Supplementary Information

Rh(II)-catalyzed denitrogenative 1-sulfonyl-1,2,3-triazole–1-alkyl-1,2,3-triazole cross-coupling as a route to 3-sulfamido-1*H*-pyrroles and 1,2,3-triazol-3-ium ylides

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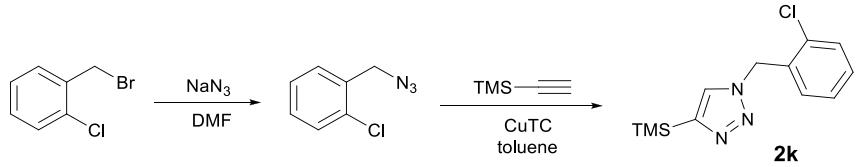
1. General experimental details

Melting points were determined on a hot stage microscope and are uncorrected. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectra were recorded on a Bruker AVANCE 400 spectrometer in solvent indicated below. Chemical shifts (δ) are reported in ppm downfield from tetramethylsilane. Crystallographic data for compound **3b** (CCDC 2044431) have been deposited with the Cambridge Crystallographic Data Centre. Column chromatography was performed on silica gel 60 M (0.04–0.063 mm). Thin-layer chromatography (TLC) was conducted on aluminum sheets precoated with SiO_2 ALUGRAM SIL G/UV254. All solvents were distilled and dried prior to use. 1,2-Dichloroethane (DCE) and dichloromethane (DCM) were washed with concentrated H_2SO_4, water, then distilled from P_2O_5 and stored over anhydrous K_2CO_3.

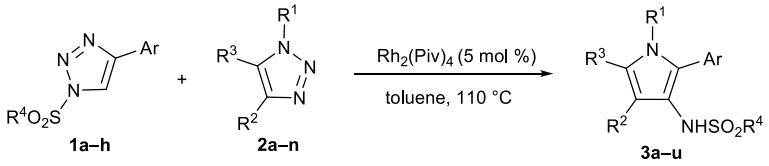
Triazoles **1a**–**h**[1] and triazoles **2a–j**, **l–p**[2] were synthesized according to the published procedures and they have full characterization data.

2. Synthesis of triazole 2k



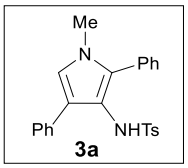
To a solution of sodium azide (650 mg, 10 mmol) in DMF (20 mL) 1-(bromomethyl)-2-chlorobenzene (2.05 g, 10 mmol) was added dropwise at 5−10 °C. The resulting reaction mixture was stirred overnight, followed by the addition of cold water (40 mL) and toluene (25 mL). The water phase was extracted once with toluene (25 mL), and the combined organic phases were washed with water, brine and dried over anhydrous Na_2SO_4 at 3−5 °C. A cold toluene solution of azide was filtered, the insoluble material was washed with toluene (10 mL). To the combined cold phases ethynyltrimethylsilane (980 mg, 10 mmol) and copper thiophene-2-carboxylate (CuTC) (191 mg, 1 mmol) were added, and the resulting mixture was stirred overnight at room temperature. The reaction mixture was filtered through the pad of celite using DCM as eluent. The residue obtained after evaporation of the solvent was crystallized from Et_2O/hexane mixture (1:1, 2 mL) to give 0.929 g (35%) of 1-(2-chlorobenzyl)-4-(trimethylsilyl)-1*H*-1,2,3-triazole **2k** as a white solid. M.p. 74−76 °C (Et_2O/hexane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.45–7.43 (m, 1H), 7.33–7.25 (m, 2H), 7.16–7.14 (m, 1H), 5.71 (s, 2H), 0.33 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.3, 132.9, 130.2, 130.0, 129.8, 129.3 (br), 127.6, 50.7, -1.1. HRMS−ESI: $[M + H]^+$ calcd for $C_{12}H_{17}{}^{35}ClN_3Si^+$ 266.0875, found 266.0881.

3. Synthesis of pyrroles 3



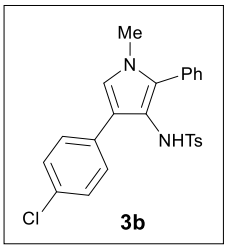
General procedure: A screw-cap tube was charged with 1-sulfonyl-1*H*-1,2,3-triazole **1a–h** (0.54 mmol), 1-alkyl-4-aryl-1*H*-1,2,3-triazole **2a–n** (0.3 mmol), and toluene (0.6 mL). To the mixture heated to 110 °C $Rh_2(Piv)_4$ (9.1 mg, 0.015 mmol) was added, and the cap was immediately screwed. The reaction mixture was heated at this temperature under stirring until full consumption of the starting materials (~15 min, control by TLC). The solvent was removed under reduced pressure, and the product was purified by column chromatography on silica gel.

4-Methyl-*N*-(1-methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)benzenesulfonamide (3a)



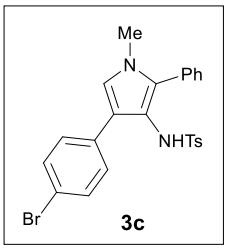
Compound **3a** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (110 mg, yield 91%). M.p. 131−132 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.36 (m, 2H), 7.36–7.30 (m, 3H), 7.27–7.15 (m, 7H), 6.85–6.80 (m, 2H), 6.70 (s, 1H), 6.45 (s, 1H), 3.48 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 136.7, 134.2, 132.9, 130.2, 130.2, 128.8, 128.2, 128.1, 127.6, 127.4, 127.0, 125.6, 122.5, 119.4, 113.6, 35.2, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{24}H_{22}N_2NaO_2S^+$ 425.1294, found 425.1286.

***N*-(4-(4-Chlorophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3b)**



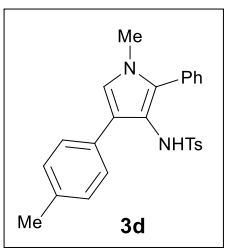
Compound **3b** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 4-(4-chlorophenyl)-1-methyl-1*H*-1,2,3-triazole **2b** (58 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (84 mg, yield 64%). Mp: 193−194 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.34 (m, 3H), 7.31–7.29 (m, 2H), 7.26–7.24 (m, 2H), 7.22–7.19 (m, 2H), 7.18–7.16 (m, 2H), 6.87–6.85 (m, 2H), 6.69 (s, 1H), 6.40 (s, 1H), 3.48 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 136.8, 133.3, 132.8, 131.4, 130.1, 129.9, 128.8, 128.6, 128.3, 128.2, 127.7, 127.0, 121.3, 119.4, 113.5, 35.2, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{24}H_{21}{}^{35}ClN_2NaO_2S^+$ 459.0904, found 459.0896.

_N_-(4-(4-Bromophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3c)



Compound **3c** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 4-(4-bromophenyl)-1-methyl-1*H*-1,2,3-triazole **2c** (71 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (76 mg, yield 53%). M.p. 196−197 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.34 (m, 3H), 7.32–7.30 (m, 2H), 7.25–7.20 (m, 6H), 6.89–6.87 (m, 2H), 6.70 (s, 1H), 6.18 (s, 1H), 3.49 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 136.8, 133.34, 133.25, 131.1, 130.2, 129.9, 128.91, 128.86, 128.3, 127.8, 127.0, 121.3, 119.6, 119.3, 113.5, 35.2, 21.5. HRMS−ESI: $[M + Na]^+$ calcd for $C_{24}H_{21}{}^{79}BrN_2NaO_2S^+$ 503.0399, found 503.0399.

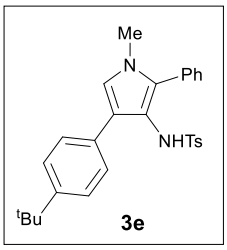
4-Methyl-_N_-(1-methyl-2-phenyl-4-(*p*-tolyl)-1*H*-pyrrol-3-yl)benzenesulfonamide (3d)



Compound **3d** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-methyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole **1d** (52 mg, 0.3

mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (54 mg, yield 43%). M.p. 185−186 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34–7.32 (m, 3H), 7.27–7.23 (m, 4H), 7.22–7.20 (m, 2H), 7.07–7.05 (m, 2H), 6.84–6.82 (m, 2H), 6.68 (s, 1H), 6.31 (s, 1H), 3.48 (s, 3H), 2.37 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 136.9, 135.2, 132.8, 131.2, 130.3, 130.2, 128.9, 128.7, 128.2, 127.5, 127.3, 127.0, 122.5, 119.1, 113.6, 35.2, 21.4, 21.1. HRMS−ESI: $[M + H]^+$ calcd for $C_{25}H_{25}N_2O_2S^+$ 417.1631, found 417.1616.

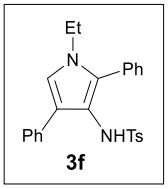
_N_-(4-(4-(*tert*-Butyl)phenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3e)



3e

Compound **3e** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 4-(4-(*tert*-butyl)phenyl)-1-methyl-1*H*-1,2,3-triazole **2e** (65 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (70 mg, yield 51%). M.p. 223−225 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.32 (m, 3H), 7.26–7.21 (m, 8H), 6.85–6.80 (m, 2H), 6.65 (s, 1H), 6.09 (s, 1H), 3.50 (s, 3H), 2.31 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.5, 142.2, 136.6, 132.8, 131.1, 130.4, 130.2, 128.7, 128.2, 127.5, 127.1, 127.0, 125.0, 122.4, 119.2, 113.5, 35.2, 34.3, 31.4, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{28}H_{30}N_2NaO_2S^+$ 481.1920, found 481.1912.

_N_-(1-Ethyl-2,4-diphenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3f)

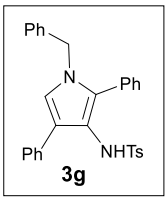


3f

Compound **3f** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-ethyl-4-phenyl-1*H*-1,2,3-triazole **2f** (52 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (75 mg, yield 60%). M.p. 153−154 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.38 (m, 2H), 7.33–7.32 (m, 3H), 7.26–7.22 (m, 4H), 7.20–7.17 (m, 3H), 6.85–6.83 (m, 2H), 6.77 (s, 1H), 6.26 (s, 1H), 3.81 (q, 2H, *J* 7.2 Hz), 2.31 (s, 3H), 1.24 (t, 3H, *J* 7.2 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3,

136.7, 134.4, 132.4, 130.4, 130.2, 128.8, 128.2, 128.1, 127.6, 127.3, 127.0, 125.6, 122.6, 117.2, 113.5, 42.3, 21.4, 16.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{25}H_{24}N_2NaO_2S^+$ 439.1456, found 439.1448.

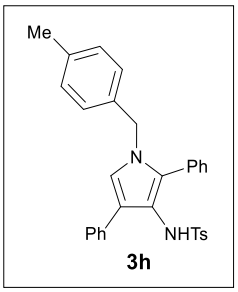
_N_-(1-Benzyl-2,4-diphenyl-1_H_-pyrrol-3-yl)-4-methylbenzenesulfonamide (3g)



3g

Compound **3g** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-benzyl-4-phenyl-1*H*-1,2,3-triazole **2g** (71 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (83 mg, yield 58%). M.p. 194−195 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42–7.40 (m, 2H), 7.31–7.24 (m, 10H), 7.20–7.16 (m, 1H), 7.09–7.08 (m, 2H), 7.00–6.96 (m, 2H), 6.86–6.84 (m, 2H), 6.75 (s, 1H), 6.31 (s, 1H), 4.95 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 137.7, 136.4, 134.1, 133.0, 130.2, 130.0, 128.8, 128.6, 128.3, 128.1, 127.8, 127.6, 127.4, 127.1, 126.7, 125.8, 123.0, 118.7, 114.0, 51.1, 21.4; HRMS−ESI: $[M + Na]^+$ calcd for $C_{30}H_{26}N_2NaO_2S^+$ 501.1613, found 501.1598.

4-Methyl-_N_-(1-(4-methylbenzyl)-2,4-diphenyl-1_H_-pyrrol-3-yl)benzenesulfonamide (3h)

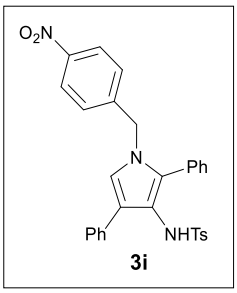


3h

Compound **3h** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-(4-methylbenzyl)-4-phenyl-1*H*-1,2,3-triazole **2h** (75 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (86 mg, yield 58%). M.p. 186−187 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.37 (m, 2H), 7.30–7.23 (m, 7H), 7.18–7.15 (m, 1H), 7.12–7.09 (m, 4H), 6.88–6.83 (m, 4H), 6.72 (s, 1H), 6.23 (s, 1H), 4.90 (s, 2H), 2.35 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.4, 137.3, 136.4, 134.7, 134.2, 133.0, 130.3, 130.1, 129.3, 128.8, 128.2, 128.1, 127.7, 127.4, 127.1, 126.7,

125.7, 122.9, 118.6, 113.8, 50.9, 21.4, 21.0. HRMS−ESI: $[M + Na]^+$ calcd for $C_{31}H_{28}N_2NaO_2S^+$ 515.1769, found 515.1786.

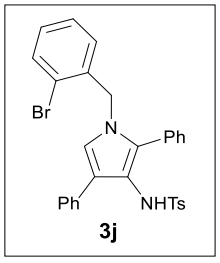
4-Methyl-*N*-(1-(4-nitrobenzyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)benzenesulfonamide (3i)



3i

Compound **3i** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-(4-nitrobenzyl)-4-phenyl-1*H*-1,2,3-triazole **2i** (84 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. Yellow solid (89 mg, yield 57%). M.p. 207−209 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14–8.12 (m, 2H), 7.37–7.35 (m, 2H), 7.30–7.17 (m, 8H), 7.07–7.03 (m, 4H), 6.87–6.85 (m ,2H), 6.76 (s, 1H), 6.13 (s, 1H), 5.06 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 145.1, 142.6, 136.5, 133.7, 133.2, 130.2, 129.6, 128.9, 128.4, 128.2, 128.1, 127.4, 127.2, 127.1, 126.1, 123.9, 123.8, 118.6, 114.8, 50.7, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{30}H_{25}N_3NaO_4S^+$ 546.1463, found 546.1476.

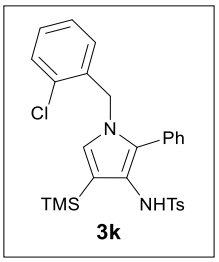
***N*-(1-(2-Bromobenzyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3j)**



3j

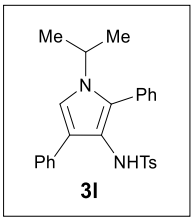
Compound **3j** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-(2-bromobenzyl)-4-phenyl-1*H*-1,2,3-triazole **2j** (94 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (92 mg, yield 55%). M.p. 195−196 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.51 (m, 1H), 7.42–7.39 (m, 2H), 7.30–7.23 (m, 8H), 7.20–7.14 (m, 2H), 7.06–7.04 (m, 2H), 6.86–6.84 (m, 2H), 6.73 (s, 1H), 6.71–6.69 (m, 1H), 6.17 (s, 1H), 5.01 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 137.2, 136.4, 134.0, 133.1, 132.7, 130.0, 129.7, 129.1, 128.8, 128.3, 128.2, 128.1, 127.9, 127.8, 127.4, 127.1, 125.9, 123.3, 122.0, 118.7, 114.2, 51.4, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{30}H_{25}{}^{79}BrN_2NaO_2S^+$ 579.0718, found 579.0703.

***N*-(1-(2-Chlorobenzyl)-2-phenyl-4-(trimethylsilyl)-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3k)**



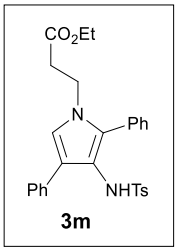
Compound **3k** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-(2-chlorobenzyl)-4-(trimethylsilyl)-1*H*-1,2,3-triazole **2k** (80 mg, 0.3 mmol) and using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (102 mg, yield 67%). M.p. 146−147 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32–7.30 (m,1H), 7.24–7.19 (m, 4H), 7.18–7.14 (m, 1H), 7.07–7.03 (m, 2H), 6.91–6.89 (m, 2H), 6.65 (s, 1H), 6.59–6.57 (m, 2H), 6.51–6.49 (m, 1H), 6.10 (s, 1H), 4.92 (s, 2H), 2.32 (s, 3H), 0.40 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.4, 136.3, 135.9, 131.9, 131.8, 129.6, 129.4, 129.3, 128.9, 128.6, 128.2, 127.7, 127.4, 127.2, 127.1, 127.0, 121.2, 118.1, 48.7, 21.4, 0.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{27}H_{29}{}^{35}ClN_2NaO_2SSi^+$ 531.1305, found 531.1307.

***N*-(1-Isopropyl-2,4-diphenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3l)**



Compound **3l** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-isopropyl-4-phenyl-1*H*-1,2,3-triazole **2l** (56 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (44 mg, yield 34%). M.p. 169−171 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42–7.40 (m, 2H), 7.34–7.32 (m, 3H), 7.26–7.21 (m, 4H), 7.18–7.13 (m, 3H), 6.85–6.84 (m, 3H), 6.19 (s, 1H), 4.21 (sept, 1H, *J* 6.7 Hz), 2.32 (s, 3H), 1.35 (d, 6H, *J* 6.7 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 136.7, 134.6, 132.3, 130.5, 130.4, 128.8, 128.3, 128.1, 127.6, 127.2, 127.0, 125.5, 122.6, 113.6, 113.1, 47.7, 23.7, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{26}H_{26}N_2NaO_2S^+$ 453.1613, found 453.1611.

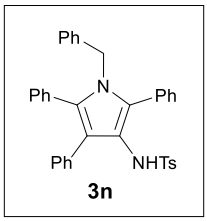
Ethyl 3-(3-((4-methylphenyl)sulfonamido)-2,4-diphenyl-1*H*-pyrrol-1-yl)propanoate (3m)



3m

Compound **3m** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and ethyl 3-(4-phenyl-1*H*-1,2,3-triazol-1-yl)propanoate **2m** (74 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (73 mg, yield 50%). M.p. 123−125 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.32 (m, 5H), 7.25–7.15 (m, 7H), 6.85–6.83 (m, 2H), 6.76 (s, 1H), 6.06 (s, 1H), 4.09 (m, 4H), 2.51 (t, 2H, *J* 7.1 Hz), 2.31 (s, 3H), 1.21 (t, 3H, *J* 7.1 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 142.4, 136.6, 134.1, 132.4, 130.2, 130.0, 128.8, 128.4, 128.1, 127.9, 127.3, 127.0, 125.7, 122.8, 118.2, 114.1, 60.8, 43.1, 35.8, 21.4, 14.1. HRMS−ESI: $[M + Na]^+$ calcd for $C_{28}H_{28}N_2NaO_4S^+$ 511.1667, found 511.1666.

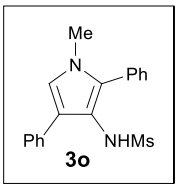
***N*-(1-Benzyl-2,4,5-triphenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3n)**



3n

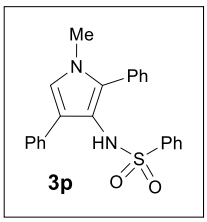
Compound **3n** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-benzyl-4,5-diphenyl-1*H*-1,2,3-triazole **2n** (93 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. Pale yellow oil (67 mg, yield 40%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28–7.25 (m, 3H), 7.20–7.18 (m, 7H), 7.14–7.12 (m, 3H), 7.09–7.06 (m, 5H), 6.95–6.92 (m, 2H), 6.86–6.84 (m, 2H), 6.60–6.57 (m, 2H), 6.15 (s, 1H), 4.98 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 138.6, 136.5, 133.7, 132.7, 132.0, 131.14, 131.06, 130.7, 130.5, 129.8, 128.8, 128.2 (2C), 128.1, 127.7, 127.7, 127.4, 127.0, 126.9, 126.0, 125.5, 121.8, 115.2, 48.6, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{36}H_{30}N_2NaO_2S^+$ 577.1926, found 577.1928.

***N*-(1-Methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)methanesulfonamide (3o)**



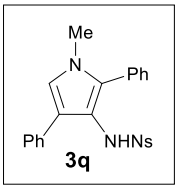
Compound **3o** was prepared according to the general procedure from 1-(methylsulfonyl)-4-phenyl-1*H*-1,2,3-triazole **1b** (120 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (39 mg, yield 42%). M.p. 144−146 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60–7.57 (m, 2H), 7.50–7.48 (m, 4H), 7.45–7.40 (m, 3H), 7.31–7.27 (m, 1H), 6.81 (s, 1H), 5.93 (s, 1H), 3.59 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.1, 132.9, 130.5, 130.3, 128.7 (2C), 128.3, 127.9, 126.4, 122.6, 119.4, 113.8, 40.6, 35.3. HRMS−ESI: $[M + Na]^+$ calcd for $C_{18}H_{18}N_2NaO_2S^+$ 349.0987, found 349.0977.

***N*-(1-Methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)benzenesulfonamide (3p)**



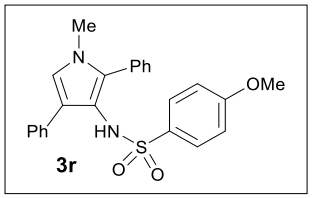
Compound **3p** was prepared according to the general procedure from 4-phenyl-1-(phenylsulfonyl)-1*H*-1,2,3-triazole **1c** (154 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (55 mg, yield 47%). M.p. 188−189 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.17 (m, 13H), 7.09–7.05 (m, 2H), 6.71 (s, 1H), 6.29 (s, 1H), 3.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 134.1, 132.8, 131.9, 130.2, 130.1, 128.4, 128.3, 128.2, 127.7, 127.4, 127.0, 125.9, 122.5, 119.4, 113.5, 35.2. HRMS−ESI: $[M + Na]^+$ calcd for $C_{23}H_{20}N_2NaO_2S^+$ 411.1143, found 411.1136.

***N*-(1-Methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)-4-nitrobenzenesulfonamide (3q)**



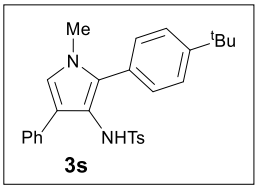
Compound **3q** was prepared according to the general procedure from 1-((4-nitrophenyl)sulfonyl)-4-phenyl-1*H*-1,2,3-triazole **1d** (178 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (74 mg, yield 57%). M.p. 208−210 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84–7.82 (m, 2H), 7.52–7.50 (m, 2H), 7.38–7.36 (m, 3H), 7.28–7.13 (m, 7H), 6.70 (s, 1H), 6.29 (s 1H), 3.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 145.4, 133.9, 133.6, 130.2, 130.0, 128.5, 128.4, 128.2, 128.1, 127.4, 126.1, 123.3, 122.6, 119.7, 112.4, 35.3. HRMS−ESI: $[M + H]^+$ calcd for $C_{23}H_{20}N_3O_4S^+$ 434.1169, found 434.1156.

4-Methoxy-*N*-(1-methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)benzenesulfonamide (3r)



Compound **3r** was prepared according to the general procedure from 1-((4-methoxyphenyl)sulfonyl)-4-phenyl-1*H*-1,2,3-triazole **1e** (170 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (30 mg, yield 24%). M.p. 180−181 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.31 (m, 5H), 7.28–7.23 (m, 6H), 7.18–7.14 (m, 1H), 6.70 (s, 1H), 6.52–6.49 (m, 2H), 6.14 (s, 1H), 3.80 (s, 3H), 3.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 134.2, 132.9, 131.3, 130.3, 130.2, 129.1, 128.3, 128.2, 127.7, 127.4, 125.8, 122.5, 119.4, 113.7, 113.4, 55.3, 35.2. HRMS−ESI: $[M + Na]^+$ calcd for $C_{24}H_{22}N_2NaO_3S^+$ 441.1243, found 441.1227.

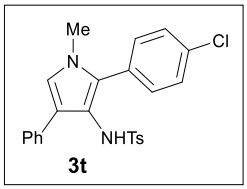
***N*-(2-(4-(*tert*-Butyl)phenyl)-1-methyl-4-phenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3s)**



Compound **3s** was prepared according to the general procedure from 4-(4-(*tert*-butyl)phenyl)-1-tosyl-1*H*-1,2,3-triazole **1f** (192 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (85 mg, yield 62%). M.p. 223−224 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.40 (m, 2H), 7.34–7.32 (m, 2H), 7.26–7.22 (m, 4H), 7.18–7.15 (m, 1H), 7.09–7.07 (m, 2H), 6.84–6.82

(m, 2H), 6.70 (s, 1H), 6.20 (s, 1H), 3.48 (s, 3H), 2.31 (s, 3H), 1.39 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 142.2, 136.6, 134.3, 132.9, 129.6, 128.7, 128.1, 127.3, 127.1, 127.0, 125.6, 125.1, 122.4, 119.2, 113.4, 35.2, 34.5, 31.3, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{28}H_{30}N_2NaO_2S^+$ 481.1926, found 481.1915.

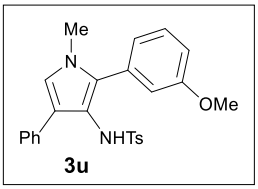
***N*-(2-(4-Chlorophenyl)-1-methyl-4-phenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3t)**



3t

Compound **3t** was prepared according to the general procedure from 4-(4-chlorophenyl)-1-tosyl-1*H*-1,2,3-triazole **1g** (180 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (56 mg, yield 43%). M.p. 195−196 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.29 (m, 3H), 7.26–7.22 (m, 4H), 7.20–7.17 (m, 3H), 6.87–6.85 (m, 2H), 6.70 (s, 1H), 6.12 (s, 1H), 3.50 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 136.9, 133.9, 133.8, 131.7, 131.5, 128.81, 128.76, 128.5, 128.2, 127.5, 127.0, 125.8, 122.9, 119.7, 113.9, 35.2, 21.4. HRMS−ESI: $[M + Na]^+$ calcd for $C_{24}H_{21}{}^{35}ClN_2NaO_2S^+$ 459.0904, found 459.0905.

***N*-(2-(3-Methoxyphenyl)-1-methyl-4-phenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (3u)**

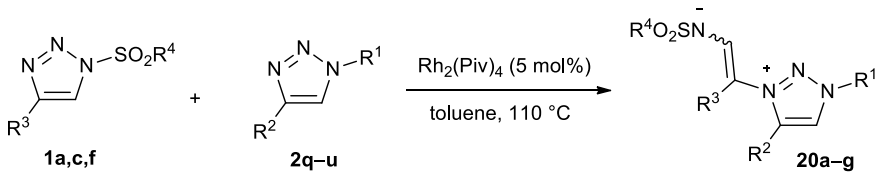


3u

Compound **3u** was prepared according to the general procedure from 4-(3-methoxyphenyl)-1-tosyl-1*H*-1,2,3-triazole **1h** (178 mg, 0.54 mmol) and 1-methyl-4-phenyl-1*H*-1,2,3-triazole **2a** (48 mg, 0.3 mmol) using benzene/EtOAc mixture (50:1) as eluent for chromatography. White solid (91 mg, yield 70%). 1 mmol scale synthesis of compound **3u** (0.263 g, yield 61%) was carried out according to the general procedure from triazole **1h** (0.159 g, 1 mmol) and triazole **2a** (0.592 g, 1.8 mmol). M.p. 167−168 °C ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.38 (m, 2H), 7.27–7.15 (m, 6H), 6.88–6.75 (m, 5H), 6.70 (s, 1H), 6.31 (s, 1H), 3.82 (s, 3H), 3.50 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 142.4, 136.8, 134.2, 132.6, 131.4, 129.2, 128.8,

128.2, 127.4, 127.0, 125.6, 122.6, 122.4, 119.5, 115.5, 113.6, 113.4, 55.2, 35.2, 21.3. HRMS−ESI: $[M + Na]^+$ calcd for $C_{25}H_{24}N_2NaO_3S^+$ 455.1400, found 455.1395.

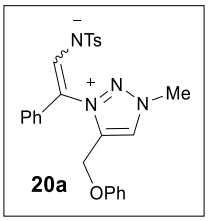
4. Synthesis of triazolium ylides 20



General procedure

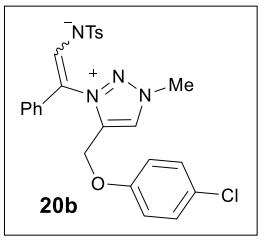
General procedure: A screw-cap tube was charged with 1-sulfonyl-1*H*-1,2,3-triazole **1a**,**c**,**f** (0.54 mmol), 1-alkyl-4-alkyl-1*H*-1,2,3-triazole **2q–u** (0.3 mmol), and toluene (0.6 mL). To the mixture heated to 110 °C $Rh_2(Piv)_4$ (9.1 mg, 0.015 mmol) was added, and the cap was immediately screwed. The reaction mixture was heated at this temperature under stirring until full consumption of the starting materials (~15 min, control by TLC). After cooling the reaction to room temperature, benzene (3 mL) and hexane (6 mL) were added (in some cases Et_2O (3 mL) was additionally added). The resulting precipitate was filtered off and washed with benzene/hexane mixture (1:2).

(2-(1-Methyl-4-(phenoxymethyl)-1*H*-1,2,3-triazol-3-ium-3-yl)-2-phenylvinyl)(tosyl)amide (20a)



Compound **20a** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-methyl-4-(phenoxymethyl)-1*H*-1,2,3-triazole **2q** (57 mg, 0.3 mmol). Brown solid (123 mg, yield 89%). Mp: 152 °C (benzene/hexane, dec.). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.03 (s, 1H), 7.87 (s, 1H), 7.56–7.54 (m, 2H), 7.25–7.18 (m, 6H), 7.06–7.03 (m, 1H), 7.00–6.93 (m, 3H), 6.68–6.66 (m, 2H), 4.94 (s, 2H), 4.35 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.4, 142.0, 136.6, 130.7, 130.0, 129.5, 129.1, 125.8, 124.8, 122.2, 121.6, 115.2, 114.9, 59.4, 40.7, 21.3. HRMS−ESI: $[M + H]^+$ calcd for $C_{25}H_{25}N_4O_3S^+$ 461.1642, found 461.1627.

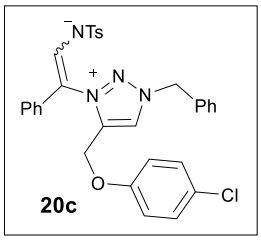
(2-(4-((4-Chlorophenoxy)methyl)-1-methyl-1*H*-1,2,3-triazol-3-ium-3-yl)-2-phenylvinyl)-(tosyl)amide (20b)



20b

Compound **20b** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 4-((4-chlorophenoxy)methyl)-1-methyl-1*H*-1,2,3-triazole **2r** (67 mg, 0.3 mmol). Brown-yellow solid (110 mg, yield 74%). Mp: 154 °C (benzene/hexane, dec.). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.01 (s, 1H), 7.87 (s, 1H), 7.55–7.53 (m, 2H), 7.27–7.16 (m, 6H), 7.06–7.03 (m, 1H), 6.94–6.93 (m, 2H), 6.75–6.73 (m, 2H), 4.98 (s, 2H), 4.34 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.2, 143.6, 141.7, 140.7, 140.4, 136.6, 130.7, 130.2, 129.8, 129.5, 129.3, 129.1, 128.5, 128.4, 127.0, 126.0, 126.0, 125.8, 125.8, 124.9, 123.5, 121.6, 117.0, 116.9, 106.4, 59.9, 40.7, 21.3. HRMS−ESI: $[M + H]^+$ calcd for $C_{25}H_{24}{}^{35}ClN_4O_3S^+$ 495.1252, found 495.1257.

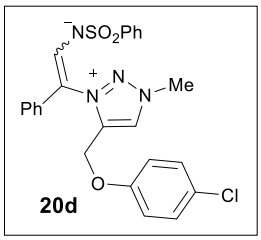
(2-(1-Benzyl-4-((4-chlorophenoxy)methyl)-1*H*-1,2,3-triazol-3-ium-3-yl)-2-phenylvinyl)-(tosyl)amide (20c)



20c

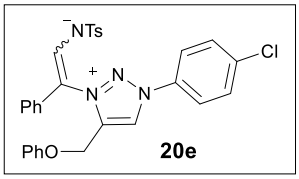
Compound **20c** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-benzyl-4-((4-chlorophenoxy)methyl)-1*H*-1,2,3-triazole **2s** (90 mg, 0.3 mmol). Yellow-orange solid (140 mg, yield 82%). M.p. 182 °C (benzene/hexane, dec.). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.18 (s, 1H), 7.85 (s, 1H), 7.53–7.42 (m, 7H), 7.27–7.15 (m, 6H), 7.06–7.02 (m, 1H), 6.89–6.87 (m, 2H), 6.74–6.72 (m, 2H), 5.92 (s, 2H), 4.99 (s, 2H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.2, 142.2, 133.5, 130.0, 129.74, 129.71, 129.6, 129.5, 129.3, 129.2, 128.8, 127.0, 126.0, 125.8, 121.5, 116.9, 60.1, 57.0, 21.3. HRMS−ESI: $[M + H]^+$ calcd for $C_{31}H_{28}{}^{35}ClN_4O_3S^+$ 571.1565, found 571.1567.

(2-(4-((4-Chlorophenoxy)methyl)-1-methyl-1*H*-1,2,3-triazol-3-ium-3-yl)-2-phenylvinyl)-(phenylsulfonyl)amide (20d)



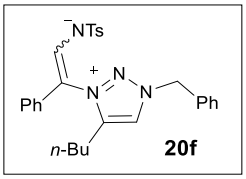
Compound **20d** was prepared according to the general procedure from 4-phenyl-1-(phenylsulfonyl)-1*H*-1,2,3-triazole **2c** (154 mg, 0.54 mmol) and 4-((4-chlorophenoxy)methyl)-1-methyl-1*H*-1,2,3-triazole **2r** (67 mg 0.3 mmol). Pale yellow solid (143 mg, yield 99%). M.p. 203 °C (benzene/hexane, dec.). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.01 (s, 1H), 7.88 (s, 1H), 7.71–7.65 (m, 2H), 7.46–7.38 (m, 3H), 7.28–7.18 (m, 4H), 7.09–7.02 (m, 1H), 6.97–6.91 (m, 2H), 6.72–6.67 (m, 2H), 4.98 (s, 2H), 4.34 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.2, 146.5, 141.6, 141.1, 136.6, 130.7, 130.6, 129.8, 129.13, 129.10, 128.9, 126.0, 125.7, 124.9, 121.6, 117.0, 116.8, 106.6, 59.8, 40.7. HRMS−ESI: $[M + H]^+$ calcd for $C_{24}H_{22}{}^{35}ClN_4O_3S^+$ 481.1096, found 481.1087.

(2-(1-(4-Chlorophenyl)-4-(phenoxymethyl)-1*H*-1,2,3-triazol-3-ium-3-yl)-2-phenylvinyl)-(tosyl)amide (20e)



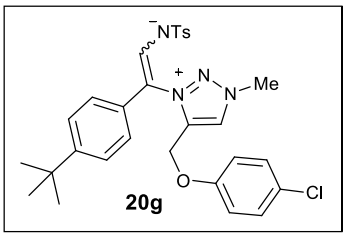
Compound **20e** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg, 0.54 mmol) and 1-(4-chlorophenyl)-4-(phenoxymethyl)-1*H*-1,2,3-triazole **2t** (86 mg, 0.3 mmol). Orange solid (140 mg, yield 84%). M.p. 180 °C (benzene/hexane, dec.). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.85 (s, 1H), 8.10–8.08 (m, 2H), 7.95 (s, 1H), 7.80–7.78 (m, 2H), 7.60–7.58 (m, 2H), 7.27–7.19 (m, 6H), 7.11–7.09 (m, 3H), 7.01–6.98 (m, 1H), 6.73–6.71 (m, 2H), 5.03 (s, 2H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.5, 143.3, 136.6, 134.3, 130.6, 130.2, 130.1, 130.0, 129.6, 129.3, 129.2, 128.8, 128.4, 127.0, 125.9, 125.1, 123.9, 122.4, 122.3, 121.9, 115.3, 115.1, 60.1, 21.3. HRMS−ESI: $[M + H]^+$ calcd for $C_{30}H_{26}{}^{35}ClN_4O_3S^+$ 557.1409, found 557.1414.

(2-(1-Benzyl-4-butyl-1*H*-1,2,3-triazol-3-ium-3-yl)-2-phenylvinyl)(tosyl)amide (20f)



Compound **20f** was prepared according to the general procedure from 4-phenyl-1-tosyl-1*H*-1,2,3-triazole **1a** (162 mg 0.54 mmol) and 1-benzyl-4-butyl-1*H*-1,2,3-triazole **2u** (65 mg 0.3 mmol). Brown solid (45 mg, yield 30%). M.p. 86 °C (benzene/hexane/Et_2O, dec.). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.94 (s, 1H), 7.90 (s, 1H), 7.52–7.42 (m, 7H), 7.23–7.18 (m, 4H), 7.04–7.00 (m, 1H), 6.81–6.79 (m, 2H), 5.87 (s, 2H), 2.41–2.27 (m, 2H), 2.31 (s, 3H), 1.43–1.35 (m, 2H), 1.08–0.99 (m, 2H), 0.68 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 146.8, 133.6, 129.7, 129.63, 129.55, 129.44, 129.38, 129.3, 129.2, 128.6, 125.8, 125.7, 120.7, 56.7, 28.7, 23.0, 21.9, 21.3, 13.7. HRMS−ESI: $[M + H]^+$ calcd for $C_{28}H_{31}N_4O_2S^+$ 487.2162, found 487.2150.

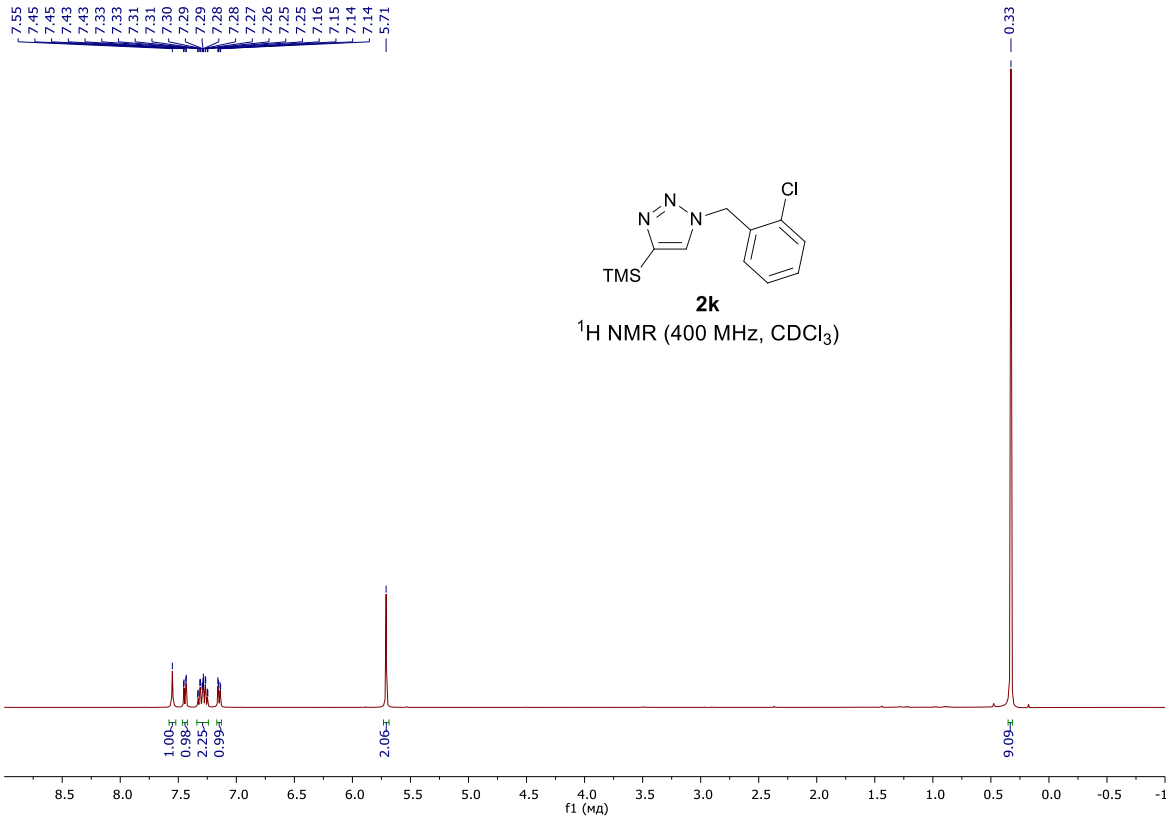
(2-(4-(*tert*-Butyl)phenyl)-2-(4-((4-chlorophenoxy)methyl)-1-methyl-1*H*-1,2,3-triazol-3-ium-3-yl)vinyl)(tosyl)amide (20g)

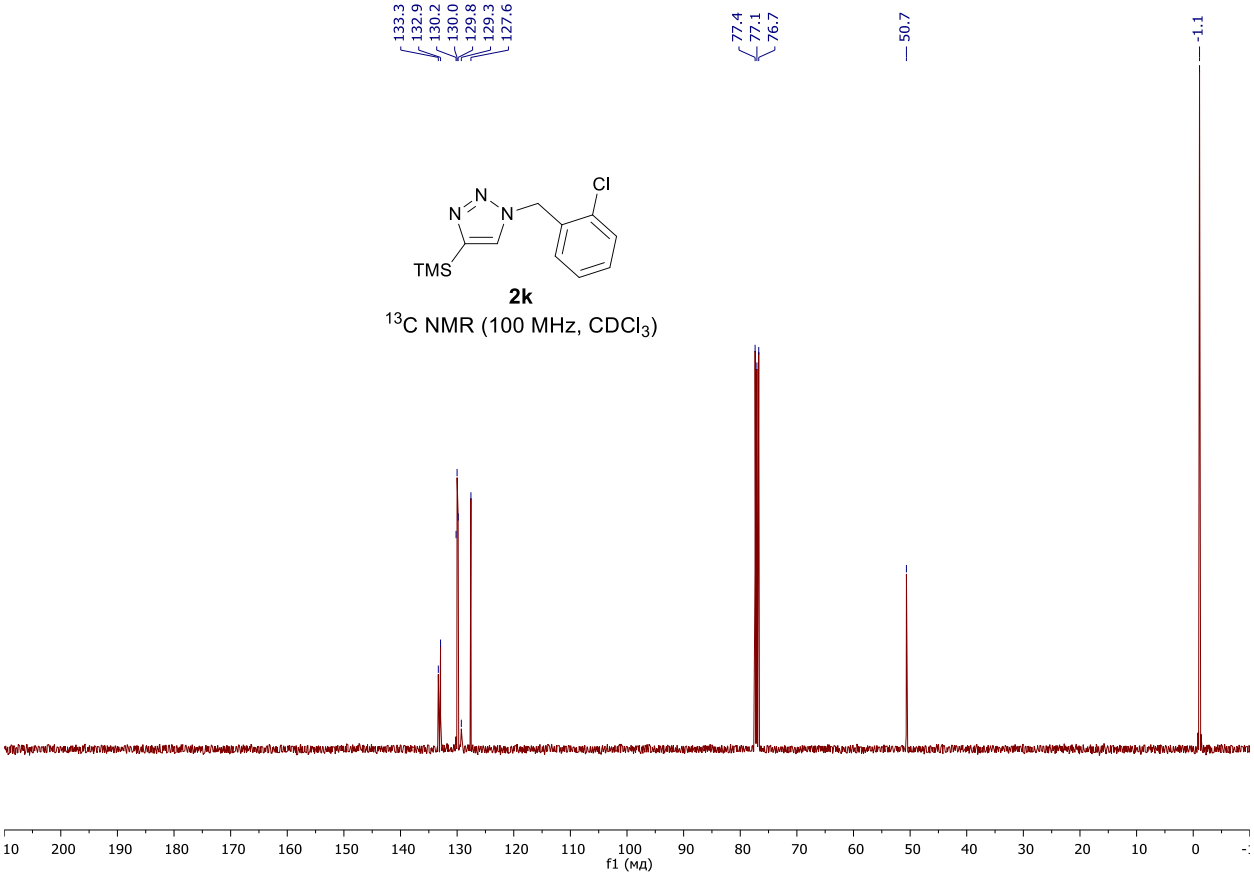


Compound **20g** was prepared according to the general procedure from 4-(4-(*tert*-butyl)phenyl)-1-tosyl-1*H*-1,2,3-triazole **1f** (192 mg, 0.54 mmol) and 4-((4-chlorophenoxy)methyl)-1-methyl-1*H*-1,2,3-triazole **2r** (67 mg, 0.3 mmol). Brown solid (83 mg, yield 50%). M.p. 110 °C (benzene/hexane, dec.). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.01 (s, 1H), 7.79 (s, 1H), 7.55–7.53 (m, 2H), 7.26–7.22 (m, 4H), 7.18–7.16 (m, 2H), 6.88–6.85 (m, 2H), 6.76–6.73 (m, 2H), 4.98 (s, 2H), 4.33 (s, 3H), 2.28 (s, 3H), 1.24 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.2, 141.7, 140.4, 130.6, 129.7, 129.5, 129.2, 126.0, 125.9, 125.8, 121.6, 116.9, 60.1, 40.7, 34.5, 31.5, 21.3. HRMS−ESI: $[M + H]^+$ calcd for $C_{29}H_{32}{}^{35}ClN_4O_3S^+$ 551.1878, found 551.1878.

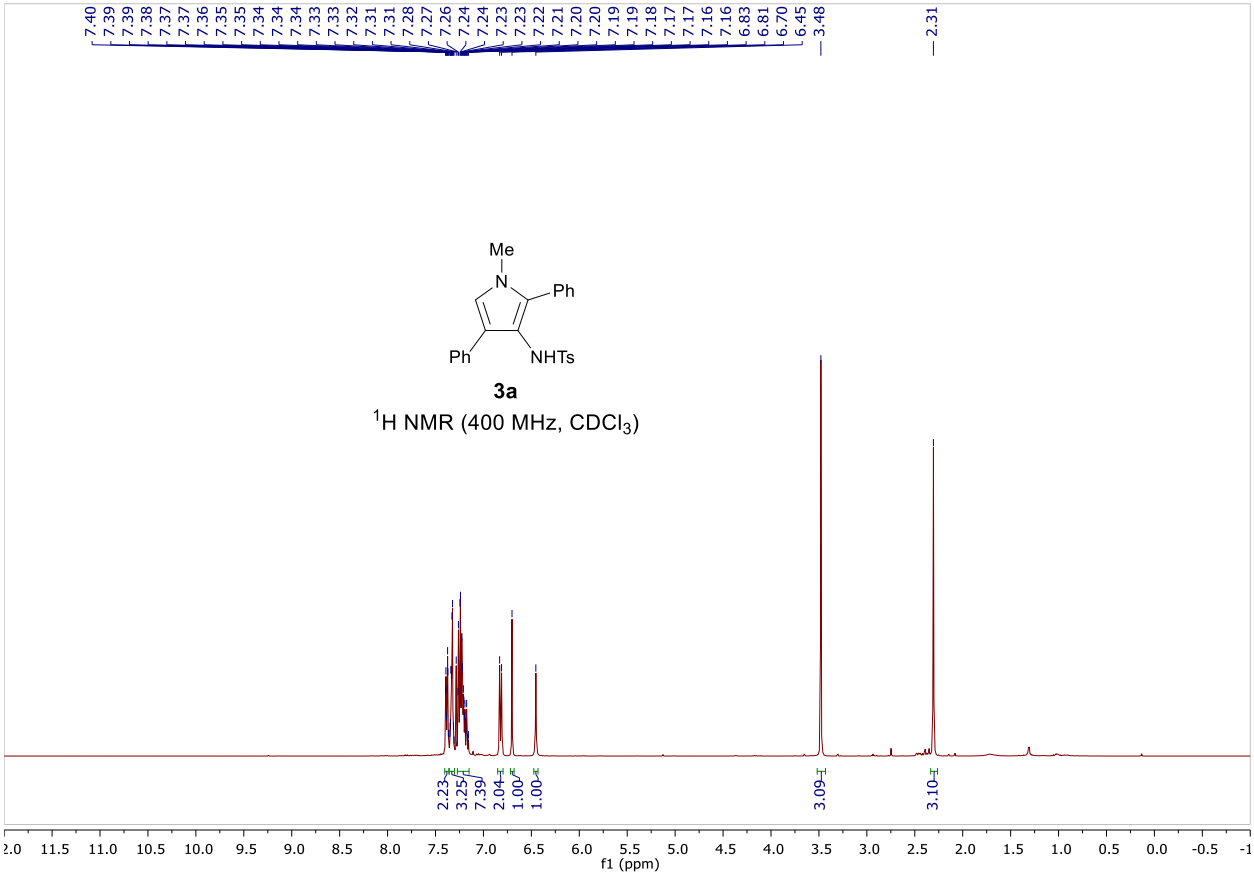
5. ^{1}H and ^{13}C NMR spectra

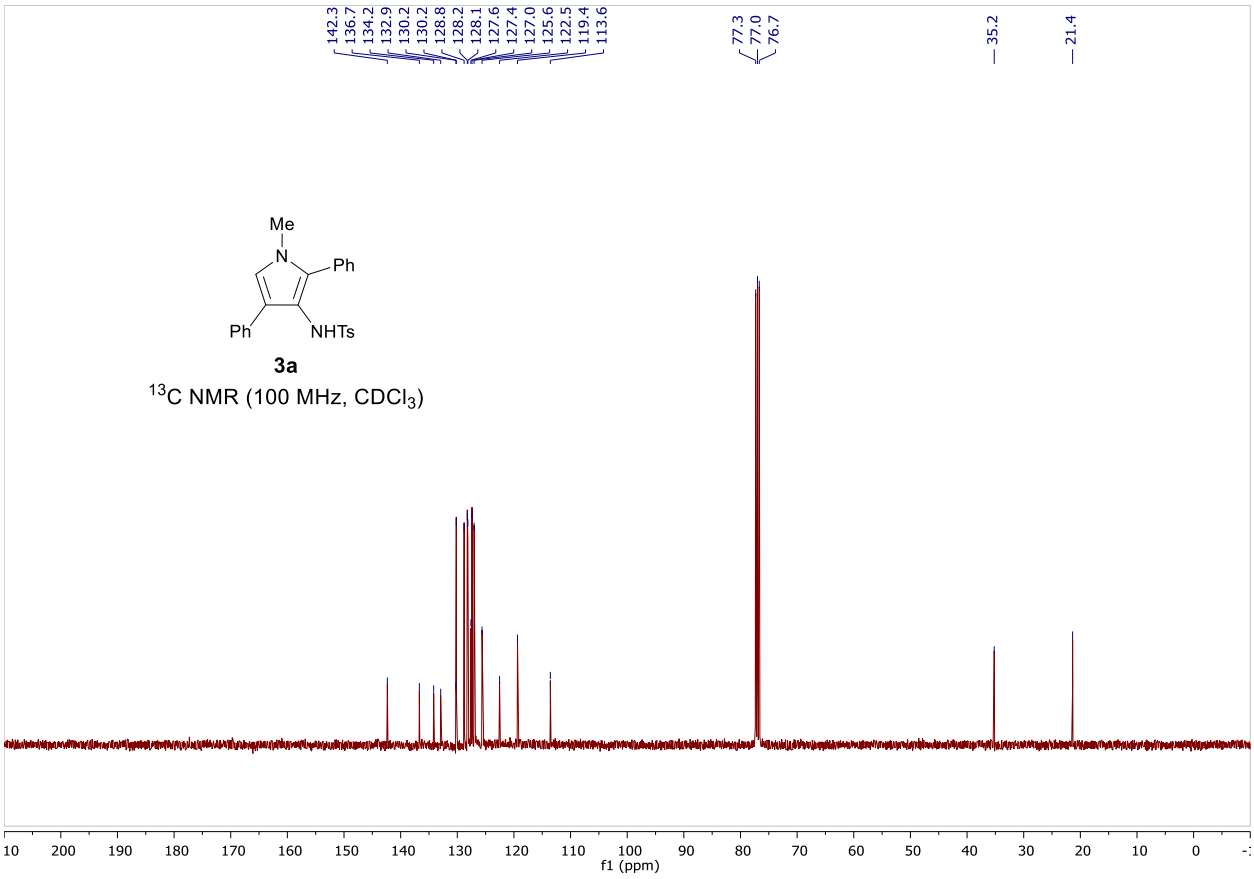
^{1}H and ^{13}C NMR spectra of compound **2k**



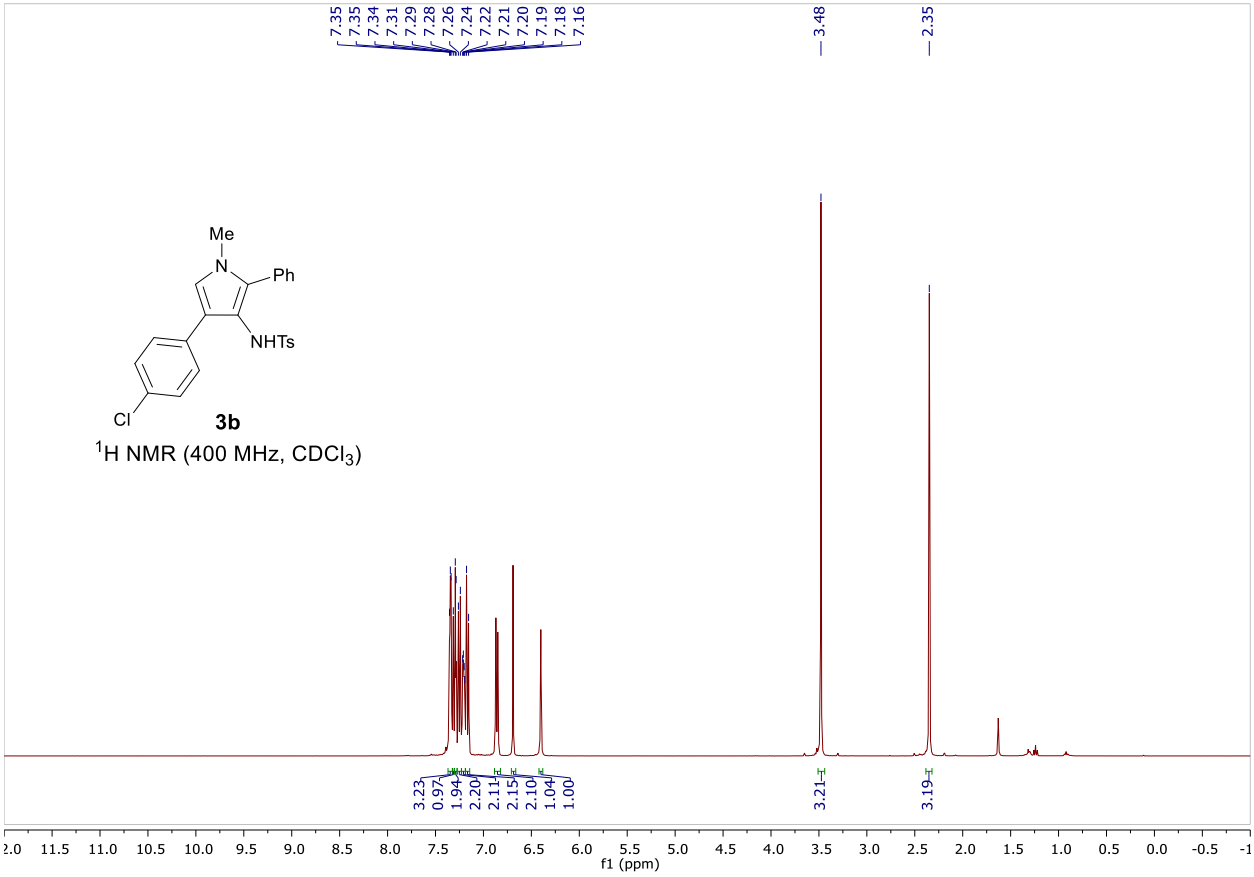


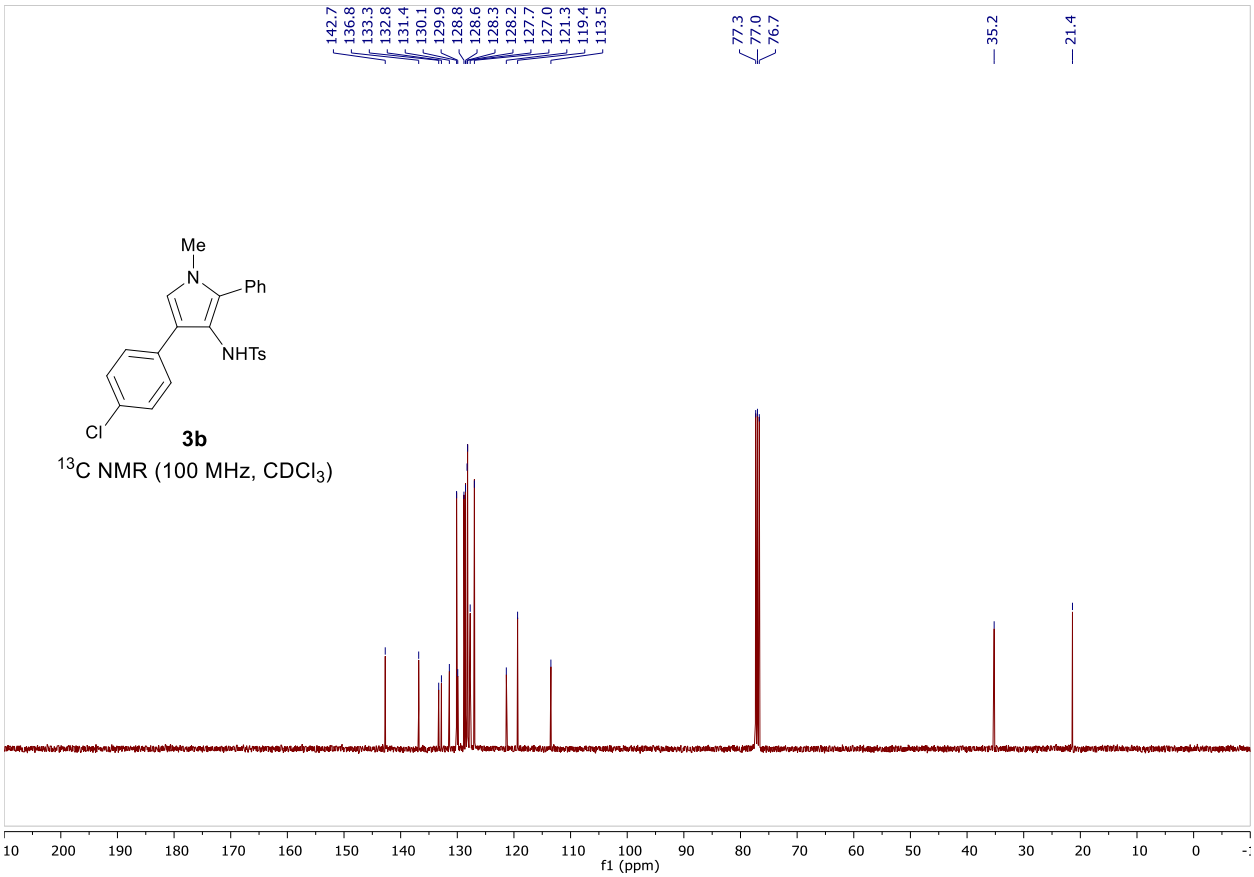
^{1}H and ^{13}C NMR spectra of compound **3a**



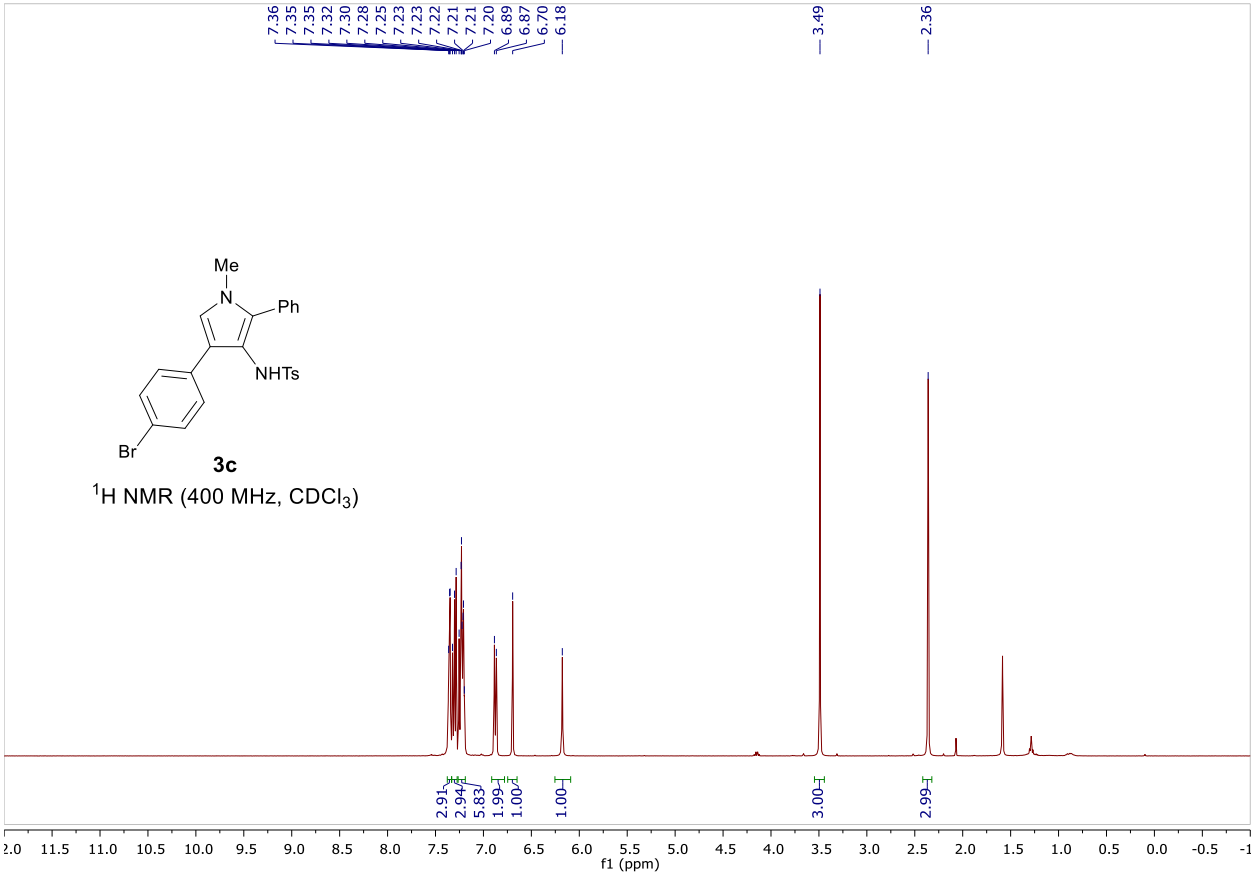


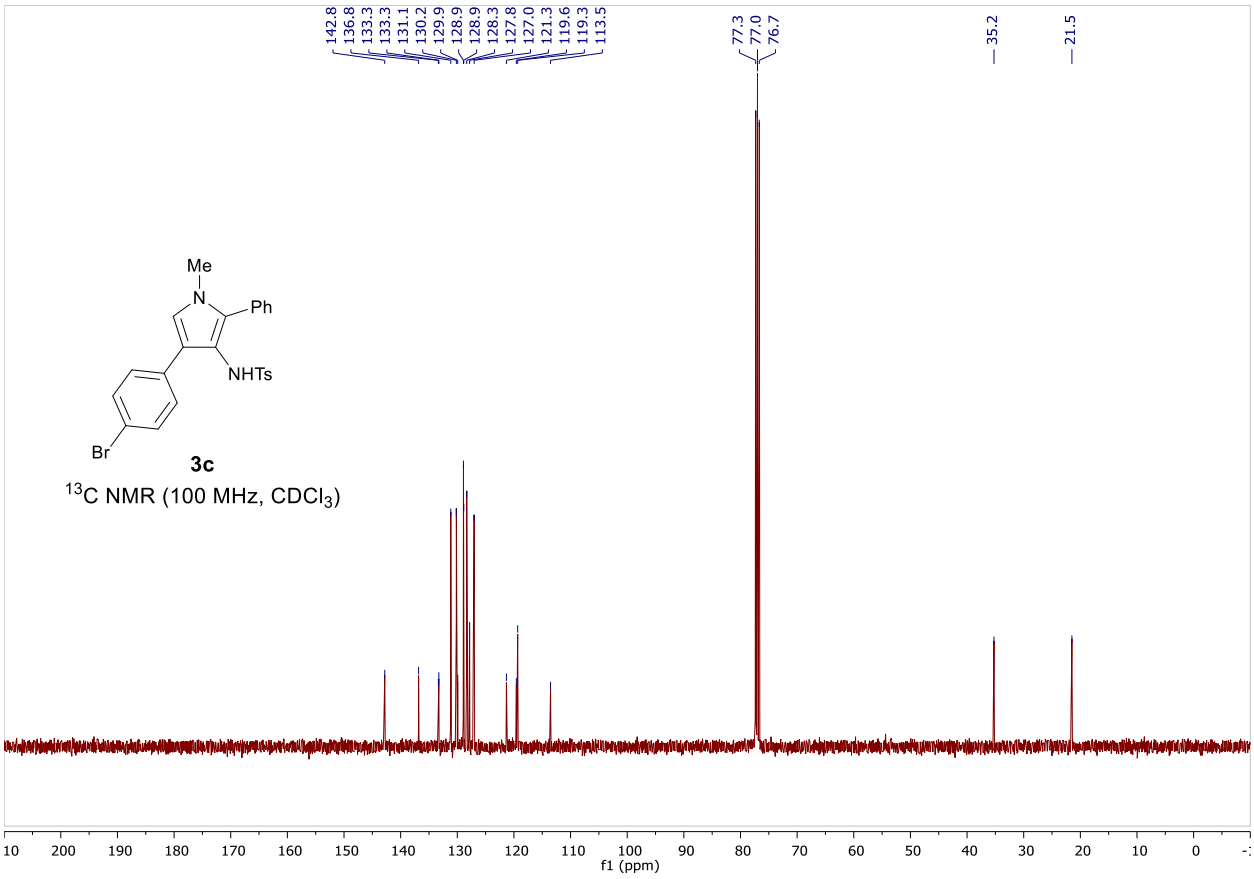
^{1}H and ^{13}C NMR spectra of compound **3b**



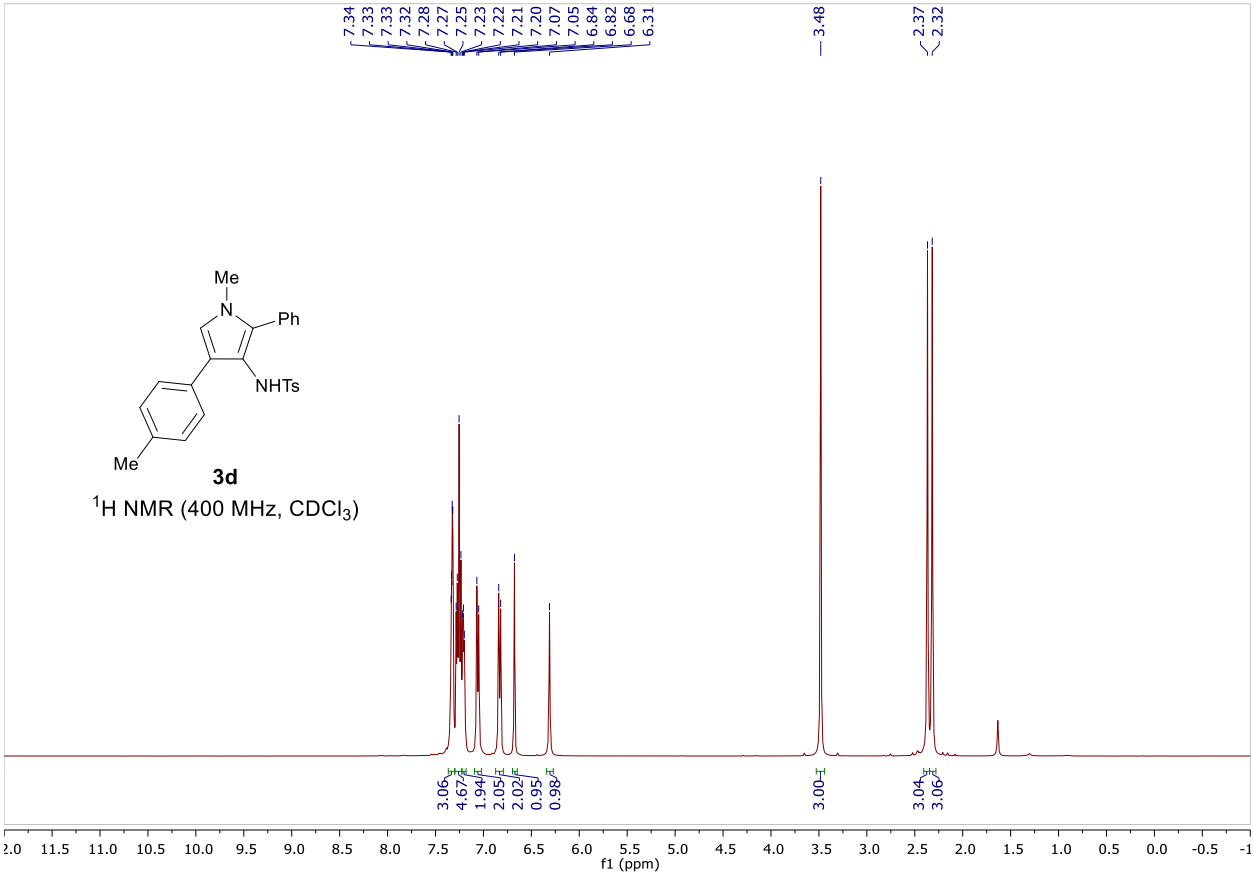


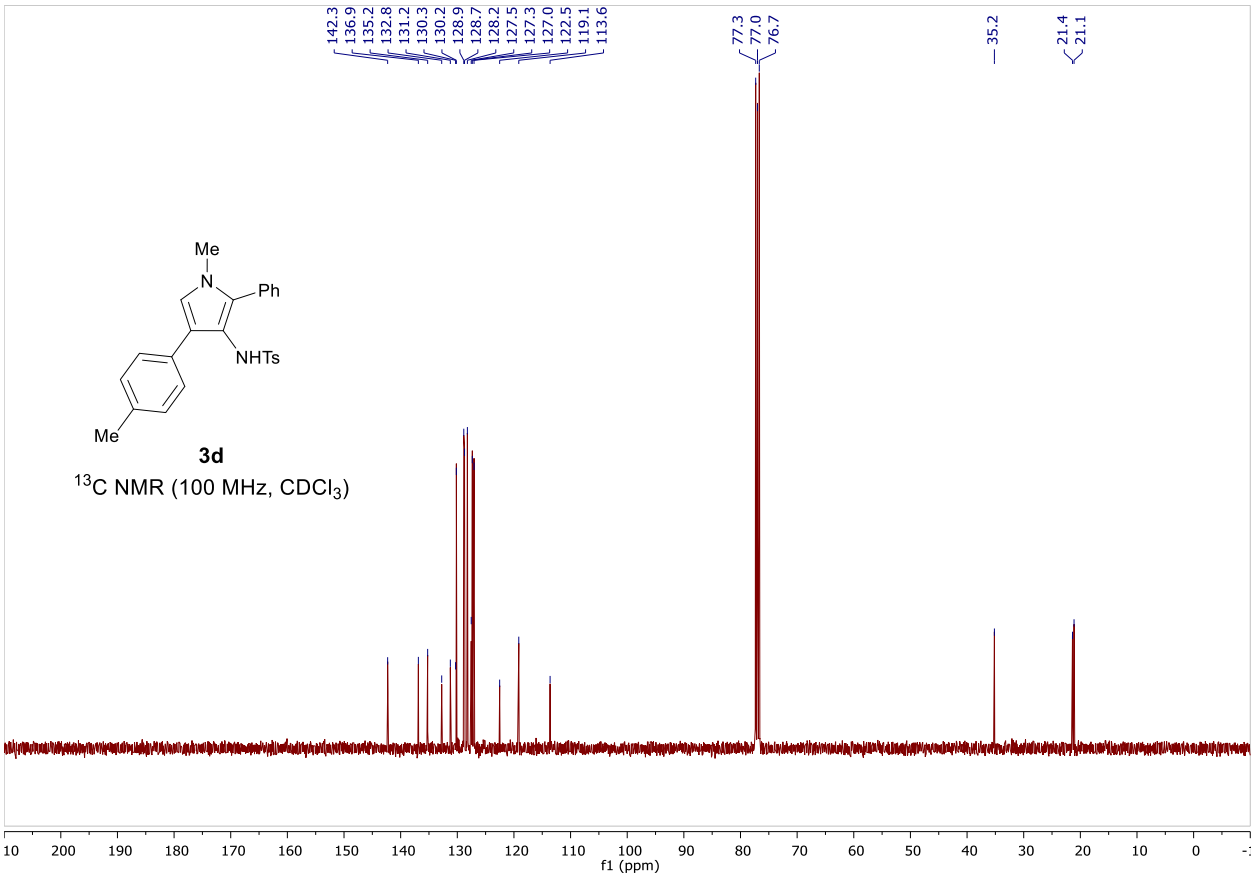
^{1}H and ^{13}C NMR spectra of compound **3c**



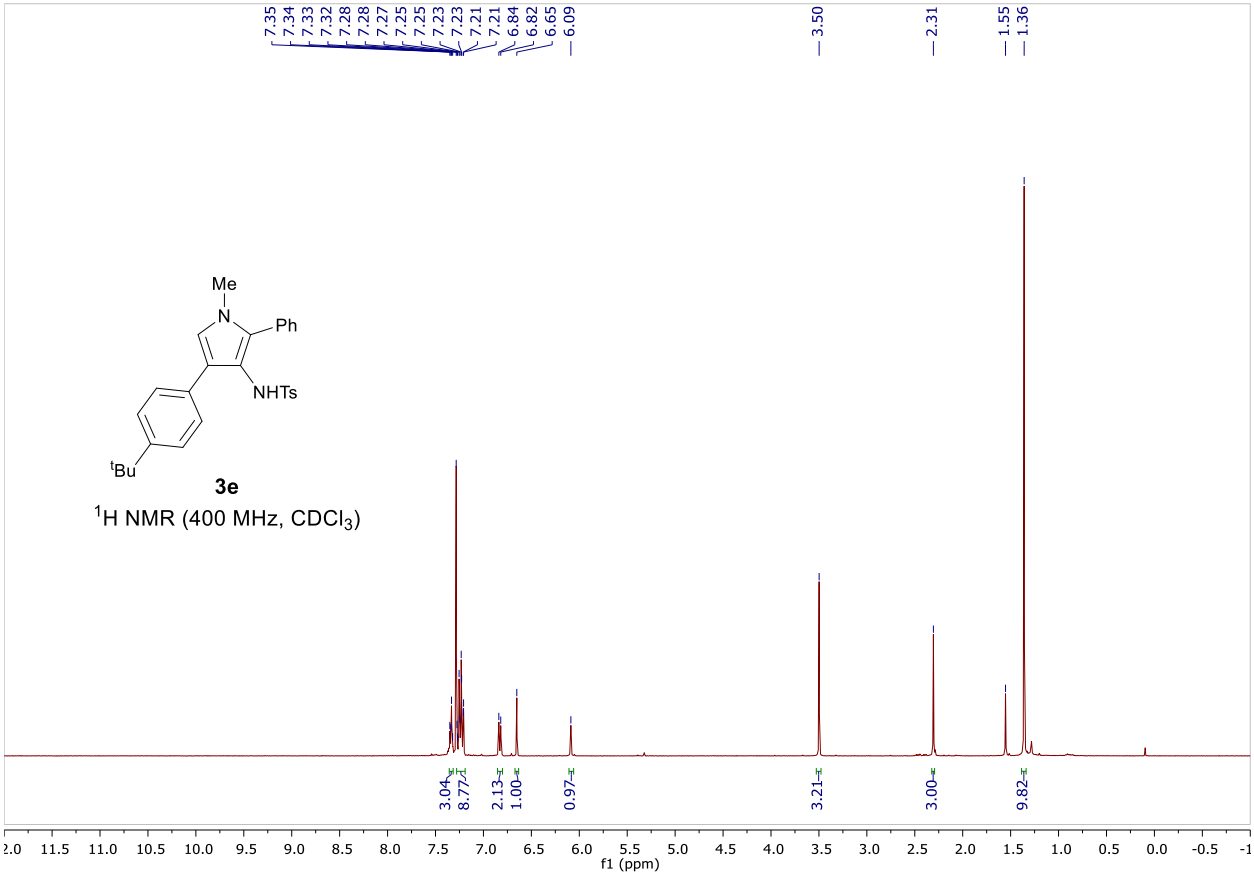


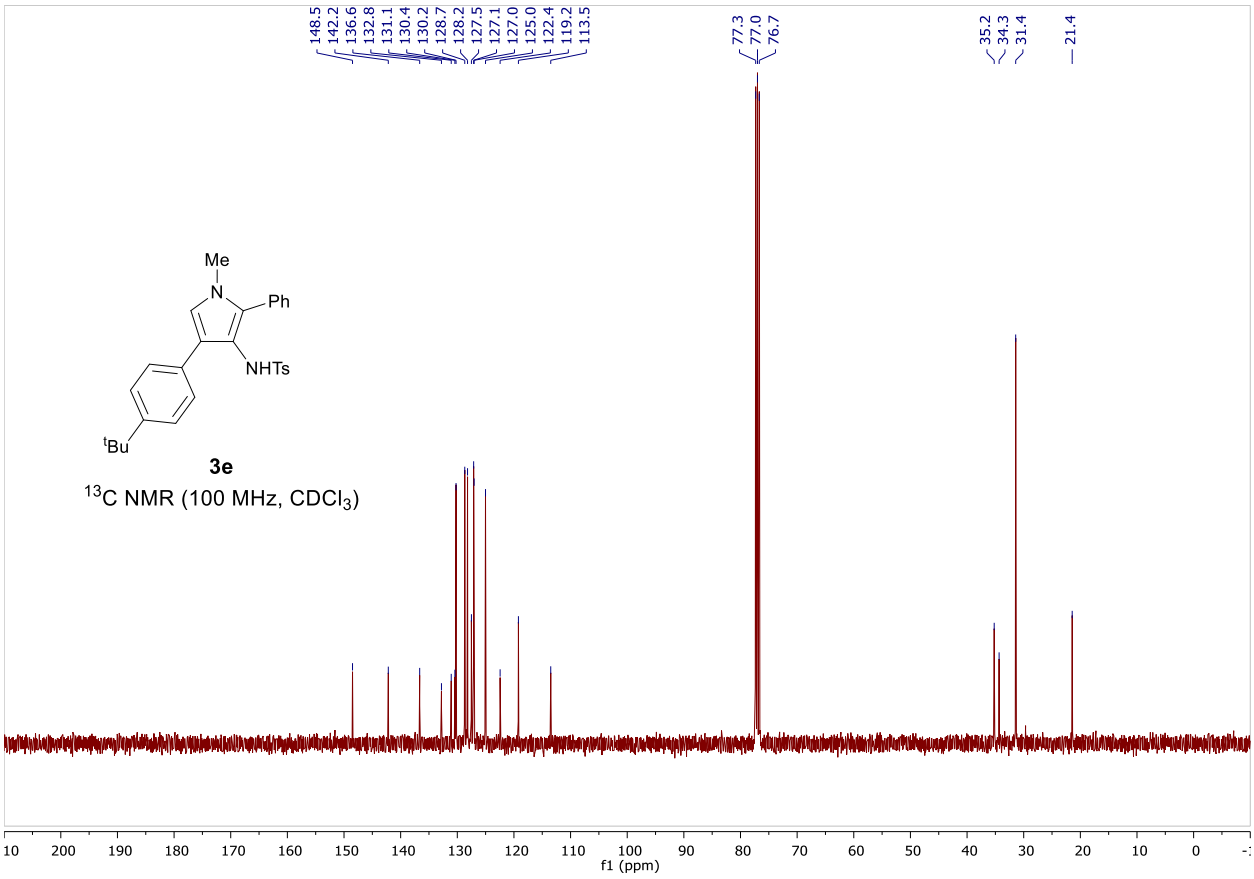
^{1}H and ^{13}C NMR spectra of compound **3d**



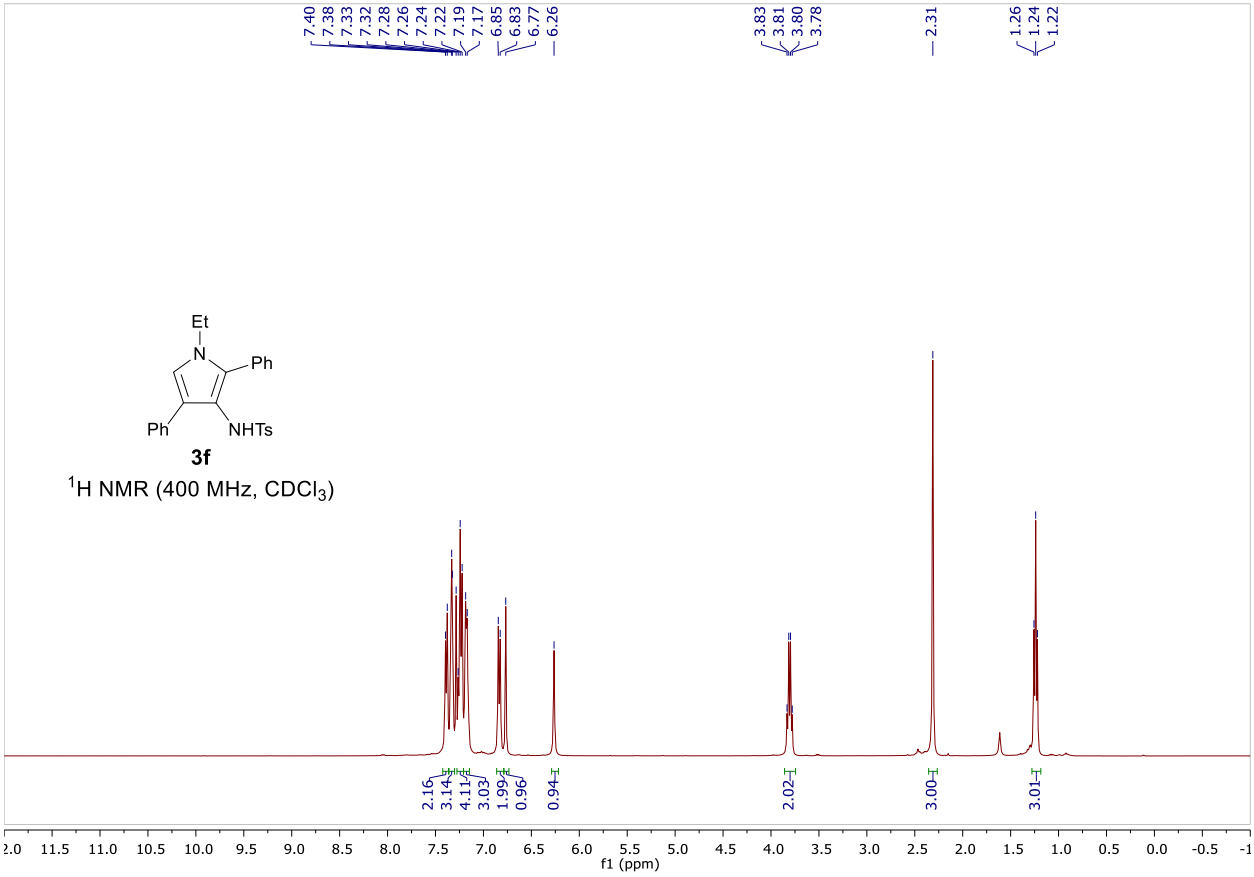


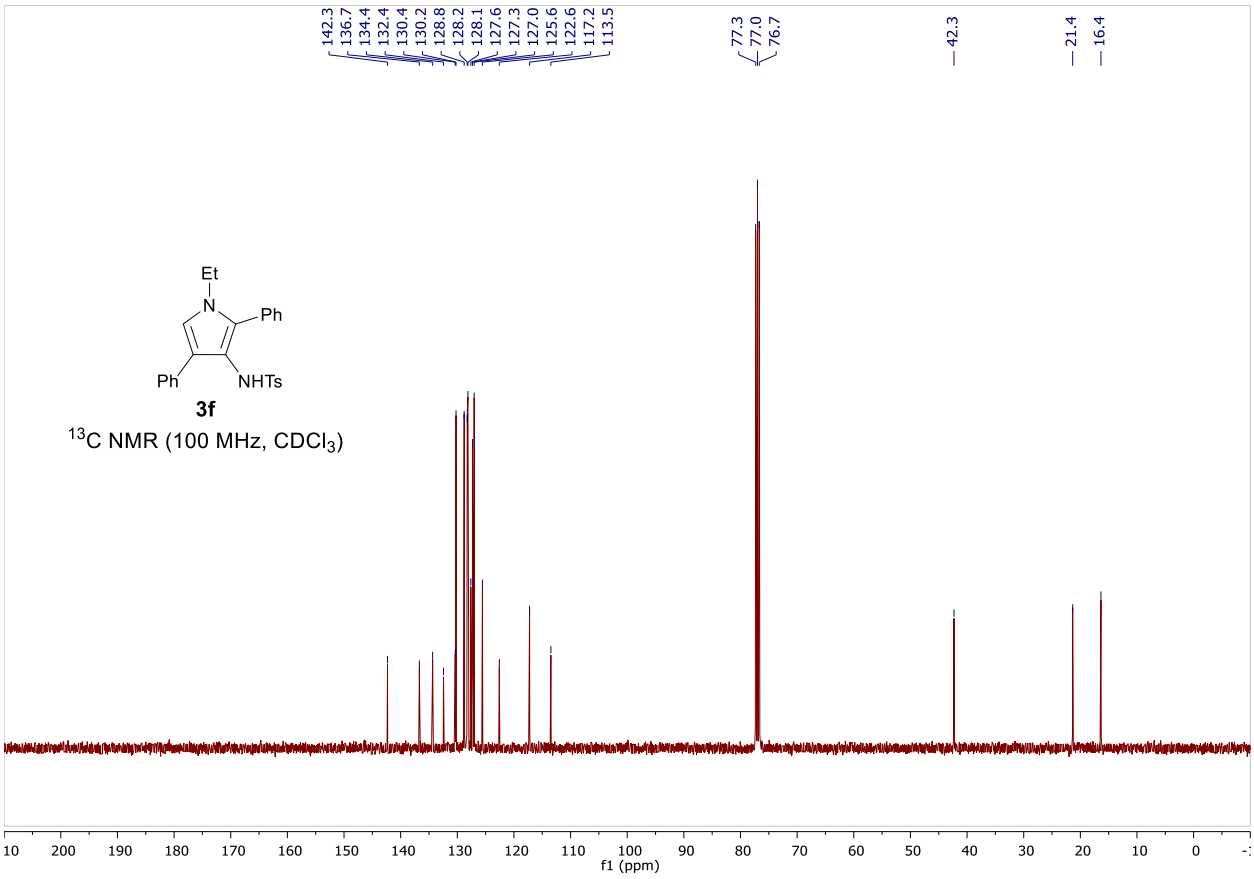
^{1}H and ^{13}C NMR spectra of compound **3e**



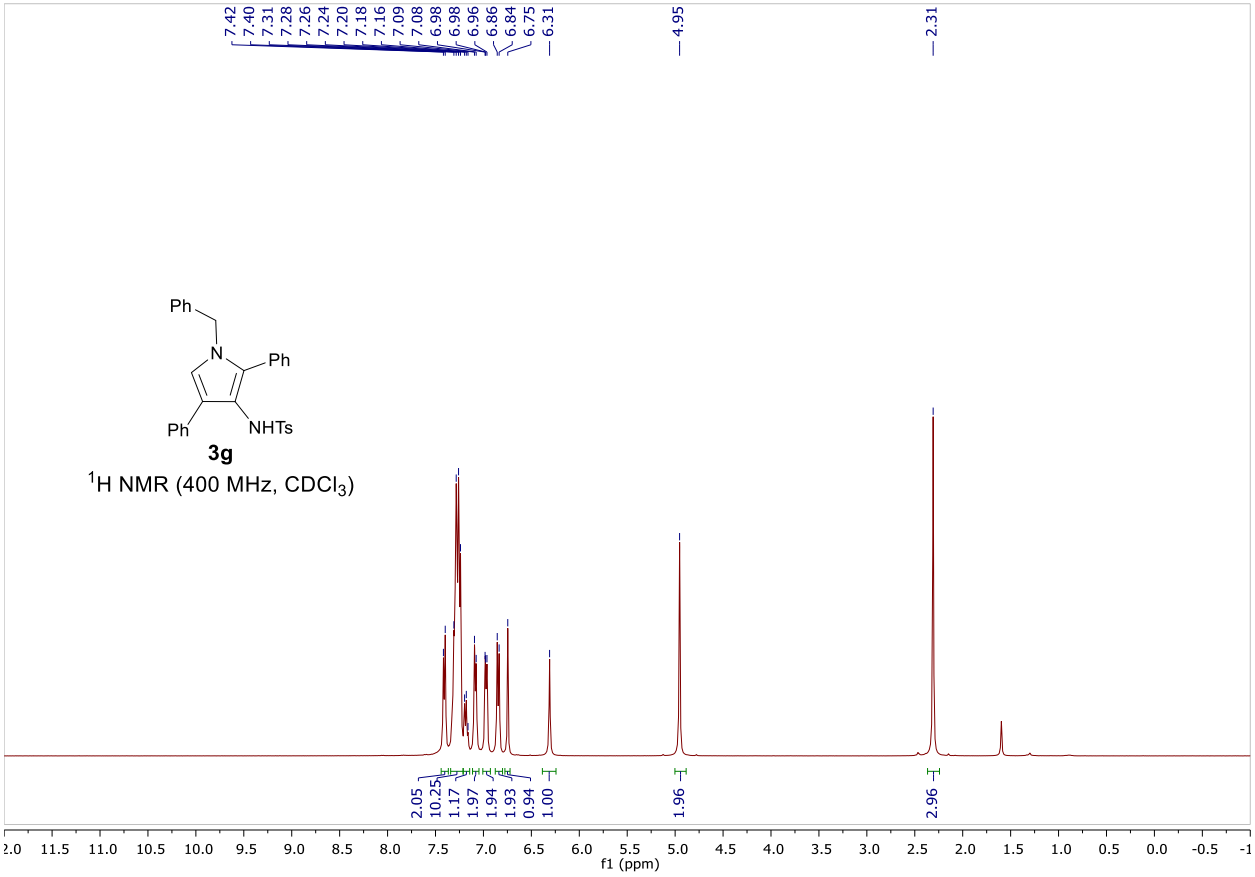


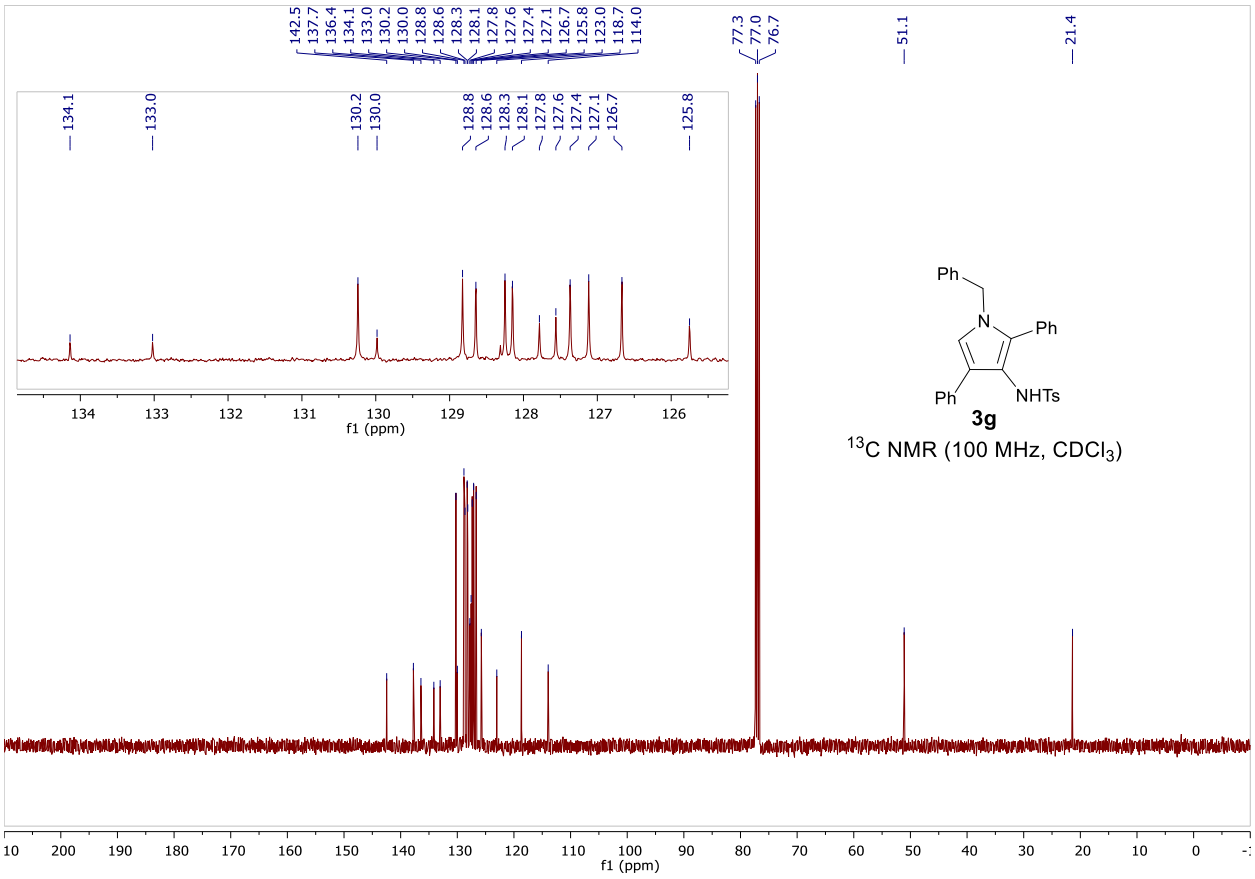
^{1}H and ^{13}C NMR spectra of compound **3f**



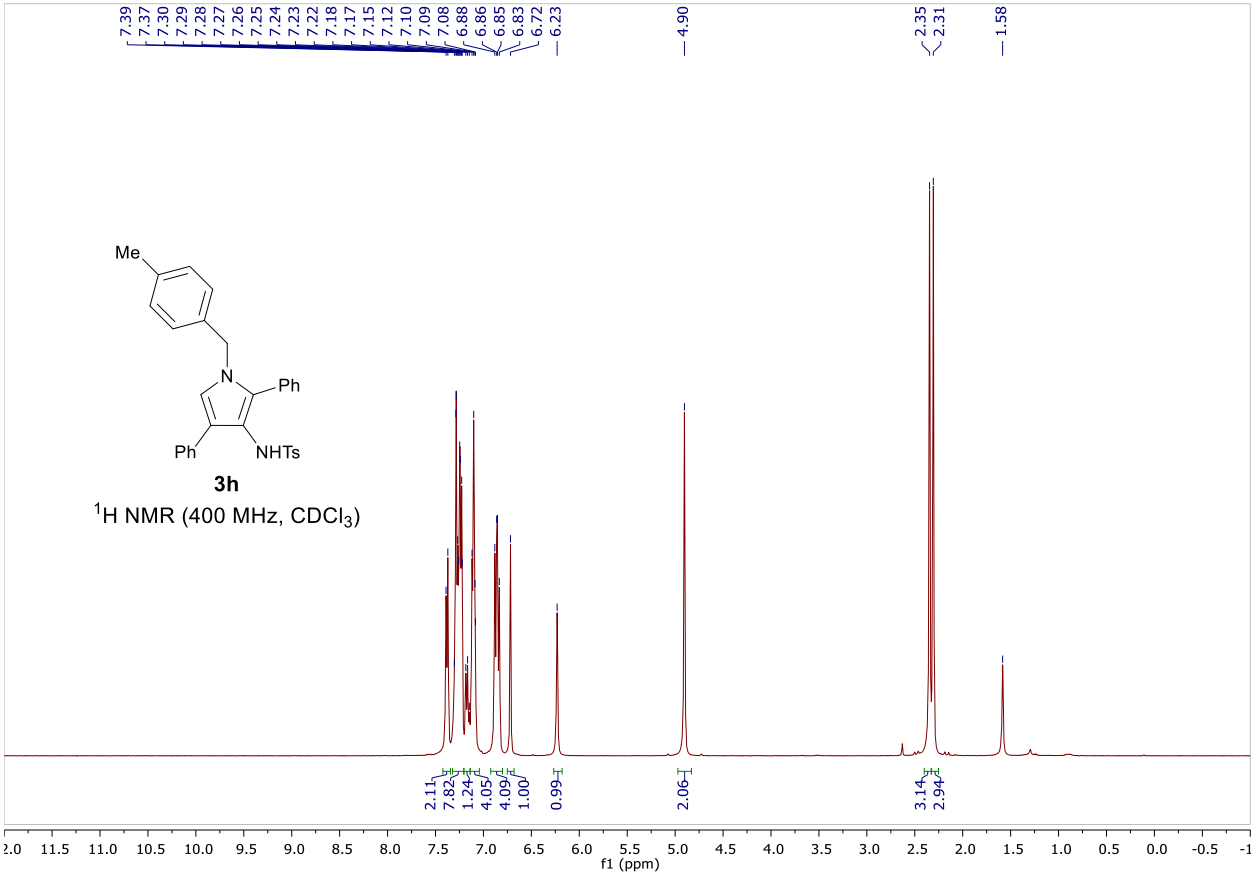


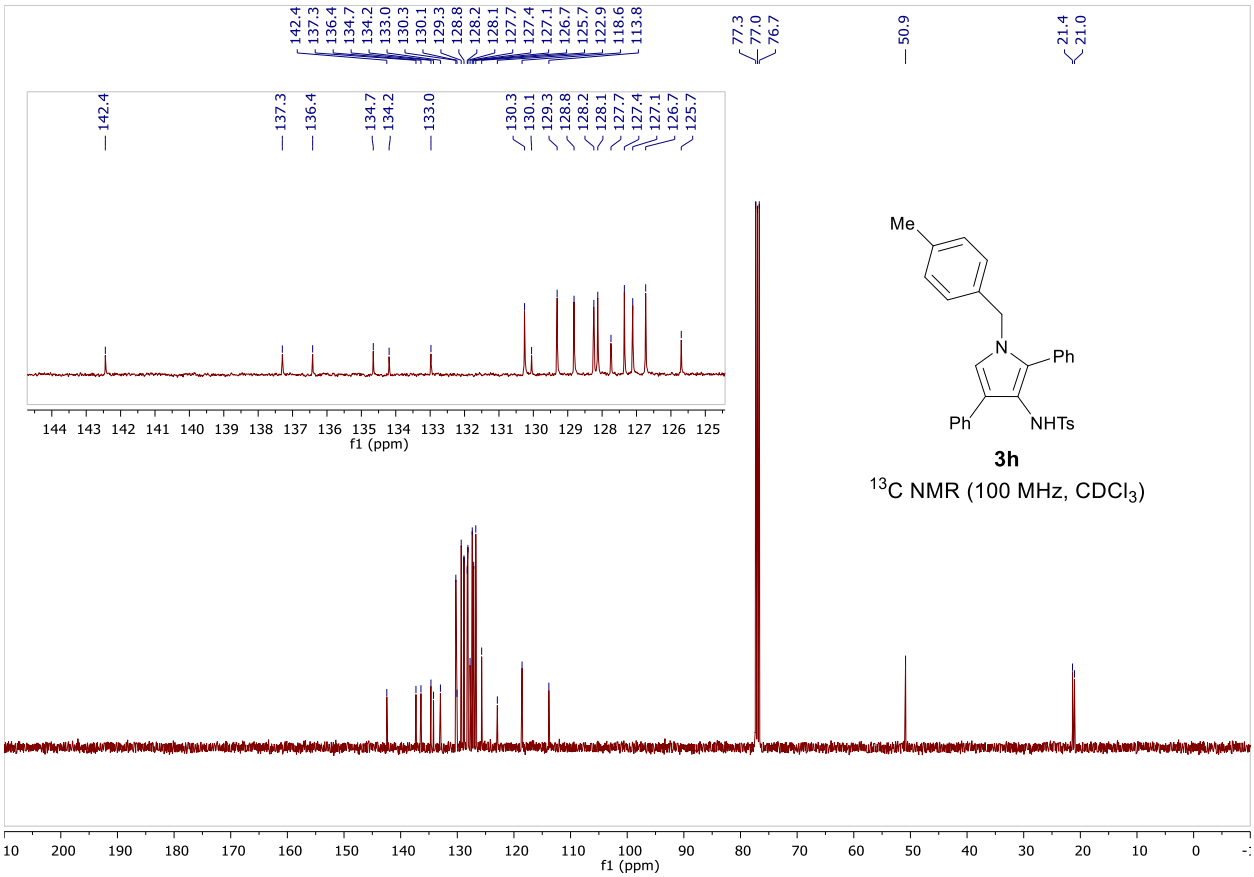
^{1}H and ^{13}C NMR spectra of compound **3g**



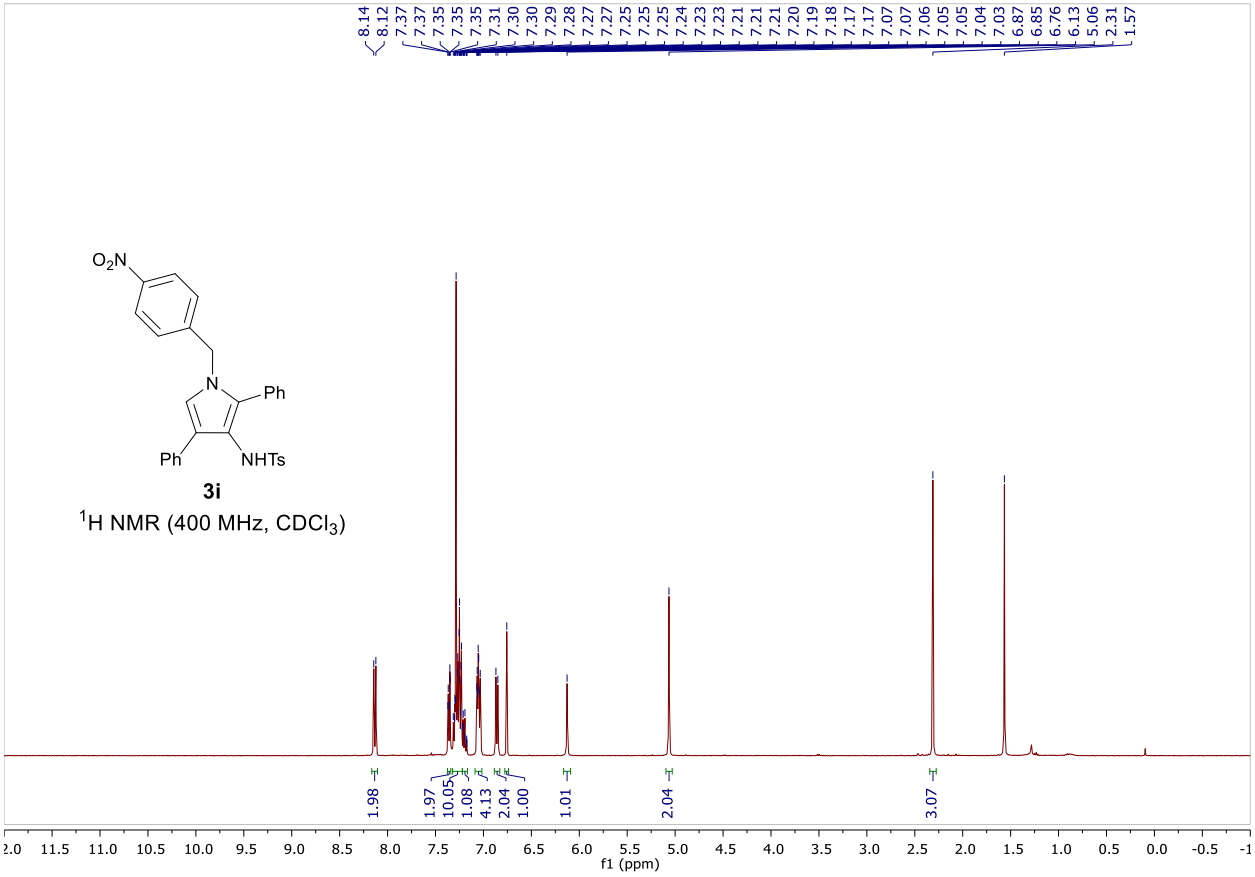


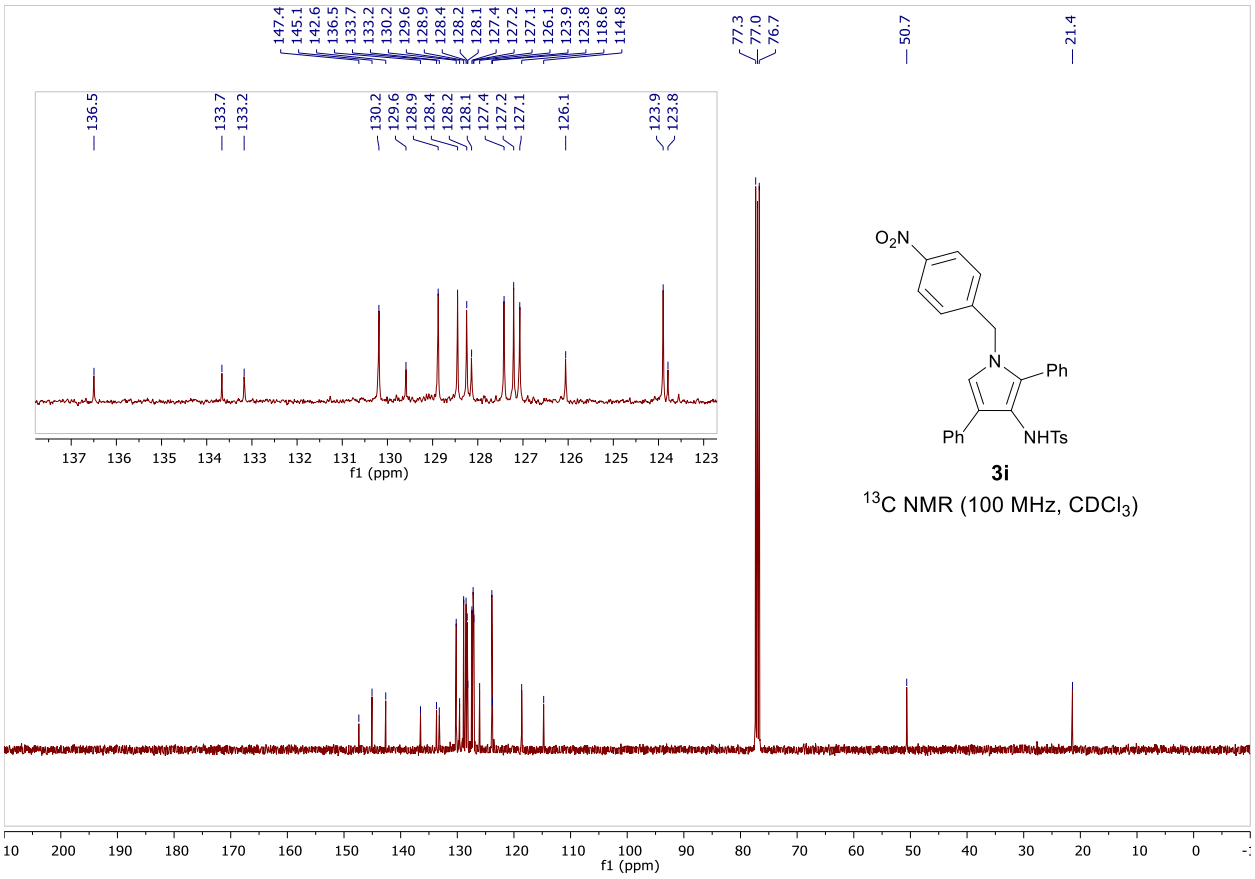
^{1}H and ^{13}C NMR spectra of compound **3h**



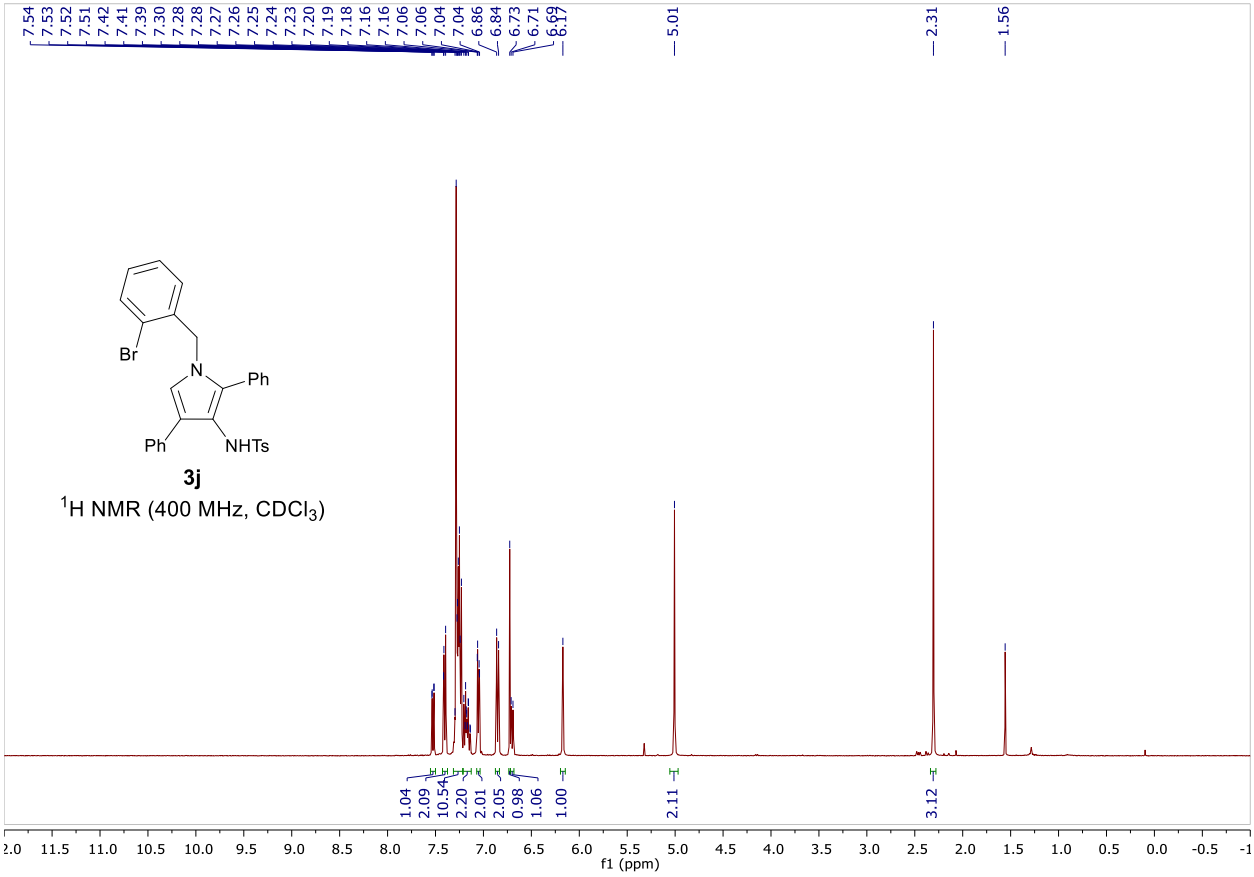


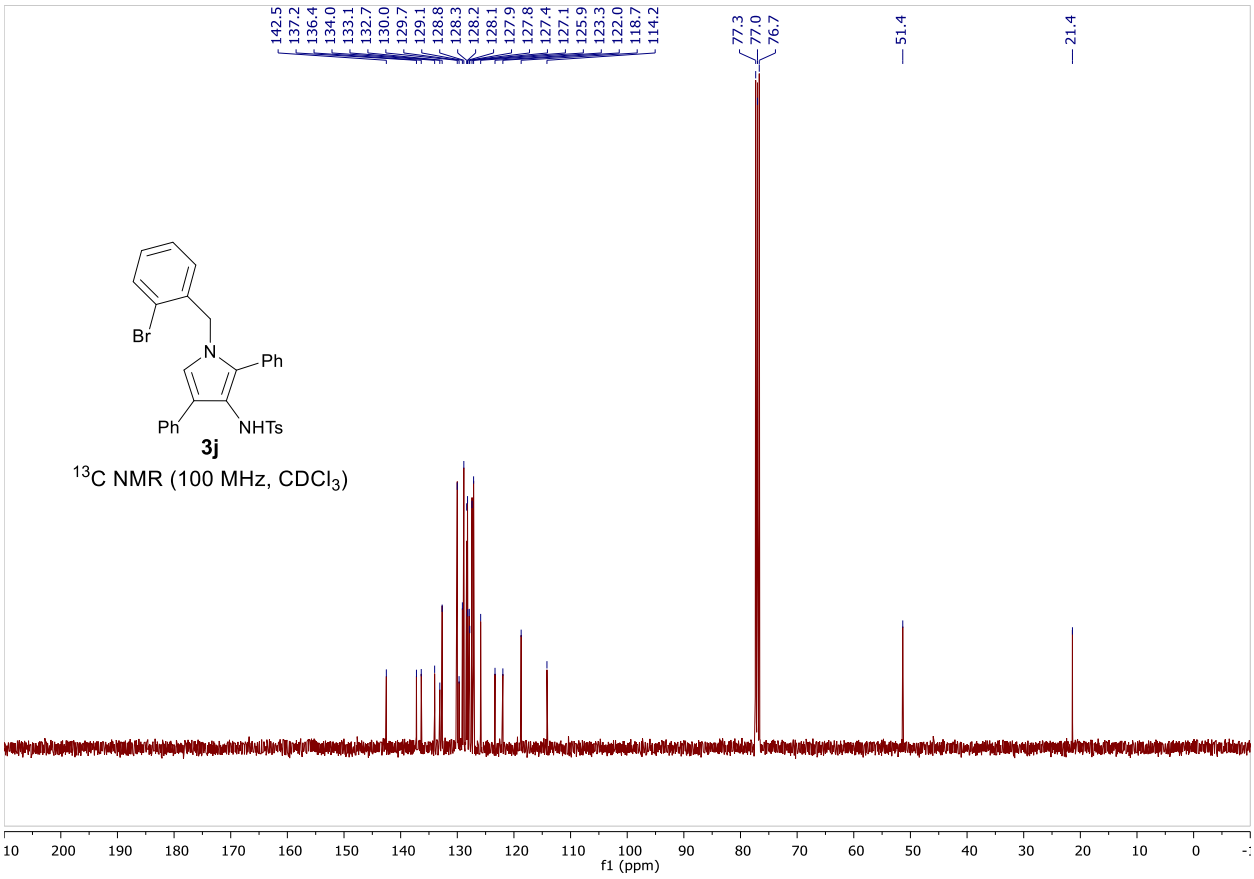
^{1}H and ^{13}C NMR spectra of compound **3i**



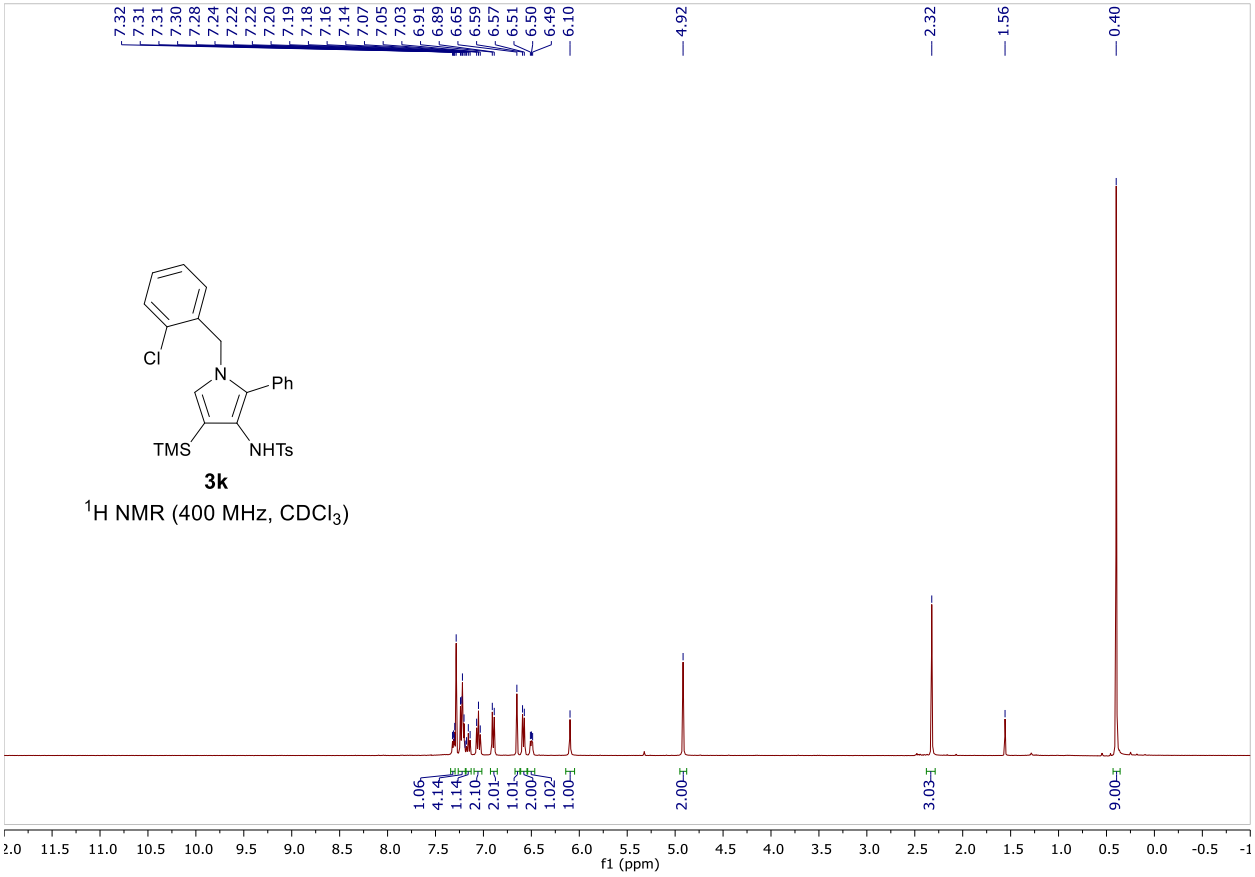


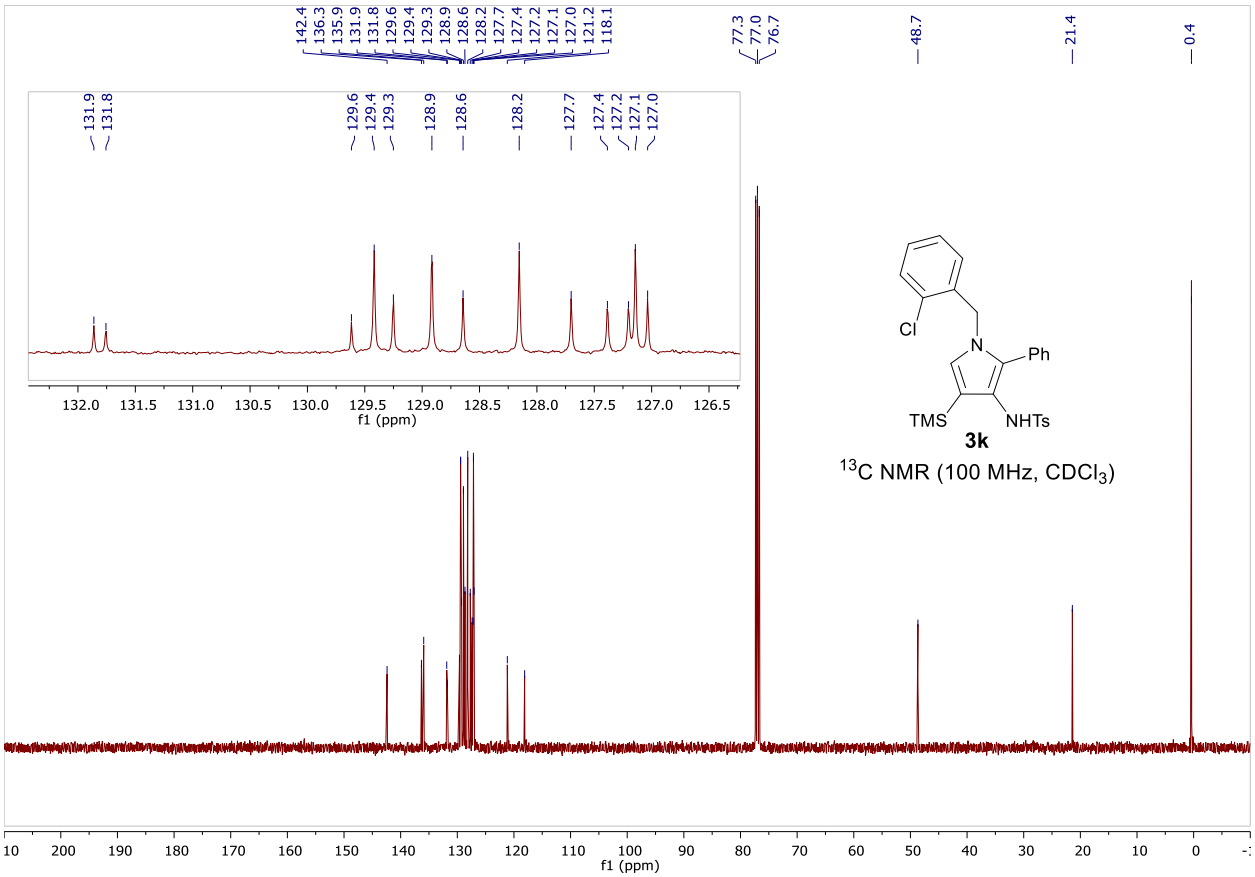
^{1}H and ^{13}C NMR spectra of compound **3j**



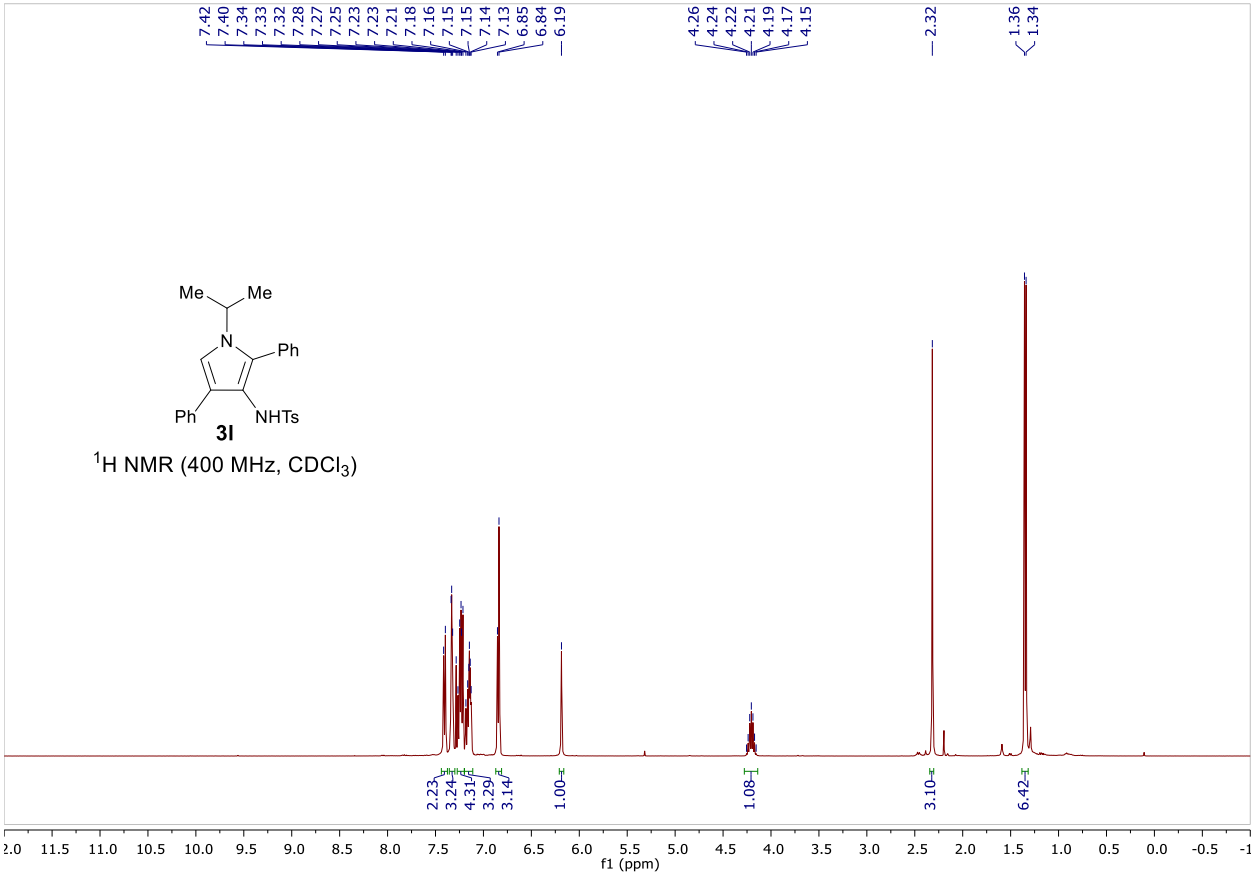


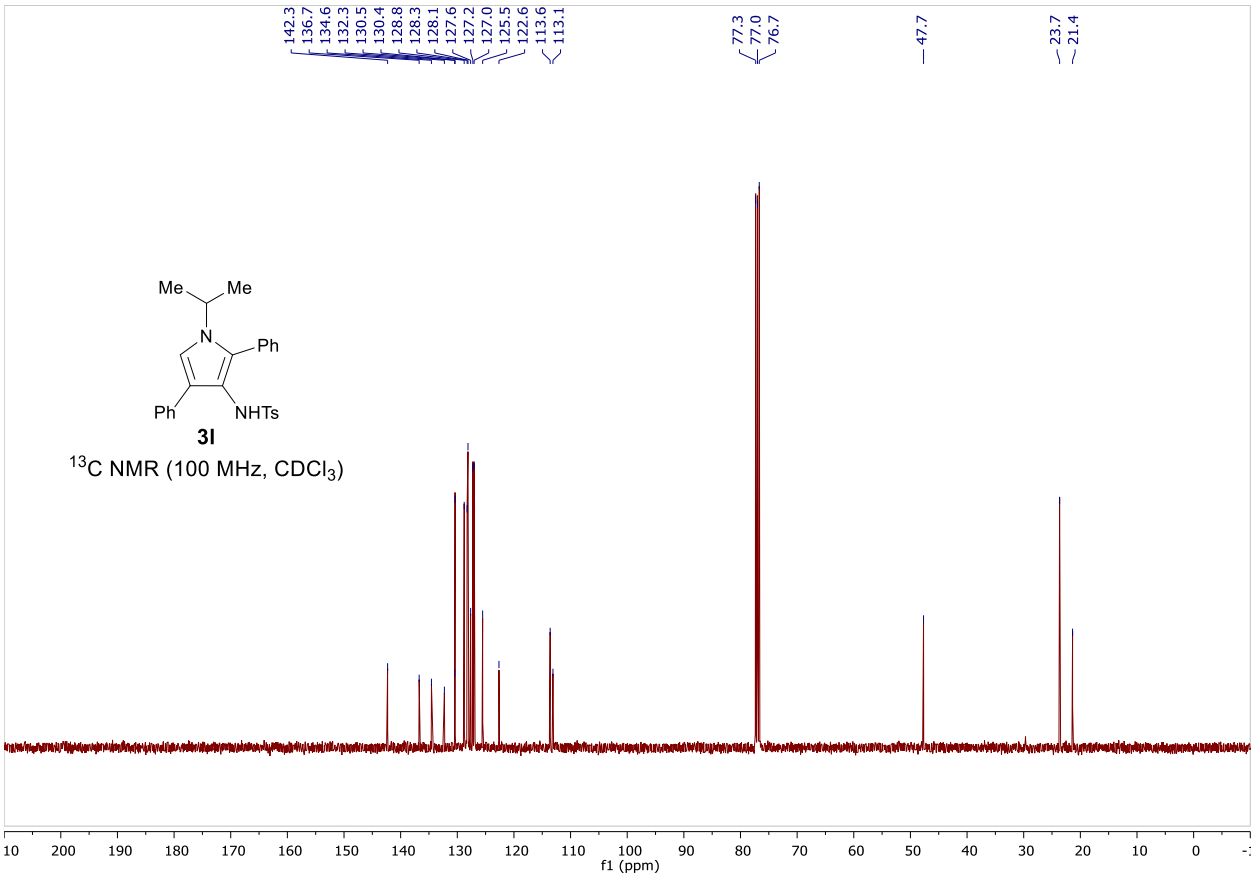
^{1}H and ^{13}C NMR spectra of compound **3k**



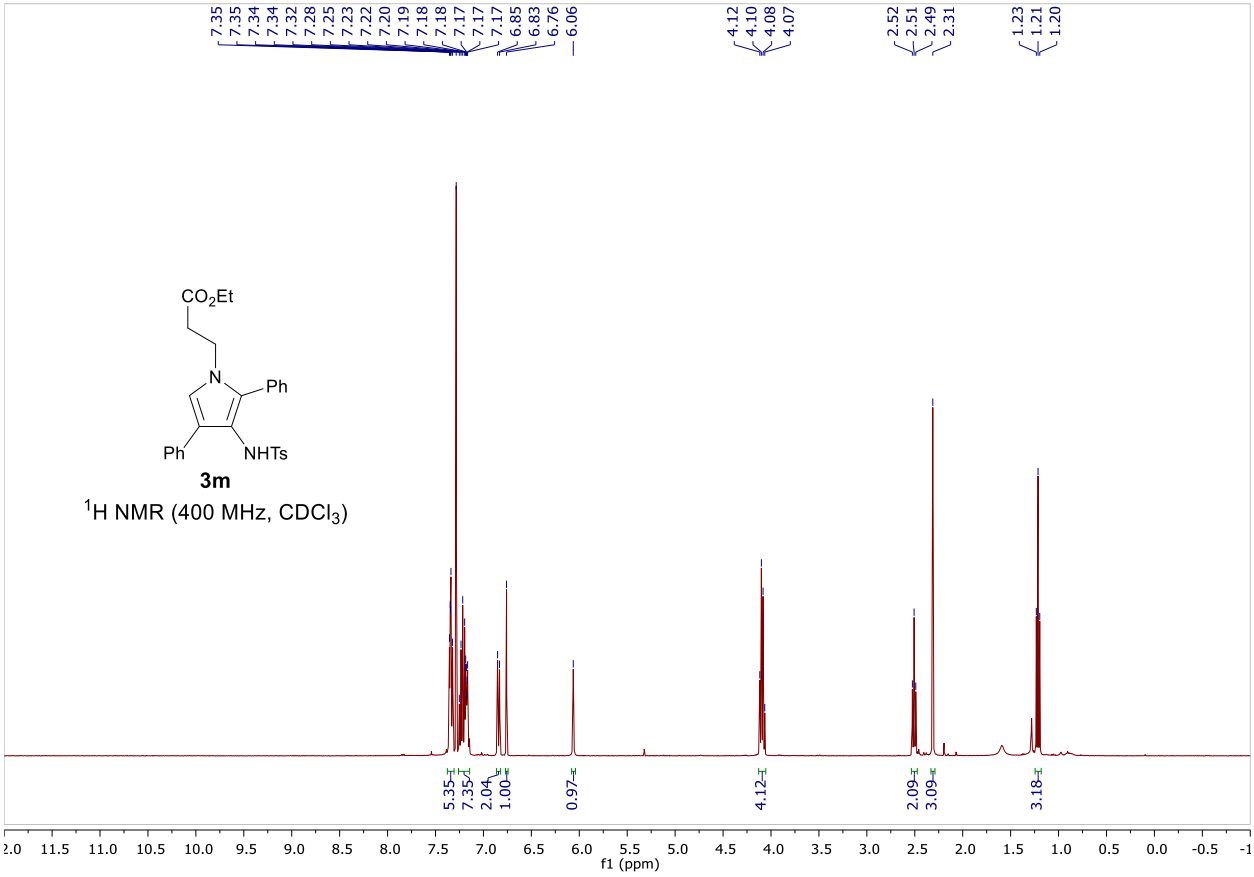


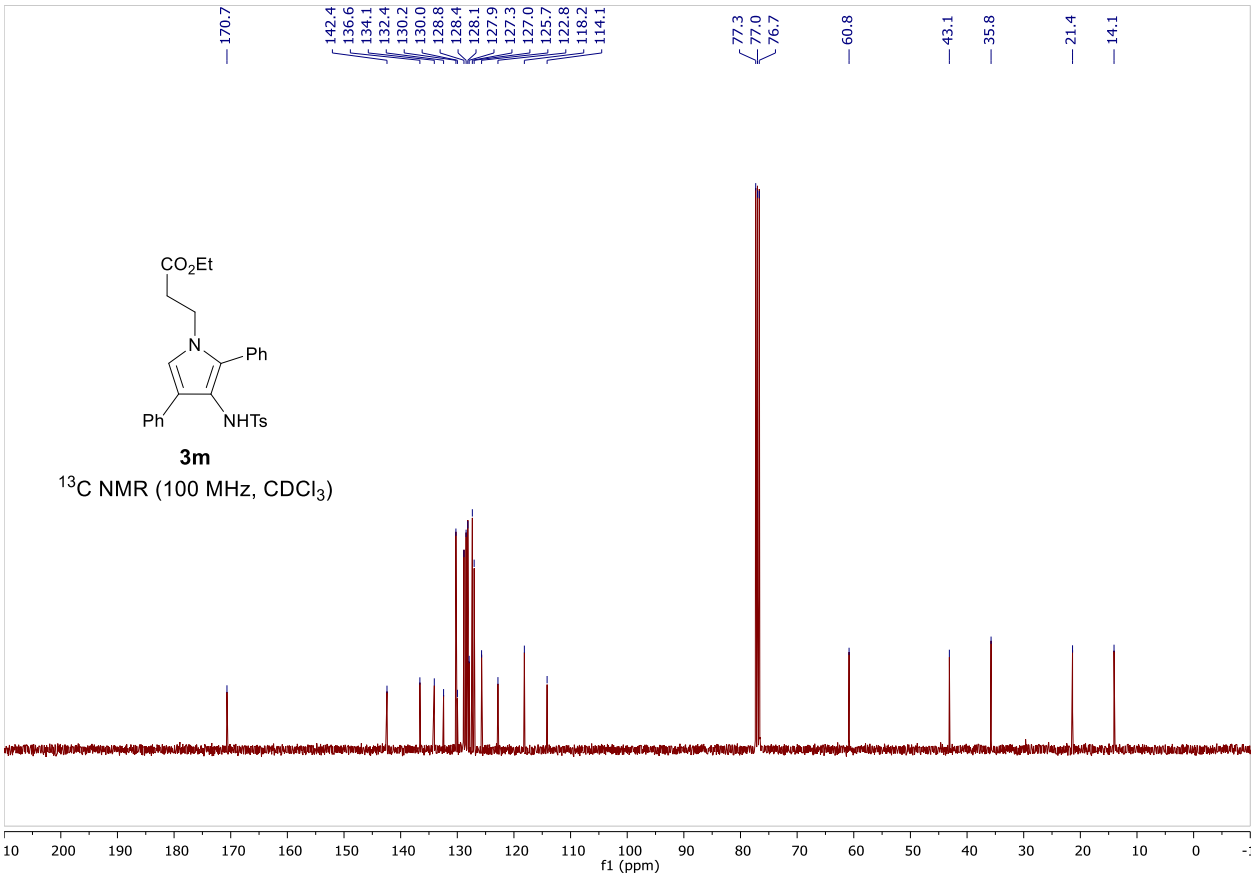
^{1}H and ^{13}C NMR spectra of compound **3l**



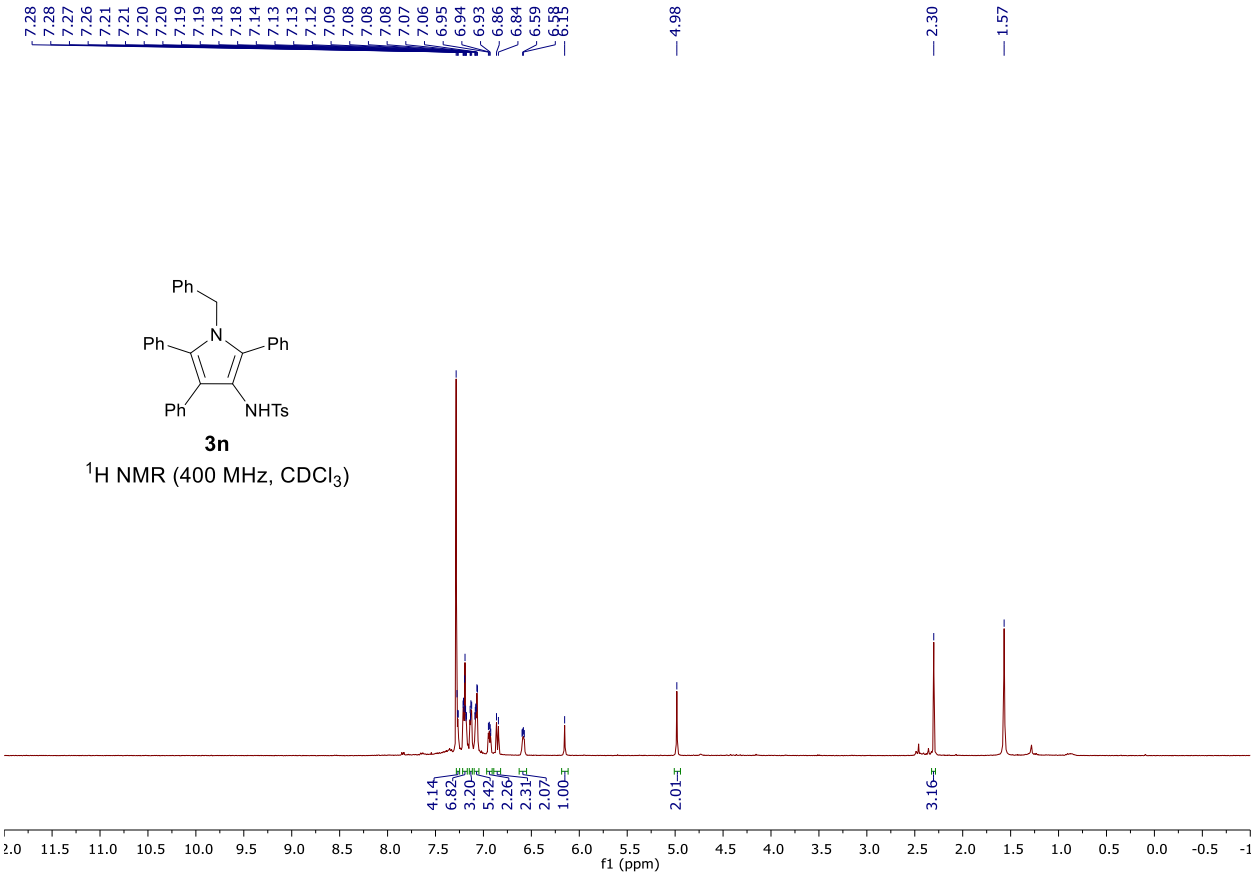


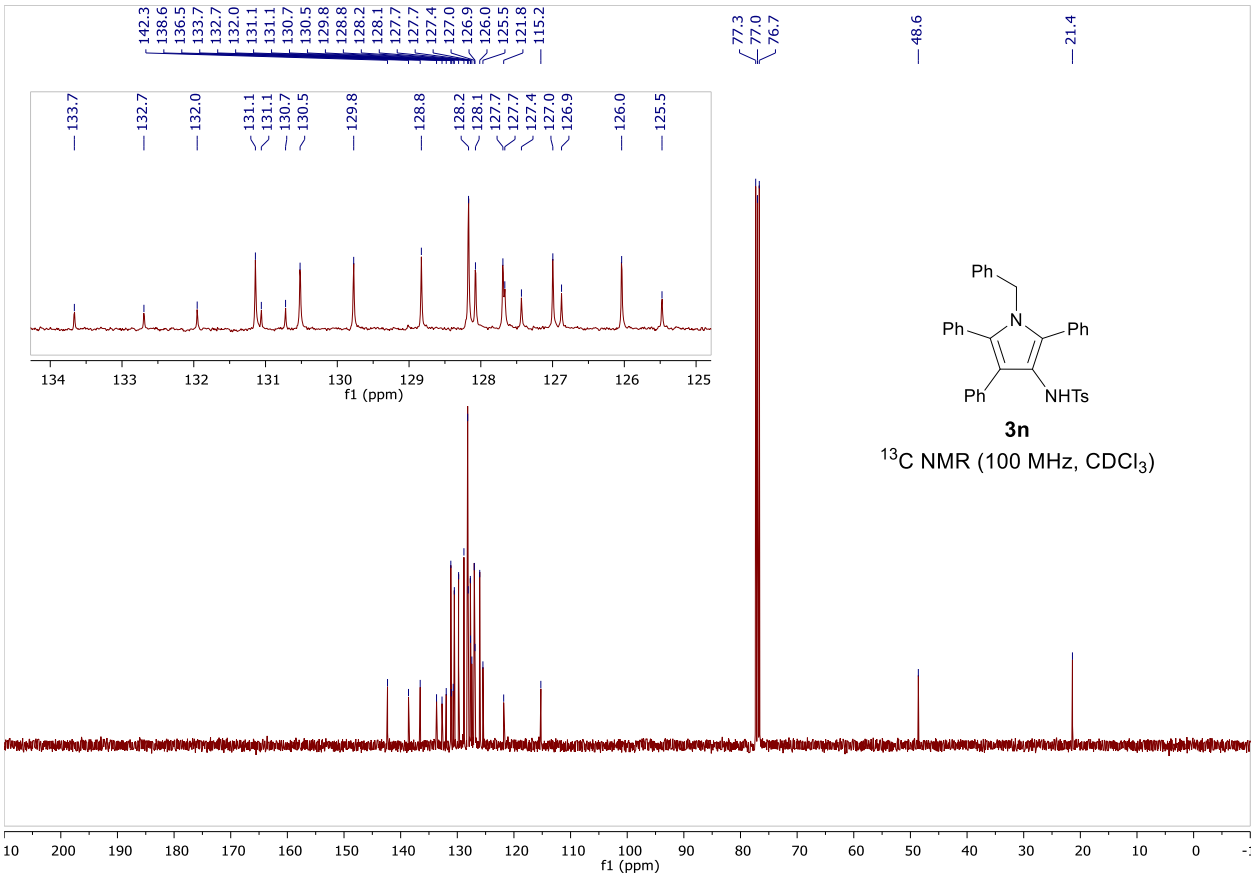
^{1}H and ^{13}C NMR spectra of compound **3m**



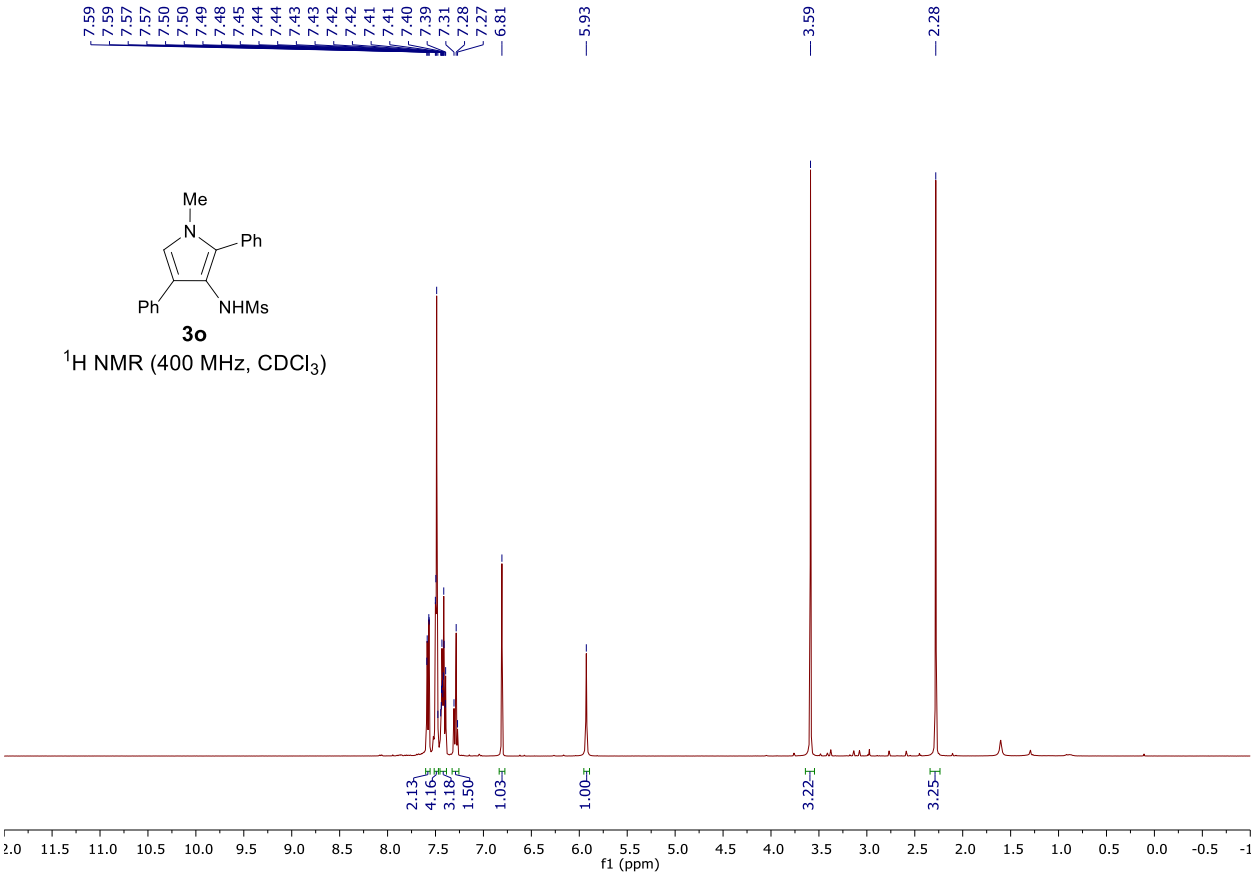


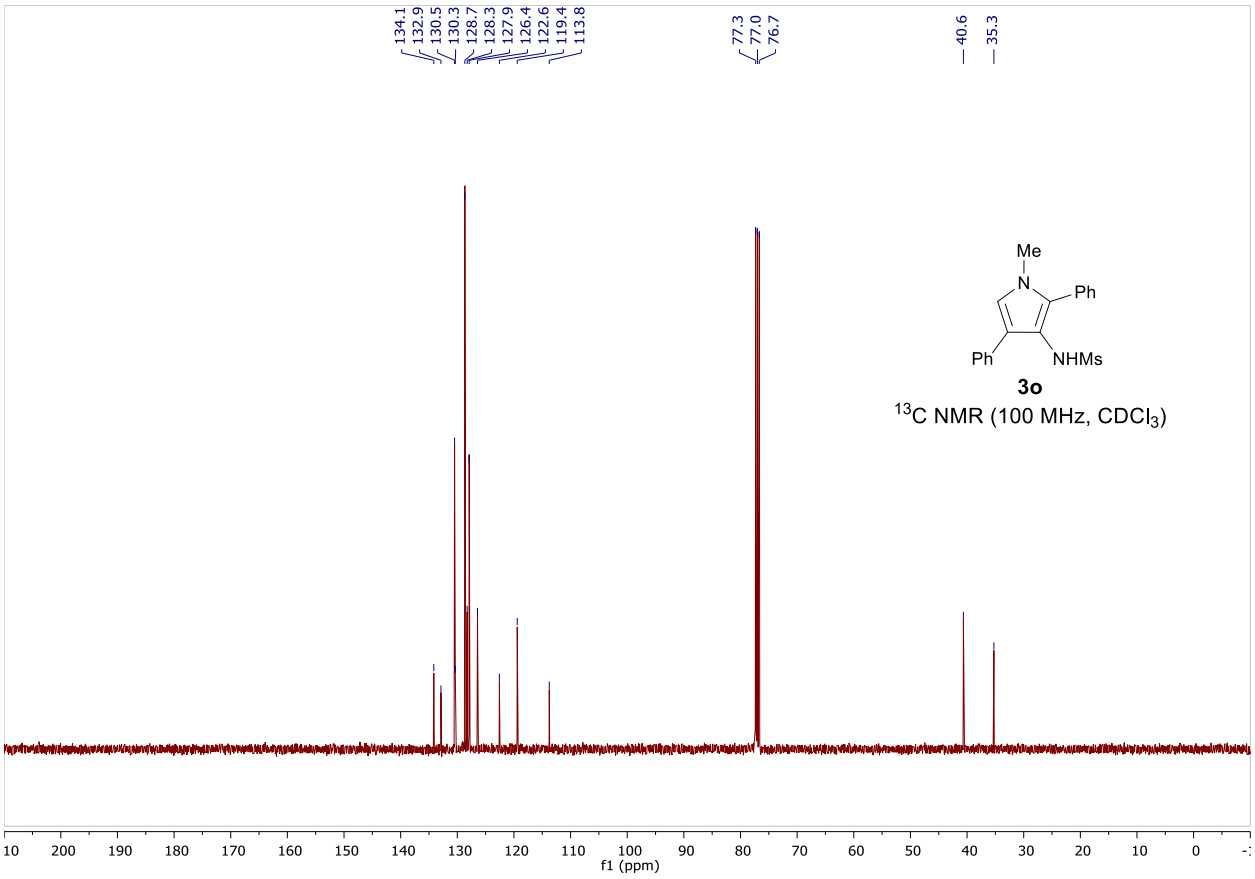
^{1}H and ^{13}C NMR spectra of compound **3n**



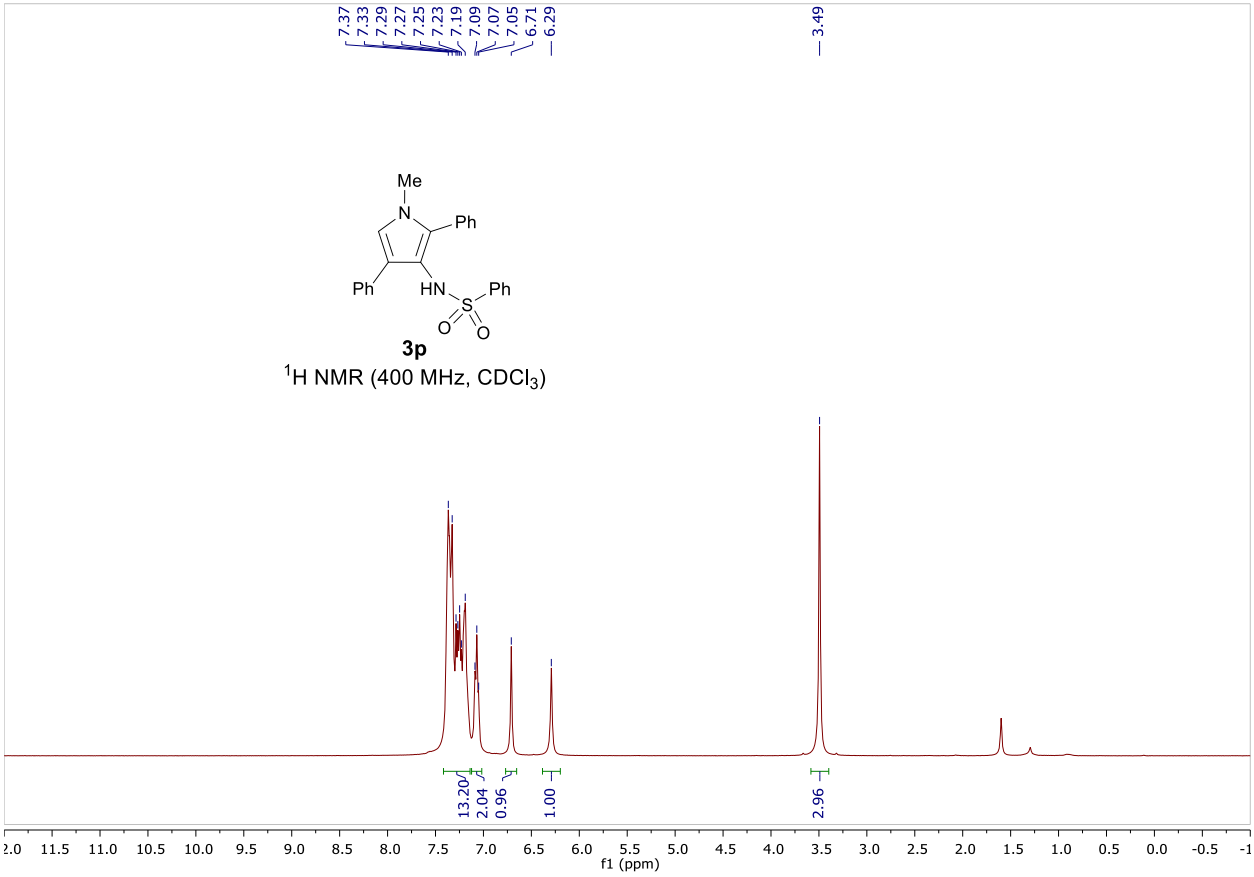


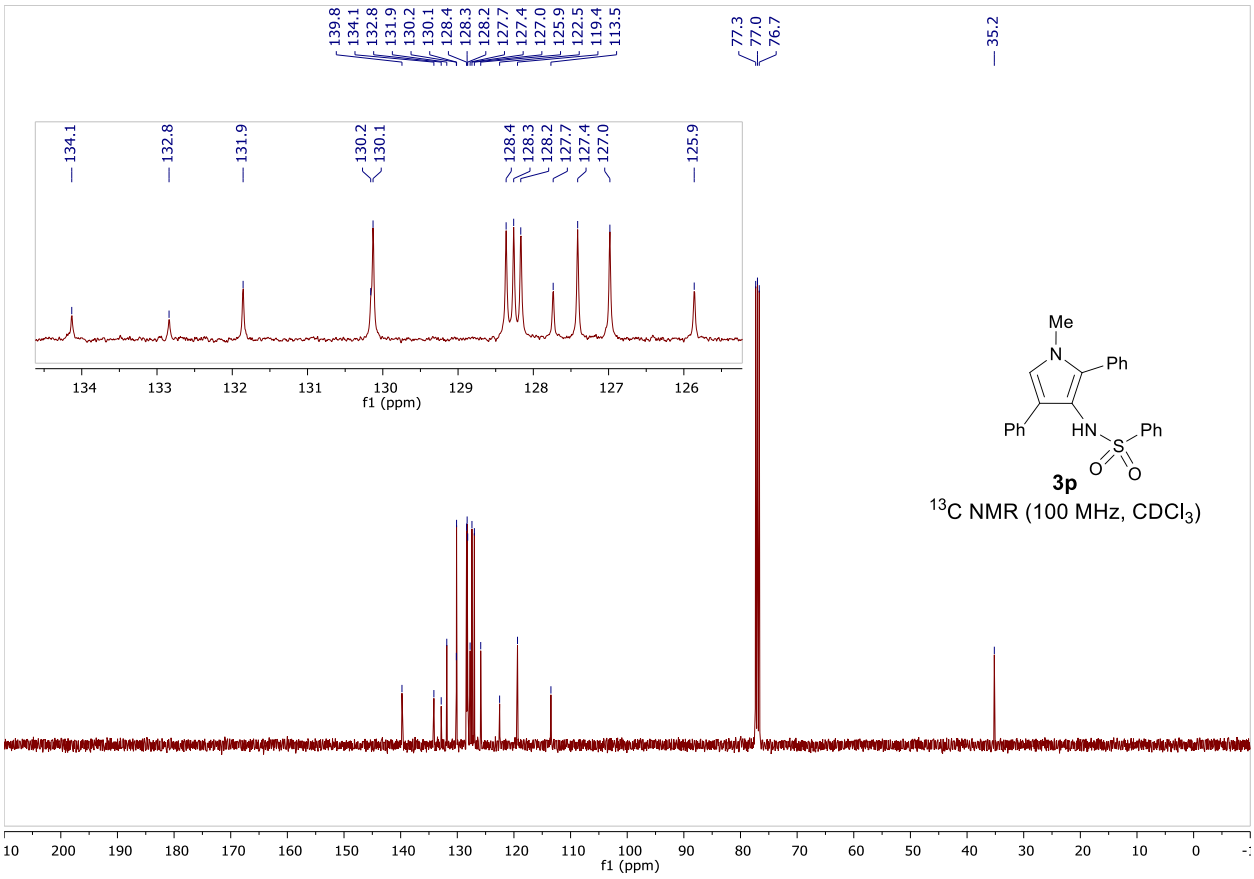
^{1}H and ^{13}C NMR spectra of compound **3o**



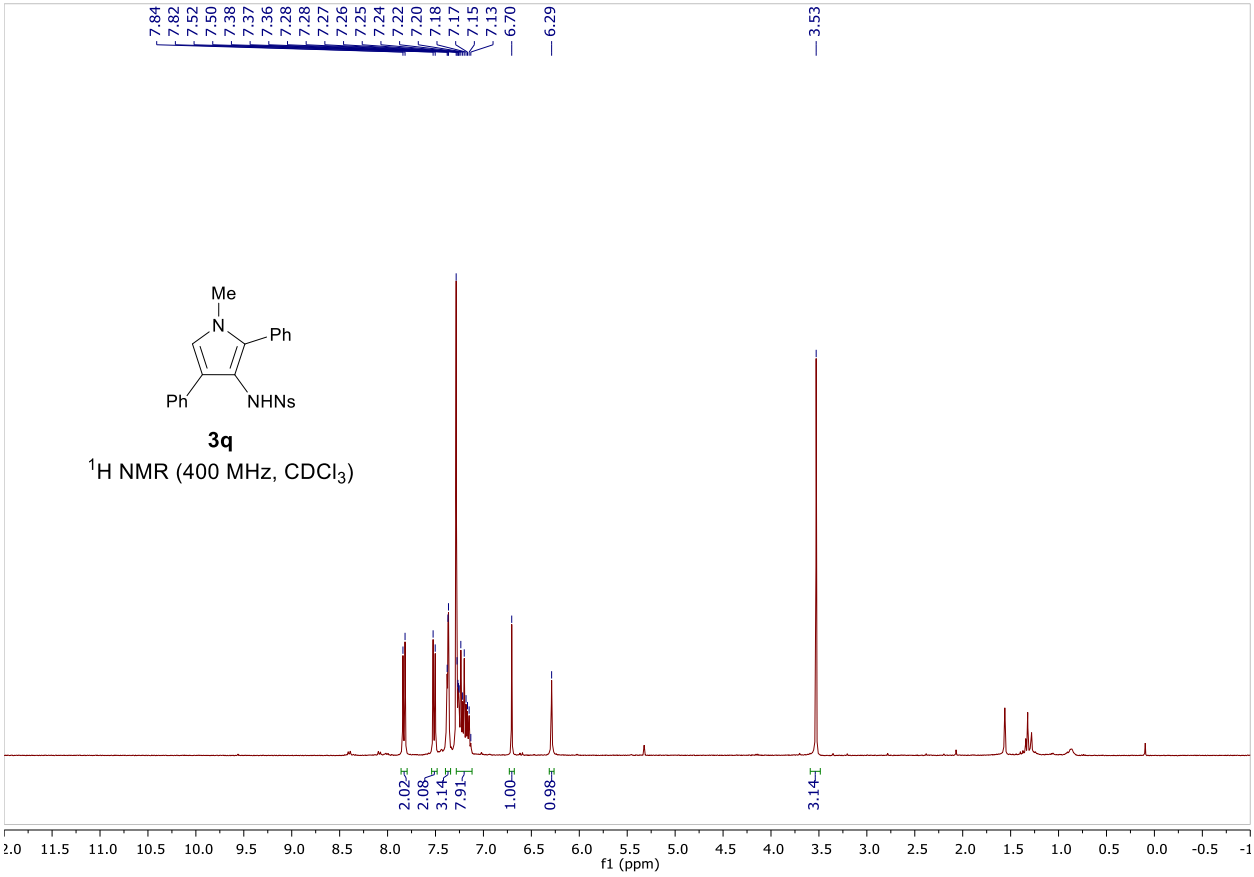


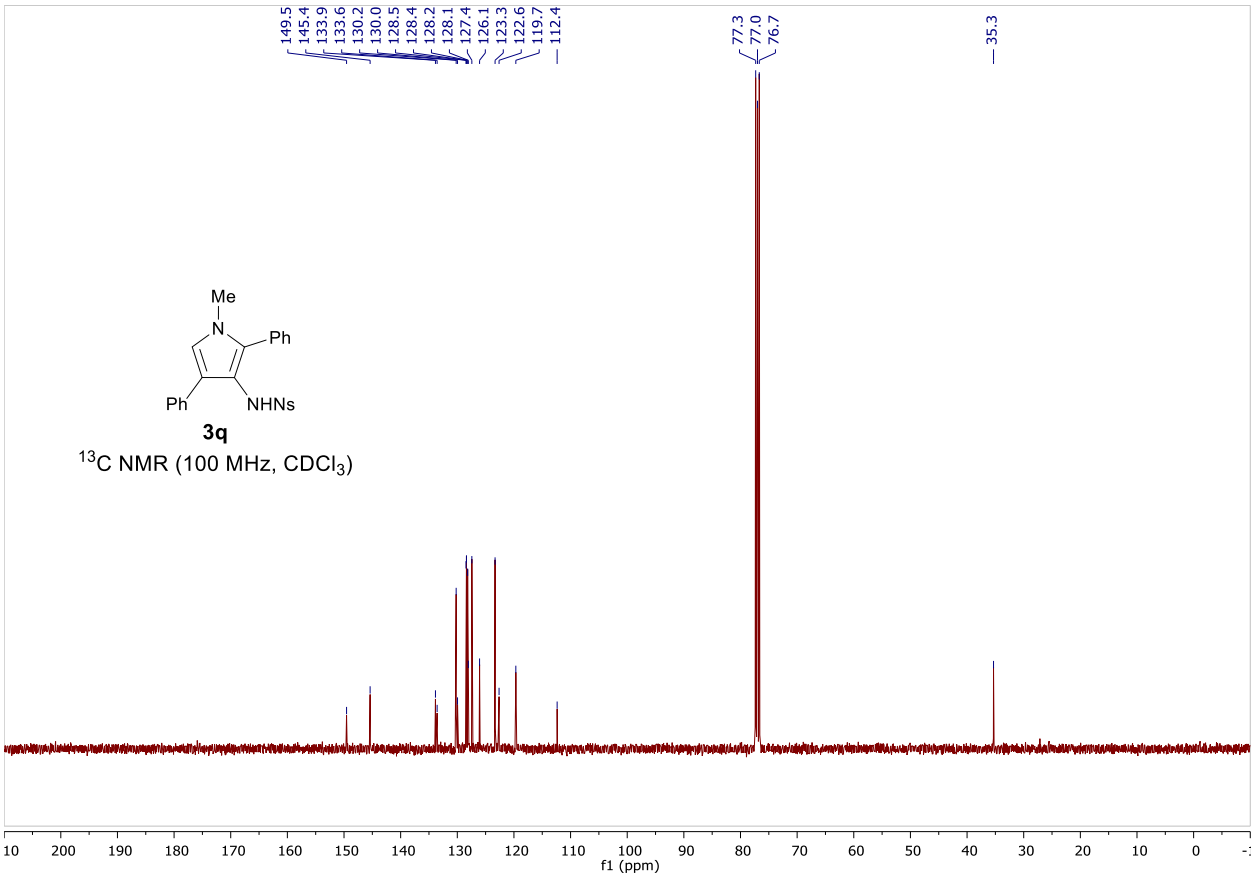
^{1}H and ^{13}C NMR spectra of compound **3p**



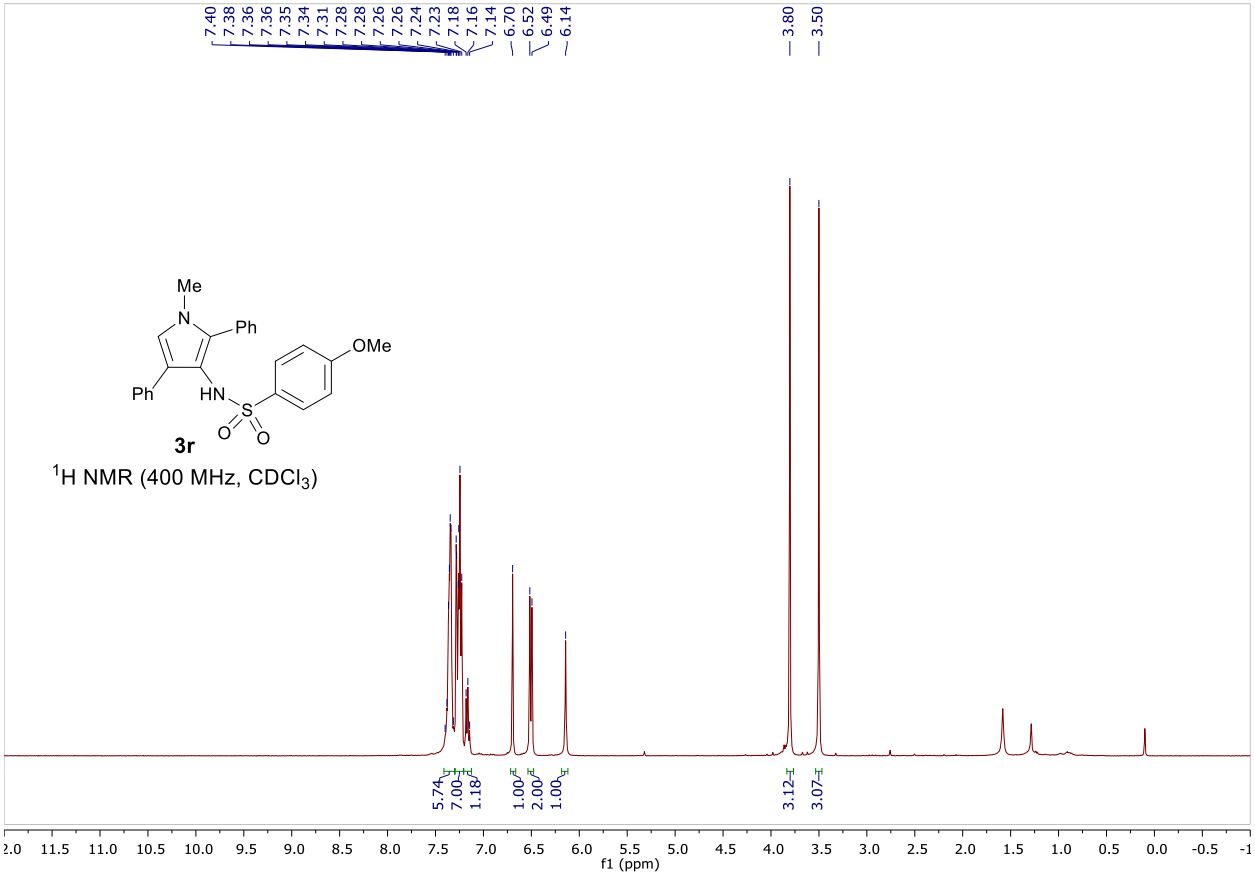


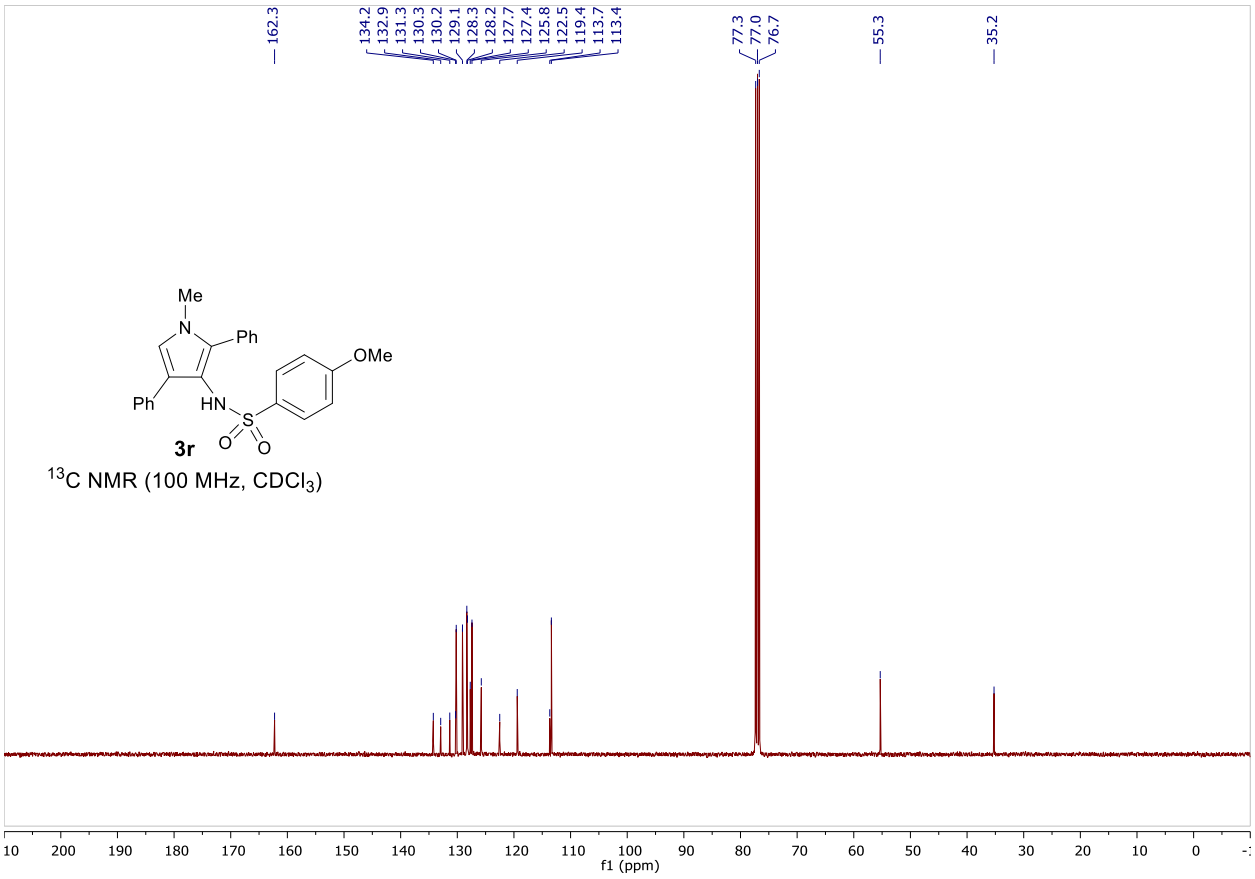
^{1}H and ^{13}C NMR spectra of compound **3q**



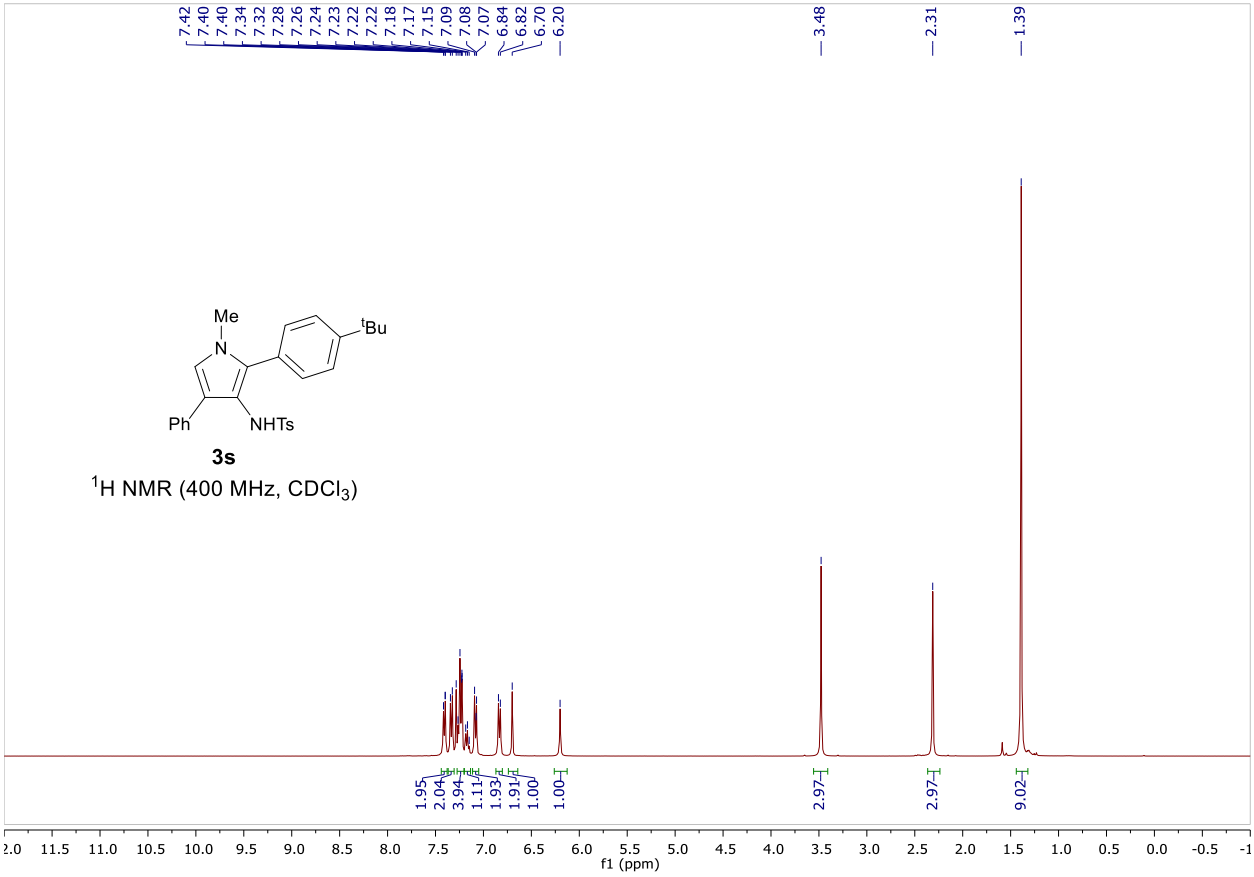


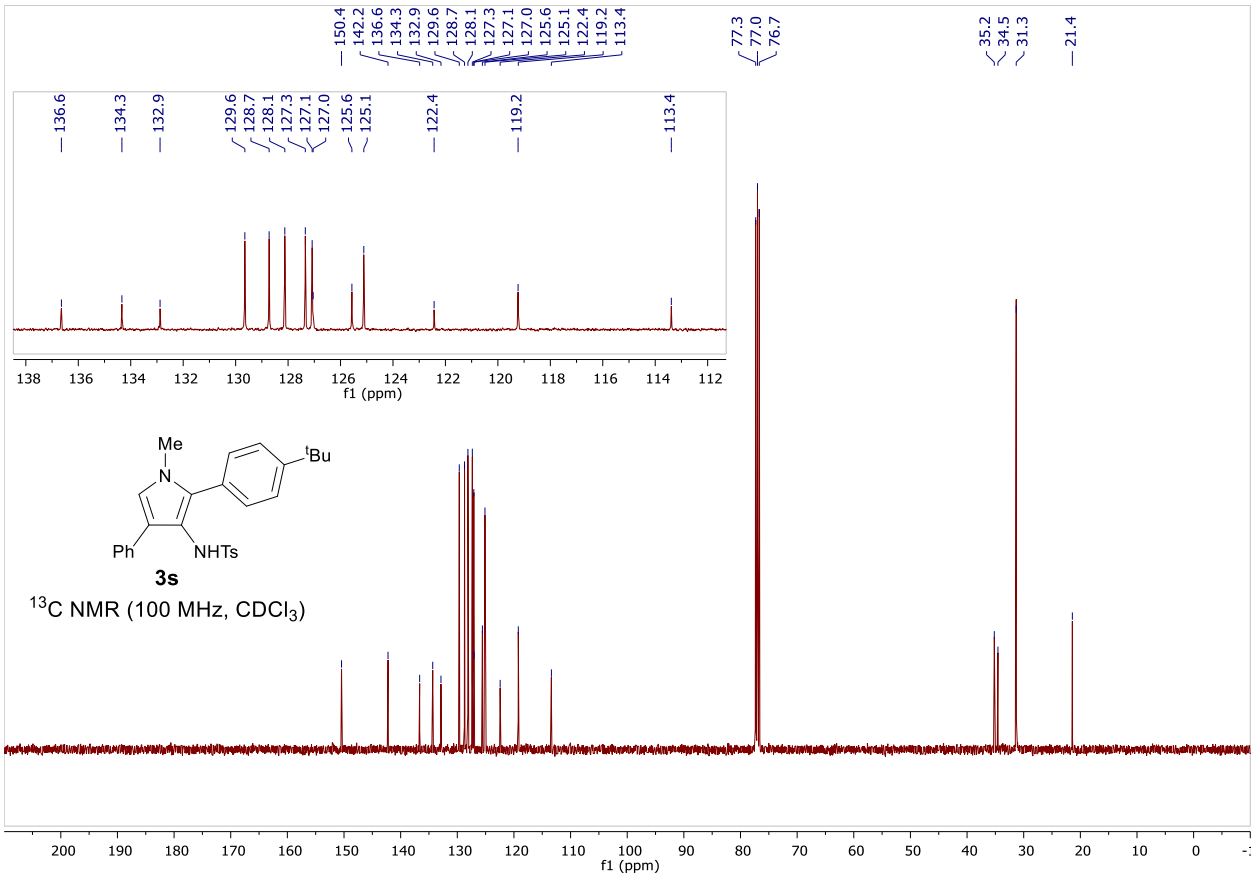
^{1}H and ^{13}C NMR spectra of compound **3r**



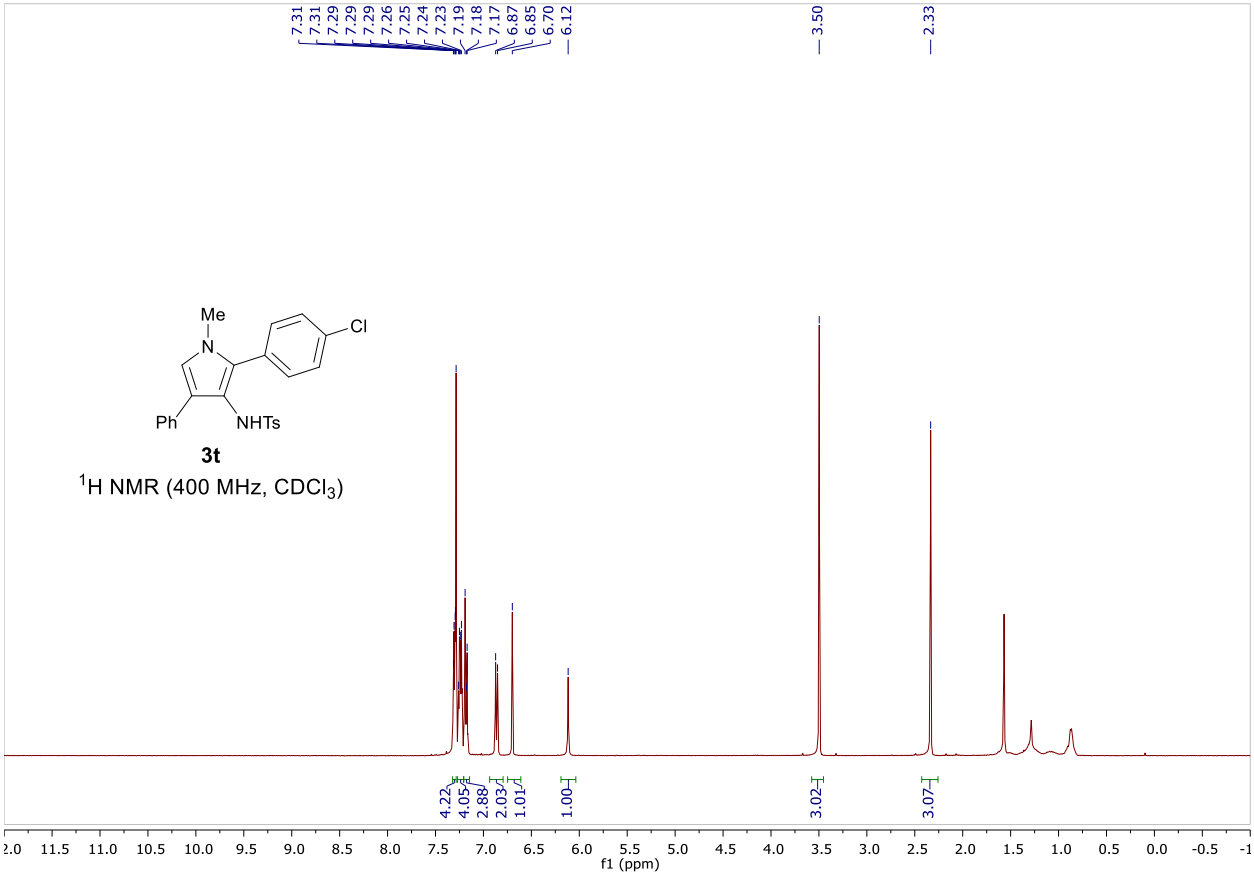


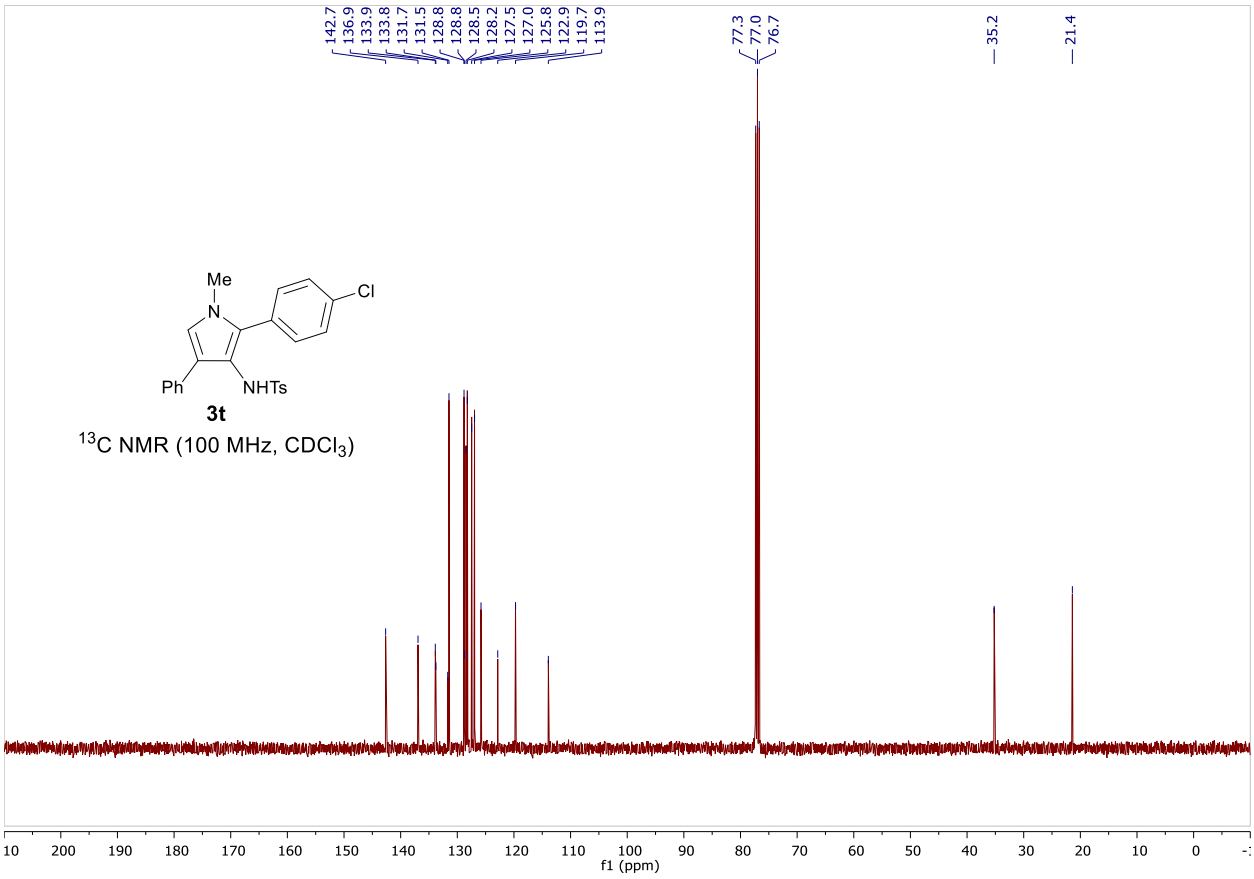
^{1}H and ^{13}C NMR spectra of compound **3s**



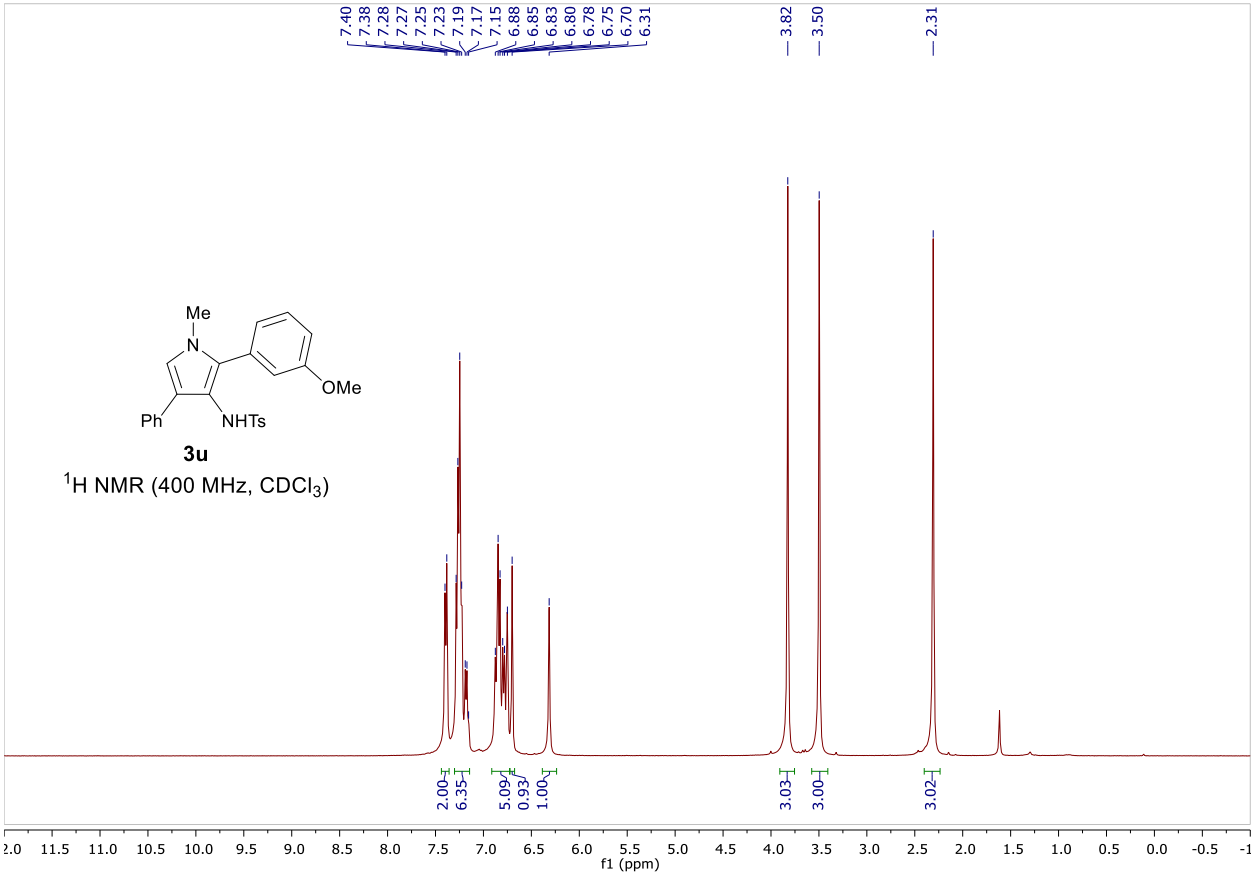


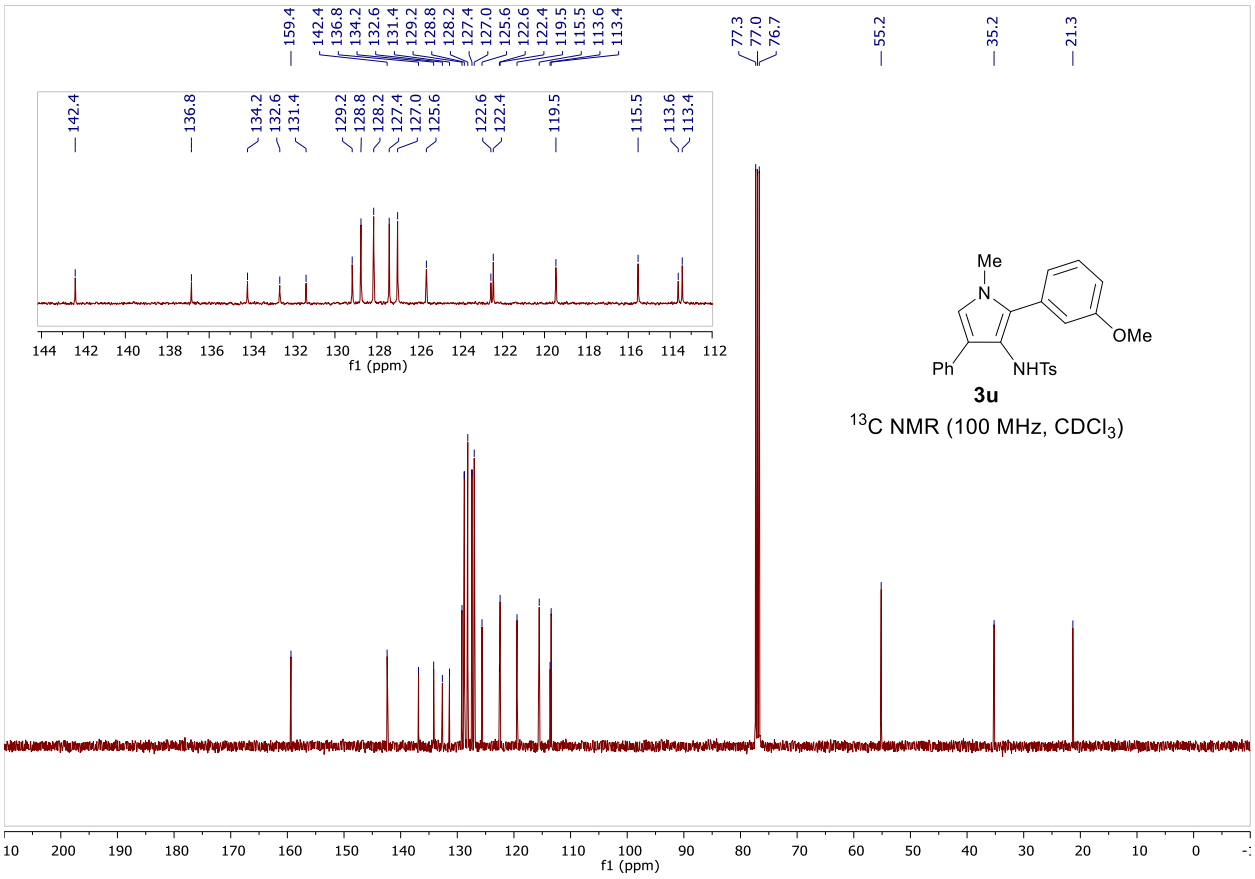
^{1}H and ^{13}C NMR spectra of compound **3t**



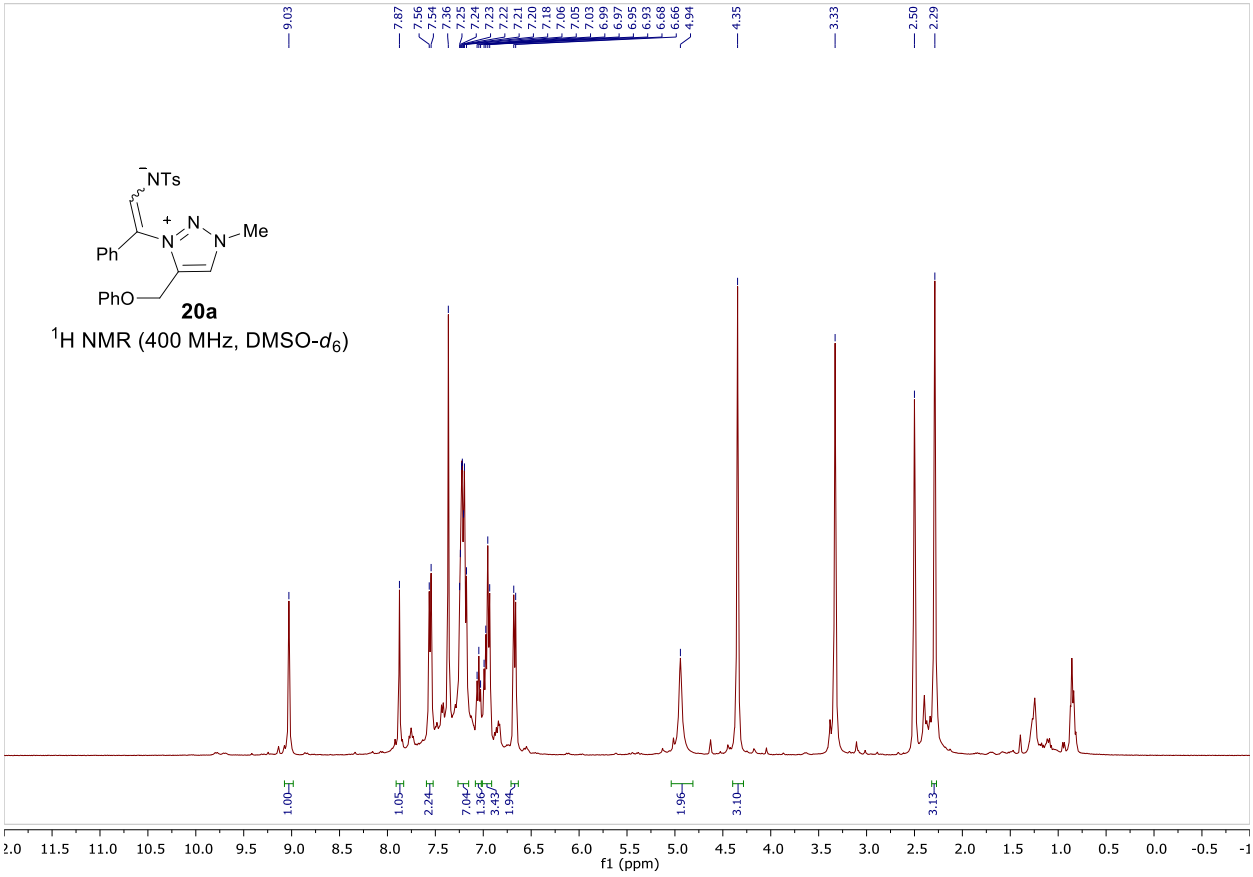


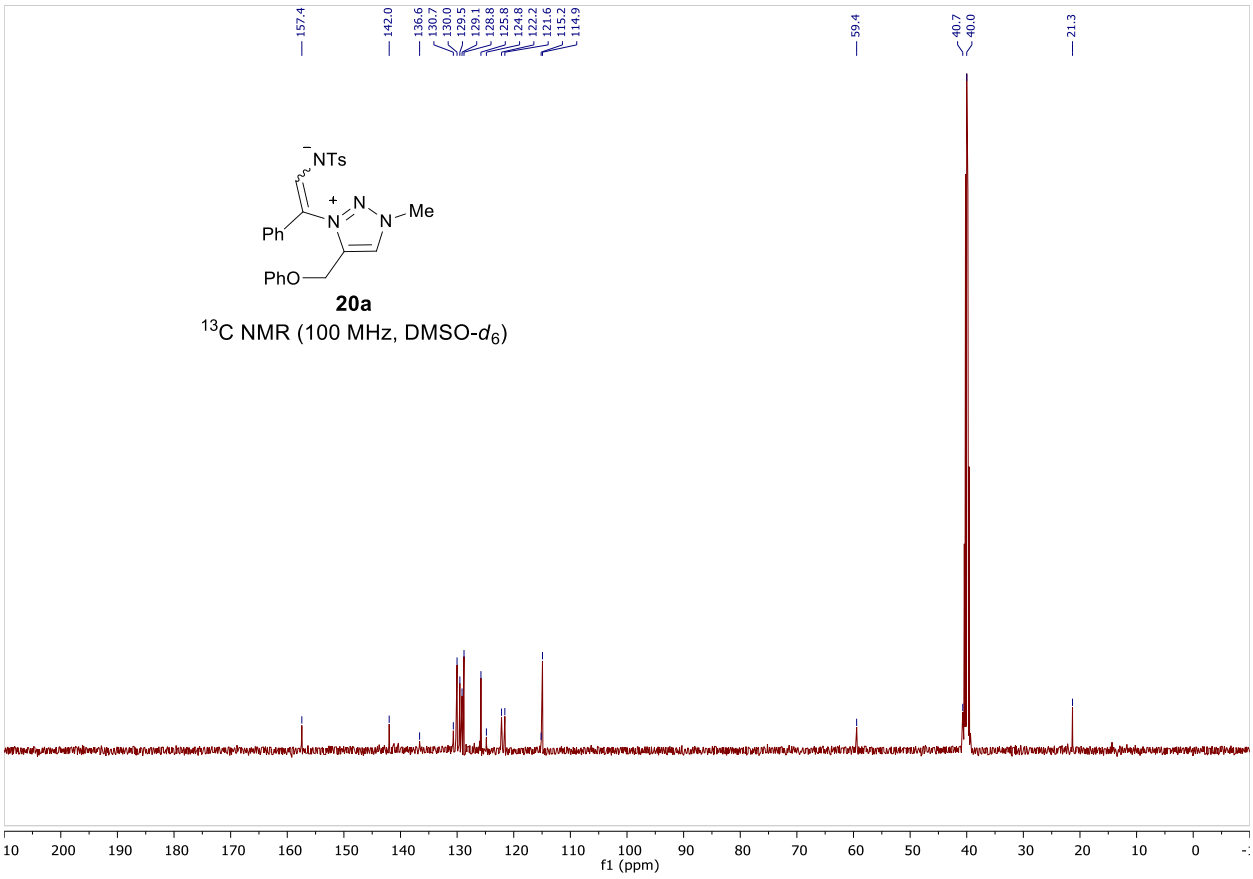
^{1}H and ^{13}C NMR spectra of compound **3u**



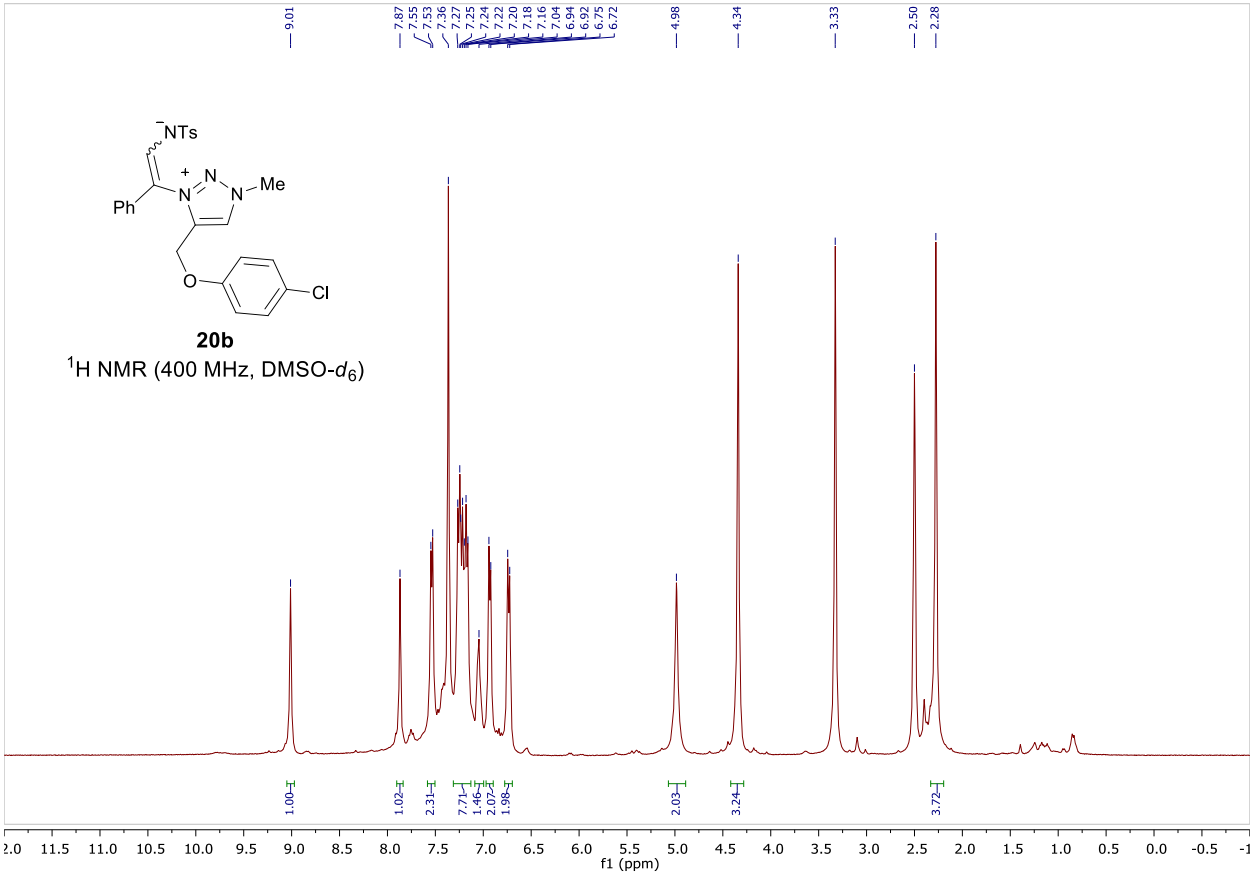


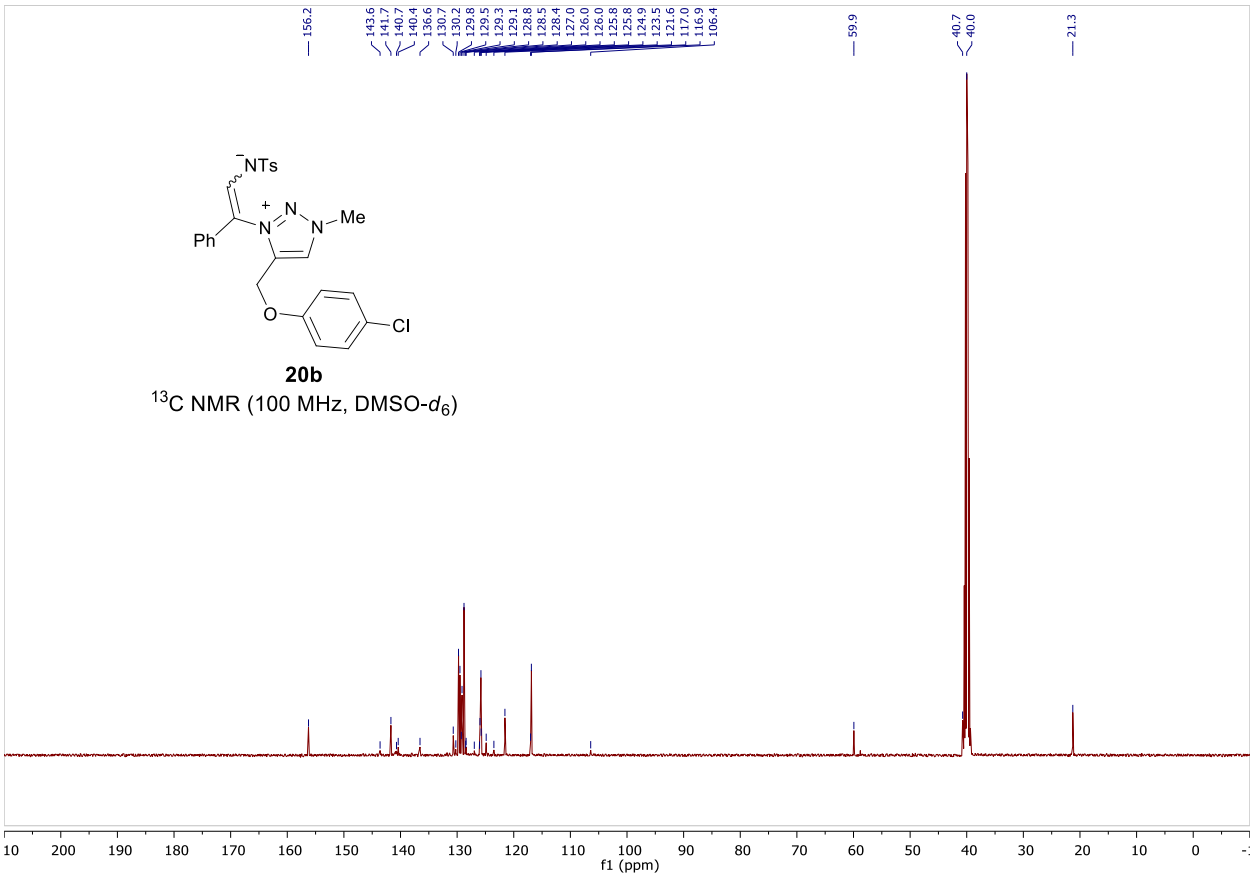
^{1}H and ^{13}C NMR spectra of compound **20a**



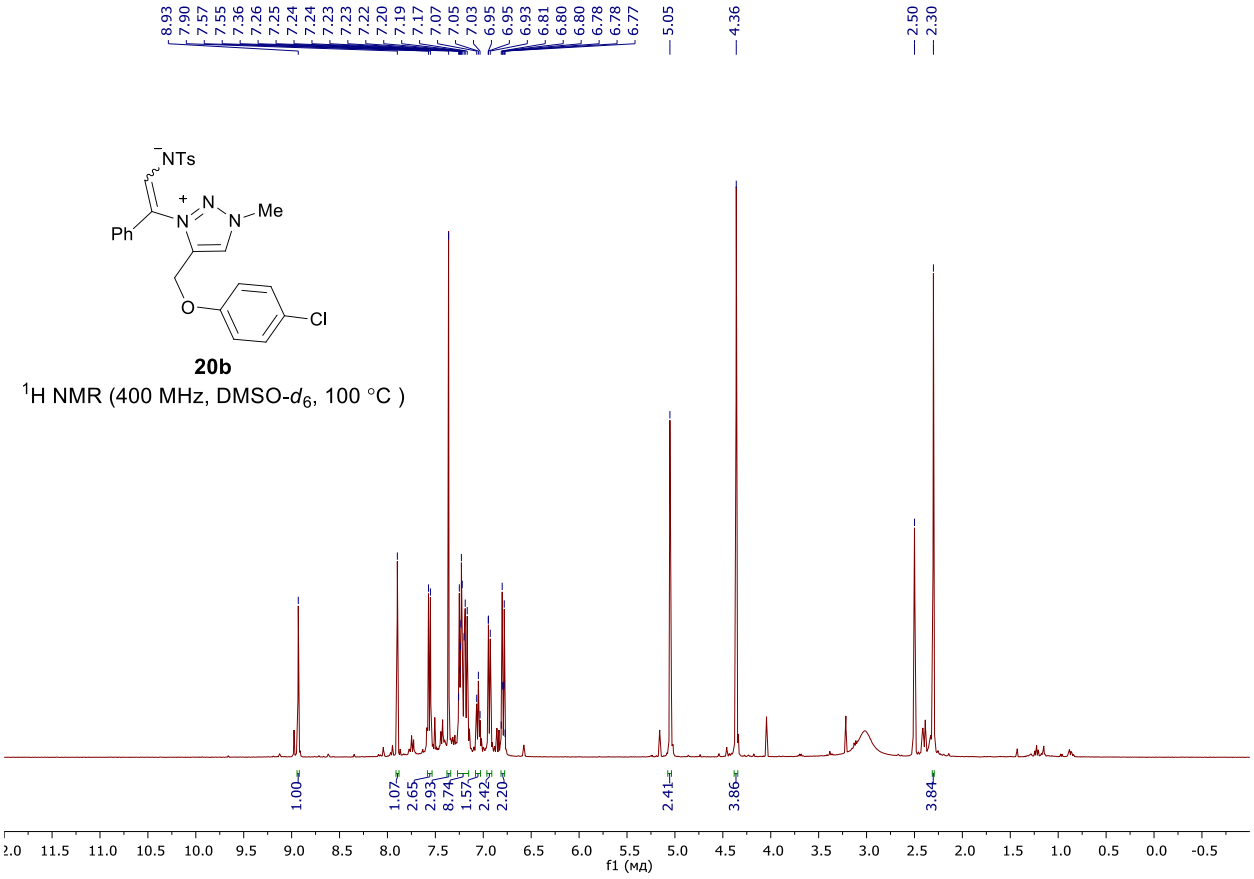


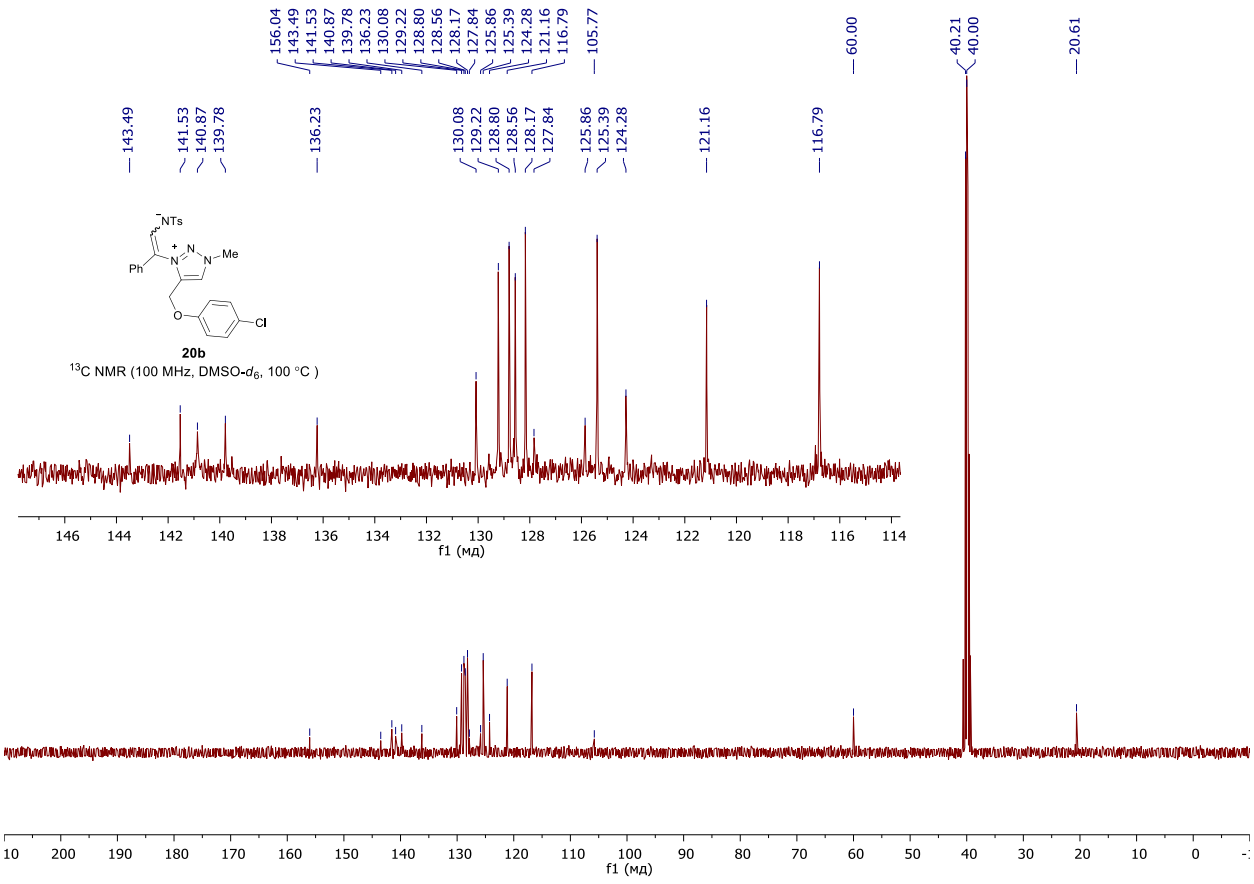
^{1}H and ^{13}C NMR spectra of compound **20b**





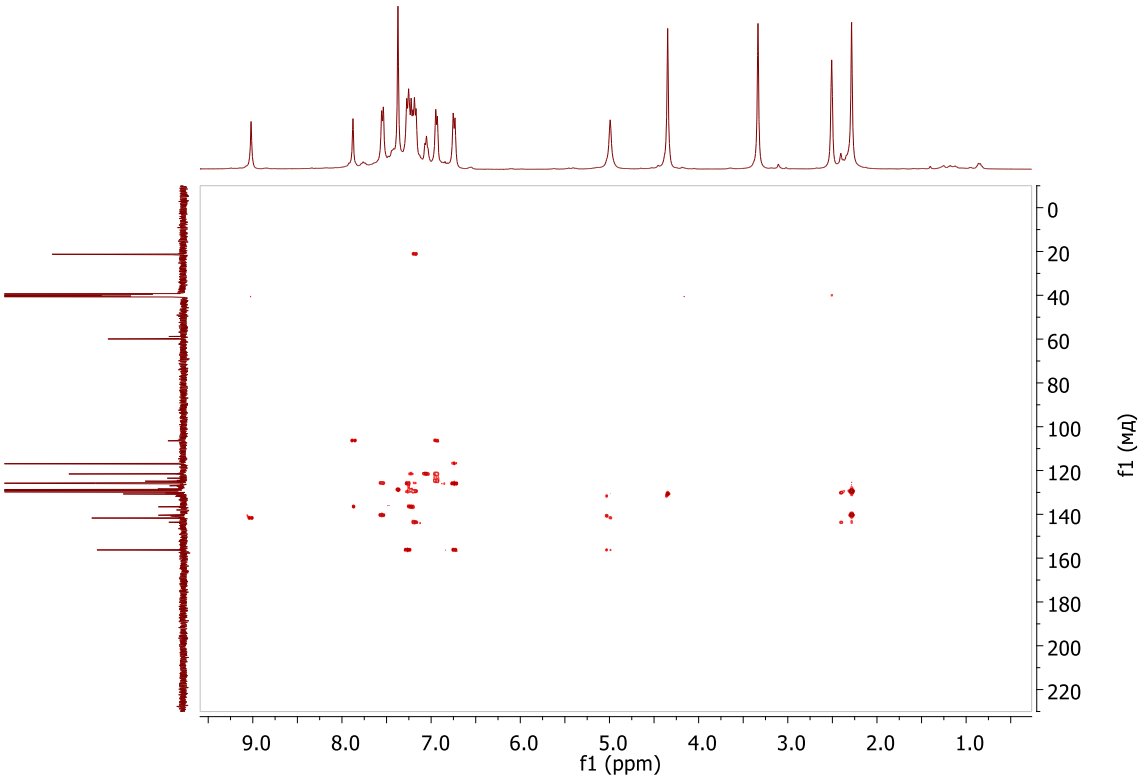
^{1}H and ^{13}C NMR spectra of compound **20b** at 100 °C



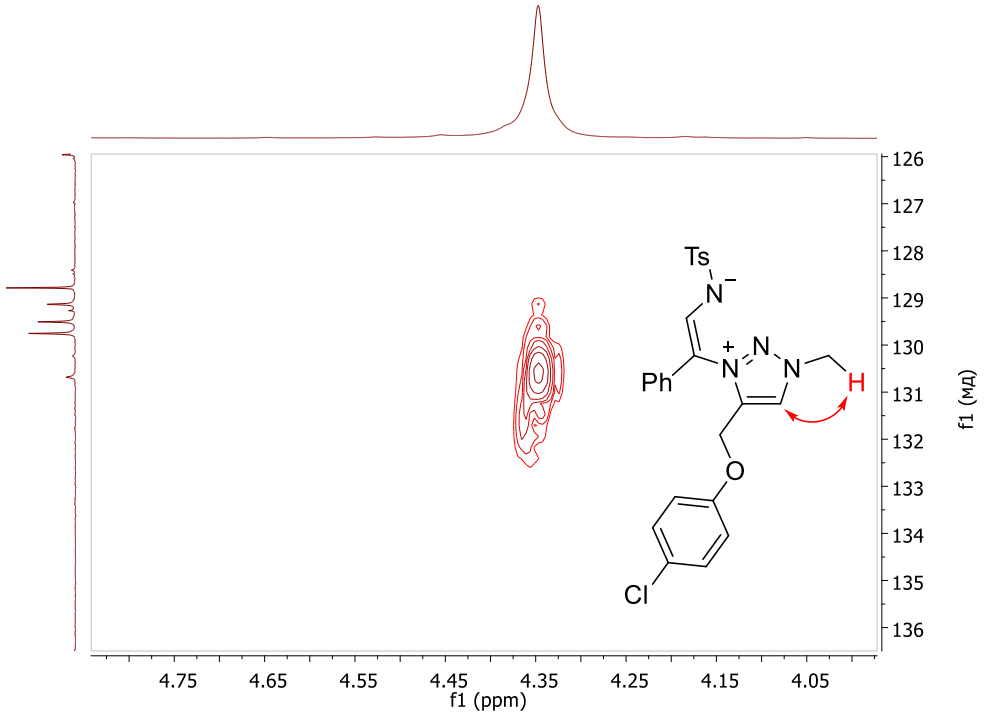


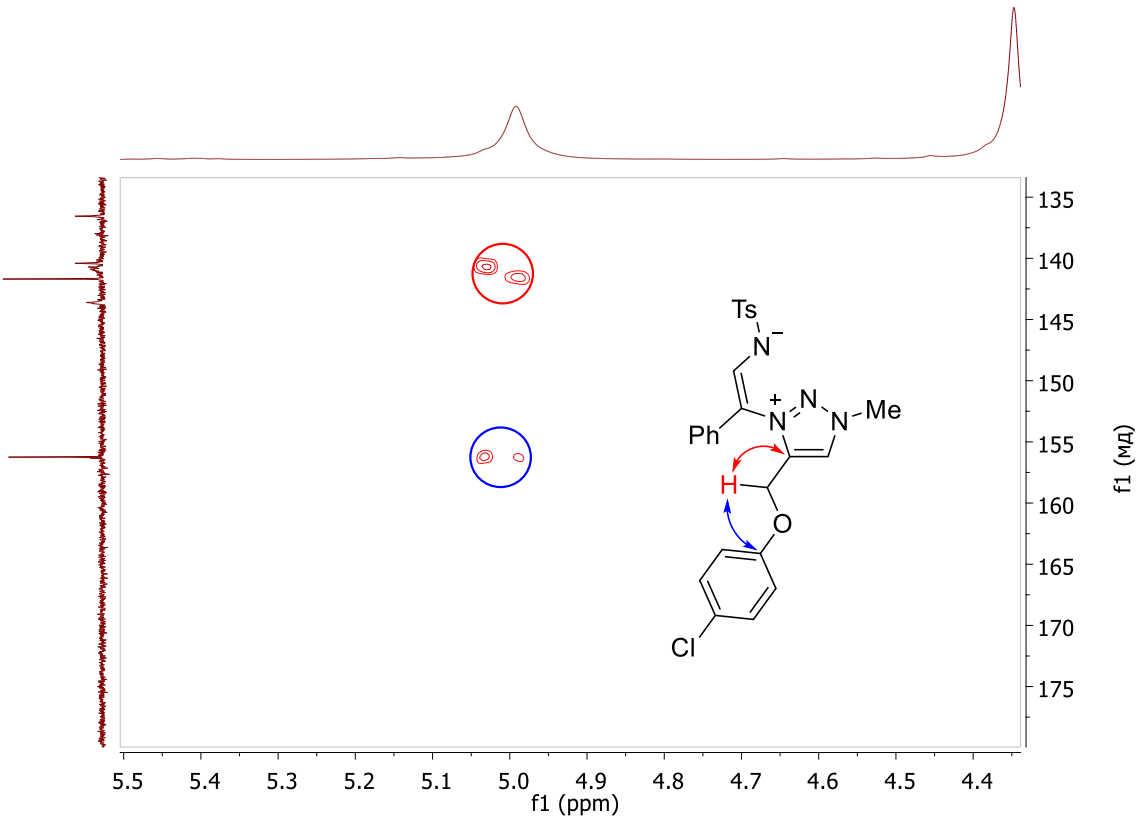
2D NMR spectra of compound **20b**

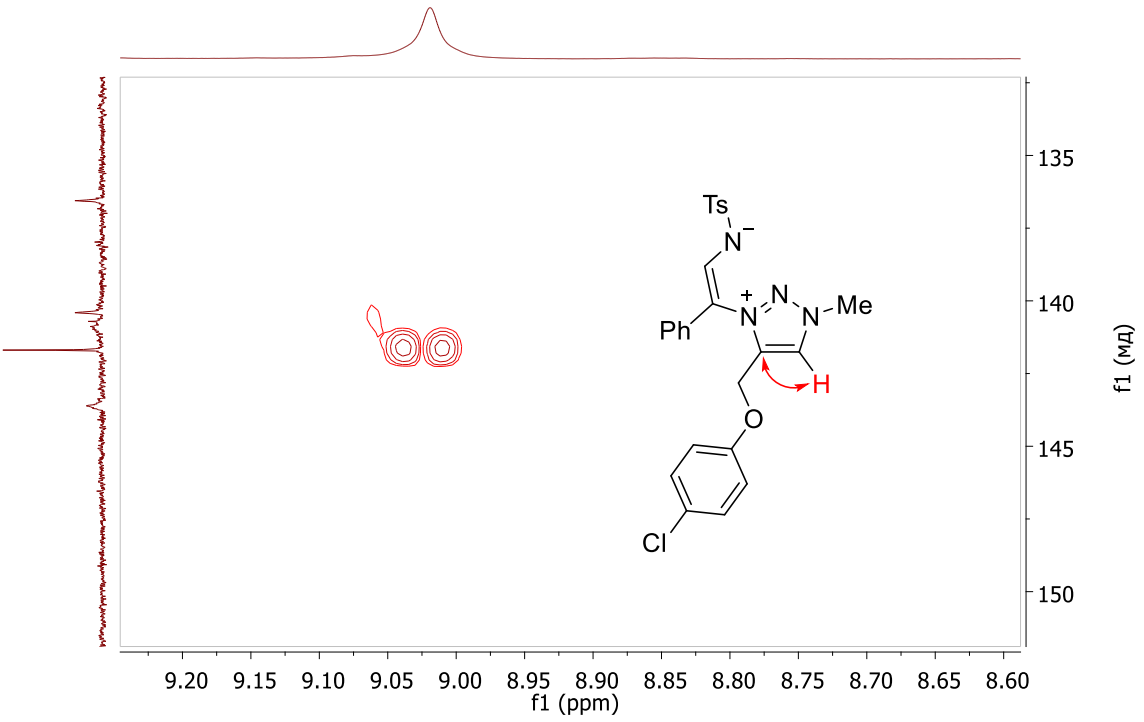
^{1}H-^{13}C HMBC spectrum

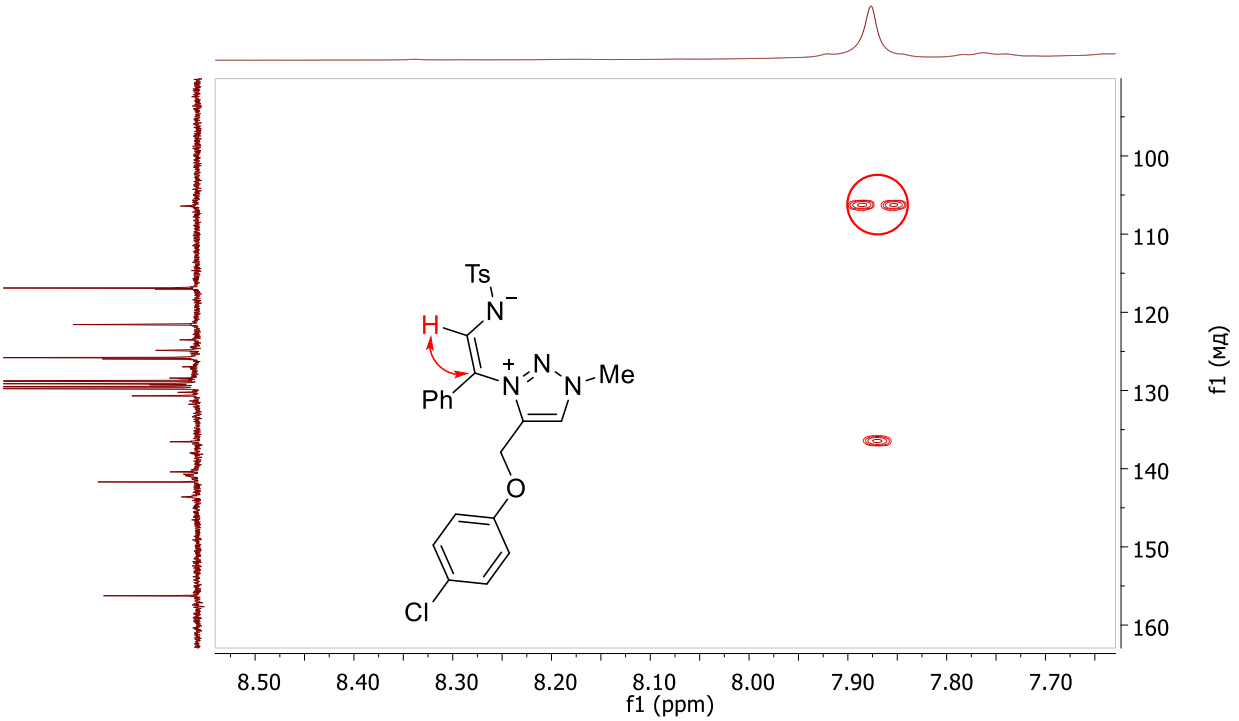


Key cross-peaks in ^{1}H-^{13}C HMBC spectrum

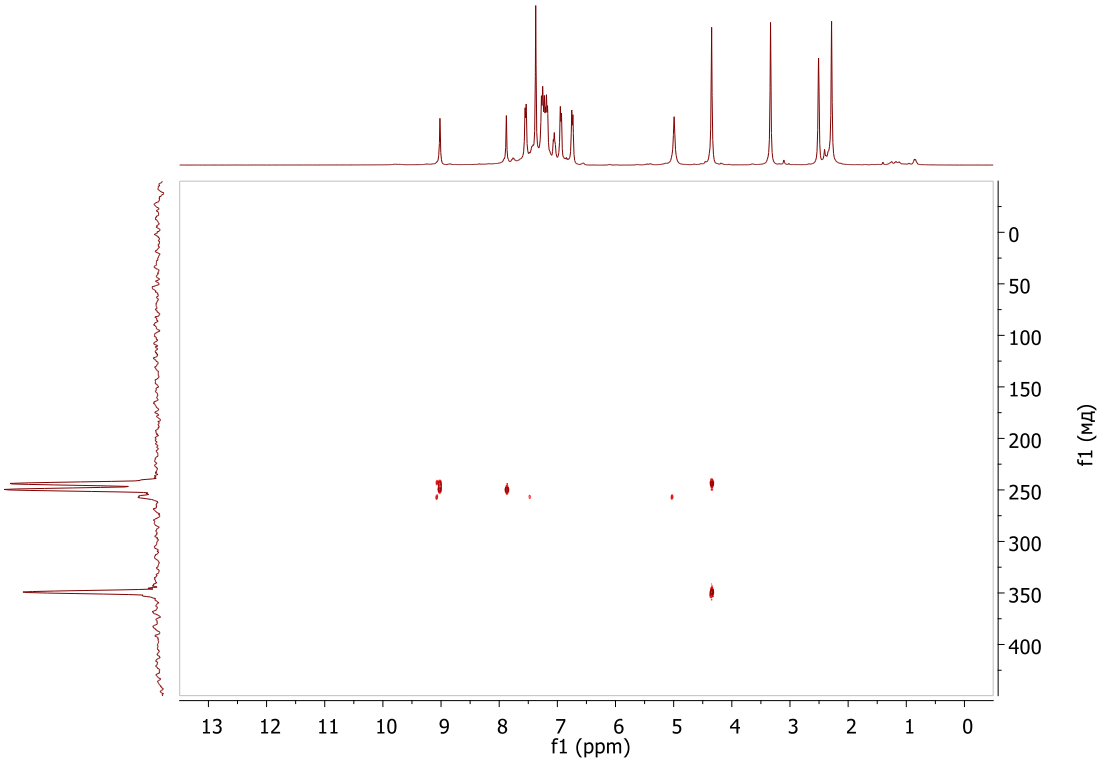



Ts
N
Ph
N
N
Me
H
O
Cl
135
140
145
150
155
160
165
170
175
f1 (мд)
5.5
5.4
5.3
5.2
5.1
5.0
4.9
4.8
4.7
4.6
4.5
4.4
f1 (ppm)

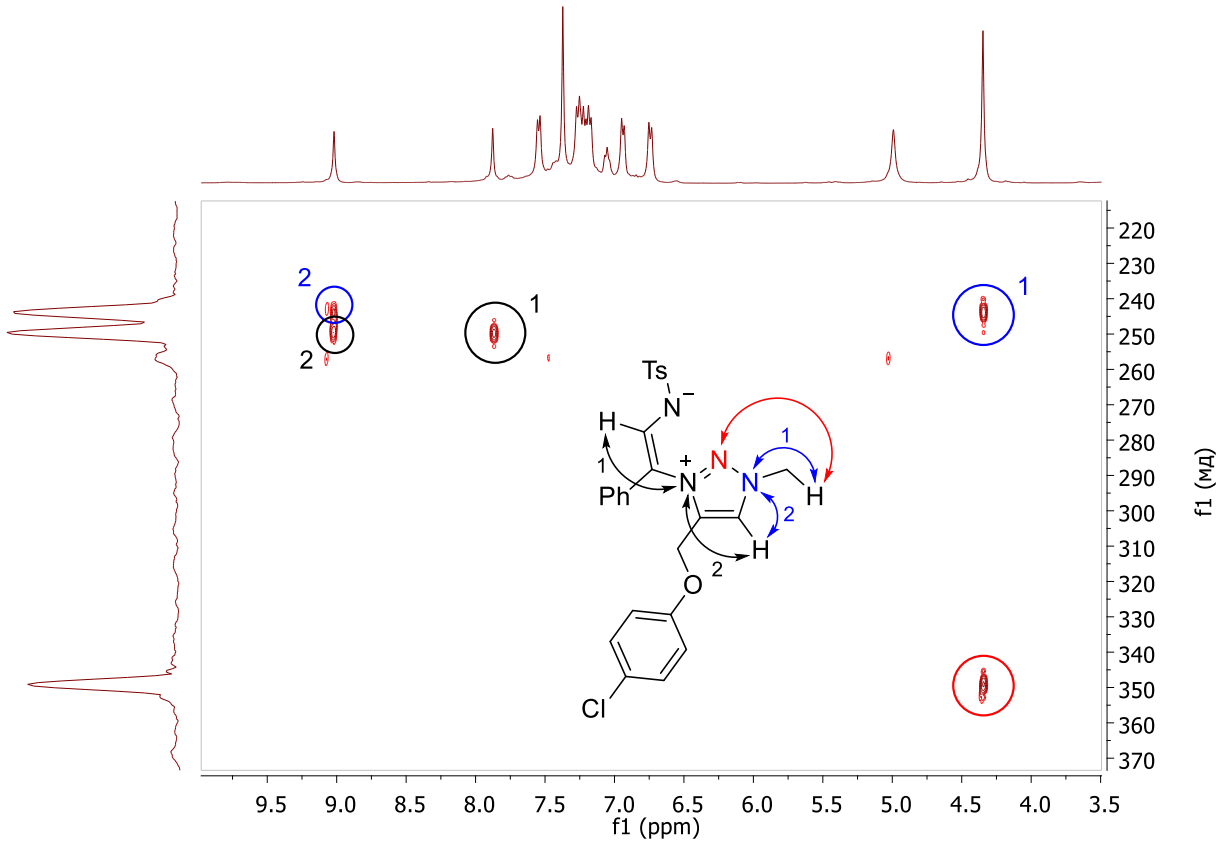

Ts
N
Ph
N
N
Me
H
O
Cl
135
140
145
150
f1 (мд)
9.20
9.15
9.10
9.05
9.00
8.95
8.90
8.85
8.80
8.75
8.70
8.65
8.60
f1 (ppm)


Ts
N
H
Ph
N
N
Me
O
Cl
8.50
8.40
8.30
8.20
8.10
8.00
7.90
7.80
7.70
f1 (ppm)
100
110
120
130
140
150
160
f1 (мд)

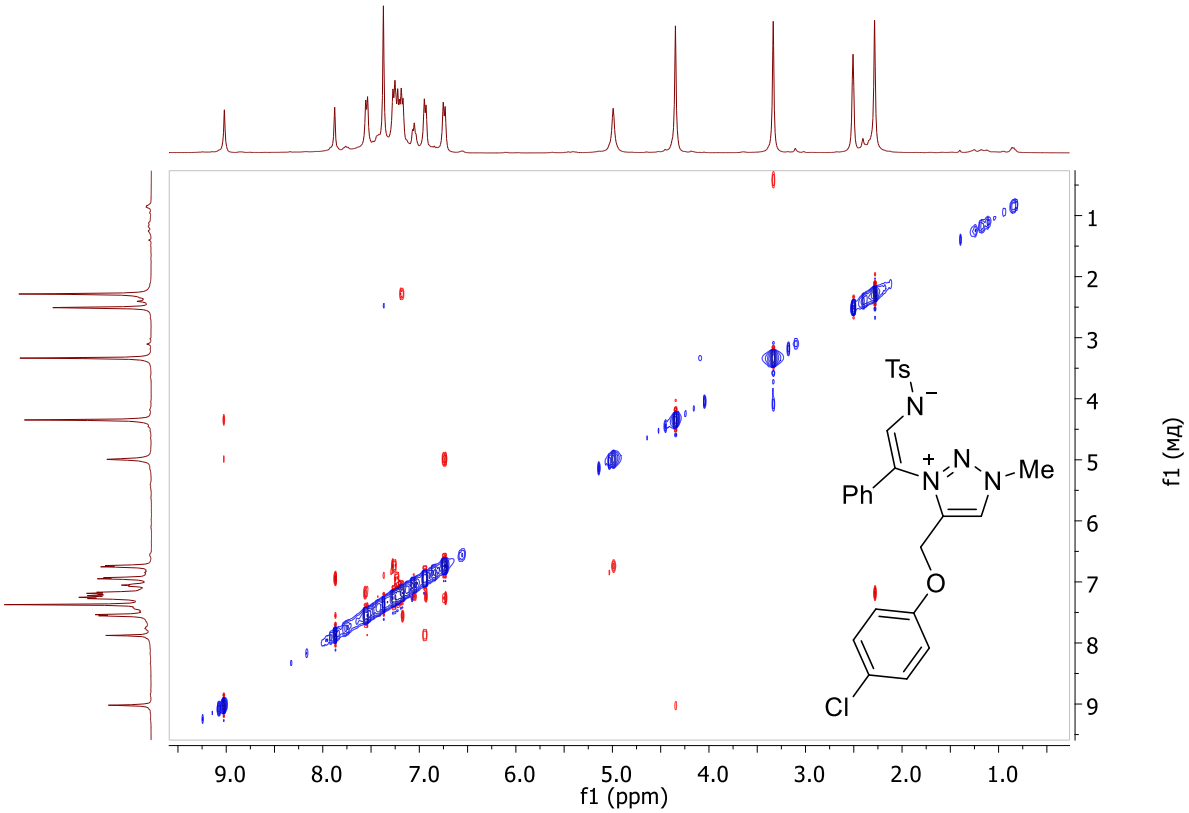
^{1}H-^{15}N HMBC spectrum



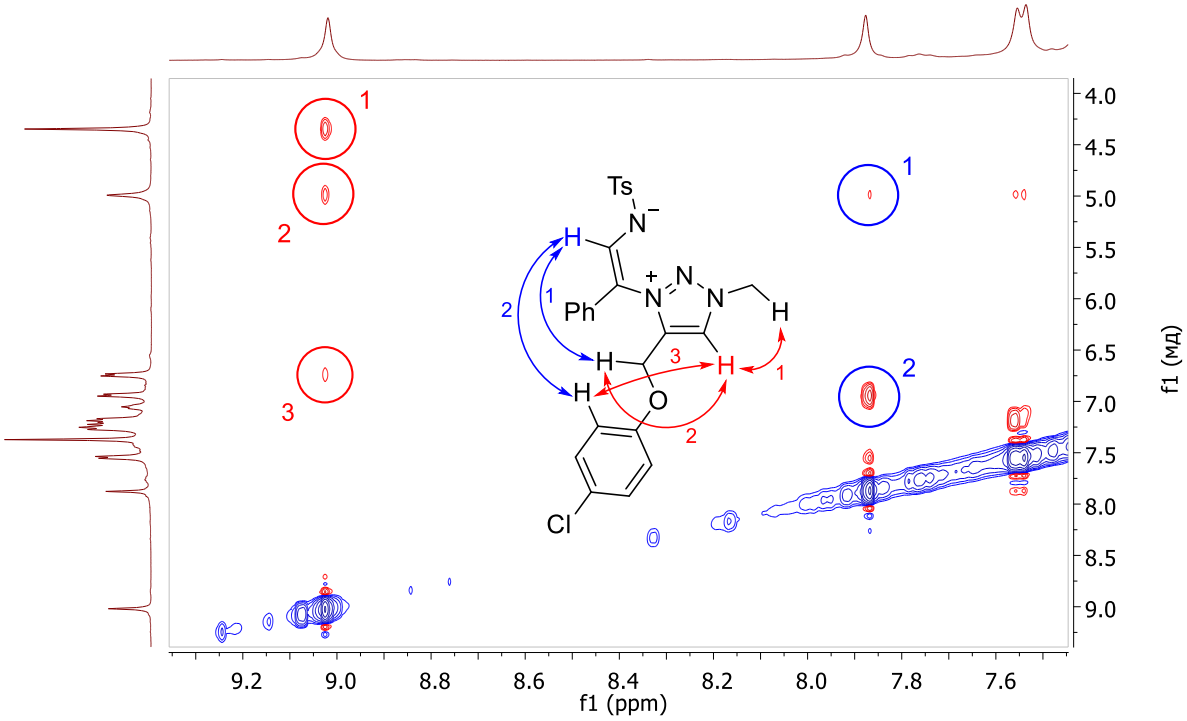
Key cross-peaks in ^{1}H-^{15}N HMBC spectrum



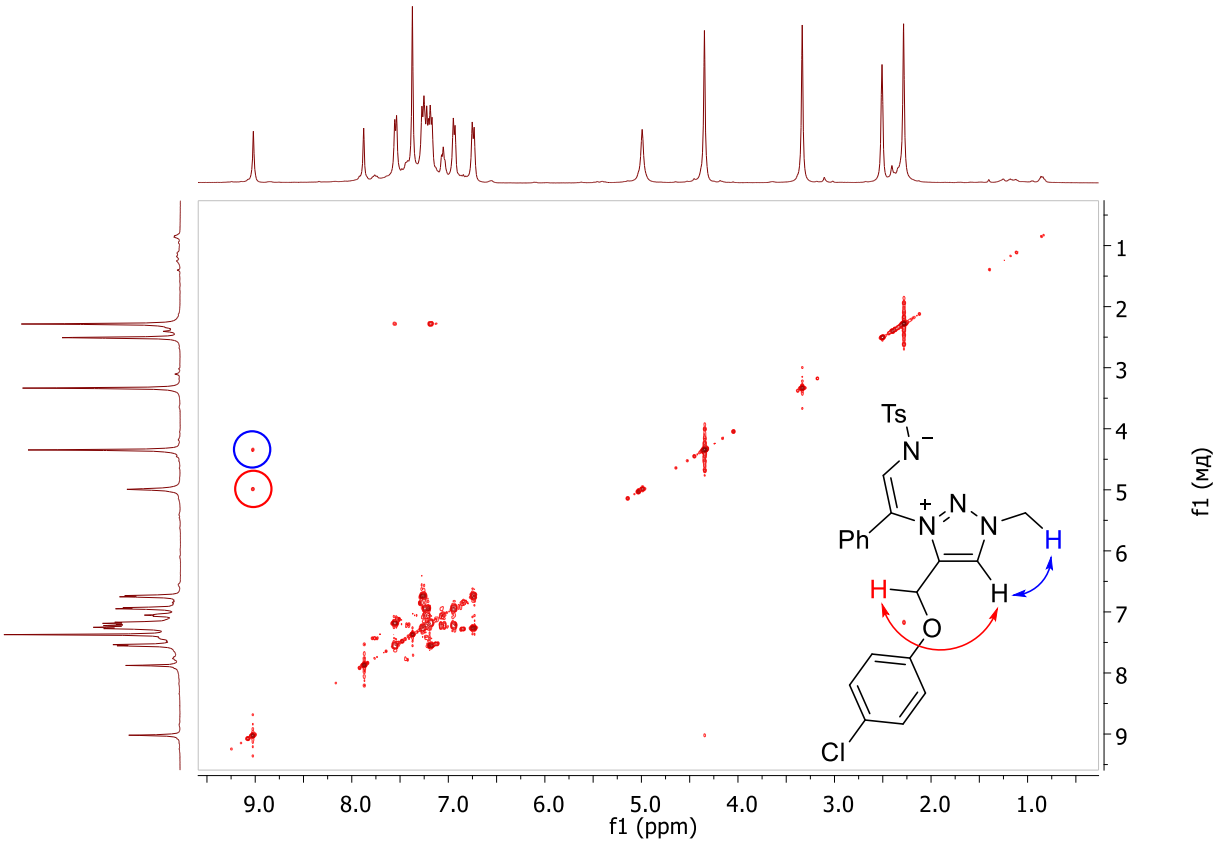
2D NOESY spectrum



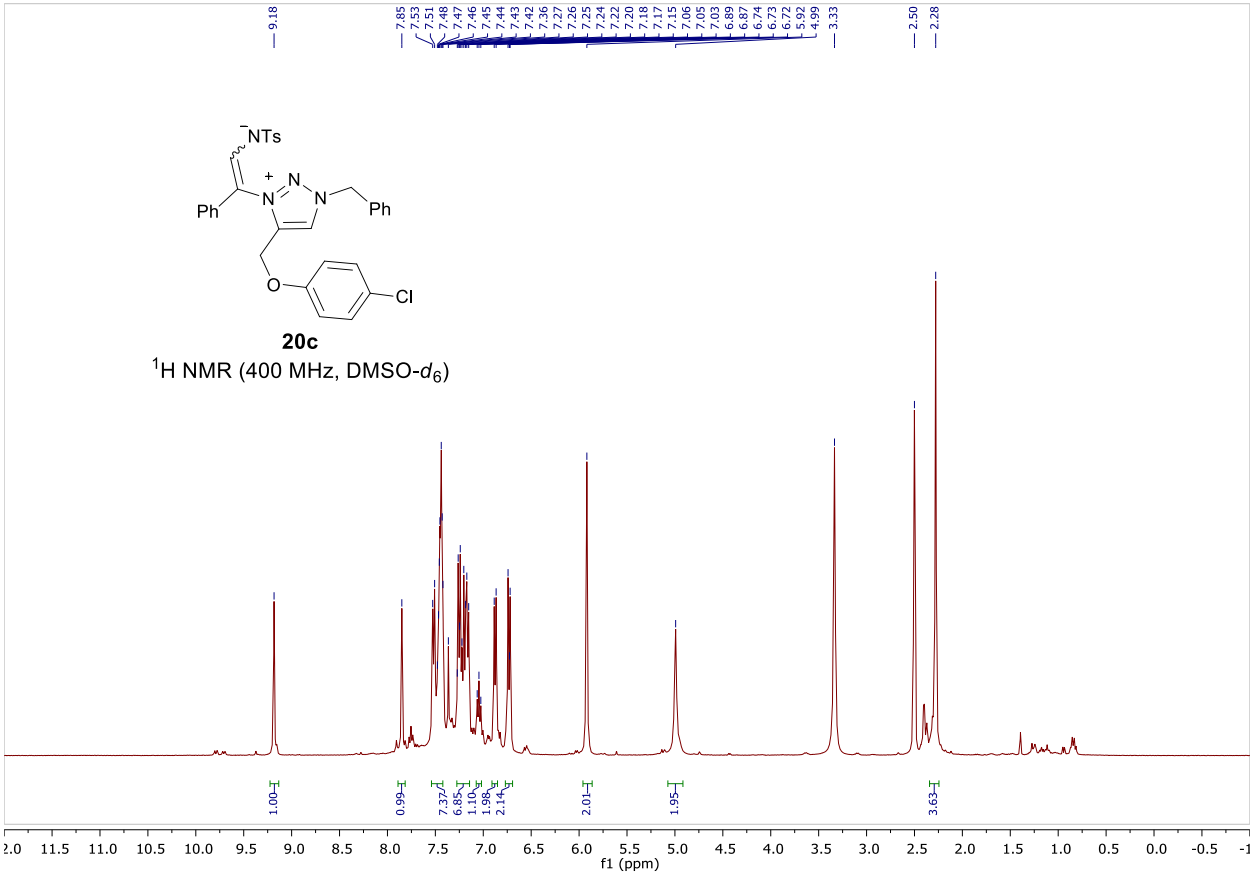
Key cross-peaks in 2D NOESY spectrum



Key cross-peaks in COSY ^{1}H-^{1}H spectrum

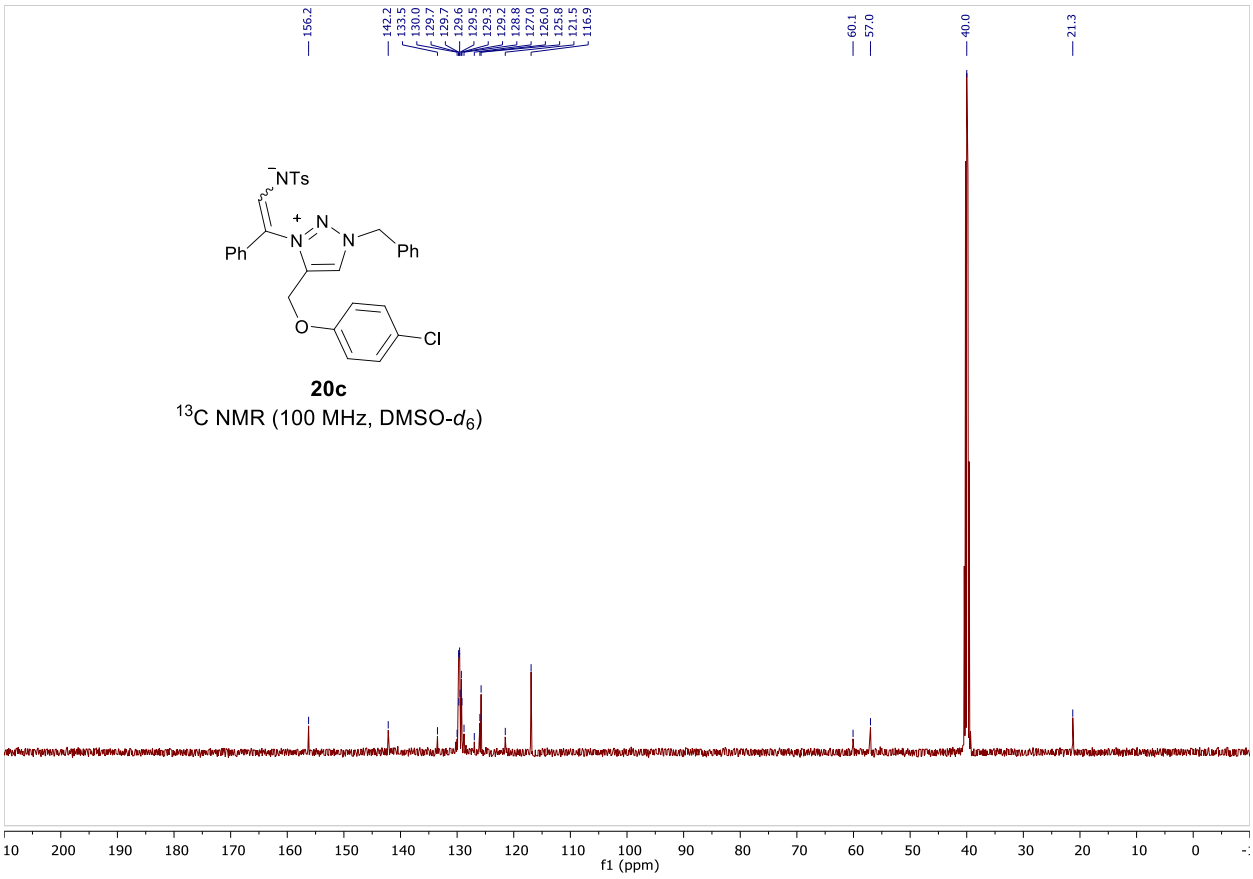


^{1}H and ^{13}C NMR spectra of compound **20c**



20c

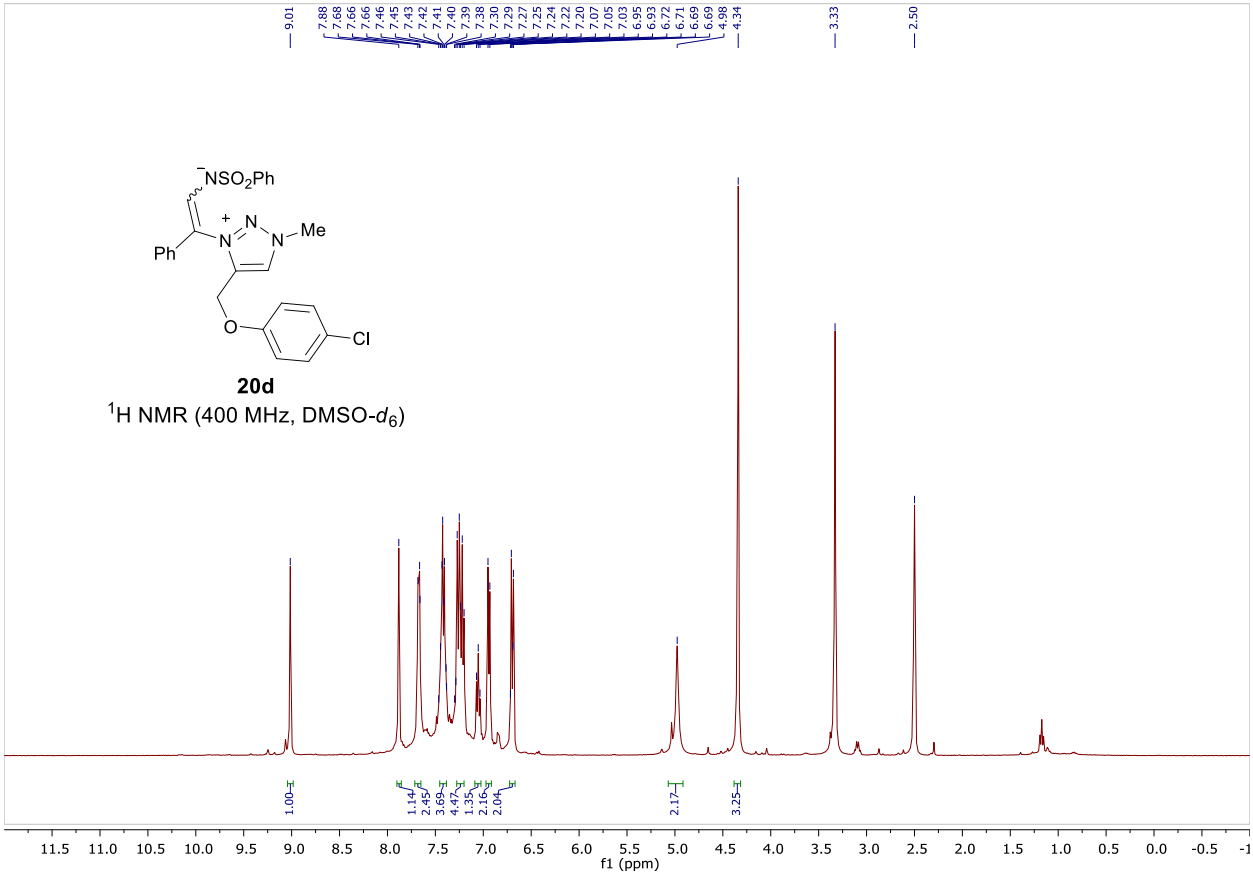
^{1}H NMR (400 MHz, DMSO-d_6)



20c

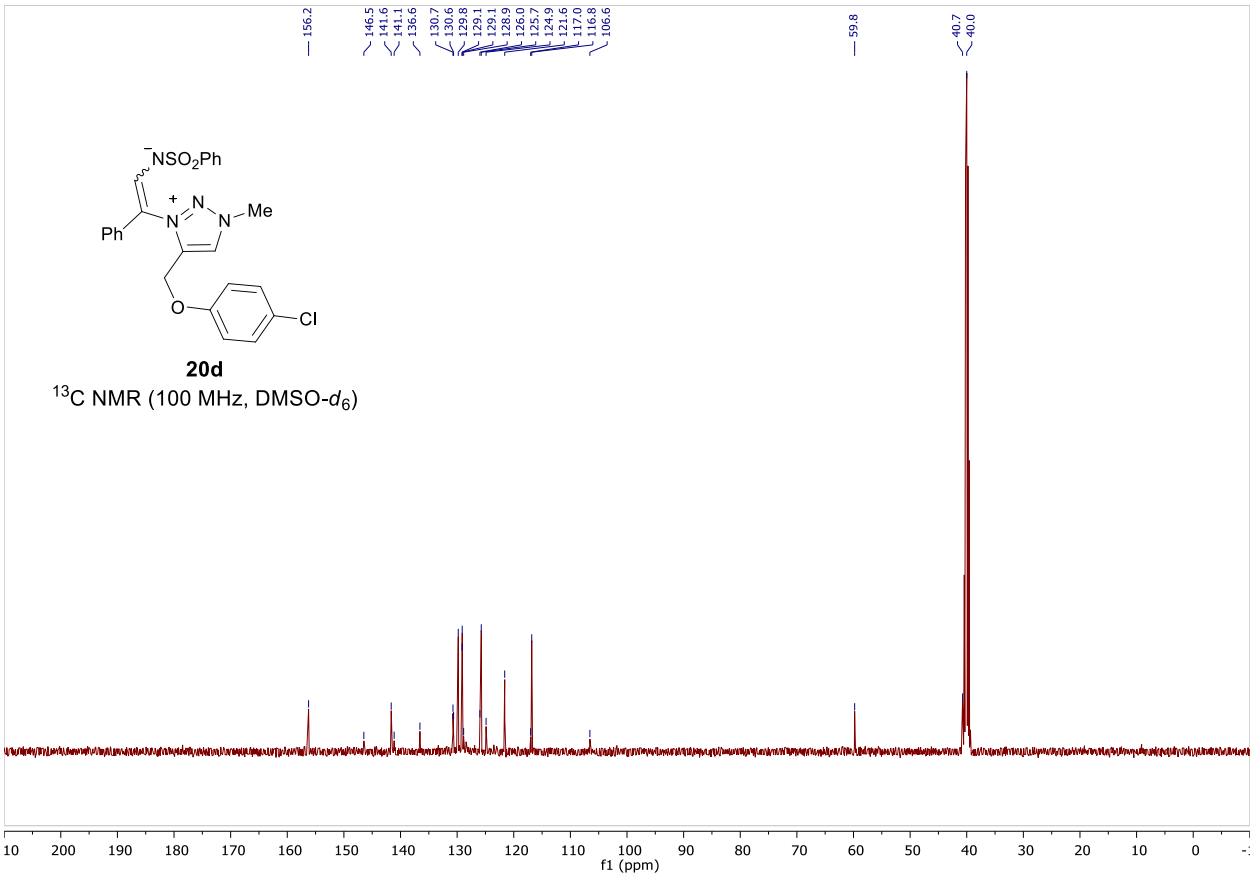
^{13}C NMR (100 MHz, DMSO-d_6)

^{1}H and ^{13}C NMR spectra of compound **20d**



20d

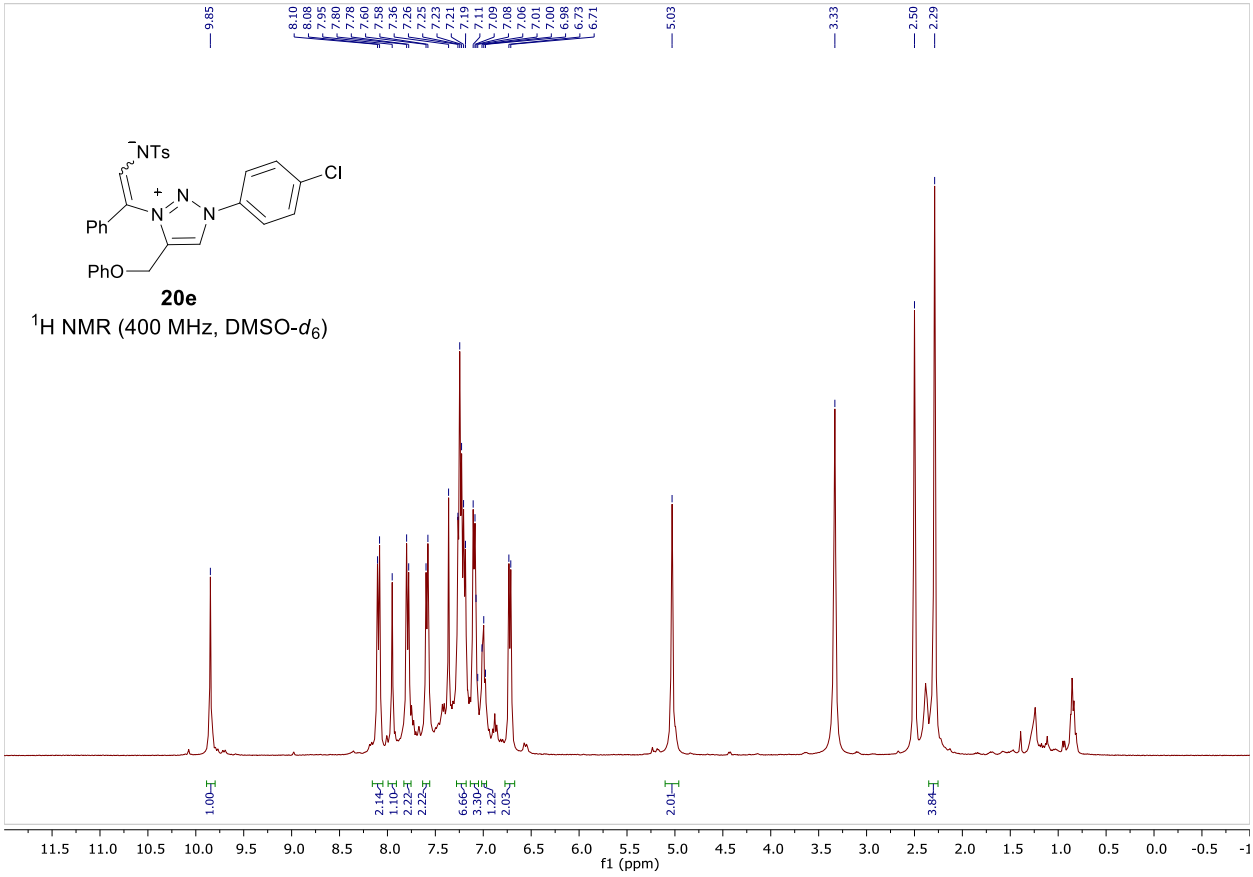
^{1}H NMR (400 MHz, DMSO-d_6)

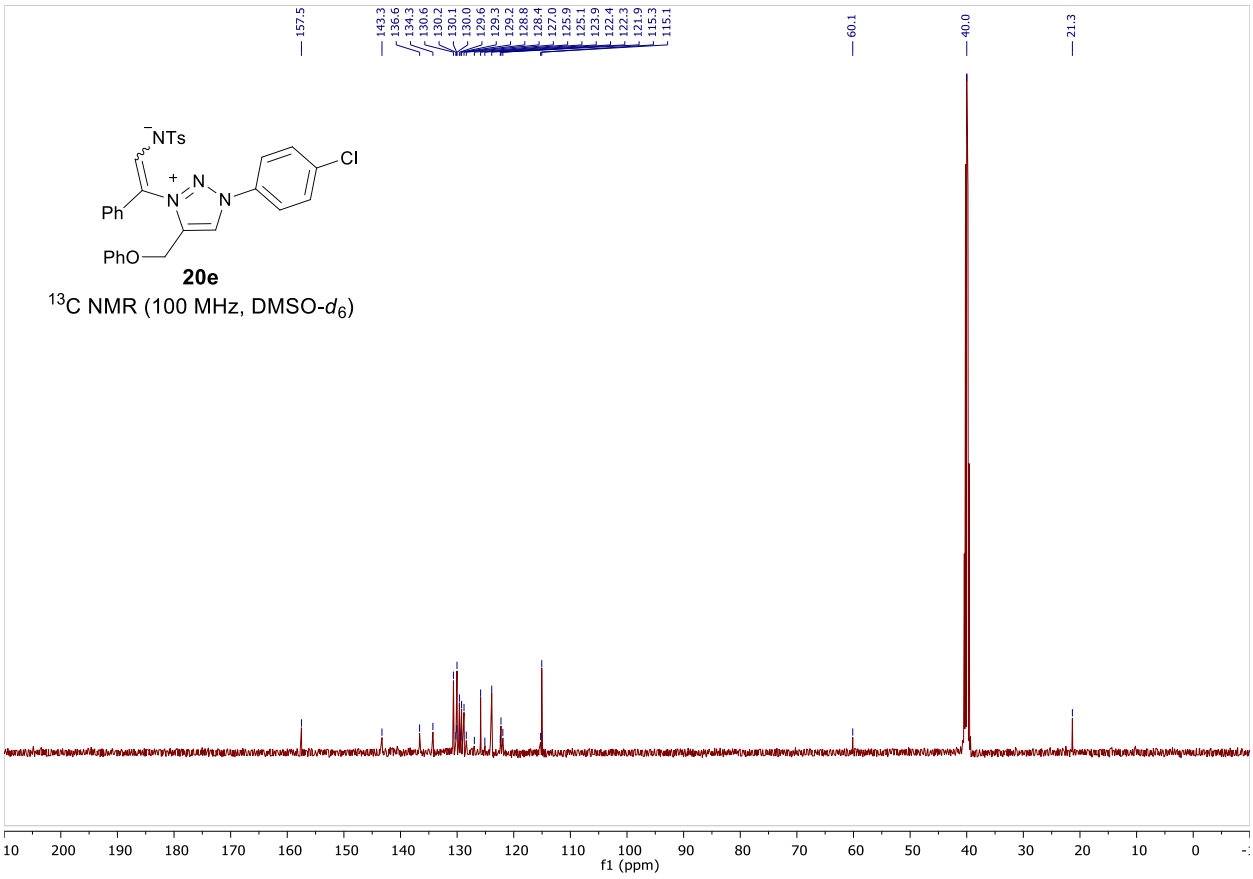


20d

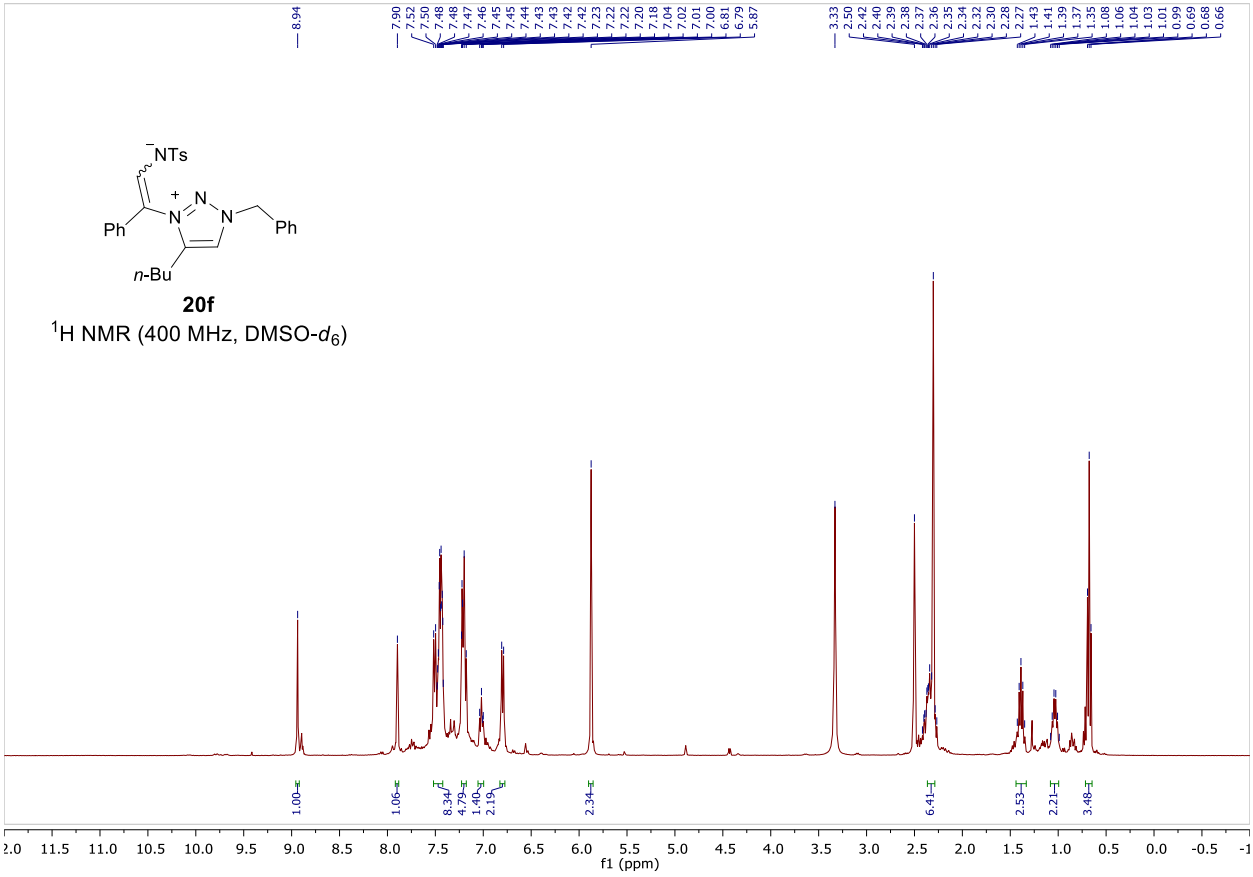
^{13}C NMR (100 MHz, DMSO-d_6)

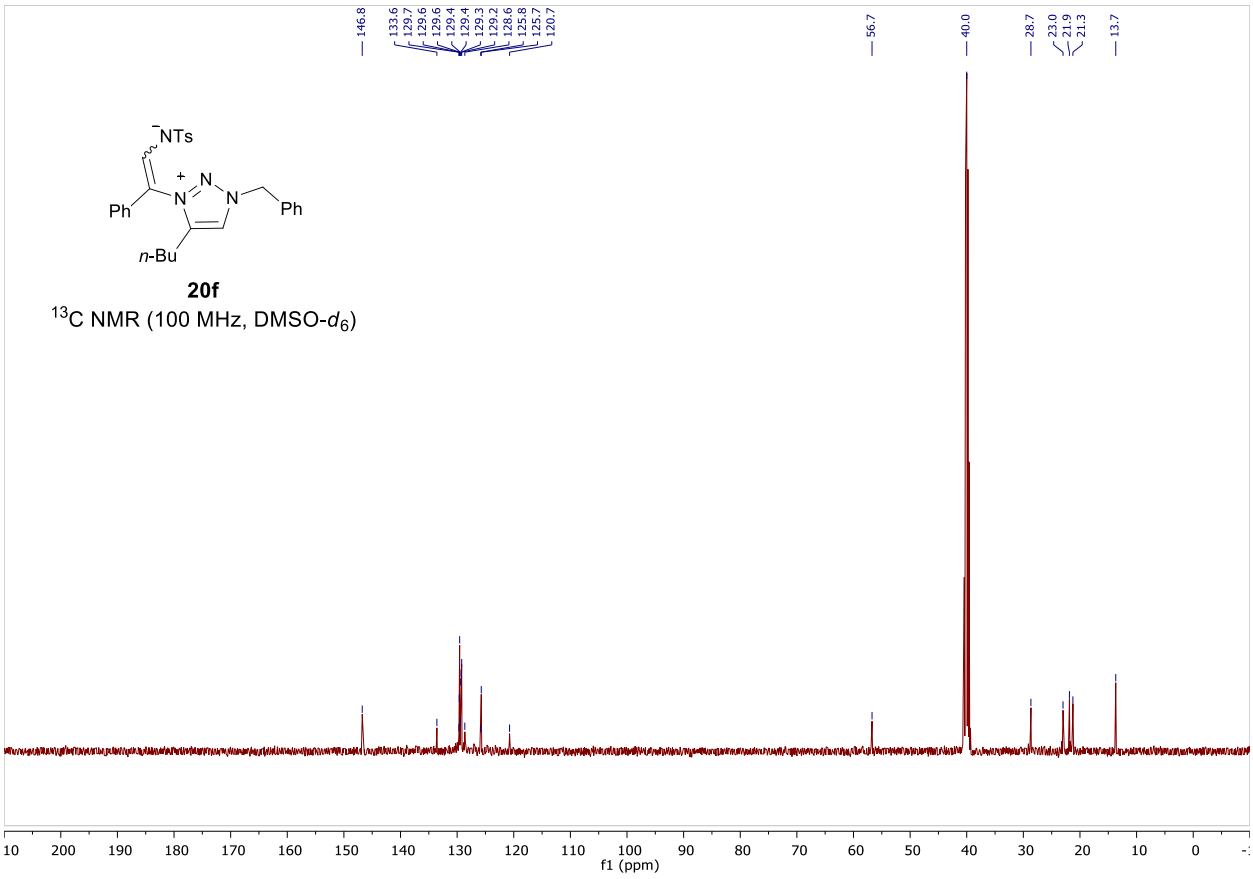
^{1}H and ^{13}C NMR spectra of compound **20e**



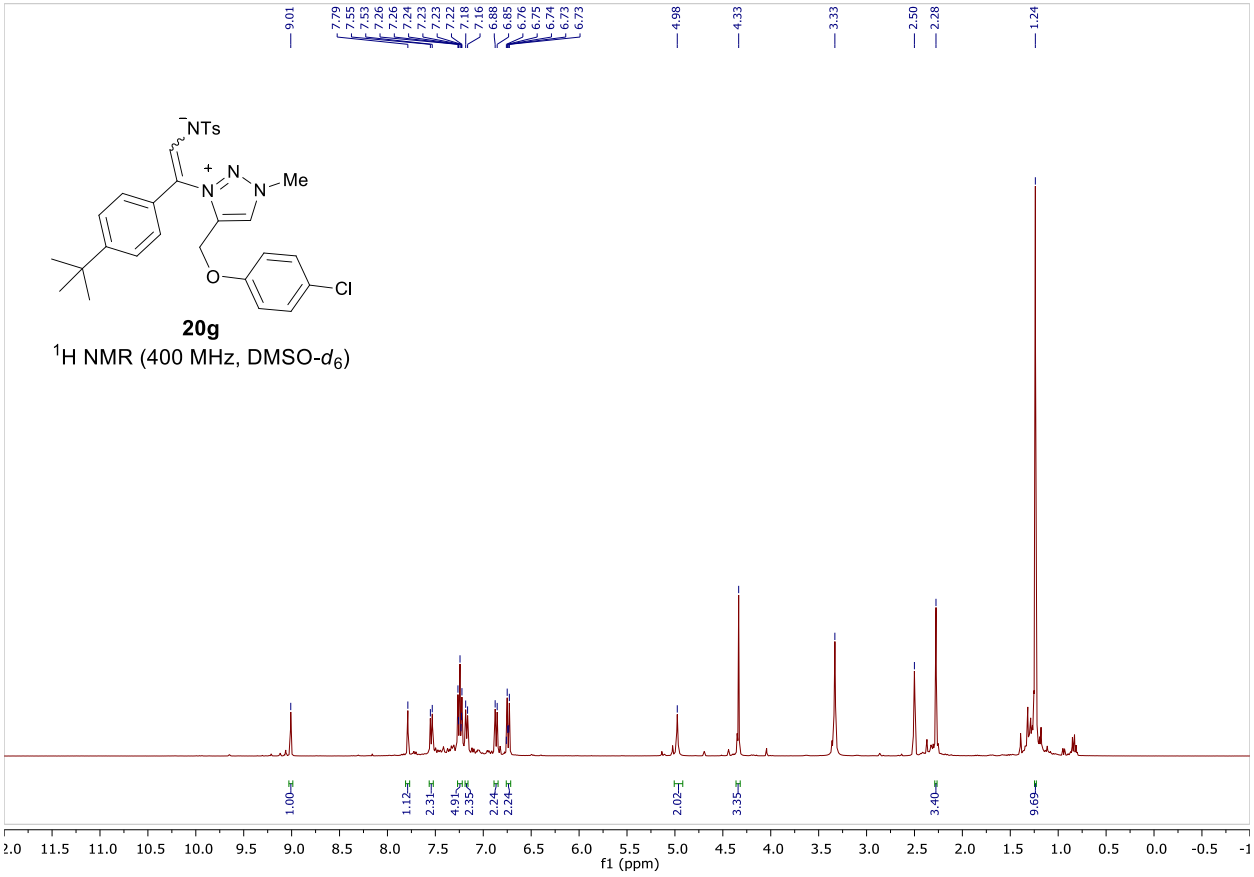


^{1}H and ^{13}C NMR spectra of compound **20f**



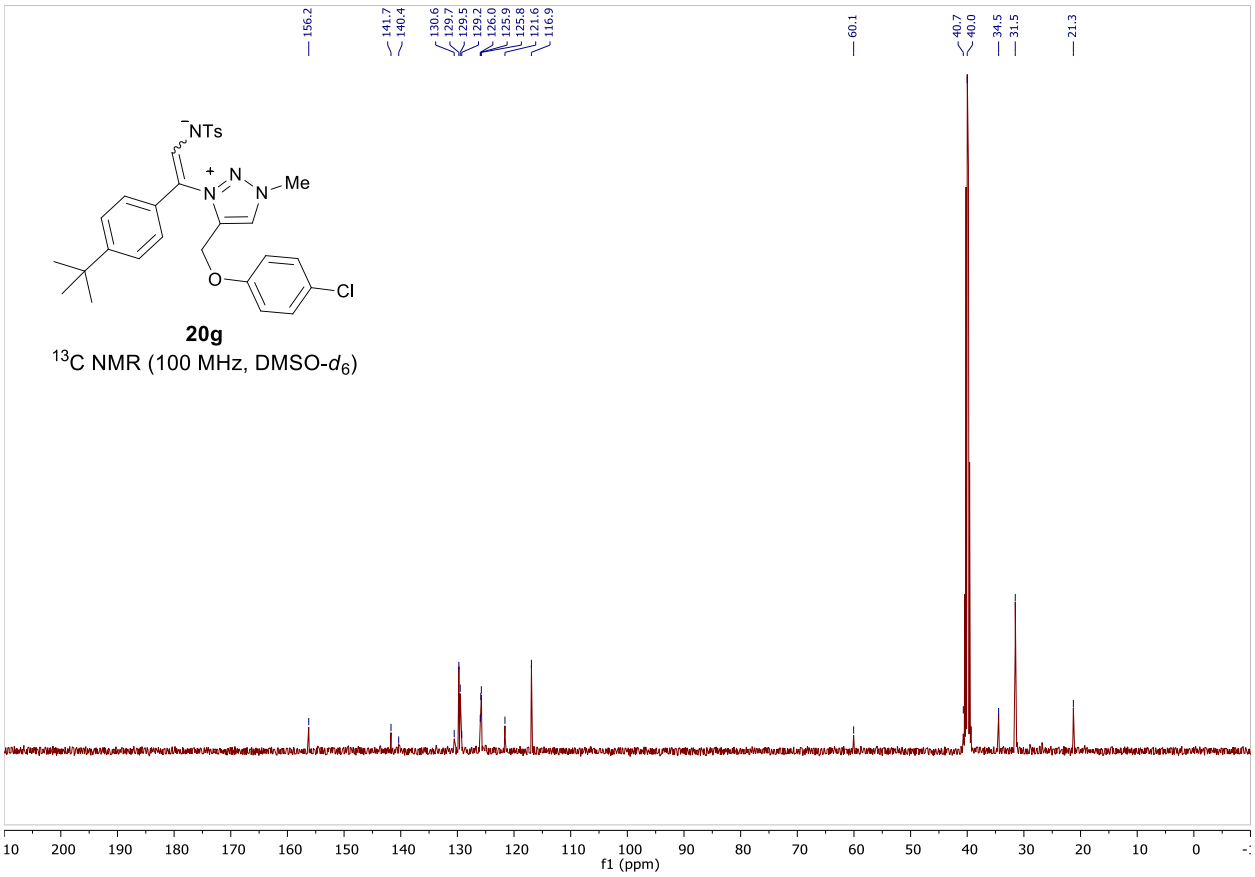


^{1}H and ^{13}C NMR spectra of compound **20g**



20g

^{1}H NMR (400 MHz, DMSO-d_6)



20g

^{13}C NMR (100 MHz, DMSO-d_6)

6. X-ray data of compound 3b

Single crystals of $C_{24}H_{21}ClN_2O_2S$ (**3b**) were grown from chloroform by slow evaporation. A suitable crystal was selected and intensity data were collected on a SuperNova, Single source at offset/far, HyPix3000 diffractometer. The crystal was kept at 100.2(4) K during data collection. Using Olex2,[3] the structure was solved with the ShelXT[4] structure solution program using Intrinsic Phasing and refined with the ShelXL[5] refinement package using Least Squares minimisation.

Figure S1. X-Ray crystal structure of *N*-(4-(4-chlorophenyl)-1-methyl-2-phenyl-1*H*-pyrrol-3-yl)-4-methylbenzenesulfonamide (**3b**) with 50% ellipsoid probability (CCDC Number 2044431)

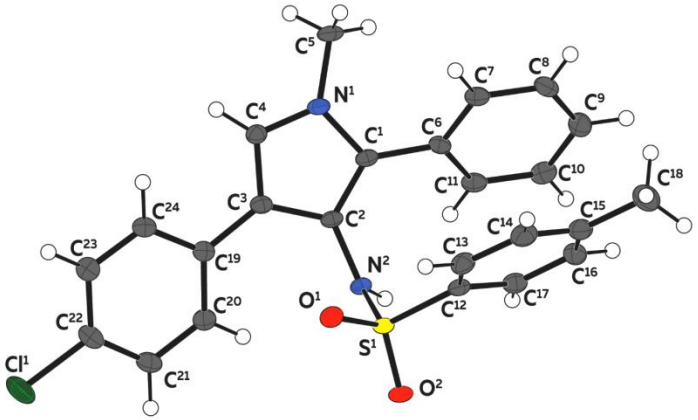


Table S1. Crystal data and structure refinement for **3b.**

Identification code	RNV52
Empirical formula	$C_{24}H_{21}ClN_2O_2S$
Formula weight	436.94
Temperature/K	100.2(4)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.98800(10)
b/Å	13.0920(2)
c/Å	13.6788(2)
α/°	90
β/°	94.2570(10)
γ/°	90
Volume/Å^3	2140.92(5)

Z	4
ρ_{calc}g/cm^3	1.356
μ/mm^{-1}	2.678
F(000)	912.0
Crystal size/mm^3	0.18 × 0.13 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.394 to 141
Index ranges	$-14 \leq h \leq 14$, $-16 \leq k \leq 15$, $-16 \leq l \leq 16$
Reflections collected	13479
Independent reflections	4059 [R_{int} = 0.0586, R_{sigma} = 0.0482]
Data/restraints/parameters	4059/0/277
Goodness-of-fit on F^2	1.084
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.1191
Final R indexes [all data]	R_1 = 0.0487, wR_2 = 0.1247
Largest diff. peak/hole / e Å^{-3}	0.29/-0.58

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **3b**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
S1	8329.6(3)	5817.5(3)	4559.3(3)	14.02(14)
Cl1	5640.8(4)	6064.9(5)	9097.3(4)	37.54(18)
O2	9390.7(10)	6178.4(10)	5002.3(9)	17.9(3)
O1	7321.2(10)	6309.8(10)	4799.0(9)	18.8(3)
N1	6042.2(12)	2950.7(12)	3995.4(11)	17.1(3)
N2	8286.1(12)	4621.8(11)	4868.5(10)	14.1(3)
C4	5626.5(14)	3319.0(14)	4822.7(13)	16.5(4)
C19	6227.9(14)	4511.2(14)	6213.4(13)	16.0(4)
C1	7077.3(14)	3375.0(14)	3880.8(13)	15.4(4)
C3	6384.6(14)	3986.1(14)	5284.9(13)	15.1(4)
C6	7750.9(14)	3135.9(13)	3049.5(13)	15.8(4)
C2	7303.3(14)	4020.1(13)	4679.9(13)	14.3(4)

C7	7289.1(14)	3163.5(14)	2077.1(13)	18.7(4)
C17	9245.5(15)	5353.6(14)	2856.6(14)	19.0(4)
C24	5147.1(14)	4639.0(14)	6518.7(13)	16.8(4)
C12	8393.2(14)	5879.4(13)	3274.6(13)	16.3(4)
C11	8885.9(14)	2895.8(14)	3218.5(14)	18.2(4)
C9	9069.8(16)	2747.1(15)	1480.0(14)	22.6(4)
C10	9540.0(15)	2713.1(14)	2440.6(14)	21.6(4)
C23	4964.7(15)	5099.7(14)	7404.9(14)	19.6(4)
C8	7942.8(16)	2971.2(15)	1304.7(14)	21.2(4)
C22	5872.0(16)	5465.9(16)	7988.2(14)	22.9(4)
C16	9312.4(16)	5403.8(15)	1851.0(14)	22.3(4)
C13	7621.6(14)	6460.1(16)	2704.1(14)	21.6(4)
C20	7124.5(15)	4869.6(17)	6833.3(14)	24.3(4)
C14	7713.5(15)	6510.9(17)	1698.2(14)	25.2(4)
C21	6950.5(16)	5354.9(17)	7709.1(14)	26.5(5)
C5	5478.1(15)	2178.1(15)	3370.5(14)	23.7(4)
C15	8552.3(16)	5978.8(16)	1257.4(14)	24.2(4)
C18	8644.5(19)	6021.0(19)	167.7(15)	33.4(5)

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3b**

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
S1	11.8(2)	14.1(3)	15.7(2)	-0.86(15)	-2.77(16)	-1.67(15)
Cl1	32.8(3)	53.4(4)	25.9(3)	-19.8(2)	-1.6(2)	6.9(2)
O2	14.4(6)	17.4(7)	21.0(7)	-2.3(5)	-3.9(5)	-3.4(5)
O1	14.9(6)	18.2(7)	23.1(7)	-0.6(5)	-0.2(5)	0.9(5)
N1	14.9(7)	16.6(8)	19.5(8)	-3.1(6)	-1.6(6)	-4.1(6)
N2	11.3(7)	14.6(8)	16.1(7)	0.9(6)	-2.5(5)	-1.4(6)
C4	15.2(8)	18.5(9)	15.6(8)	1.4(7)	-1.1(6)	-1.7(7)
C19	18.6(8)	14.2(9)	14.8(8)	3.0(7)	-1.8(6)	0.1(7)
C1	12.4(7)	14.9(9)	18.2(9)	0.8(7)	-3.1(6)	-1.4(6)
C3	14.3(8)	15.3(8)	15.0(8)	2.0(7)	-3.9(6)	-0.3(7)

C6	17.9(8)	12.1(8)	17.1(9)	-2.8(7)	-0.8(6)	-0.3(7)
C2	12.3(8)	13.5(9)	16.5(9)	1.7(7)	-3.7(6)	-1.3(6)
C7	16.4(8)	17.4(9)	21.5(9)	-2.5(7)	-3.3(7)	0.1(7)
C17	19.9(9)	14.7(9)	21.9(9)	0.9(7)	-2.0(7)	-1.6(7)
C24	17.1(8)	14.8(9)	17.9(9)	1.8(7)	-3.9(6)	1.5(7)
C12	15.5(8)	15.5(9)	17.4(9)	0.6(7)	-2.0(6)	-4.7(7)
C11	18.3(8)	13.7(9)	22.0(9)	-1.2(7)	-3.4(7)	0.7(7)
C9	26.4(9)	16.2(9)	25.9(10)	-4.1(8)	6.7(8)	1.1(7)
C10	16.4(8)	16.3(9)	31.9(10)	-2.6(8)	0.1(7)	2.8(7)
C23	19.3(9)	18.0(9)	21.4(9)	0.9(7)	-0.1(7)	4.4(7)
C8	26.2(9)	19.9(10)	17.0(9)	-3.7(7)	-1.4(7)	-2.3(8)
C22	27.5(10)	23.4(10)	17.3(9)	-3.3(8)	-1.7(7)	2.4(8)
C16	26.2(9)	19.9(10)	21.0(9)	-2.7(8)	3.3(7)	-4.2(8)
C13	14.6(8)	27.0(11)	22.8(10)	2.4(8)	-2.2(7)	-1.4(7)
C20	17.8(9)	34.6(12)	20.1(10)	-2.6(8)	-0.8(7)	-4.7(8)
C14	18.5(9)	33.9(12)	22.0(10)	6.7(8)	-6.3(7)	-3.3(8)
C21	22.0(9)	37.3(12)	19.3(10)	-5.8(9)	-4.5(7)	-4.5(8)
C5	20.2(9)	22.3(10)	28.2(10)	-8.3(8)	-0.8(7)	-9.5(8)
C15	24.9(10)	28.2(11)	19.0(10)	1.3(8)	-1.7(7)	-9.2(8)
C18	38.1(12)	42.6(13)	18.9(10)	1.1(9)	-2.5(9)	-6.6(10)

Table S4. Bond lengths for **3b**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
S1	O2	1.4471(12)	C6	C11	1.399(2)
S1	O1	1.4294(13)	C7	C8	1.384(3)
S1	N2	1.6234(15)	C17	C12	1.390(3)
S1	C12	1.7666(19)	C17	C16	1.385(3)
Cl1	C22	1.7482(19)	C24	C23	1.386(3)
N1	C4	1.358(2)	C12	C13	1.391(3)
N1	C1	1.379(2)	C11	C10	1.389(3)
N1	C5	1.458(2)	C9	C10	1.391(3)

N2	C2	1.425(2)	C9	C8	1.386(3)
C4	C3	1.380(2)	C23	C22	1.386(3)
C19	C3	1.468(2)	C22	C21	1.383(3)
C19	C24	1.401(2)	C16	C15	1.395(3)
C19	C20	1.400(2)	C13	C14	1.390(3)
C1	C6	1.476(2)	C20	C21	1.385(3)
C1	C2	1.392(2)	C14	C15	1.396(3)
C3	C2	1.427(2)	C15	C18	1.504(3)
C6	C7	1.403(2)			

Table S5. Bond angles for **3b**

Atom	**Atom**	**Atom**	**Angle/**°	**Atom**	**Atom**	**Atom**	**Angle/**°
O2	S1	N2	104.48(7)	C1	C2	N2	126.00(16)
O2	S1	C12	107.46(8)	C1	C2	C3	108.85(15)
O1	S1	O2	119.27(8)	C8	C7	C6	120.87(17)
O1	S1	N2	109.33(8)	C16	C17	C12	118.91(17)
O1	S1	C12	107.89(8)	C23	C24	C19	121.49(16)
N2	S1	C12	107.94(8)	C17	C12	S1	118.29(14)
C4	N1	C1	109.91(14)	C17	C12	C13	121.23(17)
C4	N1	C5	123.49(15)	C13	C12	S1	120.47(15)
C1	N1	C5	126.51(15)	C10	C11	C6	120.64(17)
C2	N2	S1	121.88(12)	C8	C9	C10	119.44(18)
N1	C4	C3	109.67(15)	C11	C10	C9	120.40(17)
C24	C19	C3	119.63(15)	C24	C23	C22	119.09(17)
C20	C19	C3	122.62(16)	C7	C8	C9	120.41(17)
C20	C19	C24	117.71(17)	C23	C22	Cl1	119.12(15)
N1	C1	C6	123.39(15)	C21	C22	Cl1	119.90(14)
N1	C1	C2	106.23(15)	C21	C22	C23	120.98(17)
C2	C1	C6	130.38(16)	C17	C16	C15	121.33(18)
C4	C3	C19	124.79(16)	C14	C13	C12	118.89(18)
C4	C3	C2	105.34(16)	C21	C20	C19	121.30(17)

C2	C3	C19	129.87(16)	C13	C14	C15	121.06(18)
C7	C6	C1	121.67(16)	C22	C21	C20	119.39(17)
C11	C6	C1	120.08(16)	C16	C15	C14	118.56(18)
C11	C6	C7	118.24(16)	C16	C15	C18	120.25(19)
N2	C2	C3	125.16(16)	C14	C15	C18	121.19(19)

Table S6. Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) for **3b**

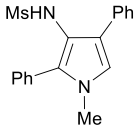
Atom	***x***	***y***	***z***	**U(eq)**
H4	4936	3147	5044	20
H7	6534	3313	1950	22
H17	9762	4974	3246	23
H24	4538	4410	6118	20
H11	9206	2858	3858	22
H9	9508	2621	960	27
H10	10297	2567	2562	26
H23	4243	5162	7605	24
H8	7624	2992	664	25
H16	9875	5047	1566	27
H13	7054	6808	2991	26
H20	7851	4780	6654	29
H14	7208	6906	1313	30
H21	7554	5604	8106	32
H5A	5048	1739	3761	36
H5B	6025	1780	3060	36
H5C	4990	2506	2878	36
H18A	9413	6114	36	50
H18B	8208	6582	-104	50
H18C	8371	5394	-125	50
H2	8950(20)	4317(18)	4892(17)	27(6)

7. Calculation details

All calculations were performed by using the Gaussian 09 suite of quantum chemical programs.[6] Geometry optimizations of compounds **3o**, **12–17**, **19**, dinitrogen and transition states TS2, TS4–TS9, TS11 were performed at the DFT B3LYP/6-31+G(d,p) level using PCM model for 1,2-dichloroethane. Complexes **11, 18**, $Rh_2(OAc)_4$, and transition states TS1, TS3, TS10 were optimized employing a Stuttgart RSC 1997 ECP basis set for rhodium and a 6-31+G(d,p) basis set for other atoms. Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

Table S7. Energies (au) and cartesian coordinates of stationary points for compounds **3o**, **11–19**, and transition states TS1–TS11 (DFT B3LYP/6-31+G(d,p)/Stuttgart RSC 1997 ECP, PCM for DCE, 357 K).

Pyrrole **3o**



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Thermal correction to Enthalpy = 0.356857
Thermal correction to Gibbs Free Energy = 0.257958
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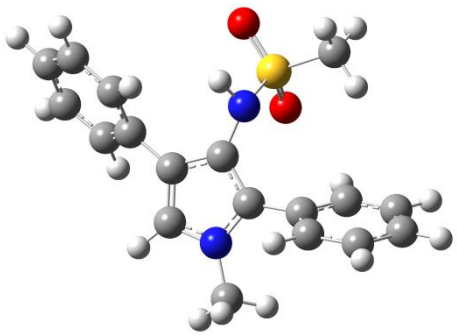
H = -1354.551879, G = -1354,650779.
Imaginary frequency = 0.



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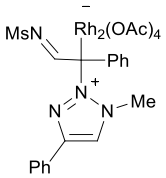
O	1.53106293	3.47581801	-0.01476140
O	-0.01957407	2.28230501	1.61913060
S	0.25633193	2.78191601	0.26175360
N	0.07907893	1.47918201	-0.83337640

Complex **11**



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H = -2599.053970, G = -2599.227925.
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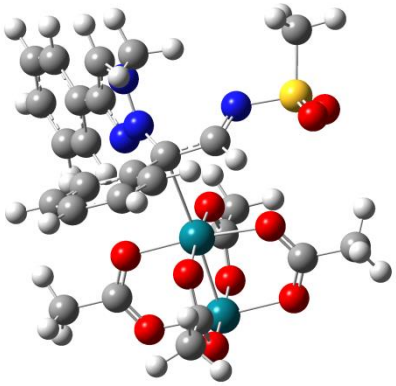

C	-4.66332300	-1.19131100	-0.12965500
C	-3.01452700	3.30143100	1.45490300
N	-2.51069500	-0.07457400	0.33990100
N	-2.09505800	1.09787100	0.74541700
N	-3.15223600	1.92032400	0.98444000

C	-2.51915507	-0.17873899	-0.21004640
C	0.06625093	0.13715301	-0.35797940
C	-1.09807007	-0.57745399	-0.08684340
C	2.63208893	-0.40154999	-0.20273640
C	-1.60439407	-2.91634999	0.73608960
N	-0.71268407	-1.82393999	0.35855460
C	0.65854893	-1.90586499	0.36645260
C	1.19309893	-0.70682899	-0.07169440
C	3.52064193	-0.68600399	0.85124860
C	4.88757493	-0.42568599	0.72899860
C	5.39599393	0.13656101	-0.44630840
C	4.52558193	0.42583201	-1.50180740
C	3.16043593	0.15451501	-1.38274940
C	-3.08106707	0.75511201	0.67693460
C	-4.42316007	1.12900201	0.55997360
C	-5.22285207	0.57339801	-0.44317240
C	-4.67409707	-0.35843099	-1.33045540
C	-3.33244207	-0.73055399	-1.21545140
H	-1.00667507	4.76719001	0.40957960
H	-2.02184307	3.36870001	-0.09245540
H	-0.92291507	4.15813901	-1.27684140
H	0.70463093	1.64560901	-1.61778140
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H	-2.43480607	-2.53244299	1.33119360
H	-2.00345807	-3.42588699	-0.14590440
H	1.15496593	-2.81830699	0.66403360
H	3.13005493	-1.10045499	1.77607760
H	5.55362493	-0.65218599	1.55690060
H	6.45759293	0.34628801	-0.53887240
H	4.90972993	0.85381901	-2.42347240
H	2.50619193	0.34725201	-2.22863940
H	-2.46258207	1.17759801	1.46278360
H	-4.84359107	1.84999901	1.25524360
H	-6.26568407	0.86327901	-0.53306740
H	-5.28802407	-0.79168399	-2.11475540
H	-2.90871807	-1.44668499	-1.91384740

C	-4.26814500	1.23728500	0.70790700
C	-3.85806600	-0.03650900	0.29426300
C	-4.03183800	-2.38052700	-0.53284200
C	-4.79391500	-3.47705100	-0.93717000
C	-6.19125600	-3.40165600	-0.94646600
C	-6.82419700	-2.22008700	-0.54724000
C	-6.06630400	-1.12058900	-0.14049700
H	-2.43909100	3.31238100	2.38063600
H	-2.51802900	3.89247900	0.68586600
H	-4.01854500	3.68144600	1.63411900
H	-5.24220100	1.68749000	0.81969900
H	-2.94862400	-2.43645300	-0.53001400
H	-4.29588500	-4.39080600	-1.24746100
H	-6.78189100	-4.25610200	-1.26314200
H	-7.90789900	-2.15216500	-0.55202800
H	-6.57458900	-0.21145900	0.16622900
C	-0.71134500	1.51160300	0.94571700
C	-0.24959100	2.41452000	-0.04099900
N	-0.94903700	2.73926100	-1.11211800
S	-0.20298400	3.74440900	-2.21533300
O	0.01101900	3.01591300	-3.48811900
O	0.96979100	4.45921100	-1.64630600
C	-1.50017300	4.95473700	-2.50916200
C	-0.33484800	1.59832300	2.38438200
C	0.55447600	2.57863600	2.86899200
C	0.88711100	2.63944900	4.22300800
C	0.32722600	1.73983400	5.13639500
C	-0.56799700	0.77170200	4.67150000
C	-0.89096400	0.69833500	3.31514700
H	0.73732900	2.84782800	0.12146900
H	-1.13296900	5.62410400	-3.28935500
H	-1.68573900	5.50482700	-1.58610600
H	-2.39553400	4.42910900	-2.84198300
H	0.99324500	3.30489300	2.19317500
H	1.57758000	3.40527900	4.56574500
H	0.58070700	1.79600400	6.19090600
H	-1.01303300	0.06203400	5.36362500
H	-1.56343100	-0.08195300	2.97429900
Rh	2.54778900	-1.98218800	-0.65703500
Rh	0.96636700	-0.28546700	0.03897500
O	1.96334100	1.00707700	-1.23000600
C	2.93742200	0.58828900	-1.93855100
O	3.39128800	-0.60319300	-1.93095400
O	2.30219200	0.20372100	1.53785000
C	3.41408400	-0.41286000	1.62450400
O	3.80066800	-1.35034300	0.85041300
O	0.12088700	-1.72483300	1.26671600
C	0.63181200	-2.89014300	1.32140800
O	1.63692300	-3.29054400	0.64441400
O	-0.21791800	-0.88607500	-1.54662900
C	0.15700100	-1.84764300	-2.29162200
O	1.22888300	-2.52569600	-2.14218600
C	0.01497900	-3.87268300	2.28948400
H	0.15295700	-4.89590600	1.93552000

H	0.51850900	-3.77426900	3.25789900
H	-1.04528900	-3.65703100	2.43218700
C	4.34467100	-0.02193600	2.74825600
H	4.06483600	0.94688900	3.16303800
H	4.28020200	-0.77735400	3.53912800
H	5.37665600	-0.00045400	2.39037500
C	3.61118000	1.59287400	-2.84109100
H	2.85760600	2.18496900	-3.36514000
H	4.20635100	2.27805500	-2.22775100
H	4.26770400	1.09021900	-3.55236800
C	-0.72371200	-2.20005400	-3.46709100
H	-0.37878500	-1.63727100	-4.34183700
H	-0.64691300	-3.26483300	-3.69566800
H	-1.76045500	-1.92392700	-3.26894300

$Rh_2(OAc)_4$

Zero-point correction = 0.209750
Thermal correction to Energy = 0.238756
Thermal correction to Enthalpy = 0.239887
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H = -1135.100961, G = -1135.201173.
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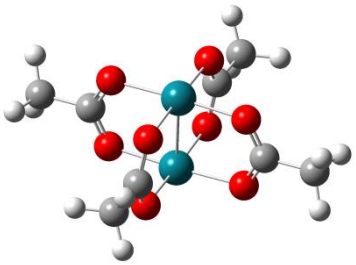

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C	1.87668000	-1.86734300	-0.00004500
O	1.45507300	-1.45502100	1.13214600
O	1.45497100	1.45506600	-1.13220400
C	1.87660100	1.86741300	-0.00003000
O	1.45496800	1.45509300	1.13215000
O	-1.45505600	1.45503300	-1.13215700
C	-1.87666700	1.86735700	0.00002900
O	-1.45504200	1.45498600	1.13219600
O	-1.45500400	-1.45507600	-1.13218300
C	-1.87660900	-1.86742500	-0.00000300
O	-1.45495900	-1.45510100	1.13217100
C	2.97705600	2.89854300	0.00003400
H	2.91929800	3.51889500	0.89597000
H	3.94238200	2.37980700	0.00297400
H	2.92269500	3.51556400	-0.89838200
C	-2.97707700	2.89853800	0.00002100
H	-3.94244100	2.37987400	-0.00139300
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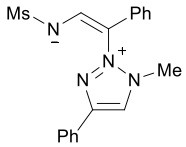
H	-2.92015000	3.51804600	-0.89654600

Ylide **12**



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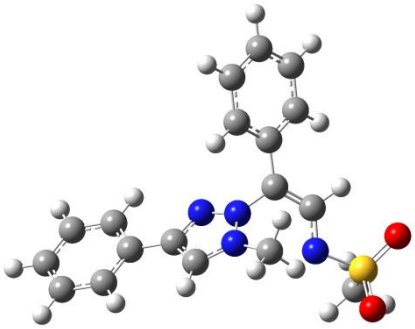

C	3.90261283	-4.36877107	-1.26147169
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O	5.34909283	-2.60647207	0.10916031
S	4.19136983	-3.52435907	0.30495031
N	2.77829683	-2.73383707	0.59029931
C	1.68461883	0.88166793	0.68335131
C	2.81324983	-1.39268007	0.54867831
C	1.72418883	-0.58347607	0.80514031
C	-2.89588717	-2.11373307	0.60339331
C	1.35845783	-2.12817107	3.31321231
N	-0.60123317	-1.21384907	0.44661231
N	0.50123883	-1.23118007	1.16761331
N	0.31468683	-1.94714707	2.30340331
C	-0.94115117	-2.41436007	2.28970331
C	-1.52938317	-1.92992507	1.11457531
C	-3.30556617	-1.45201607	-0.56684269
C	-4.60132417	-1.62298107	-1.05407569

C	2.97715100	-2.89845700	-0.00002100
H	3.94247100	-2.37970600	0.00227900
H	2.91978000	-3.51846200	0.89617600
H	2.92242100	-3.51582700	-0.89817800
C	-2.97705200	-2.89856700	0.00004800
H	-2.92015400	-3.51805400	0.89663000
H	-3.94238800	-2.37984300	0.00147300
H	-2.92181300	-3.51645600	-0.89772600

C	-5.50433917	-2.45338107	-0.38190469
C	-5.10249317	-3.11395707	0.78311731
C	-3.80694217	-2.94655607	1.27421731
C	0.75095983	1.65385293	1.40638331
C	0.73674883	3.04589593	1.30966531
C	1.65962883	3.71137993	0.49661031
C	2.58855883	2.95930793	-0.23043269
C	2.59392483	1.56634293	-0.15102369
H	4.78522683	-4.97594507	-1.47075669
H	3.75537483	-3.61766707	-2.03842669
H	3.01766383	-4.99672307	-1.15477769
H	3.75332683	-0.88599107	0.32428531
H	2.10452283	-2.82470707	2.92727331
H	1.81791483	-1.16109907	3.51919731
H	0.87775283	-2.51778407	4.20830631
H	-1.31530317	-3.03172207	3.09072231
H	-2.60820617	-0.80584107	-1.08891569
H	-4.90589417	-1.10610707	-1.95903169
H	-6.51246417	-2.58499207	-0.76298369
H	-5.79602417	-3.76172307	1.31043131
H	-3.51177517	-3.47134307	2.17751631
H	0.03156083	1.16604093	2.05776731
H	0.00515783	3.61163493	1.87986531
H	1.64952483	4.79462393	0.42372531
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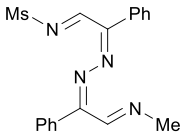
H	3.29947483	1.00662193	-0.75671469

Tetraazatetraene **13**



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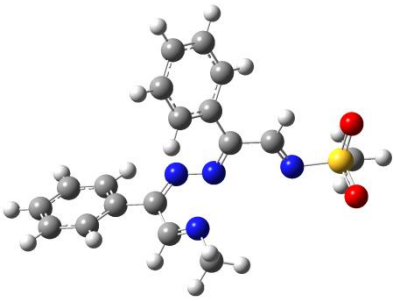
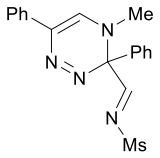
Thermal correction to Enthalpy = 0.366665
Thermal correction to Gibbs Free Energy = 0.258298
E_0 = -1464.007942, E = -1463.975062,
H = -1463.973931, G = -1464.082298.
Imaginary frequency = 0.

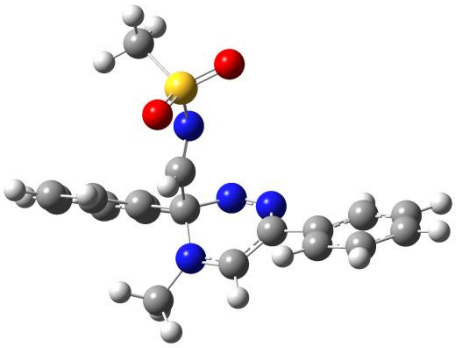


C	5.15820056	-2.21986206	-1.88401838
O	5.09301456	-2.73911006	0.73439362
O	5.48257156	-0.34742706	-0.00358138
S	4.81178956	-1.64882506	-0.21881338
N	3.10619256	-1.49514506	-0.29102038

Dihydrotriazine **14**



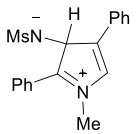
Zero-point correction = 0.334433
Thermal correction to Energy = 0.366132
Thermal correction to Enthalpy = 0.367263
Thermal correction to Gibbs Free Energy = 0.262741
E_0 = -1464.002104, E = -1463.970406,
H = -1463.969275, G = -1464.073796.
Imaginary frequency = 0.



C	-2.33120077	3.69109812	-0.23117138
O	0.30434323	3.31326112	-0.46501538
O	-0.77094877	2.89203512	1.79166262
S	-0.85074077	2.83975012	0.31655562

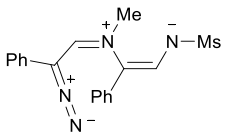
C	0.78521556	1.35594994	0.36909662	N	-1.19292977	1.24196312	-0.24682038
C	2.64123356	-0.33742906	0.02994362	C	-2.94955177	-1.33519788	0.11538062
C	1.20002156	-0.03851606	0.07357562	C	-1.12726677	0.32233612	0.63451862
C	-3.20728244	-1.44873106	-0.24346538	C	-1.44078277	-1.13716788	0.25519662
C	-0.26082944	-3.06410406	3.30701762	C	2.64832223	-1.22686788	0.16855962
N	-0.90033644	-0.85776006	-0.33707438	C	-1.58836677	-2.98524888	2.06825762
N	0.39532356	-1.03917506	-0.12969538	N	0.50031823	-1.49784888	-1.00630738
N	-0.51505244	-2.15274606	2.20411862	N	-0.76048777	-1.46965288	-1.05772038
C	-1.54345444	-2.35530006	1.47793662	N	-0.84037377	-2.00071588	1.27685962
C	-1.82531544	-1.52177106	0.28598162	C	0.50743423	-1.96175388	1.28850862
C	-3.43777144	-1.13388706	-1.59622138	C	1.19259023	-1.45304288	0.19168462
C	-4.73654644	-1.05958606	-2.09495838	C	3.33276723	-0.88491288	1.34999862
C	-5.83039444	-1.29513606	-1.25266338	C	4.71514323	-0.68531988	1.34417462
C	-5.61390944	-1.60473406	0.09243762	C	5.44015723	-0.80314488	0.15472062
C	-4.31257944	-1.68316006	0.59441062	C	4.76608623	-1.12326788	-1.02949438
C	-0.27795844	1.62265394	1.25022962	C	3.38704723	-1.33503488	-1.02551238
C	-0.66305044	2.93796494	1.51549762	C	-3.83329277	-0.72061488	1.01681062
C	0.00371456	4.00401294	0.90423862	C	-5.21118577	-0.91840388	0.90676062
C	1.06605156	3.74982694	0.03042762	C	-5.72369077	-1.73322188	-0.10718438
C	1.45938356	2.43652994	-0.23013138	C	-4.84914177	-2.34698788	-1.00740938
H	6.22994856	-2.42250406	-1.92519638	C	-3.46934977	-2.14923888	-0.89943638
H	4.88438756	-1.43185206	-2.58614838	H	-3.18886777	3.27569712	0.29873762
H	4.58184756	-3.12779006	-2.06115338	H	-2.42367977	3.55397112	-1.30846238
H	3.31225656	0.48393394	0.29651662	H	-2.19174277	4.74436912	0.01886962
H	0.73024356	-3.50982606	3.16916062	H	-0.90314577	0.52626012	1.68767462
H	-0.22318744	-2.48951606	4.23885762	H	-2.38076777	-2.50098088	2.64002162
H	-1.00835844	-3.86481506	3.40126062	H	-2.02676977	-3.75185988	1.42399262
H	-2.24900744	-3.17204806	1.67850962	H	-0.88865377	-3.46345488	2.75455262
H	-2.59010144	-0.95432106	-2.24900838	H	1.01539123	-2.44871088	2.11475862
H	-4.89759844	-0.82209006	-3.14231338	H	2.77954323	-0.75203888	2.27552162
H	-6.84197044	-1.23810006	-1.64338238	H	5.22165923	-0.42159688	2.26826062
H	-6.45611944	-1.78221206	0.75435562	H	6.51370323	-0.63955188	0.14814262
H	-4.16521244	-1.90887706	1.64583962	H	5.31763223	-1.21372188	-1.96114538
H	-0.78083744	0.80231794	1.74945262	H	2.87306223	-1.59265188	-1.94499038
H	-1.48026644	3.12938594	2.20441862	H	-3.45756277	-0.08702388	1.81534262
H	-0.29871244	5.02633294	1.11062462	H	-5.88087677	-0.43528488	1.61178062
H	1.58773656	4.57252294	-0.44902538	H	-6.79518977	-1.88620388	-0.19492838
H	2.27833256	2.25310094	-0.91975138	H	-5.23779577	-2.98010688	-1.79952138
				H	-2.79421477	-2.61690588	-1.60568938

Betaine **15**

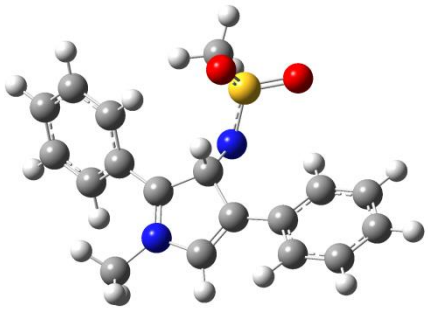


Zero-point correction = 0.326121
Thermal correction to Energy = 0.354858
Thermal correction to Enthalpy = 0.355989
Thermal correction to Gibbs Free Energy = 0.261151
E_0 = -1354.530564, E = -1354.501828,
H = -1354.500696, G = -1354.595535.
Imaginary frequency = 0.

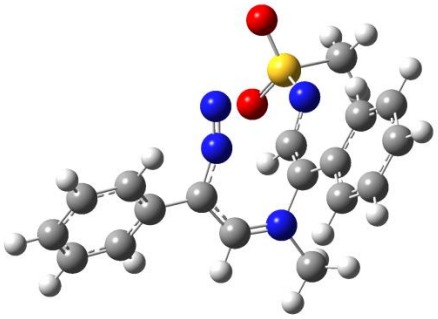
Diazo ylide s*yn*-**16**



Zero-point correction = 0.333374
Thermal correction to Energy = 0.366117
Thermal correction to Enthalpy = 0.367248
Thermal correction to Gibbs Free Energy = 0.260683
E_0 = -1463.990987, E = -1463.958243,
H = -1463.957112, G = -1464.063678.
Imaginary frequency = 0.

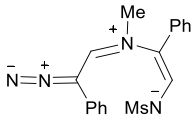


C	-1.65924036	3.01938771	-0.66953568
O	0.94519464	3.07044771	-0.46819668
O	-0.35371636	2.14645271	1.48610732
S	-0.18676136	2.20506471	-0.00817268
N	-0.15875236	0.75971771	-0.69772568
C	-2.63573336	-0.97525329	0.12523232
C	-0.05237036	-0.37939529	0.17576332
C	-1.22660336	-1.34631329	0.07060932
C	2.57103264	-0.95140929	0.04902532
C	-1.49625036	-3.83508929	-0.11813168
N	-0.75782336	-2.56646329	-0.07687068
C	0.66680864	-2.56931529	-0.12861568
C	1.14905364	-1.31741229	-0.00460168
C	3.51456664	-1.87514629	0.54744232
C	4.87243164	-1.56262329	0.57823932
C	5.31728864	-0.31716029	0.11938432
C	4.39074264	0.60964971	-0.36582568
C	3.02891764	0.30080971	-0.40307468
C	-3.04933136	0.00447071	1.05067132
C	-4.39264536	0.36694371	1.13132332
C	-5.33250736	-0.21407229	0.27331532
C	-4.92469836	-1.16163829	-0.67099568
C	-3.58697936	-1.54691729	-0.74369068
H	-2.54146836	2.46814671	-0.34376868
H	-1.58678836	3.01862671	-1.75798768
H	-1.67514936	4.04228771	-0.28893968
H	-0.03381336	-0.07949629	1.24645832
H	-2.48942836	-3.69907529	0.30396632
H	-1.57160136	-4.18444529	-1.15058068
H	-0.94352536	-4.56755029	0.47091932
H	1.16915664	-3.51690329	-0.25664468
H	3.17941864	-2.83250929	0.93500232
H	5.58177064	-2.28504529	0.97138232
H	6.37479964	-0.07119729	0.14763232
H	4.72627064	1.57996471	-0.72023968
H	2.31974264	1.02383171	-0.78632368
H	-2.32121536	0.47250871	1.70467432
H	-4.70446336	1.10894771	1.85953832
H	-6.37651236	0.07764871	0.33357432
H	-5.64611936	-1.59784429	-1.35453468
H	-3.27782136	-2.25910929	-1.50065068

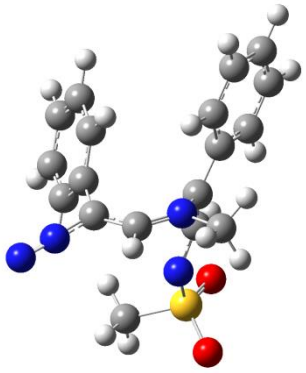


C	5.28169011	-1.24878601	1.00880854
O	3.60374111	-1.84136901	-0.95112746
O	2.86807511	-2.28846701	1.42568754
S	3.57042411	-1.39335601	0.46290554
N	3.02565811	0.16794599	0.50311054
C	1.73015811	2.95797799	0.94666254
C	2.06242111	0.43379199	1.39083754
C	1.42954211	1.66137399	1.56000454
C	-2.69812389	0.52394199	0.65433354
C	0.72263211	1.99469199	3.95310554
N	-0.42145589	0.88067099	-0.08626346
N	-0.02591989	0.76743599	-1.14558546
N	0.38415011	1.64358999	2.56355154
C	-0.83993589	1.27899099	2.22746654
C	-1.28904189	0.89835099	0.95696454
C	-3.44054889	-0.21548501	1.59169754
C	-4.77368589	-0.54058401	1.33449954
C	-5.37573289	-0.15635401	0.13283754
C	-4.63497989	0.56073499	-0.81124846
C	-3.30673189	0.90358999	-0.55295446
C	2.78819611	3.11462499	0.01949254
C	3.05181911	4.35600699	-0.56295246
C	2.27920611	5.47760399	-0.24829746
C	1.22672911	5.33888499	0.66326154
C	0.95391011	4.10314099	1.24790754
H	5.28908411	-0.89674501	2.04106754
H	5.79352411	-0.54425301	0.35281154
H	5.72838611	-2.24204901	0.93464154
H	1.68988711	-0.37926001	2.02140154
H	1.39449811	1.23621499	4.36380054
H	1.22925311	2.96191799	3.96477454
H	-0.18346089	2.04931099	4.55815954
H	-1.58582889	1.28905599	3.01555654
H	-2.97679489	-0.55317601	2.51347254
H	-5.33417989	-1.11120101	2.06877554
H	-6.40940989	-0.41957601	-0.06892046
H	-5.09134989	0.86292899	-1.74884946
H	-2.75244289	1.47636099	-1.29052646
H	3.39545711	2.25648199	-0.23607846
H	3.87210711	4.44292299	-1.27047046
H	2.49058211	6.44032499	-0.70406046
H	0.61052511	6.19619199	0.92004454
H	0.12339711	4.03033099	1.94267554

Diazo ylide *anti*-**16**

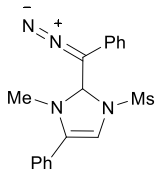


Zero-point correction = 0.333778
Thermal correction to Energy = 0.366445
Thermal correction to Enthalpy = 0.367576
Thermal correction to Gibbs Free Energy = 0.261073
E_0 = -1463.986736, E = -1463.954070,
H = -1463.952939, G = -1464.059441.
Imaginary frequency = 0.

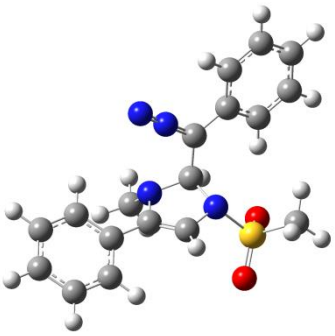


C	-4.05766296	-0.32844915	-1.01045233
O	-3.89509296	-2.50398315	0.46828867
O	-2.56088196	-2.41816115	-1.67634133
S	-3.04017796	-1.70932715	-0.45387133
N	-1.83769996	-1.01426215	0.41512567
C	1.93504704	-1.05245415	0.19291767
C	-0.58262696	-1.17624815	-0.04909133
C	0.55748104	-0.79478315	0.62654367
C	-0.13520796	2.21337785	-0.09779433
C	0.63740604	-1.18263715	3.07206667
N	-1.26934996	2.90775685	1.88286267
N	-1.90491196	3.74316785	2.30554667
N	0.37830804	-0.25076515	1.95286767
C	-0.22144896	0.89179685	2.20983867
C	-0.53593496	1.94373985	1.31616767
C	-1.11382696	2.37122685	-1.09019033
C	-0.74086196	2.68060785	-2.39936033
C	0.61023404	2.83520285	-2.72486933
C	1.58726804	2.68974185	-1.73505233
C	1.21783704	2.39134985	-0.42230533
C	2.23708204	-1.90740615	-0.89391633
C	3.55176004	-2.12514215	-1.29974733
C	4.62134004	-1.51752315	-0.62917333
C	4.34528504	-0.68189715	0.45530567
C	3.02733104	-0.44841315	0.85534767
H	-3.47251396	0.27723885	-1.70256933
H	-4.36012596	0.25282285	-0.13882733
H	-4.93027396	-0.75117415	-1.51186633
H	-0.44120496	-1.65539015	-1.01804133
H	-0.11882496	-1.97189215	3.05402567
H	1.62455904	-1.62592015	2.94005067

Diazo imidazoline *syn*-**17**



Zero-point correction = 0.334666
Thermal correction to Energy = 0.366659
Thermal correction to Enthalpy = 0.367790
Thermal correction to Gibbs Free Energy = 0.263459
E_0 = -1463.993329, E = -1463.961335,
H = -1463.960204, G = -1464.064535.
Imaginary frequency = 0.

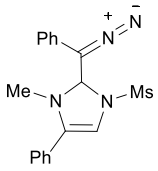


C	2.26667976	3.56111023	-1.52133817
O	1.93732976	3.18563423	1.09316983
O	0.02833376	4.21365023	-0.24566317
S	1.14553176	3.25670523	-0.15245217
N	0.57504676	1.64744123	-0.51633717
C	-2.89658724	0.33201923	-0.21551917
C	-0.79572324	1.55717323	-0.92313417
C	-1.48594524	0.73645423	-0.10368017
C	2.99328576	-0.66757077	-0.11827017
C	-1.00894924	0.38586823	2.30230783
N	0.83120876	-1.60796277	-0.46505917
N	0.23357876	-2.51075777	-0.84095017
N	-0.63486024	0.18329823	0.89199183
C	0.73422076	0.57547823	0.53293983
C	1.52837576	-0.60230177	-0.01825217
C	3.79832076	0.36115523	0.41456783
C	5.19117976	0.28842223	0.33615783
C	5.81865776	-0.80067177	-0.27351817
C	5.02934876	-1.82513877	-0.80824617
C	3.63909276	-1.76196677	-0.73496817
C	-3.85371524	1.22368723	-0.73448517
C	-5.18569324	0.83276323	-0.87370017
C	-5.58846824	-0.44956477	-0.48372117
C	-4.64727824	-1.33893277	0.04426083
C	-3.31200124	-0.95330877	0.17745283
H	1.69699576	3.51089623	-2.44978417
H	3.04831376	2.80189423	-1.49625617
H	2.68163876	4.55946123	-1.37225017
H	-1.12320724	2.03130623	-1.83623517
H	-0.93515124	1.43984023	2.60670383

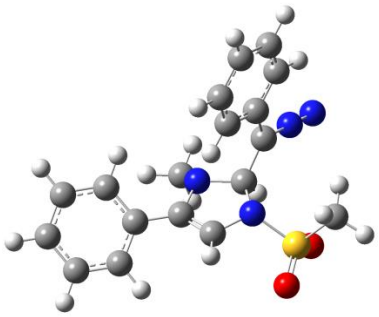
H	0.60399604	-0.64997715	4.02313467
H	-0.50214796	1.04678685	3.24803467
H	-2.16182096	2.24613985	-0.83806633
H	-1.50363296	2.79722685	-3.16304133
H	0.90008504	3.07288385	-3.74389233
H	2.63703904	2.81616385	-1.98125333
H	1.97708604	2.29510085	0.34611167
H	1.44050404	-2.41943715	-1.42314233
H	3.74309204	-2.78729815	-2.13985833
H	5.64476904	-1.69716215	-0.94413033
H	5.15695504	-0.19929115	0.99315967
H	2.84597404	0.22124985	1.69078867

H	-2.03580624	0.05053423	2.45214983
H	-0.35538824	-0.21825177	2.93580383
H	1.26290076	0.98841923	1.39319883
H	3.34970376	1.22366523	0.89358683
H	5.78558276	1.09431023	0.75736883
H	6.90146276	-0.85161177	-0.33223817
H	5.49686476	-2.68025877	-1.28797817
H	3.05416576	-2.57114277	-1.16168317
H	-3.55346424	2.22913423	-1.01369917
H	-5.91206524	1.53340923	-1.27496417
H	-6.62697724	-0.75017477	-0.58597817
H	-4.95084124	-2.33637677	0.34855683
H	-2.58168924	-1.65197277	0.57286083

Diazo imidazoline *anti*-**17**

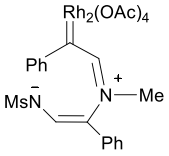


Zero-point correction = 0.334951
Thermal correction to Energy = 0.366792
Thermal correction to Enthalpy = 0.367923
Thermal correction to Gibbs Free Energy = 0.264674
E_0 = -1463.992797, E = -1463.960956,
H = -1463.959825, G = -1464.063074.
Imaginary frequency = 0.

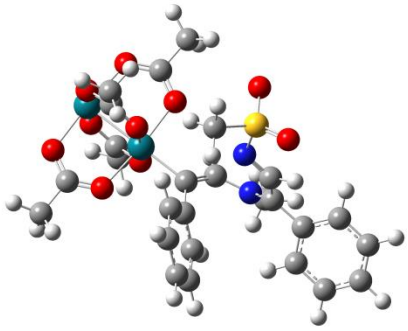


C	-2.53873716	-3.04885077	-1.51532471
O	-1.36220516	-4.13049377	0.60733229
O	-0.19096216	-4.30164577	-1.64718171
S	-1.01766916	-3.53691677	-0.69948871
N	-0.22995116	-2.02251177	-0.46938471
C	3.18597984	-0.67416677	0.00673529
C	1.15600784	-1.93127077	-0.80746071
C	1.79778484	-1.16035077	0.09299329
C	-1.79456716	0.78487223	-0.00052871
C	1.31069784	-0.69346877	2.49282429
N	-2.47329316	-0.62804077	1.80078429
N	-3.25262216	-0.84736177	2.61222529
N	0.89931584	-0.69685977	1.08570029
C	-0.40813216	-1.34212977	0.85303429
C	-1.58452516	-0.37820877	0.87667029
C	-0.85591716	1.11108523	-1.00066471
C	-1.05943316	2.21362023	-1.83262271

Complex **18**



Zero-point correction = 0.535378
Thermal correction to Energy = 0.596199
Thermal correction to Enthalpy = 0.597330
Thermal correction to Gibbs Free Energy = 0.427290
E_0 = -2489.602611, E = -2489.541791,
H = -2489.540660, G = -2489.710700.
Imaginary frequency = 0.

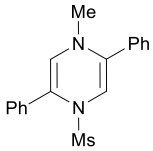


C	0.33758748	3.32562774	1.92728568
O	0.79254948	3.46801874	-0.69618332
O	2.79004648	3.39313374	0.85895968
S	1.41088548	2.95949974	0.54329968
N	1.27503748	1.24596774	0.48189268
C	3.96173848	-1.28273426	-0.04938332
C	2.40019348	0.62531874	0.32974768
C	2.57836248	-0.76061226	-0.05990032
C	0.17473548	-1.15029226	2.16071968
C	1.88721848	-2.54496626	-1.59623932
N	1.57977248	-1.51108826	-0.56854632
C	0.21837148	-1.32590826	-0.34294932
C	-0.44235852	-1.03443726	0.83501968
C	-0.06325252	-0.18316826	3.15956068
C	0.50729248	-0.30849626	4.42658368
C	1.28776848	-1.42513526	4.74543968
C	1.48953348	-2.42134026	3.78250068
C	0.94714648	-2.28329226	2.50530568

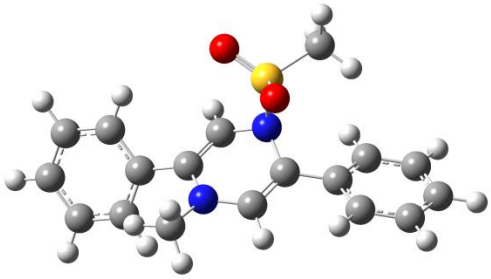
C	-2.19527416	3.01614923	-1.69438071
C	-3.13330816	2.70010923	-0.70608771
C	-2.93824316	1.60124223	0.12978529
C	4.20638284	-1.52567377	-0.45394071
C	5.51648184	-1.06044477	-0.58025471
C	5.83320084	0.25749523	-0.23428171
C	4.82708484	1.10904323	0.23425829
C	3.51431684	0.64950623	0.35356229
H	-2.27931616	-2.56449977	-2.45639171
H	-3.08321416	-2.36924277	-0.85928571
H	-3.10954816	-3.96344877	-1.68536771
H	1.50017484	-2.29139377	-1.76382171
H	1.39333084	-1.71331077	2.89998629
H	2.27395284	-0.19408477	2.59430029
H	0.57591784	-0.13655777	3.07972829
H	-0.59127116	-2.10129477	1.62753529
H	0.03508284	0.51125623	-1.13360471
H	-0.31972616	2.44350923	-2.59426471
H	-2.34744516	3.87247123	-2.34417471
H	-4.02331616	3.31031323	-0.58207571
H	-3.68452416	1.38046523	0.88716429
H	3.97084584	-2.55683177	-0.70001271
H	6.29231784	-1.73156677	-0.93705871
H	6.85420984	0.61610023	-0.32497471
H	5.06254784	2.13506223	0.50189629
H	2.73453684	1.32122723	0.69894629

C	5.04228448	-0.50883326	-0.52129332
C	6.34372948	-1.00796026	-0.47381132
C	6.59252248	-2.28027126	0.05152668
C	5.52928648	-3.05547026	0.52715568
C	4.22576648	-2.56439026	0.47548668
H	0.80193848	2.94143174	2.83581168
H	-0.62568652	2.84936874	1.73937768
H	0.24469348	4.41264874	1.96631568
H	3.34429848	1.16558674	0.43609068
H	1.12353948	-2.46624726	-2.37114232
H	2.87030848	-2.37025926	-2.02593932
H	1.83819948	-3.54073826	-1.15265432
H	-0.37227552	-1.53900526	-1.22706832
H	-0.70236452	0.65891374	2.92716368
H	0.32513048	0.45810274	5.17490568
H	1.71752548	-1.52870226	5.73757268
H	2.06842948	-3.30735126	4.02813168
H	1.08994848	-3.07417126	1.77527668
H	4.86652448	0.46882374	-0.95838732
H	7.16219648	-0.40466526	-0.85409932
H	7.60720648	-2.66461326	0.09060968
H	5.71517448	-4.03999026	0.94531368
H	3.41244048	-3.16598626	0.86671268
Rh	-2.46991752	-0.73373726	0.61958068
Rh	-4.90482752	-0.47417426	0.27907368
O	-5.16905952	-1.46695126	2.07682068
C	-4.15461252	-1.86500926	2.73221868
O	-2.93287852	-1.70129826	2.39381568
O	-4.87331852	-2.28419226	-0.72094532
C	-3.77506152	-2.90620426	-0.85743332
O	-2.63832252	-2.52165526	-0.41187332
O	-4.45363952	0.50120474	-1.49292932
C	-3.24107652	0.64866374	-1.84337632
O	-2.21867752	0.25000574	-1.18606432
O	-4.78033452	1.31331974	1.30559768
C	-3.65656652	1.71551374	1.73789068
O	-2.54011052	1.10339574	1.60317368
C	-2.96741152	1.33278774	-3.16374932
H	-2.09860752	1.98900874	-3.07763132
H	-2.73981352	0.57092674	-3.91771932
H	-3.84093752	1.89863574	-3.49051832
C	-3.78937352	-4.20572226	-1.63007732
H	-4.80584552	-4.59381426	-1.70733432
H	-3.40398952	-4.02345226	-2.63937932
H	-3.13787452	-4.93997526	-1.15065632
C	-4.40580952	-2.62510226	4.01534168
H	-5.36408152	-2.33457126	4.44932668
H	-4.44094552	-3.69667726	3.78823668
H	-3.59606952	-2.45564626	4.72743268
C	-3.62178352	3.04676674	2.45482268
H	-4.61091452	3.29512874	2.84221168
H	-2.89165652	3.02856074	3.26660068
H	-3.32271452	3.82533574	1.74408668

Dihydropyrazine **19**

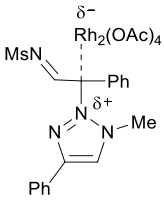


Zero-point correction = 0.325124
Thermal correction to Energy = 0.354560
Thermal correction to Enthalpy = 0.355691
Thermal correction to Gibbs Free Energy = 0.257849
E_0 = -1354.545996, E = -1354.516561,
H = -1354.515430, G = -1354.613272.
Imaginary frequency = 0.

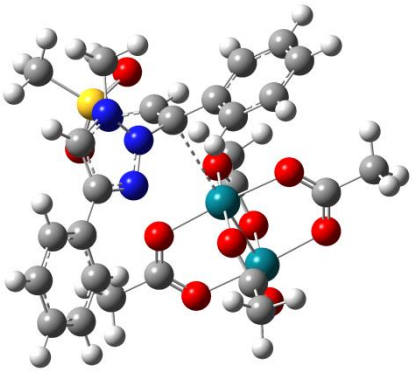


C	2.28020990	2.76336742	-0.47757195
O	1.44401590	1.72833342	1.82624005
O	-0.24201010	2.94702442	0.34801405
S	0.92916390	2.05294742	0.47611005
N	0.55039790	0.53916442	-0.46634495
C	-3.11463210	-0.44410958	-0.20974895
C	-0.85032210	0.41145042	-0.73506095
C	-1.65638610	-0.33515058	0.06018805
C	2.50057490	-1.00026658	-0.17349895
C	-1.77582910	-1.63832258	2.22466705
N	-1.06775210	-1.13555158	1.04425905
C	0.28976790	-1.38497358	0.94040105
C	1.10035490	-0.64612258	0.14197605
C	3.30353790	-1.71446558	0.73802105
C	4.61327090	-2.06887758	0.41308905
C	5.15867890	-1.71019458	-0.82482695
C	4.37711990	-0.98881158	-1.73254295
C	3.06551090	-0.63424258	-1.41006995
C	-3.88910510	0.71982742	-0.33986395
C	-5.24987610	0.63598342	-0.64816195
C	-5.85369310	-0.61171758	-0.82602495
C	-5.08963310	-1.77754358	-0.69763395
C	-3.73057110	-1.69527158	-0.39219695
H	2.54629390	3.70197242	0.01220405
H	1.92516590	2.93738542	-1.49319495
H	3.11662190	2.06513742	-0.46489795
H	-1.22777110	0.90815142	-1.62010395
H	-1.51729410	-1.04588258	3.10909605

TS1



Zero-point correction = 0.547520
Thermal correction to Energy = 0.609124
Thermal correction to Enthalpy = 0.610255
Thermal correction to Gibbs Free Energy = 0.437707
E_0 = -2599.116926, E = -2599.055322,
H = -2599.054191, G = -2599.226740.
Imaginary frequency = 1.

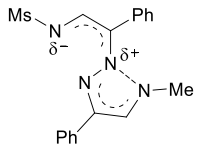


C	-4.31970180	-1.42805830	-0.51418493
C	-3.44094380	3.33280070	0.90171107
N	-2.38975380	0.02261070	0.00826107
N	-2.18349480	1.26194570	0.38275607
N	-3.36267780	1.92027570	0.52097907
C	-4.34509380	1.06511270	0.21842607
C	-3.72257880	-0.14792230	-0.10698093
C	-3.52023680	-2.42252130	-1.10369093
C	-4.08604180	-3.63738430	-1.49207693
C	-5.45190680	-3.87391330	-1.29992493
C	-6.25124480	-2.88747430	-0.71323793
C	-5.68963580	-1.67112830	-0.32047093
H	-2.96143080	3.47381670	1.87077807
H	-2.94683780	3.93204670	0.13657907
H	-4.49635280	3.59136070	0.96456107
H	-5.38059580	1.36744670	0.23936307
H	-2.46291080	-2.23604030	-1.25883193
H	-3.46063980	-4.39835330	-1.94930193
H	-5.88974980	-4.81983530	-1.60454093
H	-7.31087280	-3.06497730	-0.55605893
H	-6.31971680	-0.92058930	0.14745307
C	-0.90137180	1.88661570	0.61468207
C	-0.44285380	2.68166370	-0.43634593
N	-1.11930880	2.84300370	-1.57171593
S	-0.40379280	3.75951870	-2.74691193
O	-0.07527980	2.91357970	-3.92199893
O	0.69339420	4.62361670	-2.22991793
C	-1.76209780	4.83156970	-3.24062693
C	-0.48248980	1.96848970	2.02779507

H	-2.85090910	-1.58428358	2.06919605
H	-1.49688210	-2.68115858	2.40266805
H	0.63833990	-2.26899458	1.46403205
H	2.90984990	-1.97690958	1.71536105
H	5.21399390	-2.61477158	1.13507805
H	6.18001890	-1.98239658	-1.07379995
H	4.78724790	-0.70231558	-2.69697295
H	2.46263890	-0.07884058	-2.12114695
H	-3.42238610	1.68801142	-0.18771295
H	-5.83702110	1.54469342	-0.74244895
H	-6.91145010	-0.67719358	-1.06319295
H	-5.55092110	-2.75000258	-0.84261395
H	-3.13927410	-2.60275658	-0.30969895

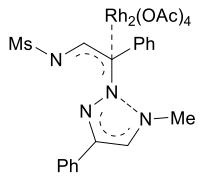
C	0.38562320	2.98422670	2.48404007
C	0.77384320	3.04991370	3.82195807
C	0.29087620	2.12312570	4.75324207
C	-0.58425480	1.12297070	4.31974307
C	-0.96188280	1.04230470	2.97783307
H	0.50810920	3.19431270	-0.29002893
H	-1.40279080	5.43231970	-4.07824893
H	-2.03357580	5.46769970	-2.39742293
H	-2.60182580	4.20726670	-3.54735593
H	0.75539120	3.73634170	1.79473207
H	1.44532820	3.84264270	4.14068807
H	0.58673820	2.18427370	5.79630607
H	-0.97071680	0.39227470	5.02511207
H	-1.62030480	0.23761870	2.66530407
Rh	3.06184520	-1.51834630	-1.00003493
Rh	1.29964520	-0.05630030	-0.28008393
O	2.32832820	1.49096970	-1.16648493
C	3.43155820	1.25626170	-1.76128293
O	3.97718320	0.10674770	-1.86670293
O	2.37015820	0.25148870	1.45517407
C	3.49035320	-0.33429030	1.61547007
O	4.03652220	-1.12034030	0.77049607
O	0.40231720	-1.70635830	0.58108707
C	0.97074620	-2.84377630	0.50844607
O	2.07135420	-3.08000330	-0.09496093
O	0.35063920	-0.44422630	-2.06647793
C	0.89402320	-1.23212230	-2.90705193
O	2.00386020	-1.84223230	-2.73490593
C	0.30599820	-4.00073830	1.21475807
H	0.54839720	-4.94224430	0.71881507
H	0.68409320	-4.04704030	2.24233607
H	-0.77479380	-3.85518030	1.25420207
C	4.21874020	-0.10422730	2.91727007
H	3.92761420	0.85128570	3.35570407
H	3.94805720	-0.90304730	3.61684907
H	5.29841820	-0.14181230	2.76034907
C	4.16142720	2.43264970	-2.35992993
H	3.45280020	3.20770270	-2.65536493
H	4.83404720	2.84990570	-1.60181793
H	4.76300020	2.11384270	-3.21294193
C	0.18611020	-1.44331730	-4.22265993
H	0.55370220	-0.70036830	-4.93912593
H	0.40301020	-2.43746530	-4.61774193
H	-0.88925480	-1.30147730	-4.10544093

TS2



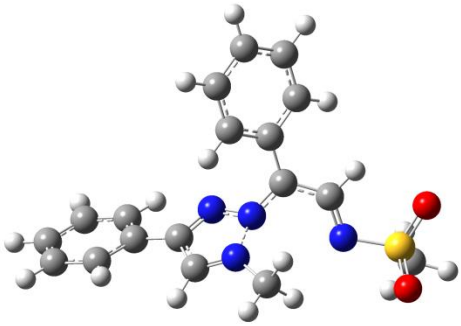
Zero-point correction = 0.332330
Thermal correction to Energy = 0.364043
Thermal correction to Enthalpy = 0.365174

TS3



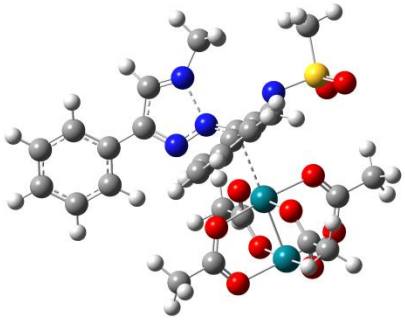
Zero-point correction = 0.543427
Thermal correction to Energy = 0.606495
Thermal correction to Enthalpy = 0.607626

Thermal correction to Gibbs Free Energy = 0.260622
E_0 = -1463.987030, E = -1463.955317,
H = -1463.954186, G = -1464.058738.
Imaginary frequency = 1.



C	4.65750081	-3.47084904	-1.59625855
O	4.83209581	-3.53405504	1.05360745
O	5.38258481	-1.36677304	-0.12640355
S	4.53019381	-2.58065004	-0.03918555
N	2.89516981	-2.22842404	0.02971945
C	0.94254281	0.97012496	0.30872145
C	2.57853481	-0.95284504	0.09426945
C	1.24667181	-0.47535804	0.20308645
C	-3.24632219	-2.08169004	0.11872345
C	0.91399581	-2.77582004	2.84459545
N	-0.93931919	-1.31636704	-0.12233855
N	0.28115281	-1.41298804	0.31315545
N	-0.06450919	-2.19865504	1.94721445
C	-1.29560919	-2.53458204	1.77504045
C	-1.86014319	-1.94093604	0.58887845
C	-3.57550919	-1.83389604	-1.22668355
C	-4.89242719	-1.96231304	-1.66559055
C	-5.90121819	-2.34318604	-0.77296455
C	-5.58279019	-2.59027704	0.56548645
C	-4.26608619	-2.45862604	1.01016845
C	-0.12694319	1.43031096	1.10106945
C	-0.40763819	2.79393896	1.20502845
C	0.37589181	3.73201996	0.52574345
C	1.44125481	3.28871896	-0.26469855
C	1.71860481	1.92522796	-0.37756455
H	5.69095081	-3.81150804	-1.68235155
H	4.40414581	-2.78923404	-2.40886355
H	3.97087981	-4.31693704	-1.56467655
H	3.36709481	-0.19690004	0.07897745
H	1.59715781	-3.40350504	2.26735145
H	1.49111181	-1.97481804	3.31265245
H	0.41940981	-3.37645204	3.61513445
H	-1.80583219	-3.26858004	2.39553945
H	-2.79449519	-1.54411104	-1.92179555
H	-5.13152719	-1.76962104	-2.70715855
H	-6.92562519	-2.44517704	-1.11810655
H	-6.35906819	-2.88030104	1.26701745
H	-4.04093819	-2.63849404	2.05703745
H	-0.73457519	0.72096696	1.65330445

Thermal correction to Gibbs Free Energy = 0.429537
E_0 = -2599.087298, E = -2599.024229,
H = -2599.023098, G = -2599.201188.
Imaginary frequency = 1.

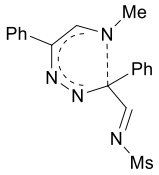


C	-3.21917619	-0.63442745	-0.60985525
C	-1.47497219	4.05849455	-0.24314325
N	-1.03016119	0.27813455	-0.03002925
N	-0.26856119	1.31882955	0.02202775
N	-1.60761419	2.62576355	-0.07808525
C	-2.60546219	1.88478855	-0.39819225
C	-2.29965219	0.47499755	-0.31901125
C	-2.71865619	-1.90448145	-0.95173525
C	-3.59248919	-2.95734145	-1.22030125
C	-4.97724819	-2.76056245	-1.15631425
C	-5.48223719	-1.50129145	-0.81823025
C	-4.61096019	-0.44466545	-0.54523325
H	-1.04422719	4.48925755	0.66364075
H	-0.79900719	4.25625555	-1.07757625
H	-2.45253519	4.51169955	-0.44099825
H	-3.54638619	2.28444255	-0.77171825
H	-1.64585519	-2.05553645	-1.00916925
H	-3.19296619	-3.93166145	-1.48604325
H	-5.65570019	-3.58137945	-1.36892425
H	-6.55464419	-1.34031545	-0.76152225
H	-5.02128919	0.52191455	-0.26842825
C	0.75808381	1.54530955	0.90250475
C	1.74693681	2.47914355	0.43980275
N	1.68390281	3.09578855	-0.71120425
S	2.97044181	4.12193955	-1.07043725
O	3.56945381	3.69670555	-2.35449425
O	3.88788381	4.32233255	0.07902275
C	2.10255581	5.66897055	-1.36644325
C	0.55460681	1.33914455	2.36975875
C	1.04383581	2.27958755	3.29897975
C	0.83975281	2.11177955	4.67084475
C	0.12479681	1.01028255	5.14901375
C	-0.37900719	0.07697655	4.23682075
C	-0.16467819	0.23568455	2.86645075
H	2.58343781	2.66613555	1.11459975
H	2.85972681	6.40056455	-1.65473925
H	1.60091881	5.97410755	-0.44752625
H	1.38845581	5.51599455	-2.17594025
H	1.57582181	3.16209455	2.95894075
H	1.22941681	2.85343555	5.36259475

H	-1.23642019	3.12308196	1.82544745
H	0.15721481	4.79247496	0.60764645
H	2.05228781	4.00448196	-0.80723955
H	2.53143081	1.60255096	-1.02118655

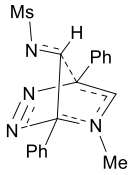
H	-0.04102119	0.88301455	6.21489775
H	-0.93427919	-0.78669745	4.59246375
H	-0.52982819	-0.51727345	2.17941175
Rh	4.02248081	-2.32031245	-0.29577825
Rh	2.51729281	-0.51146345	0.20496675
O	3.96299981	0.76554655	-0.51571425
C	5.06735281	0.29972755	-0.95111425
O	5.37142781	-0.93932045	-0.99669325
O	3.38903081	-0.40642145	2.06941675
C	4.33283781	-1.20955445	2.36950775
O	4.80802381	-2.10810345	1.59736975
O	1.18921281	-1.93425845	0.89388275
C	1.51103881	-3.16675345	0.87111975
O	2.61295481	-3.63171845	0.42520375
O	1.76000881	-0.71427945	-1.70037725
C	2.23457981	-1.61200045	-2.47130025
O	3.16716281	-2.42874645	-2.16530725
C	0.52397181	-4.15499045	1.44401675
H	0.62313281	-5.12353445	0.95064475
H	0.74264681	-4.28972545	2.50940475
H	-0.49571219	-3.77850345	1.34857775
C	4.91782281	-1.10947745	3.75732675
H	4.75276481	-0.11436645	4.17268775
H	4.42036181	-1.84267945	4.40208475
H	5.98382281	-1.34459245	3.73712475
C	6.09761581	1.29312755	-1.42525625
H	5.60560581	2.13345355	-1.91849325
H	6.63708581	1.68020055	-0.55336925
H	6.81393881	0.81134055	-2.09253225
C	1.62794481	-1.74001345	-3.84756025
H	1.16701781	-0.79942945	-4.15243525
H	2.38777481	-2.04524045	-4.56968925
H	0.85397781	-2.51531945	-3.82070025

TS4

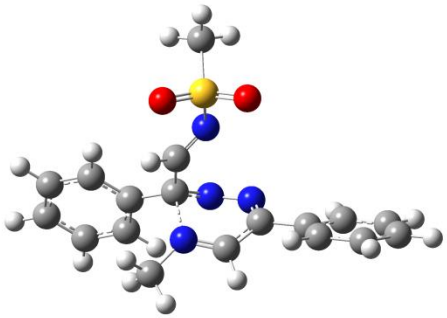


Zero-point correction = 0.332294
Thermal correction to Energy = 0.363809
Thermal correction to Enthalpy = 0.364940
Thermal correction to Gibbs Free Energy = 0.261776
E_0 = -1463.976830, E = -1463.945315,
H = -1463.944184, G = -1464.047348.
Imaginary frequency = 1.

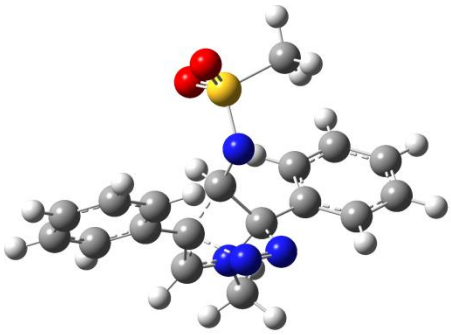
TS5



Zero-point correction = 0.333762
Thermal correction to Energy = 0.364435
Thermal correction to Enthalpy = 0.365566
Thermal correction to Gibbs Free Energy = 0.265906
E_0 = -1463,973969, E = -1463,943296,
H = -1463,942165, G = -1464,041825.
Imaginary frequency = 1.

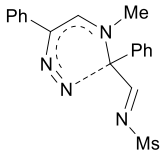


C	-0.59838687	3.39984919	-0.73038500
O	1.29160613	2.40907219	0.87987000
O	-1.05839387	2.64857019	1.79750300
S	-0.16358087	2.35226719	0.65843400
N	-0.48936087	0.79619019	-0.02191400
C	-3.06336887	-1.70744181	0.24102200
C	-1.27250187	0.05726519	0.66450200
C	-1.60892587	-1.34937981	0.23262300
C	2.57869713	-2.08533081	0.45161100
C	-1.61018387	-2.62945881	2.98979400
N	0.44407313	-1.96145581	-0.66823400
N	-0.87498487	-1.96077881	-0.72318200
N	-0.83523487	-1.98791481	1.93467400
C	0.40632413	-2.31337081	1.71692100
C	1.09910813	-2.01534181	0.49158200
C	3.33229713	-1.75750881	1.59330300
C	4.72822113	-1.81309481	1.57052700
C	5.39801713	-2.18856681	0.40295400
C	4.65794613	-2.50703781	-0.74239400
C	3.26441313	-2.45842481	-0.71979000
C	-4.06138087	-0.79847481	0.63007700
C	-5.40698187	-1.17618681	0.61823100
C	-5.77252887	-2.46466581	0.22281500
C	-4.78449987	-3.37750581	-0.16474300
C	-3.44222587	-3.00271181	-0.15470100
H	-1.66442787	3.28850219	-0.93046100
H	0.00240313	3.09606119	-1.58757000
H	-0.36341087	4.42268719	-0.43032000
H	-1.73342387	0.39888319	1.59437600
H	-2.07297287	-1.86668481	3.62148000
H	-2.40807087	-3.22679581	2.53745200
H	-0.98212887	-3.28643581	3.60175700
H	0.91264713	-2.96207581	2.43695600
H	2.82887413	-1.43529981	2.50074700
H	5.29010413	-1.55131781	2.46246700
H	6.48310313	-2.22904081	0.38294300
H	5.16904113	-2.80088781	-1.65491800
H	2.69343613	-2.71157881	-1.60631600
H	-3.81149287	0.21262219	0.93241000
H	-6.16643787	-0.45943081	0.91500800
H	-6.81839287	-2.75656781	0.21544300
H	-5.06027187	-4.38118881	-0.47385100
H	-2.67480687	-3.70555681	-0.46042000

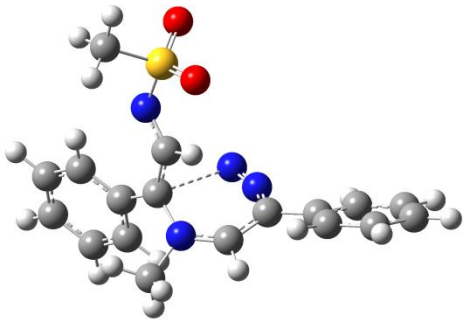


C	1.36329633	2.88163641	0.52618704
O	-1.25827267	3.00675641	0.53561704
O	-0.13114267	1.93030941	-1.45270296
S	-0.18970167	2.09753841	0.03528004
N	-0.23940467	0.69734041	0.83448204
C	2.42742133	-1.13021459	0.40660304
C	-0.17220767	-0.46961059	0.08880904
C	0.98311633	-1.51242859	0.44870504
C	-2.75962867	-1.24754459	0.31446004
C	1.46129133	-3.72491159	-0.75373096
N	-0.72533367	-1.92415059	1.99389704
N	0.45806033	-1.85329259	1.96978704
N	0.56963133	-2.64894359	-0.30584996
C	-0.75968467	-2.69642759	-0.35332096
C	-1.31284767	-1.56647359	0.31724404
C	-3.62420667	-1.77688959	-0.65880596
C	-4.98323667	-1.45769859	-0.64753596
C	-5.49505667	-0.60399259	0.33449804
C	-4.63965067	-0.06668759	1.30117104
C	-3.27961267	-0.38136859	1.29096004
C	2.93970433	-0.52587659	-0.75378296
C	4.28257333	-0.15150359	-0.81819496
C	5.12609333	-0.37154759	0.27561504
C	4.61941133	-0.96722659	1.43306004
C	3.27593133	-1.34686859	1.50155704
H	2.19166333	2.25786141	0.18875104
H	1.36939133	2.97449341	1.61293004
H	1.40093033	3.86659241	0.05700204
H	-0.11137767	-0.30902559	-0.99886196
H	2.26683233	-3.30231859	-1.35368796
H	1.88231033	-4.23746659	0.11445304
H	0.88048233	-4.42592959	-1.35189396
H	-1.26557967	-3.55110259	-0.78423996
H	-3.24072967	-2.42675359	-1.43967396
H	-5.63848067	-1.87201459	-1.40781896
H	-6.55209767	-0.35513259	0.34252004
H	-5.02926267	0.60284541	2.06203604
H	-2.61517667	0.04521941	2.03354904
H	2.29133733	-0.34118959	-1.60499496
H	4.66630133	0.31597541	-1.71972696
H	6.16992233	-0.07686259	0.22598904
H	5.26736833	-1.13849559	2.28717504
H	2.88937033	-1.80621059	2.40357304

TS6

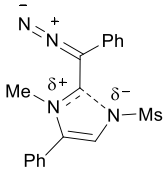


Zero-point correction = 0.332632
Thermal correction to Energy = 0.364579
Thermal correction to Enthalpy = 0.365710
Thermal correction to Gibbs Free Energy = 0.260927
E_0 = -1463.982686, E = -1463.50739,
H = -1463.949608, G = -1464.054391.
Imaginary frequency = 1.

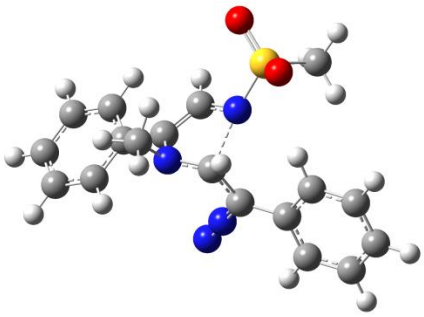


C	-3.38028310	3.60674279	1.30418637
O	-2.06099510	3.36981879	-0.98120863
O	-0.77632110	3.06395479	1.17285637
S	-2.02896810	2.83280579	0.40126537
N	-2.48603810	1.24049179	0.35509637
C	-3.05207210	-1.77002721	0.60594337
C	-1.66095710	0.37557579	0.93582437
C	-1.86363010	-1.00924121	1.02449837
C	2.60835690	-1.01371721	0.40901937
C	-1.34793810	-2.49051921	2.98068837
N	0.44742290	-1.30305321	-0.66726463
N	-0.51039810	-1.26020421	-1.29239363
N	-0.88489110	-1.70982521	1.80396737
C	0.43842490	-1.64258621	1.62567137
C	1.15850490	-1.26794321	0.46638037
C	3.27652190	-0.49377021	1.53122137
C	4.65274390	-0.26177821	1.48707837
C	5.37707490	-0.52184021	0.32022337
C	4.71425090	-1.02390721	-0.80483463
C	3.34340090	-1.27743121	-0.76111663
C	-4.31527510	-1.15976821	0.44584737
C	-5.42575810	-1.90820521	0.05415237
C	-5.31365110	-3.28122921	-0.19014463
C	-4.06804510	-3.89905021	-0.04305963
C	-2.95342310	-3.15436021	0.34371937
H	-3.39246210	3.20921979	2.31964837
H	-4.31282010	3.38304679	0.78547737
H	-3.18886510	4.68132579	1.31034437
H	-0.75237110	0.75296379	1.41421337
H	-2.37331510	-2.20823921	3.20883337
H	-1.29452610	-3.56321121	2.78633237
H	-0.70699810	-2.24495121	3.83065837

TS7



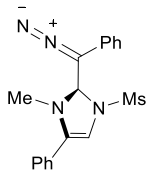
Zero-point correction = 0.332666
Thermal correction to Energy = 0.364510
Thermal correction to Enthalpy = 0.364510
Thermal correction to Gibbs Free Energy = 0.261880
E_0 = -1463.973894, E = -1463.942050,
H = -1463.940919, G = -1464.044681.
Imaginary frequency = 1.



C	2.09663384	3.06378421	-1.62137336
O	2.11131884	3.00464121	1.02744564
O	0.14449784	4.10066221	-0.15052536
S	1.14172884	3.00186721	-0.09357036
N	0.43223684	1.49949021	-0.11193536
C	-3.01635516	0.01811521	-0.02257236
C	-0.90194316	1.38900921	-0.43500636
C	-1.63570216	0.44456721	0.22555664
C	2.49446784	-1.27806579	0.08793164
C	-1.33752916	0.49049321	2.65892964
N	0.22811984	-1.86059079	-0.44455736
N	-0.45663816	-2.54719279	-1.04162436
N	-0.91601716	-0.08714179	1.36397564
C	0.42928784	-0.13585879	1.15085964
C	1.03899284	-1.10245779	0.26273864
C	3.38305884	-0.28332379	0.53797864
C	4.76230784	-0.46170479	0.40645064
C	5.27940184	-1.61669579	-0.18598736
C	4.39979584	-2.60152079	-0.64781236
C	3.02167984	-2.43860179	-0.51047836
C	-3.87931116	0.75027221	-0.86643136
C	-5.18529016	0.32370521	-1.09683436
C	-5.67363816	-0.83971579	-0.48775836
C	-4.83308016	-1.57074679	0.35462464
C	-3.52052216	-1.14988579	0.58334464
H	1.40887484	2.99656821	-2.46511836
H	2.79768884	2.22895921	-1.62055336
H	2.62696784	4.01776721	-1.63043336
H	-1.33048116	2.01769621	-1.20949236
H	-1.08682916	1.55735021	2.70991064
H	-2.41677116	0.37366221	2.75620564
H	-0.85036016	-0.04851379	3.47367664

H	1.03697990	-1.97962121	2.46711537	H	1.06358084	0.18691721	1.97064064
H	2.72116590	-0.24578321	2.43047437	H	3.00907284	0.63913721	0.96864064
H	5.15399890	0.14086779	2.36209237	H	5.43208284	0.31633521	0.76082064
H	6.44527090	-0.33130121	0.28575237	H	6.35211384	-1.74736479	-0.28985236
H	5.26667390	-1.23057721	-1.71652263	H	4.78544784	-3.50495379	-1.11078336
H	2.84514790	-1.69237421	-1.63268263	H	2.35985684	-3.22438879	-0.86248536
H	-4.41670210	-0.09726621	0.62440237	H	-3.53331716	1.66404521	-1.33916836
H	-6.38673010	-1.41377221	-0.05795663	H	-5.82864216	0.90655921	-1.74988236
H	-6.18133310	-3.85889221	-0.49461063	H	-6.69323716	-1.16680379	-0.66774936
H	-3.95868110	-4.96193121	-0.23940563	H	-5.19420216	-2.47609979	0.83430064
H	-1.99286310	-3.65363921	0.42922337	H	-2.87446616	-1.73457279	1.23045164

TS8



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Thermal correction to Energy = 0.365387
Thermal correction to Enthalpy = 0.366518
Thermal correction to Gibbs Free Energy = 0.265858
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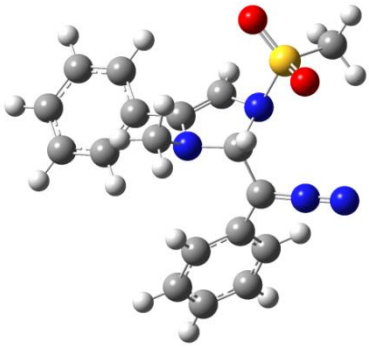
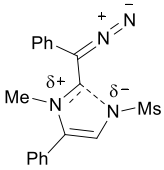
H = -1463.954378, G = -1464.055038.
Imaginary frequency = 1.



C	-3.68945593	-1.84961116	-1.63150147
O	-3.68250893	-1.23939316	0.97006753
O	-2.60866093	-3.41943916	0.22044353
S	-2.89604593	-1.99237516	-0.02668147
N	-1.43610493	-1.07070516	-0.29295247
C	2.06913707	-2.30163116	-0.03467747
C	-0.30675593	-1.81571816	-0.76204247
C	0.72366807	-1.72095316	0.10533253
C	0.46202207	1.93623784	0.11824653
C	0.52228107	-1.43503216	2.55976653
N	-1.90661393	1.80063884	0.29217553
N	-2.92855593	2.30616984	0.14925753
N	0.38368207	-0.88536316	1.20115553
C	-0.90664593	-0.28047016	0.88096953
C	-0.77094993	1.19488684	0.47687353
C	1.58282207	1.94630984	0.97006753
C	2.72418407	2.67536584	0.63092053
C	2.76486407	3.42277984	-0.55108747
C	1.65170107	3.43210884	-1.39657547

TS9



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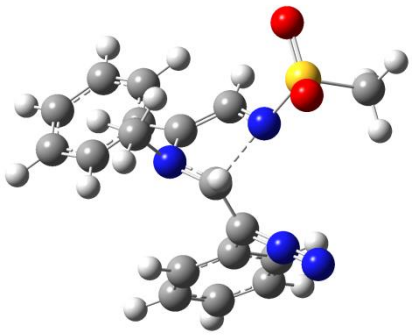
Thermal correction to Energy = 0.364420
Thermal correction to Enthalpy = 0.365551
Thermal correction to Gibbs Free Energy = 0.261024
E_0 = -1463.969449, E = -1463.937574,
H = -1463.936443, G = -1464.040970.
Imaginary frequency = 1.



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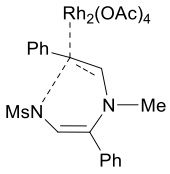
O	-3.59202893	-1.34539122	0.89823013
O	-2.55346993	-3.07275722	-0.64851987
S	-2.71599293	-1.64904522	-0.25722887
N	-1.26073293	-0.89745822	0.02728713
C	2.36320107	-1.84055322	0.22762113
C	-0.09254693	-1.51470922	-0.36658387
C	0.98678207	-1.39111822	0.46040913
C	0.85172107	1.92755078	0.37246313
C	0.47652507	-1.88139822	2.80584213
N	-1.38281393	2.08902278	1.20483913
N	-2.31657793	2.73799978	1.28415513
N	0.60862607	-0.85231322	1.74965113
C	-0.44960993	0.00982578	1.65411213
C	-0.29758793	1.34874078	1.11968813
C	0.66194707	2.50182678	-0.89544687
C	1.73534307	3.08071178	-1.57606887
C	3.01051707	3.08326278	-1.00321187
C	3.20543007	2.51153278	0.25850213

C	0.51430507	2.69086984	-1.06904347	C	2.13267307	1.94452078	0.94832113
C	2.24409907	-3.54098016	-0.67770847	C	2.70233607	-2.63088222	-0.89230787
C	3.52006207	-4.08097116	-0.84253947	C	4.01241507	-3.05629622	-1.09984387
C	4.64129707	-3.40060616	-0.35449347	C	5.02540907	-2.71302422	-0.19530687
C	4.47657507	-2.17346016	0.29581053	C	4.70489807	-1.93425022	0.91897113
C	3.20193007	-1.62637116	0.45406153	C	3.39312107	-1.50084522	1.12667413
H	-3.03604393	-2.29195116	-2.38432247	H	-2.72594693	-0.92646422	-2.53228787
H	-3.87001293	-0.79418916	-1.83203947	H	-3.47455593	0.28043878	-1.43040187
H	-4.62606693	-2.40573716	-1.56375347	H	-4.37696593	-1.20500822	-1.88452987
H	-0.32331393	-2.27600216	-1.73943847	H	-0.04933193	-2.05220422	-1.30838787
H	-0.20265993	-2.23626016	2.76274753	H	-0.36212893	-2.55602122	2.59225013
H	1.52908007	-1.83576416	2.68325153	H	1.39722907	-2.46274622	2.84650213
H	0.38140607	-0.63285916	3.28839553	H	0.32623907	-1.39294622	3.77072913
H	-1.60590893	-0.36577916	1.71504453	H	-1.23228493	-0.11022722	2.39822213
H	1.55325807	1.39193284	1.90041753	H	-0.32351793	2.49055678	-1.35210287
H	3.57886907	2.67163584	1.30154253	H	1.57534907	3.52170478	-2.55539187
H	3.65205007	3.99432184	-0.80701947	H	3.84603607	3.52926778	-1.53427987
H	1.66965807	4.00766684	-2.31757947	H	4.19188707	2.51637578	0.71241713
H	-0.33755193	2.69043584	-1.74341847	H	2.28239607	1.51955978	1.93465413
H	1.37551707	-4.08711716	-1.03315947	H	1.93839307	-2.92311422	-1.60560687
H	3.63798507	-5.03903316	-1.34025847	H	4.24323707	-3.66379522	-1.97038287
H	5.63333707	-3.82528116	-0.47646347	H	6.04502307	-3.04866822	-0.35881787
H	5.34199807	-1.63760016	0.67475953	H	5.47739307	-1.65575722	1.63034013
H	3.07855607	-0.66339316	0.93817953	H	3.16476507	-0.88423622	1.98935913

TS10



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Thermal correction to Enthalpy = 0.595705
Thermal correction to Gibbs Free Energy = 0.426395
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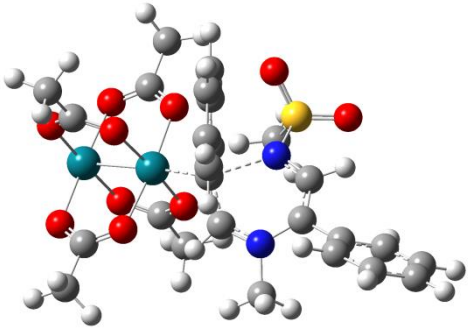
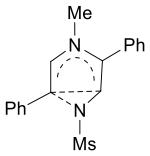
H = -2489.531724, G = -2489.701033.
Imaginary frequency = 1.



C	-0.55166917	2.73838159	-0.45812569
O	1.79503383	2.87900959	0.78848331
O	-0.20509717	2.10919559	2.11202031
S	0.52335883	2.11576859	0.83325131
N	0.81718683	0.49100659	0.36914431
C	3.95395483	-1.13761741	-0.88627469

TS11



Zero-point correction = 0.323877
Thermal correction to Energy = 0.352430
Thermal correction to Enthalpy = 0.353561
Thermal correction to Gibbs Free Energy = 0.257474
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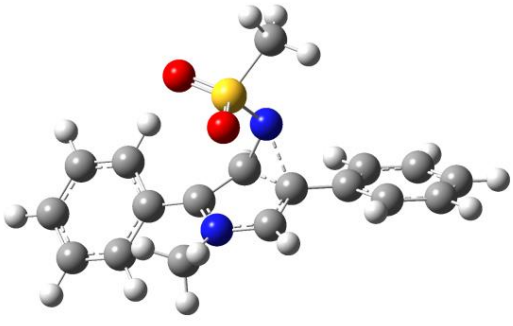
H = -1354,464619, G = -1354,560705.
Imaginary frequency = 1.

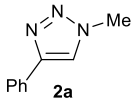


C	0.89075402	3.47563403	-0.54269795
O	-0.44516398	2.44203603	1.50873705
O	-1.63045798	2.61195103	-0.70788295
S	-0.37207198	2.32943003	0.03000305
N	0.30250602	0.90893703	-0.52510095
C	-3.01359998	-0.77385597	-0.00201795

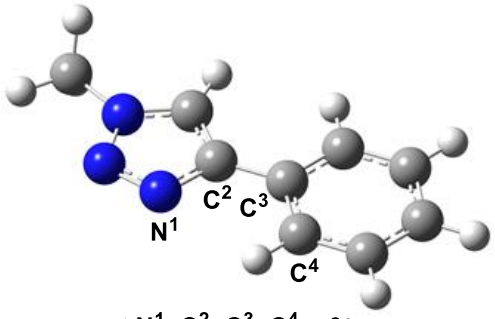
C	2.07884583	0.22793159	0.02522331	C	-0.48821898	-0.35993297	-0.48729795
C	2.50461183	-0.89091641	-0.67781169	C	-1.65109298	-0.49940097	0.42390805
C	0.01684283	-1.83247041	1.46553431	C	2.09279902	-0.90059097	0.03814605
C	1.99091683	-2.35063141	-2.59743769	C	-1.95562798	-0.50067397	2.91927705
N	1.56066583	-1.67458641	-1.34390369	N	-1.16302698	-0.56072297	1.68341405
C	0.26786083	-1.71659841	-1.04184769	C	0.20104702	-0.58439697	1.73868105
C	-0.38803117	-1.26815341	0.16711731	C	0.72421902	-0.49085497	0.42440605
C	-0.35842917	-1.18945041	2.66447931	C	3.14288502	-0.82146097	0.96940005
C	-0.02905817	-1.74215141	3.89797531	C	4.43375602	-1.22204397	0.62147705
C	0.64516983	-2.96967941	3.96693331	C	4.69857802	-1.70557897	-0.66424195
C	0.99834583	-3.63328841	2.78834931	C	3.66133502	-1.78499497	-1.59831295
C	0.70076283	-3.06426541	1.54818531	C	2.36900202	-1.38660197	-1.25005795
C	4.79657183	-0.10770641	-1.34448769	C	-3.47559598	-0.20292897	-1.21050895
C	6.17100483	-0.31696341	-1.48170369	C	-4.75550798	-0.47703797	-1.68926495
C	6.72666883	-1.56350241	-1.17739369	C	-5.61399298	-1.32034597	-0.97521095
C	5.89868383	-2.59779341	-0.72741669	C	-5.17004098	-1.89929097	0.21864405
C	4.52703183	-2.38537541	-0.57597969	C	-3.88605698	-1.64020397	0.69702805
H	-1.41681817	2.08189759	-0.52504969	H	0.55909202	4.47188303	-0.24495195
H	0.01254783	2.75313059	-1.39075769	H	0.96912702	3.39788103	-1.62672495
H	-0.83566917	3.74915159	-0.15728469	H	1.83487402	3.22133703	-0.06064095
H	2.84875783	0.95187059	0.28736031	H	-0.57311198	-0.82823197	-1.46574895
H	1.10517983	-2.68784441	-3.13130069	H	-1.44701098	0.16436703	3.61723405
H	2.55803183	-1.65118541	-3.21183569	H	-2.94533298	-0.10590597	2.70075005
H	2.61629183	-3.20826241	-2.35173669	H	-2.03872698	-1.49666997	3.35996305
H	-0.36666517	-2.15861841	-1.80196669	H	0.71122902	-0.54662097	2.68671605
H	-0.88103317	-0.24219241	2.60649931	H	2.95552302	-0.43904697	1.96789205
H	-0.30679517	-1.22316241	4.81106531	H	5.23311502	-1.15215597	1.35334605
H	0.88967083	-3.40456641	4.93190731	H	5.70312202	-2.01693297	-0.93481095
H	1.51552783	-4.58751241	2.83231431	H	3.85571702	-2.16016197	-2.59877295
H	0.98152183	-3.59064041	0.64135331	H	1.57378102	-1.45648897	-1.98523995
H	4.37134983	0.85743059	-1.60443369	H	-2.83258698	0.48399403	-1.75017495
H	6.80414083	0.49133059	-1.83598269	H	-5.08785698	-0.02069197	-2.61721295
H	7.79451283	-1.72756441	-1.28769069	H	-6.61258798	-1.52923297	-1.34691095
H	6.32255083	-3.56640641	-0.47864569	H	-5.81914298	-2.57199097	0.77178105
H	3.90044683	-3.18659441	-0.19435569	H	-3.55076298	-2.14494597	1.59581205
Rh	-2.46077917	-1.00423041	-0.21283269				
Rh	-4.86901317	-0.85555041	-0.71801769				
O	-5.22415917	-2.04884841	0.92712331				
C	-4.23708117	-2.46696441	1.61284431				
O	-3.00726117	-2.20704541	1.38654631				
O	-4.66907517	-2.54534541	-1.89078669				
C	-3.53068817	-3.09703041	-1.99746169				
O	-2.45173417	-2.68932741	-1.44112569				
O	-4.36104917	0.32468459	-2.34265269				
C	-3.13946917	0.56498859	-2.59383269				
O	-2.14297017	0.18234359	-1.88663769				
O	-4.93213717	0.81466559	0.49652431				
C	-3.87163817	1.20008559	1.08275931				
O	-2.71710617	0.66518159	0.95930031				
C	-2.82093417	1.34925859	-3.84614569				
H	-1.96531517	2.00727259	-3.68131869				
H	-2.55603317	0.64527059	-4.64321669				
H	-3.68932117	1.92602659	-4.16754169				
C	-3.42180517	-4.34738141	-2.83941269				

H	-4.36671117	-4.55745641	-3.34114869
H	-2.62454617	-4.23031841	-3.57890269
H	-3.15483317	-5.19267541	-2.19689969
C	-4.52823717	-3.36018341	2.79724131
H	-5.60236517	-3.43353441	2.97024431
H	-4.12151317	-4.35831341	2.60507031
H	-4.03077617	-2.96790941	3.68838831
C	-3.97960317	2.38210259	2.01732031
H	-4.49596417	2.06391759	2.92963031
H	-2.98959217	2.75539659	2.27994031
H	-4.57945417	3.17020459	1.55510331

Table S8. Dihedral angles and cartesian coordinates of 1-methyl-4-phenyl-1*H*-1,2,3-triazole (**2a**) and 1,4-diphenyl-1*H*-1,2,3-triazole (DFT B3LYP/6-31+G(d,p)/Stuttgart RSC 1997 ECP, PCM for DCE).

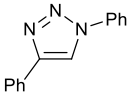


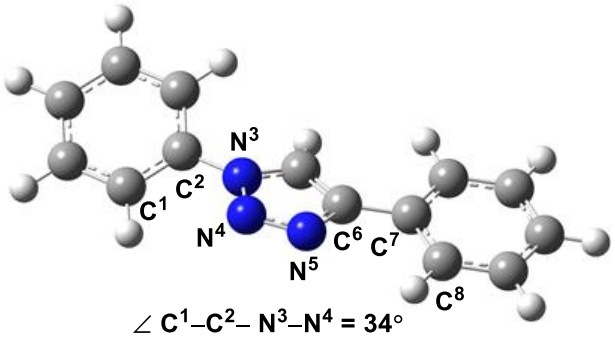
2a



∠ N^1–C^2–C^3–C^4 = 0°

C	1.00937636	-0.16387004	-0.15873610
C	-3.96773564	0.55061096	-0.15856010
N	-1.09539164	-1.49723104	-0.15888510
N	-2.39056264	-1.30816904	-0.15881810
N	-2.60827164	0.02175496	-0.15865310
C	-1.43632564	0.69746796	-0.15860110
C	-0.45649364	-0.28595704	-0.15876910
C	1.81899236	-1.31375504	-0.15860610
C	3.21039836	-1.20275404	-0.15856010
C	3.82000236	0.05623996	-0.15863610
C	3.02297936	1.20575496	-0.15876510
C	1.63140536	1.09760396	-0.15881610
H	-4.64951564	-0.29893104	-0.15862910
H	-4.13324664	1.15636896	0.73474290
H	-4.13329864	1.15653996	-1.05173810
H	-1.39692864	1.77524196	-0.15860810
H	1.35020436	-2.29181204	-0.15854410
H	3.81941636	-2.10222104	-0.15846110
H	4.90264436	0.14102096	-0.15859210
H	3.48409336	2.18916296	-0.15883510





∠ C^1–C^2– N^3–N^4 = 34°

∠ N^5–C^6– C^7–C^8 = 11°

C	2.56290409	-0.42534616	-0.27916988
N	0.67108609	-1.99332016	0.13705812
N	-0.63320191	-1.99840216	0.13988712
N	-1.04671891	-0.74905916	-0.18983788
C	0.02287509	0.06134484	-0.40357088
C	1.13001609	-0.74311716	-0.19071688
C	3.52150409	-1.45381416	-0.25392088
C	4.88272209	-1.15652416	-0.33868688
C	5.31123009	0.17008184	-0.45263988
C	4.36454909	1.19954584	-0.47815588
C	3.00297609	0.90580284	-0.38928488
H	-0.08462191	1.08806184	-0.71274288
H	3.19238709	-2.48399516	-0.17013588
H	5.60956709	-1.96341916	-0.31846088
H	6.37053209	0.39960584	-0.51944888
H	4.68557709	2.23375984	-0.56156888
H	2.28285109	1.71871284	-0.39681888
C	-2.88021191	0.83840284	0.10620212
C	-4.24063591	1.14066484	0.01658412
C	-5.15106091	0.17602784	-0.42500288

H	1.02977636	2.00172896	-0.15893210	C	-4.69549291	-1.09657416	-0.78458988
				C	-3.33652891	-1.40754416	-0.71493388
				C	-2.43687491	-0.43431516	-0.26780888
				H	-2.17895491	1.57792084	0.47799312
				H	-4.58704191	2.12784884	0.30594812
				H	-6.20843291	0.41359484	-0.48688588
				H	-5.39667791	-1.84941016	-1.13092388
				H	-2.97164591	-2.38553516	-1.00593088

8. References

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