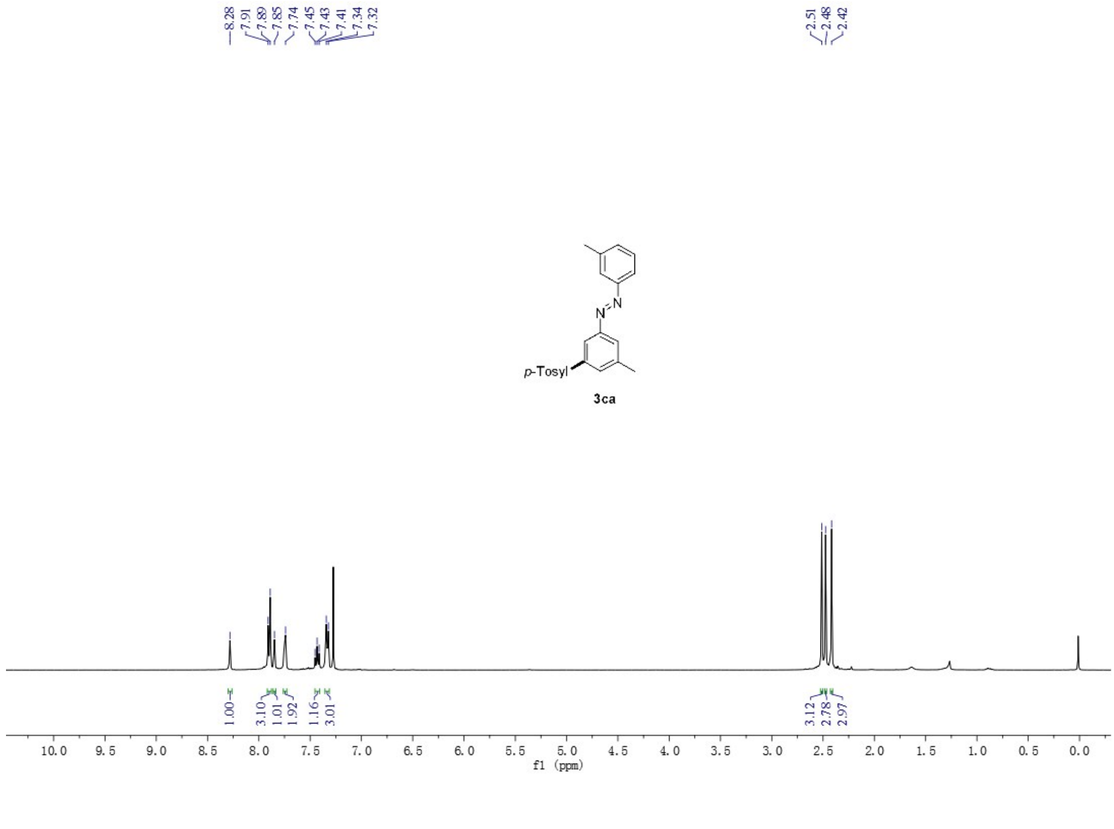
f1 (ppm)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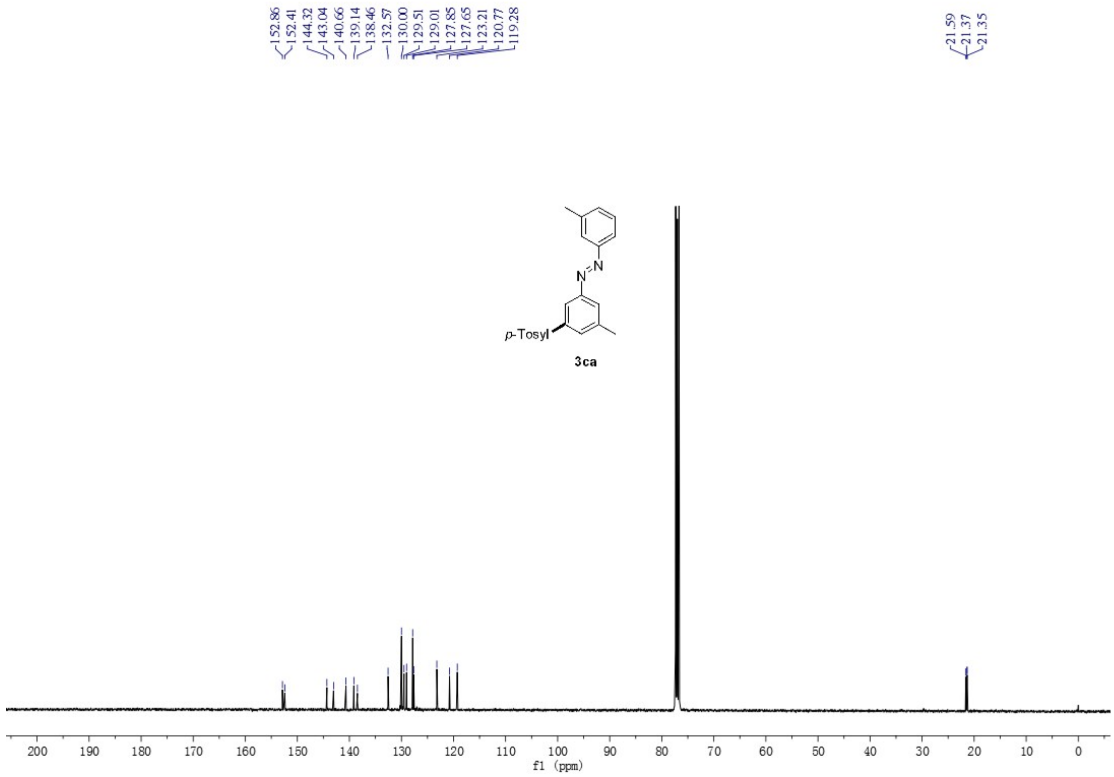
3.10
1.01
1.92
1.16
3.01
3.12
2.78
2.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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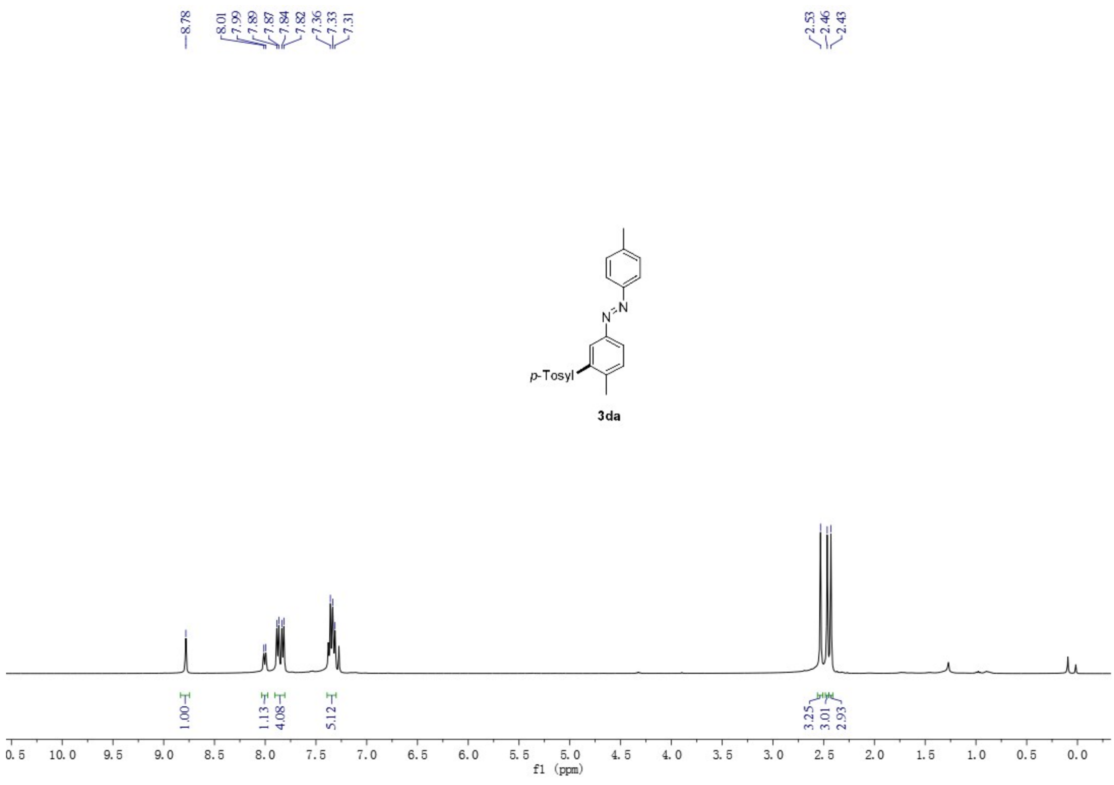
f1 (ppm)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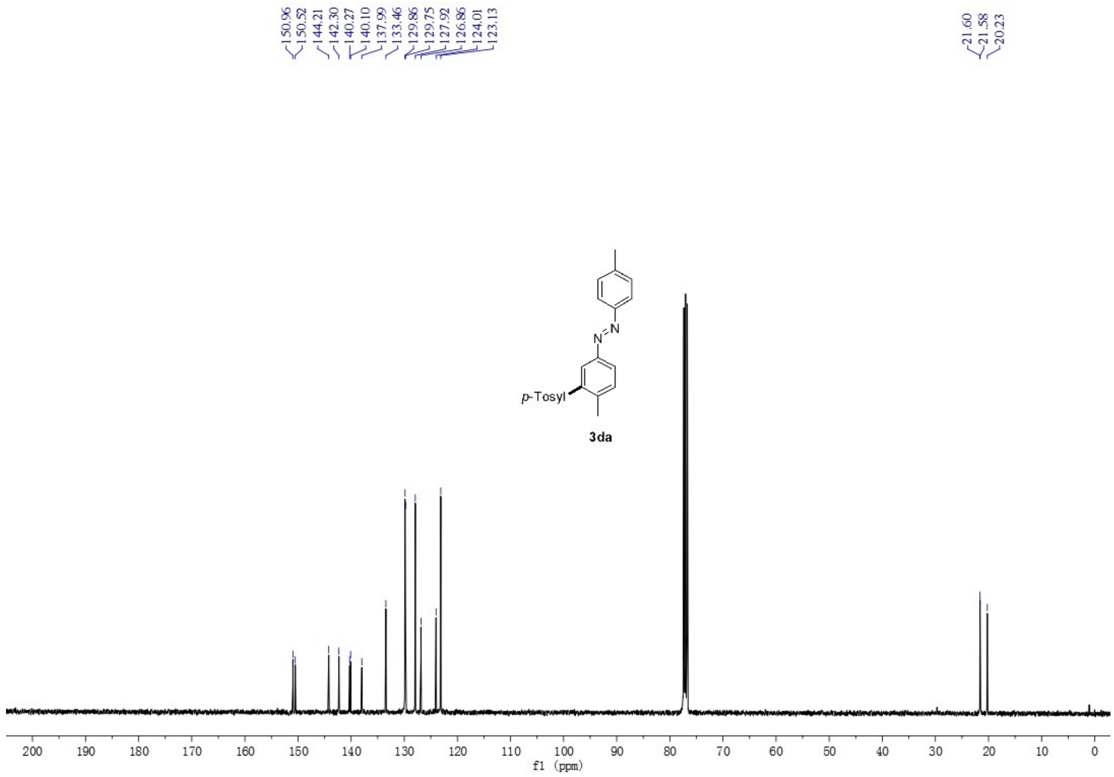

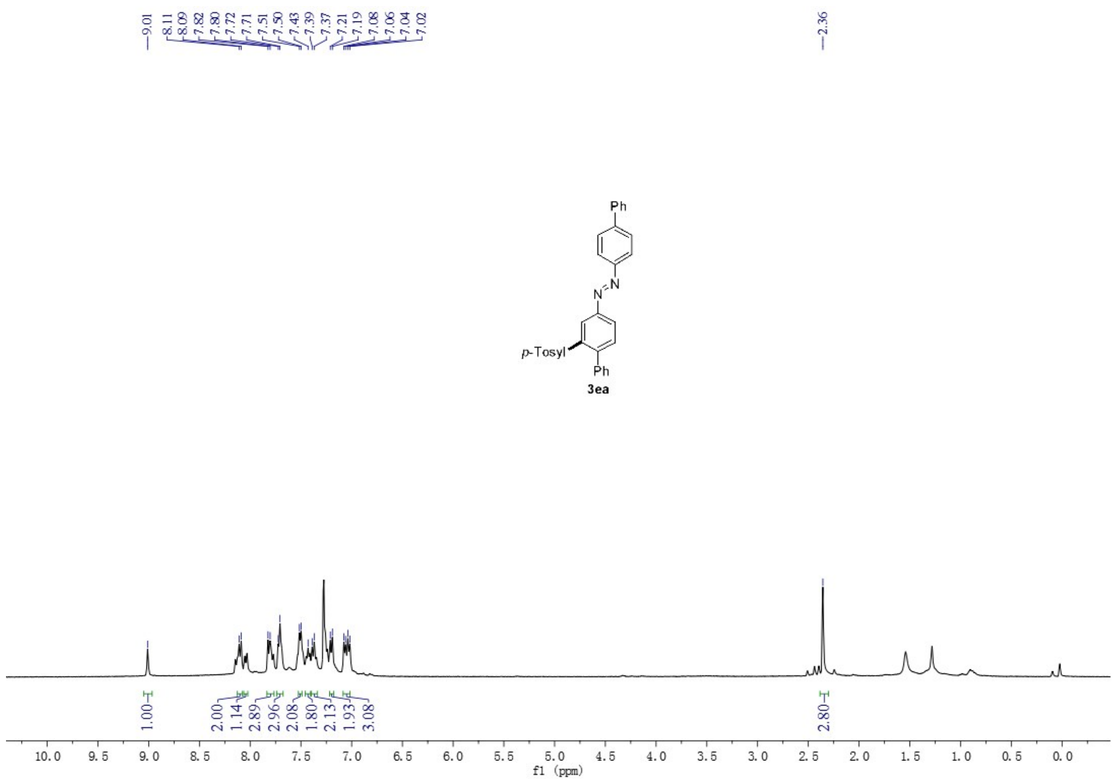

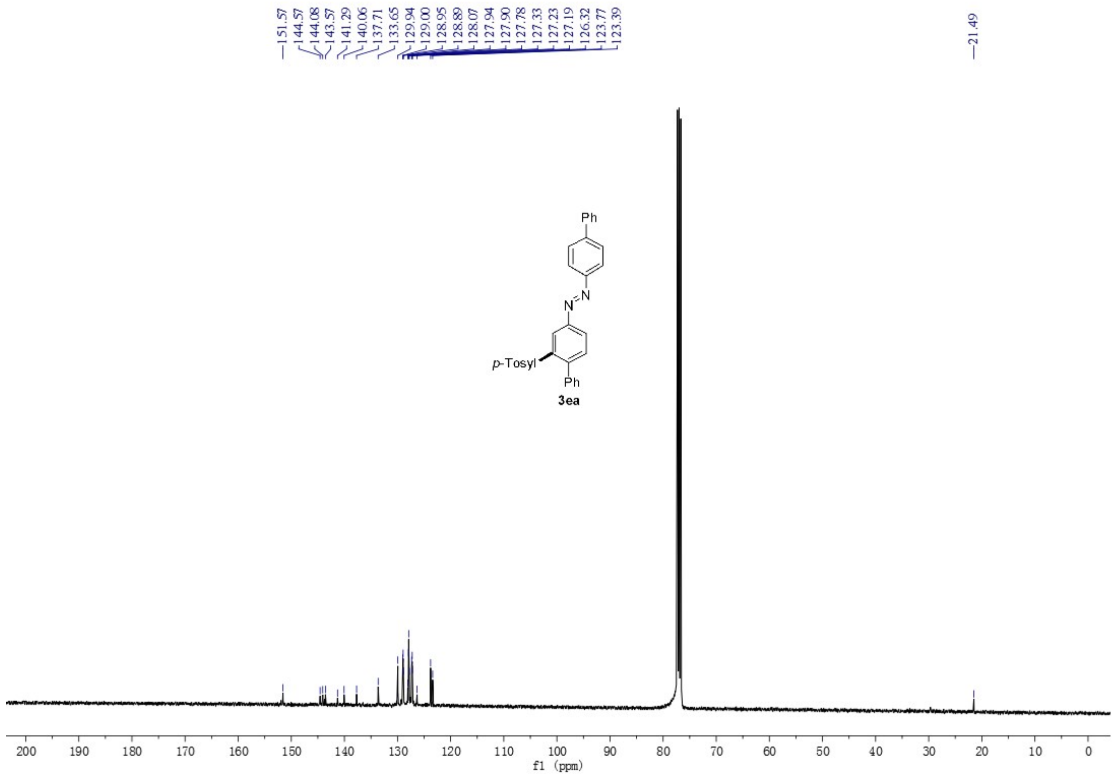

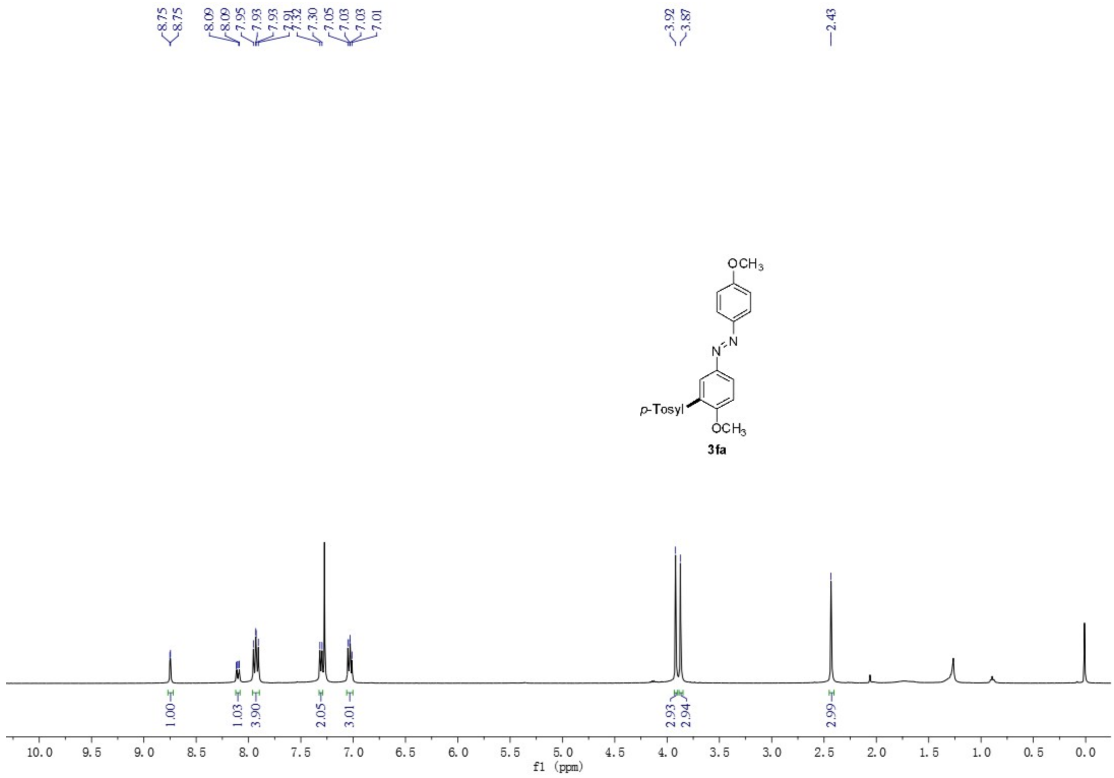

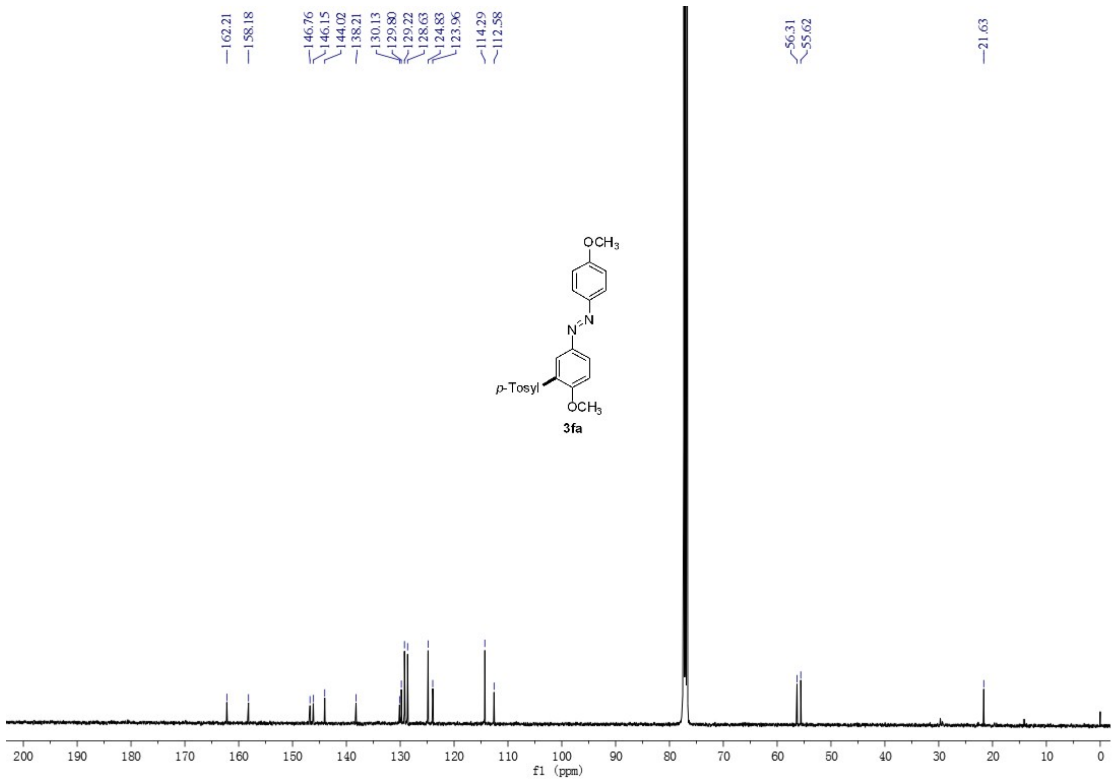

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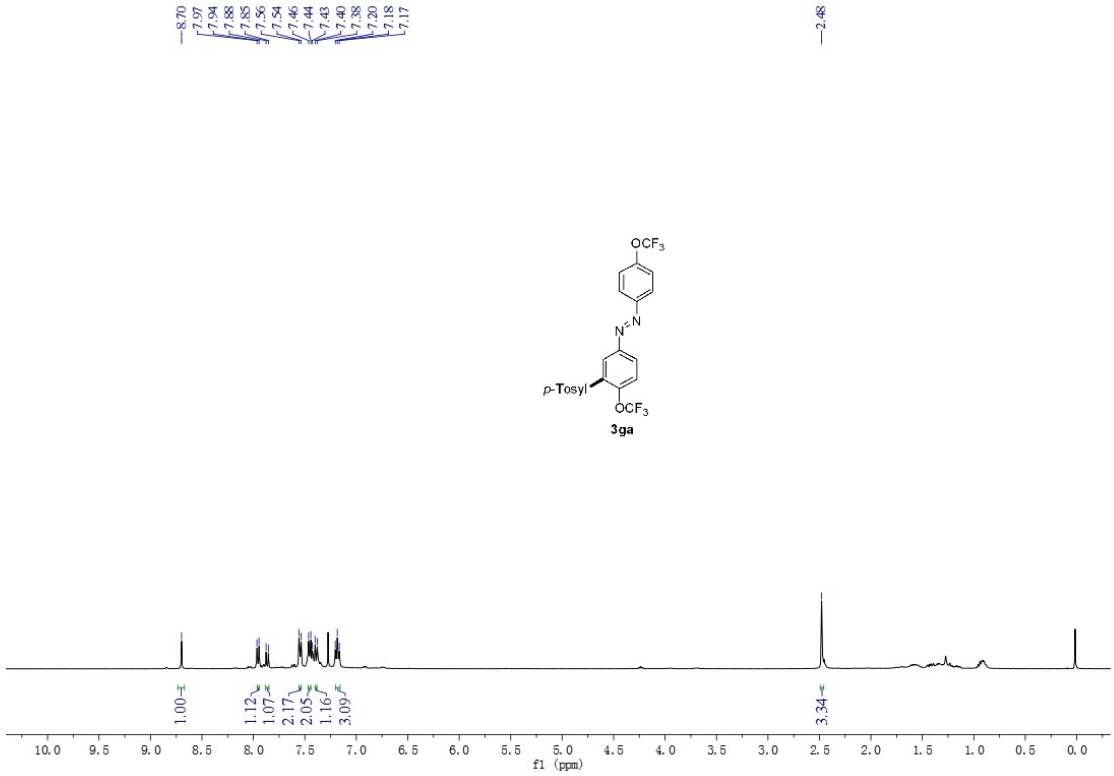
f1 (ppm)



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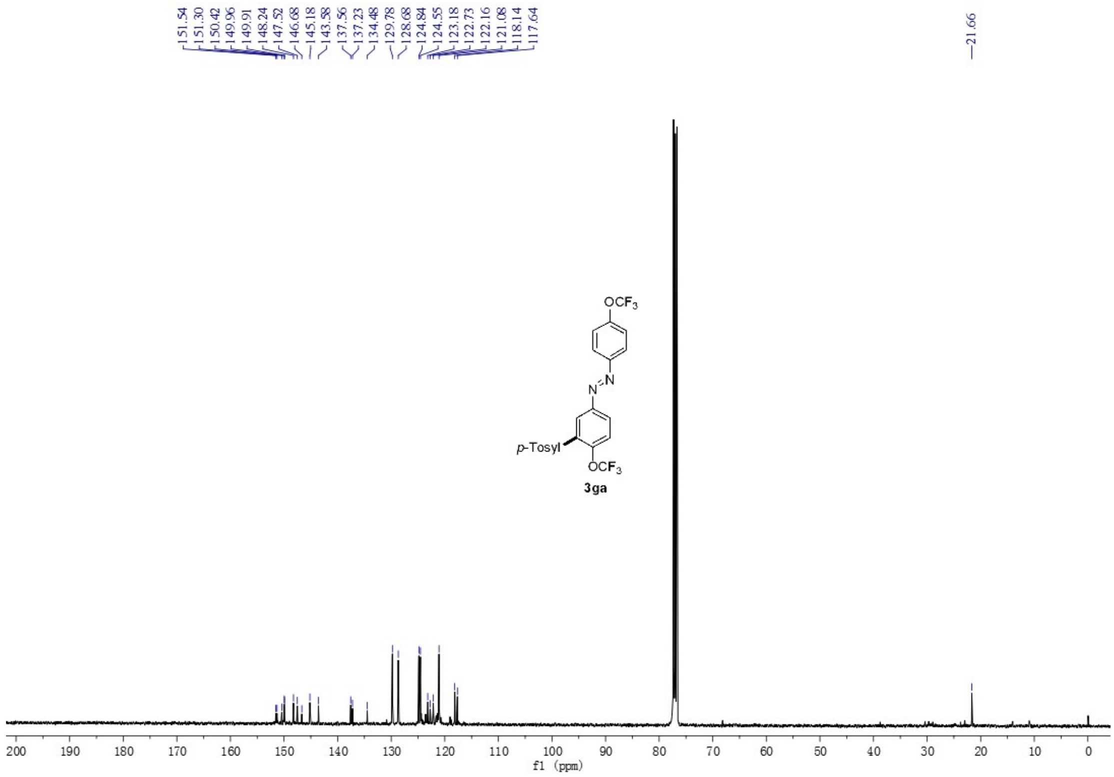
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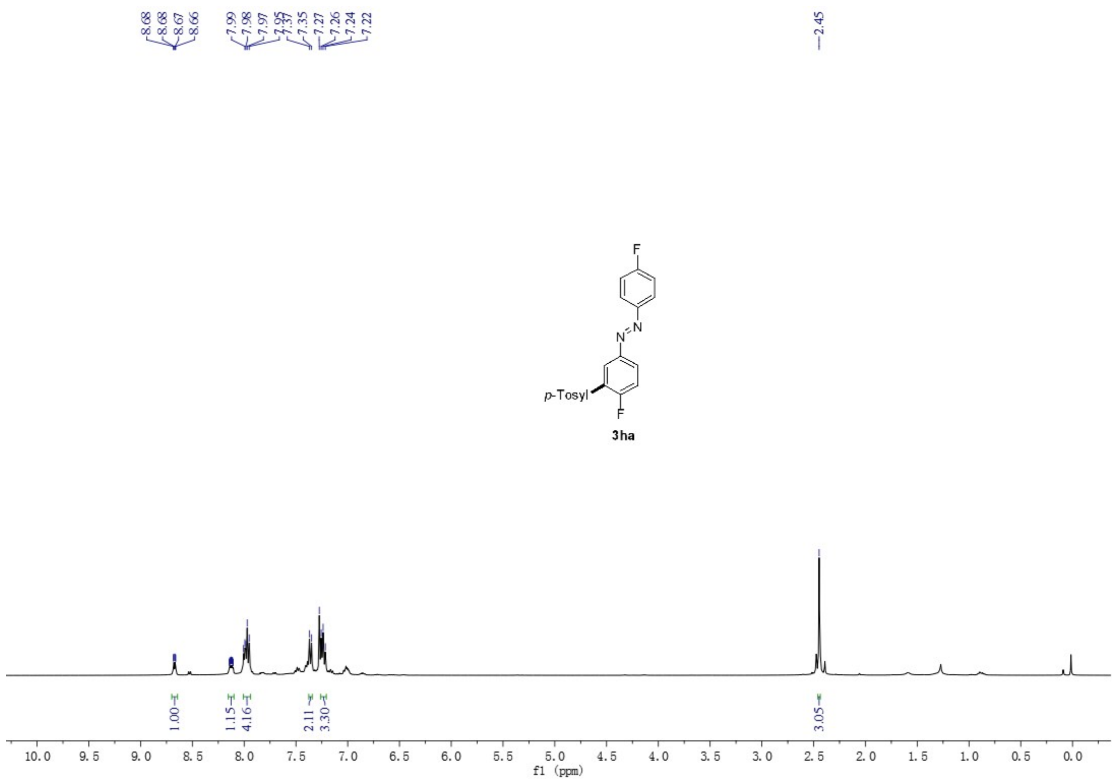
OCF3
3ga
f1 (ppm)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7.22
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F
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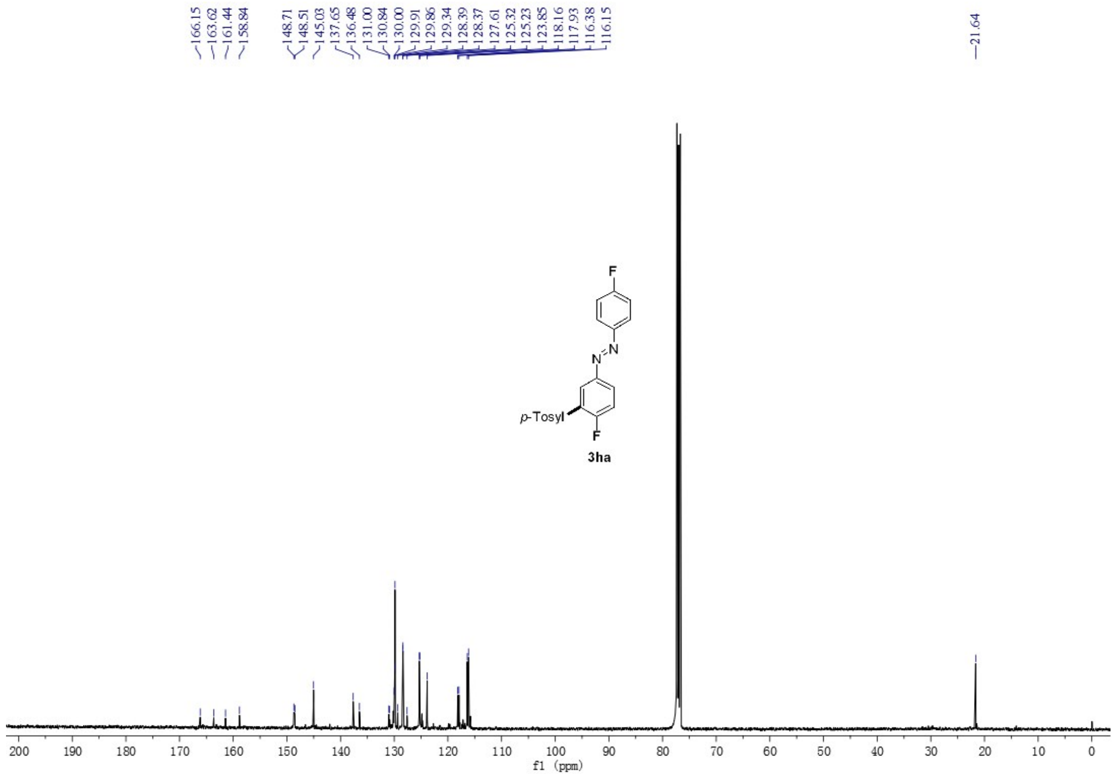
3.05
f1 (ppm)



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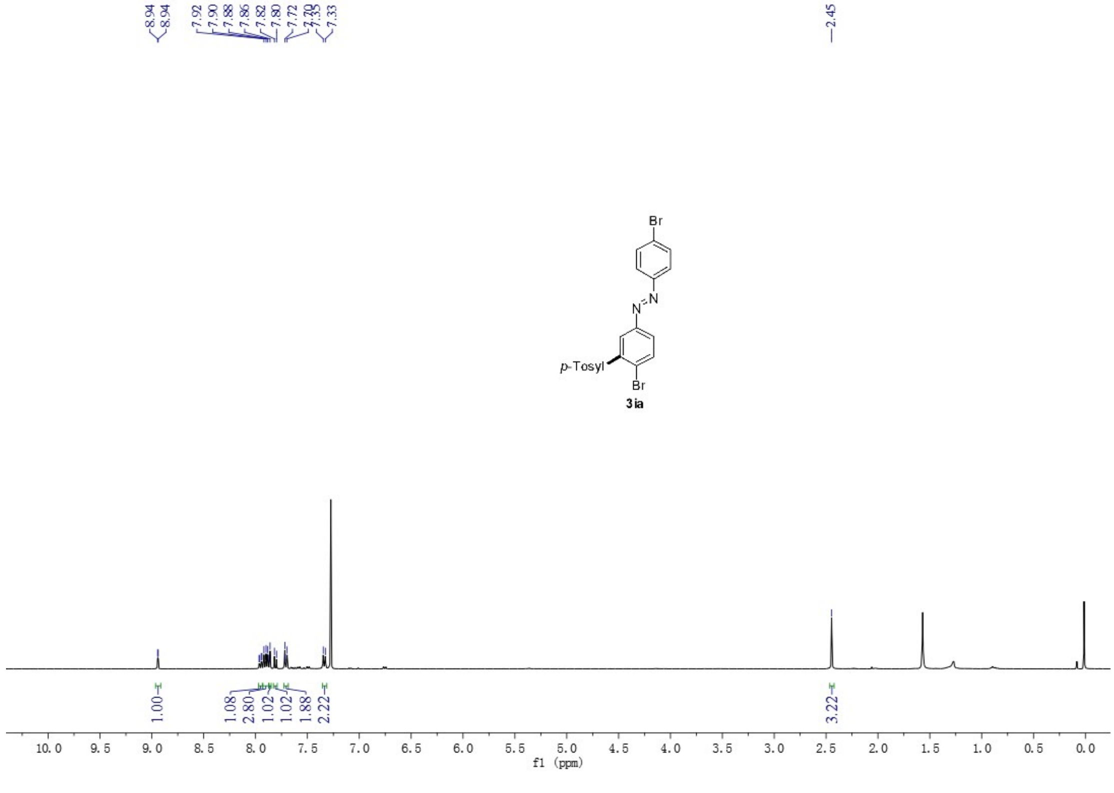

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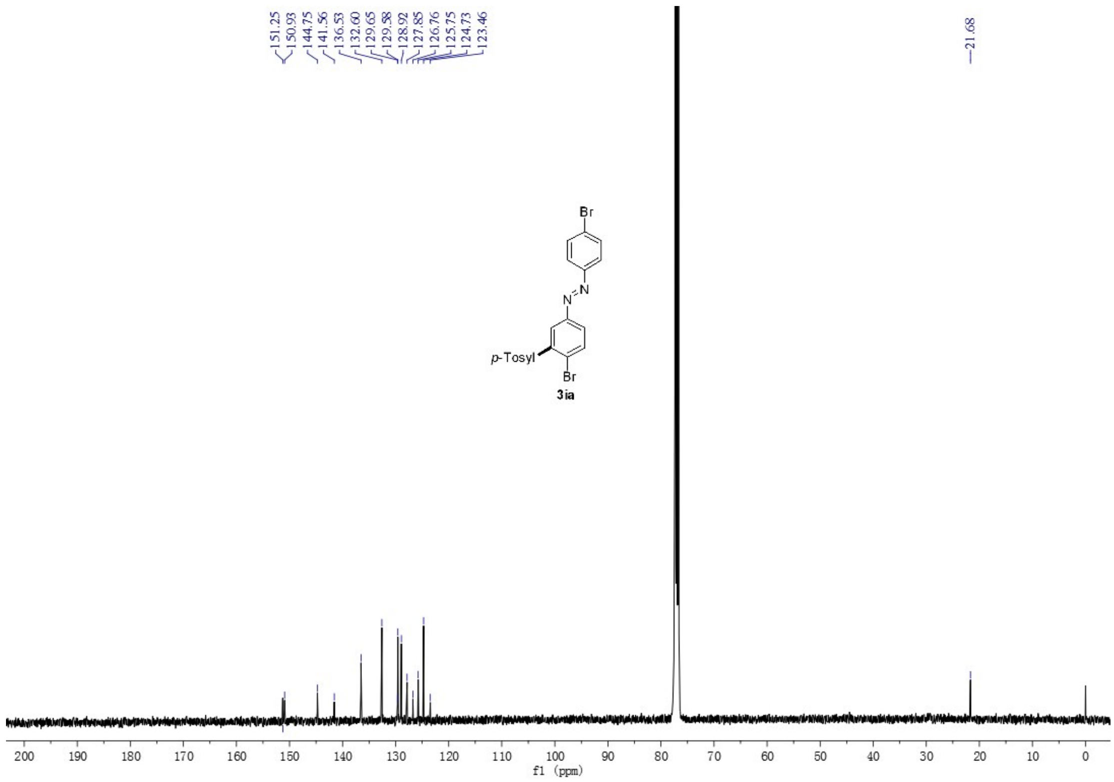

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p-Tosyl
Br
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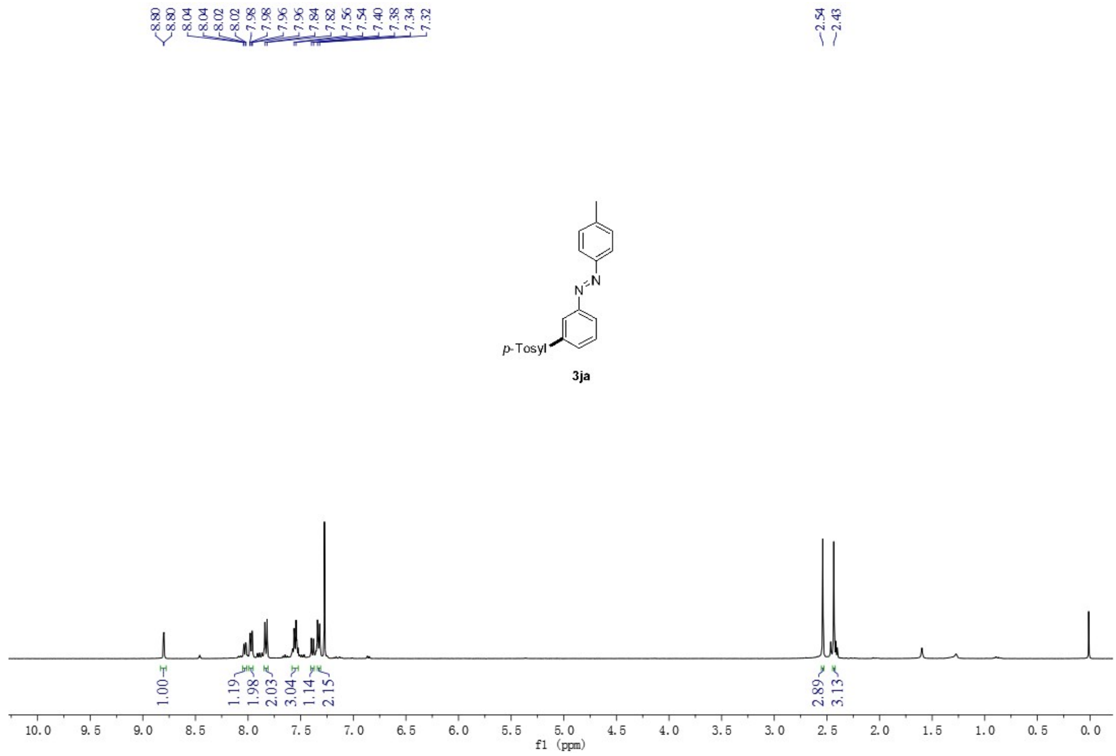

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N
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10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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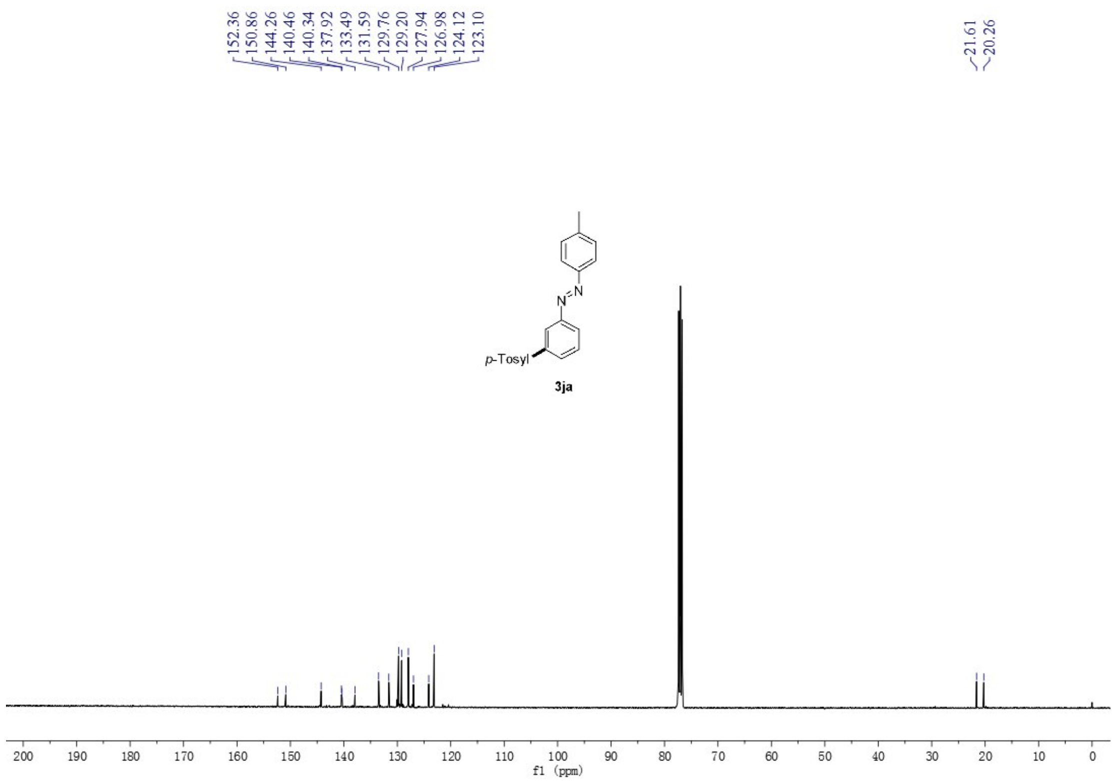

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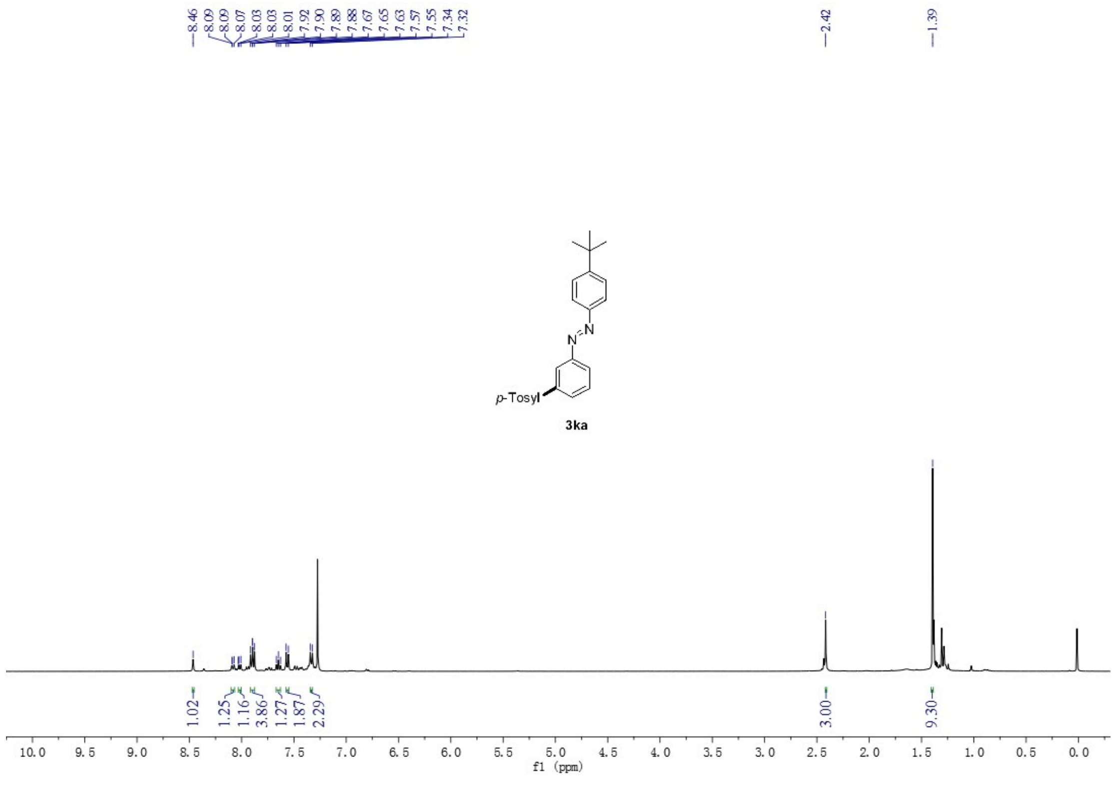

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1.02
1.25
1.16
3.86
1.27
1.87
2.29
3.00
9.30
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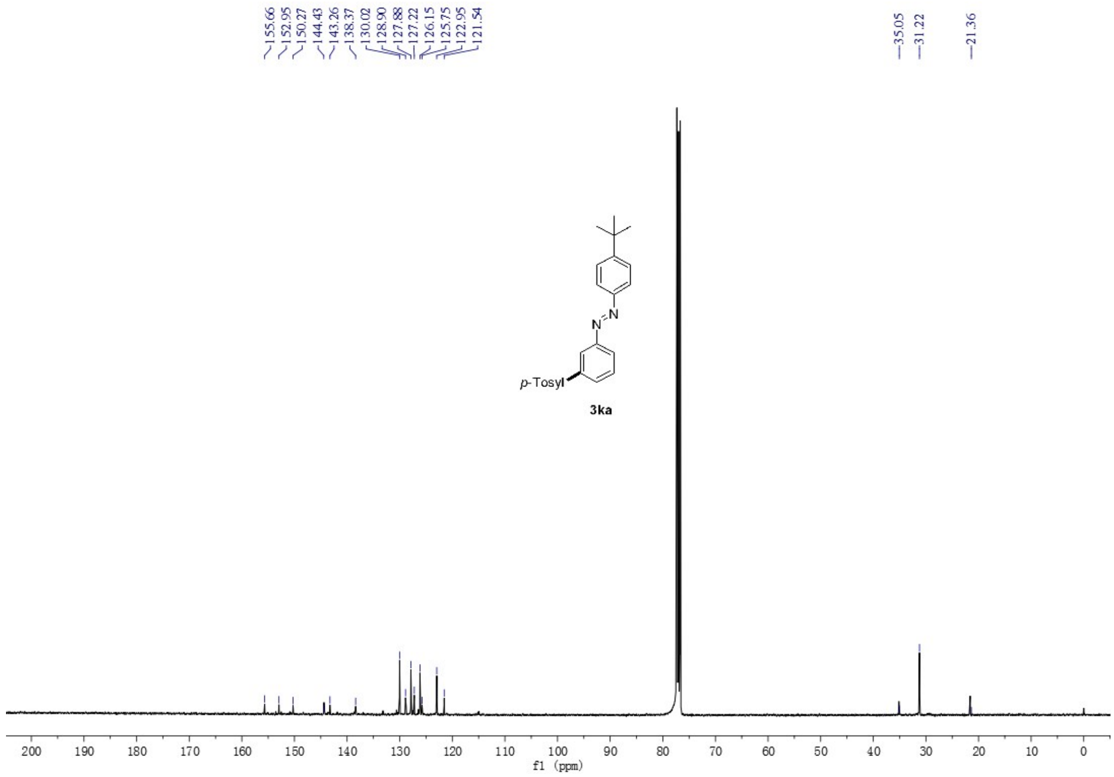
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3ka
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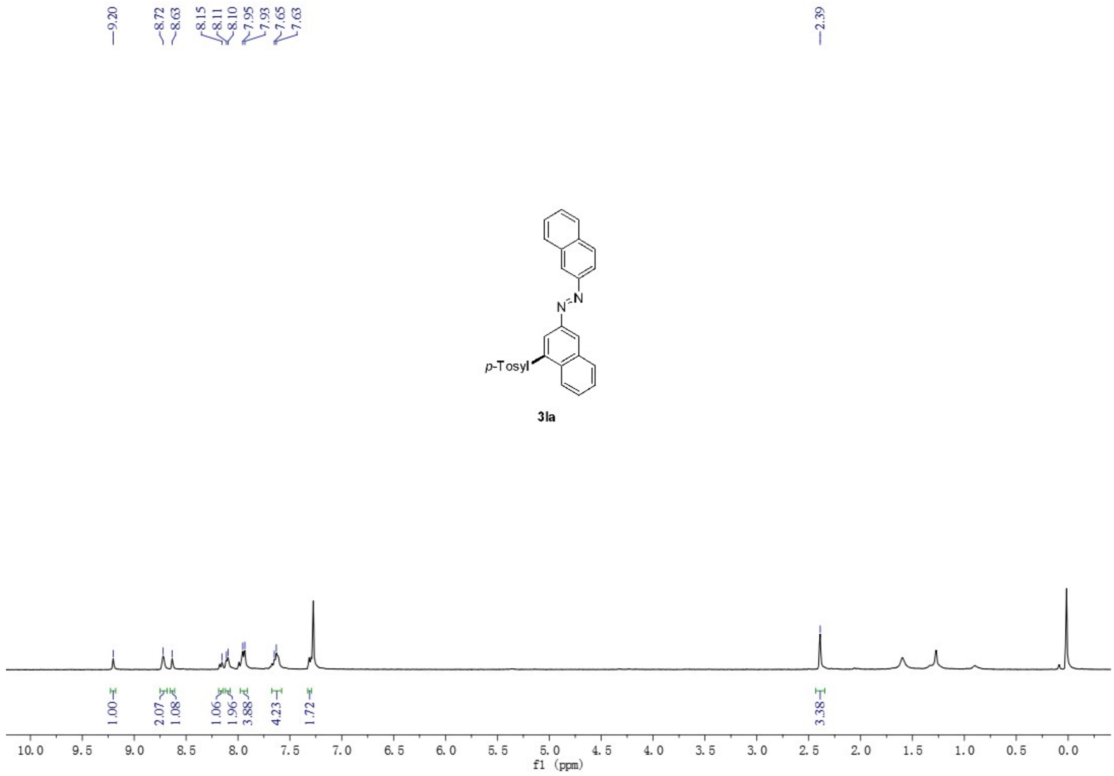
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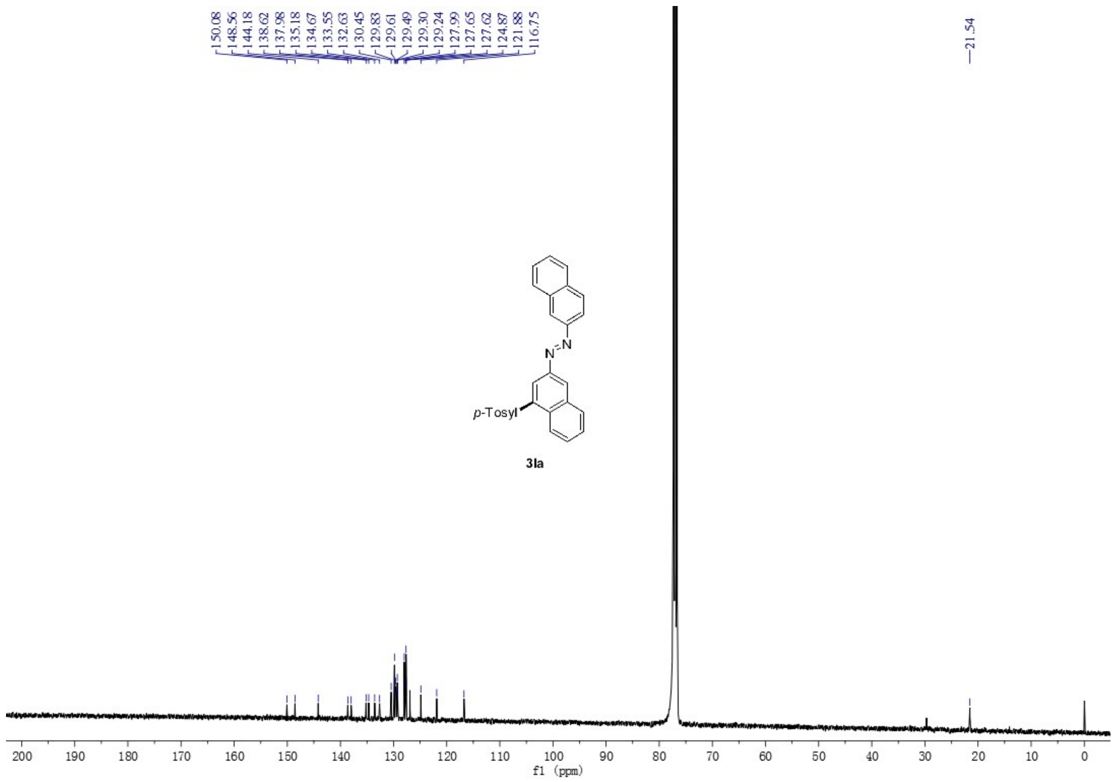
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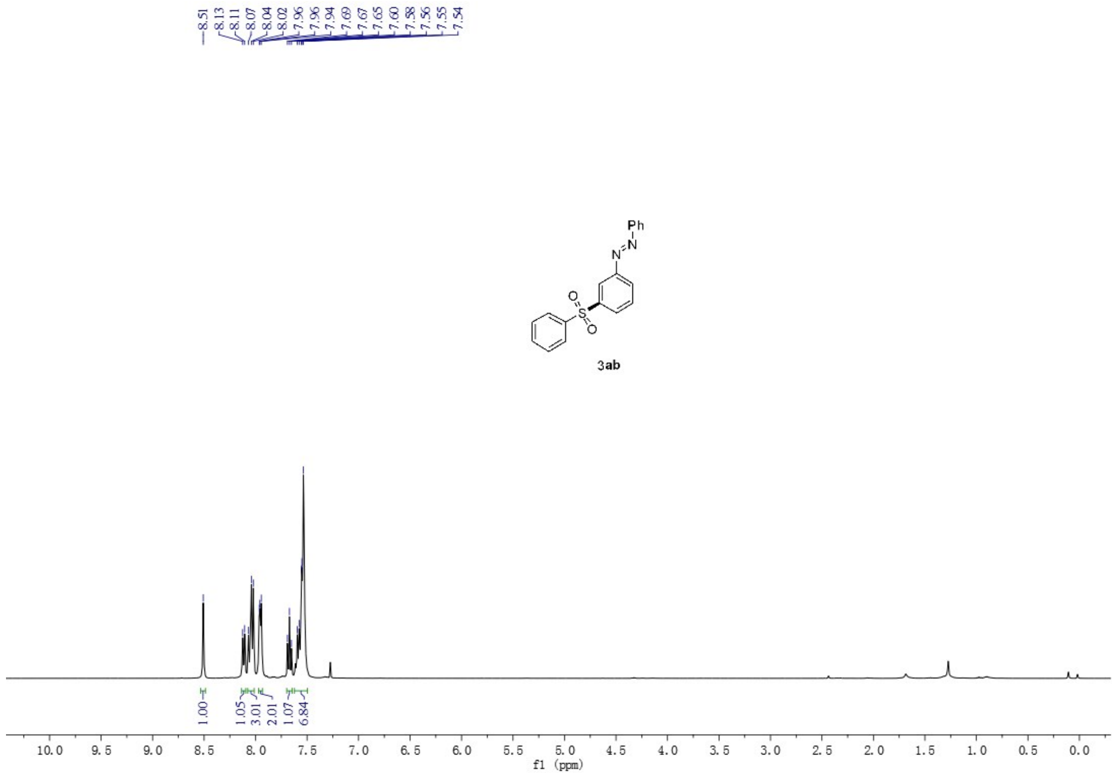
f1 (ppm)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7.56
7.55
7.54
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2.01
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6.84
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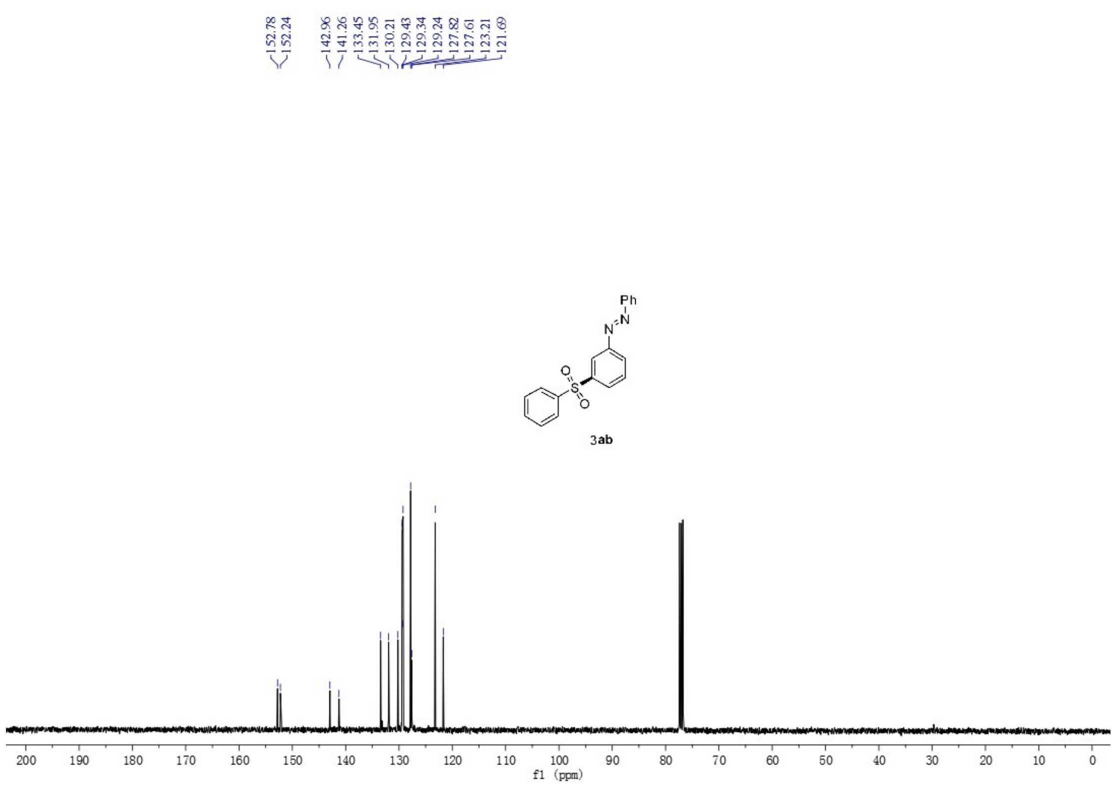
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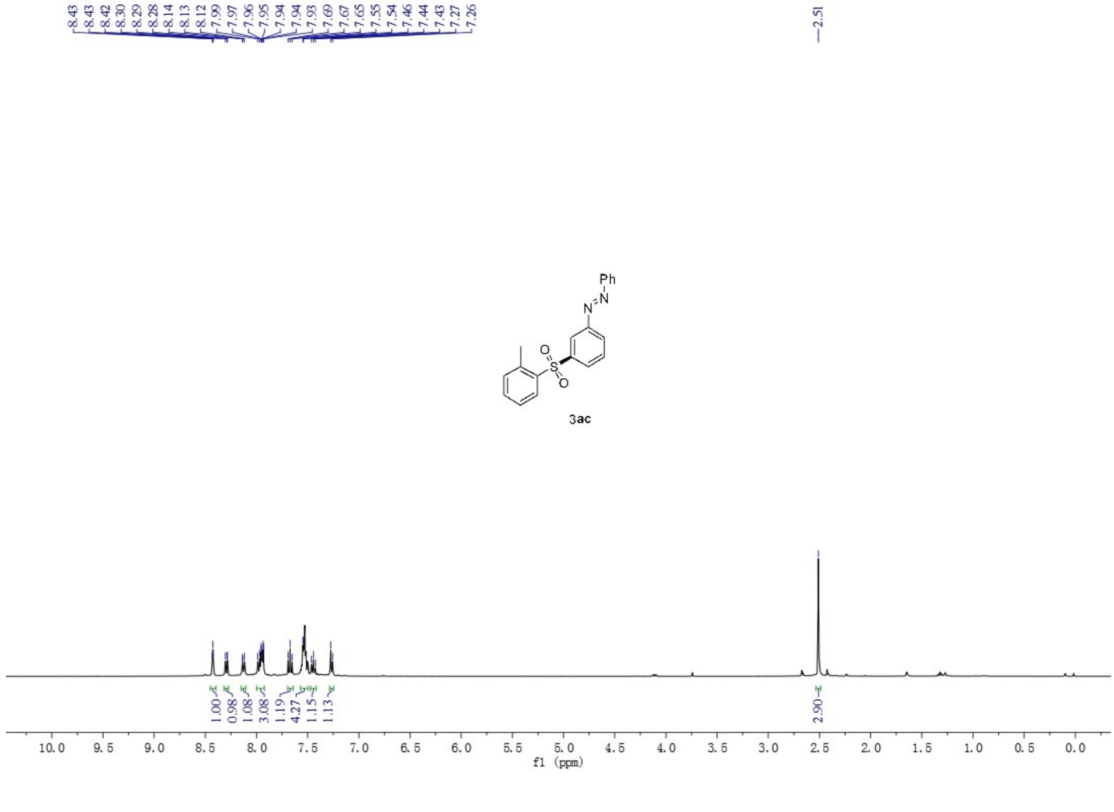
Ph
N
N
S
O
O
3ab
f1 (ppm)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7.95
7.94
7.94
7.93
7.69
7.67
7.65
7.55
7.54
7.46
7.44
7.43
7.27
7.26
2.51
Ph
N
N
S
O
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3.08
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1.15
1.13
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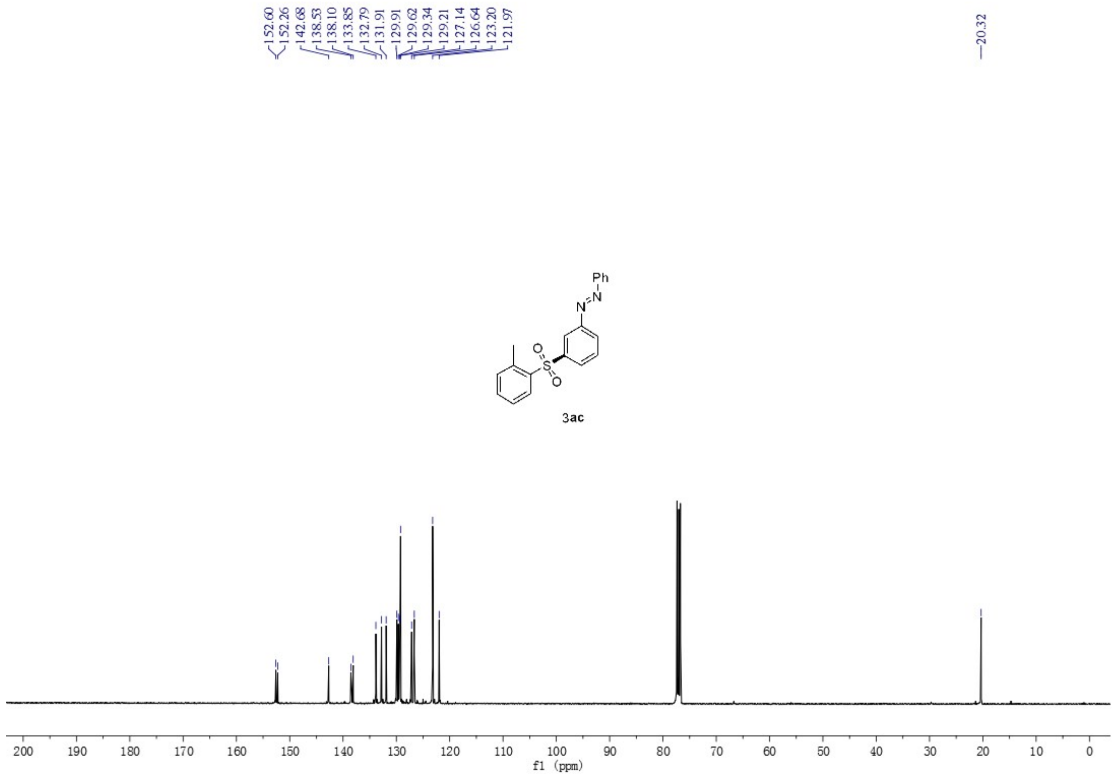
f1 (ppm)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126.64
123.20
121.97
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S
O
O
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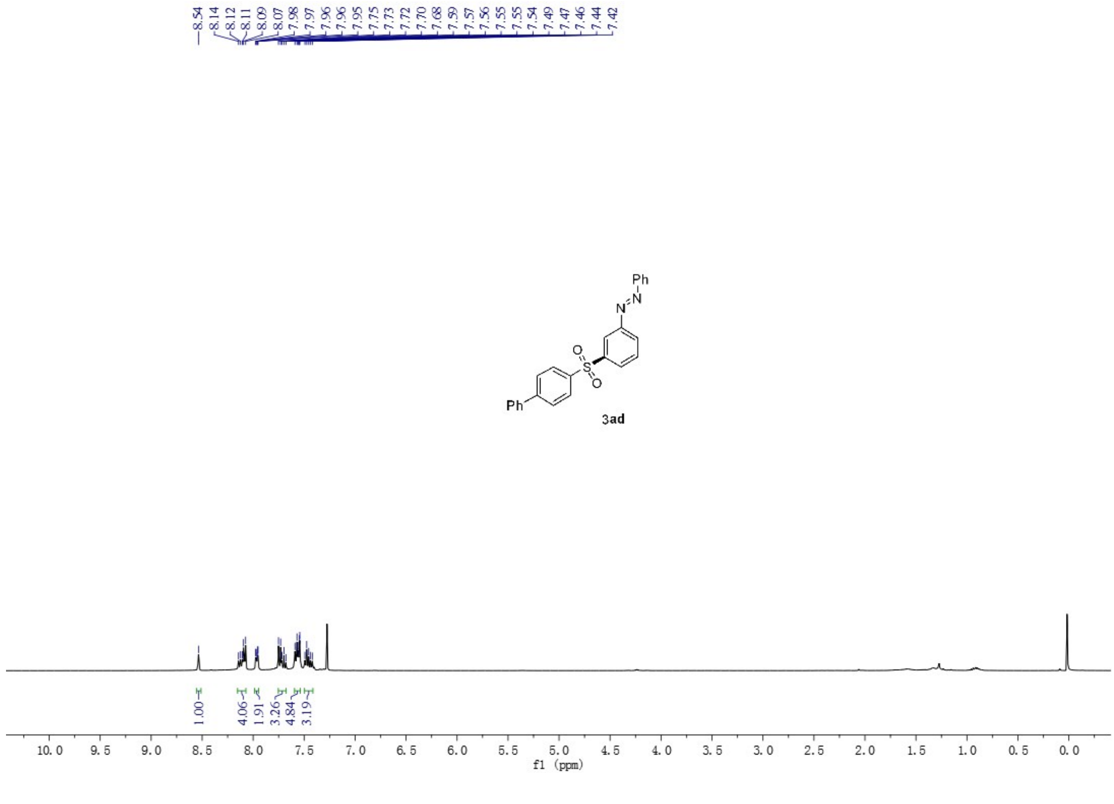
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7.72
7.70
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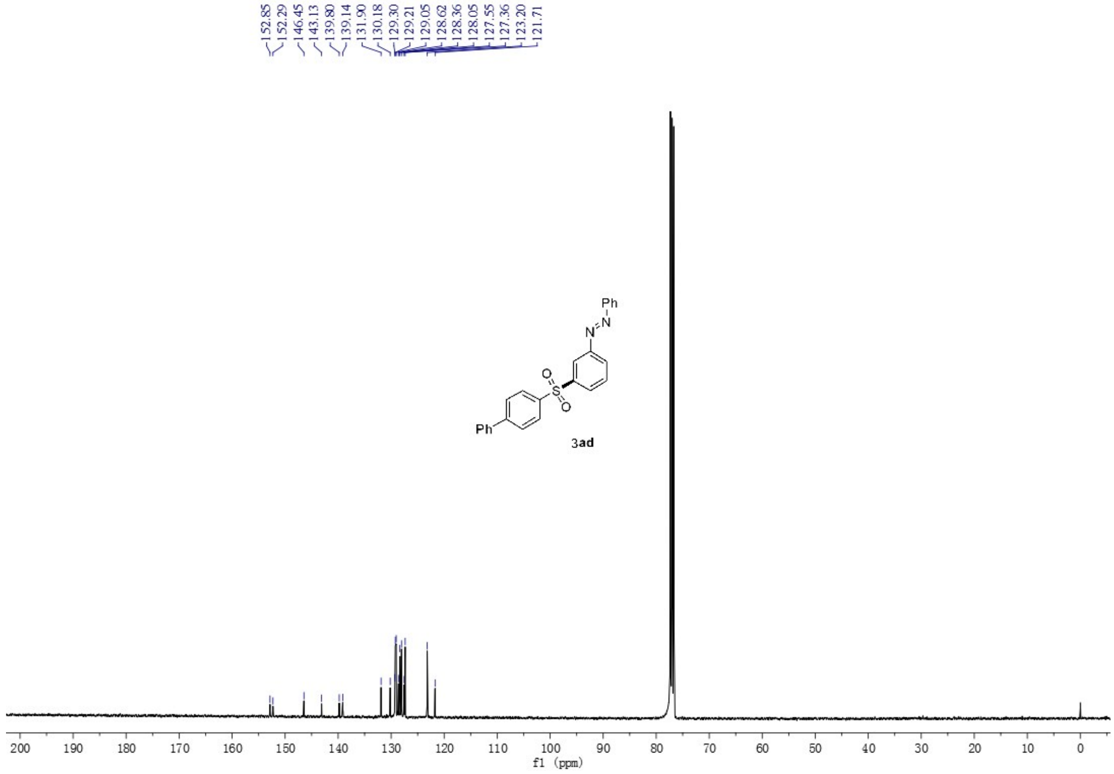
7.59
7.57
7.56
7.55
7.55
7.54
7.49
7.47
7.46
7.44
7.42
Ph
N
N
S
O
O
Ph
3ad
1.00
4.06
1.91
3.26
4.84
3.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.55
127.36
123.20
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S
O
O
Ph
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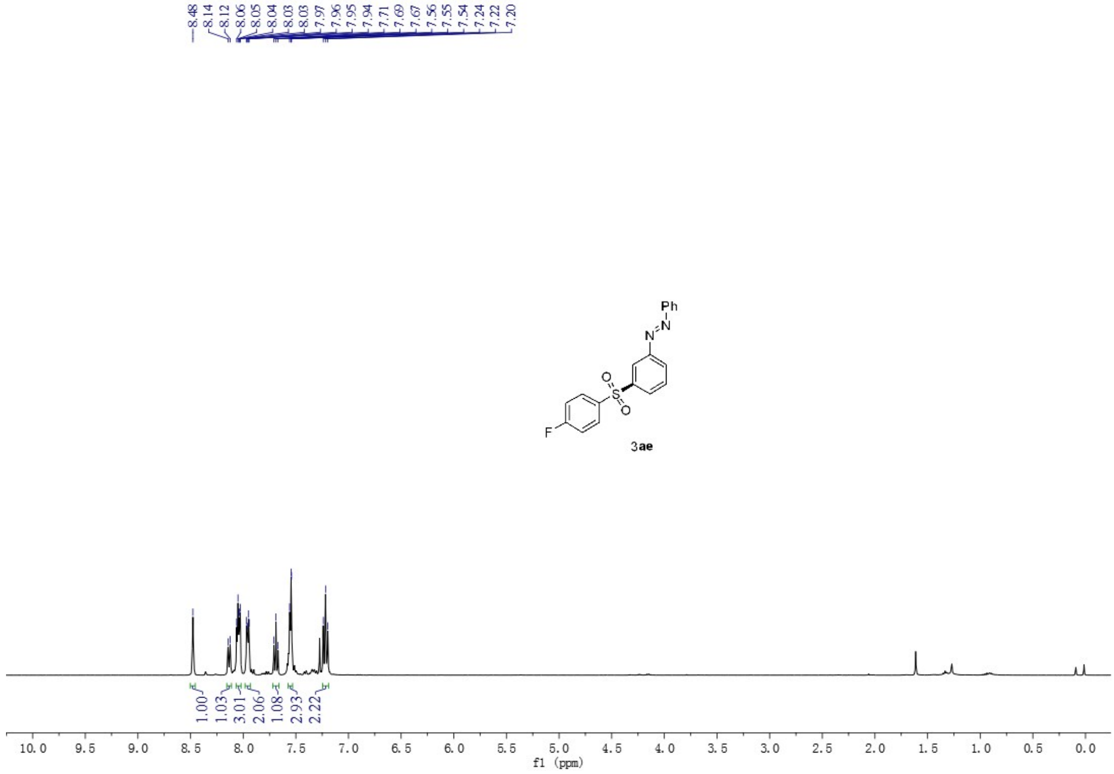
f1 (ppm)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7.71
7.69
7.67
7.56
7.55
7.54
7.24
7.22
7.20
Ph
N
N
S
O
O
F
3ae
1.00
1.03
3.01
2.06
1.08
2.93
2.22
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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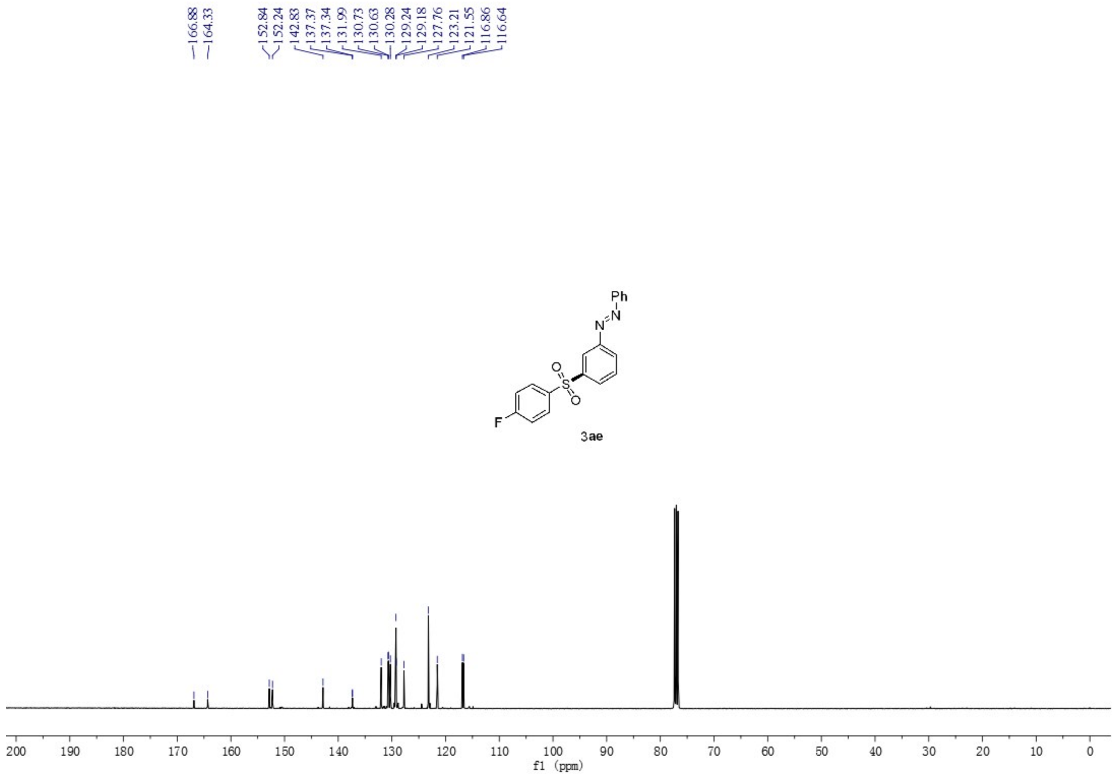
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116.64
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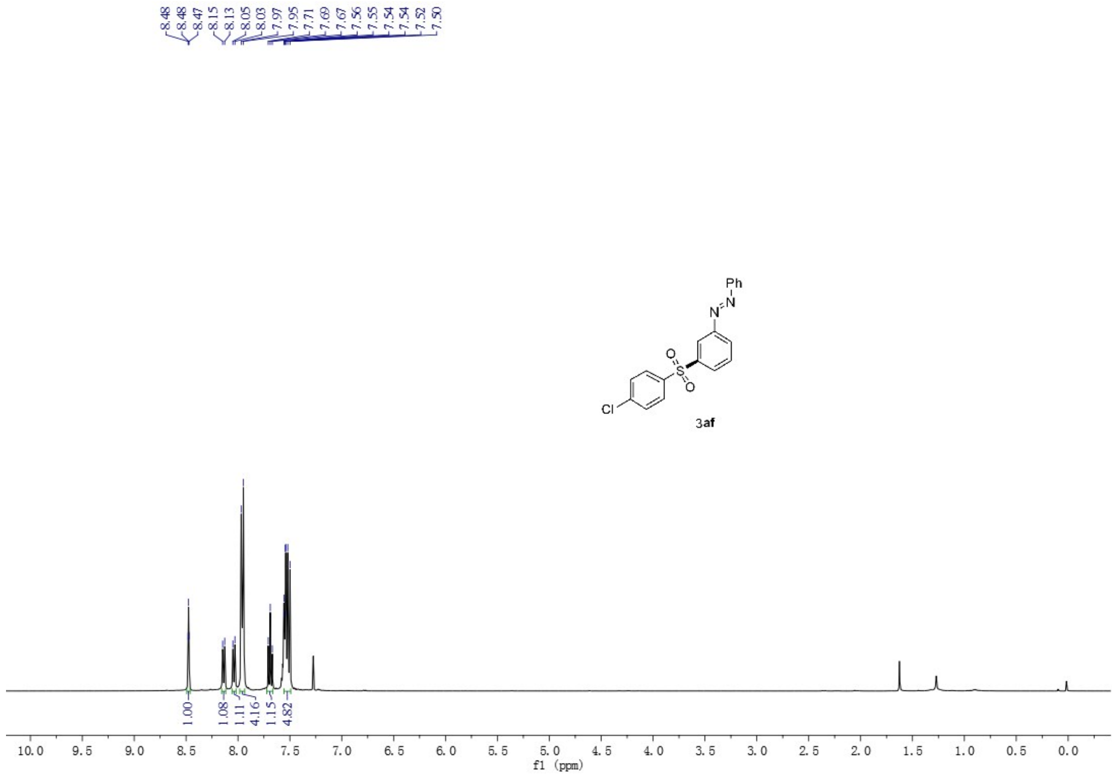
N
S
O
O
F
3ae
f1 (ppm)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7.56
7.55
7.54
7.54
7.52
7.50
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O
Cl
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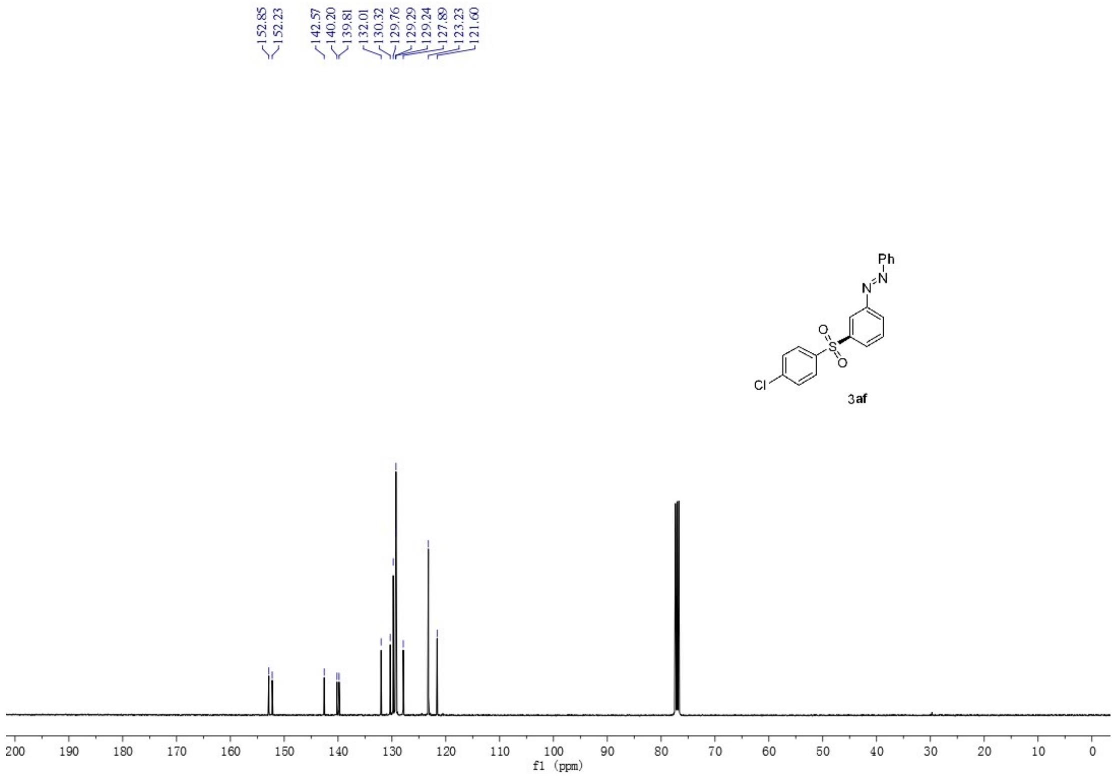
4.82
f1 (ppm)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O
S
O
Cl
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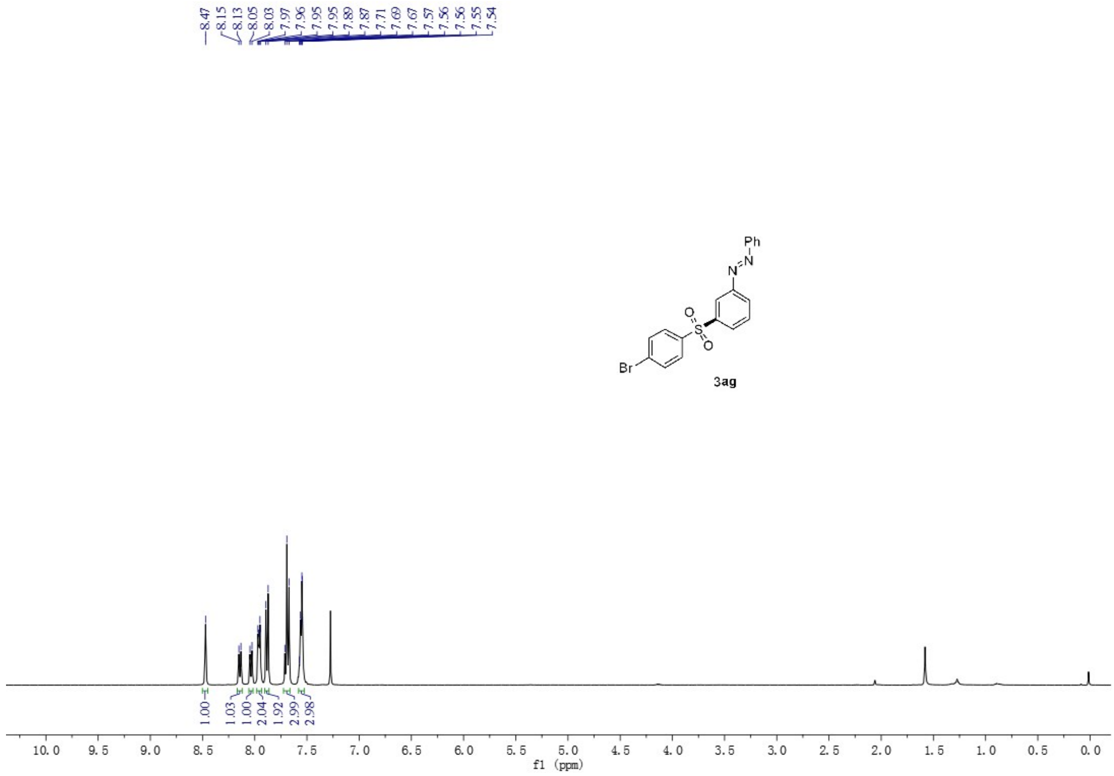
f1 (ppm)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7.89
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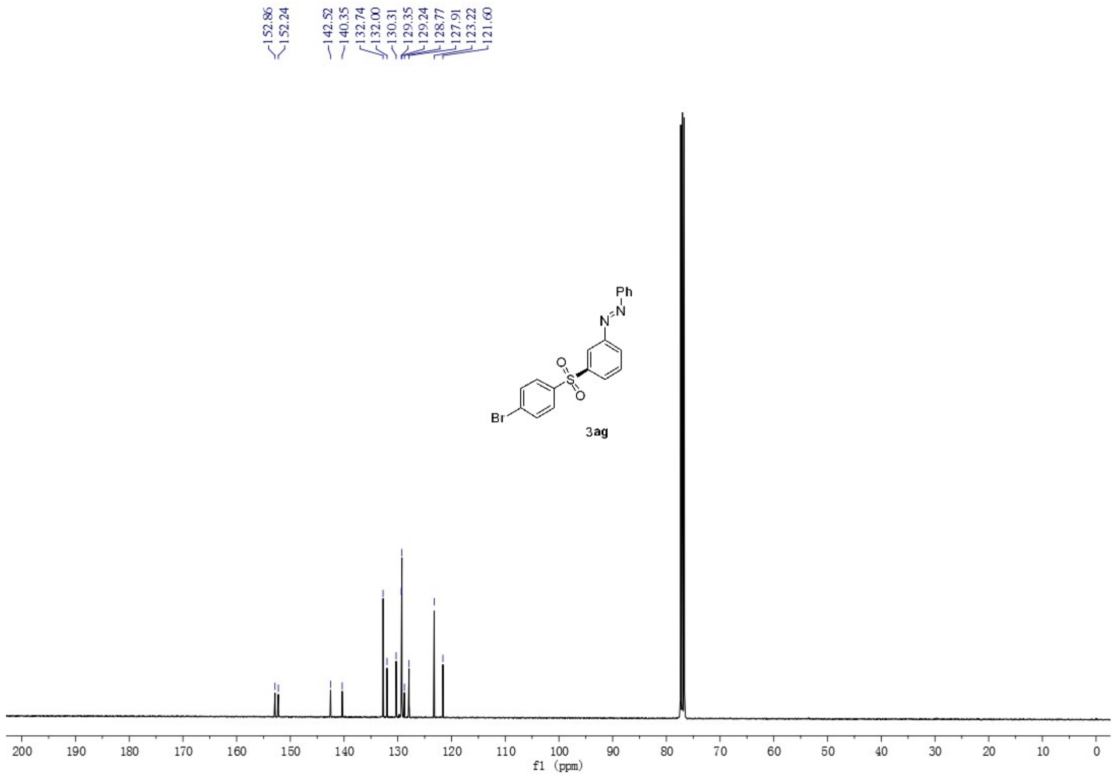
7.69
7.67
7.57
7.56
7.55
7.54
Ph
N=N
O
S
O
Br
3ag
1.00
1.03
1.00
2.04
1.92
2.99
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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O
O
Br
3ag
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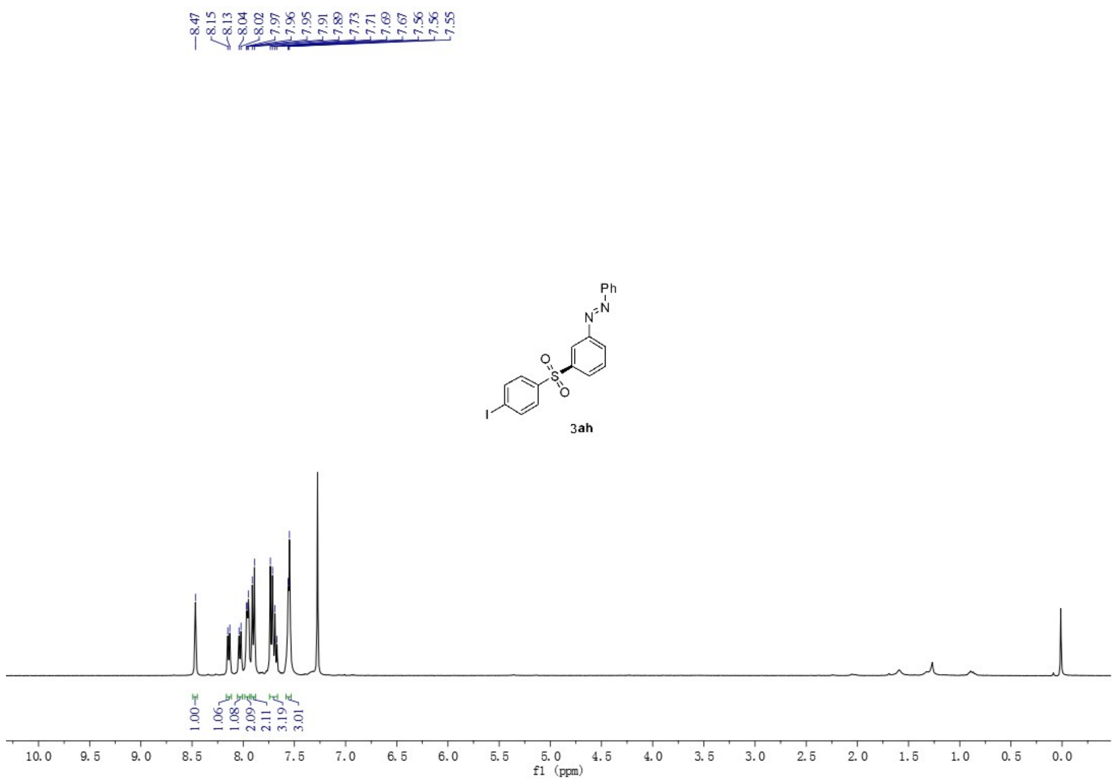
f1 (ppm)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7.69
7.67
7.56
7.56
7.55
Ph
N
N
S
O
O
I
3ah
1.00
1.06
1.08
2.09
2.11
3.19
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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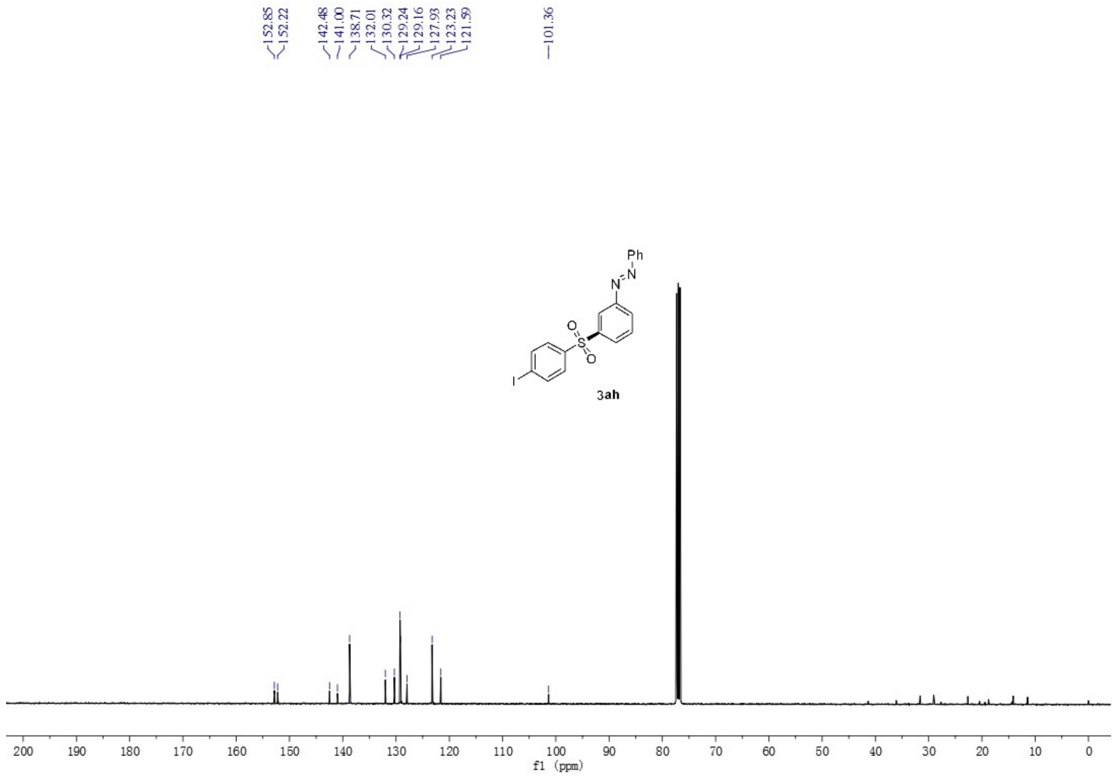
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127.93
123.23
121.59
101.36
Ph
N
N
O
S
O
I
3ah
200
190
180
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160
150
140
130
120
110
100
90
80
70
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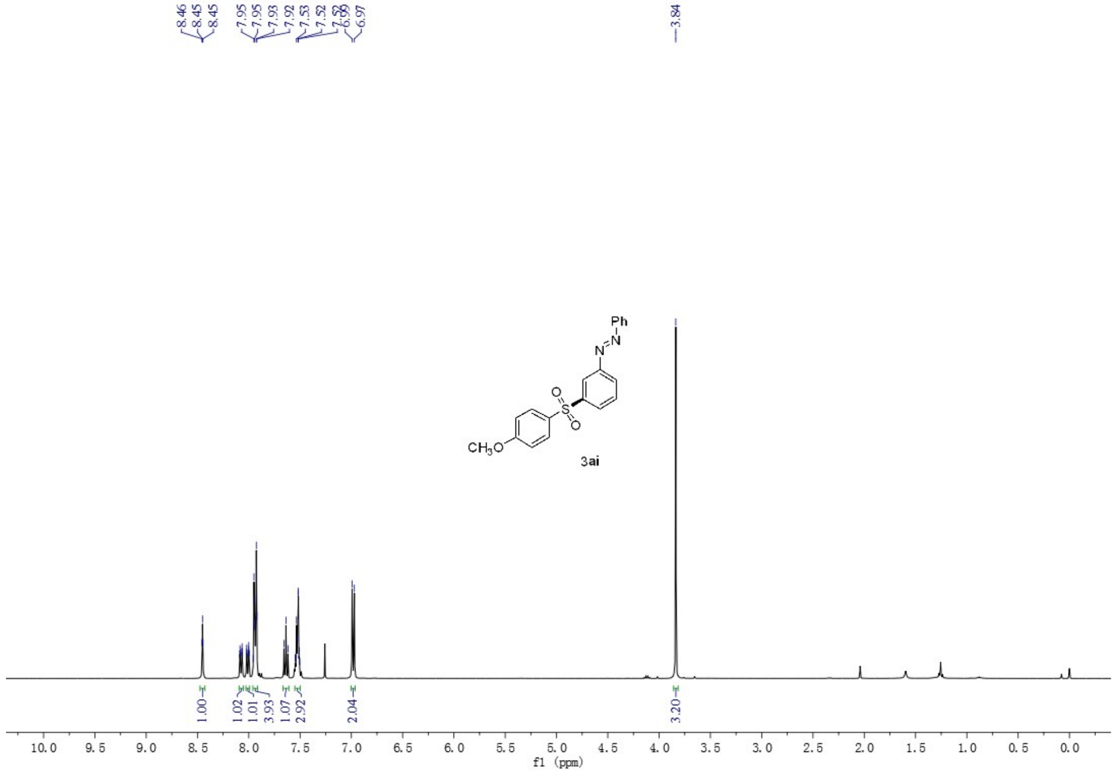
50
40
30
20
10
0
f1 (ppm)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7.52
6.99
6.97
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O
S
O
CH_3O
3ai
1.00
1.02
1.01
3.93
1.07
2.92
2.04
3.20
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
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1.0
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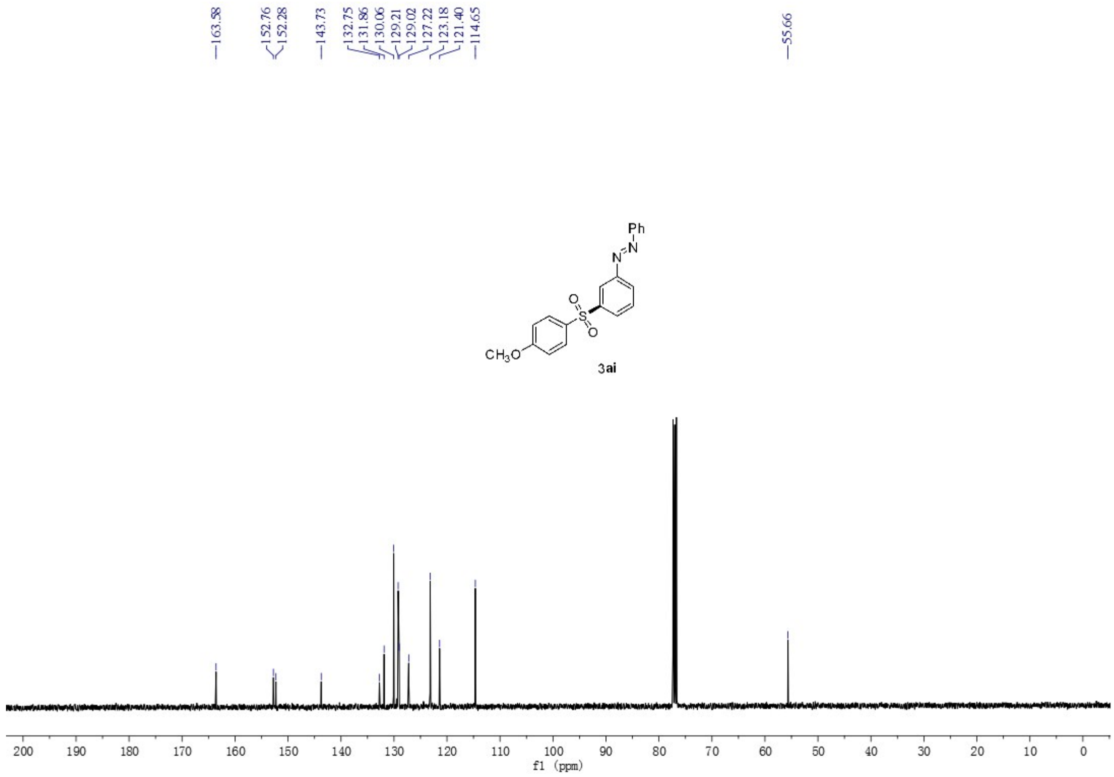
0.0
f1 (ppm)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S
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CH3O
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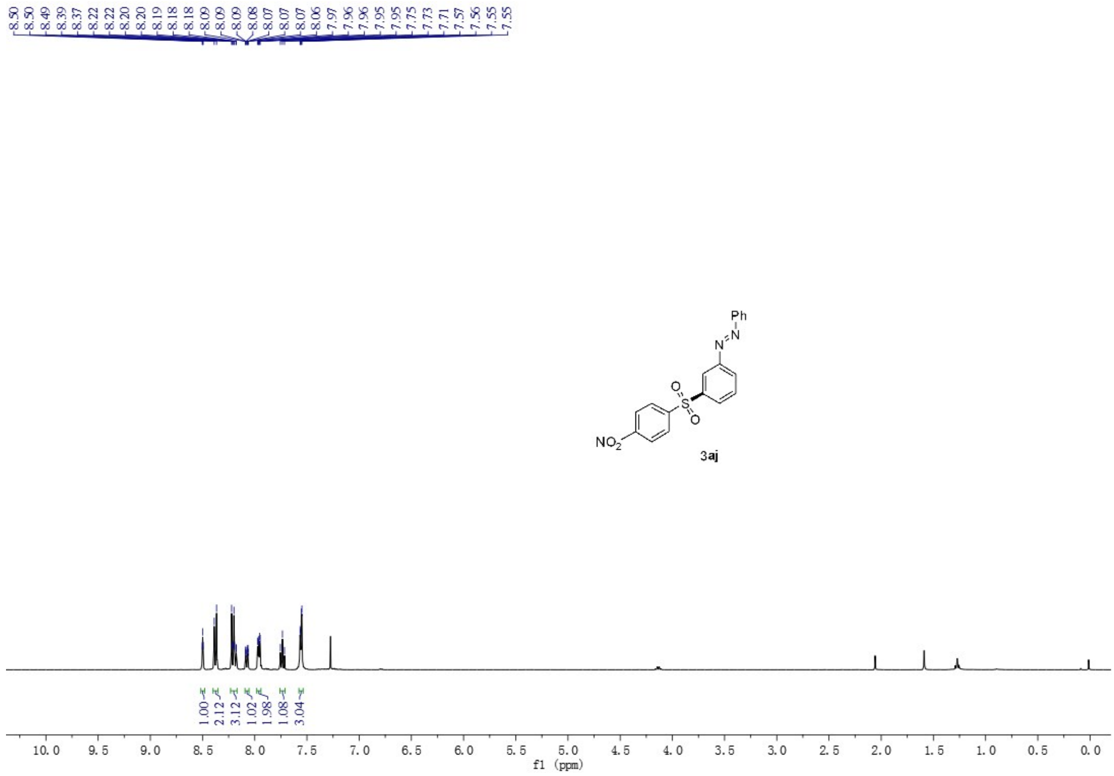
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8.06
7.97
7.96
7.96
7.95
7.95
7.75
7.73
7.71
7.57
7.56
7.55
7.55
Ph
N
N
O
S
O
NO2
3aj
1.00
2.12
3.12
1.02
1.98
1.08
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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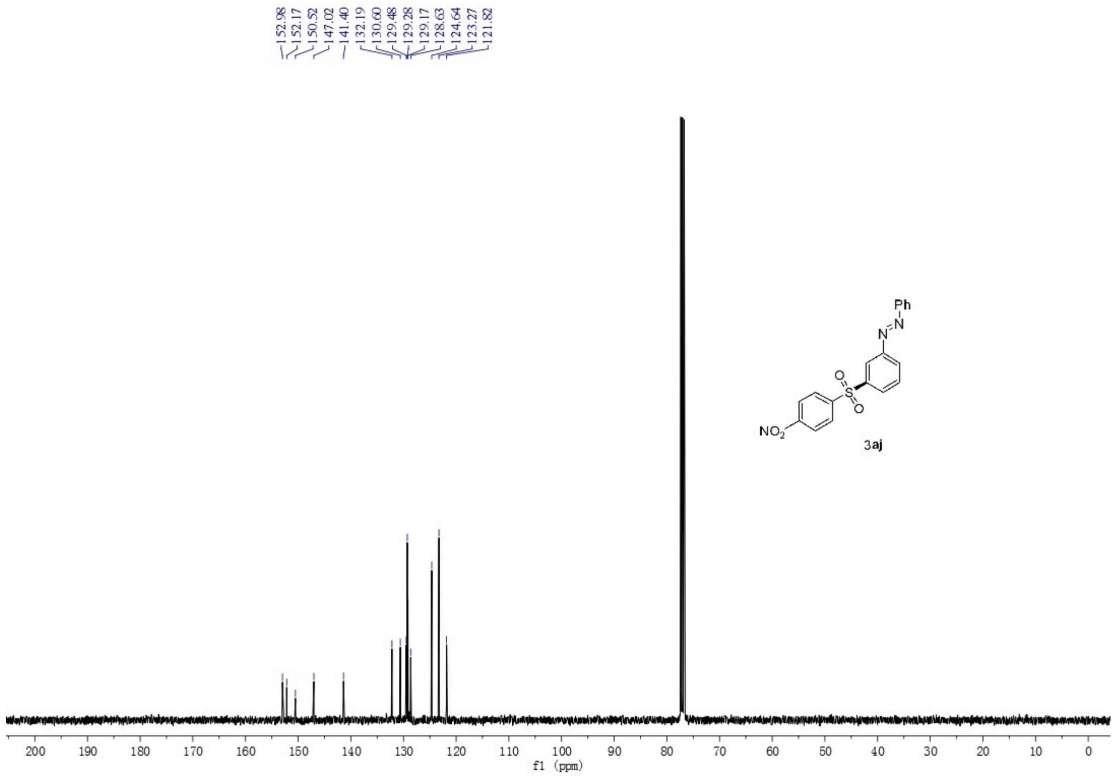
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S
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NO2
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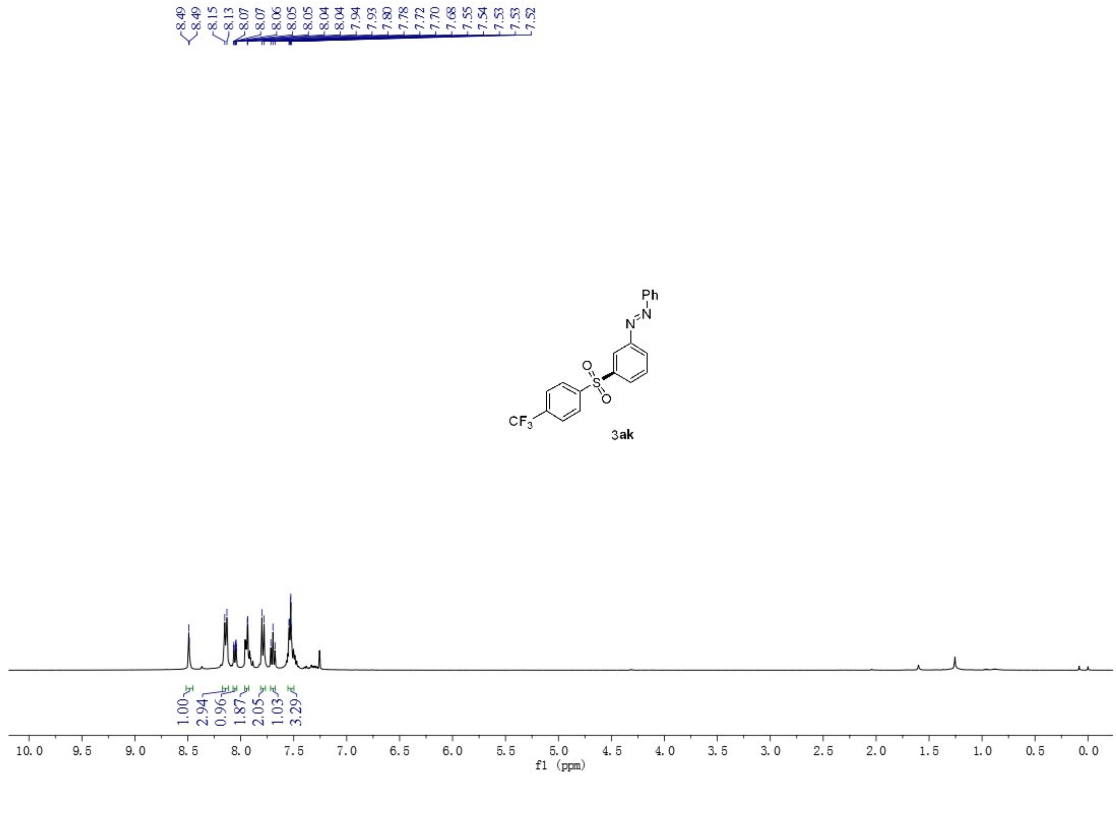
f1 (ppm)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7.68
7.55
7.54
7.53
7.52
Ph
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O
S
O
CF3
3ak
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0.96
1.87
2.05
1.03
3.29
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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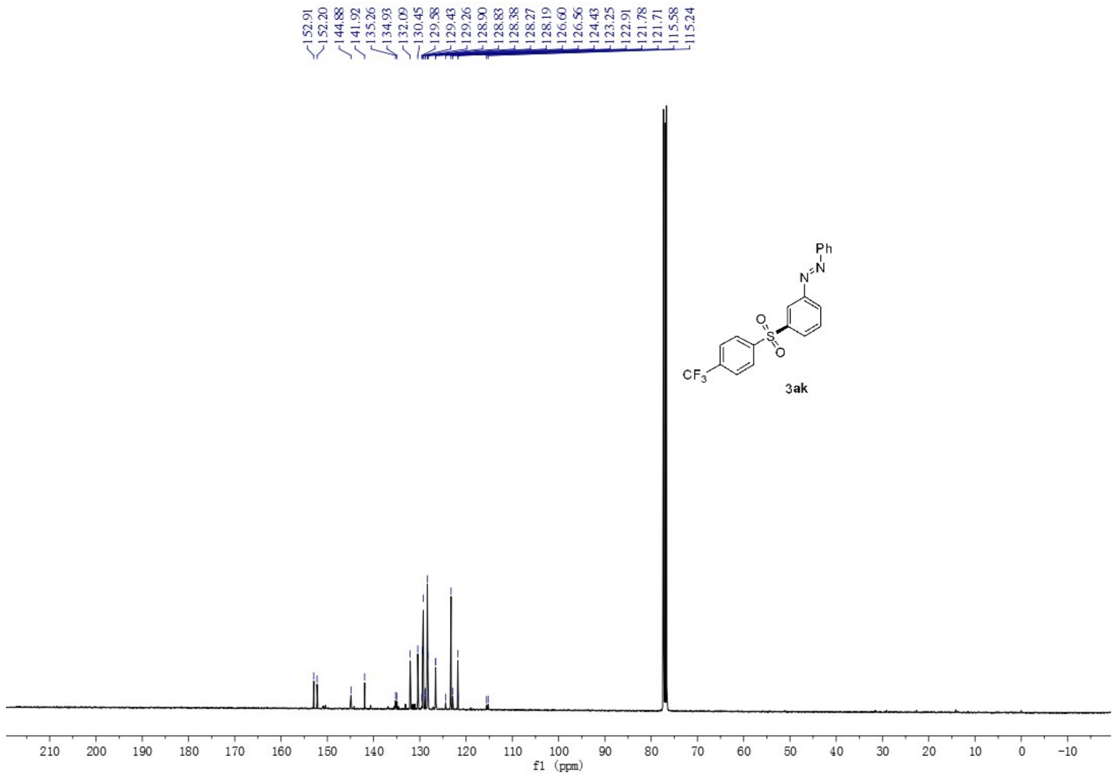
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128.19
126.60
126.56
124.43
123.25
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115.58
115.24
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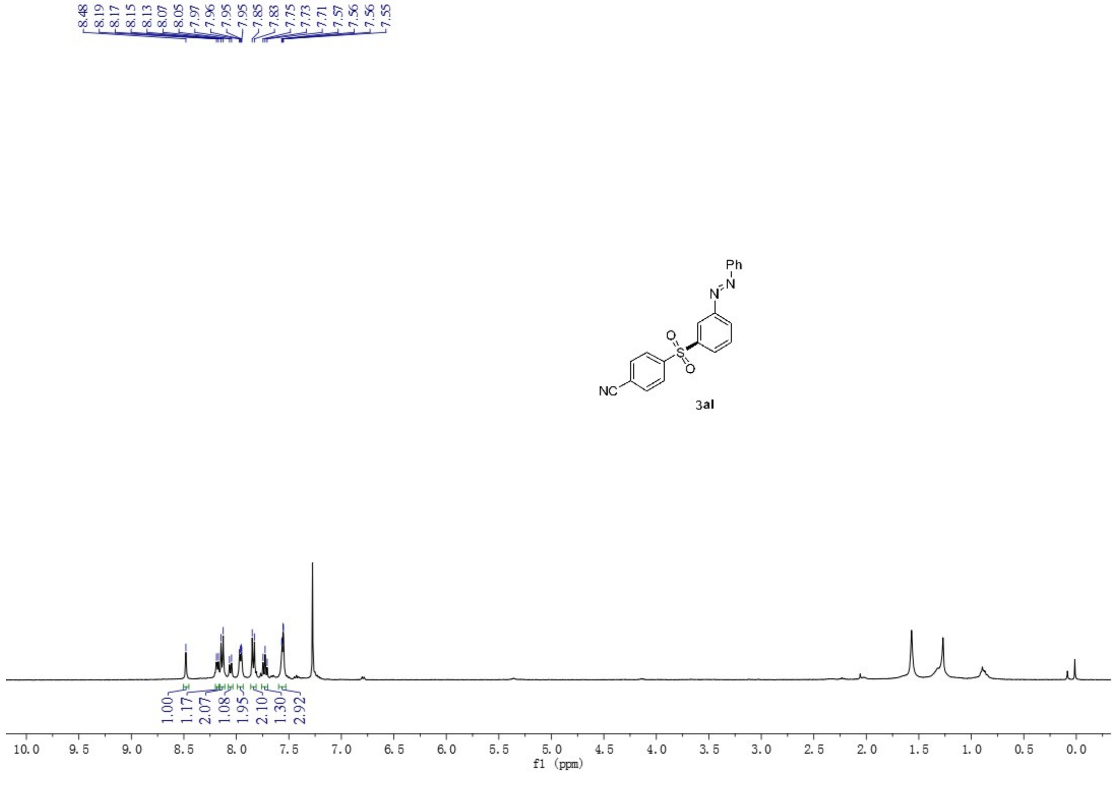
O
S
O
CF_3
3ak
f1 (ppm)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7.83
7.75
7.73
7.71
7.57
7.56
7.56
7.55
Ph
N
N
O
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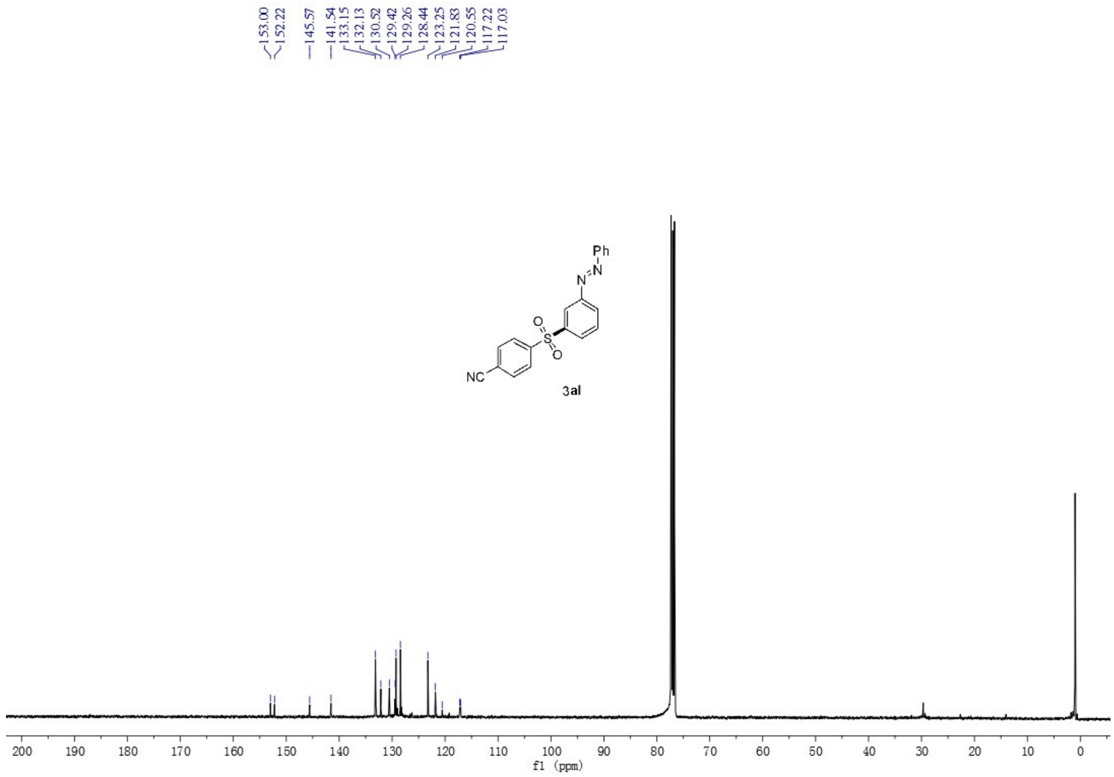
2.92
f1 (ppm)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117.03
Ph
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O
S
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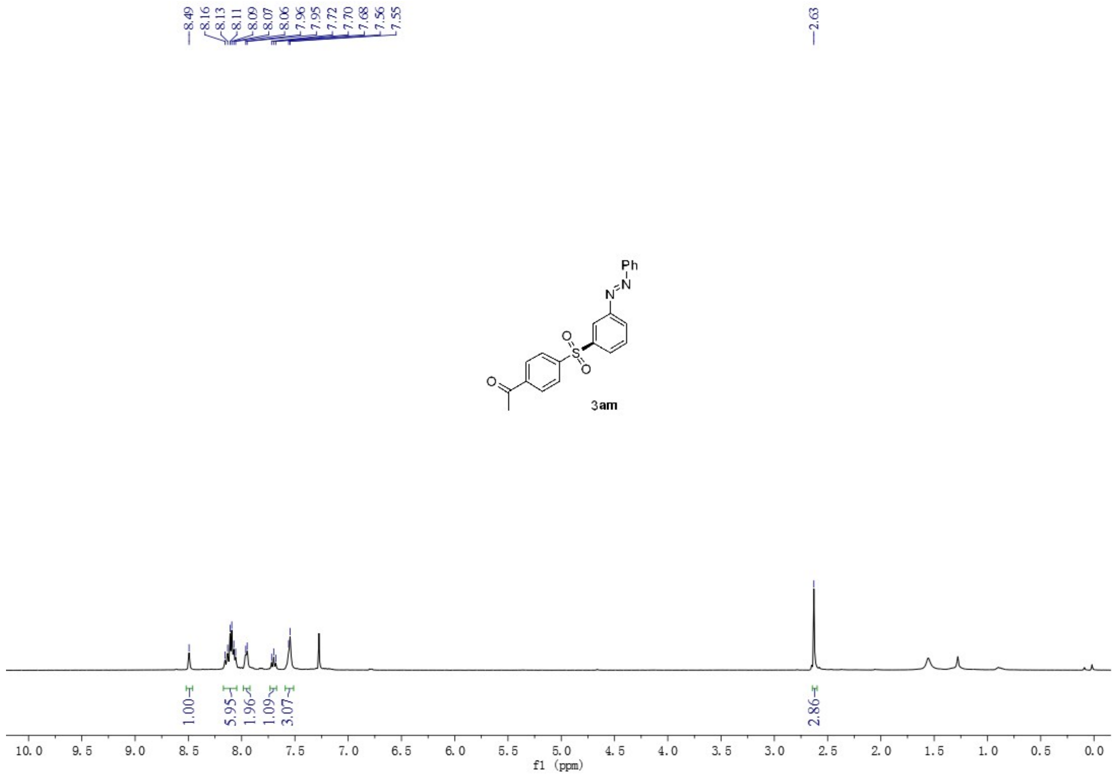
NC
3al
f1 (ppm)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7.56
7.55
2.63
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S
O
O
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1.00
5.95
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1.09
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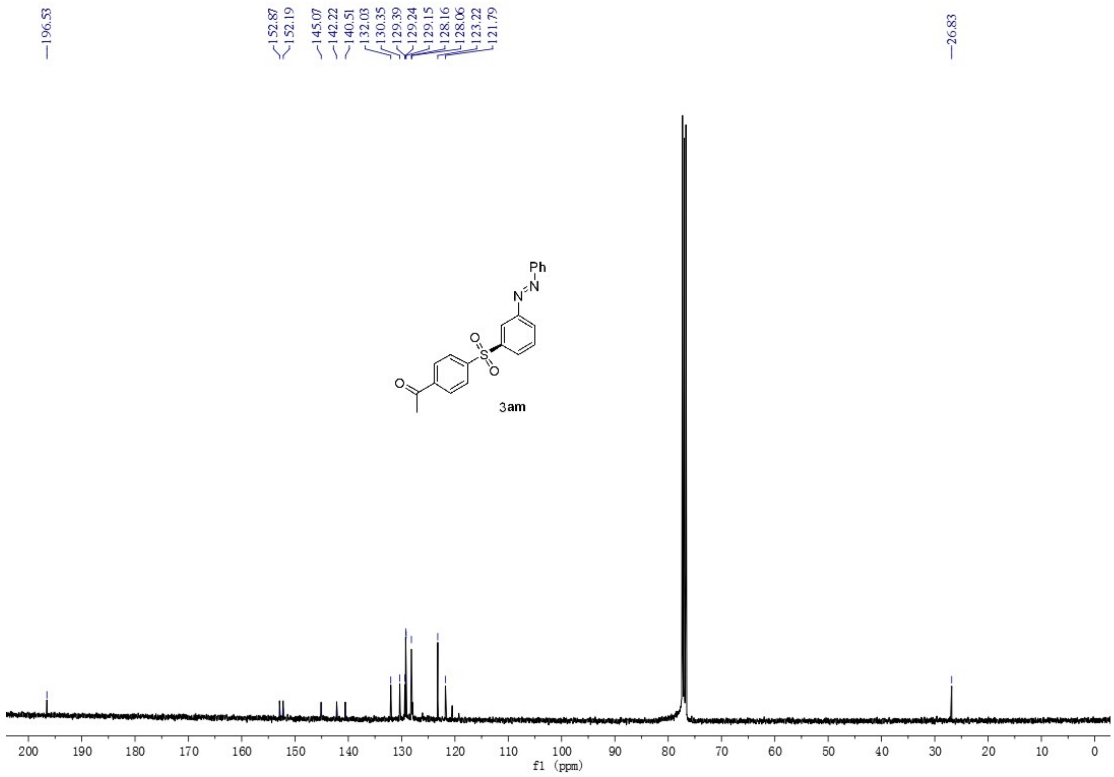

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S
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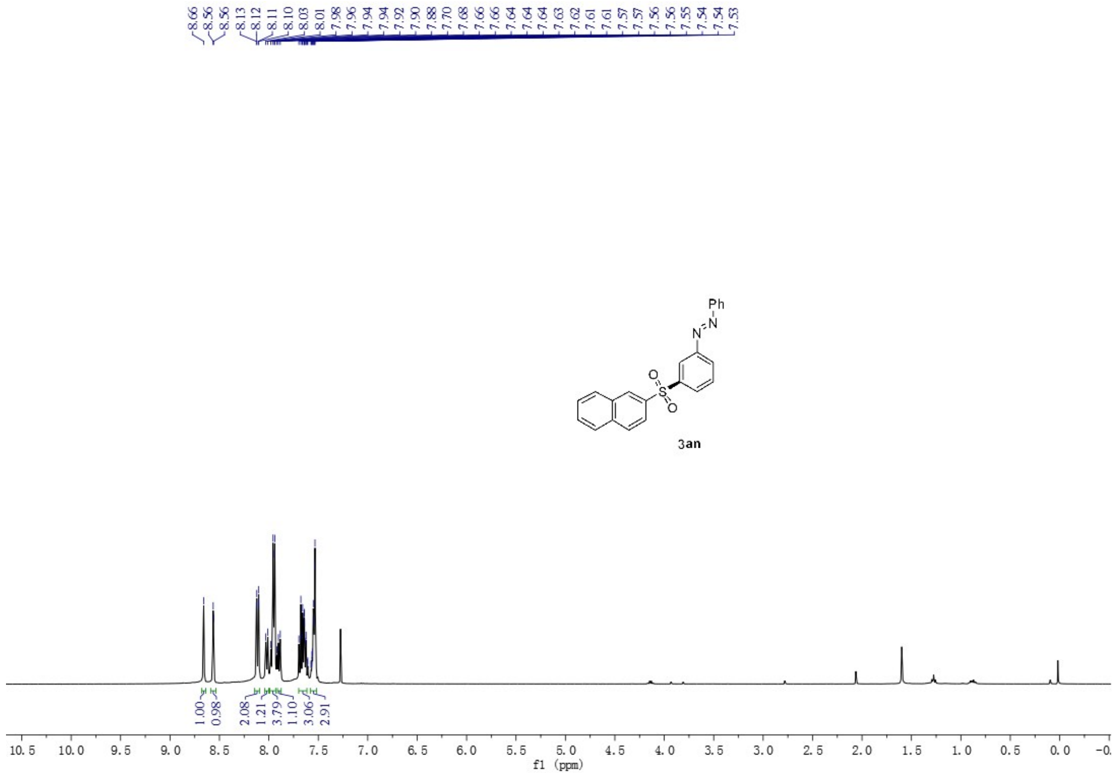
O
3am
f1 (ppm)



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7.63
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7.53
Ph
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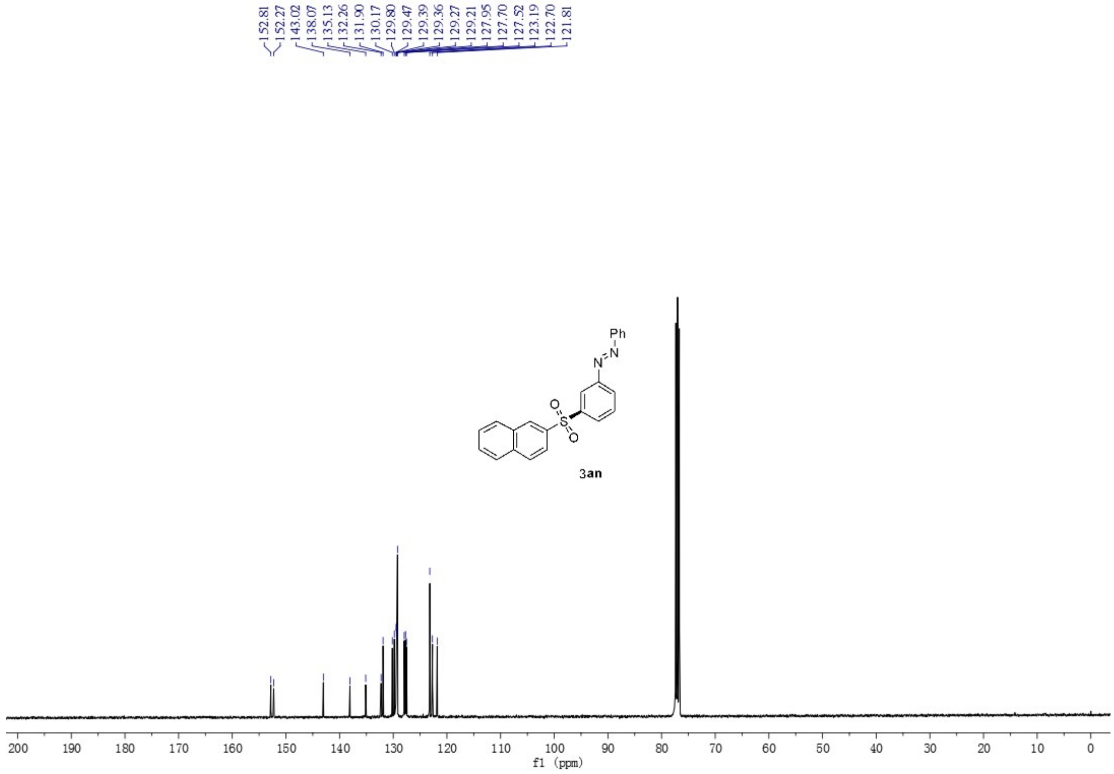
2.91
f1 (ppm)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127.52
123.19
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S
O
O
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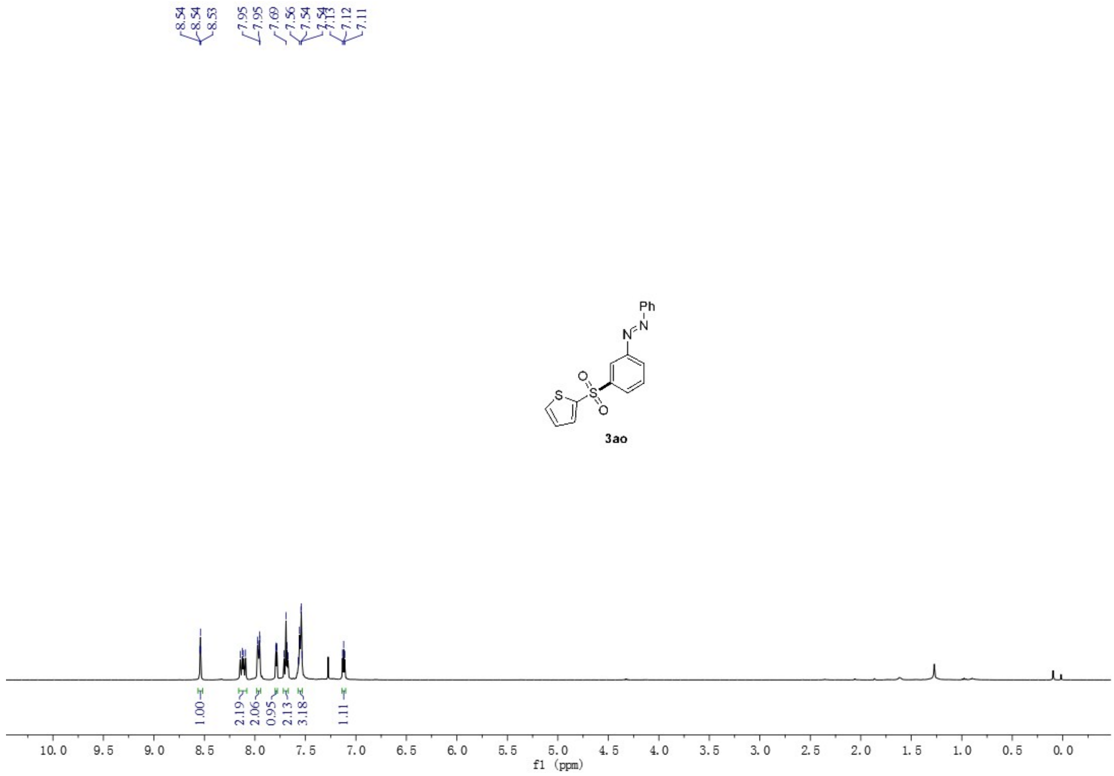
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7.12
7.11
Ph
N
N
S
S
O
O
3ao
1.00
2.19
2.06
0.95
2.13
3.18
1.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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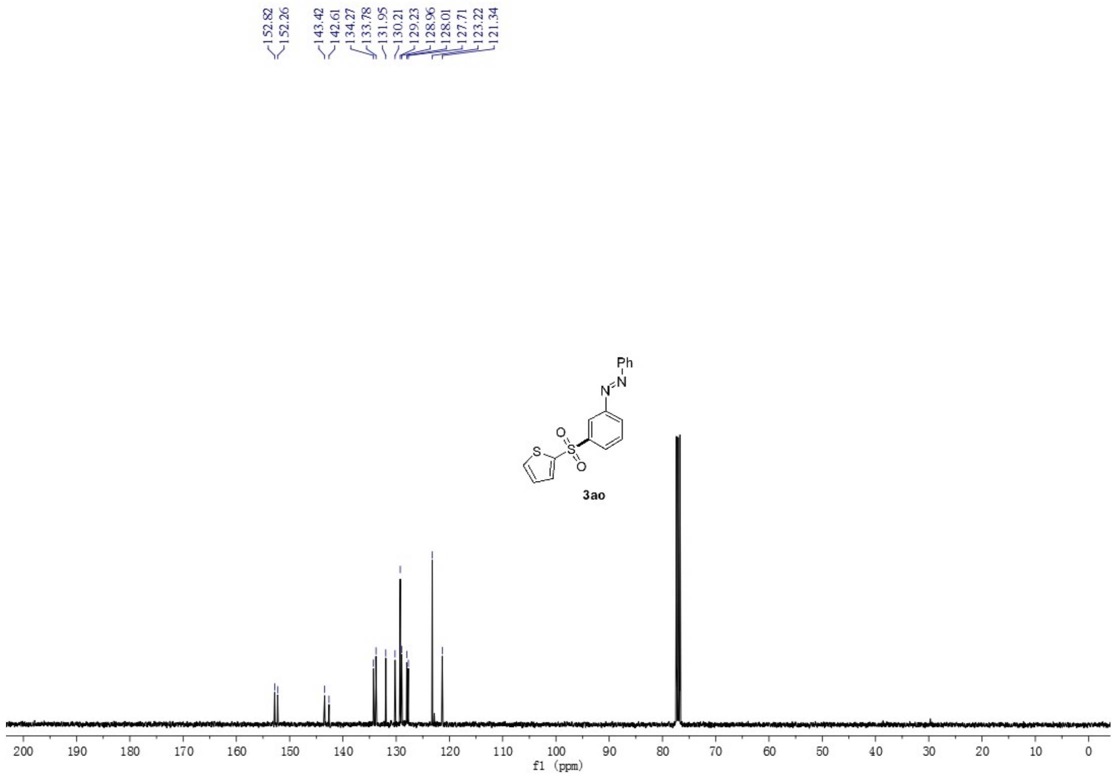
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123.22
121.34
Ph
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N
S
S
O
O
3ao
200
190
180
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110
100
90
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60
50
40
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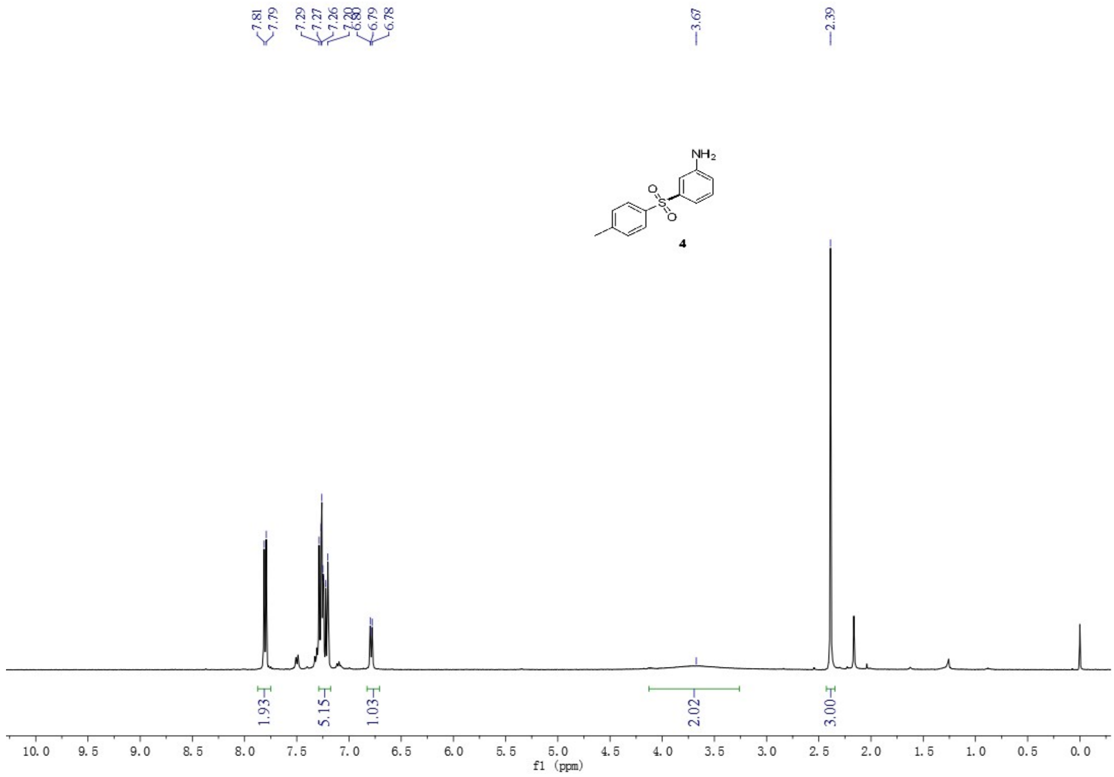
20
10
0
f1 (ppm)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NH2
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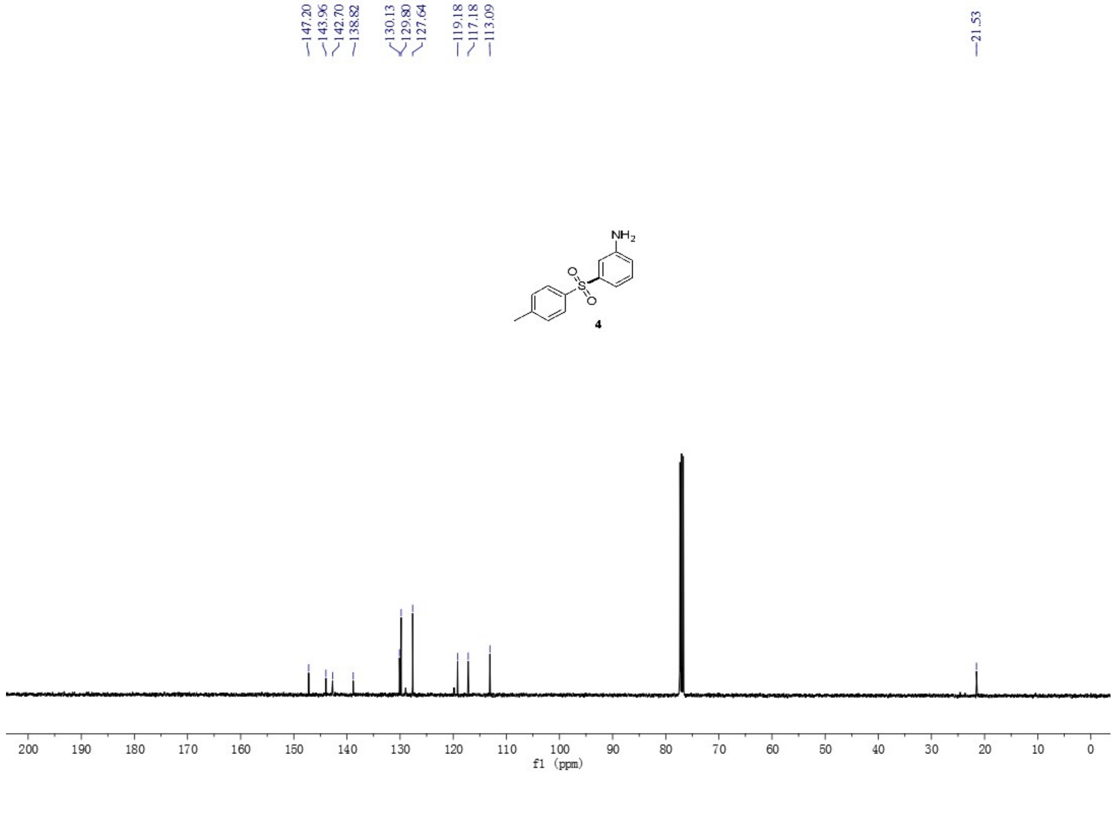
5.15
1.03
2.02
3.00
f1 (ppm)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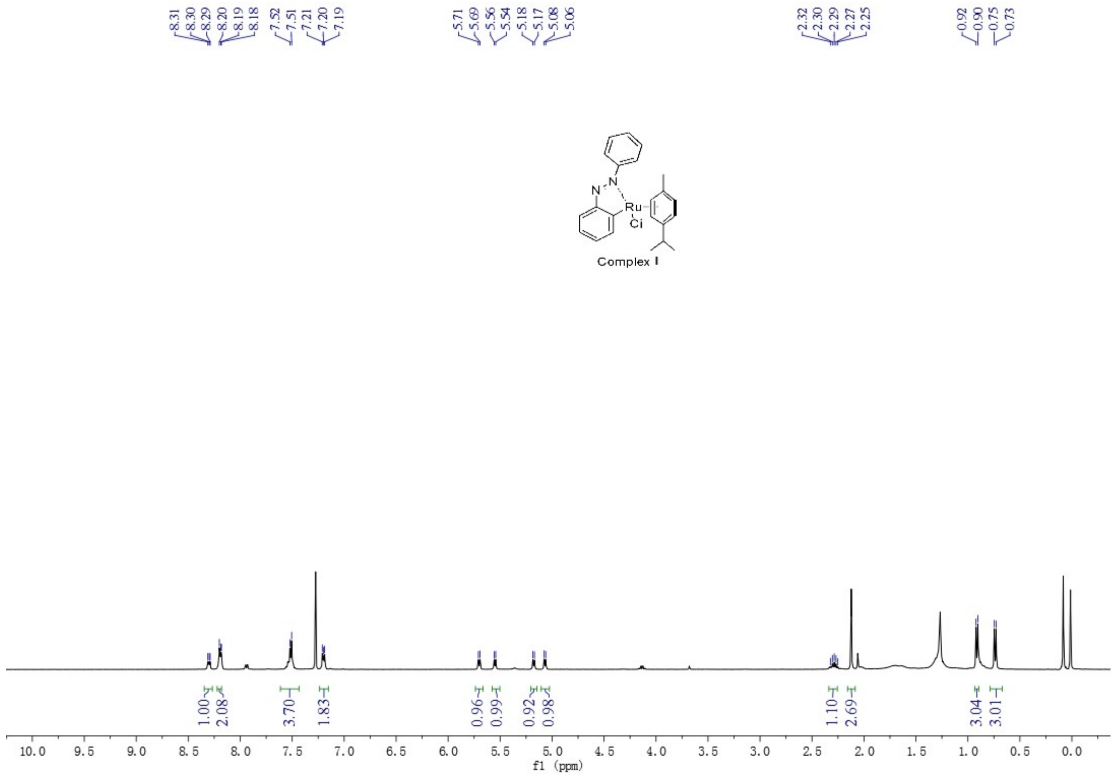
NH2
4
f1 (ppm)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5.56
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5.18
5.17
5.08
5.06
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2.30
2.29
2.27
2.25
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0.75
0.73
Ru
Cl
Complex I
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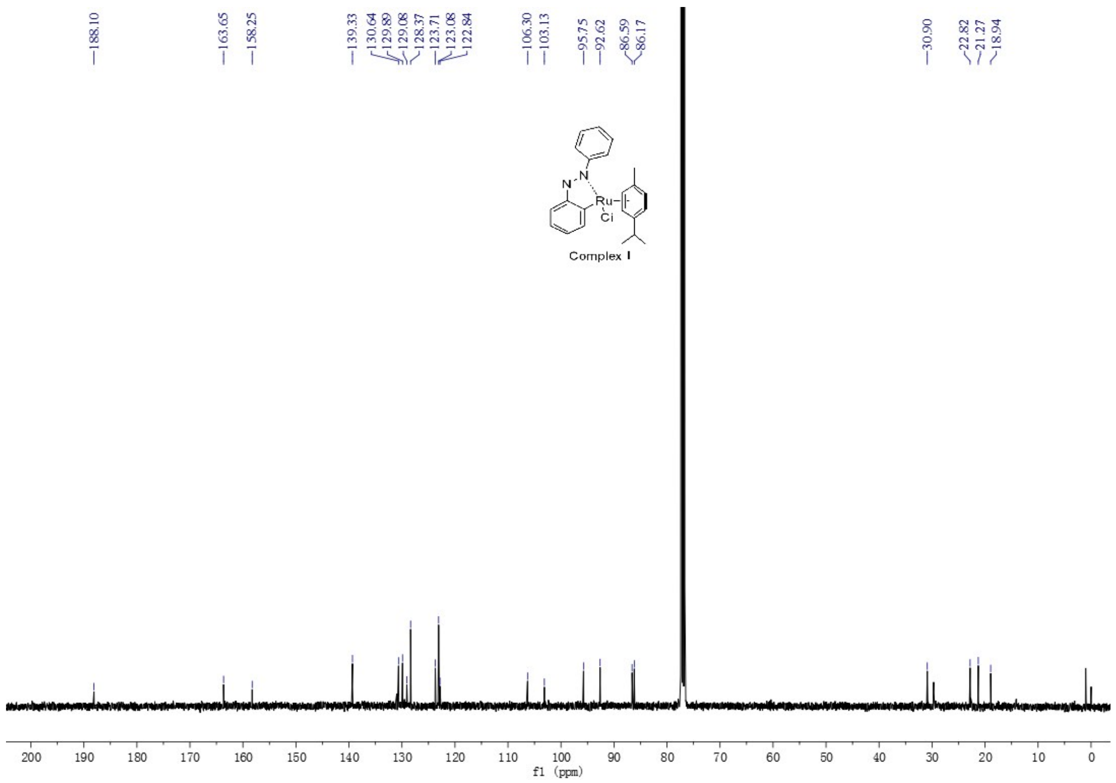
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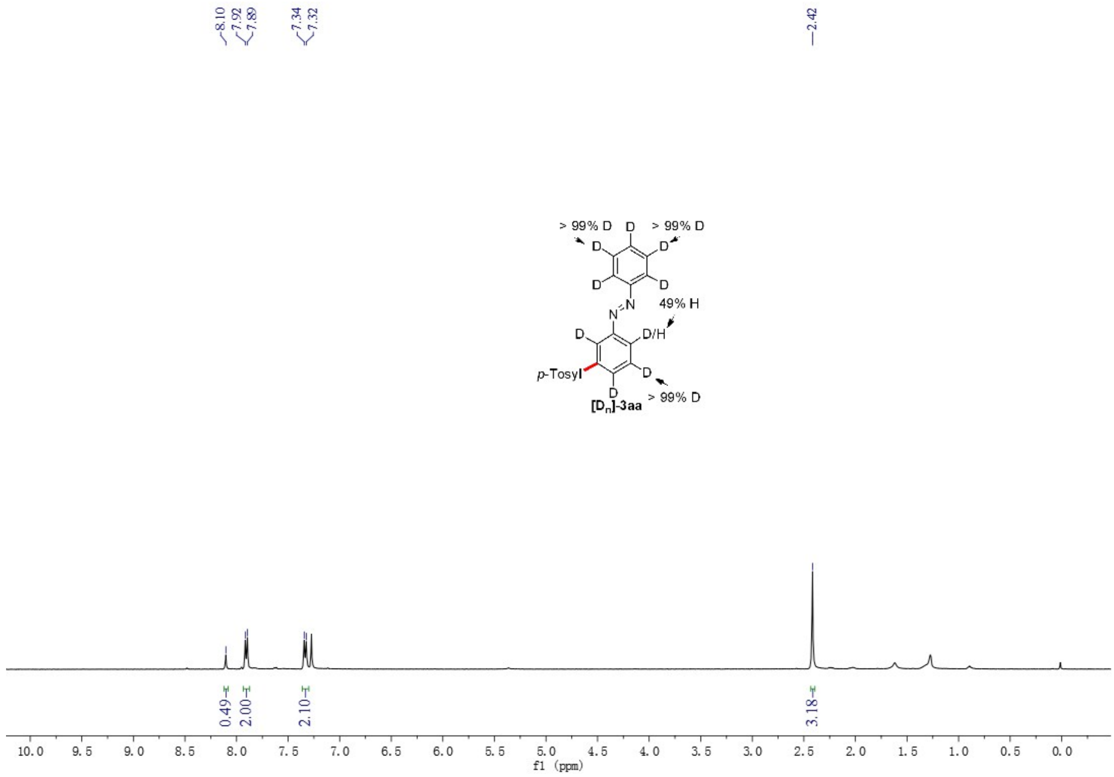
86.59
86.17
30.90
22.82
21.27
18.94
Ru
Cl
Complex I
f1 (ppm)



6.1 X-ray crystal structure and data for ruthenium-azobenzene complex

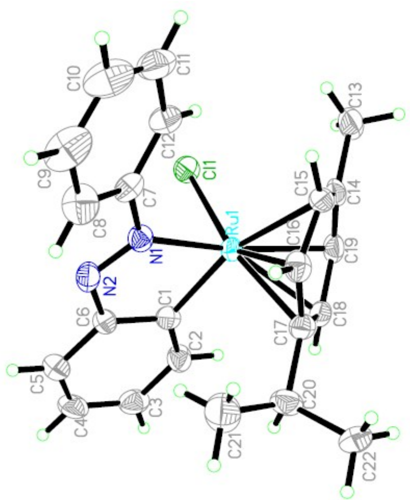


Table 1. Crystal data and structure refinement for ruthenium-azobenzene complex.

Identification code	1501752
Empirical formula	$C_{22}H_{23}ClN_2Ru$

Formula weight	451.94
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.445(2) A alpha = 82.53(3) deg.
	b = 14.347(3) A beta = 85.30(3) deg.
	c = 14.407(3) A gamma = 74.55(3) deg.
Volume	2060.8(7) A^3
Z, Calculated density	4, 1.457 Mg/m^3
Absorption coefficient	0.898 mm^-1
F(000)	920
Crystal size	0.20 x 0.20 x 0.20 mm
Theta range for data collection	3.12 to 25.01 deg.
Limiting indices	-12<=h<=12, -17<=k<=17, -17<=l<=17
Reflections collected / unique	20937 / 7196 [R(int) = 0.0450]
Completeness to theta = 25.01	99.1 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7196 / 0 / 469
Goodness-of-fit on F^2	1.105
Final R indices [I>2sigma(I)]	R1 = 0.0695, wR2 = 0.1802
R indices (all data)	R1 = 0.0817, wR2 = 0.1846
Largest diff. peak and hole	2.247 and -0.948 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1501752. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	2209(1)	6796(1)	1235(1)	36(1)

Ru(2)	-3187(1)	6893(1)	4565(1)	32(1)
Cl(2)	-4375(3)	6085(2)	3720(2)	49(1)
Cl(1)	768(3)	5949(2)	2181(2)	50(1)
C(21)	3149(15)	9017(10)	-15(12)	94(5)
N(2)	-110(8)	8458(6)	958(6)	49(2)
N(3)	-4981(7)	7777(5)	4962(5)	36(2)
C(13)	3425(13)	4310(9)	1093(13)	92(5)
N(4)	-5512(8)	8571(6)	4447(6)	41(2)
N(1)	529(8)	7677(6)	639(6)	43(2)
C(1)	1591(10)	7893(7)	2061(7)	40(2)
C(23)	-3541(9)	7976(7)	3498(7)	38(2)
C(29)	-5728(9)	7617(7)	5804(7)	38(2)
C(17)	3981(10)	7231(7)	647(7)	44(2)
C(38)	-2241(10)	6982(8)	5815(7)	44(2)
C(20)	4221(12)	8232(8)	501(9)	58(3)
C(28)	-4740(9)	8694(7)	3643(7)	42(2)
C(34)	-5843(10)	6680(8)	6116(9)	54(3)
C(24)	-2826(10)	8121(8)	2666(7)	47(2)
C(40)	-1009(9)	6623(7)	4367(7)	39(2)
C(36)	-2019(10)	5407(7)	5309(8)	46(2)
C(6)	476(10)	8589(7)	1758(7)	45(2)
C(2)	2130(11)	8037(8)	2861(8)	52(3)
C(39)	-1471(9)	7277(7)	5047(6)	38(2)
C(3)	1619(13)	8871(9)	3289(9)	63(3)
C(25)	-3242(12)	8924(8)	2032(8)	56(3)
C(33)	-6581(13)	6545(10)	6867(7)	71(4)
C(42)	-1120(12)	8244(8)	4922(8)	56(3)
C(31)	-7120(13)	8185(11)	7124(9)	77(4)
C(15)	3361(10)	5898(8)	54(8)	51(3)
C(27)	-5190(11)	9508(8)	2994(8)	55(3)

C(35)	-2365(12)	4438(8)	5403(11)	76(4)
C(7)	9(10)	7504(8)	-190(7)	47(2)
C(5)	-69(12)	9435(8)	2188(9)	61(3)
C(26)	-4429(13)	9619(9)	2187(9)	68(3)
C(12)	144(11)	6545(9)	-364(8)	59(3)
C(41)	-1329(10)	5716(7)	4490(8)	47(3)
C(30)	-6360(12)	8377(8)	6331(8)	56(3)
C(19)	4095(9)	5703(7)	1630(8)	49(3)
C(37)	-2456(10)	6025(8)	5972(7)	51(3)
C(14)	3651(10)	5316(7)	916(9)	53(3)
C(32)	-7270(13)	7270(11)	7394(9)	70(4)
C(16)	3414(10)	6860(8)	-30(7)	49(3)
C(4)	509(13)	9562(9)	2965(10)	68(4)
C(18)	4320(9)	6632(7)	1497(7)	44(2)
C(8)	-598(13)	8281(11)	-832(9)	73(4)
C(11)	-331(13)	6367(11)	-1176(10)	73(4)
C(44)	-2200(14)	9080(9)	5254(12)	89(5)
C(9)	-1077(15)	8090(14)	-1637(9)	88(5)
C(43)	136(12)	8133(9)	5446(9)	64(3)
C(22)	5582(13)	8188(10)	2(11)	79(4)
C(10)	-910(17)	7142(14)	-1795(10)	90(5)

Table 3. Bond lengths [A] and angles [deg] for 1501752.

Ru(1)-C(1)	2.032(9)
Ru(1)-N(1)	2.049(8)
Ru(1)-C(16)	2.135(10)
Ru(1)-C(17)	2.181(10)
Ru(1)-C(18)	2.213(10)
Ru(1)-C(19)	2.229(9)
Ru(1)-C(15)	2.326(9)

Ru(1)-C(14)	2.330(9)
Ru(1)-Cl(1)	2.409(3)
Ru(2)-C(23)	2.020(10)
Ru(2)-N(3)	2.048(7)
Ru(2)-C(38)	2.157(9)
Ru(2)-C(39)	2.197(9)
Ru(2)-C(40)	2.204(9)
Ru(2)-C(41)	2.212(9)
Ru(2)-C(37)	2.309(10)
Ru(2)-C(36)	2.327(9)
Ru(2)-Cl(2)	2.397(3)
C(21)-C(20)	1.524(18)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
N(2)-N(1)	1.264(11)
N(2)-C(6)	1.404(13)
N(3)-N(4)	1.291(10)
N(3)-C(29)	1.415(12)
C(13)-C(14)	1.510(15)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
N(4)-C(28)	1.376(12)
N(1)-C(7)	1.428(12)
C(1)-C(6)	1.376(14)
C(1)-C(2)	1.385(14)
C(23)-C(24)	1.382(13)
C(23)-C(28)	1.414(13)
C(29)-C(34)	1.395(14)

C(29)-C(30)	1.396(13)
C(17)-C(16)	1.408(14)
C(17)-C(18)	1.414(14)
C(17)-C(20)	1.507(14)
C(38)-C(39)	1.401(14)
C(38)-C(37)	1.436(15)
C(38)-H(38A)	0.9800
C(20)-C(22)	1.529(16)
C(20)-H(20A)	0.9800
C(28)-C(27)	1.398(14)
C(34)-C(33)	1.301(16)
C(34)-H(34A)	0.9300
C(24)-C(25)	1.370(15)
C(24)-H(24A)	0.9300
C(40)-C(39)	1.411(13)
C(40)-C(41)	1.414(14)
C(40)-H(40A)	0.9800
C(36)-C(37)	1.357(15)
C(36)-C(41)	1.416(15)
C(36)-C(35)	1.513(14)
C(6)-C(5)	1.396(14)
C(2)-C(3)	1.377(15)
C(2)-H(2A)	0.9300
C(39)-C(42)	1.512(14)
C(3)-C(4)	1.379(18)
C(3)-H(3A)	0.9300
C(25)-C(26)	1.391(16)
C(25)-H(25A)	0.9300
C(33)-C(32)	1.376(17)
C(33)-H(33A)	0.9300

C(42)-C(44)	1.510(17)
C(42)-C(43)	1.529(15)
C(42)-H(42A)	0.9800
C(31)-C(32)	1.366(19)
C(31)-C(30)	1.378(17)
C(31)-H(31A)	0.9300
C(15)-C(16)	1.386(15)
C(15)-C(14)	1.409(16)
C(15)-H(15A)	0.9800
C(27)-C(26)	1.370(16)
C(27)-H(27A)	0.9300
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(7)-C(8)	1.396(16)
C(7)-C(12)	1.398(16)
C(5)-C(4)	1.369(17)
C(5)-H(5A)	0.9300
C(26)-H(26A)	0.9300
C(12)-C(11)	1.385(16)
C(12)-H(12A)	0.9300
C(41)-H(41A)	0.9800
C(30)-H(30A)	0.9300
C(19)-C(14)	1.395(16)
C(19)-C(18)	1.400(14)
C(19)-H(19A)	0.9800
C(37)-H(37A)	0.9800
C(32)-H(32A)	0.9300
C(16)-H(16A)	0.9800
C(4)-H(4A)	0.9300

C(18)-H(18A)	0.9800
C(8)-C(9)	1.387(18)
C(8)-H(8A)	0.9300
C(11)-C(10)	1.37(2)
C(11)-H(11A)	0.9300
C(44)-H(44A)	0.9600
C(44)-H(44B)	0.9600
C(44)-H(44C)	0.9600
C(9)-C(10)	1.37(2)
C(9)-H(9A)	0.9300
C(43)-H(43A)	0.9600
C(43)-H(43B)	0.9600
C(43)-H(43C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(10)-H(10A)	0.9300

C(1)-Ru(1)-N(1)	75.5(4)
C(1)-Ru(1)-C(16)	124.6(4)
N(1)-Ru(1)-C(16)	93.7(4)
C(1)-Ru(1)-C(17)	95.2(4)
N(1)-Ru(1)-C(17)	111.2(4)
C(16)-Ru(1)-C(17)	38.1(4)
C(1)-Ru(1)-C(18)	91.8(4)
N(1)-Ru(1)-C(18)	146.0(4)
C(16)-Ru(1)-C(18)	67.4(4)
C(17)-Ru(1)-C(18)	37.5(4)
C(1)-Ru(1)-C(19)	115.2(4)
N(1)-Ru(1)-C(19)	169.0(4)

C(16)-Ru(1)-C(19)	78.3(4)
C(17)-Ru(1)-C(19)	66.9(4)
C(18)-Ru(1)-C(19)	36.7(4)
C(1)-Ru(1)-C(15)	160.0(4)
N(1)-Ru(1)-C(15)	105.2(4)
C(16)-Ru(1)-C(15)	35.9(4)
C(17)-Ru(1)-C(15)	65.7(4)
C(18)-Ru(1)-C(15)	76.5(4)
C(19)-Ru(1)-C(15)	63.9(4)
C(1)-Ru(1)-C(14)	150.4(4)
N(1)-Ru(1)-C(14)	133.9(4)
C(16)-Ru(1)-C(14)	65.2(4)
C(17)-Ru(1)-C(14)	77.7(4)
C(18)-Ru(1)-C(14)	65.0(4)
C(19)-Ru(1)-C(14)	35.6(4)
C(15)-Ru(1)-C(14)	35.2(4)
C(1)-Ru(1)-Cl(1)	88.5(3)
N(1)-Ru(1)-Cl(1)	86.9(2)
C(16)-Ru(1)-Cl(1)	146.0(3)
C(17)-Ru(1)-Cl(1)	161.8(3)
C(18)-Ru(1)-Cl(1)	124.7(3)
C(19)-Ru(1)-Cl(1)	95.5(3)
C(15)-Ru(1)-Cl(1)	111.4(3)
C(14)-Ru(1)-Cl(1)	90.3(3)
C(23)-Ru(2)-N(3)	76.5(3)
C(23)-Ru(2)-C(38)	123.1(4)
N(3)-Ru(2)-C(38)	94.1(3)
C(23)-Ru(2)-C(39)	95.2(4)
N(3)-Ru(2)-C(39)	113.6(3)
C(38)-Ru(2)-C(39)	37.5(4)

C(23)-Ru(2)-C(40)	93.7(4)
N(3)-Ru(2)-C(40)	149.3(3)
C(38)-Ru(2)-C(40)	66.7(4)
C(39)-Ru(2)-C(40)	37.4(3)
C(23)-Ru(2)-C(41)	118.5(4)
N(3)-Ru(2)-C(41)	165.0(4)
C(38)-Ru(2)-C(41)	77.8(4)
C(39)-Ru(2)-C(41)	67.2(4)
C(40)-Ru(2)-C(41)	37.3(4)
C(23)-Ru(2)-C(37)	160.4(4)
N(3)-Ru(2)-C(37)	102.2(4)
C(38)-Ru(2)-C(37)	37.3(4)
C(39)-Ru(2)-C(37)	67.0(4)
C(40)-Ru(2)-C(37)	77.4(4)
C(41)-Ru(2)-C(37)	63.7(4)
C(23)-Ru(2)-C(36)	154.4(4)
N(3)-Ru(2)-C(36)	128.8(4)
C(38)-Ru(2)-C(36)	64.9(4)
C(39)-Ru(2)-C(36)	78.4(4)
C(40)-Ru(2)-C(36)	66.2(4)
C(41)-Ru(2)-C(36)	36.2(4)
C(37)-Ru(2)-C(36)	34.0(4)
C(23)-Ru(2)-Cl(2)	86.3(3)
N(3)-Ru(2)-Cl(2)	88.1(2)
C(38)-Ru(2)-Cl(2)	150.2(3)
C(39)-Ru(2)-Cl(2)	158.1(3)
C(40)-Ru(2)-Cl(2)	120.7(3)
C(41)-Ru(2)-Cl(2)	92.8(3)
C(37)-Ru(2)-Cl(2)	113.3(3)
C(36)-Ru(2)-Cl(2)	90.8(3)

C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(1)-N(2)-C(6)	110.5(8)
N(4)-N(3)-C(29)	113.8(7)
N(4)-N(3)-Ru(2)	120.9(6)
C(29)-N(3)-Ru(2)	125.4(6)
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(3)-N(4)-C(28)	111.3(8)
N(2)-N(1)-C(7)	113.8(9)
N(2)-N(1)-Ru(1)	122.1(7)
C(7)-N(1)-Ru(1)	124.1(7)
C(6)-C(1)-C(2)	116.8(9)
C(6)-C(1)-Ru(1)	113.6(7)
C(2)-C(1)-Ru(1)	129.6(8)
C(24)-C(23)-C(28)	115.9(9)
C(24)-C(23)-Ru(2)	131.2(7)
C(28)-C(23)-Ru(2)	112.9(7)
C(34)-C(29)-C(30)	119.0(10)
C(34)-C(29)-N(3)	119.4(9)
C(30)-C(29)-N(3)	121.6(9)
C(16)-C(17)-C(18)	117.6(10)

C(16)-C(17)-C(20)	122.7(10)
C(18)-C(17)-C(20)	119.6(9)
C(16)-C(17)-Ru(1)	69.2(6)
C(18)-C(17)-Ru(1)	72.5(6)
C(20)-C(17)-Ru(1)	128.9(7)
C(39)-C(38)-C(37)	122.7(9)
C(39)-C(38)-Ru(2)	72.8(5)
C(37)-C(38)-Ru(2)	77.1(6)
C(39)-C(38)-H(38A)	118.6
C(37)-C(38)-H(38A)	118.6
Ru(2)-C(38)-H(38A)	118.6
C(17)-C(20)-C(21)	115.1(11)
C(17)-C(20)-C(22)	109.9(9)
C(21)-C(20)-C(22)	110.1(11)
C(17)-C(20)-H(20A)	107.1
C(21)-C(20)-H(20A)	107.1
C(22)-C(20)-H(20A)	107.1
N(4)-C(28)-C(27)	118.7(9)
N(4)-C(28)-C(23)	118.4(9)
C(27)-C(28)-C(23)	122.9(9)
C(33)-C(34)-C(29)	119.1(12)
C(33)-C(34)-H(34A)	120.4
C(29)-C(34)-H(34A)	120.4
C(25)-C(24)-C(23)	121.8(10)
C(25)-C(24)-H(24A)	119.1
C(23)-C(24)-H(24A)	119.1
C(39)-C(40)-C(41)	119.5(9)
C(39)-C(40)-Ru(2)	71.1(5)
C(41)-C(40)-Ru(2)	71.7(5)
C(39)-C(40)-H(40A)	119.8

C(41)-C(40)-H(40A)	119.8
Ru(2)-C(40)-H(40A)	119.8
C(37)-C(36)-C(41)	118.9(9)
C(37)-C(36)-C(35)	120.6(11)
C(41)-C(36)-C(35)	120.3(11)
C(37)-C(36)-Ru(2)	72.3(6)
C(41)-C(36)-Ru(2)	67.4(5)
C(35)-C(36)-Ru(2)	128.1(7)
C(1)-C(6)-C(5)	123.1(10)
C(1)-C(6)-N(2)	118.3(9)
C(5)-C(6)-N(2)	118.5(10)
C(3)-C(2)-C(1)	121.0(11)
C(3)-C(2)-H(2A)	119.5
C(1)-C(2)-H(2A)	119.5
C(38)-C(39)-C(40)	117.1(9)
C(38)-C(39)-C(42)	123.3(9)
C(40)-C(39)-C(42)	119.6(9)
C(38)-C(39)-Ru(2)	69.7(5)
C(40)-C(39)-Ru(2)	71.5(5)
C(42)-C(39)-Ru(2)	129.6(7)
C(2)-C(3)-C(4)	120.9(11)
C(2)-C(3)-H(3A)	119.5
C(4)-C(3)-H(3A)	119.5
C(24)-C(25)-C(26)	121.2(10)
C(24)-C(25)-H(25A)	119.4
C(26)-C(25)-H(25A)	119.4
C(34)-C(33)-C(32)	124.5(14)
C(34)-C(33)-H(33A)	117.8
C(32)-C(33)-H(33A)	117.8
C(44)-C(42)-C(39)	114.7(10)

C(44)-C(42)-C(43)	109.1(10)
C(39)-C(42)-C(43)	108.6(9)
C(44)-C(42)-H(42A)	108.1
C(39)-C(42)-H(42A)	108.1
C(43)-C(42)-H(42A)	108.1
C(32)-C(31)-C(30)	121.1(12)
C(32)-C(31)-H(31A)	119.5
C(30)-C(31)-H(31A)	119.5
C(16)-C(15)-C(14)	119.1(10)
C(16)-C(15)-Ru(1)	64.5(5)
C(14)-C(15)-Ru(1)	72.5(6)
C(16)-C(15)-H(15A)	119.0
C(14)-C(15)-H(15A)	119.0
Ru(1)-C(15)-H(15A)	119.0
C(26)-C(27)-C(28)	118.5(10)
C(26)-C(27)-H(27A)	120.7
C(28)-C(27)-H(27A)	120.7
C(36)-C(35)-H(35A)	109.5
C(36)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(36)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(8)-C(7)-C(12)	120.3(11)
C(8)-C(7)-N(1)	120.5(11)
C(12)-C(7)-N(1)	119.2(10)
C(4)-C(5)-C(6)	118.4(11)
C(4)-C(5)-H(5A)	120.8
C(6)-C(5)-H(5A)	120.8
C(27)-C(26)-C(25)	119.6(10)

C(27)-C(26)-H(26A)	120.2
C(25)-C(26)-H(26A)	120.2
C(11)-C(12)-C(7)	119.7(12)
C(11)-C(12)-H(12A)	120.1
C(7)-C(12)-H(12A)	120.1
C(40)-C(41)-C(36)	122.1(9)
C(40)-C(41)-Ru(2)	71.0(5)
C(36)-C(41)-Ru(2)	76.3(6)
C(40)-C(41)-H(41A)	118.7
C(36)-C(41)-H(41A)	118.7
Ru(2)-C(41)-H(41A)	118.7
C(31)-C(30)-C(29)	118.9(11)
C(31)-C(30)-H(30A)	120.5
C(29)-C(30)-H(30A)	120.5
C(14)-C(19)-C(18)	121.8(10)
C(14)-C(19)-Ru(1)	76.2(6)
C(18)-C(19)-Ru(1)	71.0(5)
C(14)-C(19)-H(19A)	118.9
C(18)-C(19)-H(19A)	118.9
Ru(1)-C(19)-H(19A)	118.9
C(36)-C(37)-C(38)	119.3(10)
C(36)-C(37)-Ru(2)	73.7(6)
C(38)-C(37)-Ru(2)	65.6(5)
C(36)-C(37)-H(37A)	119.3
C(38)-C(37)-H(37A)	119.3
Ru(2)-C(37)-H(37A)	119.3
C(19)-C(14)-C(15)	118.7(9)
C(19)-C(14)-C(13)	119.8(12)
C(15)-C(14)-C(13)	121.4(12)
C(19)-C(14)-Ru(1)	68.3(5)

C(15)-C(14)-Ru(1)	72.2(6)
C(13)-C(14)-Ru(1)	128.8(7)
C(31)-C(32)-C(33)	117.2(12)
C(31)-C(32)-H(32A)	121.4
C(33)-C(32)-H(32A)	121.4
C(15)-C(16)-C(17)	122.2(10)
C(15)-C(16)-Ru(1)	79.6(6)
C(17)-C(16)-Ru(1)	72.8(6)
C(15)-C(16)-H(16A)	118.9
C(17)-C(16)-H(16A)	118.9
Ru(1)-C(16)-H(16A)	118.9
C(5)-C(4)-C(3)	119.7(11)
C(5)-C(4)-H(4A)	120.1
C(3)-C(4)-H(4A)	120.1
C(19)-C(18)-C(17)	119.5(10)
C(19)-C(18)-Ru(1)	72.3(6)
C(17)-C(18)-Ru(1)	70.0(6)
C(19)-C(18)-H(18A)	119.7
C(17)-C(18)-H(18A)	119.7
Ru(1)-C(18)-H(18A)	119.7
C(9)-C(8)-C(7)	119.3(14)
C(9)-C(8)-H(8A)	120.4
C(7)-C(8)-H(8A)	120.4
C(10)-C(11)-C(12)	118.6(14)
C(10)-C(11)-H(11A)	120.7
C(12)-C(11)-H(11A)	120.7
C(42)-C(44)-H(44A)	109.5
C(42)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(42)-C(44)-H(44C)	109.5

H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(10)-C(9)-C(8)	119.0(14)
C(10)-C(9)-H(9A)	120.5
C(8)-C(9)-H(9A)	120.5
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(11)-C(10)-C(9)	123.0(13)
C(11)-C(10)-H(10A)	118.5
C(9)-C(10)-H(10A)	118.5

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1501752. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	33(1)	37(1)	36(1)	-6(1)	2(1)	-7(1)
Ru(2)	28(1)	33(1)	31(1)	-3(1)	-5(1)	-3(1)
Cl(2)	51(2)	48(1)	51(2)	-9(1)	-15(1)	-11(1)
Cl(1)	49(1)	51(2)	50(2)	-6(1)	12(1)	-17(1)
C(21)	82(10)	64(9)	123(13)	18(9)	17(9)	-16(8)

N(2)	37(5)	48(5)	57(6)	-2(4)	0(4)	-4(4)
N(3)	31(4)	34(4)	42(4)	-4(3)	-2(3)	-4(3)
C(13)	59(8)	47(7)	167(16)	-25(9)	50(9)	-21(6)
N(4)	39(4)	33(4)	44(5)	4(4)	-6(4)	1(3)
N(1)	40(4)	44(5)	43(5)	-5(4)	4(4)	-10(4)
C(1)	44(5)	42(5)	36(5)	-8(4)	6(4)	-15(4)
C(23)	33(5)	42(5)	42(5)	-6(4)	-8(4)	-11(4)
C(29)	33(5)	38(5)	39(5)	-2(4)	-3(4)	-5(4)
C(17)	45(6)	49(6)	42(6)	-10(5)	9(4)	-18(5)
C(38)	44(6)	53(6)	37(5)	-14(5)	-8(4)	-7(5)
C(20)	70(8)	42(6)	65(7)	-3(5)	7(6)	-24(6)
C(28)	37(5)	41(5)	45(6)	-2(4)	2(4)	-7(4)
C(34)	35(5)	44(6)	78(8)	13(6)	1(5)	-11(5)
C(24)	35(5)	58(7)	44(6)	-2(5)	-1(4)	-9(5)
C(40)	28(5)	45(6)	42(5)	-6(4)	-8(4)	-3(4)
C(36)	36(5)	31(5)	66(7)	8(5)	-16(5)	-6(4)
C(6)	41(5)	43(6)	51(6)	-16(5)	3(5)	-9(4)
C(2)	47(6)	57(7)	52(6)	-17(5)	-3(5)	-7(5)
C(39)	37(5)	43(5)	36(5)	-8(4)	-10(4)	-6(4)
C(3)	66(8)	72(8)	63(8)	-29(7)	12(6)	-33(7)
C(25)	58(7)	61(7)	51(7)	8(6)	2(5)	-27(6)
C(33)	87(9)	77(9)	28(6)	-12(6)	-17(6)	24(7)
C(42)	68(7)	46(6)	60(7)	-6(5)	-21(6)	-20(6)
C(31)	73(9)	98(11)	56(8)	-41(8)	14(7)	-3(8)
C(15)	42(6)	61(7)	58(7)	-36(6)	11(5)	-18(5)
C(27)	56(7)	42(6)	58(7)	9(5)	-6(5)	0(5)
C(35)	48(7)	38(6)	142(13)	12(7)	-32(8)	-13(5)
C(7)	40(5)	65(7)	39(5)	-2(5)	-4(4)	-20(5)
C(5)	57(7)	48(7)	80(9)	-21(6)	1(6)	-12(5)
C(26)	81(9)	54(7)	56(7)	21(6)	0(6)	-11(6)

C(12)	55(7)	68(8)	61(7)	-13(6)	-15(6)	-20(6)
C(41)	41(5)	41(6)	58(7)	-15(5)	-15(5)	2(4)
C(30)	69(7)	41(6)	53(7)	-11(5)	4(6)	-2(5)
C(19)	34(5)	40(6)	63(7)	4(5)	-1(5)	2(4)
C(37)	39(6)	66(7)	44(6)	12(5)	-11(5)	-16(5)
C(14)	37(5)	33(5)	83(8)	-14(5)	27(5)	-6(4)
C(32)	70(8)	88(10)	49(7)	8(7)	9(6)	-27(7)
C(16)	47(6)	58(7)	41(6)	-10(5)	0(5)	-8(5)
C(4)	72(8)	55(7)	87(9)	-39(7)	17(7)	-24(7)
C(18)	33(5)	49(6)	49(6)	-11(5)	2(4)	-8(4)
C(8)	78(9)	83(10)	52(7)	0(7)	-13(7)	-12(7)
C(11)	68(8)	94(10)	72(9)	-27(8)	-2(7)	-39(8)
C(44)	81(10)	46(7)	142(14)	-21(8)	-35(10)	-8(7)
C(9)	92(11)	125(14)	53(8)	28(9)	-31(7)	-45(10)
C(43)	62(7)	61(7)	78(9)	-14(6)	-23(6)	-24(6)
C(22)	63(8)	63(8)	119(12)	-16(8)	23(8)	-37(7)
C(10)	107(12)	123(14)	57(9)	0(9)	-27(8)	-57(11)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1501752.

	x	y	z	U(eq)
H(21A)	2304	9053	314	141
H(21B)	3112	8860	-638	141
H(21C)	3357	9634	-47	141
H(13A)	4213	3841	901	138
H(13B)	2695	4286	741	138
H(13C)	3224	4162	1749	138
H(38A)	-2706	7464	6234	53
H(20A)	4252	8429	1124	70
H(34A)	-5397	6158	5792	65

H(24A)	-2040	7660	2532	56
H(40A)	-614	6843	3766	47
H(2A)	2848	7563	3113	62
H(3A)	2029	8970	3804	75
H(25A)	-2722	9006	1487	67
H(33A)	-6649	5915	7061	85
H(42A)	-920	8406	4253	67
H(31A)	-7538	8686	7481	93
H(15A)	2857	5696	-392	61
H(27A)	-5988	9964	3108	66
H(35A)	-1697	3952	5744	114
H(35B)	-2403	4254	4791	114
H(35C)	-3213	4494	5734	114
H(5A)	-807	9900	1952	73
H(26A)	-4703	10157	1746	81
H(12A)	552	6029	63	71
H(41A)	-1167	5326	3961	57
H(30A)	-6268	9004	6149	68
H(19A)	4146	5350	2261	59
H(37A)	-3110	5888	6463	61
H(32A)	-7814	7143	7912	84
H(16A)	3034	7300	-575	59
H(4A)	154	10112	3272	81
H(18A)	4546	6909	2029	52
H(8A)	-681	8918	-719	88
H(11A)	-258	5733	-1297	88
H(44A)	-2988	9161	4920	133
H(44B)	-1906	9666	5139	133
H(44C)	-2393	8946	5913	133
H(9A)	-1505	8598	-2065	106

H(43A)	828	7604	5235	96
H(43B)	-48	8002	6106	96
H(43C)	418	8724	5324	96
H(22A)	6251	7699	338	118
H(22B)	5774	8809	-21	118
H(22C)	5574	8029	-624	118
H(10A)	-1205	7020	-2348	108

Table 6. Torsion angles [deg] for 1501752.

C(23)-Ru(2)-N(3)-N(4)	-1.7(7)
C(38)-Ru(2)-N(3)-N(4)	121.4(7)
C(39)-Ru(2)-N(3)-N(4)	88.2(7)
C(40)-Ru(2)-N(3)-N(4)	72.4(10)
C(41)-Ru(2)-N(3)-N(4)	177.9(11)
C(37)-Ru(2)-N(3)-N(4)	158.2(7)
C(36)-Ru(2)-N(3)-N(4)	-177.8(7)
Cl(2)-Ru(2)-N(3)-N(4)	-88.3(7)
C(23)-Ru(2)-N(3)-C(29)	-179.5(8)
C(38)-Ru(2)-N(3)-C(29)	-56.4(8)
C(39)-Ru(2)-N(3)-C(29)	-89.7(8)
C(40)-Ru(2)-N(3)-C(29)	-105.5(9)
C(41)-Ru(2)-N(3)-C(29)	0.0(18)
C(37)-Ru(2)-N(3)-C(29)	-19.6(8)
C(36)-Ru(2)-N(3)-C(29)	4.3(9)
Cl(2)-Ru(2)-N(3)-C(29)	93.8(7)
C(29)-N(3)-N(4)-C(28)	179.5(8)
Ru(2)-N(3)-N(4)-C(28)	1.4(11)
C(6)-N(2)-N(1)-C(7)	-178.6(8)
C(6)-N(2)-N(1)-Ru(1)	-1.7(11)
C(1)-Ru(1)-N(1)-N(2)	2.0(8)

C(16)-Ru(1)-N(1)-N(2)	-122.8(8)
C(17)-Ru(1)-N(1)-N(2)	-88.0(8)
C(18)-Ru(1)-N(1)-N(2)	-69.1(10)
C(19)-Ru(1)-N(1)-N(2)	-165.9(17)
C(15)-Ru(1)-N(1)-N(2)	-157.3(8)
C(14)-Ru(1)-N(1)-N(2)	178.7(7)
Cl(1)-Ru(1)-N(1)-N(2)	91.3(8)
C(1)-Ru(1)-N(1)-C(7)	178.7(8)
C(16)-Ru(1)-N(1)-C(7)	53.8(8)
C(17)-Ru(1)-N(1)-C(7)	88.6(8)
C(18)-Ru(1)-N(1)-C(7)	107.5(9)
C(19)-Ru(1)-N(1)-C(7)	11(2)
C(15)-Ru(1)-N(1)-C(7)	19.3(8)
C(14)-Ru(1)-N(1)-C(7)	-4.7(10)
Cl(1)-Ru(1)-N(1)-C(7)	-92.1(7)
N(1)-Ru(1)-C(1)-C(6)	-1.7(7)
C(16)-Ru(1)-C(1)-C(6)	82.7(8)
C(17)-Ru(1)-C(1)-C(6)	108.9(8)
C(18)-Ru(1)-C(1)-C(6)	146.3(8)
C(19)-Ru(1)-C(1)-C(6)	175.7(7)
C(15)-Ru(1)-C(1)-C(6)	92.9(14)
C(14)-Ru(1)-C(1)-C(6)	-176.9(7)
Cl(1)-Ru(1)-C(1)-C(6)	-89.0(7)
N(1)-Ru(1)-C(1)-C(2)	178.8(10)
C(16)-Ru(1)-C(1)-C(2)	-96.7(10)
C(17)-Ru(1)-C(1)-C(2)	-70.5(10)
C(18)-Ru(1)-C(1)-C(2)	-33.1(10)
C(19)-Ru(1)-C(1)-C(2)	-3.7(11)
C(15)-Ru(1)-C(1)-C(2)	-86.5(15)
C(14)-Ru(1)-C(1)-C(2)	3.7(14)

Cl(1)-Ru(1)-C(1)-C(2)	91.6(10)
N(3)-Ru(2)-C(23)-C(24)	-177.8(10)
C(38)-Ru(2)-C(23)-C(24)	96.1(10)
C(39)-Ru(2)-C(23)-C(24)	69.1(10)
C(40)-Ru(2)-C(23)-C(24)	31.7(10)
C(41)-Ru(2)-C(23)-C(24)	2.3(11)
C(37)-Ru(2)-C(23)-C(24)	93.5(14)
C(36)-Ru(2)-C(23)-C(24)	-4.8(15)
Cl(2)-Ru(2)-C(23)-C(24)	-88.9(9)
N(3)-Ru(2)-C(23)-C(28)	1.4(7)
C(38)-Ru(2)-C(23)-C(28)	-84.6(8)
C(39)-Ru(2)-C(23)-C(28)	-111.6(7)
C(40)-Ru(2)-C(23)-C(28)	-149.1(7)
C(41)-Ru(2)-C(23)-C(28)	-178.4(7)
C(37)-Ru(2)-C(23)-C(28)	-87.2(13)
C(36)-Ru(2)-C(23)-C(28)	174.5(7)
Cl(2)-Ru(2)-C(23)-C(28)	90.4(7)
N(4)-N(3)-C(29)-C(34)	139.8(9)
Ru(2)-N(3)-C(29)-C(34)	-42.2(12)
N(4)-N(3)-C(29)-C(30)	-39.9(13)
Ru(2)-N(3)-C(29)-C(30)	138.1(8)
C(1)-Ru(1)-C(17)-C(16)	-143.9(7)
N(1)-Ru(1)-C(17)-C(16)	-67.5(7)
C(18)-Ru(1)-C(17)-C(16)	129.8(9)
C(19)-Ru(1)-C(17)-C(16)	100.8(7)
C(15)-Ru(1)-C(17)-C(16)	30.2(6)
C(14)-Ru(1)-C(17)-C(16)	65.2(7)
Cl(1)-Ru(1)-C(17)-C(16)	114.9(9)
C(1)-Ru(1)-C(17)-C(18)	86.2(6)
N(1)-Ru(1)-C(17)-C(18)	162.7(6)

C(16)-Ru(1)-C(17)-C(18)	-129.8(9)
C(19)-Ru(1)-C(17)-C(18)	-29.0(6)
C(15)-Ru(1)-C(17)-C(18)	-99.7(7)
C(14)-Ru(1)-C(17)-C(18)	-64.7(6)
Cl(1)-Ru(1)-C(17)-C(18)	-14.9(12)
C(1)-Ru(1)-C(17)-C(20)	-28.1(10)
N(1)-Ru(1)-C(17)-C(20)	48.4(10)
C(16)-Ru(1)-C(17)-C(20)	115.9(13)
C(18)-Ru(1)-C(17)-C(20)	-114.3(12)
C(19)-Ru(1)-C(17)-C(20)	-143.3(11)
C(15)-Ru(1)-C(17)-C(20)	146.0(11)
C(14)-Ru(1)-C(17)-C(20)	-179.0(11)
Cl(1)-Ru(1)-C(17)-C(20)	-129.2(10)
C(23)-Ru(2)-C(38)-C(39)	-47.9(7)
N(3)-Ru(2)-C(38)-C(39)	-124.4(6)
C(40)-Ru(2)-C(38)-C(39)	30.7(6)
C(41)-Ru(2)-C(38)-C(39)	68.3(6)
C(37)-Ru(2)-C(38)-C(39)	130.6(9)
C(36)-Ru(2)-C(38)-C(39)	104.2(6)
Cl(2)-Ru(2)-C(38)-C(39)	142.3(5)
C(23)-Ru(2)-C(38)-C(37)	-178.6(6)
N(3)-Ru(2)-C(38)-C(37)	104.9(6)
C(39)-Ru(2)-C(38)-C(37)	-130.6(9)
C(40)-Ru(2)-C(38)-C(37)	-99.9(7)
C(41)-Ru(2)-C(38)-C(37)	-62.3(6)
C(36)-Ru(2)-C(38)-C(37)	-26.4(6)
Cl(2)-Ru(2)-C(38)-C(37)	11.6(9)
C(16)-C(17)-C(20)-C(21)	37.5(15)
C(18)-C(17)-C(20)-C(21)	-141.8(11)
Ru(1)-C(17)-C(20)-C(21)	-51.1(15)

C(16)-C(17)-C(20)-C(22)	-87.5(14)
C(18)-C(17)-C(20)-C(22)	93.2(13)
Ru(1)-C(17)-C(20)-C(22)	-176.0(9)
N(3)-N(4)-C(28)-C(27)	178.4(9)
N(3)-N(4)-C(28)-C(23)	0.0(13)
C(24)-C(23)-C(28)-N(4)	178.1(9)
Ru(2)-C(23)-C(28)-N(4)	-1.3(12)
C(24)-C(23)-C(28)-C(27)	-0.3(15)
Ru(2)-C(23)-C(28)-C(27)	-179.7(9)
C(30)-C(29)-C(34)-C(33)	3.0(16)
N(3)-C(29)-C(34)-C(33)	-176.8(10)
C(28)-C(23)-C(24)-C(25)	1.5(15)
Ru(2)-C(23)-C(24)-C(25)	-179.3(8)
C(23)-Ru(2)-C(40)-C(39)	93.8(6)
N(3)-Ru(2)-C(40)-C(39)	24.3(10)
C(38)-Ru(2)-C(40)-C(39)	-30.8(6)
C(41)-Ru(2)-C(40)-C(39)	-131.4(9)
C(37)-Ru(2)-C(40)-C(39)	-68.5(6)
C(36)-Ru(2)-C(40)-C(39)	-102.5(6)
Cl(2)-Ru(2)-C(40)-C(39)	-178.3(5)
C(23)-Ru(2)-C(40)-C(41)	-134.8(6)
N(3)-Ru(2)-C(40)-C(41)	155.7(6)
C(38)-Ru(2)-C(40)-C(41)	100.6(7)
C(39)-Ru(2)-C(40)-C(41)	131.4(9)
C(37)-Ru(2)-C(40)-C(41)	62.9(6)
C(36)-Ru(2)-C(40)-C(41)	29.0(6)
Cl(2)-Ru(2)-C(40)-C(41)	-46.9(7)
C(23)-Ru(2)-C(36)-C(37)	143.6(8)
N(3)-Ru(2)-C(36)-C(37)	-45.1(8)
C(38)-Ru(2)-C(36)-C(37)	28.8(6)

C(39)-Ru(2)-C(36)-C(37)	65.9(6)
C(40)-Ru(2)-C(36)-C(37)	103.2(7)
C(41)-Ru(2)-C(36)-C(37)	133.0(9)
Cl(2)-Ru(2)-C(36)-C(37)	-133.3(6)
C(23)-Ru(2)-C(36)-C(41)	10.6(12)
N(3)-Ru(2)-C(36)-C(41)	-178.1(5)
C(38)-Ru(2)-C(36)-C(41)	-104.1(7)
C(39)-Ru(2)-C(36)-C(41)	-67.1(6)
C(40)-Ru(2)-C(36)-C(41)	-29.8(6)
C(37)-Ru(2)-C(36)-C(41)	-133.0(9)
Cl(2)-Ru(2)-C(36)-C(41)	93.7(6)
C(23)-Ru(2)-C(36)-C(35)	-101.1(13)
N(3)-Ru(2)-C(36)-C(35)	70.2(12)
C(38)-Ru(2)-C(36)-C(35)	144.2(12)
C(39)-Ru(2)-C(36)-C(35)	-178.7(12)
C(40)-Ru(2)-C(36)-C(35)	-141.5(12)
C(41)-Ru(2)-C(36)-C(35)	-111.7(14)
C(37)-Ru(2)-C(36)-C(35)	115.4(14)
Cl(2)-Ru(2)-C(36)-C(35)	-18.0(11)
C(2)-C(1)-C(6)-C(5)	3.5(16)
Ru(1)-C(1)-C(6)-C(5)	-176.0(9)
C(2)-C(1)-C(6)-N(2)	-178.9(9)
Ru(1)-C(1)-C(6)-N(2)	1.6(12)
N(1)-N(2)-C(6)-C(1)	0.0(13)
N(1)-N(2)-C(6)-C(5)	177.7(10)
C(6)-C(1)-C(2)-C(3)	-4.2(16)
Ru(1)-C(1)-C(2)-C(3)	175.1(8)
C(37)-C(38)-C(39)-C(40)	6.2(14)
Ru(2)-C(38)-C(39)-C(40)	-55.3(7)
C(37)-C(38)-C(39)-C(42)	-173.7(9)

Ru(2)-C(38)-C(39)-C(42)	124.8(9)
C(37)-C(38)-C(39)-Ru(2)	61.5(8)
C(41)-C(40)-C(39)-C(38)	-0.4(13)
Ru(2)-C(40)-C(39)-C(38)	54.4(7)
C(41)-C(40)-C(39)-C(42)	179.5(9)
Ru(2)-C(40)-C(39)-C(42)	-125.7(8)
C(41)-C(40)-C(39)-Ru(2)	-54.8(8)
C(23)-Ru(2)-C(39)-C(38)	141.3(6)
N(3)-Ru(2)-C(39)-C(38)	63.8(6)
C(40)-Ru(2)-C(39)-C(38)	-129.5(9)
C(41)-Ru(2)-C(39)-C(38)	-99.9(7)
C(37)-Ru(2)-C(39)-C(38)	-30.0(6)
C(36)-Ru(2)-C(39)-C(38)	-63.7(6)
Cl(2)-Ru(2)-C(39)-C(38)	-125.5(7)
C(23)-Ru(2)-C(39)-C(40)	-89.2(6)
N(3)-Ru(2)-C(39)-C(40)	-166.7(5)
C(38)-Ru(2)-C(39)-C(40)	129.5(9)
C(41)-Ru(2)-C(39)-C(40)	29.6(6)
C(37)-Ru(2)-C(39)-C(40)	99.5(7)
C(36)-Ru(2)-C(39)-C(40)	65.8(6)
Cl(2)-Ru(2)-C(39)-C(40)	4.0(11)
C(23)-Ru(2)-C(39)-C(42)	24.3(10)
N(3)-Ru(2)-C(39)-C(42)	-53.2(10)
C(38)-Ru(2)-C(39)-C(42)	-117.0(12)
C(40)-Ru(2)-C(39)-C(42)	113.5(12)
C(41)-Ru(2)-C(39)-C(42)	143.1(10)
C(37)-Ru(2)-C(39)-C(42)	-147.0(10)
C(36)-Ru(2)-C(39)-C(42)	179.3(10)
Cl(2)-Ru(2)-C(39)-C(42)	117.5(9)
C(1)-C(2)-C(3)-C(4)	3.8(18)

C(23)-C(24)-C(25)-C(26)	-1.8(18)
C(29)-C(34)-C(33)-C(32)	-0.4(19)
C(38)-C(39)-C(42)-C(44)	-36.1(15)
C(40)-C(39)-C(42)-C(44)	144.0(11)
Ru(2)-C(39)-C(42)-C(44)	54.2(14)
C(38)-C(39)-C(42)-C(43)	86.2(12)
C(40)-C(39)-C(42)-C(43)	-93.7(11)
Ru(2)-C(39)-C(42)-C(43)	176.5(8)
C(1)-Ru(1)-C(15)-C(16)	-14.5(15)
N(1)-Ru(1)-C(15)-C(16)	74.9(7)
C(17)-Ru(1)-C(15)-C(16)	-31.9(6)
C(18)-Ru(1)-C(15)-C(16)	-70.1(7)
C(19)-Ru(1)-C(15)-C(16)	-106.9(7)
C(14)-Ru(1)-C(15)-C(16)	-135.6(10)
Cl(1)-Ru(1)-C(15)-C(16)	167.6(6)
C(1)-Ru(1)-C(15)-C(14)	121.1(12)
N(1)-Ru(1)-C(15)-C(14)	-149.5(6)
C(16)-Ru(1)-C(15)-C(14)	135.6(10)
C(17)-Ru(1)-C(15)-C(14)	103.7(7)
C(18)-Ru(1)-C(15)-C(14)	65.5(6)
C(19)-Ru(1)-C(15)-C(14)	28.7(6)
Cl(1)-Ru(1)-C(15)-C(14)	-56.8(6)
N(4)-C(28)-C(27)-C(26)	-179.0(11)
C(23)-C(28)-C(27)-C(26)	-0.6(18)
N(2)-N(1)-C(7)-C(8)	32.0(14)
Ru(1)-N(1)-C(7)-C(8)	-144.8(9)
N(2)-N(1)-C(7)-C(12)	-149.5(10)
Ru(1)-N(1)-C(7)-C(12)	33.7(13)
C(1)-C(6)-C(5)-C(4)	-2.1(18)
N(2)-C(6)-C(5)-C(4)	-179.7(11)

C(28)-C(27)-C(26)-C(25)	0.4(19)
C(24)-C(25)-C(26)-C(27)	1(2)
C(8)-C(7)-C(12)-C(11)	-0.2(17)
N(1)-C(7)-C(12)-C(11)	-178.7(10)
C(39)-C(40)-C(41)-C(36)	-4.7(14)
Ru(2)-C(40)-C(41)-C(36)	-59.3(8)
C(39)-C(40)-C(41)-Ru(2)	54.5(8)
C(37)-C(36)-C(41)-C(40)	4.1(14)
C(35)-C(36)-C(41)-C(40)	178.8(9)
Ru(2)-C(36)-C(41)-C(40)	56.8(8)
C(37)-C(36)-C(41)-Ru(2)	-52.7(9)
C(35)-C(36)-C(41)-Ru(2)	122.0(9)
C(23)-Ru(2)-C(41)-C(40)	53.7(7)
N(3)-Ru(2)-C(41)-C(40)	-125.7(13)
C(38)-Ru(2)-C(41)-C(40)	-67.5(6)
C(39)-Ru(2)-C(41)-C(40)	-29.6(6)
C(37)-Ru(2)-C(41)-C(40)	-104.3(7)
C(36)-Ru(2)-C(41)-C(40)	-131.4(9)
Cl(2)-Ru(2)-C(41)-C(40)	141.1(6)
C(23)-Ru(2)-C(41)-C(36)	-174.8(6)
N(3)-Ru(2)-C(41)-C(36)	5.7(17)
C(38)-Ru(2)-C(41)-C(36)	64.0(6)
C(39)-Ru(2)-C(41)-C(36)	101.8(7)
C(40)-Ru(2)-C(41)-C(36)	131.4(9)
C(37)-Ru(2)-C(41)-C(36)	27.2(6)
Cl(2)-Ru(2)-C(41)-C(36)	-87.5(6)
C(32)-C(31)-C(30)-C(29)	0(2)
C(34)-C(29)-C(30)-C(31)	-2.5(17)
N(3)-C(29)-C(30)-C(31)	177.2(10)
C(1)-Ru(1)-C(19)-C(14)	173.7(6)

N(1)-Ru(1)-C(19)-C(14)	-19(2)
C(16)-Ru(1)-C(19)-C(14)	-63.4(7)
C(17)-Ru(1)-C(19)-C(14)	-101.6(7)
C(18)-Ru(1)-C(19)-C(14)	-131.2(10)
C(15)-Ru(1)-C(19)-C(14)	-28.4(6)
Cl(1)-Ru(1)-C(19)-C(14)	82.8(6)
C(1)-Ru(1)-C(19)-C(18)	-55.1(7)
N(1)-Ru(1)-C(19)-C(18)	111.9(19)
C(16)-Ru(1)-C(19)-C(18)	67.8(7)
C(17)-Ru(1)-C(19)-C(18)	29.6(6)
C(15)-Ru(1)-C(19)-C(18)	102.7(7)
C(14)-Ru(1)-C(19)-C(18)	131.2(10)
Cl(1)-Ru(1)-C(19)-C(18)	-146.0(6)
C(41)-C(36)-C(37)-C(38)	1.7(14)
C(35)-C(36)-C(37)-C(38)	-173.1(9)
Ru(2)-C(36)-C(37)-C(38)	-48.8(8)
C(41)-C(36)-C(37)-Ru(2)	50.5(8)
C(35)-C(36)-C(37)-Ru(2)	-124.2(9)
C(39)-C(38)-C(37)-C(36)	-7.0(15)
Ru(2)-C(38)-C(37)-C(36)	52.5(9)
C(39)-C(38)-C(37)-Ru(2)	-59.5(8)
C(23)-Ru(2)-C(37)-C(36)	-130.3(11)
N(3)-Ru(2)-C(37)-C(36)	145.6(6)
C(38)-Ru(2)-C(37)-C(36)	-133.9(9)
C(39)-Ru(2)-C(37)-C(36)	-103.8(7)
C(40)-Ru(2)-C(37)-C(36)	-65.9(6)
C(41)-Ru(2)-C(37)-C(36)	-28.8(6)
Cl(2)-Ru(2)-C(37)-C(36)	52.4(7)
C(23)-Ru(2)-C(37)-C(38)	3.6(15)
N(3)-Ru(2)-C(37)-C(38)	-80.5(6)

C(39)-Ru(2)-C(37)-C(38)	30.1(6)
C(40)-Ru(2)-C(37)-C(38)	68.0(6)
C(41)-Ru(2)-C(37)-C(38)	105.1(7)
C(36)-Ru(2)-C(37)-C(38)	133.9(9)
Cl(2)-Ru(2)-C(37)-C(38)	-173.7(5)
C(18)-C(19)-C(14)-C(15)	-3.2(14)
Ru(1)-C(19)-C(14)-C(15)	53.6(8)
C(18)-C(19)-C(14)-C(13)	179.9(9)
Ru(1)-C(19)-C(14)-C(13)	-123.3(9)
C(18)-C(19)-C(14)-Ru(1)	-56.9(8)
C(16)-C(15)-C(14)-C(19)	-5.5(14)
Ru(1)-C(15)-C(14)-C(19)	-51.8(8)
C(16)-C(15)-C(14)-C(13)	171.3(9)
Ru(1)-C(15)-C(14)-C(13)	125.1(9)
C(16)-C(15)-C(14)-Ru(1)	46.3(8)
C(1)-Ru(1)-C(14)-C(19)	-11.6(11)
N(1)-Ru(1)-C(14)-C(19)	175.0(6)
C(16)-Ru(1)-C(14)-C(19)	105.3(7)
C(17)-Ru(1)-C(14)-C(19)	67.2(7)
C(18)-Ru(1)-C(14)-C(19)	29.8(6)
C(15)-Ru(1)-C(14)-C(19)	132.1(9)
Cl(1)-Ru(1)-C(14)-C(19)	-99.0(6)
C(1)-Ru(1)-C(14)-C(15)	-143.7(8)
N(1)-Ru(1)-C(14)-C(15)	42.8(8)
C(16)-Ru(1)-C(14)-C(15)	-26.9(6)
C(17)-Ru(1)-C(14)-C(15)	-64.9(6)
C(18)-Ru(1)-C(14)-C(15)	-102.4(7)
C(19)-Ru(1)-C(14)-C(15)	-132.1(9)
Cl(1)-Ru(1)-C(14)-C(15)	128.8(6)
C(1)-Ru(1)-C(14)-C(13)	99.9(14)

N(1)-Ru(1)-C(14)-C(13)	-73.5(14)
C(16)-Ru(1)-C(14)-C(13)	-143.2(15)
C(17)-Ru(1)-C(14)-C(13)	178.7(14)
C(18)-Ru(1)-C(14)-C(13)	141.3(14)
C(19)-Ru(1)-C(14)-C(13)	111.5(16)
C(15)-Ru(1)-C(14)-C(13)	-116.4(16)
Cl(1)-Ru(1)-C(14)-C(13)	12.5(13)
C(30)-C(31)-C(32)-C(33)	3(2)
C(34)-C(33)-C(32)-C(31)	-3(2)
C(14)-C(15)-C(16)-C(17)	12.1(15)
Ru(1)-C(15)-C(16)-C(17)	61.8(9)
C(14)-C(15)-C(16)-Ru(1)	-49.8(9)
C(18)-C(17)-C(16)-C(15)	-9.5(15)
C(20)-C(17)-C(16)-C(15)	171.2(10)
Ru(1)-C(17)-C(16)-C(15)	-65.2(9)
C(18)-C(17)-C(16)-Ru(1)	55.7(8)
C(20)-C(17)-C(16)-Ru(1)	-123.6(10)
C(1)-Ru(1)-C(16)-C(15)	174.1(6)
N(1)-Ru(1)-C(16)-C(15)	-111.0(7)
C(17)-Ru(1)-C(16)-C(15)	128.6(10)
C(18)-Ru(1)-C(16)-C(15)	98.2(7)
C(19)-Ru(1)-C(16)-C(15)	61.4(7)
C(14)-Ru(1)-C(16)-C(15)	26.4(6)
Cl(1)-Ru(1)-C(16)-C(15)	-21.0(10)
C(1)-Ru(1)-C(16)-C(17)	45.4(8)
N(1)-Ru(1)-C(16)-C(17)	120.4(6)
C(18)-Ru(1)-C(16)-C(17)	-30.4(6)
C(19)-Ru(1)-C(16)-C(17)	-67.3(7)
C(15)-Ru(1)-C(16)-C(17)	-128.6(10)
C(14)-Ru(1)-C(16)-C(17)	-102.2(7)

Cl(1)-Ru(1)-C(16)-C(17)	-149.6(5)
C(6)-C(5)-C(4)-C(3)	1.4(19)
C(2)-C(3)-C(4)-C(5)	-2.2(19)
C(14)-C(19)-C(18)-C(17)	5.7(14)
Ru(1)-C(19)-C(18)-C(17)	-53.6(8)
C(14)-C(19)-C(18)-Ru(1)	59.3(9)
C(16)-C(17)-C(18)-C(19)	0.5(14)
C(20)-C(17)-C(18)-C(19)	179.9(9)
Ru(1)-C(17)-C(18)-C(19)	54.7(8)
C(16)-C(17)-C(18)-Ru(1)	-54.1(8)
C(20)-C(17)-C(18)-Ru(1)	125.3(9)
C(1)-Ru(1)-C(18)-C(19)	132.1(7)
N(1)-Ru(1)-C(18)-C(19)	-161.5(7)
C(16)-Ru(1)-C(18)-C(19)	-100.9(7)
C(17)-Ru(1)-C(18)-C(19)	-131.8(9)
C(15)-Ru(1)-C(18)-C(19)	-64.3(7)
C(14)-Ru(1)-C(18)-C(19)	-28.9(6)
Cl(1)-Ru(1)-C(18)-C(19)	42.6(7)
C(1)-Ru(1)-C(18)-C(17)	-96.2(6)
N(1)-Ru(1)-C(18)-C(17)	-29.7(9)
C(16)-Ru(1)-C(18)-C(17)	30.8(6)
C(19)-Ru(1)-C(18)-C(17)	131.8(9)
C(15)-Ru(1)-C(18)-C(17)	67.5(6)
C(14)-Ru(1)-C(18)-C(17)	102.9(7)
Cl(1)-Ru(1)-C(18)-C(17)	174.4(5)
C(12)-C(7)-C(8)-C(9)	0.6(19)
N(1)-C(7)-C(8)-C(9)	179.1(11)
C(7)-C(12)-C(11)-C(10)	0.8(19)
C(7)-C(8)-C(9)-C(10)	-2(2)
C(12)-C(11)-C(10)-C(9)	-2(2)

C(8)-C(9)-C(10)-C(11)	2(3)

6.2 X-ray crystal structure and data for 3af

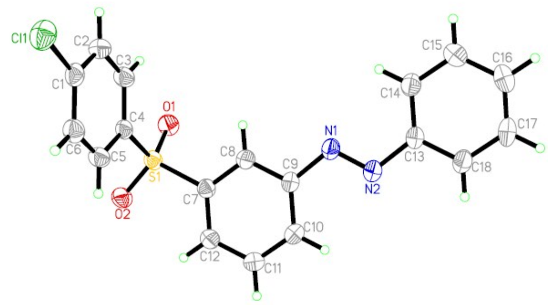


Table 1. Crystal data and structure refinement for **3af**.

Identification code	1501755
Empirical formula	C18 H13 Cl N2 O2 S
Formula weight	356.81
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 34.644(7) A alpha = 90 deg.
	b = 7.0976(14) A beta = 98.63(3) deg.
	c = 13.544(3) A gamma = 90 deg.
Volume	3292.7(11) A^3
Z, Calculated density	8, 1.440 Mg/m^3
Absorption coefficient	0.372 mm^-1
F(000)	1472
Crystal size	0.20 x 0.20 x 0.20 mm
Theta range for data collection	2.38 to 28.63 deg.
Limiting indices	-46<=h<=46, -9<=k<=9, -18<=l<=17
Reflections collected / unique	14452 / 4211 [R(int) = 0.0268]
Completeness to theta = 28.63	99.4 %
Absorption correction	None

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4211 / 0 / 217
Goodness-of-fit on F^2	1.002
Final R indices [I>2sigma(I)]	R1 = 0.0409, wR2 = 0.1337
R indices (all data)	R1 = 0.0632, wR2 = 0.1539
Largest diff. peak and hole	0.244 and -0.247 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3af**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
S(1)	1620(1)	102(1)	928(1)	48(1)
Cl(1)	2291(1)	-5543(1)	4271(1)	75(1)
N(1)	217(1)	-1732(2)	1206(1)	51(1)
C(9)	494(1)	-232(2)	1301(1)	45(1)
N(2)	-125(1)	-1203(2)	1260(1)	50(1)
O(1)	1569(1)	-905(2)	-1(1)	59(1)
C(4)	1822(1)	-1467(2)	1876(1)	44(1)
C(8)	868(1)	-717(3)	1144(1)	47(1)
C(13)	-407(1)	-2690(3)	1164(1)	47(1)
O(2)	1847(1)	1807(2)	1012(1)	60(1)
C(12)	1072(1)	2508(3)	1459(2)	54(1)
C(7)	1153(1)	666(3)	1216(1)	45(1)
C(1)	2126(1)	-3938(3)	3339(1)	51(1)
C(10)	411(1)	1616(3)	1543(2)	53(1)
C(11)	698(1)	2968(3)	1617(2)	57(1)
C(5)	1933(1)	-823(3)	2843(2)	54(1)
C(6)	2083(1)	-2069(3)	3578(2)	57(1)
C(18)	-784(1)	-2143(3)	1232(2)	58(1)
C(14)	-322(1)	-4560(3)	1001(2)	57(1)
C(2)	2028(1)	-4576(3)	2377(2)	58(1)
C(3)	1873(1)	-3340(3)	1640(2)	55(1)

C(15)	-617(1)	-5878(3)	906(2)	64(1)
C(17)	-1077(1)	-3470(4)	1138(2)	70(1)
C(16)	-996(1)	-5336(4)	977(2)	69(1)

Table 3. Bond lengths [A] and angles [deg] for **3af**.

S(1)-O(1)	1.4344(14)
S(1)-O(2)	1.4381(13)
S(1)-C(4)	1.7629(19)
S(1)-C(7)	1.7662(19)
Cl(1)-C(1)	1.733(2)
N(1)-N(2)	1.253(2)
N(1)-C(9)	1.428(2)
C(9)-C(8)	1.386(2)
C(9)-C(10)	1.392(3)
N(2)-C(13)	1.430(2)
C(4)-C(3)	1.384(3)
C(4)-C(5)	1.387(2)
C(8)-C(7)	1.386(2)
C(8)-H(8A)	0.9300
C(13)-C(18)	1.379(3)
C(13)-C(14)	1.384(3)
C(12)-C(11)	1.384(3)
C(12)-C(7)	1.387(2)
C(12)-H(12A)	0.9300
C(1)-C(2)	1.373(3)
C(1)-C(6)	1.378(3)
C(10)-C(11)	1.376(3)
C(10)-H(10A)	0.9300
C(11)-H(11A)	0.9300
C(5)-C(6)	1.374(3)

C(5)-H(5A)	0.9300
C(6)-H(6A)	0.9300
C(18)-C(17)	1.378(3)
C(18)-H(18A)	0.9300
C(14)-C(15)	1.376(3)
C(14)-H(14A)	0.9300
C(2)-C(3)	1.376(3)
C(2)-H(2A)	0.9300
C(3)-H(3A)	0.9300
C(15)-C(16)	1.387(3)
C(15)-H(15A)	0.9300
C(17)-C(16)	1.378(3)
C(17)-H(17A)	0.9300
C(16)-H(16A)	0.9300

O(1)-S(1)-O(2)	118.92(9)
O(1)-S(1)-C(4)	107.88(8)
O(2)-S(1)-C(4)	108.72(8)
O(1)-S(1)-C(7)	107.98(9)
O(2)-S(1)-C(7)	107.46(8)
C(4)-S(1)-C(7)	105.04(8)
N(2)-N(1)-C(9)	113.58(16)
C(8)-C(9)-C(10)	120.11(17)
C(8)-C(9)-N(1)	115.66(16)
C(10)-C(9)-N(1)	124.22(16)
N(1)-N(2)-C(13)	114.24(16)
C(3)-C(4)-C(5)	120.49(18)
C(3)-C(4)-S(1)	119.31(14)
C(5)-C(4)-S(1)	120.20(14)
C(7)-C(8)-C(9)	119.10(17)

C(7)-C(8)-H(8A)	120.5
C(9)-C(8)-H(8A)	120.5
C(18)-C(13)-C(14)	120.40(18)
C(18)-C(13)-N(2)	115.26(17)
C(14)-C(13)-N(2)	124.34(16)
C(11)-C(12)-C(7)	119.09(18)
C(11)-C(12)-H(12A)	120.5
C(7)-C(12)-H(12A)	120.5
C(8)-C(7)-C(12)	121.10(17)
C(8)-C(7)-S(1)	119.47(14)
C(12)-C(7)-S(1)	119.35(14)
C(2)-C(1)-C(6)	121.35(19)
C(2)-C(1)-Cl(1)	118.81(16)
C(6)-C(1)-Cl(1)	119.81(16)
C(11)-C(10)-C(9)	120.03(18)
C(11)-C(10)-H(10A)	120.0
C(9)-C(10)-H(10A)	120.0
C(10)-C(11)-C(12)	120.56(18)
C(10)-C(11)-H(11A)	119.7
C(12)-C(11)-H(11A)	119.7
C(6)-C(5)-C(4)	119.54(18)
C(6)-C(5)-H(5A)	120.2
C(4)-C(5)-H(5A)	120.2
C(5)-C(6)-C(1)	119.47(18)
C(5)-C(6)-H(6A)	120.3
C(1)-C(6)-H(6A)	120.3
C(17)-C(18)-C(13)	119.6(2)
C(17)-C(18)-H(18A)	120.2
C(13)-C(18)-H(18A)	120.2
C(15)-C(14)-C(13)	119.66(19)

C(15)-C(14)-H(14A)	120.2
C(13)-C(14)-H(14A)	120.2
C(1)-C(2)-C(3)	119.45(18)
C(1)-C(2)-H(2A)	120.3
C(3)-C(2)-H(2A)	120.3
C(2)-C(3)-C(4)	119.66(18)
C(2)-C(3)-H(3A)	120.2
C(4)-C(3)-H(3A)	120.2
C(14)-C(15)-C(16)	120.2(2)
C(14)-C(15)-H(15A)	119.9
C(16)-C(15)-H(15A)	119.9
C(16)-C(17)-C(18)	120.4(2)
C(16)-C(17)-H(17A)	119.8
C(18)-C(17)-H(17A)	119.8
C(17)-C(16)-C(15)	119.7(2)
C(17)-C(16)-H(16A)	120.1
C(15)-C(16)-H(16A)	120.1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **3af**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

Atom	U11	U22	U33	U23	U13	U12
S(1)	44(1)	51(1)	51(1)	-5(1)	14(1)	-6(1)
Cl(1)	67(1)	81(1)	77(1)	20(1)	10(1)	3(1)
N(1)	40(1)	55(1)	61(1)	1(1)	11(1)	1(1)
C(9)	39(1)	51(1)	45(1)	3(1)	6(1)	1(1)
N(2)	41(1)	57(1)	52(1)	1(1)	7(1)	2(1)
O(1)	61(1)	68(1)	50(1)	-9(1)	14(1)	-3(1)
C(4)	34(1)	49(1)	51(1)	-8(1)	11(1)	-5(1)
C(8)	45(1)	48(1)	50(1)	-1(1)	10(1)	0(1)
C(13)	39(1)	58(1)	45(1)	2(1)	5(1)	0(1)
O(2)	55(1)	52(1)	78(1)	-2(1)	22(1)	-12(1)

C(12)	51(1)	51(1)	61(1)	-6(1)	10(1)	-4(1)
C(7)	43(1)	49(1)	44(1)	-2(1)	7(1)	-2(1)
C(1)	35(1)	58(1)	60(1)	3(1)	12(1)	-3(1)
C(10)	47(1)	55(1)	59(1)	-2(1)	11(1)	7(1)
C(11)	57(1)	49(1)	66(1)	-9(1)	9(1)	4(1)
C(5)	54(1)	52(1)	57(1)	-13(1)	10(1)	-3(1)
C(6)	52(1)	68(1)	50(1)	-11(1)	7(1)	-2(1)
C(18)	44(1)	69(1)	62(1)	-2(1)	9(1)	4(1)
C(14)	47(1)	61(1)	62(1)	4(1)	10(1)	1(1)
C(2)	58(1)	49(1)	68(1)	-9(1)	10(1)	2(1)
C(3)	55(1)	55(1)	54(1)	-13(1)	8(1)	-4(1)
C(15)	68(1)	58(1)	66(1)	0(1)	8(1)	-9(1)
C(17)	38(1)	95(2)	77(2)	6(1)	9(1)	-3(1)
C(16)	57(1)	82(2)	68(2)	7(1)	4(1)	-19(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3af**.

Atom	x	y	z	U(eq)
H(8A)	926	-1953	993	57
H(12A)	1267	3421	1516	64
H(10A)	160	1936	1654	64
H(11A)	641	4202	1775	69
H(5A)	1906	444	2994	65
H(6A)	2154	-1656	4231	68
H(18A)	-840	-885	1342	70
H(14A)	-67	-4924	956	68
H(2A)	2066	-5834	2225	69
H(3A)	1803	-3760	988	65
H(15A)	-561	-7135	794	77
H(17A)	-1332	-3105	1182	84
H(16A)	-1195	-6228	916	83

Table 6. Torsion angles [deg] for **3af**.

N(2)-N(1)-C(9)-C(8)	-173.67(16)
N(2)-N(1)-C(9)-C(10)	6.9(3)
C(9)-N(1)-N(2)-C(13)	179.88(14)
O(1)-S(1)-C(4)-C(3)	-4.56(17)
O(2)-S(1)-C(4)-C(3)	-134.79(15)
C(7)-S(1)-C(4)-C(3)	110.43(15)
O(1)-S(1)-C(4)-C(5)	174.73(14)
O(2)-S(1)-C(4)-C(5)	44.50(16)
C(7)-S(1)-C(4)-C(5)	-70.28(16)
C(10)-C(9)-C(8)-C(7)	-1.0(3)
N(1)-C(9)-C(8)-C(7)	179.51(15)
N(1)-N(2)-C(13)-C(18)	179.34(17)
N(1)-N(2)-C(13)-C(14)	-1.5(3)
C(9)-C(8)-C(7)-C(12)	1.3(3)
C(9)-C(8)-C(7)-S(1)	-175.40(14)
C(11)-C(12)-C(7)-C(8)	-1.0(3)
C(11)-C(12)-C(7)-S(1)	175.62(15)
O(1)-S(1)-C(7)-C(8)	47.49(17)
O(2)-S(1)-C(7)-C(8)	176.91(14)
C(4)-S(1)-C(7)-C(8)	-67.43(16)
O(1)-S(1)-C(7)-C(12)	-129.22(16)
O(2)-S(1)-C(7)-C(12)	0.20(18)
C(4)-S(1)-C(7)-C(12)	115.86(16)
C(8)-C(9)-C(10)-C(11)	0.6(3)
N(1)-C(9)-C(10)-C(11)	-179.98(17)
C(9)-C(10)-C(11)-C(12)	-0.4(3)
C(7)-C(12)-C(11)-C(10)	0.6(3)
C(3)-C(4)-C(5)-C(6)	-2.0(3)
S(1)-C(4)-C(5)-C(6)	178.70(14)

C(4)-C(5)-C(6)-C(1)	0.9(3)
C(2)-C(1)-C(6)-C(5)	1.1(3)
Cl(1)-C(1)-C(6)-C(5)	-176.73(14)
C(14)-C(13)-C(18)-C(17)	0.0(3)
N(2)-C(13)-C(18)-C(17)	179.23(17)
C(18)-C(13)-C(14)-C(15)	0.0(3)
N(2)-C(13)-C(14)-C(15)	-179.09(18)
C(6)-C(1)-C(2)-C(3)	-1.9(3)
Cl(1)-C(1)-C(2)-C(3)	175.94(15)
C(1)-C(2)-C(3)-C(4)	0.7(3)
C(5)-C(4)-C(3)-C(2)	1.2(3)
S(1)-C(4)-C(3)-C(2)	-179.50(15)
C(13)-C(14)-C(15)-C(16)	-0.2(3)
C(13)-C(18)-C(17)-C(16)	0.1(3)
C(18)-C(17)-C(16)-C(15)	-0.3(4)
C(14)-C(15)-C(16)-C(17)	0.4(3)