

Supporting Information

Copper-catalyzed Regioselective Trifluoromethylthiolation of Pyrroles by Trifluoromethanesulfonyl Hypervalent Iodonium Ylide

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1. Figure S1, S2 and Table S1

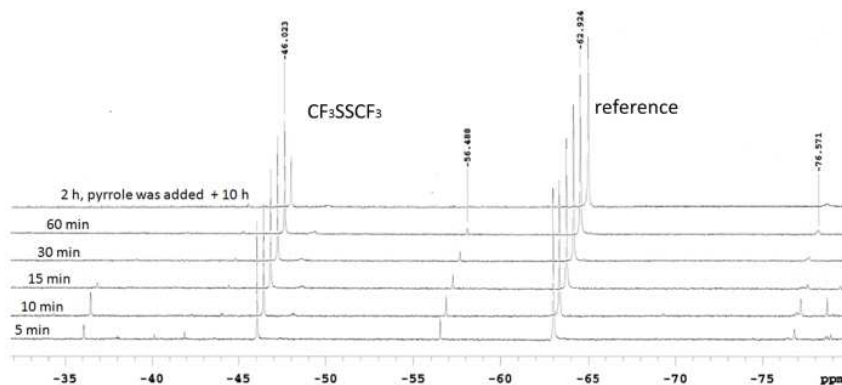


Figure S1. ^{19}F NMR experiments of reaction of **5** in the presence of CuF_2 in NMP from 5 min. to 60 min. Pyrrole **6a** was added after 2 h

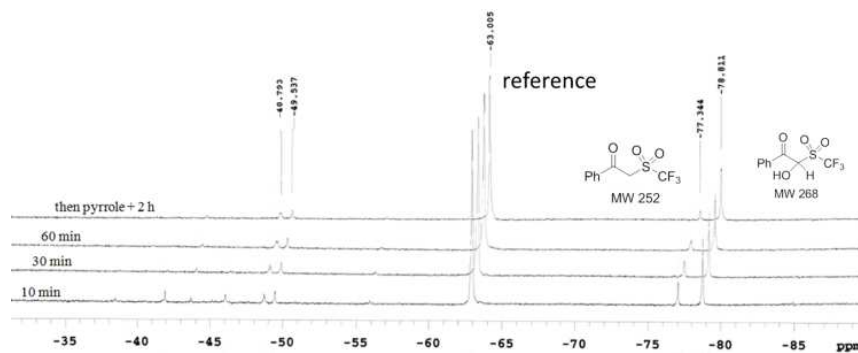


Figure S2. ^{19}F NMR experiments of reaction of **5** with TEMPO in the presence of CuF_2 in NMP from 10 min. to 60 min. Pyrrole **6a** was added after 1 h

Table S1. Prediction of Chemical Shifts (ppm, ^{19}F NMR) of the Intermediates **11-14** by Computations

Method	HF	EDF2			B3LYP			
compounds	6-31G*	6-31G*	6-31G**	6-311G*	6-31G*	6-31G**	6-311G*	Observed
11	-45.0	-57.0	-74.4	-84.8	-74.4	-74.3	-85.8	-76.6 ^a
12	-35.2	-48.2	-65.4	-73.5	-65.1	-65.0	-74.1	-56.4 ^a
13	-53.2	-86.0	-86.0	-96.8	-85.5	-85.4	-97.9	-78.8 ^a
14	-59.9	-95.7	-95.5	-107.2	-94.8	-94.6	-107.4	-77.3 ^b
CF_3SSCF_3	-24.0	-37.1	-52.7	-58.3	-52.2	-52.1	-58.9	-46.0 ^b

^aPrediction. ^bAuthentic data of **14** and CF_3SSCF_3 .

2. General Methods

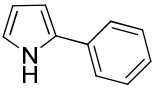
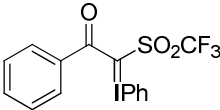
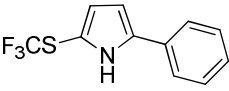
All reagents were used as received from commercial sources, unless specified otherwise, or prepared as described in the literature. Reactions requiring anhydrous conditions were performed in oven-dried glassware under a positive pressure of nitrogen. Reaction mixtures were stirred magnetically. Solvents were transferred via syringe and were introduced into the reaction vessels through a rubber septum. All of the reactions were monitored by thin-layer chromatography (TLC) carried out on 0.25 mm Merck silica-gel (60-F254). The TLC plates were visualized with UV light and 7% phosphomolybdic acid or KMnO_4 in water/heat. Column chromatography was carried out on a column packed with silica-gel 60N spherical neutral size 63-210 μm . The ^1H -NMR (300 MHz) and ^{19}F -NMR (282.3 MHz) spectra were recorded on a Varian Mercury 300. The ^{13}C -NMR (150.9 MHz) was recorded on a Bruker Avance 600. Chemical shifts (δ) are reported in parts per million and coupling constants (J) are in hertz. All the melting points are uncorrected. Mass spectra were recorded on a SHIMADZU GCMS-QP5050A(EI-MS) and SHIMADZU LCMS-2010EV (ESI-MS and APCI-MS). Infrared spectra were recorded on a JASCO FT/IR-200 spectrometer.

General procedure for trifluoromethylthiolation of pyrroles

To a mixture of pyrrole (0.2 mmol) and reagent **5** (0.4 mmol) in NMP (1.5 mL), CuF_2 (0.04 mmol) was added. The reaction was stirred at room temperature, monitored by TLC. After the reaction was complete, the reaction mixture was extracted with Et_2O , washed with water, brine and dried over Na_2SO_4 , used column chromatography on silica gel, using n-hexane and AcOEt as eluent, to give the desired product.

3. Optimization of reaction conditions

Table S2. Reaction Conditions of Pyrrole **6a** with Reagent **5**^a

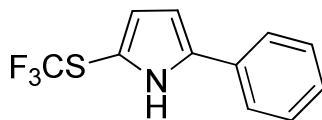
 6a +  5 $\xrightarrow[\text{THF, rt, 6 h}]{\text{additive (20 mol \%)} \\ \text{catalyst (20 mol \%)}}$  7a			
entry	catalyst	additive	yield (%) ^b
1	LiCl	-	11
2	FeCl_2	-	14
3	CaF_2	-	3

4	ZnF ₂	-	9
5	CoF ₃	-	13
6	Cu(OTf) ₂	-	3
7	CuF ₂	phthalimide	63
8 ^c	CuF ₂	phthalimide	28
9	CuF ₂	DMAP	55
10	CuF ₂	PhNMe ₂	31
11	CuF ₂	PPh ₃	32
12	CuF ₂	PhSEt	68
13	CuF ₂	Ph ₂ S	73
14	CuF ₂	PhOEt	75
15	CuF ₂	PhOH	3
16	CuF ₂	HFIP	33

^aReaction conditions: pyrrole **6a** (0.1 mmol), reagent **5** (0.2 mmol), additive (20 mol %), catalyst (20 mol %), THF (0.75 mL), stirred at room temperature for 6 h. ^bYields were determined by ¹⁹F NMR spectroscopy with trifluoromethyl benzene as the internal standard. ^cThe reaction was performed at 60 °C.

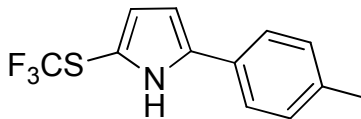
4. Experimental Data

2-Phenyl-5-[(trifluoromethyl)thio]pyrrole (**7a**)



Violet solid. m.p.: 72-73 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.59 (s, 1H), 7.50 (d, *J* = 7.2 Hz, 2H), 7.40 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 6.70 (dd, *J* = 2.7, 1.8 Hz, 1H), 6.56 (dd, *J* = 3.6, 2.7 Hz, 1H); ¹³C NMR (150.9 MHz, CDCl₃) δ 138.0, 131.6, 129.2, 128.5 (q, *J* = 312.3 Hz), 127.8, 124.6, 123.2, 108.5, 108.4 (d, *J* = 1.5 Hz); ¹⁹F NMR (282 MHz, CDCl₃) δ -4 5.1 (s, 3F); IR (KBr) 3424, 3128, 2962, 2927, 2857, 1176, 1124 cm⁻¹; MS (ESI, *m/z*) 242 [M-H]⁻; HRMS (ESI) calcd. for C₁₁H₇F₃NS [M-H]⁻: 242.0251, Found: 242.0248.

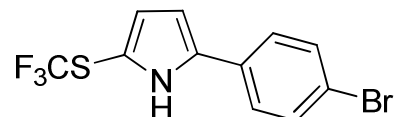
2-(4-Tolyl)-5-[(trifluoromethyl)thio]pyrrole (**7b**)



Violet solid. m.p.: 51-53 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.53 (s, 1H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 6.69 (dd, *J* = 2.7, 2.7 Hz, 1H), 6.51 (dd, *J* = 2.7, 2.7 Hz, 1H), 2.37 (s, 3H); ¹³C NMR (150.9

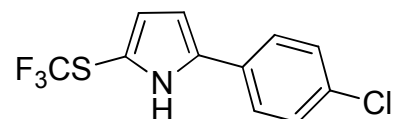
MHz, CDCl₃) δ 138.2, 137.7, 129.9, 128.7, 128.4 (q, J = 310.8 Hz), 124.5, 123.1, 107.9, 107.8 (q, J = 3.0 Hz), 21.3; ¹⁹F NMR (282 MHz, CDCl₃) δ -45.2 (s, 3F); IR (KBr) 3436, 3127, 3024, 2958, 2926, 2864, 1507, 1446, 1425, 1381, 1298, 1165, 1108 cm⁻¹; MS (ESI, m/z) 256 [M-H]⁻; HRMS (ESI) calcd. for C₁₂H₉F₃NS [M-H]⁻: 256.0408, Found: 256.0410.

2-(4-Bromophenyl)-5-[(trifluoromethyl)thio]pyrrole (**7c**)



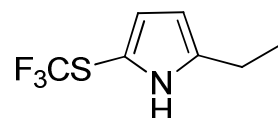
Violet solid. m.p.: 61-62 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.57 (s, 1H), 7.52 (d, J = 7.2 Hz, 2H), 7.35 (d, J = 7.2 Hz, 2H), 6.70 (t, J = 0.9 Hz, 1H), 6.55 (t, J = 0.9 Hz, 1H); ¹³C NMR (150.9 MHz, CDCl₃) δ 136.8, 132.3, 130.4, 128.4 (q, J = 310.8 Hz), 126.0, 123.3, 121.6, 109.1 (q, J = 3.0 Hz), 108.8; ¹⁹F NMR (282 MHz, CDCl₃) δ -44.9 (s, 3F); IR (KBr) 3441, 3405, 3133, 2961, 2925, 2854, 1485, 1181, 1141, 1104 cm⁻¹; MS (ESI, m/z) 320 [M-H]⁻; HRMS (ESI) calcd. for C₁₁H₆BrF₃NS [M-H]⁻: 319.9356, Found: 319.9359.

2-(4-Chlorophenyl)-5-[(trifluoromethyl)thio]pyrrole (**7d**)



Violet solid. m.p.: 39-40 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.56 (s, 1H), 7.46-7.36 (m, 4H), 6.70 (dd, J = 2.7, 2.7 Hz, 1H), 6.55 (dd, J = 2.7, 2.7 Hz, 1H); ¹³C NMR (150.9 MHz, CDCl₃) δ 136.8, 133.6, 130.0, 129.4, 128.4 (q, J = 310.8 Hz), 125.8, 123.3, 109.0 (q, J = 3.0 Hz), 108.8; ¹⁹F NMR (282 MHz, CDCl₃) δ -45.0 (s, 3F); IR (KBr) 3467, 3124, 3052, 2963, 2927, 1491, 1444, 1295, 1126 cm⁻¹; MS (ESI, m/z) 276 [M-H]⁻; HRMS (ESI) calcd. for C₁₁H₆ClF₃NS [M-H]⁻: 275.9862, Found: 275.9862.

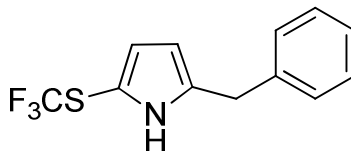
2-Ethyl-5-[(trifluoromethyl)thio]pyrrole (**7e**)



Brown liquid. ¹H NMR (600 MHz, CDCl₃) δ 8.12 (s, 1H), 6.55 (dd, J = 3.0, 3.0 Hz, 1H), 6.01 (dd, J = 3.0,

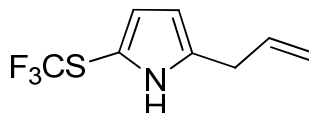
3.0 Hz, 1H), 2.65 (q, $J = 7.8$ Hz, 2H), 1.24 (t, $J = 7.8$ Hz, 3H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 140.7, 130.6 (q, $J = 310.8$ Hz), 122.1, 107.7, 105.2 (q, $J = 3.0$ Hz), 21.2, 13.3; ^{19}F NMR (282 MHz, CDCl_3) δ -45.7 (s, 3F); IR (neat) 3471, 3399, 2973, 2938, 1642, 1108 cm^{-1} ; MS (ESI, m/z) 194 $[\text{M}-\text{H}]^-$; HRMS (ESI) calcd. for $\text{C}_7\text{H}_7\text{F}_3\text{NS}$ $[\text{M}-\text{H}]^-$: 194.0251, Found: 194.0259.

2-Benzyl-5-[(trifluoromethyl)thio]pyrrole (**7f**)



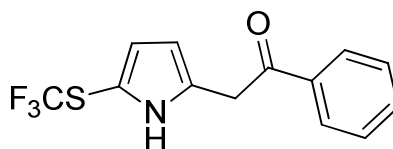
Colorless oil. ^1H NMR (300 MHz, CDCl_3) δ 8.01 (s, 1H), 7.32-7.27 (m, 3H), 7.18 (d, $J = 6.3$ Hz, 2H), 6.65 (s, 1H), 6.05 (s, 1H), 3.97 (s, 2H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 138.3, 137.3, 129.0, 128.8, 128.5 (q, $J = 310.8$ Hz), 127.0, 122.2, 109.7, 106.3 (q, $J = 3.0$ Hz), 34.4; ^{19}F NMR (282 MHz, CDCl_3) δ -45.6 (s, 3F); IR (neat) 3453, 3403, 3090, 3067, 3029, 2909, 2846, 1454, 1108 cm^{-1} ; MS (ESI, m/z) 256 $[\text{M}-\text{H}]^-$; HRMS (ESI) calcd. for $\text{C}_{12}\text{H}_9\text{F}_3\text{NS}$ $[\text{M}-\text{H}]^-$: 256.0408, Found: 256.0411.

2-Allyl-5-[(trifluoromethyl)thio]pyrrole (**7g**)



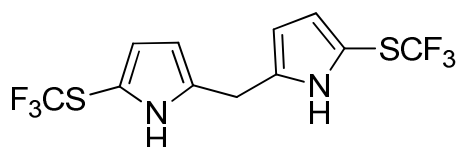
Colorless liquid. ^1H NMR (300 MHz, CDCl_3) δ 8.14 (s, 1H), 6.56 (t, $J = 3.0$ Hz, 1H), 6.03 (s, 1H), 5.99-5.86 (m, 1H), 5.17 (dd, $J = 15.3, 1.8$ Hz, 2H), 3.39 (d, $J = 6.6$ Hz, 2H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 136.2, 134.3, 130.3 (q, $J = 303.1$ Hz), 122.0, 117.5, 108.9, 105.8, 32.4; ^{19}F NMR (282 MHz, CDCl_3) δ -45.6 (s, 3F); IR (neat) 3462, 3407, 3086, 3008, 2985, 2908, 1640, 1561, 1459, 1108 cm^{-1} ; MS (ESI, m/z) 206 $[\text{M}-\text{H}]^-$; HRMS (ESI) calcd. for $\text{C}_8\text{H}_7\text{F}_3\text{NS}$ $[\text{M}-\text{H}]^-$: 206.0251, Found: 206.0250.

1-Phenyl-2-{5-[(trifluoromethyl)thio]pyrrol-2-yl}ethanone (**7h**)



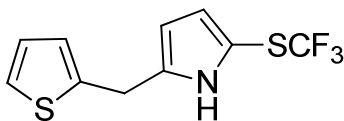
Brown solid. m.p.: 65-66 °C; ^1H NMR (300 MHz, CDCl_3) δ 9.36 (s, 1H), 8.00 (d, $J = 7.5$ Hz, 2H), 7.60 (t, $J = 7.5$ Hz, 1H), 7.49 (t, $J = 7.5$ Hz, 2H), 6.57 (dd, $J = 2.7, 2.4$ Hz, 1H), 6.14 (d, $J = 2.7$ Hz, 1H), 4.34 (s, 2H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 196.9, 136.0, 133.8, 130.4, 128.8, 128.4 (q, $J = 310.8$ Hz), 128.3, 121.4, 110.2, 107.1, 36.6; ^{19}F NMR (282 MHz, CDCl_3) δ -45.3 (s, 3F); IR (KBr) 3314, 3116, 3061, 2950, 2819, 1681, 1596, 1561, 1450, 1278, 1119 cm^{-1} ; MS (ESI, m/z) 284 $[\text{M}-\text{H}]^-$; HRMS (ESI) calcd. for $\text{C}_{13}\text{H}_9\text{F}_3\text{NOS}$ $[\text{M}-\text{H}]^-$: 284.0357, Found: 284.0348.

Bis{5-[(trifluoromethyl)thio]pyrrol-2-yl} methane (**7i**)



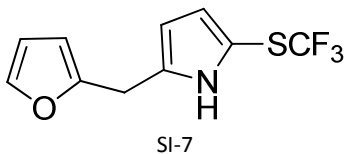
Gray solid. m.p.: 70-71 °C; ^1H NMR (300 MHz, CDCl_3) δ 8.16 (s, 2H), 6.59 (dd, $J = 3.0, 2.7$ Hz, 2H), 6.11 (dd, $J = 3.0, 2.7$ Hz, 2H), 4.00 (s, 2H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 134.2, 128.4 (q, $J = 310.8$ Hz), 122.2, 110.0, 107.4, 27.1; ^{19}F NMR (282 MHz, CDCl_3) δ -45.3 (s, 3F); IR (KBr) 3377, 1565, 1457, 1300, 1128 cm^{-1} ; MS (ESI, m/z) 345 $[\text{M}-\text{H}]^-$; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_7\text{F}_6\text{N}_2\text{S}_2$ $[\text{M}-\text{H}]^-$: 344.9955, Found: 344.9953.

2-(Thiophen-2-ylmethyl)-5-[(trifluoromethyl)thio]pyrrole (**7j**)



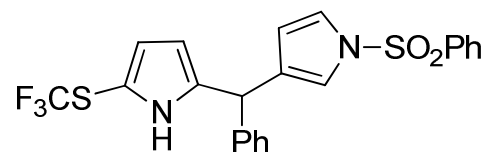
Red liquid. ^1H NMR (300 MHz, CDCl_3) δ 8.16 (s, 1H), 7.22-7.19 (m, 1H), 6.98-6.94 (m, 1H), 6.85 (dd, $J = 3.0, 3.0$ Hz, 1H), 6.59-6.56 (m, 1H), 6.11 (dd, $J = 3.0, 3.0$ Hz, 1H), 4.17 (s, 2H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 140.5, 136.2, 128.2 (q, $J = 310.8$ Hz), 127.0, 125.7, 124.6, 122.0, 109.3, 106.4 (q, $J = 3.0$ Hz), 28.5; ^{19}F NMR (282 MHz, CDCl_3) δ -45.5 (s, 3F); IR (neat) 3395, 2900, 1642, 1560, 1109 cm^{-1} ; MS (ESI, m/z) 262 $[\text{M}-\text{H}]^-$; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_7\text{F}_3\text{NS}_2$ $[\text{M}-\text{H}]^-$: 261.9972, Found: 261.9972.

2-(Furan-2-ylmethyl)-5-[(trifluoromethyl)thio]pyrrole (**7k**)



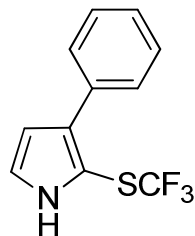
Pale yellow liquid. ^1H NMR (300 MHz, CDCl_3) δ 8.31 (s, 1H), 7.37 (d, $J = 1.2$ Hz, 1H), 6.56 (t, $J = 3.0$ Hz, 1H), 6.33 (dd, $J = 3.0, 2.1$ Hz, 1H), 6.09 (t, $J = 0.9$ Hz, 2H), 3.99 (s, 2H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 140.5, 136.2, 128.2 (q, $J = 310.8$ Hz), 127.0, 125.7, 124.6, 122.0, 109.3, 106.4 (q, $J = 3.0$ Hz), 28.5; ^{19}F NMR (282 MHz, CDCl_3) δ -45.5 (s, 3F); IR (neat) 3457, 3404, 3121, 2904, 1561, 1459, 1108 cm^{-1} ; MS (ESI, m/z) 246 $[\text{M-H}]^-$; HRMS (ESI) calcd. for $\text{C}_{10}\text{H}_7\text{F}_3\text{NOS}$ $[\text{M-H}]^-$: 246.0200, Found: 246.0201.

3-{Phenyl[5-(trifluoromethyl)thiopyrrol-2-yl]methyl}-1-phenylsulfonylpyrrole (**7l**)



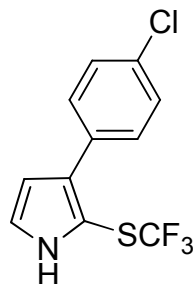
Brown oil. ^1H NMR (300 MHz, CDCl_3) δ 8.07 (s, 1H), 7.81 (d, $J = 7.5$ Hz, 2H), 7.59 (t, $J = 7.5$ Hz, 1H), 7.48 (t, $J = 7.5$ Hz, 2H), 7.31-7.23 (m, 3H), 7.20 (s, 1H), 7.16 (d, $J = 6.3$ Hz, 2H), 6.81 (s, 1H), 6.52 (t, $J = 3.0$ Hz, 1H), 6.13 (dd, $J = 1.8, 1.5$ Hz, 1H), 5.85 (t, $J = 3.0$ Hz, 1H), 5.22 (s, 1H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 141.3, 139.6, 138.9, 134.1, 130.6, 129.5, 128.9, 128.5, 128.4 (q, $J = 312.3$ Hz), 127.4, 126.9, 121.8, 121.7, 119.1, 114.6, 110.2, 106.6 (q, $J = 3.0$ Hz), 43.3; ^{19}F NMR (282 MHz, CDCl_3) δ -45.4 (s, 3F); IR (neat) 3377, 3136, 3063, 3032, 1449, 1369, 1173, 1108 cm^{-1} ; MS (ESI, m/z) 461 $[\text{M-H}]^-$; HRMS (ESI) calcd. for $\text{C}_{22}\text{H}_{16}\text{F}_3\text{N}_2\text{O}_2\text{S}_2$ $[\text{M-H}]^-$: 461.0605, Found: 461.0600.

3-Phenyl-2-[(trifluoromethyl)thio]pyrrole (**7m**)



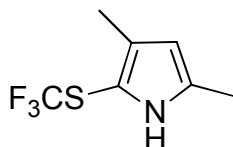
Gray oil. ^1H NMR (300 MHz, CDCl_3) δ 8.47 (s, 1H), 7.60 (d, $J = 7.5$ Hz, 2H), 7.40 (t, $J = 7.5$ Hz, 2H), 7.30 (t, $J = 7.5$ Hz, 1H), 7.03 (dd, $J = 2.7, 1.5$ Hz, 1H), 6.56 (dd, $J = 2.7, 1.5$ Hz, 1H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 134.7, 134.5, 128.8 (q, $J = 312.3$ Hz), 128.6, 128.5, 127.1, 123.4, 111.3, 108.4 (q, $J = 3.0$ Hz); ^{19}F NMR (282 MHz, CDCl_3) δ -44.1 (s, 3F); IR (neat) 3477, 3408, 3063, 3032, 1603, 1500, 1447, 1108 cm^{-1} ; MS (ESI, m/z) 242 $[\text{M-H}]^-$; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_7\text{F}_3\text{NS}$ $[\text{M-H}]^-$: 242.0251, Found: 242.0250.

3-(4-Chlorophenyl)-2-[(trifluoromethyl)thio]pyrrole (**7n**)



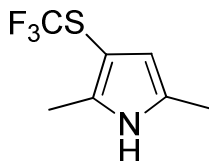
Gray oil. ^1H NMR (300 MHz, CDCl_3) δ 8.51 (s, 1H), 7.51 (dd, $J = 7.5, 2.4$ Hz, 2H), 7.36 (dd, $J = 7.5, 1.8$ Hz, 2H), 7.04 (t, $J = 3.0$ Hz, 1H), 6.48 (t, $J = 3.0$ Hz, 1H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 133.5, 133.1, 132.9, 129.7, 128.7, 128.6 (q, $J = 312.3$ Hz), 123.5, 111.2, 104.7; ^{19}F NMR (282 MHz, CDCl_3) δ -44.1 (s, 3F); IR (neat) 3427, 3217, 3063, 2962, 1497, 1158, 1108 cm^{-1} ; MS (ESI, m/z) 276 $[\text{M}-\text{H}]^-$; HRMS (ESI) calcd. for $\text{C}_{11}\text{H}_6\text{ClF}_3\text{NS}$ $[\text{M}-\text{H}]^-$: 275.9862, Found: 275.9859.

3,5-Dimethyl-2-[(trifluoromethyl)thio]pyrrole (**7o**)¹



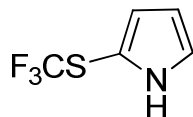
Colorless liquid. ^1H NMR (300 MHz, CDCl_3) δ 7.89 (s, 1H), 5.87 (s, 1H), 2.24 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 133.2, 131.7, 128.8 (q, $J = 312.3$ Hz), 110.4, 102.8 (q, $J = 3.0$ Hz), 13.4, 11.6; ^{19}F NMR (282 MHz, CDCl_3) δ -45.5 (s, 3F); MS (ESI, m/z) 194 $[\text{M}-\text{H}]^-$.

2,5-Dimethyl-3-[(trifluoromethyl)thio]pyrrole (**7p**)¹



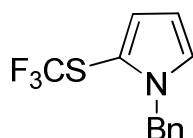
Pale yellow liquid. ^1H NMR (300 MHz, CDCl_3) δ 7.90 (s, 1H), 5.96 (s, 1H), 2.30 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (150.9 MHz, CDCl_3) δ 134.5, 129.9 (q, $J = 309.3$ Hz), 126.8, 112.7, 97.9 (q, $J = 3.0$ Hz), 13.0, 11.4; ^{19}F NMR (282 MHz, CDCl_3) δ -45.5 (s, 3F); MS (ESI, m/z) 194 $[\text{M}-\text{H}]^-$.

2-[(Trifluoromethyl)thio]pyrrole (**7q**)¹



Pale yellow liquid. ¹H NMR (300 MHz, CDCl₃) δ 8.45 (s, 1H), 7.01 (s, 1H), 6.66 (s, 1H), 6.31 (s, 1H); ¹⁹F NMR (282 MHz, CDCl₃) δ -45.7 (s, 3F); MS (ESI, m/z) 166 [M-H]⁻.

N-Benzyl-2-[(trifluoromethyl)thio]pyrrole (**7r**)

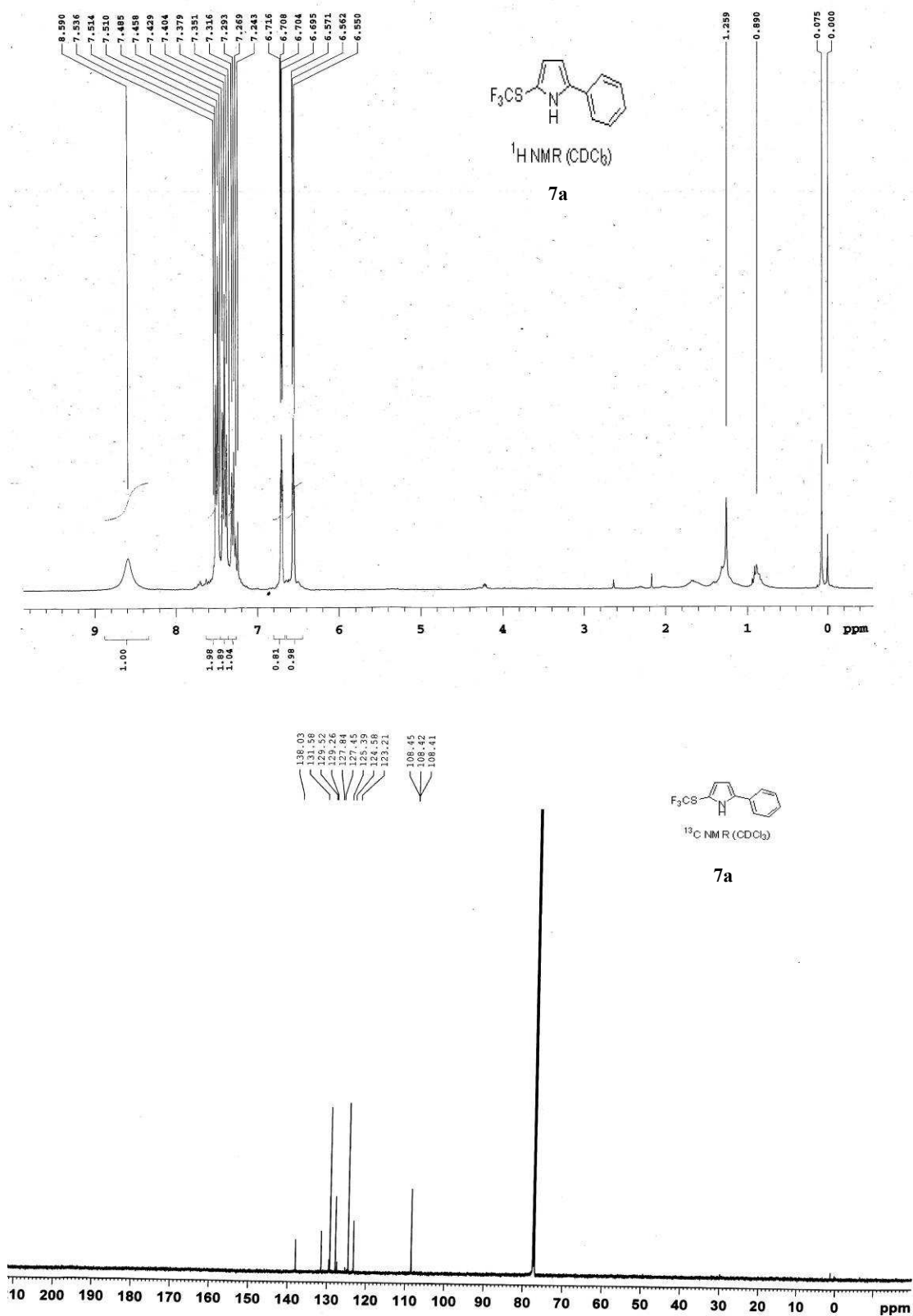


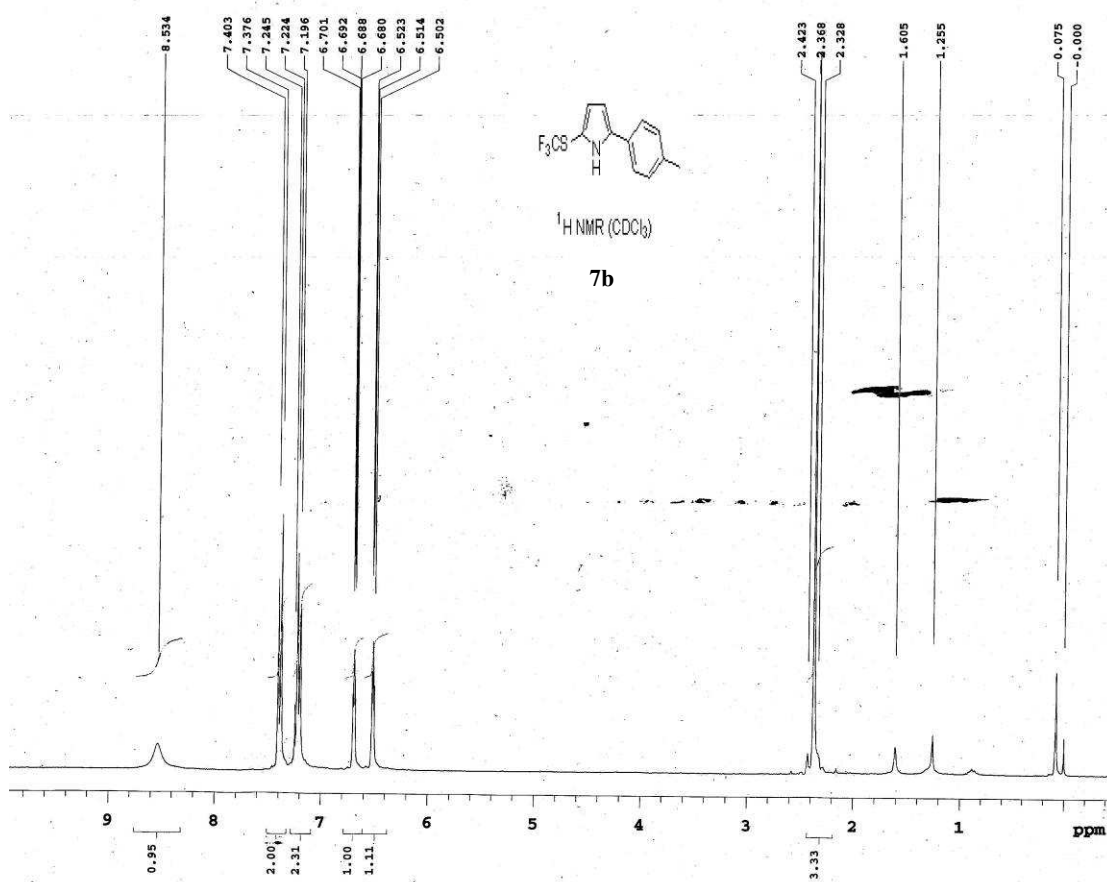
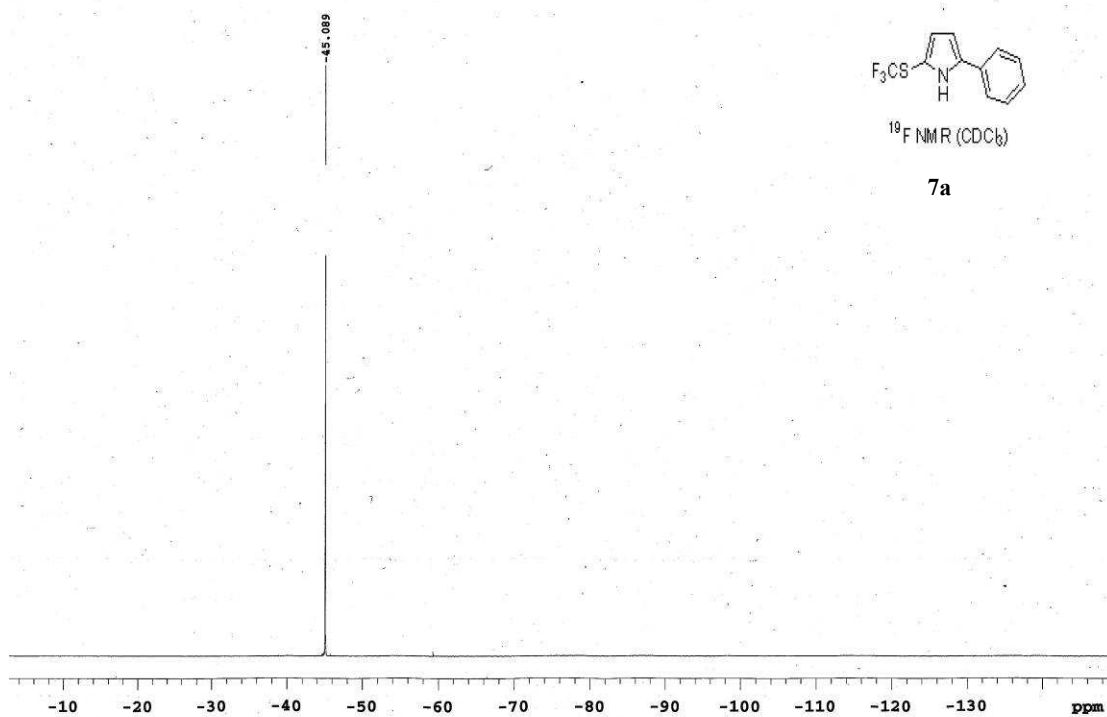
Pale yellow liquid. ¹H NMR (300 MHz, CDCl₃) δ 7.35-7.27 (m, 3H), 7.07 (d, *J* = 7.5 Hz, 2H), 6.93 (d, *J* = 1.8 Hz, 1H), 6.72 (t, *J* = 1.8 Hz, 1H), 6.27 (dd, *J* = 3.6, 3.0 Hz, 1H), 5.26 (s, 2H); ¹³C NMR (150.9 MHz, CDCl₃) δ 137.5, 128.9, 128.4 (q, *J* = 310.8 Hz), 127.9, 127.6, 127.2, 123.1, 109.9, 109.8 (q, *J* = 3.0 Hz), 50.7; ¹⁹F NMR (282 MHz, CDCl₃) δ -45.4 (s, 3F); IR (neat) 3113, 3094, 3071, 3033, 2932, 1455, 1292, 1126, 1100 cm⁻¹; MS (EI, m/z) 257 [M]; HRMS (EI) calcd. for C₁₂H₁₀F₃NS [M]: 257.0486, Found: 257.0496.

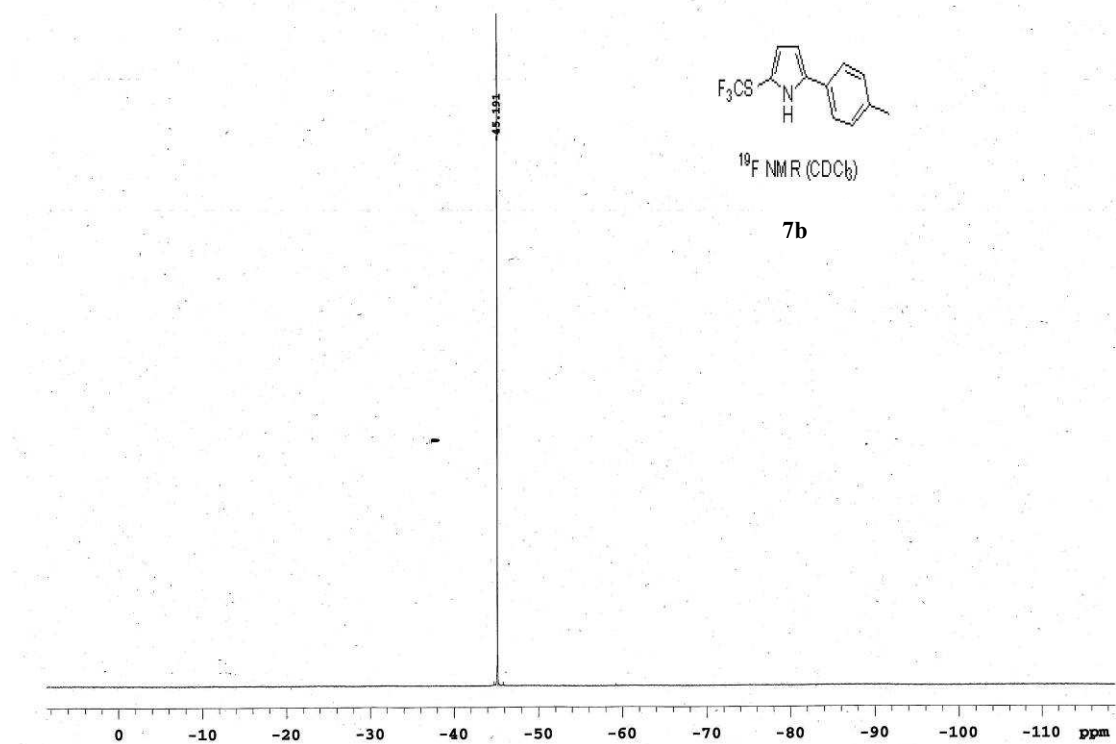
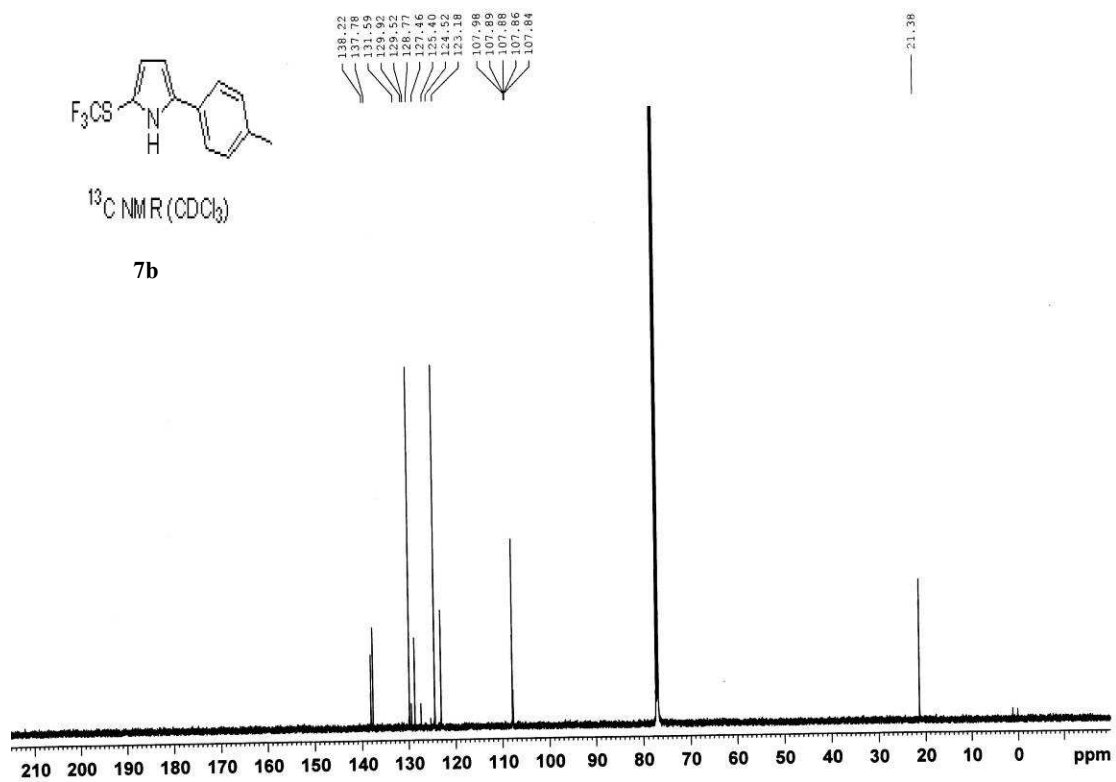
5. Reference

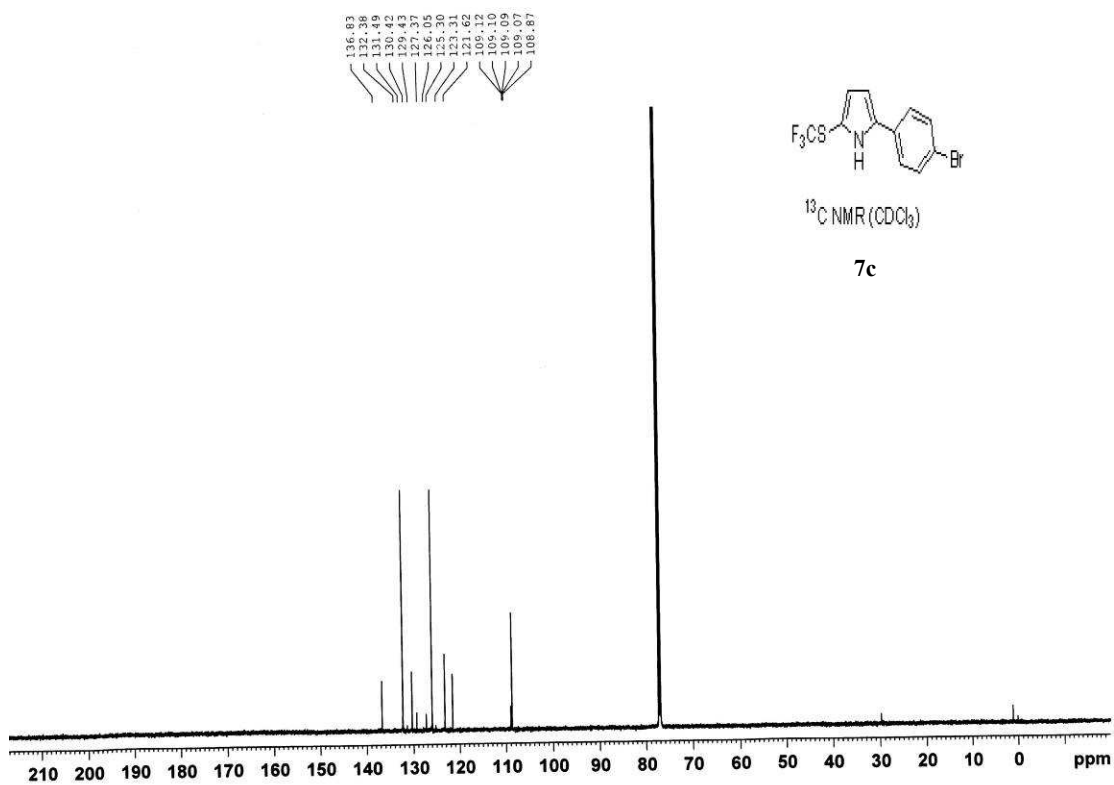
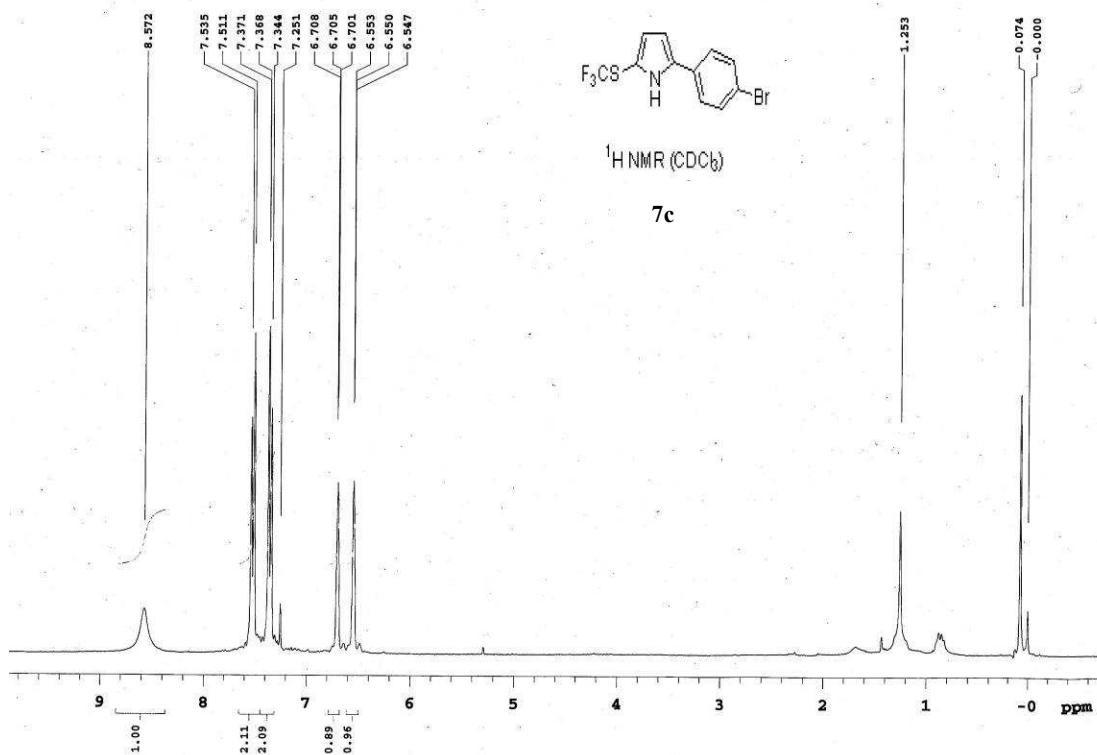
- 1 Haas, A.; Niemann, U. *Chem. Ber.* **1977**, *110*, 67.

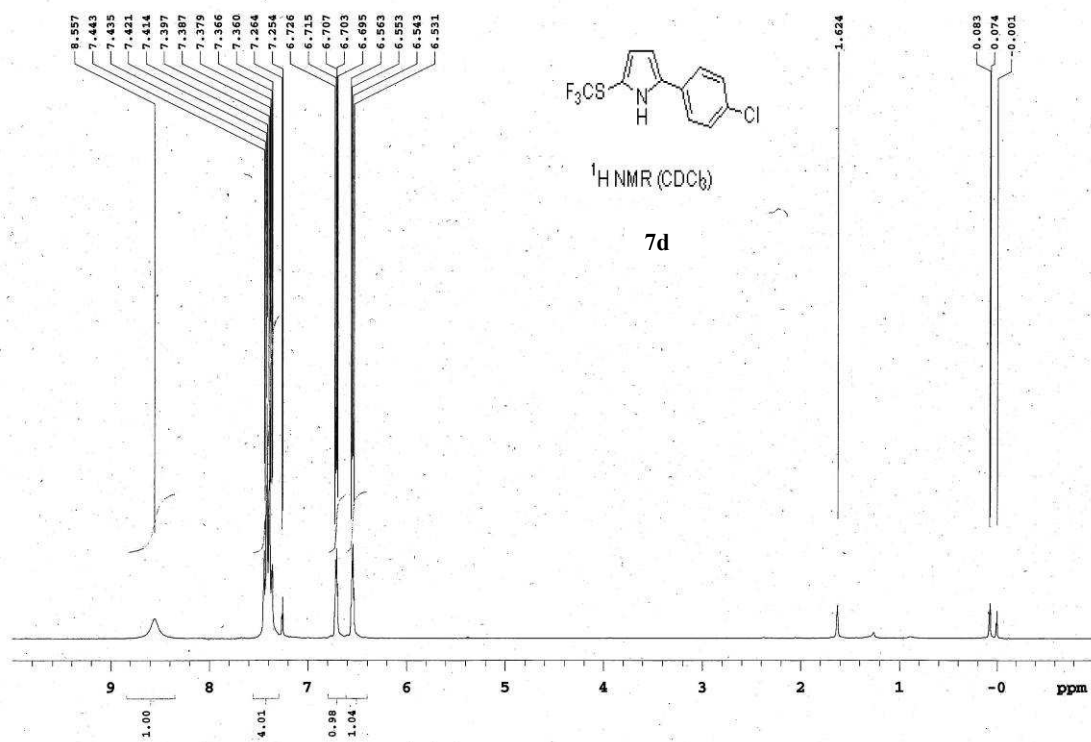
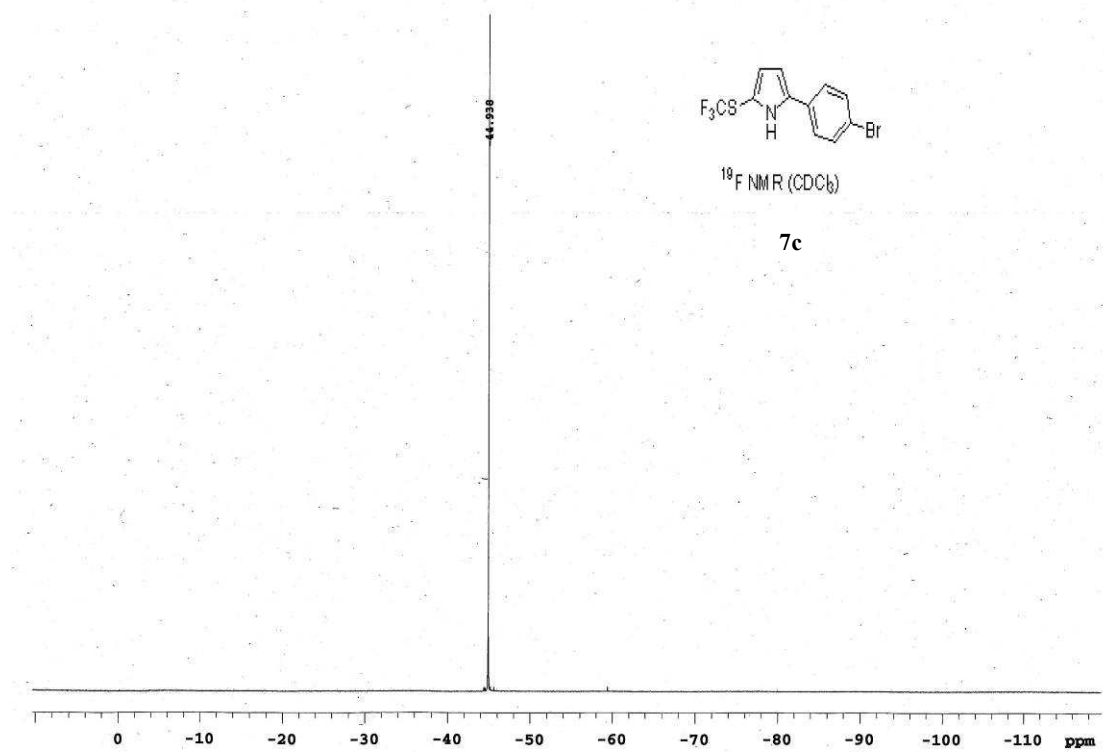
6. Copies of ^1H , ^{13}C and ^{19}F NMR spectra of unknown pyrroles 7

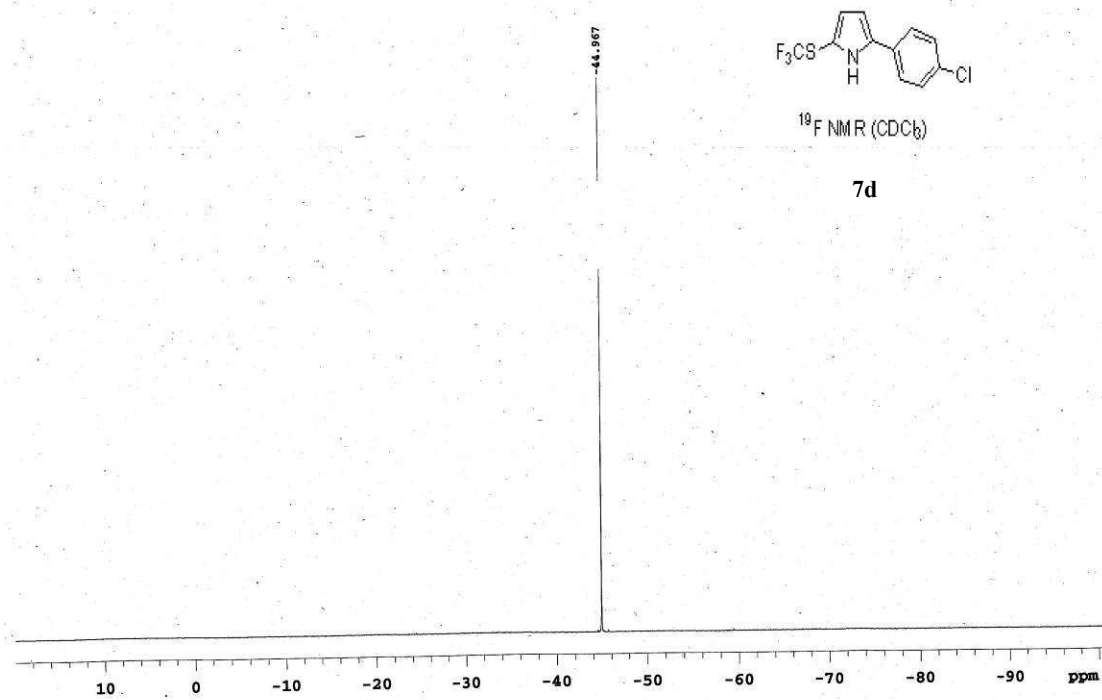
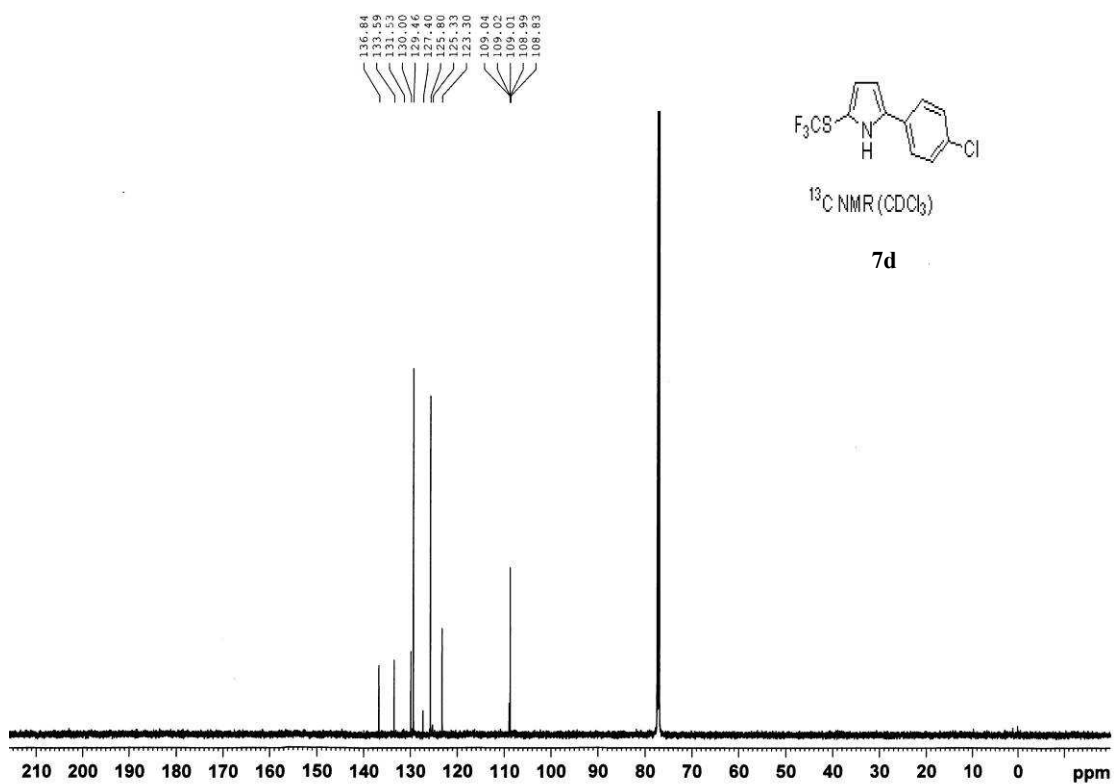


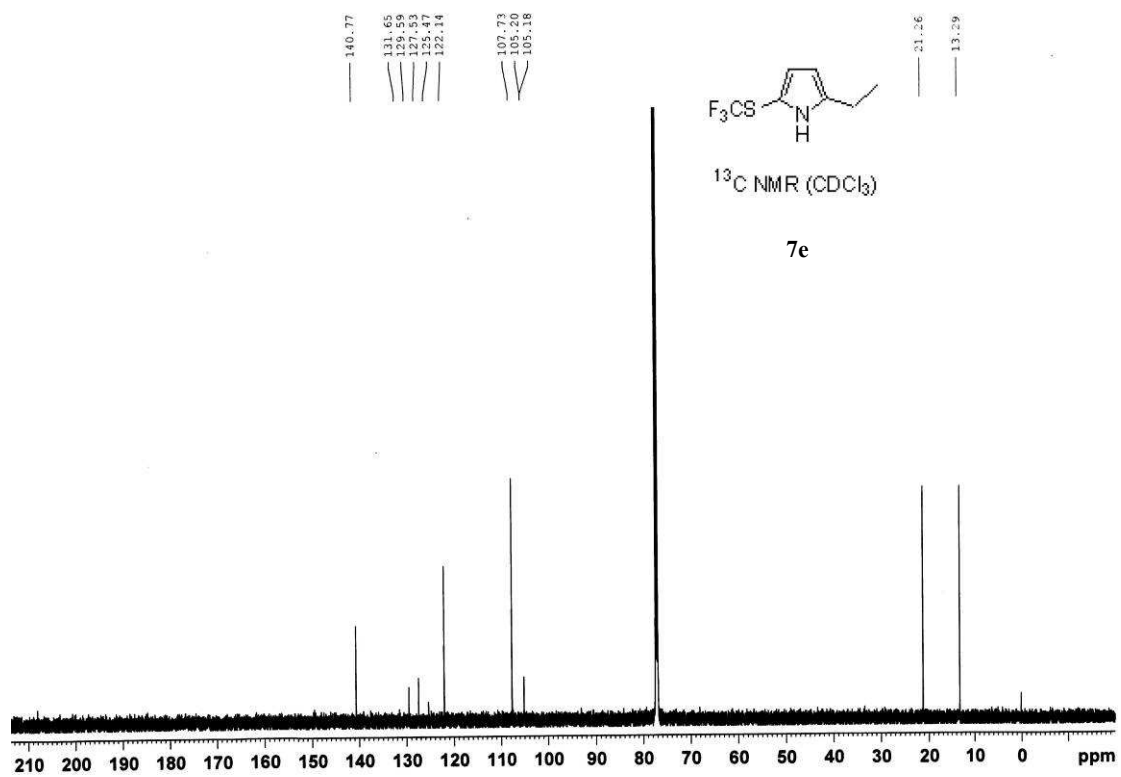
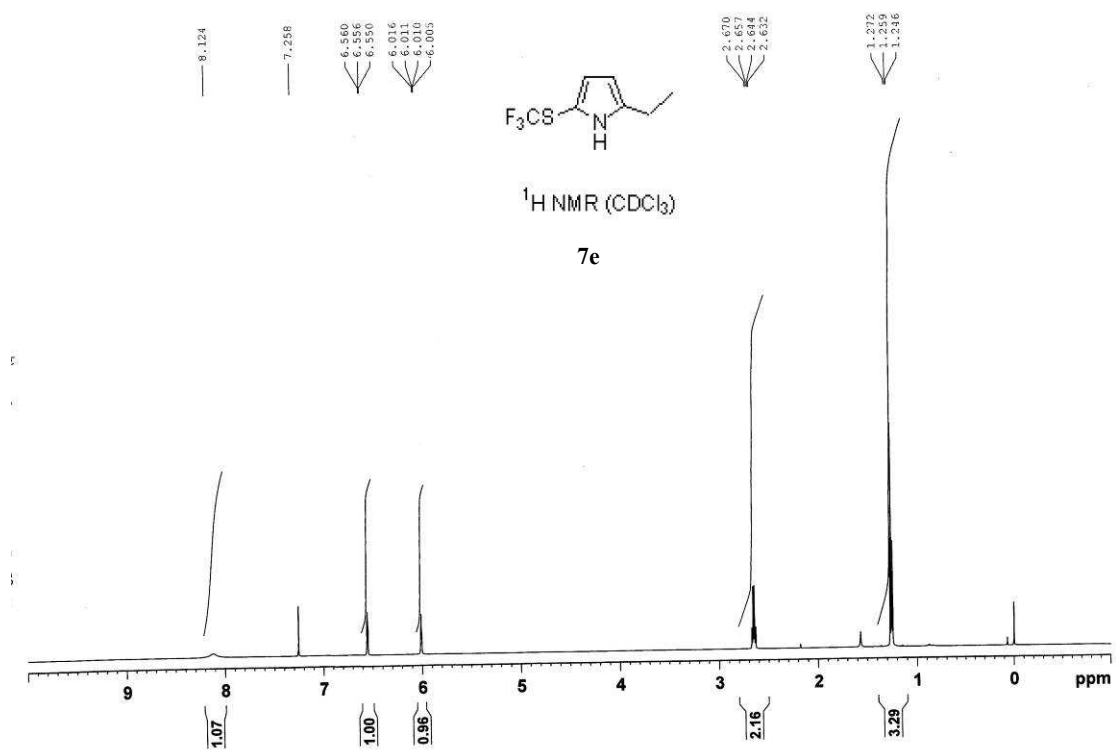


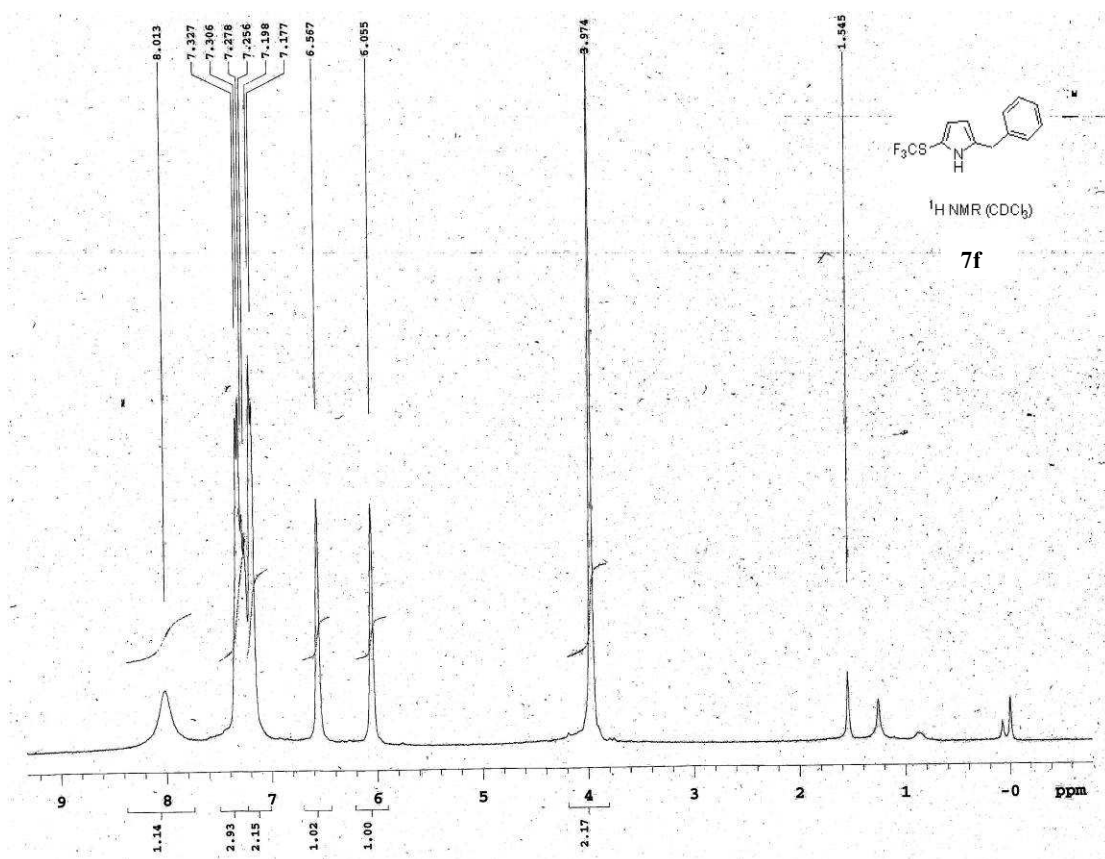
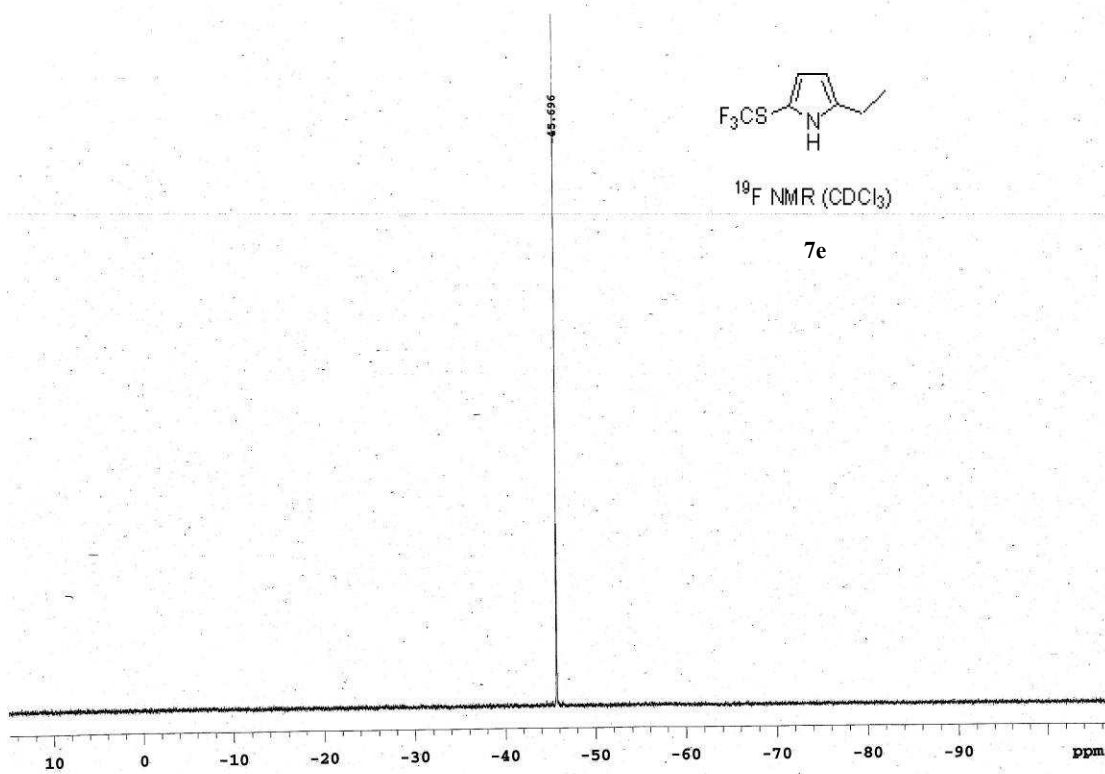


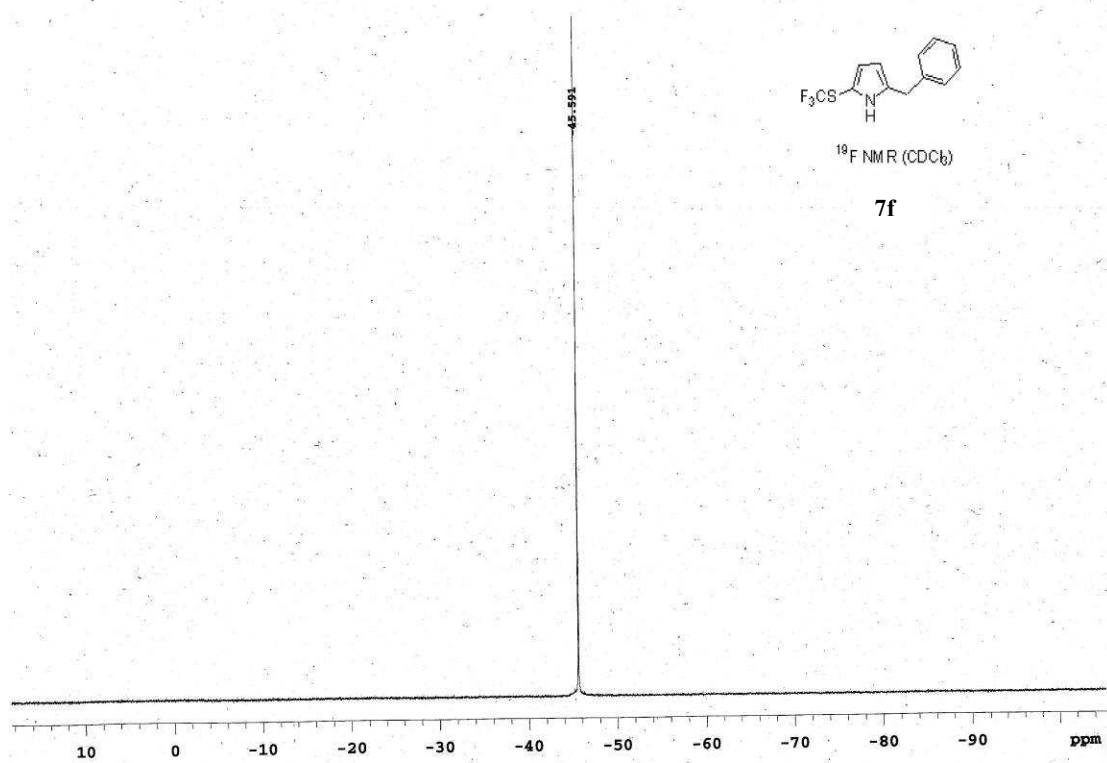
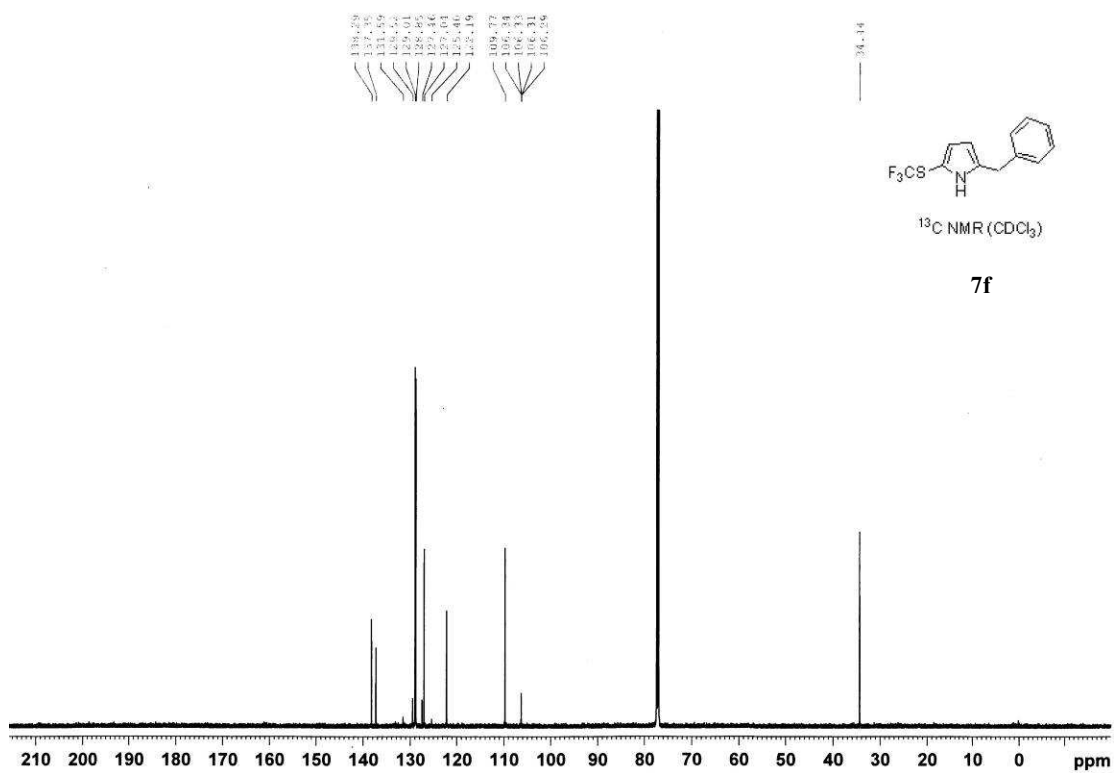


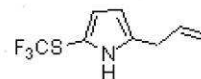






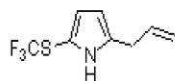
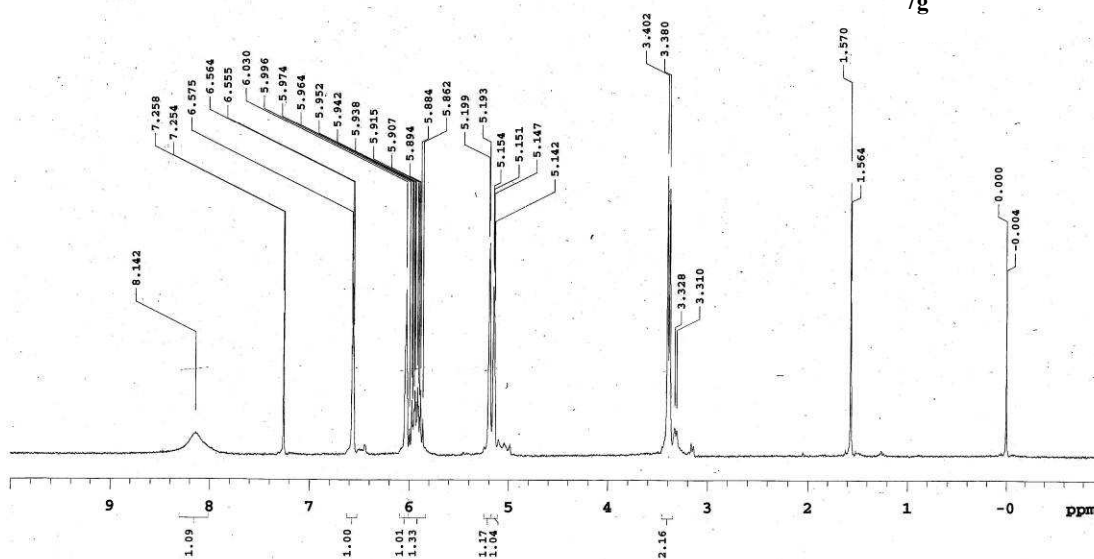






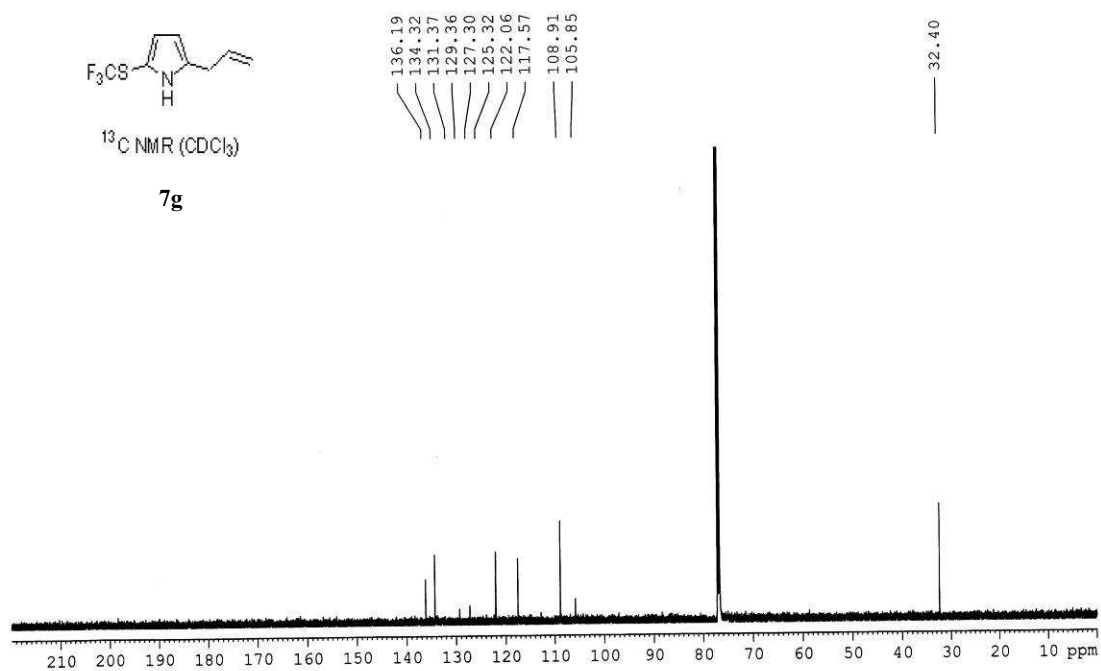
¹H NMR (CDCl₃)

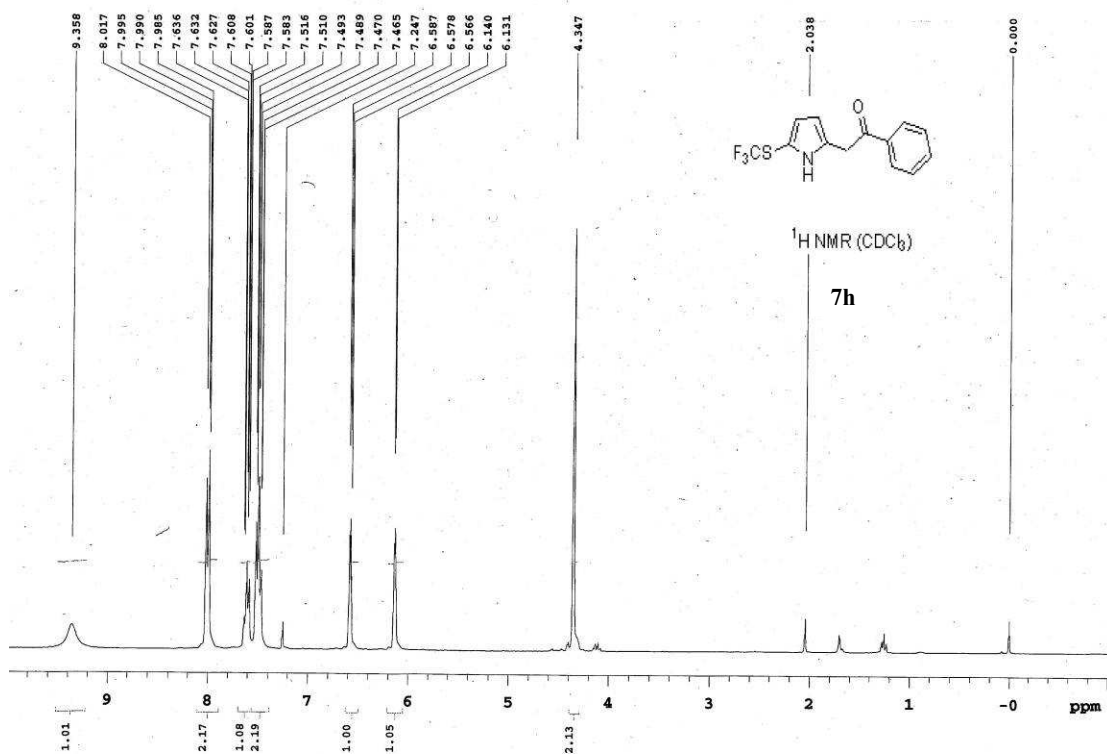
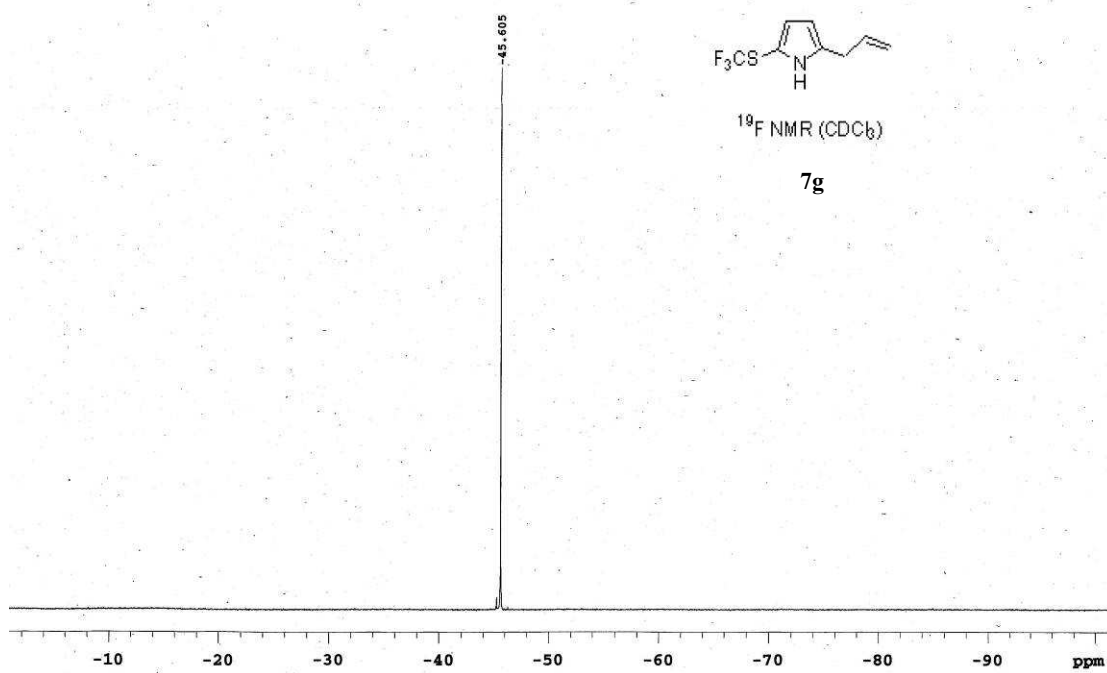
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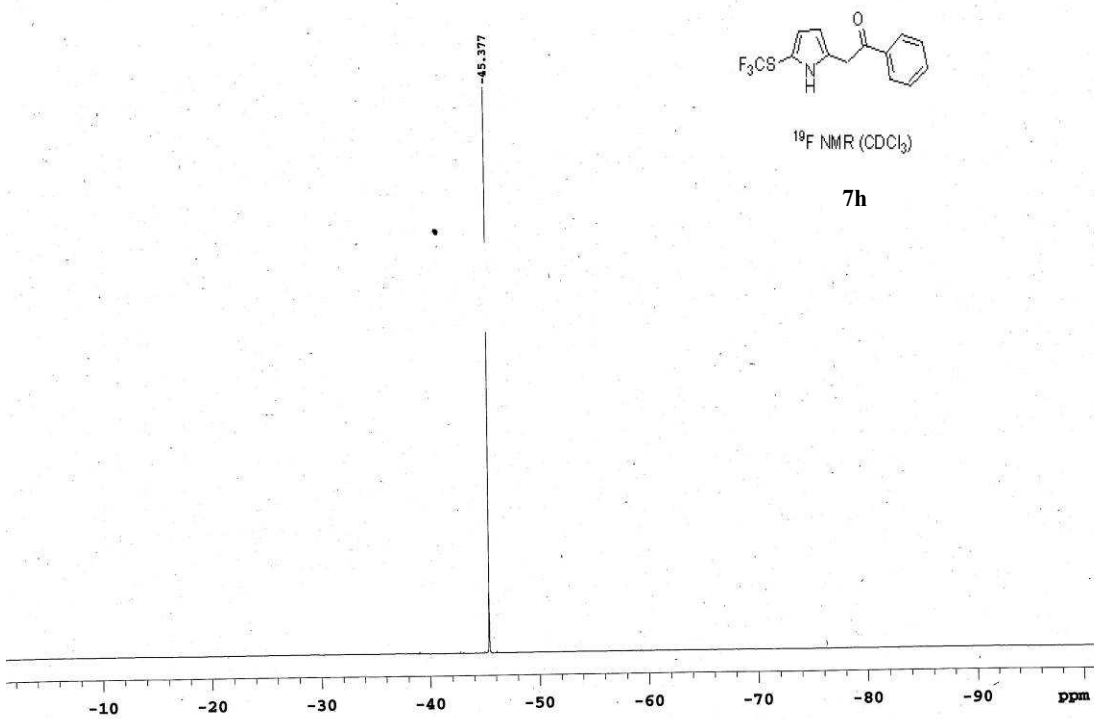
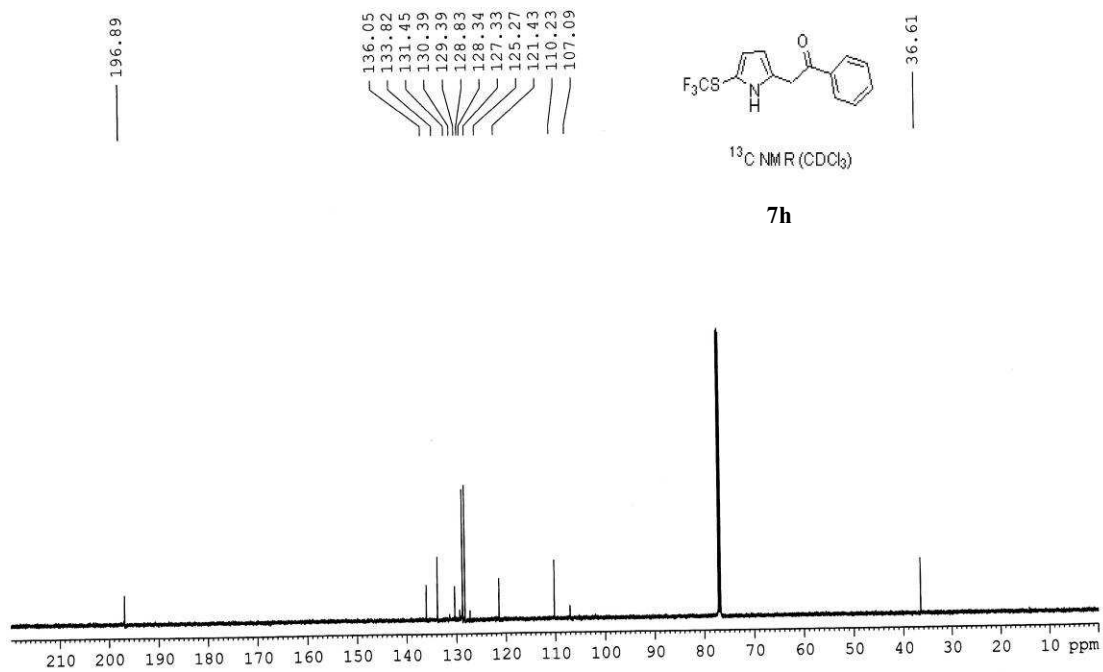


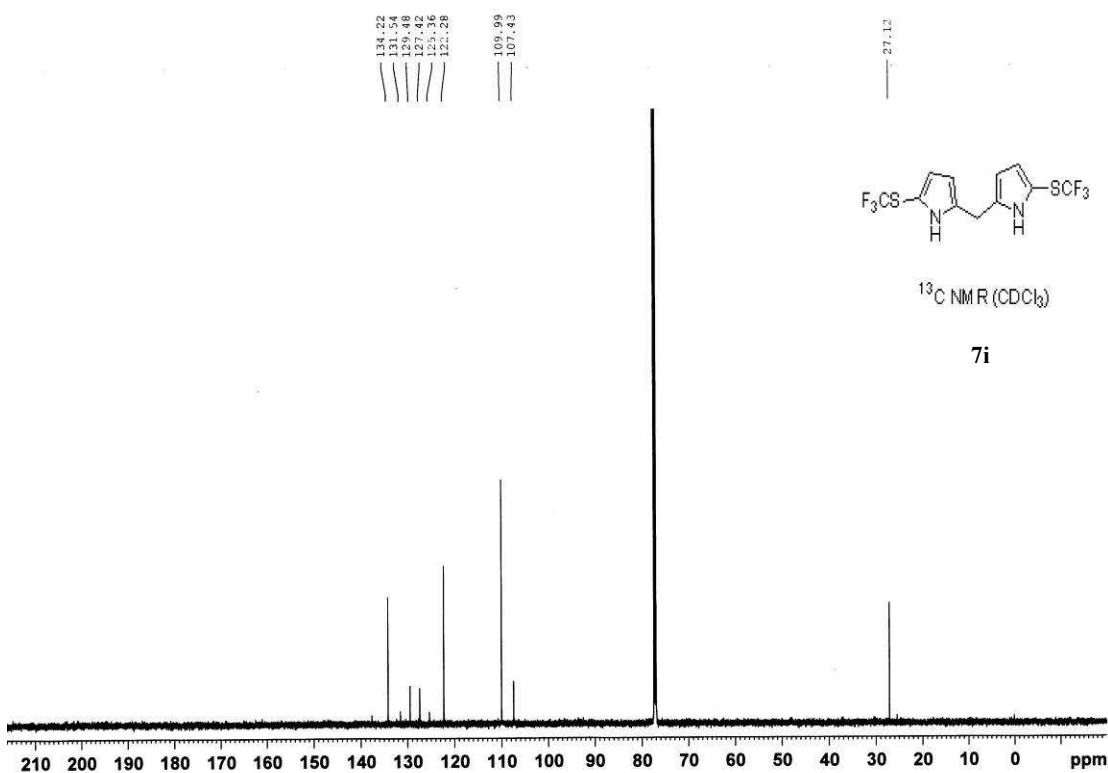
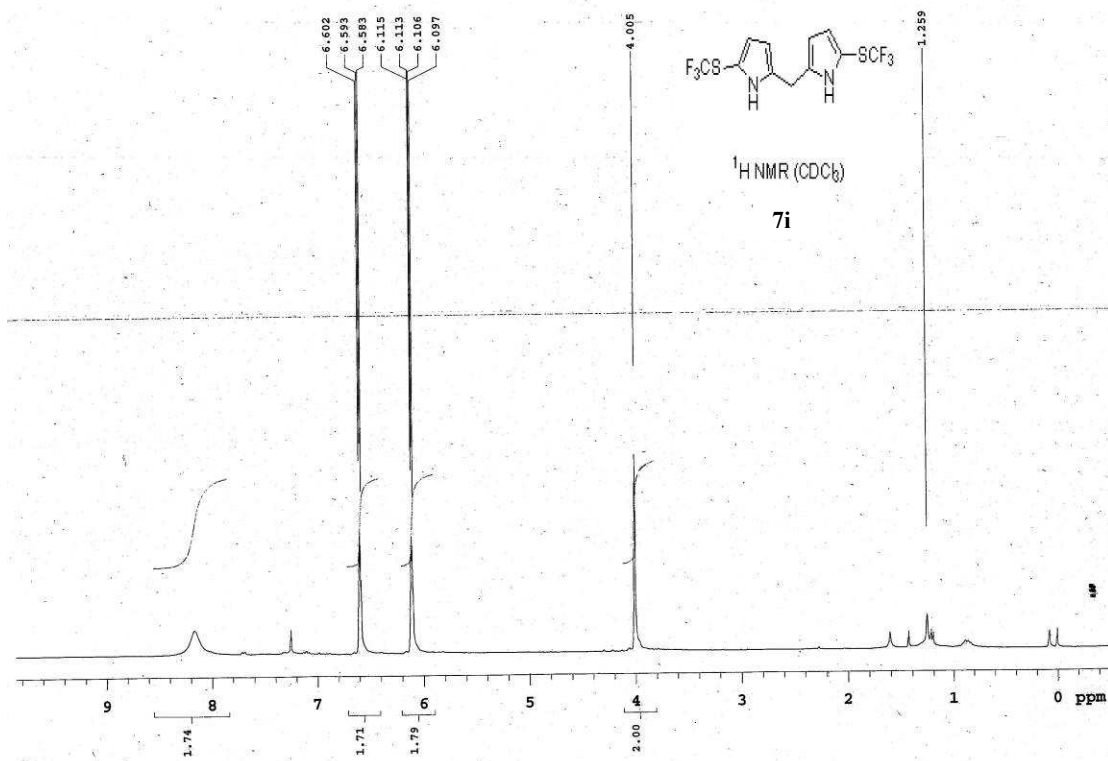
¹³C NMR (CDCl₃)

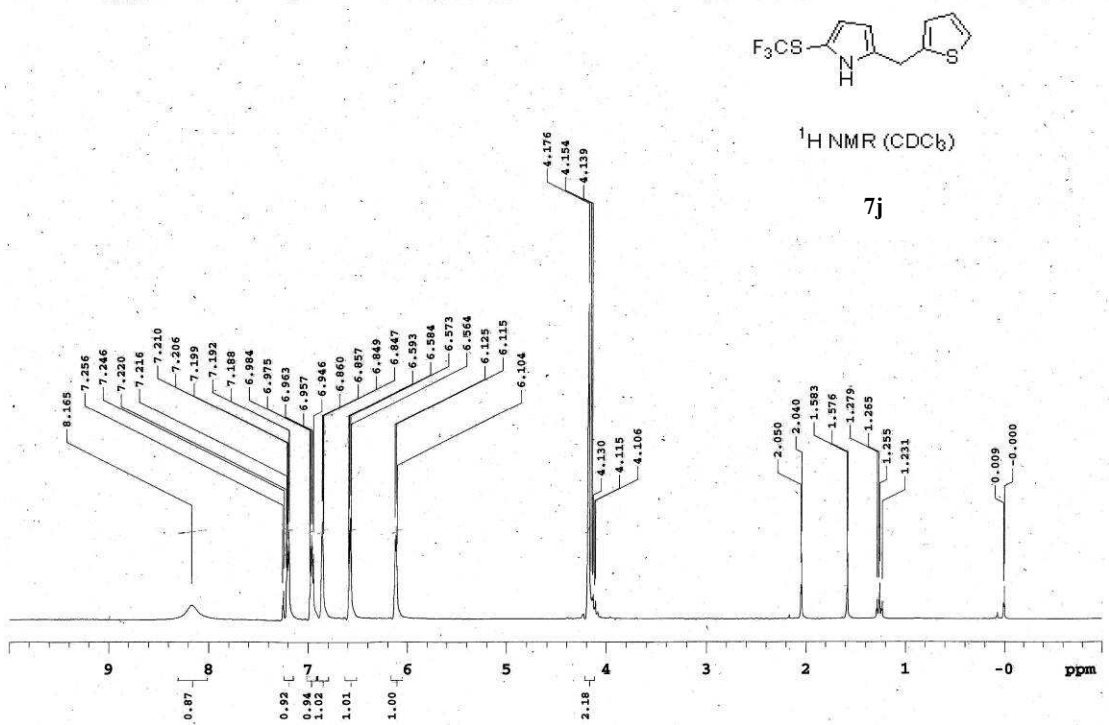
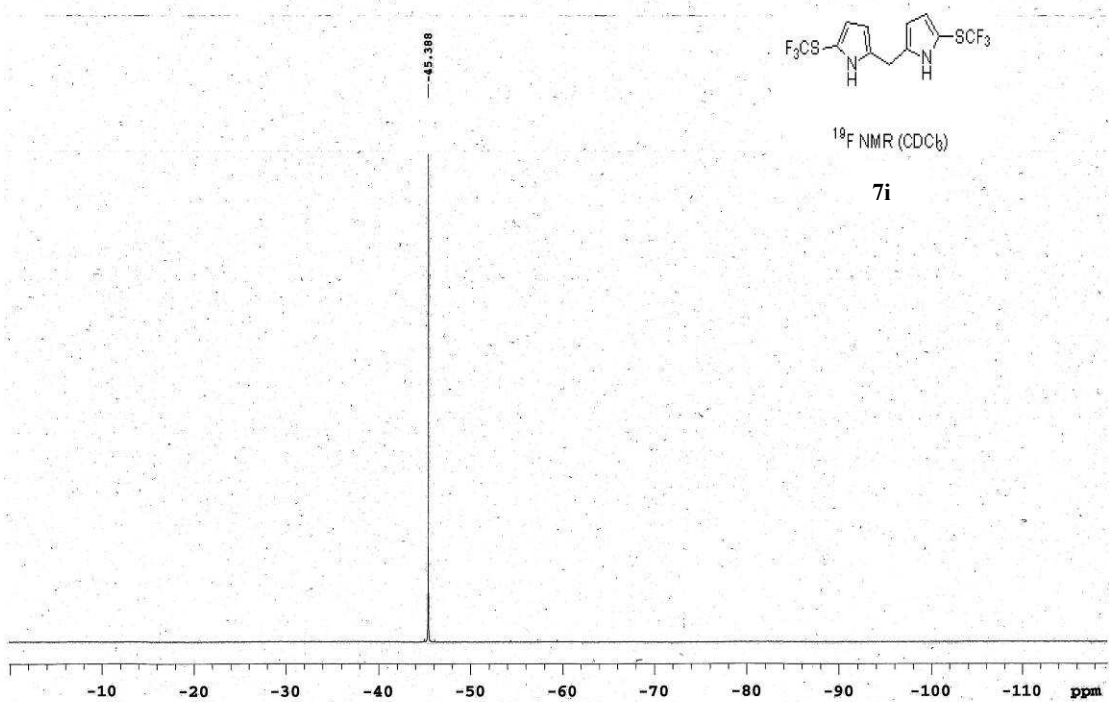
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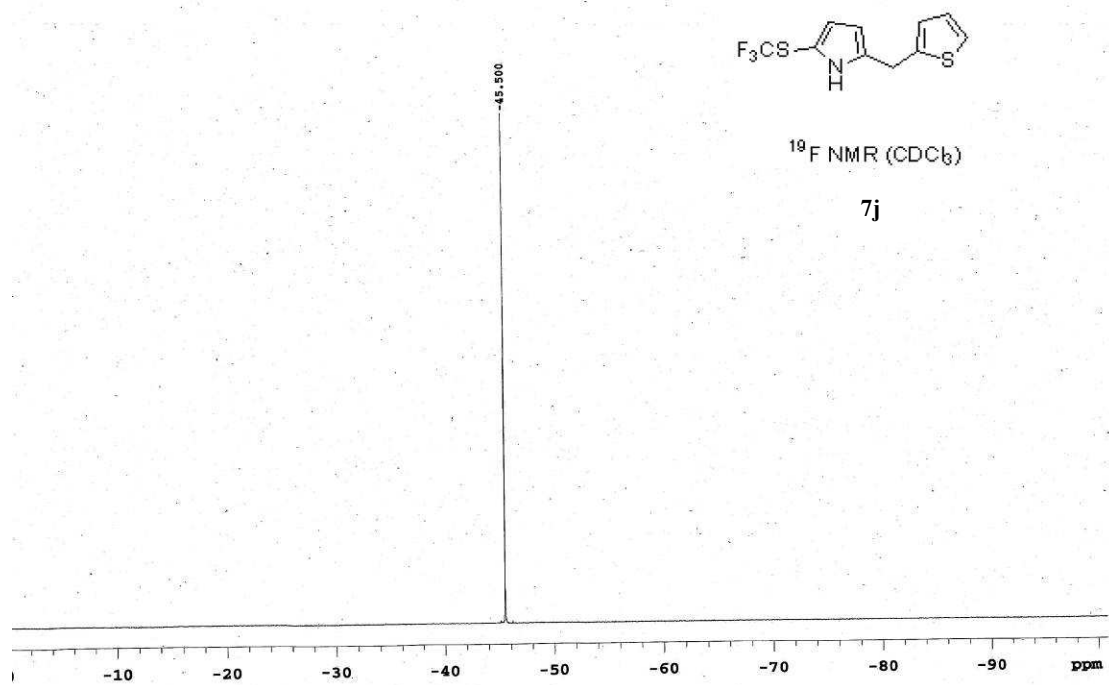
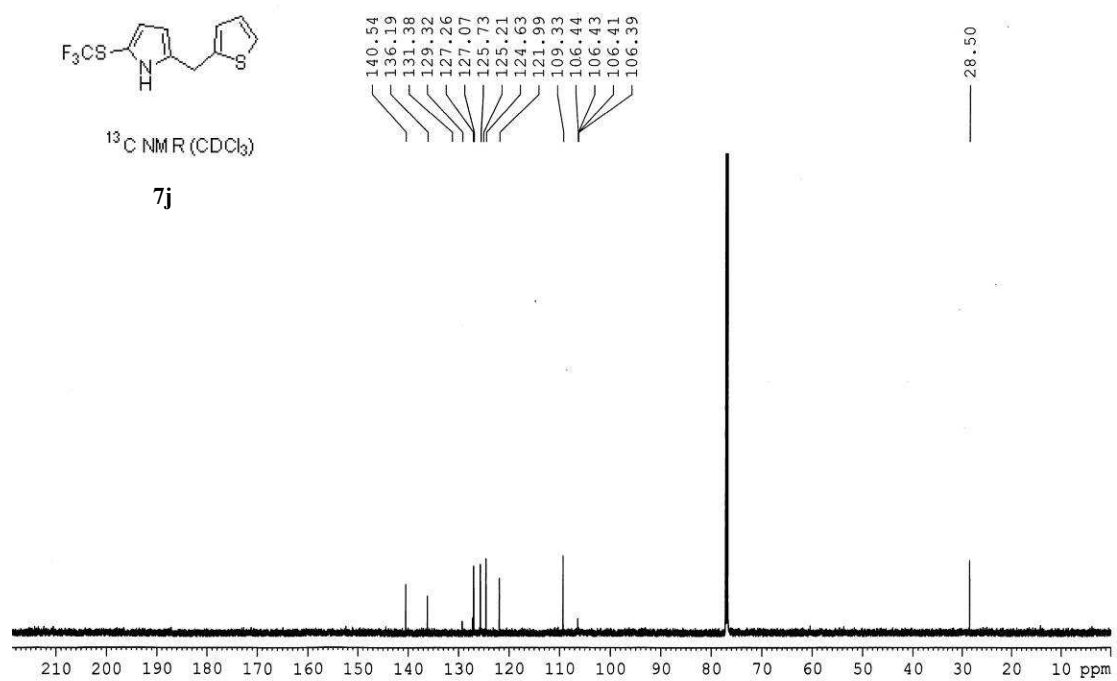


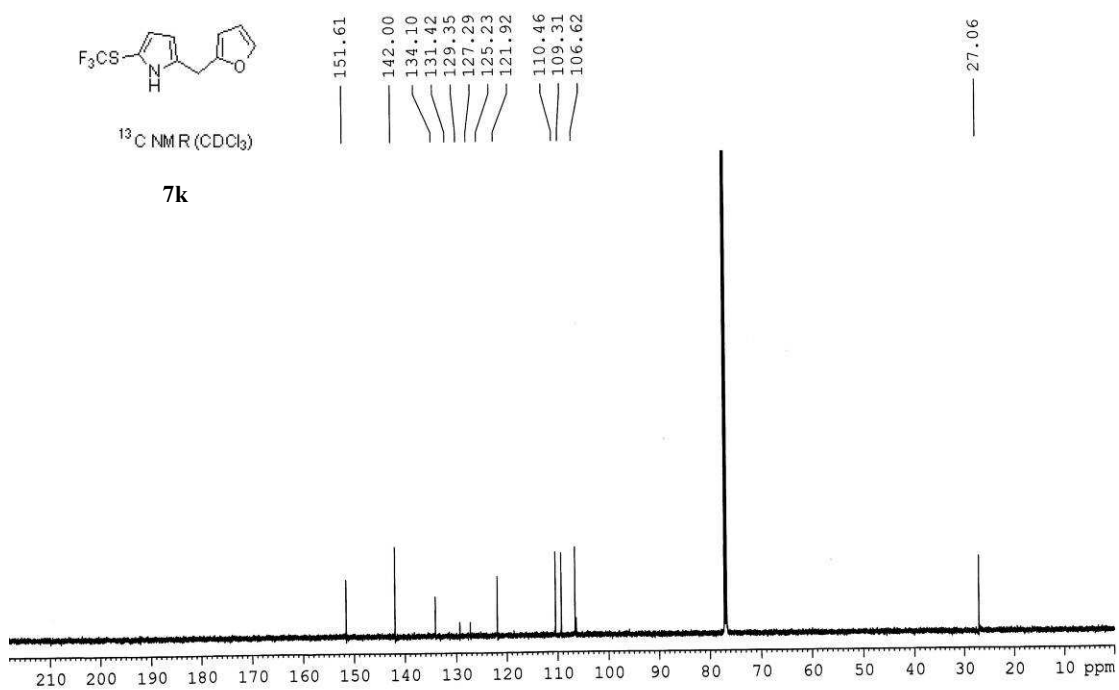
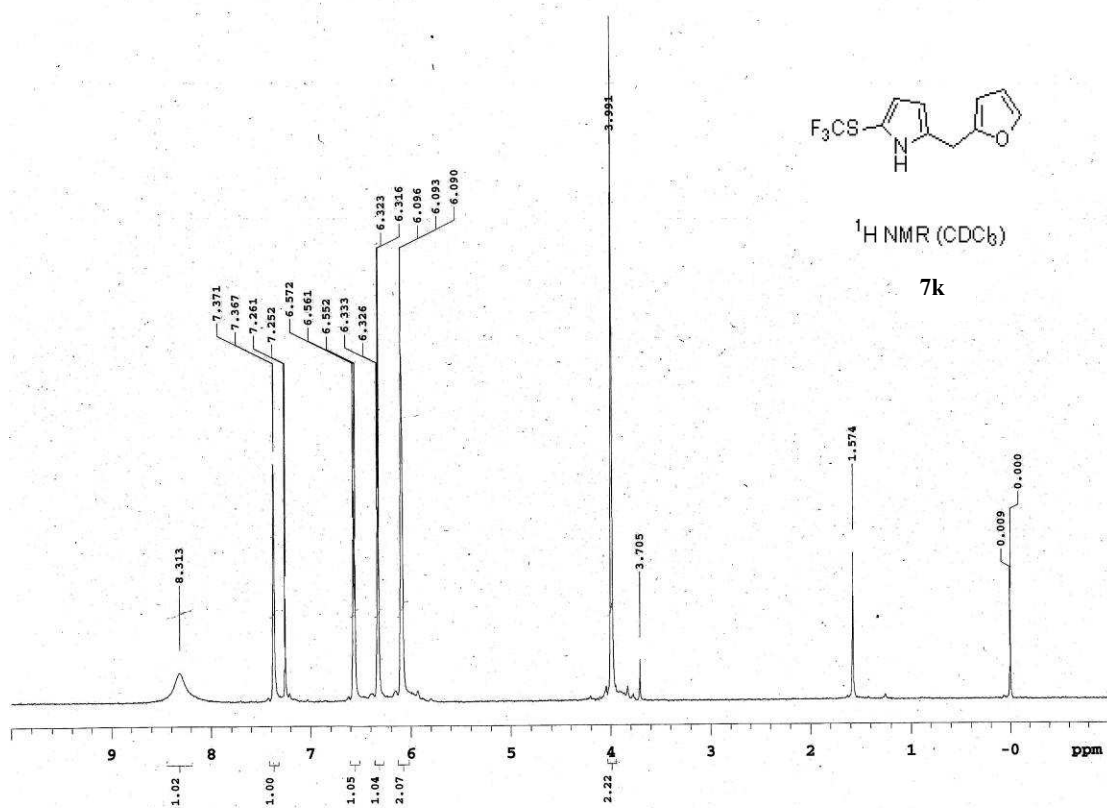


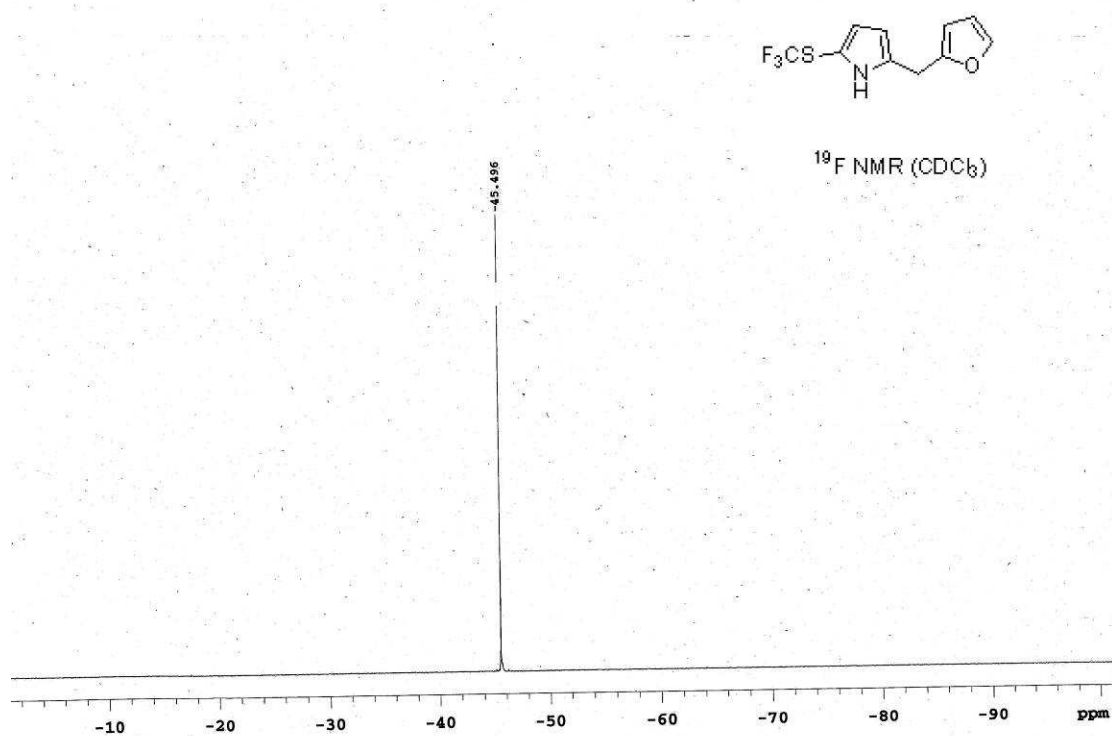


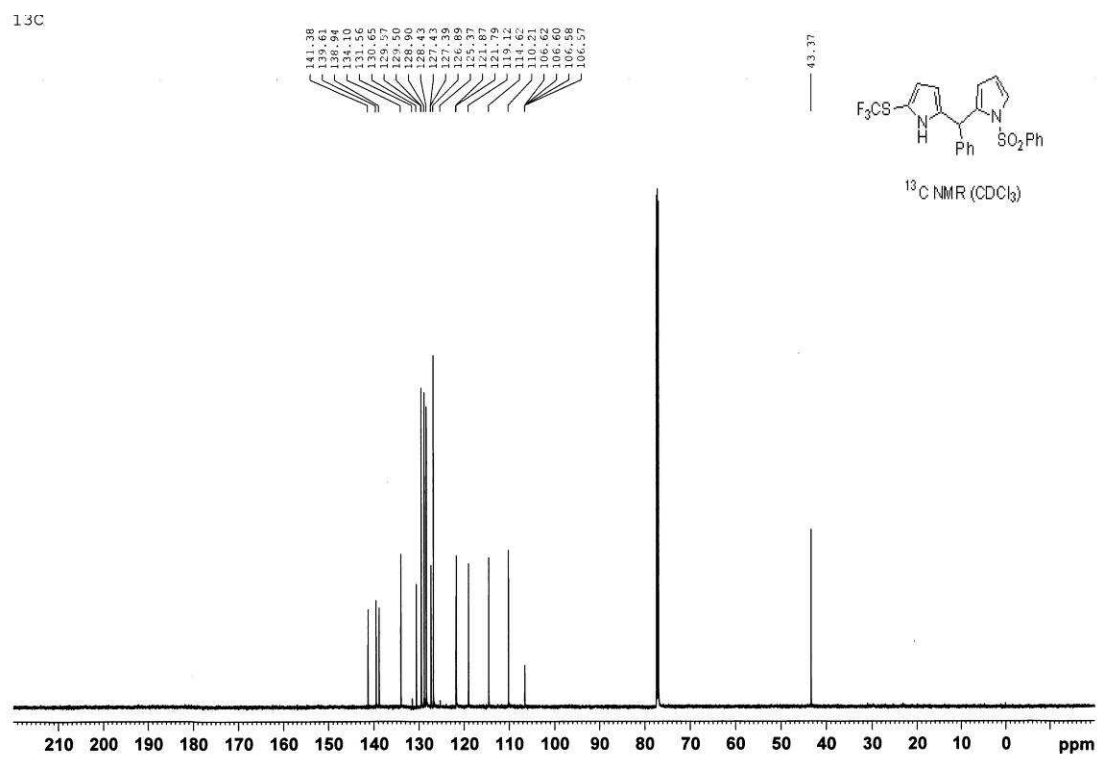
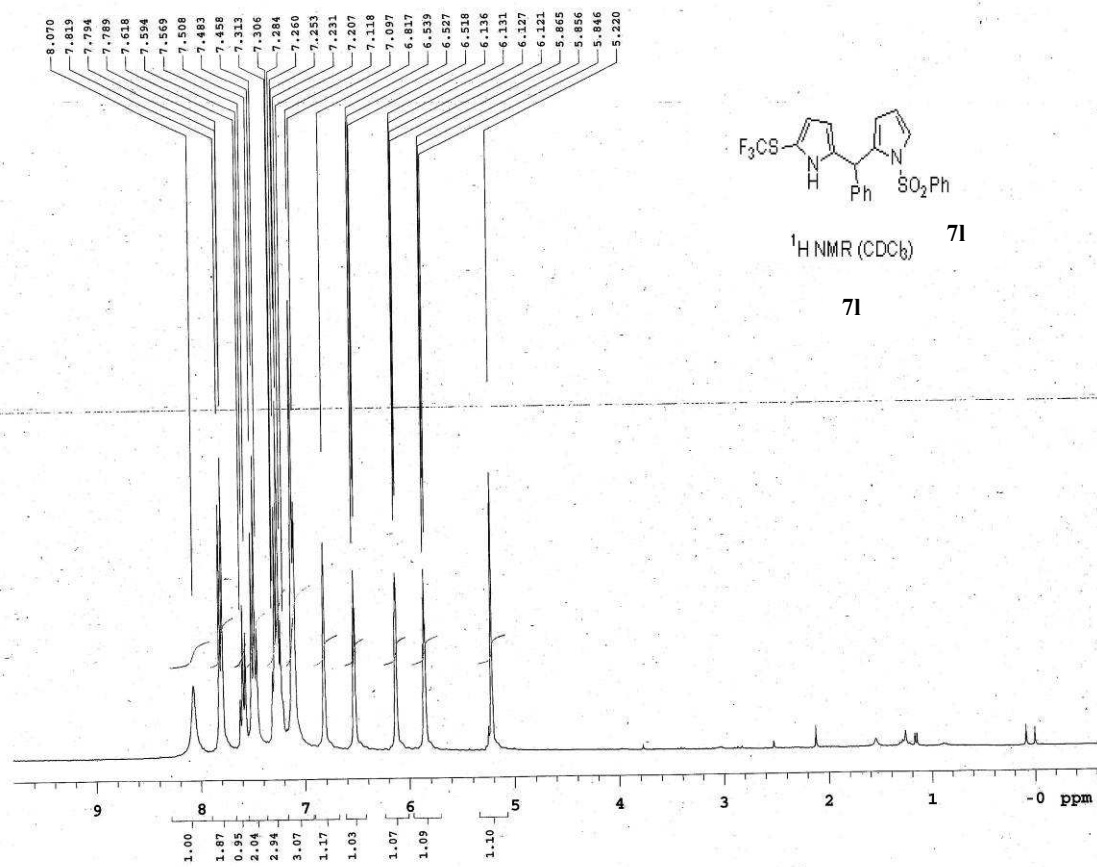


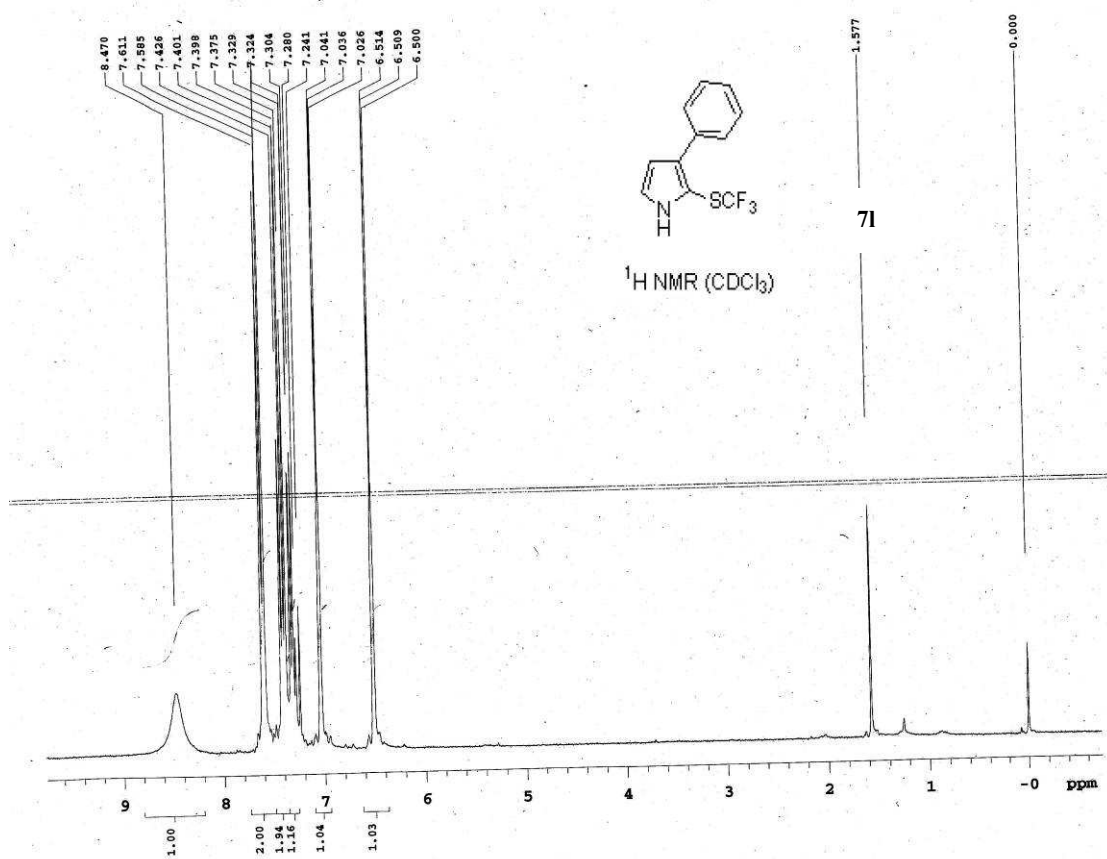
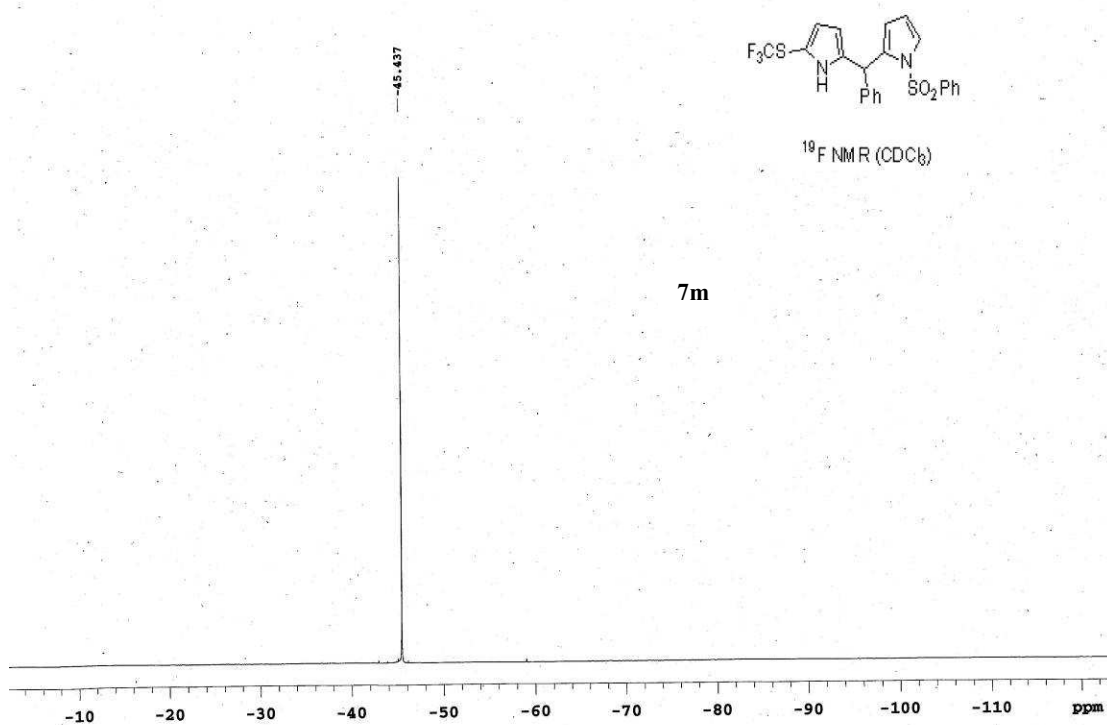


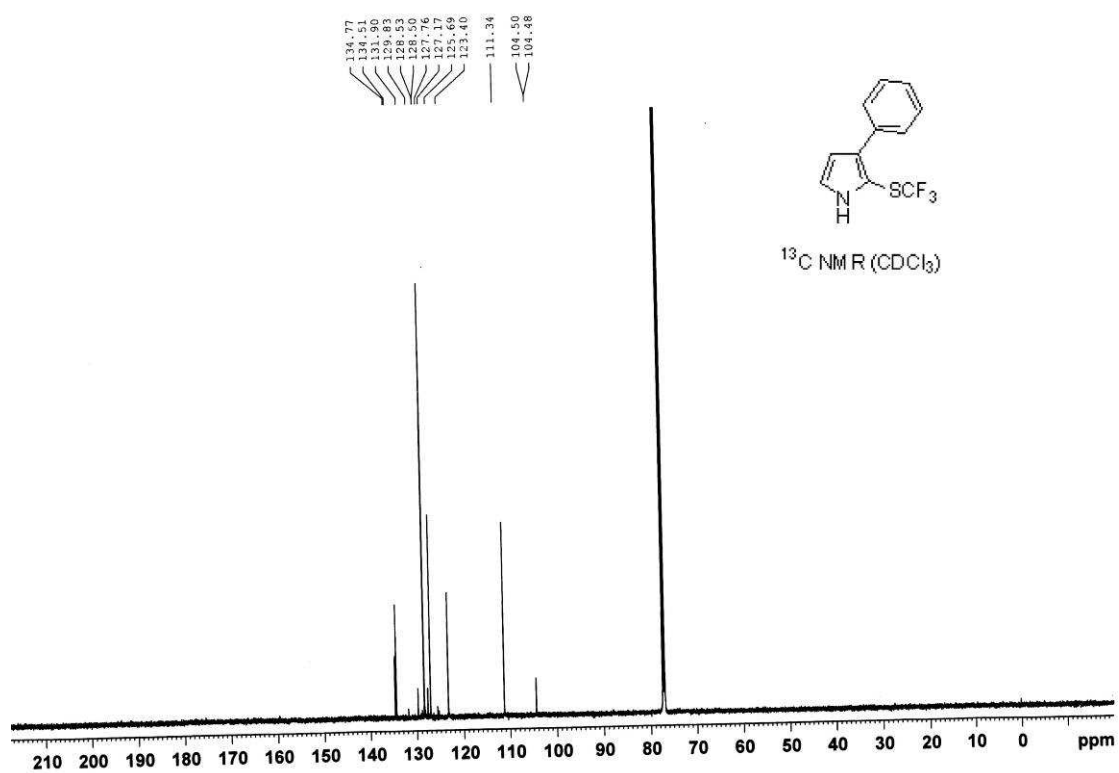




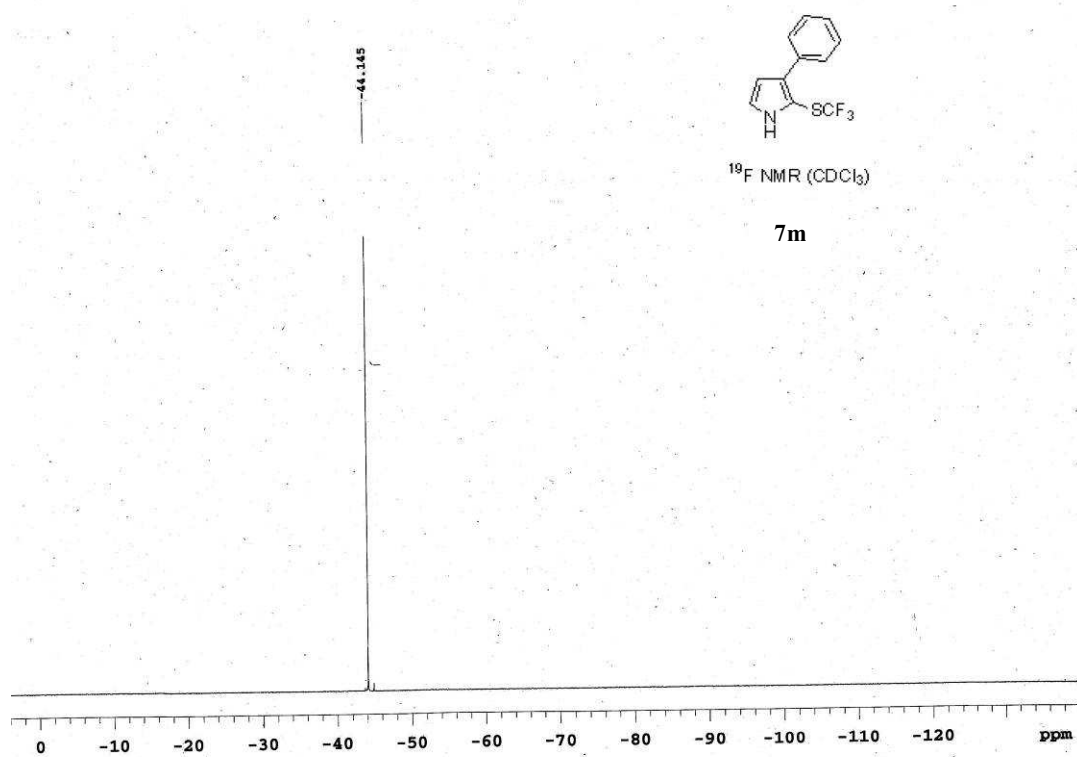


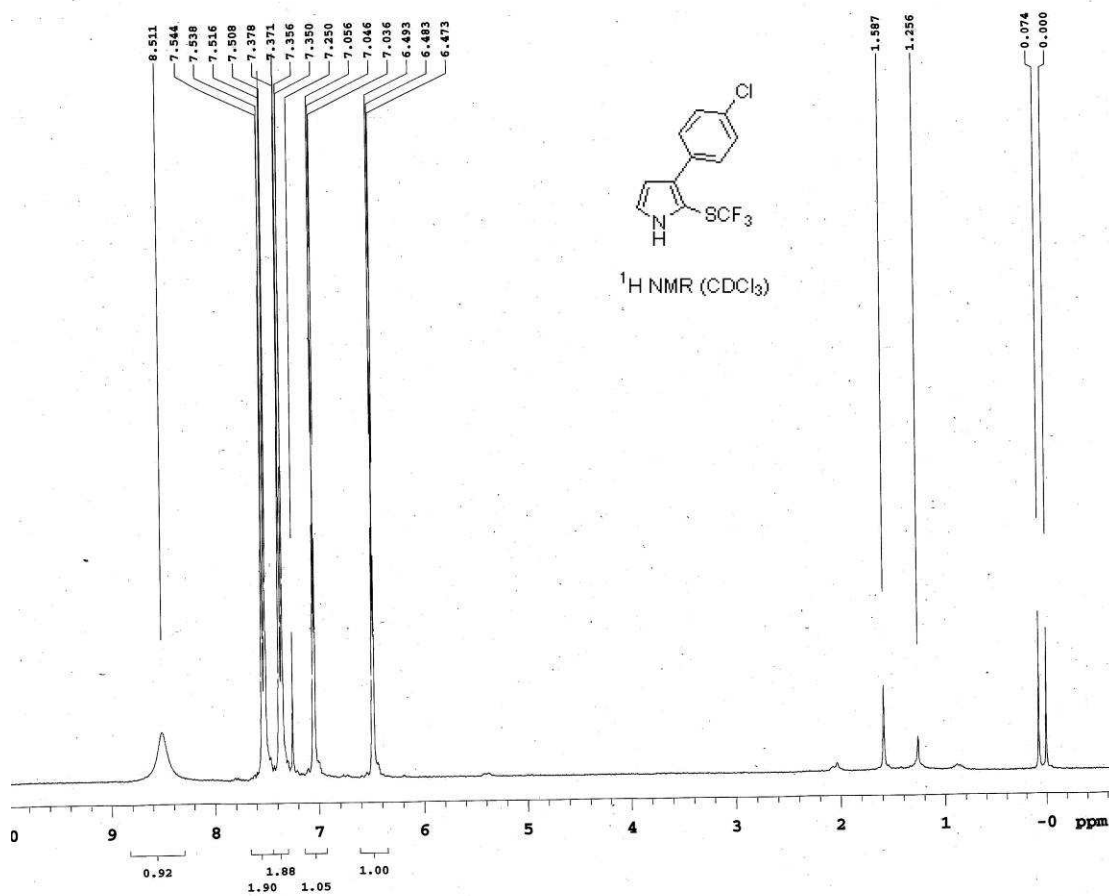




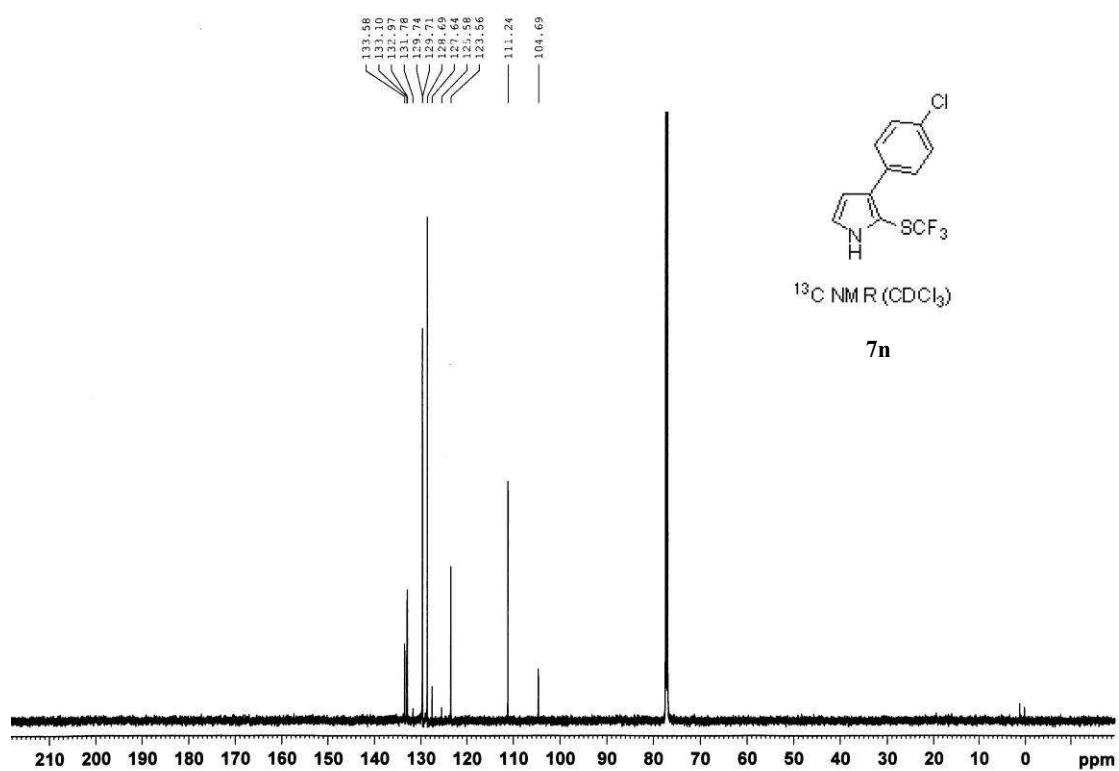


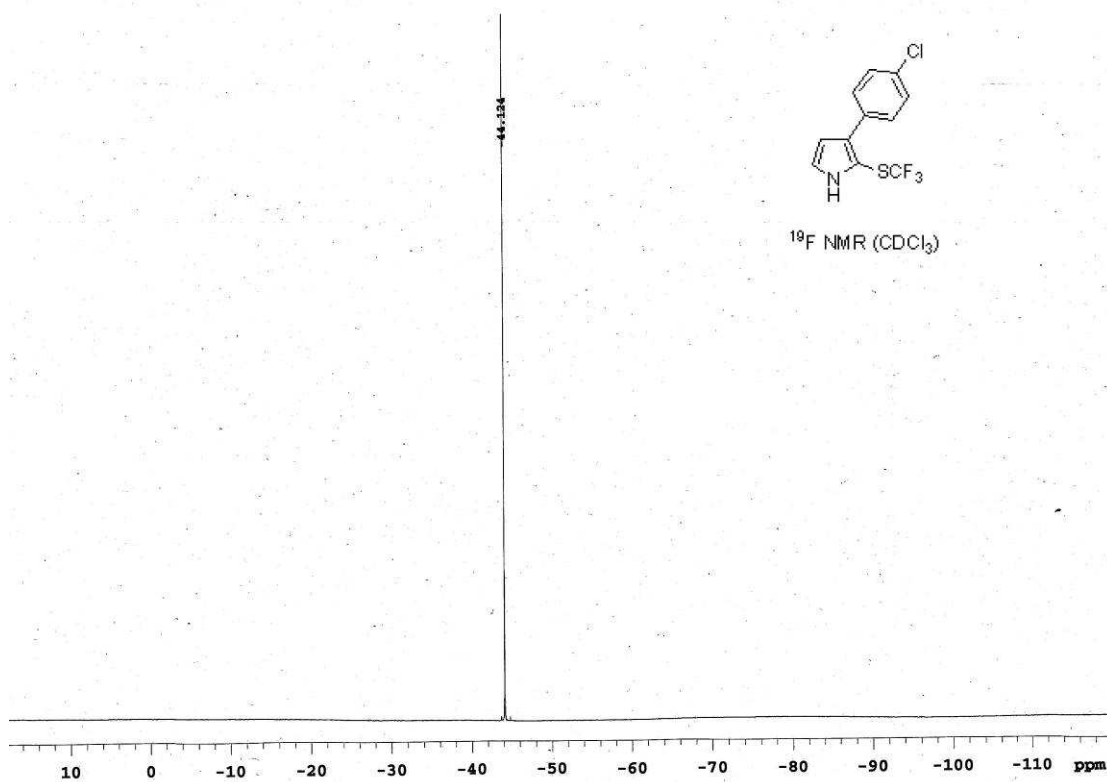
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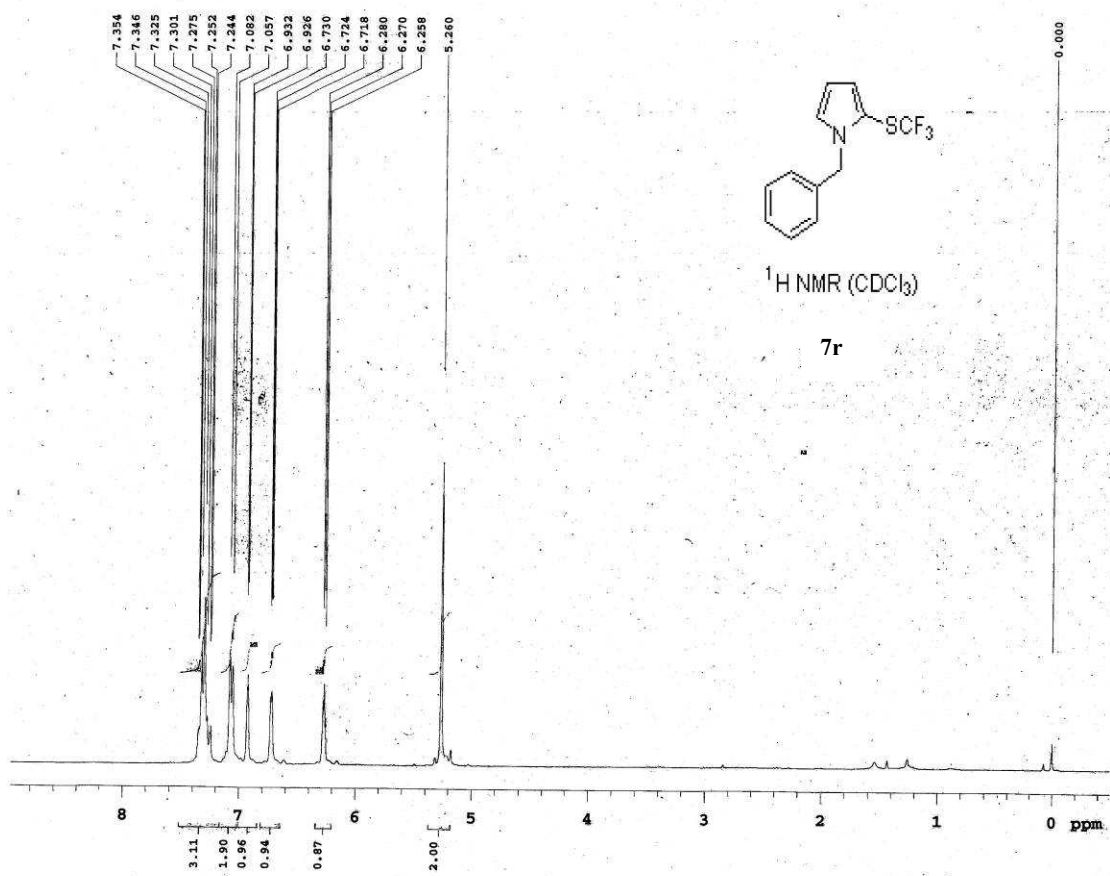


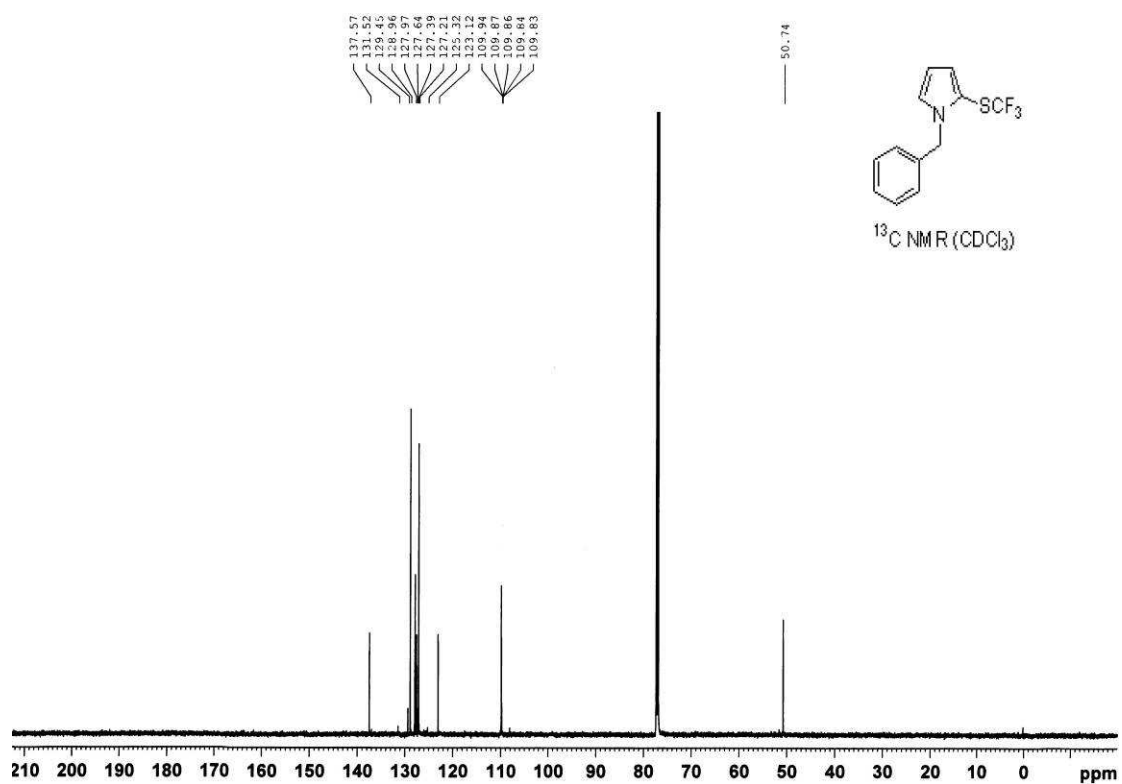
7n





7n





7r

