Supporting Information

Transannulation of 1-Sulfonyl-1,2,3-Triazoles with Heterocumulenes

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Content

General Information

^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker DRX-600, a Bruker DRX-500, and a Bruker AMX-400. Infrared spectra were recorded on a Nicolet Avatar 370 and on a Perkin-Elmer Spectrum 100 Fourier transform infrared spectrometers. Melting points were determined using a Thomas-Hoover melting point apparatus and are uncorrected. HPLC was performed on an Agilent 1100 LC/MSD equipped with an Agilent 1100 SL mass spectrometer (ES) eluting with 0.1% trifluoroacetic acid in H_2O and 0.05% trifluoroacetic acid in CH_3CN. Column chromatography was carried out employing EMD (Merck) Silica Gel 60 (40-63 μm). Precoated Merck F-254 silica gel plates were used for a thin layer analytical chromatography. Chloroform was purchased from Fischer (certified ACS grade containing *ca.* 0.75 % of ethanol) and distilled from phosphorous pentoxide under inert atmosphere. $Rh_2(Oct)_4$, $Rh_2(esp)_2$ and $Rh_2(S\text{-PTAD})_4$ were purchased from Strem Chemicals, and $Rh_2(Piv)_4$,[1] $Rh_2(TPA)_4$,[2] $Rh_2(S\text{-PTV})_4$,[2] $Rh_2(S\text{-PTTL})_4$,[3] $Rh_2(S\text{-NTV})_4$,[4] $Rh_2(S\text{-NTTL})_4$[4] were prepared using literature procedures. Sulfonyl azides were prepared using standard methods.[5] All isocyanates and isothiocyanates were purchased from Aldrich, Acros Organics, AK Scientific, TCI or Alfa Aesar and were re-distilled prior to use.

(1) Cotton, F. A.; Felthouse, T. R. *Inorg. Chem.* **1980**, *19*, 323.

(2) Hashimoto, S.; Watanabe, N.; Sato, T.; Shiro, M.; Ikegami, S. *Tetrahedron Lett.* **1993**, *34*, 5109.

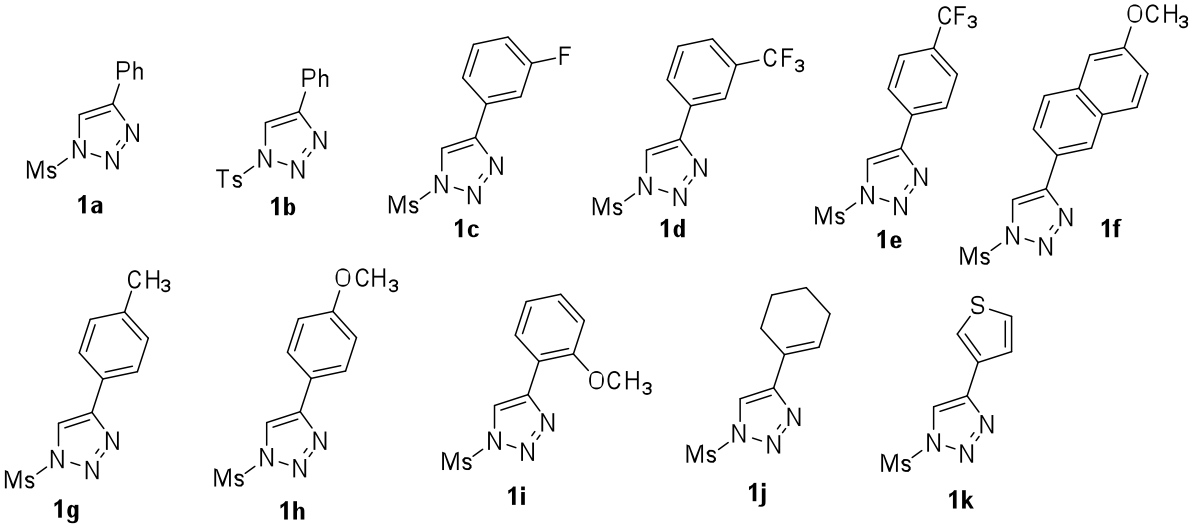
(3) Tsutsui, H.; Abe, T.; Nakamura, S.; Anada, M.; Hashimoto, S. *Chem. Pharm. Bull*. **2005**, *53*, 1366.

(4) (a) Müller, P.; Allenbach, Y. F.; Robert, E. *Tetrahedron: Asymmetry* **2003**, *14*, 779. (b) Müller, P.; Bernardinelli, G.; Allenbach, Y. F.; Ferry, M.; Flack, H. D. *Org. Lett*. **2004**, *6*, 1725.

(5) (a) Breslow, D. S.; Sloan, M. F.; Newburg, N. R.; Renfrow, W. B. *J. Am. Chem. Soc.* **1969**, *91*, 2273. (b) Danheiser, R. L.; Miller, R. F.; Brisbois, R. G.; Park, S. Z. *J. Org. Chem.* **1990**, *55*, 1959.

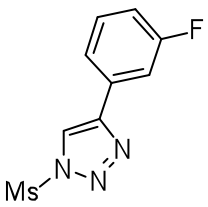
Starting Materials

N-Sulfonyl 1,2,3-triazoles **1** were prepared using the reported CuTC-catalyzed azide-alkyne cycloaddition (CuAAC) protocol.[6] However, due to the potential danger of methanesulfonyl azide, we strongly recommend to avoid isolating this compound in large quantities. Generation of mesyl azide, followed by immediate use is highly preferred. 1-Sulfonyl-1,2,3-triazoles **1**, as previously reported,[6b] may gradually hydrolyze if atmospheric moisture is not excluded; therefore, a glove box was used for prolonged storage and manipulating the triazoles. Compounds **1a-b**,[6b] **1e-f**,[6b] **1g**,[3c] **1h**,[6b] and **1j-k**[6b] were previously reported.



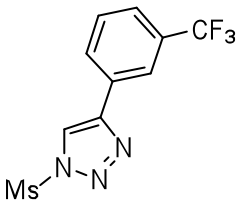
(6) (a) Raushel, J.; Fokin, V. V. *Org. Lett.* **2010**, *12*, 4952. (b) Chuprakov, S.; Kwok, S. W.; Zhang, L.; Lercher, L.; Fokin, V. V. *J. Am. Chem. Soc*. **2009**, *131*, 18034. (c) Chuprakov, S.; Malik, J. A.; Zibinsky, M.; Fokin, V. V. *J. Am. Chem. Soc*. **2011**, *133*, 10352.

4-(3-Fluorophenyl)-1-(methylsulfonyl)-1H-1,2,3-triazole (1c)



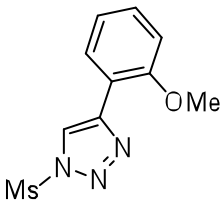
1c: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.33 (s, 1H), 7.65–7.56 (m, 2H), 7.48–7.38 (m, 1H), 7.15–7.05 (m, 1H), 3.58 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 163.1 (d, J = 246.7 Hz), 146.3 (d, J = 2.6 Hz), 130.8 (d, J = 8.3 Hz), 130.7 (d, J = 8.6 Hz), 121.8 (d, J = 2.9 Hz), 119.4, 116.2 (d, J = 21.2 Hz), 113.2 (d, J = 23.3 Hz), 42.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -112.1; FT IR: 1588, 1474, 1453, 1353, 1339, 1202, 1183, 1156, 1005, 950, 876, 855, 783, 766 cm^{-1}; mp 129–132 °C; LRMS (ESI) m/z 242.2 $[M + H]^+$.

1-(Methylsulfonyl)-4-(3-(trifluoromethyl)phenyl)-1H-1,2,3-triazole (1d)



1d: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.40 (s, 1H), 8.12 (s, 1H), 8.09–8.02 (m, 1H), 7.69–7.64 (m, 1H), 7.63–7.57 (m, 1H), 3.60 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 146.1, 131.6 (q, J = 32.6 Hz), 129.7, 129.5, 129.3, 125.9 (q, J = 3.7 Hz), 123.8 (q, J = 272.4 Hz), 123.0 (q, J = 3.8 Hz), 119.5, 42.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -63.1; FT IR: 1379, 1358, 1299, 1200, 1180, 1163, 1125, 1068, 999, 949, 800, 772 703, 695 cm^{-1}; mp 107–109 °C; LRMS (ESI–TOF) m/z 292.2 $[M + H]^+$.

4-(2-Methoxyphenyl)-1-(methylsulfonyl)-1H-1,2,3-triazole (1i)



1i: ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.56 (s, 1H), 8.36 (dd, J = 7.71, 1.49 Hz, 1H), 7.43–7.34 (m, 1H), 7.13–7.08 (m, 1H), 7.01 (d, J = 1.19 Hz, 1H), 3.97 (s, 3H), 3.54 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 156.0, 142.9, 130.1, 128.0, 122.0, 121.0, 117.4, 110.8, 55.5, 42.7; FT IR: 1372, 1326, 1175, 1128, 1023, 995, 969, 944, 770, 757 cm^{-1}; mp 93–94 °C (dec.); LRMS (ESI) m/z 254.2 $[M + H]^+$.

Optimization

Experimental procedure. To an oven-dried 0.5-2 mL micro-wave vial equipped with a stirring bar were added 0.2 mmol of 1-sulfonyl-4-phenyl-1H-1,2,3-triazole **1** and 0.002 mmol of Rh(II) carboxylate (Figure 1) under inert atmosphere (glove box). The vial was sealed, and 0.026 mL (0.24 mmol) of phenyl isocyanate was added to the vial *via* syringe, followed by 1.0 mL of anhydrous chloroform. The resulting reaction mixture was stirred at temperatures listed in Table 1, and then was analyzed by LCMS and NMR after periods of time shown in Table 1. Conversion and yield were calculated based on ^{1}H NMR integration using dibromomethane as an internal standard. Obtained results are summarized in Table 1.

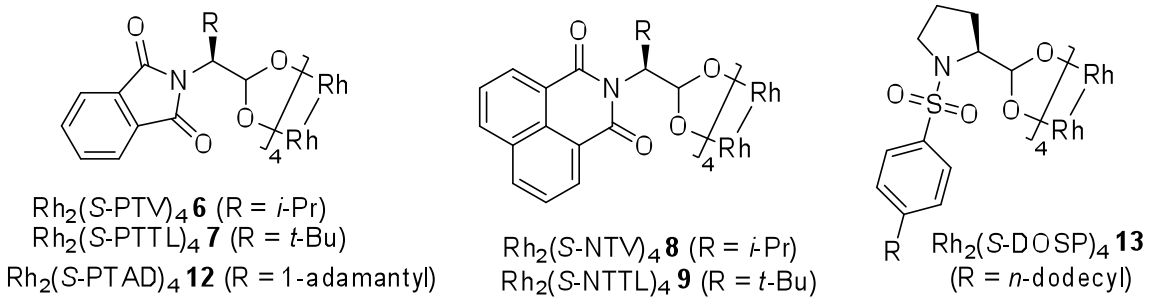
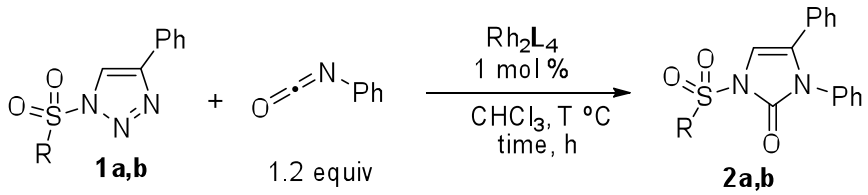


Figure 1. Rh(II) carboxylates used in this study.

Table 1. Conditions screening for transannulation with isocyanates.



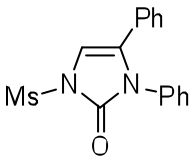
R	catalyst[a]	T, °C	time, h	yield, %	conversion, %
Ts	$Rh_2(Oct)_4$	70	0.5	<5	100
Ts	$Rh_2(Piv)_4$	70	0.5	35	100
Ts	$Rh_2(esp)_2$	70	0.5	33	100
Ts	Rh_2(*S*-PTV)$_4$	70	0.5	56	100
Ts	Rh_2(*S*-PTTL)$_4$	70	0.5	40	100
Ts	Rh_2(*S*-NTTL)$_4$	rt	24	14	25
Ts	Rh_2(*S*-NTV)$_4$	rt	24	59	100
Ts	Rh_2(*S*-PTTL)$_4$	rt	24	51	58
Ts	Rh_2(*S*-PTAD)$_4$	rt	24	58	76
Ts	Rh_2(*S*-PTV)$_4$	rt	24	55	85
Ts	Rh_2(*S*-DOSP)$_4$	rt	24	10	20
Ms	$Rh_2(Piv)_4$	rt	3	53	NA
Ms	$Rh_2(esp)_2$	rt	4	65	100
Ms	Rh_2(*S*-PTTL)$_4$	rt	3	89	95
Ms	Rh_2(*S*-PTV)$_4$	rt	4	56	91
Ms	Rh_2(*S*-NTV)$_4$	rt	3	86	100
Ms	Rh_2(*S*-NTTL)$_4$	rt	3	95	100
Ms	$Rh_2(TPA)_4$	rt	4	10	19

[a] Oct – *n*-octanoate; Piv – pivalate; $Rh_2(esp)_2$ – Bis[rhodium(α,α,α′,α′-tetramethyl-1,3-benzenedipropionic acid)]; TPA – triphenylacetate.

Rh_2(*S*-NTTL)$_4$-Catalyzed transannulation of 1-mesyl-1,2,3-triazoles with isocyanates and isothiocyanates

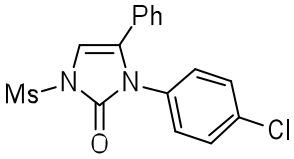
Typical preparative procedure. To an oven-dried 2-5 mL micro-wave vial equipped with a stirring bar were added 0.223 g (1.0 mmol) of 1-(methylsulfonyl)-4-phenyl-1H-1,2,3-triazole **1b** and 0.0072 g (0.005 mmol) of Rh_2(*S*-NTTL)$_4$ **9** under inert atmosphere (glove box). The vial was sealed, and phenyl isocyanate (0.130 mL, 1.2 mmol) was added to the vial *via* syringe, followed by 5.0 mL of anhydrous chloroform. The resulting green reaction mixture was stirred at ambient temperature for 2 hrs until judged complete by LC and TLC analysis. Column chromatography was directly applied to the reaction mixture using silica gel (ethyl acetate-hexanes 1:2) to afford 0.297 g (0.95 mmol, 95% yield) of 1-(methylsulfonyl)-3,4-diphenyl-1H-imidazol-2(3H)-one **2b** as white solid.

1-(Methylsulfonyl)-3,4-diphenyl-1H-imidazol-2(3H)-one (2b)



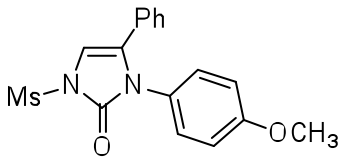
2b: (95% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.42–7.24 (m, 6H), 7.24–7.18 (m, 2H), 7.11–7.05 (m, 2H), 6.91 (s, 1H), 3.55 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 150.0, 133.9, 129.1, 128.7, 128.6, 128.0, 127.7, 127.6, 127.0, 126.6, 105.3, 40.9; FT IR: 1717, 1495, 1449, 1360, 1170, 971 cm^{-1}; mp 195–198 °C (dec.); LRMS (ESI) *m/z* 314.4 $[M + H]^+$.

3-(4-Chlorophenyl)-1-(methylsulfonyl)-4-phenyl-1H-imidazol-2(3H)-one (2c)



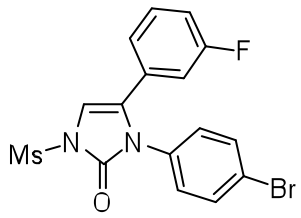
2c: (94% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.38–7.26 (m, 5H), 7.17–7.13 (m, 2H), 7.11–7.06 (m, 2H), 6.90 (s, 1H), 3.54 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 149.9, 133.8, 132.4, 129.3, 129.0, 128.8, 128.2, 127.6, 127.4, 126.3, 105.6, 40.9; FT IR : 1720, 1497, 1361, 1320, 1172, 1089, 972, 719 cm^{-1}; mp 215–216 °C ; LRMS (ESI) *m/z* 349.2 $[M + H]^+$.

3-(4-Methoxyphenyl)-1-(methylsulfonyl)-4-phenyl-1H-imidazol-2(3H)-one (2d)



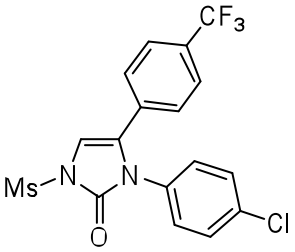
2d: (94% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.33–7.24 (m, 3H), 7.17–7.05 (m, 4H), 6.92–6.86 (m, 3H), 3.82 (s, 3H), 3.54 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 159.1, 150.2, 128.7, 128.6, 128.4, 127.7, 127.6, 126.8, 126.6, 114.4, 104.9, 55.4, 40.9; FT IR: 1714, 1519, 1363, 1299, 1259, 1175, 1165, 1105, 1028, 971, 767, 715 cm^{-1}; mp 198–200 °C; LRMS (ESI) *m/z* 345.3 $[M + H]^+$.

3-(4-Bromophenyl)-4-(3-fluorophenyl)-1-(methylsulfonyl)-1H-imidazol-2(3H)-one (2e)



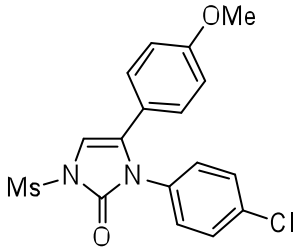
2e: (94% yield); ^{1}H NMR (DMSO-d_6, 500MHz) δ ppm 7.70–7.60 (m, 2H), 7.38–7.30 (m, 2H), 7.24–7.19 (m, 2H), 7.15 (dt, J = 8.46, 2.01 Hz, 1H), 7.09–7.00 (m, 1H), 6.96–6.86 (m, 1H), 3.63 (s, 3H); ^{13}C NMR (DMSO-d_6, 126MHz) δ ppm 161.7 (d, J = 243.9 Hz), 149.1, 133.2, 132.0, 130.5 (d, J = 8.6 Hz), 129.6 (d, J = 8.9 Hz), 129.5, 124.0 (d, J = 2.2 Hz), 123.5 (d, J = 2.5 Hz), 121.0, 115.2 (d, J = 21.0 Hz), 114.3 (d, J = 23.4 Hz), 107.2, 40.5; ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -112.0; FT IR: 1719, 1488, 1447, 1377, 1348, 1161, 1070, 970, 888, 767, 732 cm^{-1}; mp 166–167 ^{o}C; LRMS (ESI) *m/z* 411.1, 413.1 $[M + H]^+$.

3-(4-Chlorophenyl)-1-(methylsulfonyl)-4-(4-(trifluoromethyl)phenyl)-1H-imidazol-2(3H)-one (2f)



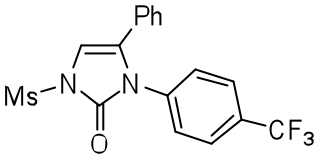
2f: (80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.61–7.54 (m, 2H), 7.41–7.35 (m, 2H), 7.23–7.18 (m, 2H), 7.17–7.12 (m, 2H), 7.00 (s, 1H), 3.56 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 149.7, 134.2, 132.0, 130.9, 130.8 (q, J = 32.8 Hz), 129.6, 128.1, 127.6, 125.8 (q, J = 3.7 Hz), 124.8, 123.6 (q, J = 272.0 Hz), 107.0, 41.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -63.1; mp 225–226 °C; LRMS (ESI) *m/z* 417.2 $[M + H]^+$.

3-(4-Chlorophenyl)-4-(4-methoxyphenyl)-1-(methylsulfonyl)-1H-imidazol-2(3H)-one (2g)



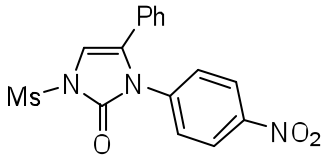
2g: (85% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.35–7.29 (m, 2H), 7.14–7.08 (m, 2H), 7.01–6.94 (m, 2H), 6.83–6.76 (m, 3H), 3.78 (s, 3H), 3.51 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 160.0, 149.8, 133.7, 132.4, 129.3, 129.1, 128.2, 126.2, 119.6, 114.2, 104.6, 55.3, 40.9; FT IR: 1719, 1511, 1494, 1364, 1249, 1176, 1165, 1090, 974, 943, 831, 736 cm^{-1}; mp 201 °C (dec.); LRMS (ESI) *m/z* 379.2 $[M + H]^+$.

1-(Methylsulfonyl)-4-phenyl-3-(4-(trifluoromethyl)phenyl)-1H-imidazol-2(3H)-one (2h)



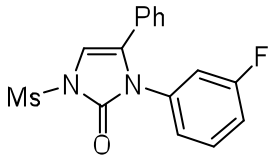
2h: (83% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.64–7.58 (m, 2H), 7.35–7.27 (m, 5H), 7.08–7.04 (m, 2H), 6.90 (s, 1H), 3.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 149.8, 137.0, 129.7 (q, J = 32.8 Hz), 129.1, 128.9, 127.6, 127.2, 126.9, 126.2 (q, J = 3.7 Hz), 126.0, 123.6 (q, J = 272.2 Hz), 106.1, 41.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -62.9; FT IR: 1719, 1361, 1335, 1156, 1115, 1071, 971, 766 cm^{-1}; mp 186–188 °C; LRMS (ESI) *m/z* 383.2 $[M + H]^+$.

1-(Methylsulfonyl)-3-(4-nitrophenyl)-4-phenyl-1H-imidazol-2(3H)-one (2i)



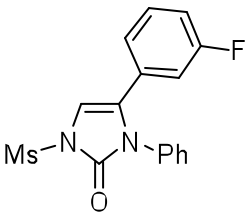
2i: (53% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.27–8.17 (m, 2H), 7.42–7.30 (m, 5H), 7.13–7.05 (m, 2H), 6.94 (s, 1H), 3.56 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 149.5, 146.3, 139.4, 129.3, 129.0, 127.6, 127.0, 125.7, 124.3, 106.7, 41.0; FT IR: 1723, 1518, 1319, 1170, 1108, 1064, 973, 943, 855, 719 cm^{-1}; mp 223–224 °C; LRMS (ESI) *m/z* 360.2 $[M + H]^+$.

3-(3-Fluorophenyl)-1-(methylsulfonyl)-4-phenyl-1H-imidazol-2(3H)-one (2j)



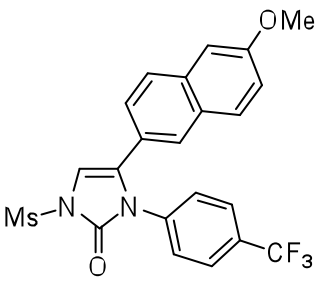
2j: (89% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.38–7.26 (m, 4H), 7.12–7.08 (m, 2H), 7.08–7.02 (m, 1H), 7.02–6.96 (m, 2H), 6.91 (s, 1H), 3.55 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 162.5 (d, J = 248.2 Hz), 149.8, 135.1 (d, J = 10.2 Hz), 130.2 (d, J = 8.9 Hz), 129.0, 128.8, 127.5, 127.3, 126.3, 122.7 (d, J = 3.1 Hz), 115.1 (d, J = 21.0 Hz), 114.5 (d, J = 24.3 Hz), 105.7, 40.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -111.0; FT IR: 1718, 1596, 1492, 1447, 1386, 1358, 1269, 1173, 1160, 1097, 986, 870 cm^{-1}; mp 173–175 ^{o}C; LRMS (ESI) *m/z* 333.2 $[M + H]^+$.

4-(3-fluorophenyl)-1-(methylsulfonyl)-3-phenyl-1H-imidazol-2(3H)-one (2k)



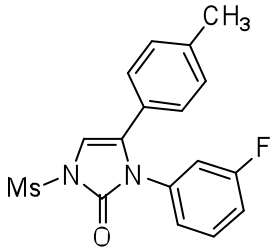
2k: (92% yield); ^{1}H NMR (500MHz, $CDCl_3$) δ ppm 7.44–7.34 (m, 3H), 7.27–7.19 (m, 3H), 7.01 (dt, J = 8.40, 2.54 Hz, 1H), 6.95 (s, 1H), 6.89–6.85 (m, 1H), 6.81–6.77 (m, 1H), 3.55 (s, 3H); ^{13}C NMR ($CDCl_3$, 126MHz) δ ppm 162.5 (d, J = 247.2 Hz), 149.9, 133.6, 130.3 (d, J = 8.4 Hz), 129.7 (d, J = 8.5 Hz), 129.3, 128.3, 127.0, 125.4 (d, J = 2.6 Hz), 123.2 (d, J = 2.9 Hz), 115.7 (d, J = 21.1 Hz), 114.5 (d, J = 23.5 Hz), 106.0, 40.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -111.9; FT IR: 1718, 1448, 1358, 1169, 1154, 986, 973, 873 720 cm^{-1}; mp 179–180 ^{o}C; LRMS (ESI) *m/z* 333.2 $[M + H]^+$.

4-(6-Methoxynaphthalen-2-yl)-1-(methylsulfonyl)-3-(4-(trifluoromethyl)phenyl)-1H-imidazol-2(3H)-one (2l)



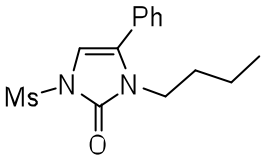
2l: (69% yield); ^{1}H NMR (400MHz, $CDCl_3$) δ ppm 7.66–7.54 (m, 5H), 7.39–7.31 (m, 2H), 7.17 (dd, J = 8.91, 2.53 Hz, 1H), 7.08 (d, J = 2.30 Hz, 1H), 7.00–6.94 (m, 2H), 3.91 (s, 3H), 3.55 (s, 3H); ^{13}C NMR ($CDCl_3$, 125MHz) δ ppm 158.6, 149.8, 137.1, 134.4, 129.7 (q, J = 32.8 Hz), 129.5, 128.4, 127.4, 126.9, 126.3, 126.2 (q, J = 3.6 Hz), 125.2, 123.6 (q, J = 272.4 Hz), 122.3, 119.9, 105.9, 105.7, 55.4, 41.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -62.9; FT IR: 1723, 1365, 1320, 1274, 1214, 1158, 1110, 1068, 965, 854, 764 cm^{-1}; mp 178–181 ^{o}C; LRMS (ESI) *m/z* 463.2 $[M + H]^+$.

3-(3-Fluorophenyl)-1-(methylsulfonyl)-4-(*p*-tolyl)-1H-imidazol-2(3H)-one (2m)



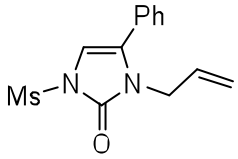
2m: (85% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.36–7.30 (m, 1H), 7.13–7.08 (m, 2H), 7.08–7.02 (m, 1H), 7.01–6.94 (m, 4H), 6.86 (s, 1H), 3.54 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 162.5 (d, J = 248.0 Hz), 149.8, 139.1, 135.2 (d, J = 10.0 Hz), 130.2 (d, J = 9.0 Hz), 129.5, 127.5, 126.4, 124.3, 122.8 (d, J = 3.3 Hz), 115.1 (d, J = 21.1 Hz), 114.6 (d, J = 24.2 Hz), 105.2, 40.9, 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -111.1; FT IR: 1718, 1595, 1491, 1359, 1268, 1160, 1173, 986, 867, 767 cm^{-1}; mp 203–205 ^{o}C; LRMS (ESI) *m/z* 347.2 $[M + H]^+$.

3-Butyl-1-(methylsulfonyl)-4-phenyl-1H-imidazol-2(3H)-one (2n)



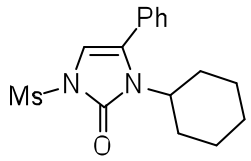
2n: (97% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.48–7.41 (m, 3H), 7.36–7.31 (m, 2H), 6.64 (s, 1H), 3.70–3.59 (m, 2H), 3.47 (s, 3H), 1.53–1.43 (m, 2H), 1.25–1.13 (m, 2H), 0.79 (t, J = 7.37 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 150.7, 129.4, 129.0, 128.5, 128.1, 127.0, 104.3, 41.8, 40.7, 30.8, 19.6, 13.4; FT IR: 1710, 1451, 1357, 1171, 1133, 1060, 967, 762 cm^{-1}; mp 54–56 °C ; LRMS (ESI) *m/z* 295.4 $[M + H]^+$.

3-Allyl-1-(methylsulfonyl)-4-phenyl-1H-imidazol-2(3H)-one (2o)



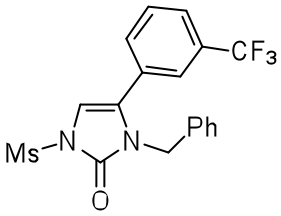
2o: (85% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.46–7.40 (m, 3H), 7.38–7.33 (m, 2H), 6.69 (s, 1H), 5.81 (ddt, J = 17.06, 10.33, 5.17 Hz, 1H), 5.18 (d, J = 10.33 Hz, 1H), 5.05 (d, J = 17.12 Hz, 1H), 4.25 (td, J = 5.11, 1.51 Hz, 2H), 3.48 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 150.6, 132.0, 129.4, 128.9, 128.5, 127.7, 127.2, 117.7, 104.4, 44.3, 40.8; FT IR: 1705, 1449, 1347, 1325, 1166, 1150, 1099, 998, 967 cm^{-1}; mp 87–91 °C ; LRMS (ESI) *m/z* 279.2 $[M + H]^+$.

3-Cyclohexyl-1-(methylsulfonyl)-4-phenyl-1H-imidazol-2(3H)-one (2p)



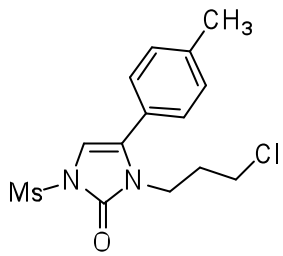
2p: (95% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.48–7.41 (m, 3H), 7.32–7.27 (m, 2H), 6.58 (s, 1H), 3.58 (tt, J = 12.16, 3.83 Hz, 1H), 3.47 (s, 3H), 2.34–2.21 (m, 2H), 1.84–1.67 (m, 4H), 1.62–1.52 (m, 1H), 1.21–1.06 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 150.0, 129.3, 129.1, 128.9, 128.3, 127.2, 104.4, 55.3, 40.7, 29.6, 25.8, 24.8; FT IR: 1711, 1372, 1358, 1173, 1125, 966, 769, 758 cm^{-1}; mp 123–126 °C; LRMS (ESI) *m/z* 321.2 $[M + H]^+$.

3-Benzyl-1-(methylsulfonyl)-4-(3-(trifluoromethyl)phenyl)-1H-imidazol-2(3H)-one (2q)



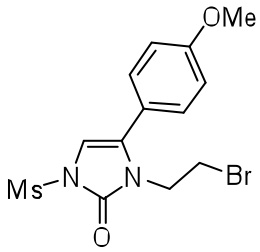
2q: (93% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.71–7.65 (m, 1H), 7.52 (t, J = 7.77 Hz, 1H), 7.44 (s, 1H), 7.42–7.38 (m, 1H), 7.31–7.25 (m, 3H), 7.09–7.03 (m, 2H), 6.78 (s, 1H), 4.84 (s, 2H), 3.55 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 151.0, 135.9, 132.0, 131.3 (q, J = 32.9 Hz), 129.5, 128.8, 128.6, 128.0, 127.2, 126.1 (q, J = 3.7 Hz), 125.8, 125.7 (q, J = 3.8 Hz), 123.4 (q, J = 272.6 Hz), 105.5, 45.8, 40.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -63.2; FT IR: 1724, 1354, 1327, 1283, 1165, 1093, 1073, 974, 761, 725 cm^{-1}; mp 99–101 ^{o}C; LRMS (ESI) *m/z* 397.2 $[M + H]^+$.

3-(3-Chloropropyl)-1-(methylsulfonyl)-4-(p-tolyl)-1H-imidazol-2(3H)-one (2r)



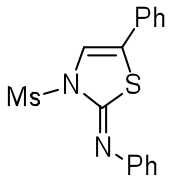
2r: (90% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.31–7.22 (m, 4H), 6.65 (s, 1H), 3.86–3.81 (m, 2H), 3.51–3.46 (m, 5H), 2.43 (s, 3H), 2.06 (qd, J = 12.92, 6.37 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 150.7, 139.8, 129.8, 128.5, 126.9, 124.5, 104.3, 41.8, 40.8, 39.8, 31.4, 21.3; FT IR: 1706, 1382, 1354, 1297, 1170, 1147, 1097, 1009, 977, 824, 772, 723 cm^{-1}; mp 142–143 ^{o}C; LRMS (ESI) *m/z* 329.2 $[M + H]^+$.

3-(2-Bromoethyl)-4-(4-methoxyphenyl)-1-(methylsulfonyl)-1H-imidazol-2(3H)-one (2s)



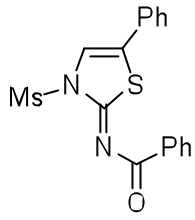
2s: (92% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.33–7.26 (m, 2H), 7.04–6.96 (m, 2H), 6.63 (s, 1H), 4.03 (t, J = 6.89 Hz, 2H), 3.88 (s, 3H), 3.49 (s, 3H), 3.46 (t, J =6.90 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 160.6, 150.5, 130.3, 126.4, 119.4, 114.6, 104.5, 55.4, 43.0, 40.1, 27.8; FT IR: 1712, 1348, 1256, 1212, 1161, 1081, 834, 767, 733 cm^{-1}; mp 128–130 °C; LRMS (ESI) *m/z* 375.1, 377.1 $[M + H]^+$.

(Z)-N-(3-(Methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)aniline (3a)



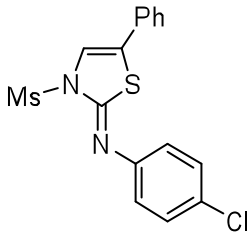
3a: (87% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.43–7.28 (m, 8H), 7.20–7.14 (m, 1H), 7.13–7.07 (m, 2H), 3.66 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 152.8, 149.6, 130.3, 129.6, 129.0, 128.5, 125.2, 124.8, 120.8, 117.8, 116.6, 41.0; FT IR: 1621, 1587, 1364, 1354, 1162, 1119, 958, 829, 748 cm^{-1}; mp 102–104 ^{o}C; LRMS (ESI) *m/z* 331.2 $[M + H]^+$.

(Z)-N-(3-(methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)benzamide (3b)



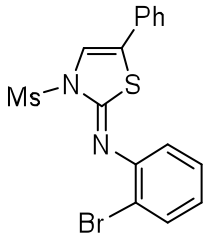
3b: (91% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.37–8.28 (m, 2H), 7.67 (s, 1H), 7.59–7.54 (m, 1H), 7.53–7.46 (m, 4H), 7.46–7.36 (m, 3H), 3.80 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 174.3, 165.9, 135.4, 132.7, 129.9, 129.7, 129.3, 129.1, 128.4, 125.9, 125.2, 115.6, 41.6; FT IR: 1609, 1573, 1464, 1368, 1328, 1231, 1175, 1152, 971, 881, 751 cm^{-1}; mp 163 ^{o}C (dec.); LRMS (ESI) *m/z* 359.2 $[M + H]^+$.

(Z)-4-chloro-N-(3-(methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)aniline (3c)



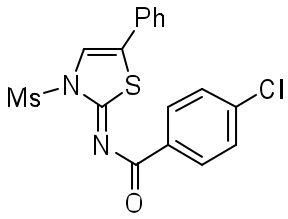
3c: (51% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.39–7.28 (m, 8H), 7.06–7.01 (m, 2H), 3.64 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 153.9, 148.5, 130.6, 130.4, 130.1, 129.5, 129.1, 125.7, 122.7, 118.4, 117.2, 41.5; mp 144–145 ^{o}C; LRMS (ESI) *m/z* 365.3 $[M + H]^{+}$.

(Z)-2-bromo-N-(3-(methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)aniline (3d)



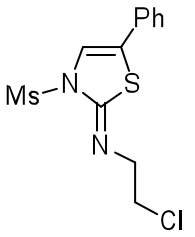
3d: (95% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.68 (dd, J = 8.02, 1.28 Hz, 1H), 7.40 (s, 1H), 7.40–7.30 (m, 6H), 7.20 (dd, J = 7.90, 1.49 Hz, 1H), 7.06 (dt, J = 7.94, 1.55 Hz, 1H), 3.81 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 154.4, 148.1, 133.3, 130.1, 129.0, 128.7, 128.6, 126.0, 125.2, 121.0, 118.1, 117.1, 117.0, 41.3; FT IR: 1620, 1574, 1469, 1364, 1162, 1117, 1028, 973, 961, 827, 745 cm^{-1}; mp 145–146 ^{o}C; LRMS (ESI) *m/z* 409.2, 411.2 $[M + H]^{+}$.

(Z)-4-chloro-N-(3-(methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)benzamide (3e)



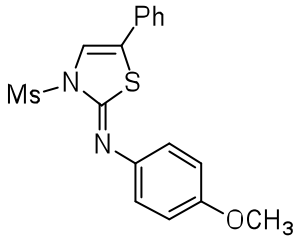
3e: (82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.26–8.22 (m, 2H), 7.67 (s, 1H), 7.52–7.48 (m, 2H), 7.47–7.37 (m, 5H), 3.78 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 173.3, 166.2, 139.0, 134.0, 131.0, 129.8, 129.3, 129.2, 128.7, 125.9, 125.4, 115.7, 41.7; FT IR: 1606, 1591, 1490, 1471, 1333, 1230, 1175, 1143, 960, 879 754 cm^{-1}; mp 180 ^{o}C (dec.); LRMS (ESI) *m/z* 393.2 $[M + H]^{+}$.

(Z)-2-chloro-N-(3-(methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)ethanamine (3f)



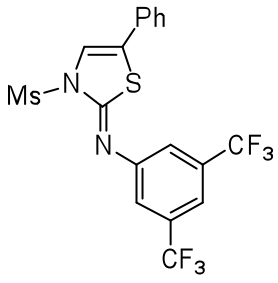
3f: (59% yield, 35% of triazole recovered); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.40–7.30 (m, 5H), 7.29 (s, 1H), 3.84 (t, J = 5.94 Hz, 2H), 3.57–3.53 (m, 5H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 153.1, 130.4, 129.0, 128.4, 125.1, 117.7, 117.0, 56.8, 44.5, 40.7; mp 100–102 ^{o}C; LRMS (ESI) *m/z* 317.1 $[M + H]^+$.

(Z)-4-methoxy-N-(3-(methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)aniline (3g)



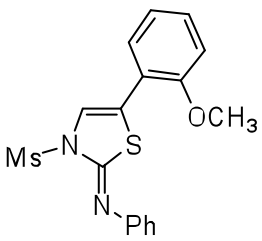
3g: (48% yield, 49% of triazole recovered); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.39–7.27 (m, 6H), 7.07–7.02 (m, 2H), 6.96–6.91 (m, 2H), 3.82 (s, 3H), 3.64 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 156.7, 152.1, 142.8, 130.4, 129.0, 128.4, 125.2, 121.9, 117.7, 116.6, 114.7, 55.4, 41.0; FT IR: 1624, 1593, 1501, 1356, 1239, 1159, 1116, 956, 821, 748 cm^{-1}; mp 129–130 ^{o}C; LRMS (ESI) *m/z* 361.2 $[M + H]^+$.

(Z)-N-(3-(methylsulfonyl)-5-phenylthiazol-2(3H)-ylidene)-3,5-bis(trifluoromethyl)aniline (3h)



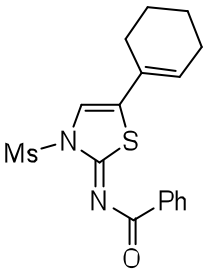
3h: (96% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.66 (s, 1H), 7.56 (s, 2H), 7.41–7.30 (m, 6H), 3.67 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 155.5, 150.6, 133.0 (q, J = 33.4 Hz), 129.6, 129.3, 128.9, 125.4, 123.1 (q, J = 272.8 Hz), 121.6, 118.2, 118.0 (septet, J = 3.8 Hz), 117.0, 41.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -63.2; FT IR: 1628, 1590, 1378, 1361, 1268, 1167, 1120, 949, 890, 749 cm^{-1}; mp 145–146 ^{o}C; LRMS (ESI) *m/z* 467.1 $[M + H]^+$.

(Z)-N-(5-(2-Methoxyphenyl)-3-(methylsulfonyl)thiazol-2(3H)-ylidene)aniline (3i)



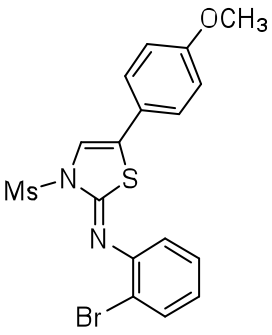
3i: (70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.70 (s, 1H), 7.45–7.39 (m, 2H), 7.32–7.26 (m, 1H), 7.21–7.11 (m, 4H), 6.99–6.92 (m, 2H), 3.93 (s, 3H), 3.68 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 156.3, 152.9, 149.7, 129.5, 129.1, 128.0, 124.5, 120.9, 120.9, 120.1, 119.1, 114.0, 111.1, 55.5, 40.9; FT IR: 1621, 1583, 1493, 1359, 1301, 1251, 1173, 1130, 1116, 1016, 972, 833, 753 cm^{-1}; mp 120–121 ^{o}C; LRMS (ESI) *m/z* 361.2 $[M + H]^+$.

(Z)-N-(5-(cyclohex-1-en-1-yl)-3-(methylsulfonyl)thiazol-2(3H)-ylidene)benzamide (3j)



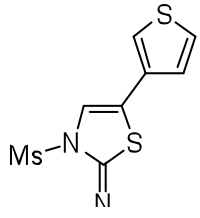
3j: (45% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 8.34–8.24 (m, 2H), 7.58–7.51 (m, 1H), 7.51–7.45 (m, 2H), 7.23 (s, 1H), 6.07 (t, J = 3.84 Hz, 1H), 3.74 (s, 3H), 2.32-2.18 (m, 4H), 1.80-1.62 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 174.2, 165.6, 135.6, 132.6, 129.6, 128.5, 128.4, 127.8, 127.0, 114.0, 41.6, 26.0, 25.7, 22.1, 21.8; mp 168 ^{o}C (dec.); LRMS (ESI) *m/z* 363.2 $[M + H]^+$.

(Z)-2-bromo-N-(5-(4-methoxyphenyl)-3-(methylsulfonyl)thiazol-2(3H)-ylidene)aniline (3k)



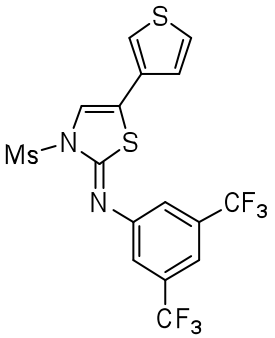
3k: (97% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.66 (dd, J = 8.01, 1.27 Hz, 1H), 7.36 (dt, J = 7.72, 1.32 Hz, 1H), 7.27–7.23 (m, 3H), 7.19 (dd, J = 7.90, 1.49 Hz, 1H), 7.05 (dt, J = 7.82, 1.52 Hz, 1H), 6.91–6.88 (m, 2H), 3.83 (s, 3H), 3.79 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 159.9, 154.6, 148.2, 133.3, 128.7, 126.7, 125.9, 122.6, 121.1, 118.0, 117.1, 115.6, 114.5, 55.4, 41.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -63.2; FT IR: 1627, 1608, 1576, 1509, 1461, 1359, 1289, 1249, 1163, 1127, 1117, 1030, 972, 962, 816, 824 cm^{-1}; mp 131–132 ^{o}C; LRMS (ESI) *m/z* 439.1, 441.0 $[M + H]^+$.

(Z)-N-(3-(methylsulfonyl)-5-(thiophen-3-yl)thiazol-2(3H)-ylidene)aniline (3l)



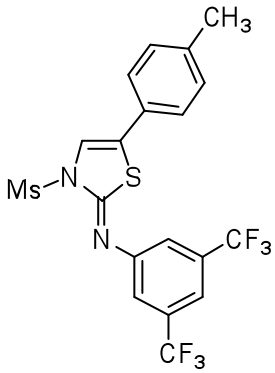
3l: (64% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.45–7.39 (m, 2H), 7.37 (dd, J = 5.02, 2.91 Hz, 1H), 7.27 (s, 1H), 7.22–7.17 (m, 1H), 7.16 (dd, J = 5.03, 0.85 Hz, 1H), 7.13–7.09 (m, 3H), 3.66 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 152.5, 149.6, 131.2, 129.6, 127.2, 124.8, 124.4, 121.2, 120.8, 116.6, 113.4, 40.9; FT IR: 1634, 1610, 1582, 1353, 1162, 1119, 955, 754, 698 cm^{-1}; mp 118–119 ^{o}C; LRMS (ESI) *m/z* 337.1 $[M + H]^+$.

(Z)-N-(3-(methylsulfonyl)-5-(thiophen-3-yl)thiazol-2(3H)-ylidene)-3,5-bis(trifluoromethyl) aniline (3m)



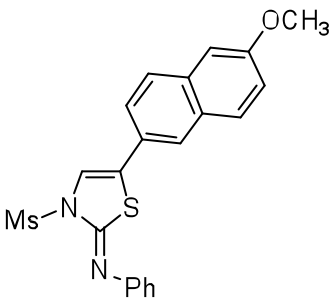
3m: (92% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.65 (s, 1H), 7.54 (s, 2H), 7.38 (dd, J = 5.08, 2.94 Hz, 1H), 7.29 (s, 1H), 7.16 (dd, J = 2.90, 1.21 Hz, 1H), 7.14 (dd, J = 5.06, 1.35 Hz, 1H), 3.65 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 155.2, 150.6, 133.0 (q, J = 33.3 Hz), 130.5, 127.5, 124.5, 123.1 (q, J = 273.0 Hz), 121.9, 121.5, 118.1 (q, J = 3.7 Hz), 116.9, 113.7, 41.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -63.2; FT IR: 1630, 1596, 1379, 1360, 1277, 1264, 1166, 1118, 962, 951 cm^{-1}mp 156–157 ^{o}C; LRMS (ESI) *m/z* 473.0 $[M + H]^+$.

(Z)-N-(3-(Methylsulfonyl)-5-(*p*-tolyl)thiazol-2(3H)-ylidene)-3,5-bis(trifluoromethyl)aniline (3n)



3n: (99% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.67 (s, 1H), 7.58 (s, 2H), 7.37 (s, 1H), 7.26–7.18 (m, 4H), 3.68 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 155.6, 150.7, 139.1, 133.0 (q, J = 33.36 Hz), 129.8, 126.8, 125.3, 123.1 (q, J = 272.84 Hz), 121.6 (q, J = 2.74 Hz), 118.3, 118.0 (septet, J = 3.43 Hz), 116.3, 41.2, 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -63.2; mp 152–153 ^{o}C; LRMS (ESI) *m/z* 481.1 $[M + H]^+$.

(Z)-N-(5-(6-methoxynaphthalen-2-yl)-3-(methylsulfonyl)thiazol-2(3H)-ylidene)aniline (3o)



3o: (50% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 7.72 (d, J = 8.62 Hz, 1H), 7.67 (d, J = 8.96 Hz, 1H), 7.56 (s, 1H), 7.50–7.41 (m, 4H), 7.24–7.11 (m, 5H), 3.94 (s, 3H), 3.69 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 158.3, 152.8, 149.7, 134.3, 129.6, 129.4, 128.6, 127.6, 125.4, 124.8, 124.4, 122.9, 120.9, 119.7, 118.2, 116.3, 105.9, 55.3, 41.0; mp 147–148 ^{o}C; LRMS (ESI) *m/z* 411.1 $[M + H]^+$.

Desulfonylation of N-mesyl-substituted products 2 and 3

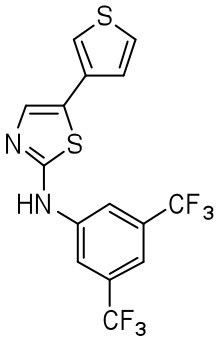
Method A.[7] A mixture of 0.094g (0.3 mmol) of 1-(methylsulfonyl)-3,4-diphenyl-1H-imidazol-2(3H)-one **2b** and 0.037g (1.5 mmol) of Mg (turnings) in 5 mL of methanol was heated to 65-70 °C in a sealed vial for 12 h, until the reaction was judged complete by LCMS and TLC analysis. The reaction mixture was poured into 5 mL of 1N HCl and extracted with DCM (2x50 mL). Organic layer were washed with $NaHCO_3$ (saturated solution) and brine, dried over Na_2SO_4. After removal of solvents the residue was purified by column chromatography on silica gel (EtOAc as an eluent) to afford 0.056 g (0.24 mmol, 79%) of 1,5-diphenyl-1H-imidazol-2(3H)-one **10** as a white solid with mp 233–235 °C (228–230 °C lit.). ^{1}H and ^{13}C NMR data were identical to those reported in literature.[8]

Method B. To a stirred solution of (Z)-N-(3-(methylsulfonyl)-5-(thiophen-3-yl)thiazol-2(3H)-ylidene)-3,5-bis(trifluoromethyl)aniline **3m** (0.142 g; 0.3 mmol) in a mixture of methanol (1 mL) and DCM (1 mL) HOBt (0.122g; 0.9 mmol) was added. The resulting mixture was stirred for 6h until judged complete by LCMS and TLC analysis. Column chromatography of the reaction mixture (silica gel, 20% EtOAc in hexanes) afforded 0.115g (98%) of compound **11** as a white solid.

N-(3,5-bis(trifluoromethyl)phenyl)-5-(thiophen-3-yl)thiazol-2-amine (11)

(7) Yoo, E. J.; Ahlquist, M.; Kim, S. H.; Bae, I.; Fokin, V.V.; Sharpless, K. B.; Chang, S. *Angew. Chem. Int. Ed.* **2007**, *46*, 1730.

(8) Lee, S. H.; Yoshida, K.; Matsushita, H.; Clapham, B.; Koch, G.; Zimmermann, J.; Janda, K. D. *J. Org. Chem.* **2004**, *69*, 8829.



11: (98% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ppm 11.01 (s, 1H), 8.32 (s, 2H), 7.71 (s, 1H), 7.66–7.62 (m, 1H), 7.62–7.59 (m, 1H), 7.58 (s, 1H), 7.44 (dd, J = 4.98, 1.35 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 160.7, 142.4, 135.1, 131.6, 130.8 (q, J = 32.6 Hz), 127.4, 125.6, 123.9, 123.2 (q, J = 272.8 Hz), 120.3, 116.2, 113.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ ppm -61.5; FT IR: 2938, 1597, 1477, 1382, 1270, 1160, 1112, 998, 964, 767 cm^{-1}; mp 179–180 ^{o}C; LRMS (ESI) *m/z* 395.1 $[M + H]^{+}$.

X-Ray crystallography analysis of 2a and 3a

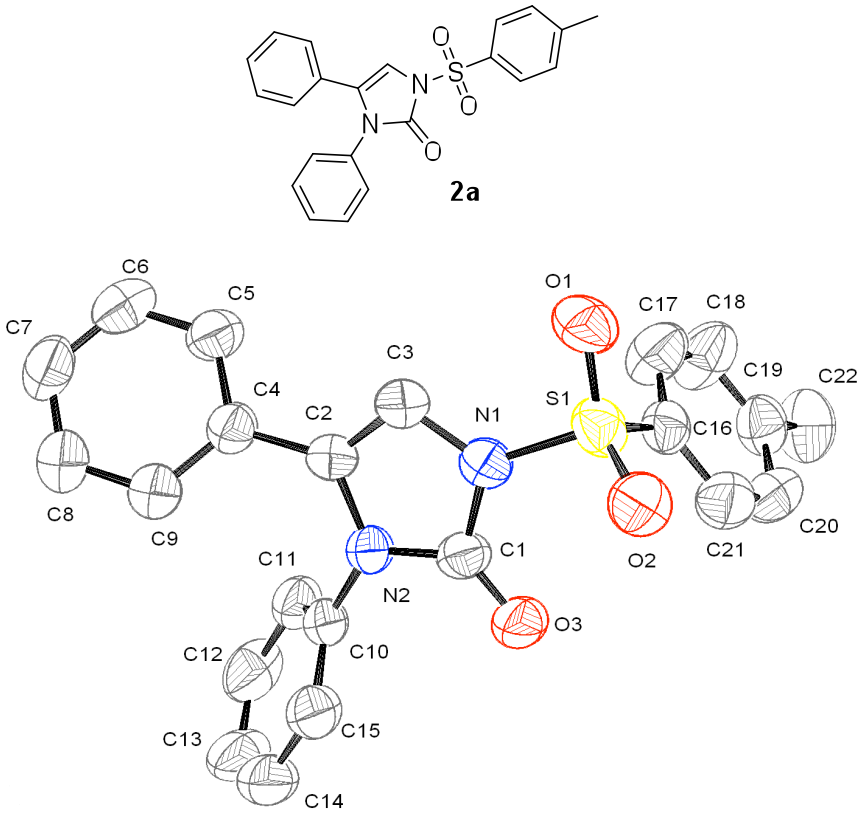


Figure 2. Crystal structure of compound **2a** (CCDC 888986).

Table 2. Crystal data and structure refinement for **2a**.

Empirical formula	C23.50 H21 N2 O4 S
Formula weight	427.48

Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 21.68(5) Å	α= 90°.
	b = 5.975(14) Å	β= 91.72(6)°.
	c = 31.44(7) Å	γ = 90°.
Volume	4070(16) $Å^3$	
Z	8	
Density (calculated)	1.395 Mg/m^3	
Absorption coefficient	0.194 mm^{-1}	
F(000)	1792	
Crystal size	0.45 x 0.10 x 0.05 mm^3	
Theta range for data collection	1.30 to 25.74°.	
Index ranges	-26<=h<=26, -7<=k<=7, -37<=l<=38	
Reflections collected	20923	
Independent reflections	3759 [R(int) = 0.0999]	
Completeness to theta = 25.00°	98.8 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9904 and 0.9180	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3759 / 0 / 255	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0745, wR2 = 0.1753	
R indices (all data)	R1 = 0.1507, wR2 = 0.2027	
Extinction coefficient	0.0013(3)	
Largest diff. peak and hole	0.206 and -0.241 $e.Å^{-3}$	

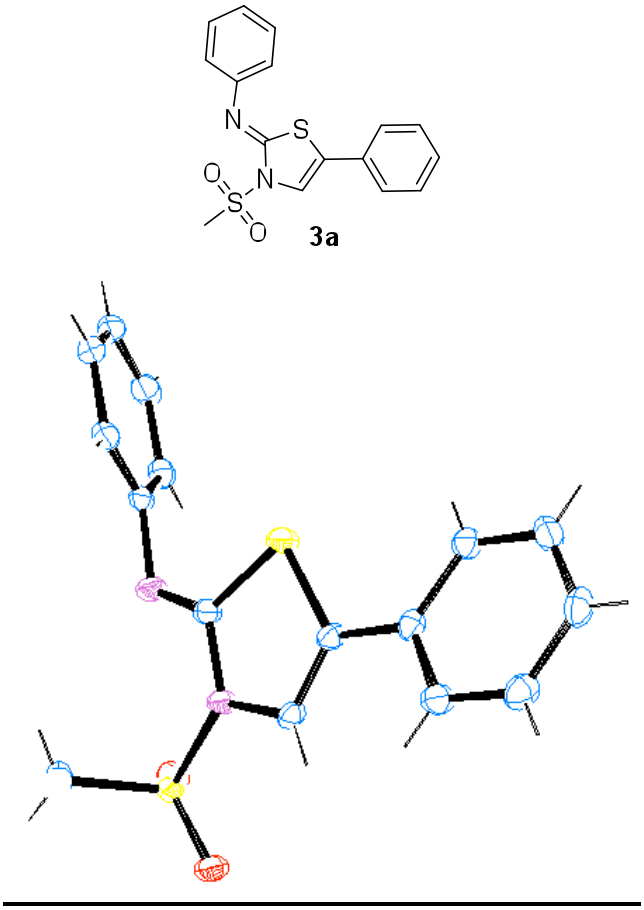
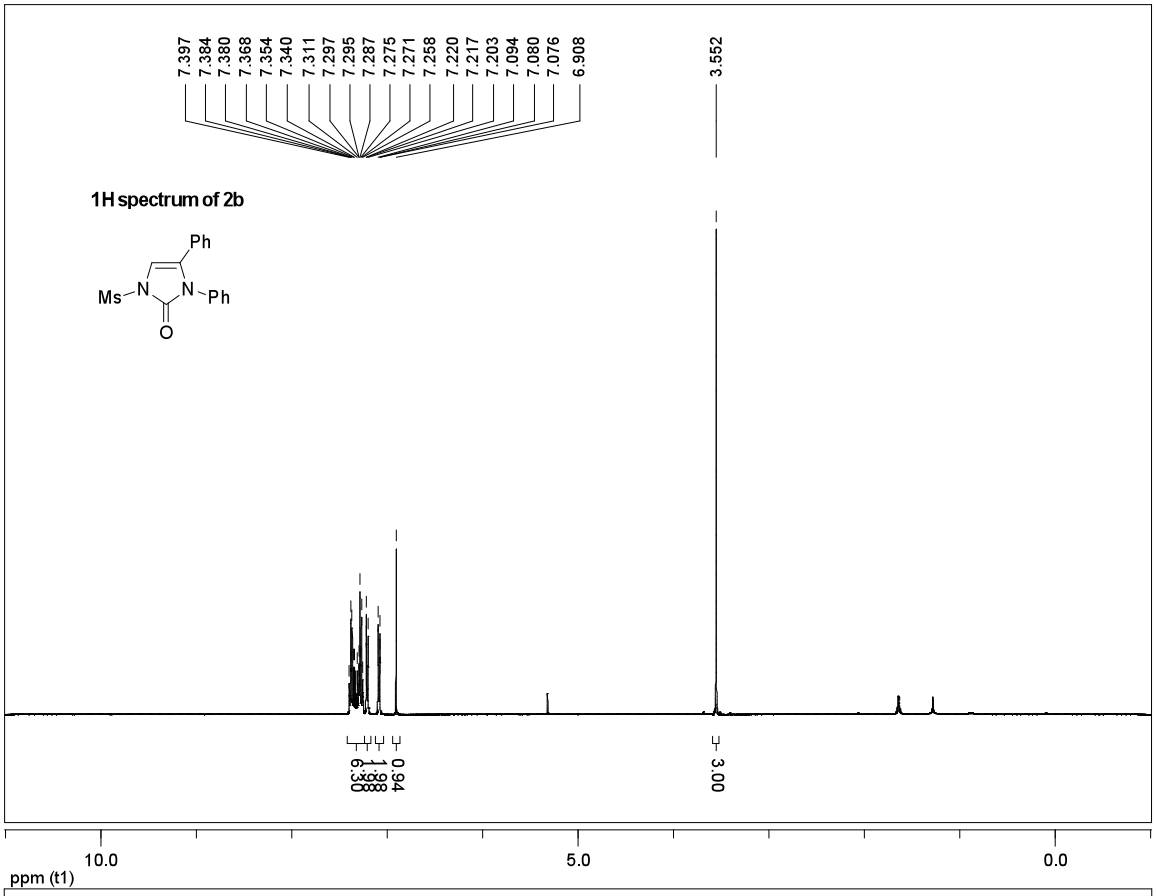


Figure 3. Crystal structure of compound **3a** (CCDC 888987).

Table 3. Crystal data and structure refinement for **3a**.

Empirical formula	C16 H14 N2 O2 S2	
Formula weight	330.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.2840(9) Å	α= 90°
	b = 8.3762(8) Å	β= 93.5250(10)°
	c = 32.860(3) Å	γ = 90°
Volume	3099.9(5) $Å^3$	
Z	8	
Density (calculated)	1.416 g/cm^3	
Absorption coefficient	0.351 mm^{-1}	

F(000)	1376
Crystal size	0.28 x 0.22 x 0.10 mm^3
Theta range for data collection	2.13 to 25.45°
Index ranges	-13<=h<=13, -8<=k<=10, -39<=l<=39
Reflections collected	24909
Independent reflections	5690 [R(int) = 0.0359]
Completeness to theta = 25.00°	99.6 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9657 and 0.9081
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5690 / 0 / 397
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R1 = 0.0309, wR2 = 0.0855
R indices (all data)	R1 = 0.0419, wR2 = 0.0917
Largest diff. peak and hole	0.302 and -0.328 e $Å^{-3}$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7.384
7.380
7.368
7.354
7.340
7.311
7.297
7.295
7.287
7.275
7.271
7.258
7.220
7.217
7.203
7.094
7.080
7.076
6.908
3.552
1H spectrum of 2b
Ph
Ms
N
N
Ph
O
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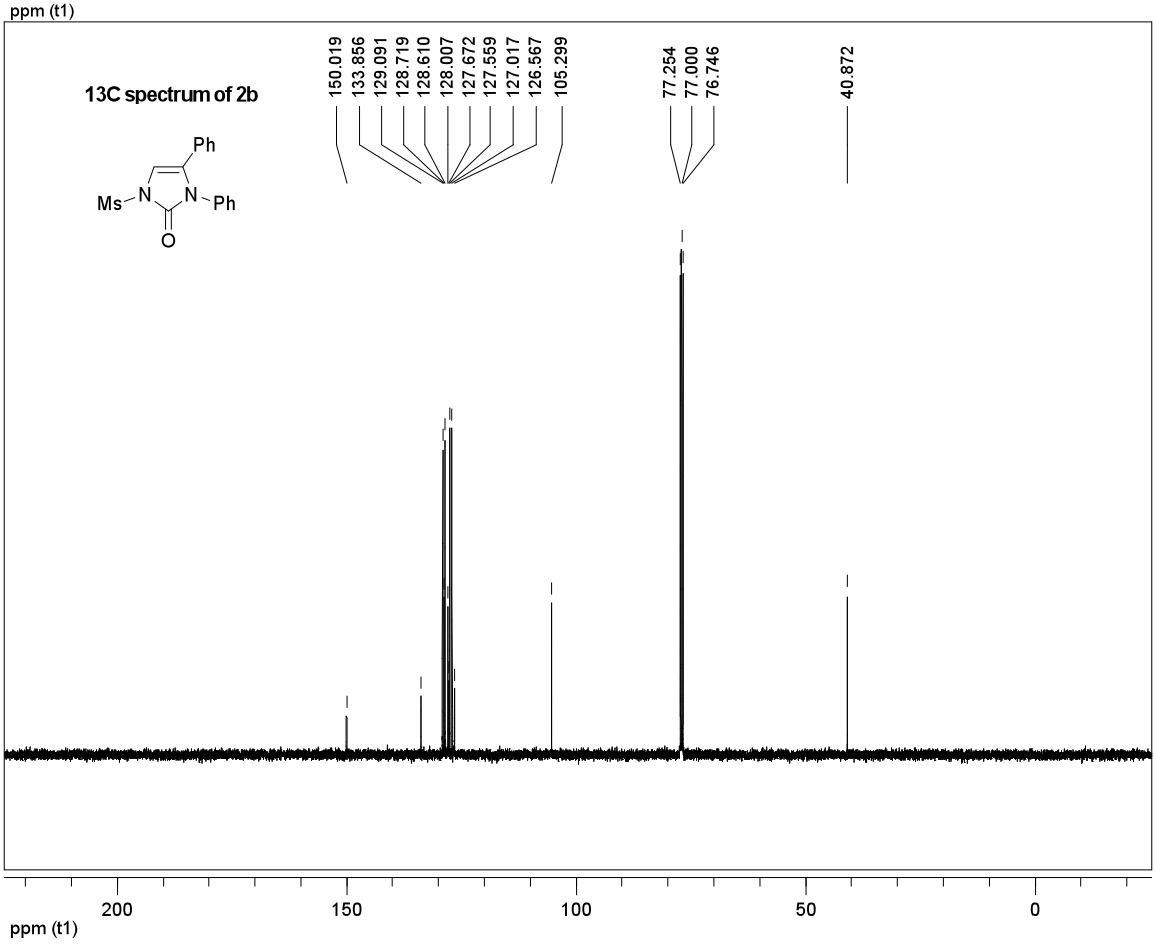
1.88
1.88
1.88
0.94
3.00
10.0
5.0
0.0
ppm (t1)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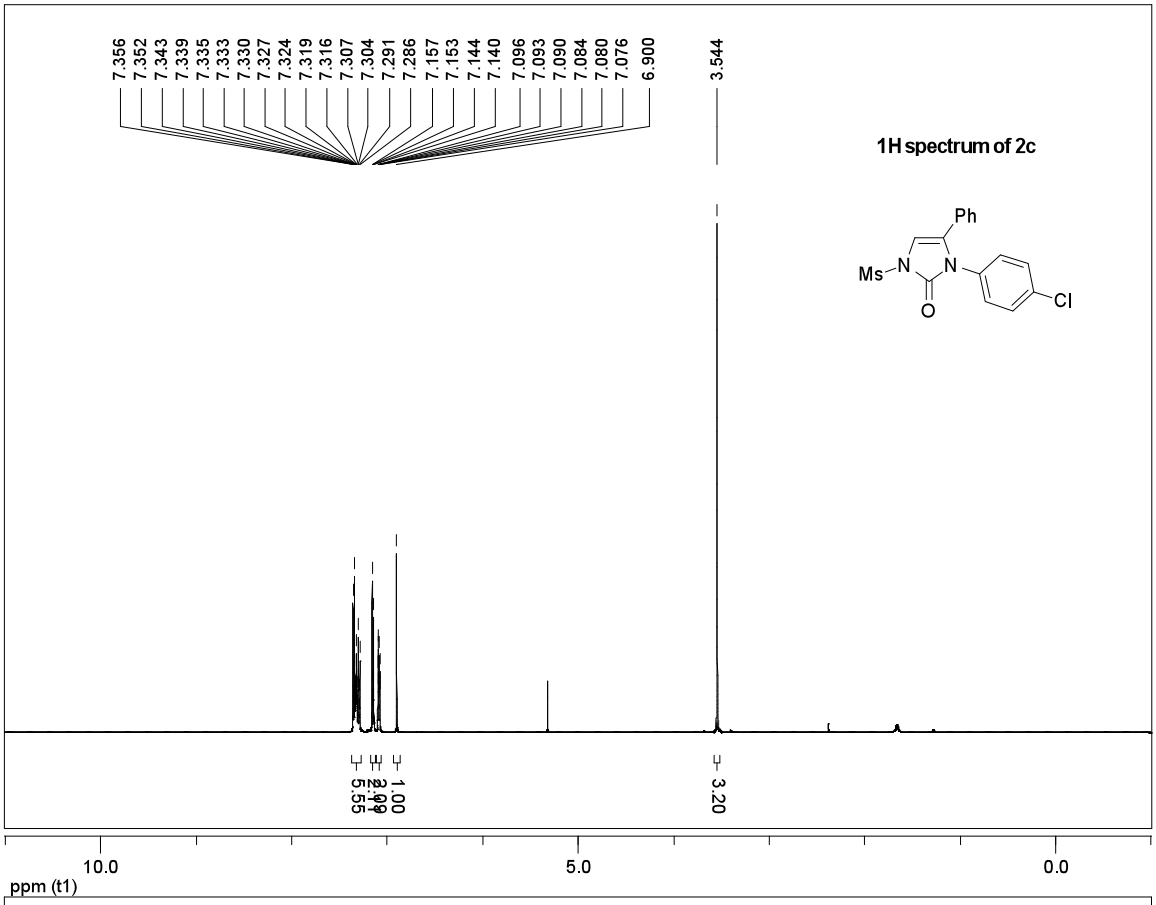
129.091
128.719
128.610
128.007
127.672
127.559
127.017
126.567
105.299
77.254
77.000
76.746
40.872
13C spectrum of 2b
Ph
Ms
N
N
Ph
O
200
150
100
50
0
ppm (t1)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7.335
7.333
7.330
7.327
7.324
7.319
7.316
7.307
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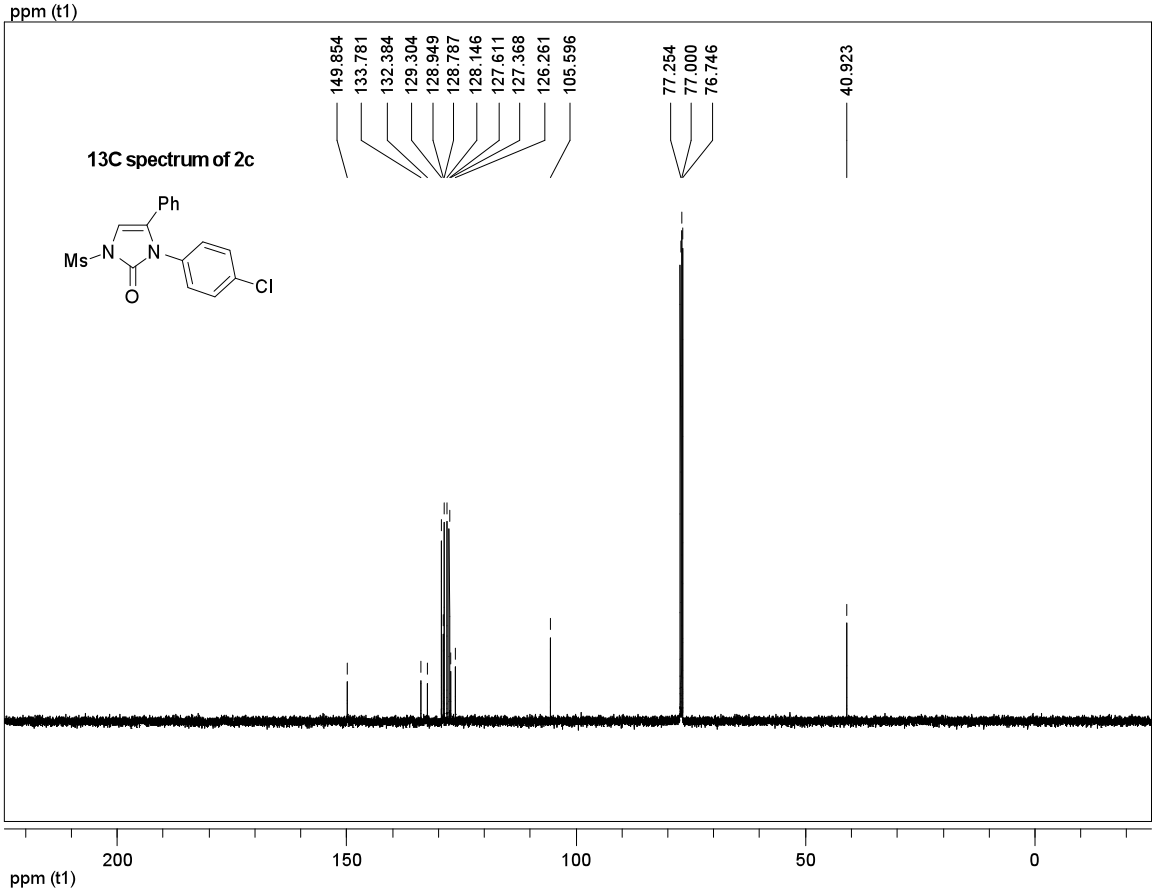
7.291
7.286
7.157
7.153
7.144
7.140
7.096
7.093
7.090
7.084
7.080
7.076
6.900
3.544
1H spectrum of 2c
Ph
Ms
N
N
O
Cl
9.55
2.09
2.09
1.00
3.20
10.0
5.0
0.0
ppm (t1)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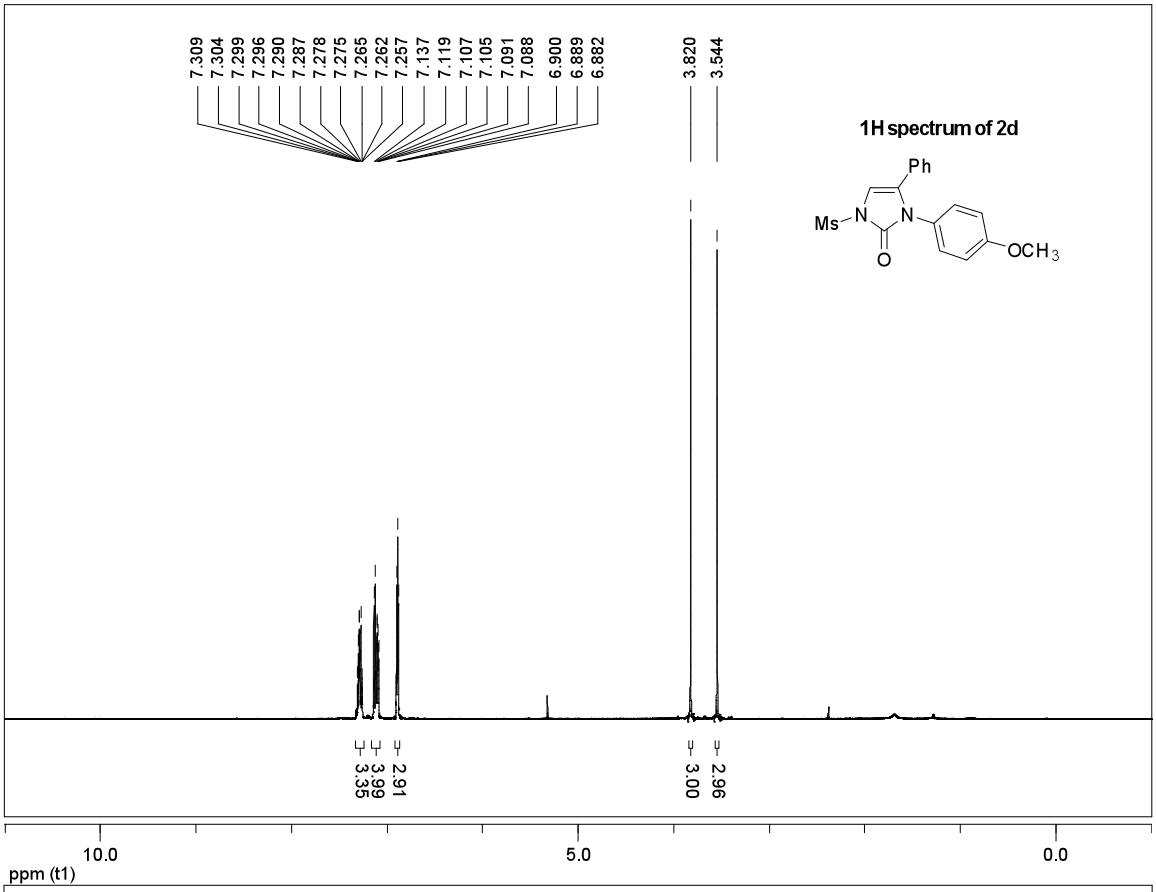
129.304
128.949
128.787
128.146
127.611
127.368
126.261
105.596
77.254
77.000
76.746
40.923
13C spectrum of 2c
Ph
Ms
N
N
O
Cl
200
150
100
50
0
ppm (t1)


7.309
7.304
7.299
7.296
7.290
7.287
7.278
7.275
7.265
7.262
7.257
7.137
7.119
7.107
7.105
7.091
7.088
6.900
6.889
6.882
3.820
3.544
1H spectrum of 2d
Ph
Ms
N
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O
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3.00
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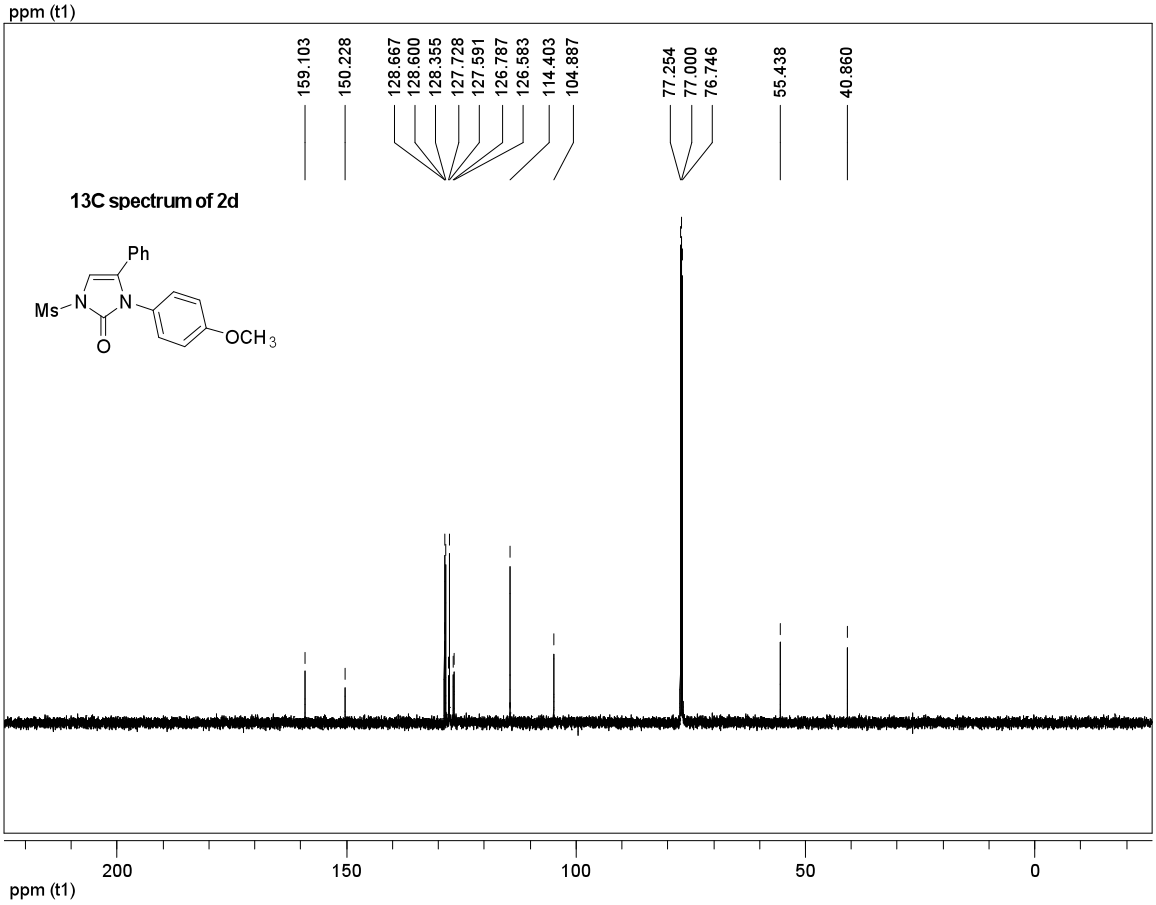
10.0
5.0
0.0
ppm (t1)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128.600
128.355
127.728
127.591
126.787
126.583
114.403
104.887
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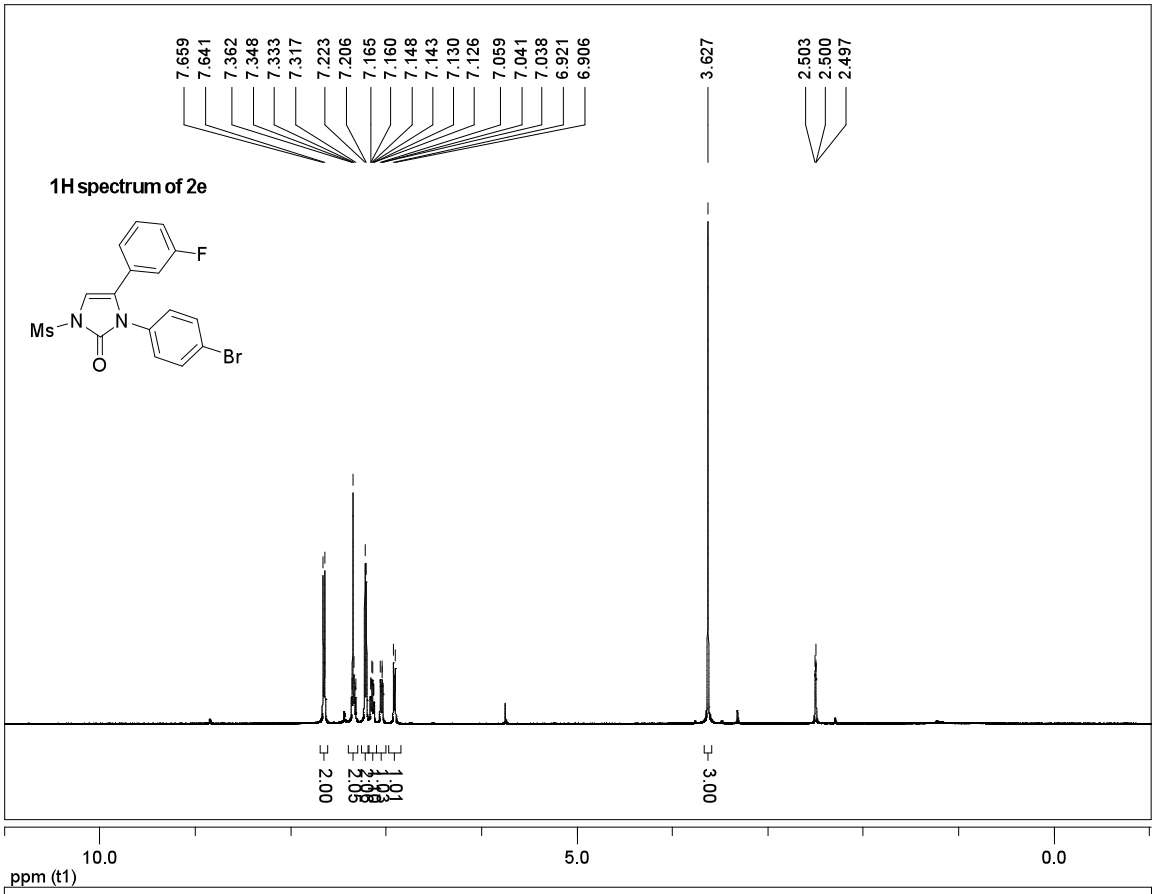
77.000
76.746
55.438
40.860
13C spectrum of 2d
Ph
Ms
N
N
O
OCH3
200
150
100
50
0
ppm (t1)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7.206
7.165
7.160
7.148
7.143
7.130
7.126
7.059
7.041
7.038
6.921
6.906
3.627
2.503
2.500
2.497
1H spectrum of 2e
F
Ms
N
N
O
Br
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3.00
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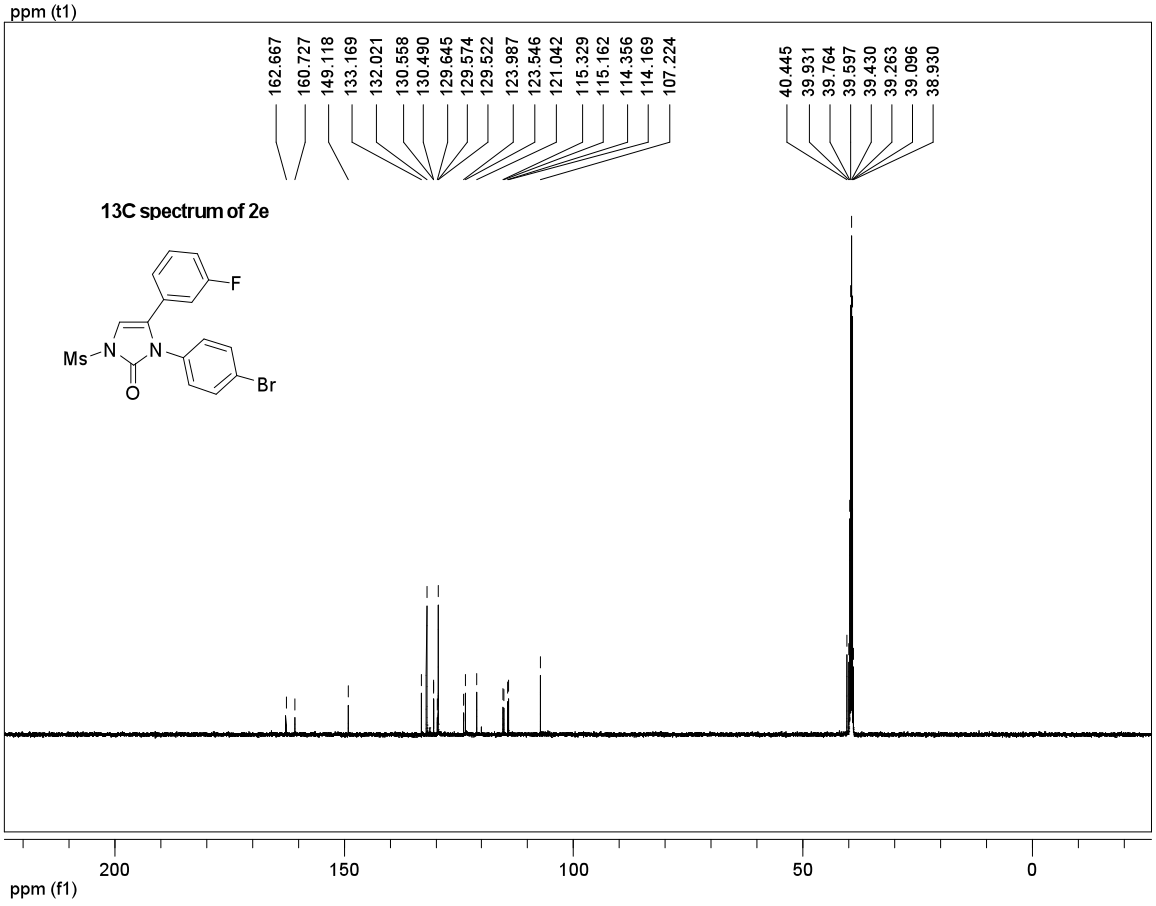
5.0
0.0
ppm (t1)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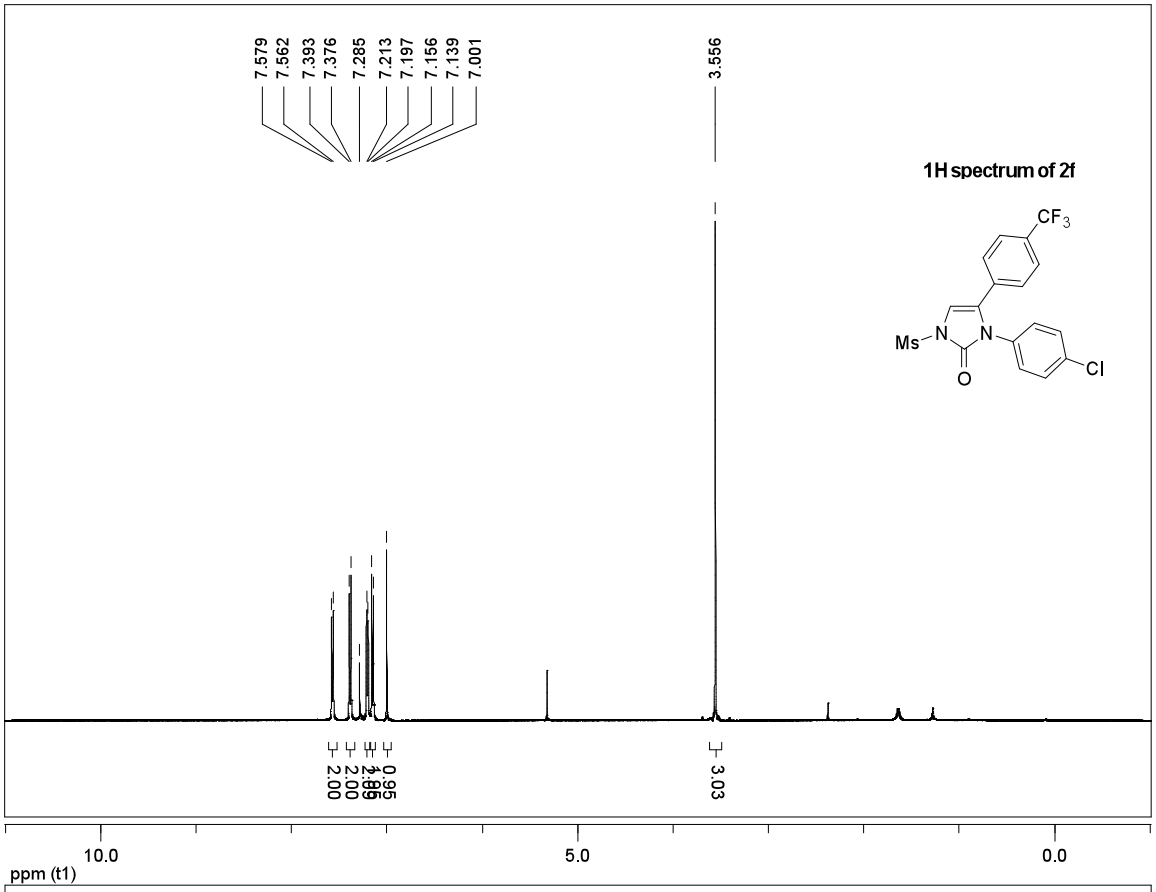
133.169
132.021
130.558
130.490
129.645
129.574
129.522
123.987
123.546
121.042
115.329
115.162
114.356
114.169
107.224
40.445
39.931
39.764
39.597
39.430
39.263
39.096
38.930
13C spectrum of 2e
F
Ms
N
N
O
Br
200
150
100
50
0
ppm (f1)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7.285
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7.156
7.139
7.001
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CF3
Ms
N
N
O
Cl
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2.00
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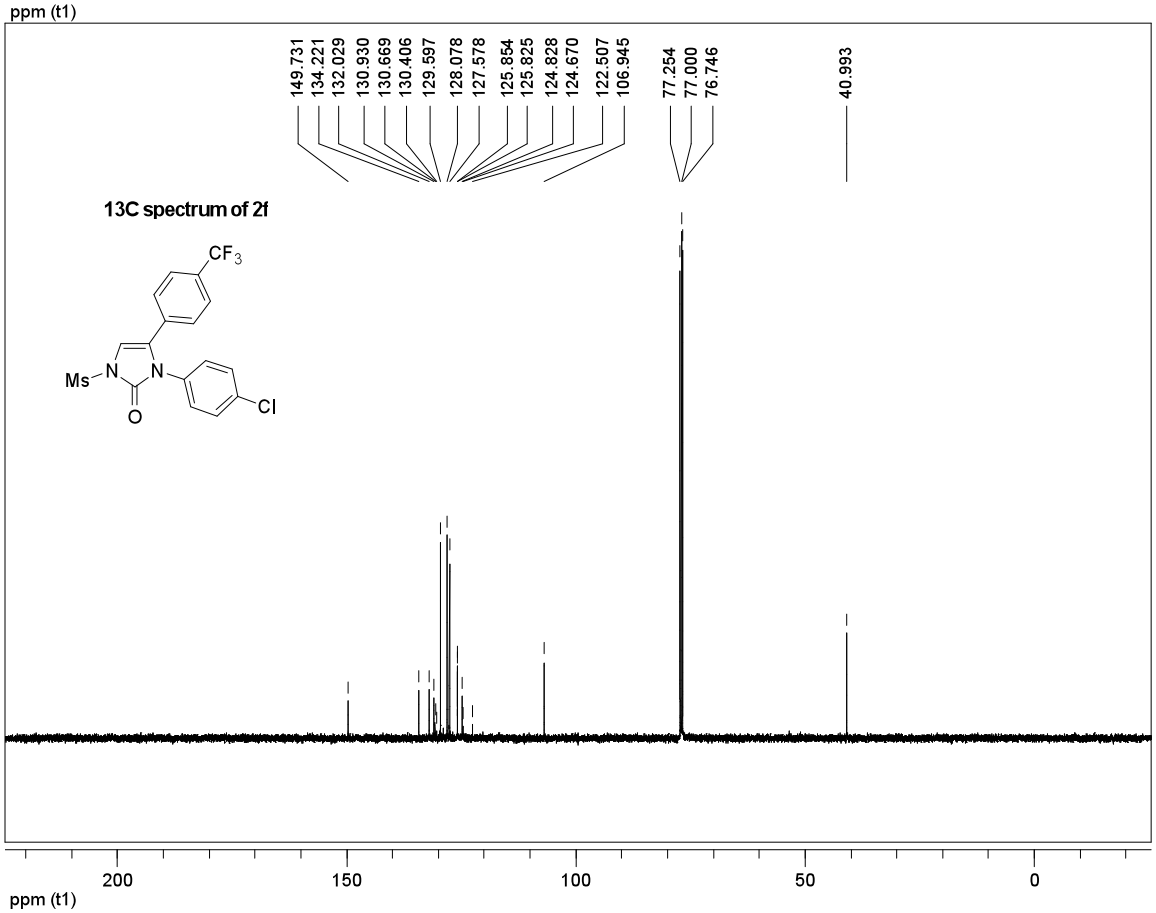
0.95
3.03
10.0
5.0
0.0
ppm (t1)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122.507
106.945
77.254
77.000
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13C spectrum of 2f
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Ms
N
N
O
Cl
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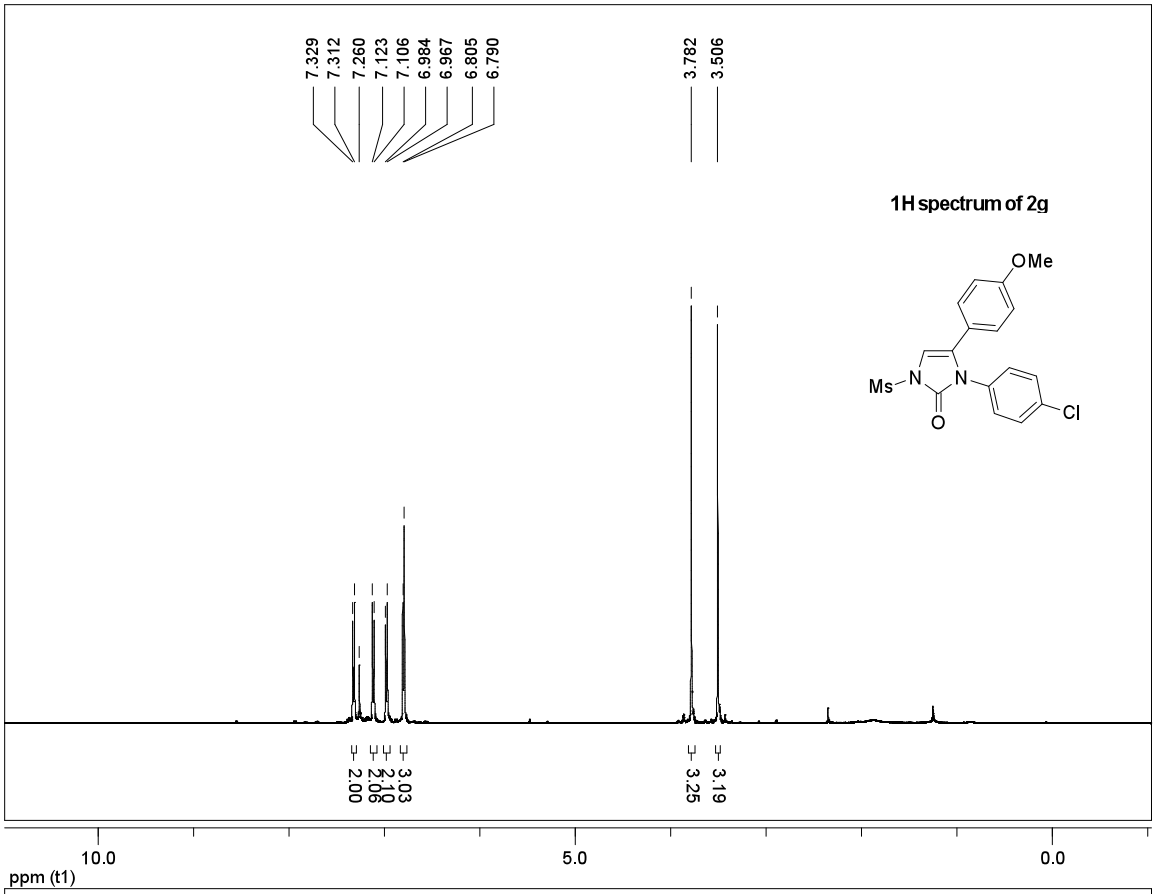
150
100
50
0
ppm (t1)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OMe
Ms
N
N
O
Cl
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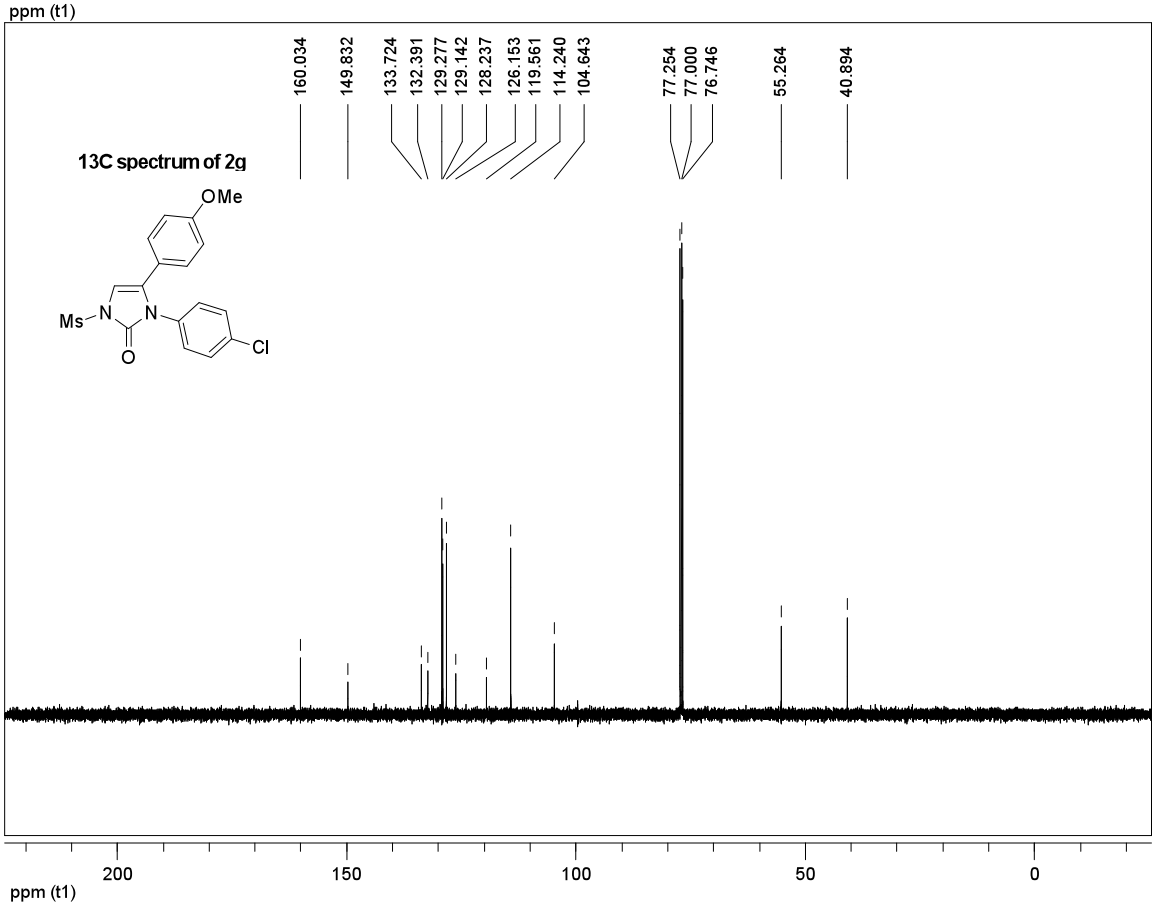
2.06
2.10
3.03
3.25
3.19
10.0
5.0
0.0
ppm (t1)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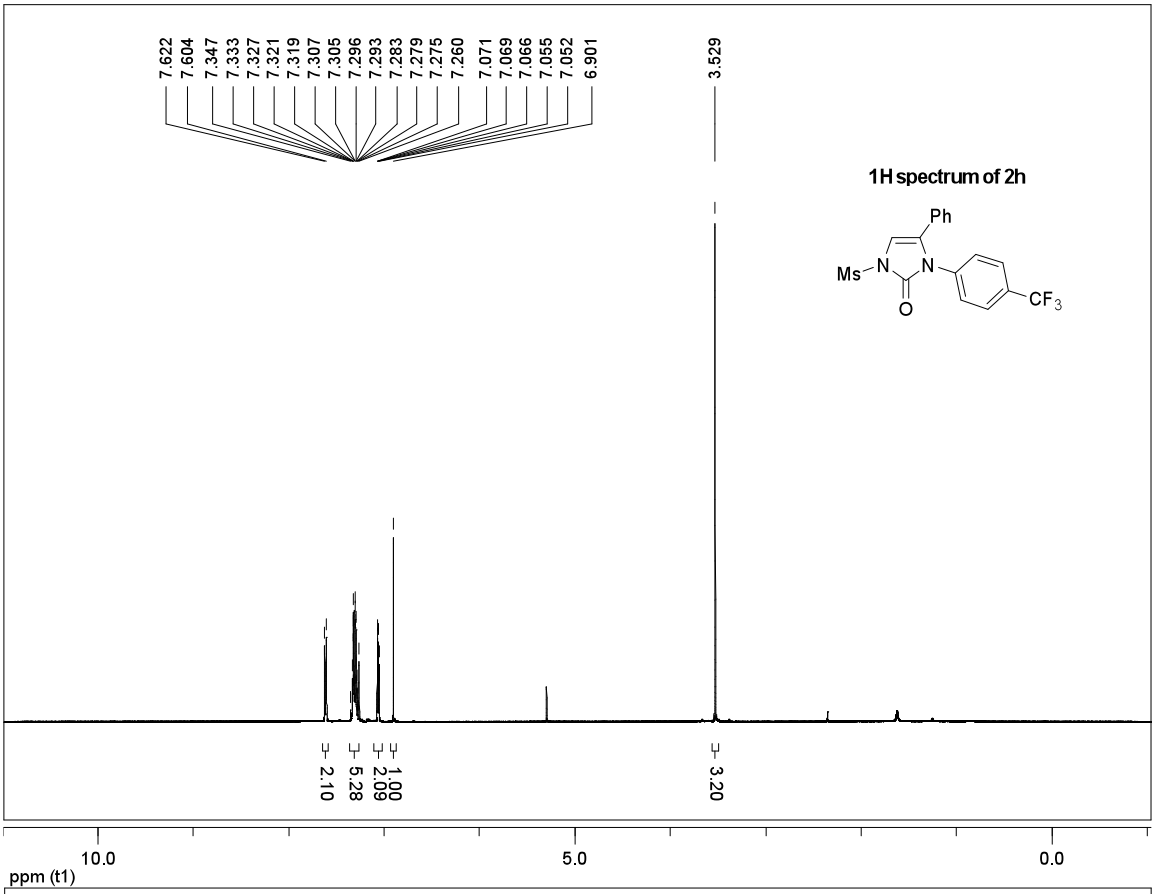
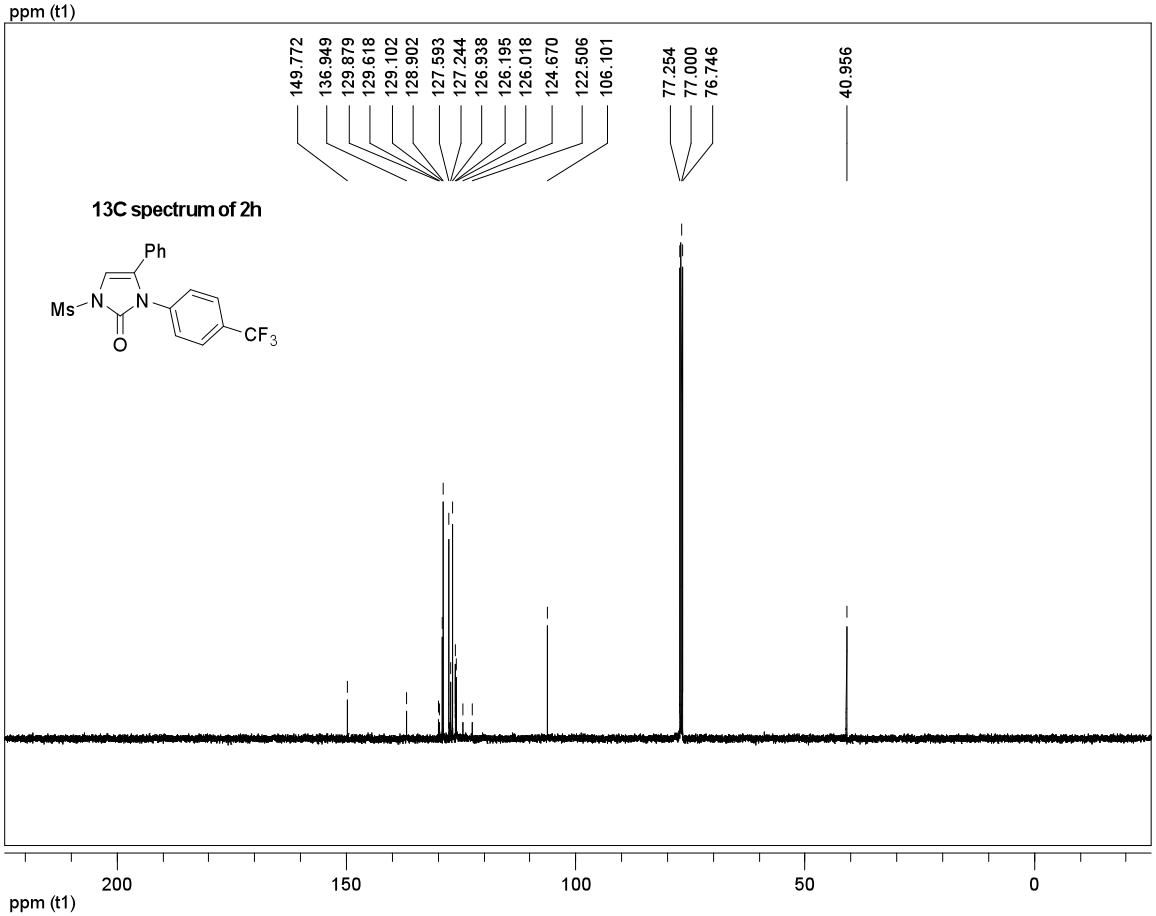
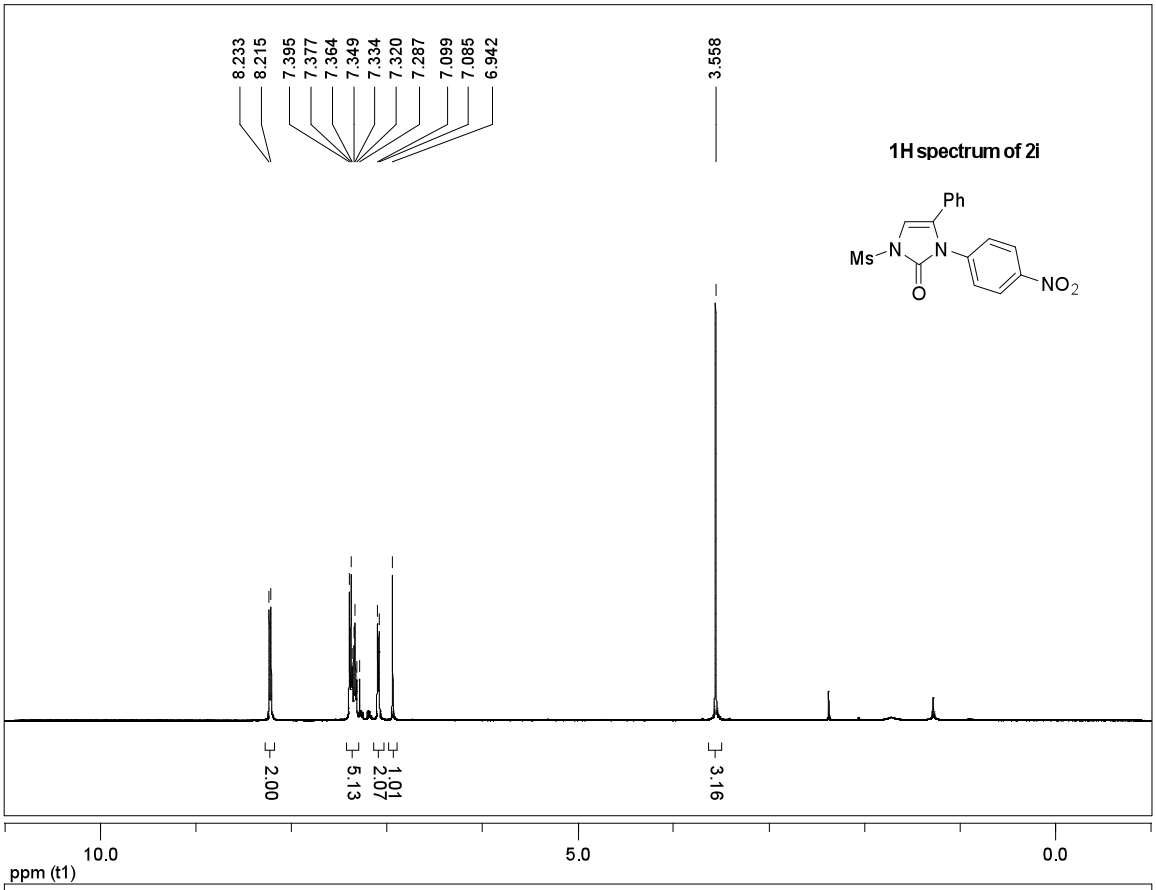
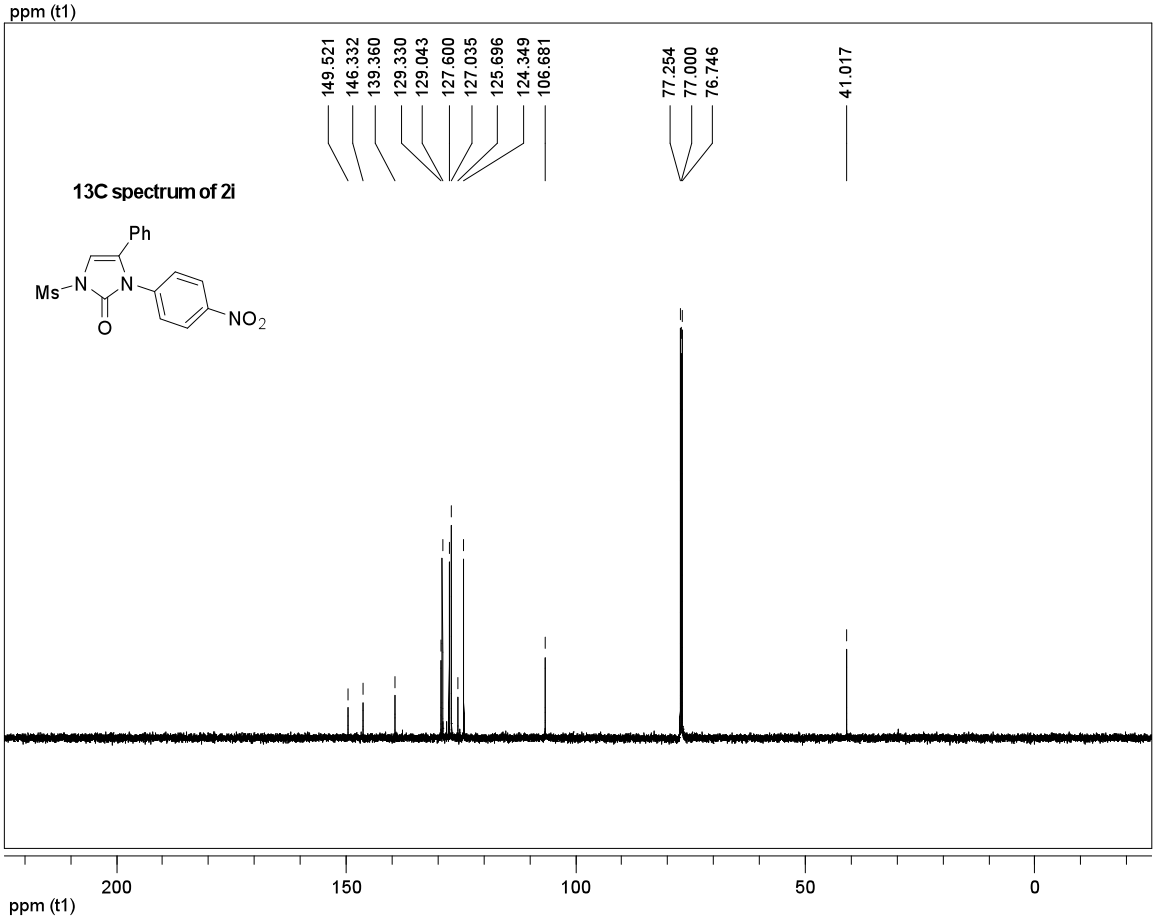
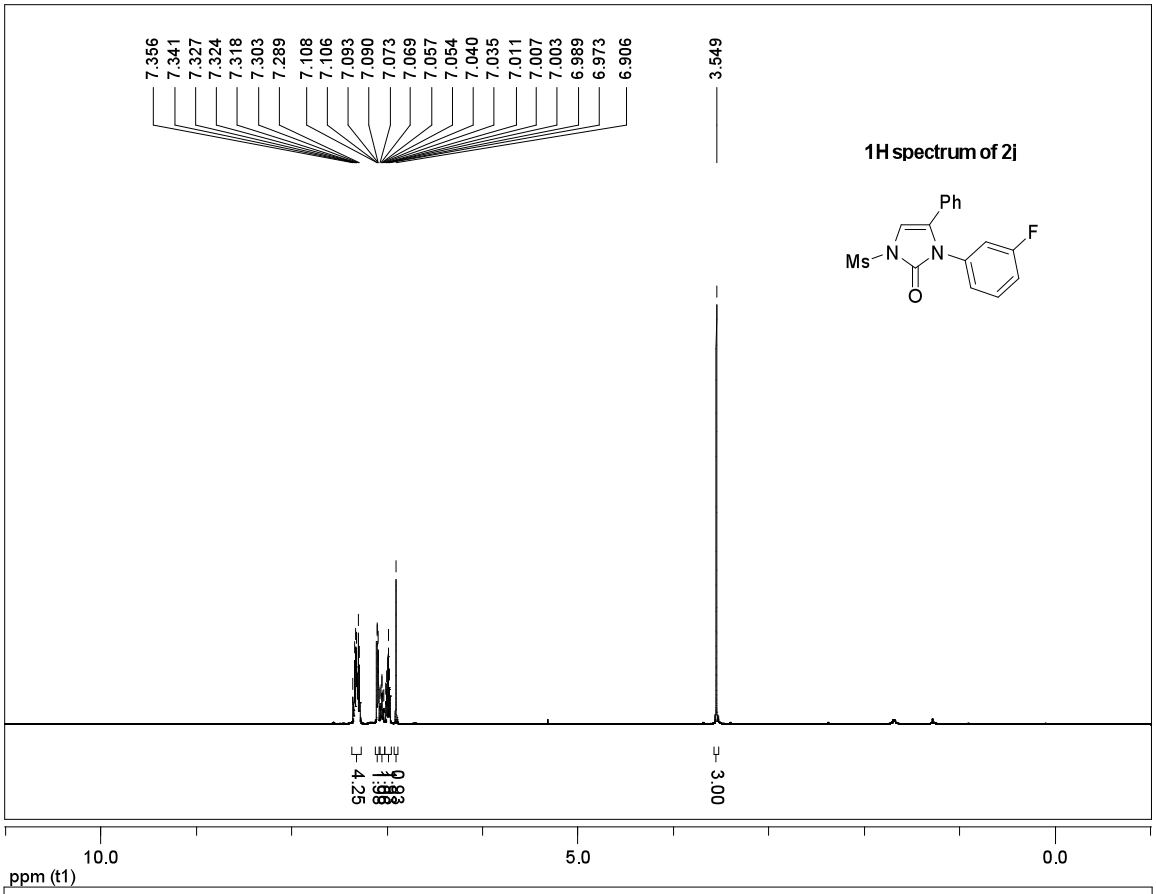
128.237
126.153
119.561
114.240
104.643
77.254
77.000
76.746
55.264
40.894
13C spectrum of 2g
OMe
Ms
N
N
O
Cl
200
150
100
50
0
ppm (t1)

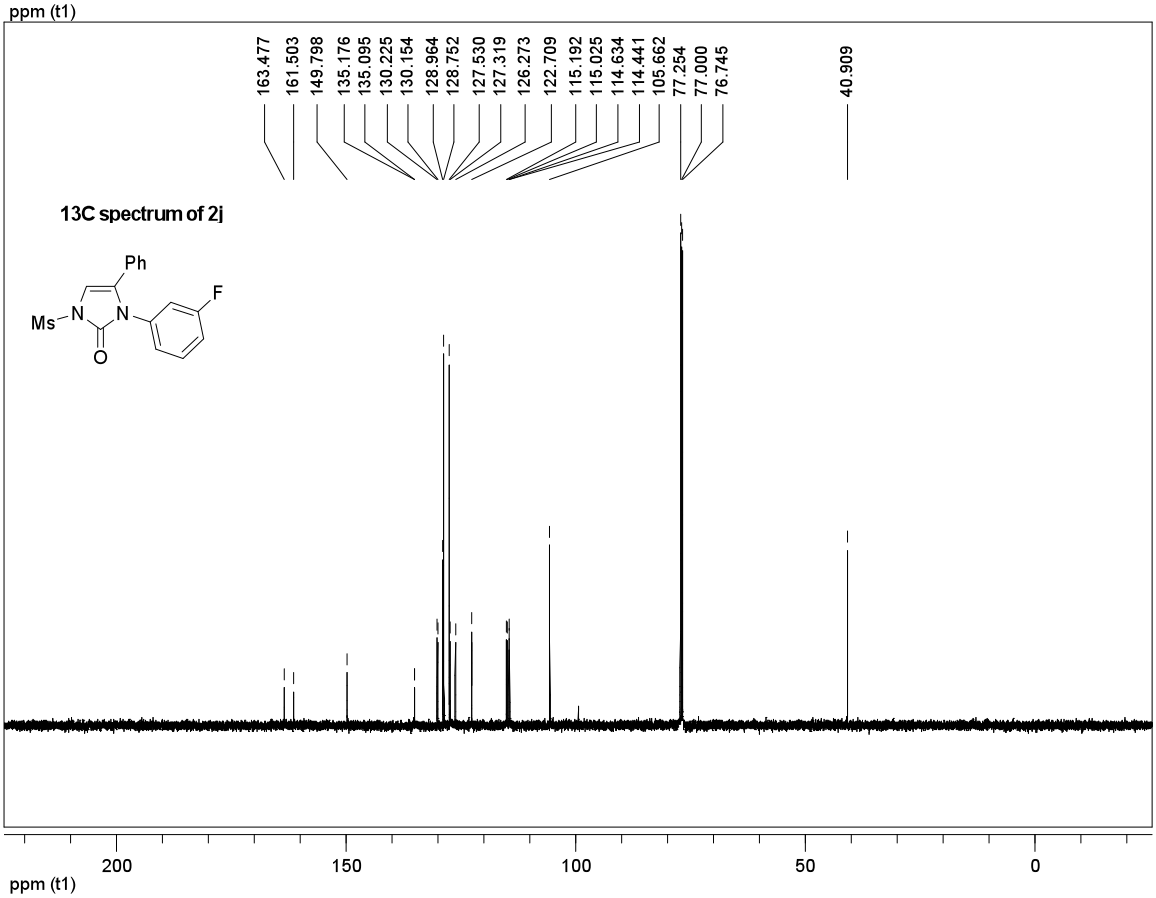

7.622
7.604
7.347
7.333
7.327
7.321
7.319
7.307
7.305
7.296
7.293
7.283
7.279
7.275
7.260
7.071
7.069
7.066
7.055
7.052
6.901
3.529
1H spectrum of 2h
Ph
Ms
N
N
O
CF3
2.10
5.28
2.09
1.00
3.20
10.0
5.0
0.0
ppm (t1)

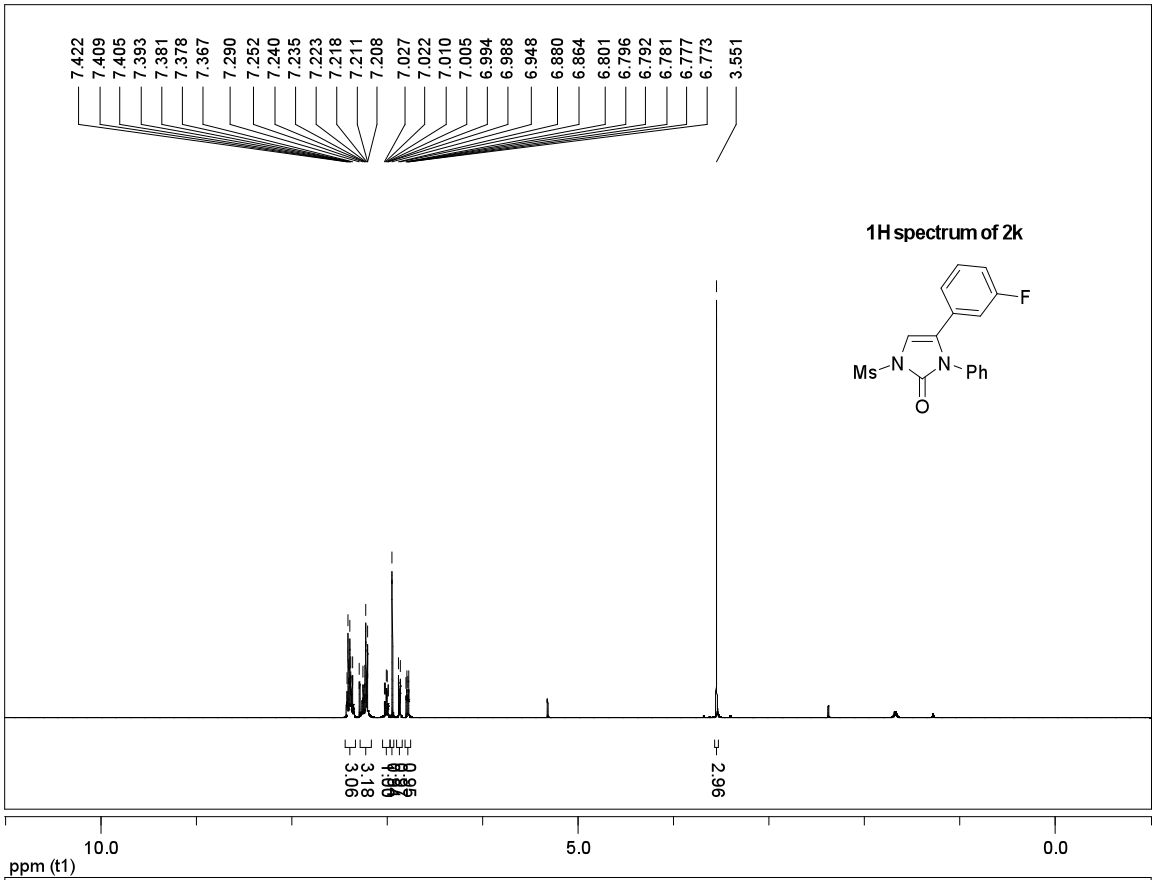

149.772
136.949
129.879
129.618
129.102
128.902
127.593
127.244
126.938
126.195
126.018
124.670
122.506
106.101
77.254
77.000
76.746
40.956
13C spectrum of 2h
Ph
Ms
N
N
O
CF3
200
150
100
50
0
ppm (t1)

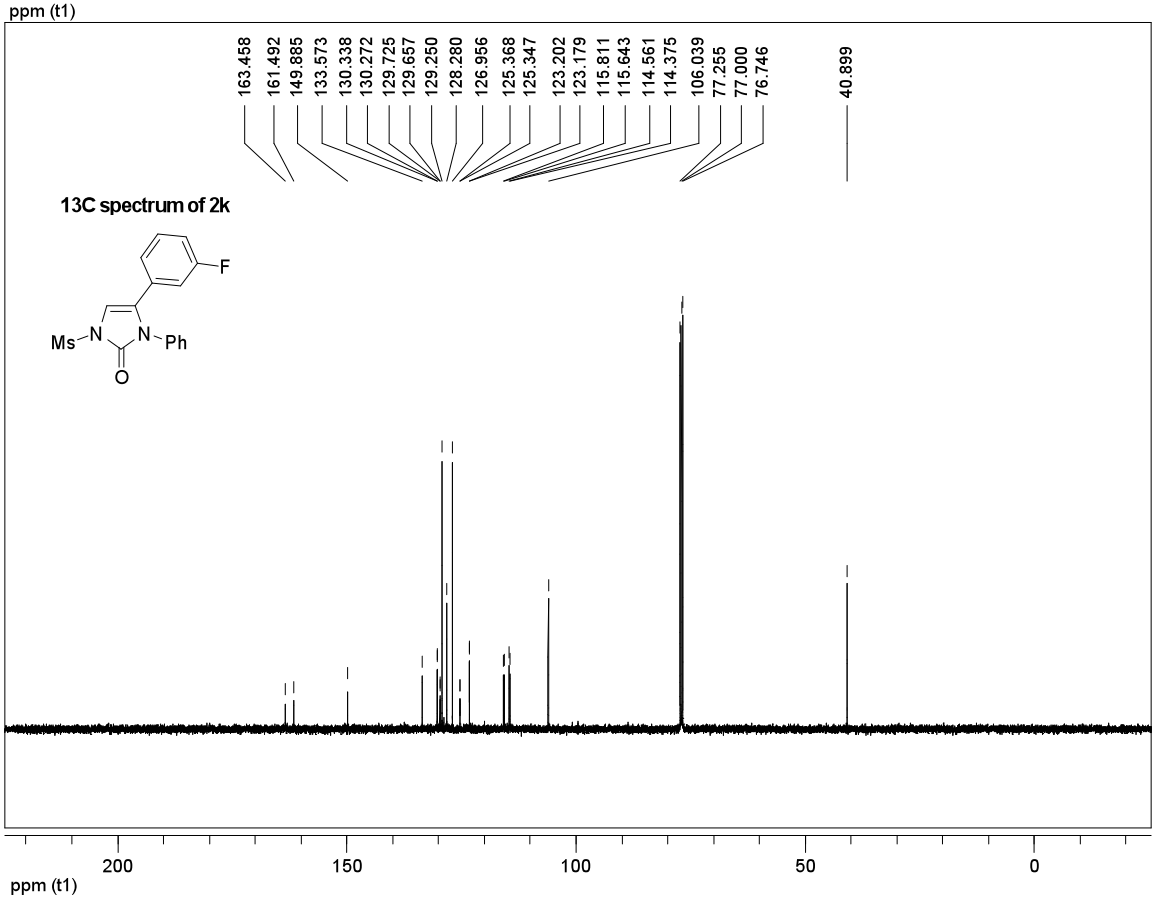

8.233
8.215
7.395
7.377
7.364
7.349
7.334
7.320
7.287
7.099
7.085
6.942
3.558
1H spectrum of 2i
Ph
Ms
N
N
O
NO2
2.00
5.13
2.07
1.01
3.16
10.0
5.0
0.0
ppm (t1)

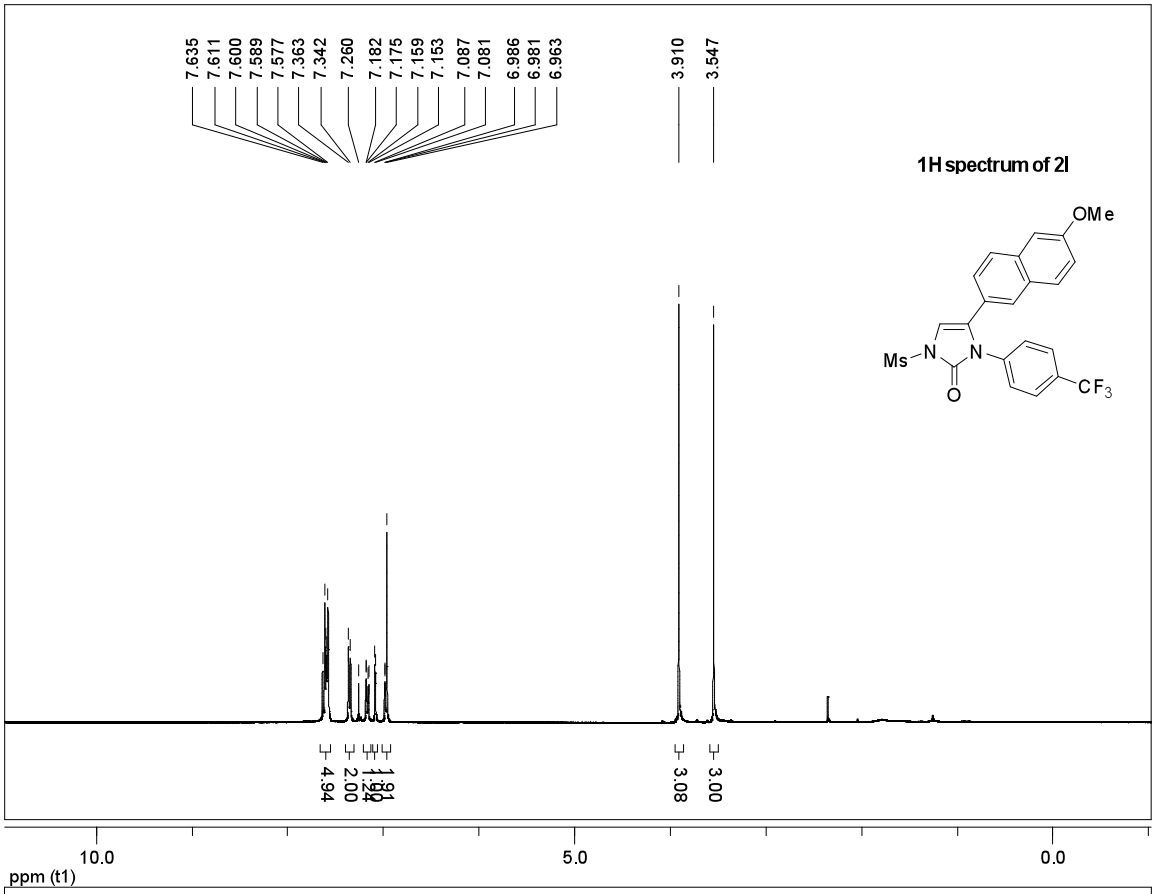

149.521
146.332
139.360
129.330
129.043
127.600
127.035
125.696
124.349
106.681
77.254
77.000
76.746
41.017
13C spectrum of 2i
Ph
Ms
N
N
O
NO2
200
150
100
50
0
ppm (t1)

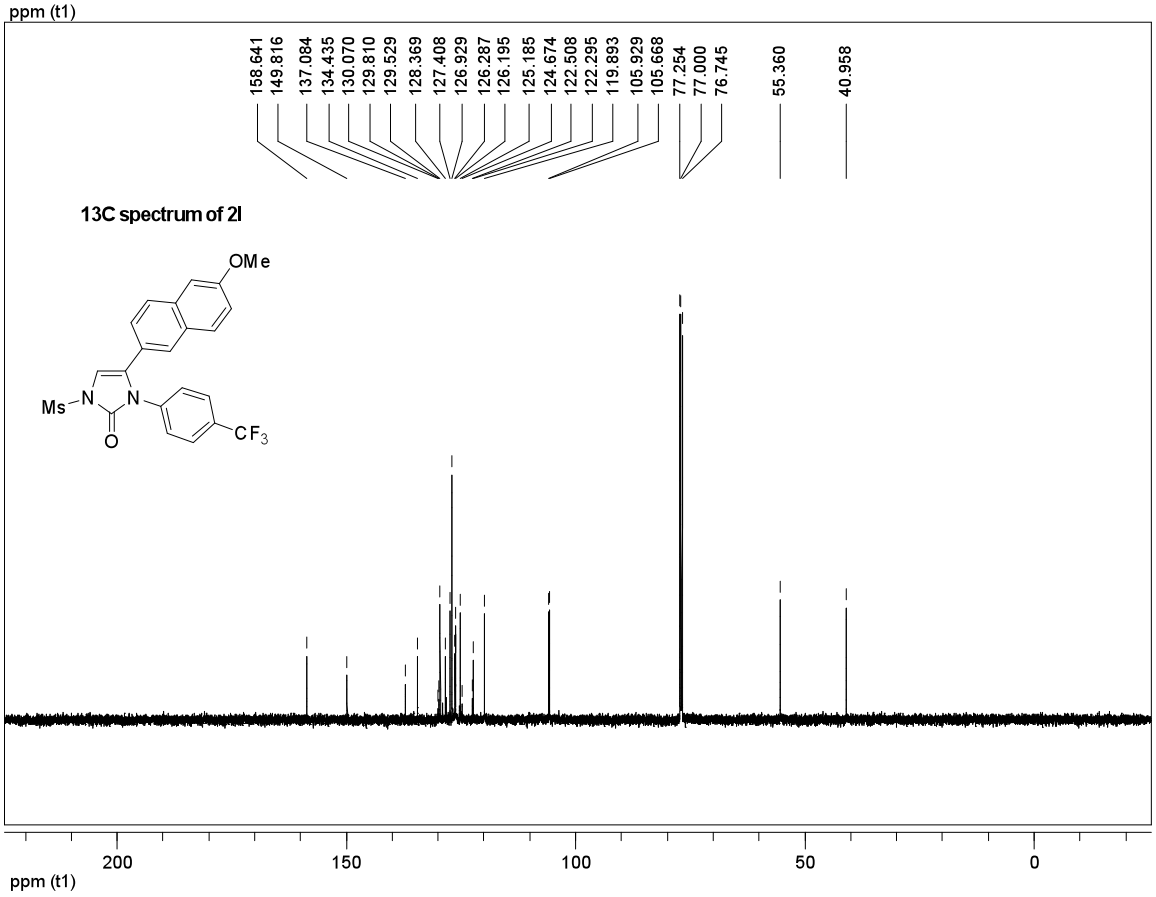

7.356
7.341
7.327
7.324
7.318
7.303
7.289
7.108
7.106
7.093
7.090
7.073
7.069
7.057
7.054
7.040
7.035
7.011
7.007
7.003
6.989
6.973
6.906
3.549
1H spectrum of 2j
Ph
F
Ms
N
N
O
4.25
3.00
10.0
5.0
0.0
ppm (t1)

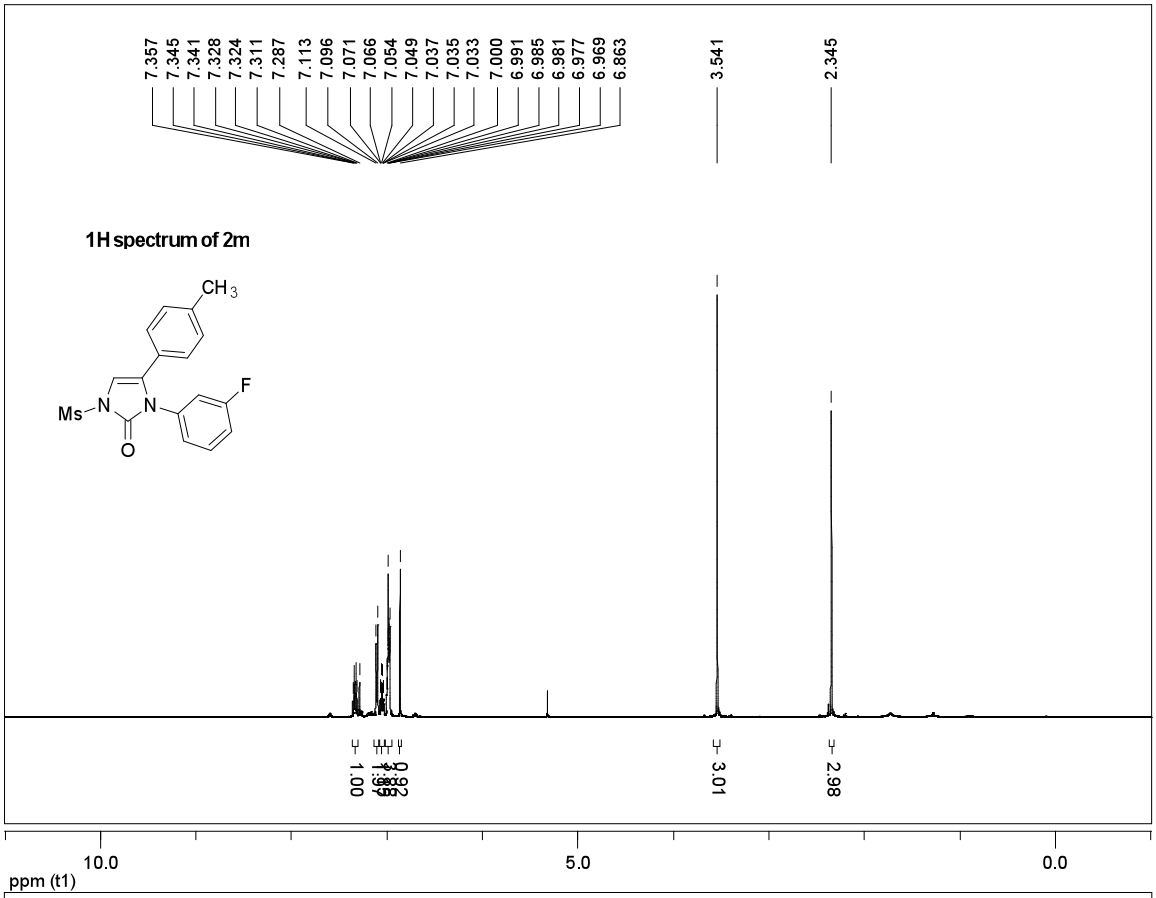

163.477
161.503
149.798
135.176
135.095
130.225
130.154
128.964
128.752
127.530
127.319
126.273
122.709
115.192
115.025
114.634
114.441
105.662
77.254
77.000
76.745
40.909
13C spectrum of 2j
Ph
F
Ms
N
N
O
200
150
100
50
0
ppm (t1)

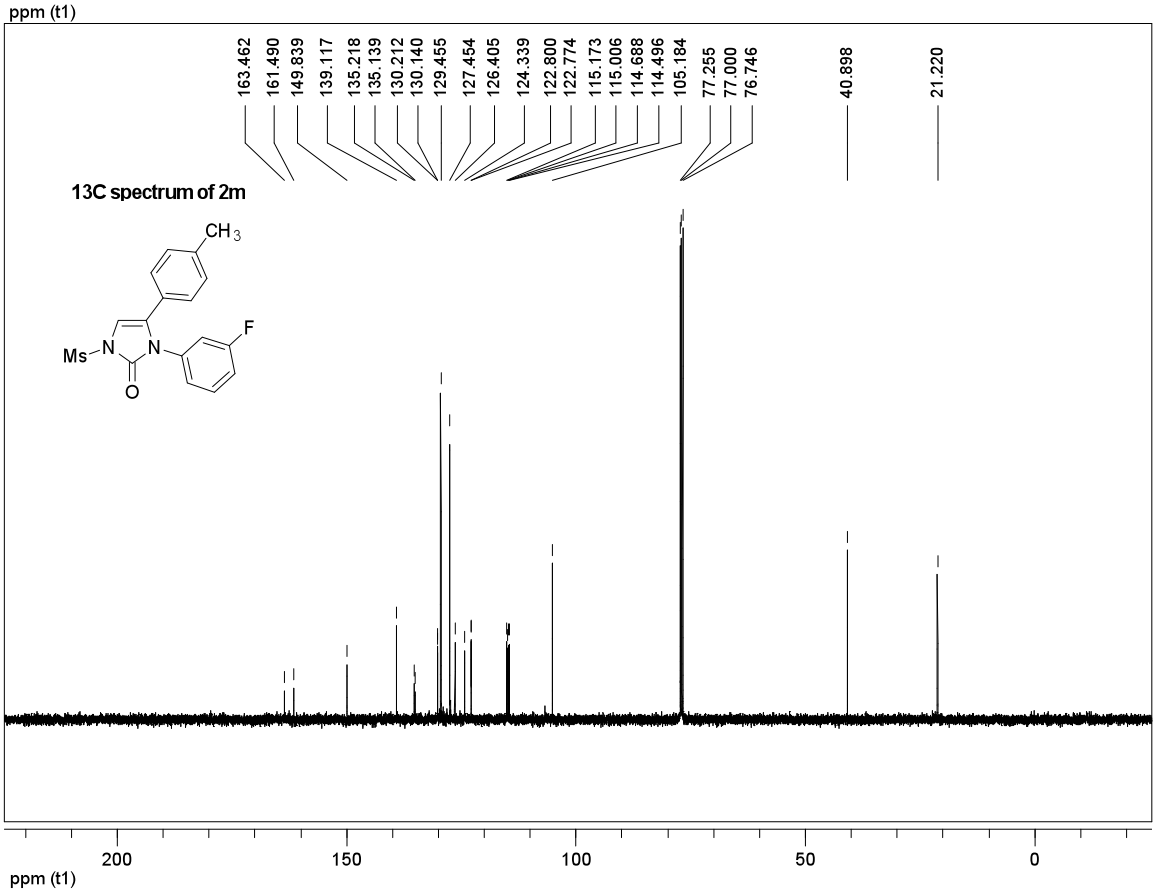

7.422
7.409
7.405
7.393
7.381
7.378
7.367
7.290
7.252
7.240
7.235
7.223
7.218
7.211
7.208
7.027
7.022
7.010
7.005
6.994
6.988
6.948
6.880
6.864
6.801
6.796
6.792
6.781
6.777
6.773
3.551
1H spectrum of 2k
F
Ms
N
N
Ph
O
3.06
3.18
2.96
10.0
5.0
0.0
ppm (t1)

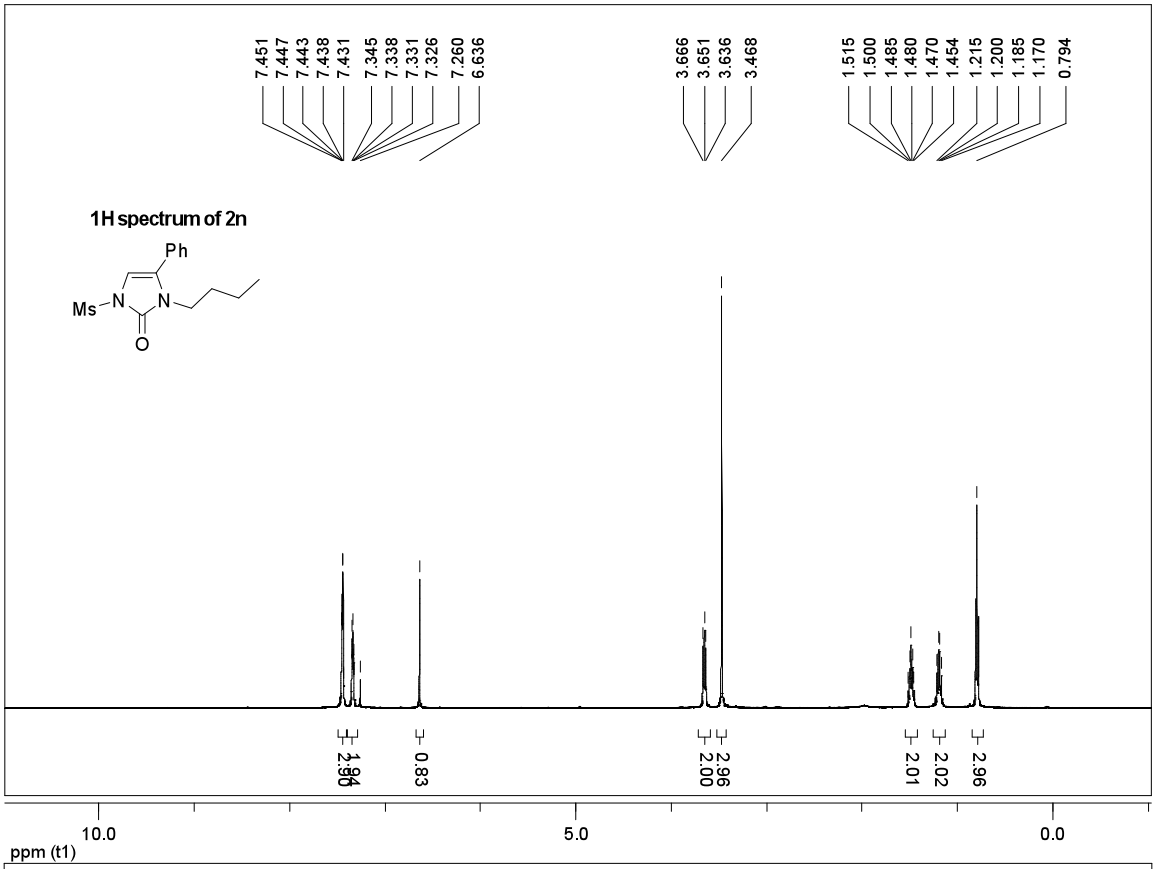

163.458
161.492
149.885
133.573
130.338
130.272
129.725
129.657
129.250
128.280
126.956
125.368
125.347
123.202
123.179
115.811
115.643
114.561
114.375
106.039
77.255
77.000
76.746
40.899
13C spectrum of 2k
F
Ms
N
N
Ph
O
200
150
100
50
0
ppm (t1)

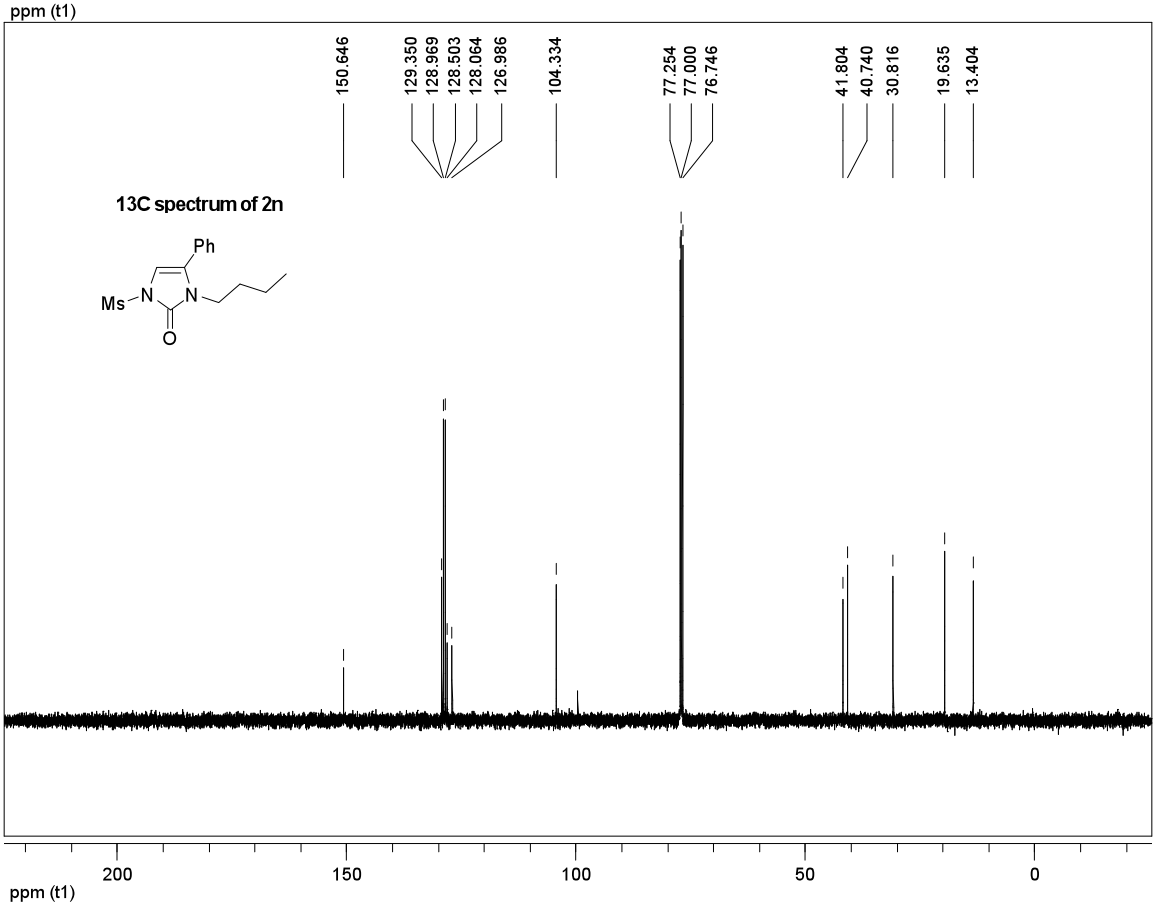

7.635
7.611
7.600
7.589
7.577
7.363
7.342
7.260
7.182
7.175
7.159
7.153
7.087
7.081
6.986
6.981
6.963
3.910
3.547
1H spectrum of 2l
OMe
Ms
N
N
O
CF3
4.94
2.00
1.91
3.08
3.00
10.0
5.0
0.0
ppm (t1)

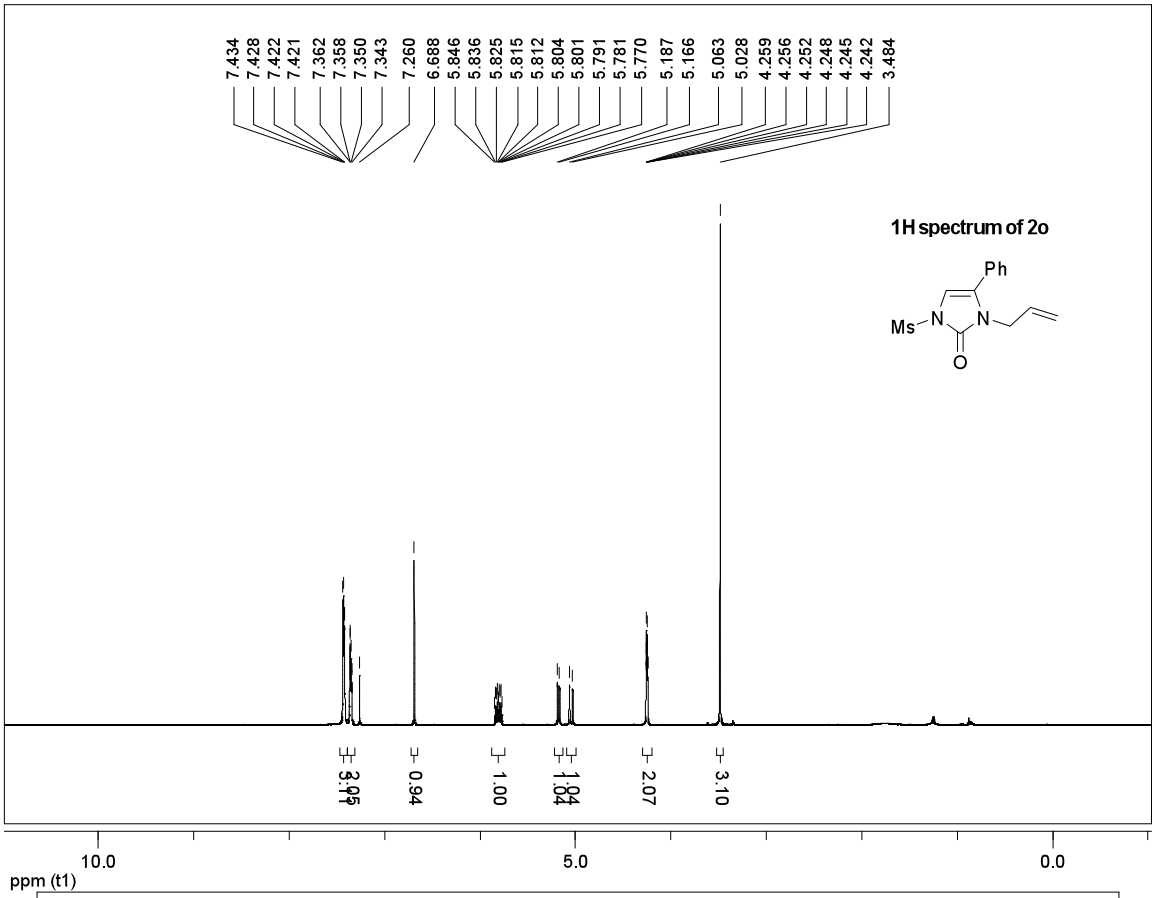

158.641
149.816
137.084
134.435
130.070
129.810
129.529
128.369
127.408
126.929
126.287
126.195
125.185
124.674
122.508
122.295
119.893
105.929
105.668
77.254
77.000
76.745
55.360
40.958
13C spectrum of 2l
OMe
Ms
N
N
O
CF3
200
150
100
50
0
ppm (t1)

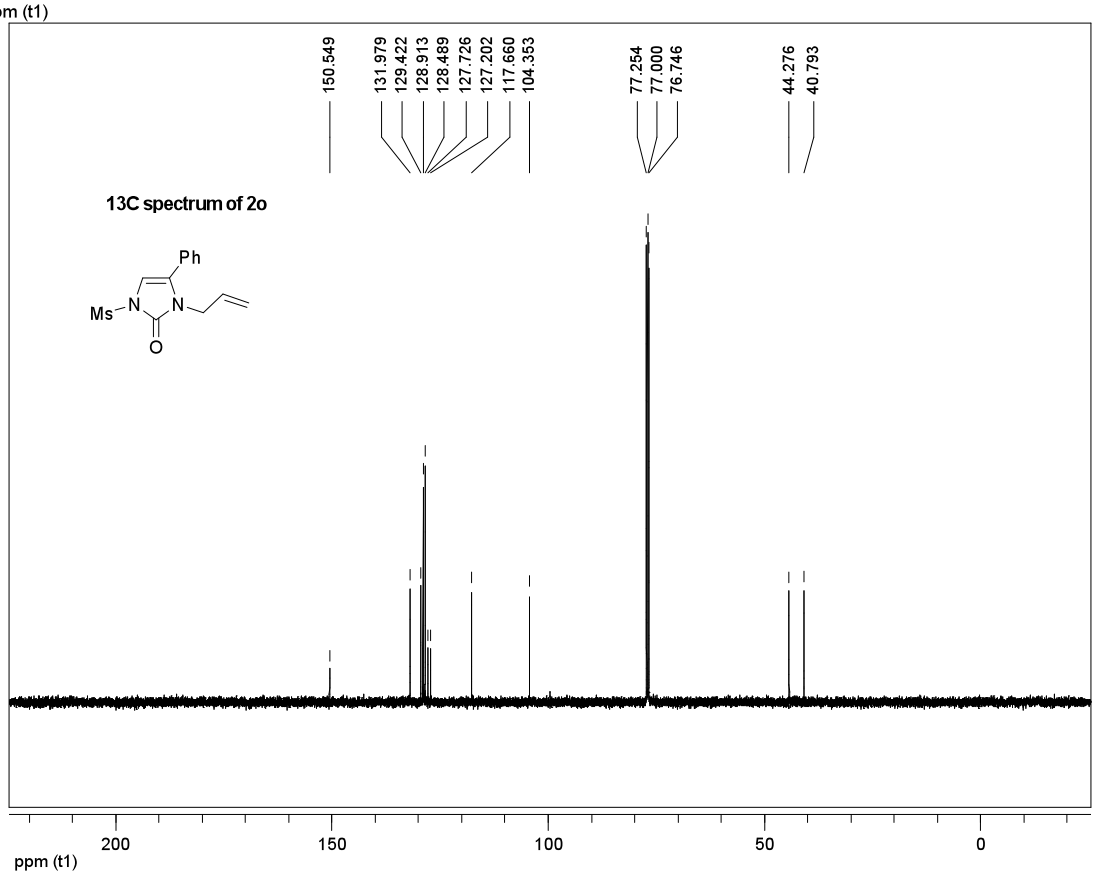

7.357
7.345
7.341
7.328
7.324
7.311
7.287
7.113
7.096
7.071
7.066
7.054
7.049
7.037
7.035
7.033
7.000
6.991
6.985
6.981
6.977
6.969
6.863
3.541
2.345
1H spectrum of 2m
CH3
Ms
N
N
F
O
1.00
3.01
2.98
10.0
5.0
0.0
ppm (t1)

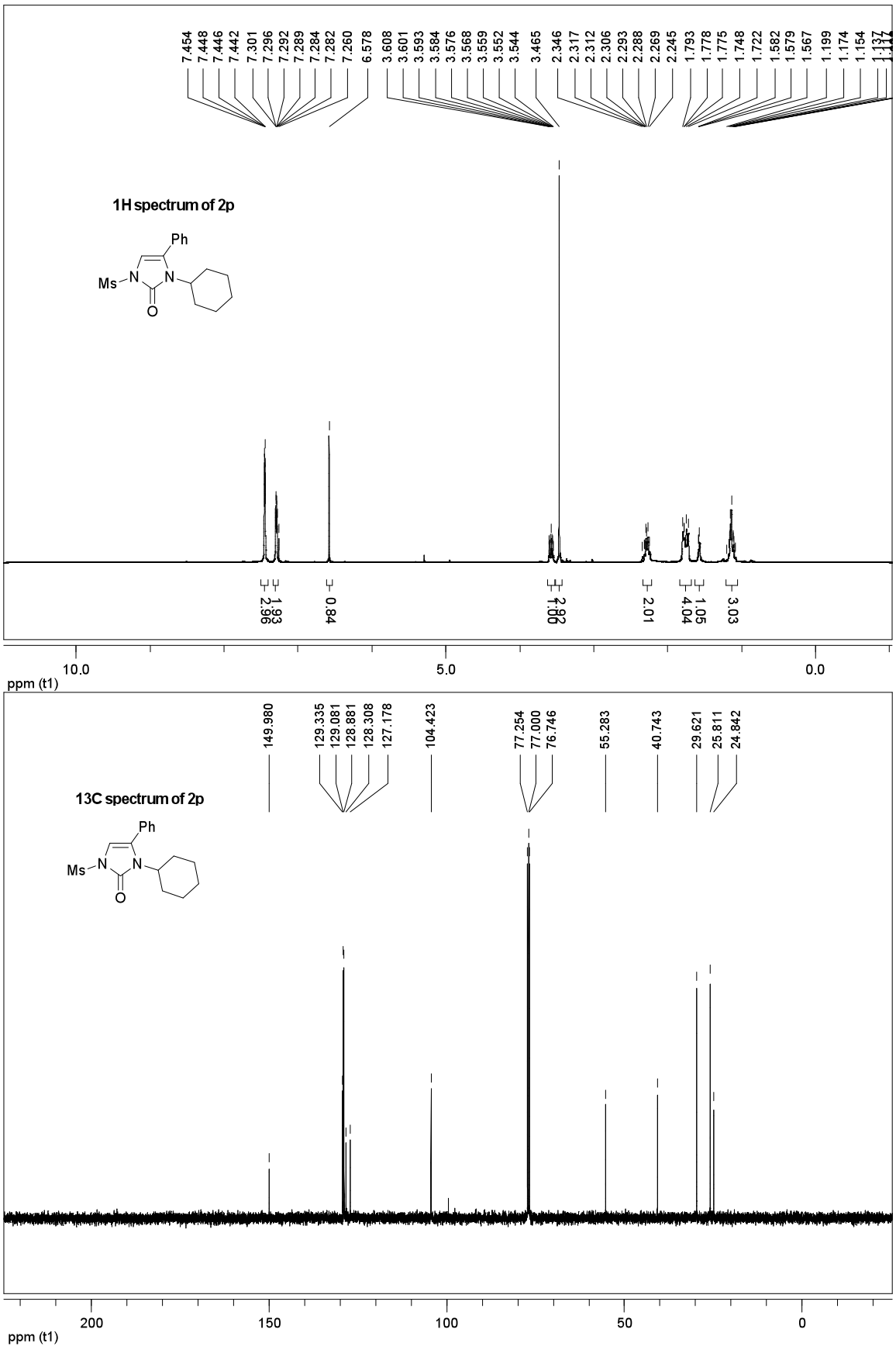

163.462
161.490
149.839
139.117
135.218
135.139
130.212
130.140
129.455
127.454
126.405
124.339
122.800
122.774
115.173
115.006
114.688
114.496
105.184
77.255
77.000
76.746
40.898
21.220
13C spectrum of 2m
CH3
Ms
N
N
F
O
200
150
100
50
0
ppm (t1)

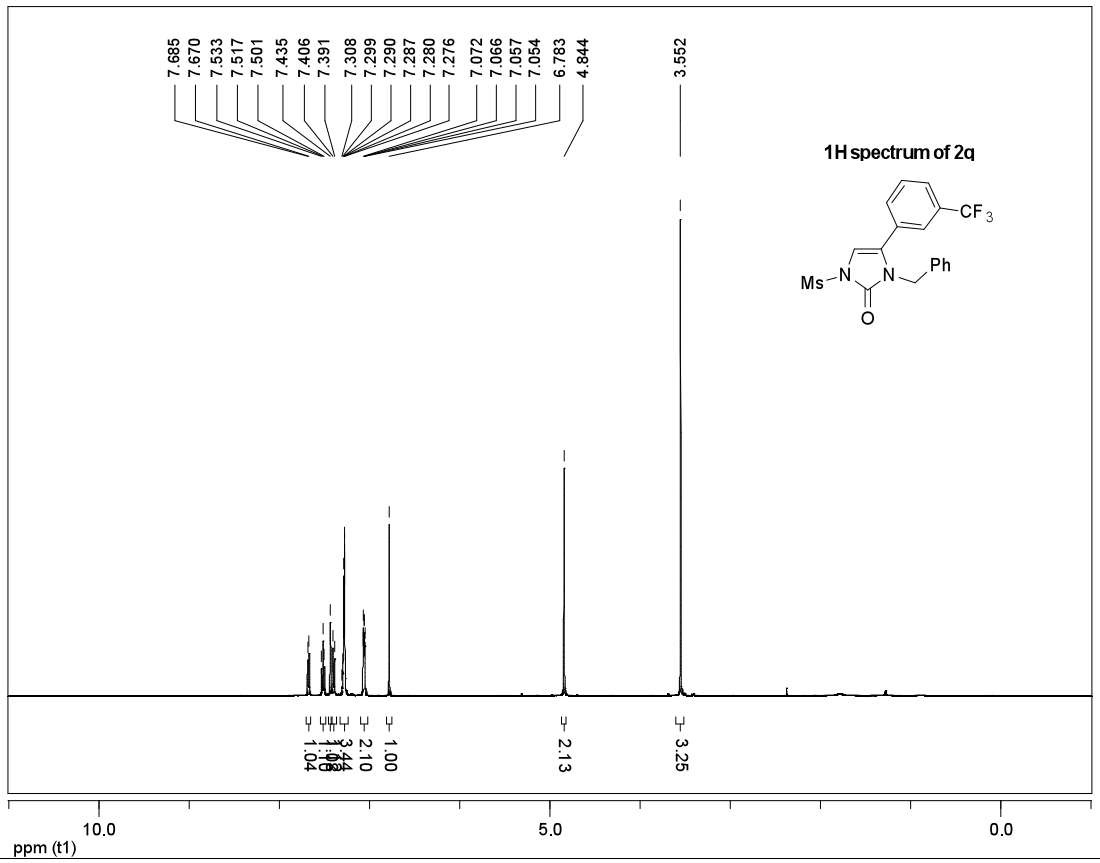

7.451
7.447
7.443
7.438
7.431
7.345
7.338
7.331
7.326
7.260
6.636
3.666
3.651
3.636
3.468
1.515
1.500
1.485
1.480
1.470
1.454
1.215
1.200
1.185
1.170
0.794
1H spectrum of 2n
Ph
Ms
N
N
O
1.90
1.94
0.83
2.00
2.96
2.01
2.02
2.96
10.0
5.0
0.0
ppm (t1)

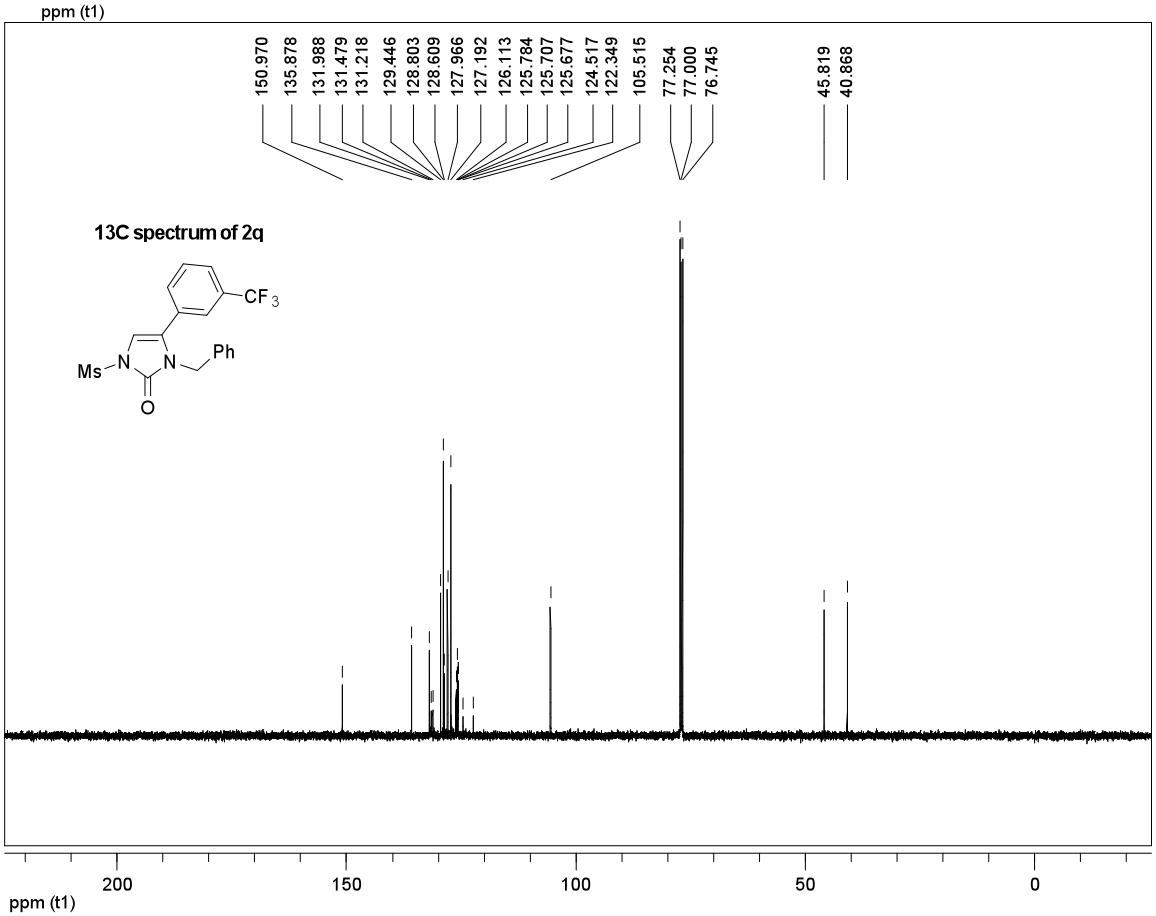

150.646
129.350
128.969
128.503
128.064
126.986
104.334
77.254
77.000
76.746
41.804
40.740
30.816
19.635
13.404
13C spectrum of 2n
Ph
Ms
N
N
O
200
150
100
50
0
ppm (t1)

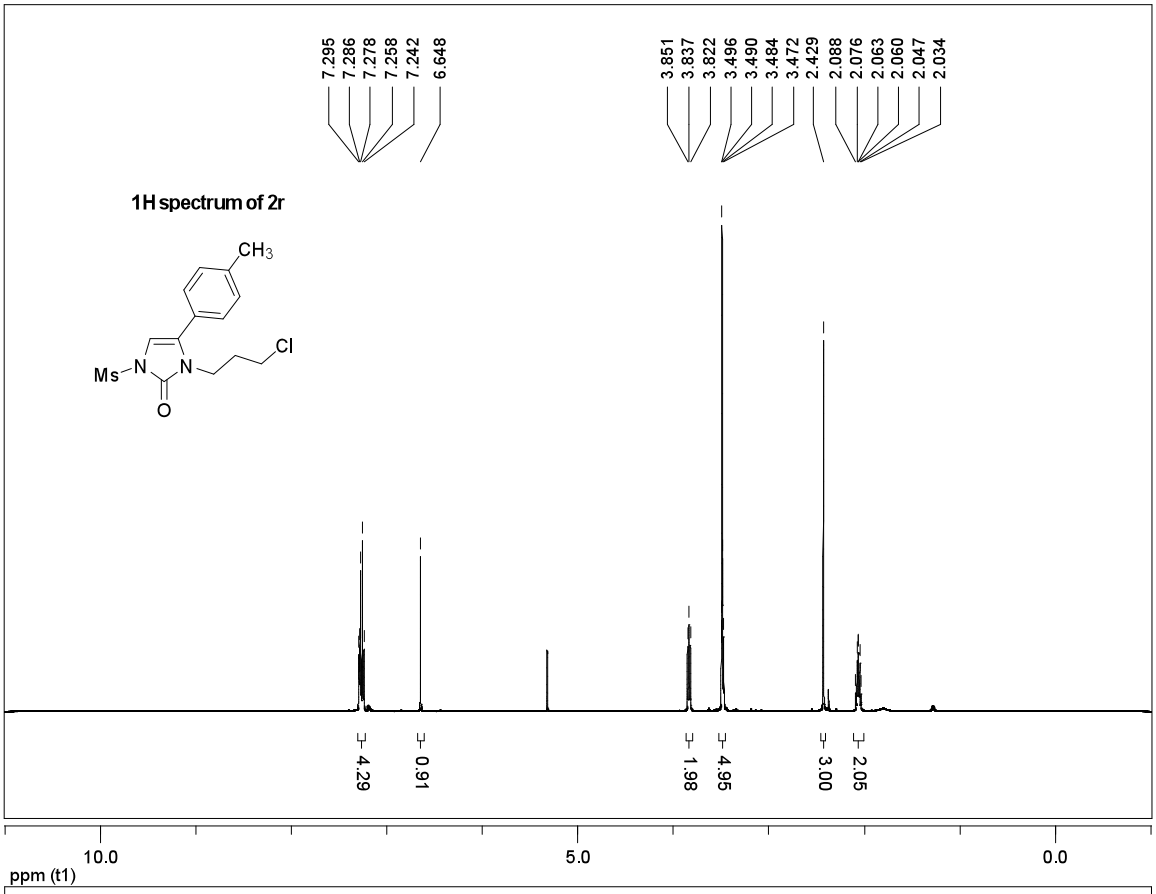

7.434
7.428
7.422
7.421
7.362
7.358
7.350
7.343
7.260
6.688
5.846
5.836
5.825
5.815
5.812
5.804
5.801
5.791
5.781
5.770
5.187
5.166
5.063
5.028
4.259
4.256
4.252
4.248
4.245
4.242
3.484
1H spectrum of 2o
Ph
Ms
N
N
O
2.05
0.94
1.00
1.04
2.07
3.10
10.0
5.0
0.0
ppm (t1)

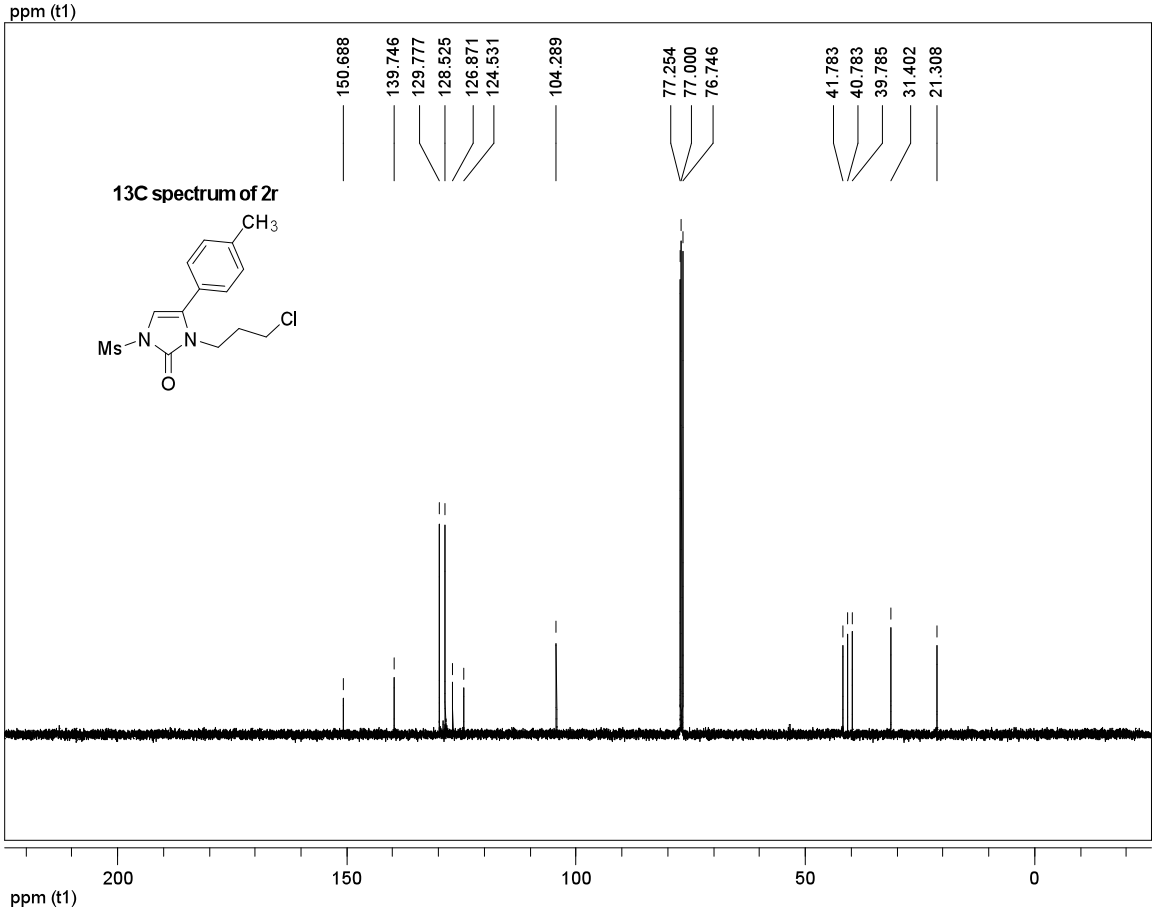

150.549
131.979
129.422
128.913
128.489
127.726
127.202
117.660
104.353
77.254
77.000
76.746
44.276
40.793
13C spectrum of 2o
Ph
Ms
N
N
O
200
150
100
50
0
ppm (t1)

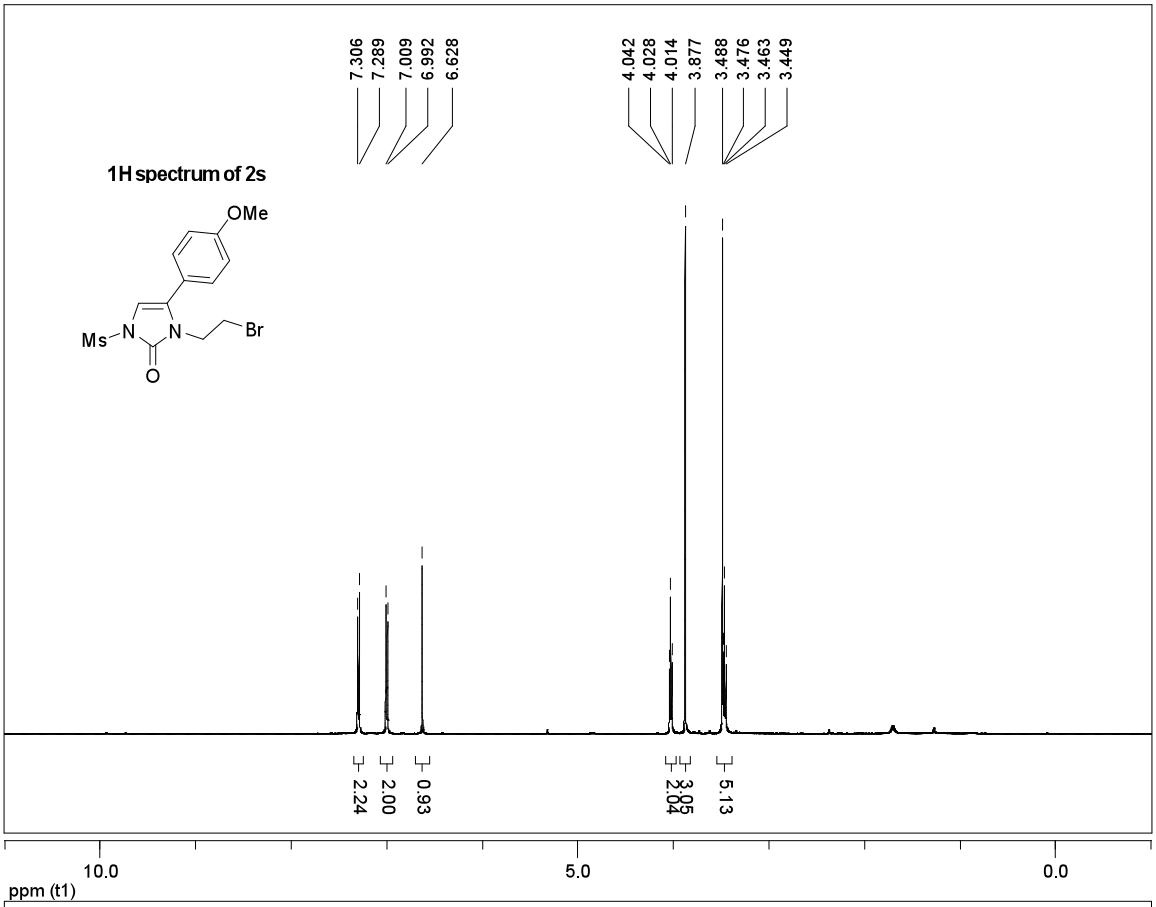

7.454
7.448
7.446
7.442
7.301
7.296
7.292
7.289
7.284
7.282
7.260
6.578
3.608
3.601
3.593
3.584
3.576
3.568
3.559
3.552
3.544
3.465
2.346
2.317
2.312
2.306
2.293
2.288
2.269
2.245
1.793
1.778
1.775
1.748
1.722
1.582
1.579
1.567
1.199
1.174
1.154
1H spectrum of 2p
Ph
Ms
N
N
O
2.96
1.93
0.84
1.00
2.01
4.04
1.05
3.03
10.0
5.0
0.0
ppm (t1)
149.980
129.335
129.081
128.881
128.308
127.178
104.423
77.254
77.000
76.746
55.283
40.743
29.621
25.811
24.842
13C spectrum of 2p
Ph
Ms
N
N
O
200
150
100
50
0
ppm (t1)

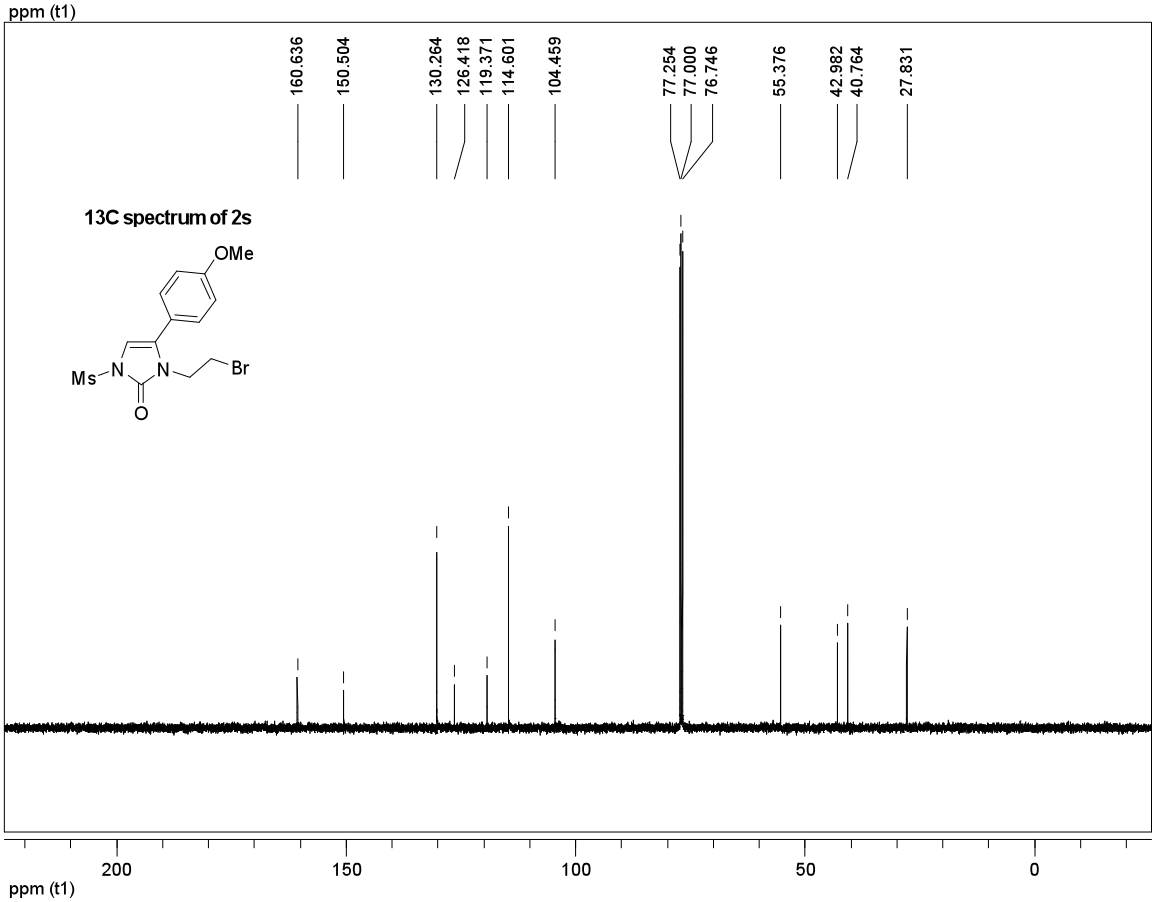

7.685
7.670
7.533
7.517
7.501
7.435
7.406
7.391
7.308
7.299
7.290
7.287
7.280
7.276
7.072
7.066
7.057
7.054
6.783
4.844
3.552
1H spectrum of 2q
CF3
Ms
N
N
Ph
O
1.04
2.10
1.00
2.13
3.25
10.0
5.0
0.0
ppm (t1)

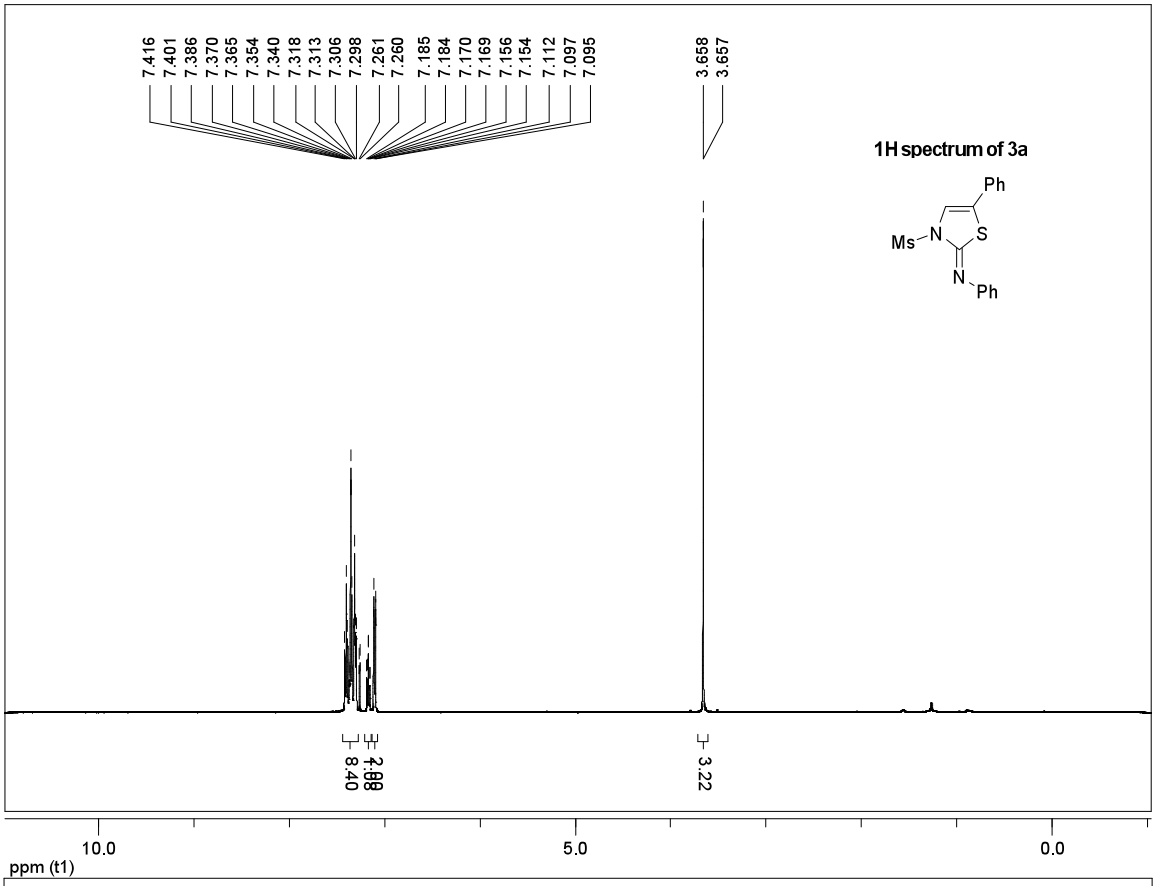

150.970
135.878
131.988
131.479
131.218
129.446
128.803
128.609
127.966
127.192
126.113
125.784
125.707
125.677
124.517
122.349
105.515
77.254
77.000
76.745
45.819
40.868
13C spectrum of 2q
CF3
Ms
N
N
Ph
O
200
150
100
50
0
ppm (t1)

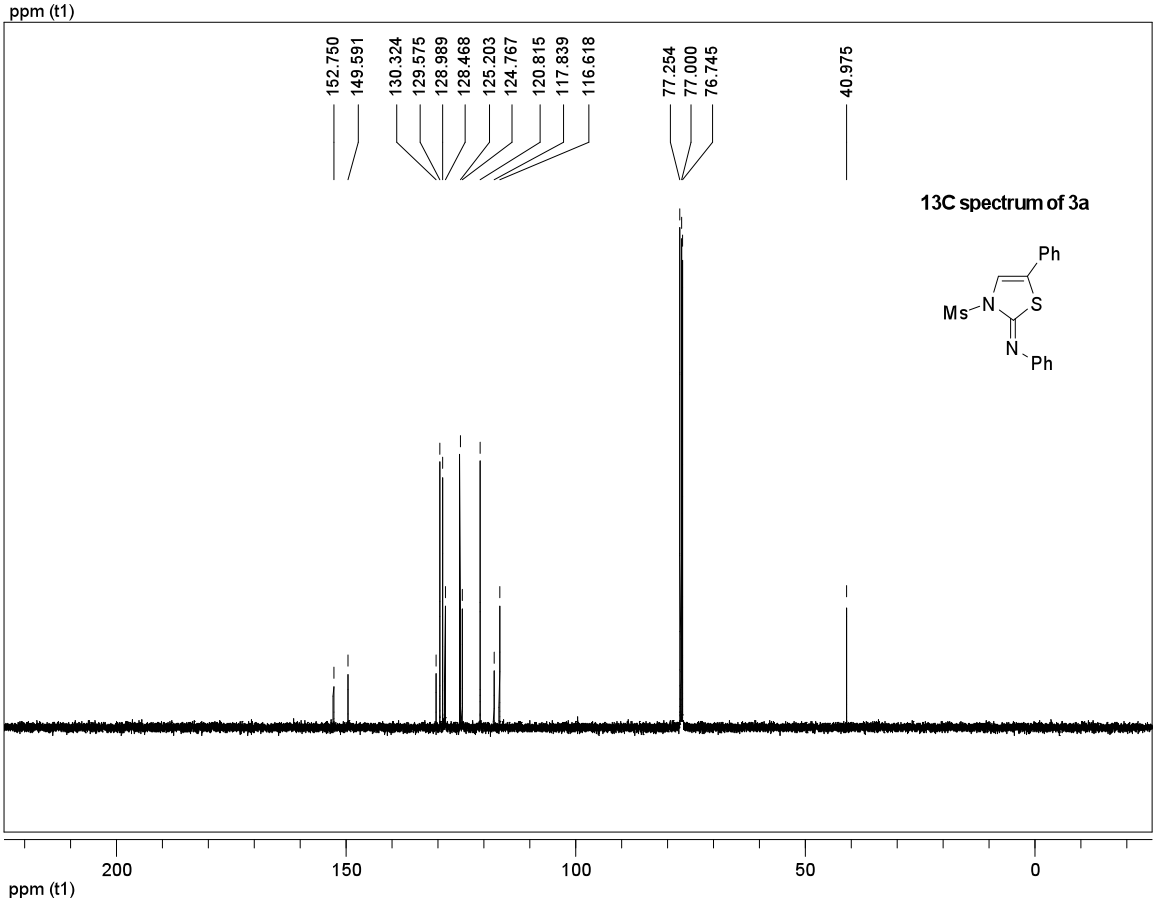

1H spectrum of 2r
7.295
7.286
7.278
7.258
7.242
6.648
3.851
3.837
3.822
3.496
3.490
3.484
3.472
2.429
2.088
2.076
2.063
2.060
2.047
2.034
CH3
Cl
Ms
N
N
O
4.29
0.91
1.98
4.95
3.00
2.05
10.0
5.0
0.0
ppm (t1)

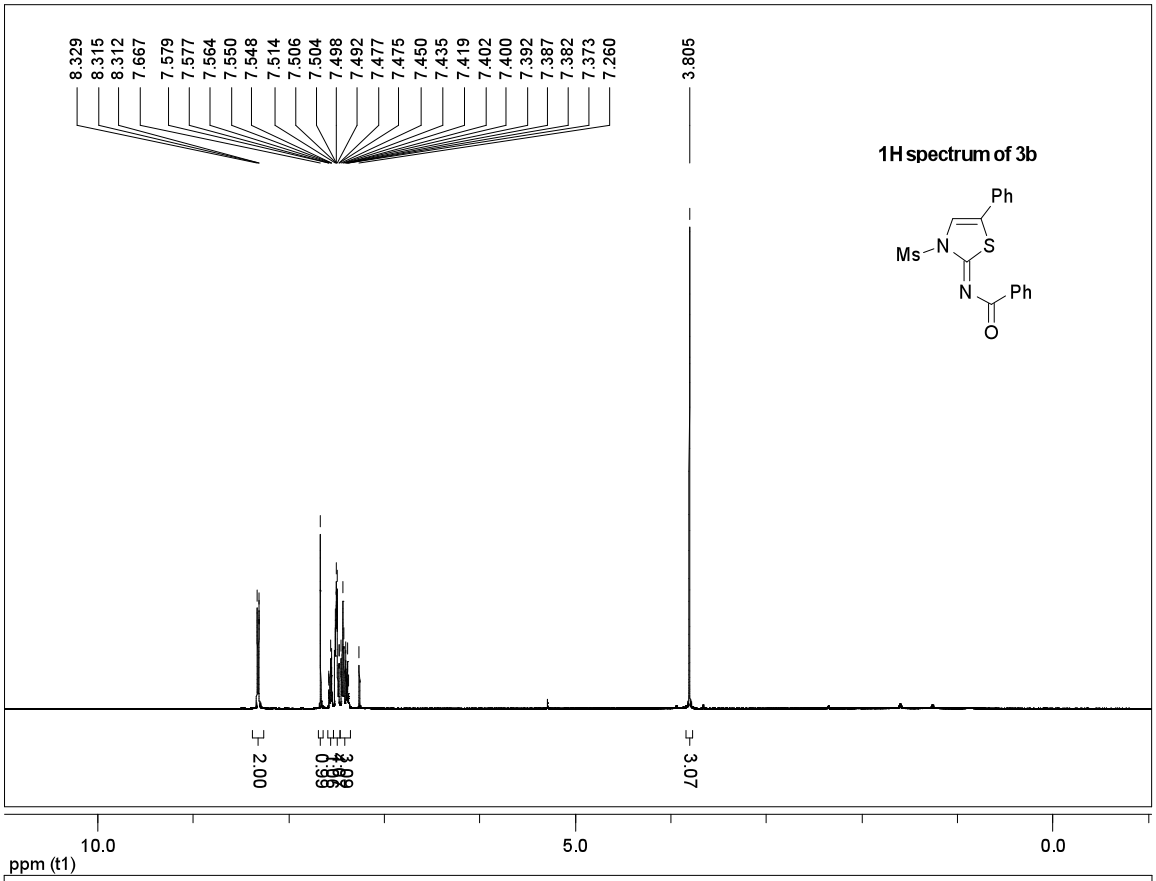

13C spectrum of 2r
150.688
139.746
129.777
128.525
126.871
124.531
104.289
77.254
77.000
76.746
41.783
40.783
39.785
31.402
21.308
CH3
Cl
Ms
N
N
O
200
150
100
50
0
ppm (t1)

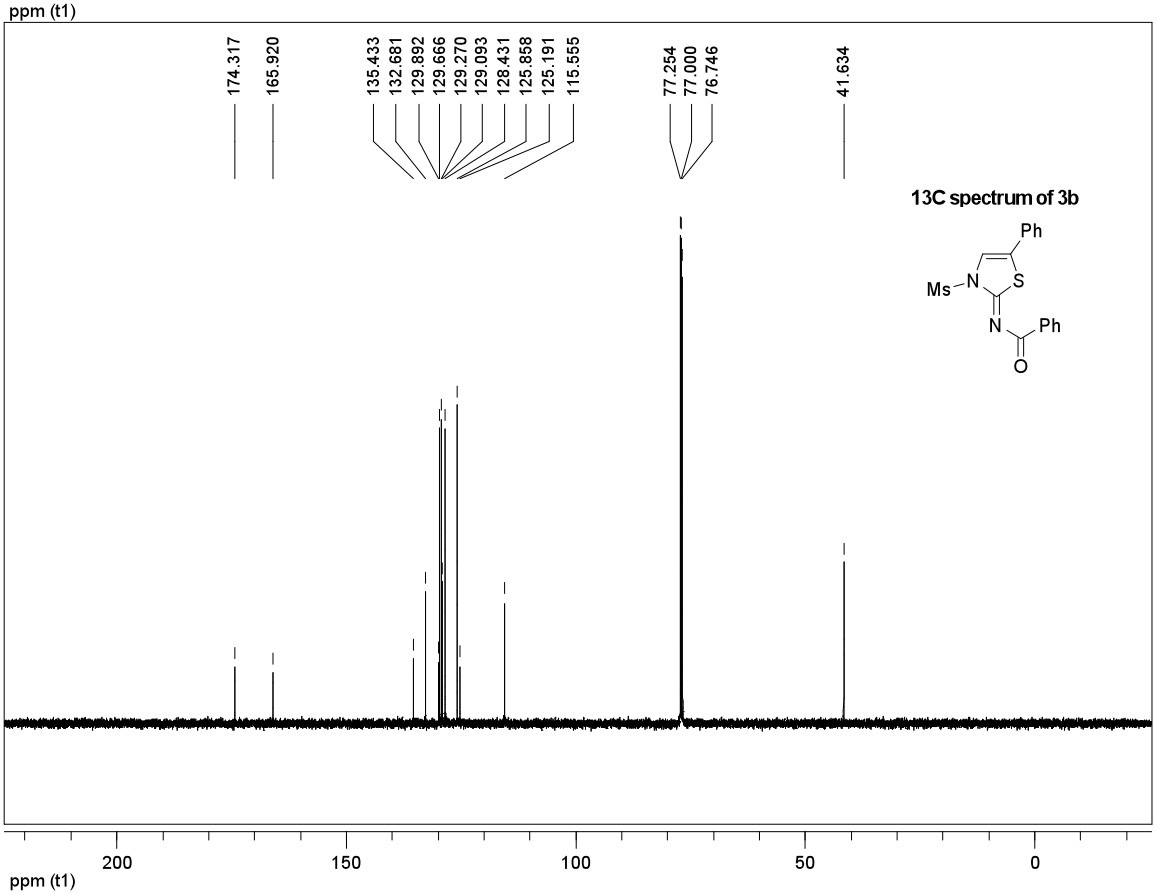

1H spectrum of 2s
7.306
7.289
7.009
6.992
6.628
4.042
4.028
4.014
3.877
3.488
3.476
3.463
3.449
OMe
Ms
N
N
Br
O
2.24
2.00
0.93
3.04
3.05
5.13
10.0
5.0
0.0
ppm (t1)


13C spectrum of 2s
160.636
150.504
130.264
126.418
119.371
114.601
104.459
77.254
77.000
76.746
55.376
42.982
40.764
27.831
OMe
Ms
N
N
Br
O
200
150
100
50
0
ppm (t1)


7.416
7.401
7.386
7.370
7.365
7.354
7.340
7.318
7.313
7.306
7.298
7.261
7.260
7.185
7.184
7.170
7.169
7.156
7.154
7.112
7.097
7.095
3.658
3.657
1H spectrum of 3a
Ph
Ms
N
S
N
Ph
8.40
7.89
3.22
10.0
5.0
0.0
ppm (t1)


152.750
149.591
130.324
129.575
128.989
128.468
125.203
124.767
120.815
117.839
116.618
77.254
77.000
76.745
40.975
13C spectrum of 3a
Ph
Ms
N
S
N
Ph
200
150
100
50
0
ppm (t1)


8.329
8.315
8.312
7.667
7.579
7.577
7.564
7.550
7.548
7.514
7.506
7.504
7.498
7.492
7.477
7.475
7.450
7.435
7.419
7.402
7.400
7.392
7.387
7.382
7.373
7.260
3.805
1H spectrum of 3b
Ph
Ms
N
S
N
Ph
O
2.00
3.07
10.0
5.0
0.0
ppm (t1)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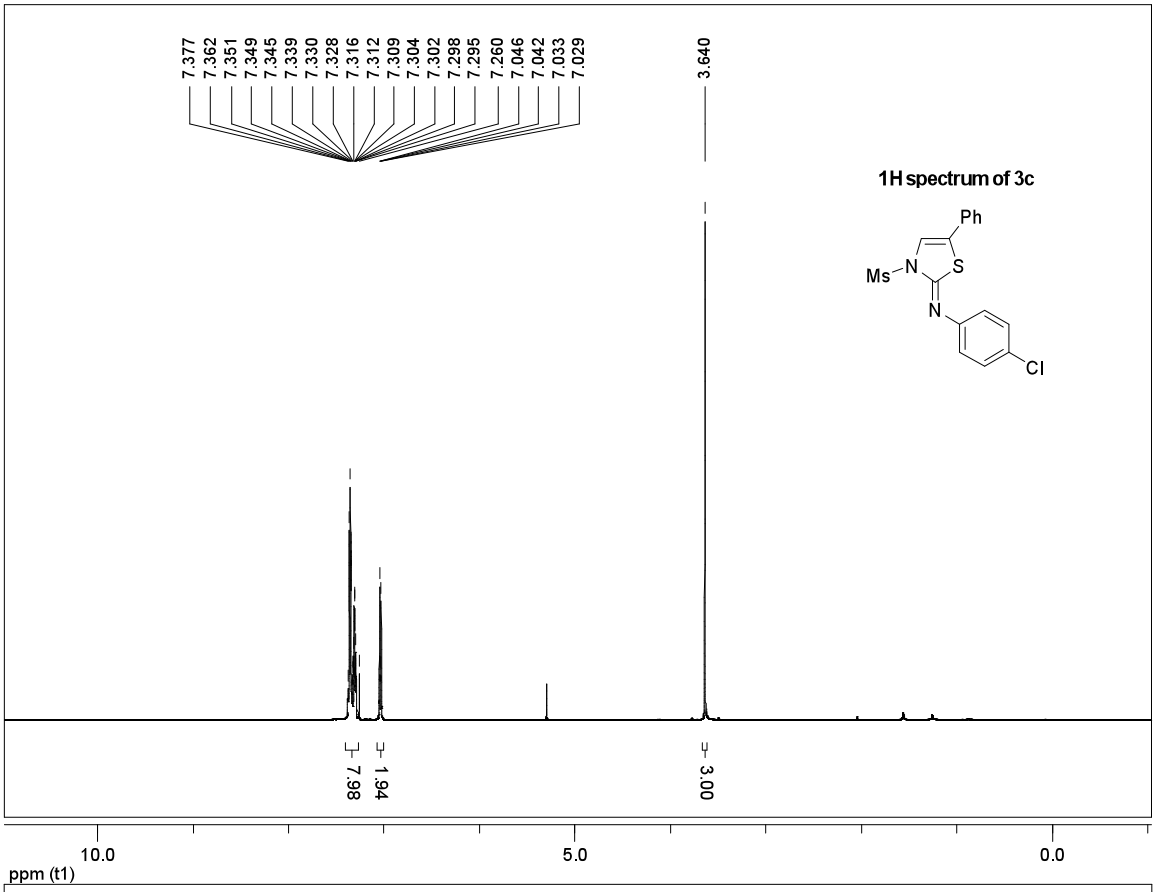
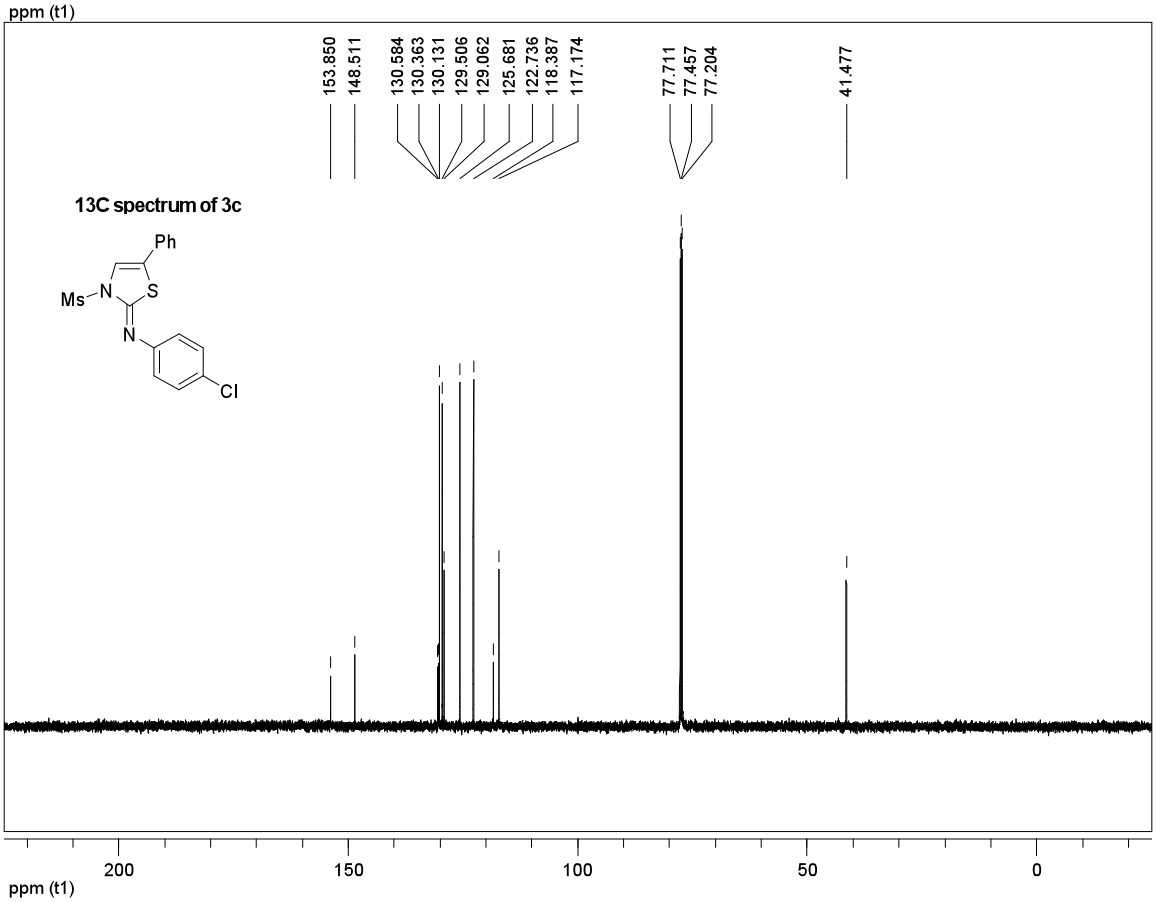
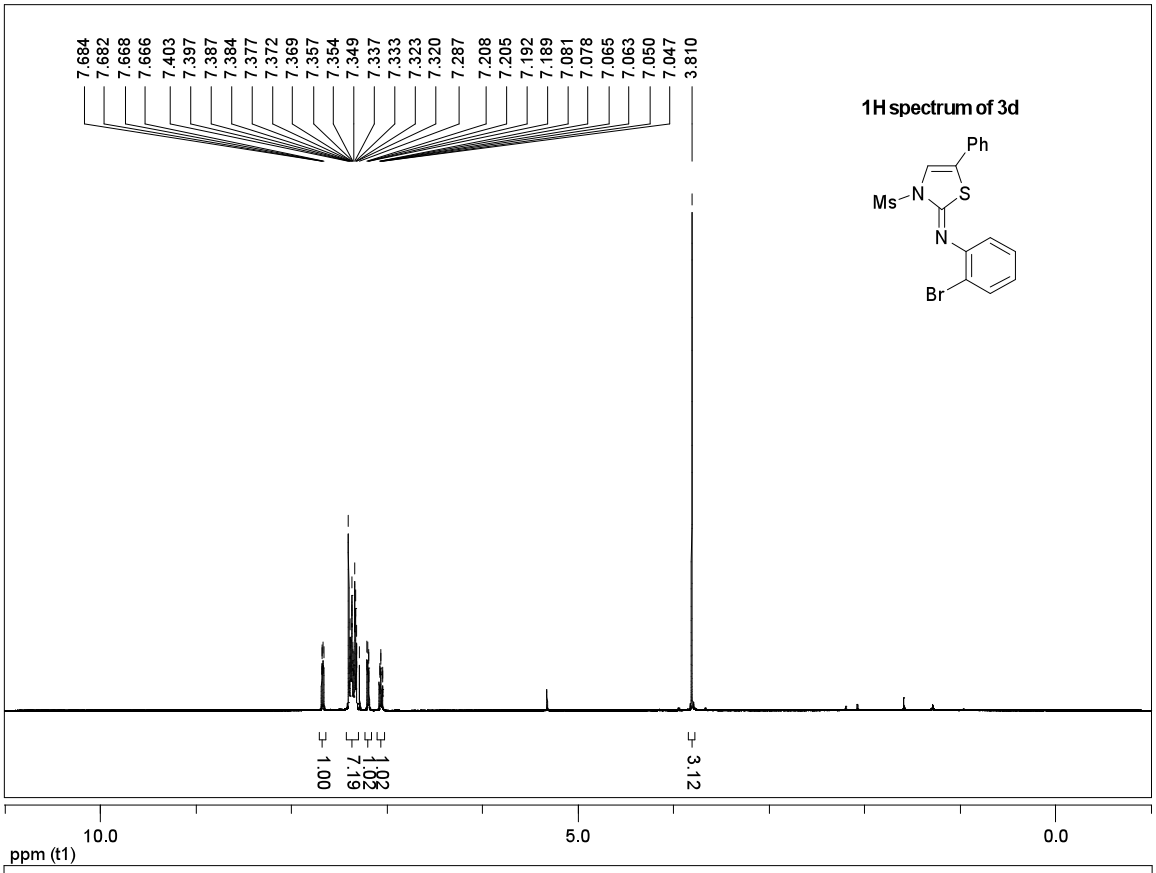
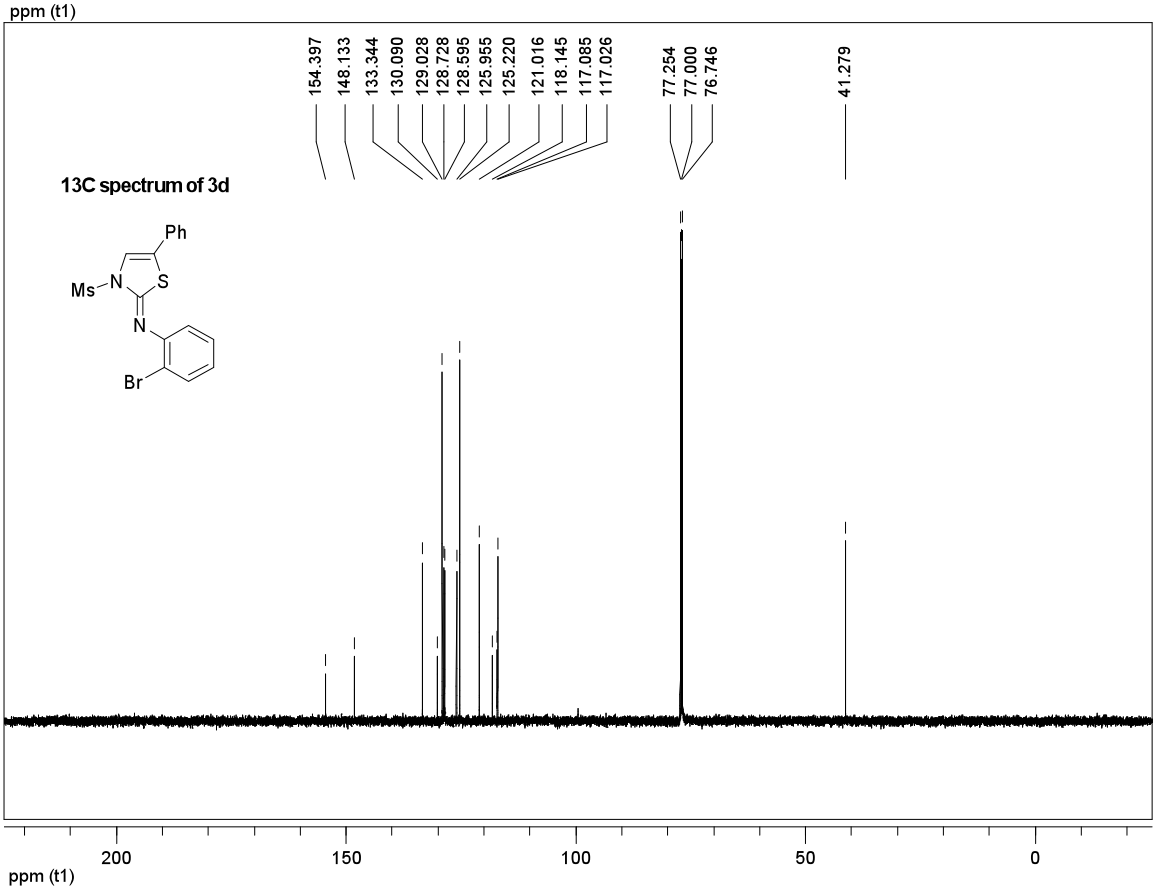
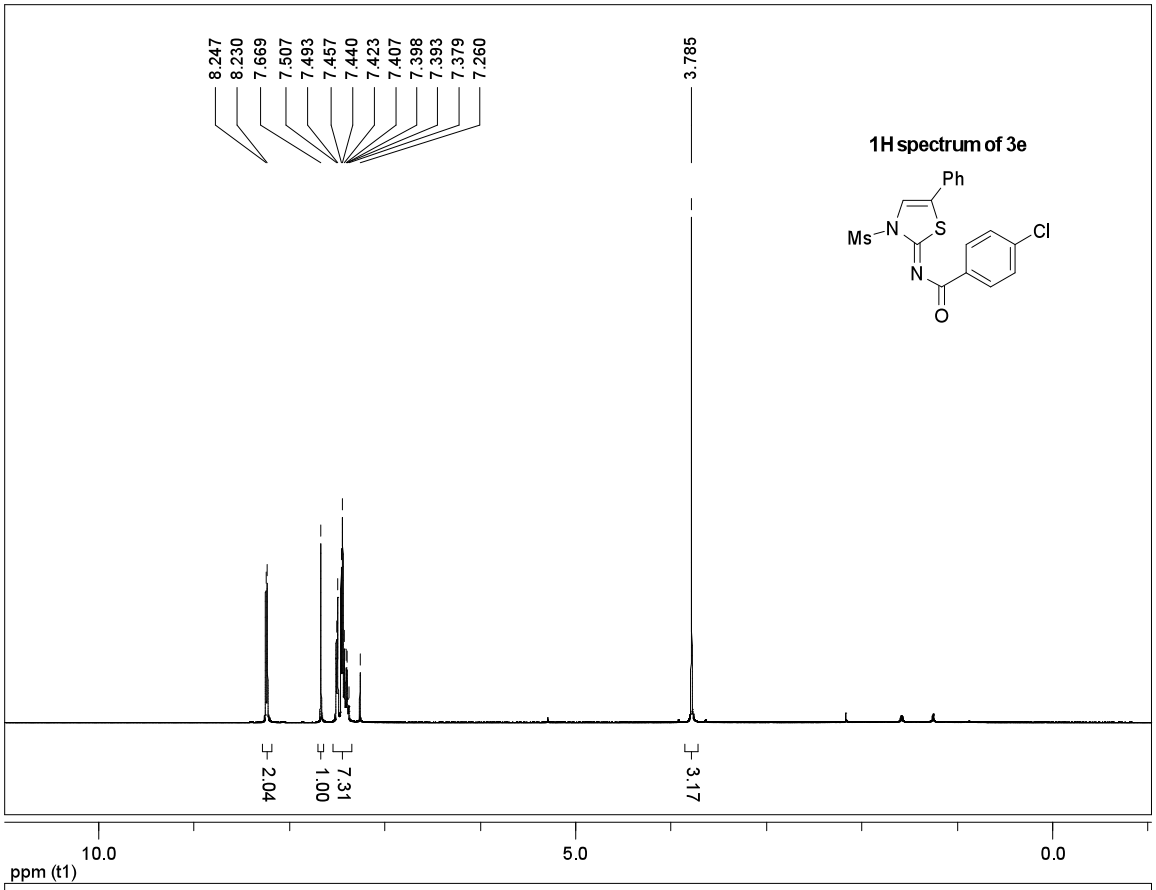
165.920
135.433
132.681
129.892
129.666
129.270
129.093
128.431
125.858
125.191
115.555
77.254
77.000
76.746
41.634
13C spectrum of 3b
Ph
Ms
N
S
N
Ph
O
200
150
100
50
0
ppm (t1)

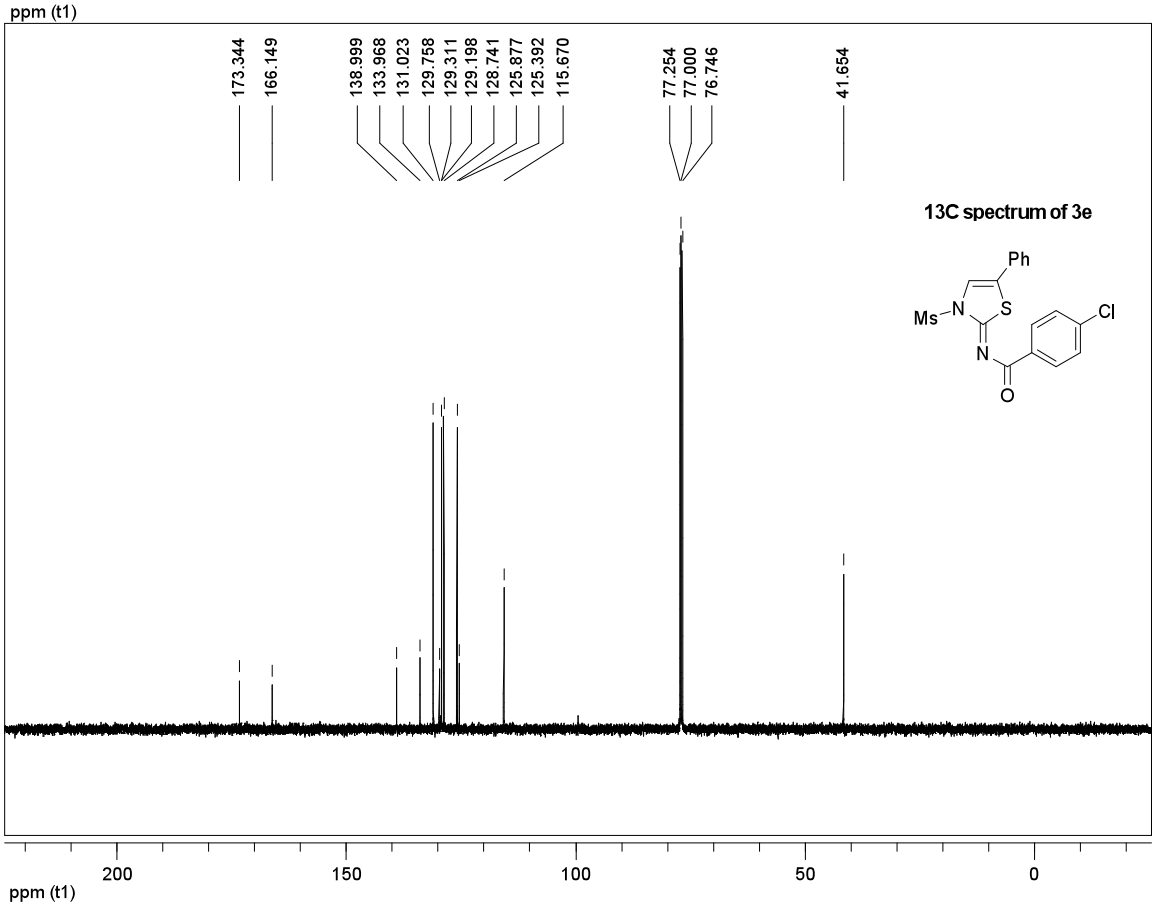

7.377
7.362
7.351
7.349
7.345
7.339
7.330
7.328
7.316
7.312
7.309
7.304
7.302
7.298
7.295
7.260
7.046
7.042
7.033
7.029
3.640
1H spectrum of 3c
Ph
Ms
N
S
N
Cl
7.98
1.94
3.00
10.0
5.0
0.0
ppm (t1)

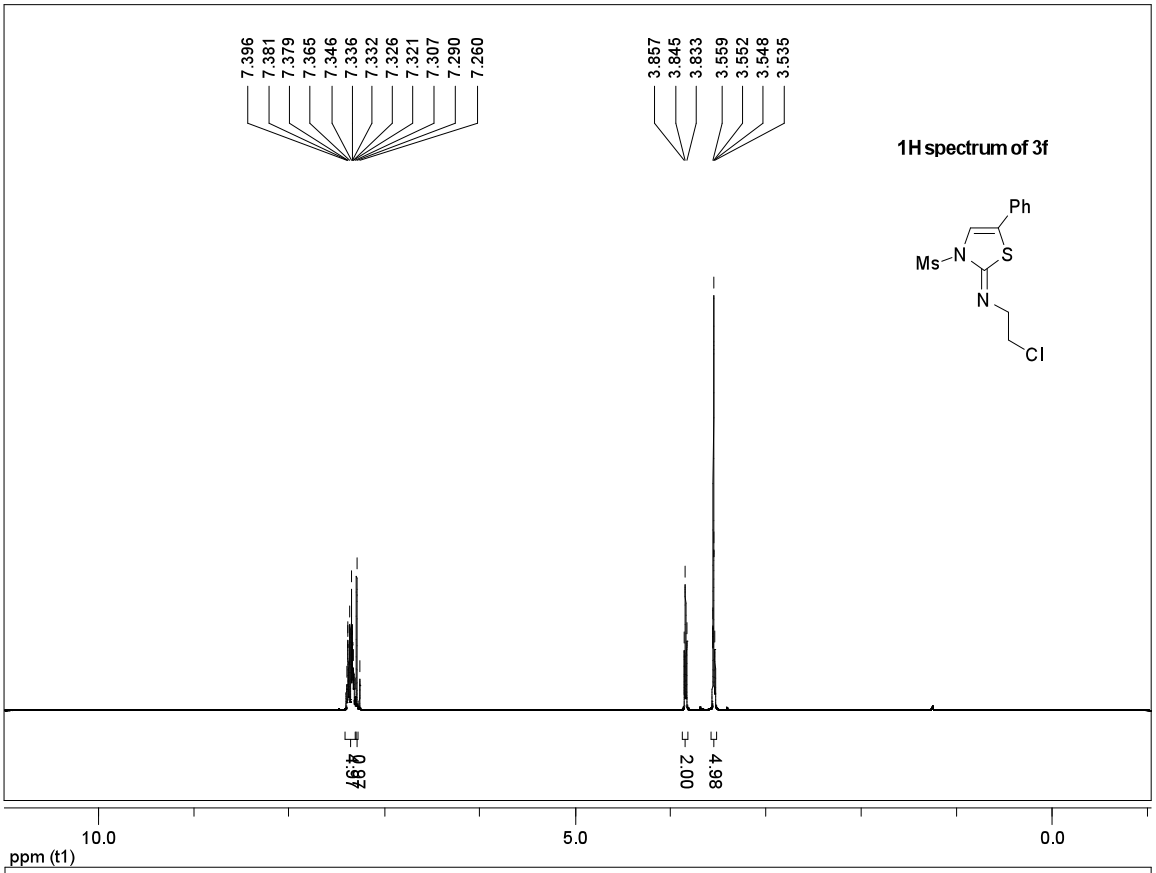

153.850
148.511
130.584
130.363
130.131
129.506
129.062
125.681
122.736
118.387
117.174
77.711
77.457
77.204
41.477
13C spectrum of 3c
Ph
Ms
N
S
N
Cl
200
150
100
50
0
ppm (t1)

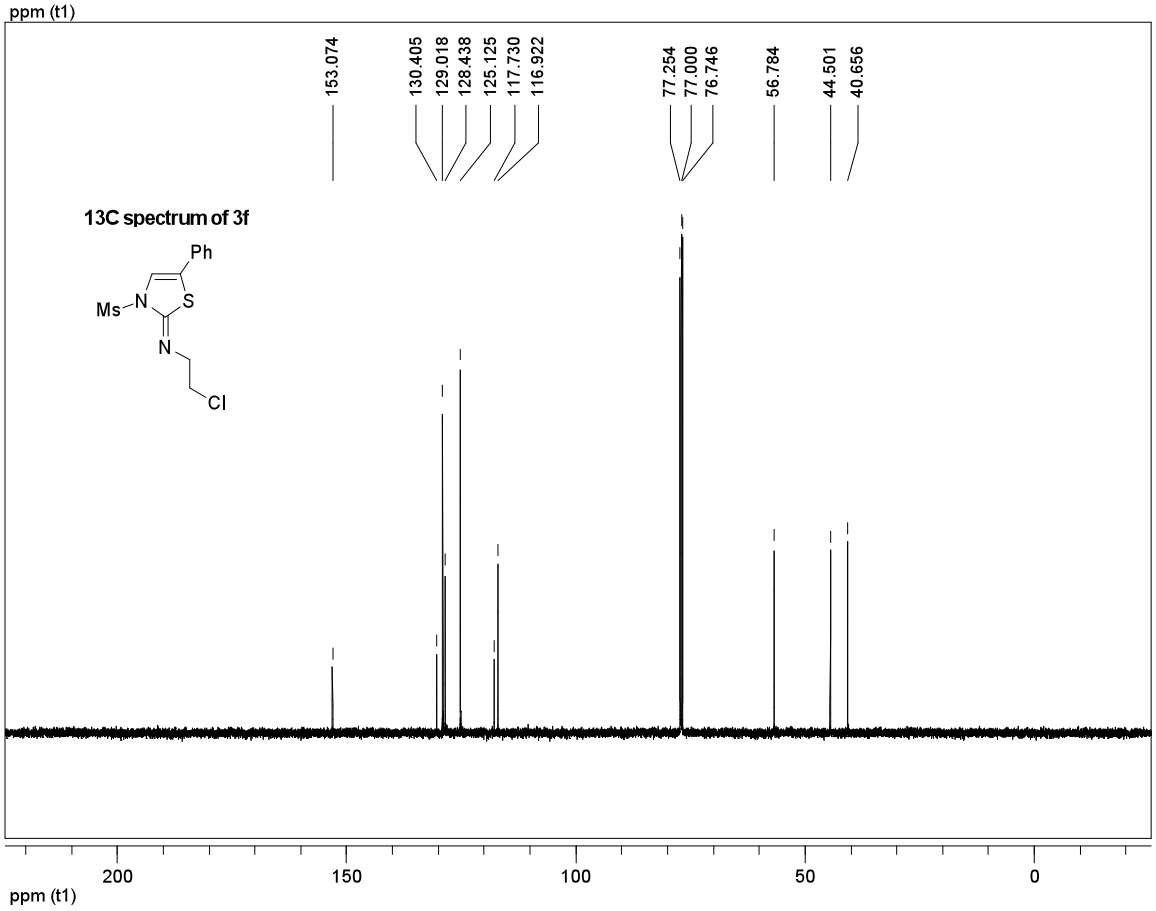

7.684
7.682
7.668
7.666
7.403
7.397
7.387
7.384
7.377
7.372
7.369
7.357
7.354
7.349
7.337
7.333
7.323
7.320
7.287
7.208
7.205
7.192
7.189
7.081
7.078
7.065
7.063
7.050
7.047
3.810
1H spectrum of 3d
Ph
Ms
N
S
N
Br
1.00
7.19
1.02
1.02
3.12
10.0
5.0
0.0
ppm (t1)

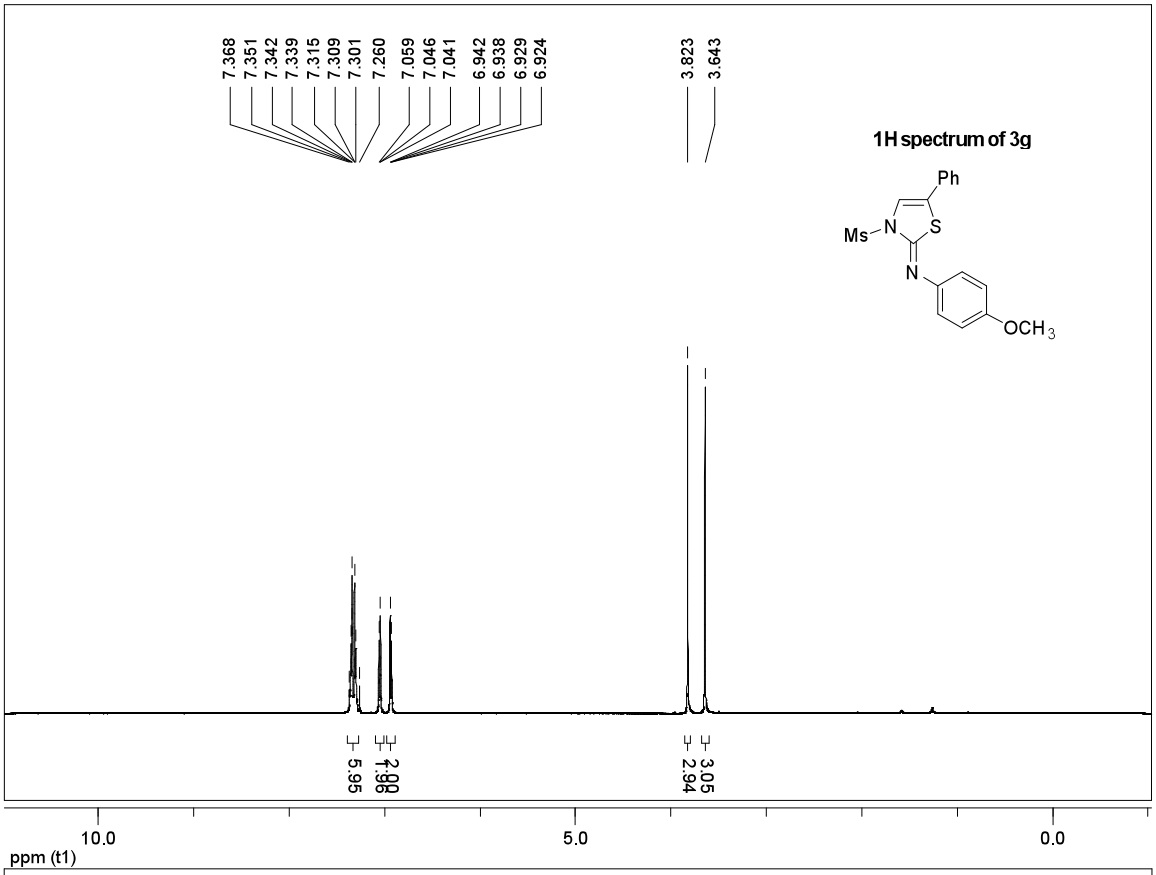

154.397
148.133
133.344
130.090
129.028
128.728
128.595
125.955
125.220
121.016
118.145
117.085
117.026
77.254
77.000
76.746
41.279
13C spectrum of 3d
Ph
Ms
N
S
N
Br
200
150
100
50
0
ppm (t1)

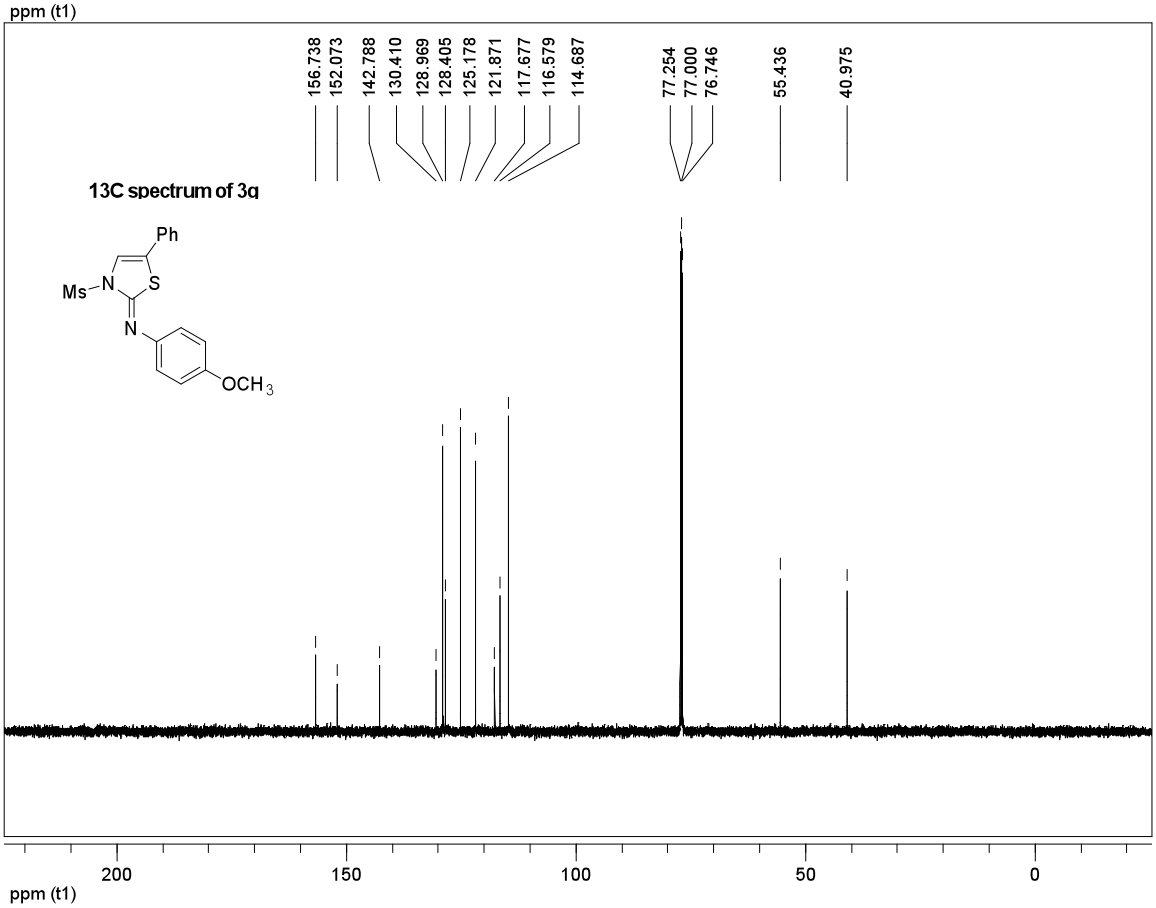

8.247
8.230
7.669
7.507
7.493
7.457
7.440
7.423
7.407
7.398
7.393
7.379
7.260
3.785
1H spectrum of 3e
Ph
Ms
N
S
Cl
N
O
2.04
1.00
7.31
3.17
10.0
5.0
0.0
ppm (t1)

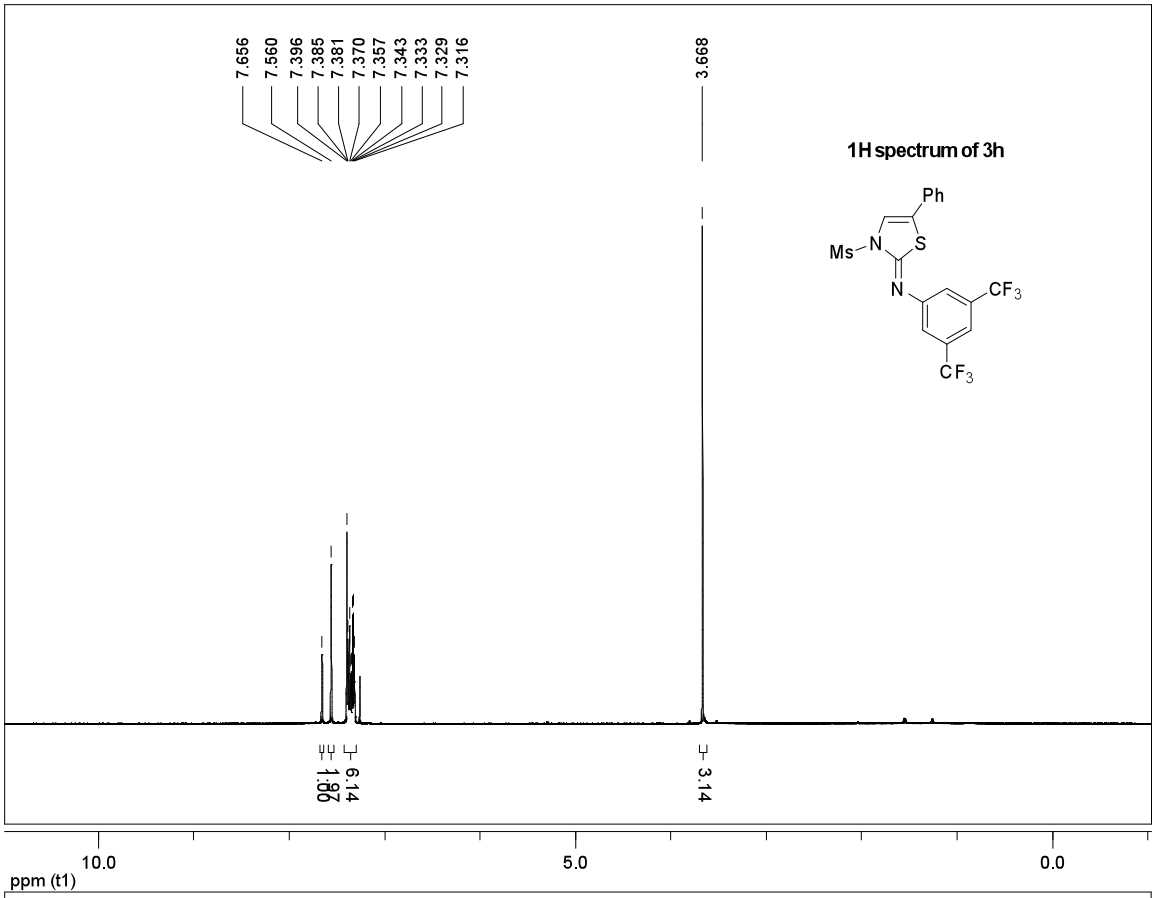

173.344
166.149
138.999
133.968
131.023
129.758
129.311
129.198
128.741
125.877
125.392
115.670
77.254
77.000
76.746
41.654
13C spectrum of 3e
Ph
Ms
N
S
Cl
N
O
200
150
100
50
0
ppm (t1)

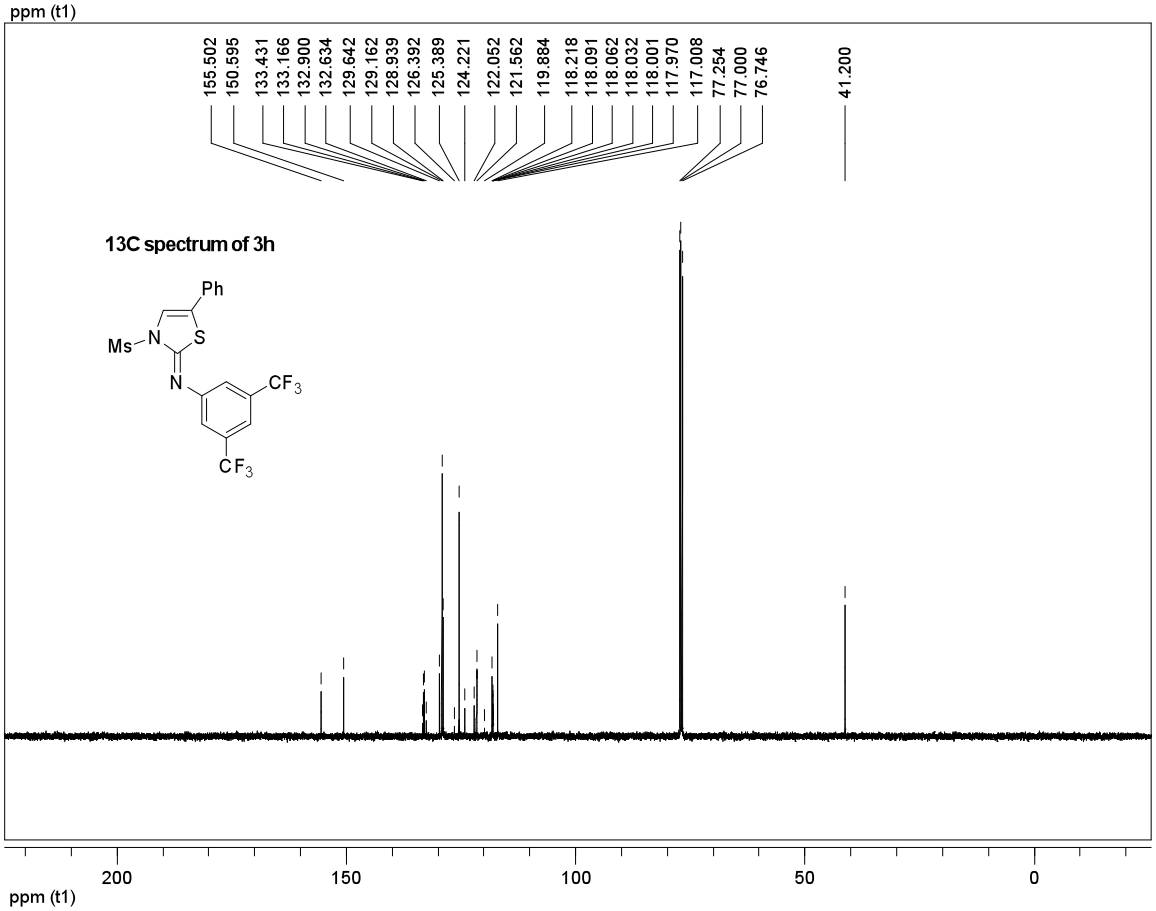

7.396
7.381
7.379
7.365
7.346
7.336
7.332
7.326
7.321
7.307
7.290
7.260
3.857
3.845
3.833
3.559
3.552
3.548
3.535
1H spectrum of 3f
Ph
Ms
N
S
N
Cl
4.97
2.00
4.98
10.0
5.0
0.0
ppm (t1)

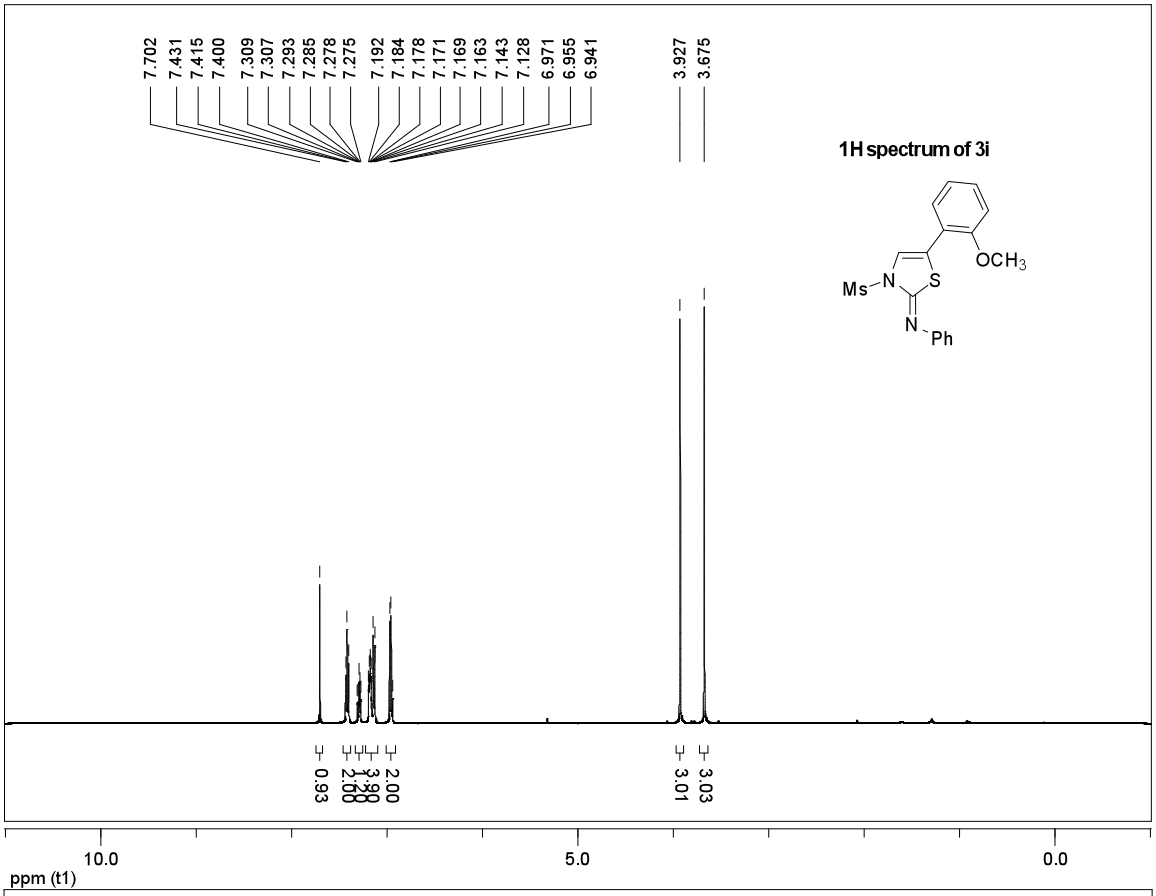

153.074
130.405
129.018
128.438
125.125
117.730
116.922
77.254
77.000
76.746
56.784
44.501
40.656
13C spectrum of 3f
Ph
Ms
N
S
N
Cl
200
150
100
50
0
ppm (t1)

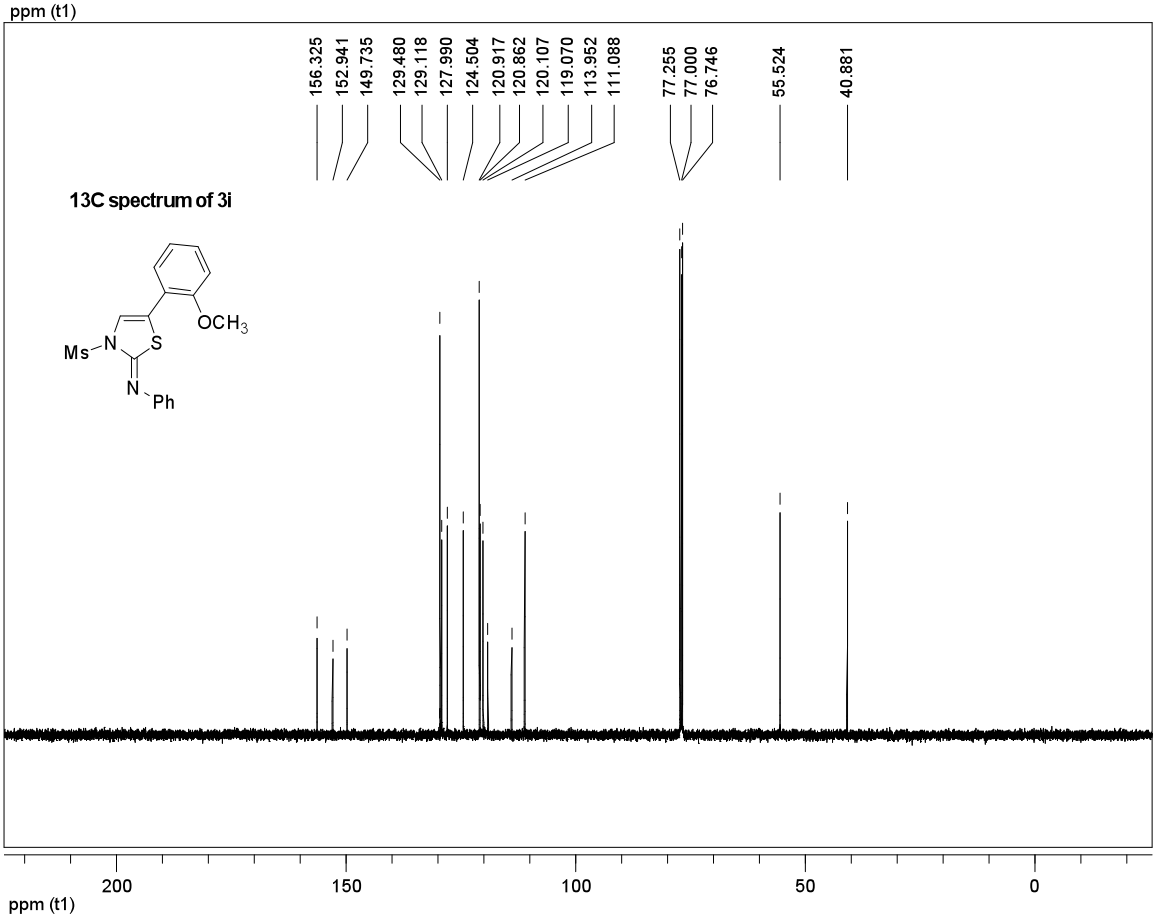

7.368
7.351
7.342
7.339
7.315
7.309
7.301
7.260
7.059
7.046
7.041
6.942
6.938
6.929
6.924
3.823
3.643
1H spectrum of 3g
Ph
Ms
N
S
N
OCH3
5.95
1.98
2.00
2.94
3.05
10.0
5.0
0.0
ppm (t1)

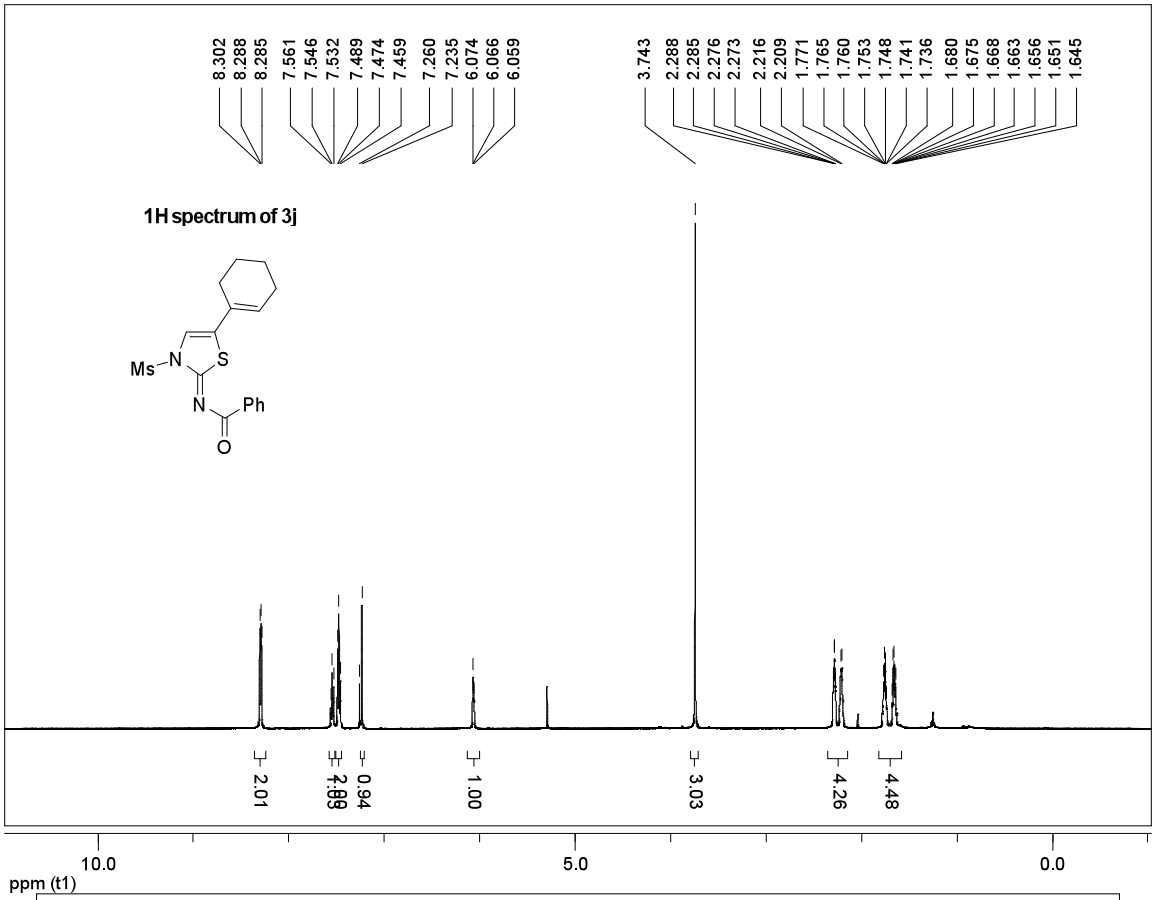

156.738
152.073
142.788
130.410
128.969
128.405
125.178
121.871
117.677
116.579
114.687
77.254
77.000
76.746
55.436
40.975
13C spectrum of 3g
Ph
Ms
N
S
N
OCH3
200
150
100
50
0
ppm (t1)

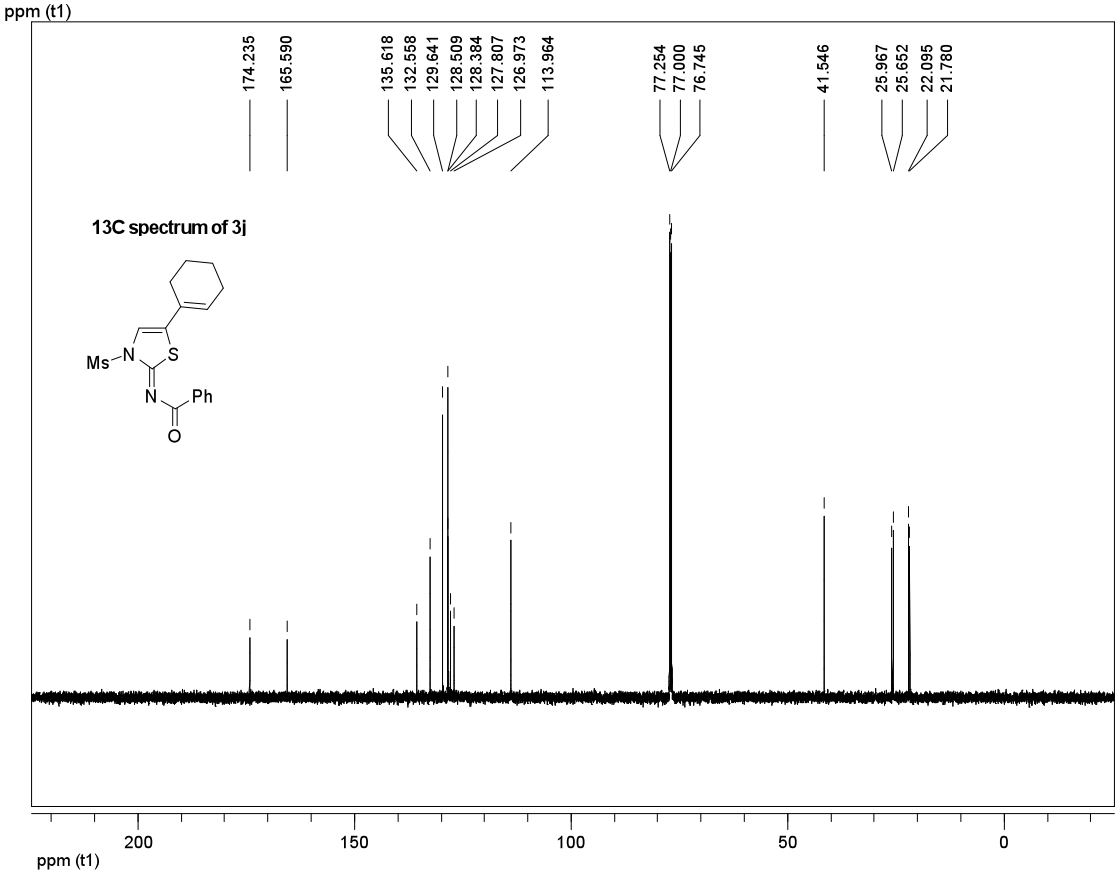

7.656
7.560
7.396
7.385
7.381
7.370
7.357
7.343
7.333
7.329
7.316
3.668
1H spectrum of 3h
Ph
Ms
N
S
N
CF3
CF3
1.00
1.97
6.14
3.14
10.0
5.0
0.0
ppm (t1)

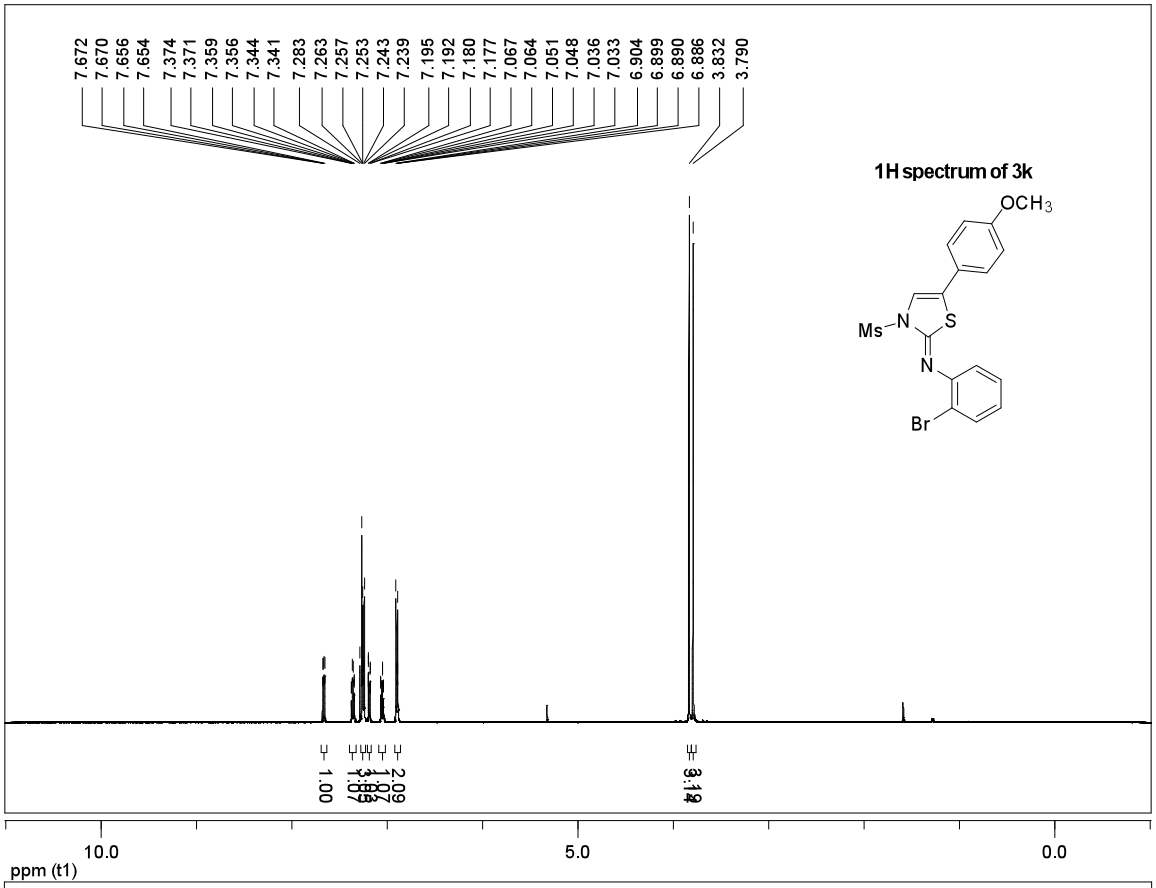

155.502
150.595
133.431
133.166
132.900
132.634
129.642
129.162
128.939
126.392
125.389
124.221
122.052
121.562
119.884
118.218
118.091
118.062
118.032
118.001
117.970
117.008
77.254
77.000
76.746
41.200
13C spectrum of 3h
Ph
Ms
N
S
N
CF3
CF3
200
150
100
50
0
ppm (t1)

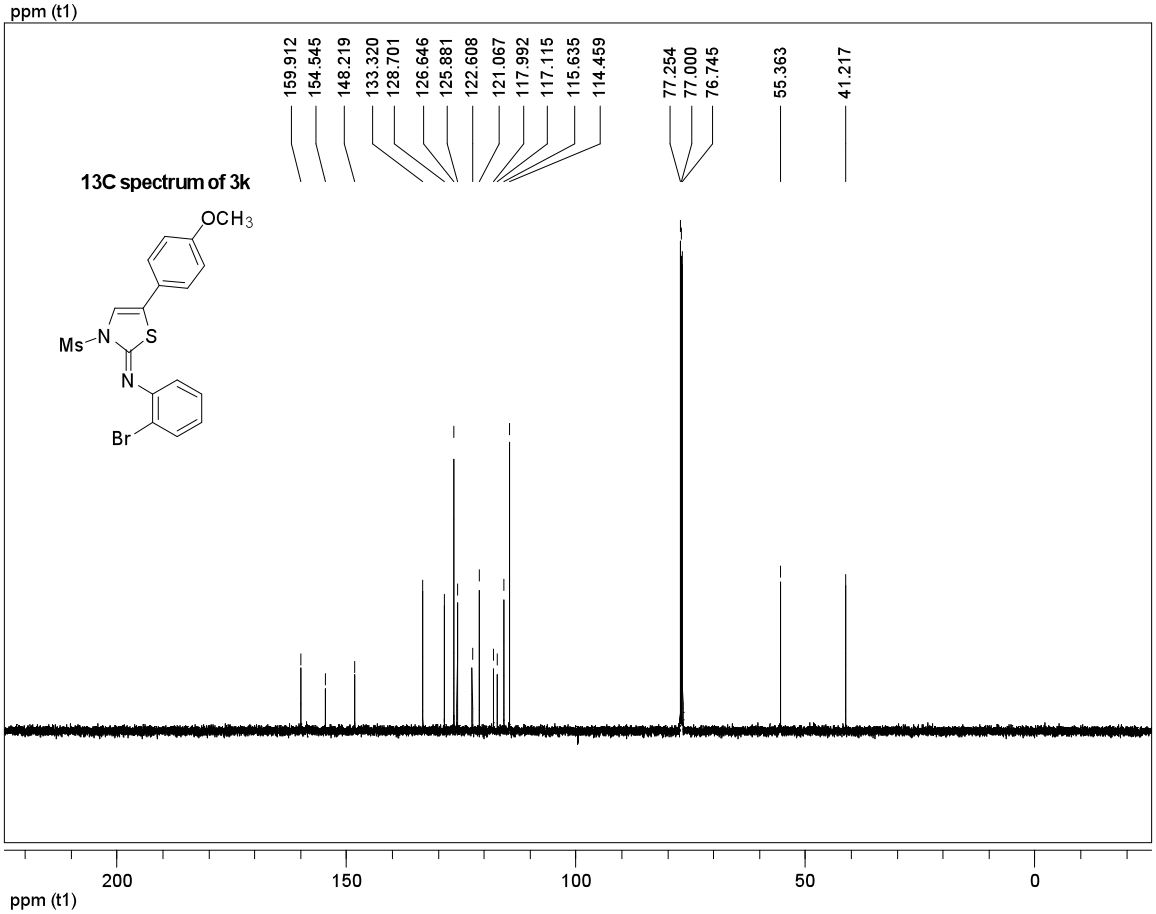

7.702
7.431
7.415
7.400
7.309
7.307
7.293
7.285
7.278
7.275
7.192
7.184
7.178
7.171
7.169
7.163
7.143
7.128
6.971
6.955
6.941
3.927
3.675
1H spectrum of 3i
OCH3
Ms
N
S
N
Ph
0.93
2.00
3.01
3.03
10.0
5.0
0.0
ppm (t1)

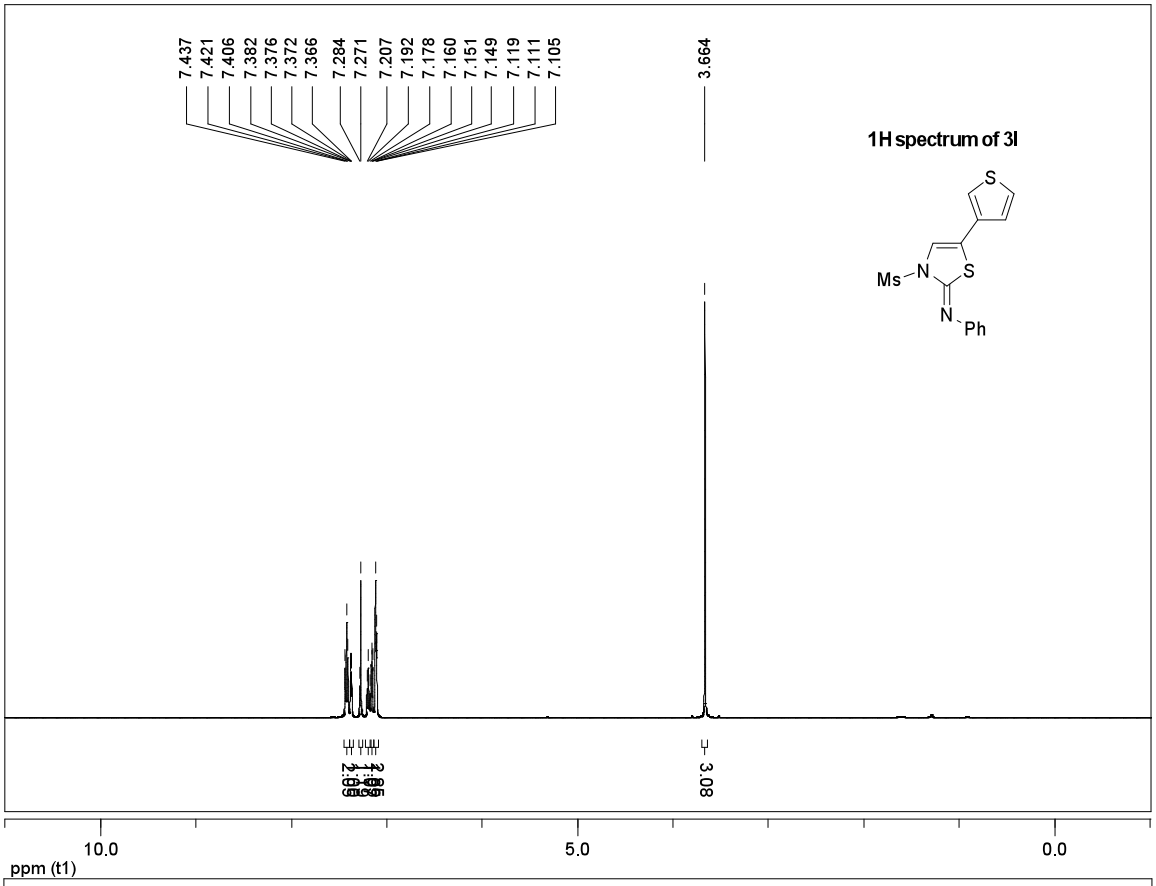

156.325
152.941
149.735
129.480
129.118
127.990
124.504
120.917
120.862
120.107
119.070
113.952
111.088
77.255
77.000
76.746
55.524
40.881
13C spectrum of 3i
OCH3
Ms
N
S
N
Ph
200
150
100
50
0
ppm (t1)

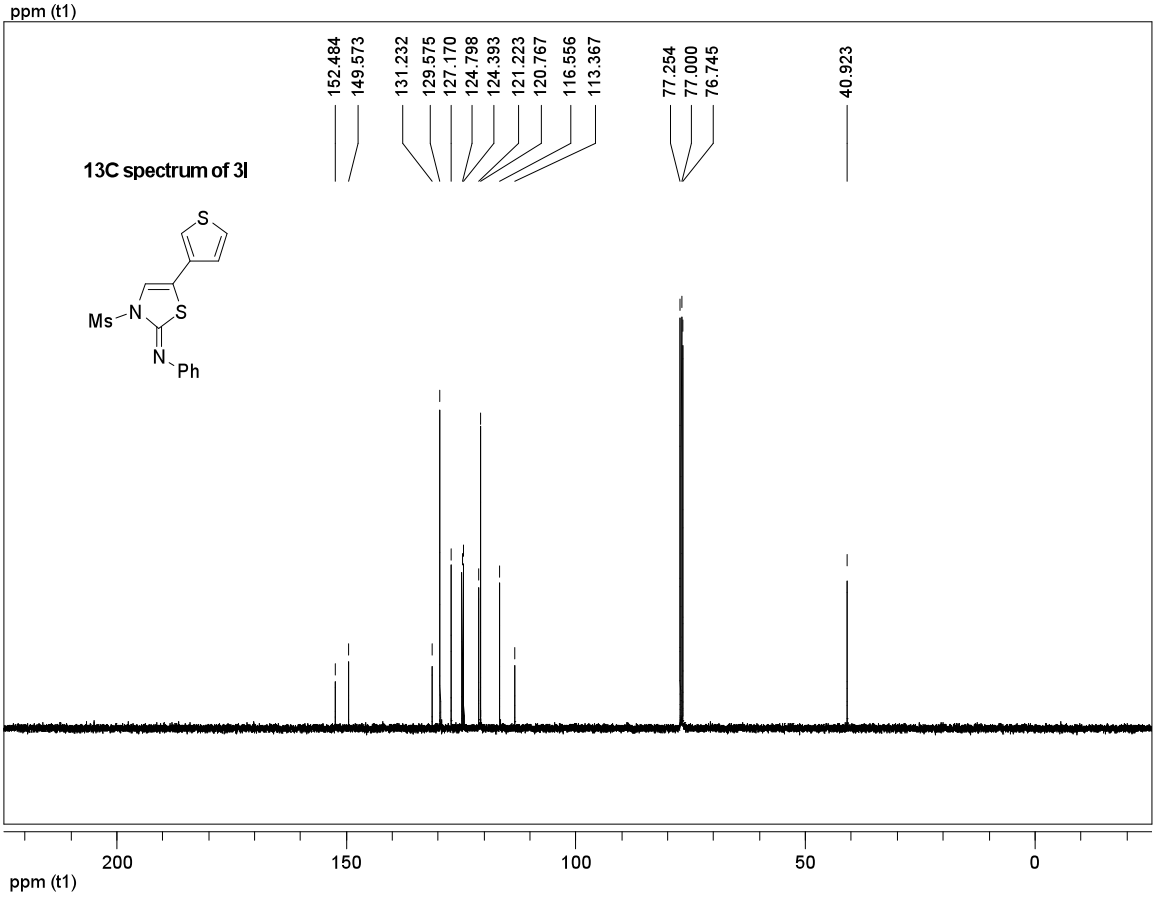

8.302
8.288
8.285
7.561
7.546
7.532
7.489
7.474
7.459
7.260
7.235
6.074
6.066
6.059
3.743
2.288
2.285
2.276
2.273
2.216
2.209
1.771
1.765
1.760
1.753
1.748
1.741
1.736
1.680
1.675
1.668
1.663
1.656
1.651
1.645
1H spectrum of 3j
Ms
N
S
N
Ph
O
2.01
2.89
0.94
1.00
3.03
4.26
4.48
10.0
5.0
0.0
ppm (t1)

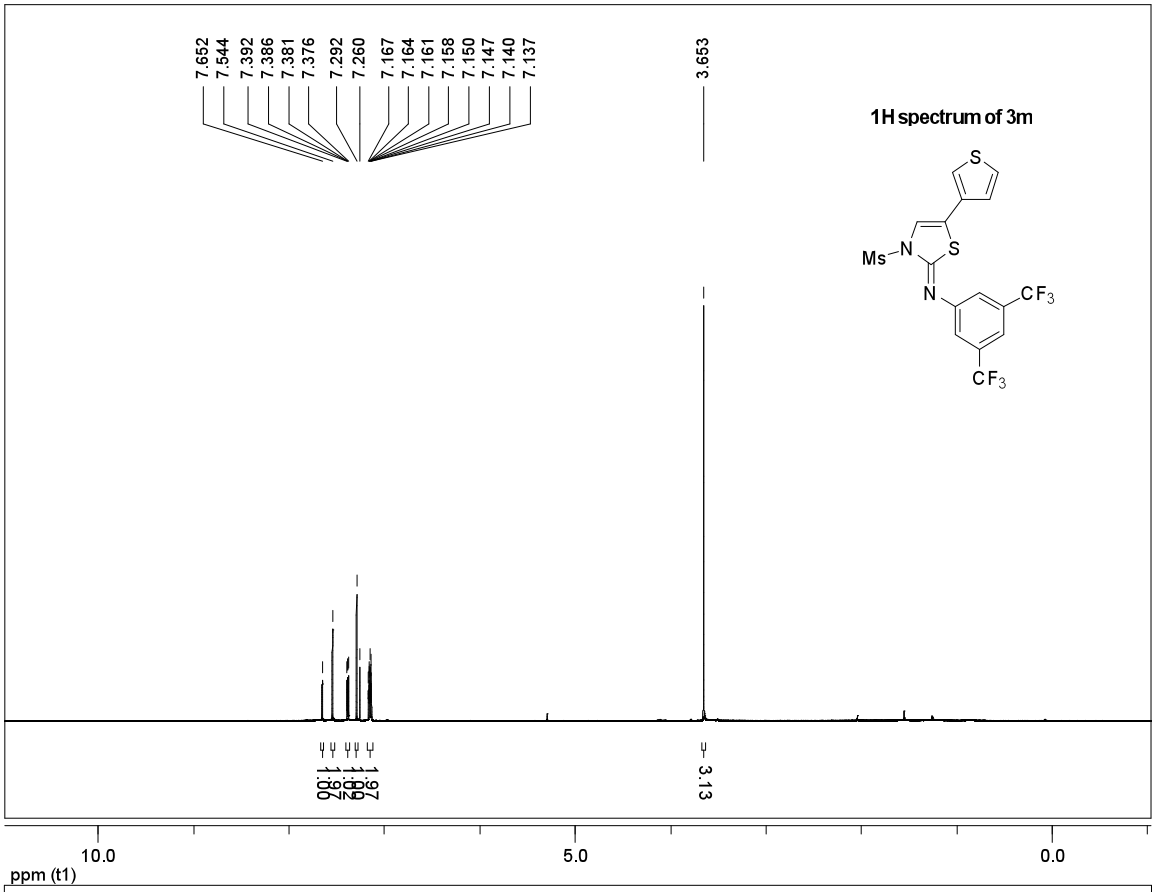

174.235
165.590
135.618
132.558
129.641
128.509
128.384
127.807
126.973
113.964
77.254
77.000
76.745
41.546
25.967
25.652
22.095
21.780
13C spectrum of 3j
Ms
N
S
N
Ph
O
200
150
100
50
0
ppm (t1)

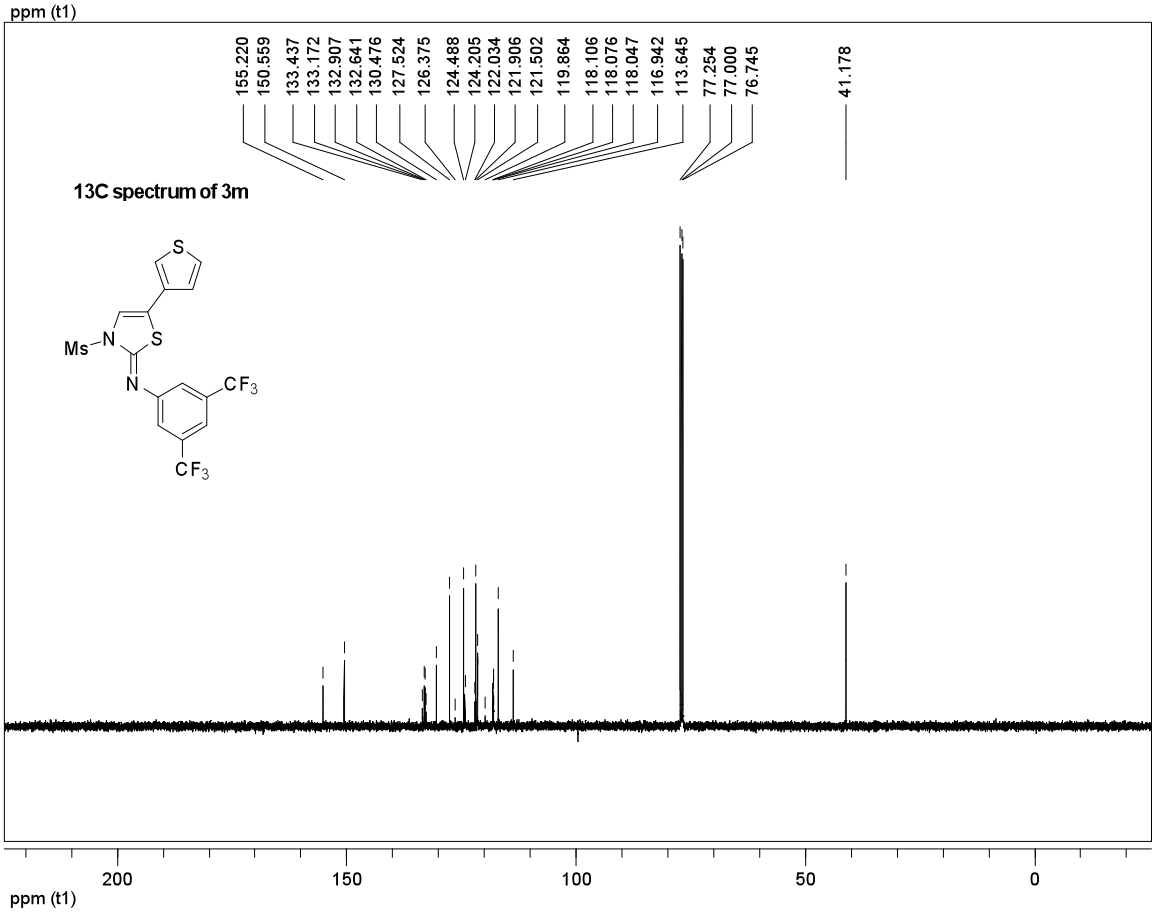

7.672
7.670
7.656
7.654
7.374
7.371
7.359
7.356
7.344
7.341
7.283
7.263
7.257
7.253
7.243
7.239
7.195
7.192
7.180
7.177
7.067
7.064
7.051
7.048
7.036
7.033
6.904
6.899
6.890
6.886
3.832
3.790
1H spectrum of 3k
OCH3
Ms
N
S
N
Br
1.00
2.09
3.14
10.0
5.0
0.0
ppm (t1)

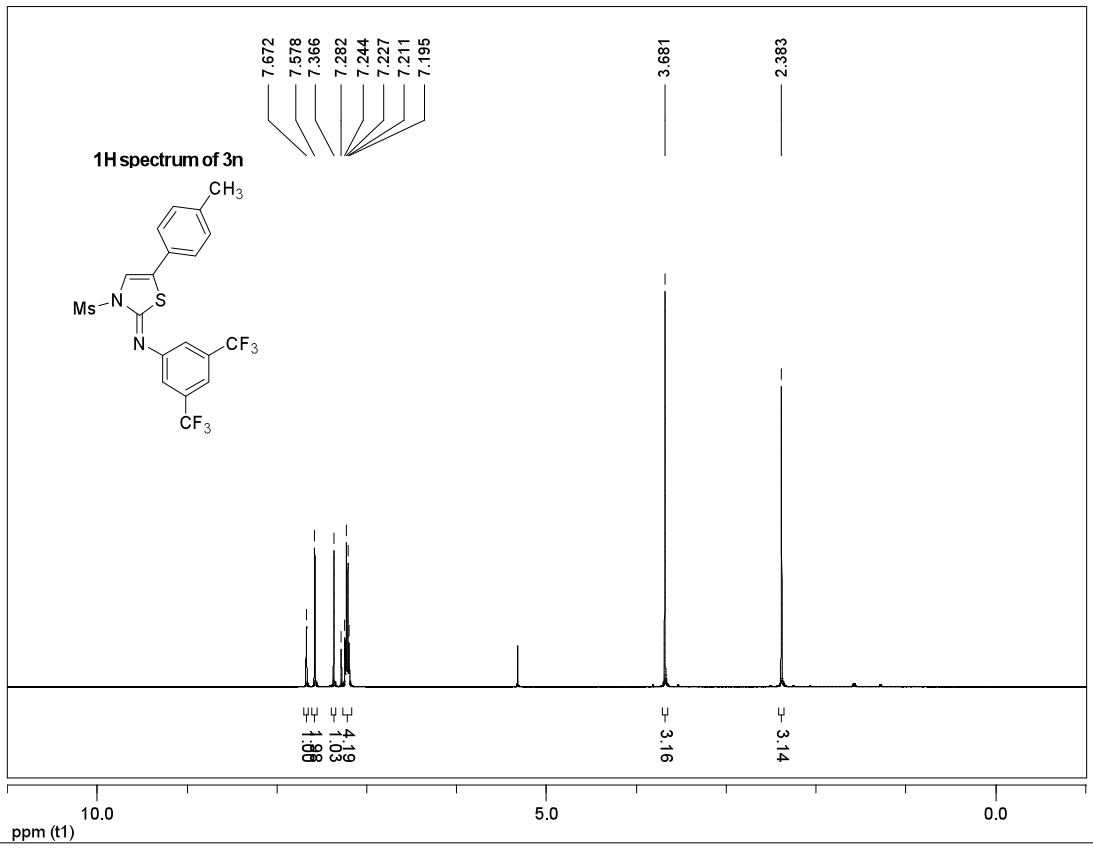

159.912
154.545
148.219
133.320
128.701
126.646
125.881
122.608
121.067
117.992
117.115
115.635
114.459
77.254
77.000
76.745
55.363
41.217
13C spectrum of 3k
OCH3
Ms
N
S
N
Br
200
150
100
50
0
ppm (t1)


7.437
7.421
7.406
7.382
7.376
7.372
7.366
7.284
7.271
7.207
7.192
7.178
7.160
7.151
7.149
7.119
7.111
7.105
3.664
1H spectrum of 3l
S
Ms
N
S
N
Ph
3.08
10.0
5.0
0.0
ppm (t1)


152.484
149.573
131.232
129.575
127.170
124.798
124.393
121.223
120.767
116.556
113.367
77.254
77.000
76.745
40.923
13C spectrum of 3l
S
Ms
N
S
N
Ph
200
150
100
50
0
ppm (t1)


7.652
7.544
7.392
7.386
7.381
7.376
7.292
7.260
7.167
7.164
7.161
7.158
7.150
7.147
7.140
7.137
3.653
1H spectrum of 3m
Ms
N
S
S
N
CF3
CF3
1.00
1.00
1.00
1.00
1.00
1.97
3.13
10.0
5.0
0.0
ppm (t1)


155.220
150.559
133.437
133.172
132.907
132.641
130.476
127.524
126.375
124.488
124.205
122.034
121.906
121.502
119.864
118.106
118.076
118.047
116.942
113.645
77.254
77.000
76.745
41.178
13C spectrum of 3m
Ms
N
S
S
N
CF3
CF3
200
150
100
50
0
ppm (t1)


1H spectrum of 3n
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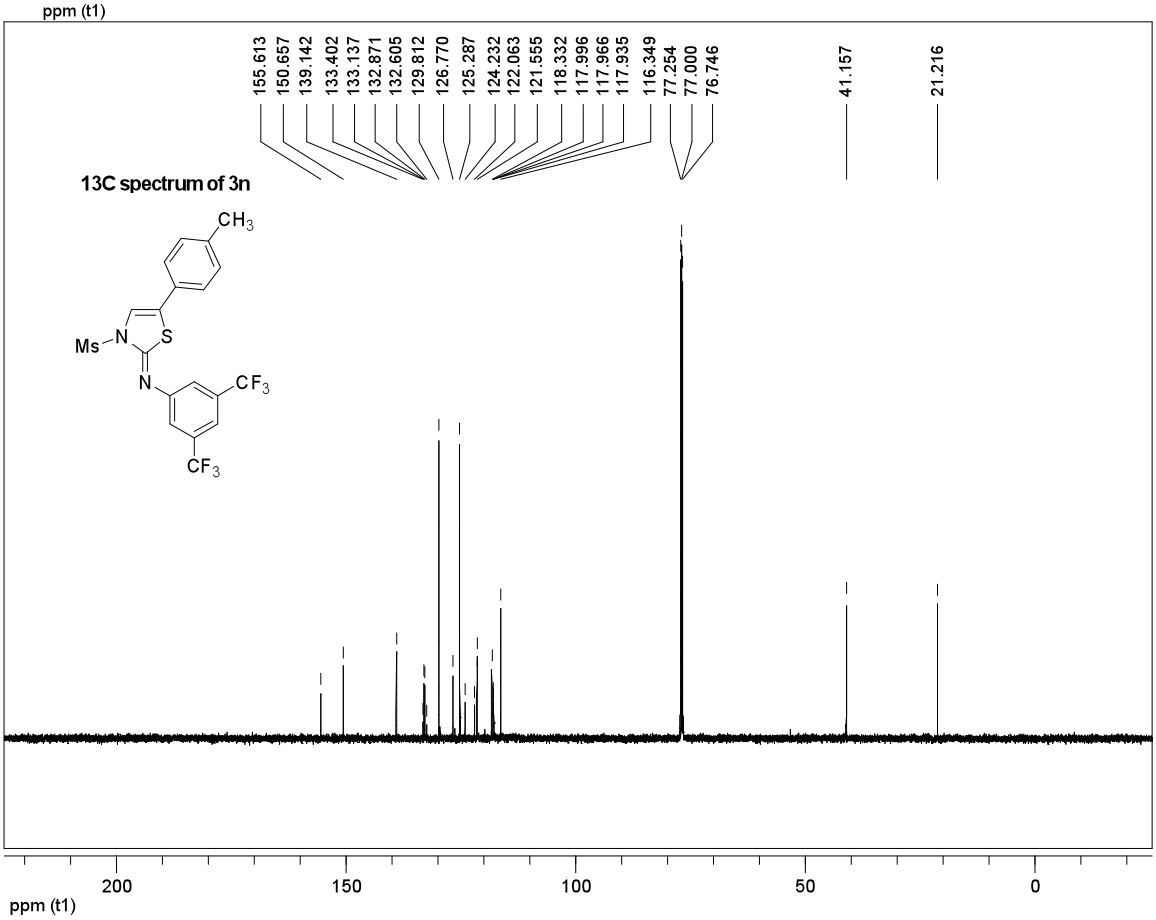
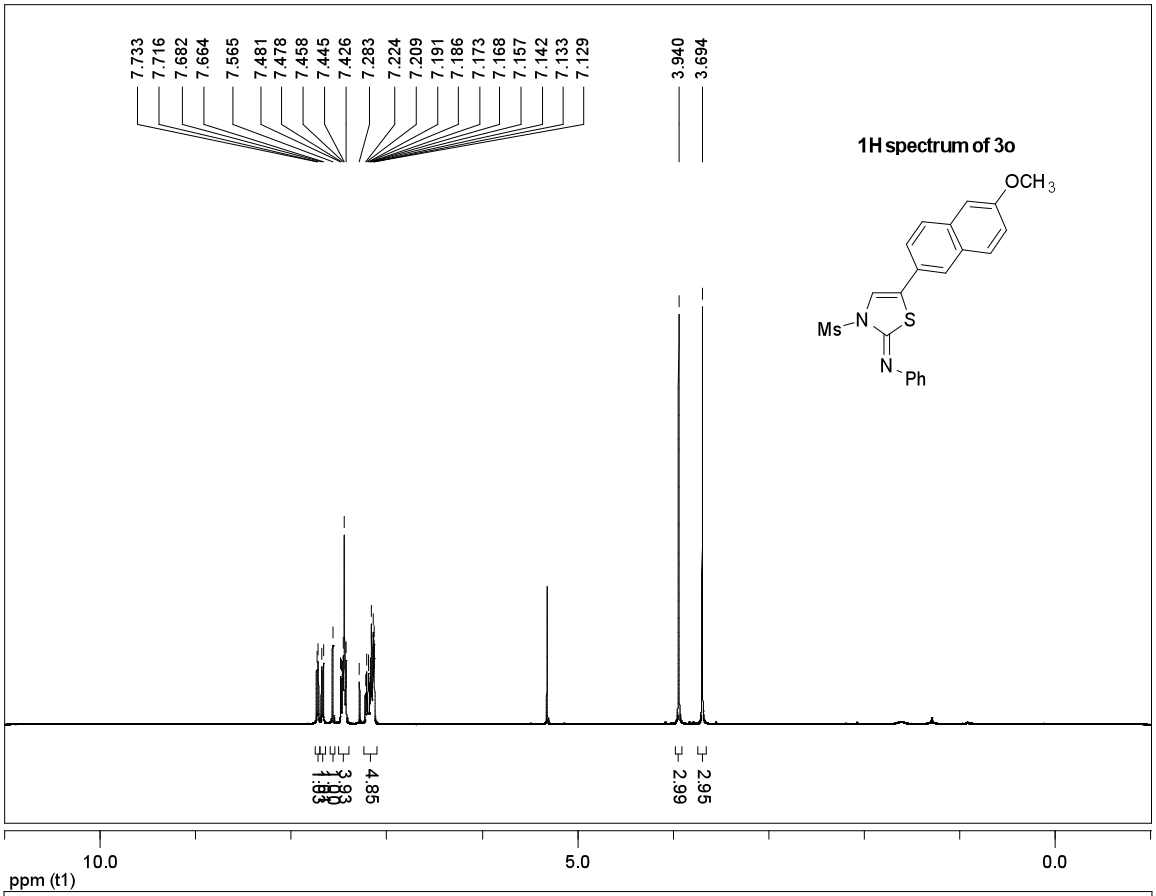
7.578
7.366
7.282
7.244
7.227
7.211
7.195
3.681
2.383
1.00
1.00
1.03
4.19
3.16
3.14
10.0
5.0
0.0
ppm (t1)


13C spectrum of 3n
155.613
150.657
139.142
133.402
133.137
132.871
132.605
129.812
126.770
125.287
124.232
122.063
121.555
118.332
117.996
117.966
117.935
116.349
77.254
77.000
76.746
41.157
21.216
200
150
100
50
0
ppm (t1)


7.733
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7.682
7.664
7.565
7.481
7.478
7.458
7.445
7.426
7.283
7.224
7.209
7.191
7.186
7.173
7.168
7.157
7.142
7.133
7.129
3.940
3.694
1H spectrum of 3o
OCH3
Ms
N
S
N
Ph
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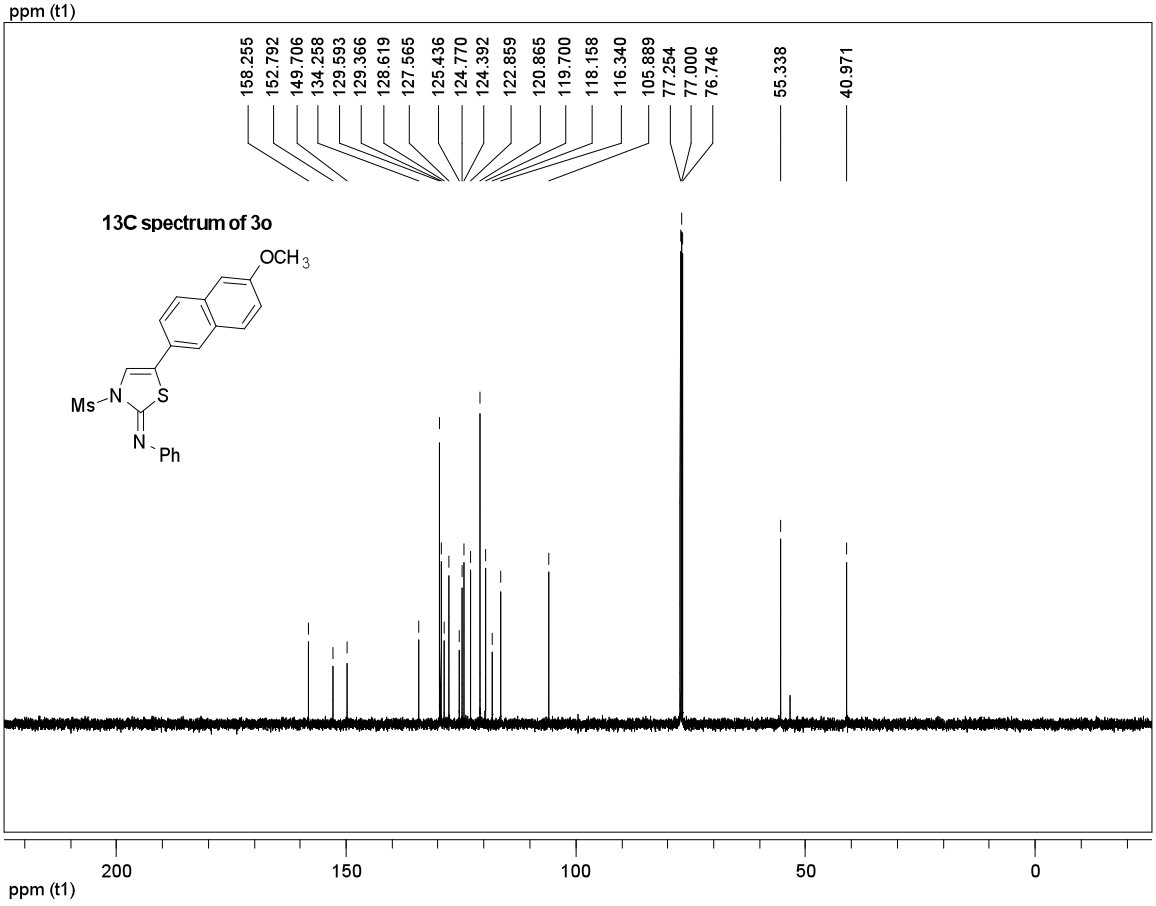
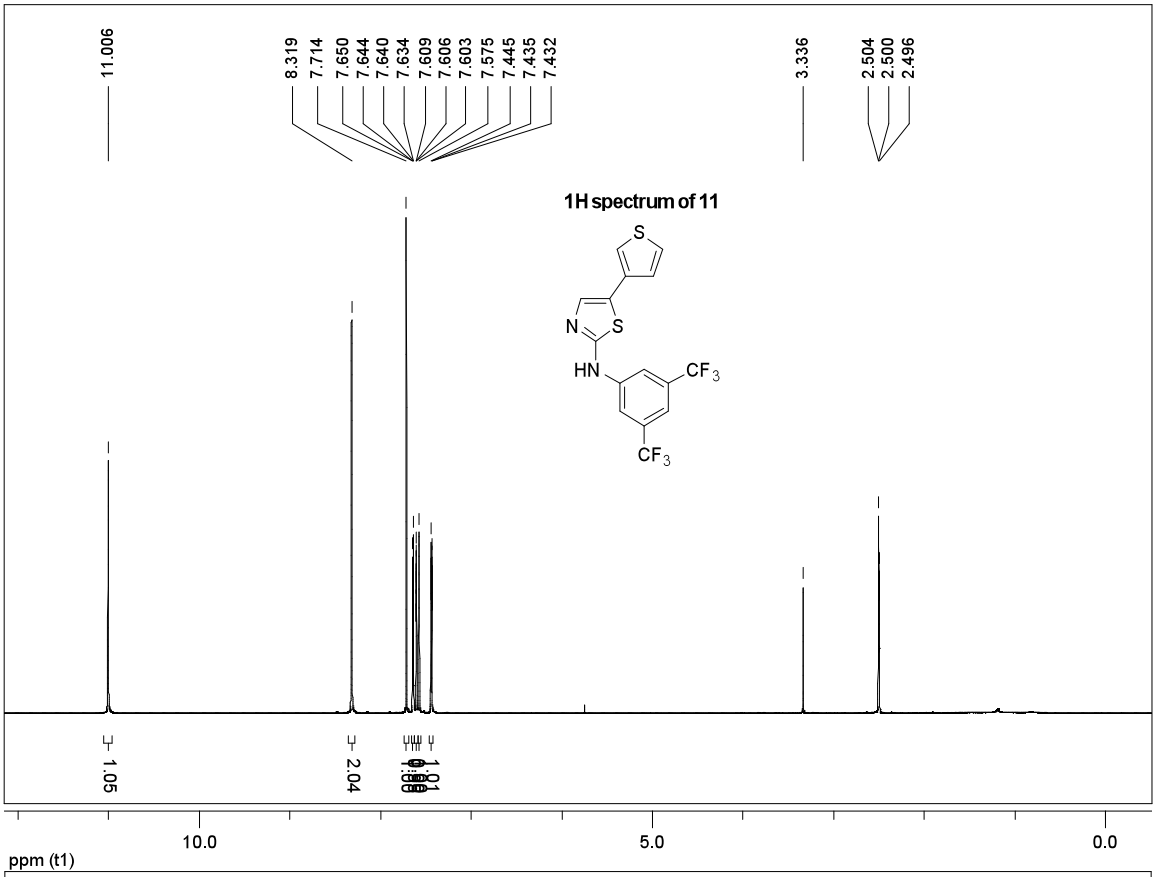
2.99
2.95
10.0
5.0
0.0
ppm (t1)


158.255
152.792
149.706
134.258
129.593
129.366
128.619
127.565
125.436
124.770
124.392
122.859
120.865
119.700
118.158
116.340
105.889
77.254
77.000
76.746
55.338
40.971
13C spectrum of 3o
OCH3
Ms
N
S
N
Ph
200
150
100
50
0
ppm (t1)


11.006
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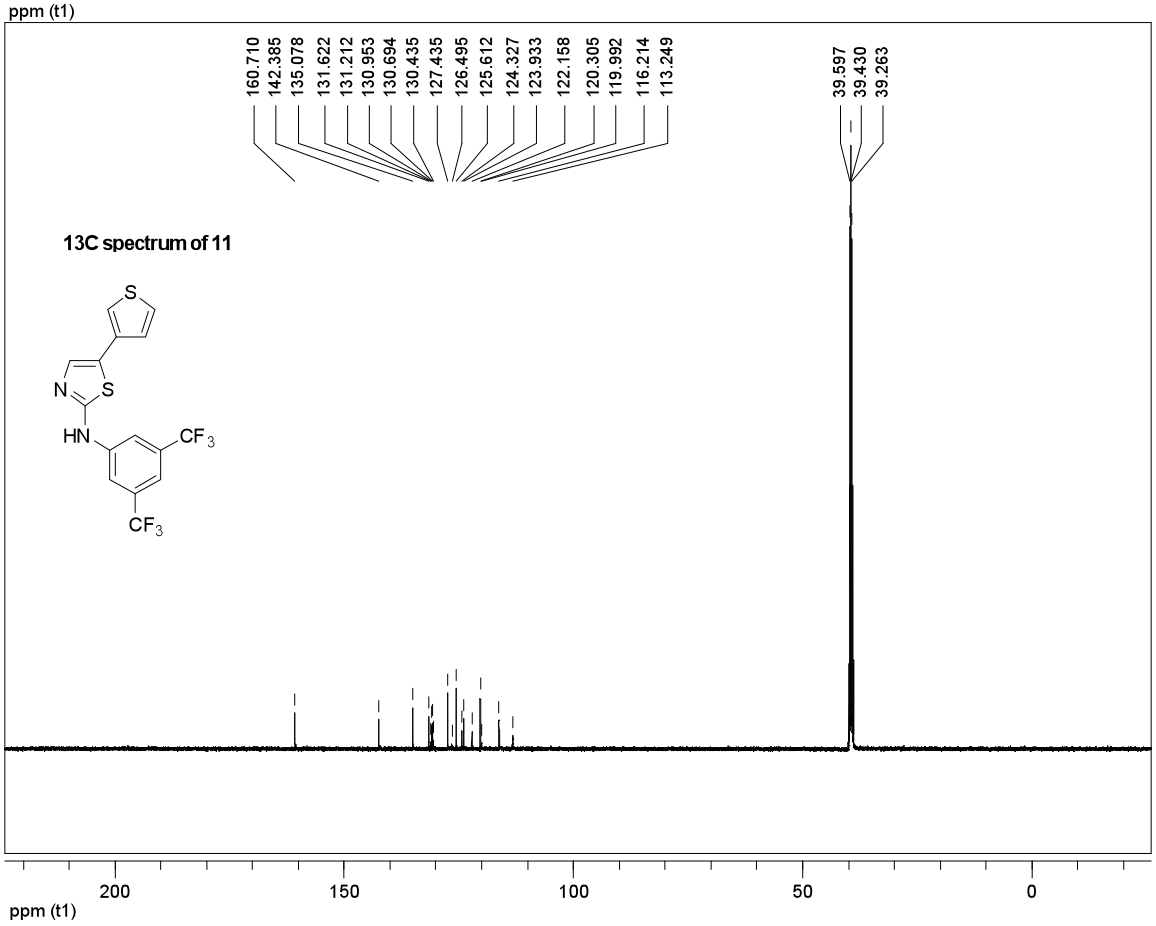
7.714
7.650
7.644
7.640
7.634
7.609
7.606
7.603
7.575
7.445
7.435
7.432
3.336
2.504
2.500
2.496
1H spectrum of 11
S
N
S
HN
CF3
CF3
1.05
2.04
10.0
5.0
0.0
ppm (t1)


160.710
142.385
135.078
131.622
131.212
130.953
130.694
130.435
127.435
126.495
125.612
124.327
123.933
122.158
120.305
119.992
116.214
113.249
39.597
39.430
39.263
13C spectrum of 11
S
N
S
HN
CF3
CF3
200
150
100
50
0
ppm (t1)