Electronic Supplementary Material (ESI) for RSC Advances.

Electronic effect Study and Quantitative Spectra Predictions of o-Methoxyaniline-terminated Monoazonaphthols: A Combined Experimental and DFT Study

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Contents

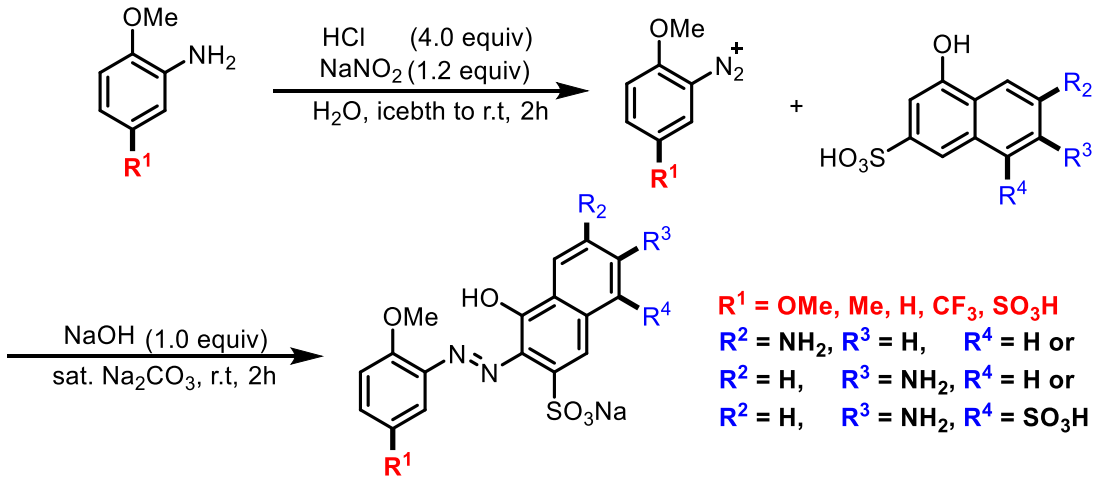
Experimental information and characterization data

Instruments and reagents

NMR spectra were recorded on Brucker 500 NMR (^{1}H 500 MHz; ^{13}C 125 MHz) in DMSO-d6. Abbreviations for data quoted are s, singlet; brs, broad singlet; d, doublet; t, triplet; dd, doublet of doublets; m, multiplet. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale (DMSO-d6: δH = 2.50 ppm, δC = 39.52 ppm). Mass spectra were measured on an Agilent TOF-G6230B mass spectrometer. UV-Vis spectra were collected on a Shimadzu UV-Vis spectrometer at the concentration of 25ppm using water as solvent.

All the reagents were purchased from Meryer Biochemical Co. Ltd., which were applied in the synthesis procedure without further purification. Deionized water was used as solvent in the synthesis and UV-Vis spectra collecting.

General procedure for the compound synthesis

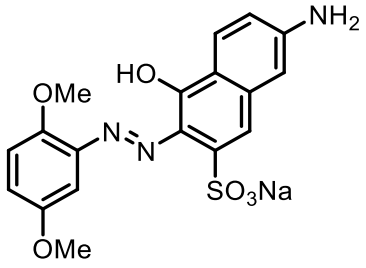


Scheme S1. Synthetic route of the azo compounds.

All the compounds were prepared in the same protocol taking different substrates. Taking the synthesis of **1a** for example, 1.53g of 2,5-dimethoxyaniline (10mmol) was blended with 40 mL water and 4 mL conc (40mmol, 4equiv). hydrochloric acid. The resulting solution was cooled to 0–5 °C and was added to a solution of 0.826 g sodium nitrite (12mmol, 1.2equiv) in 20 mL water over a period of 30 min. The resulting mixture was stirred at 0–5 °C for 30 min. 10 mmol of J acid and 10 mmol of sodium hydroxide was dissolved in 50mL saturated sodium carbonate solution, and the diazonium solution was then added in over a period of 10 min. After the resulting mixture was stirred for 2 h, 20g of sodium chloride was added in and stirred for 60min to salt out the coupled product. And the compound was separated out by centrifugal using a centrifuge at the rotating speed of 8000rpm.

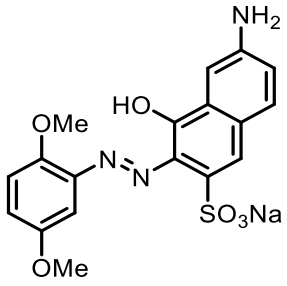
Characterization of the dyes

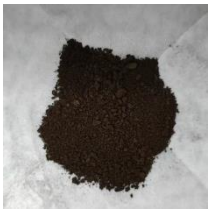
Sodium 7-amino-3-((2,5-dimethoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (1a)



Yield: 92%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.8 (s, 1H), 7.9 (d, J = 8.6 Hz, 1H), 7.6 (d, J = 3.1 Hz, 1H), 7.2 (s, 1H), 7.0 (d, J = 9.0 Hz, 1H), 6.7 (ddd, J = 8.3, 5.5, 2.6 Hz, 2H), 6.6 (s, 1H), 6.4 (s, 2H), 3.9 (s, 3H), 3.7 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.6, 154.7, 142.5, 138.5, 132.8, 129.8, 129.7, 121.9, 120.3, 114.6, 113.0, 110.7, 109.6, 102.8, 56.9, 55.9. **MS:** Calculated for **$C_{18}H_{16}N_3NaO_6S$**: 425.39, Found 401.9 [M-Na]$^-$.

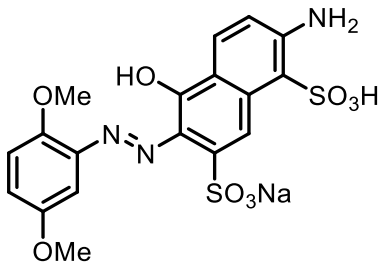
Sodium 6-amino-3-((2,5-dimethoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (1b)

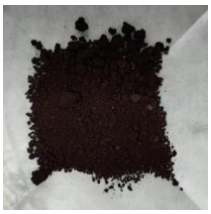




Yield: 95%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.9 (s, 1H), 7.6 (d, J = 3.1 Hz, 1H), 7.4 – 7.4 (m, 2H), 7.4 (s, 1H), 7.1 (d, J = 8.9 Hz, 1H), 7.0 (dd, J = 8.3, 2.5 Hz, 1H), 6.8 (dd, J = 8.9, 3.1 Hz, 1H), 5.7 (brs, 2H), 3.9 (s, 3H), 3.8 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 178.2, 154.7, 149.2, 143.0, 132.5, 132.4, 130.5, 130.1, 125.4, 122.1, 120.9, 113.1, 110.7, 109.8, 103.2, 57.0, 56.0. **MS:** Calculated for **$C_{18}H_{16}N_3NaO_6S$**: 425.39, Found 401.9 [M-Na]$^-$.

Sodium 7-amino-3-((2,5-dimethoxyphenyl)diazenyl)-4-hydroxy-8-sulfonaphthalene-2-sulfonate (1c)

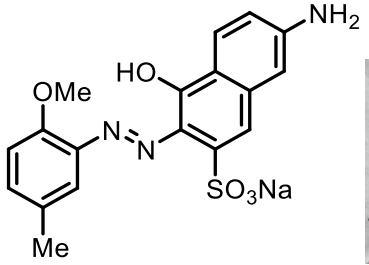




Yield: 80%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.9 (s, 1H), 8.7 (s, 1H), 7.9 (d, J = 8.8 Hz, 1H), 7.6 (d, J = 3.1 Hz, 1H), 7.3 (brs, 2H), 7.1 (d, J = 8.9 Hz, 1H), 6.8 – 6.5 (m, 2H), 3.9 (s, 3H), 3.8 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 176.9, 154.7, 150.8, 142.7, 142.5, 136.7, 132.9, 129.1, 128.8, 124.8, 122.0, 121.0, 117.2, 113.0, 109.8, 102.9, 56.9, 55.9. **MS:** Calculated for

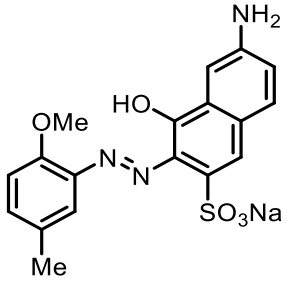
$C_{18}H_{16}N_3NaO_9S_2$: 505.45, Found 481.9 [M-Na]$^-$.

Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-methylphenyl)diazenyl)naphthalene-2-sulfonate (2a)



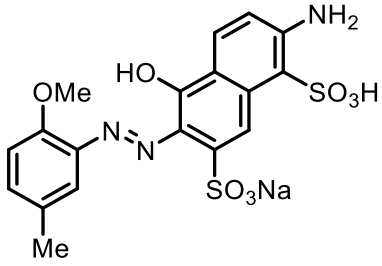
Yield: 93%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 16.1 (s, 1H), 7.9 (d, J = 8.6 Hz, 1H), 7.7 (d, J = 2.1 Hz, 1H), 7.2 (s, 1H), 7.0 (d, J = 8.3 Hz, 1H), 7.0 – 6.9 (m, 1H), 6.7 (dd, J = 8.7, 2.2 Hz, 1H), 6.6 (d, J = 2.2 Hz, 1H), 6.3 (s, 2H), 3.9 (s, 3H), 2.3 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.4, 154.5, 146.4, 144.1, 138.4, 131.6, 130.7, 129.7, 129.6, 126.0, 121.5, 120.4, 116.5, 114.7, 111.9, 110.6, 56.5, 21.2. **MS:** Calculated for **$C_{18}H_{16}N_3NaO_5S$**: 409.39, Found 386.9 [M-Na]$^-$.

Sodium 6-amino-4-hydroxy-3-((2-methoxy-5-methylphenyl)diazenyl)naphthalene-2-sulfonate (2b)



Yield: 98%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 7.8 (d, J = 2.2 Hz, 1H), 7.4 (d, J = 2.4 Hz, 1H), 7.4 (d, J = 8.4 Hz, 1H), 7.4 (s, 1H), 7.1 (d, J = 8.4 Hz, 1H), 7.0 (dd, J = 8.4, 2.1 Hz, 1H), 7.0 (dd, J = 8.3, 2.5 Hz, 1H), 5.7 (s, 2H), 4.0 (s, 3H), 2.3 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.6, 149.1, 146.9, 138.1, 132.5, 131.4, 130.8, 130.4, 130.1, 127.1, 125.3, 121.8, 120.9, 116.9, 112.1, 109.6, 56.7, 21.17. **MS:** Calculated for **$C_{18}H_{16}N_3NaO_5S$**: 409.39, Found 386.9 [M-Na]$^-$.

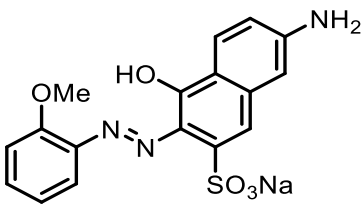
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-methylphenyl)diazenyl)-8-sulfon aphthalene-2-sulfonate (2c)

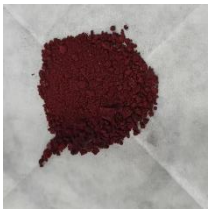


Yield: 85%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 8.7 (s, 1H), 7.9 (d, J = 8.8 Hz, 1H), 7.8 (d, J = 2.1 Hz, 1H), 7.3 (s, 1H), 7.0 (d, J = 8.3 Hz, 1H), 7.0 – 6.9 (m, 1H), 6.8 (d, J = 8.9 Hz, 1H), 3.9 (s, 1H), 2.3 (s, 1H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 176.5, 150.7, 146.5, 142.3, 136.5, 131.7, 130.7,

129.0, 128.7, 126.2, 124.6, 121.7, 121.1, 117.3, 116.6, 112.0, 56.6, 21.20. **MS:** Calculated for **$C_{18}H_{16}N_3NaO_8S_2$**: 489.45, Found 487.9 $[M-H]^-$, 465.9 $[M-Na]^-$.

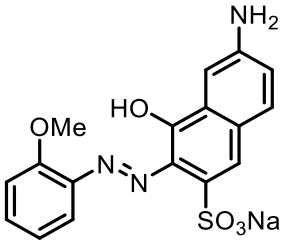
Sodium 7-amino-4-hydroxy-3-((2-methoxyphenyl)diazenyl)naphthalene-2-sulfonate (3a)

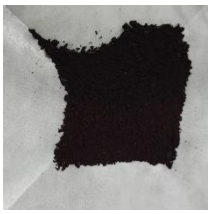




Yield: 91%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 16.0 (s, 1H), 7.9 (dd, J = 8.3, 2.9 Hz, 2H), 7.2 (s, 1H), 7.1 (d, J = 4.0 Hz, 2H), 7.0 (dd, J = 8.1, 4.1 Hz, 1H), 6.7 (dd, J = 8.7, 2.2 Hz, 1H), 6.7 (d, J = 2.2 Hz, 1H), 6.4 (s, 2H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.5, 154.7, 148.2, 144.0, 143.9, 138.4, 132.0, 129.7, 129.6, 125.5, 121.8, 121.8, 120.3, 116.2, 114.7, 112.0, 110.7, 56.5. **MS:** Calculated for **$C_{17}H_{14}N_3NaO_5S$**: 395.36, Found 371.9 $[M-Na]^-$.

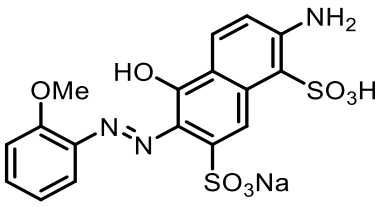
Sodium 6-amino-4-hydroxy-3-((2-methoxyphenyl)diazenyl)naphthalene-2-sulfonate (3b)





Yield: 93%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 16.2 (s, 1H), 8.0 (dd, J = 7.9, 1.5 Hz, 1H), 7.5 – 7.3 (m, 3H), 7.2 – 7.2 (m, 2H), 7.1 – 7.0 (m, 1H), 7.0 (dd, J = 8.3, 2.5 Hz, 1H), 5.7 (s, 2H), 4.0 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d6) δ 177.9, 149.1, 148.7, 138.2, 138.2, 132.4, 131.8, 130.4, 130.1, 126.6, 125.4, 122.0, 121.9, 120.9, 116.7, 112.2, 109.7, 56.6. **MS:** Calculated for **$C_{17}H_{14}N_3NaO_5S$**: 395.36, Found 371.9 $[M-Na]^-$

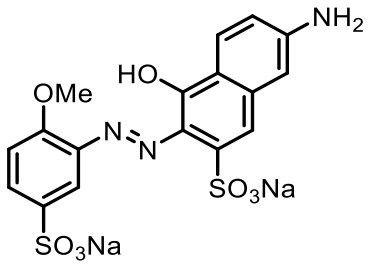
Sodium 7-amino-4-hydroxy-3-((2-methoxyphenyl)diazenyl)-8-sulfonaphthalene-2-sulfonate (3c)

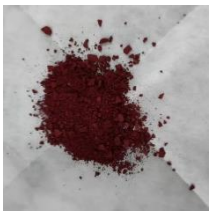


Yield: 78%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 16.2 (s, 1H), 8.7 (s, 1H), 8.0 (t, J = 9.2 Hz, 2H), 7.4 – 7.3 (brs, 2H), 7.2 (d, J = 5.8 Hz, 2H), 7.1 – 7.0 (m, 1H), 6.8 (d, J = 8.8 Hz, 1H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 176.7, 150.8, 148.4, 142.3, 136.6, 132.1, 129.0, 128.7, 125.8, 124.6, 121.9, 121.8, 121.1, 117.3, 116.4, 112.0, 56.5. **MS:** Calculated for **$C_{17}H_{14}N_3NaO_8S_2$**: 475.42, Found 473.8 $[M-H]^-$, 451.9 $[M-Na]^-$.

Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)naphthalene

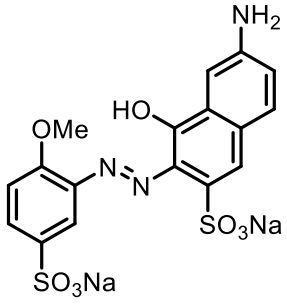
-2-sulfonate (4a)

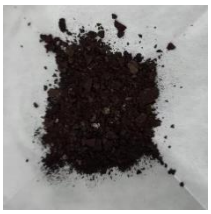




Yield: 85%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 16.1 (s, 1H), 8.2 (d, J = 2.2 Hz, 1H), 8.0 (d, J = 8.6 Hz, 1H), 7.4 (dd, J = 8.5, 2.2 Hz, 1H), 7.3 (s, 1H), 7.1 (d, J = 8.5 Hz, 1H), 6.7 (dd, J = 8.6, 2.2 Hz, 1H), 6.7 (d, J = 2.2 Hz, 1H), 6.4 (s, 2H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.5, 154.8, 148.4, 143.4, 141.8, 138.2, 131.1, 129.8, 129.8, 123.0, 122.3, 120.3, 114.7, 113.8, 111.0, 110.8, 56.8. **MS:** Calculated for **$C_{17}H_{13}N_3Na_2O_8S_2$**: 497.40, Found 451.9 $[M-2Na+H]^-$.

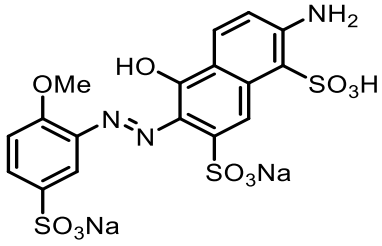
Sodium 6-amino-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)naphthalene -2-sulfonate (4b)

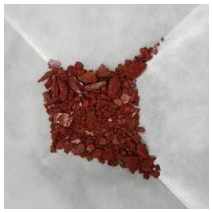




Yield: 88%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 8.2 (d, J = 2.2 Hz, 1H), 7.5 (dd, J = 8.5, 2.2 Hz, 1H), 7.43-7.4 (m, 3H), 7.1 (d, J = 8.5 Hz, 1H), 7.0 (dd, J = 8.3, 2.4 Hz, 1H), 5.8 (s, 2H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.8, 149.3, 148.9, 141.9, 137.5, 132.5, 130.9, 130.5, 130.3, 125.1, 124.0, 122.5, 121.0, 114.2, 111.2, 109.7, 56.9. **MS:** Calculated for **$C_{17}H_{13}N_3Na_2O_8S_2$**: 497.40, Found 451.9 $[M-2Na+H]^-$.

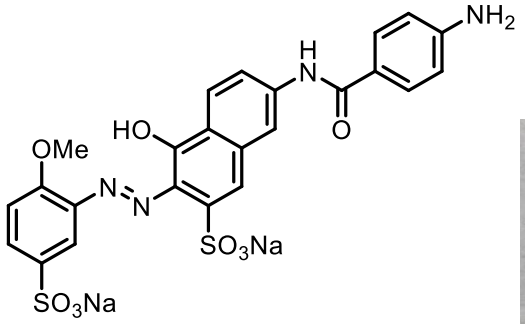
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)-8-sulfon aphthalene-2-sulfonate (4c)





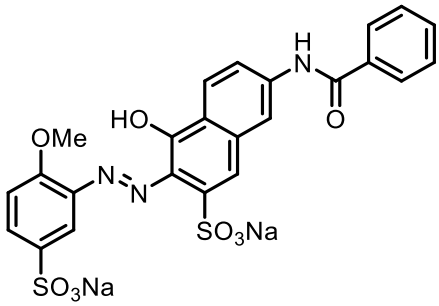
Yield: 70%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 8.8 (s, 1H), 8.2 (s, 1H), 8.0 (d, J = 8.8 Hz, 1H), 7.4 (d, J = 8.4 Hz, 1H), 7.3 (brs, 2H), 7.1 (d, J = 8.5 Hz, 1H), 6.8 (d, J = 8.9 Hz, 1H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 176.6, 150.9, 148.6, 141.7, 141.7, 136.4, 131.1, 129.2, 128.9, 124.5, 123.2, 122.4, 121.1, 117.5, 114.0, 111.1, 56.8. **MS:** Calculated for **$C_{17}H_{13}N_3Na_2O_{11}S_3$**: 577.46, Found 575.8 $[M-H]^-$, 553.8 $[M-Na]^-$.

Sodium 7-(4-aminobenzamido)-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl) diazenyl) naphthalene-2-sulfonate (4d)



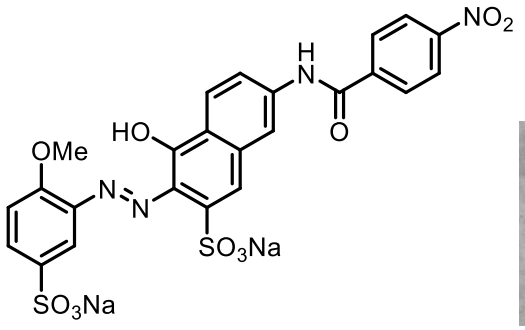
Yield: 75%, ^{1}H NMR (500 MHz, DMSO-d6) δ 10.4 (s, 1H), 8.3 (d, J = 8.7 Hz, 1H), 8.2 (d, J = 2.1 Hz, 1H), 8.1 (d, J = 2.1 Hz, 1H), 8.0 (dd, J = 8.8, 2.0 Hz, 1H), 7.9 – 7.8 (m, 2H), 7.5 (dd, J = 8.5, 2.2 Hz, 1H), 7.5 (s, 1H), 7.2 (d, J = 8.6 Hz, 1H), 6.9 (d, J = 8.1 Hz, 2H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.0, 166.0, 149.1, 144.7, 143.8, 142.1, 136.8, 130.7, 130.1, 129.9, 128.3, 126.4, 124.5, 121.3, 119.8, 118.4, 116.1, 114.2, 111.2, 56.9, 40.5, 40.3, 40.1, 40.0, 39.8, 39.6, 39.5. **MS:** Calculated for **$C_{24}H_{18}N_4Na_2O_9S_2$**: 616.53, Found 592.9 [M-Na]$^-$.

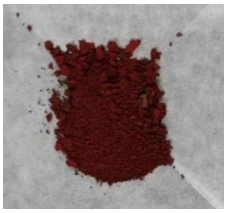
Sodium 7-benzamido-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl) naphthalene-2-sulfonate (4e)



Yield: 86%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 10.7 (s, 1H), 8.3 (d, J = 8.7 Hz, 1H), 8.2 (s, 1H), 8.2 (d, J = 2.0 Hz, 1H), 8.0 – 8.0 (m, 2H), 8.0 (dd, J = 8.7, 2.0 Hz, 1H), 7.6 (t, J = 7.3 Hz, 1H), 7.6 (t, J = 7.5 Hz, 2H), 7.5 – 7.5 (m, 2H), 7.2 (d, J = 8.5 Hz, 1H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 176.8, 166.7, 149.2, 144.2, 144.0, 142.2, 136.8, 135.1, 132.4, 130.6, 129.9, 129.0, 128.4, 128.4, 126.8, 124.6, 121.1, 120.0, 118.7, 114.3, 111.2, 57.0, 40.5, 40.3, 40.1, 40.0, 39.8, 39.6, 40.0. **MS:** Calculated for **$C_{24}H_{17}N_3NaO_9S_2$**: 601.51, Found 577.9 [M-Na]$^-$.

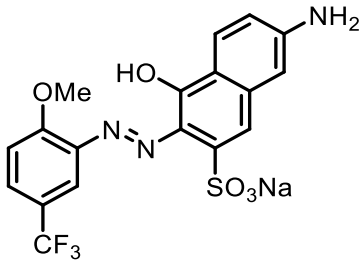
Sodium 4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)-7-(4-nitrobenzamido) naphthalene-2-sulfonate (4f)

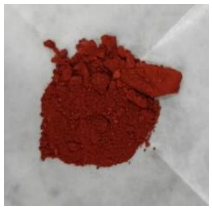




Yield: 90%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 10.4 (s, 1H), 8.3 (d, J = 8.7 Hz, 1H), 8.2 (d, J = 2.1 Hz, 1H), 8.1 (d, J = 2.1 Hz, 1H), 8.0 (dd, J = 8.8, 2.0 Hz, 1H), 7.9 – 7.8 (m, 2H), 7.5 (dd, J = 8.5, 2.2 Hz, 1H), 7.5 (s, 1H), 7.2 (d, J = 8.6 Hz, 1H), 6.9 (d, J = 8.1 Hz, 1H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.0, 166.0, 149.1, 144.7, 143.8, 142.1, 136.8, 130.7, 130.1, 129.9, 128.3, 126.4, 124.5, 121.3, 119.8, 118.4, 116.1, 114.2, 111.2, 56.9, 40.5, 40.3, 40.14 40.0, 39.8, 39.6, 39.5. **MS:** Calculated for **$C_{24}H_{17}N_3NaO_9S_2$**: 601.51, Found 600.9 [M-H]$^-$.

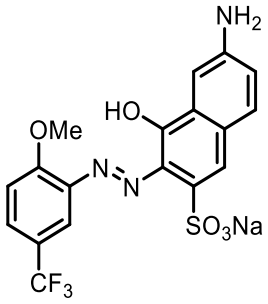
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-(trifluoromethyl)phenyl)diazenyl) naphthalene-2-sulfonate (5a)





Yield: 94%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.8 (s, 1H), 8.2 (d, J = 2.3 Hz, 1H), 7.9 (d, J = 8.6 Hz, 1H), 7.5 (dd, J = 8.7, 2.3 Hz, 1H), 7.3 (d, J = 8.6 Hz, 1H), 7.3 (s, 1H), 6.7 (dd, J = 8.6, 2.2 Hz, 1H), 6.7 (d, J = 2.2 Hz, 1H), 6.5 (s, 2H), 4.1 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 178.2, 155.2, 150.4, 143.9, 138.5, 132.7, 130.5, 130.1, 122.9, 122.5, 120.0, 114.7, 112.4, 111.0, 57.1. **MS:** Calculated for **$C_{18}H_{13}F_3N_3NaO_5S$**: 463.36, Found 439.9 [M-Na]$^-$.

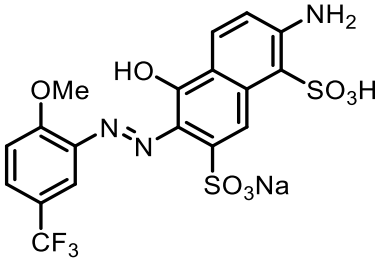
Sodium 6-amino-4-hydroxy-3-((2-methoxy-5-(trifluoromethyl)phenyl)diazenyl) naphthalene-2-sulfonate (5b)



Yield: 99%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.9 (s, 1H), 8.3 (d, J = 2.3 Hz, 1H), 7.5 (dd, J = 8.6, 2.3 Hz, 1H), 7.4 – 7.3 (m, 4H), 7.0 (dd, J = 8.3, 2.5 Hz, 1H), 5.8 (s, 2H), 4.1 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 179.3, 150.8, 149.34, 138.1, 132.4, 132.2, 130.8, 130.6, 125.3, 123.1, 122.6, 121.1, 113.0, 112.6, 110.1, 57.2. **MS:** Calculated for **$C_{18}H_{13}F_3N_3NaO_5S$**: 463.36, Found

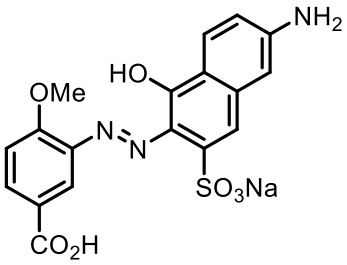
439.9 [M-Na]$^-$.

Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-(trifluoromethyl)phenyl)diazenyl)-8-sulfonaphthalene-2-sulfonate (5c)



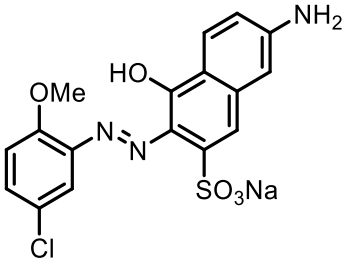
Yield: 86%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.9 (s, 1H), 8.8 (s, 1H), 8.2 (d, J = 2.3 Hz, 1H), 7.9 (d, J = 8.8 Hz, 1H), 7.5 (dd, J = 8.5, 2.3 Hz, 1H), 7.3 (d, J = 8.6 Hz, 1H), 6.8 (d, J = 8.8 Hz, 1H), 4.1 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.5, 151.3, 150.5, 142.2, 136.7, 132.7, 129.8, 129.0, 126.0, 125.0, 123.8, 123.0, 122.8, 122.5, 121.9, 120.7, 117.3, 112.6, 112.4, 57.1, 40.1. **MS:** Calculated for **$C_{18}H_{13}F_3N_3NaO_8S_2$**: 543.42, Found 519.8 [M-Na]$^-$.

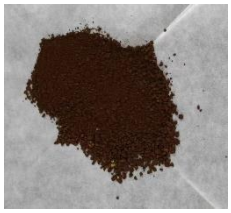
Sodium 7-amino-3-((5-carboxy-2-methoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (6a)



Yield: 87%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 8.5 (d, J = 2.1 Hz, 1H), 8.0 (d, J = 8.8 Hz, 1H), 7.8 (dd, J = 8.6, 2.1 Hz, 1H), 7.3 (s, 1H), 7.2 (d, J = 8.6 Hz, 1H), 6.8 (d, J = 6.9 Hz, 2H), 4.1 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.6, 167.4, 152.7, 151.6, 143.9, 138.2, 131.8, 130.2, 129.8, 127.3, 124.6, 122.1, 121.4, 117.1, 115.7, 112.3, 111.7, 57.0. **MS:** Calculated for **$C_{18}H_{14}N_3NaO_7S$**: 439.37, Found 415.9 [M-Na]$^-$.

Sodium 7-amino-3-((5-chloro-2-methoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (7a)

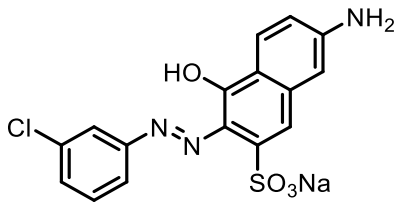


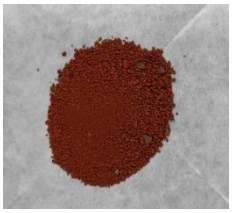


Yield: 86%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.8 (s, 1H), 8.0 (d, J = 8.4 Hz, 1H), 7.9 (d, J = 2.0 Hz, 1H), 7.3 (s, 1H), 7.2 (d, J = 2.4 Hz, 2H), 6.7 (s, 2H), 4.0 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 178.0, 172.5, 154.2, 146.9, 144.0, 138.4, 133.3, 130.3, 130.0, 126.1, 124.3, 122.6,

120.5, 115.3, 115.0, 113.6, 111.4, 60.2. **MS:** Calculated for **$C_{17}H_{13}ClN_3NaO_5S$**: 429.81, Found 405.9 $[M-Na]^-$.

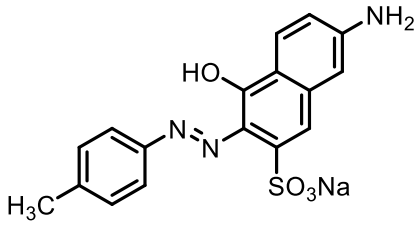
Sodium 7-amino-3-((3-chlorophenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (8a)

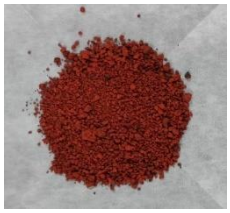




Yield: 80%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 15.7 (s, 1H), 7.9 (d, J = 7.8 Hz, 1H), 7.8 (s, 1H), 7.6 (d, J = 7.1 Hz, 1H), 7.4 (t, J = 7.6 Hz, 1H), 7.3 (s, 1H), 7.2 (d, J = 7.0 Hz, 1H), 6.8 (s, 1H), 6.7 (s, 1H). **^{13}C NMR (125 MHz, DMSO-d6)** δ 177.7, 153.5, 144.9, 138.4, 134.5, 131.4, 129.9, 129.5, 124.5, 122.6, 120.8, 116.3, 115.8, 115.4, 112.1. **MS:** Calculated for **$C_{16}H_{11}ClN_3NaO_4S$**: 399.78, Found 375.9 $[M-Na]^-$.

Sodium 7-amino-4-hydroxy-3-(p-tolyldiazenyl)naphthalene-2-sulfonate (9a)





Yield: 80%, **^{1}H NMR (500 MHz, DMSO-d6)** δ 8.0 (d, J = 8.5 Hz, 1H), 7.6 (d, J = 8.0 Hz, 2H), 7.3 (s, 1H), 7.2 (d, J = 8.0 Hz, 2H), 7.0 – 6.6 (m, 2H), 2.3 (s, 3H). **^{13}C NMR (125 MHz, DMSO-d6)** δ. 176.0, 144.2, 141.2, 138.1, 135.2, 130.4, 129.3, 128.5, 121.9, 120.9, 117.4, 116.2, 112.8, 21.2. **MS:** Calculated for **$C_{17}H_{14}N_3NaO_4S$**: 379.37, Found 355.9 $[M-Na]^-$.

Experimental UV-Vis spectra of the compounds

Qualitative UV-Vis Spectra

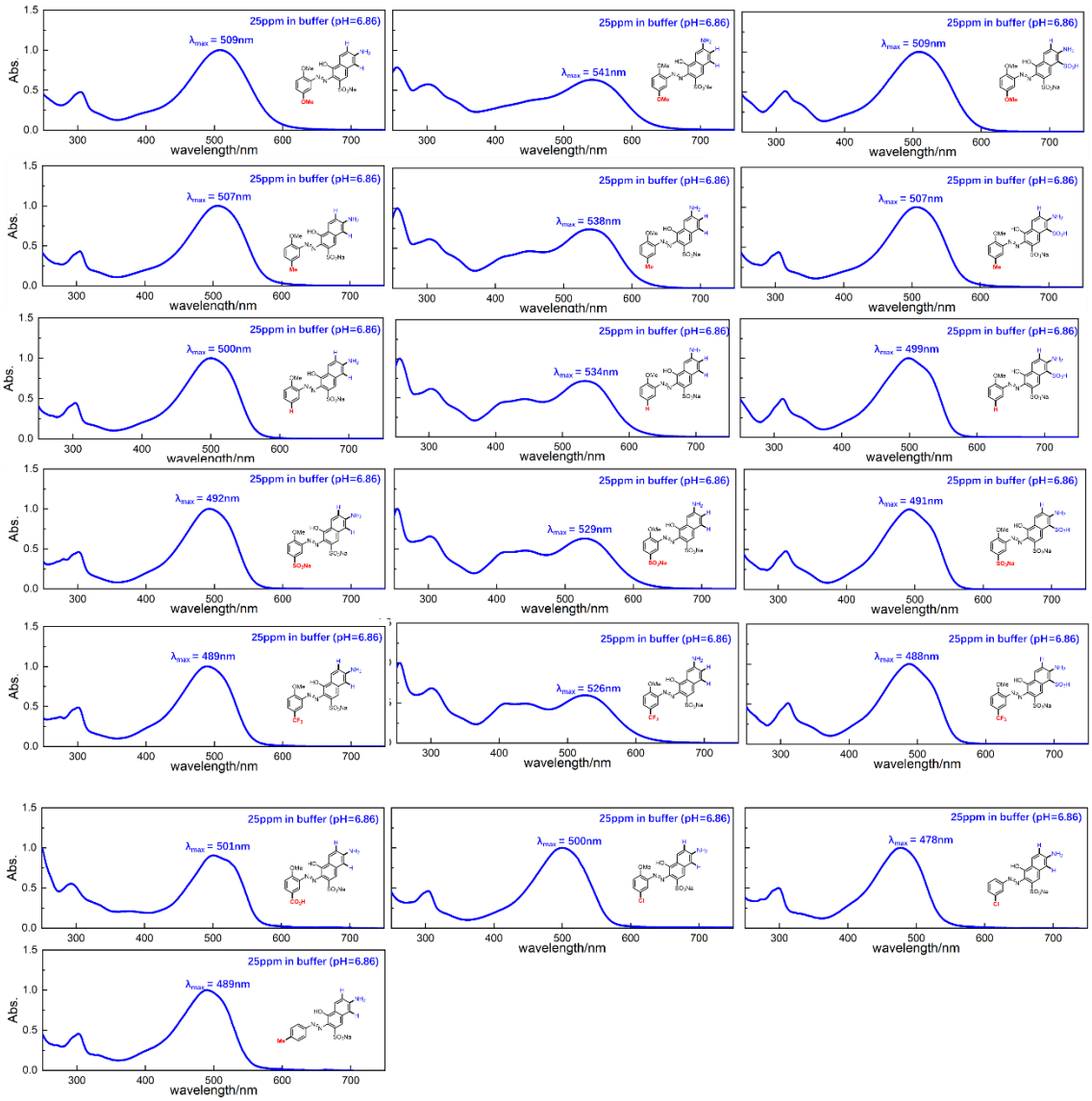


Figure S1. Normalized UV-Vis spectra of **1a-5c and 6a-9a.**

Quantitative UV-Vis Spectra

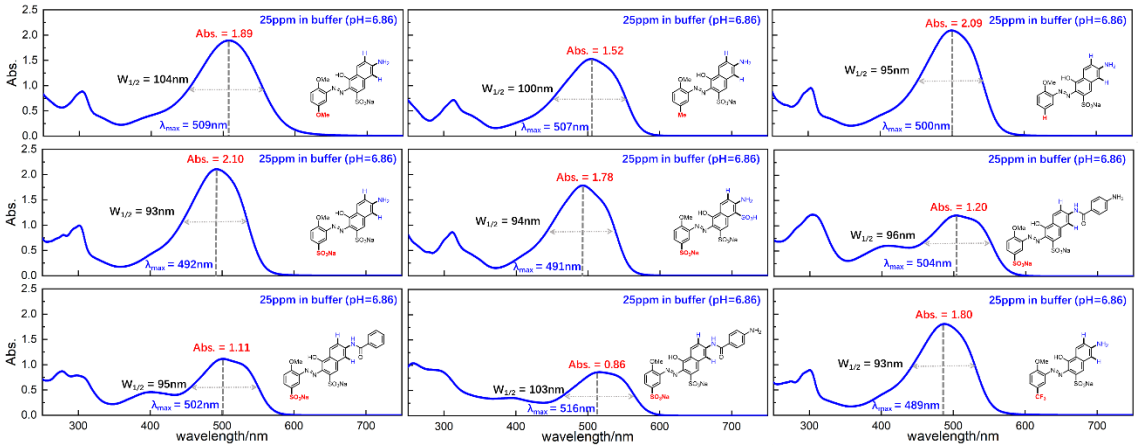


Figure S2. Quantitative UV-Vis spectra of the selected azo compounds.

Parameterization of the electronic effects

Determinations of the experimental chemical shifts of 1a-5a

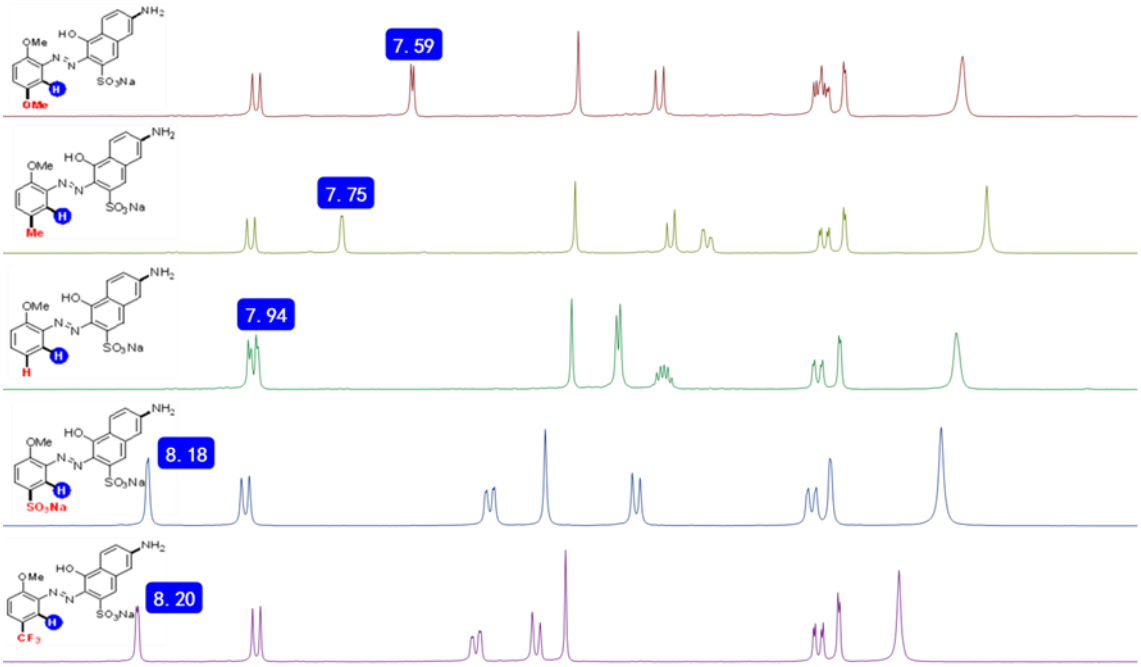


Figure S3. Stacked NMR spectra of **1a-5a.**

As we known, the NMR shifts had been widely applied in characterizing functional group electronegativity that EWG shifted the signals to high field while EDG shifted the signals to low field. As shown in Figure S3, chemical shifts of the hydrogen located between the azo functional groups and the substituents were the most charactermatic ones in the benzene rings, which were **7.59**, **7.75**, **7.94**, **8.18** and **8.20** for **1a-5a**, respectively. As a result, those chemical shifts were applied to parameterize the electron densities of aromatic rings and to draw Figure 5 directly.

Theoretical chemical shifts of 1a-5a

Theoretical NMR were calculated by Oliveira's method as described in the part of DFT calculation, and the calculated chemical shifts of the hydrogens were **6.56, 6.82, 7.01, 7.37** and **7.99** for **1a-5a**, respectively. And the calculated chemical shifts were applied for drawing **Figure 5** in the manuscript directly.

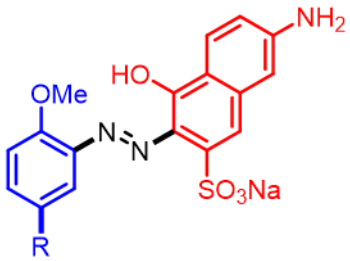
Hammett constants of 1a-5a

According to the paper reported by Taft, Hammett constants of methoxyl, methyl, hydrogen, sulfonic acid and trifluoromethyl were **0.12**, **-0.07**, **0**, **0.30** and **0.43**, respectively. And these values were applied for drawing Figure 5 directly.

Fragmented charge population of 1a-5a

The compounds were divided into three pieces as shown in Scheme S2. Charge populations

of the atoms were calculated by Multiwfn using the wavefunctions of the optimized structures. ome well-defined charge population methods including Mulliken[1-3], Hirshfeld[4], Lowdin[5], atomic dipole corrected Hirshfeld atomic charge (ADCH)[6] and CM5 atomic charge[7], were applied to measure the atomic charge population. Fragmented charge populations were calculated by adding the values of atoms which constituting in the fragments. The results were summarized in Table S1, and these values were applied for drawing Figure S4 directly.



R = OMe (1a), Me (2a), H (3a), SO_3H (4a), CF_3 (5a)
Fragment colored in black was named as Azo
Fragment colored in red was named as Naph
Fragment colored in blue was named as Ph

Scheme S2. Fragments definitions of the compounds.

Table S1. Fragmented charge populations of the Ph among 1a-5a

Compound	ADCH	CM5	Hirshfeld	Lowdin	Mulliken
1a	0.1976	0.2106	0.1727	0.1885	0.1376
2a	0.2148	0.2265	0.1862	0.1990	0.1497
3a	0.2056	0.2171	0.1729	0.1842	0.1443
4a	0.1927	0.1950	0.1726	0.2301	0.1468
5a	-0.0769	0.0532	-0.0694	-0.1147	-0.0269

Clearly, CM5 charge populations owned the best linearity to Hammett constants (R^2=0.984), hence, fragmented charge populations calculated by CM5 were applied for the discussion of electronic effect parameterization.

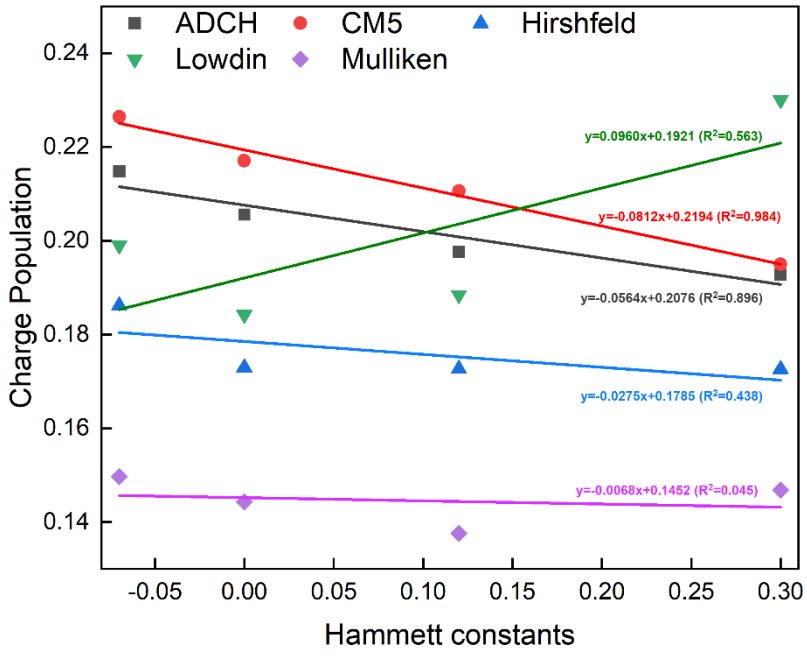


Figure S4. Linear fitting for the fragmented charge populations and Hammett constants.

Details of DFT calculation

Structure optimizations and involved software

Structures were constructed by the Open Babel Program, which were performed preoptimization tasks by using the built-in MM94 force field. DFT and TD-DFT calculations were carried out by ORCA5 computational suite, and the resolution of identity (RI) approximation and tight SCF criteria were employed in the calculation. The preoptimized structures were further optimized by the B3LYP functional, using the Ahlrichs double-zeta basis set def2-SVP (standard) and def2-SVP/J (auxiliary), combining D3 version of Grimme's dispersion. CPCM model were applied to reproduce the solvent environment. Frequency analysis was performed after optimization at the same level and no virtual frequency was found, which ensured the optimization of the structures to a minimum point.

The keywords of the mentioned optimization task were listed as follow:

! B3LYP D3 def2-SVP def2/J CPCM(water) RIJCOSX OPT FREQ TightSCF NoAutoStart MiniPrint NoPop

The extractions of energies, thermal correction values and coordinates were realized by Shermo program.

Excited states calculations

The optimized structures were applied for excited states (ES) calculation at TD-TPSS/def2-SVP CPCM(water) level, with def2/J auxiliary basis set and RI approximation. And the results calculated at TD-TPSS/def2-SVP level were applied in the latter wavefunction analysis.

The keywords of the mentioned excited states calculation were listed as follow:

```
! TPSS def2-SVP def2/J CPCM(water) RIJCOSX TightSCF NoAutoStart MiniPrint NoPop
%tddft    nroots 50
          dosoc false
          tda true
          printlevel 3
          tprint 1e-8
end
```

Theoretical NMR calculations

The optimized structures were applied for NMR calculation at revTPSS/pcSseg-1 [8-10] CPCM(DMSO) level, and the results were applied in the parameterization of the electronic effects.

The keywords of the mentioned NMR calculation were listed as follow:

```
! pcSseg-1 CPCM(DMSO) NMR TightSCF NoAutoStart MiniPrint NoPop
%method FUNCTIONAL revTPSS end
```

Details of model constructions

The detailed procedure of the building of models was described as follow (3a was taken as an example):
Firstly, the chemical structures were drawn by ChemDraw and the Simplified molecular input line entry system (SMILES) string was obtained through selecting the structures and right click->Molecule->Copy As->SMILES. For example, the obtained SMILES string of **3a** was
OC1=C2C(C=C(N)C=C2)=CC(S(=O)(O[Na])=O)=C1/N=N/C3=C(OC)C=CC=C3.

Secondly, the SMILES string was converted into 3D-structure by the Open Babel Program by typing keywords into the command line. Take 3a as example, by typing
obabel -:" OC1=C2C(C=C(N)C=C2)=CC(S(=O)(O[Na])=O)=C1/N=N/C3=C(OC)C=CC=C3" --gen3d --ff –O 3a.xyz.
we obtained the 3D-coordinates of 3a pre-optimized by MMFF94 force field in a pure text file named 3a.xyz.

Thirdly, the pre-optimized structures were further optimized by the B3LYP functional, using the Ahlrichs double-zeta basis set def2-SVP (standard) and def2-SVP/J (auxiliary), combining D3 version of Grimme's dispersion. The applied keywords were summarized in the supporting information (p15), which were:
! B3LYP D3 def2-SVP def2/J CPCM(water) RIJCOSX OPT FREQ TightSCF NoAutoStart MiniPrint NoPop

Through this structure constructing procedure, all the bond lengths, bond angles, torsion angles, and dihedral angles have been fully optimized. A frequency analysis was performed for the optimized structure at the same level and no virtual frequency was found, which ensured the optimization of the structures to a minimum point.

Results of DFT functional screening for UV-Vis spectra fitting

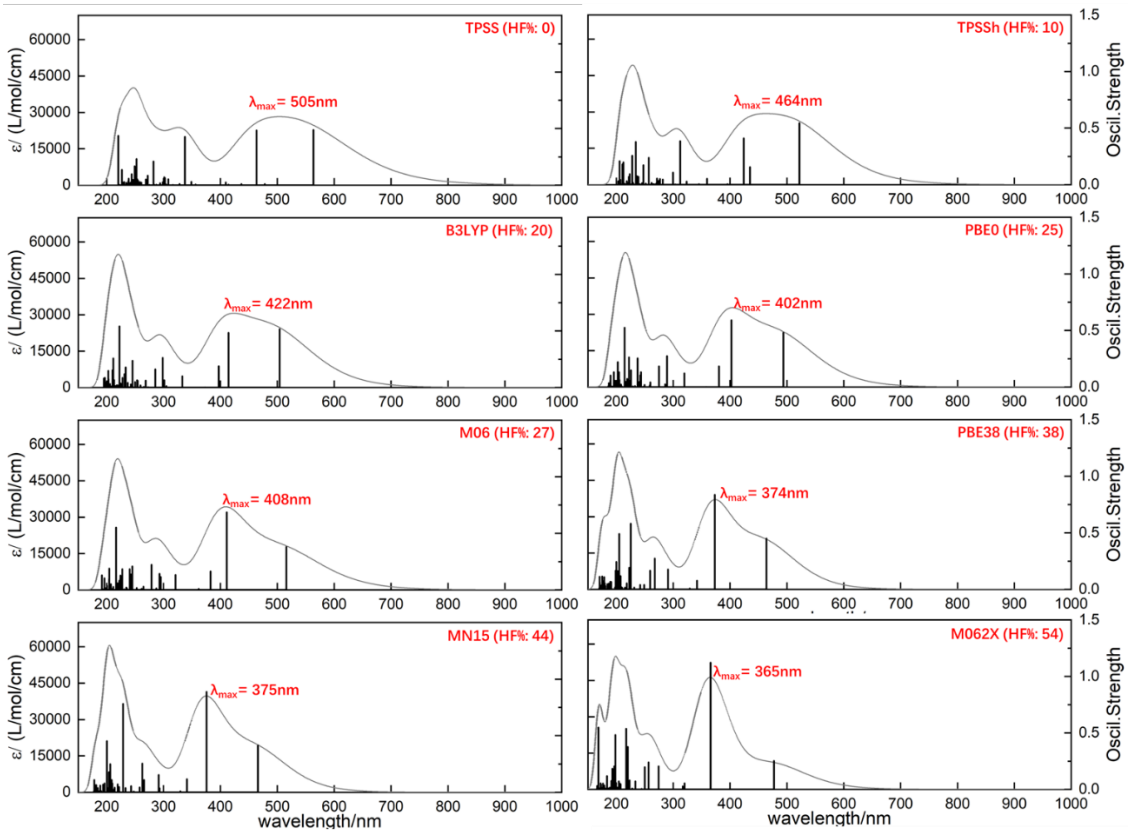


Figure S5. Theoretical UV-Vis spectra of **1a** generated by different DFT methods.

Varied DFT methods with different HF ratio (HF%) including TPSS(0)[11], THSSh(10%)[12], B3LYP(20%)[13-15], PBE0(25%)[16-18], M06(27%)[19], PBE38(38%)[20], MN15(44%)[21], M06-2X(54%)[19] were screened to pick out the optimal DFT method for fitting experimental UV-Vis spectra. The calculated theoretical UV-Vis spectra were shown in Figure S1. Clearly, UV-Vis calculated by pure DFT method TPSS matched the experimental one best in both maximum absorption wavelength (λ_{max}) and peak shape. Hence, TPSS were applied in the latter UV-Vis spectra fitting. The keywords for the calculating of UV-Vis spectra were listed as follow:

And some calculated excited energies were listed as follow:

TPSS(HF%: 0)

Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.20051	563.43430	17.74830	0.48721
2	2.59490	477.79912	20.92930	0.00964
3	2.67594	463.32982	21.58290	0.48393
4	2.83853	436.78999	22.89430	0.01010
5	2.99249	414.31719	24.13610	0.00439

6	3.02952	409.25410	24.43470	0.02408
7	3.47932	356.34621	28.06260	0.00645
8	3.55525	348.73587	28.67500	0.03046
9	3.67133	337.70895	29.61130	0.42807
10	3.77736	328.22940	30.46650	0.00937

TPSSh(HF%: 10)

Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.37598	521.82268	19.16360	0.54524
2	2.85019	435.00394	22.98830	0.15546
3	2.92232	424.26638	23.57010	0.41065
4	3.13658	395.28508	25.29820	0.00430
5	3.45011	359.36325	27.82700	0.05290
6	3.59203	345.16446	28.97170	0.00482
7	3.83172	323.57332	30.90490	0.02805
8	3.96973	312.32435	32.01800	0.38559
9	4.08667	303.38705	32.96120	0.00312
10	4.13977	299.49538	33.38950	0.10715

B3LYP(HF%: 20)

Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.46095	503.80631	19.84890	0.51593
2	2.99242	414.32749	24.13550	0.48519
3	3.12346	396.94515	25.19240	0.18907
4	3.32558	372.81998	26.82260	0.00146
5	3.72396	332.93607	30.03580	0.10089
6	4.06757	304.81117	32.80720	0.01331
7	4.11578	301.24115	33.19600	0.06449
8	4.15201	298.61268	33.48820	0.26272
9	4.34449	285.38246	35.04070	0.15975
10	4.54118	273.02192	36.62710	0.00294

PBE0(HF%: 25)

Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.51087	493.79064	20.25150	0.48122
2	3.08192	402.29473	24.85740	0.59155
3	3.25931	380.40030	26.28810	0.18326
4	3.46459	357.86117	27.94380	0.00143
5	3.87702	319.79230	31.27030	0.12092
6	4.28808	289.13687	34.58570	0.27330
7	4.32236	286.84366	34.86220	0.01859
8	4.33863	285.76820	34.99340	0.02457
9	4.51087	274.85669	36.38260	0.18358
10	4.77307	259.75783	38.49740	0.04214

M06(HF%: 27)

Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.40244	516.07582	19.37700	0.37970
2	3.01520	411.19778	24.31920	0.68639
3	3.24167	382.47065	26.14580	0.16381
4	3.42510	361.98706	27.62530	0.00792
5	3.86100	321.11907	31.14110	0.13188
6	4.20120	295.11586	33.88500	0.11504
7	4.23103	293.03517	34.12560	0.14328
8	4.31501	287.33241	34.80290	0.01340
9	4.39698	281.97612	35.46400	0.00146
10	4.44834	278.72004	35.87830	0.22175

PBE38(HF%: 38)

Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.67296	463.84561	21.55890	0.45084
2	3.32348	373.05502	26.80570	0.83587
3	3.62567	341.96222	29.24300	0.07681
4	3.76835	329.01451	30.39380	0.00870
5	4.26187	290.91505	34.37430	0.17670
6	4.63612	267.43119	37.39280	0.27465
7	4.78095	259.32940	38.56100	0.16639
8	4.98028	248.95008	40.16870	0.03977
9	5.12866	241.74796	41.36540	0.04050
10	5.15859	240.34535	41.60680	0.00375

MN15(HF%: 44)

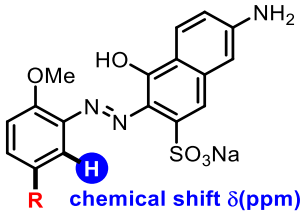
Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.66023	466.06580	21.45620	0.41335
2	3.30066	375.63486	26.62160	0.88771
3	3.63608	340.98275	29.32700	0.11669
4	3.76344	329.44374	30.35420	0.00909
5	4.23090	293.04462	34.12450	0.03610
6	4.25407	291.44835	34.31140	0.15281
7	4.66464	265.79559	37.62290	0.10928
8	4.72193	262.57128	38.08490	0.25373
9	4.80723	257.91213	38.77290	0.04324
10	4.97841	249.04370	40.15360	0.00354

M062X(HF%: 54)

Index	Excit.energy(eV	nm	1000 cm^-1)	Oscil.str.
1	2.59818	477.19719	20.95570	0.25239
2	3.39052	365.67889	27.34640	1.12102

3	3.87494	319.96420	31.25350	0.05432
4	3.91476	316.70930	31.57470	0.02811
5	4.51983	274.31158	36.45490	0.20409
6	4.83174	256.60372	38.97060	0.24062
7	4.96159	249.88820	40.01790	0.19810
8	5.07678	244.21816	40.94700	0.00526
9	5.31141	233.43000	42.83940	0.07266
10	5.44618	227.65355	43.92640	0.00833

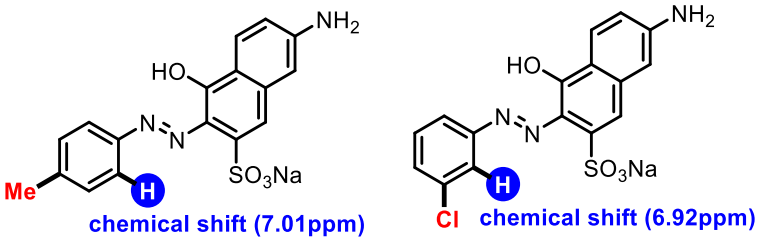
Results of theoretical NMR calculation



R = H:	δ = 7.01	R = CH_2Br:	δ = 7.30	R = CO_2H:	δ = 8.33
R = F:	δ = 6.88	R = CF_3:	δ = 7.99	R = CO_2Na:	δ = 7.95
R = Cl:	δ = 7.05	R = OH:	δ = 6.53	R = CO_2Me:	δ = 8.27
R = Br:	δ = 7.09	R = OMe:	δ = 6.56	R = $CONH_2$:	δ = 8.07
R = Me:	δ = 6.82	R = NH_2:	δ = 6.24	R = CHO:	δ = 7.60
R = CH_2OH:	δ = 7.44	R = NMe_2:	δ = 5.94	R = Ac:	δ = 7.60
R = CH_2Cl:	δ = 7.24	R = SO_3Na:	δ = 7.37		

Scheme S3. Calculated chemical shifts of the selected *o*-methoxyanilines terminated azos.

The theoretical NMR were calculated for some substituted *o*-methoxyanilines terminated azo compounds, and the chemical shifts of the hydrogen located between the azo functional groups and the substituents were summarized in Scheme S3. Accompaniedly, some selected anilines terminated azos were also calculated and the results were summarized in Scheme S4.



Scheme S4. Calculated chemical shifts of some selected anilines terminated azos.

Results of the predicted UV-Vis parameters and curves

As mentioned in the paper, λ_{max} and $W_{1/2}$ could be calculated by the following formulars, where CCS represented for the calculated chemical shifts:

λ_{max} = -0.0597*CCS + 36.9589 (R^2 = 0.9020); $W_{1/2}$ = -0.0938*CCS + 16.1334 (R^2 = 0.7309)

With the calculated chemical shifts shown in Scheme S3, λ_{max} and $W_{1/2}$ were shown in **Figure S6.**

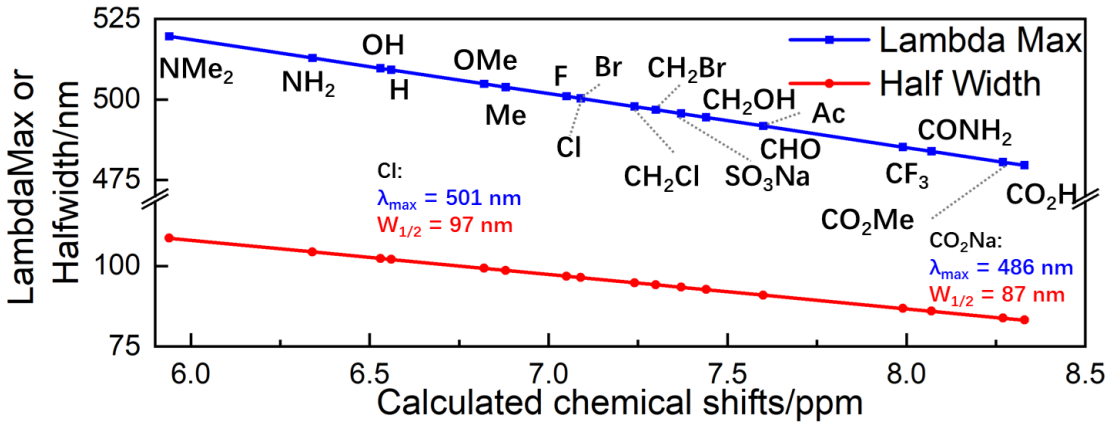


Figure S6. Predicted UV-Vis parameters.

With the calculated λ_{max} and $W_{1/2}$ in hand, predicted UV-Vis curve could be generated by the gaussian broadening using the following equation:

$$G(w) = \frac{1}{c\sqrt{2\pi}} e^{-\frac{(\lambda-\lambda max)^2}{2c^2}}$$

Where λ represented for the wavelength, λmax represented for the calculated λ_{max}. And **c** was connected to $W_{1/2}$.

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Energies of the optimized structures

1a

Electronic energy:	-1869.8125631 a.u.
Sum of electronic energy and ZPE, namely U/H/G at 0 K:	-1869.4855260 a.u.
Sum of electronic energy and thermal correction to U:	-1869.4584869 a.u.
Sum of electronic energy and thermal correction to H:	-1869.4575427 a.u.
Sum of electronic energy and thermal correction to G:	-1869.5434513 a.u.

2a

Electronic energy:	-1794.6923529 a.u.
Sum of electronic energy and ZPE, namely U/H/G at 0 K:	-1794.3704017 a.u.
Sum of electronic energy and thermal correction to U:	-1794.3441942 a.u.
Sum of electronic energy and thermal correction to H:	-1794.3432501 a.u.
Sum of electronic energy and thermal correction to G:	-1794.4275419 a.u.

3a

Electronic energy:	-1755.4269654 a.u.
Sum of electronic energy and ZPE, namely U/H/G at 0 K:	-1755.1320721 a.u.
Sum of electronic energy and thermal correction to U:	-1755.1077277 a.u.
Sum of electronic energy and thermal correction to H:	-1755.1067835 a.u.
Sum of electronic energy and thermal correction to G:	-1755.1866093 a.u.

3b

Electronic energy:	-1755.4248225 a.u.
Sum of electronic energy and ZPE, namely U/H/G at 0 K:	-1755.1298180 a.u.
Sum of electronic energy and thermal correction to U:	-1755.1055736 a.u.
Sum of electronic energy and thermal correction to H:	-1755.1046295 a.u.
Sum of electronic energy and thermal correction to G:	-1755.1844041 a.u.

3c

Electronic energy:	-2378.8013888 a.u.
Sum of electronic energy and ZPE, namely U/H/G at 0 K:	-2378.4919925 a.u.
Sum of electronic energy and thermal correction to U:	-2378.4633204 a.u.
Sum of electronic energy and thermal correction to H:	-2378.4623762 a.u.
Sum of electronic energy and thermal correction to G:	-2378.5522283 a.u.

4a

Electronic energy:	-2092.1028915 a.u.
Sum of electronic energy and ZPE, namely U/H/G at 0 K:	-2091.8033957 a.u.
Sum of electronic energy and thermal correction to U:	-2091.7753597 a.u.
Sum of electronic energy and thermal correction to H:	-2091.7744155 a.u.
Sum of electronic energy and thermal correction to G:	-2091.8635001 a.u.

5a

Electronic energy:	-2540.5462982 a.u.
Sum of electronic energy and ZPE, namely U/H/G at 0 K:	-2540.2467191 a.u.
Sum of electronic energy and thermal correction to U:	-2540.2168728 a.u.
Sum of electronic energy and thermal correction to H:	-2540.2159286 a.u.
Sum of electronic energy and thermal correction to G:	-2540.3070851 a.u.

Results of the frequency analysis

1a

There are 129 frequencies (cm^-1):

17.8	25.2	35.5	54.2	63.6	78.4	81.2	95.9	101.8
118.7	120.5	142.7	160.9	164.2	180.9	193.8	200.2	221.4
236.9	245.6	258.6	262.3	270.9	282.5	290.3	293.5	325.3
333.8	340.1	372.5	382.9	392.4	400.4	422.3	434.9	463.6
469.3	477.6	500.9	515.5	517.4	527.8	549.9	579.4	595.8
615.8	627.7	635.0	644.7	652.0	677.6	717.1	723.8	737.2
760.1	780.1	782.7	821.3	836.4	839.1	875.6	903.0	919.5
926.8	963.8	966.7	975.4	980.6	1001.8	1019.1	1054.4	1067.0
1078.7	1106.3	1149.6	1161.6	1166.8	1167.8	1179.0	1193.0	1201.1
1207.2	1210.9	1223.5	1235.7	1245.8	1267.5	1299.1	1305.2	1330.1
1357.5	1366.1	1402.9	1414.4	1438.6	1451.6	1452.8	1453.2	1459.1
1465.0	1466.9	1469.5	1475.5	1488.7	1515.5	1537.7	1552.0	1604.8
1609.8	1623.0	1651.8	1657.7	1666.4	3011.1	3012.5	3090.9	3092.3
3152.3	3152.6	3170.0	3180.8	3181.5	3189.7	3215.7	3217.7	3229.2
3580.4	3700.4	3762.5						

2a

There are 126 frequencies (cm^-1):

19.3	25.7	38.5	45.4	62.9	69.0	83.2	97.5	102.0
121.6	123.5	141.4	161.7	169.2	194.7	200.9	219.4	241.8
243.8	252.4	260.7	269.7	281.8	288.5	304.2	333.1	337.6
353.0	359.3	381.2	393.1	416.1	423.4	464.0	465.3	471.4
485.6	504.6	517.2	524.9	528.4	576.8	587.8	605.8	613.4
625.0	644.0	650.8	674.4	713.5	726.6	738.6	766.0	780.0
782.3	822.7	836.5	843.5	875.5	911.4	926.4	929.7	969.1
975.7	980.5	986.5	999.1	1016.9	1027.7	1049.2	1061.3	1069.8
1106.3	1147.3	1161.0	1166.0	1173.0	1191.3	1201.5	1210.3	1223.2
1234.4	1247.4	1269.4	1291.8	1307.0	1310.1	1356.7	1365.3	1390.9
1402.3	1414.0	1417.8	1441.7	1450.8	1453.8	1458.4	1461.4	1469.9
1474.7	1488.5	1517.2	1539.7	1552.0	1604.9	1610.3	1621.2	1650.5
1653.0	1666.6	3015.4	3025.4	3097.1	3097.2	3124.0	3155.0	3165.6
3169.5	3180.4	3180.8	3189.4	3215.6	3222.1	3577.8	3696.3	3763.6

3a

There are 117 frequencies (cm^-1):

20.6	27.5	39.8	59.1	67.5	86.2	103.4	106.5	126.5
129.4	157.3	162.1	189.9	192.0	197.0	213.3	242.2	255.9
261.0	277.1	279.2	287.5	303.8	329.4	333.6	342.1	384.3
392.5	421.0	425.1	464.1	468.4	474.0	503.2	510.8	517.3

527.5	550.8	574.6	577.7	594.0	609.5	624.7	641.3	650.6
672.9	715.2	724.2	765.2	778.1	780.3	782.2	816.1	836.3
858.4	875.5	887.7	926.5	932.5	974.7	975.9	979.8	998.6
1017.2	1019.4	1055.5	1066.8	1068.2	1106.6	1128.2	1160.5	1162.1
1165.7	1184.3	1199.1	1208.5	1214.5	1226.8	1247.4	1269.0	1279.7
1308.3	1311.6	1359.2	1368.6	1402.9	1414.7	1450.1	1454.3	1455.0
1461.6	1473.4	1478.3	1490.4	1517.2	1524.3	1552.8	1605.1	1610.3
1625.4	1637.5	1652.6	1666.6	3017.4	3100.1	3156.9	3169.9	3173.8
3180.7	3189.0	3189.8	3201.9	3215.9	3224.6	3579.8	3699.3	3763.0

3b

There are 117 frequencies (cm^-1):

20.2	27.8	34.8	51.2	62.1	86.1	106.4	118.1	127.2
133.3	148.3	167.7	190.0	194.9	216.9	227.6	239.4	261.0
265.2	269.6	286.3	303.0	326.3	335.6	345.6	378.5	395.6
399.9	405.0	421.8	429.5	462.7	474.8	503.7	508.6	512.3
527.1	549.5	558.6	569.6	590.9	595.1	610.0	642.4	645.6
664.3	720.9	736.2	767.0	776.7	779.1	806.9	828.7	846.8
848.1	856.0	886.8	927.7	932.9	947.4	978.8	999.8	1004.7
1019.8	1029.7	1054.8	1066.5	1098.6	1101.0	1128.9	1135.9	1163.3
1165.2	1174.7	1196.0	1203.8	1218.6	1228.2	1266.4	1268.9	1279.0
1300.0	1314.4	1348.6	1368.1	1371.8	1426.2	1453.2	1454.3	1459.8
1465.2	1469.4	1479.1	1480.8	1520.3	1543.3	1556.6	1603.5	1613.5
1625.8	1638.6	1651.2	1672.8	3020.0	3104.0	3159.2	3171.7	3175.1
3178.0	3190.2	3192.6	3204.6	3213.7	3227.0	3569.2	3680.8	3755.7

3c

There are 129 frequencies (cm^-1):

17.7	23.0	36.2	38.9	51.2	58.3	77.9	95.0	98.9
107.9	110.1	129.1	143.2	156.5	162.6	189.1	198.7	209.5
223.9	237.3	255.3	259.2	263.7	274.9	289.3	306.6	308.8
317.4	320.8	329.3	346.9	349.3	376.1	400.9	412.1	429.3
434.6	441.6	466.1	491.4	496.1	508.9	525.4	532.8	537.9
560.2	567.0	573.2	593.8	600.0	601.5	615.2	633.3	652.7
658.0	714.1	730.8	743.4	767.5	768.6	778.8	797.6	805.6
828.7	845.7	872.9	889.1	911.8	936.5	978.1	997.1	1003.0
1009.1	1019.5	1023.8	1054.6	1066.9	1106.9	1112.0	1112.6	1129.3
1138.8	1163.3	1165.6	1174.8	1196.6	1203.7	1219.2	1225.0	1247.8
1259.8	1276.6	1289.9	1295.2	1314.2	1349.0	1368.8	1397.7	1416.1
1439.2	1453.4	1454.9	1459.6	1464.3	1478.5	1498.8	1519.1	1525.2
1547.2	1592.8	1601.6	1625.6	1638.1	1651.2	1672.3	3019.1	3102.8
3159.1	3174.2	3183.8	3190.3	3199.1	3204.2	3226.6	3270.4	3530.9
3678.4	3682.6	3765.6						

4a

There are 126 frequencies (cm^-1):

14.8	23.4	33.8	42.4	53.0	60.1	74.9	78.7	100.3
105.9	112.7	122.9	150.3	162.8	167.6	174.4	197.9	203.3
211.7	240.4	248.9	262.2	270.5	279.9	286.4	299.7	313.4
327.5	333.0	343.8	388.3	391.3	403.3	420.5	425.4	432.0
466.6	472.8	484.6	508.6	517.0	521.2	528.1	537.8	559.9
576.9	592.8	618.4	630.0	630.9	643.1	651.3	662.3	677.2
718.5	732.0	748.3	769.8	781.3	784.5	822.7	838.3	850.5
876.2	904.9	927.7	940.0	953.0	975.2	981.7	986.0	1002.4
1020.0	1052.8	1060.0	1066.4	1106.7	1115.1	1144.0	1161.8	1164.6
1184.5	1192.0	1199.8	1207.8	1215.2	1226.4	1248.0	1264.0	1272.6
1307.6	1317.5	1347.3	1361.9	1385.8	1403.7	1414.6	1437.1	1454.5
1456.6	1457.9	1470.0	1476.2	1488.7	1511.4	1547.9	1552.2	1604.4
1609.6	1629.3	1649.2	1653.1	1666.2	3023.1	3109.2	3162.3	3172.9
3181.2	3181.8	3191.1	3214.1	3217.3	3230.5	3581.9	3702.8	3761.1

5a

There are 129 frequencies (cm^-1):

20.3	30.6	49.8	61.8	70.8	74.8	84.8	90.5	99.0
104.4	115.2	125.7	136.6	142.2	150.6	153.2	160.0	164.9
190.8	207.2	217.9	240.8	249.0	252.1	266.3	278.3	282.7
285.4	292.1	308.1	321.2	342.8	355.2	379.1	384.9	390.2
406.3	421.4	424.5	472.9	476.1	486.9	498.8	504.0	516.5
519.3	531.6	535.5	569.3	583.1	600.2	615.5	619.9	626.3
645.0	652.0	665.7	689.2	720.0	729.1	762.7	779.6	786.8
819.5	839.7	845.5	875.4	899.7	927.9	928.7	943.6	973.4
977.7	981.7	983.3	1008.6	1022.3	1056.1	1067.7	1077.9	1098.4
1121.5	1145.1	1164.1	1164.3	1186.9	1200.7	1207.0	1215.7	1225.4
1242.0	1250.1	1273.6	1289.5	1311.4	1316.3	1363.9	1384.5	1404.9
1413.7	1423.2	1454.2	1455.7	1460.7	1468.8	1476.4	1490.2	1509.8
1533.8	1552.7	1604.4	1611.1	1624.7	1637.9	1652.1	1666.2	3021.3
3106.2	3161.5	3165.6	3182.2	3190.2	3208.2	3210.8	3221.1	3228.0
3585.0	3706.8	3766.0						

Coordinates of the optimized structures

1a

C	-4.55678156	-2.67611750	-0.51254486
C	-3.20883429	-2.56940414	-0.31236759
C	-2.60922218	-1.30150434	-0.03481424
C	-3.44895678	-0.14064261	0.02535608
C	-4.85634370	-0.26823995	-0.19229557
C	-5.43452283	-1.53141101	-0.47448575
H	-0.60189990	-2.08035063	0.12742825
H	-2.58302838	-3.46005942	-0.36925550
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H	-11.81635410	-0.52625452	-2.62203250
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H	1.30089925	-0.62866877	0.70766094

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Na	-7.91262421	-3.98042832	-1.09541025

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C	-3.45207570	-0.13622066	0.03432992
C	-4.85758199	-0.26541098	-0.19708807
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H	-2.57292187	-3.44852292	-0.39151590
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4a

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S	-5.27573593	-4.32478264	-0.72864362
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O	-6.06829136	-4.26852321	-2.00874953
Na	-8.01778135	-4.09729871	-0.84727692
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5a

C	-4.77841768	-2.59856806	-0.11801401
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O	-6.79312059	-4.14696148	0.79613016
O	-6.00238659	-4.49110142	-1.51006326
Na	-8.18651337	-4.24476664	-1.35405442
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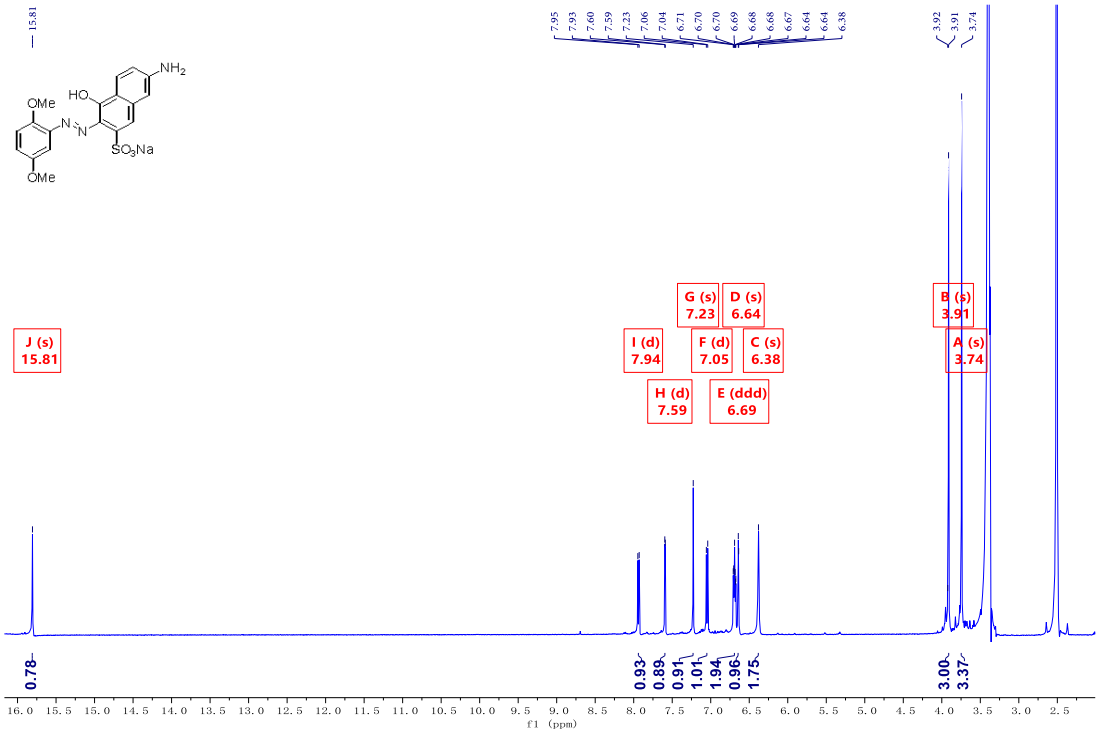
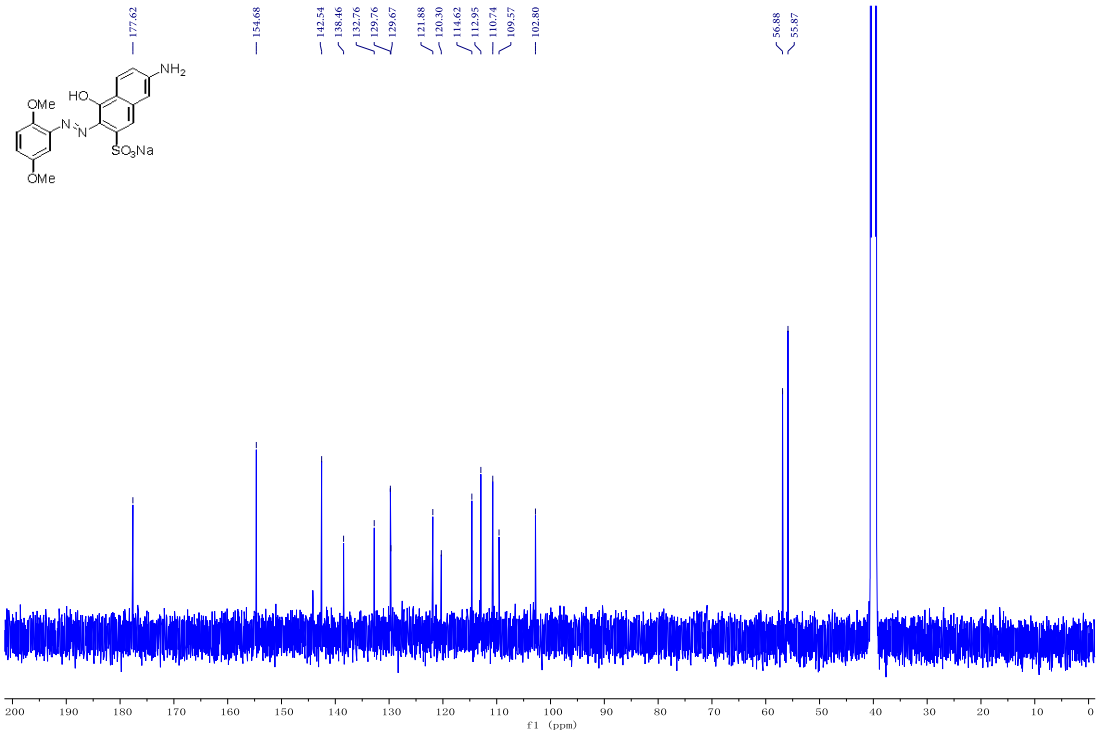
O	-10.48108667	-4.07163187	2.02520764
O	-12.28954850	-4.65614127	0.37219900
O	-9.85414612	-5.10265597	-0.09237204
Na	-8.44692399	-5.09213725	1.85921149
H	1.22618674	-0.93163810	0.90190271

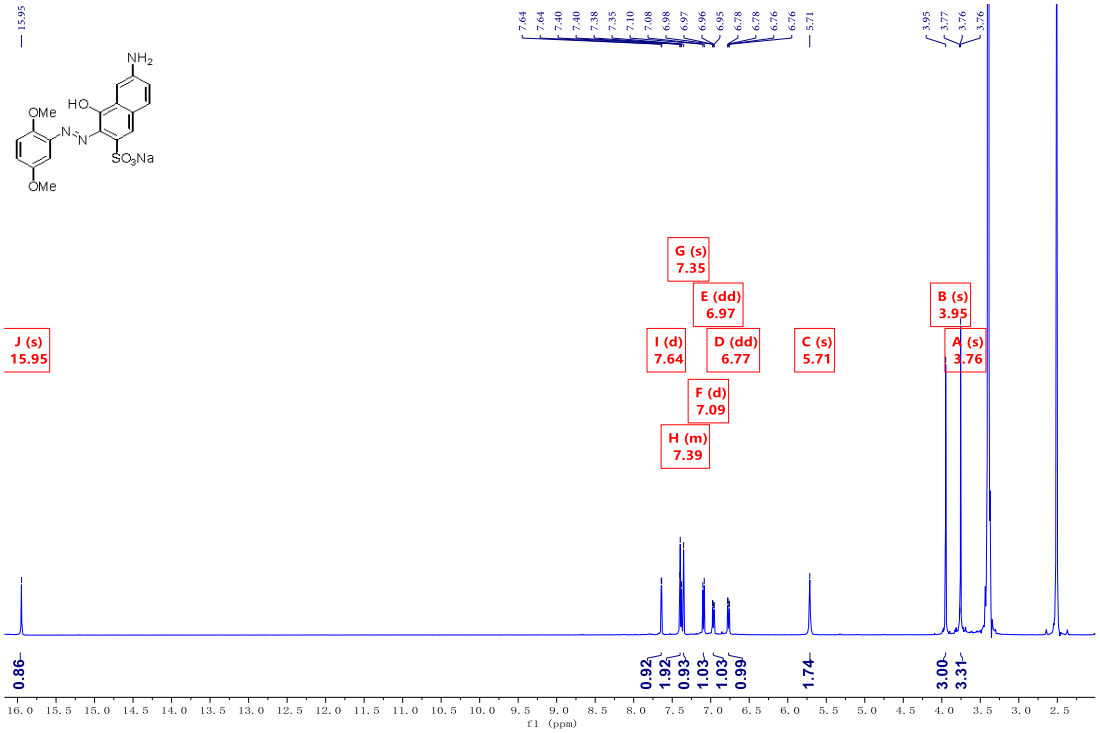
Copies of ^{1}H and ^{13}C NMR Spectra

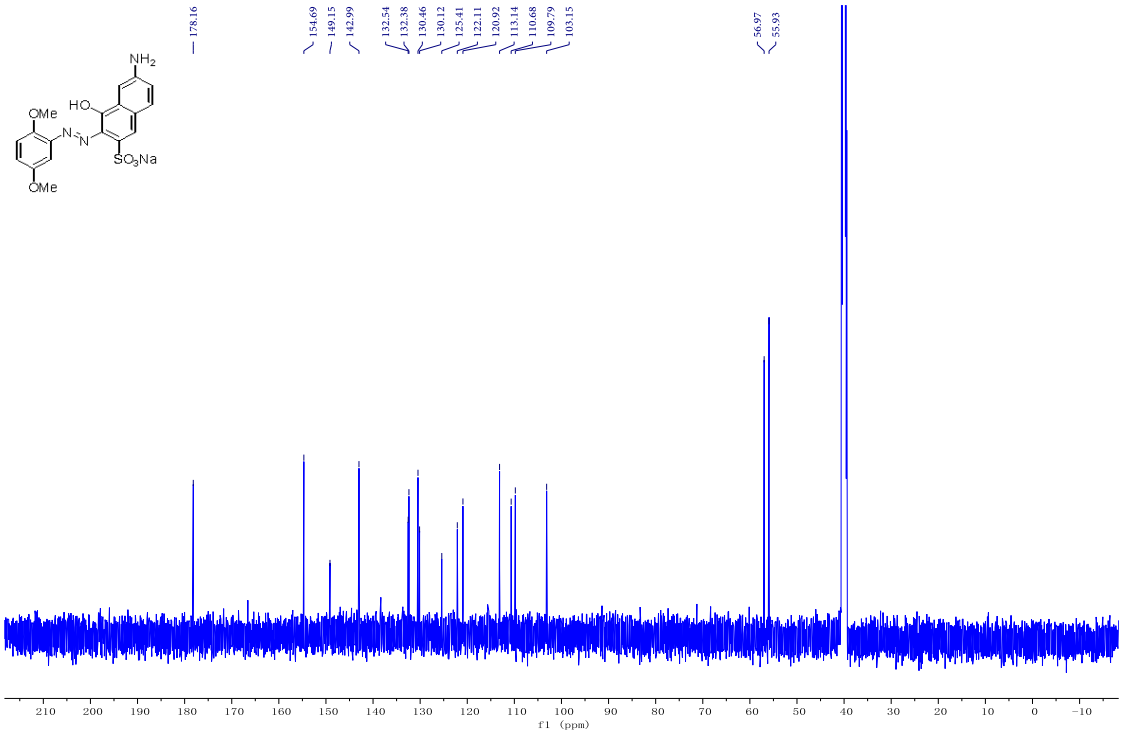
Sodium 7-amino-3-((2,5-dimethoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (1a)



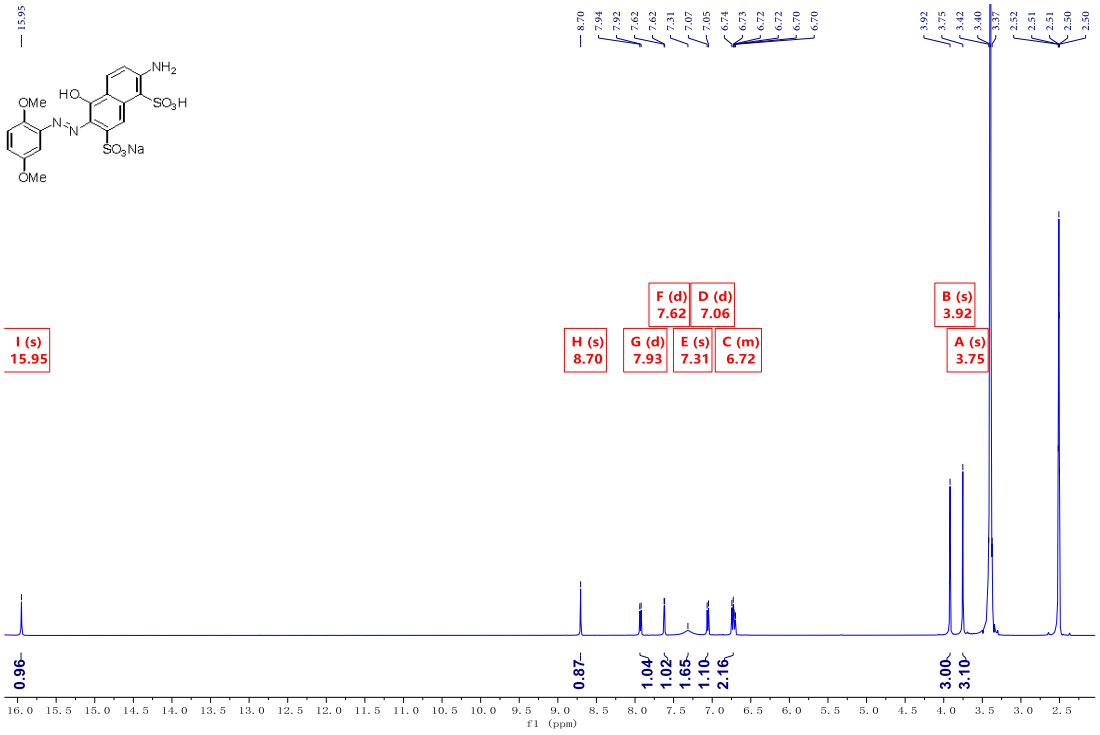


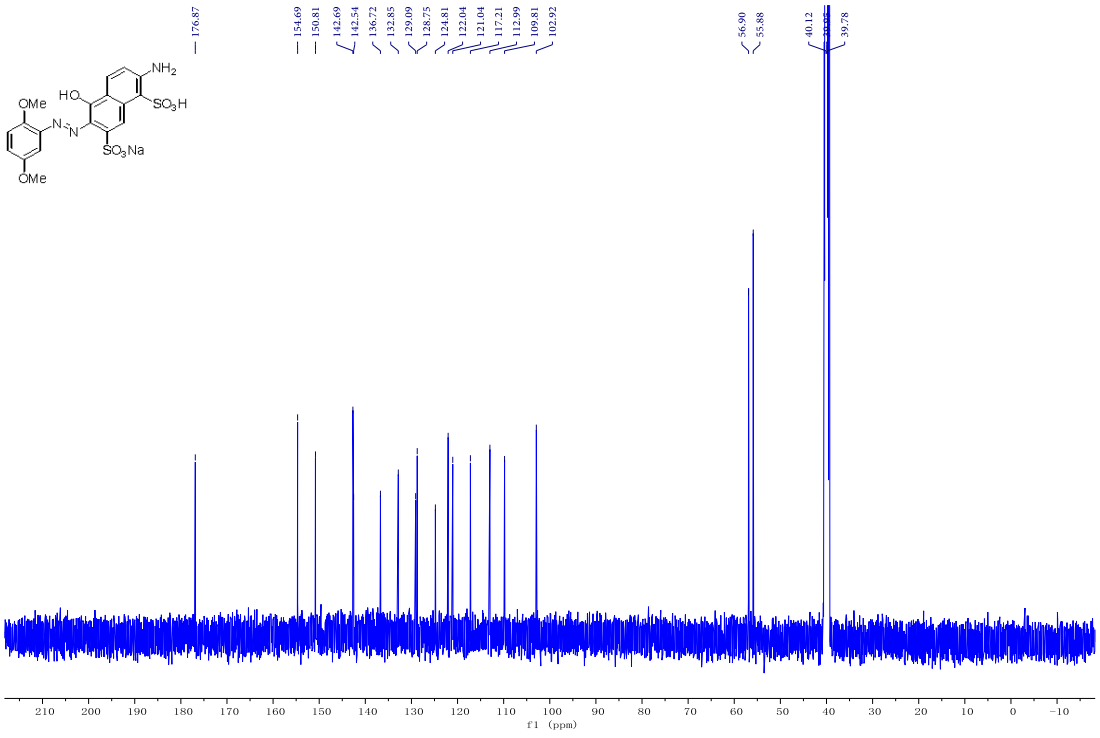
Sodium 6-amino-3-((2,5-dimethoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (1b)



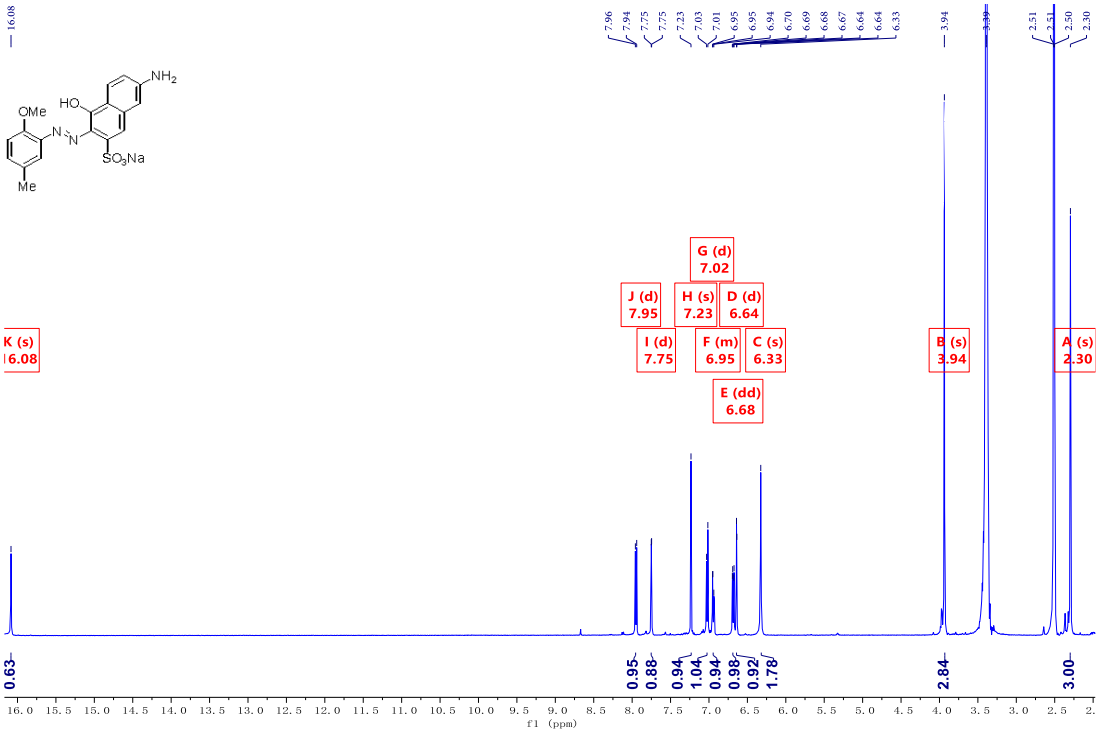


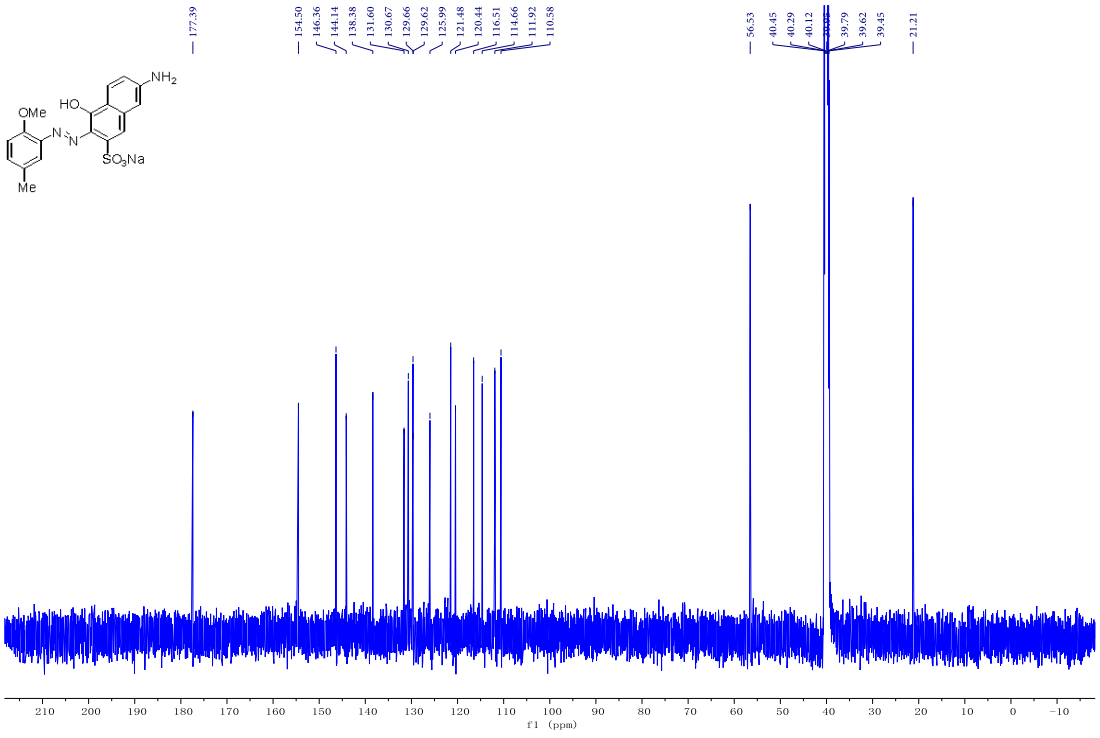
Sodium 7-amino-3-((2,5-dimethoxyphenyl)diazenyl)-4-hydroxy-8-sulfonaphthalene-2-sulfonate (1c)



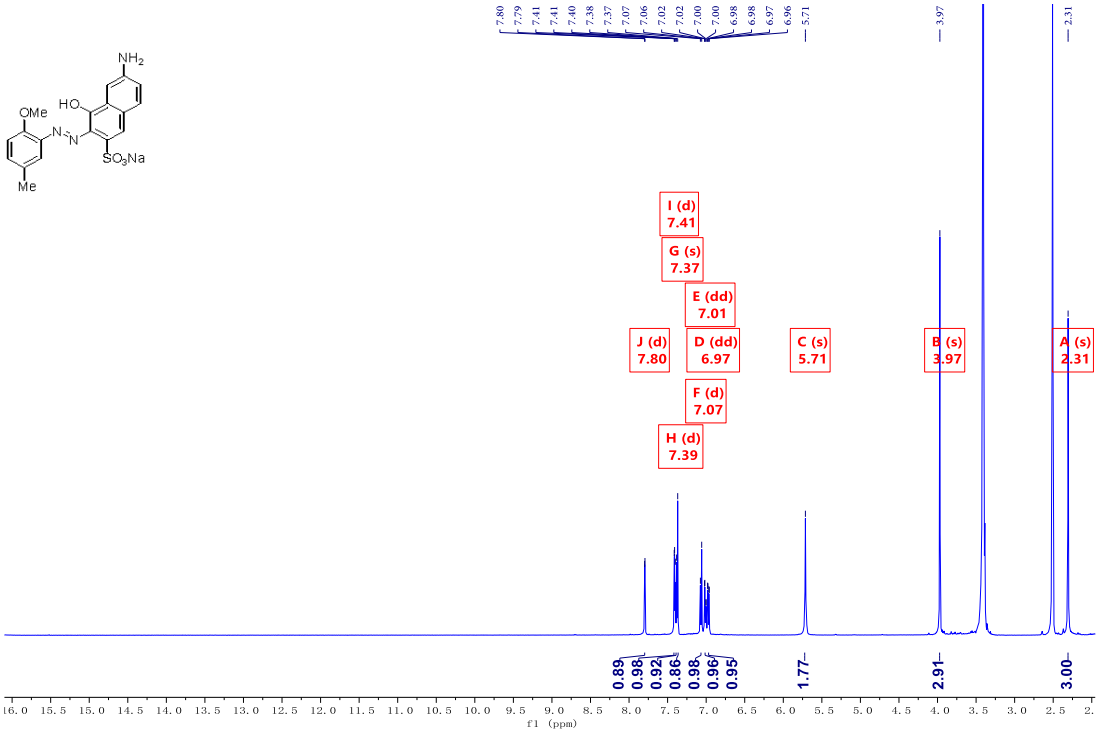


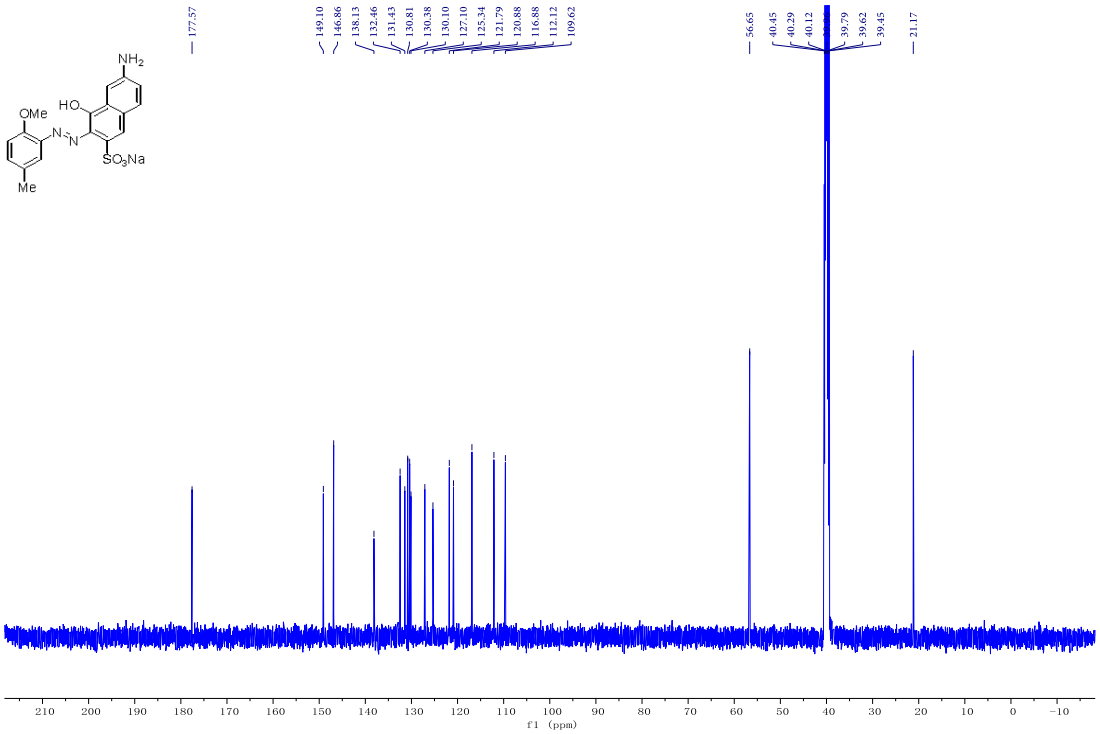
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-methylphenyl)diazenyl)naphthalene-2-sulfonate (2a)



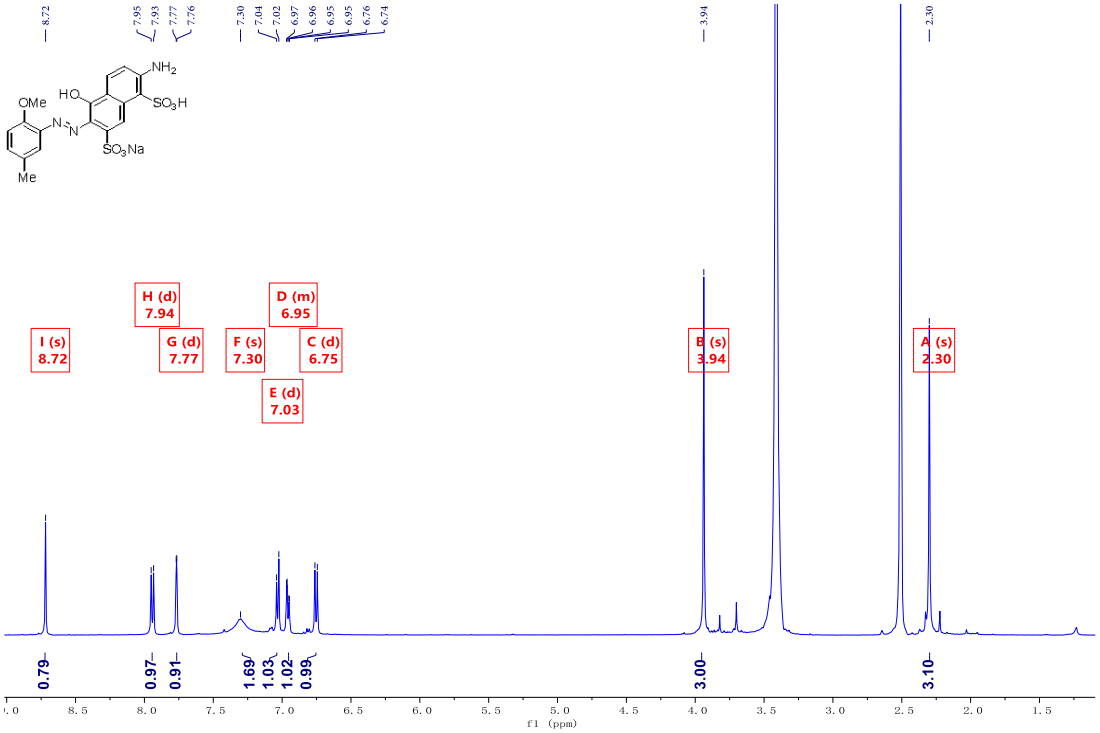


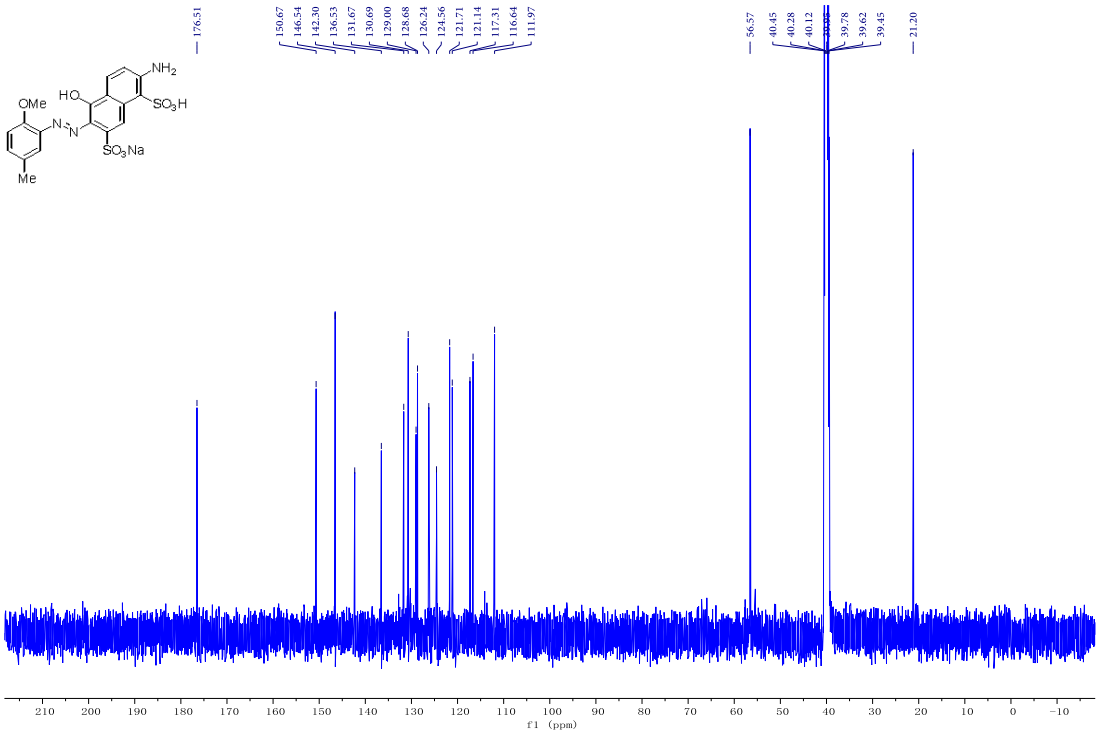
Sodium 6-amino-4-hydroxy-3-((2-methoxy-5-methylphenyl)diazenyl)naphthalene-2-sulfonate (2b)



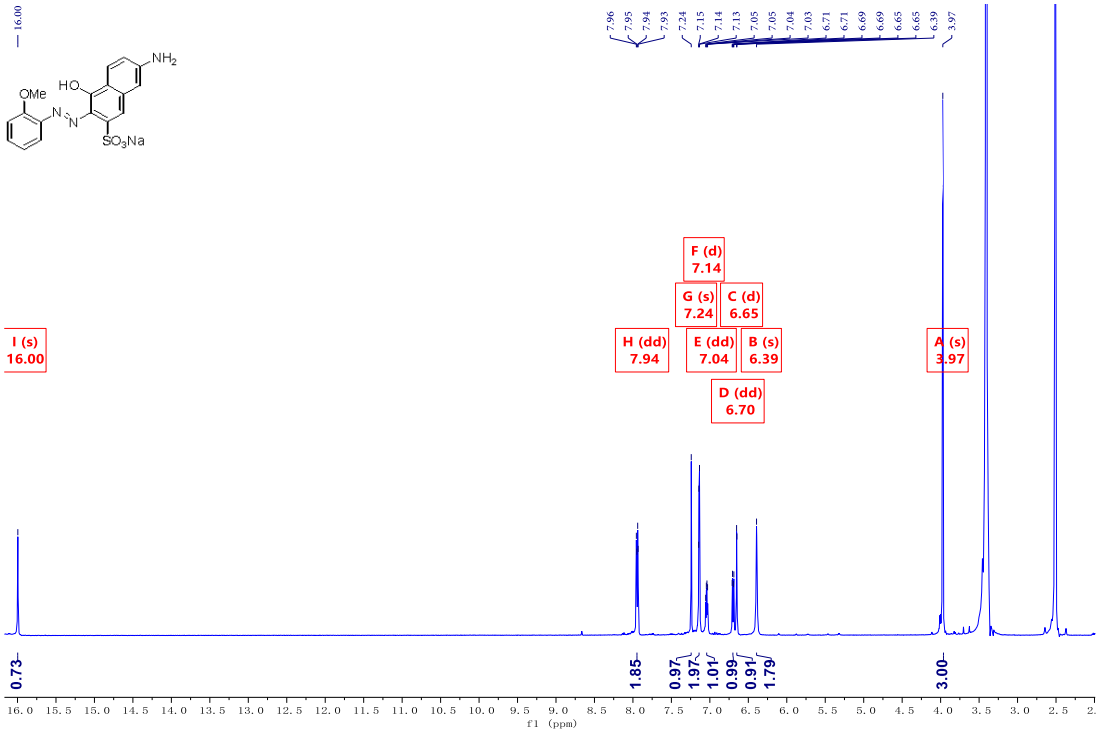


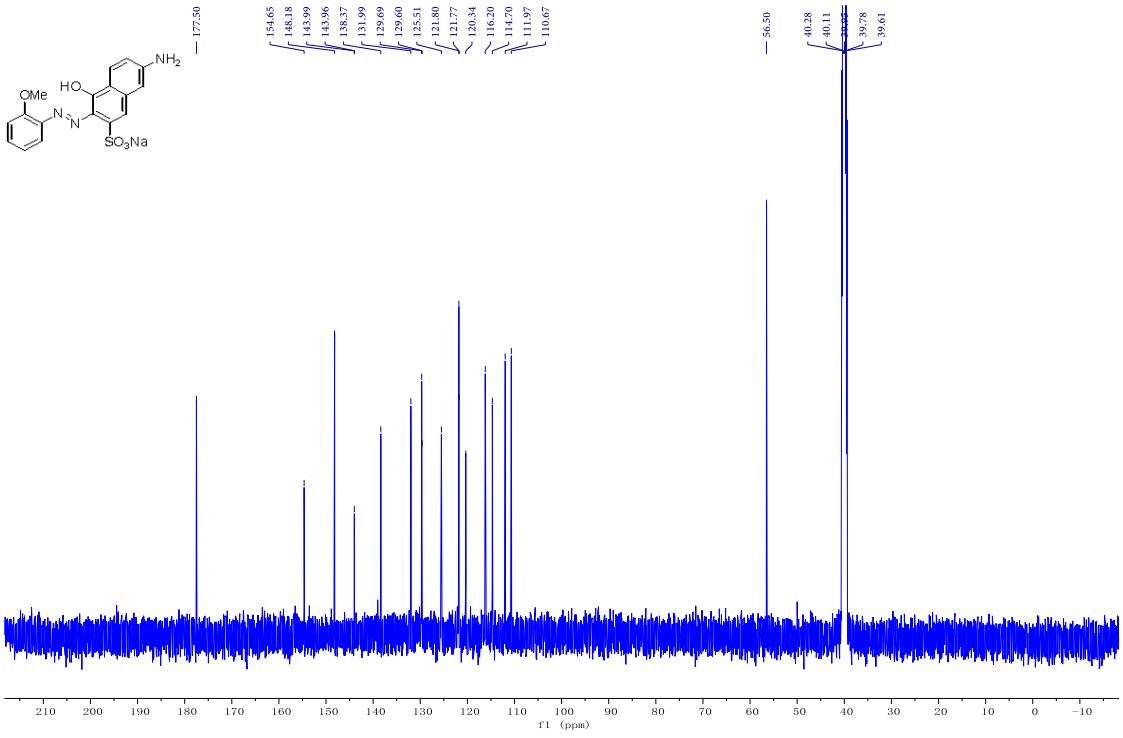
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-methylphenyl)diazenyl)-8-sulfonaphthalene-2-sulfonate (2c)



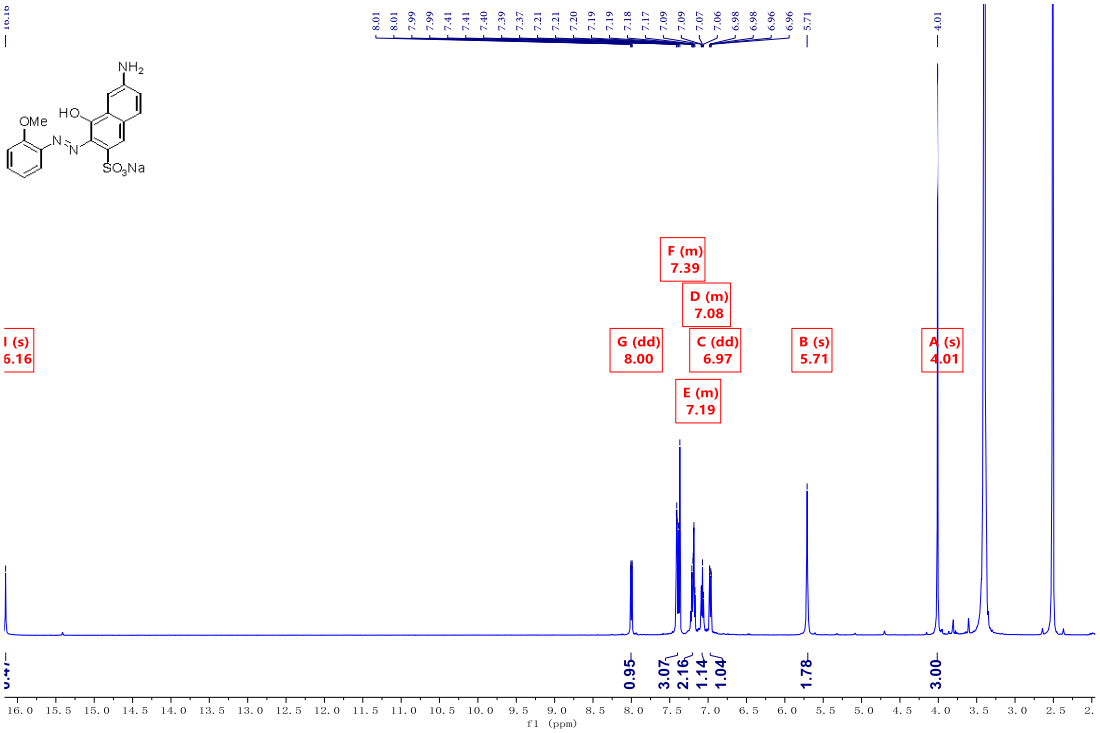


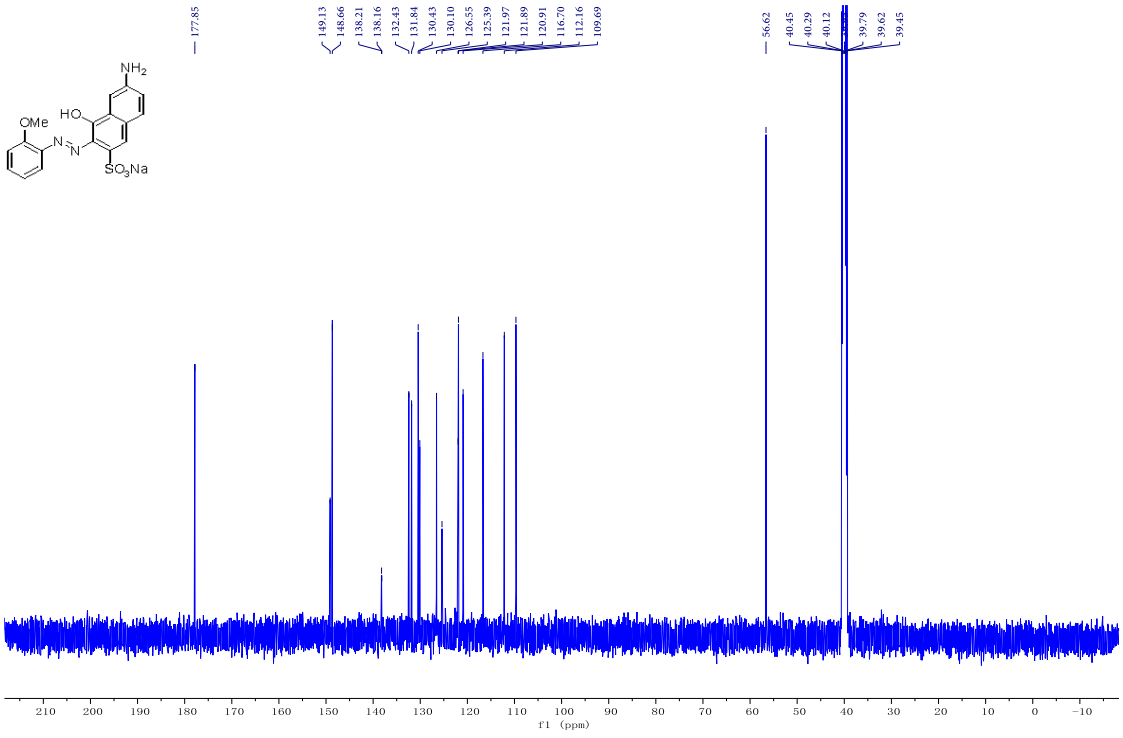
Sodium 7-amino-4-hydroxy-3-((2-methoxyphenyl)diazenyl)naphthalene-2-sulfonate (3a)



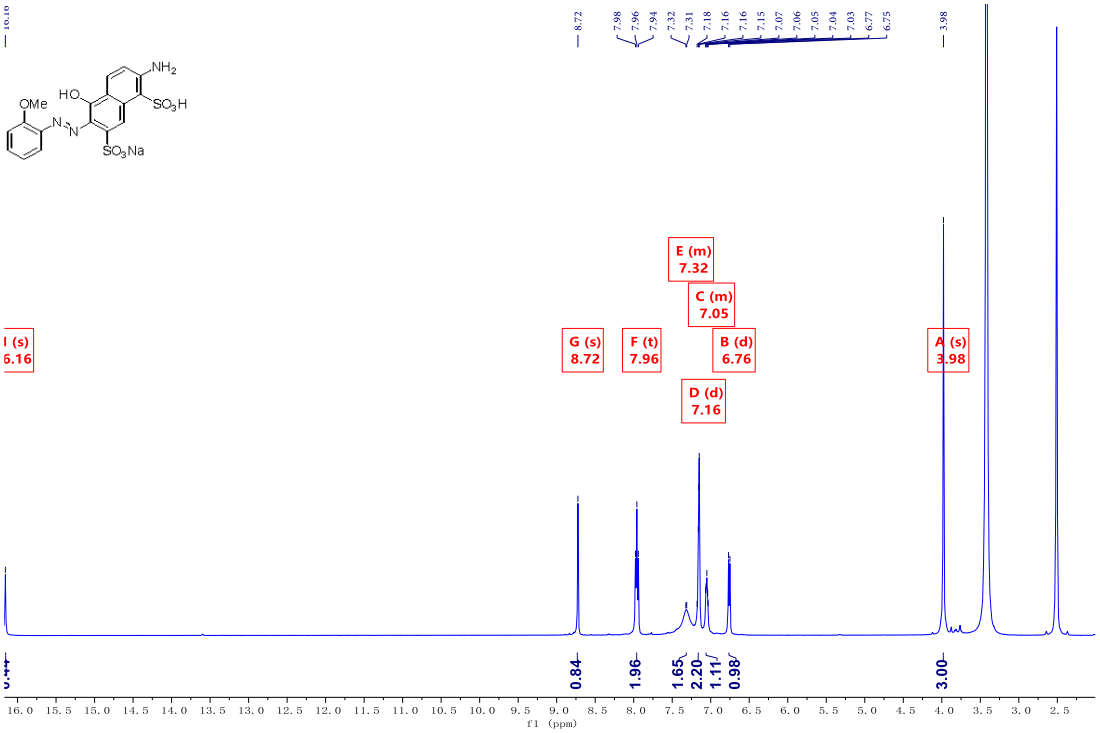


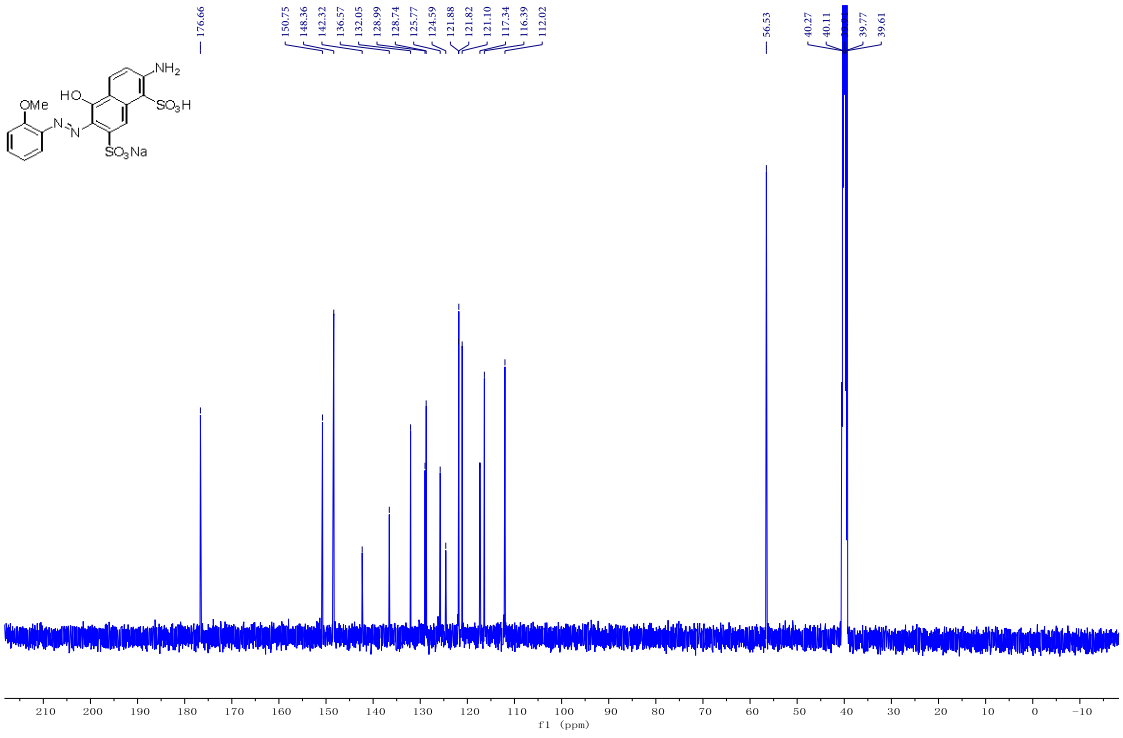
Sodium 6-amino-4-hydroxy-3-((2-methoxyphenyl)diazenyl)naphthalene-2-sulfonate (3b)



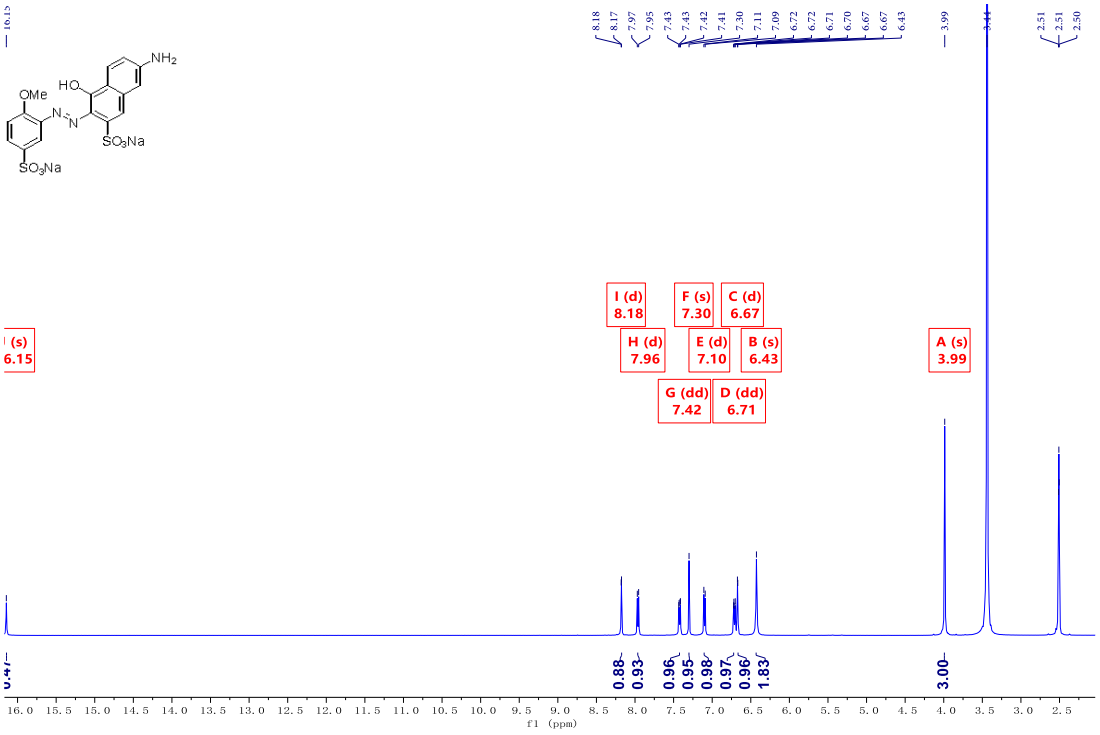


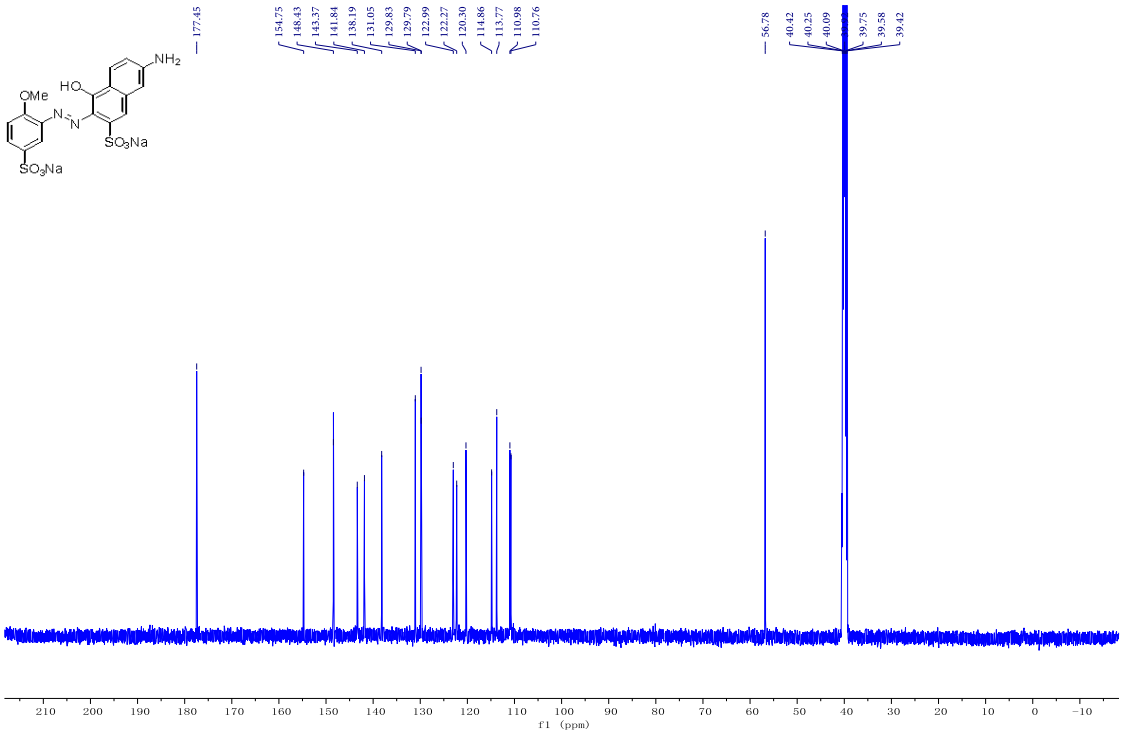
Sodium 7-amino-4-hydroxy-3-((2-methoxyphenyl)diazenyl)-8-sulfonaphthalene-2-sulfonate (3c)



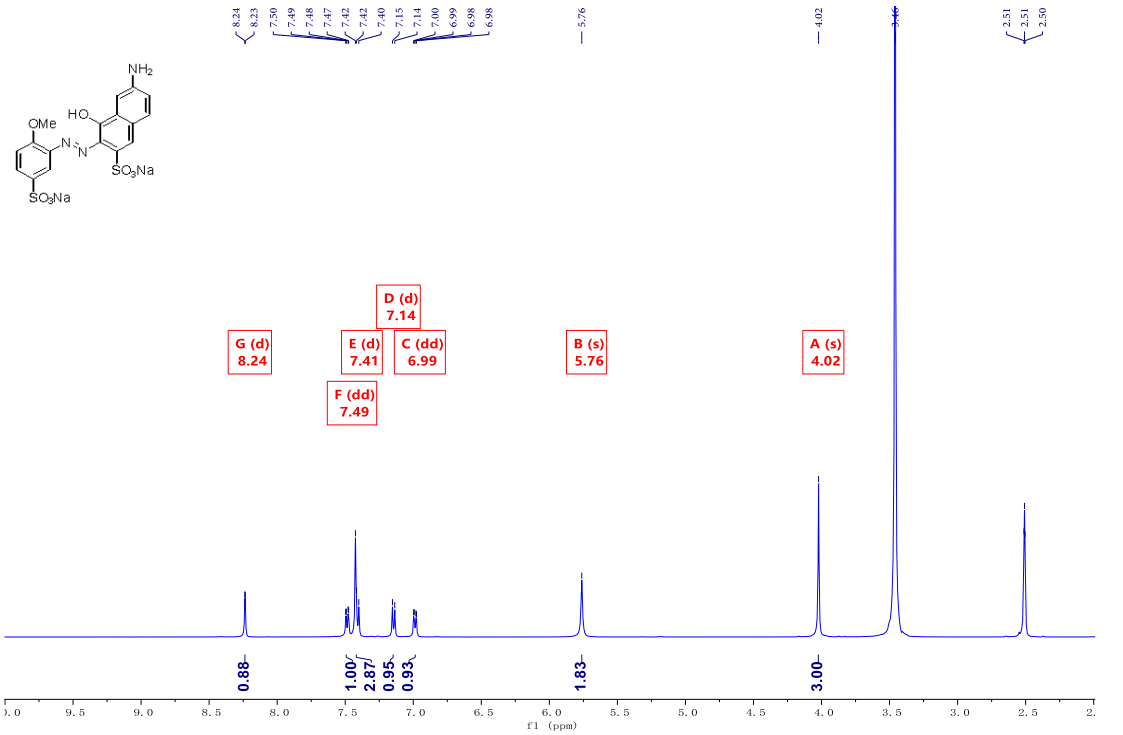


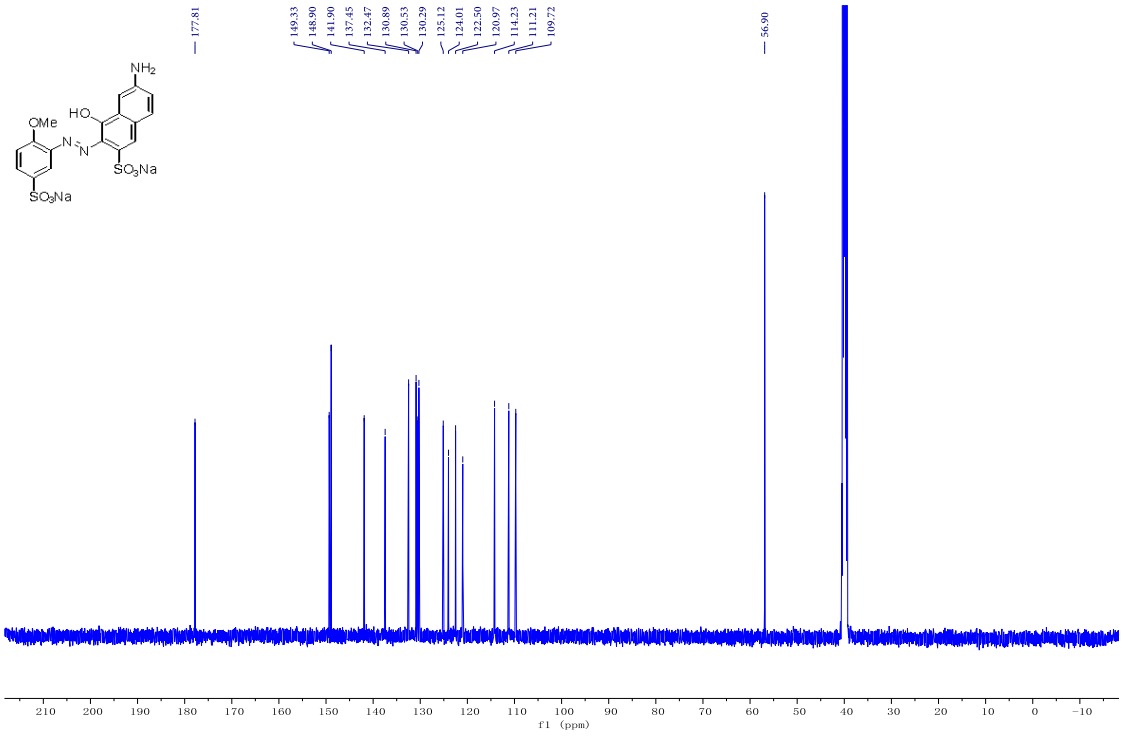
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)naphthalene-2-sulfonate (4a)



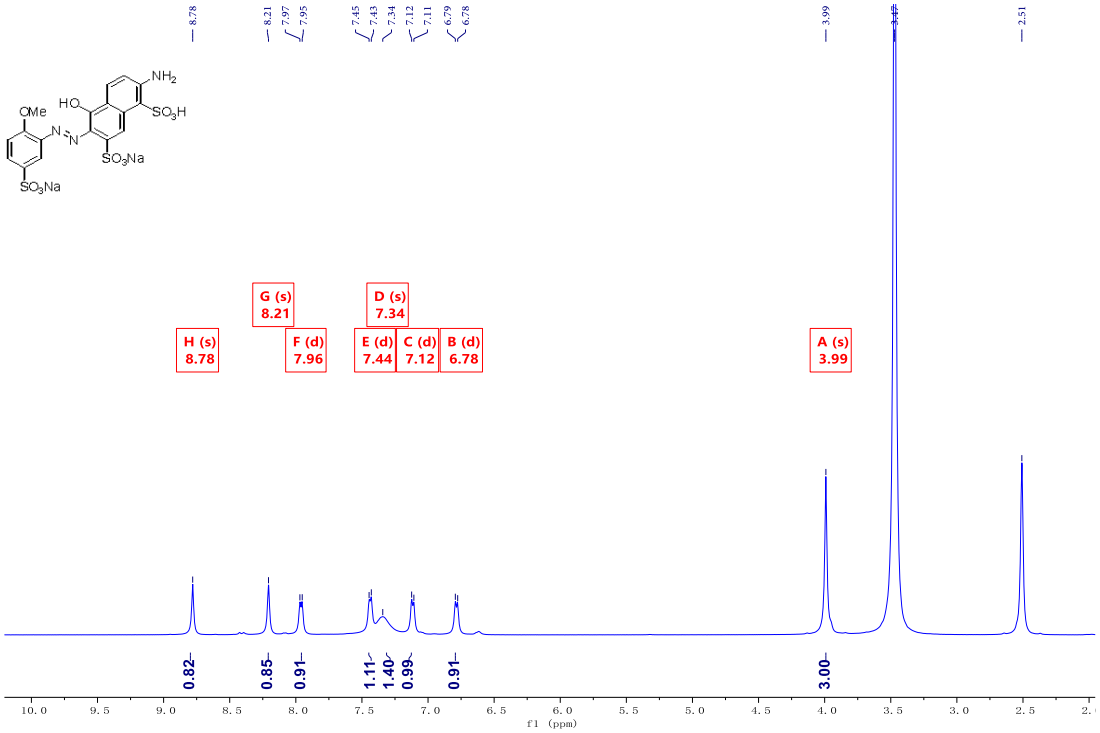


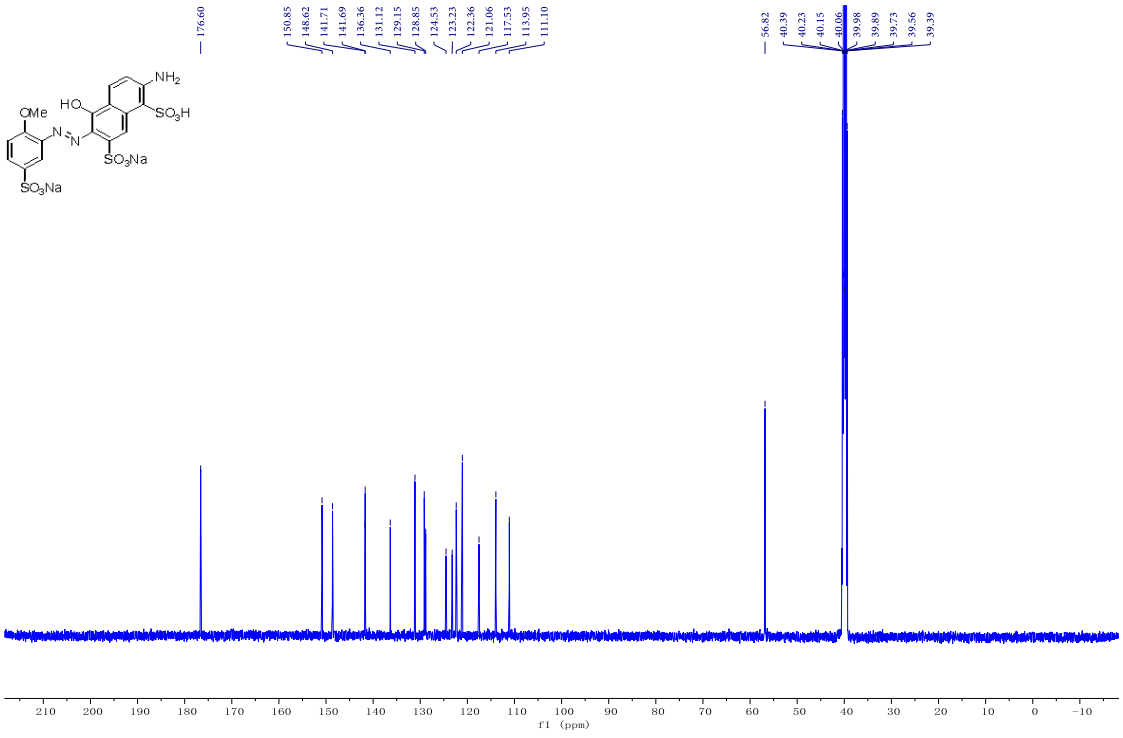
Sodium 6-amino-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)naphthalene-2-sulfonate (4b)



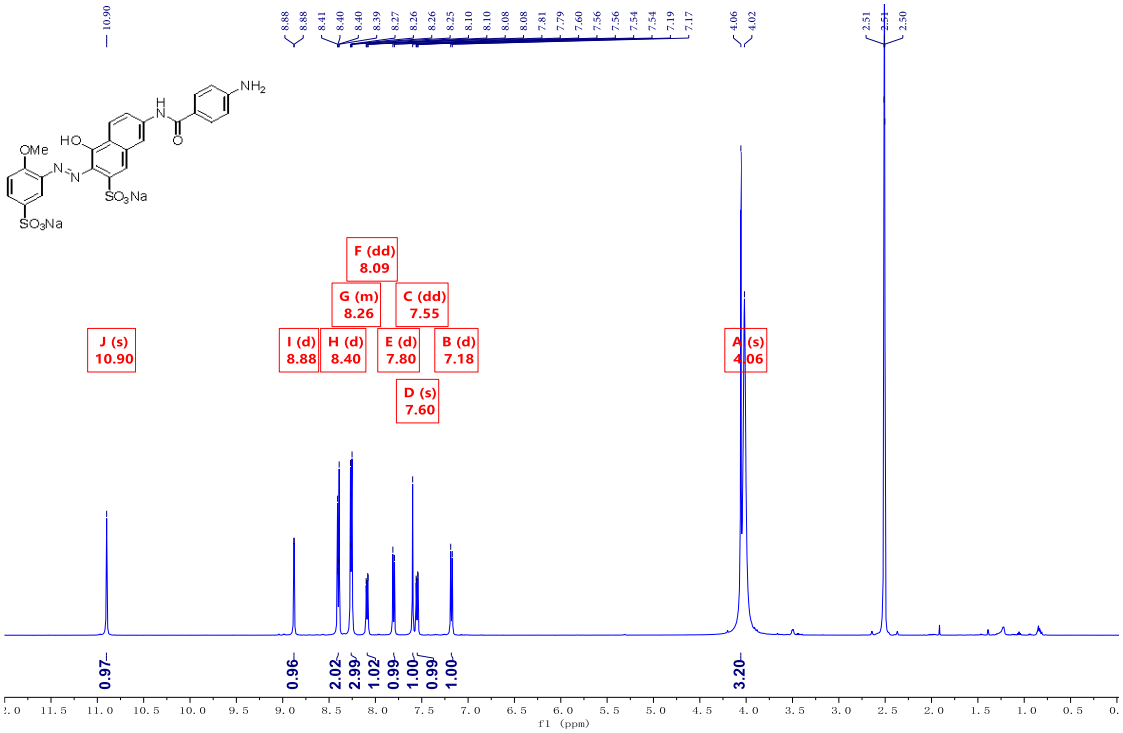


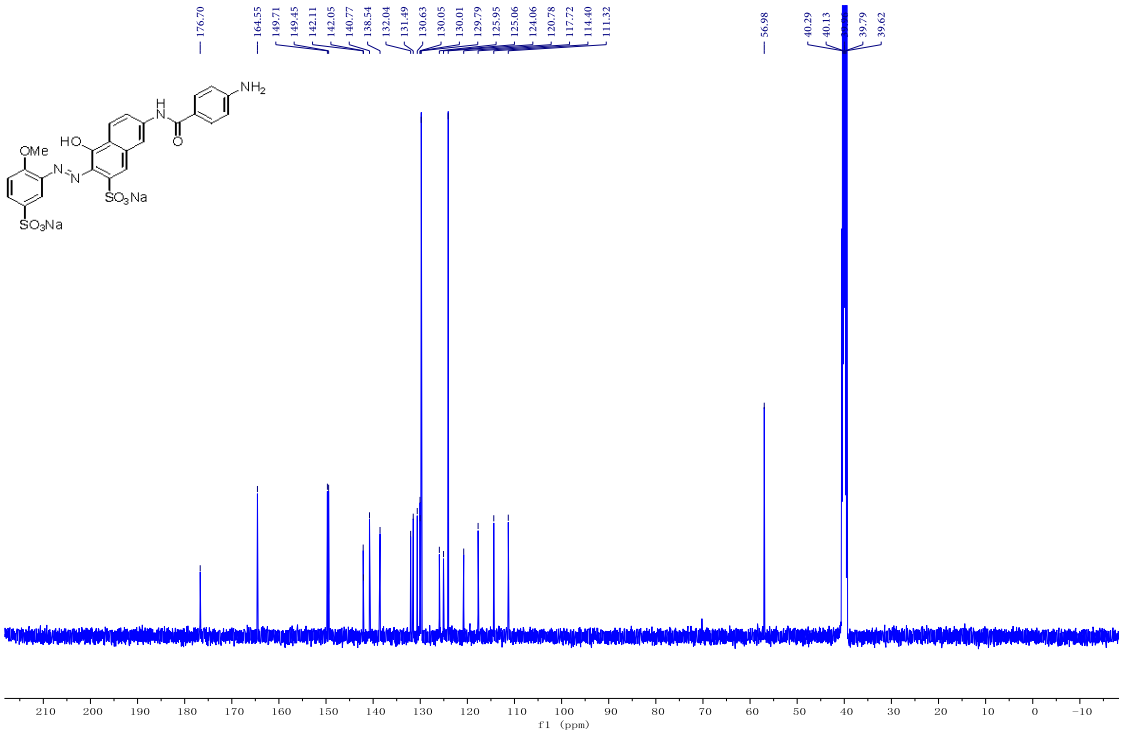
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)-8-sulfonaphthalene-2-sulfonate (4c`)



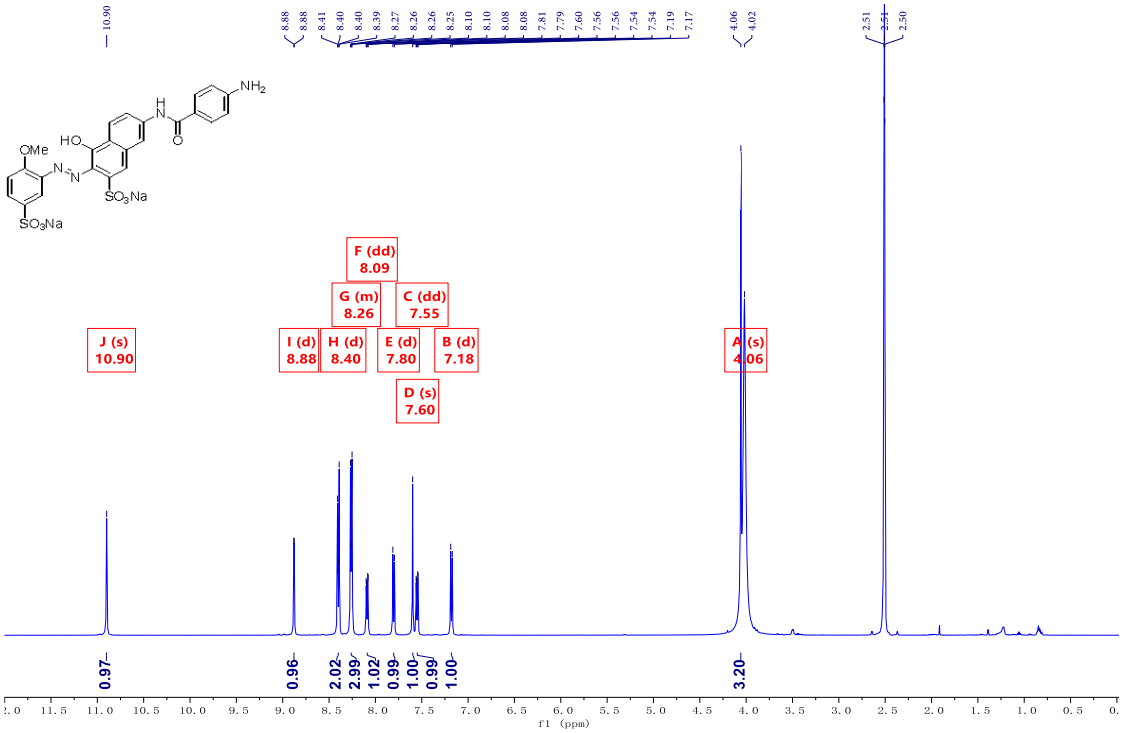


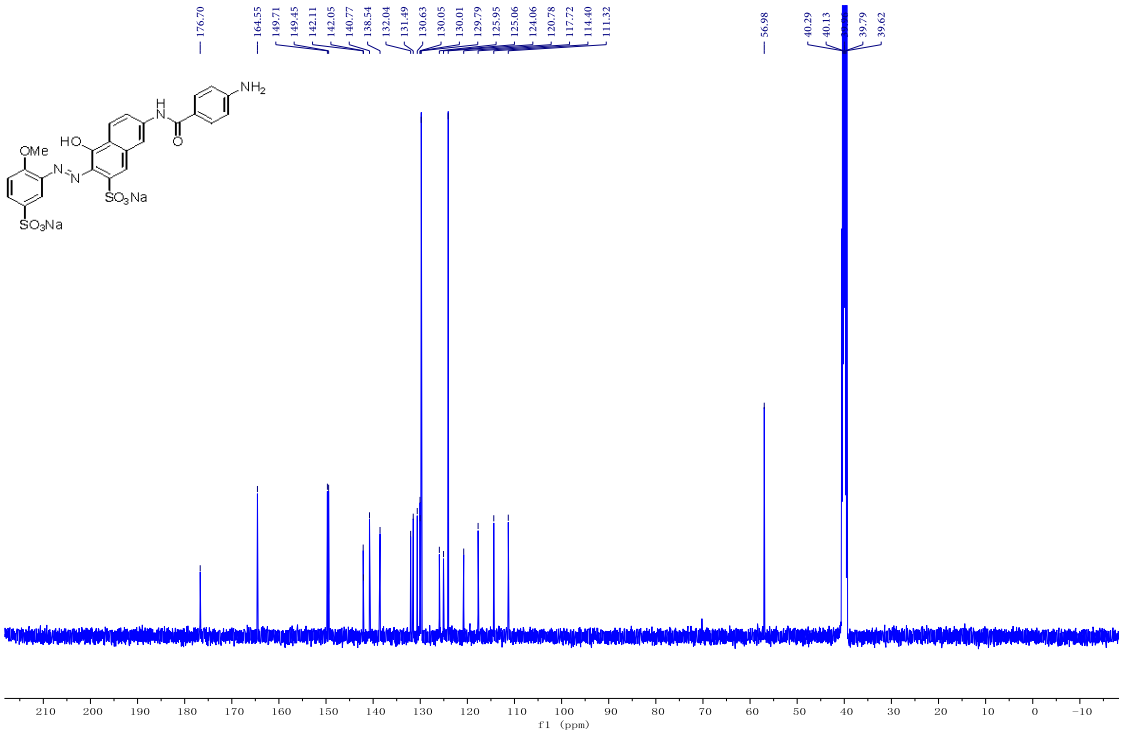
Sodium 7-(4-aminobenzamido)-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl) diazenyl) naphthalene-2-sulfonate (4d)



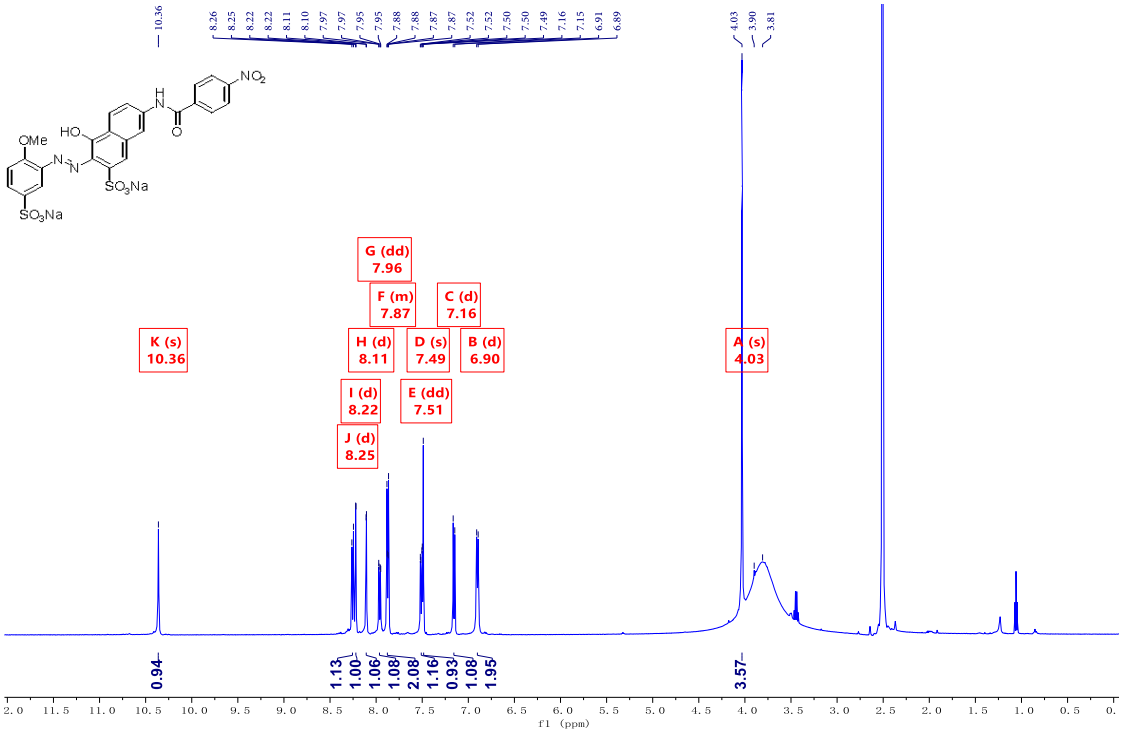


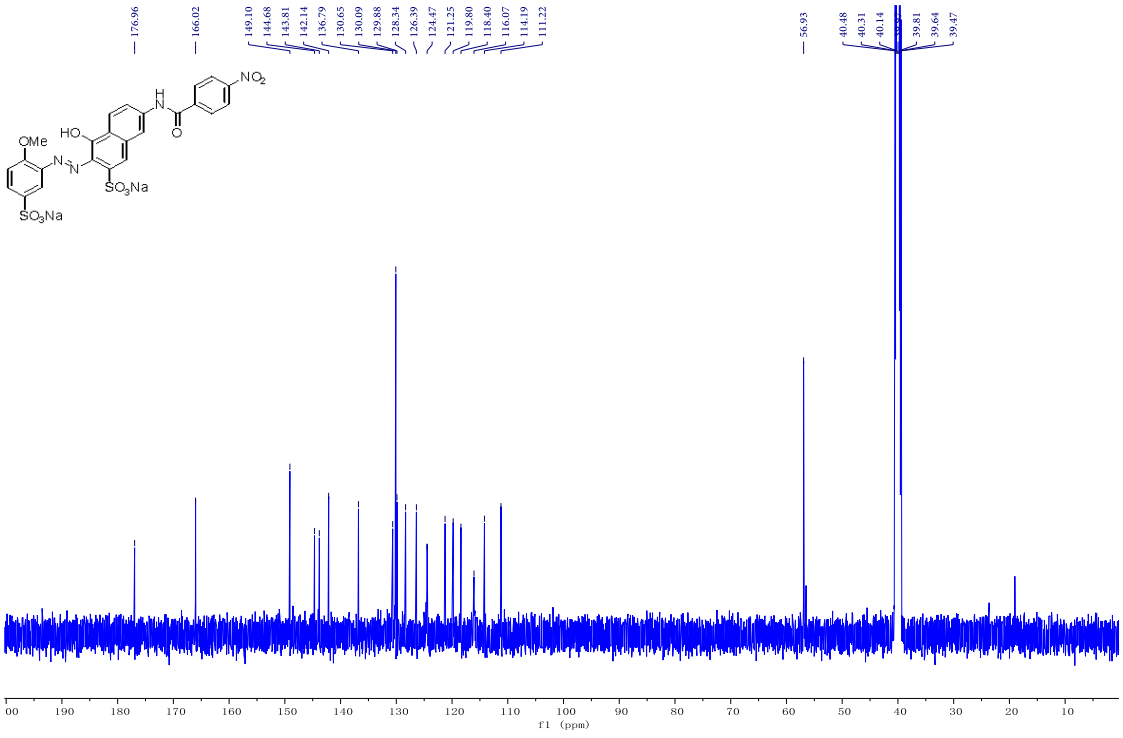
Sodium 7-benzamido-4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl) naphthalene-2-sulfonate (4e)



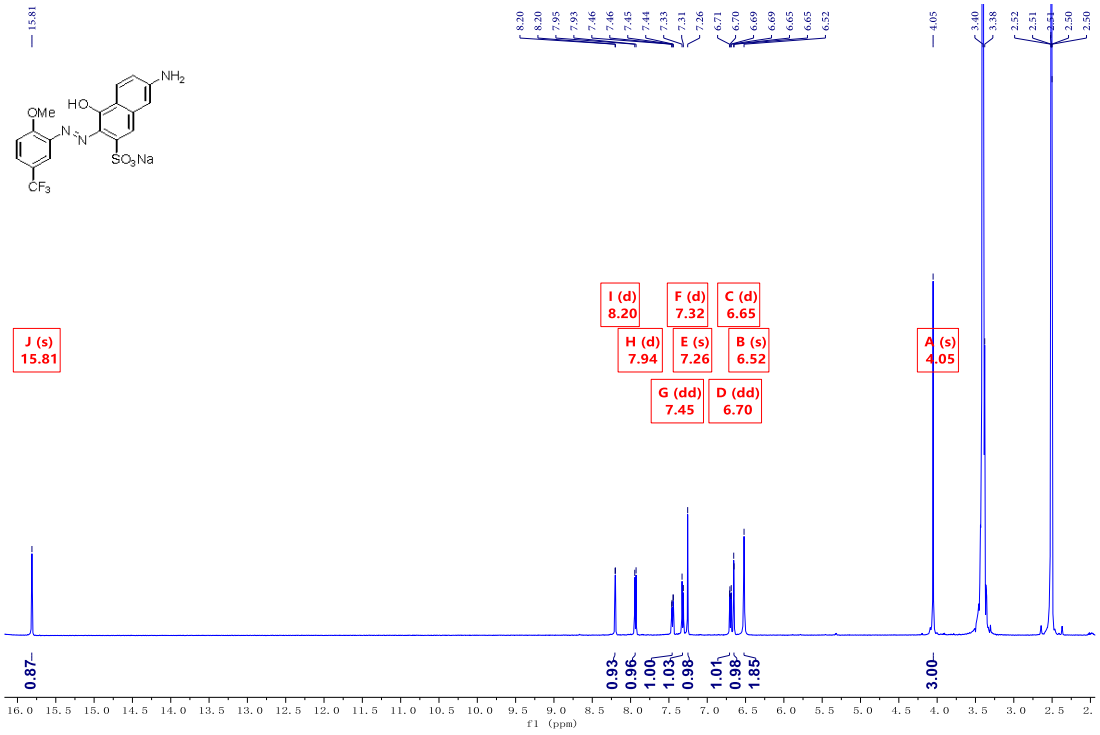


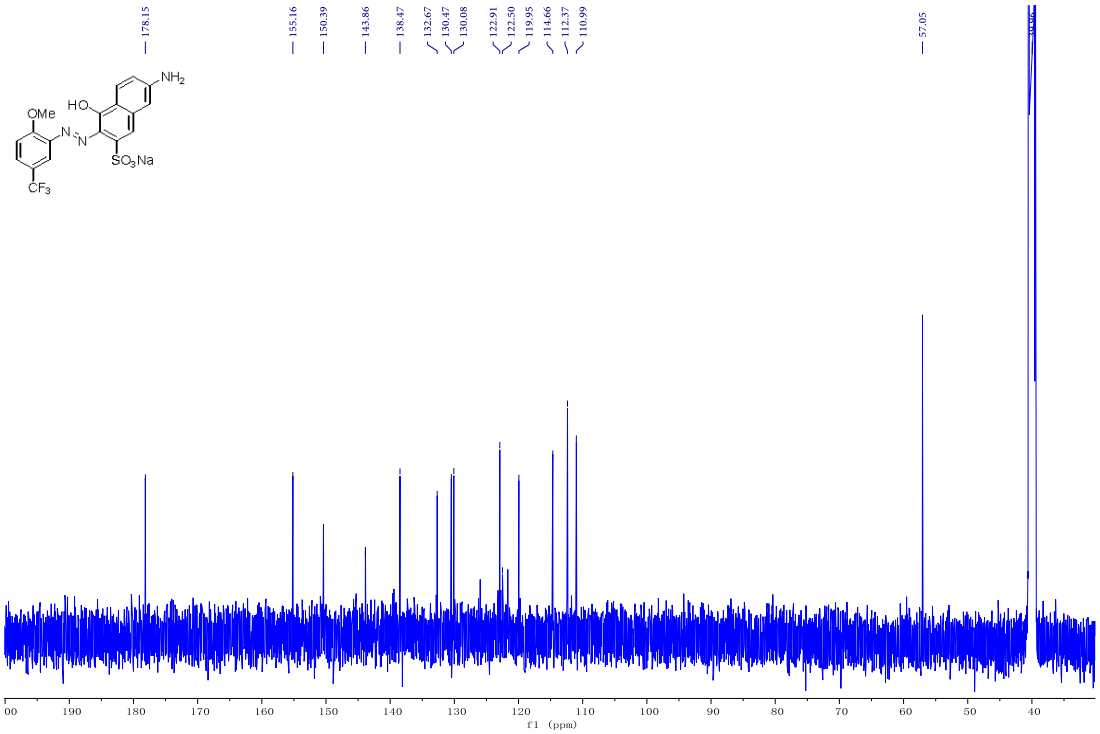
Sodium 4-hydroxy-3-((2-methoxy-5-sulfonatophenyl)diazenyl)-7-(4-nitrobenzamido) naphthalene-2-sulfonate (4f)



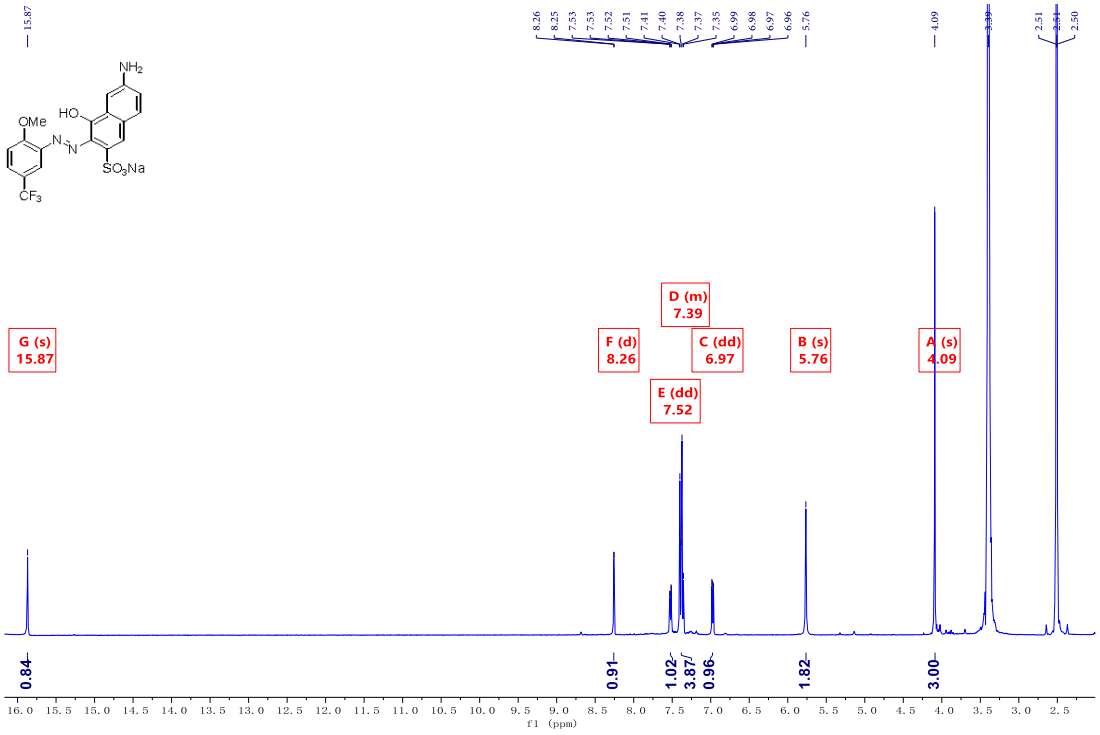


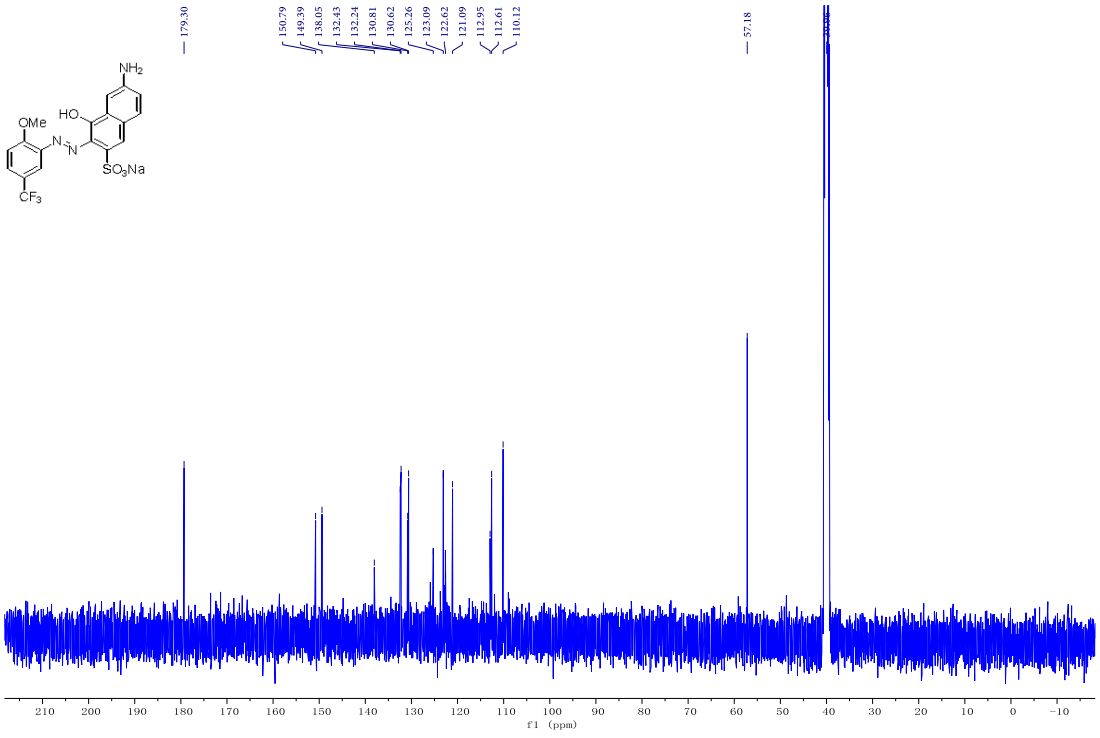
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-(trifluoromethyl)phenyl)diazenyl) naphthalene-2-sulfonate (5a)



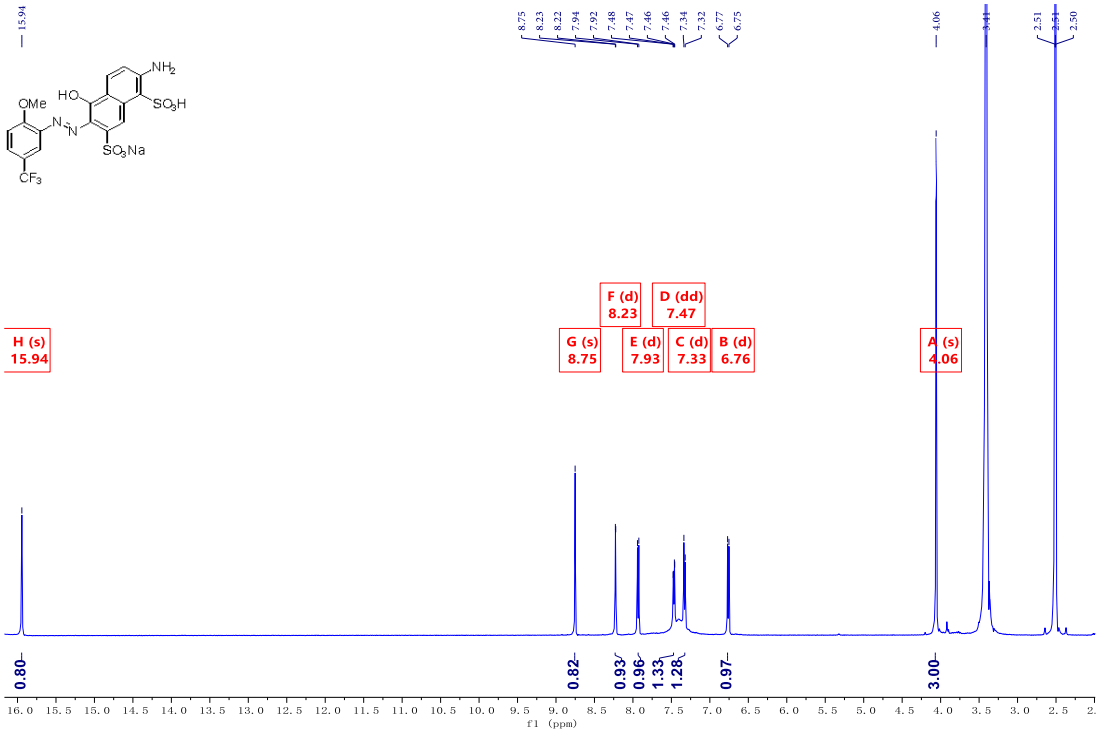


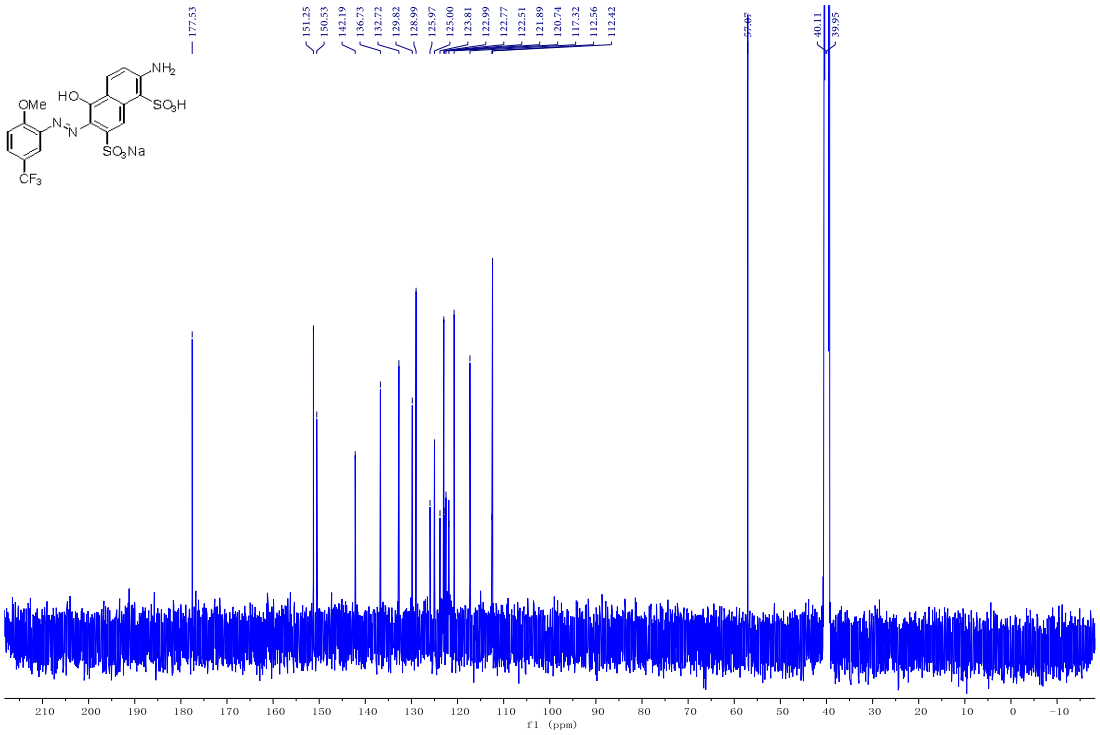
Sodium 6-amino-4-hydroxy-3-((2-methoxy-5-(trifluoromethyl)phenyl)diazenyl) naphthalene-2-sulfonate (5b)



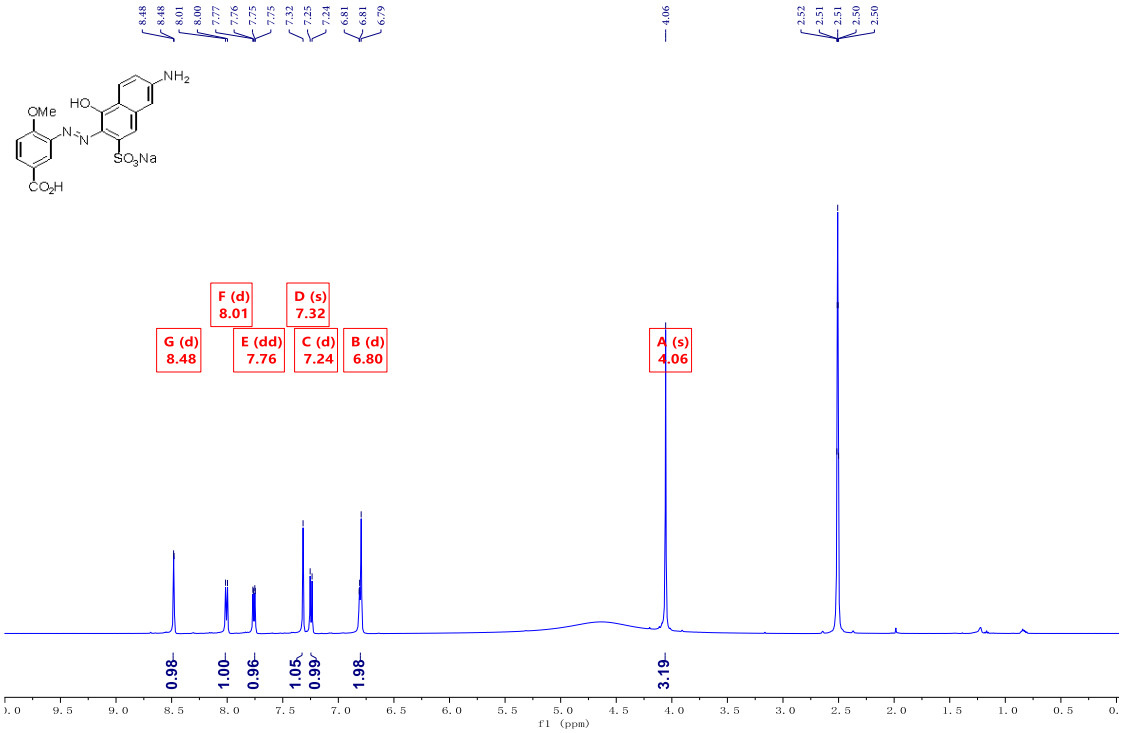


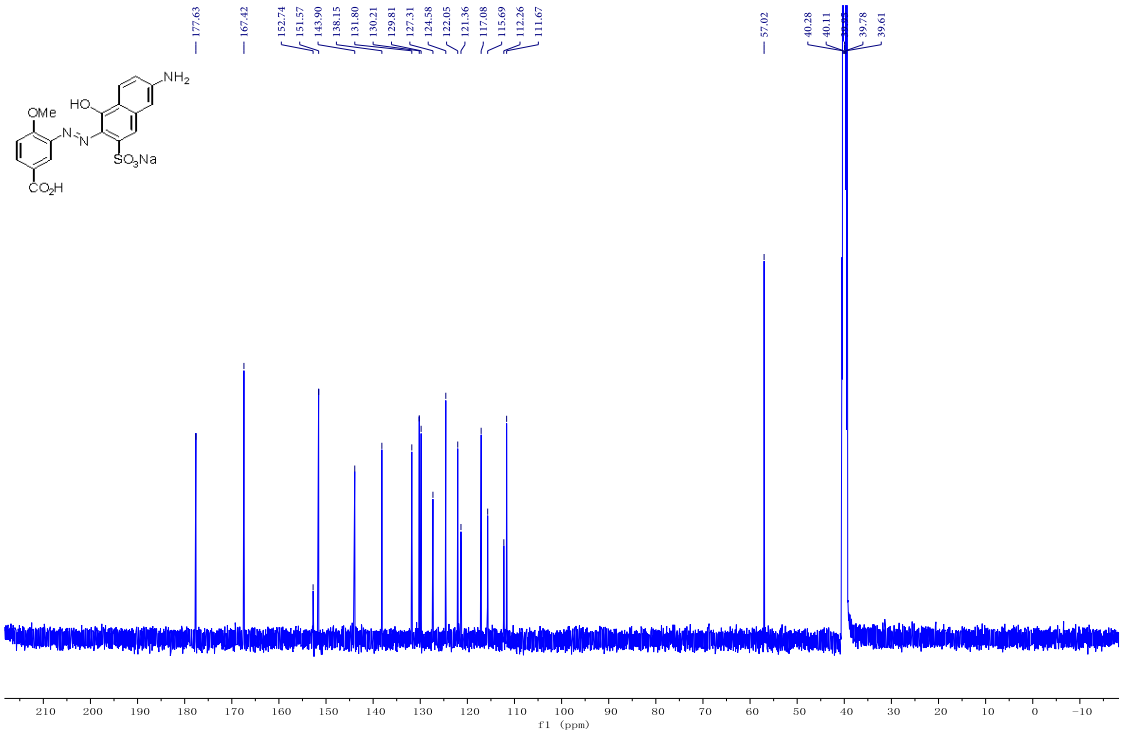
Sodium 7-amino-4-hydroxy-3-((2-methoxy-5-(trifluoromethyl)phenyl)diazenyl)-8-sulfonaphthalene-2-sulfonate (5c)



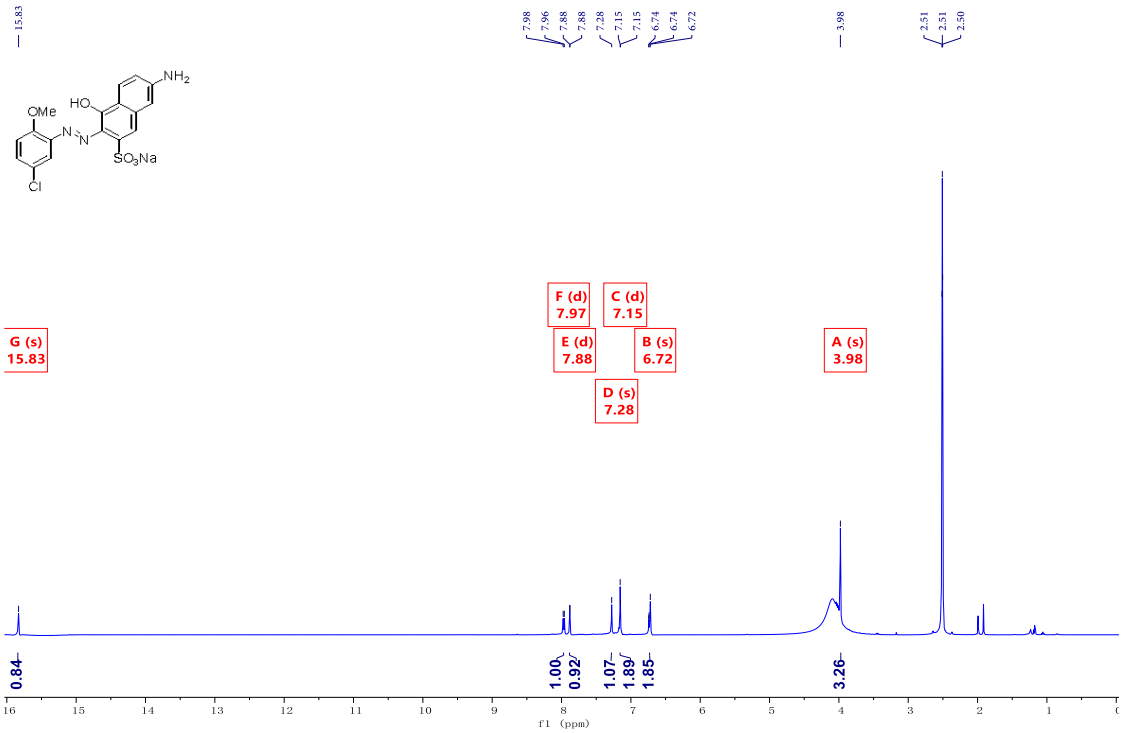


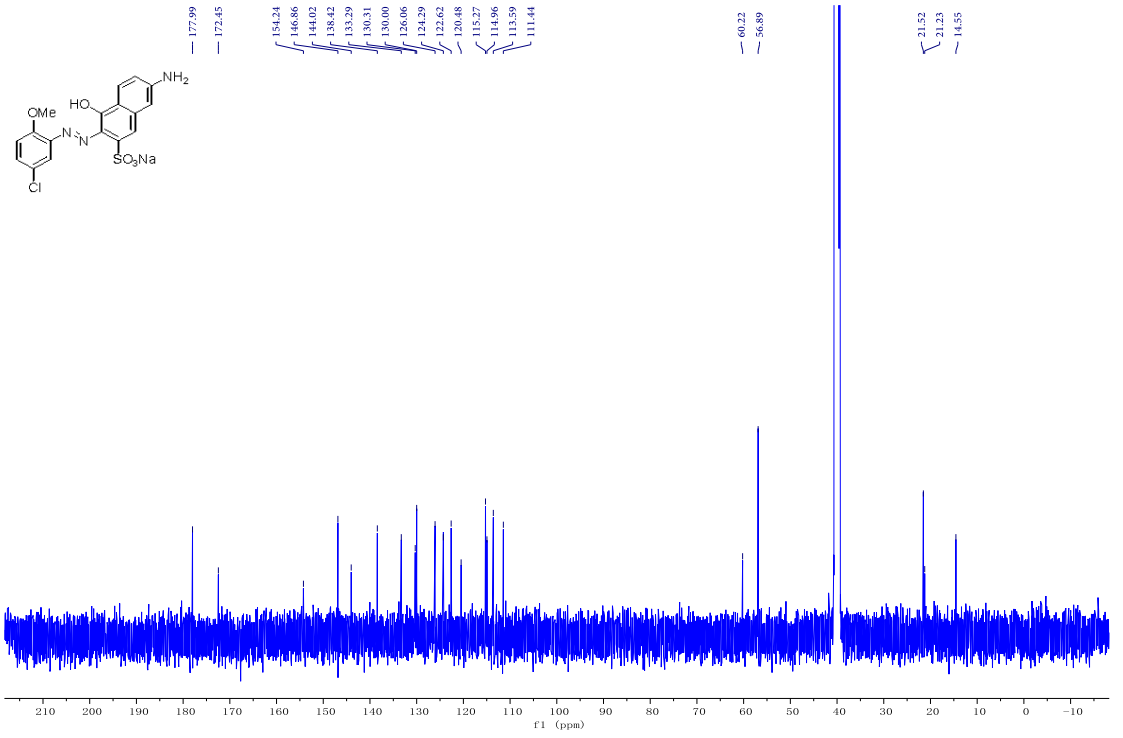
Sodium 7-amino-3-((5-carboxy-2-methoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (6a)



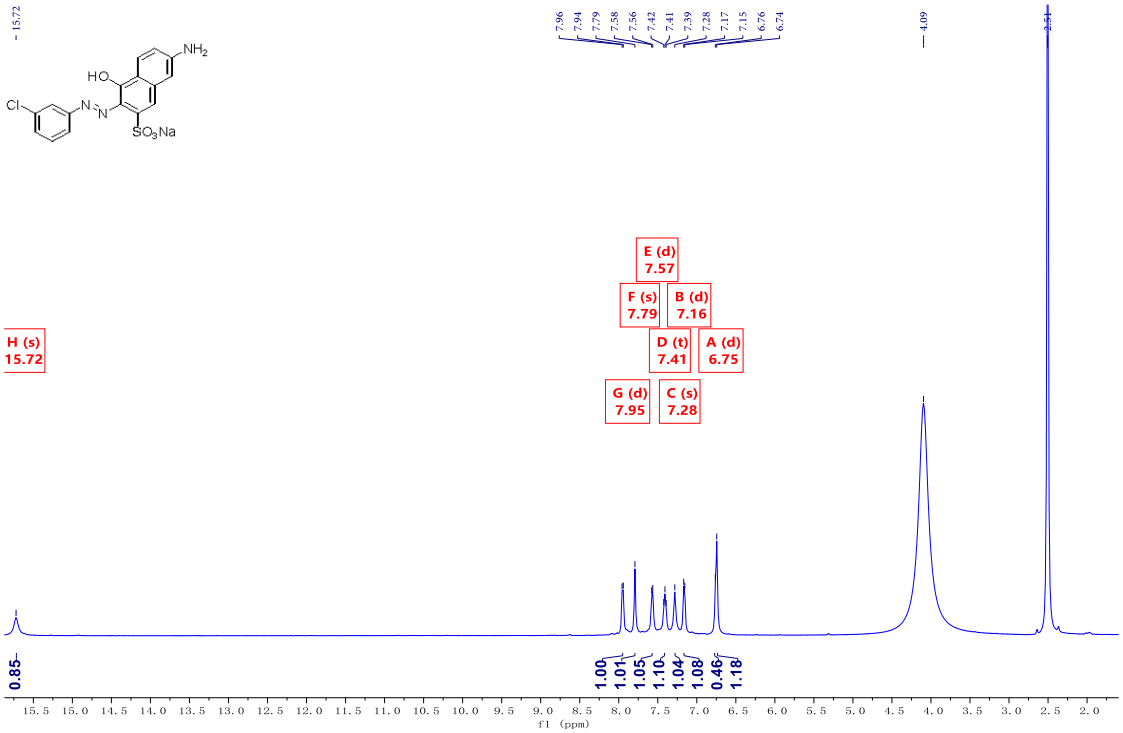


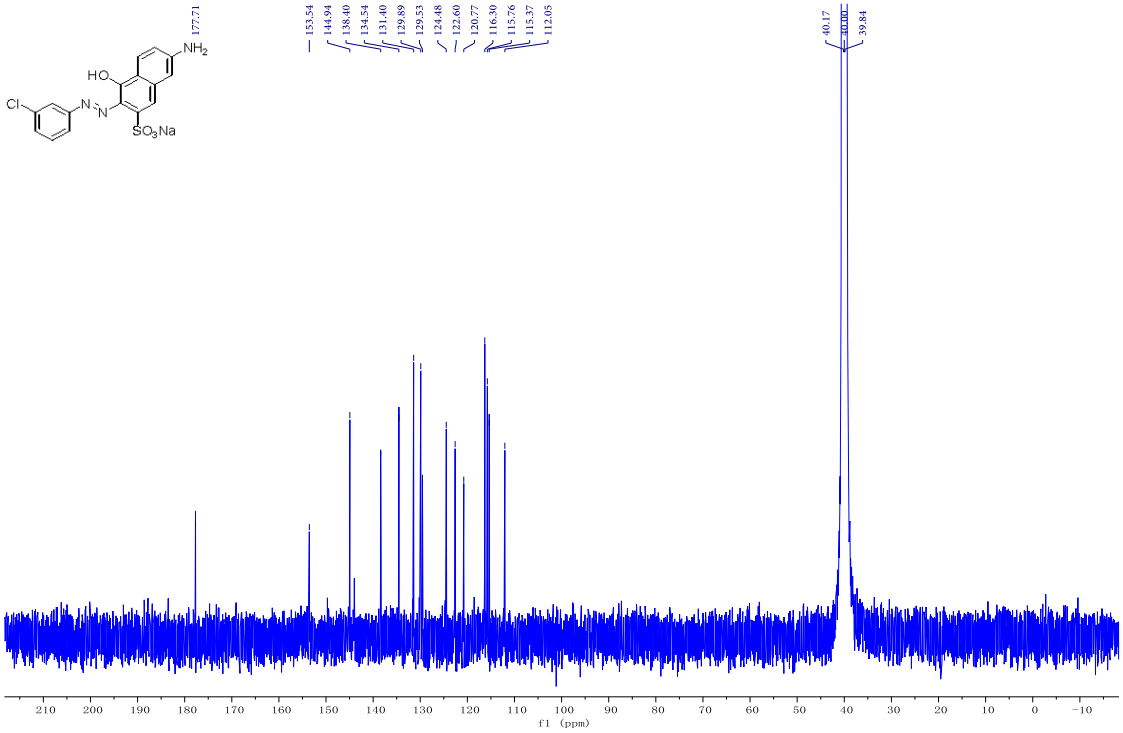
Sodium 7-amino-3-((5-chloro-2-methoxyphenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (7a)





Sodium 7-amino-3-((3-chlorophenyl)diazenyl)-4-hydroxynaphthalene-2-sulfonate (8a)





Sodium 7-amino-4-hydroxy-3-(p-tolyldiazenyl)naphthalene-2-sulfonate (9a)