

## Supporting Information

### Base-Mediated Ynone-Isocyanide [3+2] Cycloaddition: A General Method to 2,3,4-Tri-Substituted 1-*H*-Pyrroles and Bis-Pyrroles

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## **General Information.**

All reagents were purchased (unless specified) at highest commercial quality and used as received. Reaction mixtures were stirred magnetically. All reaction temperatures for reactions were achieved using a IKA heating plate and oil bath.

**Rf:** LC analysis was performed on commercially prepared 60 F254 silica gel plates and visualized by either UV irradiation or by staining with I<sub>2</sub>. Column chromatography was performed using 100- 200 mesh silica gel. Melting Point: Melting points were measured on a Kofler hot-stage melting point apparatus and are uncorrected.

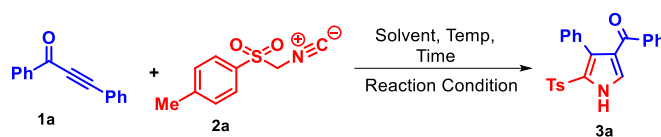
**<sup>1</sup>H NMR:** Spectra were recorded on JEOL ECS (400 MHz) instruments. Chemical shifts ( $\delta$  H) are quoted in parts per million (ppm) and referenced to TMS. Spin-spin coupling constants (*J*) are reported in Hertz (Hz).

**<sup>13</sup>C NMR:** Spectra were recorded on JEOL ECS (100 MHz) instruments. Chemical shifts ( $\delta$  C) are quoted in parts per million (ppm) and referenced to the appropriate solvent peak(s). Spin-spin coupling constants (*J*) are reported in Hertz (Hz).

**HRMS:** High resolution mass spectra were recorded on an Agilent 6500 series B5125 mass spectrometer (ESI-TOF).

## Optimization of Reaction

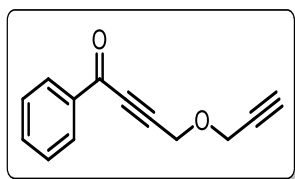
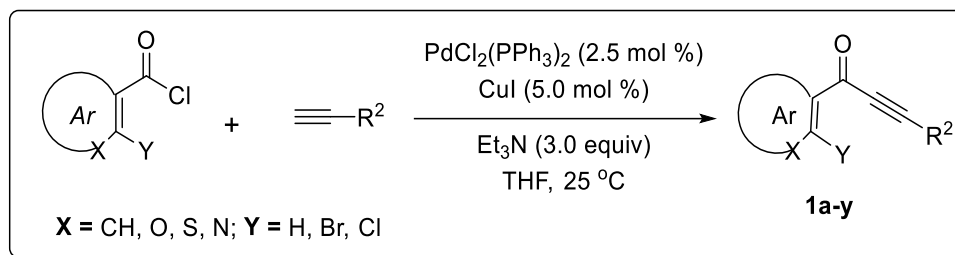
**Table S1. Optimization of Reaction Conditions** <sup>a, b</sup>



entry	base	solvent	t (min)	temp (°C)	Yield (%) <sup>b</sup>
					3a
1	<sup>t</sup> BuOK (2.0)	DMSO	60	100	65
2	<sup>t</sup> BuOK (2.0)	DMSO	60	80	74
3	<sup>t</sup> BuOK (2.0)	DMSO	60	25	82
4	<sup>t</sup> BuOK (2.0)	DMSO	30	25	82
5	<b><sup>t</sup>BuOK (2.0)</b>	<b>DMSO</b>	<b>15</b>	<b>25</b>	<b>85</b>
6	<sup>t</sup> BuOK (3.0)	DMSO	15	25	80
7	<sup>t</sup> BuOK (2.0)	DMF	15	25	75
8	<sup>t</sup> BuOK (2.0)	DMA	15	25	45
9	<sup>t</sup> BuOK (2.0)	NMP	15	25	55
10	<sup>t</sup> BuOK (2.0)	CH <sub>3</sub> CN	15	25	40
11	<sup>t</sup> BuOK (2.0)	THF	15	25	15
12	<sup>t</sup> BuOK (2.0)	toluene	15	25	10
13 <sup>c</sup>	–	DMSO	15	25	0
14	LiO <sup>t</sup> Bu (2.0)	DMSO	15	25	68
15	Cs <sub>2</sub> CO <sub>3</sub> (2.0)	DMSO	15	25	73
16	KOH (2.0)	DMSO	15	25	60
17	NaOH (2.0)	DMSO	15	25	25
18	K <sub>3</sub> PO <sub>4</sub> (2.0)	DMSO	15	25	45

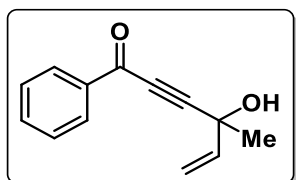
<sup>a</sup>Reactions were performed using 1a (0.5 mmol, 1.0 equiv), 2a (0.6 mmol) and base (2.0 equiv) in 2.0 mL of solvent. <sup>b</sup>Isolated yield. <sup>c</sup>without base, DMF = dimethylformamide, DMA = dimethylacetamide, NMP = N-Methyl-2-pyrrolidone

**General Procedure for the Synthesis of ynones 1a–ai:** The starting materials (**1a–ai**) were prepared by Sonogashira coupling using the standard procedure. The structure and purity of known starting materials **1a–y** were confirmed by comparison of their physical and spectral data ( $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR) with those reported in literature.<sup>1–2</sup>



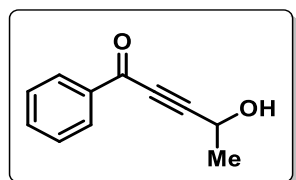
**1-Phenyl-4-(prop-2-yn-1-yloxy)but-2-yn-1-one (1q):** The product was obtained as a brown liquid (150 mg, 70%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.15–8.13 (m, 2H), 7.63 (t,  $J = 7.4$  Hz, 1H), 7.50 (t,  $J = 7.7$  Hz, 2H), 4.57 (s, 2H), 4.36 (d,  $J = 2.3$  Hz, 2H), 2.53 (t,  $J = 2.3$  Hz, 1H);

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  177.4, 136.3, 134.5, 129.7, 128.8, 89.1, 84.5, 78.3, 76.0, 57.3, 56.6; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{13}\text{H}_{11}\text{O}_2$ : 199.0759, found 199.0754.



**4-Hydroxy-4-methyl-1-phenylhex-5-en-2-yn-1-one (1r):** The product was obtained as a brown liquid (151 mg, 75%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.12 (d,  $J = 8.1$  Hz, 2H), 7.60 (t,  $J = 7.4$  Hz, 1H), 7.46 (t,  $J = 7.6$  Hz, 2H), 6.06 (dd,  $J = 17.1, 10.4$  Hz, 1H), 5.60 (d,  $J = 17.2$  Hz, 1H), 5.23 (d,  $J = 10.3$  Hz, 1H), 3.71 (s, 1H), 1.72 (s, 3H);

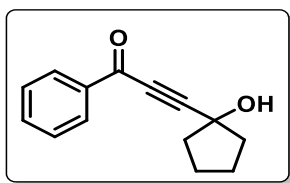
$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  178.1, 140.4, 136.3, 134.4, 129.7, 128.6, 114.9, 95.8, 81.9, 68.3, 29.5 ; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{13}\text{H}_{13}\text{O}_2$ : 201.0916, found 201.0910.



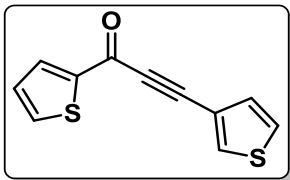
**4-Hydroxy-1-phenylpent-2-yn-1-one (1s):** The product was obtained as a brown liquid (120.8 mg, 68%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.11 (d,  $J = 7.3$  Hz, 2H), 7.59 (t,  $J = 7.4$  Hz, 1H), 7.45 (t,  $J = 7.7$  Hz, 2H), 4.83 (q,  $J = 6.6$  Hz, 1H), 4.03 (s, 1H), 1.61 (d,  $J = 6.7$  Hz, 3H);

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  178.4, 136.3, 134.6, 129.8, 128.8, 96.5, 81.5, 58.2, 23.5, ; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{11}\text{H}_{11}\text{O}_2$ : 175.0759, found 175.0754.

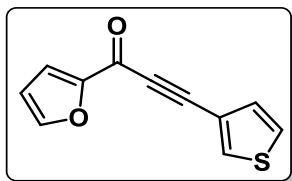




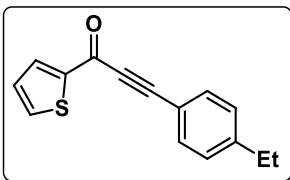
**3-(1-Hydroxycyclopentyl)-1-phenylprop-2-yn-1-one (1t):** The product was obtained as a brown liquid (130 mg, 60%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.12-8.10 (m, 2H), 7.58 (t,  $J = 7.4$  Hz, 1H), 7.44 (t,  $J = 7.7$  Hz, 2H), 3.59 (s, 1H), 2.14-2.11 (m, 4H), 1.95-1.87 (m, 2H), 1.82-1.78 (m, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  178.4, 136.5, 134.4, 129.8, 128.7, 98.6, 81.0, 74.3, 42.3, 23.7; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{14}\text{H}_{14}\text{NaO}_2$ : 237.0891, found 237.0886.



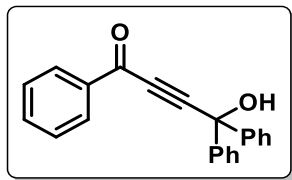
**1-(thiophen-2-yl)-3-(thiophen-3-yl)prop-2-yn-1-one (1ad):** The product was obtained as a brown solid (180 mg, 82%); mp: 61–63 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07-7.68 (m, 3H), 7.42-7.14 (m, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  169.9, 144.9, 135.4, 135.2, 134.1, 130.3, 128.5, 126.5, 119.2, 87.3, 86.8; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{11}\text{H}_7\text{OS}_2$ : 218.9938, found 218.9933.



**1-(Furan-2-yl)-3-(thiophen-3-yl)prop-2-yn-1-one (1ae):** The product was obtained as a brown solid (170.8 mg, 84%); mp: 58–60 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (dd,  $J = 2.9, 1.2$  Hz, 1H), 7.70 (t,  $J = 0.8$  Hz, 1H), 7.43 (dd,  $J = 3.6, 0.5$  Hz, 1H), 7.37 (dd,  $J = 5.0, 3.0$  Hz, 1H), 7.29 (dd,  $J = 4.9, 1.1$  Hz, 1H), 6.61 (q,  $J = 1.7$  Hz, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  164.8, 153.1, 148.1, 134.1, 130.2, 126.3, 121.0, 119.0, 112.7, 87.4, 86.4; HRMS (ESI): HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{11}\text{H}_7\text{O}_2\text{S}$ : 203.0167, found 203.0161.



**3-(4-Ethylphenyl)-1-(thiophen-2-yl)prop-2-yn-1-one (1af) :** The product was obtained as a brown solid (200 mg, 82%); mp: 67–69 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (dd,  $J = 3.8, 1.2$  Hz, 1H), 7.72 (dd,  $J = 4.9, 1.2$  Hz, 1H), 7.58 (dd,  $J = 6.5, 1.7$  Hz, 2H), 7.27-7.23 (m, 2H), 7.18 (dd,  $J = 4.8, 3.8$  Hz, 1H), 2.69 (q,  $J = 7.6$  Hz, 2H), 1.25 (t,  $J = 7.6$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.1, 148.0, 145.1, 135.3, 135.2, 133.3, 128.5, 117.1, 92.7, 86.4, 29.2, 15.3; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{15}\text{H}_{13}\text{OS}$ : 241.0687, found 241.0682.



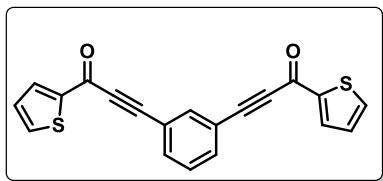
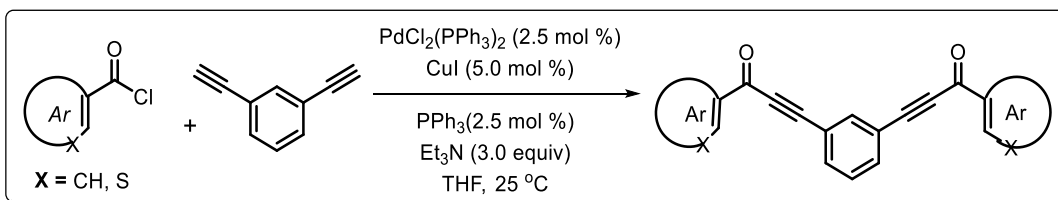
**4-Hydroxy-1,4,4-triphenylbut-2-yn-1-one (1ah):** The product was obtained as a brown solid (204 mg, 65%); mp: 50–52 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (s, 2H), 7.57 (d,  $J = 34.8$  Hz, 5H), 7.34 (d,  $J = 28.3$  Hz, 8H), 3.89 (s, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  178.0, 143.6, 136.6, 134.6, 129.8, 128.8, 128.7, 128.5, 128.4, 128.1, 127.8, 126.2, 96.0, 84.4, 74.8; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{22}\text{H}_{16}\text{NaO}_2$ : 335.1048, found 335.1043.

### General Procedure for the Synthesis of 1,3 bis-yrones :

The starting materials 1,3 bis-yrones were prepared by Sonogashira coupling using the standard procedure. Into a 250 mL two-necked round-bottom flask purged with nitrogen were added  $\text{PdCl}_2(\text{PPh}_3)_2$ , CuI,  $\text{PPh}_3$ , THF and triethylamine. Then, 1,3-diethynylbenzene was injected by syringe. The mixture was cooled to 0° C in an ice water bath, after which benzoyl chloride was injected dropwise. After stirring at room temperature for 12 h the mixture was poured into ice water. The structure and purity of known starting materials **1al–1am** were confirmed by comparison of their physical and spectral data ( $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR) with those reported in

literatur

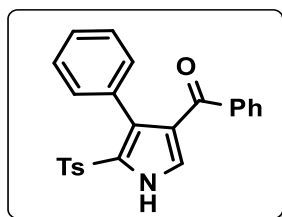
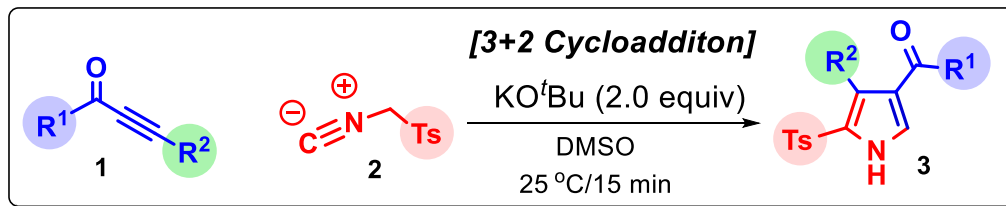
e.<sup>3</sup>



**3,3'-(1,3-Phenylene)bis(1-(thiophen-2-yl)prop-2-yn-1-one) (1ao):** The product was obtained as a brown solid (400 mg, 58%); mp: 60–62 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03–8.02 (m, 2H), 7.93 (s, 1H), 7.78–7.74 (m, 4H), 7.50 (t,  $J = 7.8$  Hz, 1H), 7.23–7.21 (m, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  169.4, 144.5, 136.9, 136.6, 135.8, 135.5, 134.8, 134.5, 129.3, 129.1, 128.5, 120.9, 89.3, 87.1; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{20}\text{H}_{11}\text{O}_2\text{S}_2$ : 347.0200, found 347.0195.

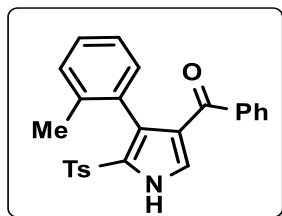
## General Procedure for the Synthesis of Functionalized 2,3,4-Trisubstituted 1-H-Pyrroles derivatives (3 &4) and 5.

To the solution of ynone **1** (0.5 mmol), isocyanide **2** (0.6mmol) and 2.0 equiv. of anhydrous <sup>t</sup>BuOK in 2.0 mL of DMSO were added. The resulting reaction mixture was stirred at 25°C for 0.15 h. Progress of the reaction was monitored by TLC analysis, after completion of starting materials; the reaction mixture was poured in water and extracted by ethyl acetate (3X10 mL). The organic layer was washed with saturated brine solution and dried over Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography on silica gel (100–200 mesh) (hexane–ethylacetate, 8:2). The structure and purity of known product **3**, **4**, **5** were confirmed by their physical and spectral data such as <sup>1</sup>H NMR, <sup>13</sup>C NMR, HRMS.

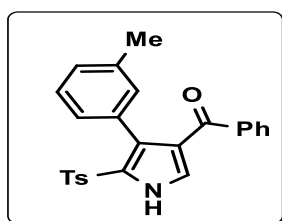


**Phenyl(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3a)** : The product was obtained a pale–yellow solid (176 mg, 88%); mp: 150–152 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.66 (s, 1H), 7.69–7.67 (m, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.32–7.26 (m, 5H), 7.20–7.16 (m, 5H), 7.04 (d, *J* = 8.1 Hz, 2H), 2.31 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.0, 144.4, 138.7, 138.0, 132.3, 131.4, 130.9, 130.6, 129.5, 128.2, 127.8, 127.6, 127.6, 127.3, 125.2, 21.6; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>24</sub>H<sub>20</sub>NO<sub>3</sub>S: 402.1164, found 402.1156.

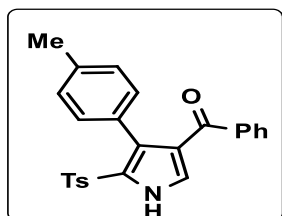
**Gram-scale experiment for 3a:** In an oven-dried 100 mL round bottom flask, a solution of ynone **1a** (1.03 g, 5.0 mmol), isocyanide **2a** (1.17 g, 6.0 mmol), and 2.0 equiv. of anhydrous <sup>t</sup>BuOK (1.12 g, 2.0 equiv) in 10 mL of DMSO were added. The resulting reaction mixture was stirred at 25°C for 0.15 h. Progress of the reaction was monitored by TLC analysis, after completion of starting materials; the reaction mixture was poured in water and extracted by ethyl acetate (3X10 mL). The organic layer was washed with saturated brine solution and dried over Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography on silica gel (100–200 mesh) (hexane–ethylacetate, 8:2) to deliver the desired product **3a** (1.60 g, 80%).



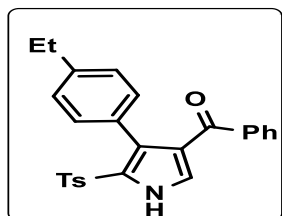
**Phenyl(4-(o-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3b)** : The product was obtained a pale–yellow solid (176 mg, 84%); mp: 145–147 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.25 (s, 1H), 7.70-7.67 (m, 2H), 7.47 (t,  $J = 7.4$  Hz, 1H), 7.37-7.33 (m, 3H), 7.24 (d,  $J = 8.4$  Hz, 2H), 7.18 (td,  $J = 7.1, 2.1$  Hz, 1H), 7.14-7.07 (m, 4H), 6.99 (d,  $J = 7.4$  Hz, 1H), 2.36 (s, 3H), 1.61 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.2, 144.4, 138.7, 137.4, 137.3, 132.1, 131.0, 130.8, 129.8, 129.3, 129.2, 129.2, 128.1, 127.7, 127.5, 127.1, 125.2, 125.0, 21.6, 19.7; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_3\text{S}$ : 416.1320, found 416.1315.



**Phenyl(4-(m-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3c)** : The product was obtained a pale–yellow solid (172 mg, 82%); mp: 135–137 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.32 (s, 1H), 7.67 (dd,  $J = 8.2, 1.2$  Hz, 2H), 7.45-7.41 (m, 1H), 7.35-7.29 (m, 5H), 7.12-7.06 (m, 3H), 7.02 (d,  $J = 7.6$  Hz, 1H), 6.97 (d,  $J = 7.4$  Hz, 1H), 6.85 (s, 1H), 2.34 (s, 3H), 2.21 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.7, 144.3, 138.6, 137.9, 136.9, 132.1, 131.0, 130.9, 129.3, 128.4, 128.0, 127.6, 127.4, 127.3, 127.0, 125.3, 21.6, 21.2 ; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_3\text{S}$ : 416.1320, found 416.1313.

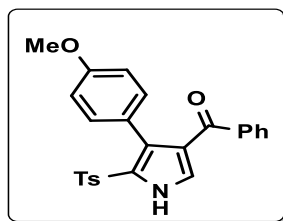


**Phenyl(4-(p-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3d)** : The product was obtained a pale–yellow solid (180 mg, 86%); mp: 155–157 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.06 (s, 1H), 7.69-7.67 (m, 2H), 7.46-7.42 (m, 1H), 7.35 (d,  $J = 3.3$  Hz, 1H), 7.33-7.29 (m, 3H), 7.09-7.02 (m, 7H), 2.34 (s, 3H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.6, 144.3, 138.5, 138.0, 137.5, 132.2, 130.9, 130.4, 129.4, 128.3, 128.1, 127.5, 127.2, 126.8, 125.4, 21.6, 21.3, ; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_3\text{S}$ : 416.1320, found 416.1312.



**(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3e)** : The product was obtained a pale–yellow solid (190 mg, 88%); mp: 190–192 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.42 (s, 1H), 7.66 (d,  $J = 7.7$  Hz, 2H), 7.42 (t,  $J = 7.4$  Hz, 1H), 7.34 (d,  $J = 3.4$  Hz, 1H), 7.31-7.26 (m, 4H), 7.08-7.01 (m, 6H), 2.60 (q,  $J = 7.6$  Hz, 2H), 2.32 (s, 3H), 1.21

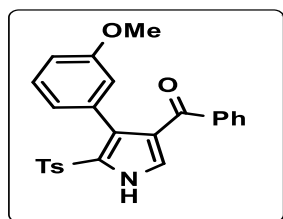
(t,  $J = 7.6$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.8, 144.2, 143.8, 138.6, 137.9, 132.1, 131.0, 130.5, 129.4, 129.3, 128.4, 128.0, 127.5, 127.2, 127.0, 125.2, 28.6, 21.6, 15.7; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{26}\text{H}_{24}\text{NO}_3\text{S}$ : 430.1477, found 430.1469.



**(4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone**

**(3f):** The product was obtained a pale-yellow solid (196 mg, 90%); mp: 186–188 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.60 (s, 1H), 7.68 (d,  $J = 7.4$  Hz, 2H), 7.43 (t,  $J = 7.4$  Hz, 1H), 7.30 (d,  $J = 8.2$  Hz, 5H), 7.12 (d,  $J = 8.7$  Hz, 2H), 7.07 (d,  $J = 8.1$  Hz, 2H), 6.76 (d,  $J = 8.5$  Hz, 2H), 3.77

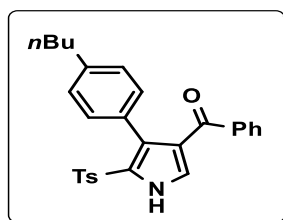
(s, 3H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  191.1, 159.3, 144.4, 138.7, 138.2, 132.3, 131.9, 130.9, 129.8, 129.5, 128.2, 127.7, 127.5, 127.2, 125.2, 123.6, 113.1, 55.3, 21.7; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_4\text{S}$ : 432.1270, found 432.1264.



**(4-(3-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone**

**(3g):** The product was obtained a pale-yellow solid (174 mg, 80%); mp: 192–194 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.33 (s, 1H), 7.68-7.66 (m, 2H), 7.45-7.41 (m, 1H), 7.37 (d,  $J = 3.3$  Hz, 1H), 7.32-7.28 (m, 4H), 7.09 (q,  $J = 7.8$  Hz, 3H), 6.78-6.72 (m, 2H), 6.69-6.68 (m, 1H), 3.69 (s,

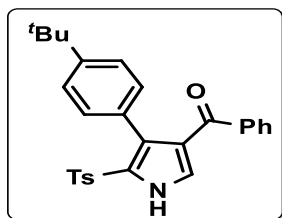
3H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.9, 158.8, 144.5, 138.6, 137.9, 132.6, 132.3, 130.5, 129.5, 128.6, 128.2, 127.7, 127.4, 127.0, 125.5, 123.2, 115.7, 114.2, 55.2, 21.7, ; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{25}\text{H}_{22}\text{NO}_4\text{S}$ : 432.1270, found 432.1261.



**(4-(4-Butylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3h) :**

The product was obtained a pale-yellow solid (189 mg, 82%); mp: 175–177 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.31 (s, 1H), 7.66-7.64 (m, 2H), 7.42-7.37 (m, 2H), 7.29-7.25 (m, 5H), 7.07-7.04 (m, 2H), 7.02-6.98 (m, 3H), 2.56 (t,  $J = 7.6$  Hz, 2H), 2.32 (s, 3H), 1.60-1.52 (m, 2H),

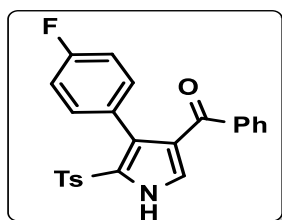
1.36-1.26 (m, 2H), 0.94 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.9, 144.2, 142.4, 138.5, 137.8, 132.1, 130.9, 130.4, 129.4, 129.3, 128.3, 128.0, 127.6, 127.4, 127.2, 127.0, 125.4, 35.3, 33.6, 22.1, 21.6, 14.0 ; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{28}\text{H}_{28}\text{NO}_3\text{S}$ : 458.1790, found 458.1789.



**(4-(4-(tert-butyl)phenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone**

**(3i)** : The product was obtained a pale–yellow solid (194 mg, 84%); mp: 180–182 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.56 (s, 1H), 7.66–7.64 (m, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.36 (d, *J* = 3.3 Hz, 1H), 7.29–7.19 (m, 6H), 7.08 (d, *J* = 8.2 Hz, 2H), 7.00 (d, *J* = 8.2 Hz, 2H), 2.30 (s,

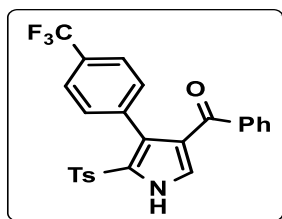
3H), 1.29 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.1, 150.7, 144.3, 138.7, 137.8, 132.1, 131.0, 130.4, 129.4, 129.3, 128.3, 128.1, 127.7, 127.5, 127.4, 127.2, 125.2, 124.4, 34.6, 31.4, 21.6; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>28</sub>H<sub>28</sub>NO<sub>3</sub>S: 458.1790, found 458.1779.



**(4-(4-Fluorophenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone**

**(3j)**: The product was obtained a pale–yellow solid (137 mg, 65%); mp: 186–188 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.23 (s, 1H), 7.67–7.65 (m, 2H), 7.48–7.43 (m, 1H), 7.38 (d, *J* = 3.4 Hz, 1H), 7.31 (dd, *J* = 15.0, 8.0 Hz, 4H), 7.17–7.13 (m, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 6.93–6.89 (m, 2H),

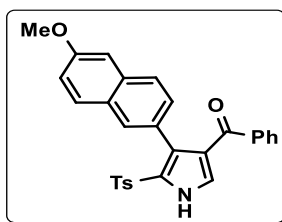
2.35 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.7, 162.6 (d, *J*<sub>C-F</sub> = 247.57 Hz), 144.7, 138.5, 137.8, 132.4 (d, *J*<sub>C-F</sub> = 7.71 Hz), 129.6, 129.4, 128.3, 128.0, 127.3, 127.0, 125.4, 114.6 (d, *J*<sub>C-F</sub> = 21.19 Hz), 21.7; <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>) δ -113.98 HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>24</sub>H<sub>19</sub>FNO<sub>3</sub>S: 420.1070, found 420.1063.



**Phenyl(5-tosyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrol-3-yl)methanone (3k)**

The product was obtained a pale–yellow solid (160 mg, 68%); mp: 177–178 °C; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 13.30 (s, 1H), 7.70–7.64 (m, 4H), 7.60 (s, 1H), 7.57–7.51 (m, 3H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 8.2 Hz, 4H), 2.35 (s, 3H); <sup>13</sup>C NMR (125 MHz,

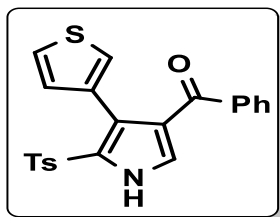
DMSO-*D*<sub>6</sub>) δ 189.8, 144.8, 139.1, 139.0, 137.3, 132.7, 131.6, 130.4, 130.0, 129.5, 129.0, 128.8, 128.4, 128.2 (q, *J*<sub>C-F</sub> = 31.7 Hz 1C), 127.2, 124.9 (q, *J*<sub>C-F</sub> = 271.6 Hz 1C), 124.49 (d, *J*<sub>C-F</sub> = 2.89 Hz 1C), 21.5; <sup>19</sup>F NMR (470 MHz, CDCl<sub>3</sub>) δ -62.38; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>25</sub>H<sub>19</sub>F<sub>3</sub>O<sub>3</sub>S: 470.1038, found 470.1051.



**(4-(6-Methoxynaphthalen-2-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3l)**

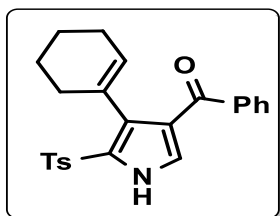
The product was obtained a pale–yellow solid (216 mg, 89%); mp: 180–182 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ

10.58 (s, 1H), 7.67 (d,  $J = 7.1$  Hz, 2H), 7.58-7.53 (m, 3H), 7.37 (t,  $J = 7.4$  Hz, 1H), 7.31-7.22 (m, 6H), 7.09 (dd,  $J = 11.1, 2.2$  Hz, 2H), 6.94 (d,  $J = 8.1$  Hz, 2H), 3.90 (s, 3H), 2.26 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.9, 157.9, 144.4, 138.7, 138.1, 134.0, 132.3, 131.0, 129.7, 129.7, 129.5, 129.0, 128.2, 127.9, 127.7, 127.4, 126.7, 126.0, 125.3, 118.8, 105.7, 55.4, 21.6; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{29}\text{H}_{24}\text{NO}_4\text{S}$ : 482.1426, found 482.1420.



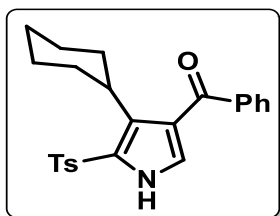
**Phenyl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3m) :**

The product was obtained a pale-yellow solid (177 mg, 86%); mp: 160–162 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.32 (s, 1H), 7.68-7.66 (m, 2H), 7.47-7.43 (m, 1H), 7.38 (d,  $J = 3.3$  Hz, 1H), 7.33-7.30 (m, 5H), 7.12-7.08 (m, 3H), 6.87 (dd,  $J = 4.9, 1.1$  Hz, 1H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.9, 144.5, 138.3, 137.6, 132.3, 130.5, 129.9, 129.5, 129.4, 128.1, 127.7, 127.1, 127.0, 126.2, 125.5, 125.2, 124.2, 21.6; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{22}\text{H}_{18}\text{NO}_3\text{S}_2$ : 408.0728, found 408.0728.



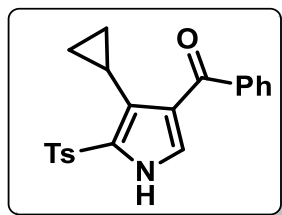
**(4-(Cyclohex-1-en-1-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3n):**

The product was obtained a pale-yellow solid (164 mg, 80%); mp: 147–149 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.95 (s, 1H), 7.75-7.70 (m, 4H), 7.52 (t,  $J = 7.4$  Hz, 1H), 7.40 (t,  $J = 7.6$  Hz, 2H), 7.33 (d,  $J = 3.3$  Hz, 1H), 7.29-7.27 (m, 2H), 5.62-5.60 (m, 1H), 2.42 (s, 3H), 2.03-2.01 (m, 2H), 1.68 (d,  $J = 1.8$  Hz, 2H), 1.45-1.41 (m, 2H), 1.37-1.34 (m, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  191.1, 144.5, 139.0, 138.3, 133.1, 132.1, 130.2, 129.4, 129.2, 129.1, 128.1, 127.7, 127.1, 126.8, 124.7, 29.4, 25.4, 22.4, 21.7, 21.5; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{24}\text{H}_{24}\text{NO}_3\text{S}$ : 406.1477, found 406.1493.



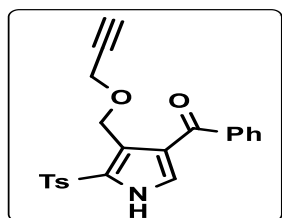
**(4-Cyclohexyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3o):**

The product was obtained a pale-yellow solid (154 mg, 75%); mp: 131–133 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.91 (s, 1H), 7.82 (d,  $J = 8.2$  Hz, 2H), 7.72-7.70 (m, 2H), 7.56-7.52 (m, 1H), 7.45-7.41 (m, 2H), 7.32 (d,  $J = 8.4$  Hz, 2H), 7.14 (d,  $J = 3.4$  Hz, 1H), 2.43 (s, 3H), 2.00-1.92 (m, 2H), 1.71-1.62 (m, 3H), 1.33-1.22 (m, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  191.8, 144.5, 140.0, 139.1, 136.5, 132.1, 129.9, 129.4, 129.3, 128.3, 127.1, 126.6, 124.7, 36.2, 30.4, 26.9, 25.6, 21.7; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{24}\text{H}_{26}\text{NO}_3\text{S}$ : 408.1633, found 408.1625.



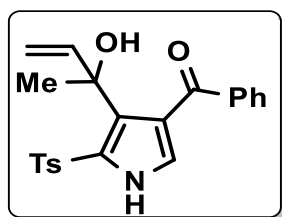
**(4-Cyclopropyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3p):**

The product was obtained a pale-yellow solid (132 mg, 72%); mp: 136–138 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.41 (s, 1H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.77-7.75 (m, 2H), 7.55-7.52 (m, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.31-7.27 (m, 2H), 7.18 (d, *J* = 3.4 Hz, 1H), 2.41 (s, 3H), 1.88-1.81 (m, 1H), 0.75-0.71 (m, 2H), 0.56-0.52 (m, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.4, 144.5, 139.2, 138.5, 132.5, 129.8, 129.5, 128.3, 128.1, 127.5, 127.3, 125.9, 21.7, 8.0, 7.1; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>21</sub>H<sub>20</sub>NO<sub>3</sub>S: 366.1164, found 366.1157.



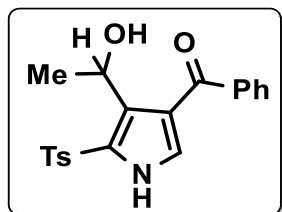
**Phenyl (4-((prop-2-yn-1-yloxy)methyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3q) :**

The product was obtained a pale-yellow solid (140 mg, 70%); mp: 117–119 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.19 (s, 1H), 7.92 (d, *J* = 8.2 Hz, 2H), 7.72 (d, *J* = 7.3 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 2.7 Hz, 1H), 5.00 (s, 2H), 4.15 (d, *J* = 2.3 Hz, 2H), 2.45 (t, *J* = 2.3 Hz, 1H), 2.40 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.9, 144.7, 139.2, 138.3, 132.2, 129.9, 129.4, 129.1, 128.4, 127.6, 126.0, 124.7, 79.7, 74.6, 60.8, 58.1, 21.6; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>22</sub>H<sub>20</sub>NO<sub>4</sub>S: 394.1113, found 394.1132.



**(4-(2-Hydroxybut-3-en-2-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3r) :**

The product was obtained a pale-yellow solid (148 mg, 74%); mp: 121–123 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.20 (s, 1H), 7.76-7.70 (m, 3H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.28 (t, *J* = 8.2 Hz, 3H), 7.21 (s, 1H), 6.31 (dd, *J* = 17.3, 10.6 Hz, 1H), 5.07 (d, *J* = 16.9 Hz, 2H), 4.87 (d, *J* = 10.6 Hz, 1H), 2.42 (s, 3H), 1.62 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 192.8, 144.5, 143.7, 139.6, 139.2, 137.6, 132.6, 130.1, 130.0, 129.8, 129.7, 129.5, 129.0, 128.6, 128.4, 127.2, 127.0, 124.6, 112.4, 72.8, 28.9, 21.7; HRMS (ESI): (M+Na)<sup>+</sup> Calcd for C<sub>22</sub>H<sub>21</sub>NNaO<sub>4</sub>S: 418.1091, found 418.1091.

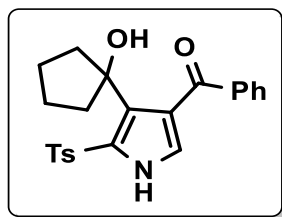


**(4-(1-Hydroxyethyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3s) :**

The product was obtained a pale-yellow solid (138 mg, 75%); mp:



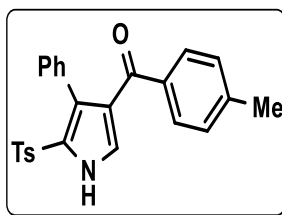
111–113 °C;  $^1\text{H}$  NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  13.04 (s, 1H), 7.81 (d, *J* = 8.1 Hz, 2H), 7.67 (d, *J* = 7.3 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.40 (d, *J* = 7.4 Hz, 3H), 5.48 (d, *J* = 10.4 Hz, 1H), 5.40–5.35 (m, 1H), 2.32 (s, 3H), 1.27 (d, *J* = 6.5 Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  193.2, 145.0, 139.4, 136.0, 133.5, 133.0, 130.8, 129.7, 129.1, 127.3, 126.7, 122.5, 61.6, 24.9, 21.6; HRMS (ESI): (M+Na)<sup>+</sup> Calcd for C<sub>20</sub>H<sub>19</sub>NNaO<sub>4</sub>S: 392.0932, found 392.0922.



**(4-(1-Hydroxycyclopentyl)-5-tosyl-1*H*-pyrrol-3-**

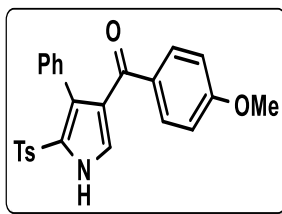
**yl)(phenyl)methanone (3t)** : The product was obtained a pale–yellow solid (149 mg, 72%); mp: 121–123 °C;  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  10.44 (s, 1H), 7.75–7.67 (m, 4H), 7.59–7.55 (m, 1H), 7.42 (dt, *J* = 21.6, 7.6 Hz, 2H), 7.26 (t, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 3.3 Hz, 1H), 4.40 (s,

1H), 2.40 (s, 3H), 2.19–2.05 (m, 2H), 1.82–1.68 (m, 6H);  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  193.0, 144.4, 139.6, 139.2, 138.2, 133.6, 132.6, 132.2, 130.1, 129.7, 129.6, 129.2, 128.5, 128.3, 127.6, 127.0, 126.5, 124.4, 80.4, 41.1, 24.1, 21.7; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>23</sub>H<sub>23</sub>NNaO<sub>4</sub>S: 432.1245, found 432.1240



**(4-Phenyl-5-tosyl-1*H*-pyrrol-3-yl)(p-tolyl)methanone (3u)** : The product was obtained a pale–yellow solid (178 mg, 85%); mp: 142–144 °C;  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  10.26 (s, 1H), 7.60 (d, *J* = 8.1 Hz, 2H), 7.34 (q, *J* = 1.6 Hz, 1H), 7.28–7.26 (m, 2H), 7.24–7.15 (m, 5H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 2.33 (d, *J* = 5.4 Hz,

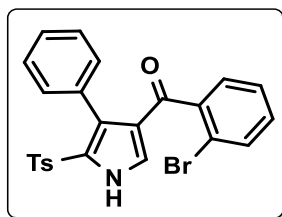
6H);  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  190.5, 144.4, 143.1, 138.0, 135.9, 131.4, 130.8, 130.7, 130.1, 129.7, 129.5, 128.9, 128.4, 127.8, 127.6, 127.3, 126.8, 125.6, 21.7; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>25</sub>H<sub>22</sub>NO<sub>3</sub>S: 416.1320, found 416.1334.



**(4-Methoxyphenyl)(4-phenyl-5-tosyl-1*H*-pyrrol-3-yl)methanone**

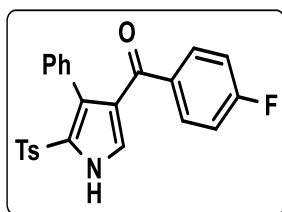
**(3v)** : The product was obtained a pale–yellow solid (187 mg, 86%); mp: 162–164 °C;  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  10.25 (s, 1H), 7.69 (dd, *J* = 6.9, 1.9 Hz, 2H), 7.33 (d, *J* = 3.2 Hz, 1H), 7.28–7.26 (m, 2H), 7.23–7.16 (m, 5H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.78 (dd, *J* = 6.8, 2.0 Hz,

2H), 3.80 (s, 3H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  189.5, 163.0, 144.3, 137.9, 131.8, 131.3, 131.1, 130.6, 129.4, 127.7, 127.5, 127.2, 127.2, 126.2, 125.7, 113.3, 55.4, 21.6; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>25</sub>H<sub>22</sub>NO<sub>4</sub>S: 432.1270, found 432.1262.



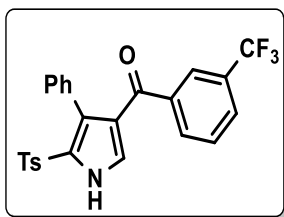
**(2-Bromophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3w):**

The product was obtained a pale–yellow solid (188 mg, 78%); mp: 147–149 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.41 (s, 1H), 7.39-7.36 (m, 1H), 7.33 (d, *J* = 3.4 Hz, 1H), 7.23-7.20 (m, 3H), 7.18-7.13 (m, 4H), 7.11-7.07 (m, 3H), 7.04 (d, *J* = 8.1 Hz, 2H), 2.32 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.4, 144.5, 141.1, 137.7, 133.0, 131.0, 130.7, 130.6, 130.5, 129.5, 129.1, 128.5, 128.3, 127.8, 127.4, 127.3, 126.9, 125.4, 119.5, 21.7; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>24</sub>H<sub>19</sub>BrNO<sub>3</sub>S: 480.0269, found 480.0261.



**(4-Fluorophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3x) :**

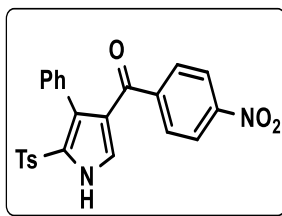
The product was obtained a pale–yellow solid (158 mg, 75%); mp: 209–211 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.62 (s, 1H), 7.71-7.67 (m, 2H), 7.35 (d, *J* = 3.3 Hz, 1H), 7.27 (d, *J* = 8.2 Hz, 2H), 7.23-7.13 (m, 5H), 7.05 (d, *J* = 8.1 Hz, 2H), 6.97-6.93 (m, 2H), 2.32 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 189.5, 165.1 (d, *J*<sub>C-F</sub>=253.35 Hz), 144.4, 137.8, 134.6, 132.0, 131.9 (d, *J*<sub>C-F</sub>=8.67 Hz), 130.6, 129.4, 127.8, 127.5, 127.1, 127.0, 125.2, 115.1 (d, *J*<sub>C-F</sub>=21.19 Hz), 21.6; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>24</sub>H<sub>19</sub>FNO<sub>3</sub>S: 420.1070, found 420.1067.



**(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(3-**

**(trifluoromethyl)phenyl)methanone (3y) :** The product was obtained a

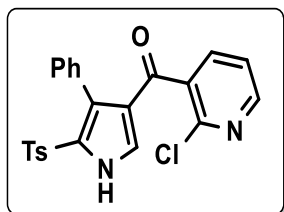
pale–yellow solid (167 mg, 71%); mp: 161–163 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.55 (s, 1H), 7.82 (t, *J* = 7.7 Hz, 2H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.45 (s, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.26 (t, *J* = 4.1 Hz, 2H), 7.20-7.15 (m, 3H), 7.12-7.09 (m, 2H), 7.05 (d, *J* = 8.1 Hz, 2H), 2.32 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 189.8, 144.6, 139.0, 137.7, 132.4, 131.0, 130.7, 130.7, 130.4, 130.2, 129.9, 129.6, 128.9, 128.6, 128.4, 128.0, 127.7, 127.3, 127.3, 126.2 (q, *J*<sub>C-F</sub>=3.8 Hz 1C), 122.3 (q, *J*<sub>C-F</sub>=272.6 Hz 1C), 21.7; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>25</sub>H<sub>19</sub>F<sub>3</sub>NO<sub>3</sub>S: 470.1038, found 470.1030.



**(4-Nitrophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3z) :**

The product was obtained a pale–yellow solid (157 mg, 70%); mp: 130–

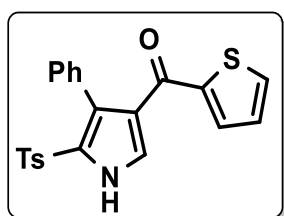
132 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.51 (s, 1H), 8.07 (dd,  $J = 6.9, 1.9$  Hz, 2H), 7.71 (dd,  $J = 6.9, 1.9$  Hz, 2H), 7.48 (d,  $J = 3.3$  Hz, 1H), 7.25 (d,  $J = 8.4$  Hz, 2H), 7.22-7.14 (m, 3H), 7.10-7.04 (m, 4H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  189.1, 149.4, 144.6, 143.5, 142.0, 137.5, 130.7, 130.6, 130.4, 130.0, 129.5, 128.6, 128.3, 128.2, 128.1, 127.8, 127.7, 127.3, 127.2, 124.9, 123.3, 123.2, 21.6; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{24}\text{H}_{19}\text{N}_2\text{O}_5\text{S}$ : 447.1015, found 447.1040.



**(2-Chloropyridin-3-yl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone**

**(3aa)** : The product was obtained a pale-yellow solid (150 mg, 68%); mp: 125–127 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.57 (s, 1H), 8.22 (dd,  $J = 4.8, 1.9$  Hz, 1H), 7.56 (d,  $J = 3.4$  Hz, 1H), 7.42 (dd,  $J = 7.6, 1.9$  Hz, 1H), 7.21-7.16 (m, 3H), 7.14-7.10 (m, 2H), 7.05-6.99 (m, 5H), 2.33 (s,

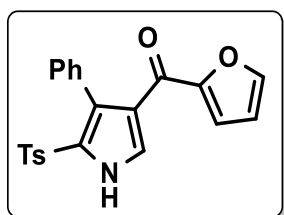
3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  187.9, 150.3, 147.3, 144.5, 137.5, 135.3, 130.4, 130.2, 130.0, 129.4, 128.5, 128.0, 127.6, 127.5, 127.3, 125.5, 121.7, 21.6; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{23}\text{H}_{18}\text{ClN}_2\text{O}_3\text{S}$ : 437.0727, found 437.0724.



**(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone** **(3ab)**:

The product was obtained a pale-yellow solid (175 mg, 85%); mp: 134–136 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.48 (s, 1H), 7.56 (dd,  $J = 4.9, 1.0$  Hz, 1H), 7.52 (dd,  $J = 3.8, 1.1$  Hz, 1H), 7.47 (d,  $J = 3.4$  Hz, 1H), 7.30-7.20 (m, 7H), 7.06 (d,  $J = 8.2$  Hz, 2H), 7.00 (dd,  $J = 4.8, 3.8$  Hz,

1H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  181.9, 144.6, 144.5, 137.9, 133.7, 133.6, 131.2, 130.6, 130.5, 129.5, 127.9, 127.9, 127.7, 127.7, 127.3, 126.1, 125.3, 21.6; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{22}\text{H}_{18}\text{NO}_3\text{S}_2$ : 408.0728, found 408.0720.

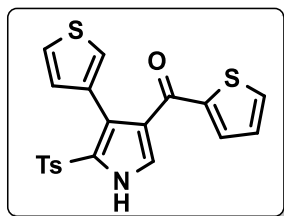


**Furan-2-yl(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone** **(3ac)**:

The product was obtained a pale-yellow solid (164 mg, 84%); mp: 122–126 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.48 (s, 1H), 7.79 (d,  $J = 3.4$  Hz, 1H), 7.51 (t,  $J = 0.8$  Hz, 1H), 7.31-7.26 (m, 5H), 7.19-7.17 (m, 2H), 7.10-7.05 (m, 3H), 6.45 (q,  $J = 1.7$  Hz, 1H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR

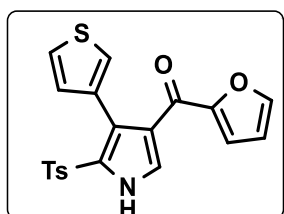
(125 MHz,  $\text{CDCl}_3$ )  $\delta$  176.1, 153.2, 145.9, 144.3, 137.8, 131.4, 130.9, 130.4, 129.4, 127.7, 127.6,

127.5, 127.2, 126.9, 123.7, 118.5, 112.2, 21.6; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>22</sub>H<sub>18</sub>NO<sub>4</sub>S: 392.0957, found 392.0949.



**Thiophen-2-yl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3ad)** : The product was obtained a pale–yellow solid (180 mg, 86%); mp: 137–139 °C; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 13.07 (s, 1H), 7.85 (d, *J* = 4.7 Hz, 1H), 7.70 (s, 1H), 7.61 (s, 1H), 7.40 (d, *J* = 3.2 Hz, 3H),

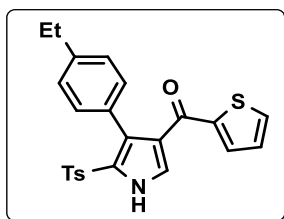
7.26 (d, *J* = 26.9 Hz, 3H), 7.08 (s, 1H), 6.86 (s, 1H), 2.23 (s, 3H); <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ 181.5, 145.0, 144.6, 139.1, 134.9, 134.5, 131.5, 130.6, 130.3, 129.0, 128.1, 128.0, 127.0, 126.0, 124.7, 124.4, 21.5; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>20</sub>H<sub>16</sub>NO<sub>3</sub>S<sub>3</sub>: 414.0292, found 414.0283.



**Furan-2-yl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3ae)** :

The product was obtained a pale–yellow solid (171 mg, 85%); mp: 163–165 °C; <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 13.09 (s, 1H), 7.95 (d, *J* = 1.1 Hz, 1H), 7.82 (d, *J* = 3.4 Hz, 1H), 7.45–7.40 (m, 3H), 7.30 (dd, *J* = 4.2, 3.0 Hz, 3H), 7.22 (d, *J* = 3.4 Hz, 1H), 6.87 (dd, *J* = 4.9, 0.8

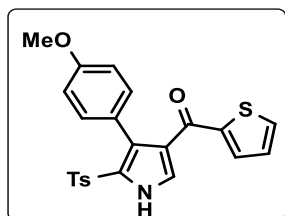
Hz, 1H), 6.66 (q, *J* = 1.7 Hz, 1H), 2.33 (s, 3H); <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>) δ 176.0, 152.7, 147.9, 144.6, 139.0, 131.5, 130.6, 130.3, 128.5, 127.9, 127.0, 125.8, 125.0, 124.6, 123.5, 119.5, 112.9, 21.5; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>20</sub>H<sub>16</sub>NO<sub>4</sub>S<sub>2</sub>: 398.0521, found 398.0545.



**(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-**

**yl)methanone (3af)**: The product was obtained a pale–yellow solid (196 mg, 89%); mp: 161–163 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.65 (s, 1H), 7.55–7.51 (m, 2H), 7.44 (s, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.06 (dd, *J* = 10.0, 8.4 Hz, 4H), 6.99 (dd, *J* = 4.8,

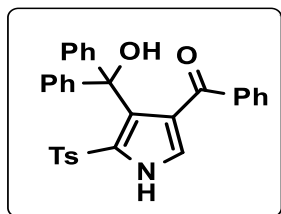
3.8 Hz, 1H), 2.62 (q, *J* = 7.6 Hz, 2H), 2.31 (s, 3H), 1.22 (t, *J* = 7.6 Hz, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 182.0, 144.8, 144.4, 144.0, 138.0, 133.7, 133.6, 130.8, 130.6, 129.5, 128.5, 127.9, 127.6, 127.4, 127.2, 126.5, 125.0, 28.7, 21.7, 15.8; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>24</sub>H<sub>22</sub>NO<sub>3</sub>S<sub>2</sub>: 436.1041, found 436.1035.



**(4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-**

**yl)methanone (3ag)** : The product was obtained a pale–yellow solid (198

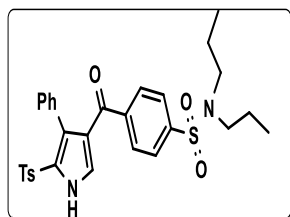
mg, 90%); mp: 185–187 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.10 (s, 1H), 7.56 (dd,  $J = 4.9, 1.1$  Hz, 1H), 7.51–7.48 (m, 2H), 7.31 (d,  $J = 8.4$  Hz, 2H), 7.17 (dd,  $J = 6.6, 2.1$  Hz, 2H), 7.09 (d,  $J = 8.1$  Hz, 2H), 7.01 (dd,  $J = 4.9, 3.8$  Hz, 1H), 6.81 (dd,  $J = 6.7, 2.1$  Hz, 2H), 3.81 (s, 3H), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  182.0, 159.4, 144.7, 144.5, 138.0, 133.7, 133.6, 132.0, 130.3, 129.5, 127.9, 127.7, 127.3, 125.7, 125.5, 123.3, 113.2, 55.3, 21.7; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{23}\text{H}_{20}\text{NO}_4\text{S}_2$ : 438.0834, found 438.0828.



**(4-(Hydroxydiphenylmethyl)-5-tosyl-1H-pyrrol-3-**

**yl)(phenyl)methanone (3ah):** The product was obtained a pale–yellow solid (218 mg, 85%); mp: 115–117 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.14 (s, 1H), 7.47 (q,  $J = 7.3$  Hz, 3H), 7.31–7.19 (m, 9H), 7.06 (d,  $J = 8.4$  Hz, 2H), 7.03–7.00 (m, 5H), 6.89 (d,  $J = 3.3$  Hz, 1H), 5.84 (s, 1H),

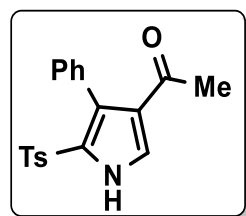
2.37 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  190.5, 145.0, 144.0, 138.7, 137.9, 137.8, 132.6, 129.6, 129.6, 128.4, 127.9, 127.4, 127.3, 126.8, 126.7, 126.5, 125.5, 79.1, 21.6; HRMS (ESI):  $(\text{M}+\text{Na})^+$  Calcd for  $\text{C}_{31}\text{H}_{25}\text{NNaO}_4\text{S}$ : 530.1402, found 530.1414.



**4-(4-Phenyl-5-tosyl-1H-pyrrole-3-carbonyl)-N,N-**

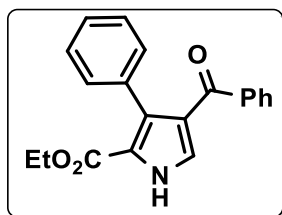
**dipropylbenzenesulfonamide (3ai):** The product was obtained a pale–yellow solid (176 mg, 65%); mp: 175–177 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.53 (s, 1H), 7.70 (dd,  $J = 12.0, 8.8$  Hz, 4H), 7.44 (d,  $J = 3.0$  Hz, 1H), 7.27–7.24 (m, 2H), 7.22–7.15 (m, 3H), 7.12–7.10 (m, 2H), 7.05

(d,  $J = 8.1$  Hz, 2H), 3.02 (t,  $J = 7.7$  Hz, 4H), 2.32 (s, 3H), 1.52 (td,  $J = 15.0, 7.5$  Hz, 4H), 0.86 (t,  $J = 7.4$  Hz, 6H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  189.9, 144.7, 143.0, 141.7, 137.8, 131.2, 130.8, 130.6, 129.9, 129.6, 128.2, 128.1, 127.8, 127.6, 127.4, 126.8, 125.1, 50.2, 22.2, 21.7, 11.4; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{30}\text{H}_{33}\text{N}_2\text{O}_5\text{S}_2$ : 565.1831, found 565.1863.

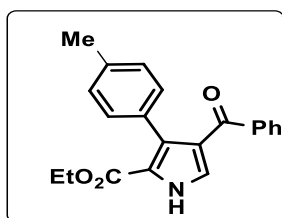


**1-(4-phenyl-5-tosyl-1H-pyrrol-3-yl)ethan-1-one (3aj):** The product was obtained a colourless liquid (52 mg, 30%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39–7.37 (m, 2H), 7.32 (t,  $J = 7.6$  Hz, 1H), 7.24–7.19 (m, 4H), 7.12 (d,  $J = 8.1$  Hz, 2H), 7.02–7.00 (m, 2H), 2.30 (s, 3H), 1.84 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO}-d_6$ )  $\delta$  198.2, 148.7, 145.0, 135.1, 134.0, 129.8, 129.6, 129.4,

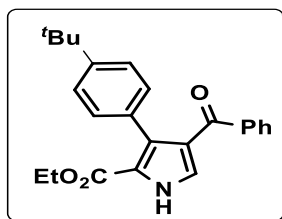
128.3, 128.1, 30.5, 21.0; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>19</sub>H<sub>18</sub>NO<sub>3</sub>S: 340.1007, found 340.1002.



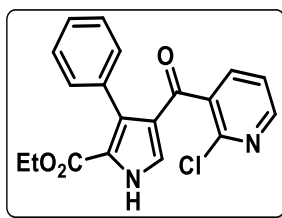
**Ethyl 4-benzoyl-3-phenyl-1H-pyrrole-2-carboxylate (4a)** : The product was obtained a pale–yellow solid (131 mg, 82%); mp: 235–237 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.90 (s, 1H), 7.72-7.70 (m, 2H), 7.47-7.42 (m, 1H), 7.36 (d, *J* = 13.2 Hz, 1H), 7.32-7.29 (m, 4H), 7.26-7.20 (m, 3H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.12 (t, *J* = 7.1 Hz, 3H) ; <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.3, 161.2, 139.1, 133.4, 132.1, 130.5, 129.6, 128.2, 127.7, 127.4, 126.4, 125.2, 121.0, 60.9, 14.1,; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>20</sub>H<sub>18</sub>NO<sub>3</sub>: 320.1287, found 320.1293.



**Ethyl 4-benzoyl-3-(p-tolyl)-1H-pyrrole-2-carboxylate (4b)**: The product was obtained a pale–yellow solid (143 mg, 85%); mp: 160–162 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.03 (s, 1H), 7.73 (d, *J* = 7.7 Hz, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.27-7.25 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 4.19 (q, *J* = 7.1 Hz, 2H), 2.28 (s, 3H), 1.15 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.4, 161.3, 139.3, 136.9, 132.8, 132.1, 130.3, 129.6, 128.2, 128.1, 124.9, 120.9, 60.8, 21.4, 14.2; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>21</sub>H<sub>20</sub>NO<sub>3</sub>: 334.1443, found 334.1436.

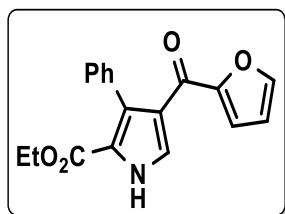


**Ethyl 4-benzoyl-3-(4-(tert-butyl)phenyl)-1H-pyrrole-2-carboxylate (4c)** : The product was obtained a pale–yellow solid (167 mg, 88%); mp: 184–186 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.73 (s, 1H), 7.67 (dd, *J* = 8.2, 1.2 Hz, 2H), 7.43-7.38 (m, 2H), 7.31-7.26 (m, 2H), 7.23 (s, 4H), 4.20 (q, *J* = 7.1 Hz, 2H), 1.27 (s, 9H), 1.14 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.5, 161.2, 150.0, 139.1, 132.7, 131.9, 130.2, 130.1, 129.5, 128.0, 127.8, 125.3, 124.2, 120.8, 60.8, 34.6, 31.4, 14.0; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>24</sub>H<sub>26</sub>NO<sub>3</sub>: 376.1913, found 376.1905.



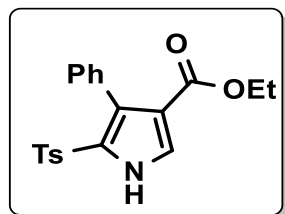
**Ethyl 4-(2-chloronicotinoyl)-3-phenyl-1H-pyrrole-2-carboxylate (4d)** : The product was obtained a pale–yellow solid (134 mg, 75%);

mp: 189–191 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.41 (s, 1H), 8.25 (dd,  $J = 4.9, 1.9$  Hz, 1H), 7.53 (d,  $J = 3.6$  Hz, 1H), 7.47 (dd,  $J = 7.5, 1.9$  Hz, 1H), 7.20–7.14 (m, 5H), 7.04 (dd,  $J = 7.6, 4.8$  Hz, 1H), 4.13 (q,  $J = 7.1$  Hz, 2H), 1.04 (t,  $J = 7.1$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  188.4, 161.0, 150.1, 147.3, 137.5, 135.9, 132.6, 131.8, 130.1, 128.6, 127.3, 127.2, 125.1, 121.8, 121.6, 60.8, 13.8; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{19}\text{H}_{16}\text{ClN}_2\text{O}_3$ : 355.0849, found 355.0844.



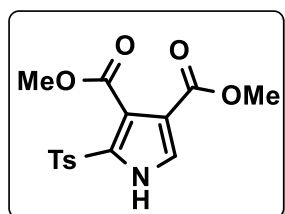
**Ethyl 4-(furan-2-carbonyl)-3-phenyl-1H-pyrrole-2-carboxylate (4e):**

The product was obtained a pale–yellow solid (124 mg, 80%); mp: 152–154 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.16 (s, 1H), 7.72 (d,  $J = 3.4$  Hz, 1H), 7.52 (d,  $J = 0.8$  Hz, 1H), 7.36–7.25 (m, 5H), 7.10 (d,  $J = 3.6$  Hz, 1H), 6.47 (q,  $J = 1.7$  Hz, 1H), 4.16 (q,  $J = 7.1$  Hz, 2H), 1.09 (t,  $J = 7.1$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  176.9, 161.3, 153.6, 145.9, 133.8, 132.6, 130.2, 128.0, 127.3, 127.2, 123.4, 121.0, 118.4, 112.2, 60.8, 14.0; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{18}\text{H}_{16}\text{NO}_4$ : 310.1079, found 310.1074.



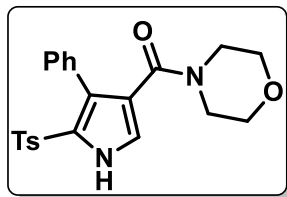
**Ethyl 4-phenyl-5-tosyl-1H-pyrrole-3-carboxylate (5a):**

The product was obtained a pale–yellow solid (140 mg, 75%); mp: 140–142 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.10 (s, 1H), 7.58 (d,  $J = 3.4$  Hz, 1H), 7.37–7.24 (m, 5H), 7.15–7.13 (m, 2H), 7.07 (d,  $J = 8.1$  Hz, 2H), 4.07 (q,  $J = 7.1$  Hz, 2H), 2.34 (s, 3H), 1.07 (t,  $J = 7.1$  Hz, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  163.3, 152.3, 144.2, 141.9, 138.0, 131.3, 130.6, 130.5, 130.0, 129.3, 128.3, 127.8, 127.5, 127.2, 126.3, 117.7, 60.0, 21.6, 14.0; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{20}\text{H}_{19}\text{NNaO}_4\text{S}$ : 3392.0932, found 3392.0927.



**Dimethyl 2-tosyl-1H-pyrrole-3,4-dicarboxylate (5b) :**

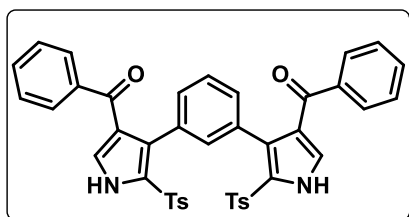
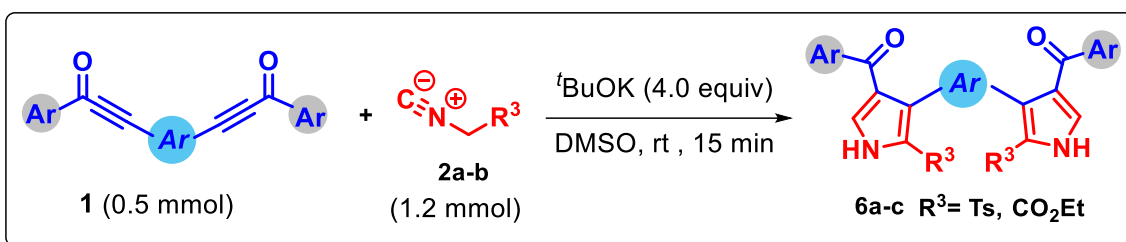
The product was obtained a pale–yellow solid (144 mg, 82%); mp: 156–158 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  10.72 (s, 1H), 7.86 (d,  $J = 8.2$  Hz, 2H), 7.46 (d,  $J = 3.3$  Hz, 1H), 7.28 (d,  $J = 8.4$  Hz, 2H), 3.94 (s, 3H), 3.78 (s, 3H), 2.38 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  164.2, 162.8, 145.1, 137.5, 130.0, 128.6, 127.7, 126.9, 121.7, 116.7, 53.0, 51.9, 21.6; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{15}\text{H}_{16}\text{NO}_6\text{S}$ : 338.0698, found 338.0693.



**Morpholino(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (5c)** :The product was obtained a colourless solid (125 mg, 60%); mp: 176–178 °C;  $^1\text{H}$  NMR (500 MHz, DMSO-*d*6)  $\delta$  12.75 (s, 1H), 7.43 (d,  $J$  = 8.2 Hz, 2H), 7.39-7.38 (m, 3H), 7.32 (d,  $J$  = 3.3 Hz, 1H), 7.28 (d,  $J$  = 8.2 Hz, 2H), 7.21-7.19 (m, 2H), 3.38-3.33 (m, 4H), 3.27 (s, 1H), 3.05-3.01 (m, 2H), 2.51 (d,  $J$  = 1.6 Hz, 1H), 2.30 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz, DMSO-*d*6)  $\delta$  164.1, 143.8, 139.2, 131.8, 130.0, 129.7, 127.7, 127.2, 126.2, 124.3, 123.6, 120.6, 65.5, 39.1, 20.9; HRMS (ESI): (M+H) $^+$  Calcd for C<sub>22</sub>H<sub>23</sub>N<sub>2</sub>O<sub>4</sub>S: 411.1379, found 411.1370.

### Scheme 3. Scope of 1,3-Bis-Arylones

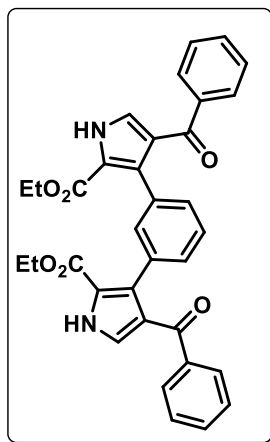
To the solution of ynone **1** (0.5 mmol), isocyanide **2** (1.2 mmol) and 4.0 equiv. of anhydrous  $^t\text{BuOK}$  in 3.0 mL of DMSO were added. The resulting reaction mixture was stirred at 25°C for 0.15 h. Progress of the reaction was monitored by TLC analysis, after completion of starting materials; the reaction mixture was poured in water and extracted by ethyl acetate (3X10 mL). The organic layer was washed with saturated brine solution and dried over Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography on silica gel (100–200 mesh) (hexane–ethylacetate, 7:3). The structure and purity of known product **6** were confirmed by their physical and spectral data such as  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, HRMS.



**(6a)**: The product was obtained a pale–yellow solid (285 mg, 78%); mp: 150–152 °C;  $^1\text{H}$  NMR (500 MHz, DMSO-*d*6)  $\delta$  13.20 (s, 2H), 7.66 (d,  $J$  = 7.1 Hz, 4H), 7.54-7.52 (m, 4H), 7.46-7.42 (m, 8H), 7.35 (d,  $J$  = 8.5 Hz, 4H), 7.19 (d,  $J$  = 7.3

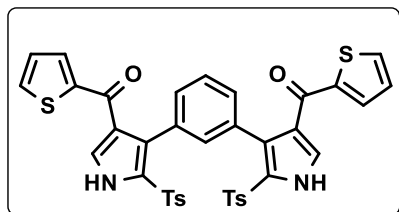


Hz, 4H), 2.36 (s, 6H);  $^{13}\text{C}$  NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  189.7, 144.2, 139.2, 139.2, 139.0, 137.0, 132.7, 132.2, 131.4, 130.3, 130.1, 129.8, 129.6, 129.5, 129.4, 128.9, 128.8, 128.0, 127.4, 127.4, 127.1, 126.6, 124.2, 21.4; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>42</sub>H<sub>32</sub>N<sub>2</sub>NaO<sub>6</sub>S<sub>2</sub>: 747.1599, found 747.1594.



**Diethyl 3,3'-(1,3-phenylene)bis(4-benzoyl-1H-pyrrole-2-carboxylate)**

**(6b)**: The product was obtained a pale–yellow solid (312 mg, 80%); mp: 170–172 °C;  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  9.85 (s, 2H), 7.70 (d,  $J$  = 7.3 Hz, 4H), 7.42–7.36 (m, 3H), 7.32–7.28 (m, 6H), 7.19 (dd,  $J$  = 7.7, 1.5 Hz, 2H), 7.09 (t,  $J$  = 7.6 Hz, 1H), 4.14 (q,  $J$  = 7.1 Hz, 4H), 1.07 (t,  $J$  = 7.1 Hz, 6H);  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  191.0, 161.5, 139.0, 132.8, 132.1, 132.0, 129.7, 129.6, 129.4, 128.1, 127.8, 127.5, 125.9, 125.1, 121.0, 60.9, 14.0; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>34</sub>H<sub>29</sub>N<sub>2</sub>O<sub>6</sub>: 561.2026, found 561.2022.



**Thiophen-2-yl(4-(3-(4-(thiophene-2-carbonyl)-2-tosyl-1H-pyrrol-3-yl)phenyl)-5-tosyl-1H-pyrrol-3-yl)methanone (6c)**

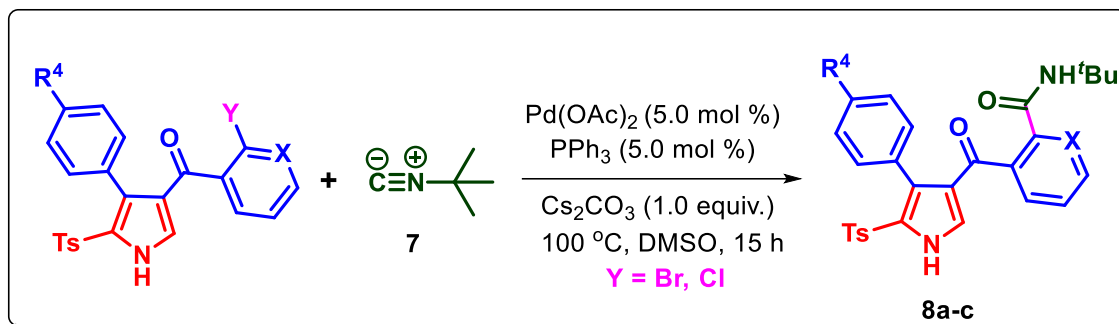
The product was obtained a pale–yellow solid (320 mg, 82%); mp: 140–142 °C;  $^1\text{H}$  NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  13.04 (s, 2H), 7.94 (dd,  $J$  = 4.9, 0.8 Hz, 2H), 7.76 (d,  $J$  = 3.3 Hz, 2H), 7.73 (d,  $J$  = 3.2 Hz, 2H), 7.46 (d,  $J$  = 8.2 Hz, 4H), 7.19–7.12 (m, 7H), 7.01 (dd,  $J$  = 7.7, 1.4 Hz, 2H), 6.94 (s, 1H), 2.26 (s, 6H);  $^{13}\text{C}$  NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  181.3, 145.1, 144.3, 139.2, 134.8, 134.6, 132.4, 131.3, 130.1, 129.8, 129.1, 128.2, 128.0, 127.5, 126.8, 124.1, 21.5; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>38</sub>H<sub>29</sub>N<sub>2</sub>O<sub>6</sub>S<sub>4</sub>: 737.0908, found 737.0904.

#### Scheme 4. Synthetic Utility

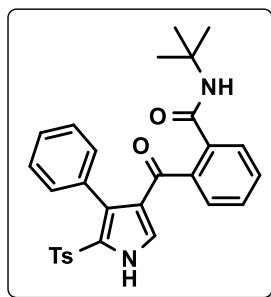
##### Synthetic Transformation via Isocyanide Insertion

In an oven-dried flask, products **3** (1.0 mmol), Pd(OAc)<sub>2</sub> (5.0 mol%), PPh<sub>3</sub> (5.0 mol%), and Cs<sub>2</sub>CO<sub>3</sub> 1.0 equiv. were dissolved in DMSO (2 mL) at room temperature, then tert-butyl isocyanides (1.2 mmol) were added using a syringe. The mixture was stirred at 100 °C and

monitored by TLC. After completion of starting materials (about 12 h), the reaction mixture was poured in water and extracted by ethyl acetate (3X10 mL). The organic layer was washed with saturated brine solution and dried over Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography on silica gel (100–200 mesh) (hexane–ethylacetate, 7:3). The structure and purity of known product **8a-c** was confirmed by their physical and spectral data such as <sup>1</sup>H NMR, <sup>13</sup>C NMR, HRMS.

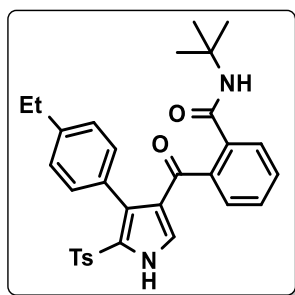


**N-(tert-butyl)-2-(4-phenyl-5-tosyl-1H-pyrrole-3-carbonyl)benzamide (8a)**



**(8a)** : The product was obtained a pale–yellow solid (186 mg, 74%); mp: 141–143 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.49 (s, 1H), 7.48 (d, *J* = 7.1 Hz, 1H), 7.38–7.32 (m, 1H), 7.30–7.24 (m, 3H), 7.23–7.20 (m, 5H), 7.14 (d, *J* = 8.2 Hz, 2H), 7.00 (d, *J* = 8.2 Hz, 2H), 5.88 (s, 1H), 2.31 (s, 3H), 1.20 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.5, 168.0, 144.2, 139.0, 137.8, 136.6, 131.0, 130.7, 130.0, 130.0, 129.7, 129.3, 128.7,

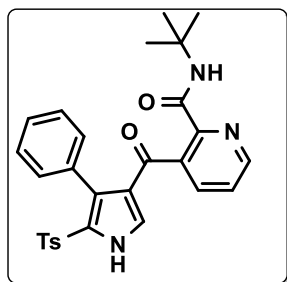
128.4, 128.3, 127.7, 127.4, 127.2, 125.4, 51.9, 28.3, 21.5, ; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>29</sub>H<sub>29</sub>N<sub>2</sub>O<sub>4</sub>S: 501.1848, found 501.1833.



**N-(tert-butyl)-2-(4-(4-ethylphenyl)-5-tosyl-1H-pyrrole-3-carbonyl)benzamide (8b)**

**(8b)**: The product was obtained a pale–yellow solid (191 mg, 72%); mp: 144–146 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.58 (s, 1H), 7.49–7.47 (m, 1H), 7.36–7.24 (m, 3H), 7.20 (d, *J* = 3.3 Hz, 1H), 7.13 (t, *J* = 8.3 Hz, 4H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.99 (d, *J* = 8.1 Hz, 2H), 5.89 (s, 1H), 2.63 (q, *J* = 7.6 Hz, 2H), 2.31 (s, 3H), 1.24 (t, *J* = 7.6 Hz, 3H), 1.19 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 191.6, 168.1, 144.0, 143.8, 139.1,

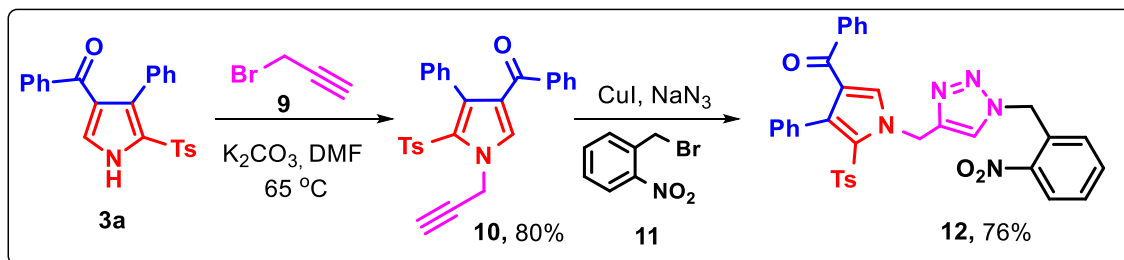
137.9, 136.5, 130.6, 130.2, 130.0, 129.7, 129.2, 128.8, 128.4, 128.3, 128.1, 127.5, 127.3, 126.8, 125.3, 51.9, 28.3, 21.5, 15.8; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>31</sub>H<sub>33</sub>N<sub>2</sub>O<sub>4</sub>S: 529.2161, found 529.2155.



### N-(*tert*-butyl)-3-(4-phenyl-5-tosyl-1*H*-pyrrole-3-

carbonyl)picolinamide (**8c**): The product was obtained a pale-yellow solid (176 mg, 70%); mp: 149–151 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.03 (s, 1H), 8.20 (dd, *J* = 4.7, 1.6 Hz, 1H), 7.71 (d, *J* = 3.3 Hz, 1H), 7.53 (s, 1H), 7.37 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.18-7.11 (m, 3H), 7.08-7.01 (m, 3H), 6.93 (t, *J* = 7.7 Hz, 2H), 6.79-6.77 (m, 2H), 2.31 (s, 3H), 1.38 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.2, 162.4, 147.8, 147.5, 144.1, 137.9, 136.7, 135.6, 130.7, 130.4, 129.4, 129.3, 127.8, 127.4, 126.9, 126.7, 126.2, 124.7, 50.9, 28.7, 21.5; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>28</sub>H<sub>28</sub>N<sub>3</sub>O<sub>4</sub>S: 502.1801, found 502.1779.

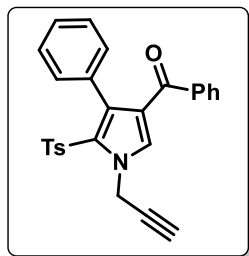
### Synthesis of Pyrrole-triazole hybrid



In a round-bottomed flask, the respective pyrrole **3** and K<sub>2</sub>CO<sub>3</sub> were solubilized in DMF (2 mL) at room temperature. Pure propargyl bromide was then added slowly under ice bath at 0-5 °C. The mixture was magnetically stirred at 65 °C for 5 h. After completion of starting materials, the reaction mixture was poured in water and extracted by ethyl acetate (3X10 mL). The organic layer was washed with saturated brine solution and dried over Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography on silica gel (100–200 mesh) (hexane–ethylacetate, 7:3). The structure and purity of known product **9a** was confirmed by their physical and spectral data such as <sup>1</sup>H NMR, <sup>13</sup>C NMR, HRMS. Procedure followed those reported in literature.<sup>4</sup>

To a stirred solution of H<sub>2</sub>O/BuOH 1:1 at room temperature, the respective pyrrole (**9a**), 1-(bromomethyl)-2-nitrobenzene (**10**), and NaN<sub>3</sub> were added as one portion. After 30 min under magnetic stirring, CuI was also added at room temperature. The reaction mixture was then heated

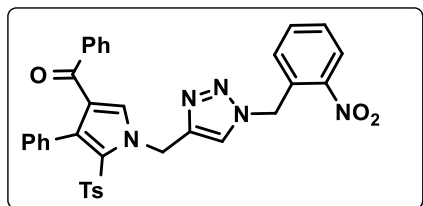
at 80 °C for 4 h. After completion of starting materials, the reaction mixture was poured in water and extracted by ethyl acetate (3X10 mL). The organic layer was washed with saturated brine solution and dried over Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography on silica gel (100–200 mesh) (hexane–ethylacetate, 6:4). The structure and purity of known product **12** was confirmed by their physical and spectral data such as <sup>1</sup>H NMR, <sup>13</sup>C NMR, HRMS. Procedure followed those reported in literature.<sup>4</sup>



**Phenyl(4-phenyl-1-(prop-2-yn-1-yl)-5-tosyl-1H-pyrrol-3-yl)methanone**

**(10):** The product was obtained a pale–yellow solid (175 mg, 80%); mp: 135–137 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.64–7.61 (m, 3H), 7.43–7.39 (m, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.30–7.26 (m, 2H), 7.22–7.16 (m, 3H), 7.14–7.09 (m, 4H), 5.29 (d, *J* = 2.5 Hz, 2H), 2.58 (t, *J* = 2.5 Hz, 1H), 2.34

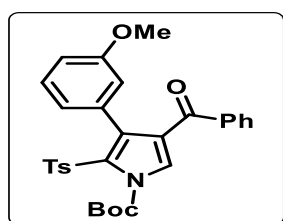
(s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.2, 144.2, 138.8, 138.4, 134.5, 132.2, 131.8, 131.1, 130.8, 129.8, 129.4, 129.3, 129.0, 128.2, 128.0, 127.7, 127.2, 127.1, 126.8, 123.7, 76.5, 76.4, 39.5, 21.5; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>27</sub>H<sub>22</sub>NO<sub>3</sub>S: 440.1320, found 440.1315.



**(1-((1-(2-Nitrobenzyl)-1H-1,2,3-triazol-4-yl)methyl)-4-phenyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone** **(12):**

The product was obtained a pale–yellow solid (236 mg, 76%); mp: 148–150 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.16

(dd, *J* = 8.1, 1.2 Hz, 1H), 7.98 (s, 1H), 7.65–7.60 (m, 3H), 7.56–7.52 (m, 2H), 7.44–7.40 (m, 1H), 7.31–7.23 (m, 4H), 7.20–7.13 (m, 3H), 7.09–7.04 (m, 5H), 5.94 (s, 2H), 5.75 (s, 2H), 2.33 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 190.0, 147.4, 144.1, 143.5, 138.9, 138.5, 134.5, 134.3, 132.6, 132.2, 131.9, 130.7, 130.3, 129.8, 129.3, 129.3, 128.1, 127.6, 127.2, 126.9, 126.5, 125.5, 124.9, 123.8, 51.1, 44.8, 21.5; HRMS (ESI): (M+H)<sup>+</sup> Calcd for C<sub>34</sub>H<sub>28</sub>N<sub>5</sub>O<sub>5</sub>S: 618.1811, found 618.1806.



**tert-butyl 4-benzoyl-3-(3-methoxyphenyl)-2-tosyl-1H-pyrrole-1-carboxylate** **(14):** The product was obtained a pale–yellow solid (22 mg, 84%); mp: 198–200 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.63–7.59

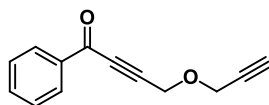
(m, 3H), 7.39 (t,  $J = 7.4$  Hz, 1H), 7.33 (d,  $J = 8.2$  Hz, 2H), 7.25 (t,  $J = 7.7$  Hz, 2H), 6.91 (t,  $J = 8.0$  Hz, 3H), 6.61-6.56 (m, 2H), 6.29 (d,  $J = 1.5$  Hz, 1H), 3.55 (s, 3H), 2.22 (s, 3H), 1.60 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  189.8, 158.5, 147.7, 143.7, 138.2, 137.8, 135.8, 132.6, 132.4, 130.3, 129.5, 129.3, 128.6, 128.4, 128.2, 128.0, 124.1, 123.0, 115.0, 114.0, 87.8, 54.9, 27.5, 21.4; HRMS (ESI):  $(\text{M}+\text{H})^+$  Calcd for  $\text{C}_{30}\text{H}_{30}\text{NO}_6\text{S}$ : 532.1794, found 532.1790.

#### References:

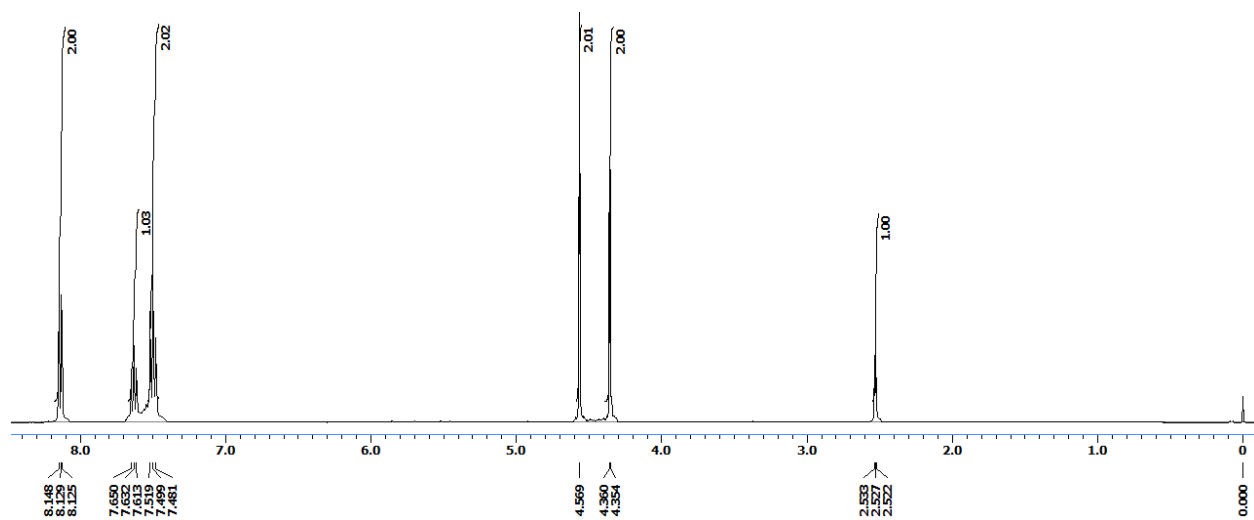
1. Okamoto, K.; Shimbayashi, T.; Tamura, E.; Ohe, K. *Org. Lett.* **2015**, *17*, 5843–5845
2. Whittaker, R. E.; Dermenci, A.; Dong, G. *Synthesis*, **2016**, *48*, 161–183.
3. Wei, Q; Deng, H; Qin, A; Tang, B.E.; *Macromol. Rapid Commun.* **2012**, *33*, 1356–1361
4. Bonacorso, H.G., Magalhães, H.T., Forno, G.M.D., Libero, F.M., Hoerner, M., Frizzo, C.P., Martins, M.A. and Zanatta, N; *Journal of the Brazilian Chemical Society* **2019.**, *30*, pp.1189-1202.

# **Copies of $^1\text{H}$ , $^{13}\text{C}$ NMR and HRMS**

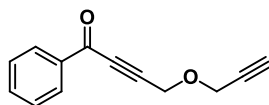
<sup>1</sup>H NMR



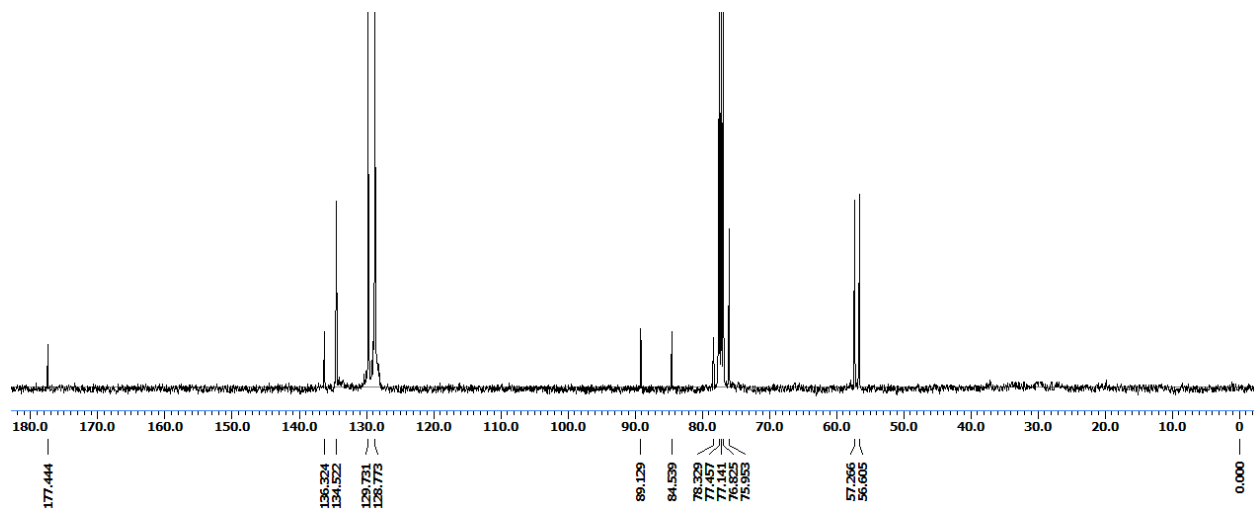
1-Phenyl-4-(prop-2-yn-1-yloxy)but-2-yn-1-one (1q)



<sup>13</sup>C NMR

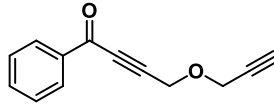


1-Phenyl-4-(prop-2-yn-1-yloxy)but-2-yn-1-one (1q)





# HRMS



## 1-Phenyl-4-(prop-2-yn-1-yloxy)but-2-yn-1-one (1q)

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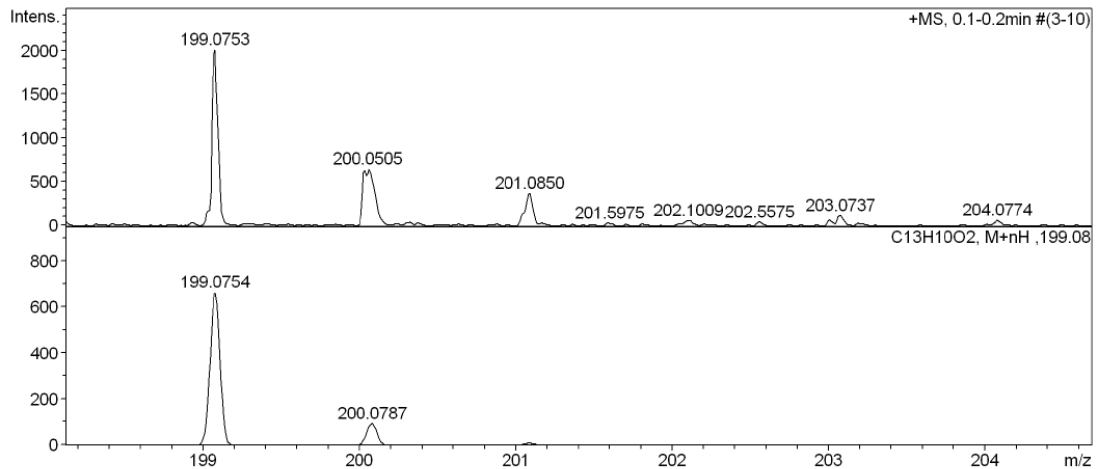
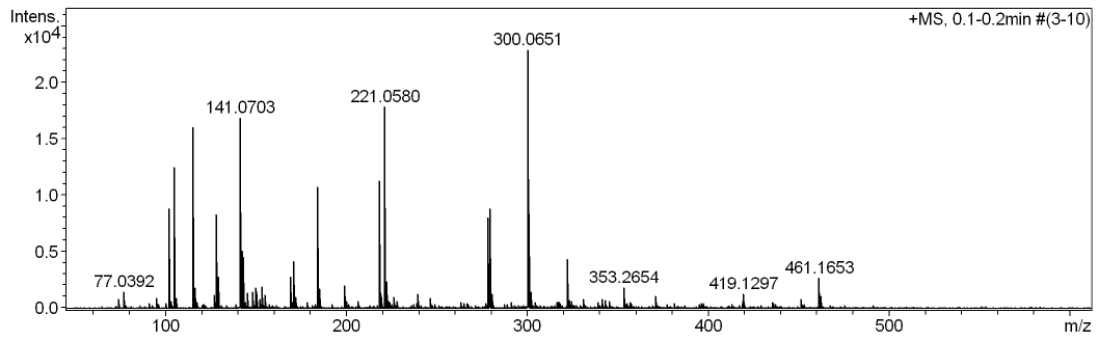
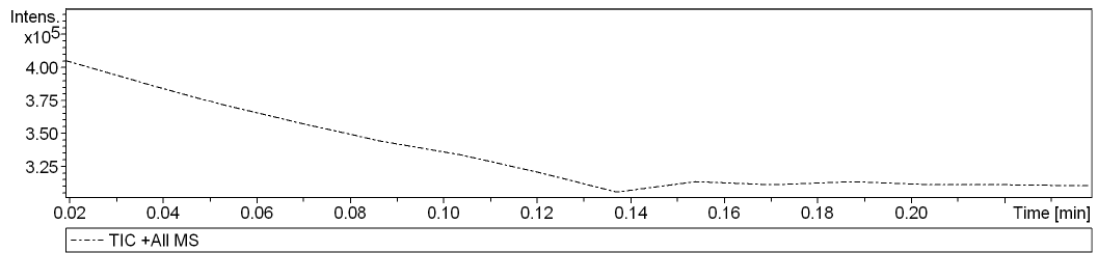
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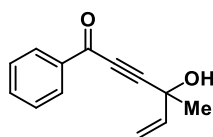
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

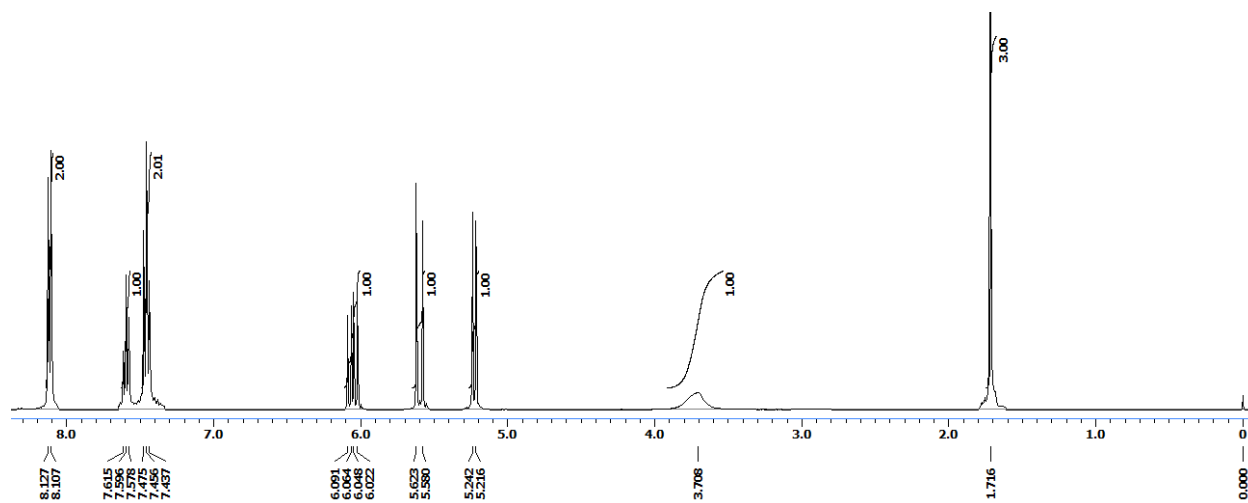
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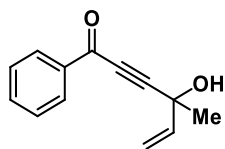
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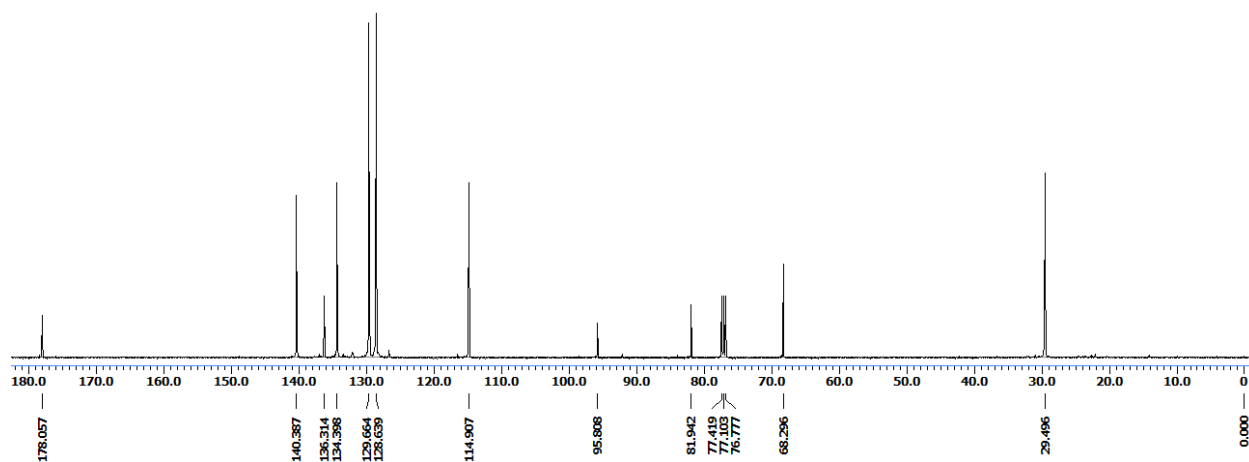
4-Hydroxy-4-methyl-1-phenylhex-5-en-2-yn-1-one (1r)



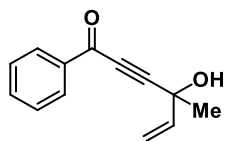
<sup>13</sup>C NMR



4-Hydroxy-4-methyl-1-phenylhex-5-en-2-yn-1-one (1r)



# HRMS



## 4-Hydroxy-4-methyl-1-phenylhex-5-en-2-yn-1-one (1r)

### Analysis Info

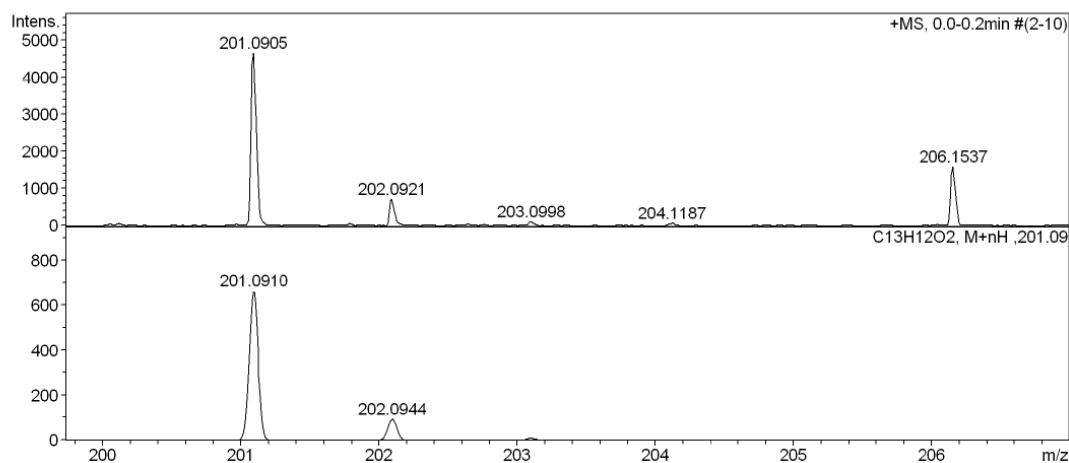
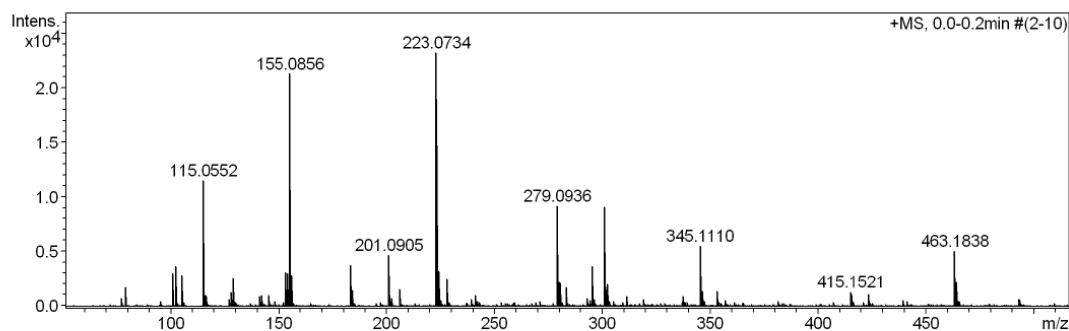
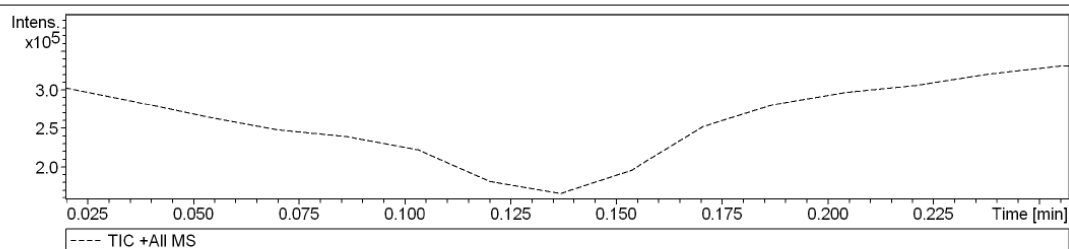
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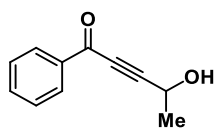
Operator Amit S.Sahu  
 Instrument micrOTOF-Q II 10337

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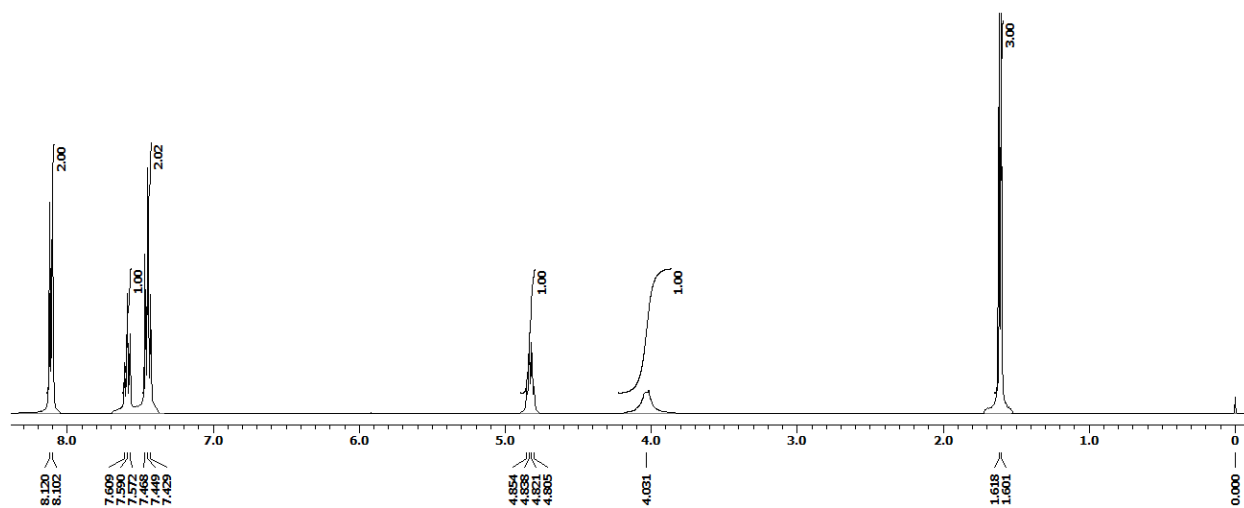
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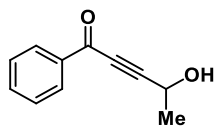
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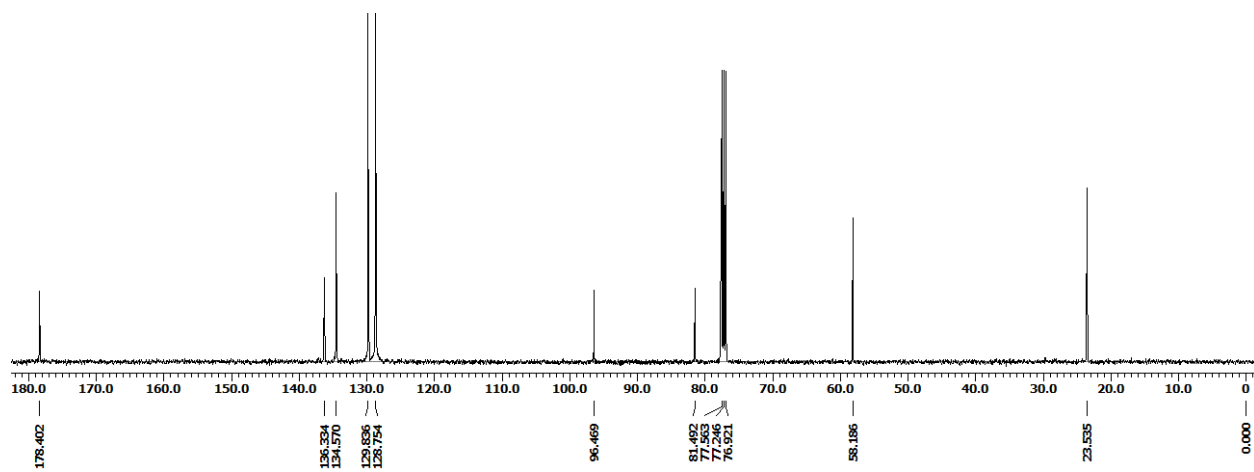
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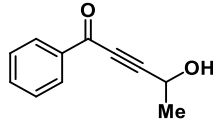
<sup>13</sup>C NMR



4-Hydroxy-1-phenylpent-2-yn-1-one (1s)



# HRMS



## 4-Hydroxy-1-phenylpent-2-yn-1-one (1s)

### Analysis Info

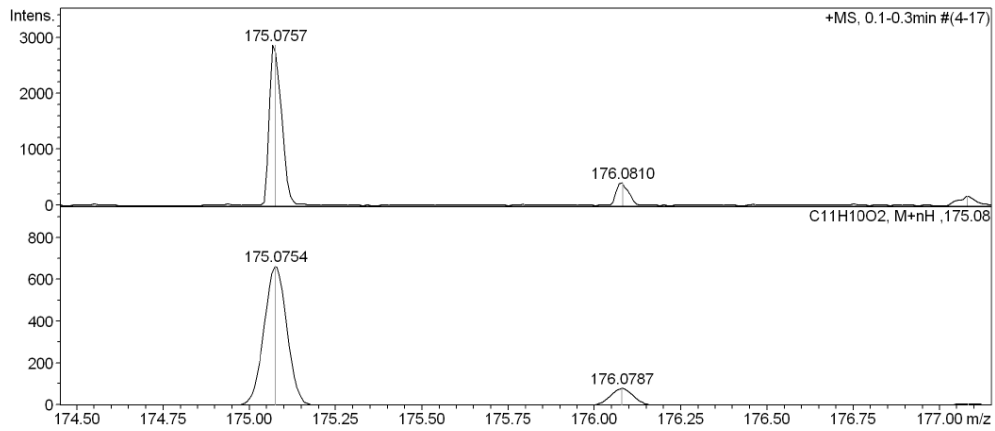
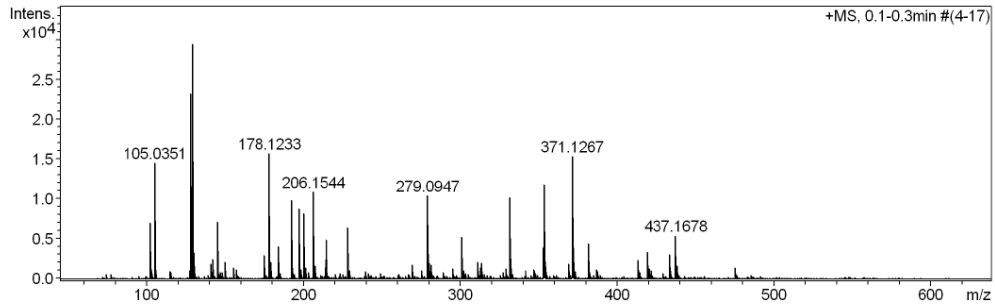
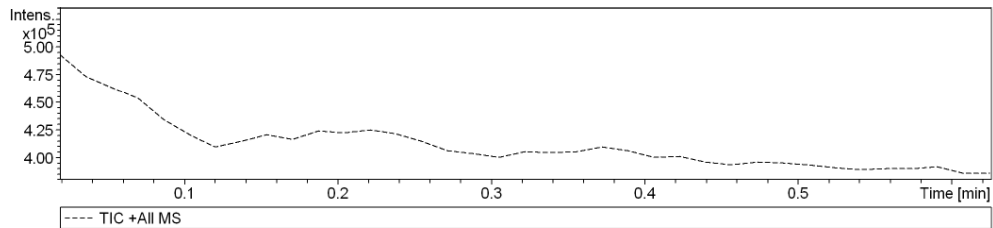
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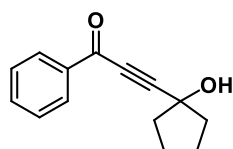
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

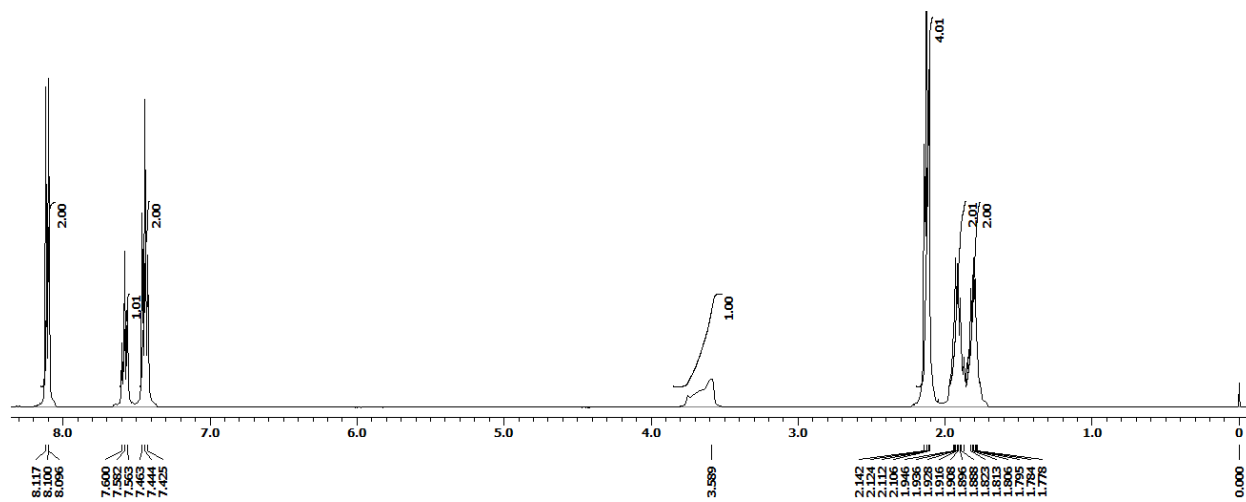
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<sup>1</sup>H NMR

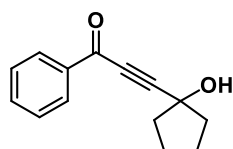


3-(1-Hydroxycyclopentyl)-1-phenylprop-2-yn-1-one (1t)

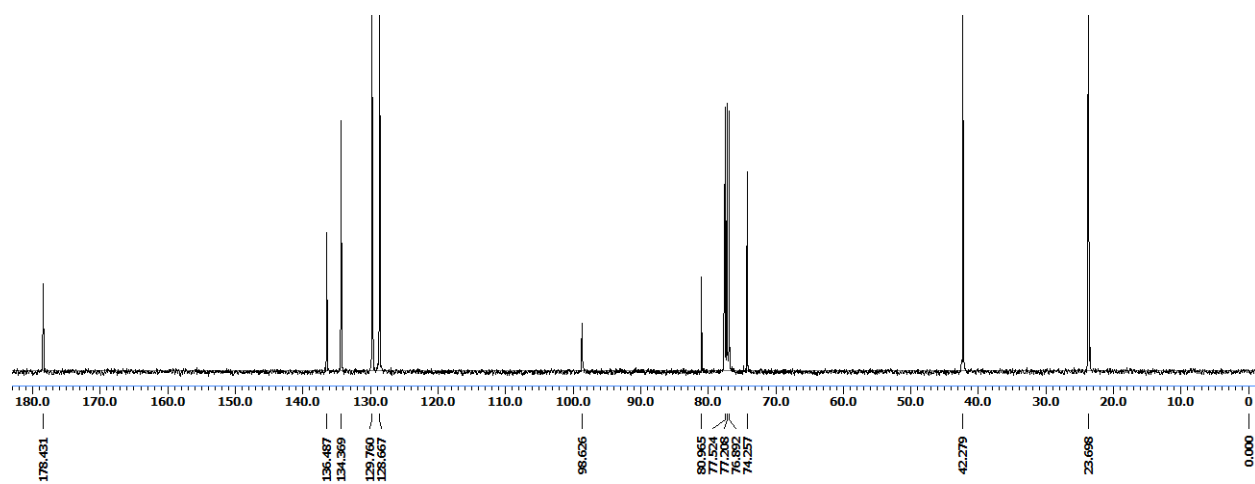




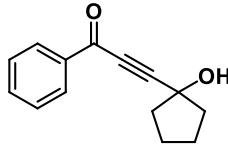
<sup>13</sup>C NMR



**3-(1-Hydroxycyclopentyl)-1-phenylprop-2-yn-1-one (1t)**



# HRMS



## 3-(1-Hydroxycyclopentyl)-1-phenylprop-2-yn-1-one (1t)

### Analysis Info

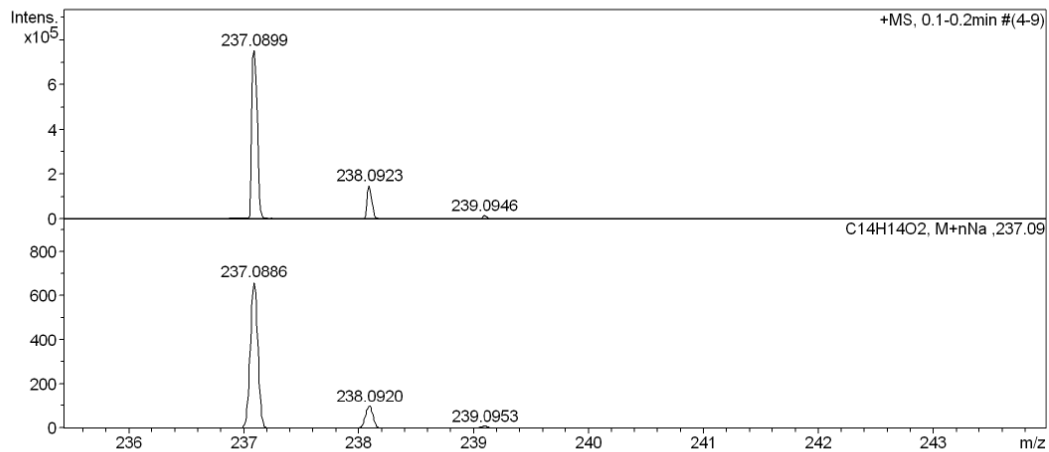
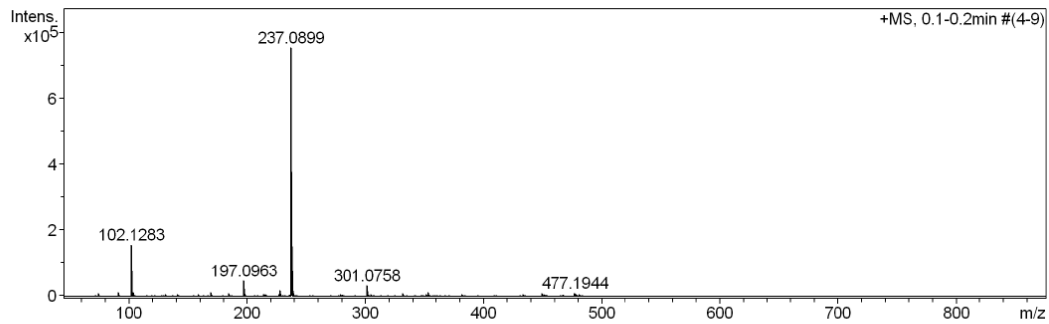
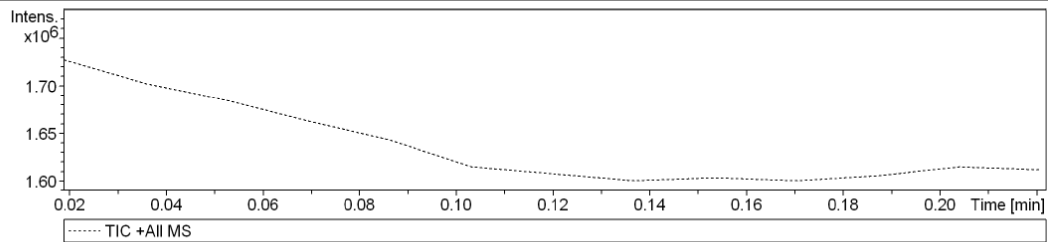
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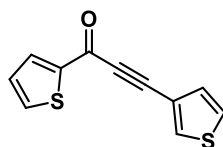
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

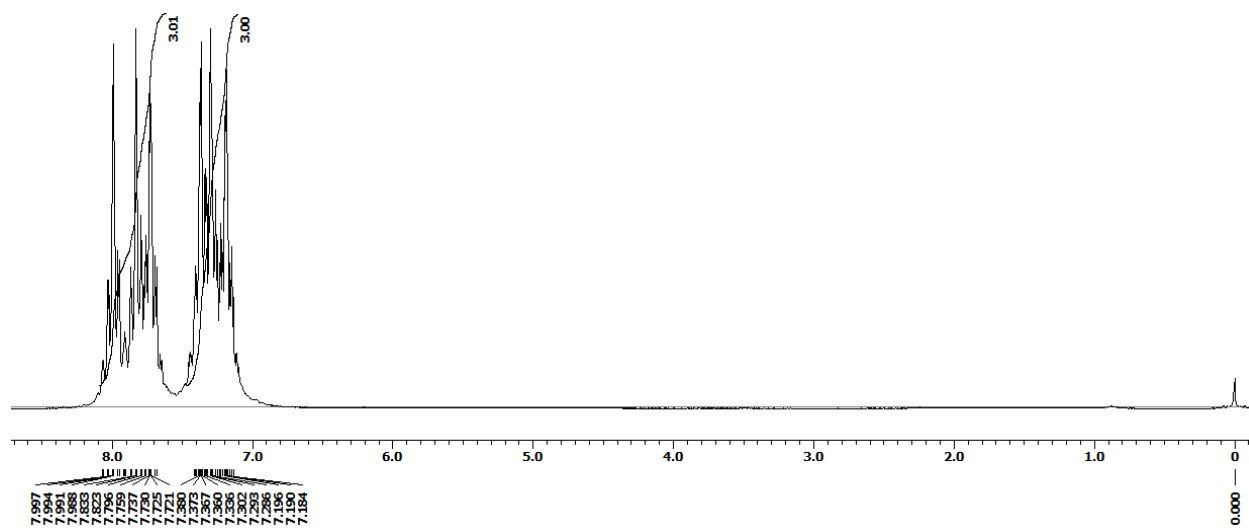
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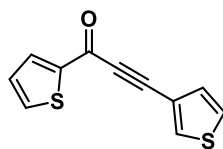
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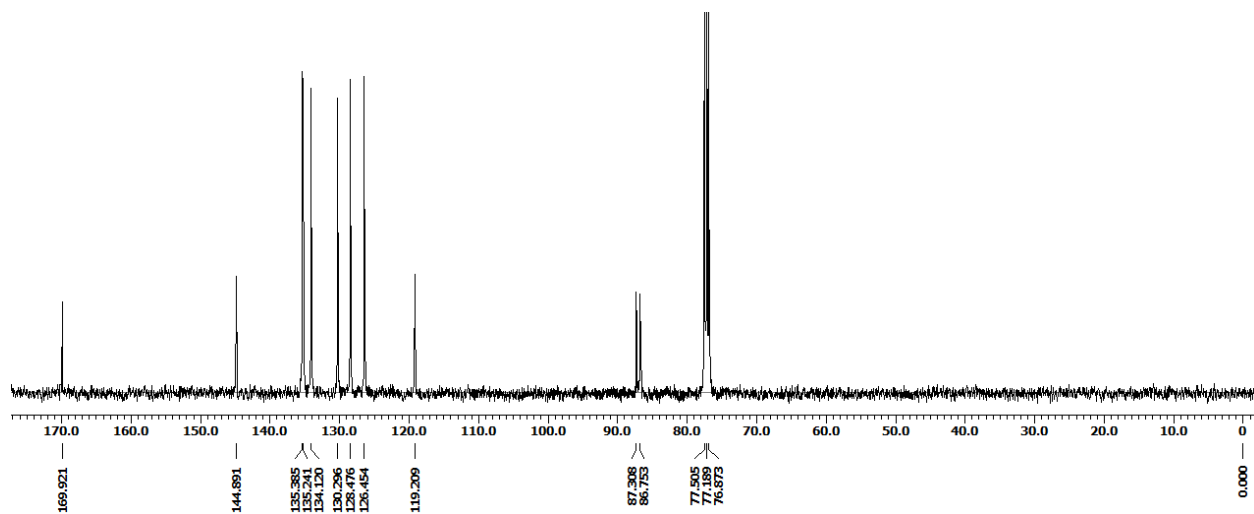
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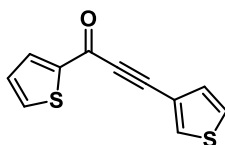
<sup>13</sup>C NMR



1-(thiophen-2-yl)-3-(thiophen-3-yl)prop-2-yn-1-one (1ad)



# HRMS



## 1-(thiophen-2-yl)-3-(thiophen-3-yl)prop-2-yn-1-one (1ad)

### Analysis Info

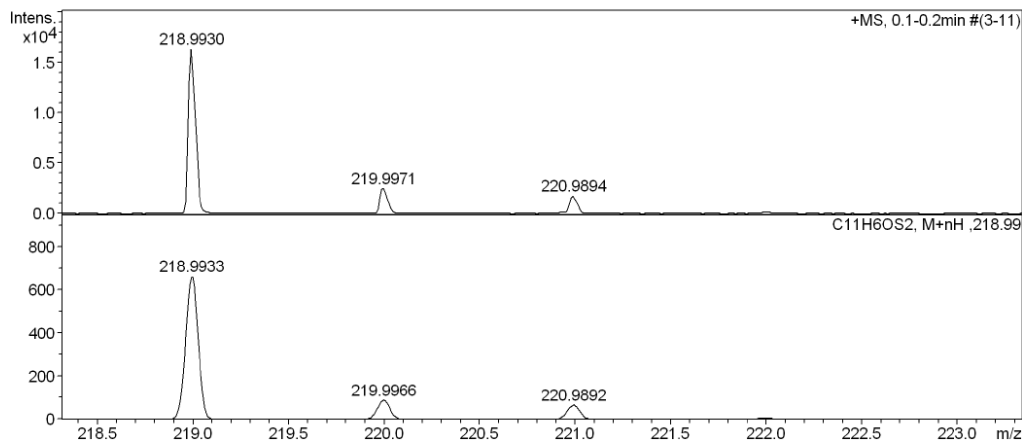
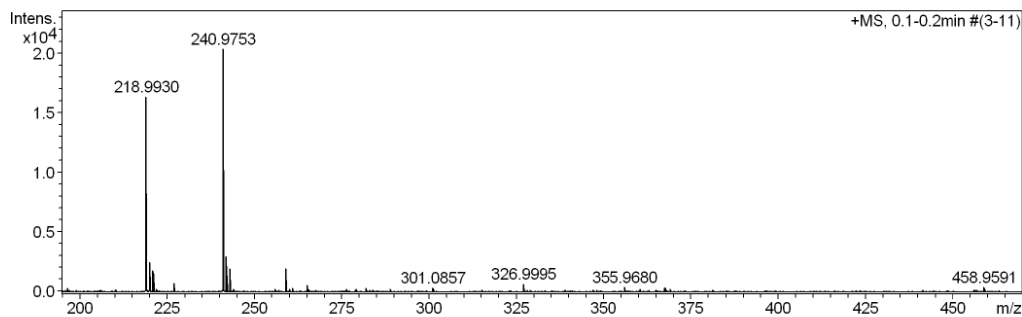
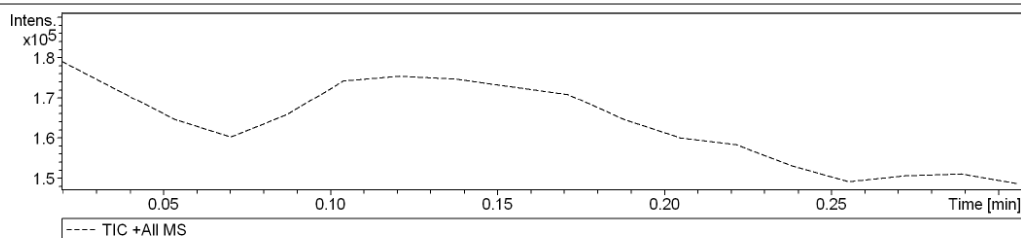
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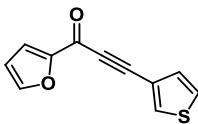
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 Instrument micrOTOF-Q II 10337

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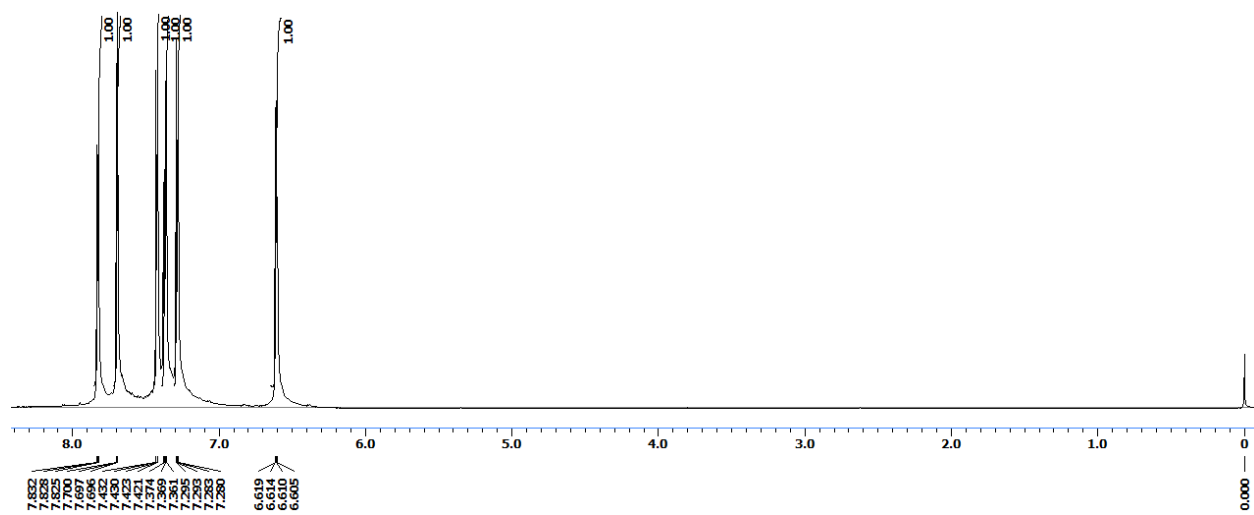
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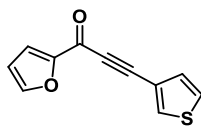
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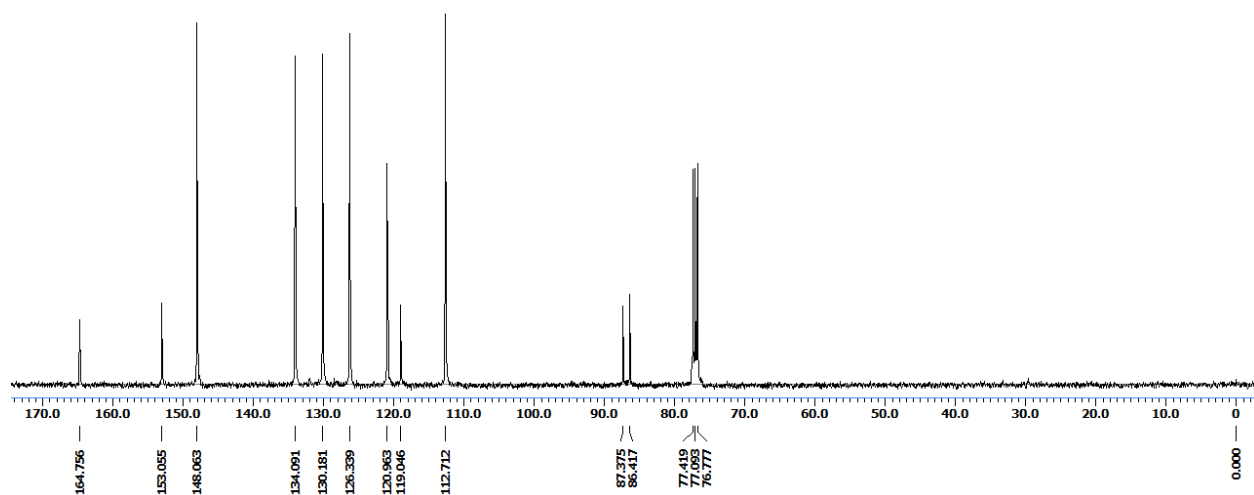
1-(Furan-2-yl)-3-(thiophen-3-yl)prop-2-yn-1-one (1ae)



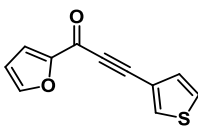
<sup>13</sup>C NMR



1-(Furan-2-yl)-3-(thiophen-3-yl)prop-2-yn-1-one (1ae)



# HRMS



## 1-(Furan-2-yl)-3-(thiophen-3-yl)prop-2-yn-1-one (1ae)

### Analysis Info

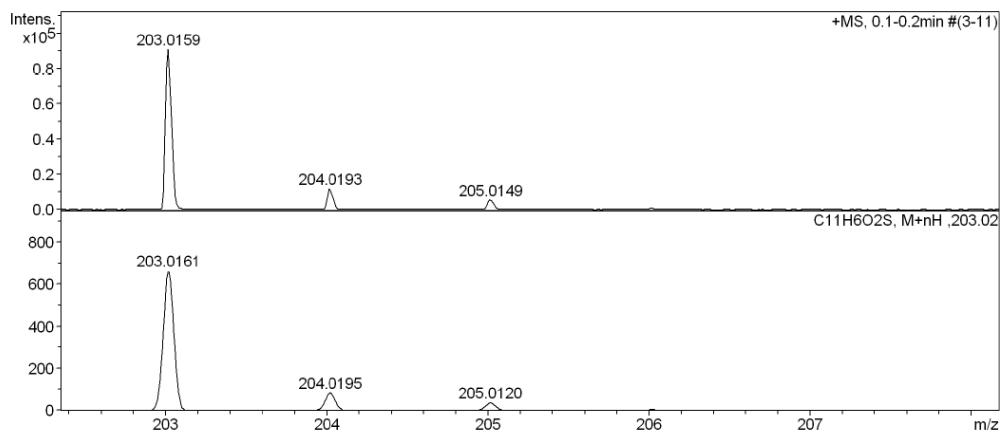
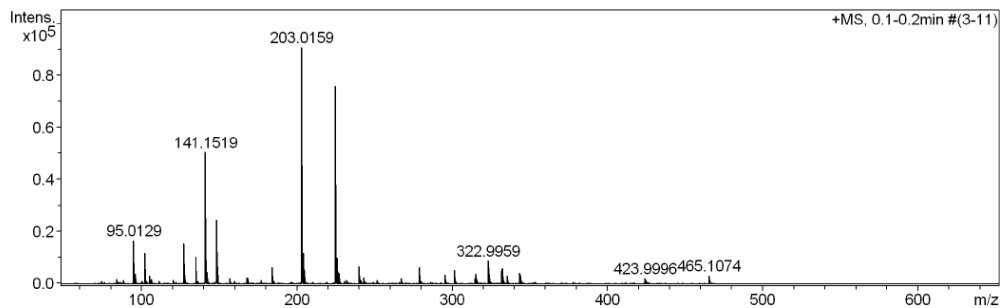
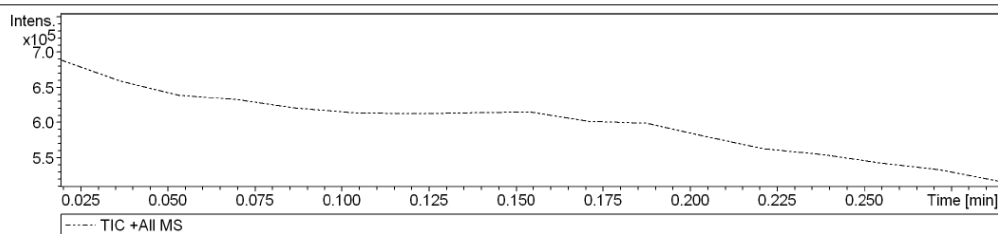
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Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

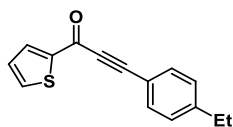
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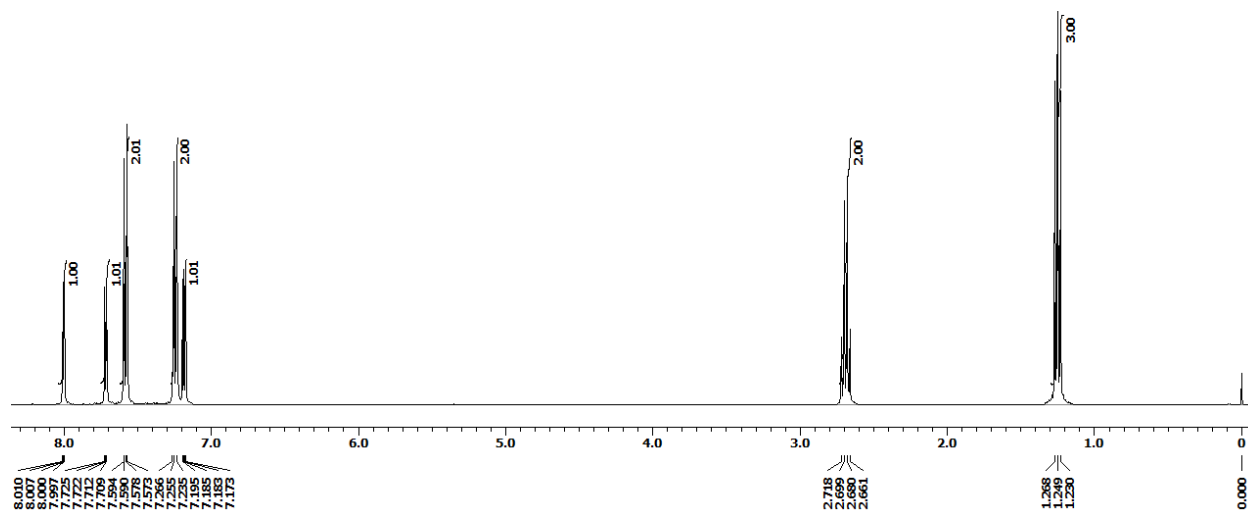




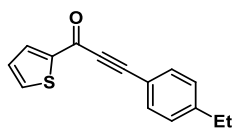
<sup>1</sup>H NMR



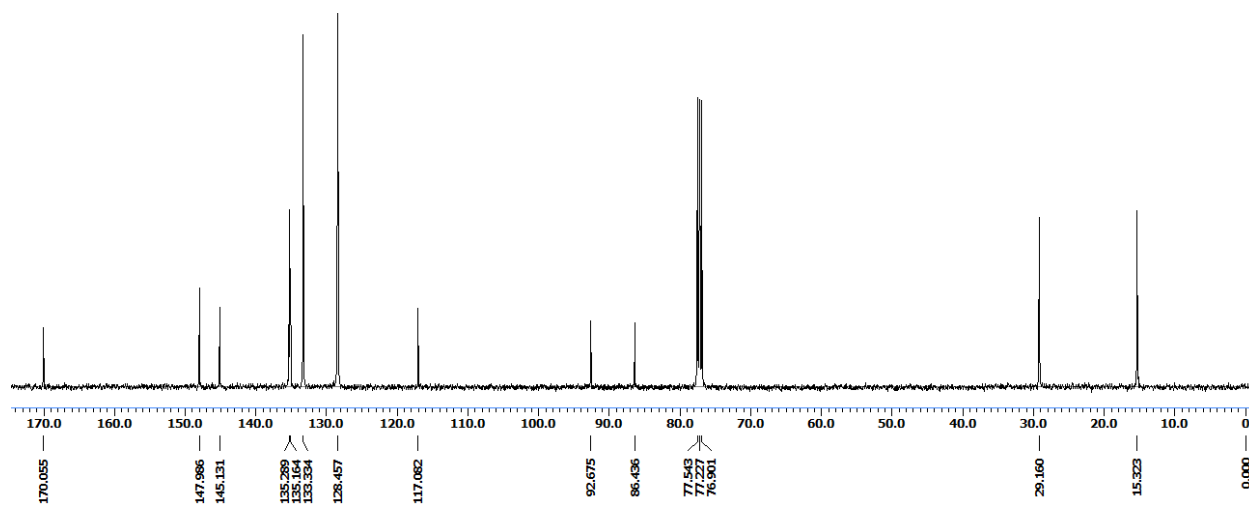
**3-(4-Ethylphenyl)-1-(thiophen-2-yl)prop-2-yn-1-one (1af)**



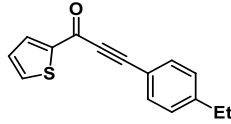
<sup>13</sup>C NMR



3-(4-Ethylphenyl)-1-(thiophen-2-yl)prop-2-yn-1-one (1af)



# HRMS



## 3-(4-Ethylphenyl)-1-(thiophen-2-yl)prop-2-yn-1-one (1af)

### Analysis Info

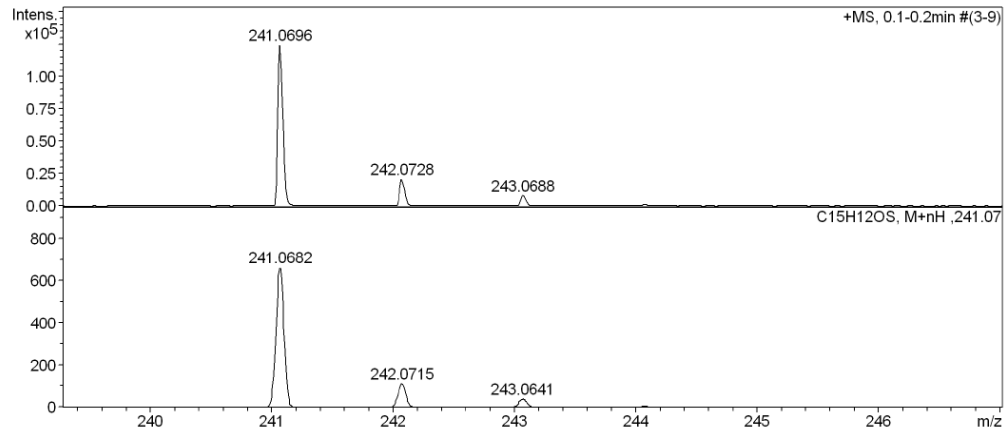
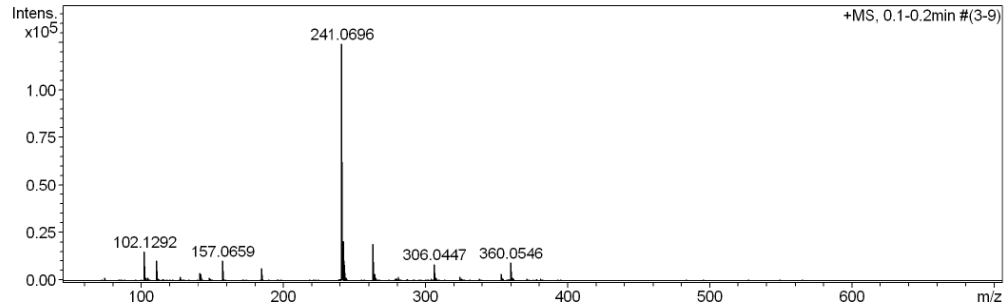
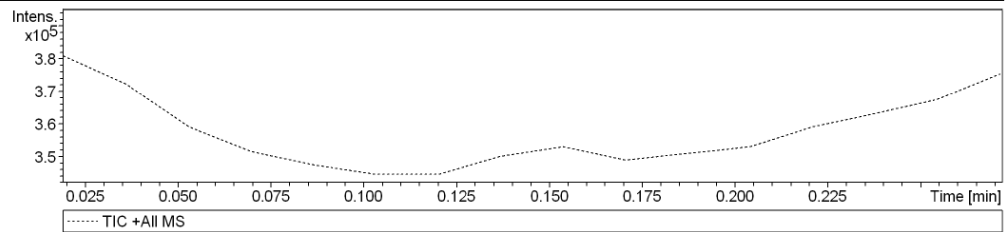
Analysis Name D:\Data\DEC-2020\NKS\29122020-NKS-AN-29.d  
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Sample Name Tmix-131118  
Comment

Acquisition Date 12/30/2020 12:15:40 AM

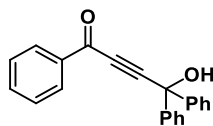
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

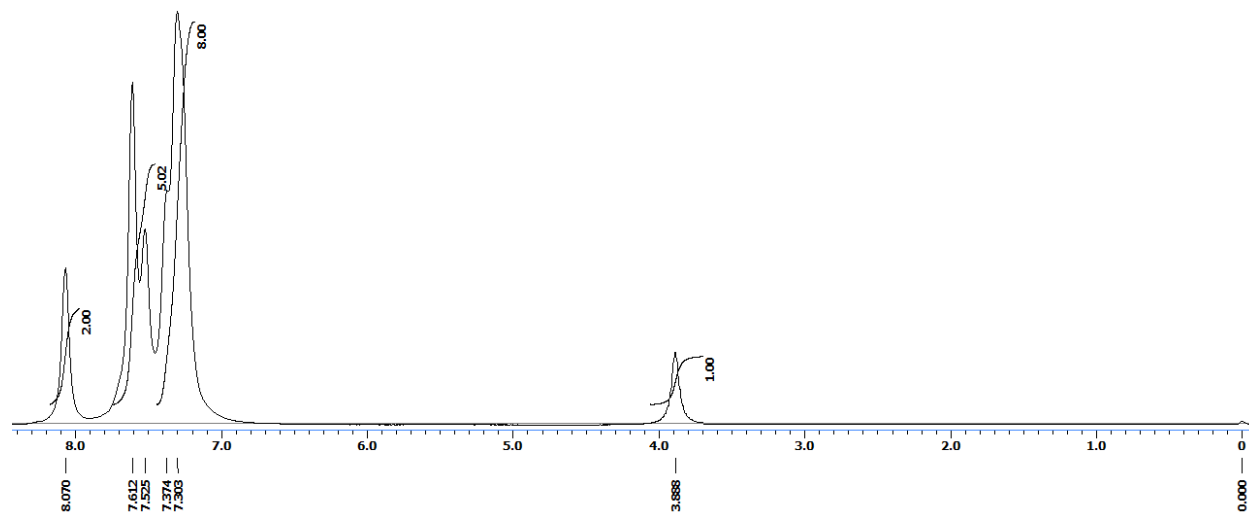
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



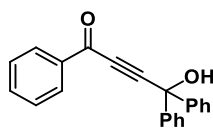
<sup>1</sup>H NMR



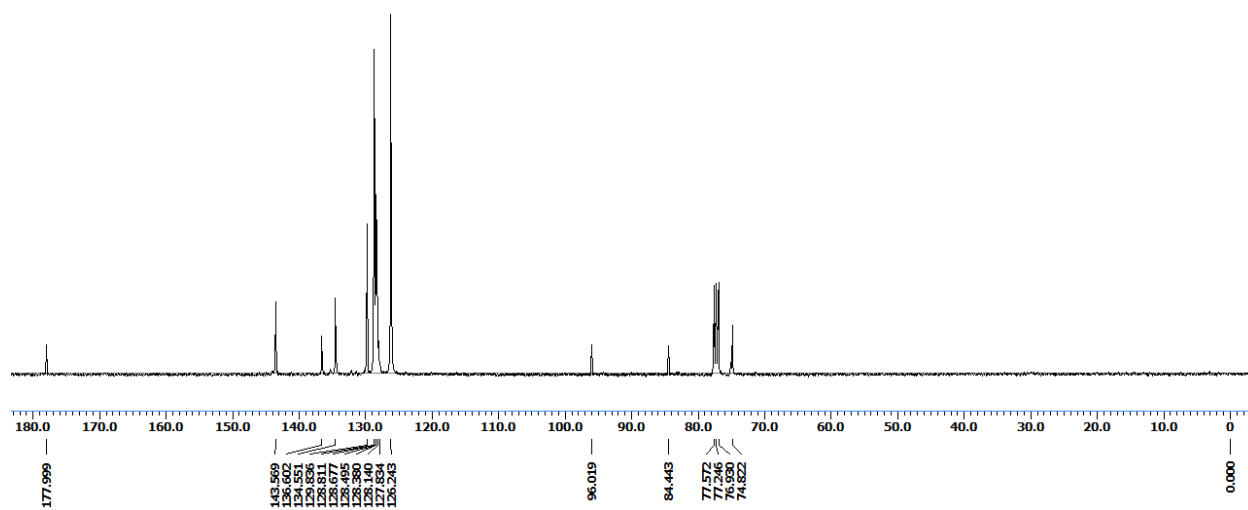
4-Hydroxy-1,4,4-triphenylbut-2-yn-1-one (1ah)



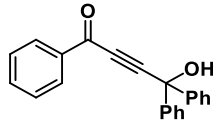
<sup>13</sup>C NMR



4-Hydroxy-1,4,4-triphenylbut-2-yn-1-one (1ah)



# HRMS



## 4-Hydroxy-1,4,4-triphenylbut-2-yn-1-one (1ah)

### Analysis Info

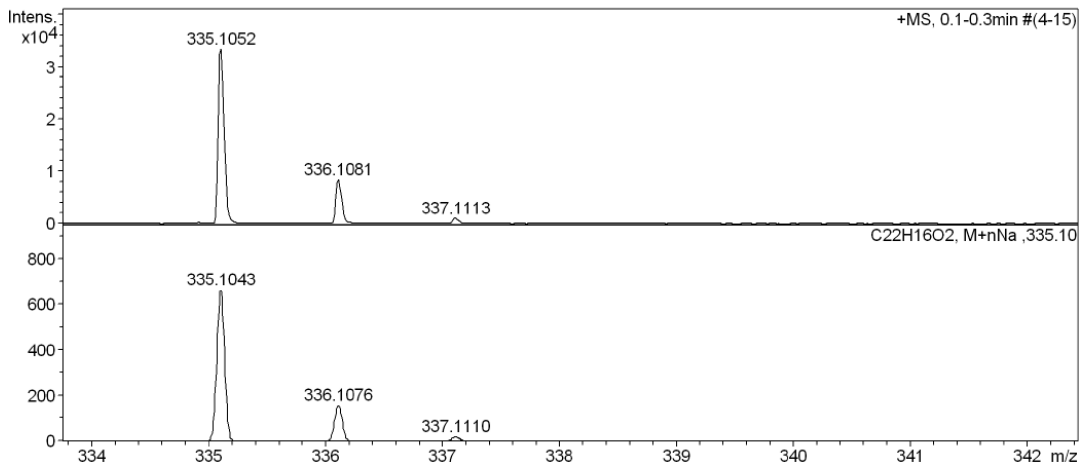
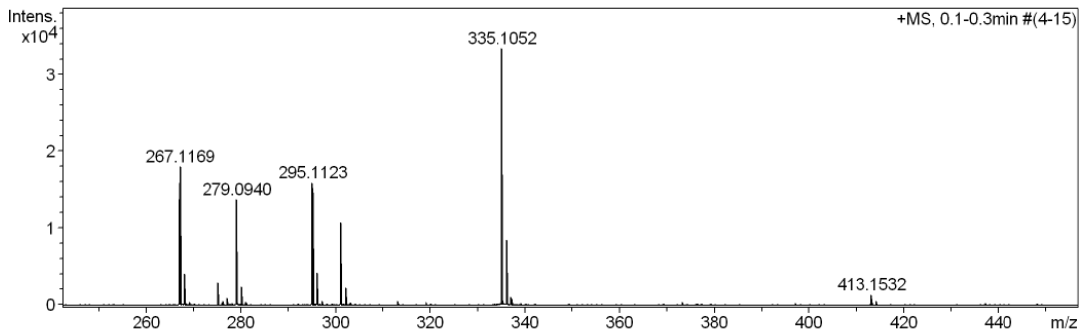
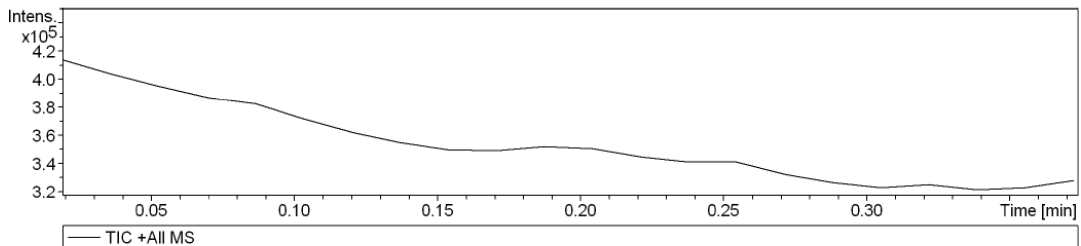
Analysis Name D:\Data\DEC-2020\NKS\29122020\_NKS\_AN\_13.d  
Method Pos\_tune\_low.m  
Sample Name Tmix-131118  
Comment

Acquisition Date 12/29/2020 9:21:35 PM

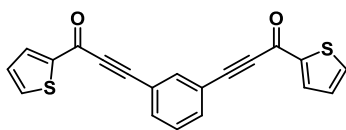
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

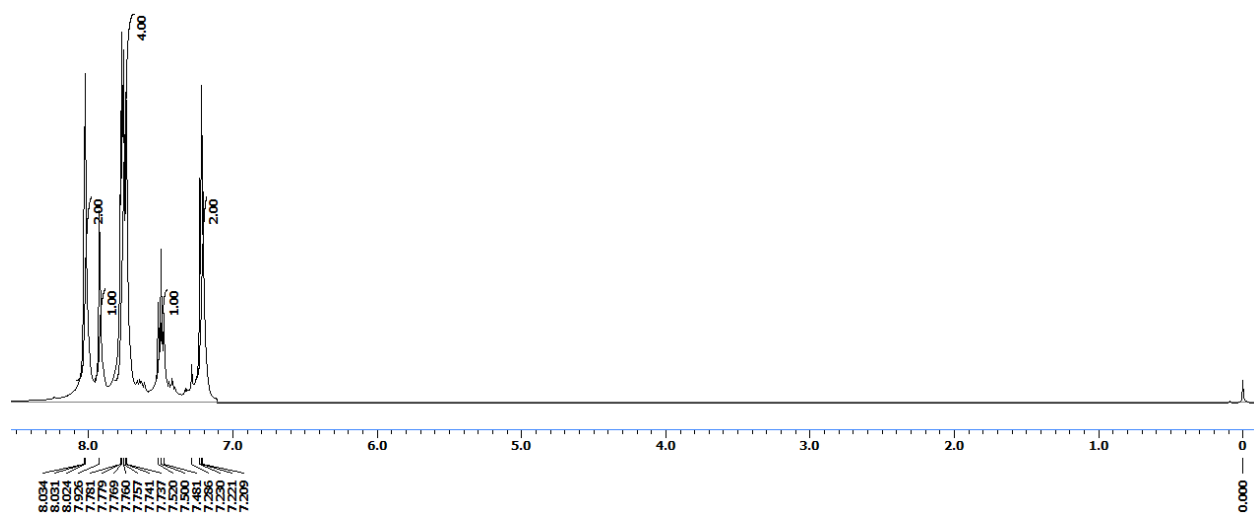
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



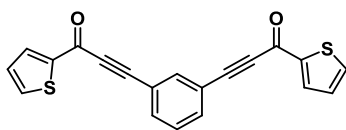
<sup>1</sup>H NMR



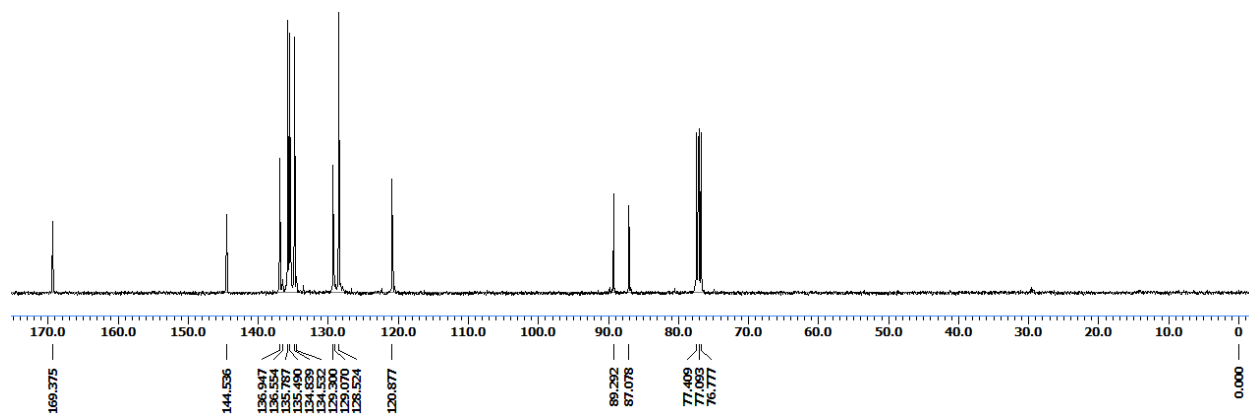
3,3'-(1,3-Phenylene)bis(1-(thiophen-2-yl)prop-2-yn-1-one) (1am)



<sup>13</sup>C NMR

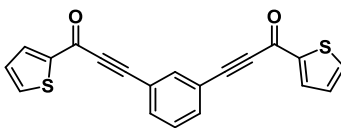


**3,3'-(1,3-Phenylene)bis(1-(thiophen-2-yl)prop-2-yn-1-one) (1am)**





# HRMS



## 3,3'-(1,3-Phenylene)bis(1-(thiophen-2-yl)prop-2-yn-1-one) (1am)

### Analysis Info

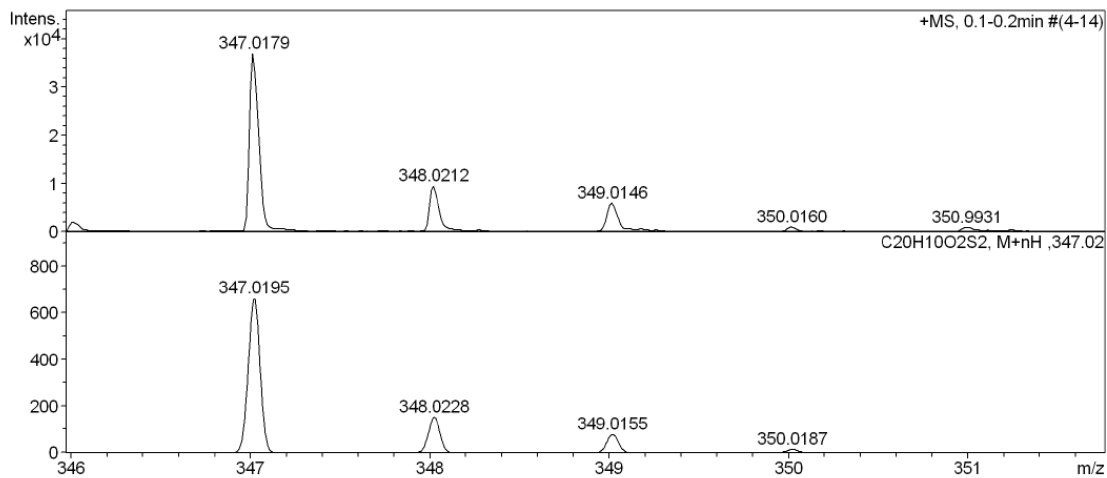
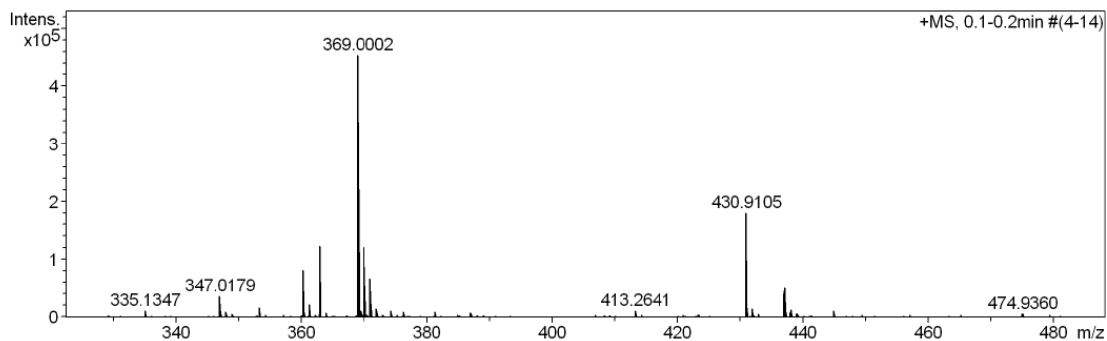
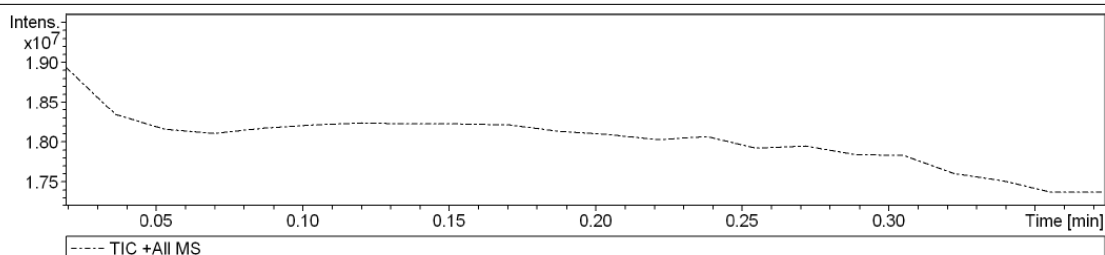
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 Comment

Acquisition Date 12/29/2020 7:35:58 PM

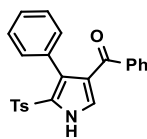
Operator Amit S.Sahu  
 Instrument microTOF-Q II 10337

### Acquisition Parameter

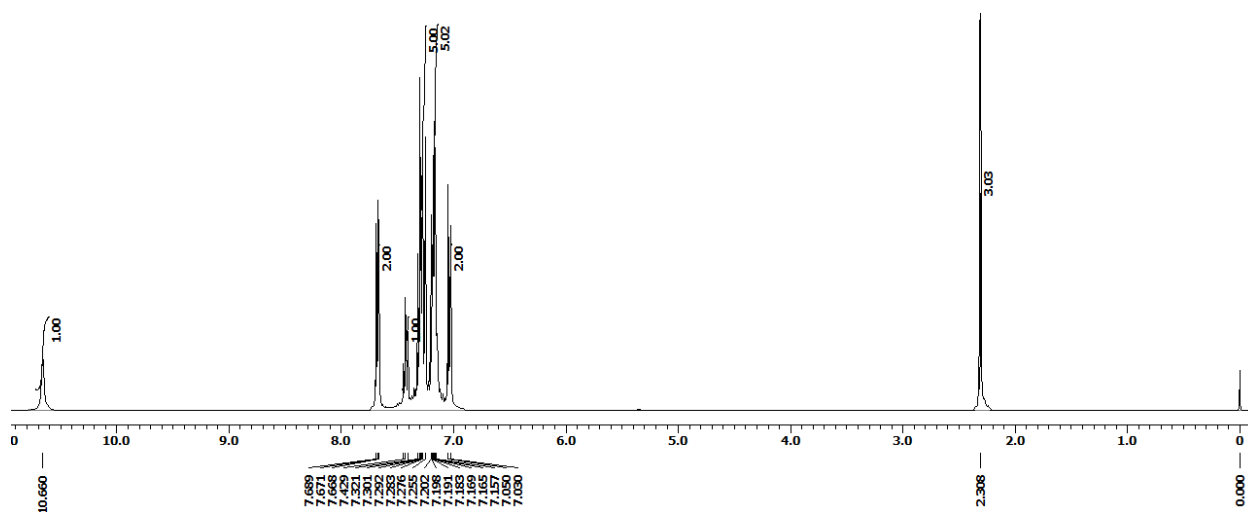
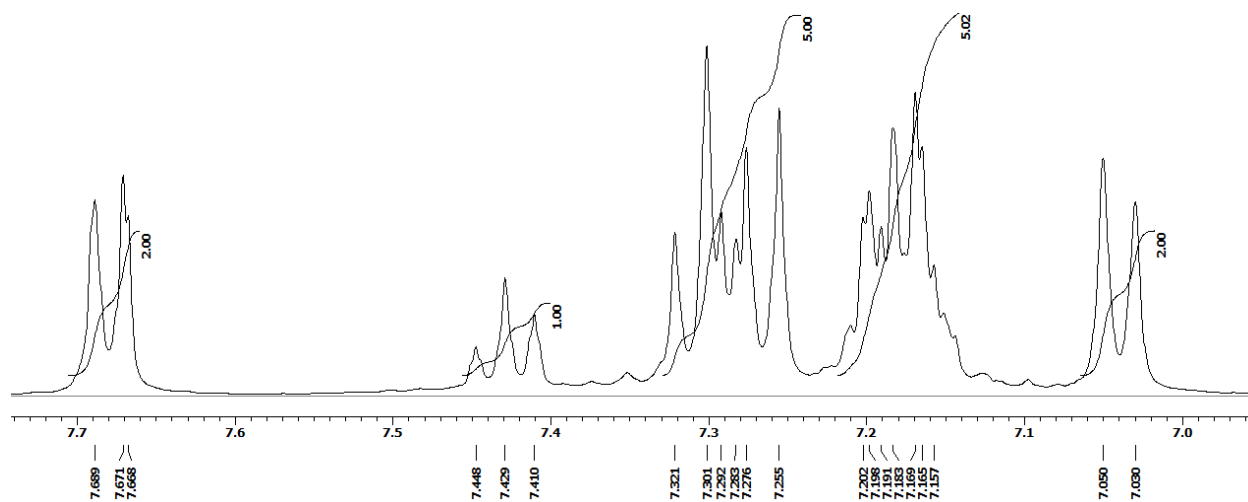
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



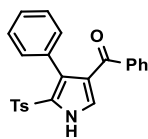
# <sup>1</sup>H NMR



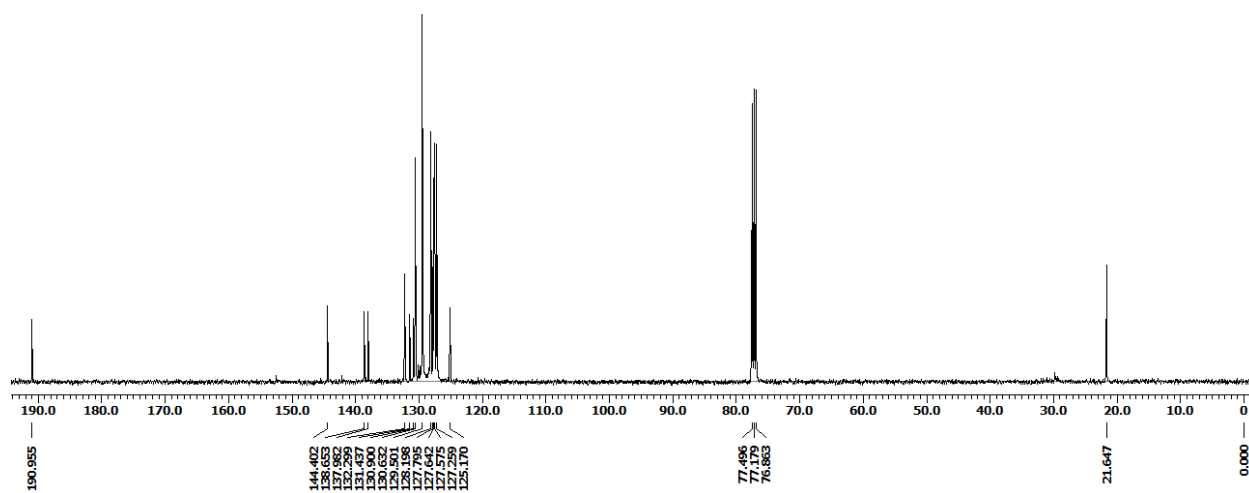
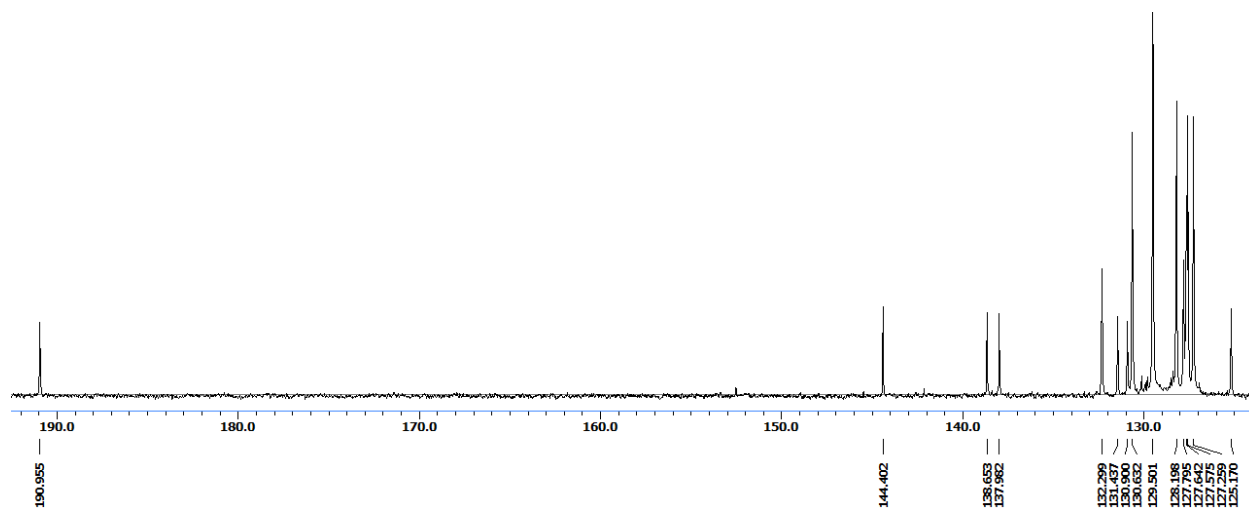
Phenyl(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3a)



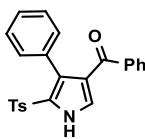
<sup>13</sup>C NMR



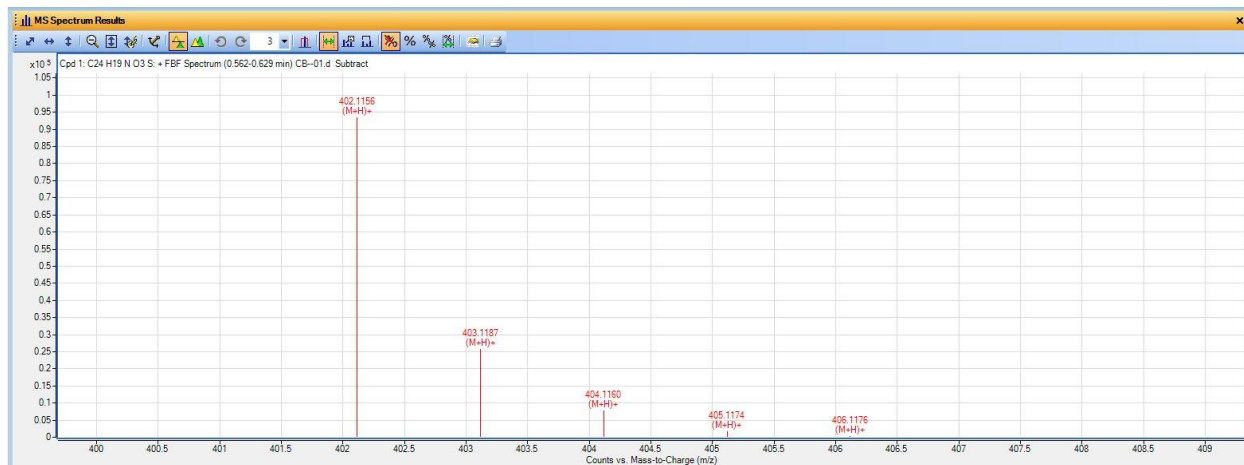
Phenyl(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3a)



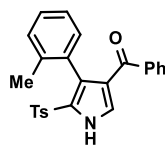
## HRMS



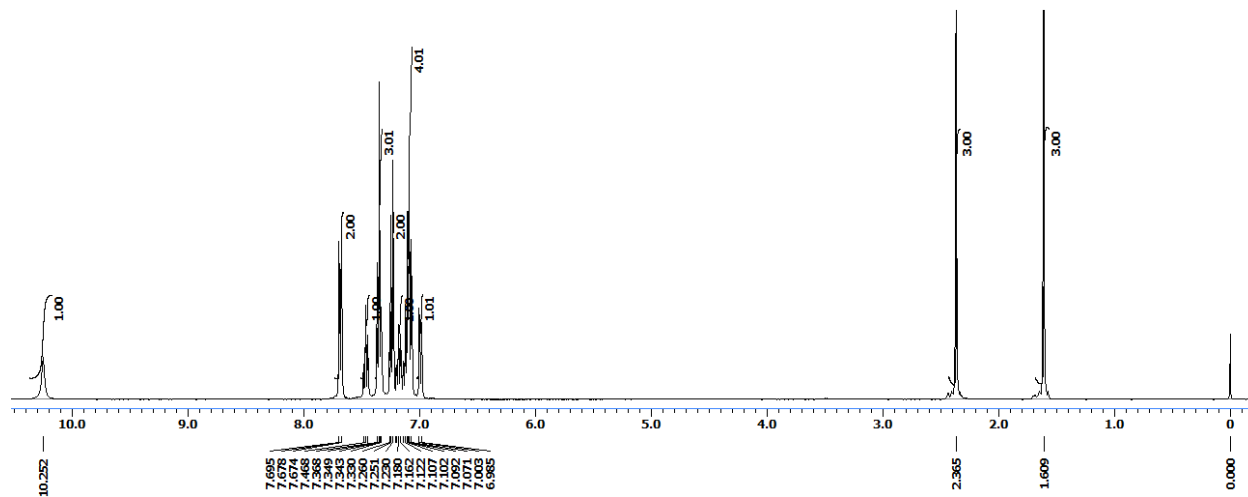
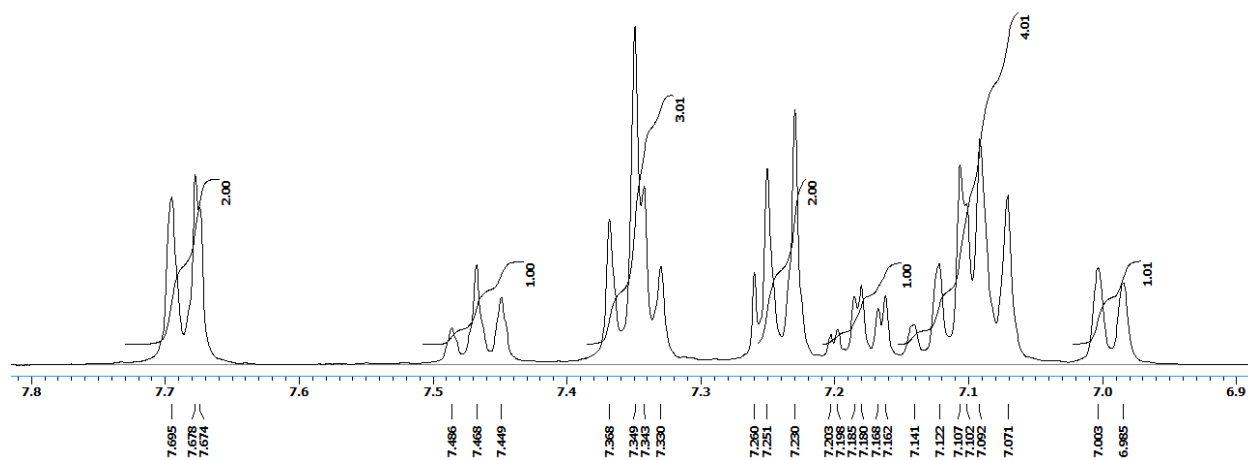
Phenyl(4-phenyl-5-tosyl-1*H*-pyrrol-3-yl)methanone (3a)



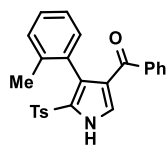
# <sup>1</sup>H NMR



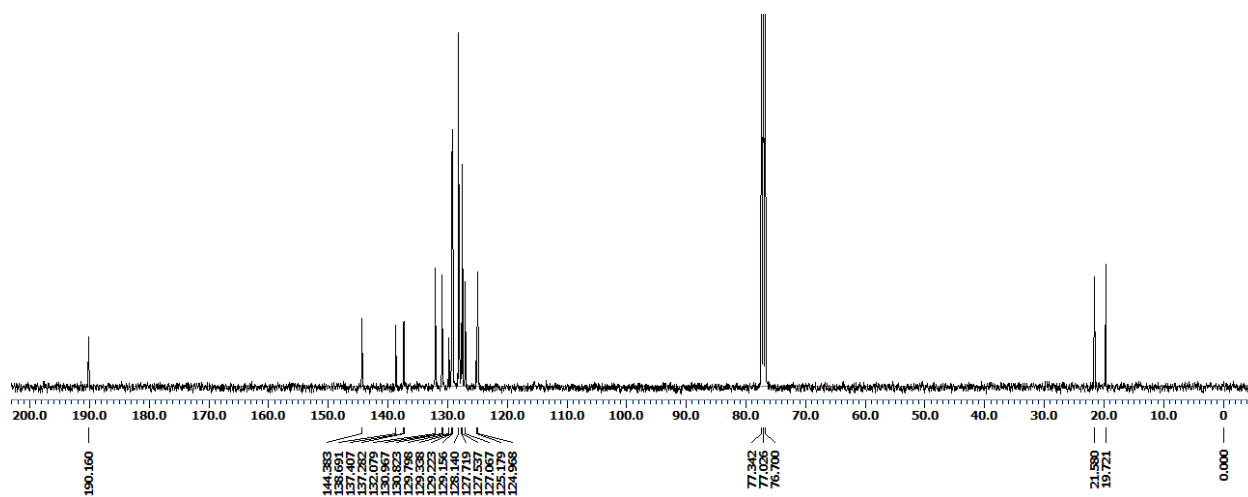
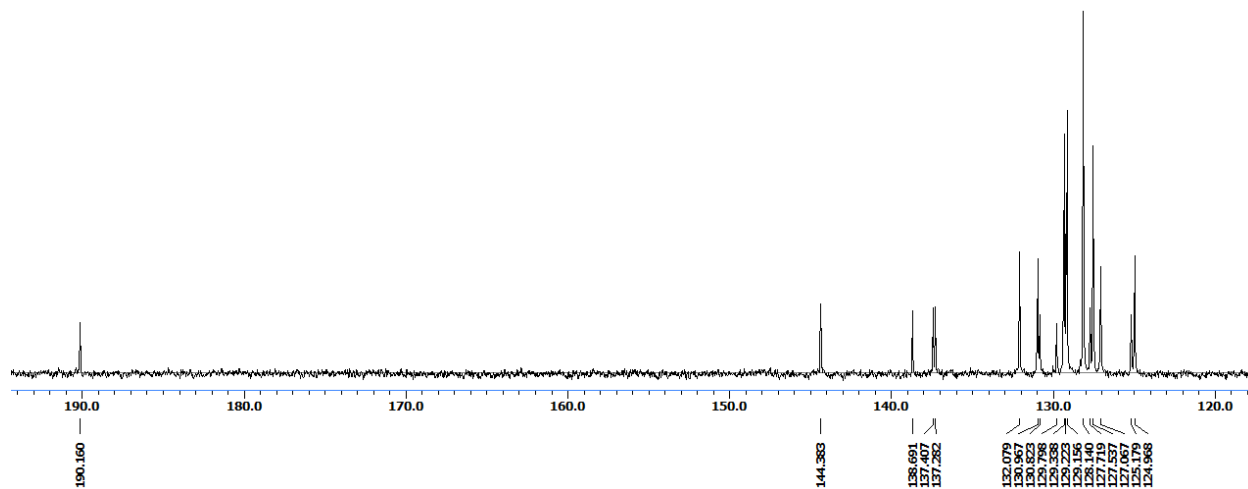
Phenyl(4-(o-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3b)



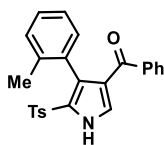
<sup>13</sup>C NMR



Phenyl(4-(o-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3b)



# HRMS



## Phenyl(4-(o-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3b)

### Analysis Info

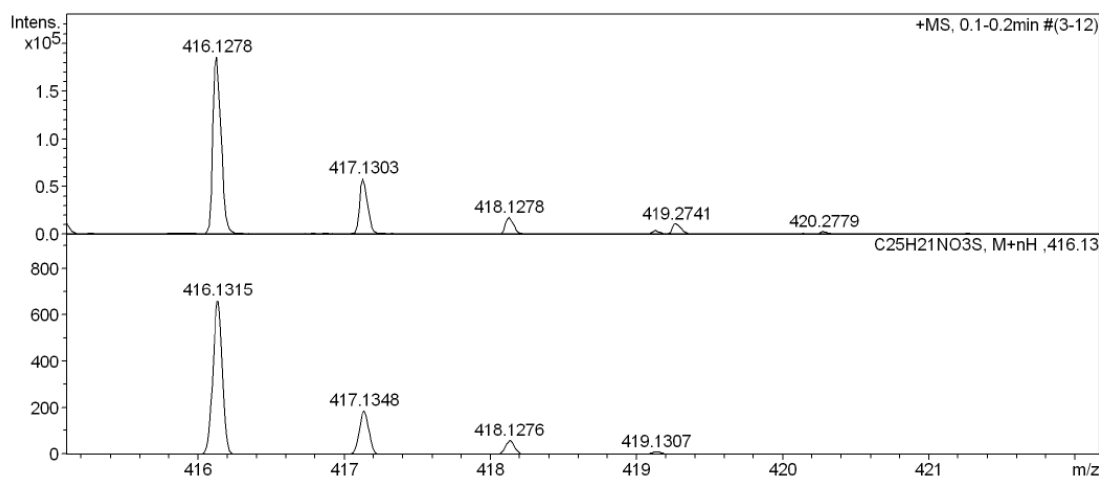
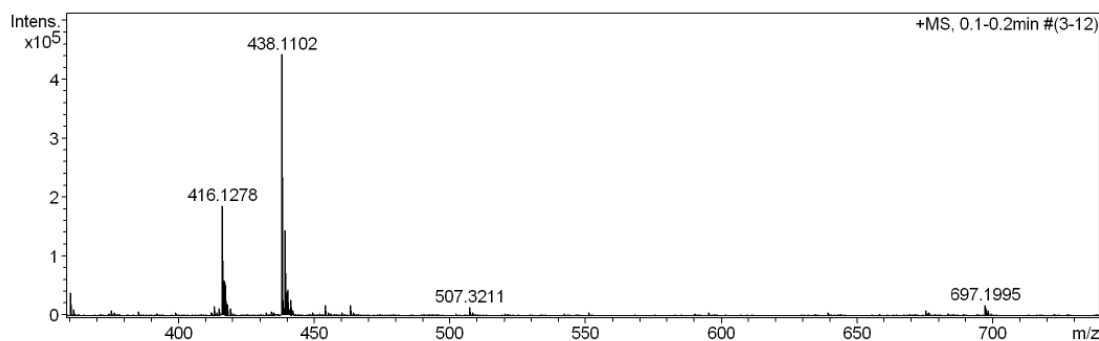
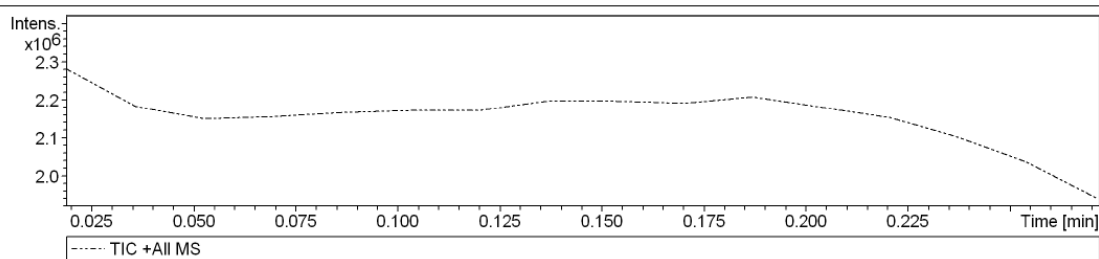
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 Sample Name Tmix-131118  
 Comment

Acquisition Date 12/29/2020 7:46:38 PM

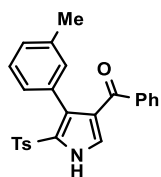
Operator Amit S.Sahu  
 Instrument micrOTOF-Q II 10337

### Acquisition Parameter

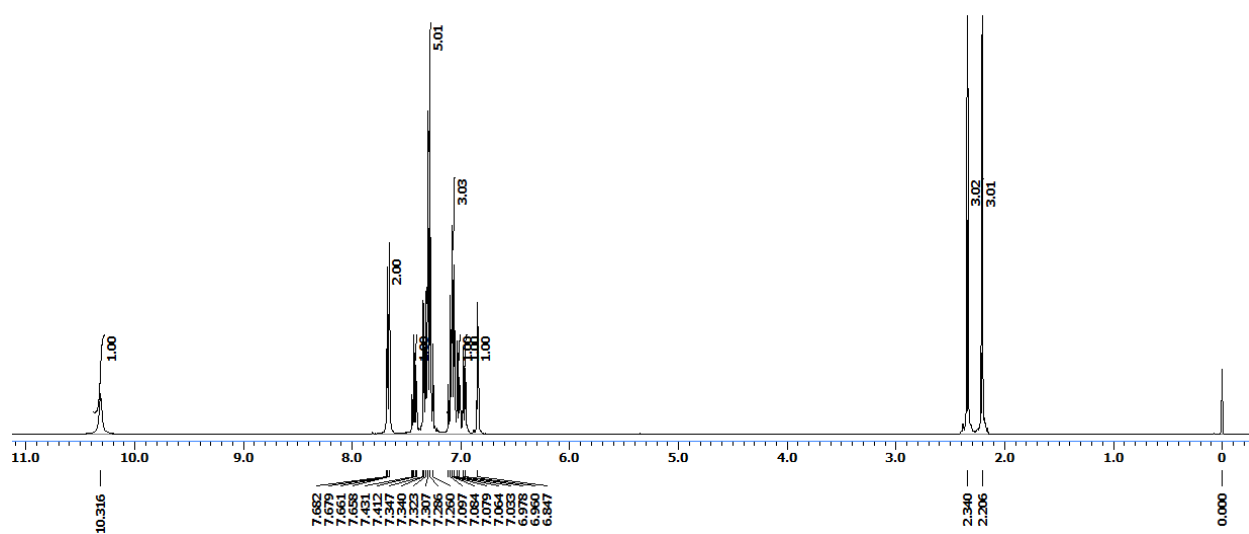
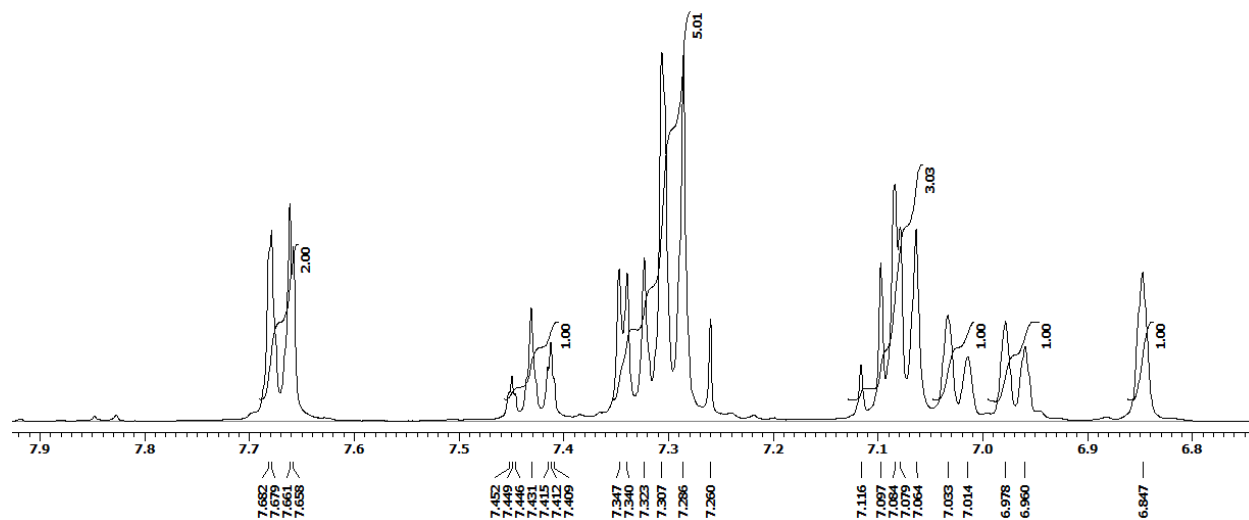
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



# <sup>1</sup>H NMR

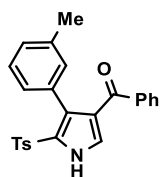


Phenyl(4-(m-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3c)

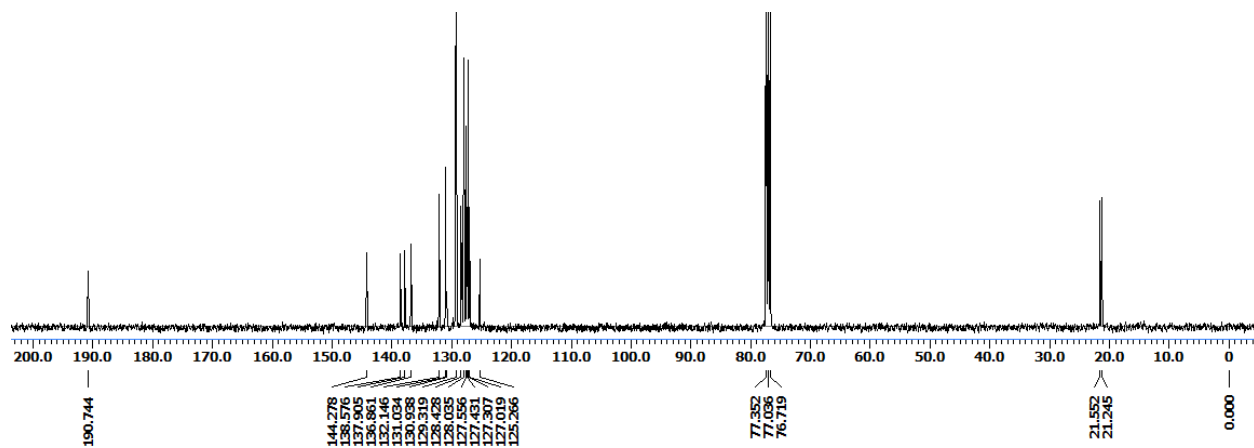
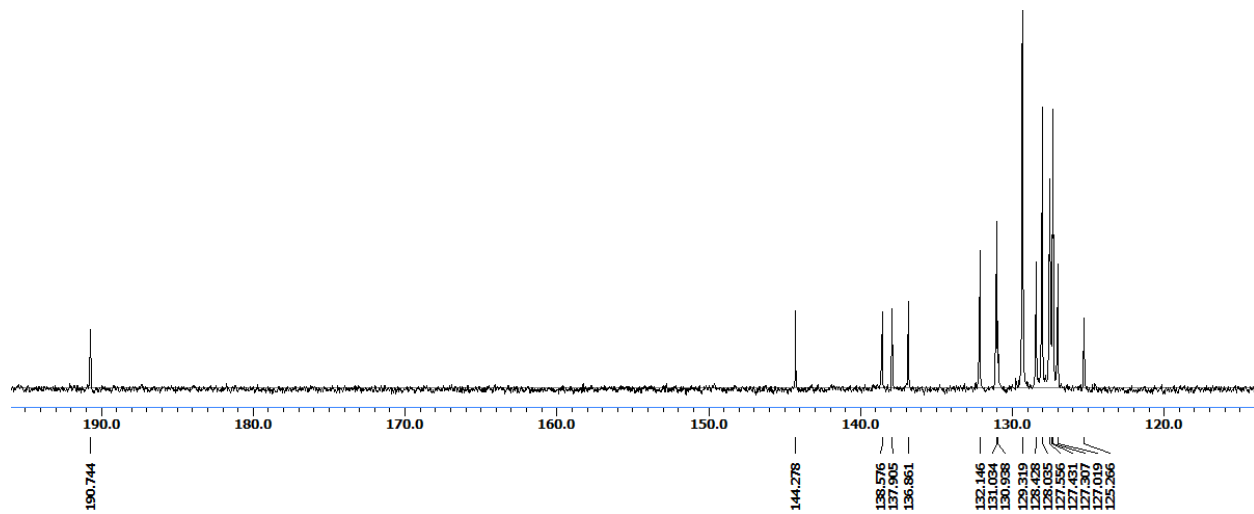




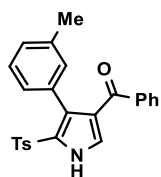
<sup>13</sup>C NMR



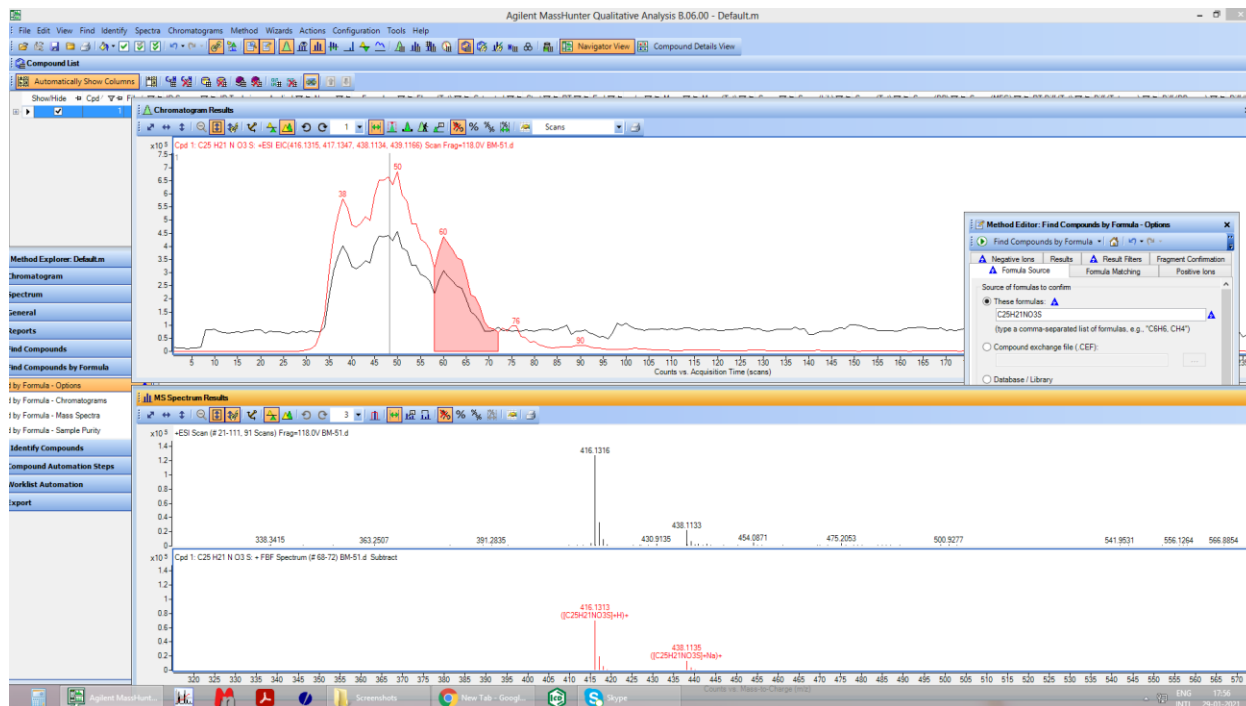
Phenyl(4-(m-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3c)



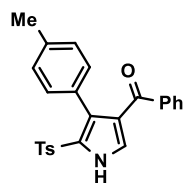
# HRMS



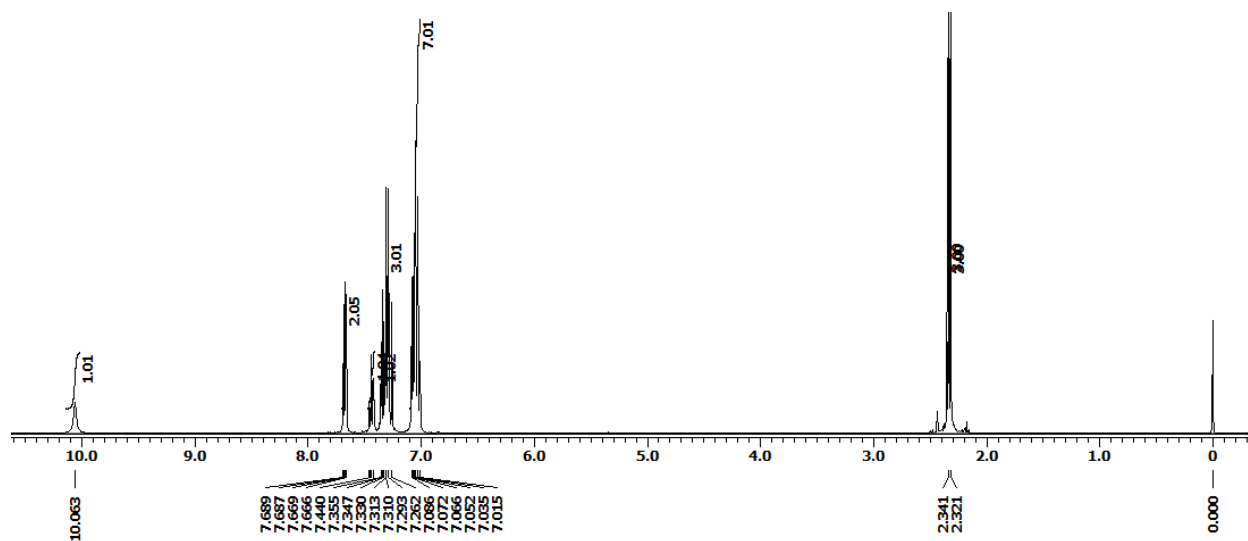
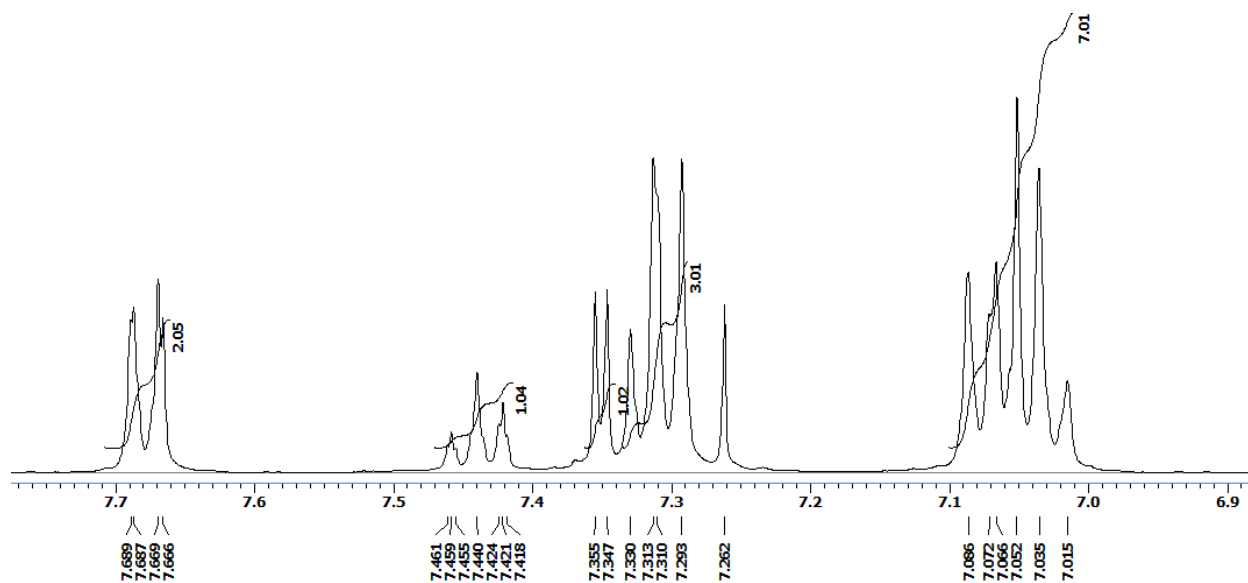
Phenyl(4-(m-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3c)



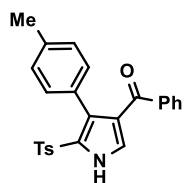
# <sup>1</sup>H NMR



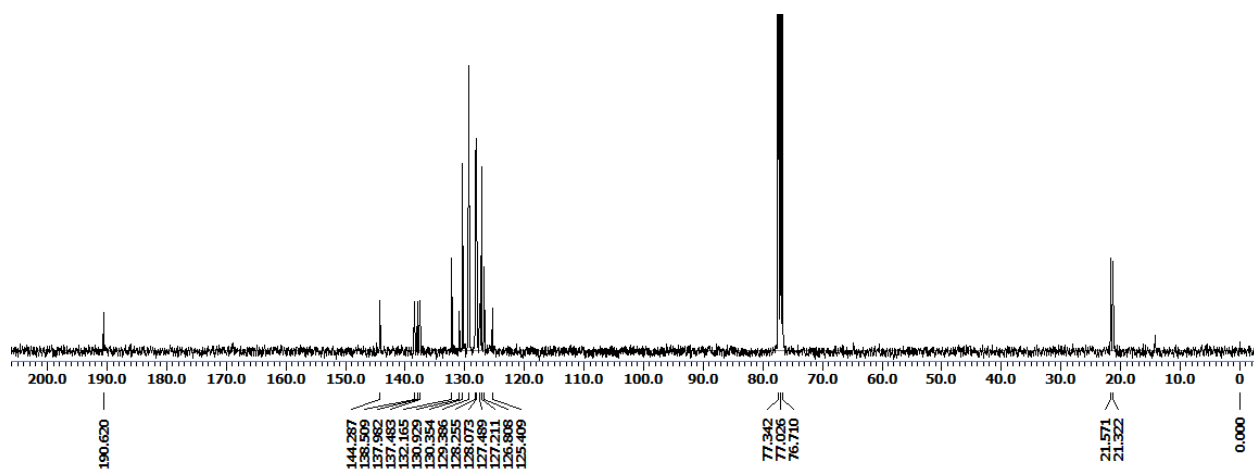
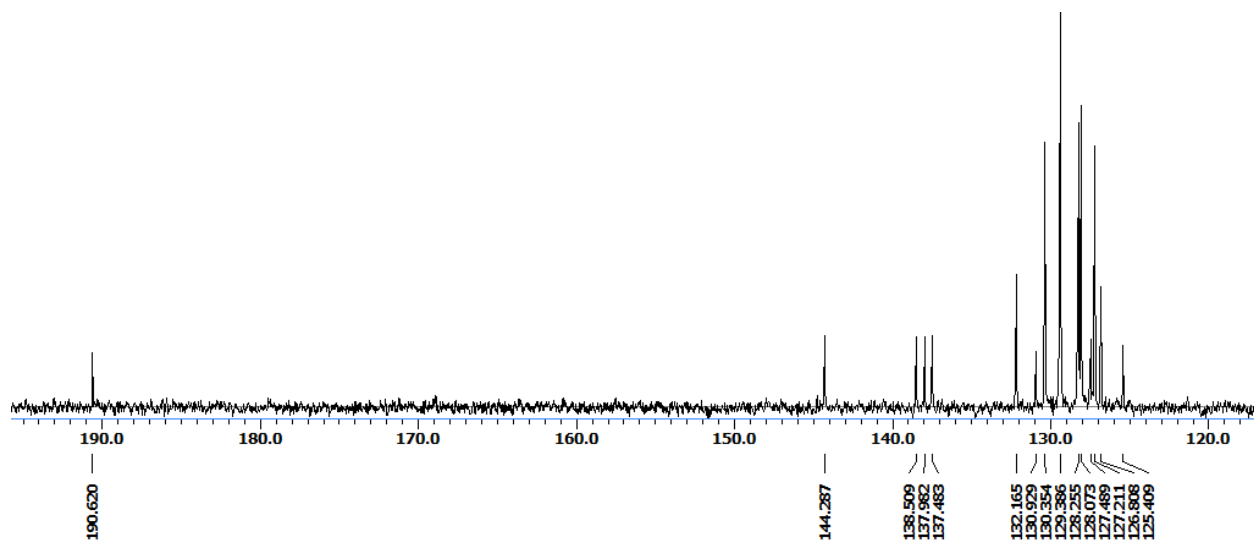
Phenyl(4-(p-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3d)



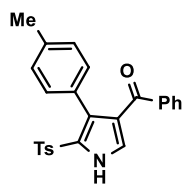
<sup>13</sup>C NMR



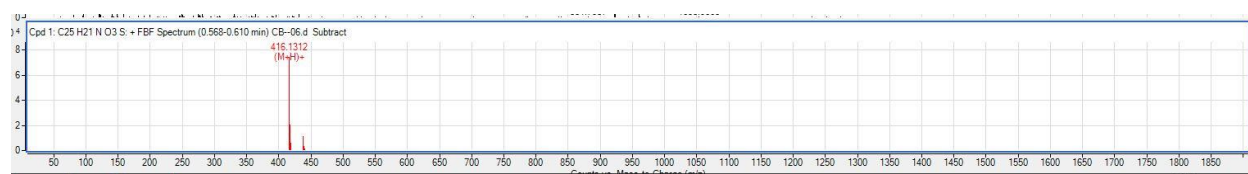
Phenyl(4-(p-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3d)



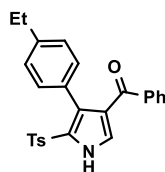
## HRMS



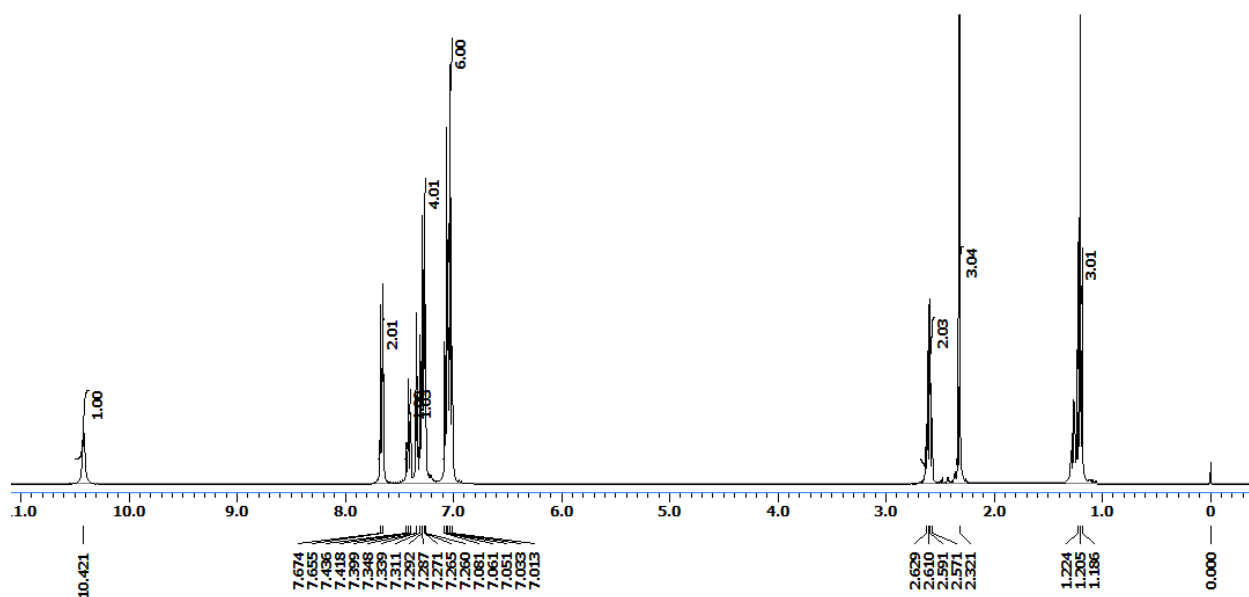
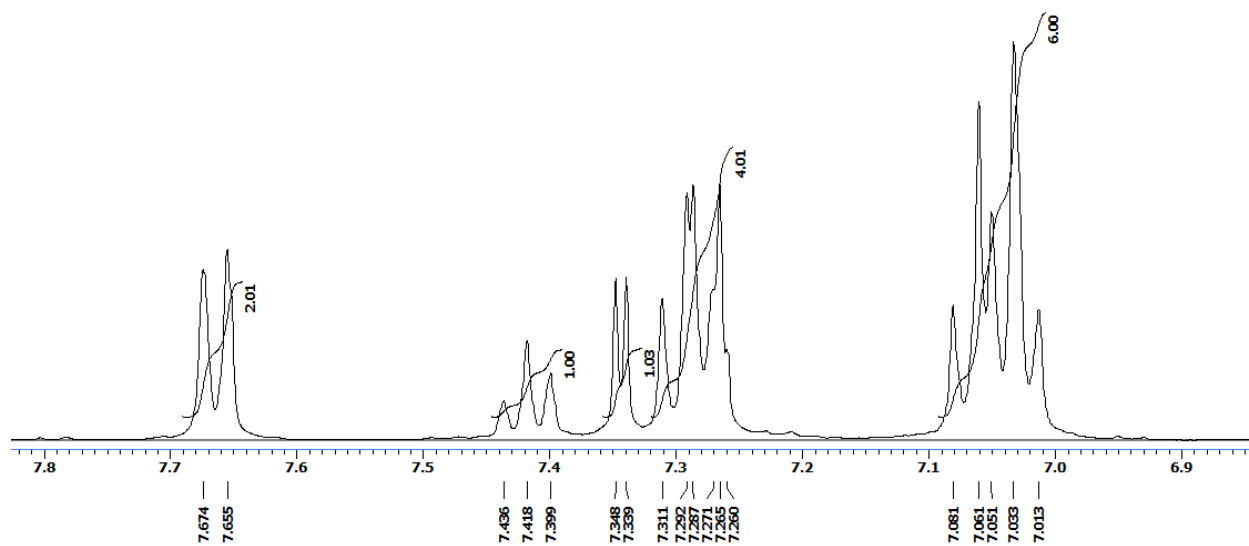
**Phenyl(4-(p-tolyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3d)**



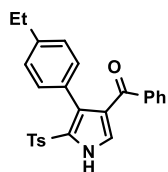
# <sup>1</sup>H NMR



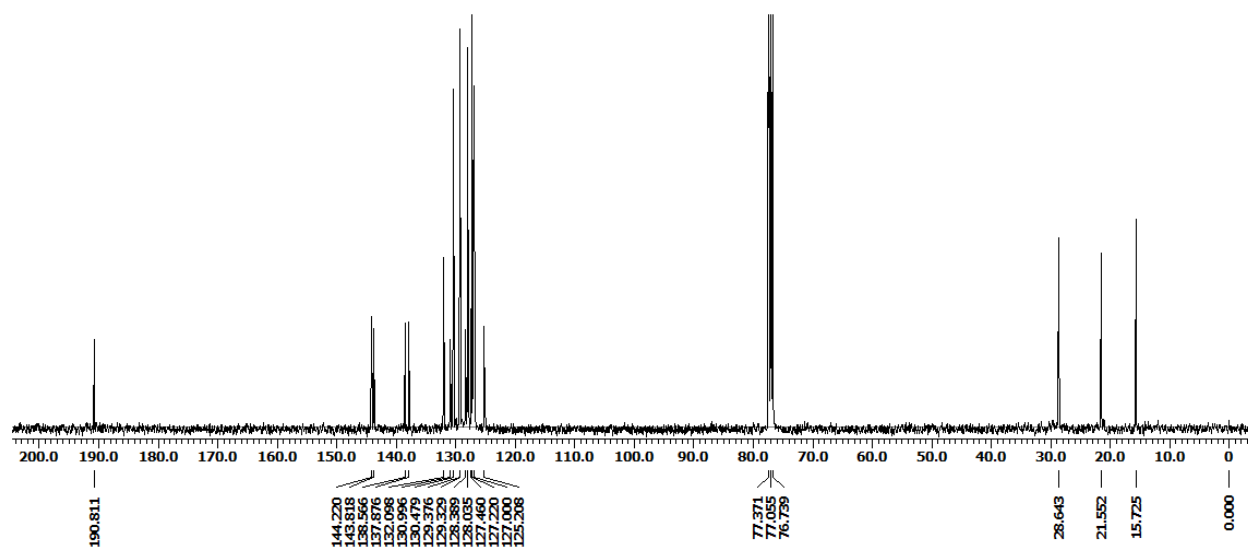
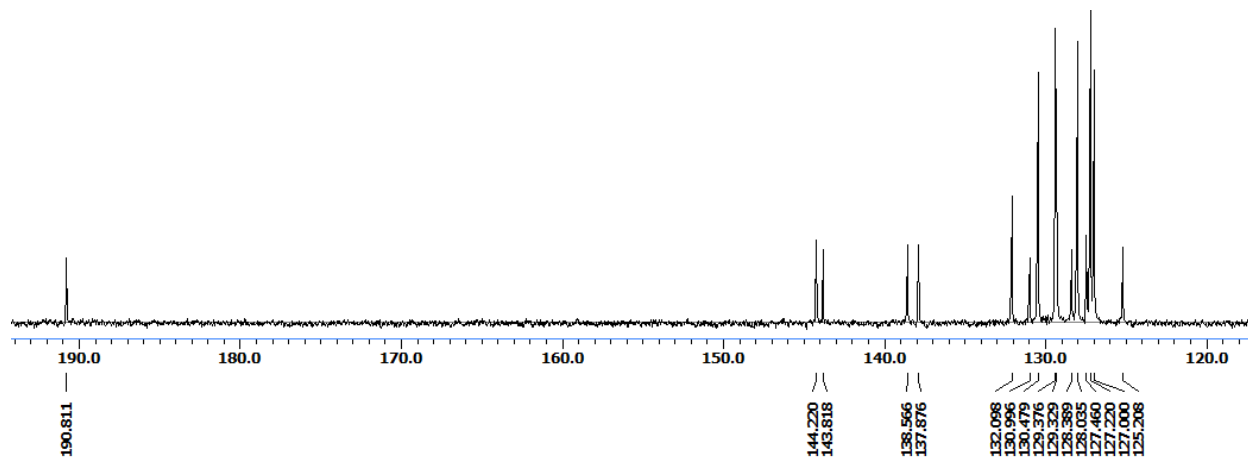
(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3e)



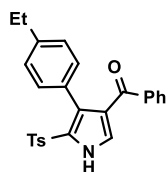
<sup>13</sup>C NMR



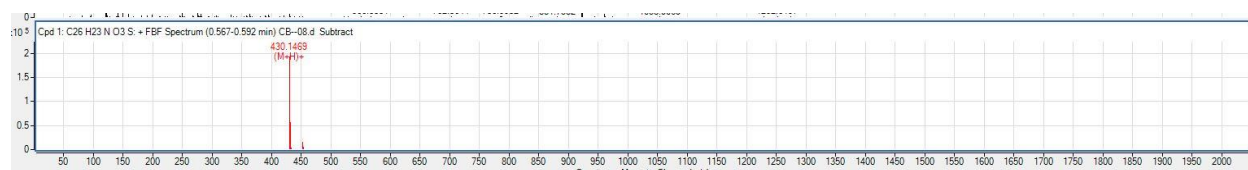
(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3e)



## HRMS

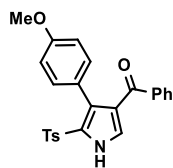


**(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3e)**

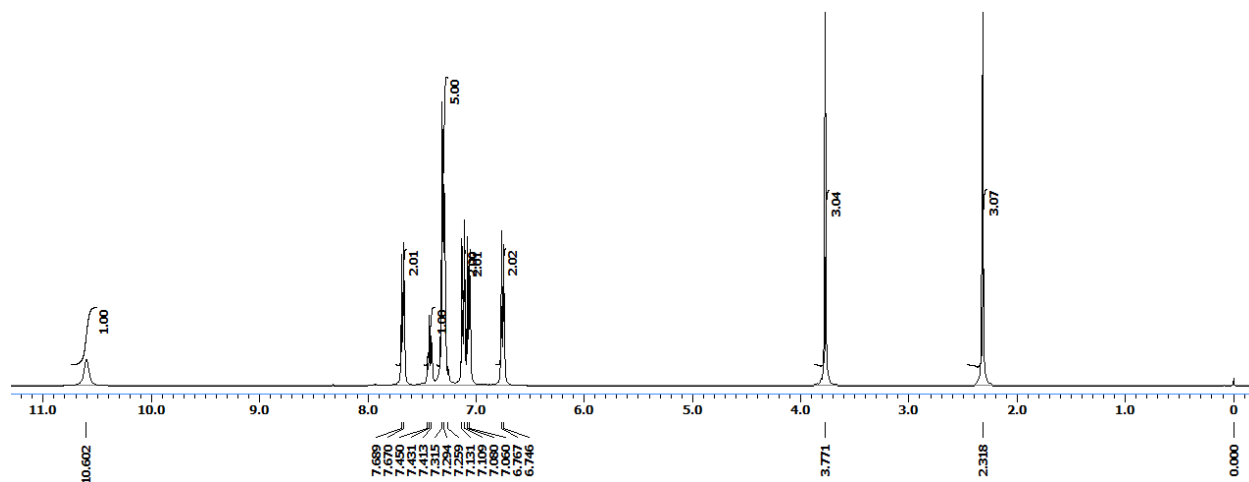
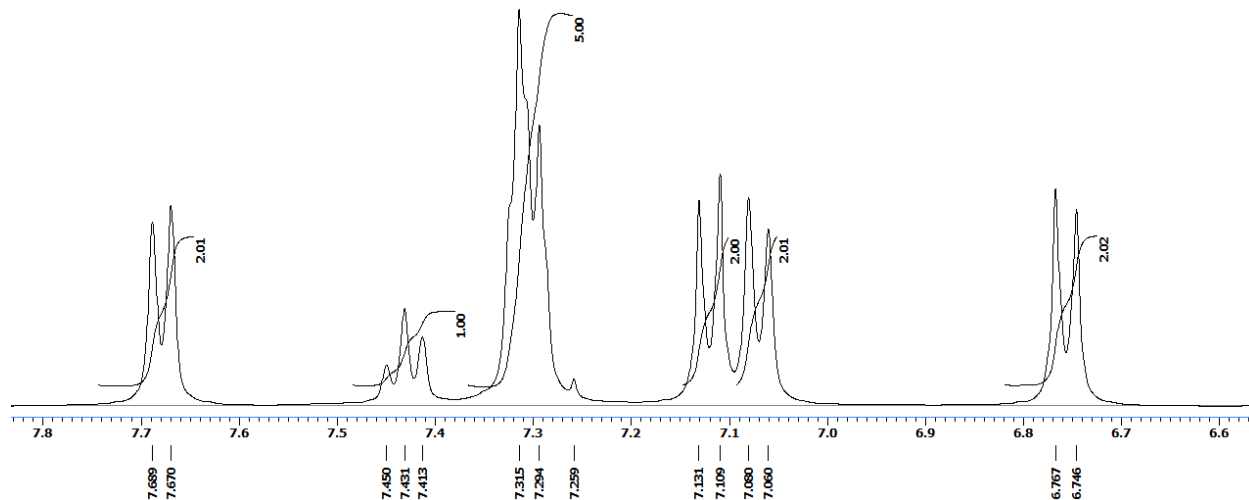




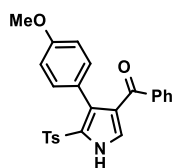
# <sup>1</sup>H NMR



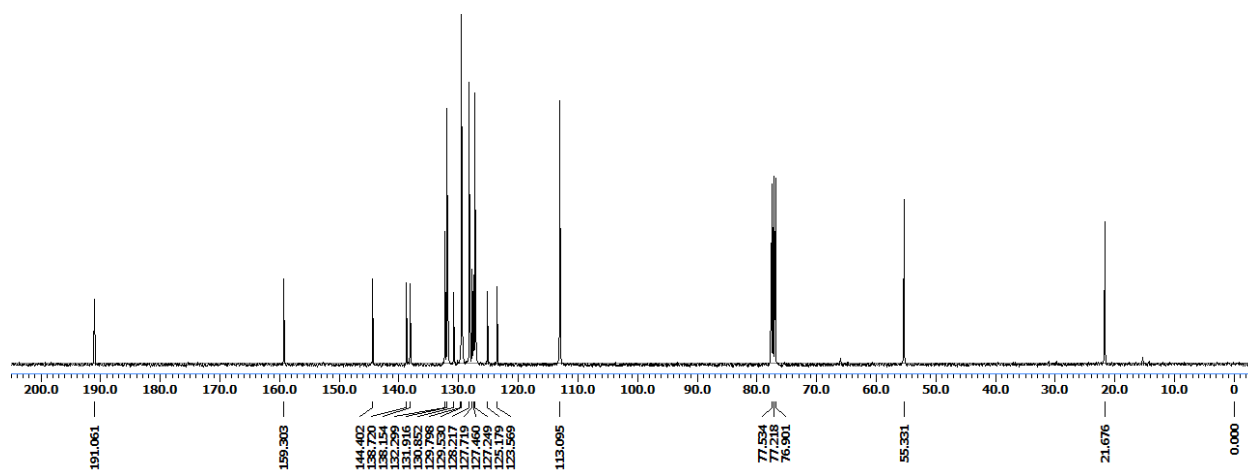
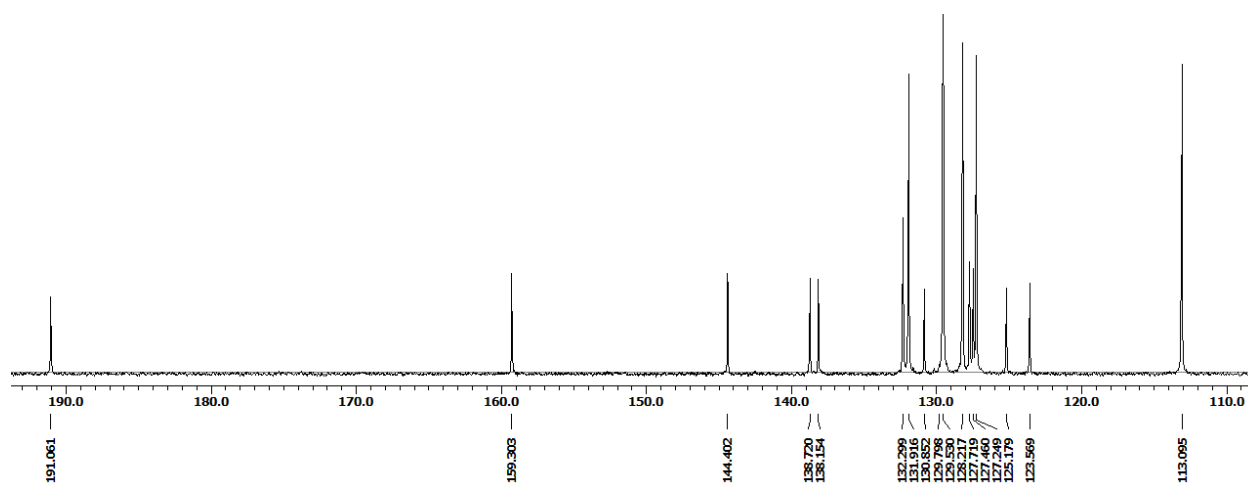
(4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3f)



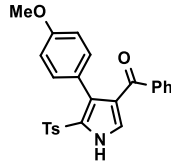
<sup>13</sup>C NMR



(4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3f)



# HRMS



## (4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3f)

### Analysis Info

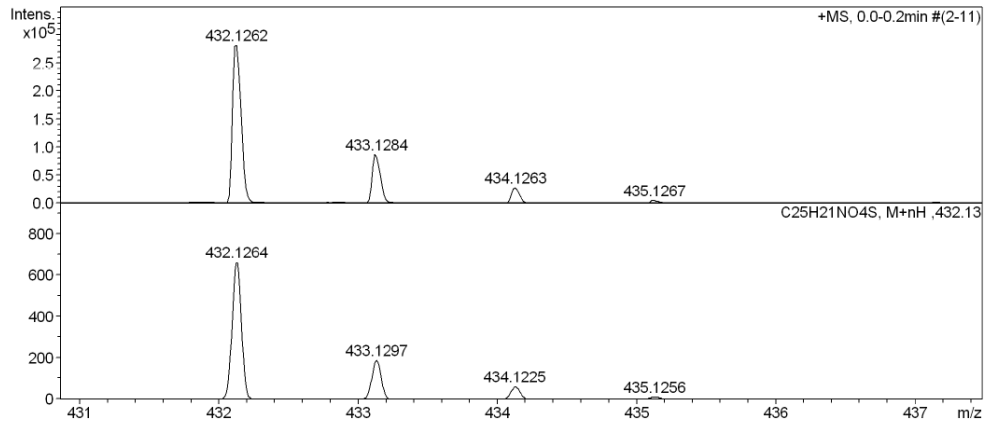
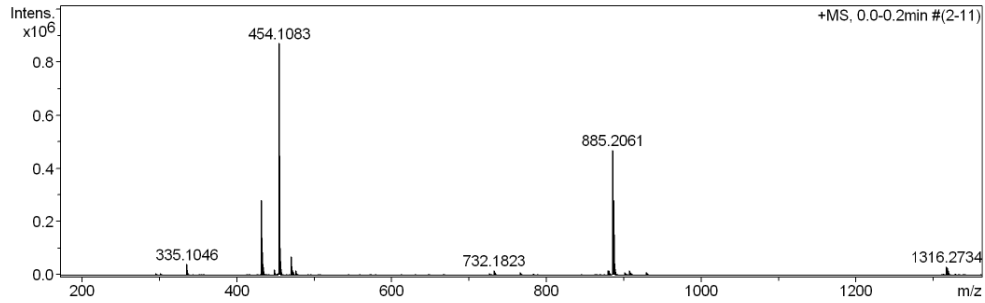
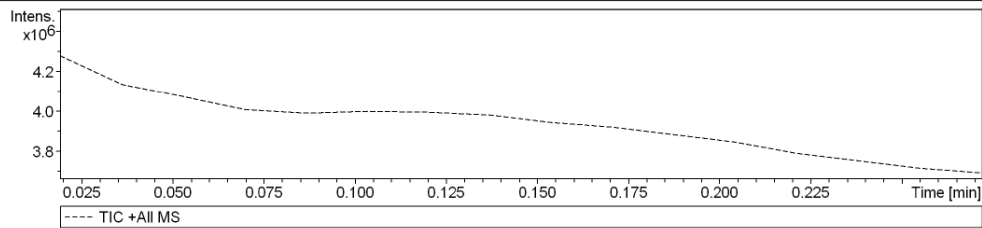
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Comment

Acquisition Date 12/29/2020 9:26:06 PM

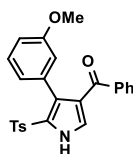
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

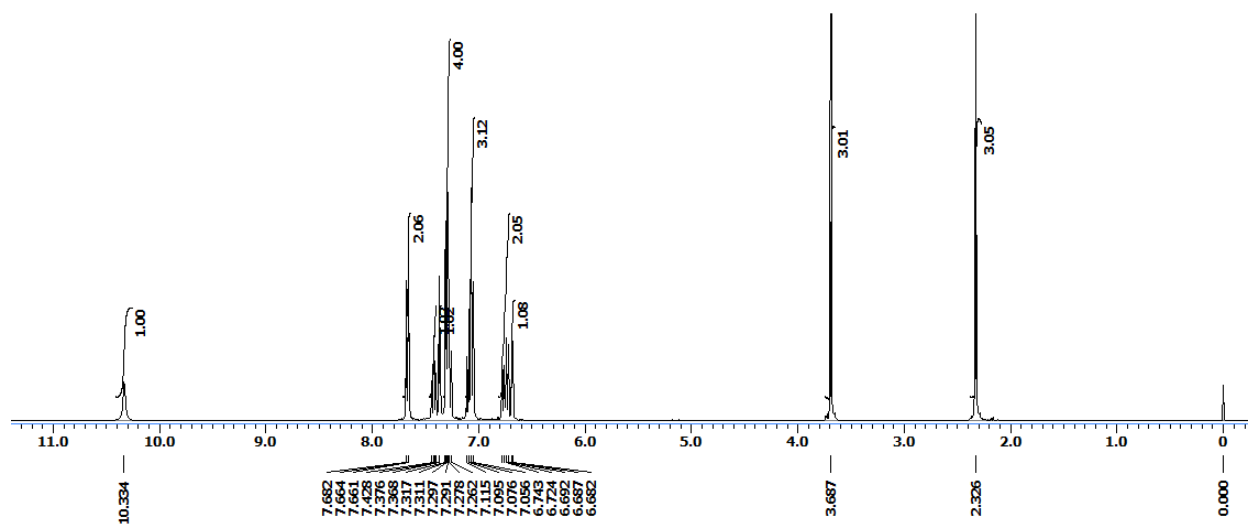
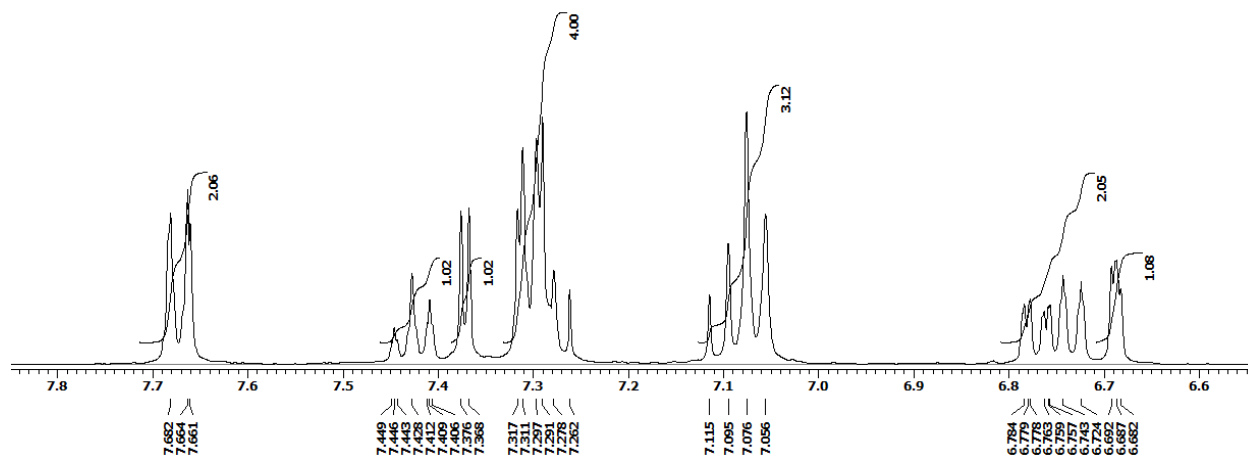
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



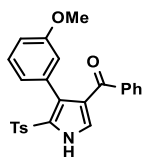
# <sup>1</sup>H NMR



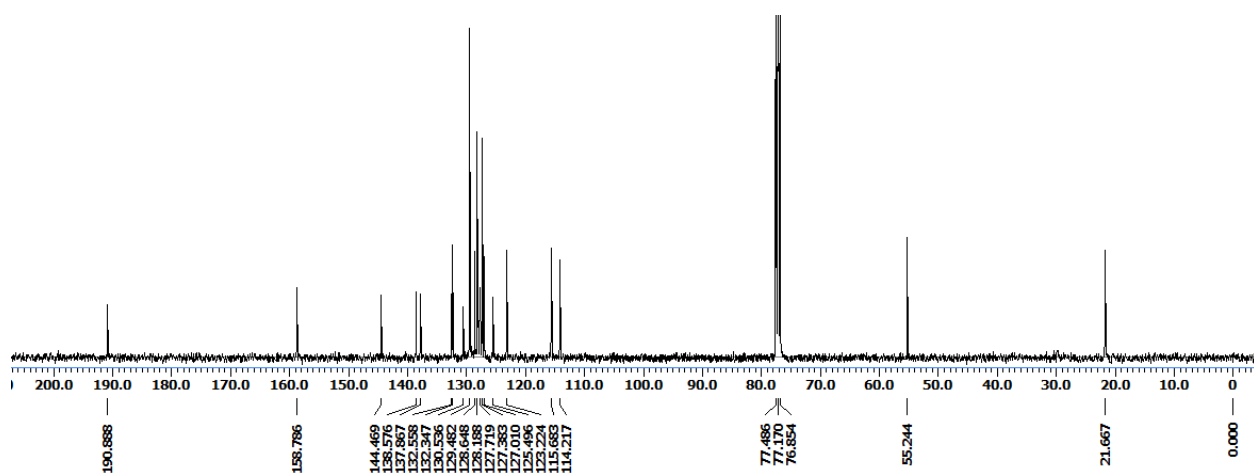
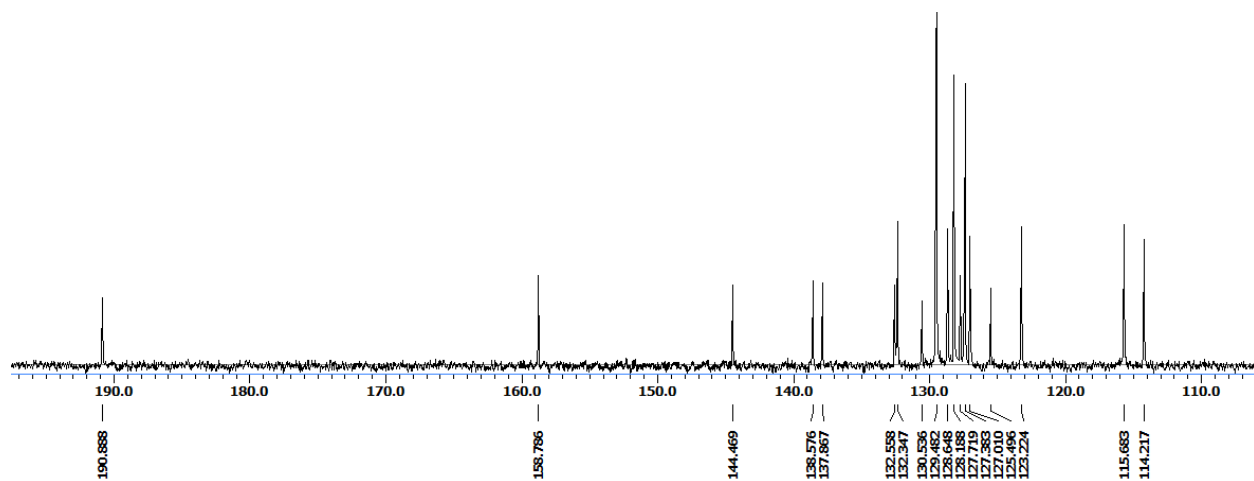
(4-(3-Methoxyphenyl)-5-tosyl-1*H*-pyrrol-3-yl)(phenyl)methanone (3g)



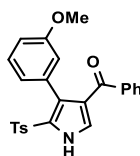
<sup>13</sup>C NMR



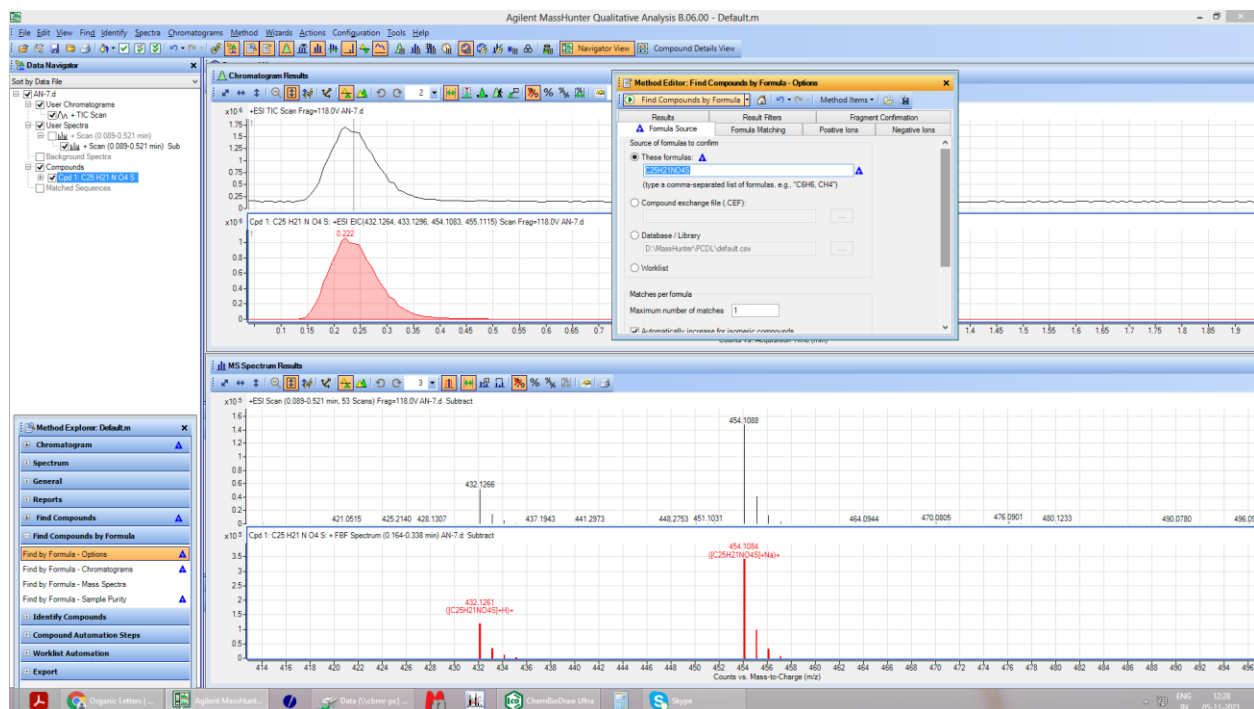
(4-(3-Methoxyphenyl)-5-tosyl-1*H*-pyrrol-3-yl)(phenyl)methanone (3g)



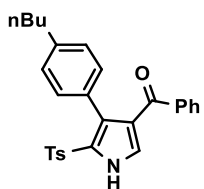
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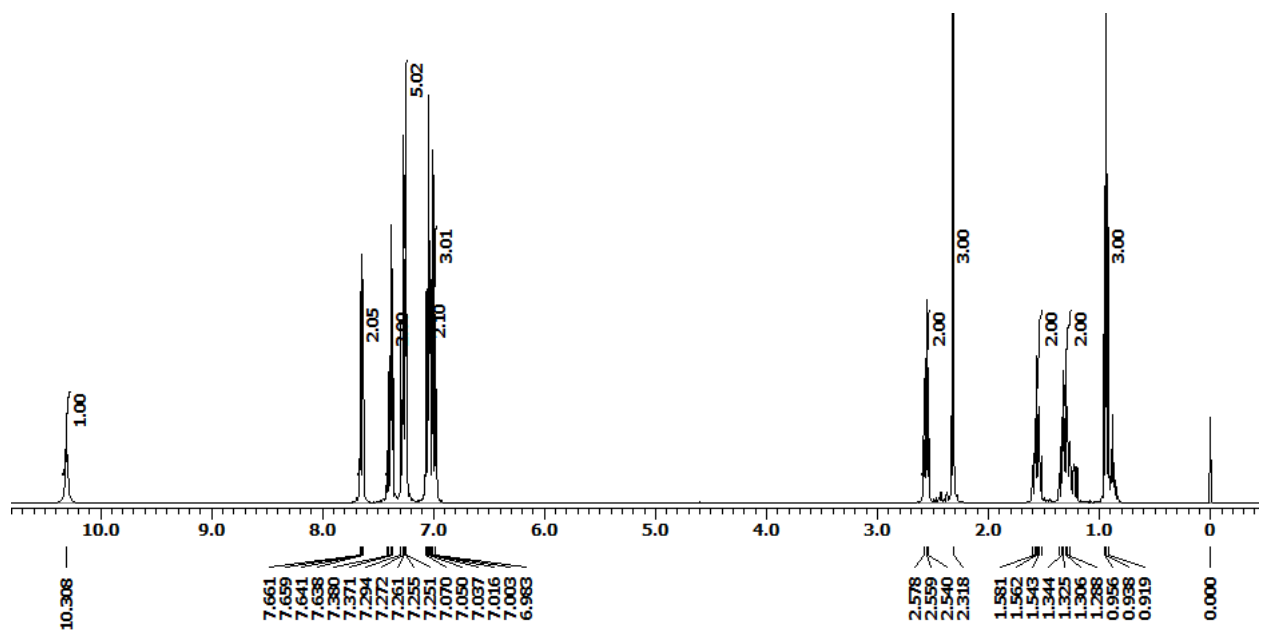
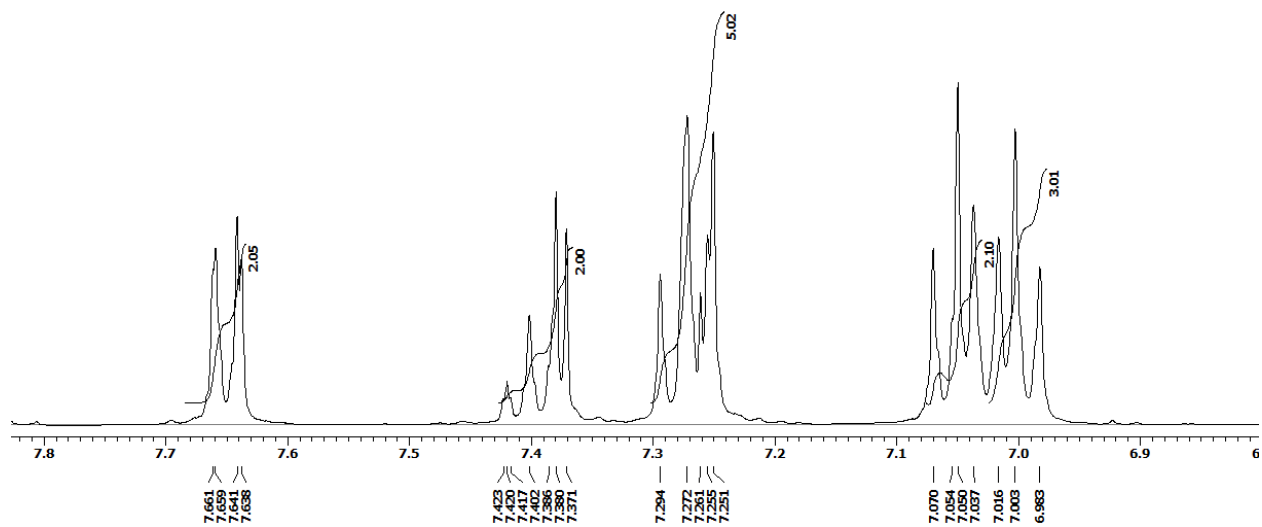
(4-(3-Methoxyphenyl)-5-tosyl-1*H*-pyrrol-3-yl)(phenyl)methanone (3g)



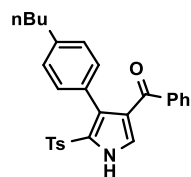
# <sup>1</sup>H NMR



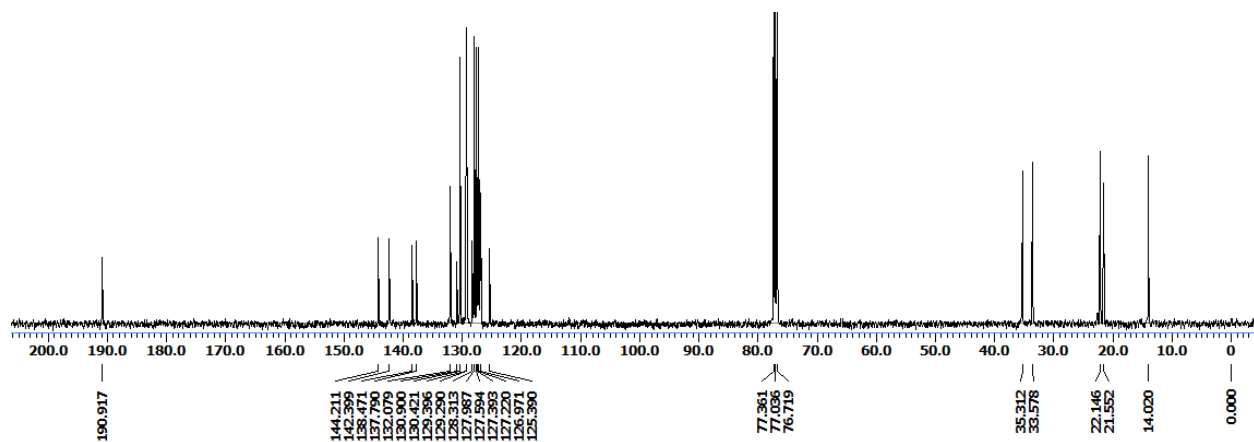
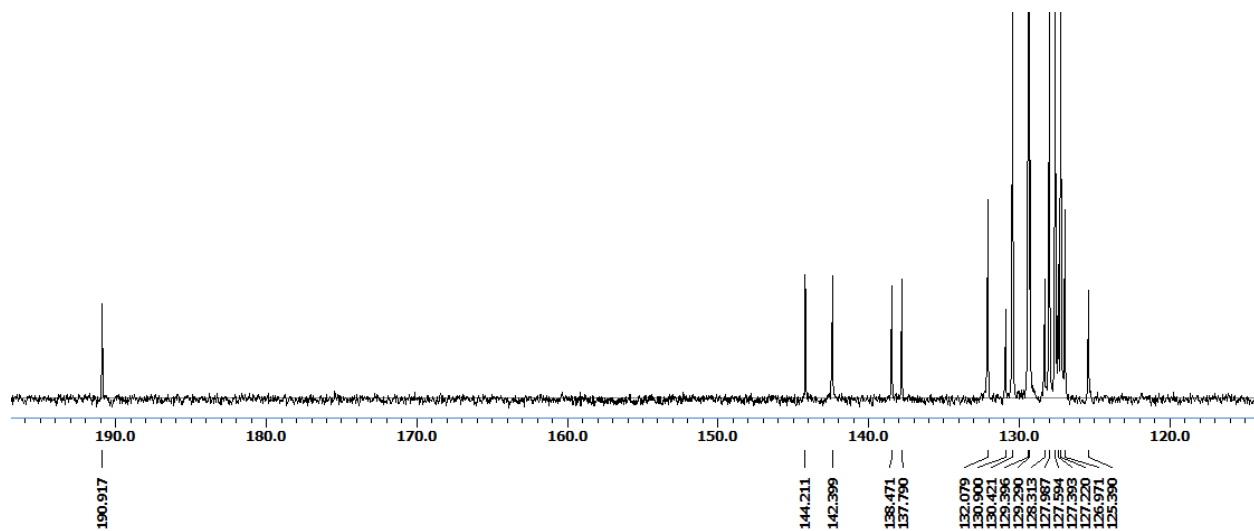
(4-(4-Butylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3h)



<sup>13</sup>C NMR

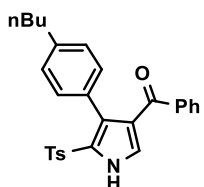


(4-(4-Butylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3h)

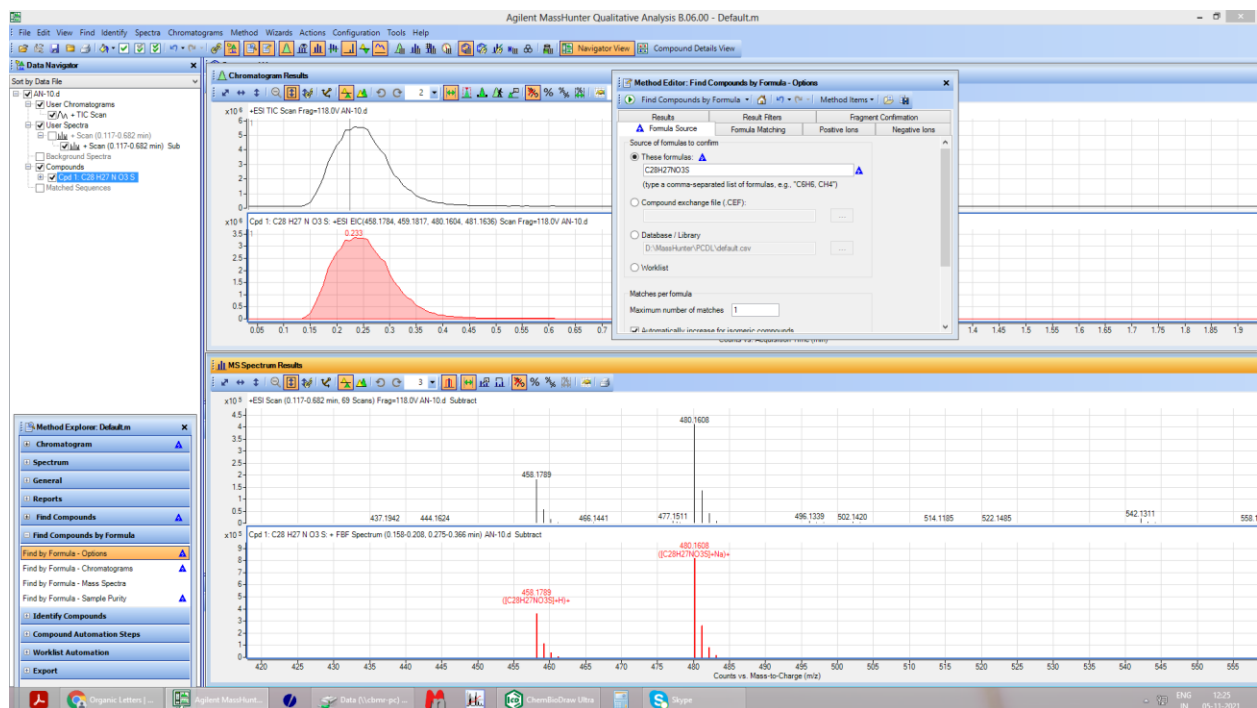




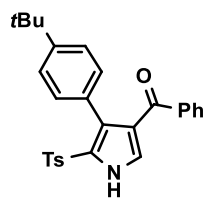
# HRMS



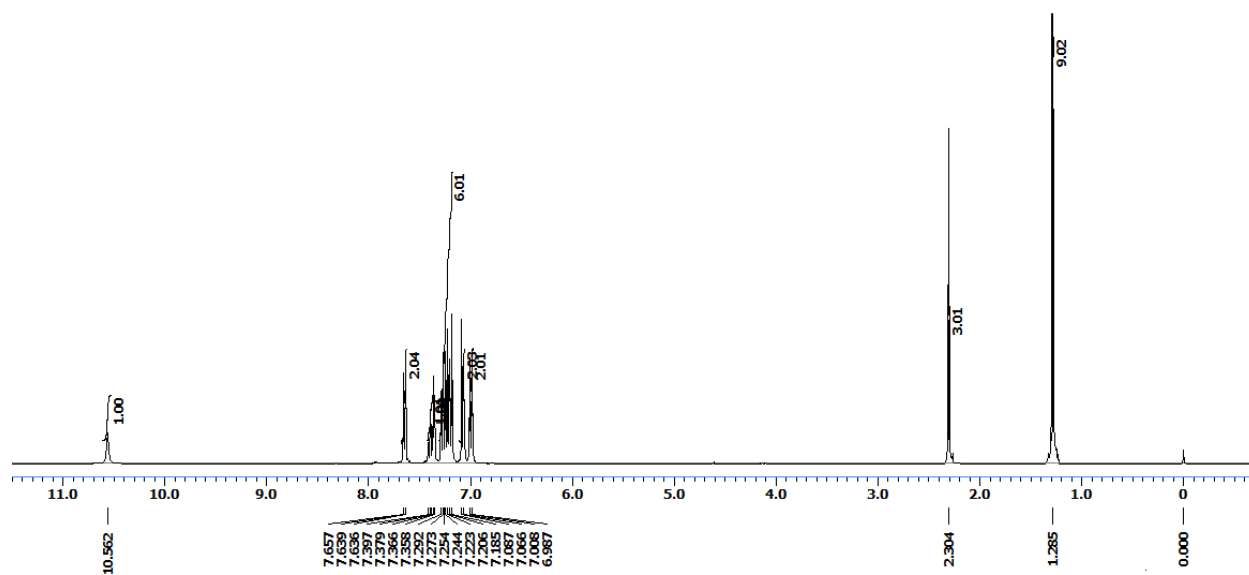
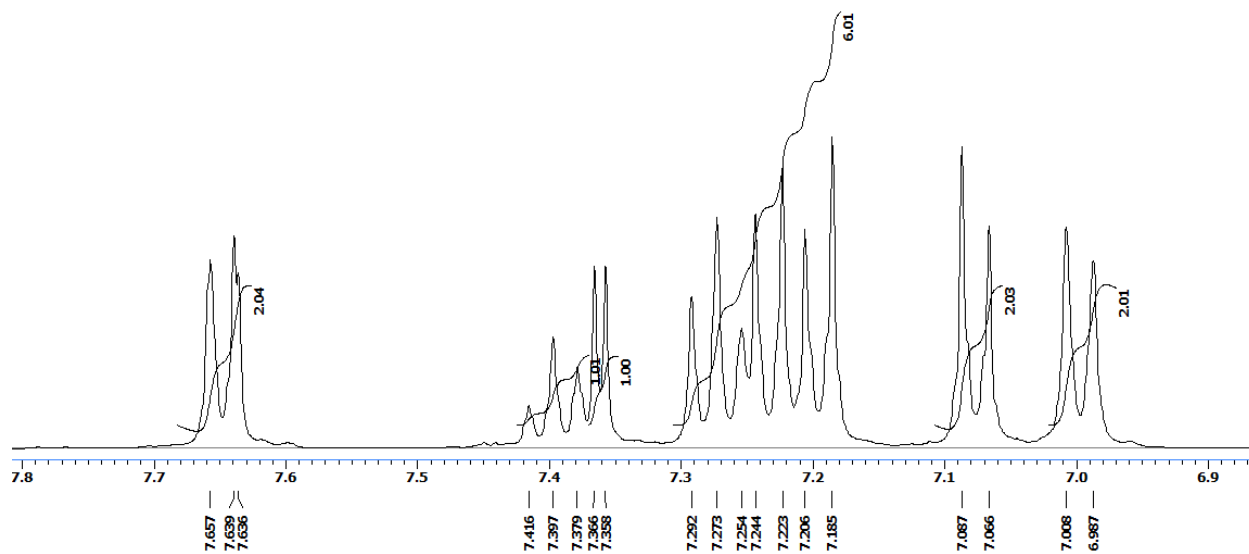
**(4-(4-Butylphenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3h)**



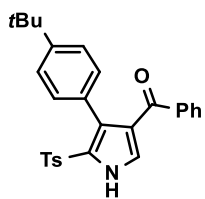
<sup>1</sup>H NMR



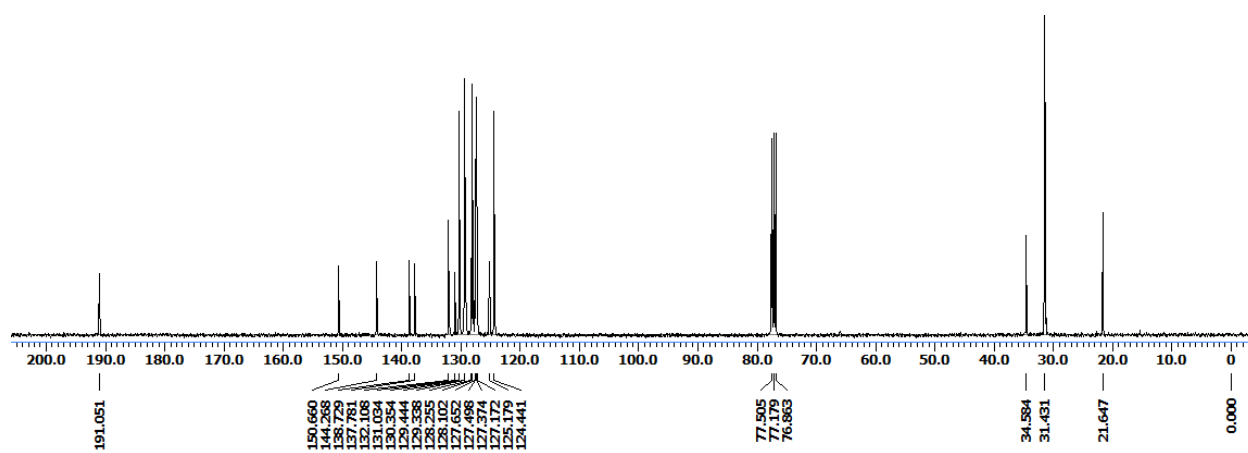
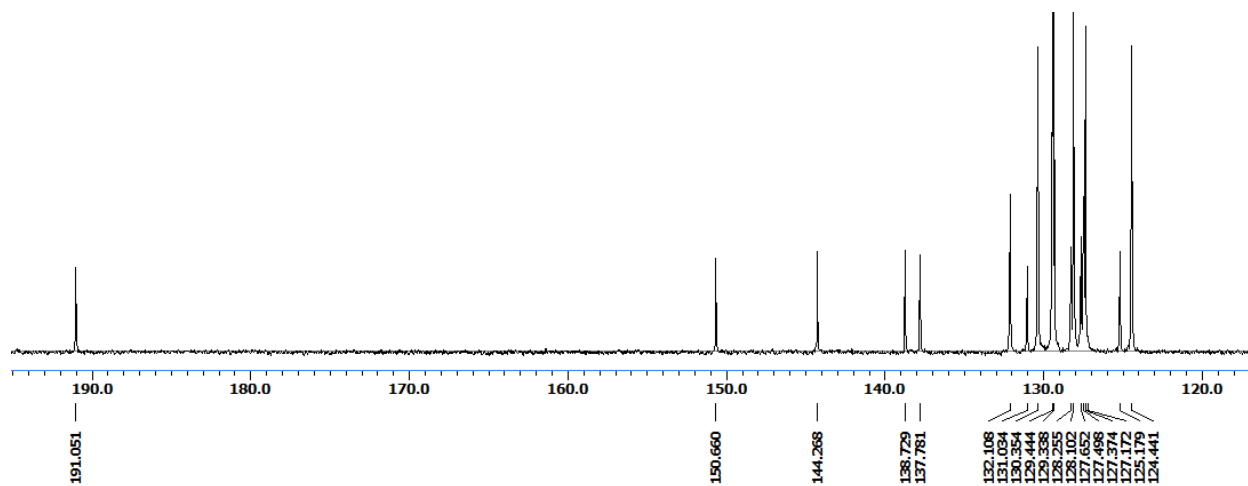
(4-(4-(tert-butyl)phenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3i)



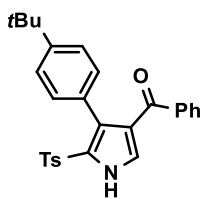
<sup>13</sup>C NMR



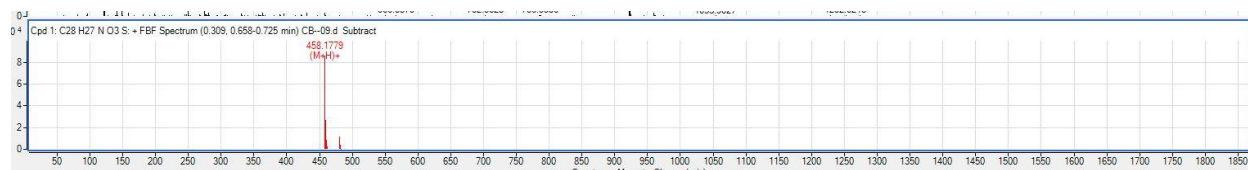
(4-(4-(tert-butyl)phenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3i)



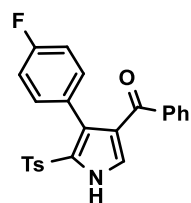
## HRMS



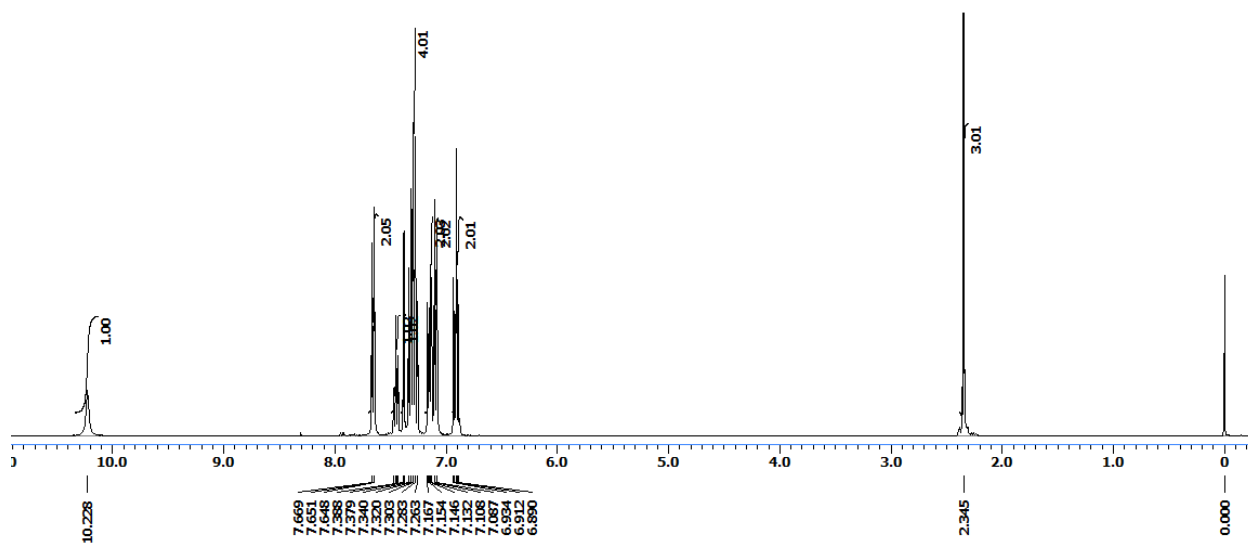
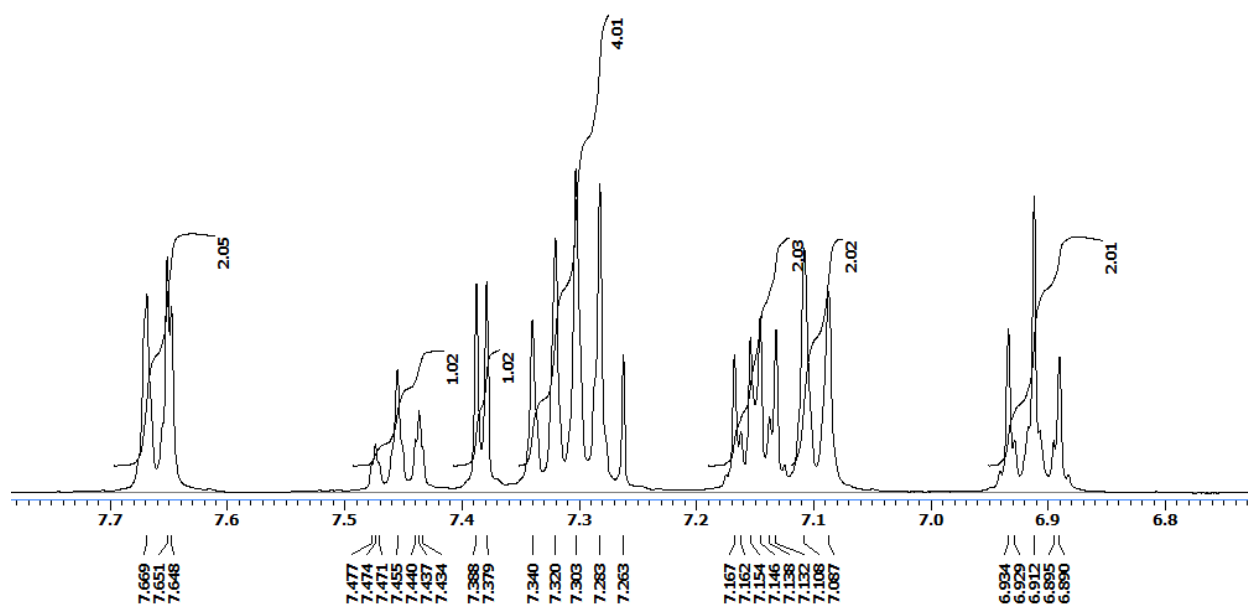
**(4-(4-(tert-butyl)phenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3i)**



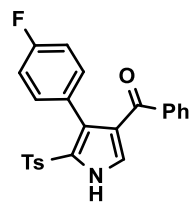
# <sup>1</sup>H NMR



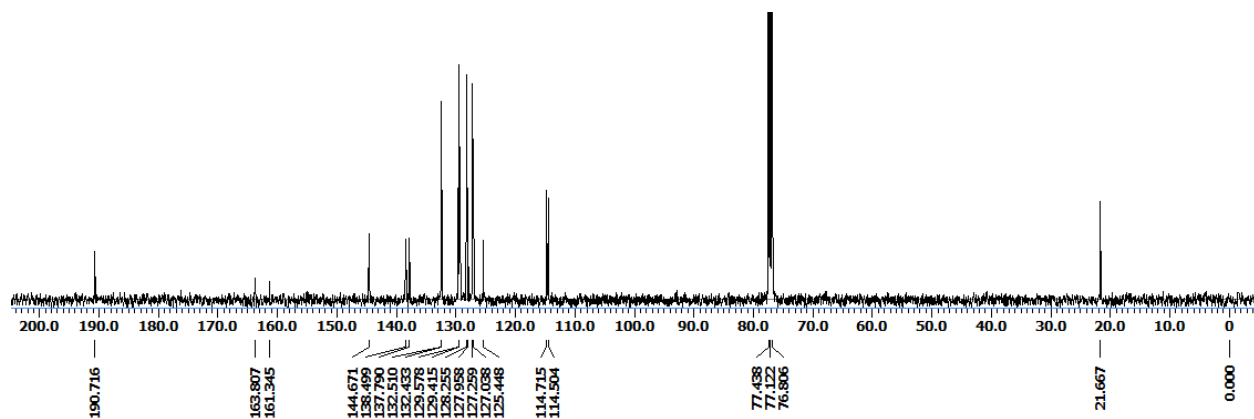
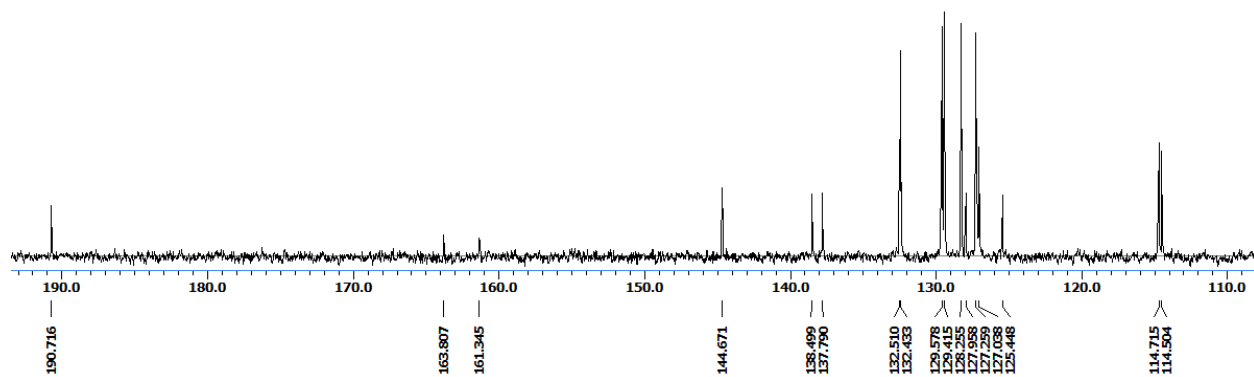
(4-(4-Fluorophenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3j)



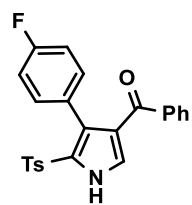
<sup>13</sup>C NMR



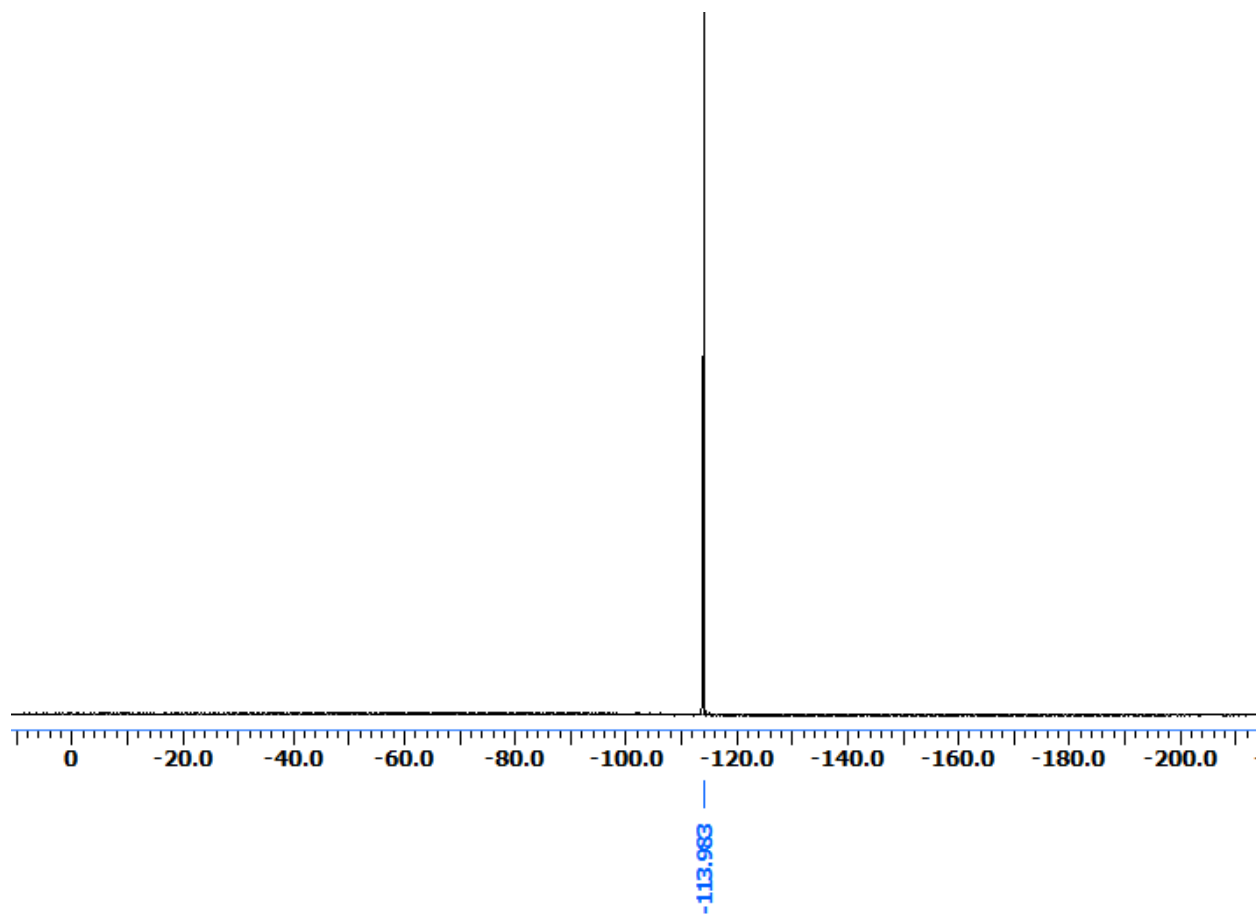
(4-(4-Fluorophenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3j)



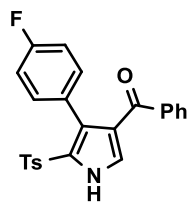
**<sup>19</sup>F NMR**



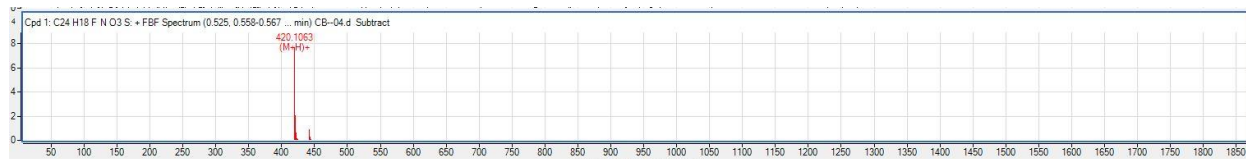
**(4-(4-Fluorophenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3j)**



# HRMS

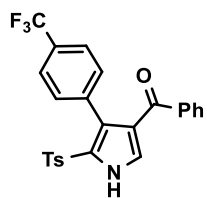


**(4-(4-Fluorophenyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3j)**

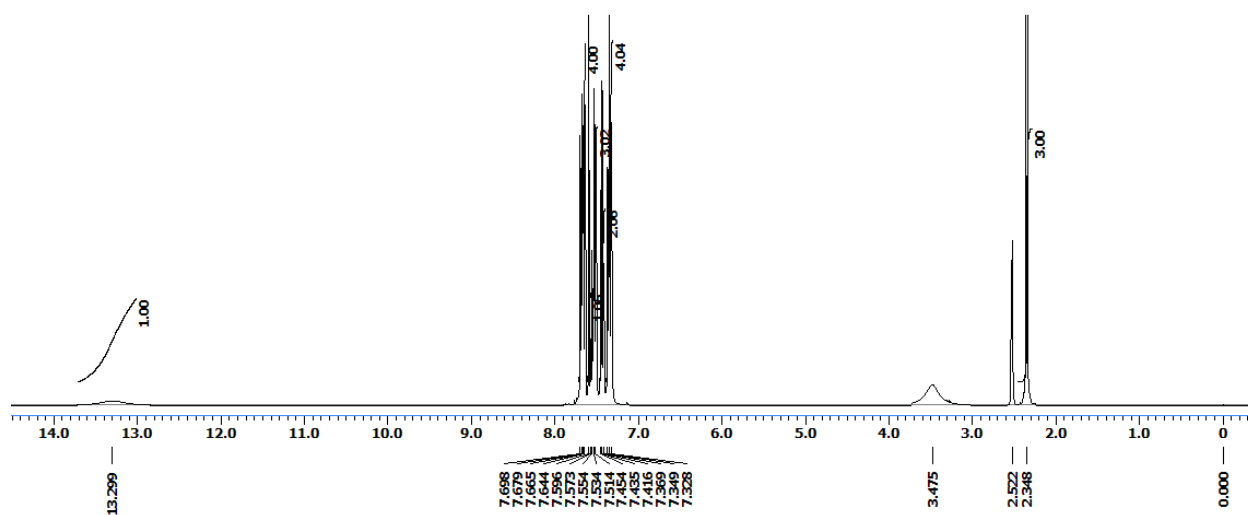
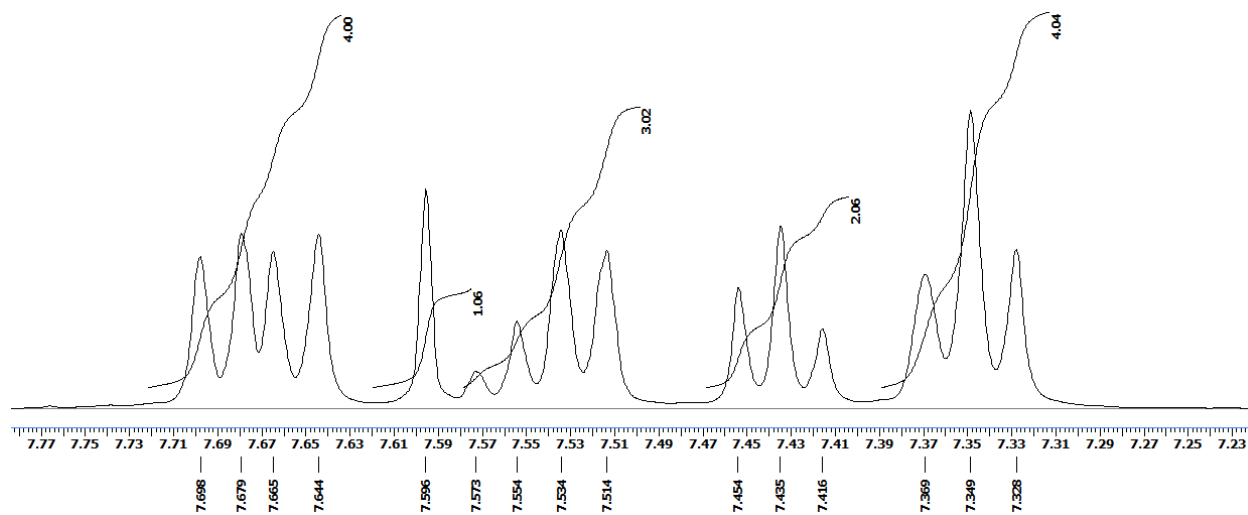




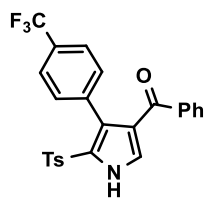
# <sup>1</sup>H NMR



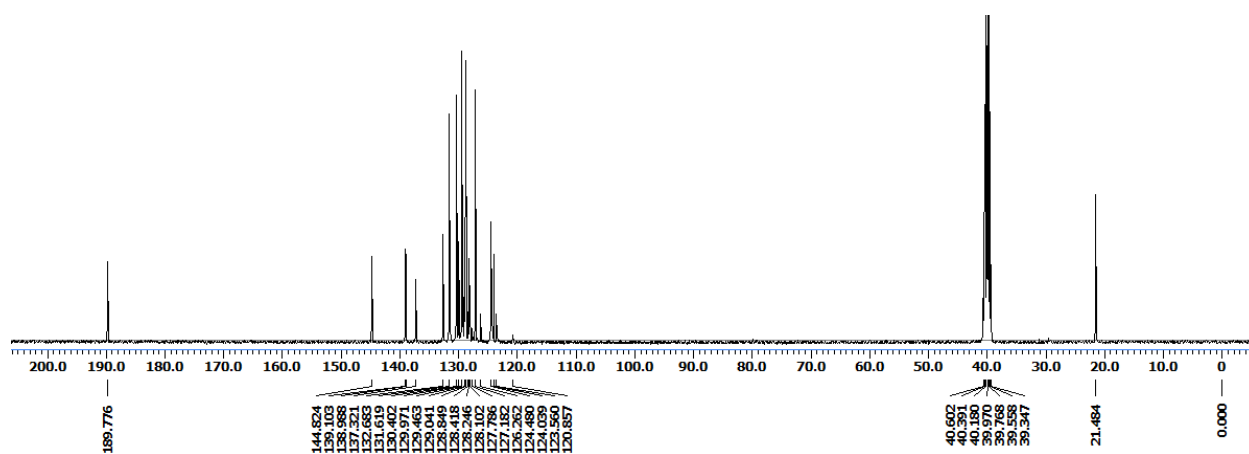
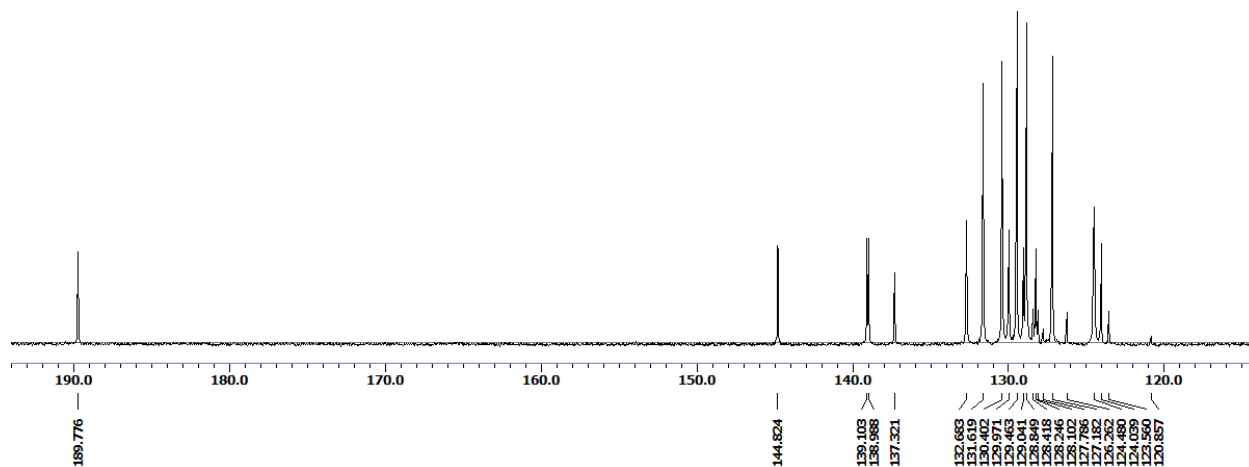
Phenyl(5-tosyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrol-3-yl)methanone (3k)



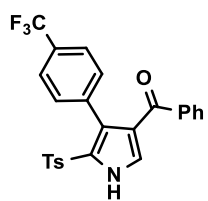
<sup>13</sup>C NMR



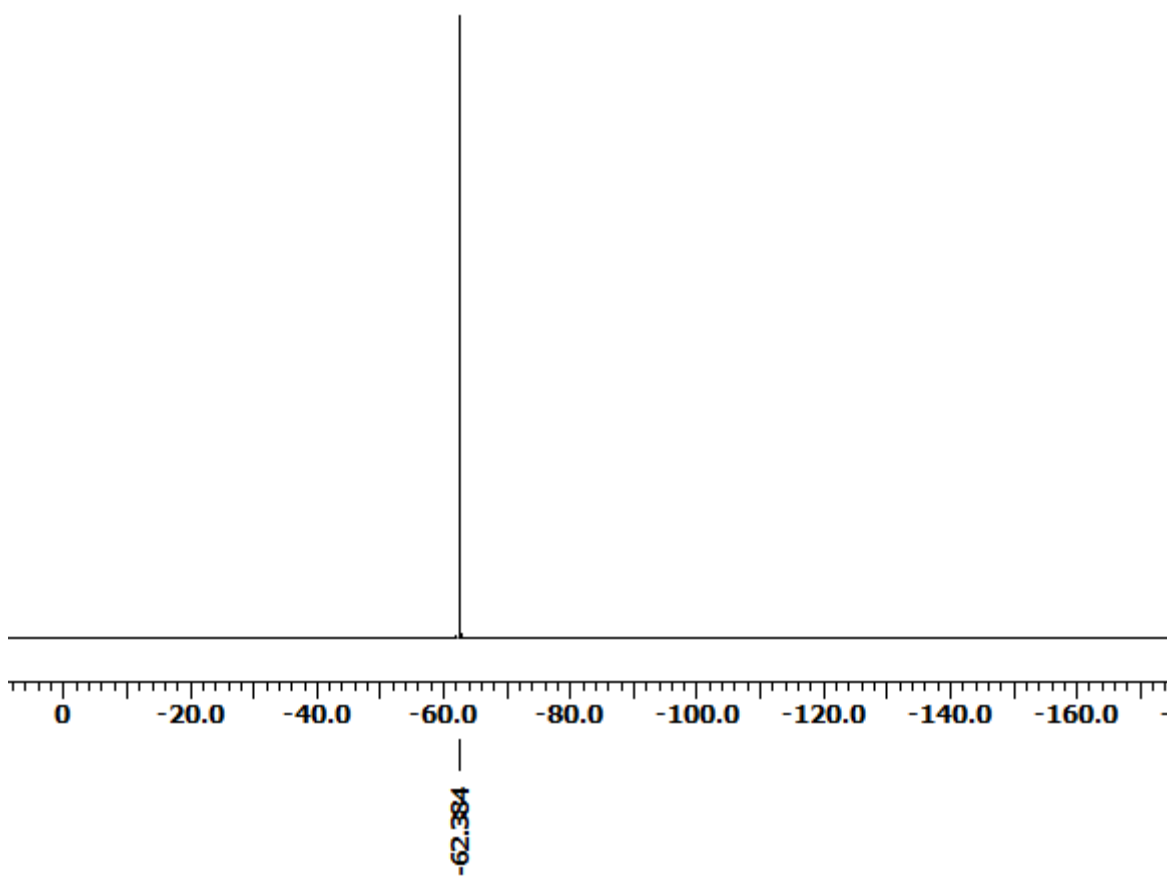
Phenyl(5-tosyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrol-3-yl)methanone (3k)



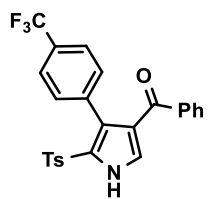
**<sup>19</sup>F NMR**



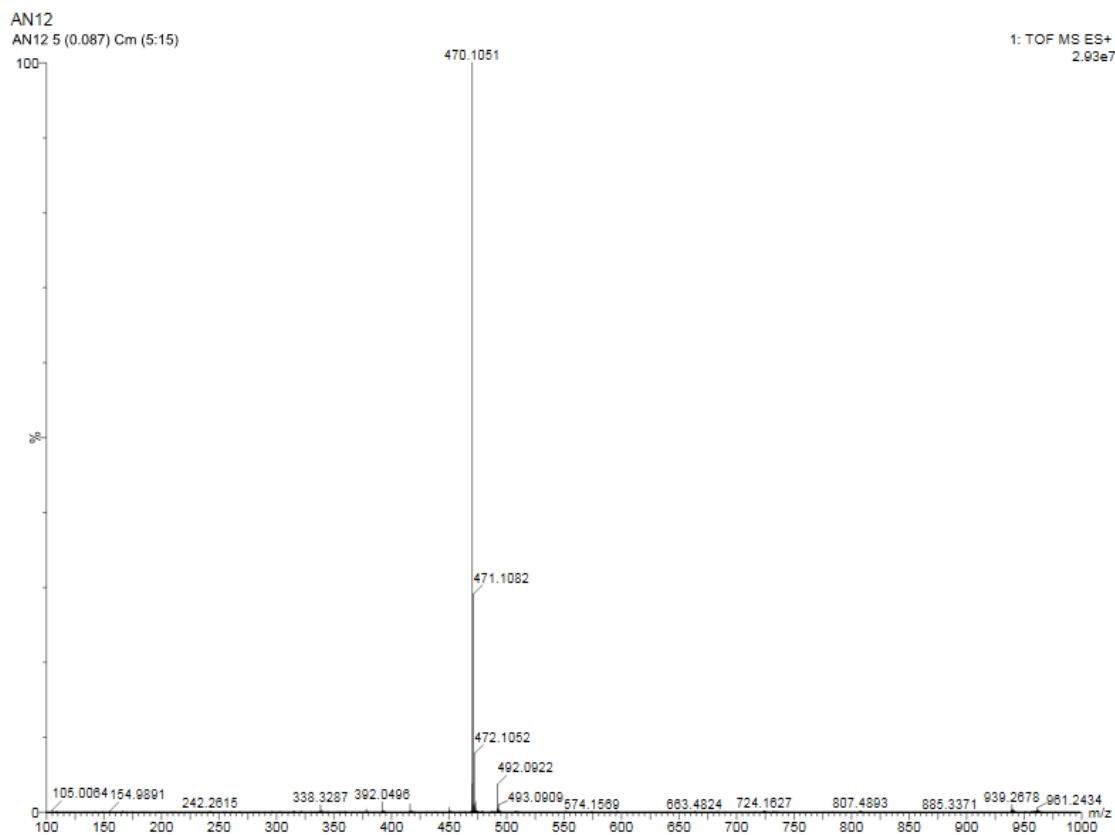
**Phenyl(5-tosyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrol-3-yl)methanone (3k)**



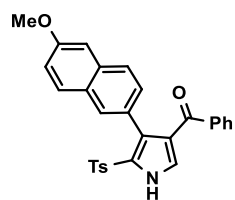
# HRMS



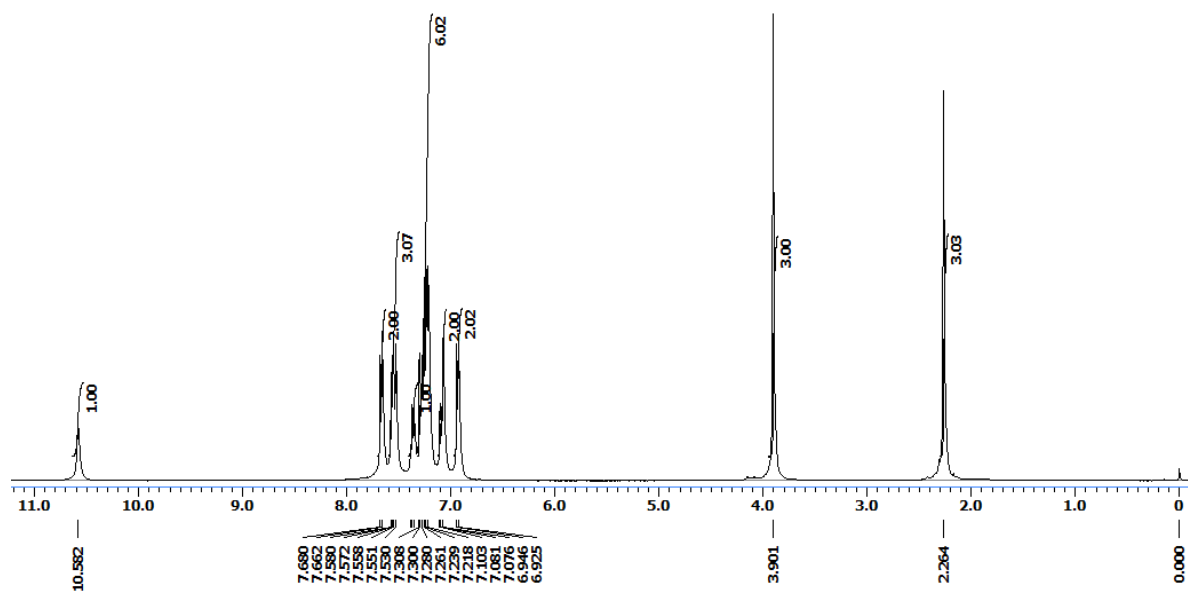
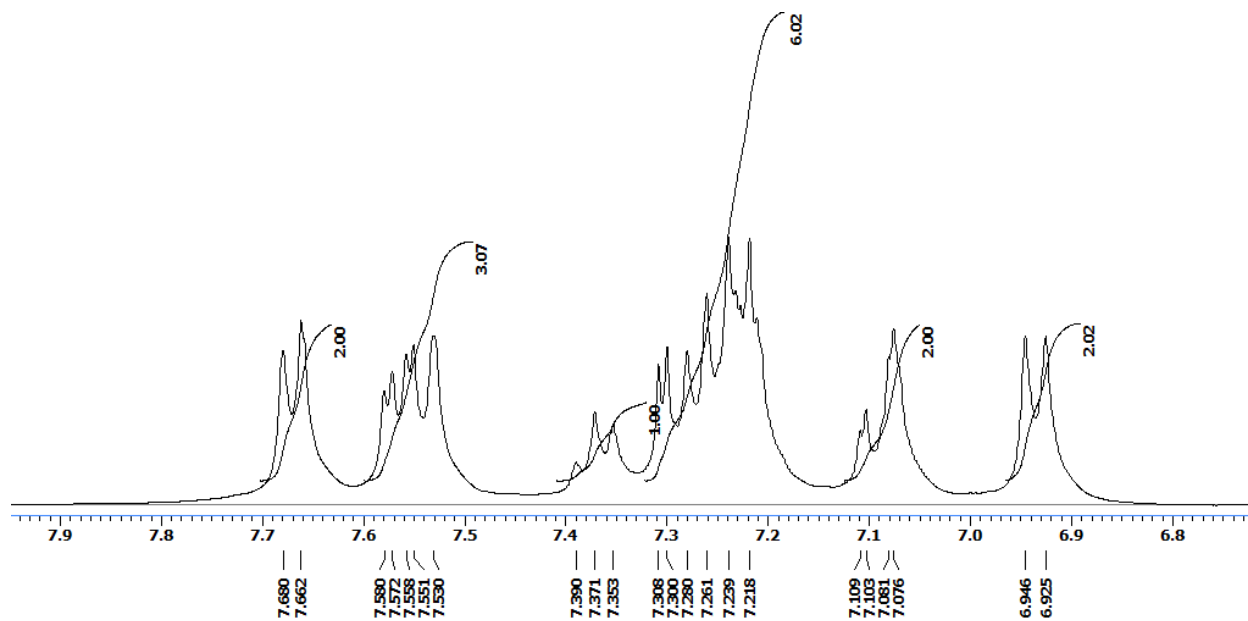
**Phenyl(5-tosyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrrol-3-yl)methanone (3k)**



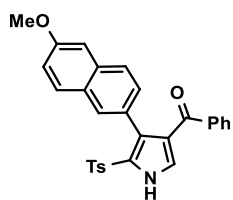
# <sup>1</sup>H NMR



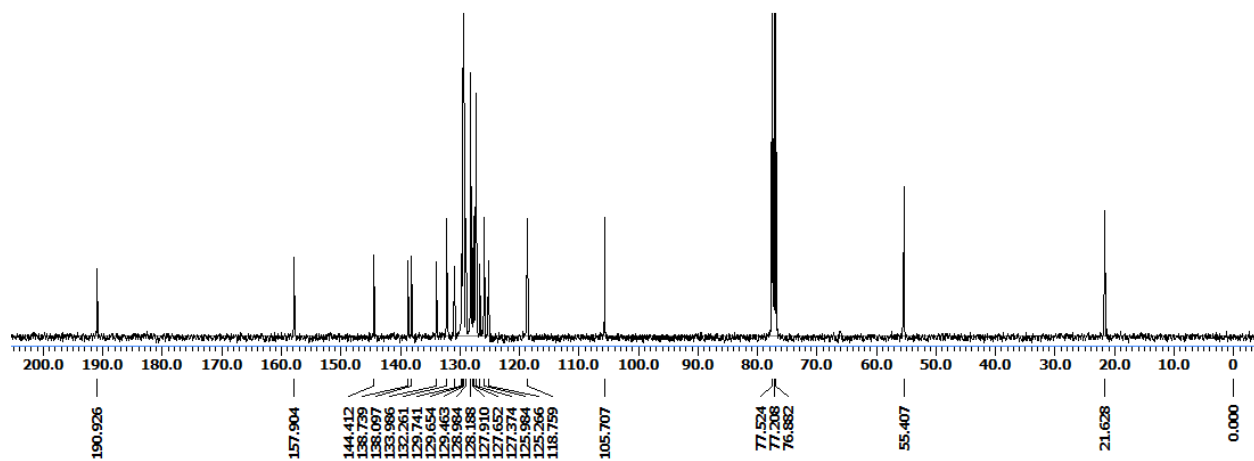
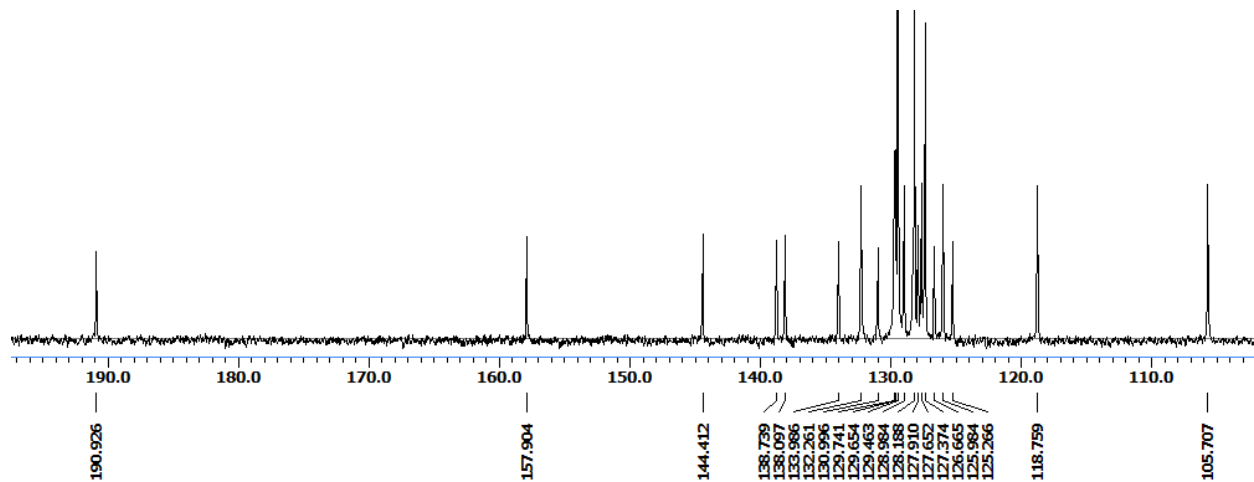
(4-(6-Methoxynaphthalen-2-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (31)



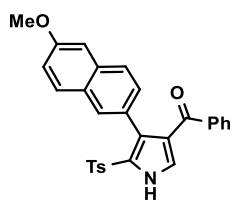
<sup>13</sup>C NMR



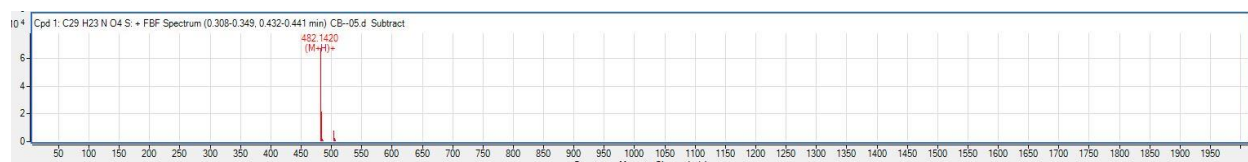
(4-(6-Methoxynaphthalen-2-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (31)



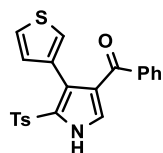
## HRMS



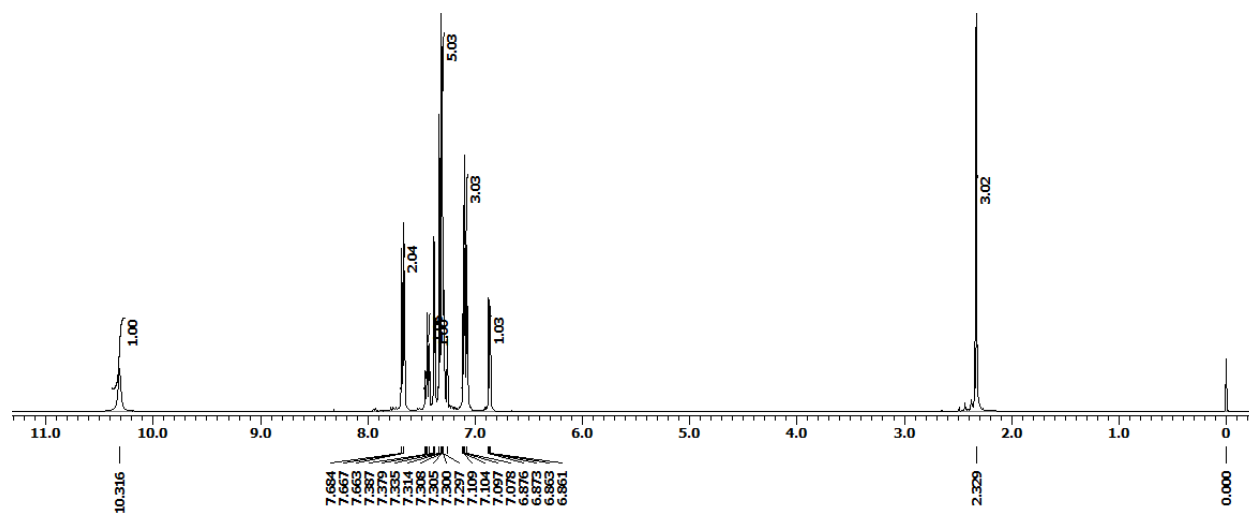
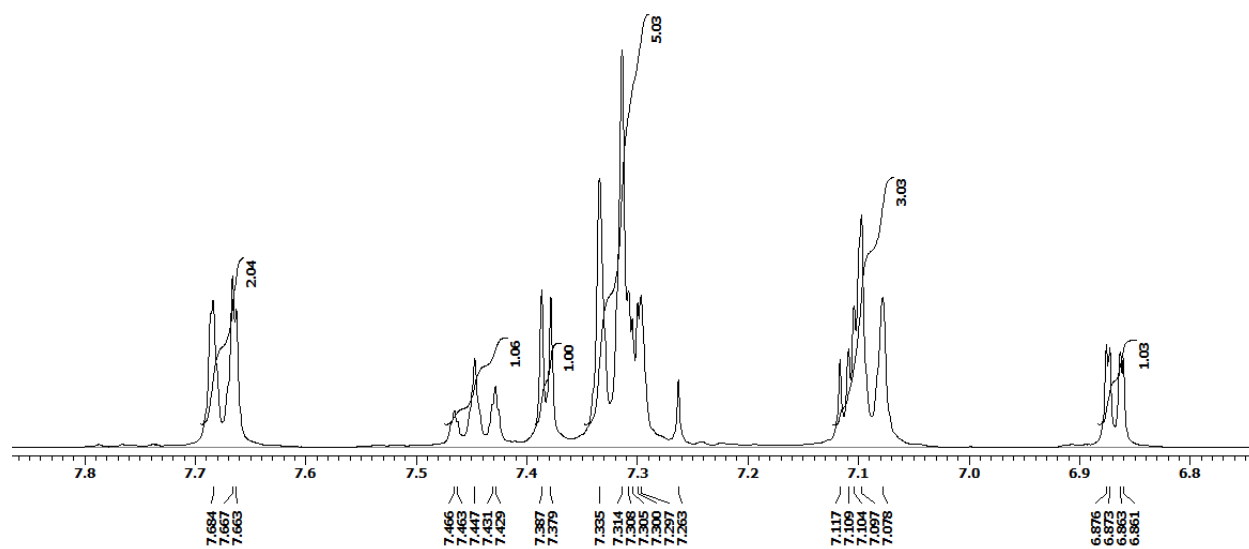
**(4-(6-Methoxynaphthalen-2-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (31)**



# <sup>1</sup>H NMR

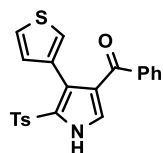


Phenyl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3m)

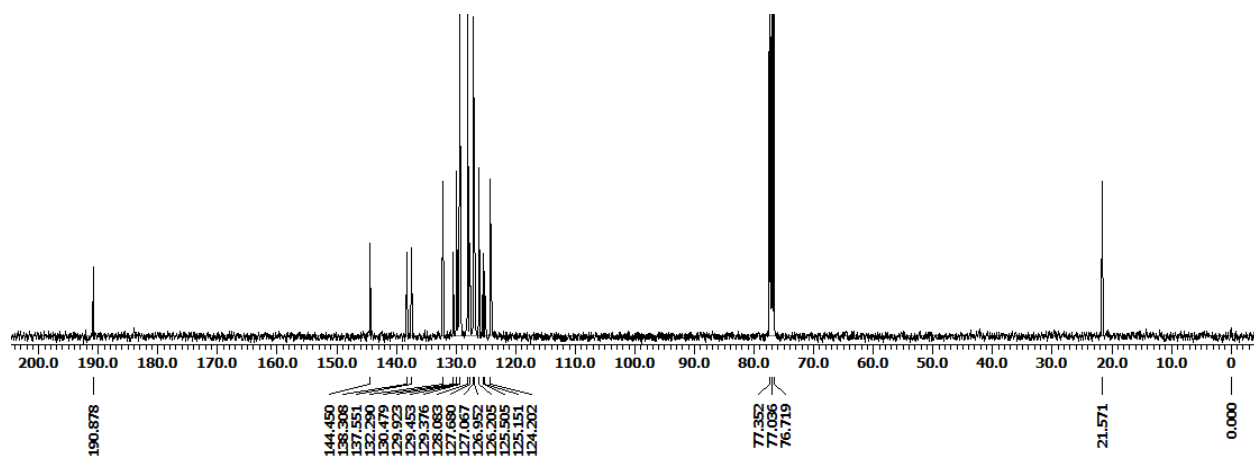
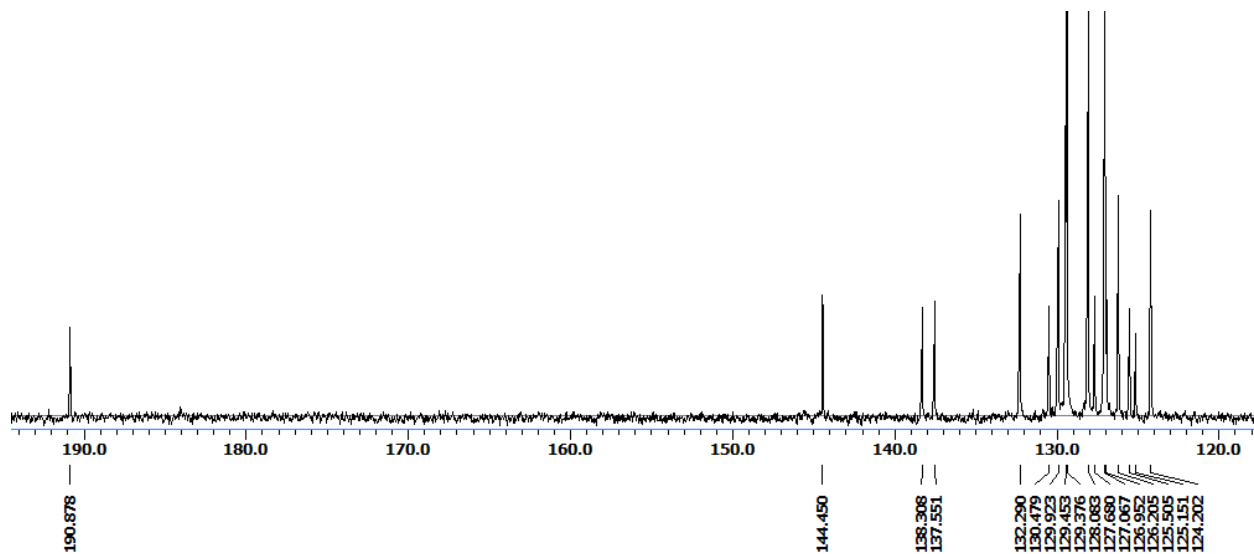




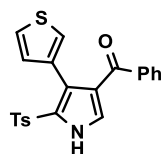
<sup>13</sup>C NMR



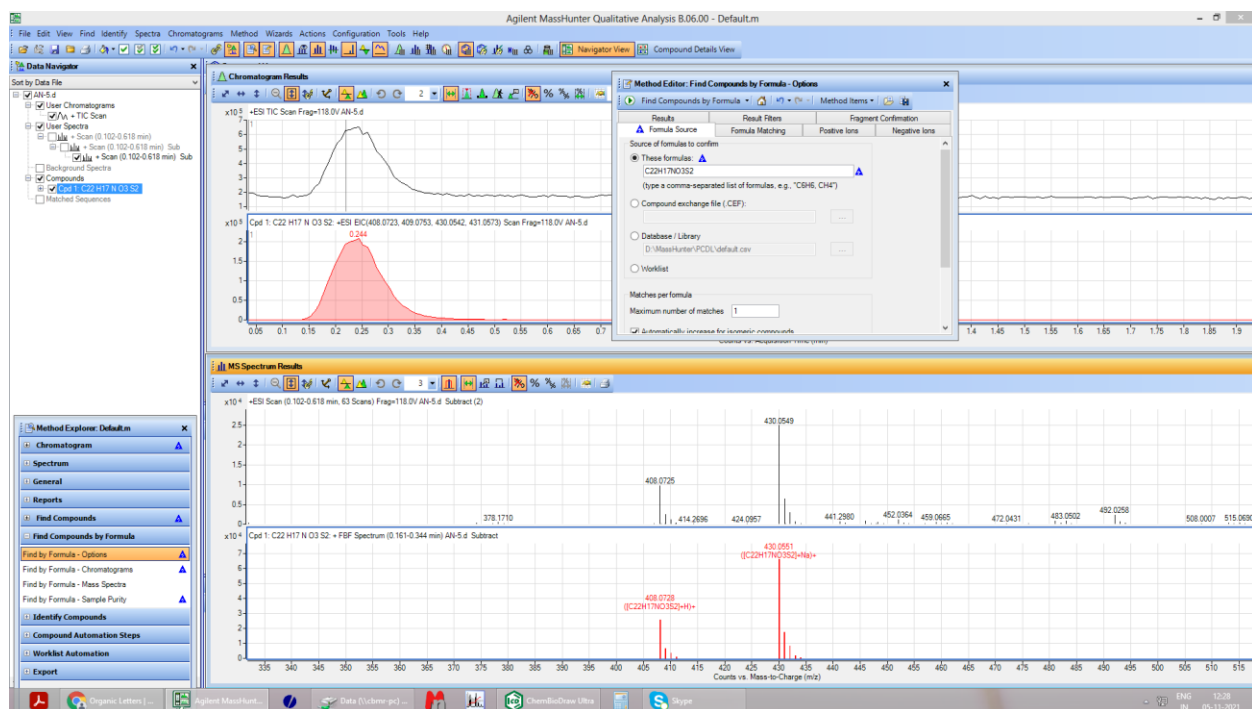
Phenyl(4-(thiophen-3-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (3m)



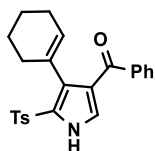
# HRMS



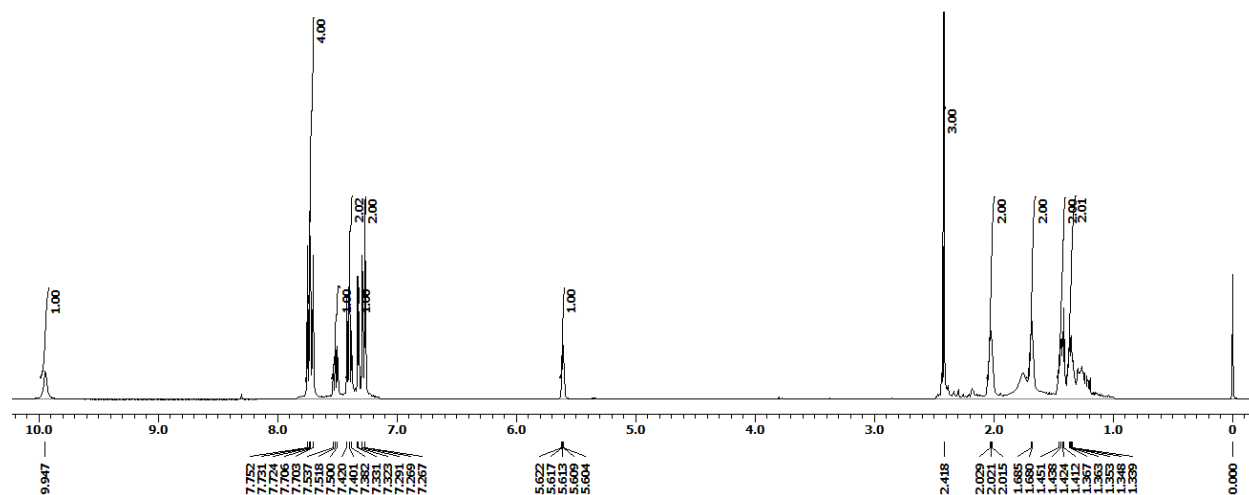
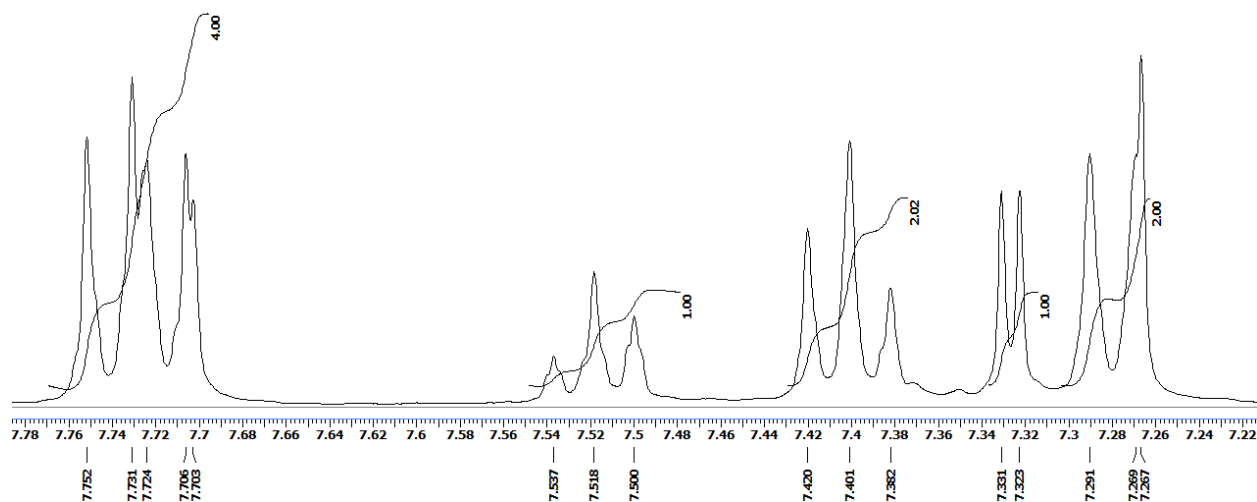
## Phenyl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3m)



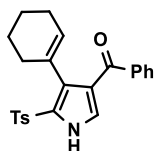
# <sup>1</sup>H NMR



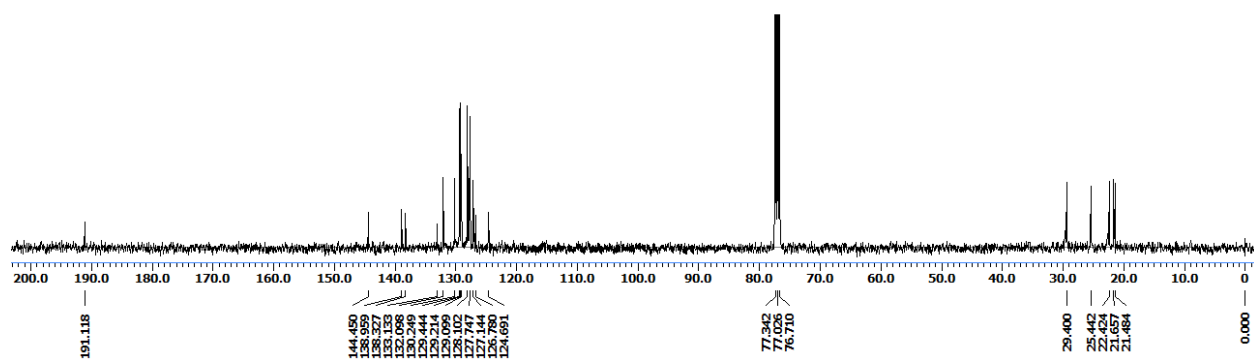
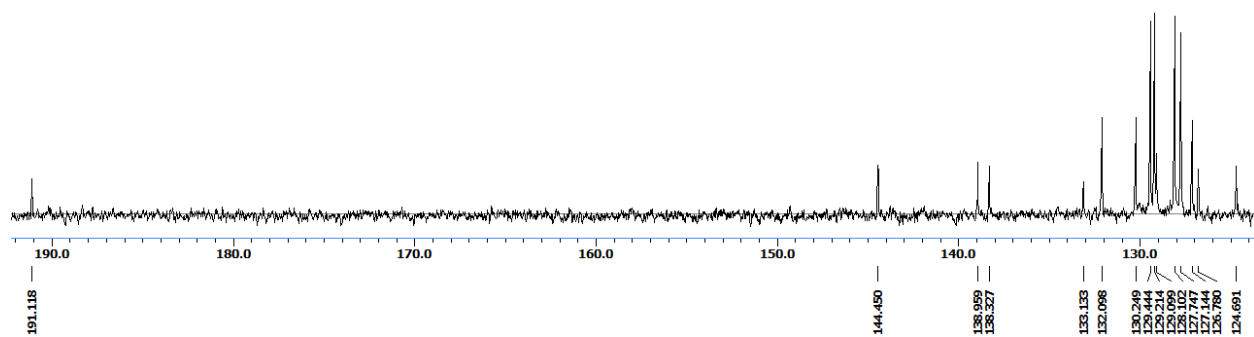
(4-(Cyclohex-1-en-1-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3n)



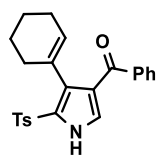
<sup>13</sup>C NMR



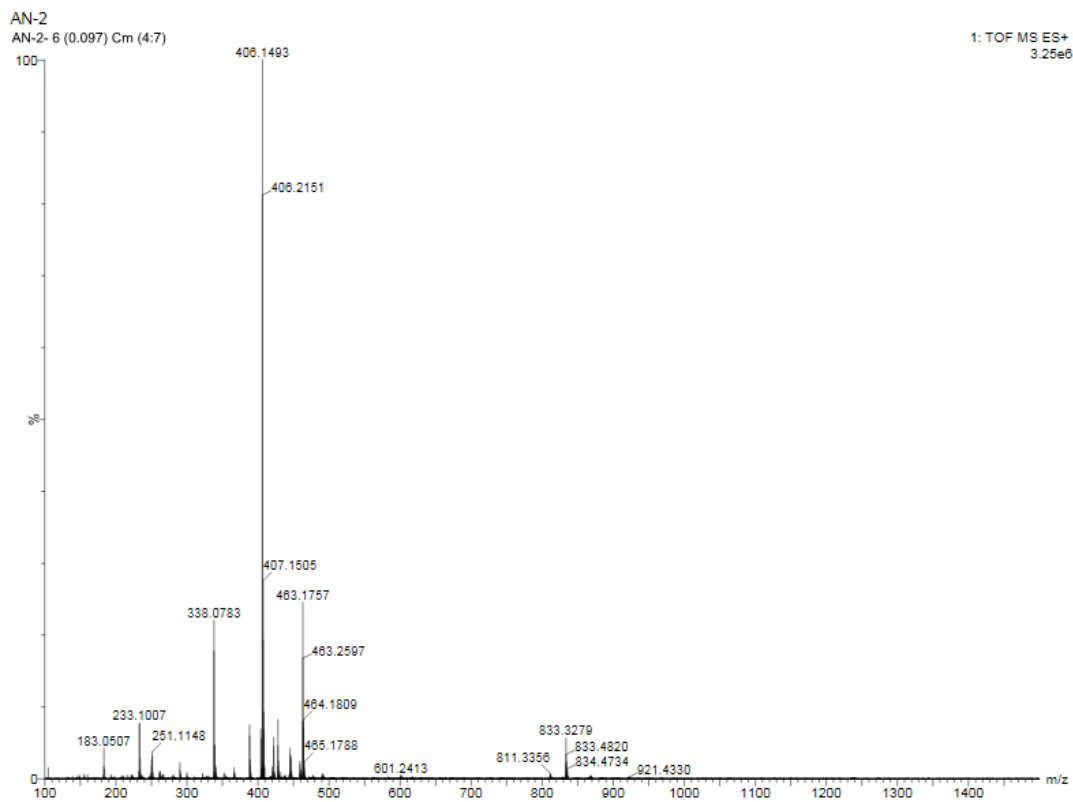
(4-(Cyclohex-1-en-1-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3n)



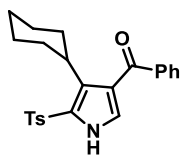
# HRMS



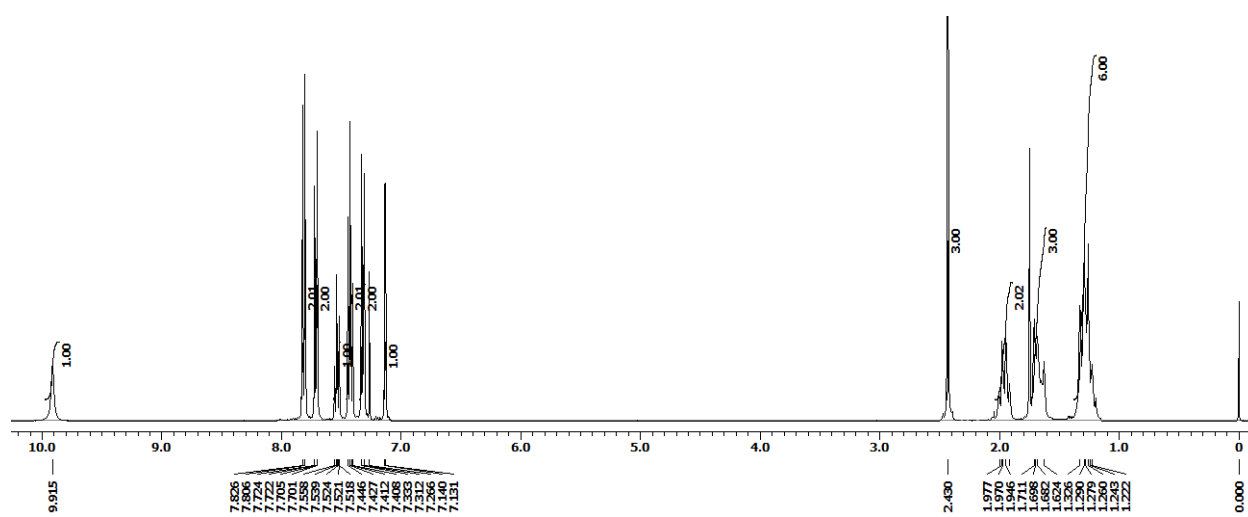
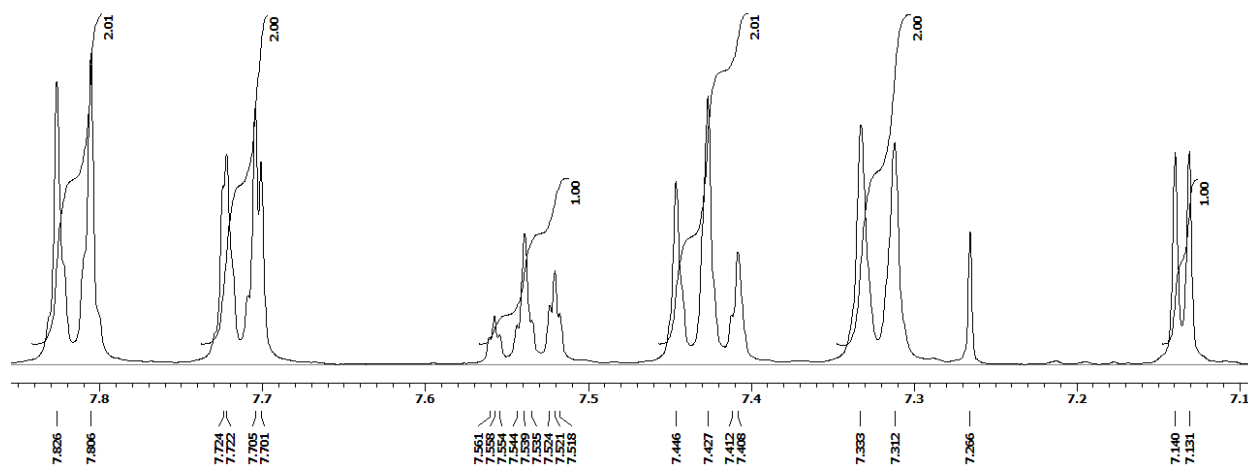
(4-(Cyclohex-1-en-1-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3n)



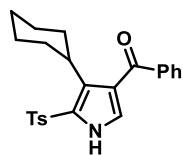
# $^1\text{H}$ NMR



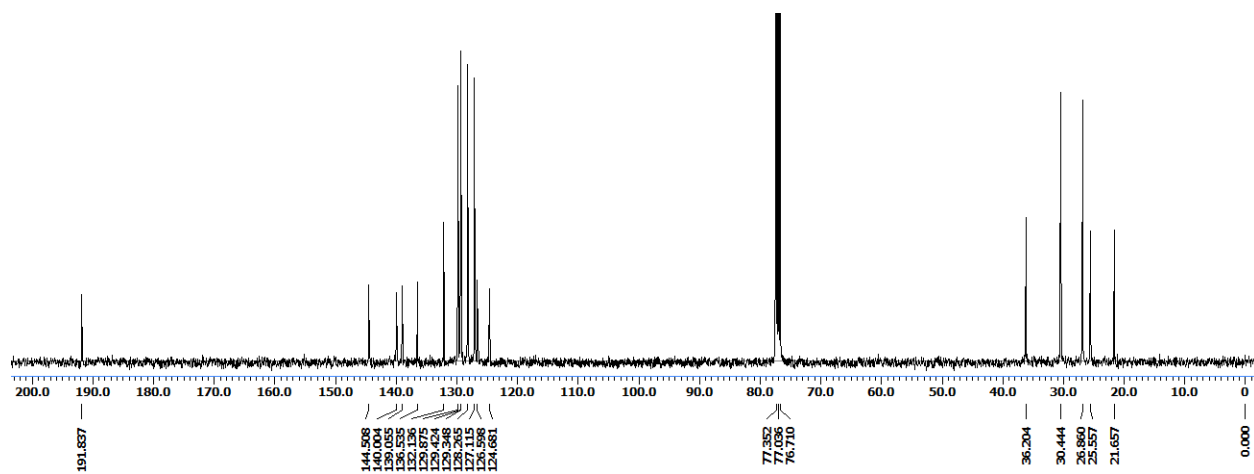
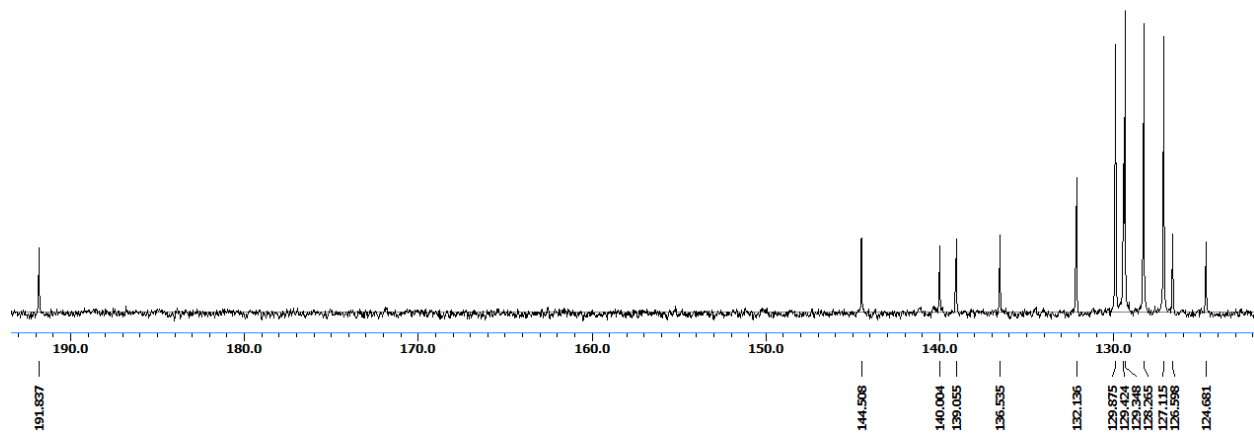
(4-Cyclohexyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3o)



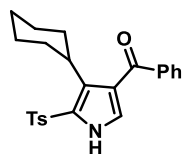
<sup>13</sup>C NMR



(4-Cyclohexyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3o)



# HRMS

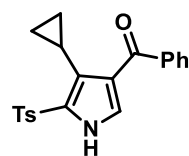


**(4-Cyclohexyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3o)**

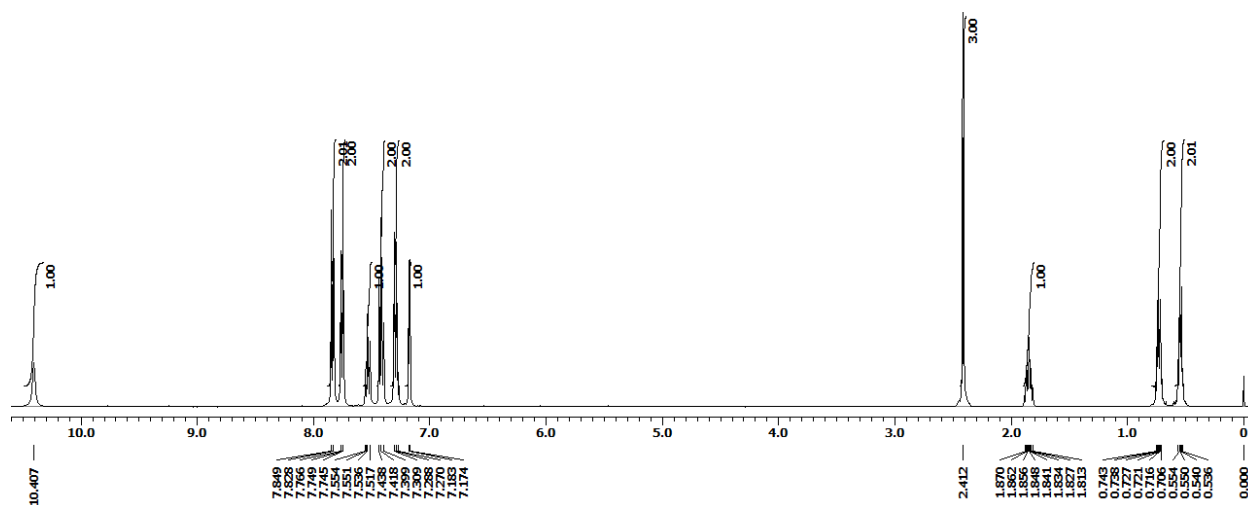
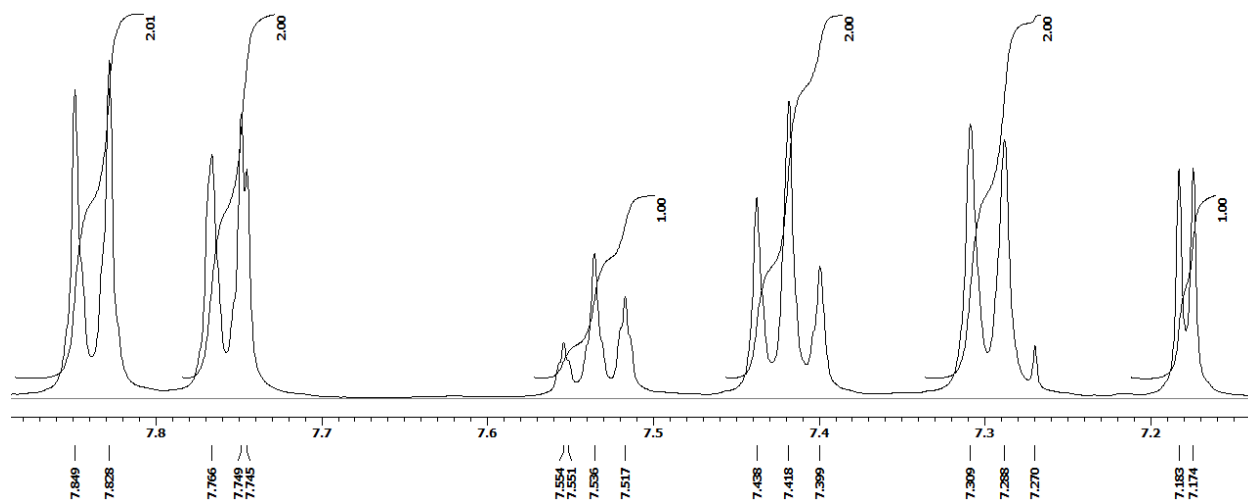




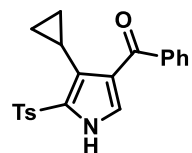
<sup>1</sup>H NMR



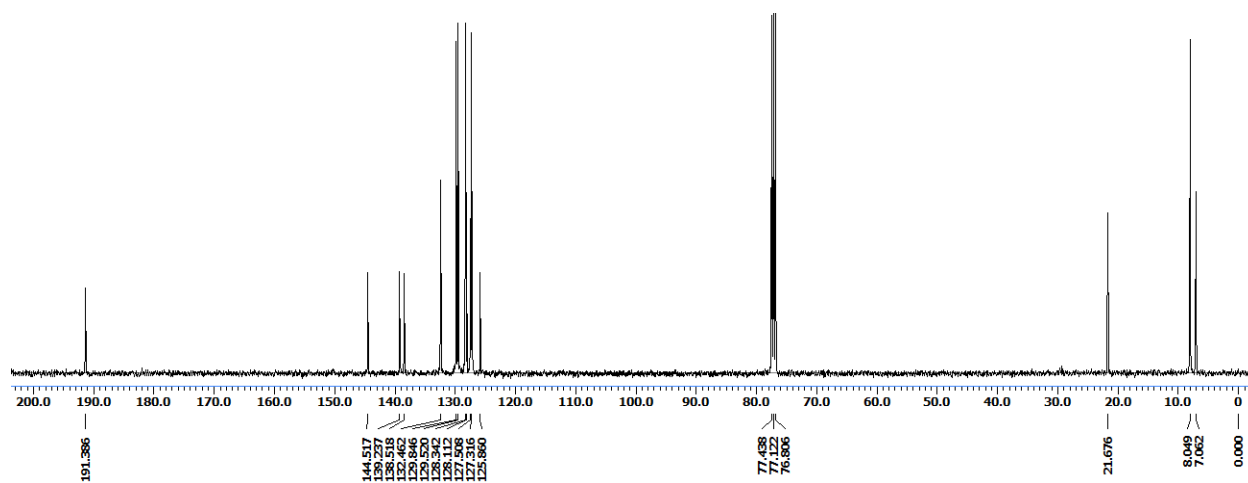
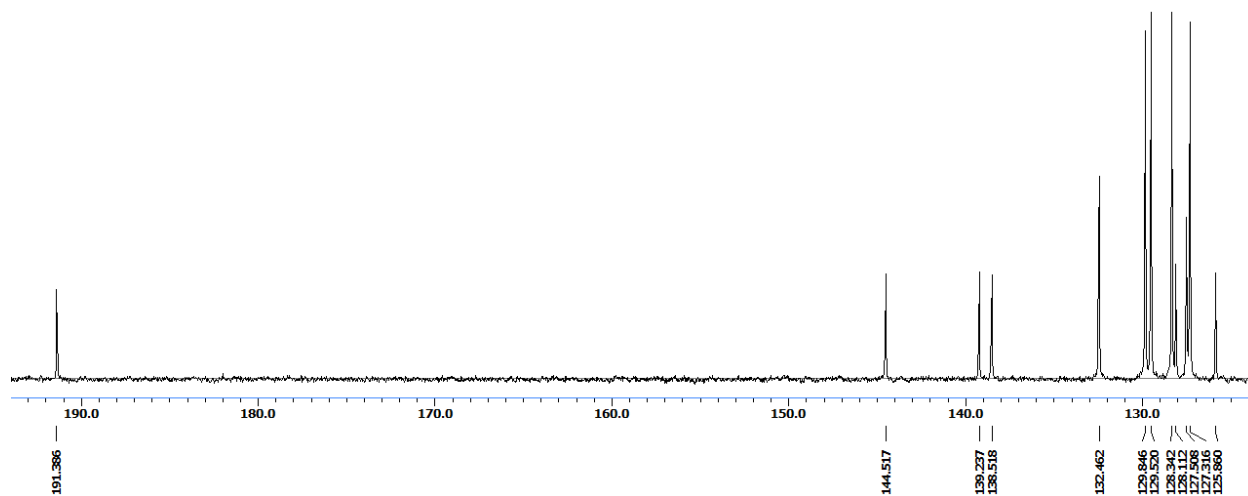
(4-Cyclopropyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3p)



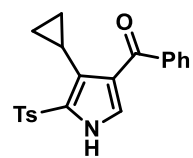
<sup>13</sup>C NMR



(4-Cyclopropyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3p)



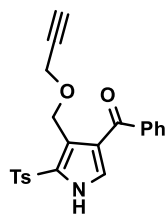
## HRMS



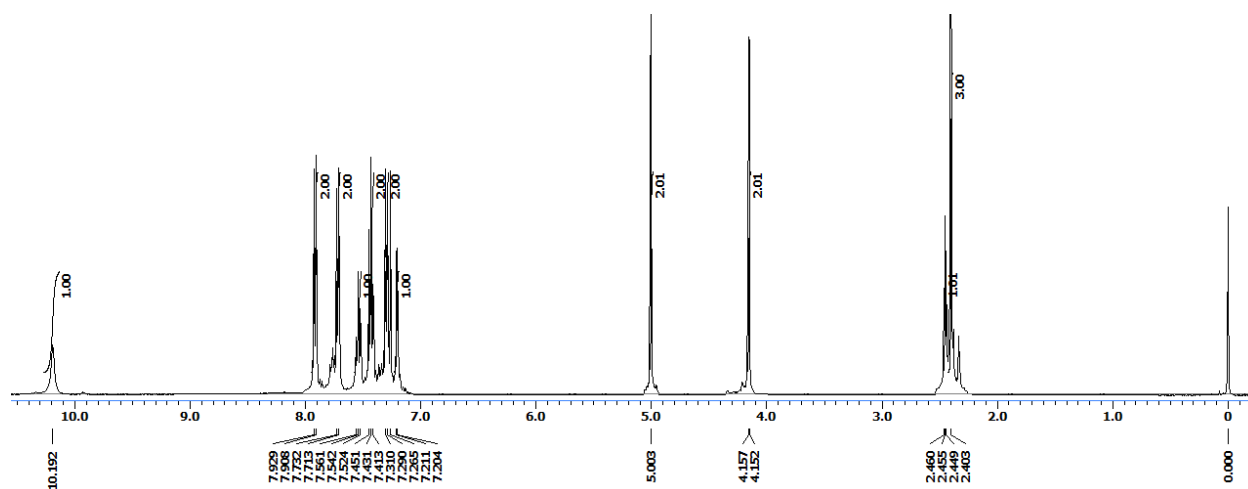
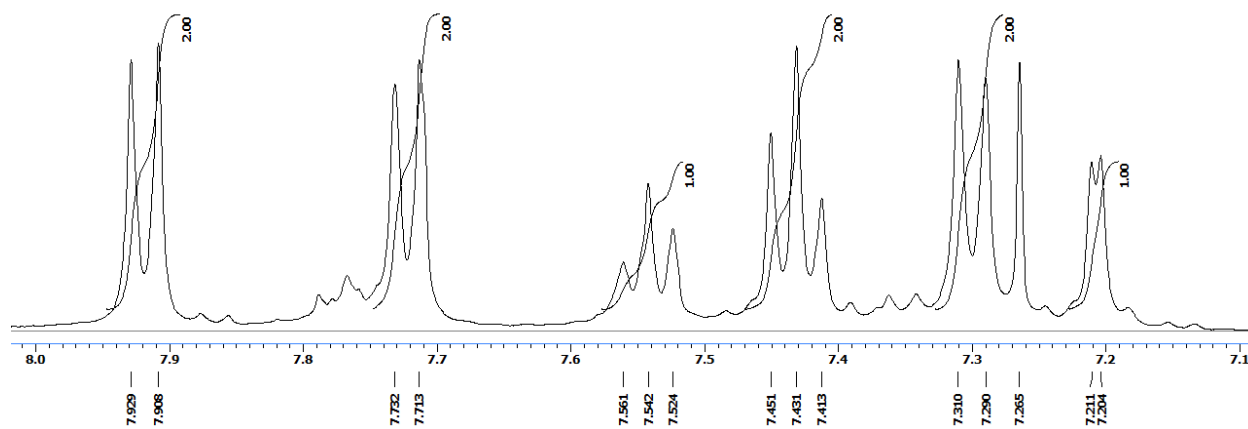
**(4-Cyclopropyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3p)**



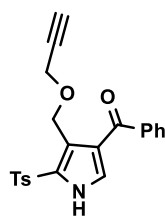
# <sup>1</sup>H NMR



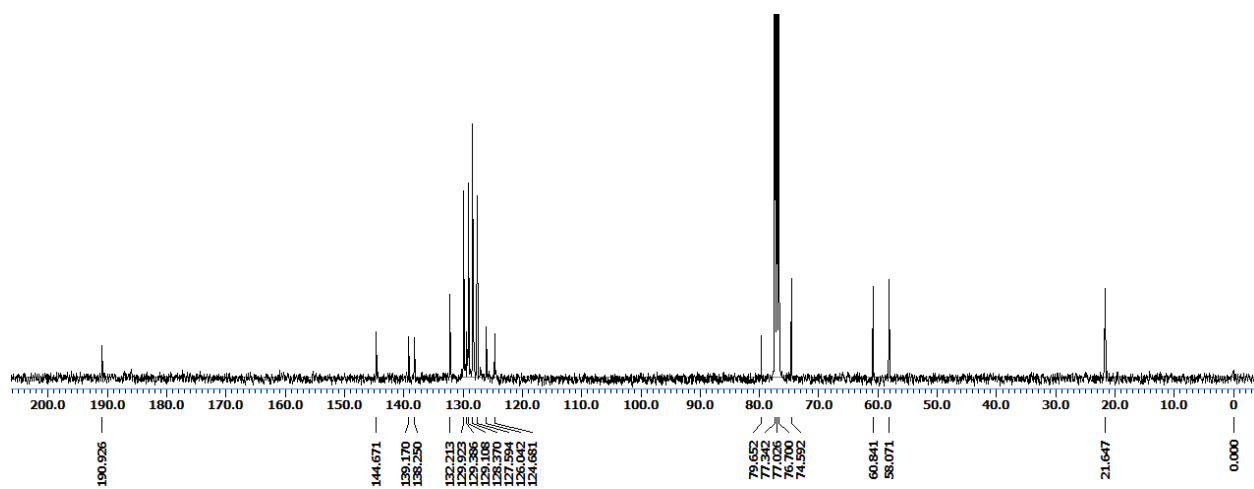
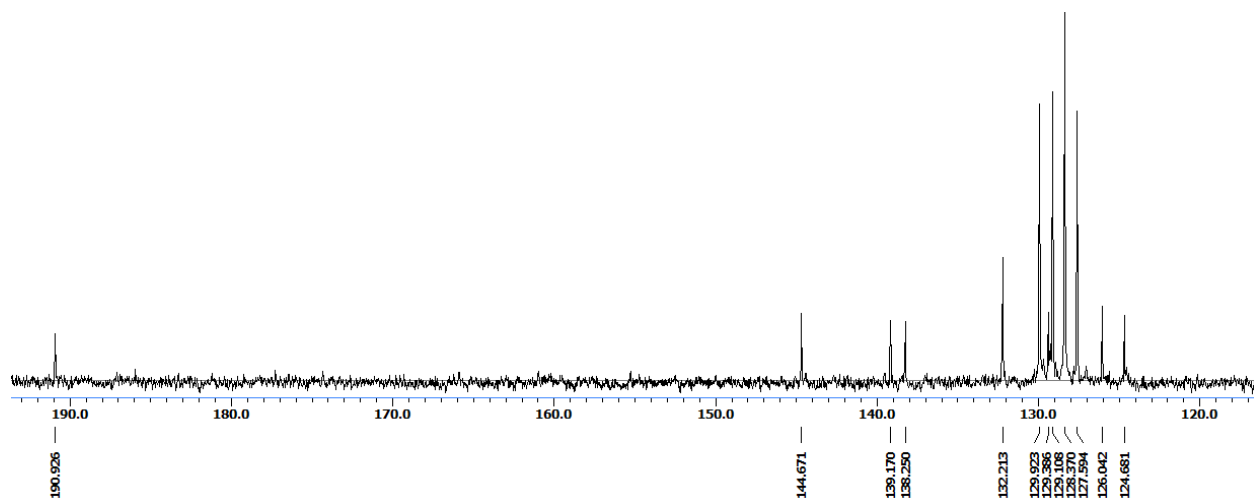
Phenyl (4-((prop-2-yn-1-yloxy)methyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3q)



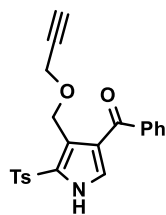
<sup>13</sup>C NMR



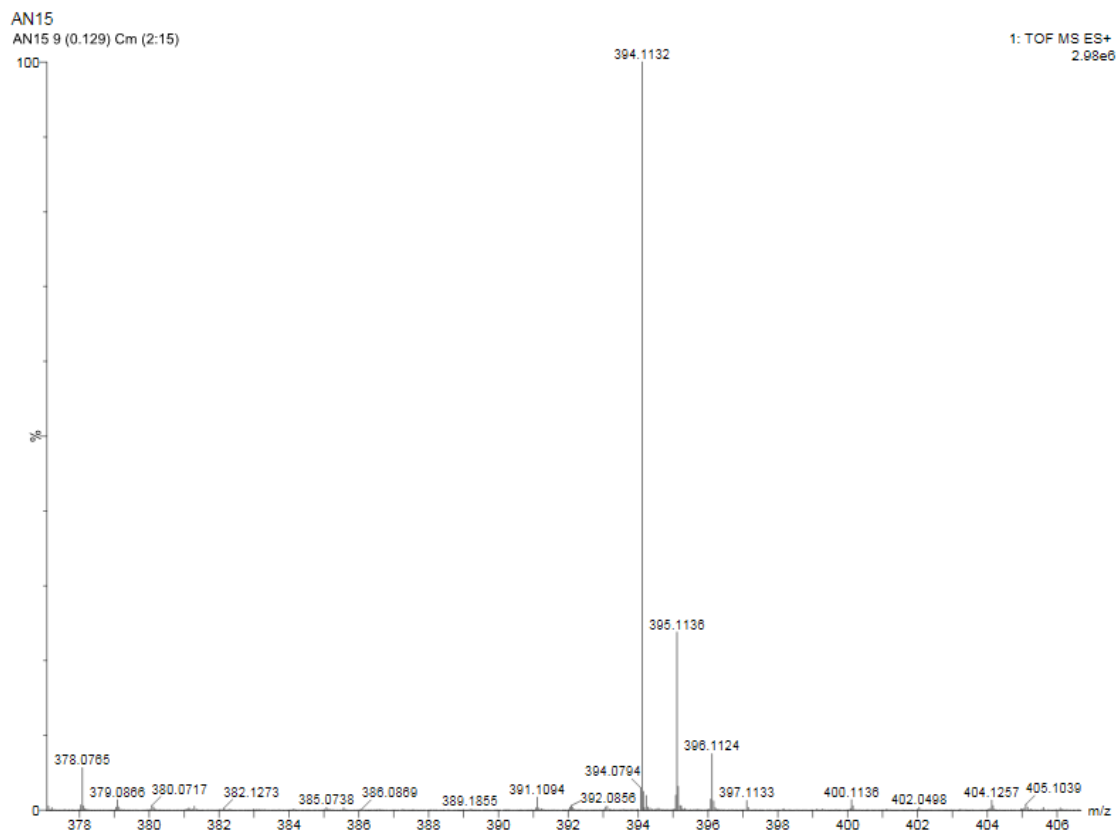
Phenyl (4-((prop-2-yn-1-yloxy)methyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3q)



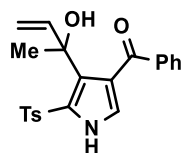
# HRMS



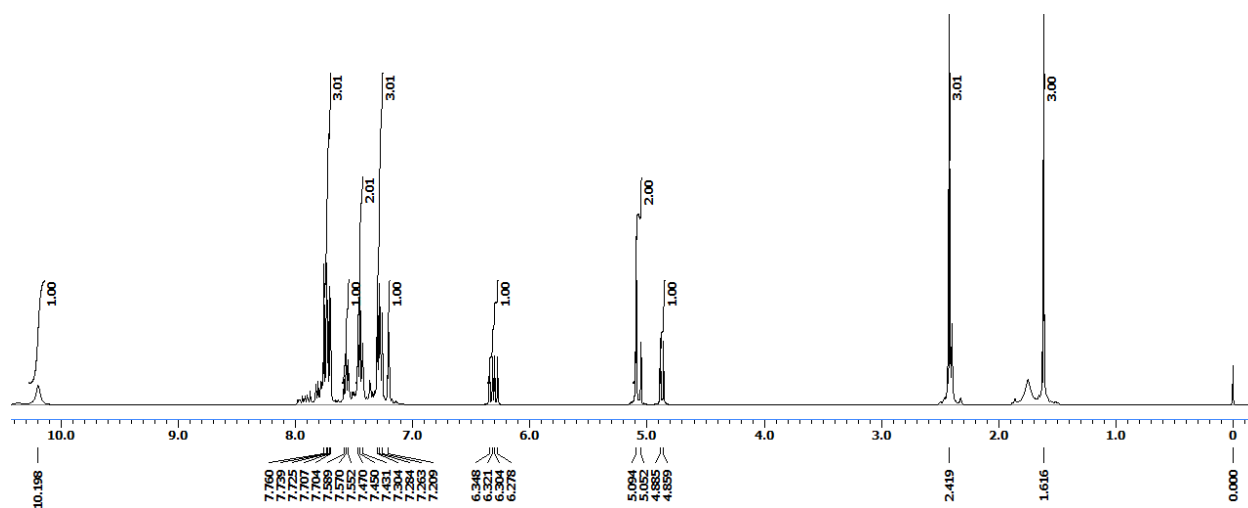
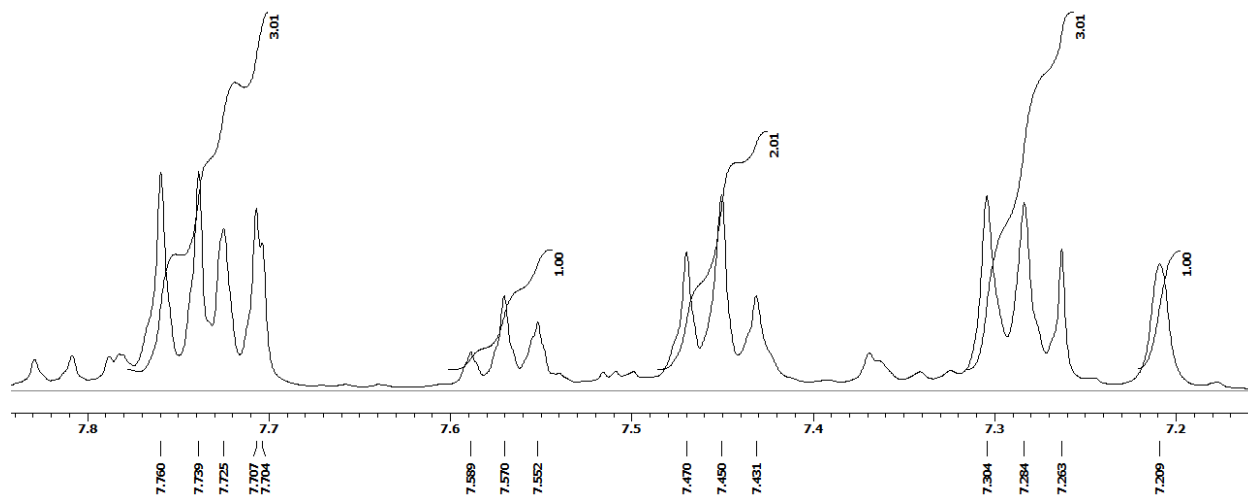
**Phenyl (4-((prop-2-yn-1-yloxy)methyl)-5-tosyl-1H-pyrrol-3-yl)methanone (3q)**



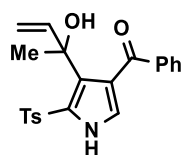
<sup>1</sup>H NMR



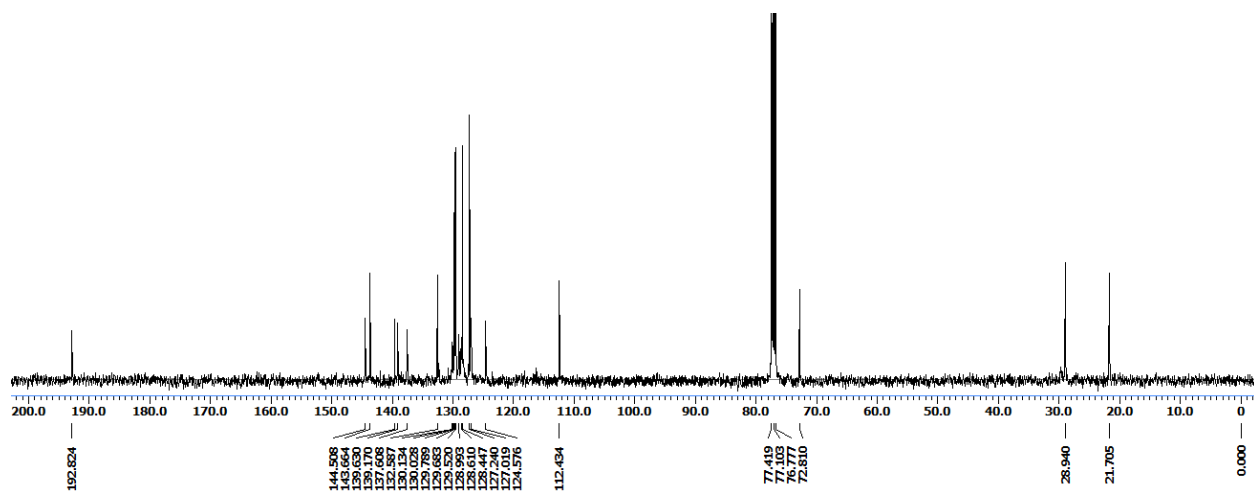
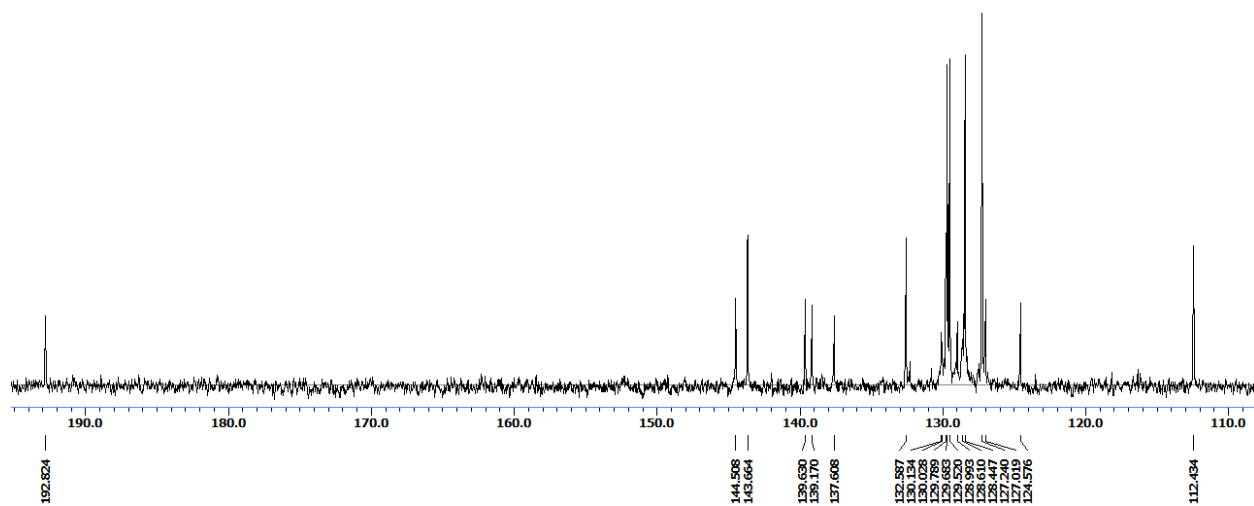
(4-(2-Hydroxybut-3-en-2-yl)-5-tosyl-1*H*-pyrrol-3-yl)(phenyl)methanone (3r)



<sup>13</sup>C NMR

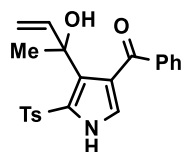


(4-(2-Hydroxybut-3-en-2-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3r)

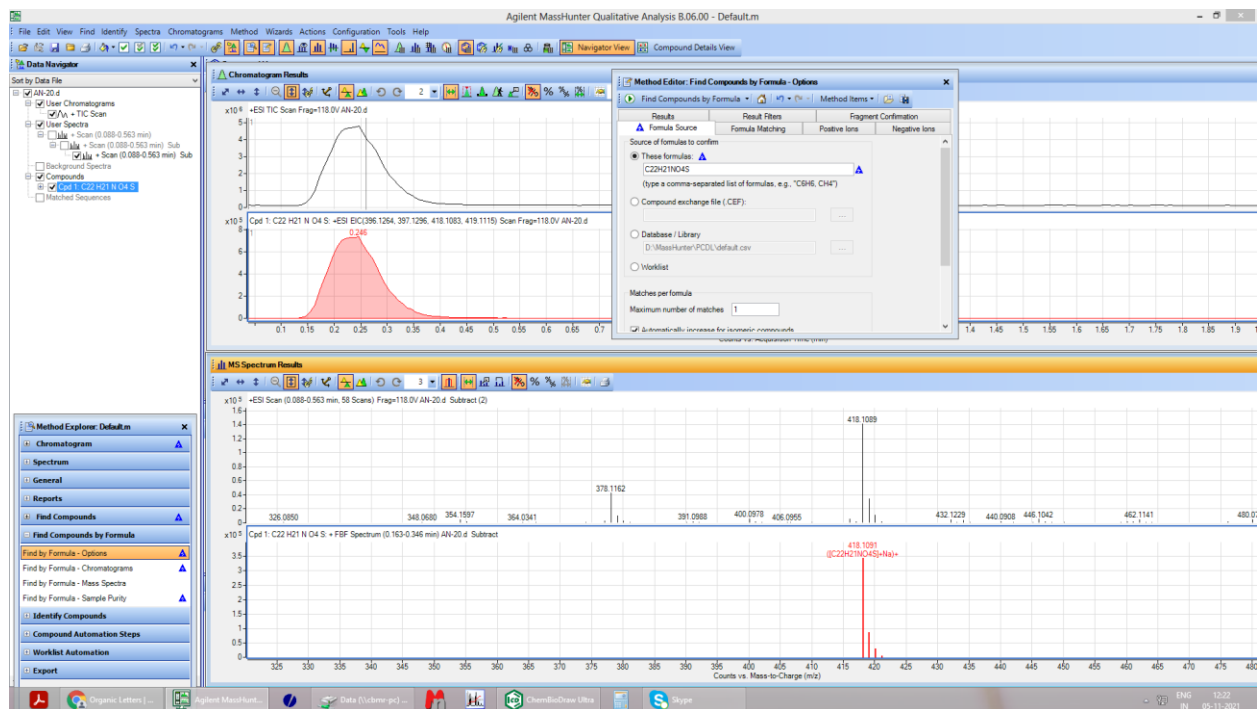




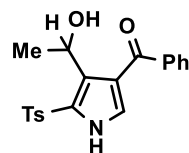
# HRMS



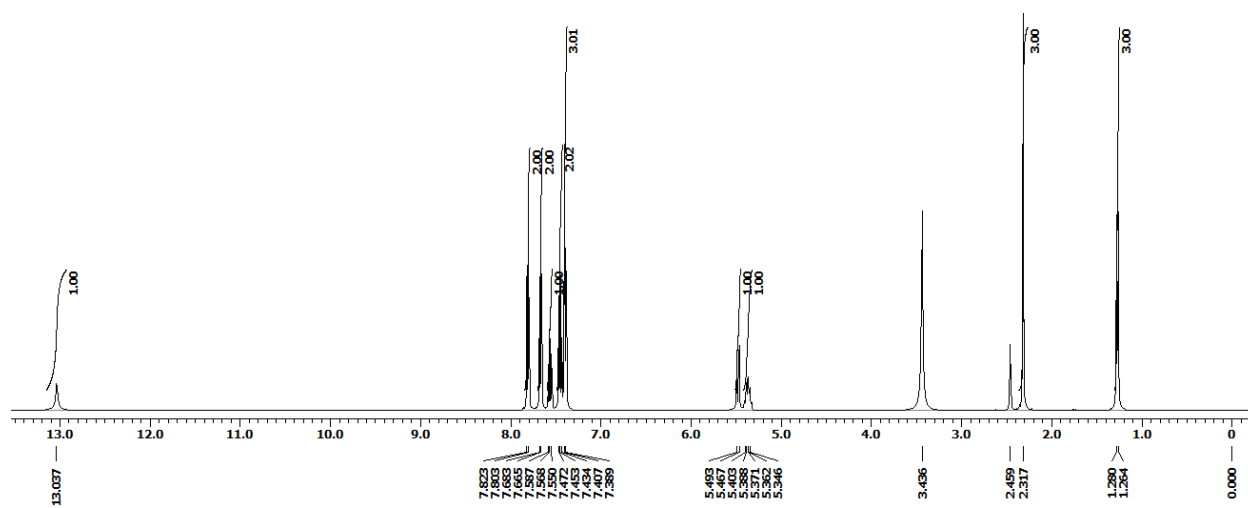
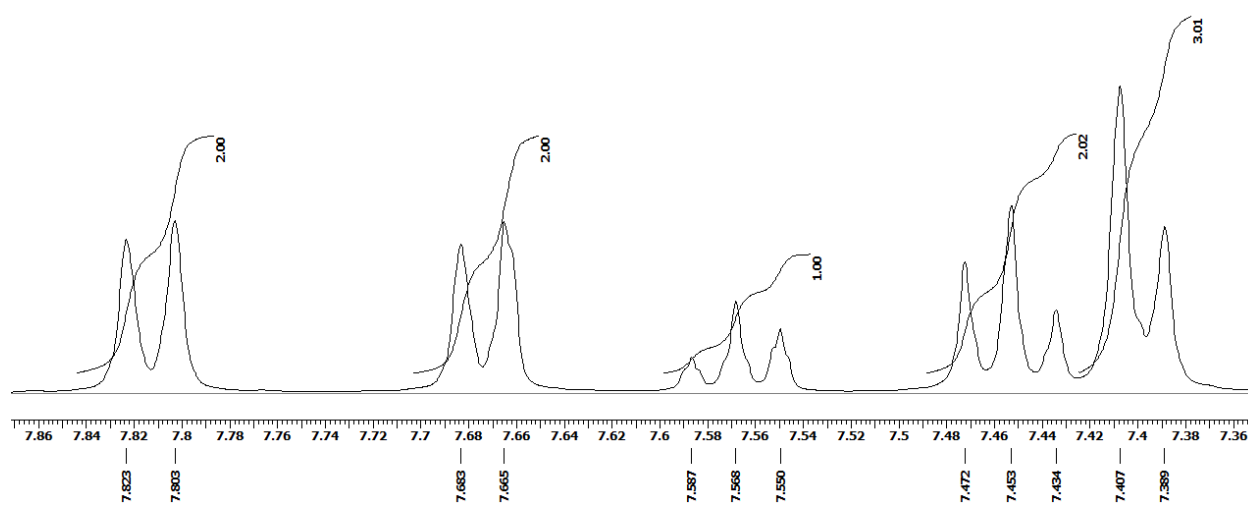
(4-(2-Hydroxybut-3-en-2-yl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3r)



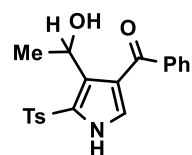
# <sup>1</sup>H NMR



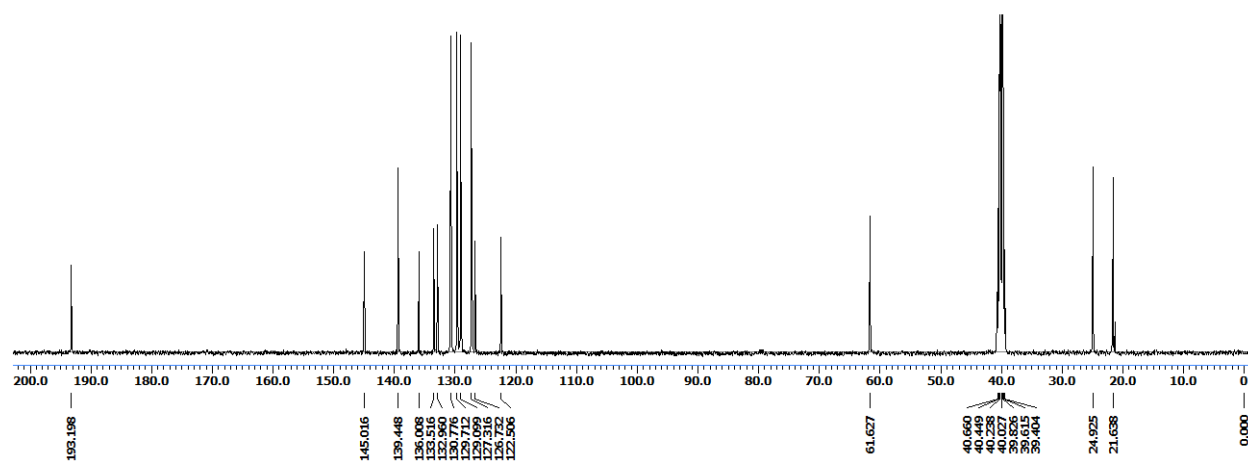
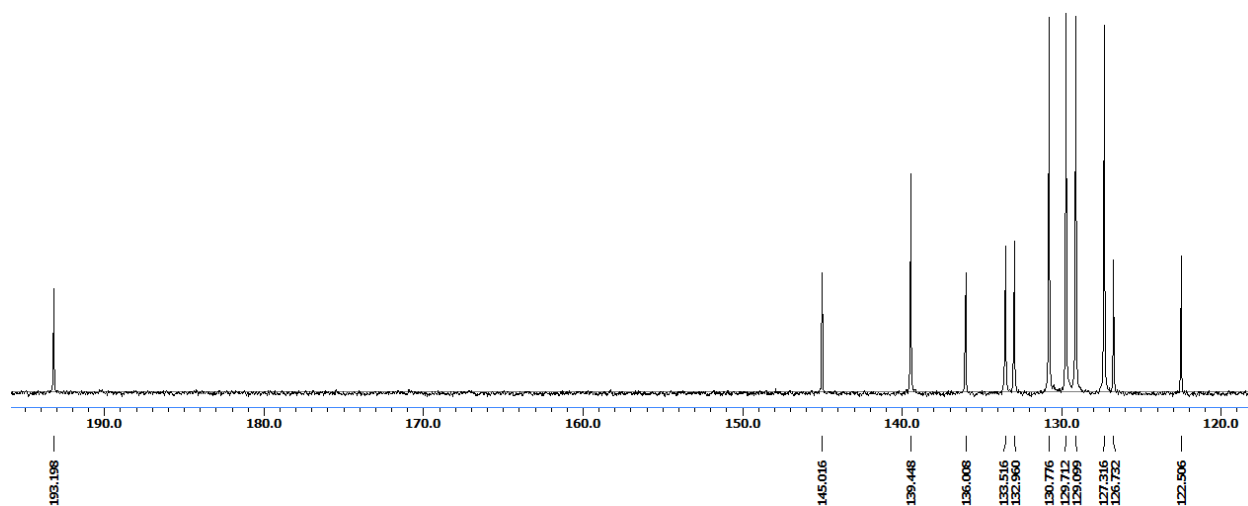
(4-(1-Hydroxyethyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3s)



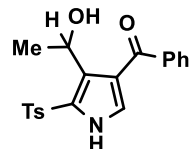
<sup>13</sup>C NMR



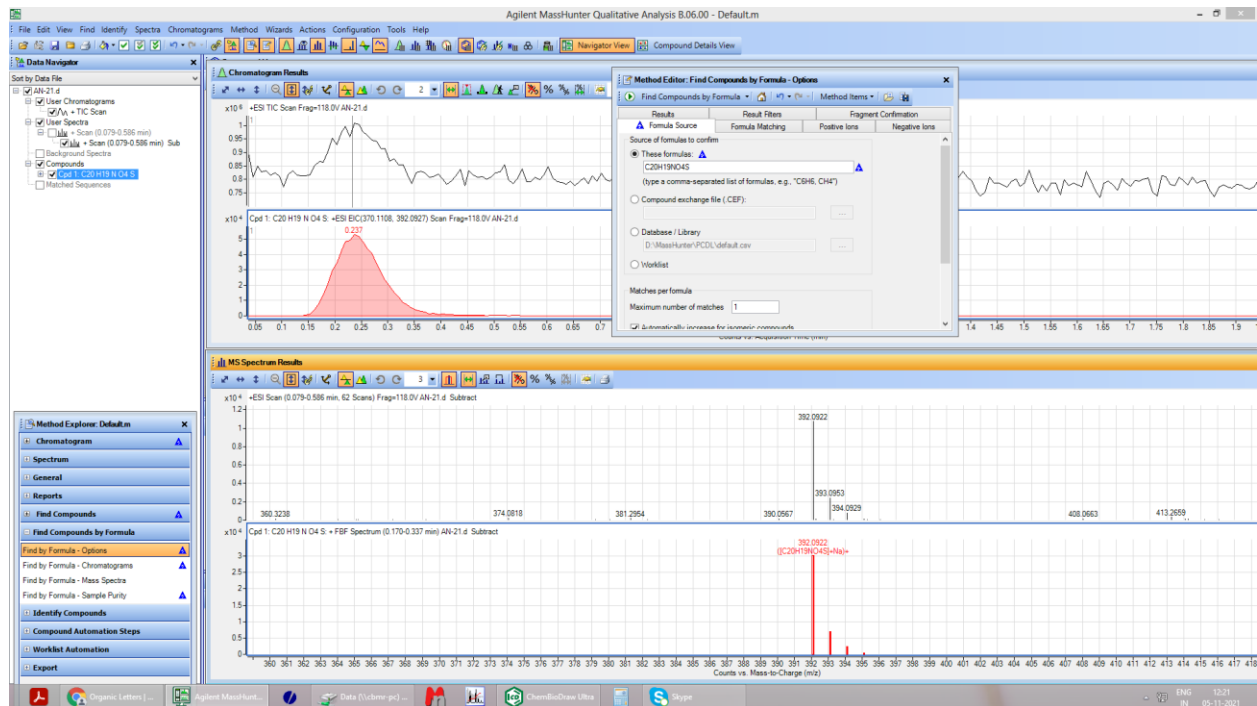
(4-(1-Hydroxyethyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3s)



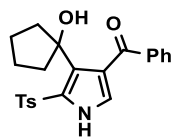
# HRMS



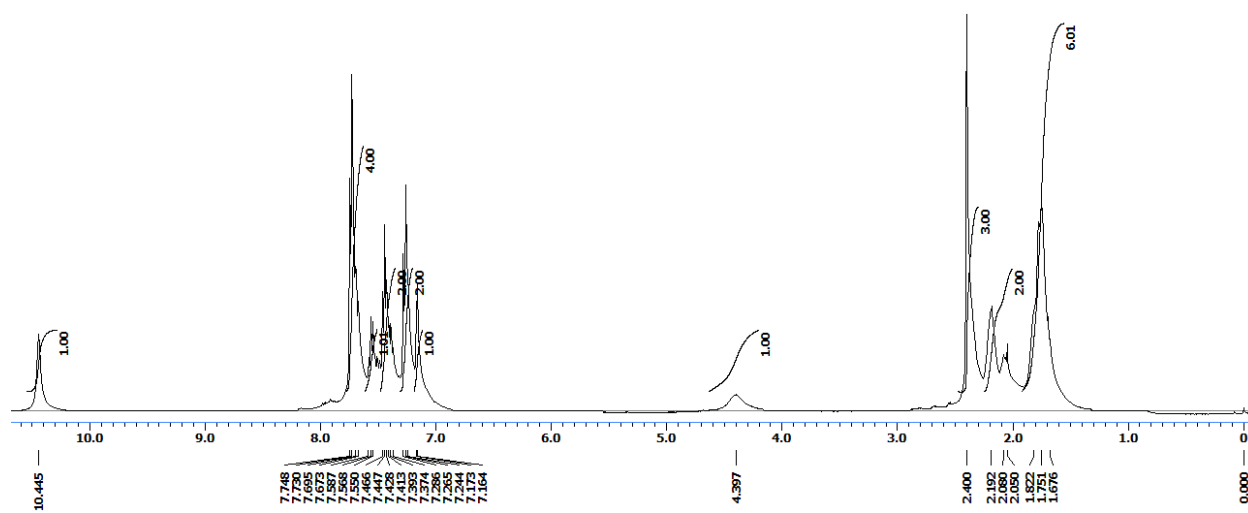
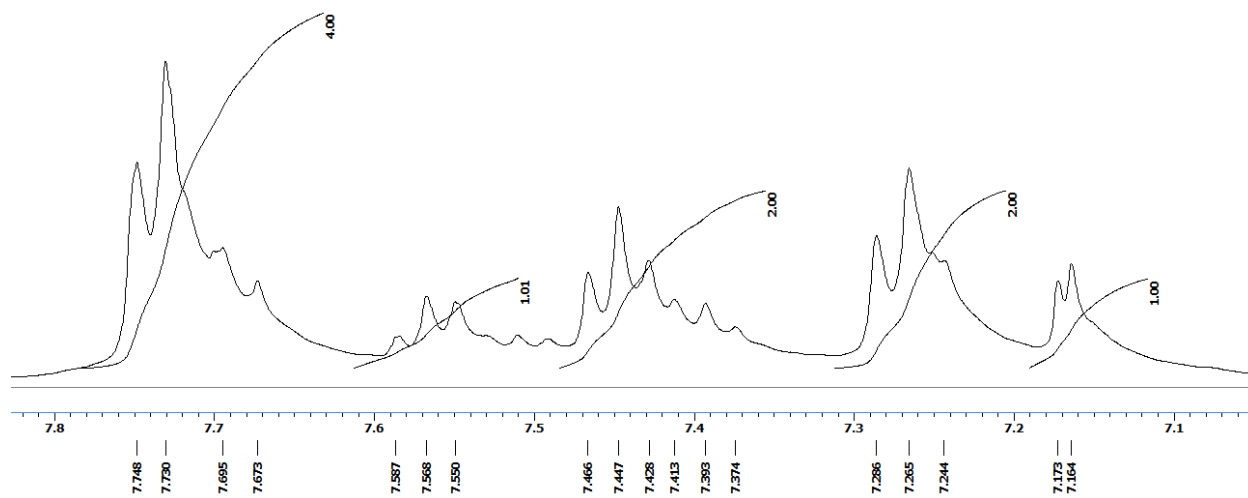
(4-(1-Hydroxyethyl)-5-tosyl-1*H*-pyrrol-3-yl)(phenyl)methanone (3s)



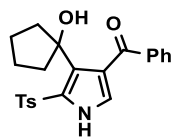
# <sup>1</sup>H NMR



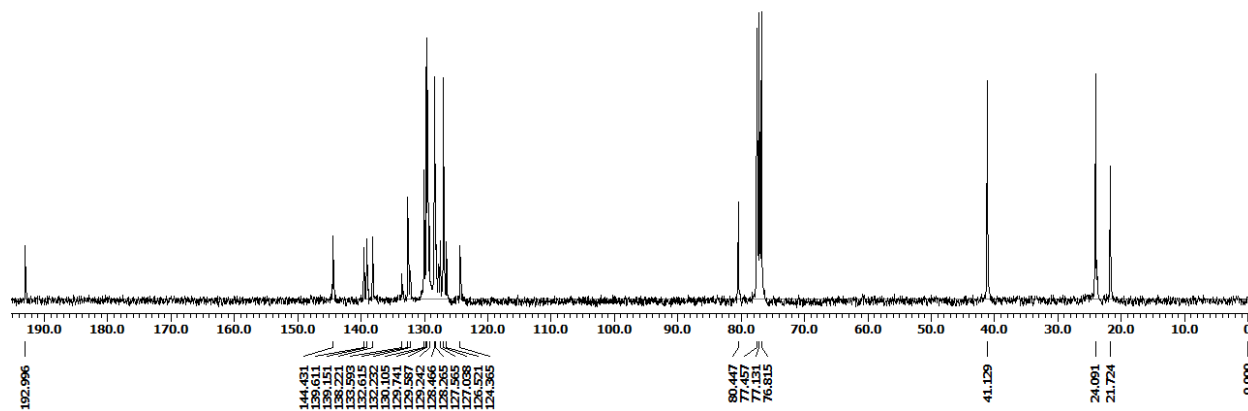
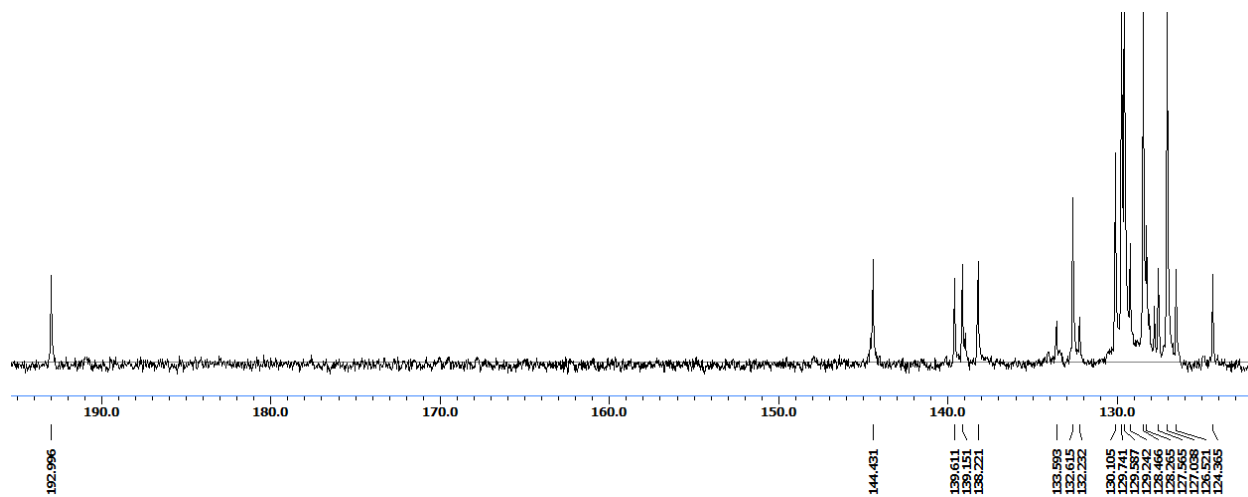
(4-(1-Hydroxycyclopentyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3t)



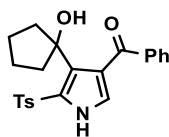
<sup>13</sup>C NMR



(4-(1-Hydroxycyclopentyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3t)



# HRMS



## (4-(1-Hydroxycyclopentyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3t)

### Analysis Info

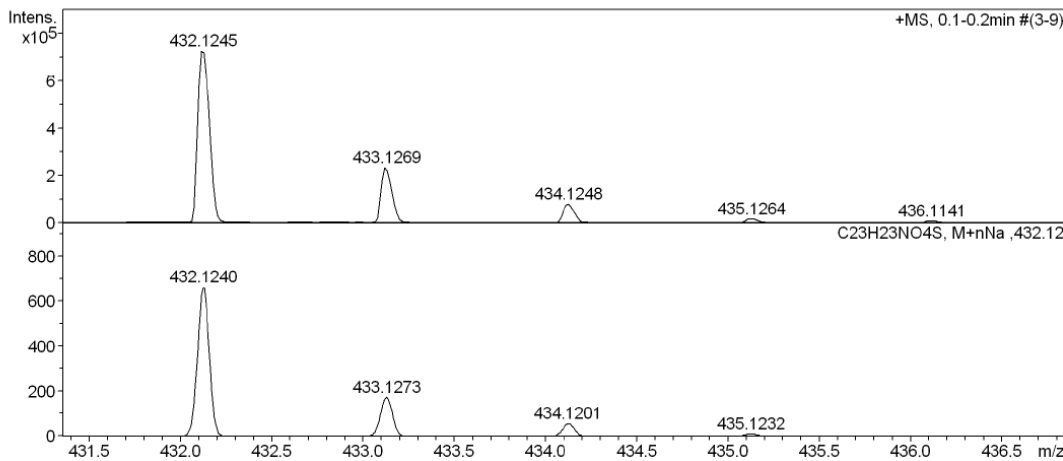
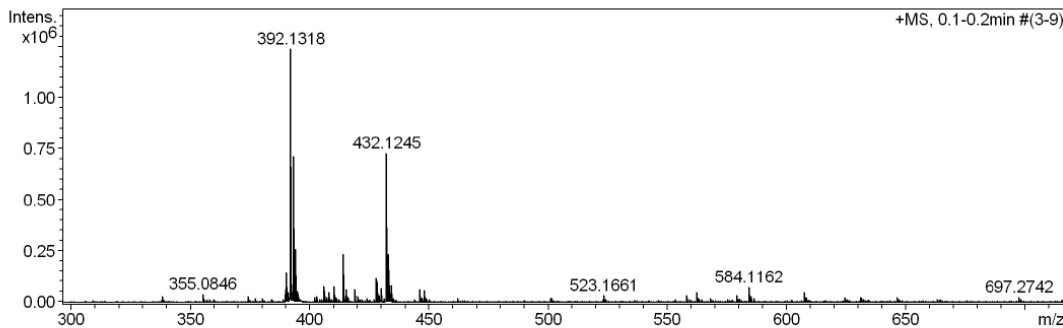
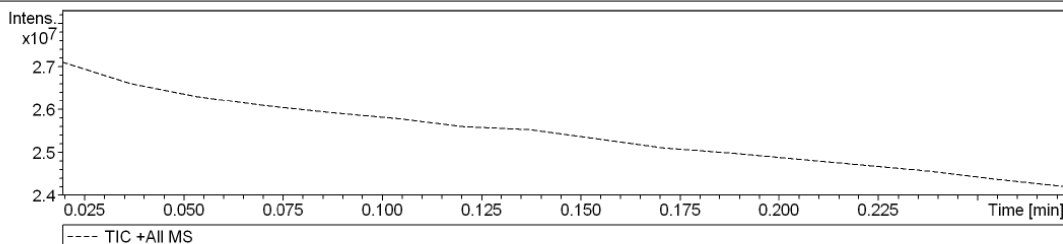
Analysis Name D:\Data\DEC-2020\NKS\29122020-NKS-AN-48.d  
 Method pos tune\_wide\_030118.m  
 Sample Name Tmix-131118  
 Comment

Acquisition Date 12/30/2020 2:22:59 PM

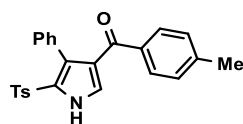
Operator Amit S.Sahu  
 Instrument micrOTOF-Q II 10337

### Acquisition Parameter

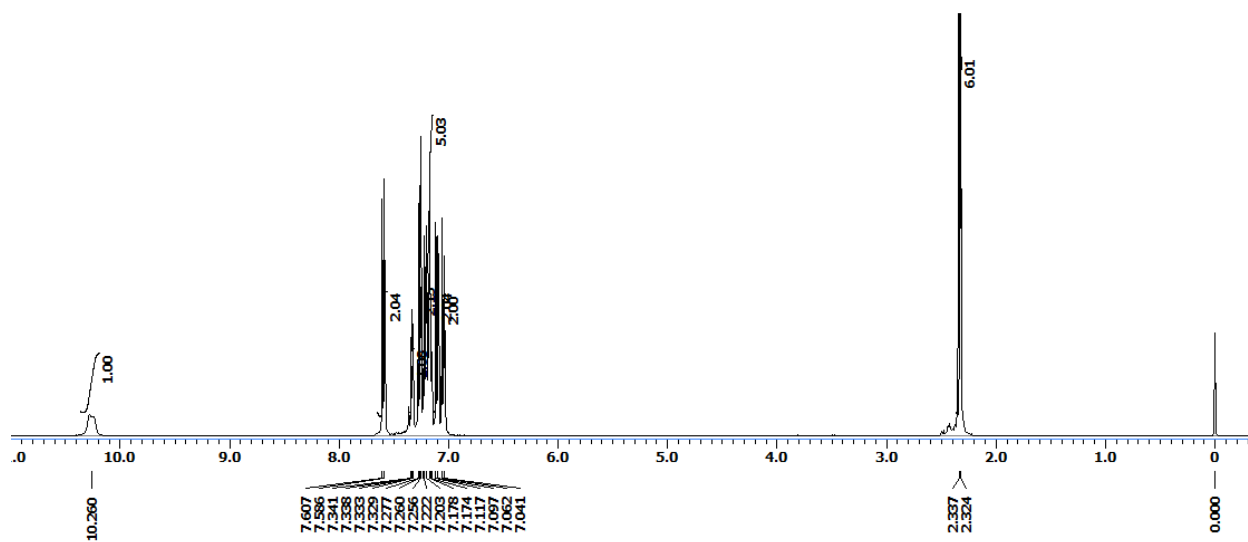
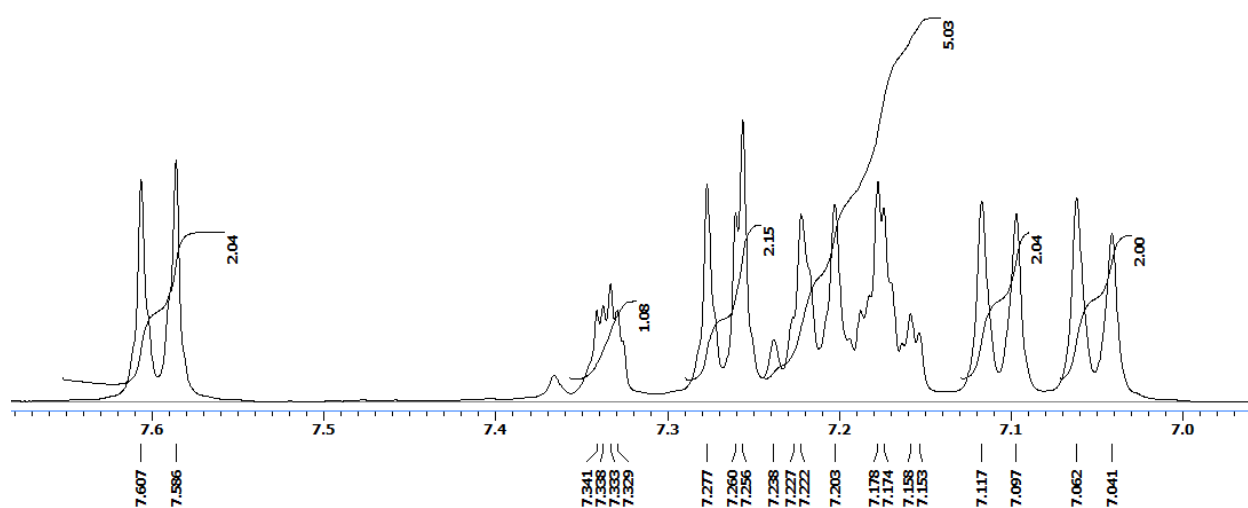
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



# <sup>1</sup>H NMR

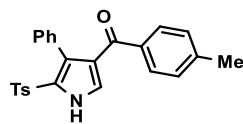


(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(p-tolyl)methanone (3u)

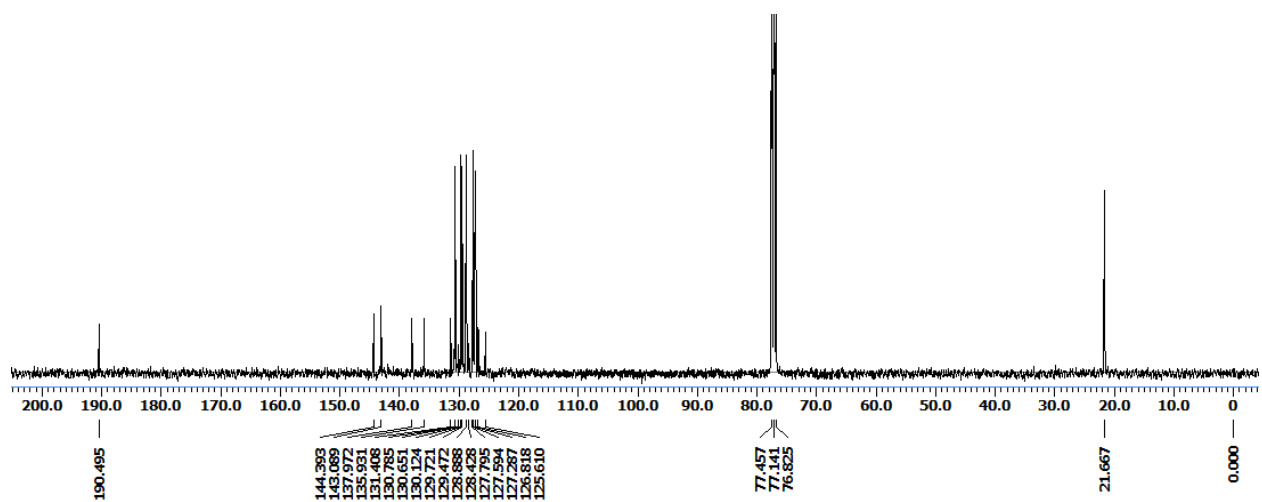
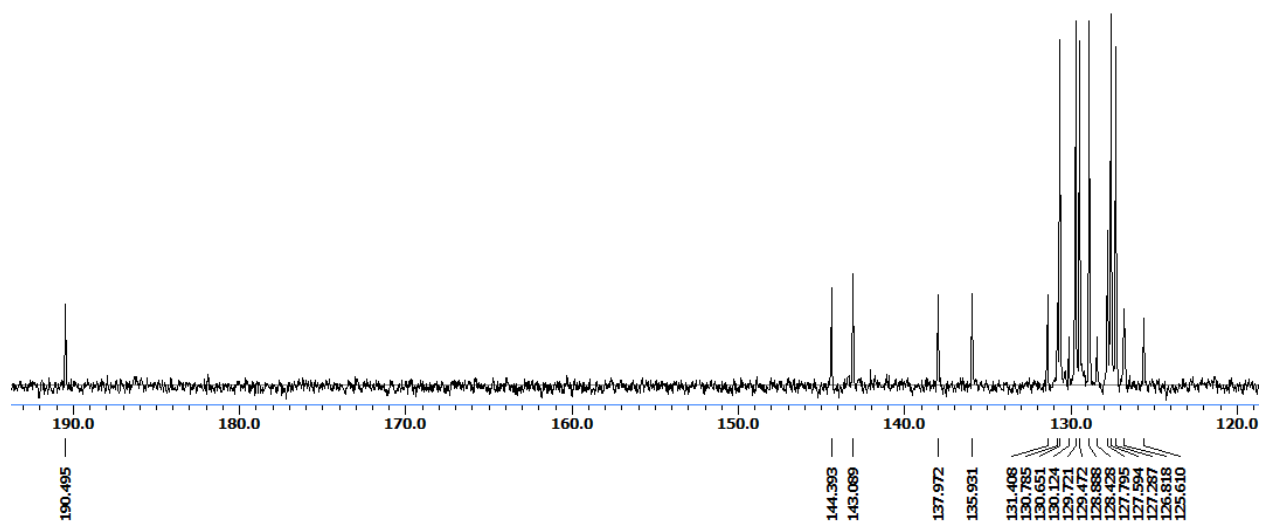




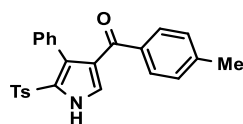
<sup>13</sup>C NMR



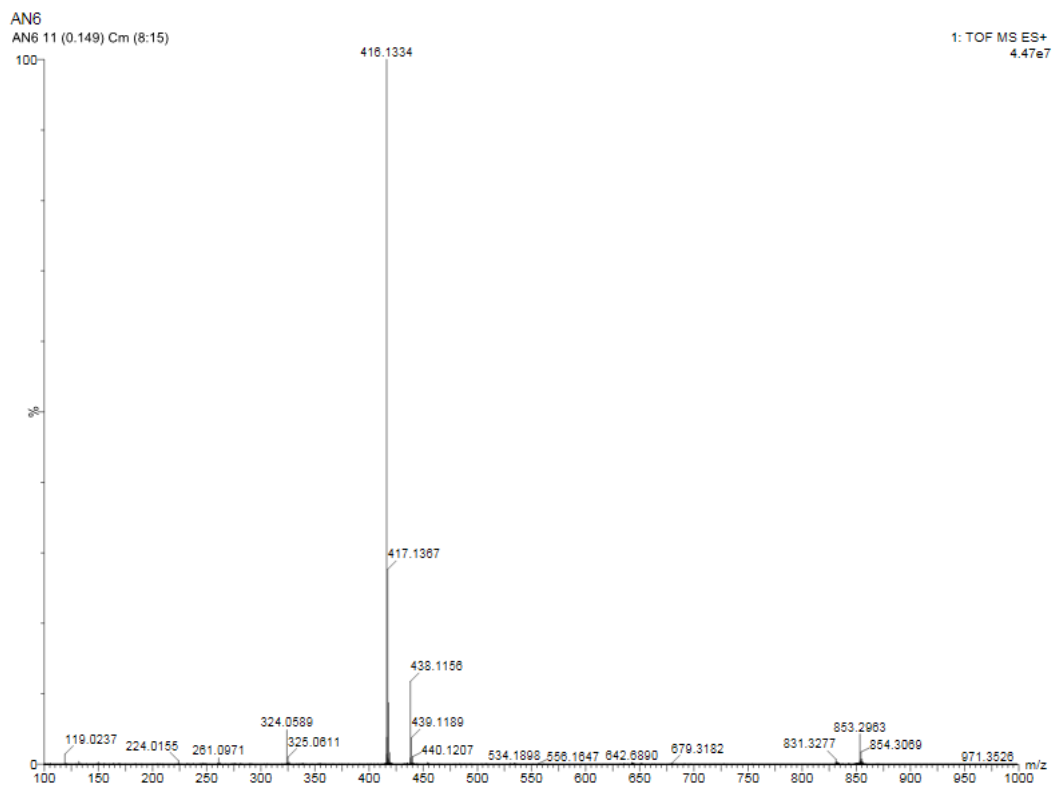
(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(p-tolyl)methanone (3u)



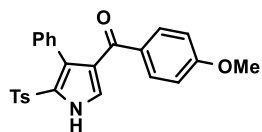
# HRMS



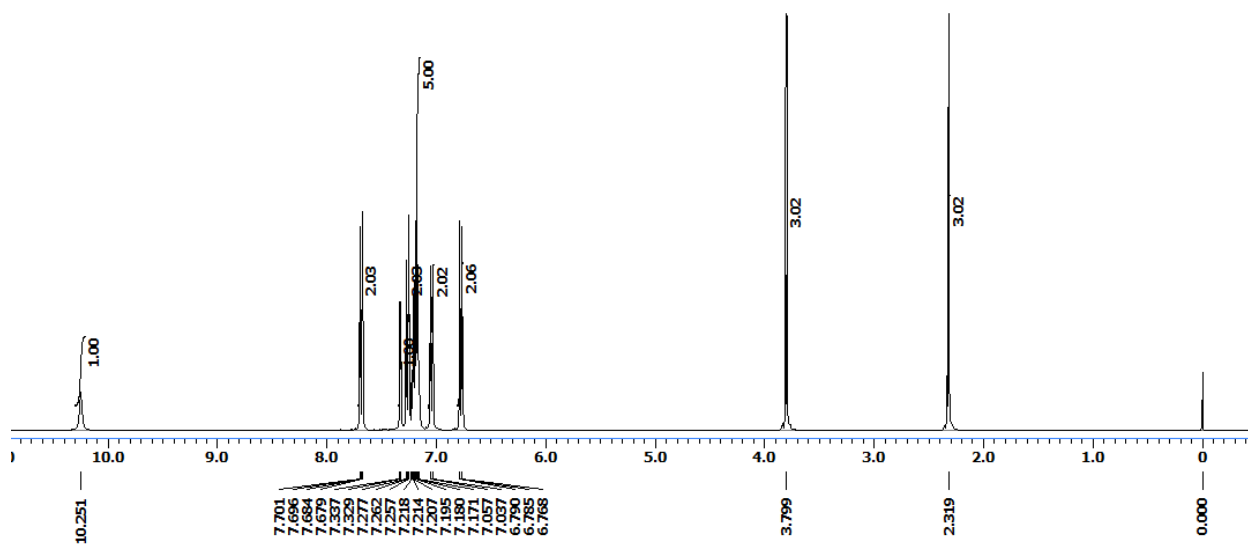
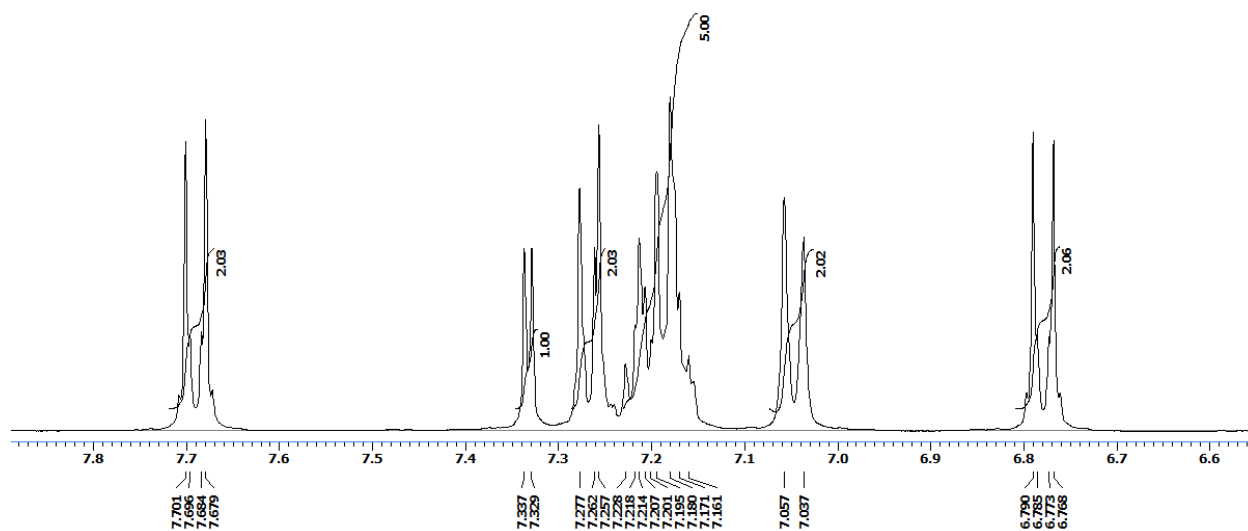
**(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(p-tolyl)methanone (3u)**



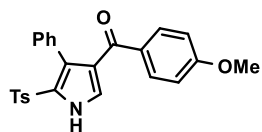
# <sup>1</sup>H NMR



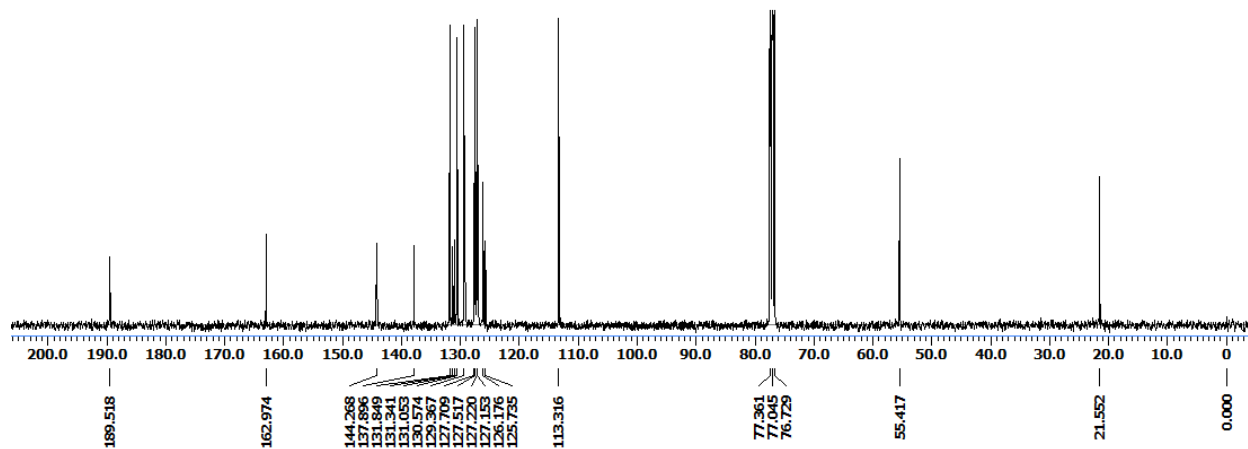
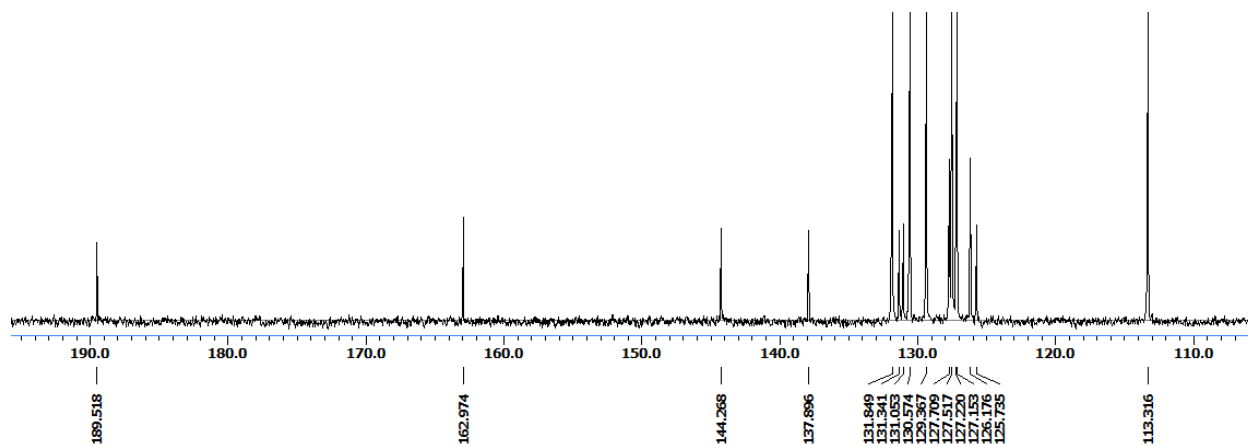
(4-Methoxyphenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3v)



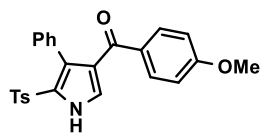
<sup>13</sup>C NMR



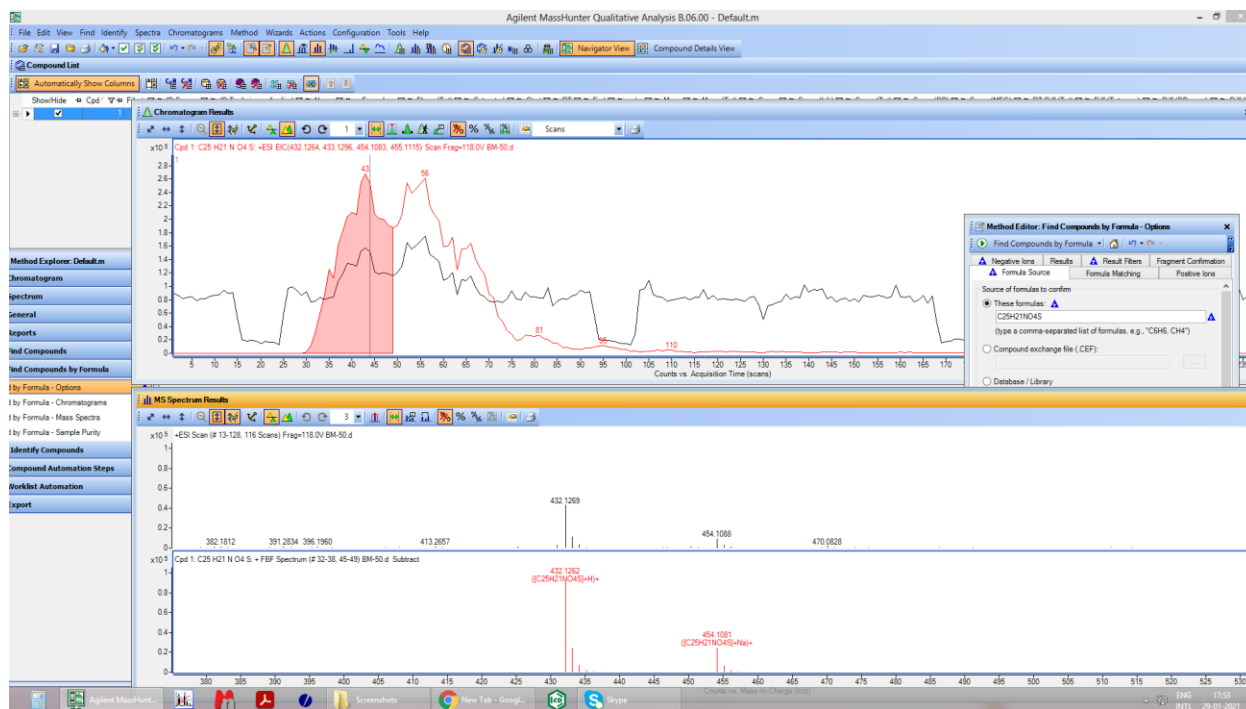
(4-Methoxyphenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3v)



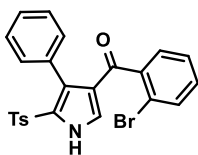
## HRMS



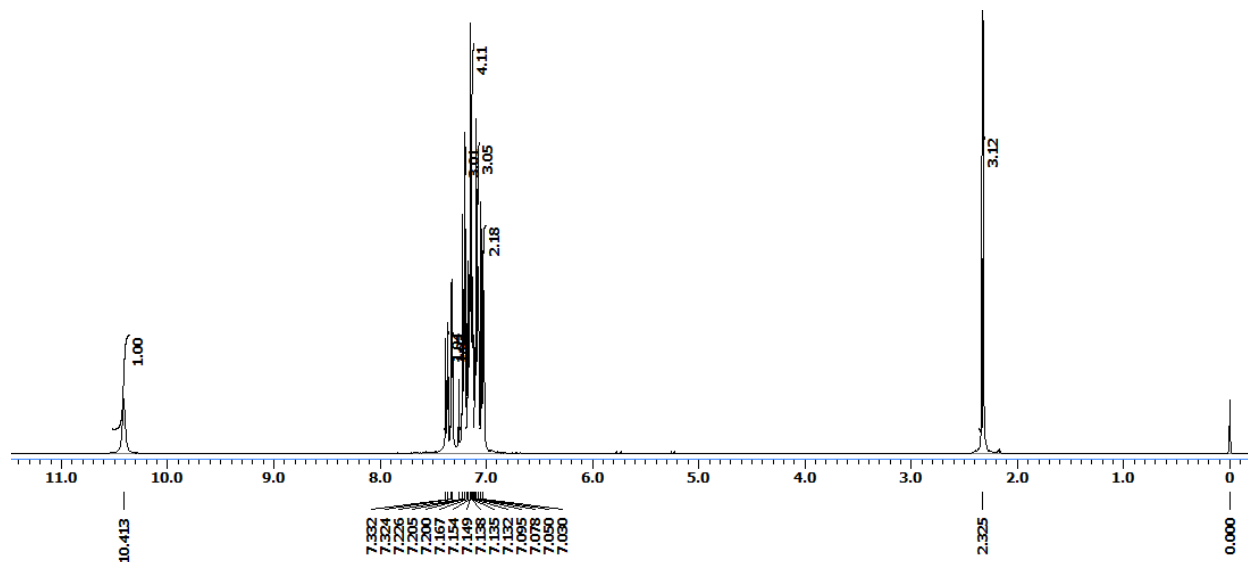
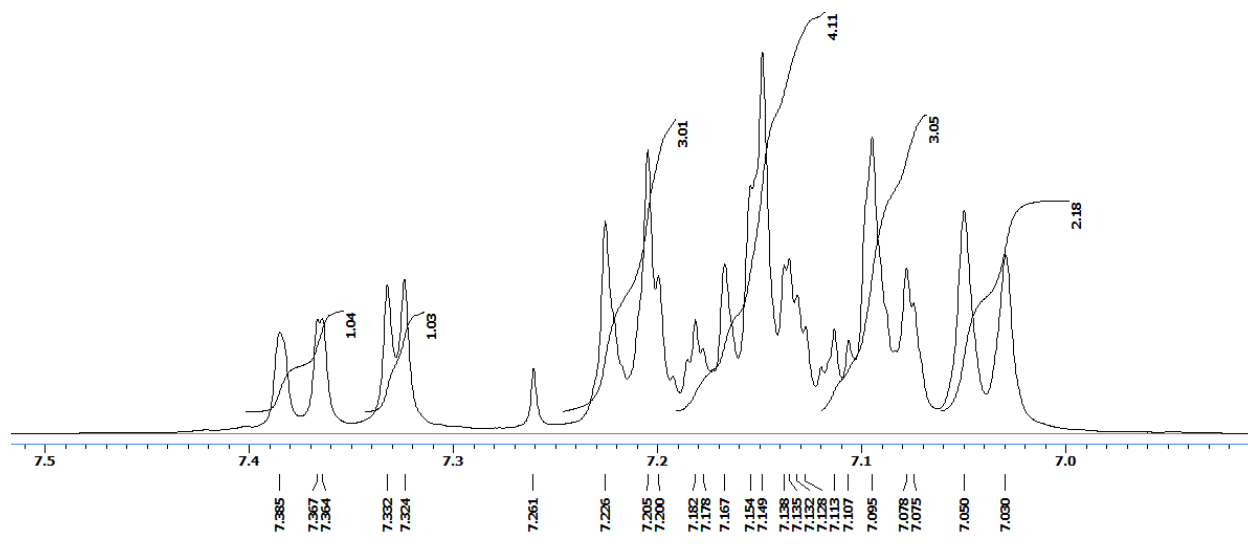
(4-Methoxyphenyl)(4-phenyl-5-tosyl-1*H*-pyrrol-3-yl)methanone (3v)



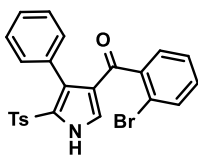
# <sup>1</sup>H NMR



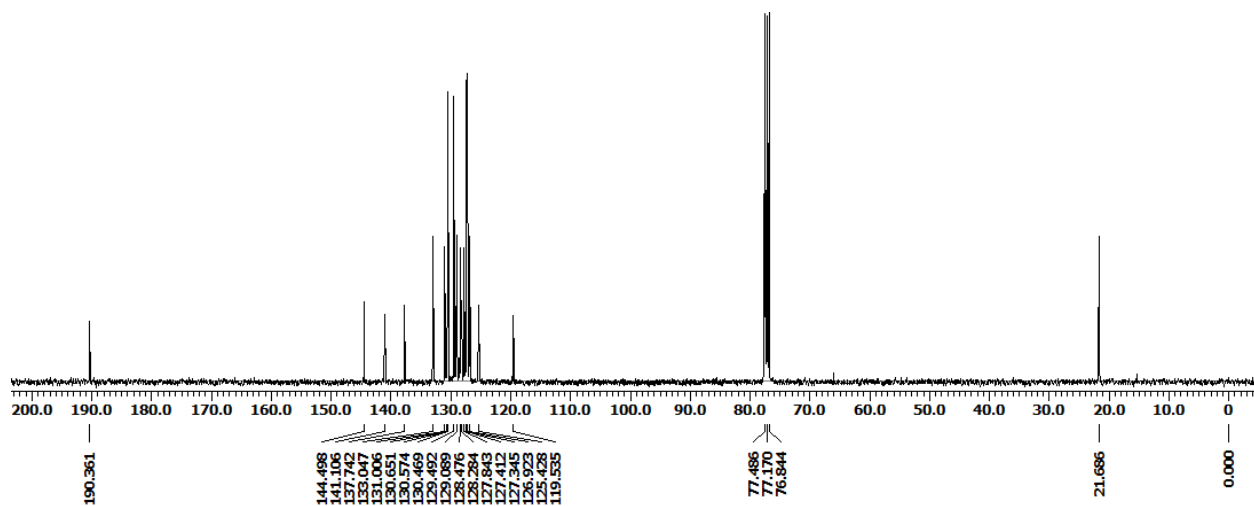
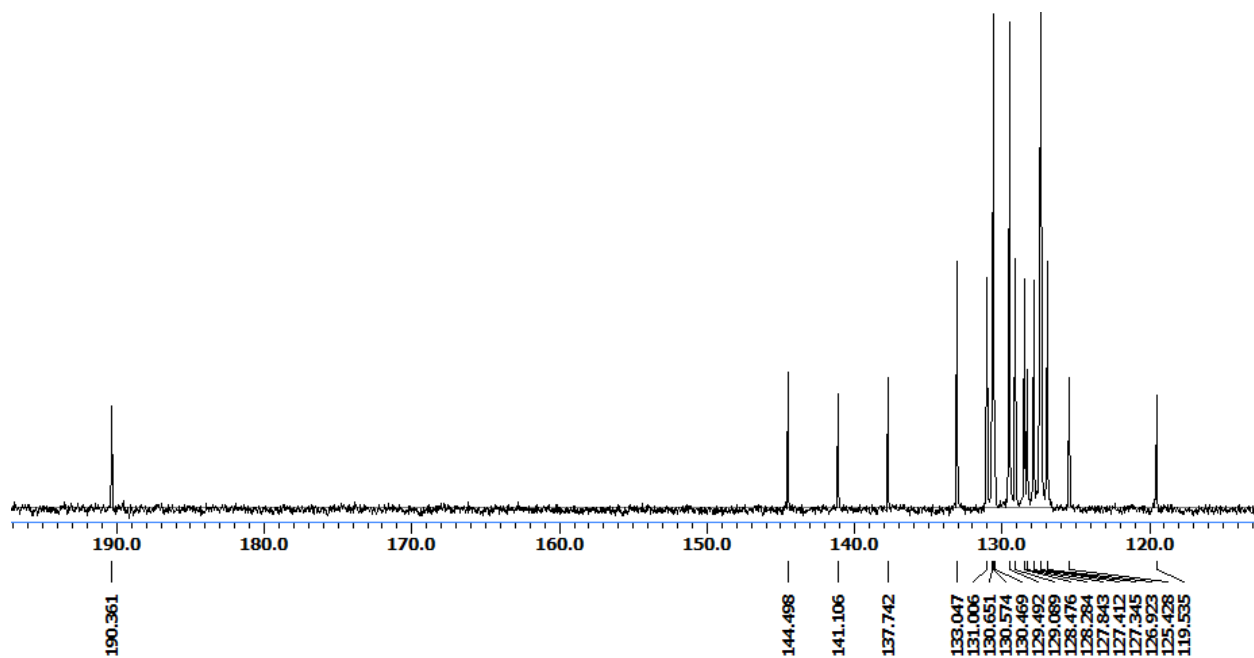
(2-Bromophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3w)



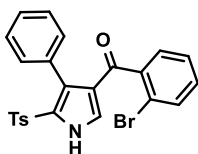
<sup>13</sup>C NMR



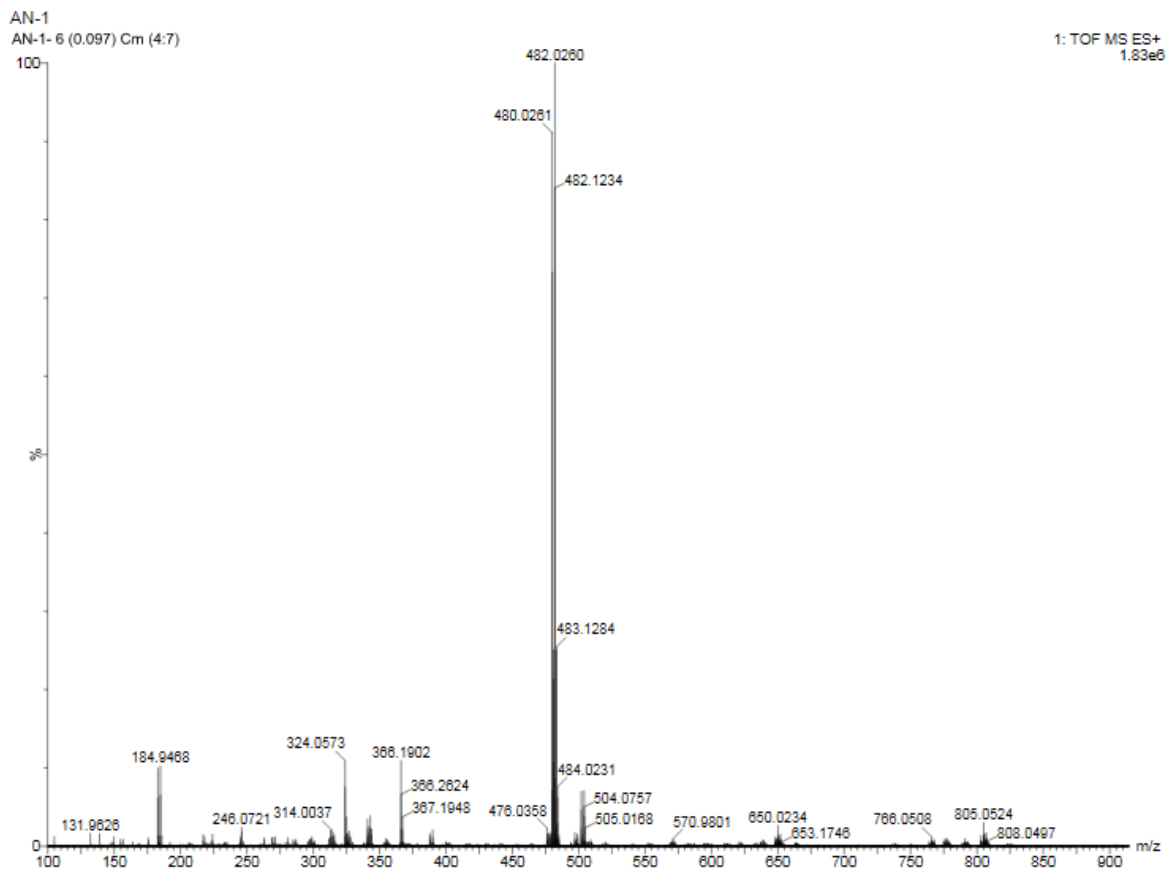
(2-Bromophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3w)



# HRMS

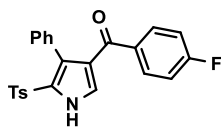


(2-Bromophenyl)(4-phenyl-5-tosyl-1*H*-pyrrol-3-yl)methanone (3w)

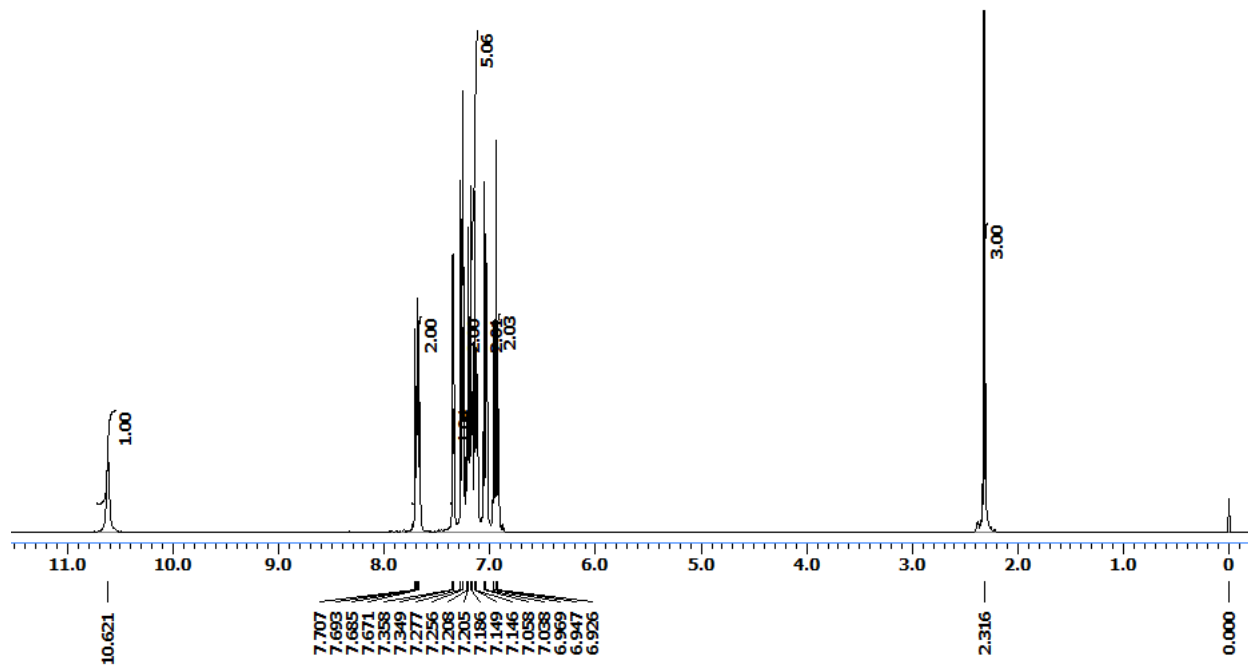
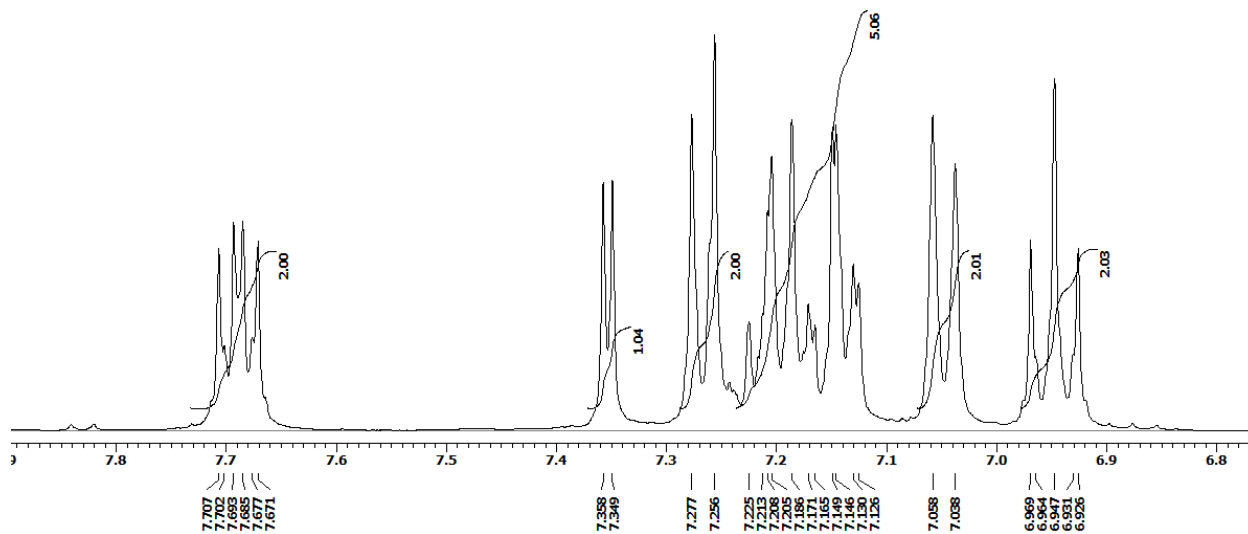




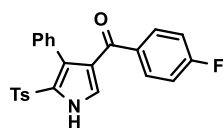
<sup>1</sup>H NMR



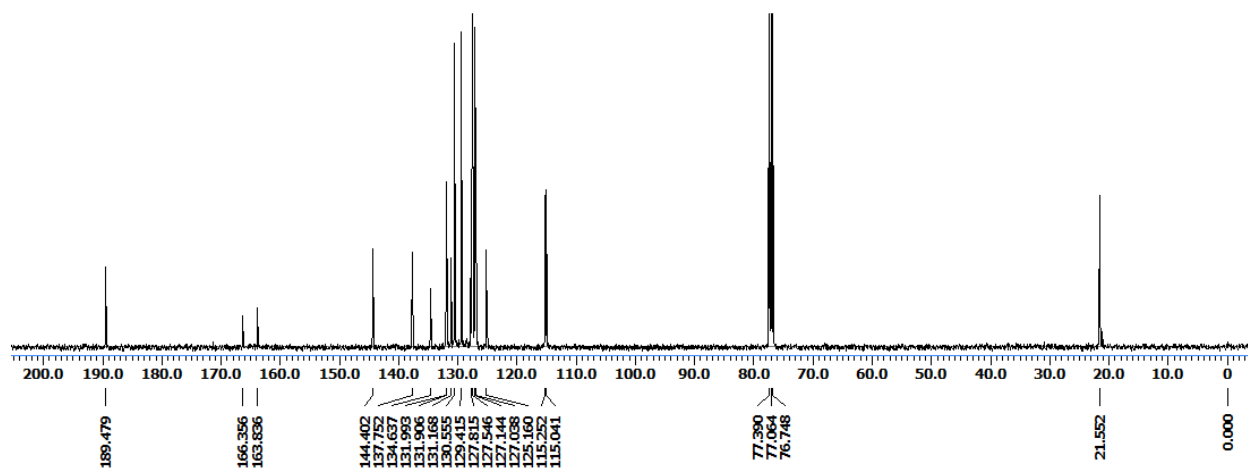
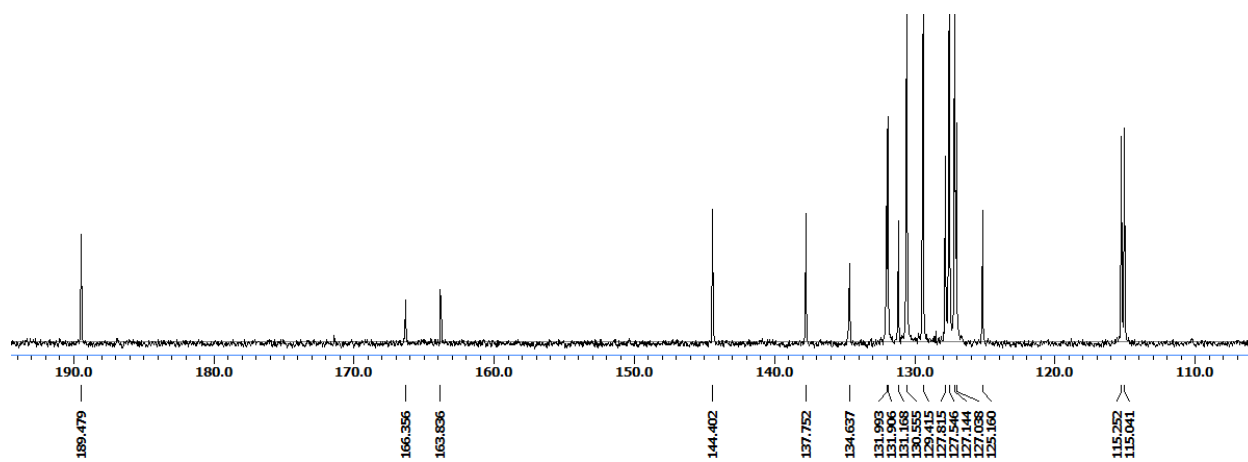
(4-Fluorophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3x)



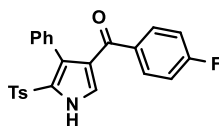
<sup>13</sup>C NMR



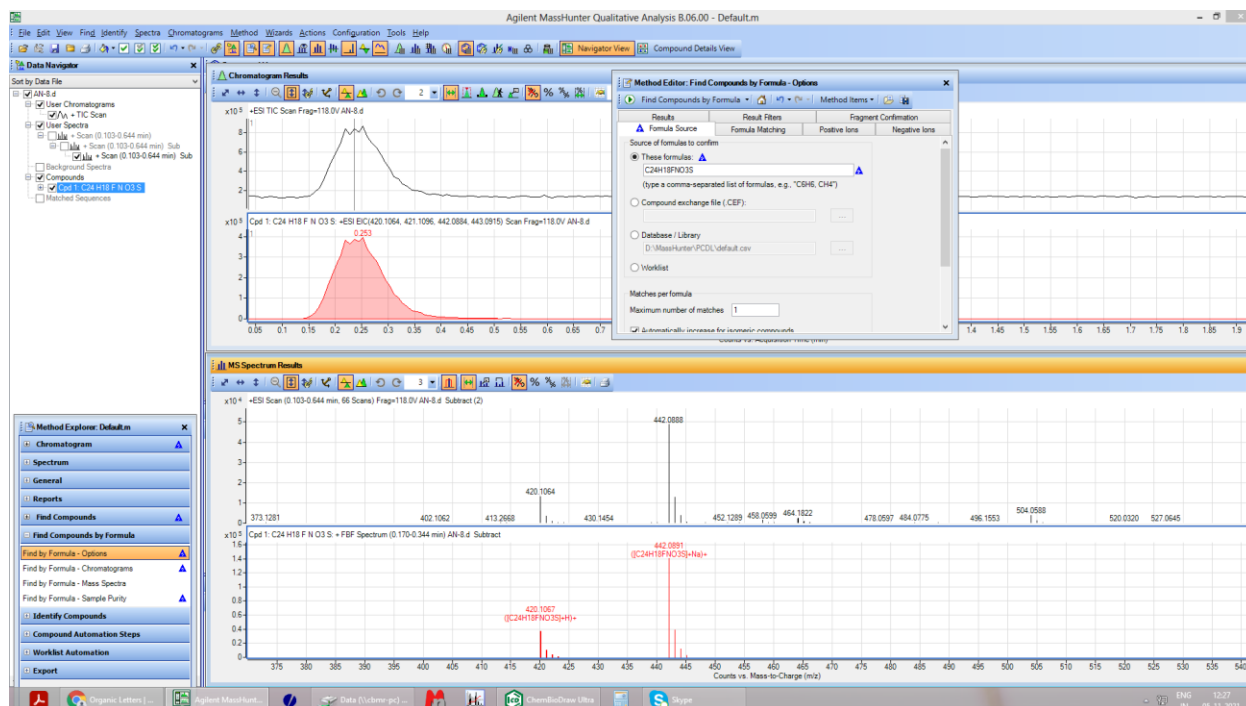
(4-Fluorophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3x)



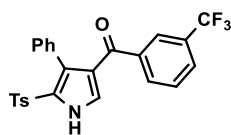
# HRMS



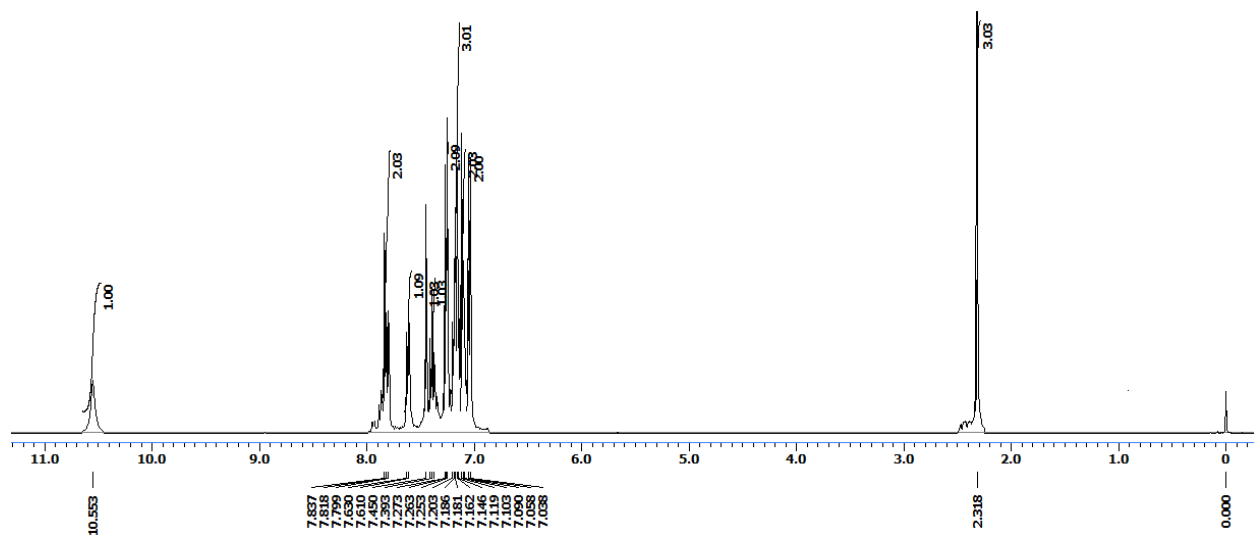
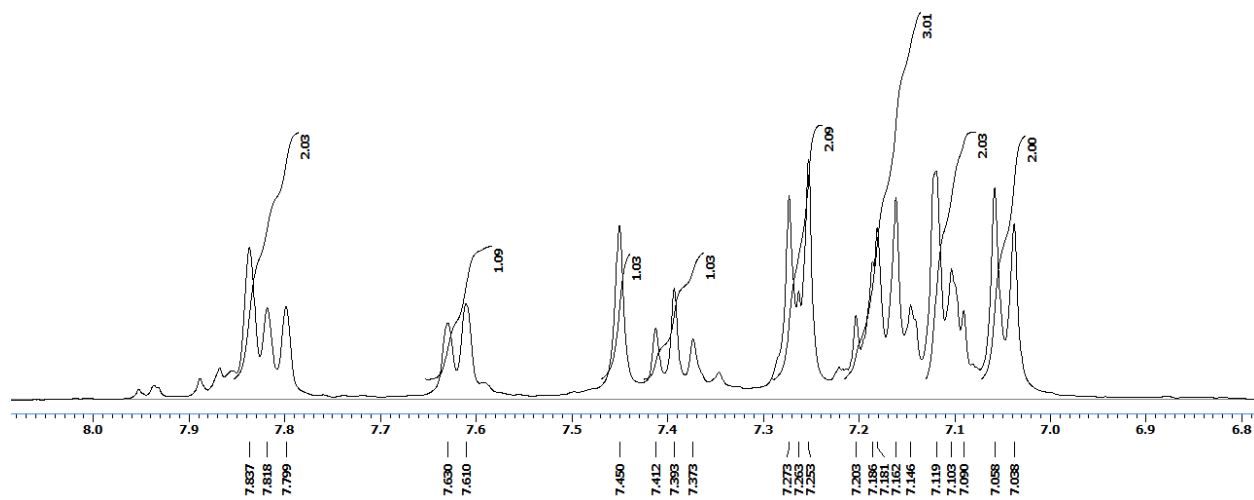
(4-Fluorophenyl)(4-phenyl-5-tosyl-1*H*-pyrrol-3-yl)methanone (3x)



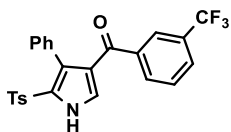
# <sup>1</sup>H NMR



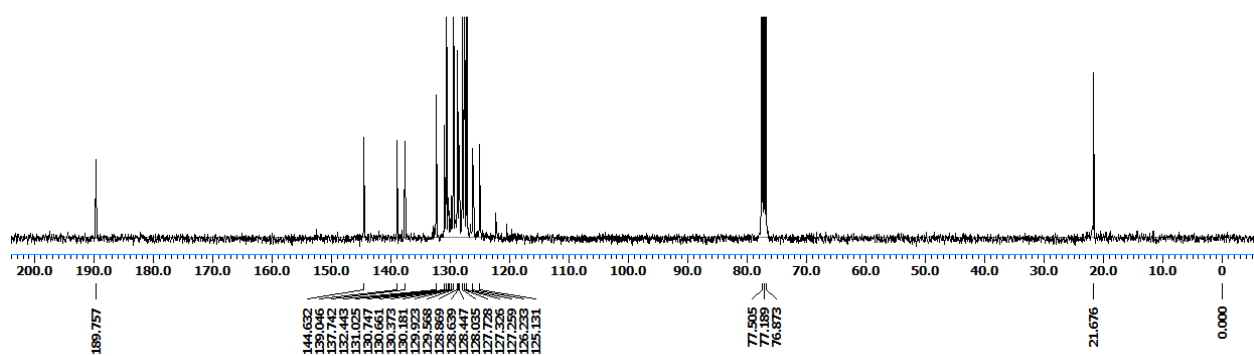
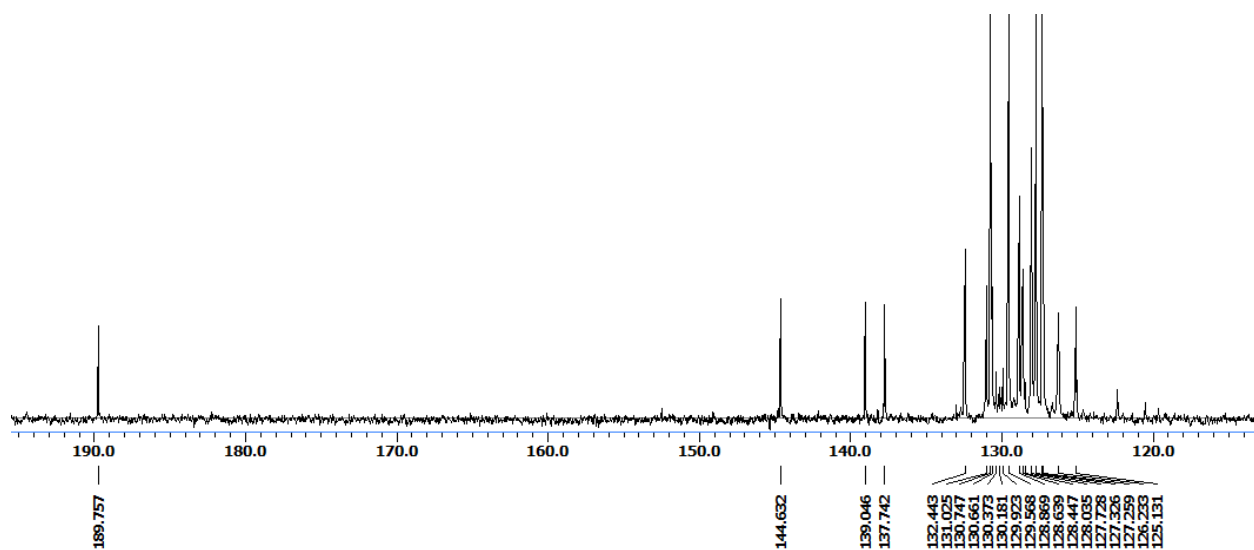
(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(3-(trifluoromethyl)phenyl)methanone (3y)



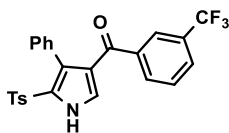
<sup>13</sup>C NMR



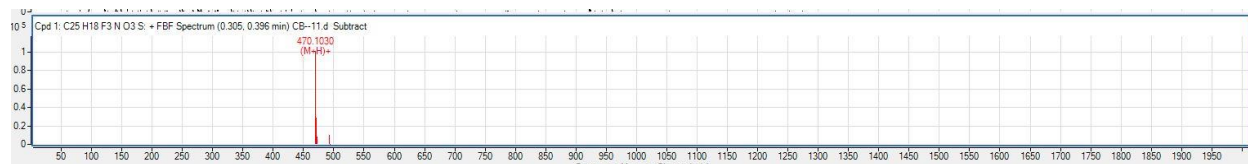
(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(3-(trifluoromethyl)phenyl)methanone (3y)



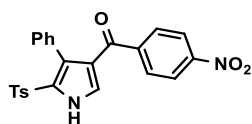
## HRMS



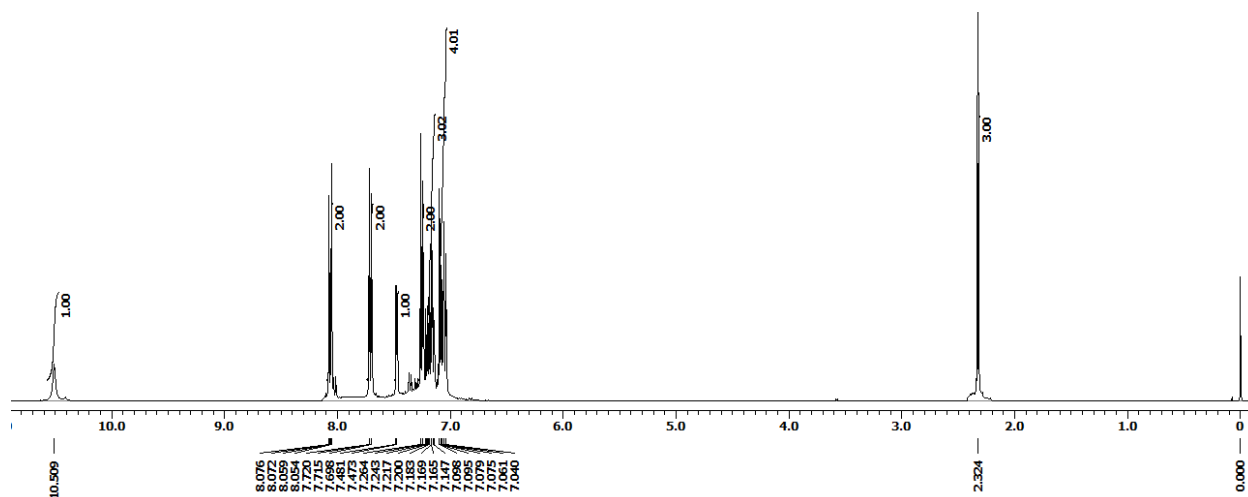
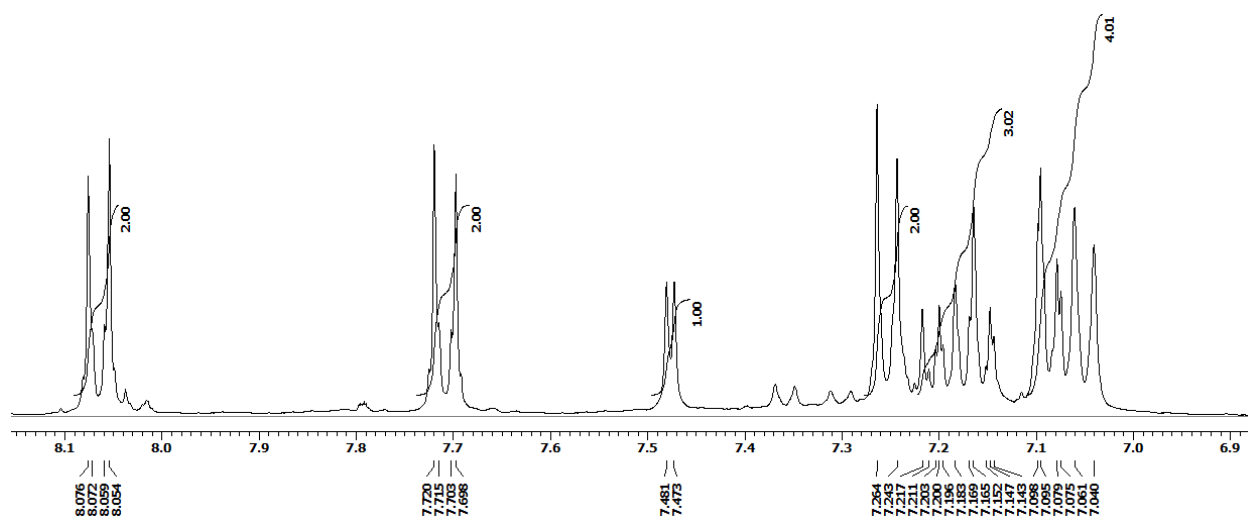
**(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(3-(trifluoromethyl)phenyl)methanone (3y)**



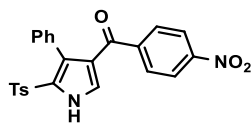
# <sup>1</sup>H NMR



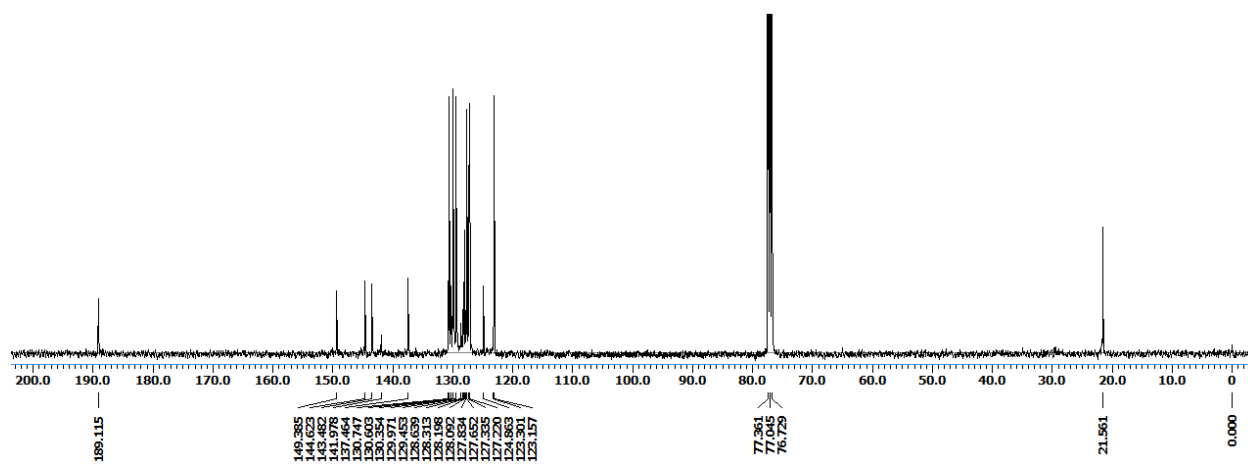
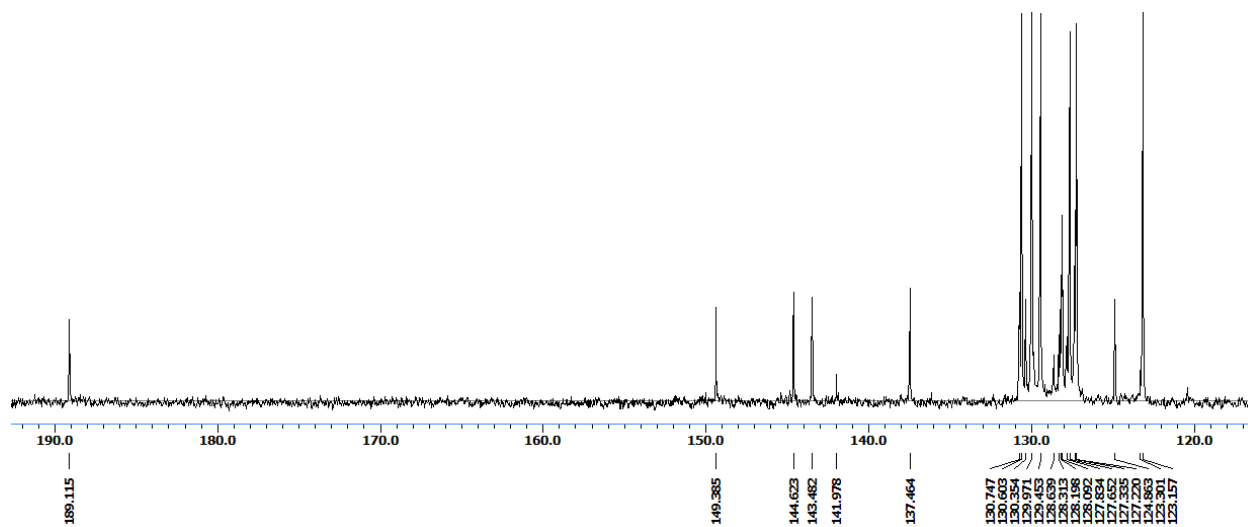
(4-Nitrophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3z)



<sup>13</sup>C NMR

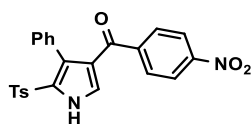


(4-Nitrophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3z)

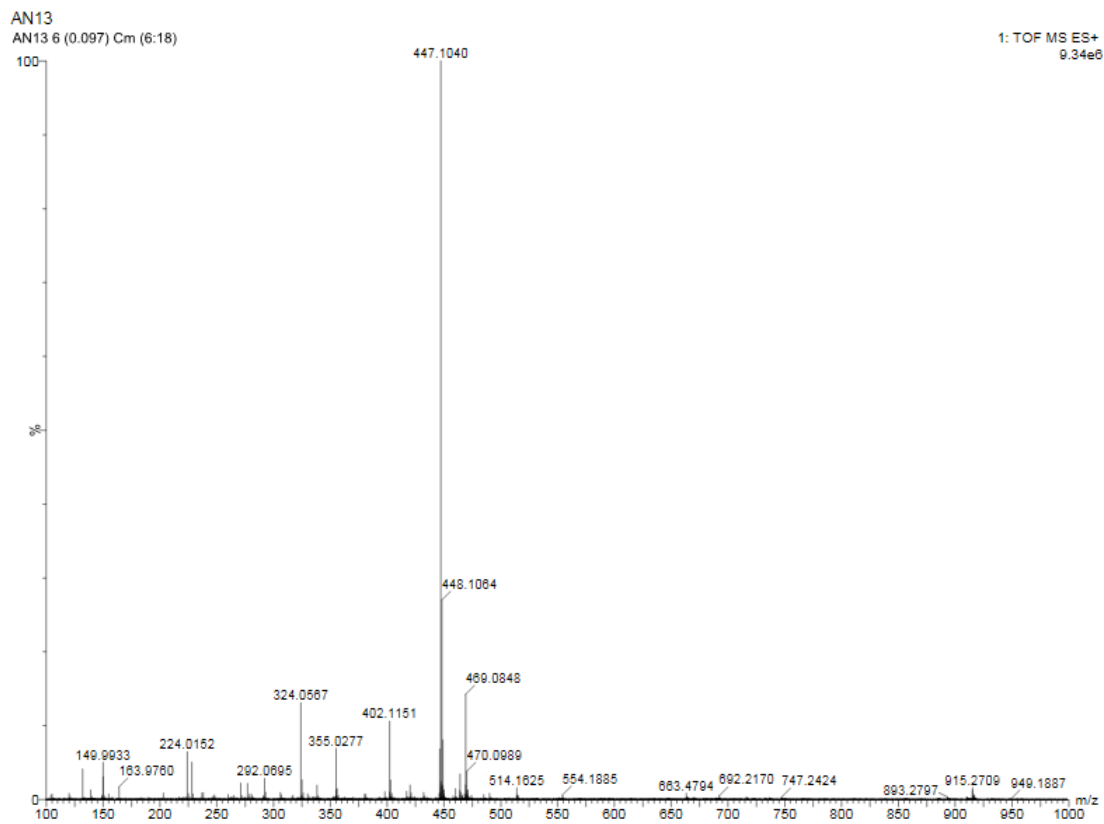




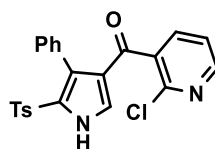
# HRMS



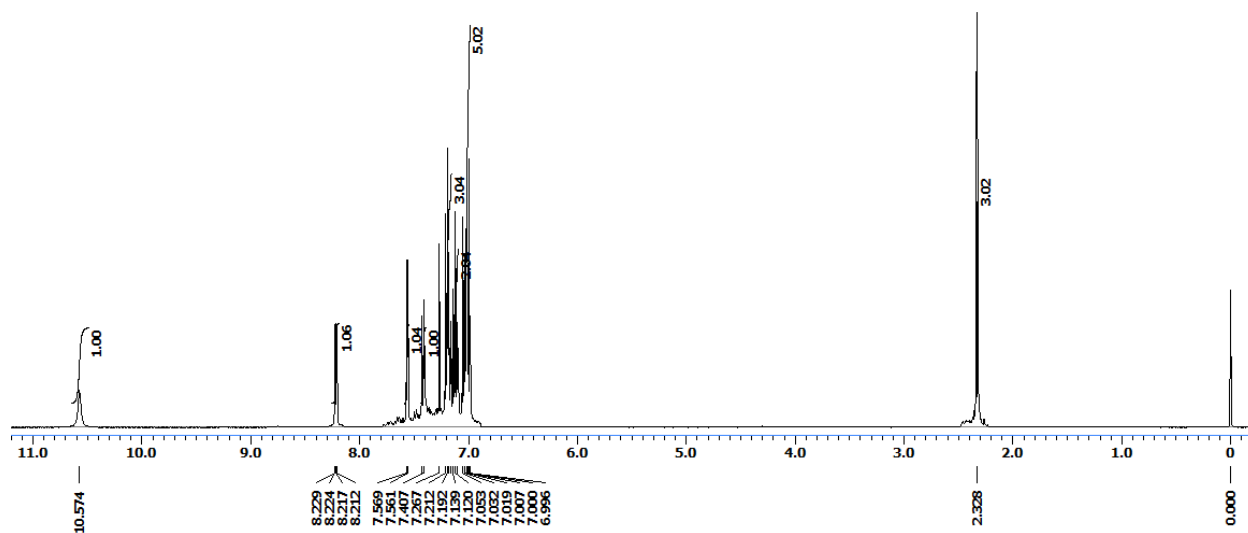
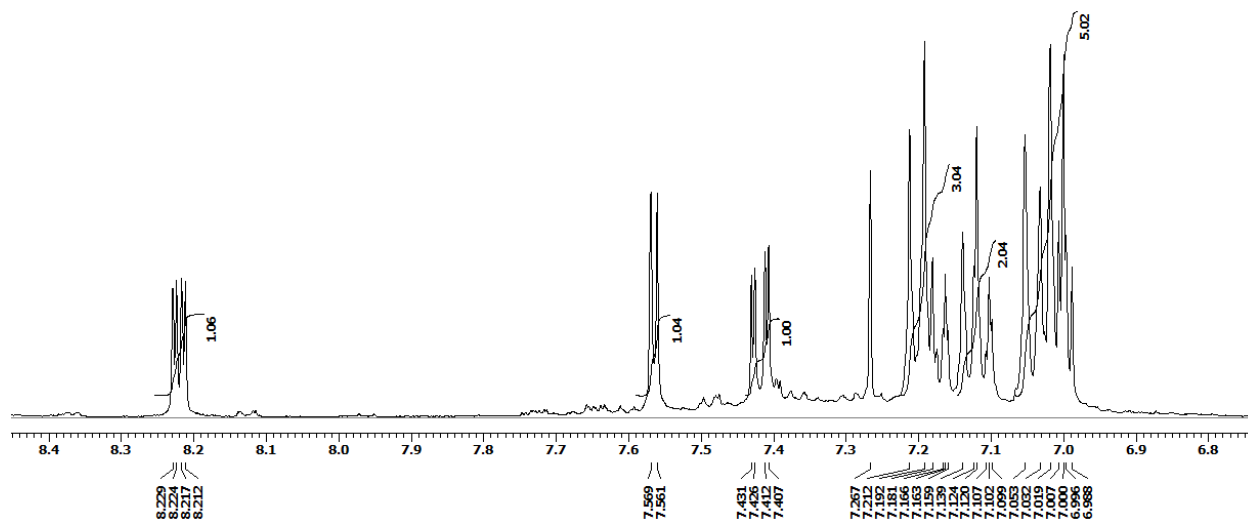
**(4-Nitrophenyl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3z)**



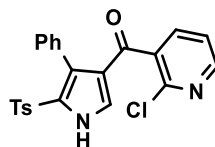
# <sup>1</sup>H NMR



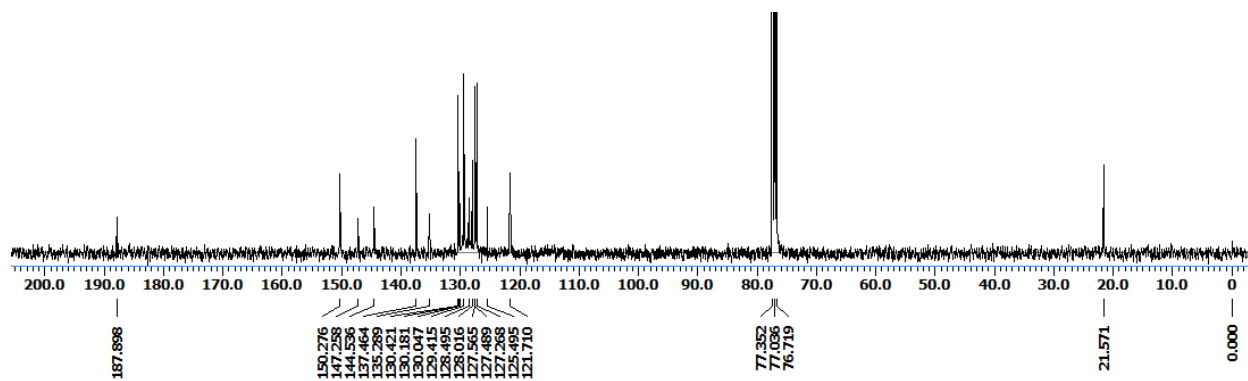
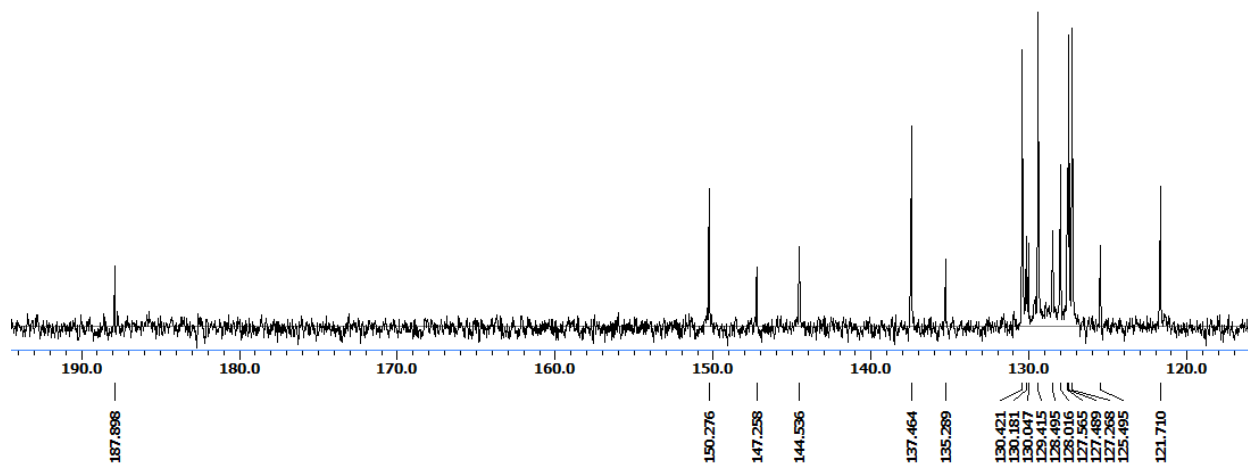
(2-Chloropyridin-3-yl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3aa)



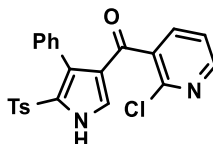
<sup>13</sup>C NMR



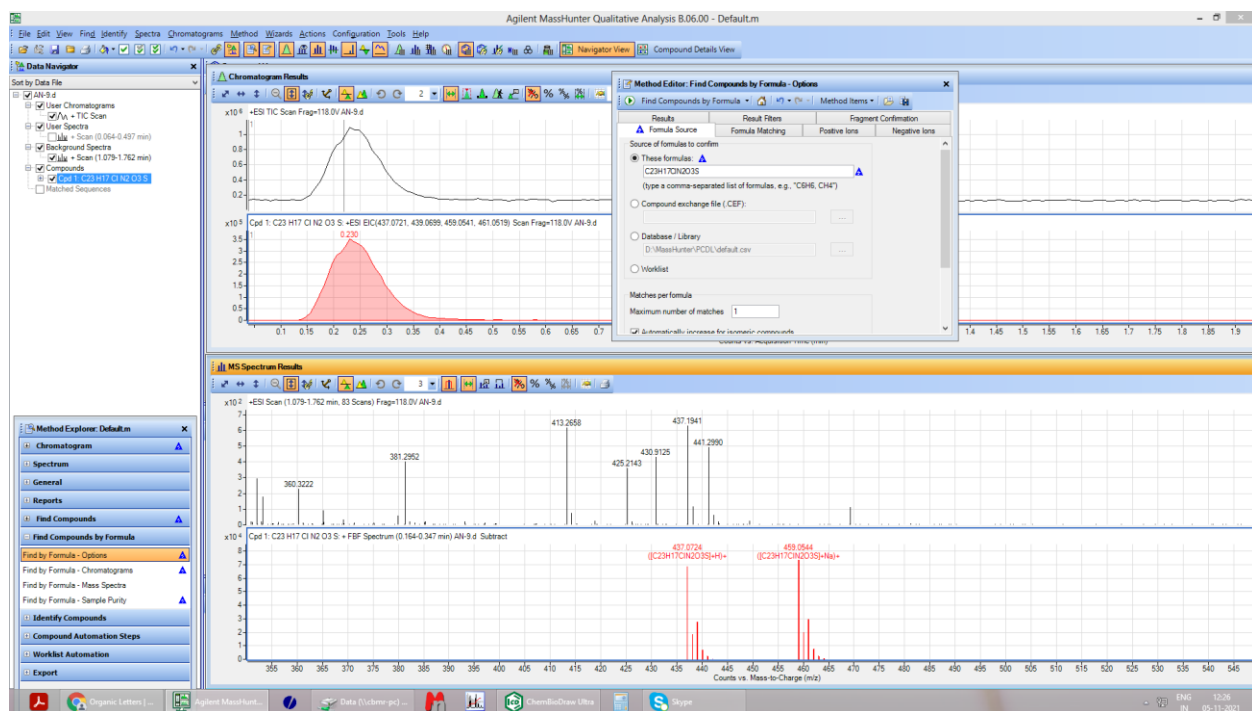
(2-Chloropyridin-3-yl)(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3aa)



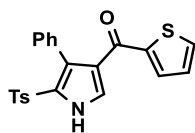
# HRMS



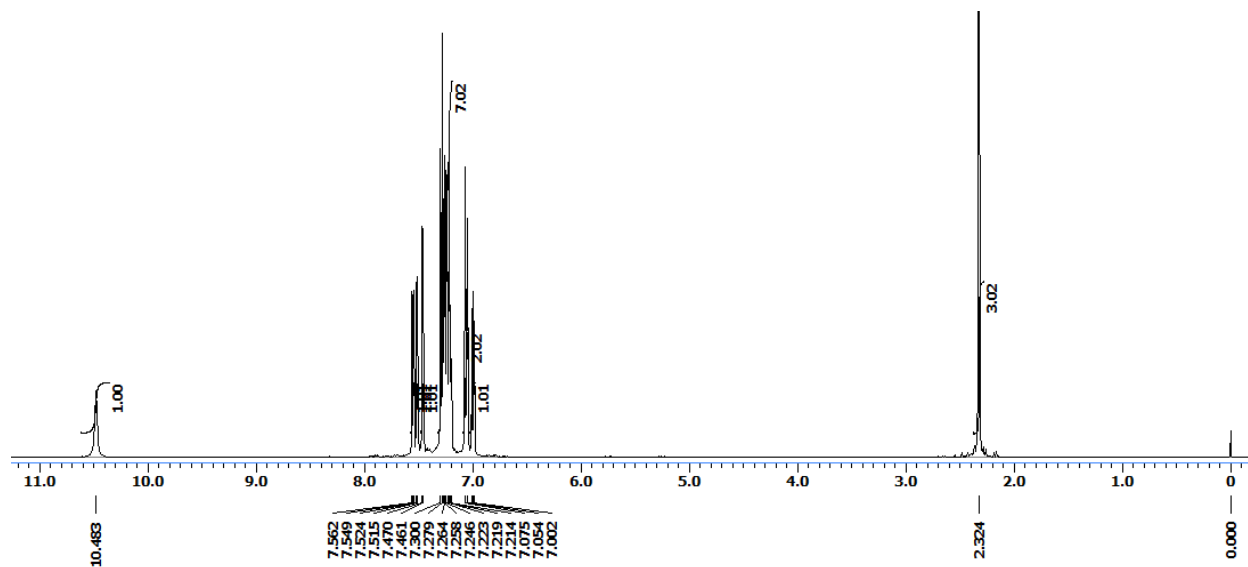
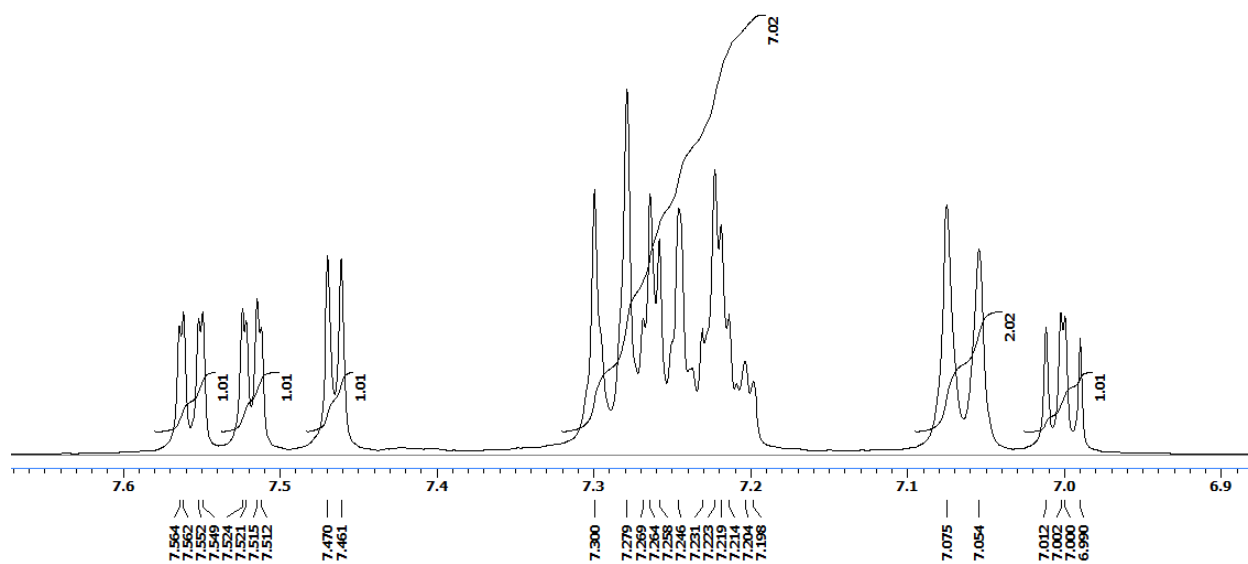
(2-Chloropyridin-3-yl)(4-phenyl-5-tosyl-1*H*-pyrrol-3-yl)methanone (3aa)



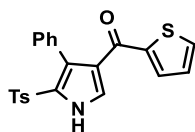
# <sup>1</sup>H NMR



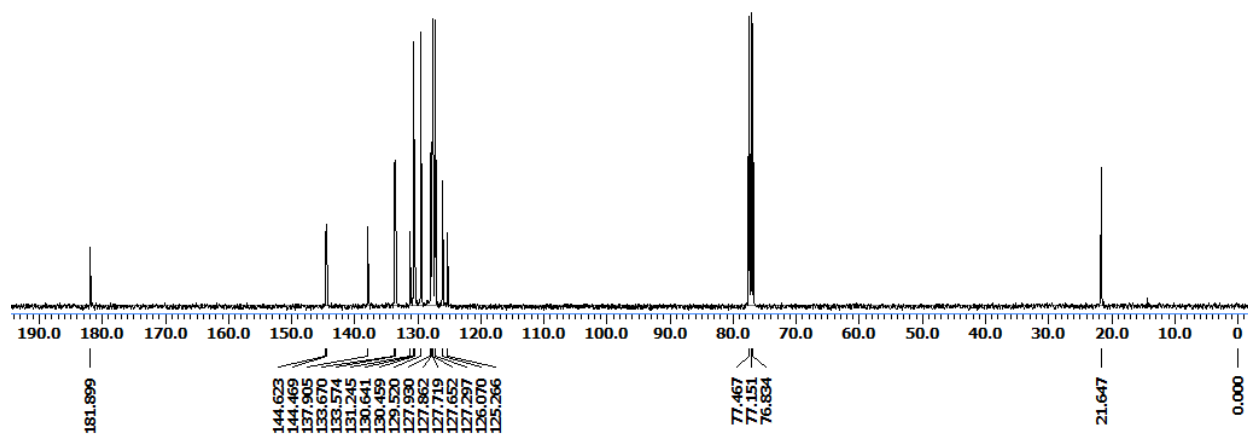
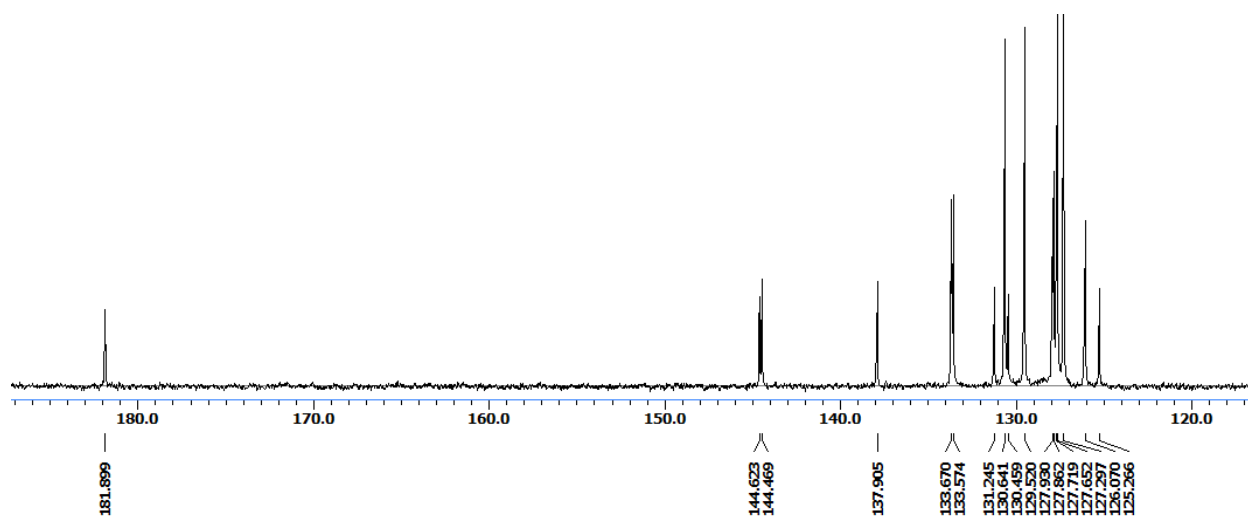
(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3ab)



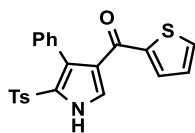
<sup>13</sup>C NMR



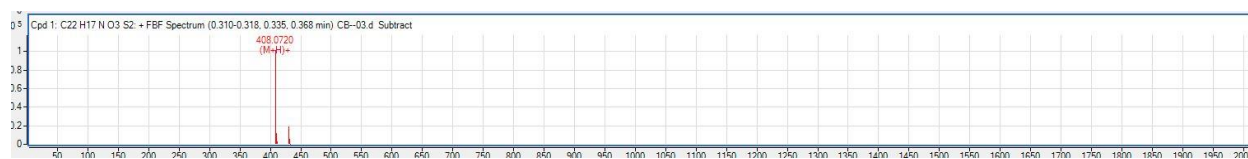
(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3ab)



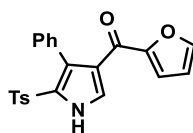
## HRMS



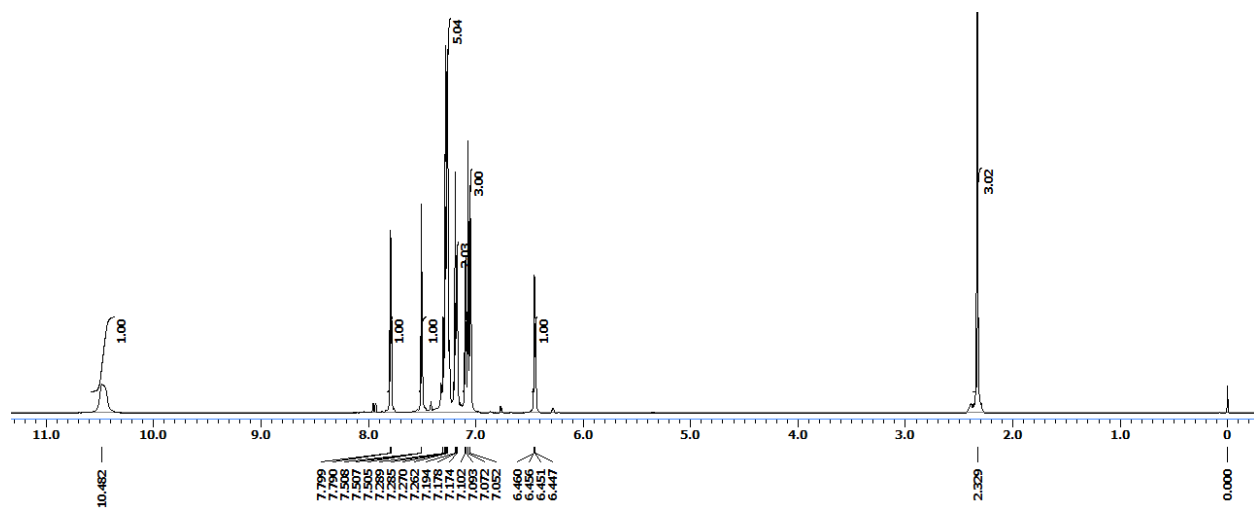
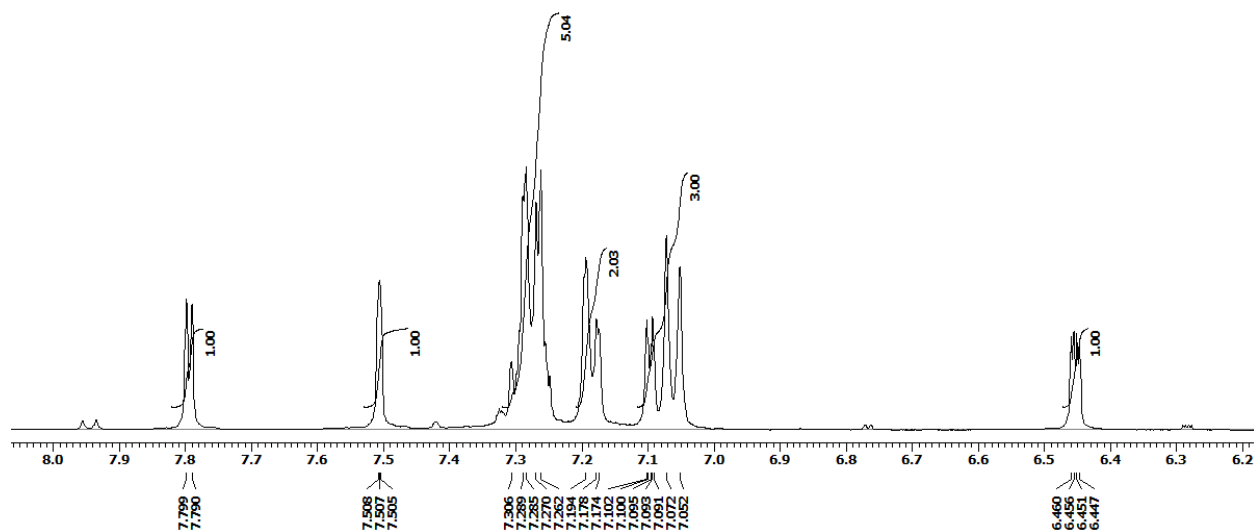
**(4-Phenyl-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3ab)**



<sup>1</sup>H NMR

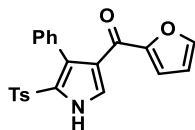


Furan-2-yl(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3ac)

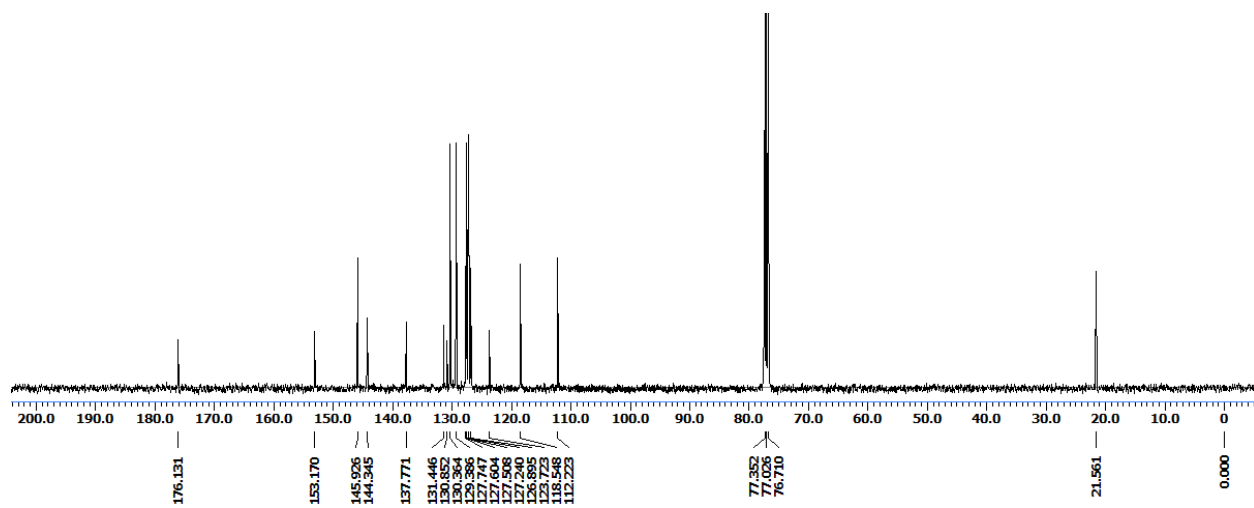
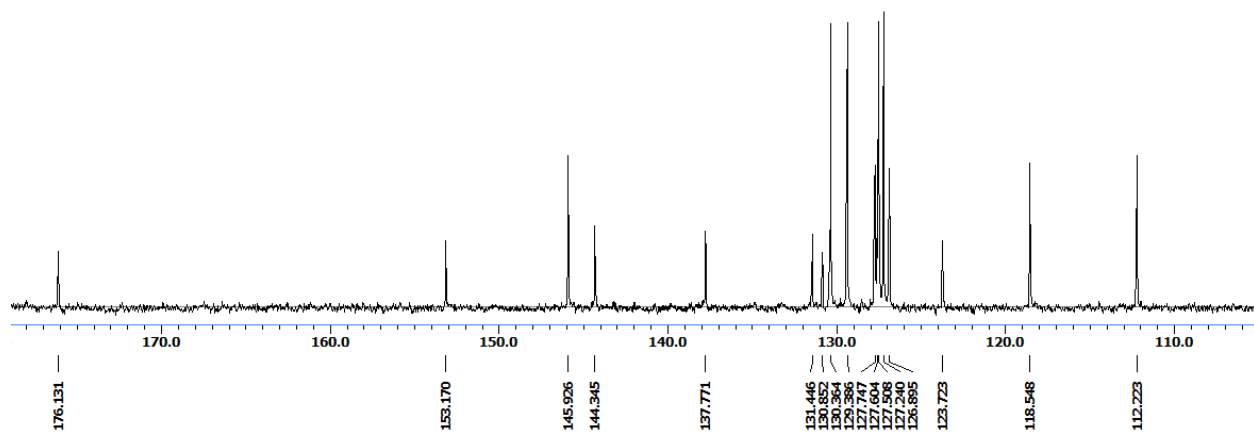




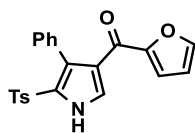
<sup>13</sup>C NMR



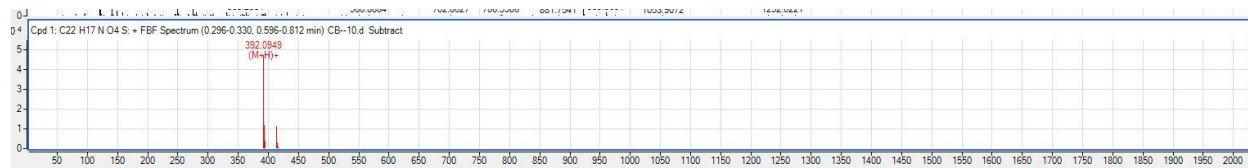
Furan-2-yl(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3ac)



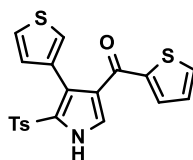
## HRMS



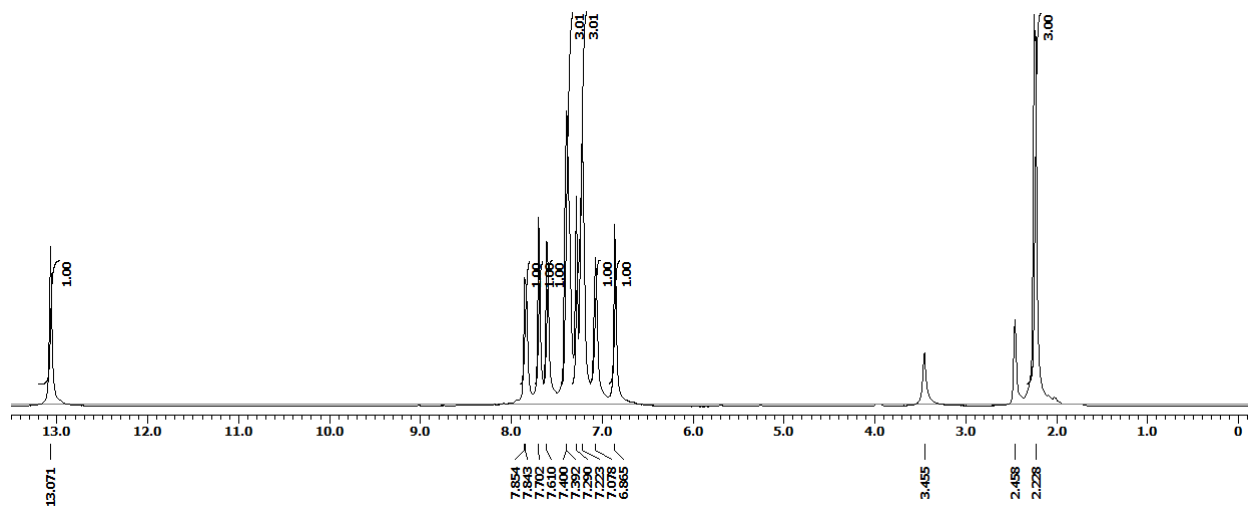
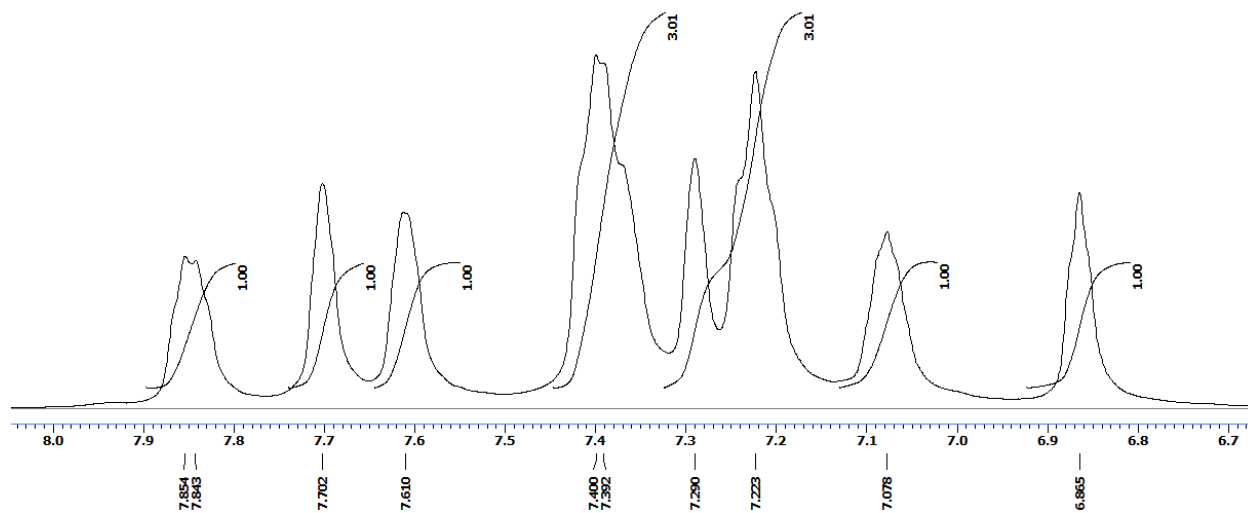
**Furan-2-yl(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (3ac)**



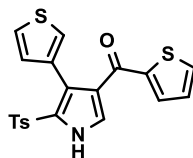
# <sup>1</sup>H NMR



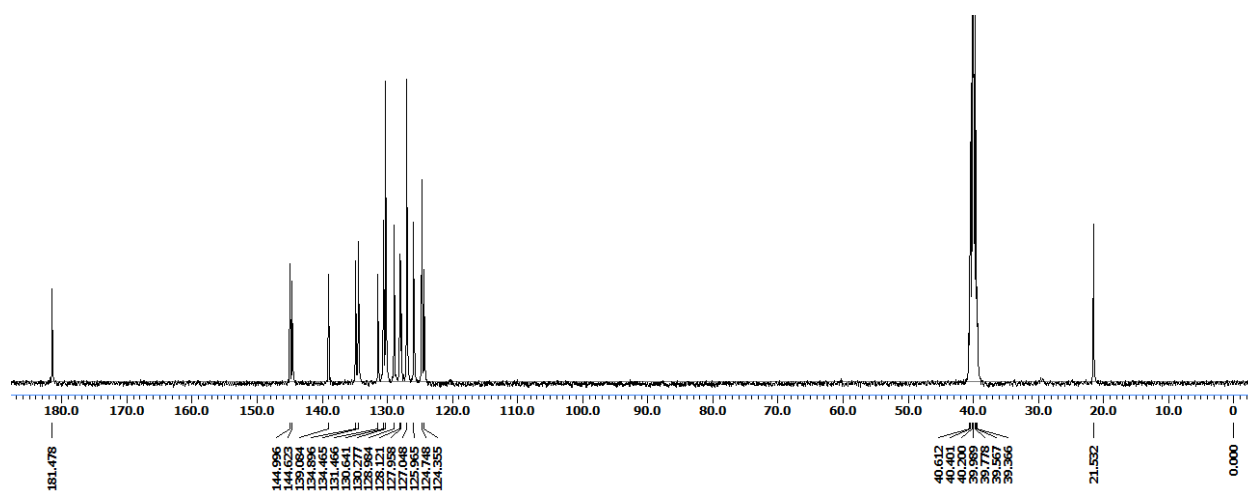
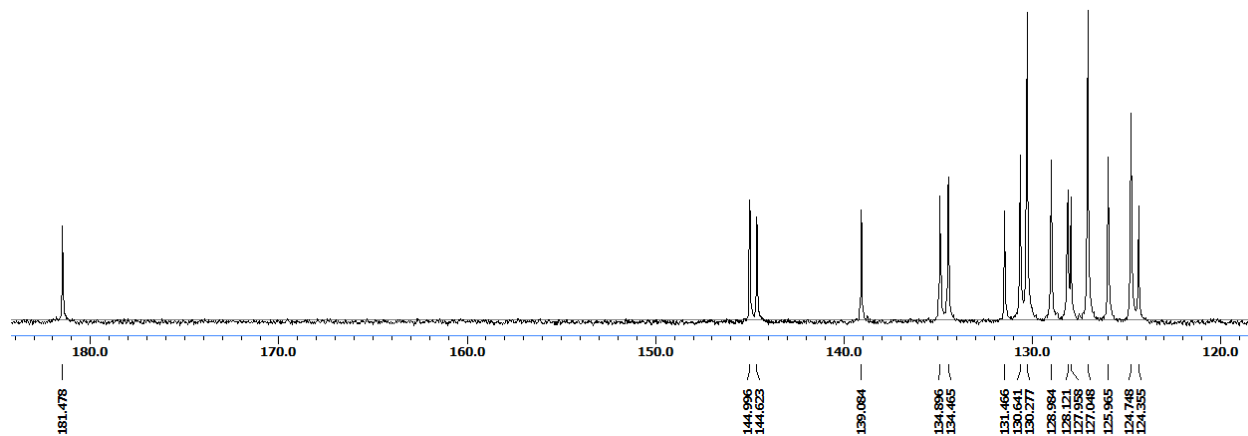
Thiophen-2-yl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3ad)



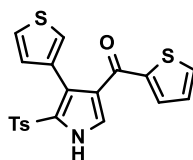
<sup>13</sup>C NMR



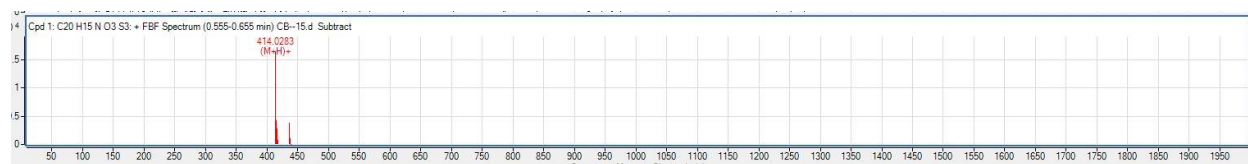
Thiophen-2-yl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3ad)



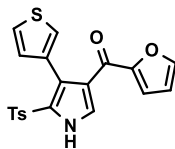
## HRMS



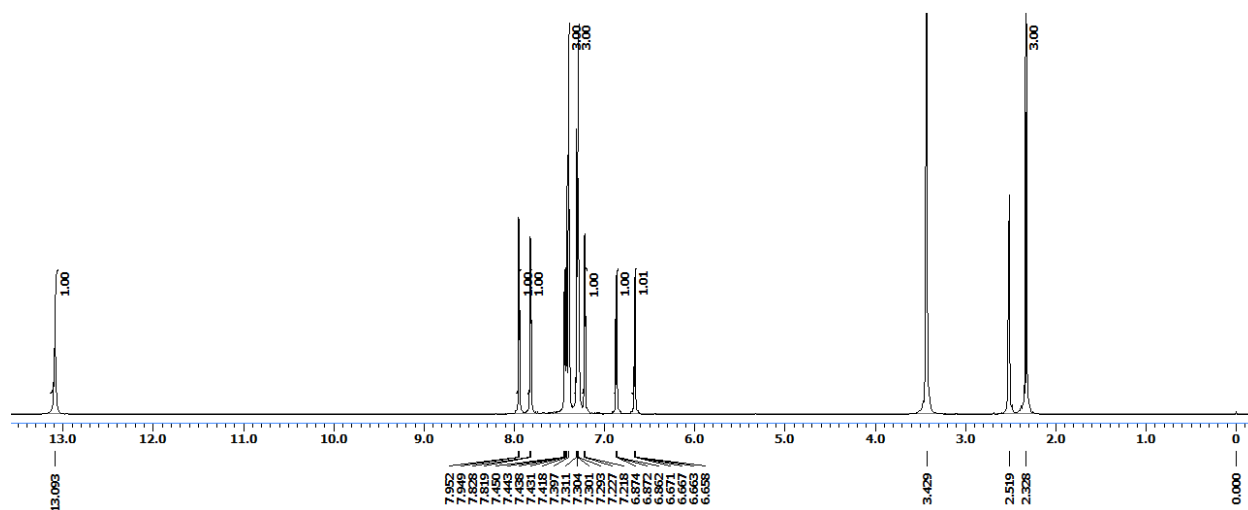
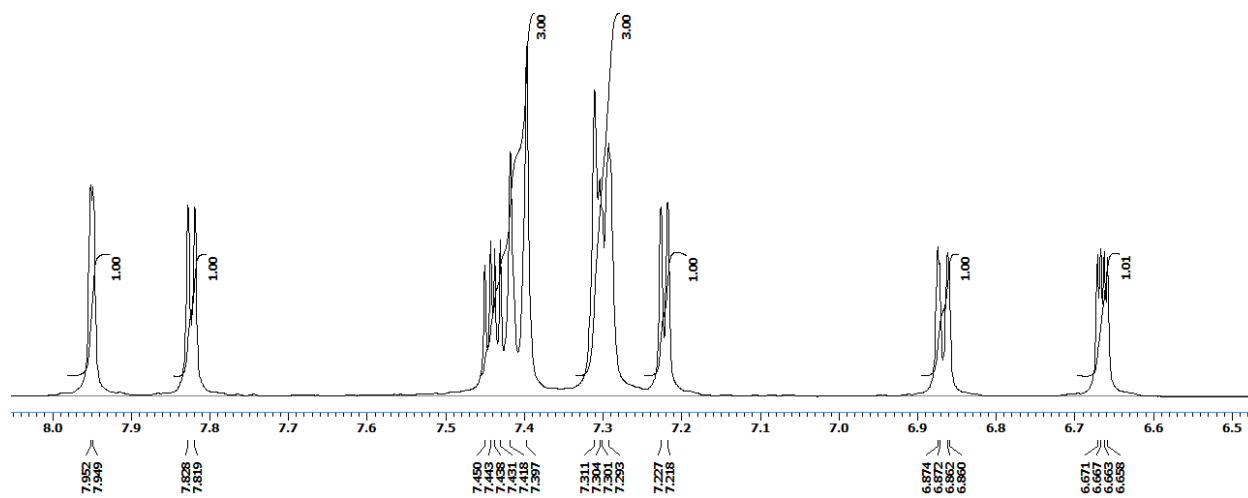
**Thiophen-2-yl(4-(thiophen-3-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (3ad)**



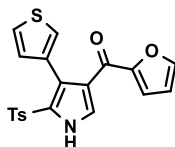
# <sup>1</sup>H NMR



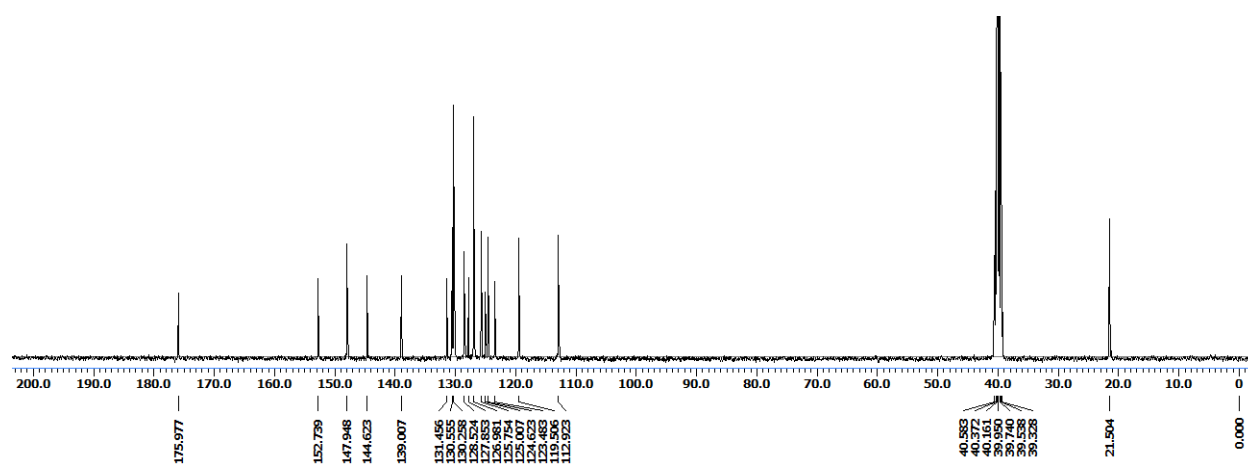
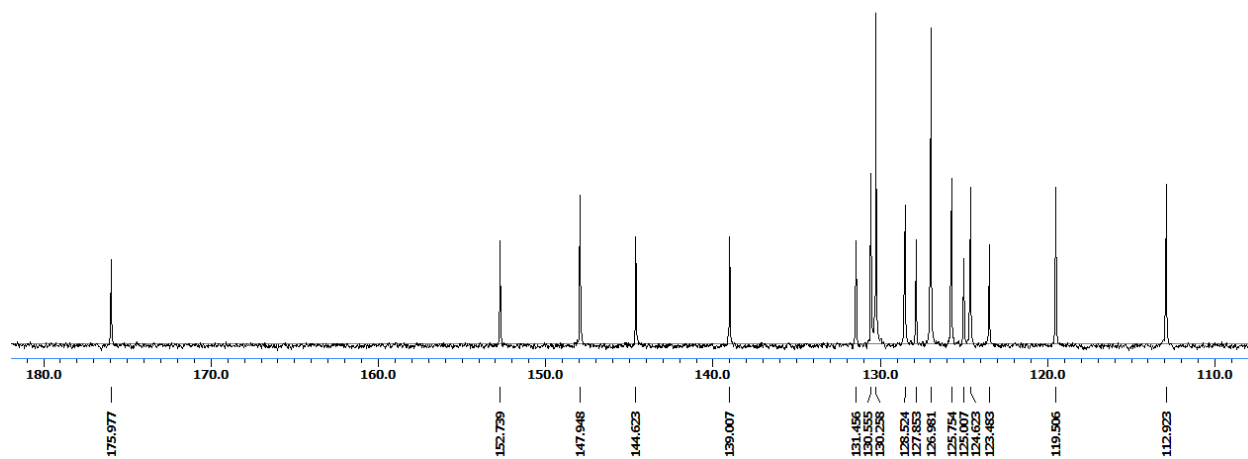
Furan-2-yl(4-(thiophen-3-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (3ae)



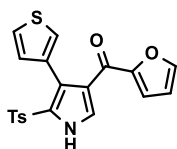
<sup>13</sup>C NMR



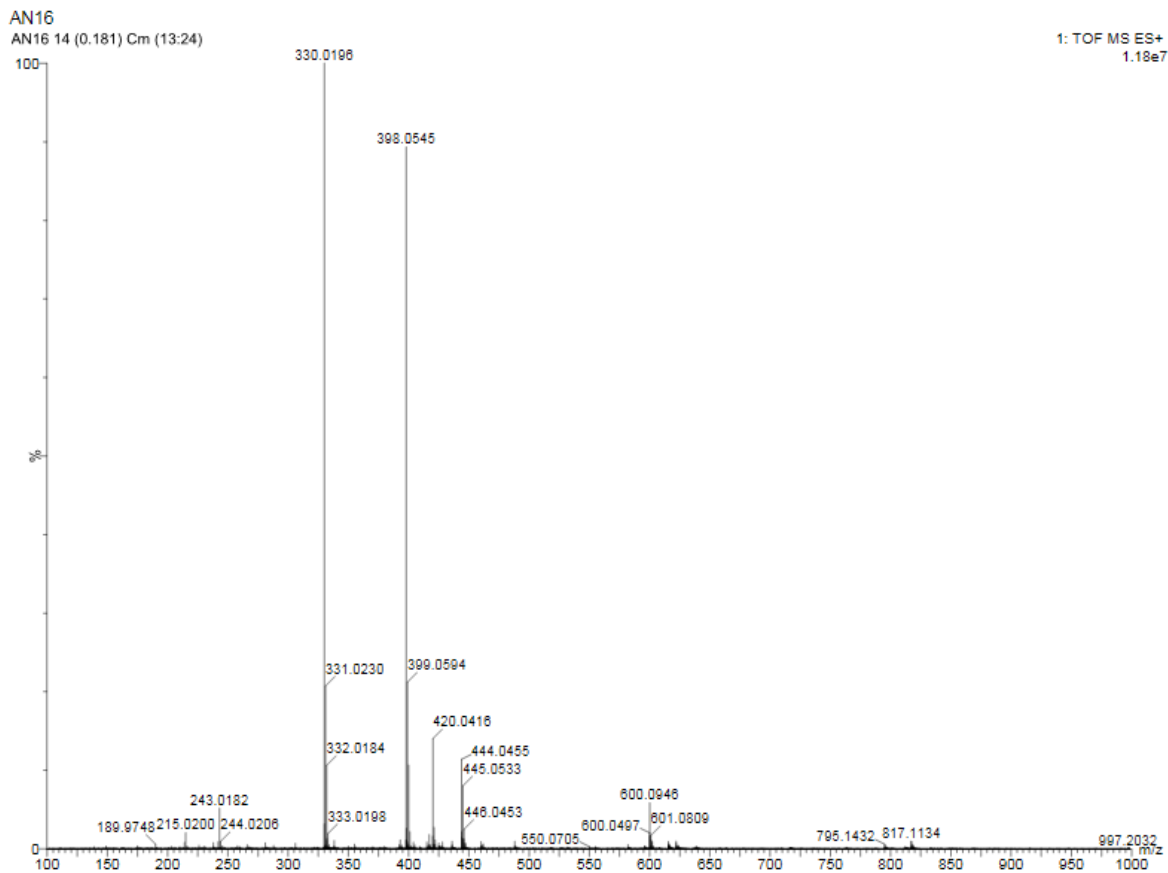
Furan-2-yl(4-(thiophen-3-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (3ae)



# HRMS

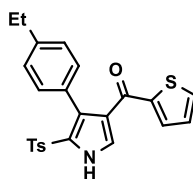


**Furan-2-yl(4-(thiophen-3-yl)-5-tosyl-1*H*-pyrrol-3-yl)methanone (3ae)**

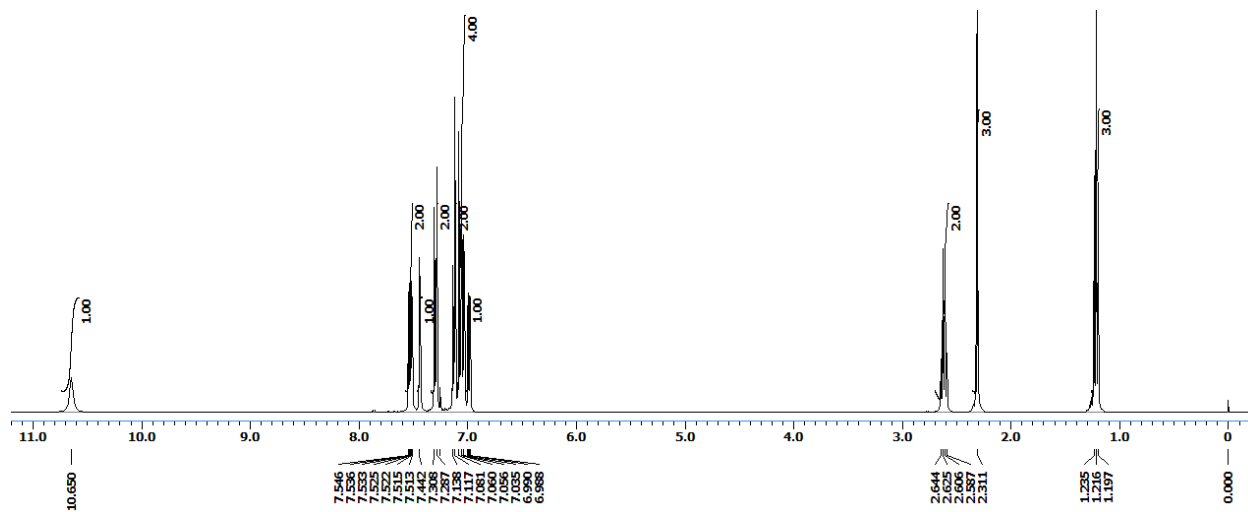
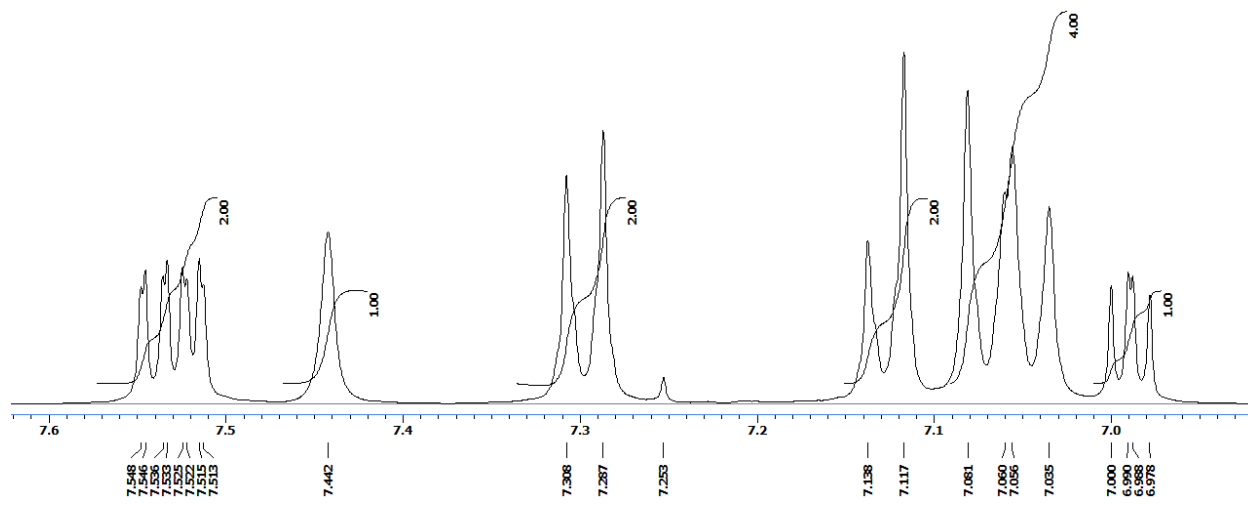




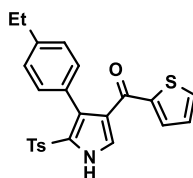
# <sup>1</sup>H NMR



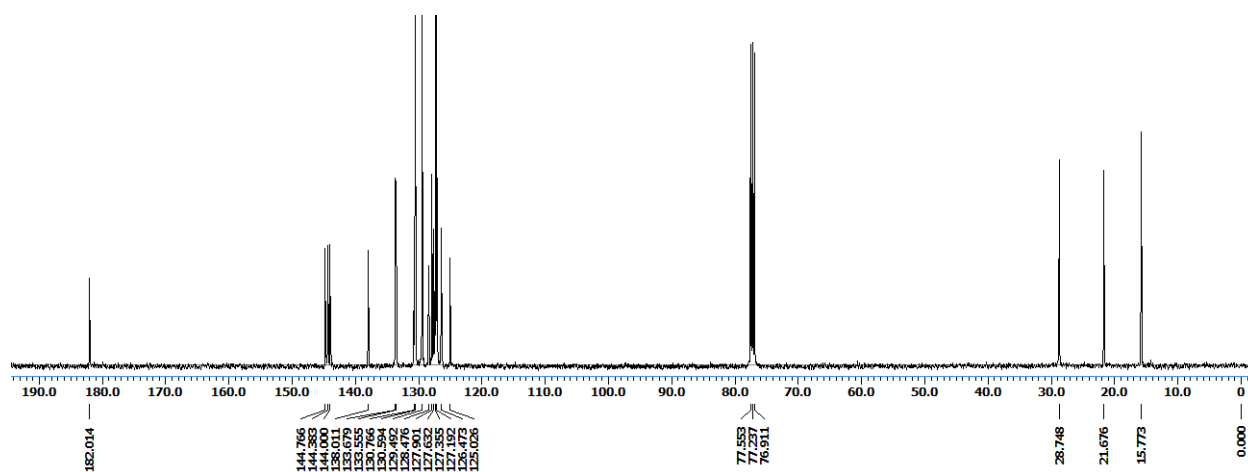
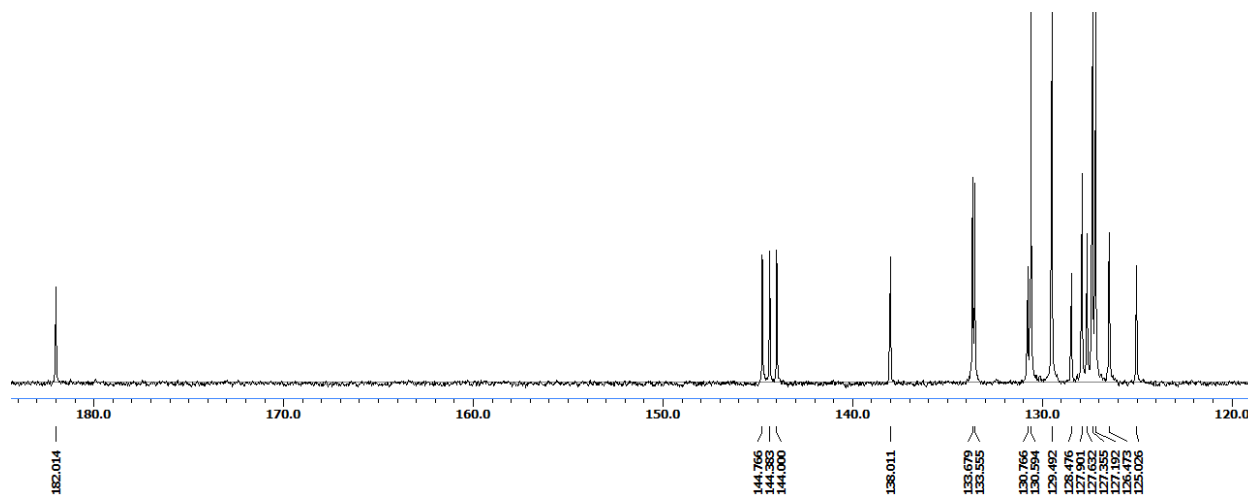
(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3af)



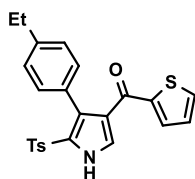
<sup>13</sup>C NMR



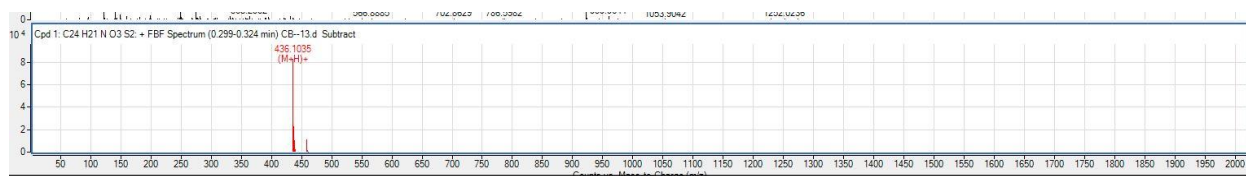
(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3af)



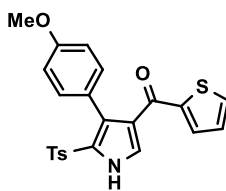
## HRMS



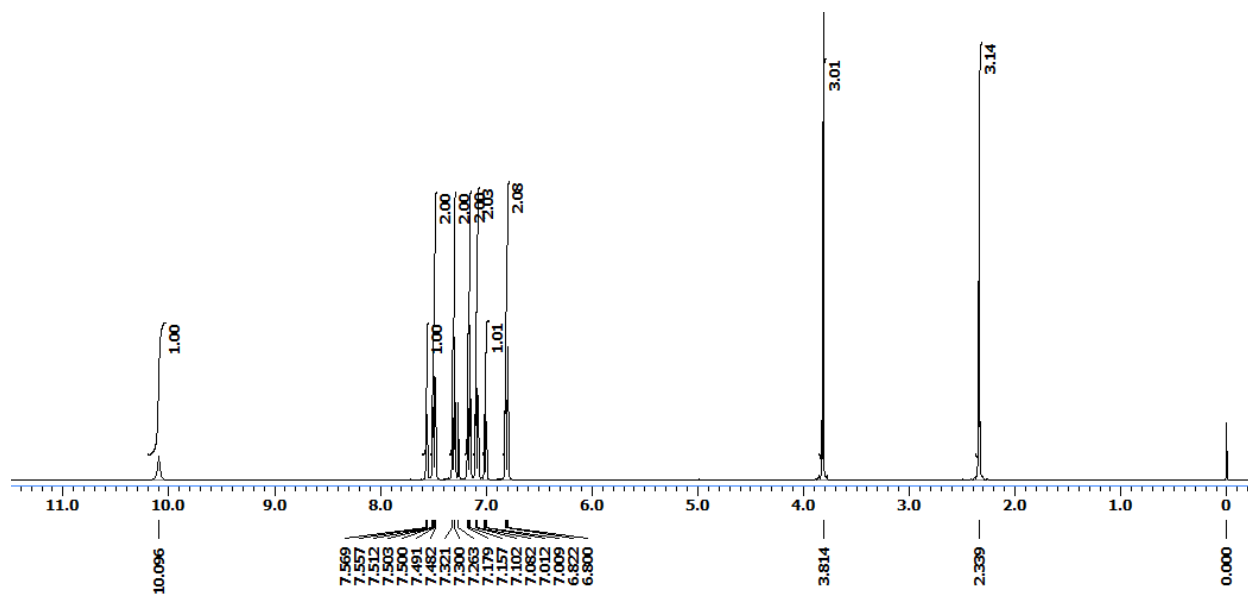
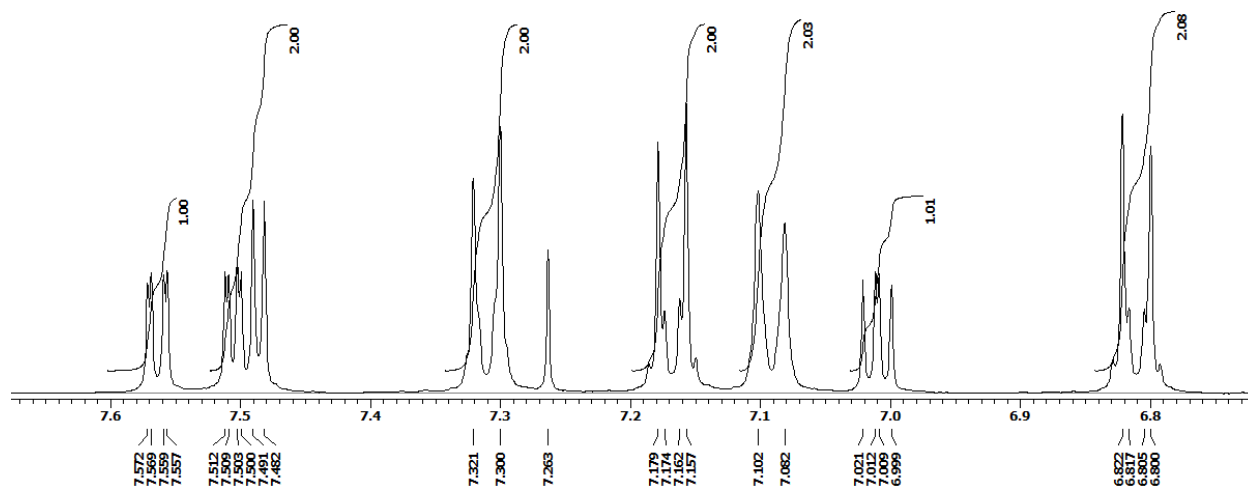
**(4-(4-Ethylphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3af)**



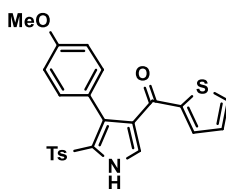
# <sup>1</sup>H NMR



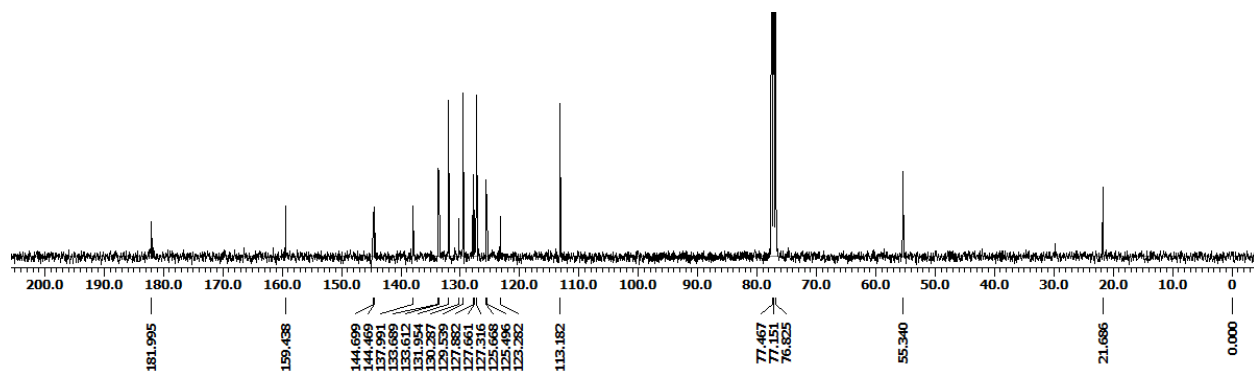
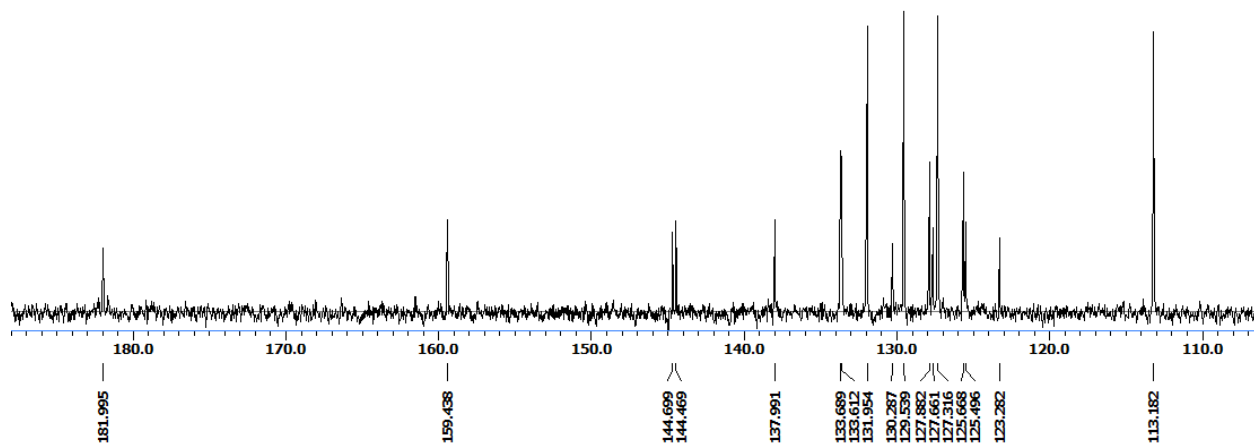
(4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3ag)



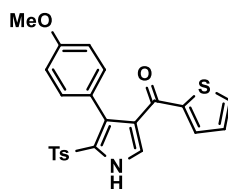
<sup>13</sup>C NMR



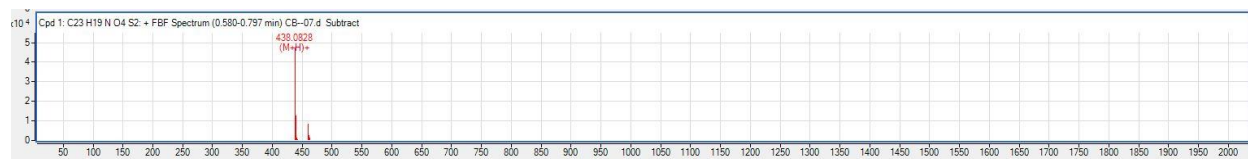
(4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3ag)



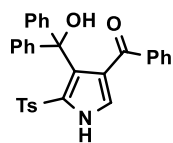
## HRMS



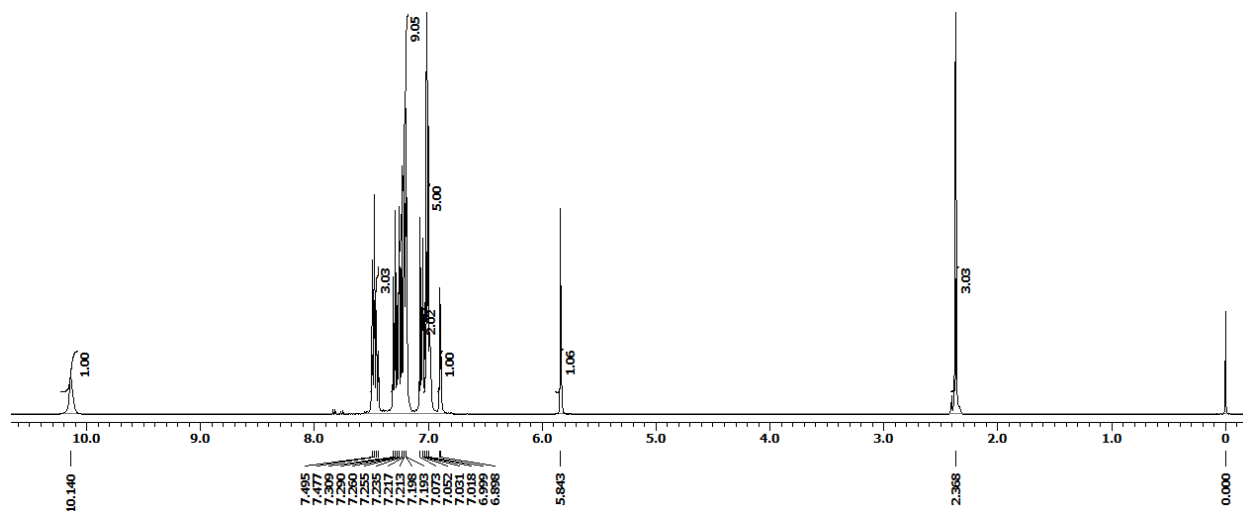
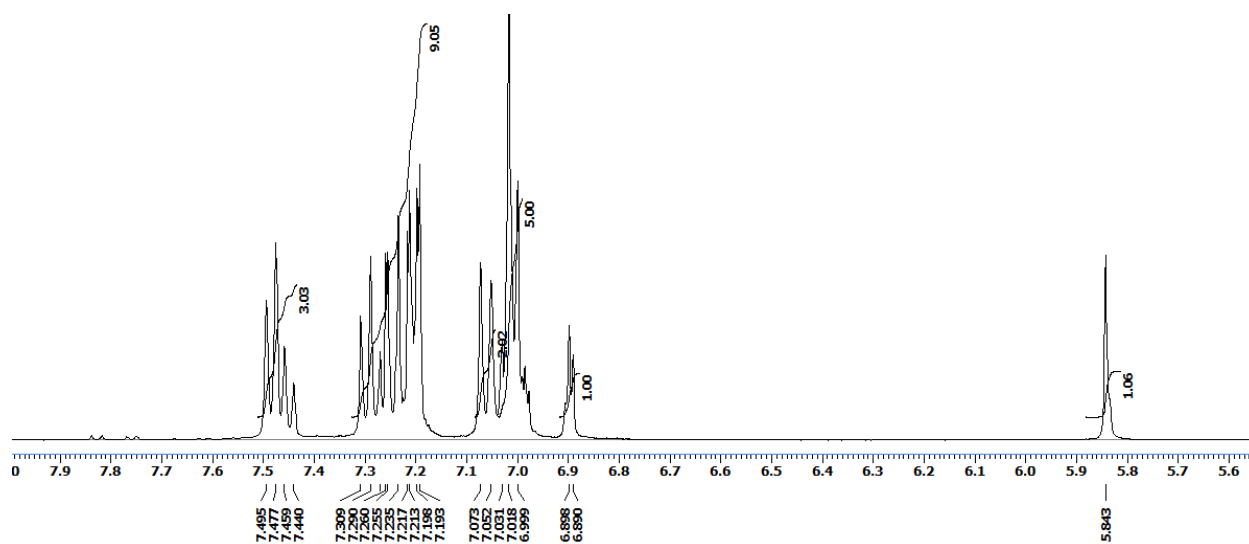
**(4-(4-Methoxyphenyl)-5-tosyl-1H-pyrrol-3-yl)(thiophen-2-yl)methanone (3ag)**



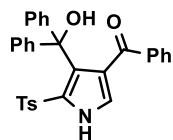
<sup>1</sup>H NMR



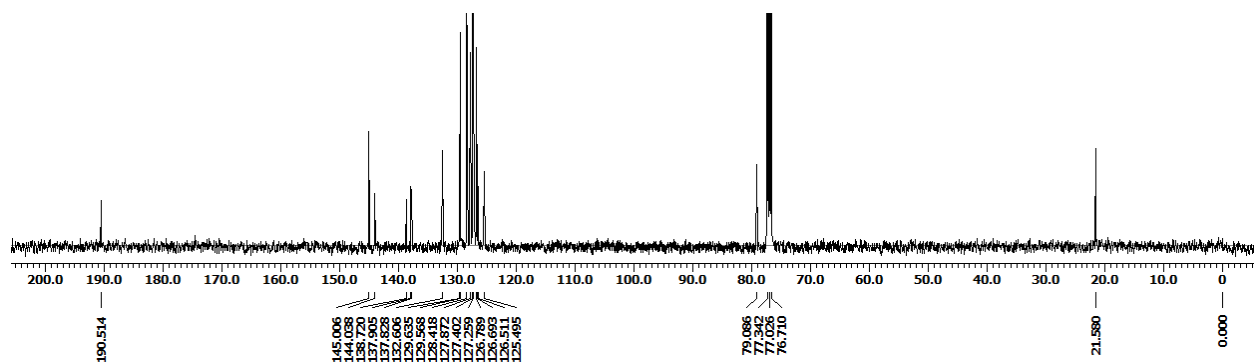
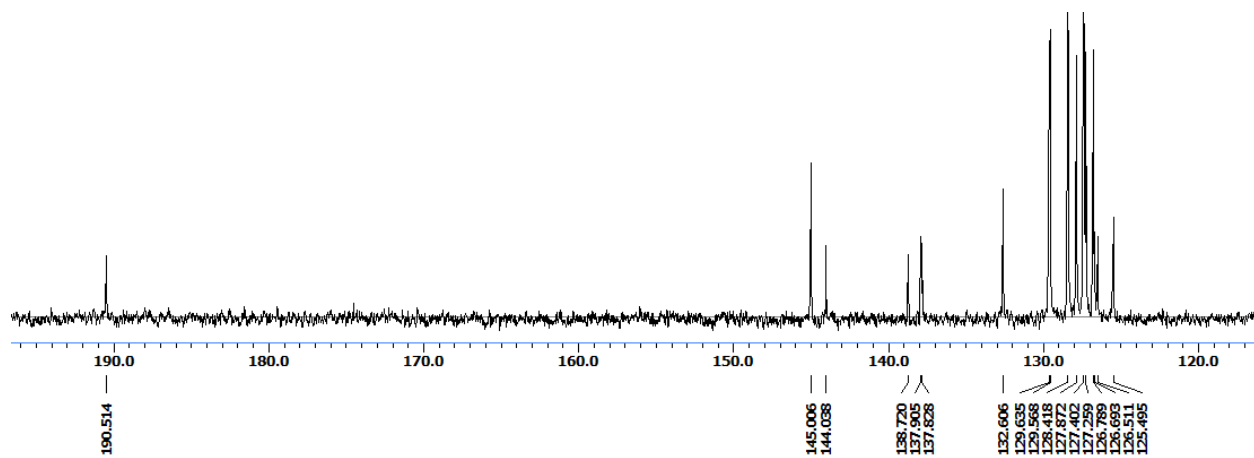
(4-(Hydroxydiphenylmethyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3ah)



<sup>13</sup>C NMR

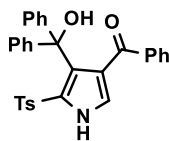


(4-(Hydroxydiphenylmethyl)-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (3ah)

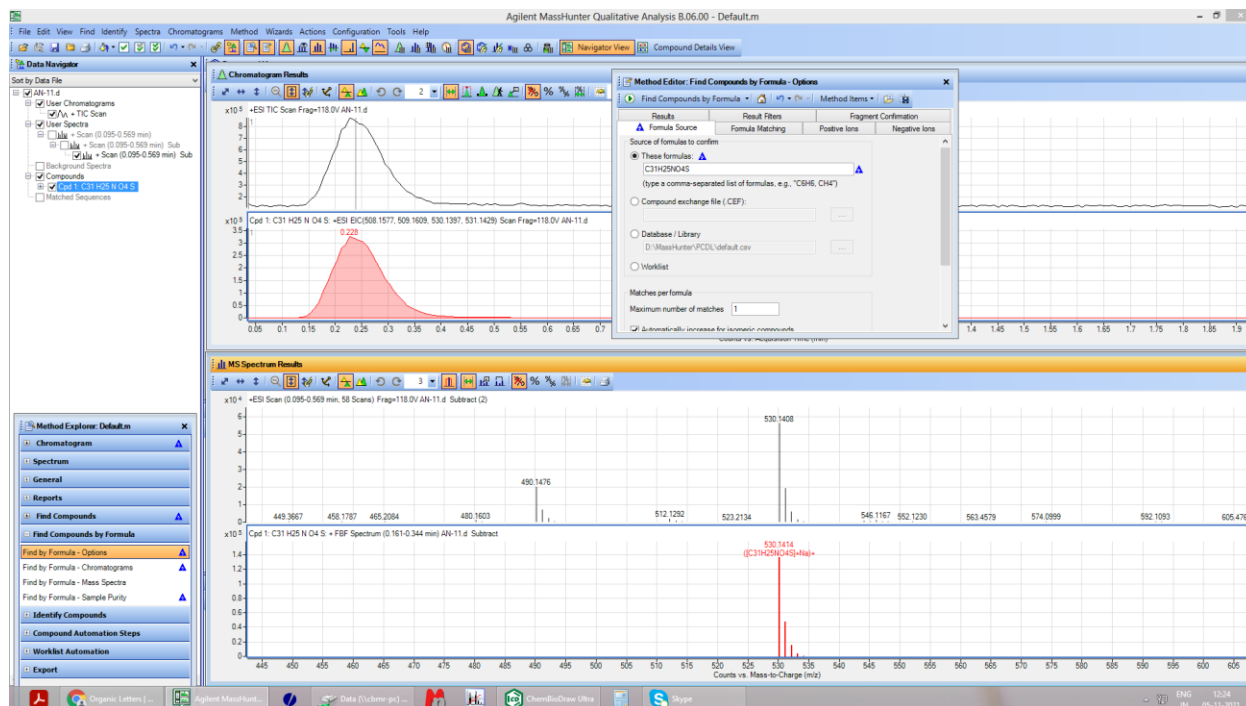




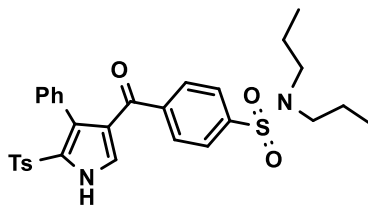
# HRMS



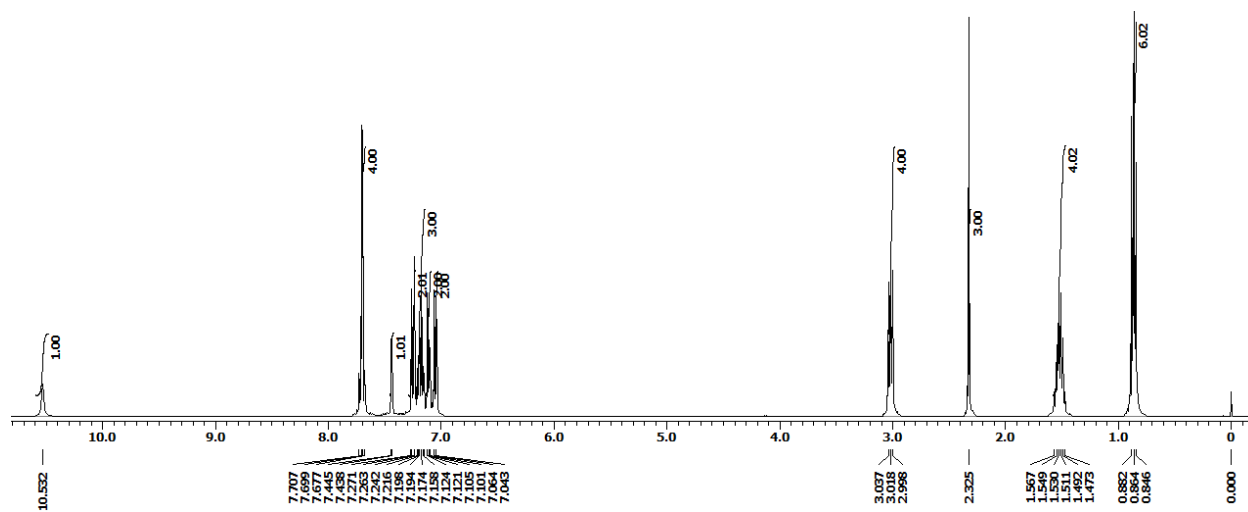
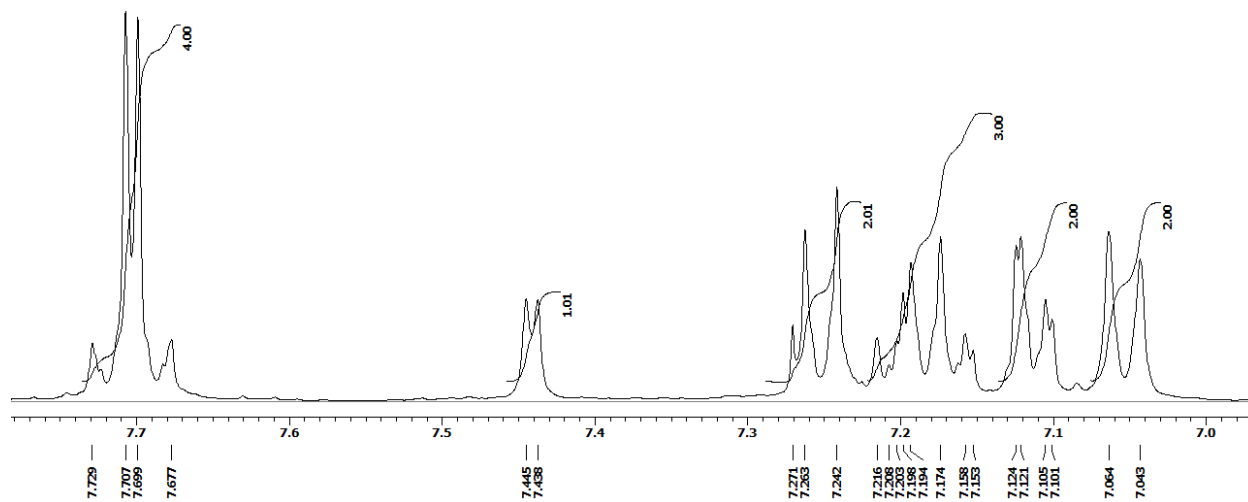
(4-(Hydroxydiphenylmethyl)-5-tosyl-1*H*-pyrrol-3-yl)(phenyl)methanone (3ah)



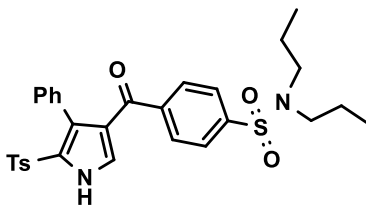
# <sup>1</sup>H NMR



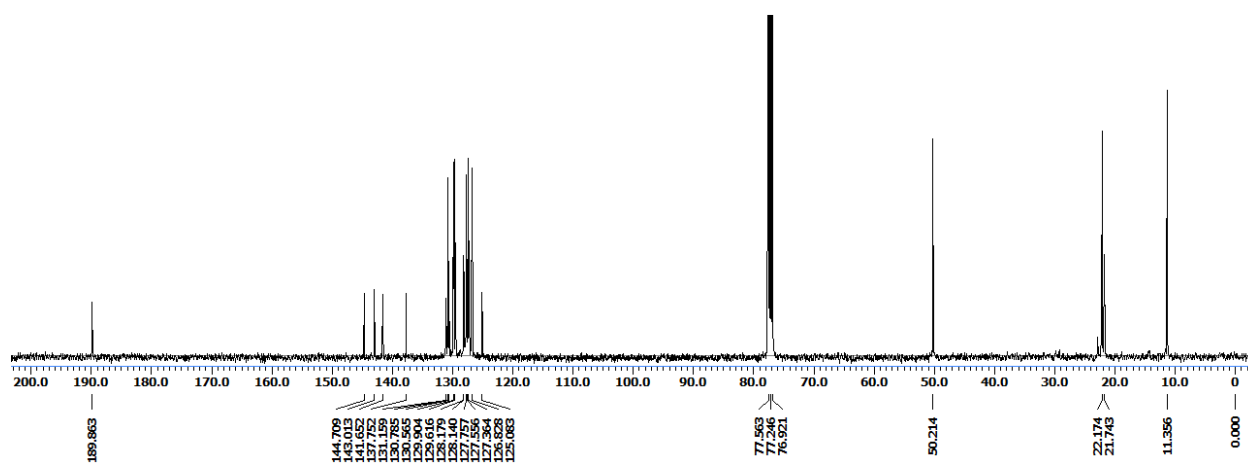
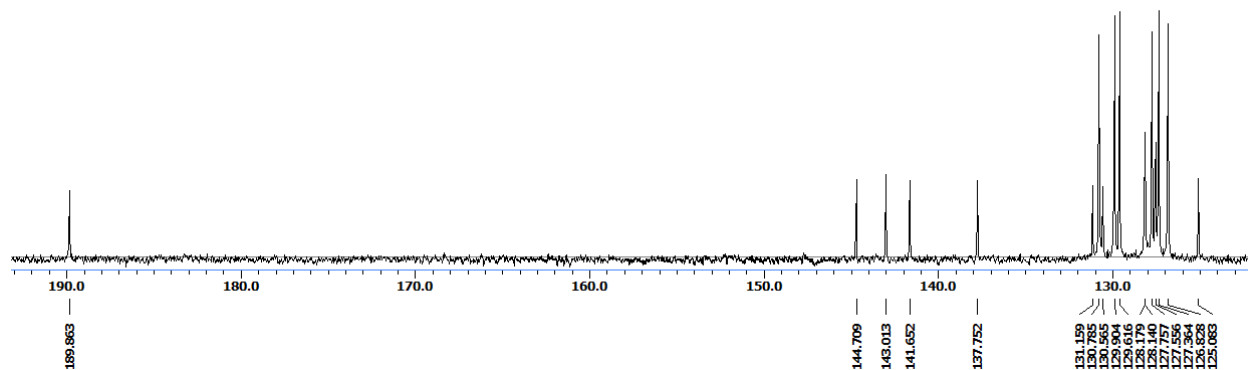
4-(4-Phenyl-5-tosyl-1H-pyrrole-3-carbonyl)-N,N-dipropylbenzenesulfonamide (3ai)



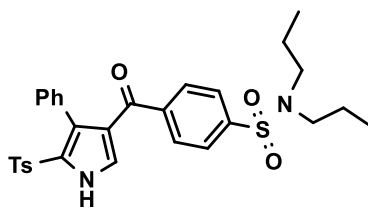
<sup>13</sup>C NMR



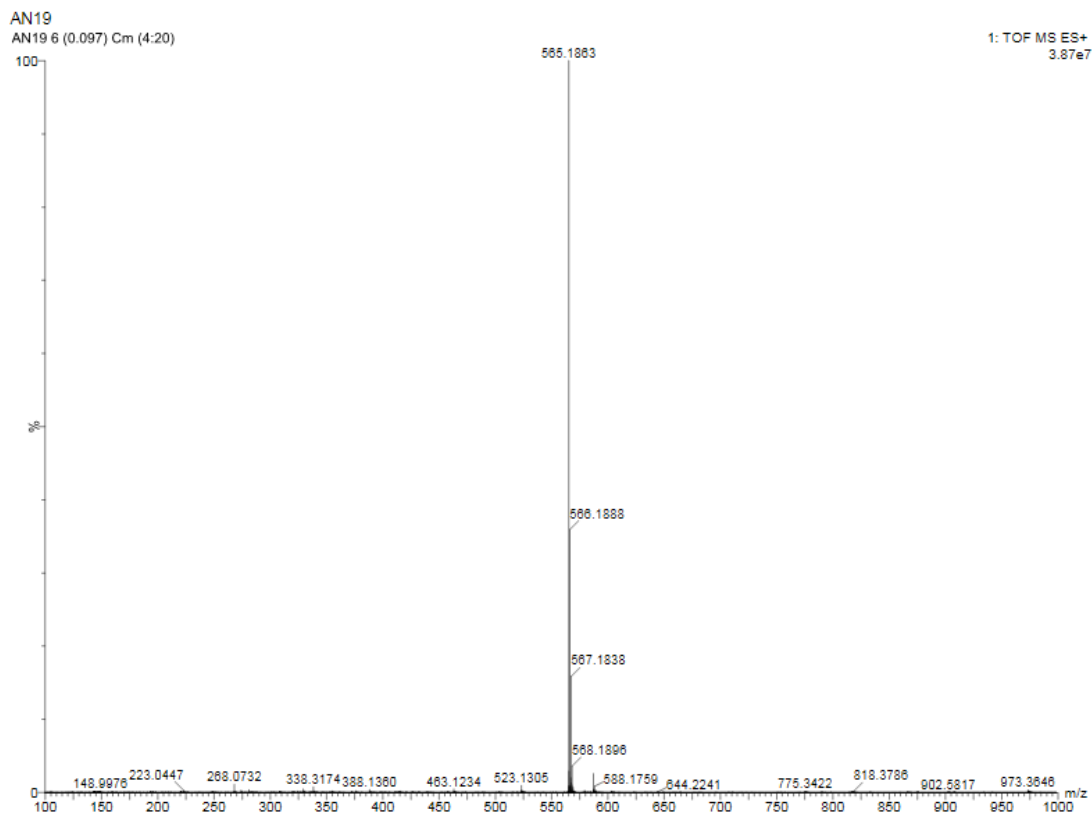
4-(4-Phenyl-5-tosyl-1H-pyrrole-3-carbonyl)-N,N-dipropylbenzenesulfonamide (3ai)



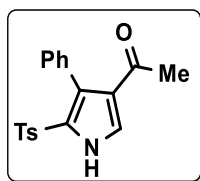
# HRMS



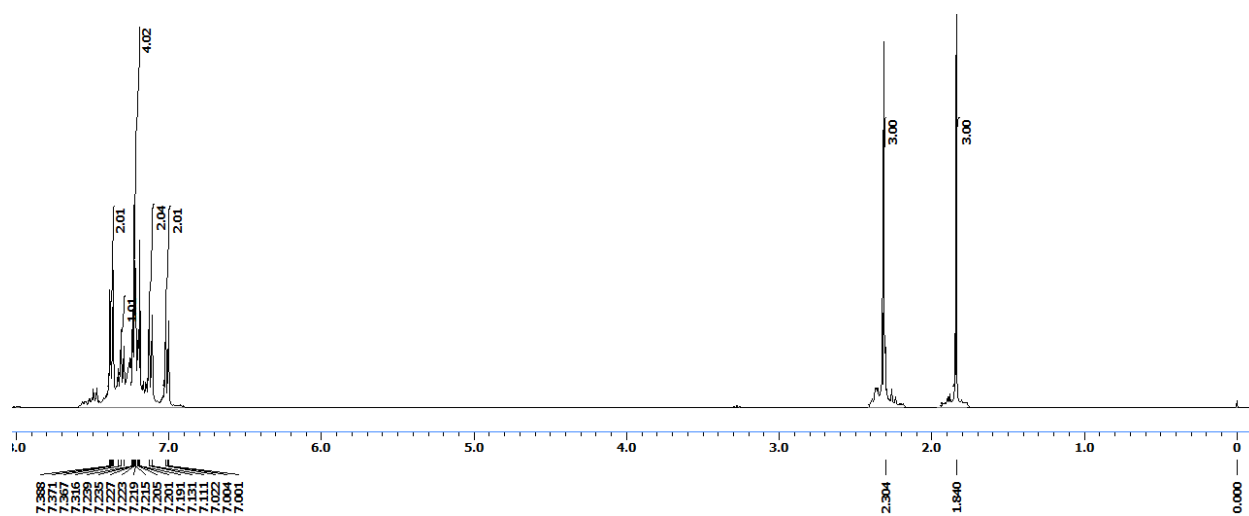
**4-(4-Phenyl-5-tosyl-1H-pyrrole-3-carbonyl)-N,N-dipropylbenzenesulfonamide (3ai)**



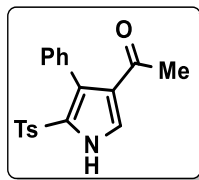
<sup>1</sup>H NMR



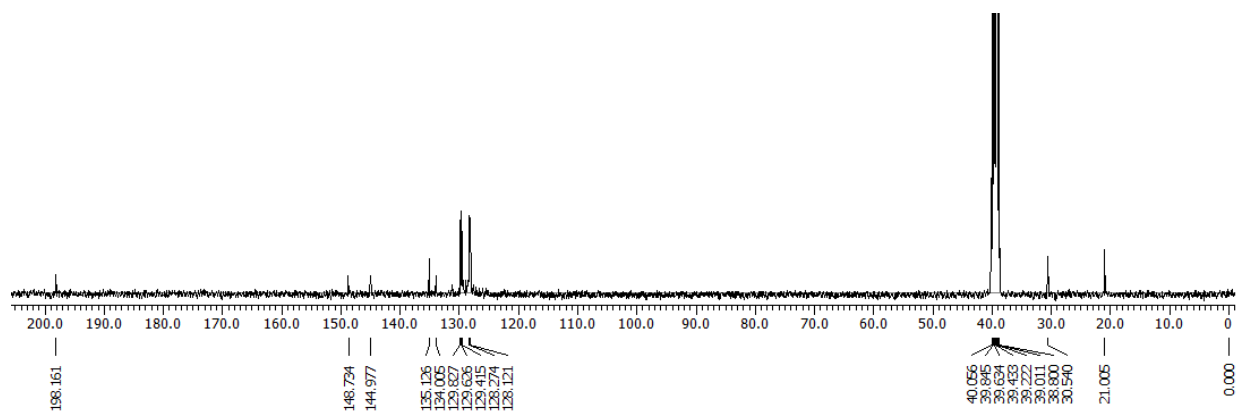
1-(4-phenyl-5-tosyl-1H-pyrrol-3-yl)ethan-1-one (3aj)



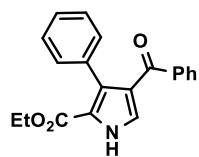
<sup>13</sup>C NMR



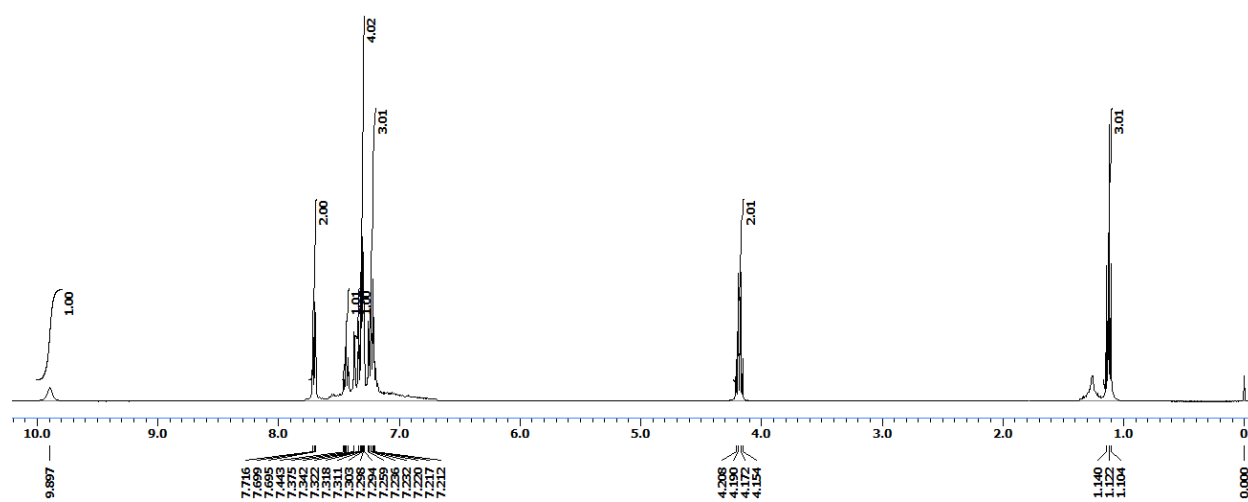
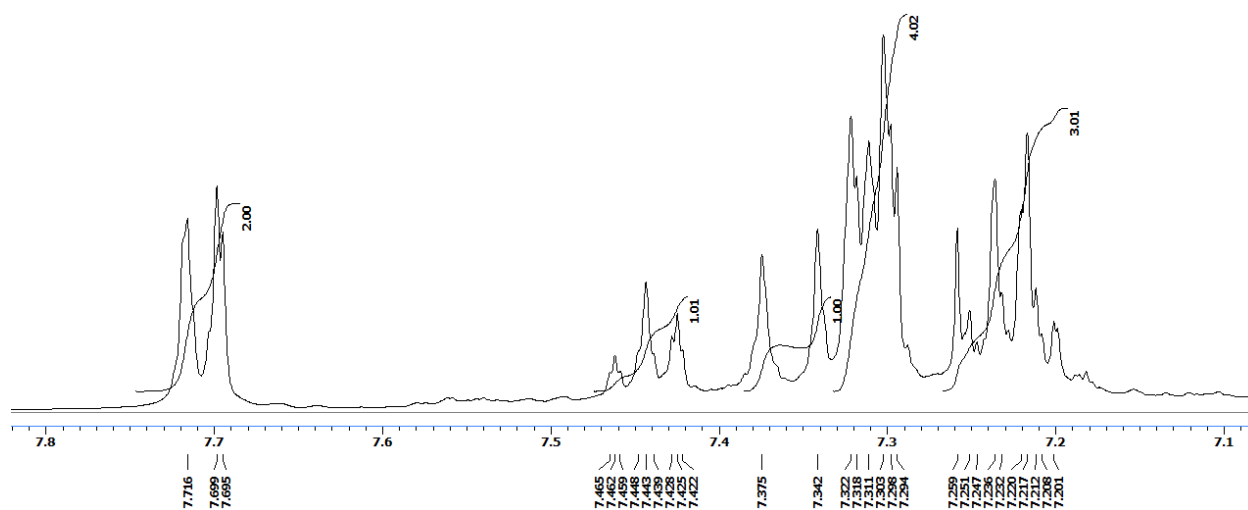
1-(4-phenyl-5-tosyl-1H-pyrrol-3-yl)ethan-1-one (3aj)



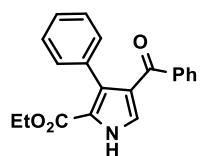
<sup>1</sup>H NMR



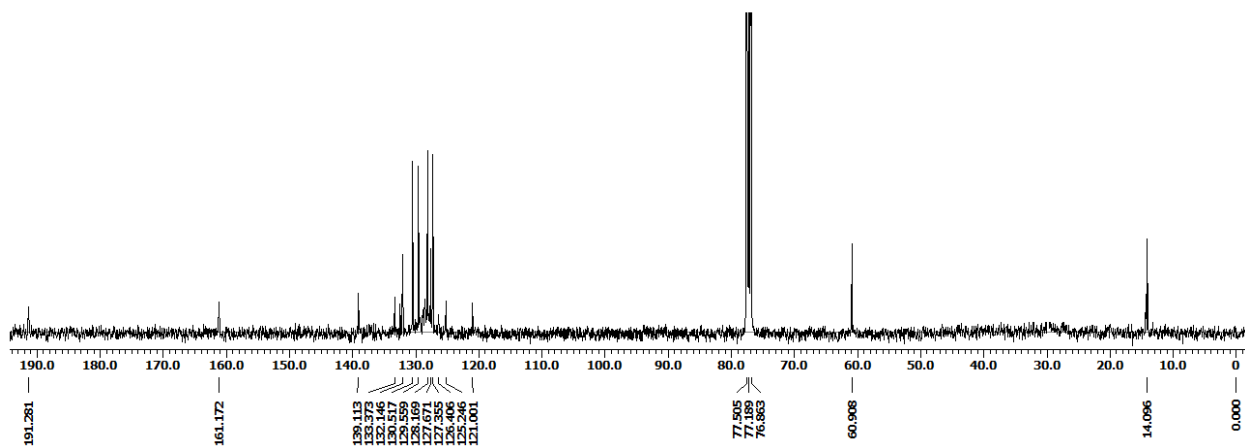
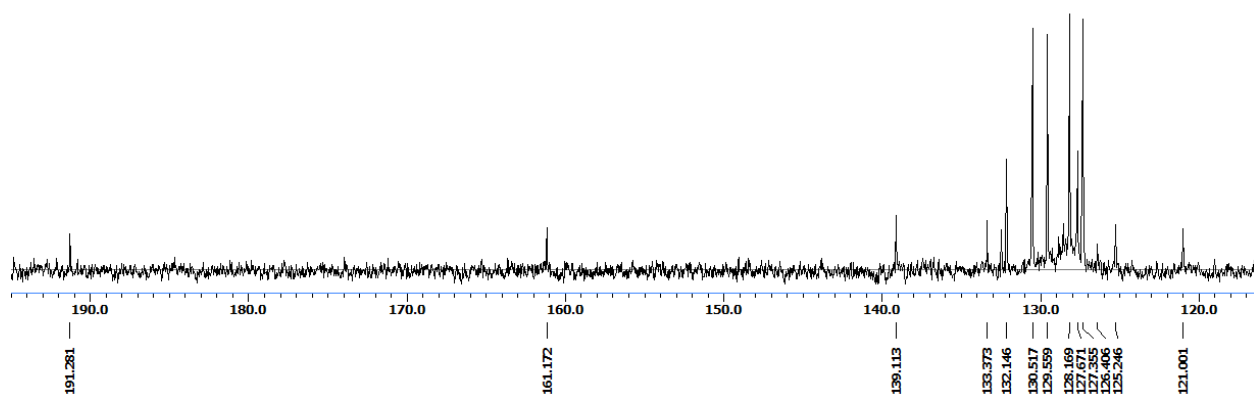
Ethyl 4-benzoyl-3-phenyl-1H-pyrrole-2-carboxylate (4a)



<sup>13</sup>C NMR

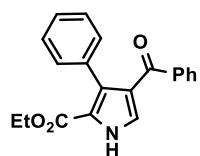


Ethyl 4-benzoyl-3-phenyl-1H-pyrrole-2-carboxylate (4a)

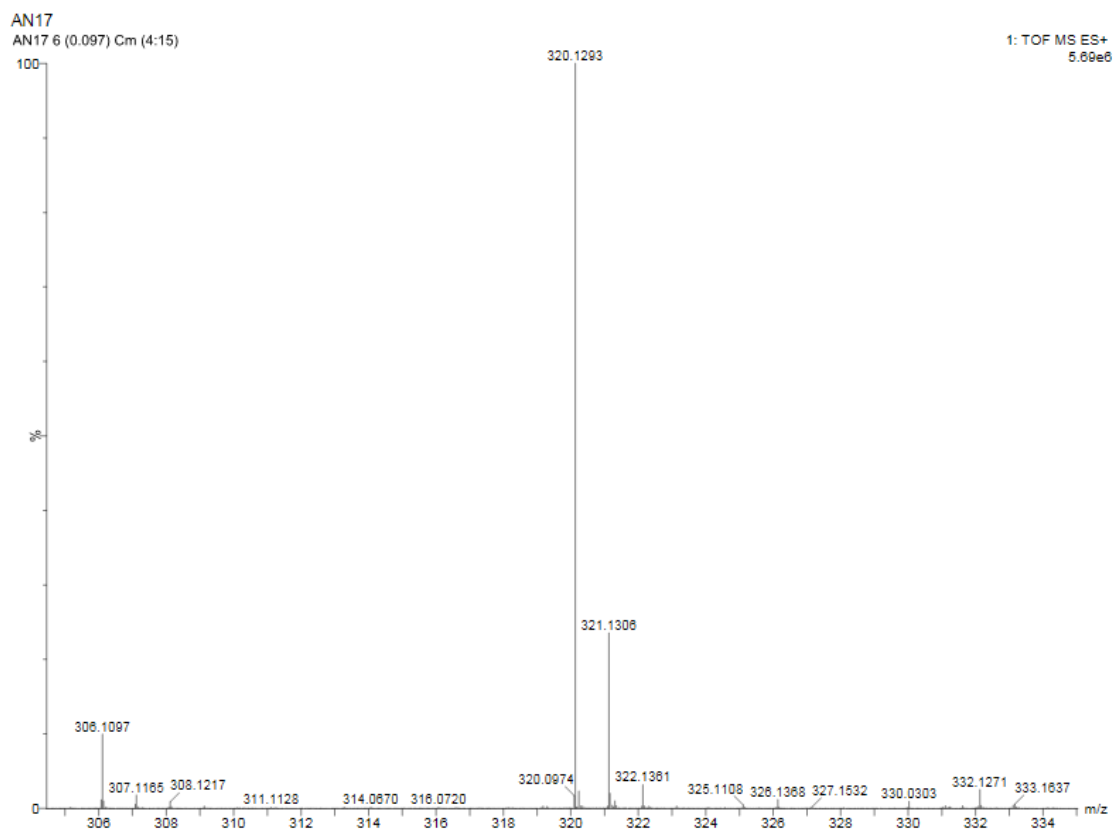




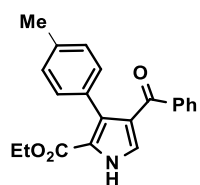
# HRMS



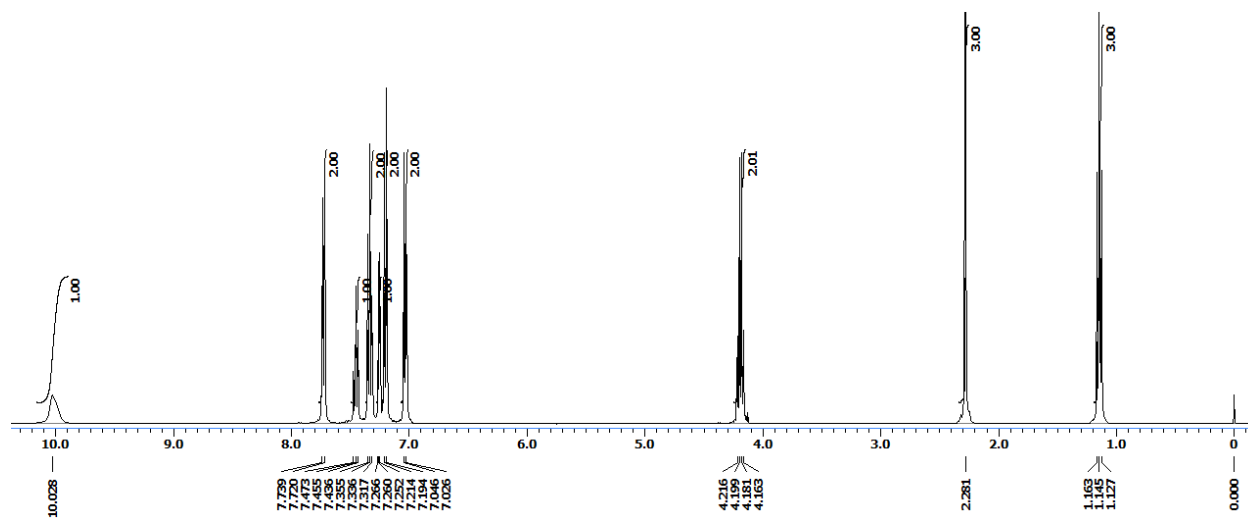
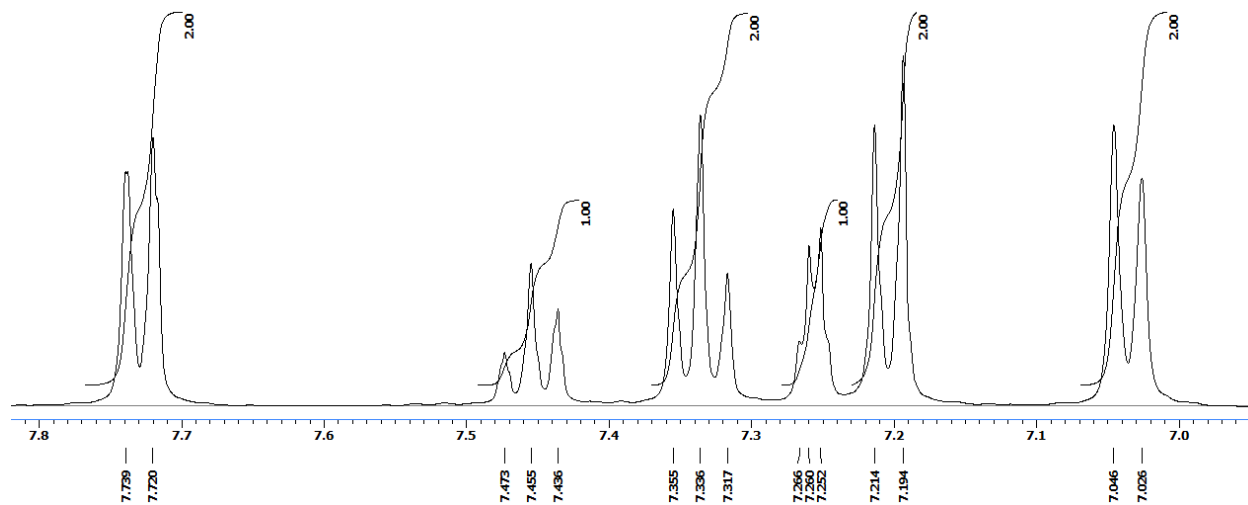
**Ethyl 4-benzoyl-3-phenyl-1H-pyrrole-2-carboxylate (4a)**



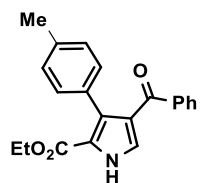
# <sup>1</sup>H NMR



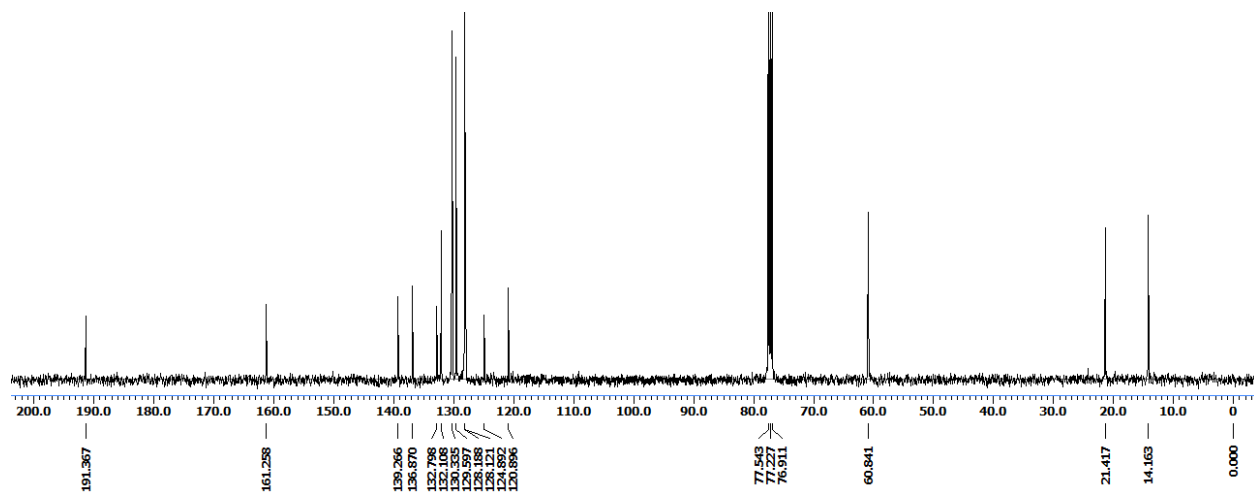
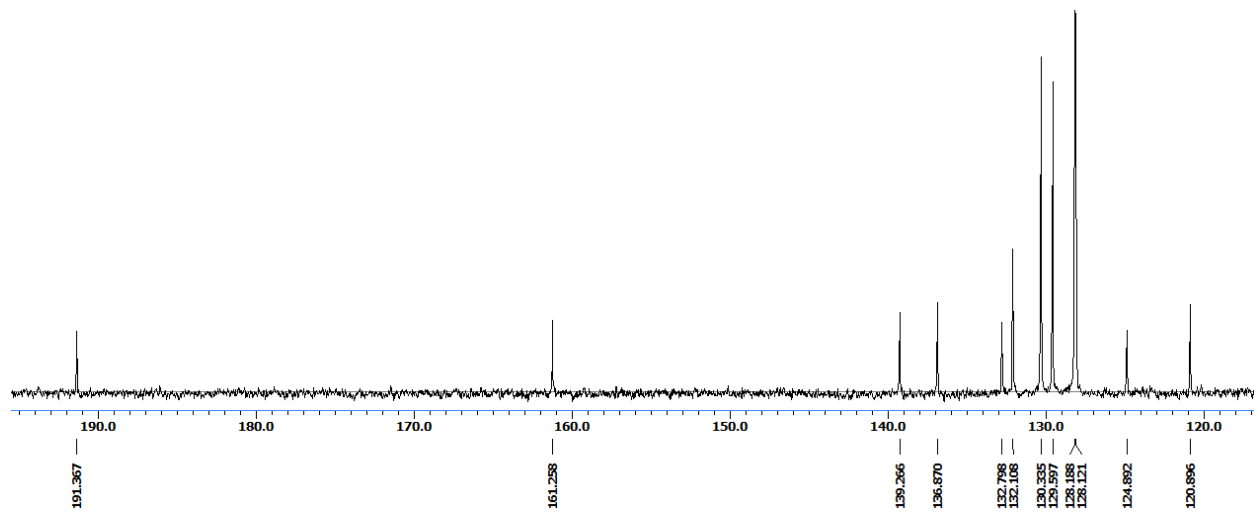
Ethyl 4-benzoyl-3-(p-tolyl)-1H-pyrrole-2-carboxylate (4b)



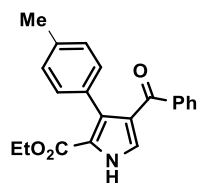
<sup>13</sup>C NMR



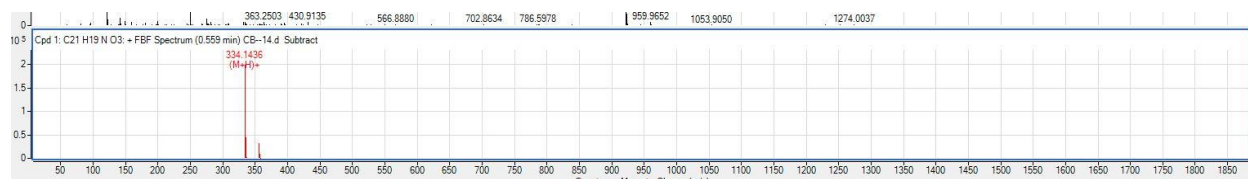
Ethyl 4-benzoyl-3-(p-tolyl)-1H-pyrrole-2-carboxylate (4b)



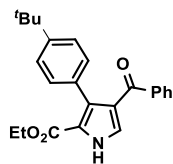
## HRMS



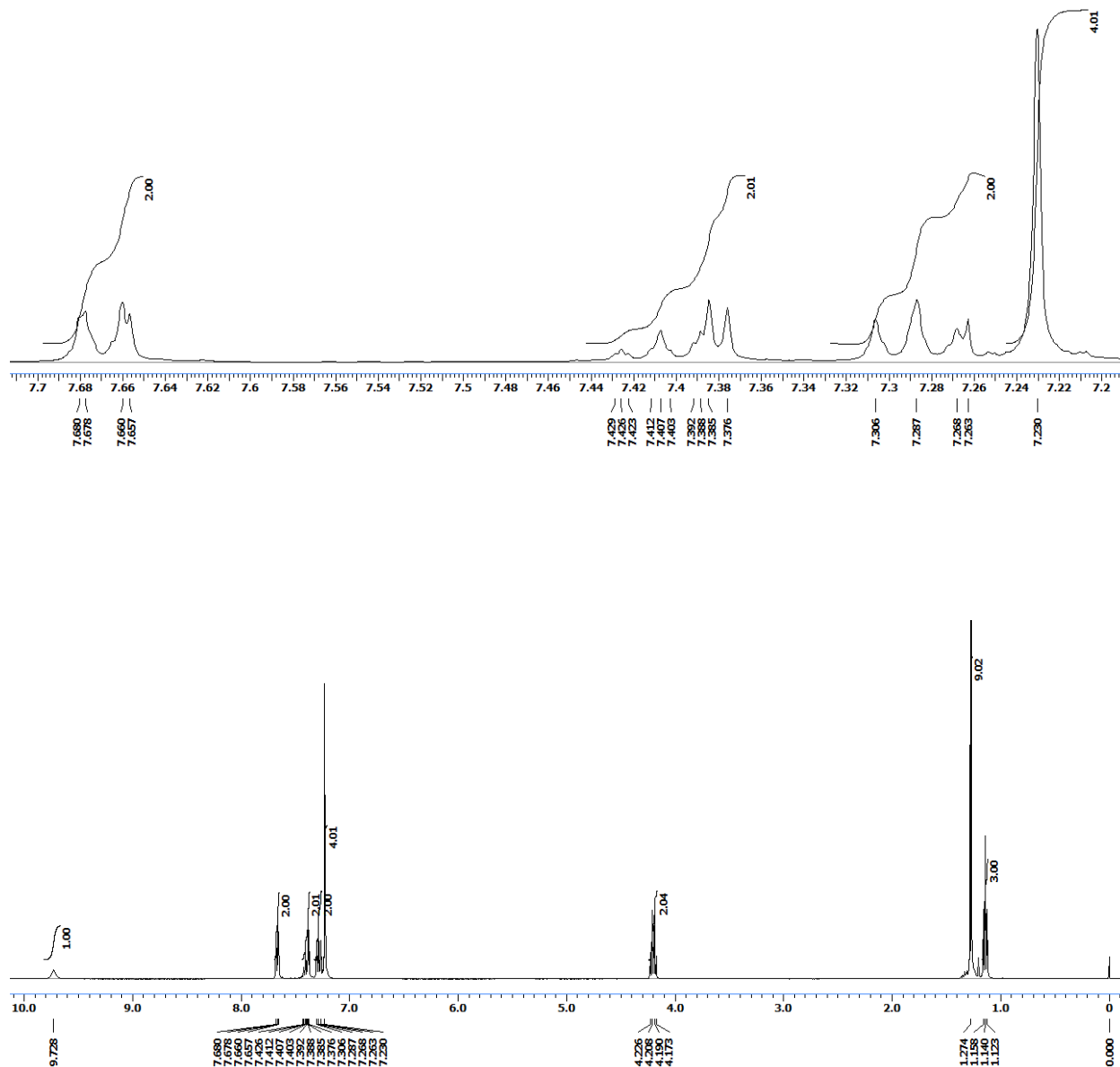
**Ethyl 4-benzoyl-3-(p-tolyl)-1H-pyrrole-2-carboxylate (4b)**



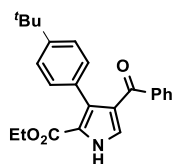
# <sup>1</sup>H NMR



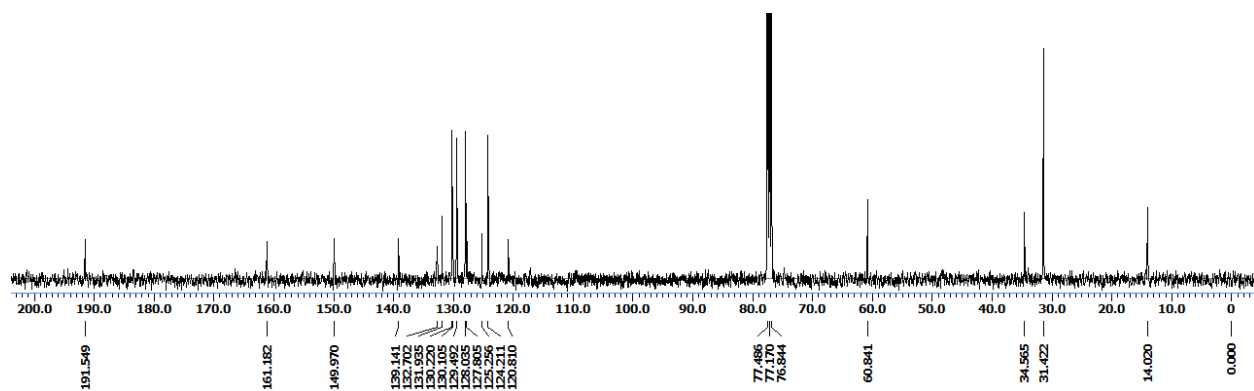
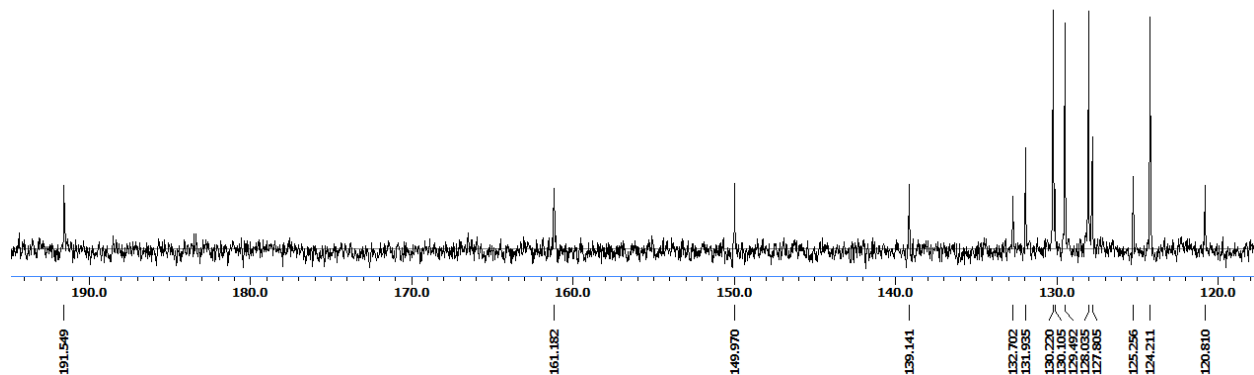
Ethyl 4-benzoyl-3-(4-(tert-butyl)phenyl)-1H-pyrrole-2-carboxylate (4c)



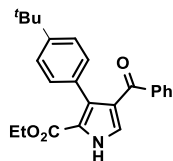
# <sup>13</sup>C NMR



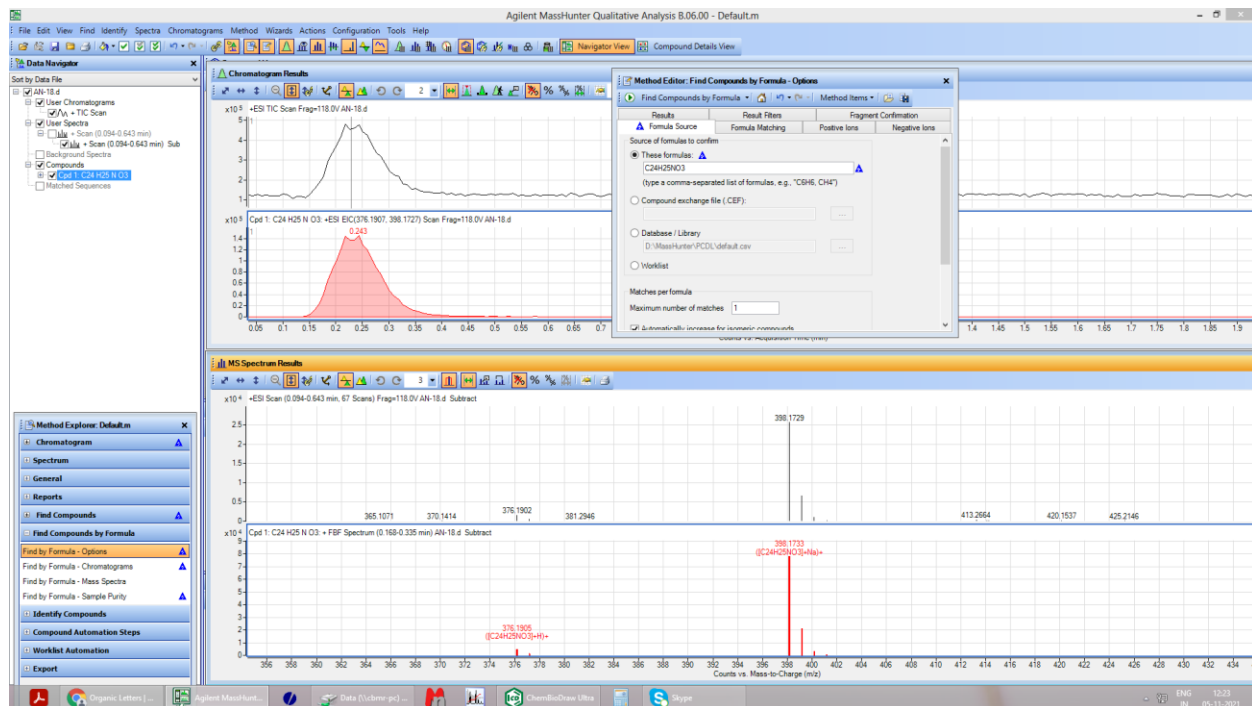
Ethyl 4-benzoyl-3-(4-(tert-butyl)phenyl)-1H-pyrrole-2-carboxylate (4c)



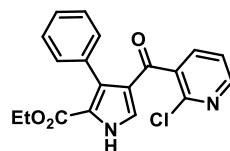
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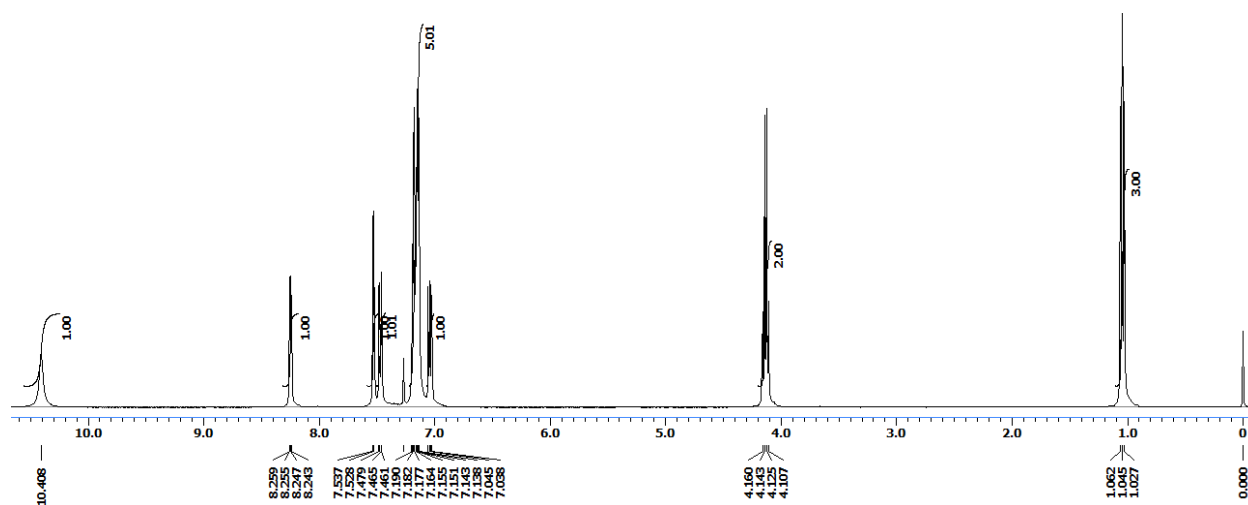
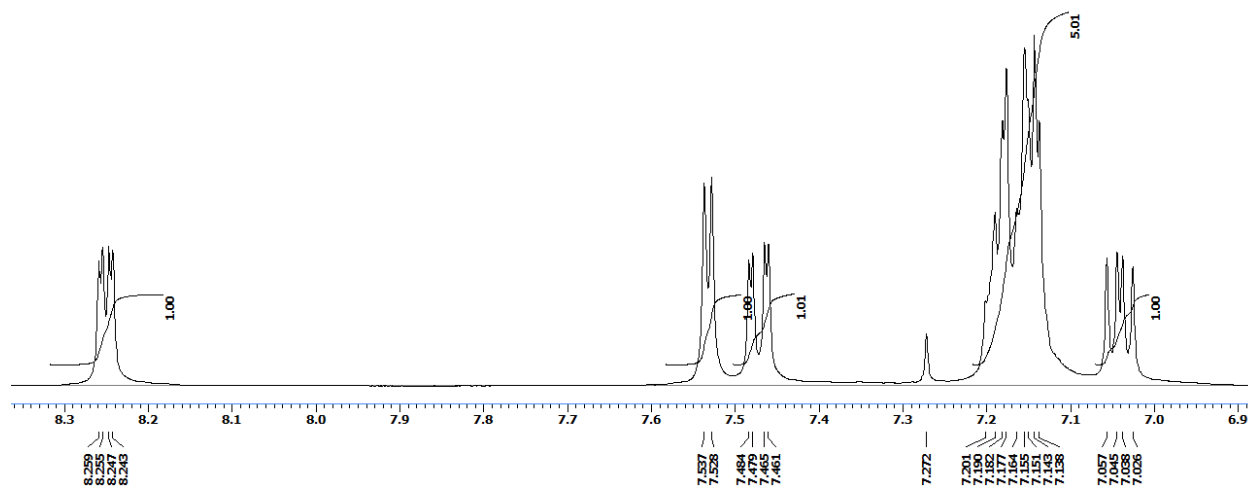
**Ethyl 4-benzoyl-3-(4-(tert-butyl)phenyl)-1H-pyrrole-2-carboxylate (4c)**



# <sup>1</sup>H NMR

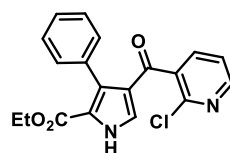


Ethyl 4-(2-chloronicotinoyl)-3-phenyl-1H-pyrrole-2-carboxylate (4d)

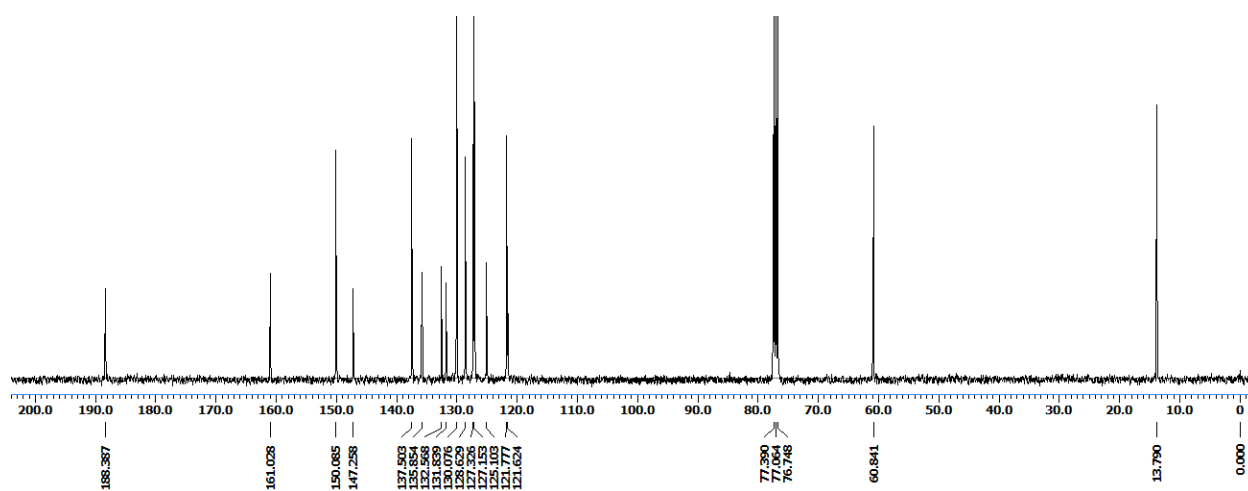
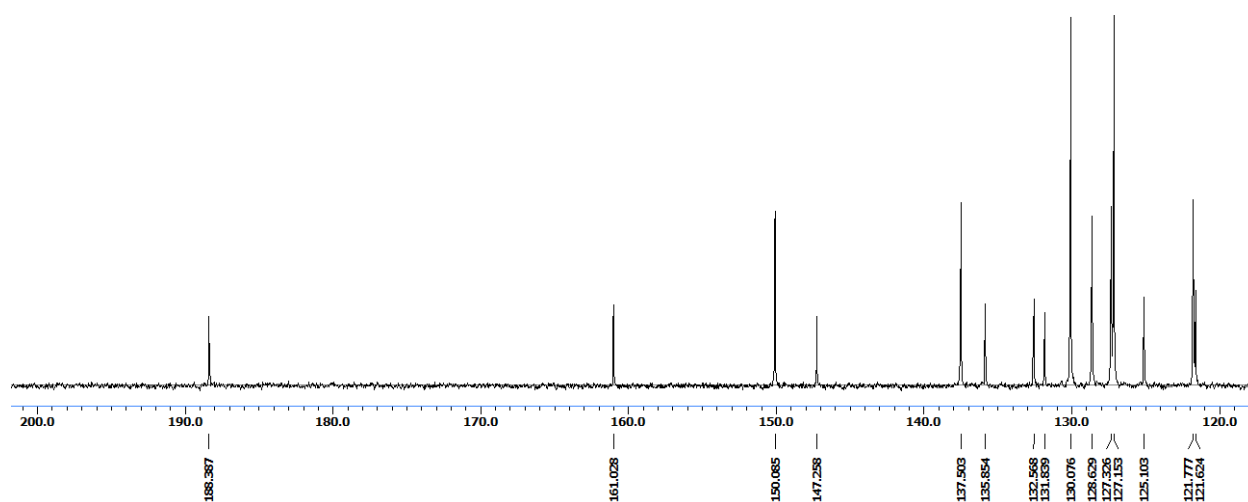




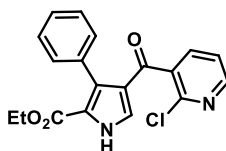
<sup>13</sup>C NMR



Ethyl 4-(2-chloronicotinoyl)-3-phenyl-1H-pyrrole-2-carboxylate (4d)



# HRMS



## Ethyl 4-(2-chloronicotinoyl)-3-phenyl-1H-pyrrole-2-carboxylate (4d)

### Analysis Info

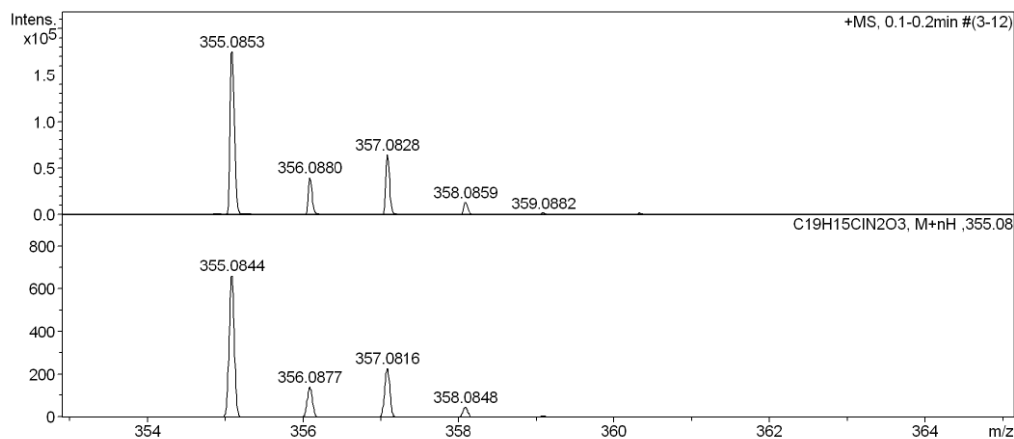
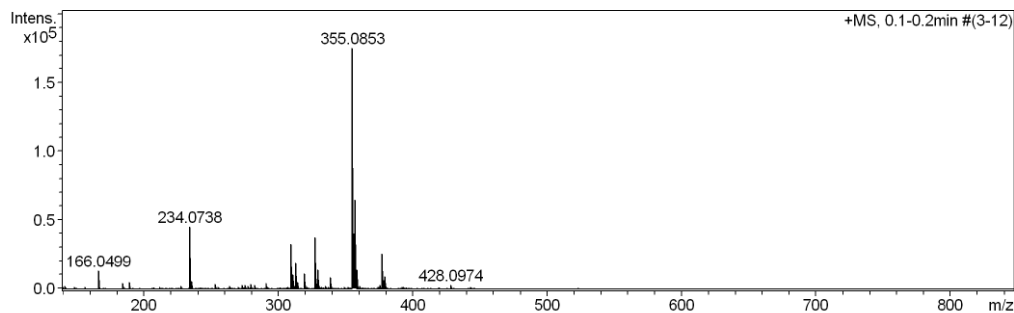
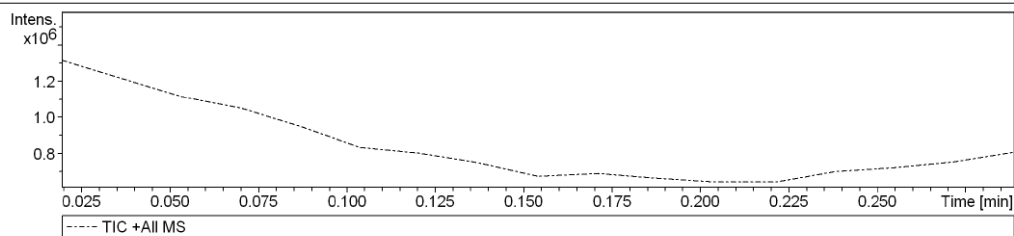
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Sample Name Tmix-131118  
Comment

Acquisition Date 12/30/2020 2:19:21 PM

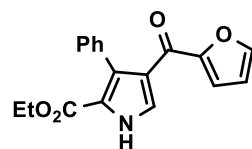
Operator Amit S.Sahu  
Instrument microTOF-Q II 10337

### Acquisition Parameter

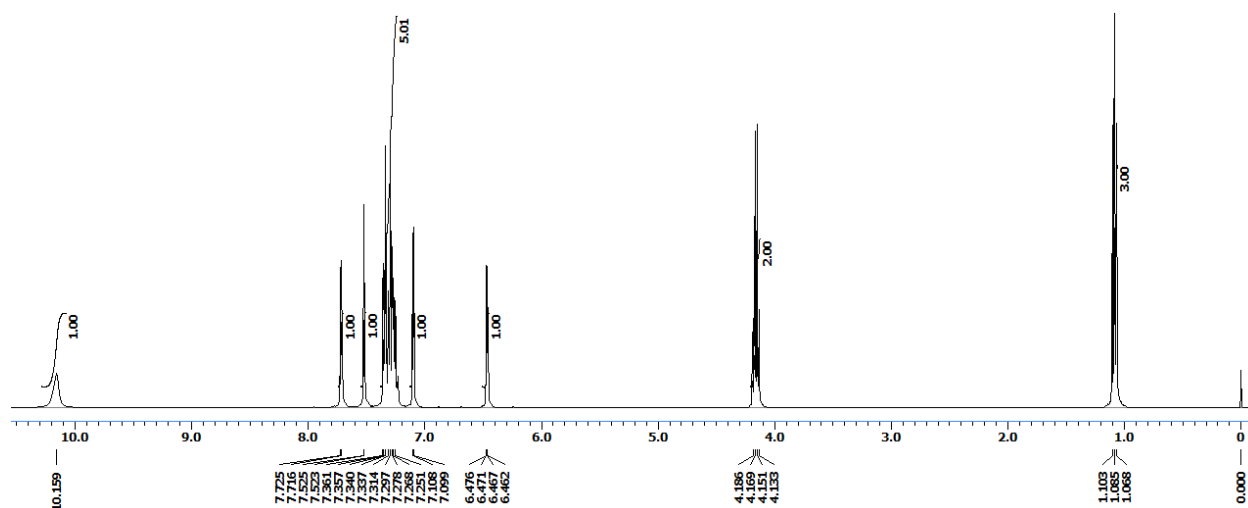
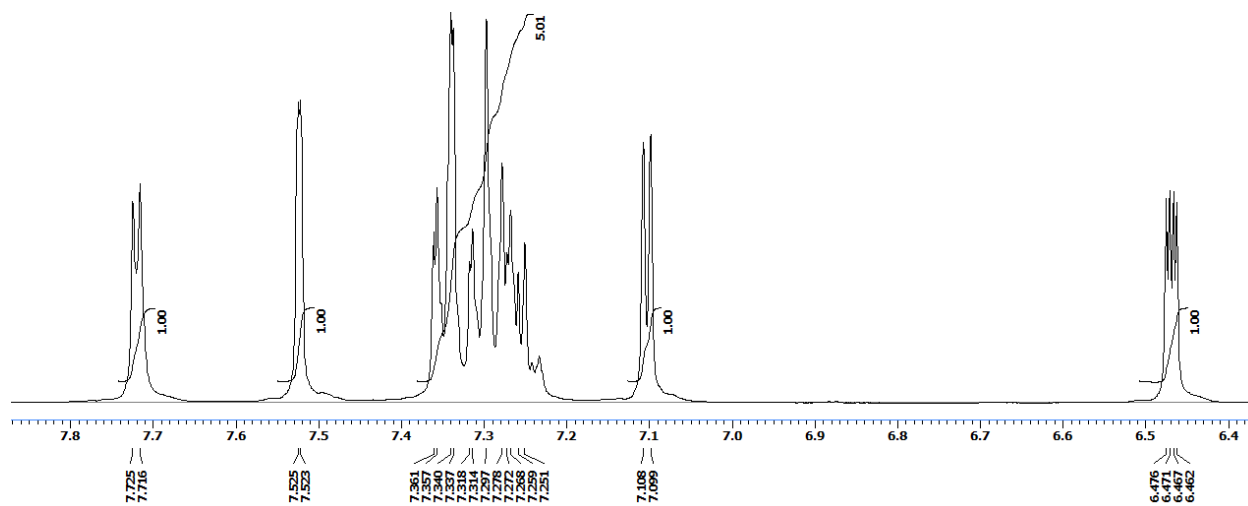
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



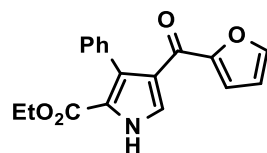
<sup>1</sup>H NMR



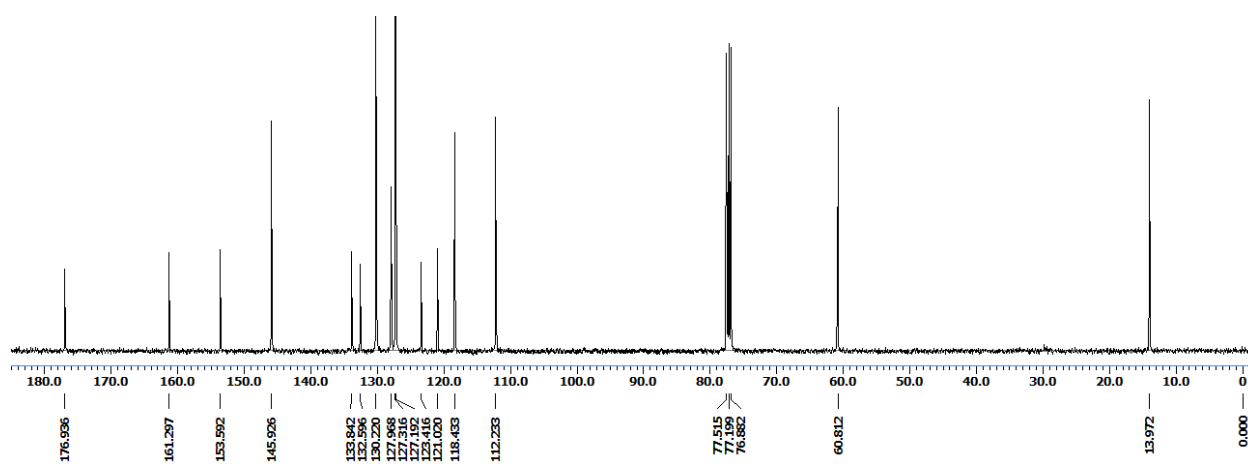
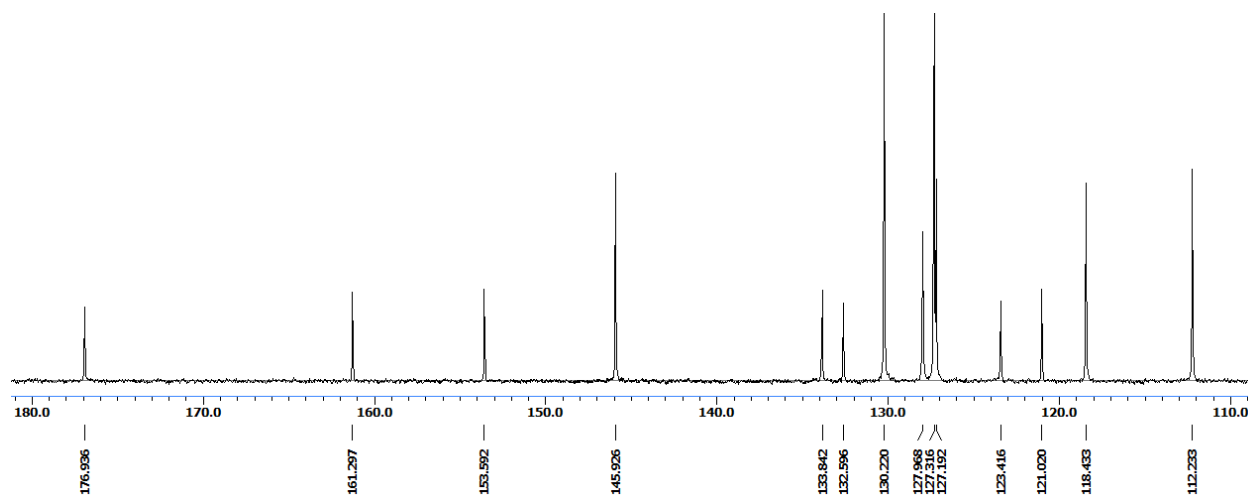
Ethyl 4-(furan-2-carbonyl)-3-phenyl-1H-pyrrole-2-carboxylate (4e)



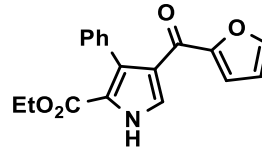
<sup>13</sup>C NMR



**Ethyl 4-(furan-2-carbonyl)-3-phenyl-1H-pyrrole-2-carboxylate (4e)**



# HRMS



## Ethyl 4-(furan-2-carbonyl)-3-phenyl-1H-pyrrole-2-carboxylate (4e)

### Analysis Info

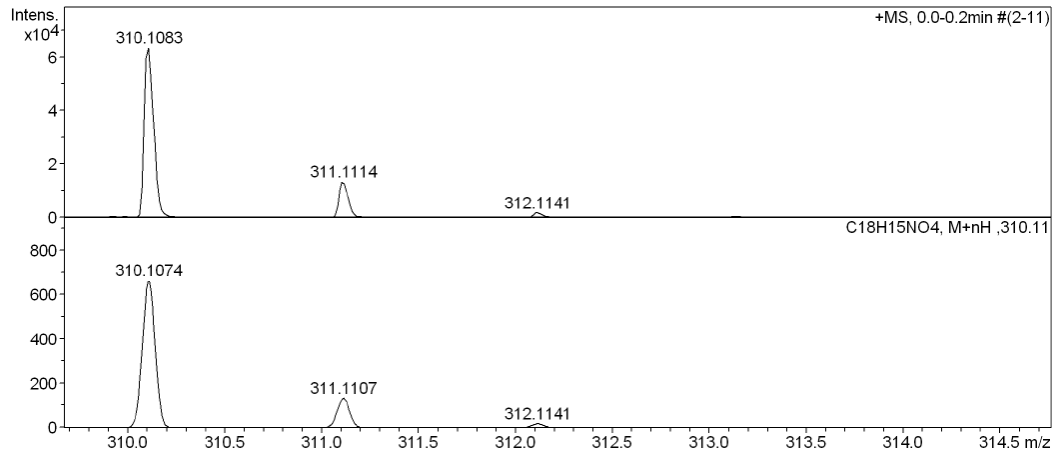
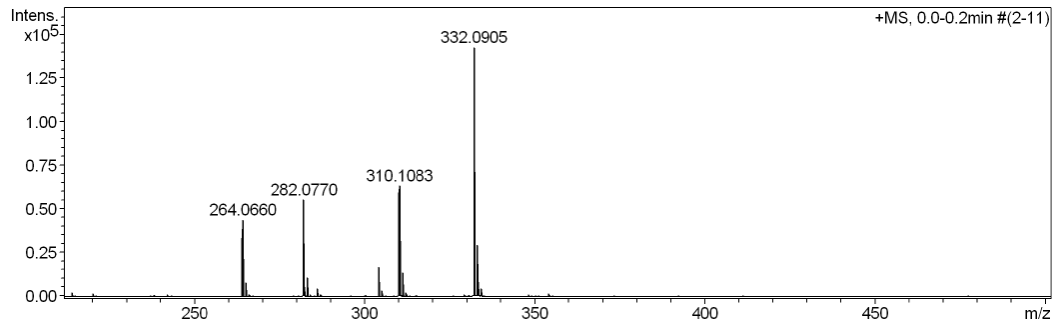
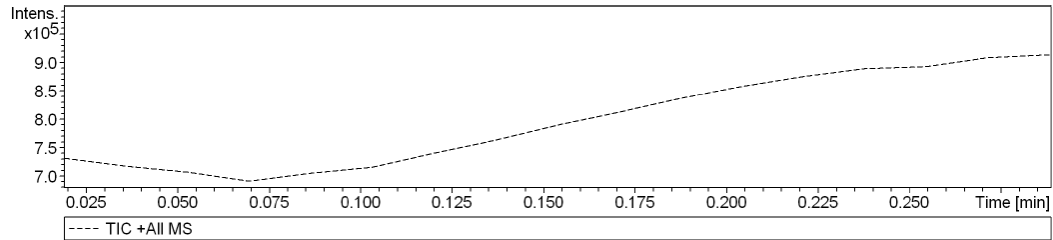
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Method Pos\_tune\_low.m  
Sample Name Tmix-131118  
Comment

Acquisition Date 12/30/2020 5:38:07 PM

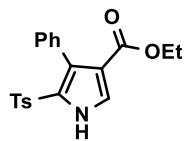
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

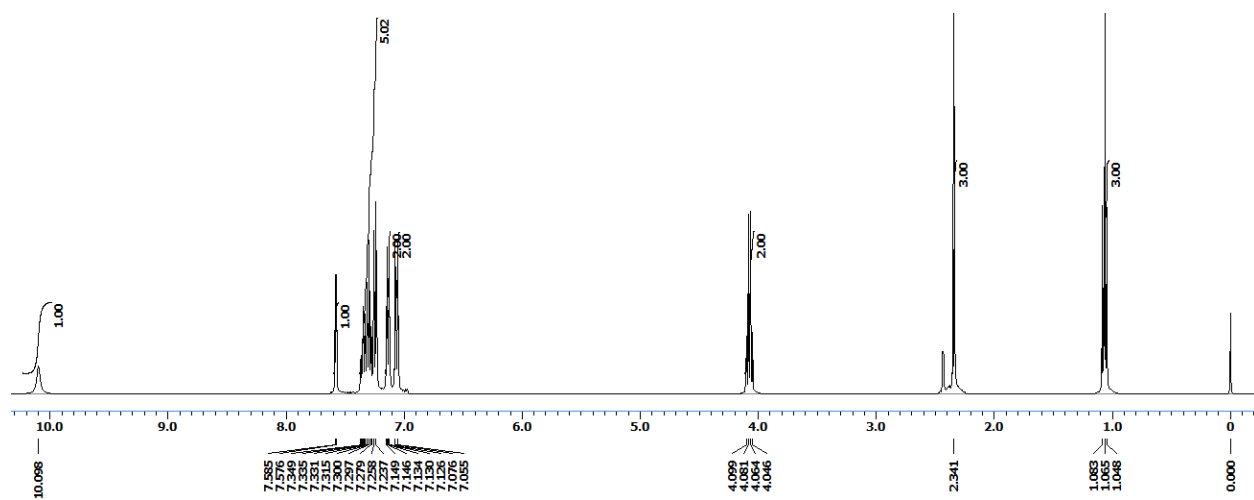
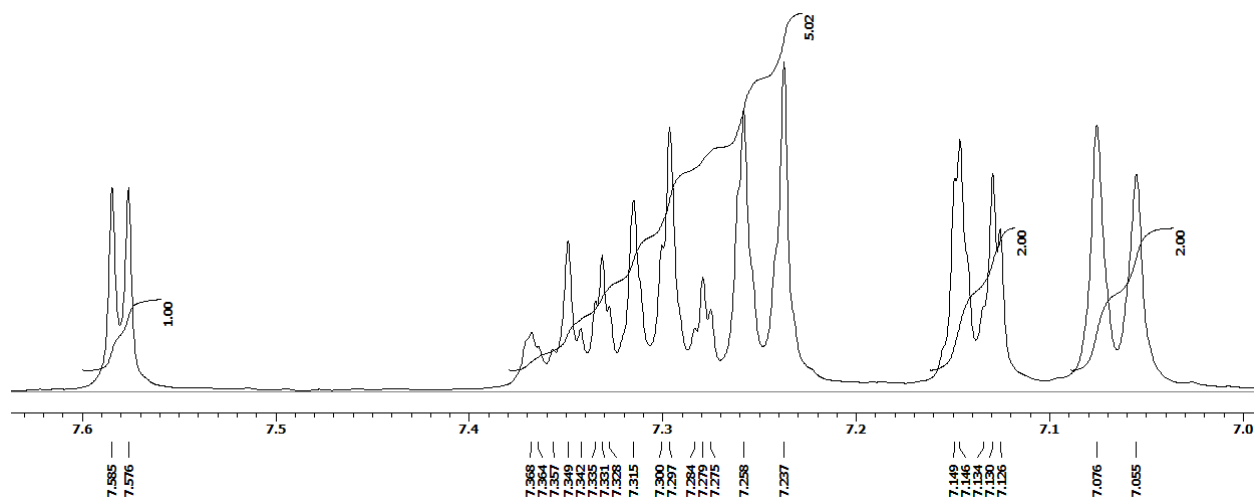
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



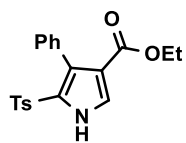
**<sup>1</sup>H NMR**



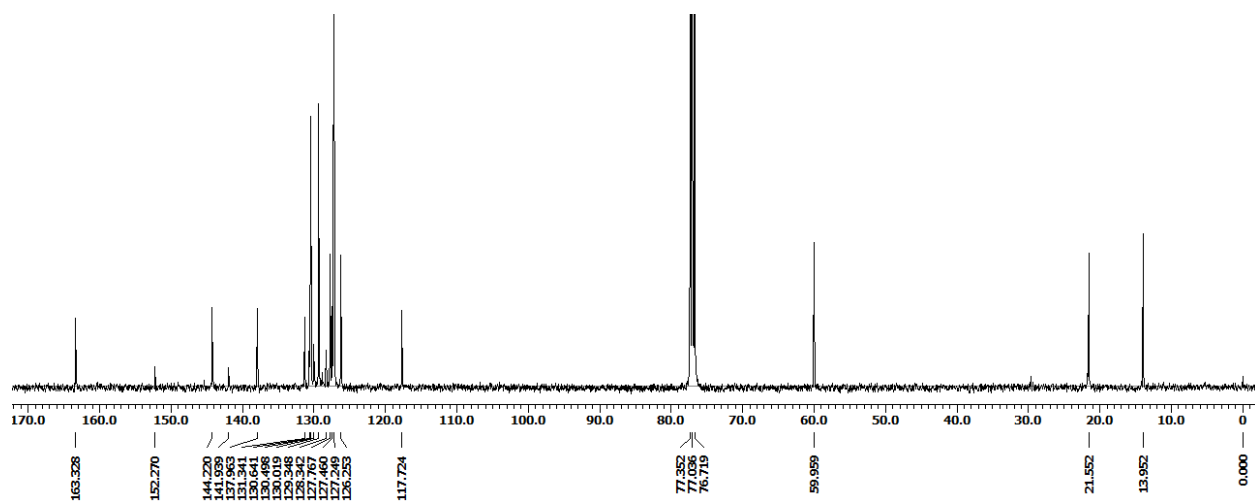
**Ethyl 4-phenyl-5-tosyl-1H-pyrrole-3-carboxylate (5a)**



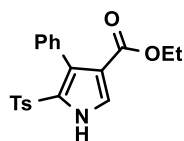
<sup>13</sup>C NMR



Ethyl 4-phenyl-5-tosyl-1H-pyrrole-3-carboxylate (5a)



# HRMS



## Ethyl 4-phenyl-5-tosyl-1H-pyrrole-3-carboxylate (5a)

### Analysis Info

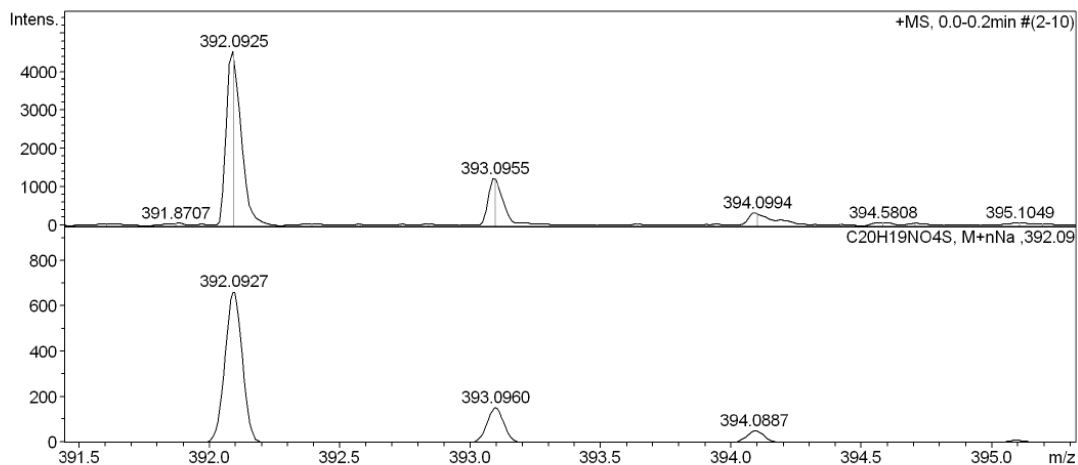
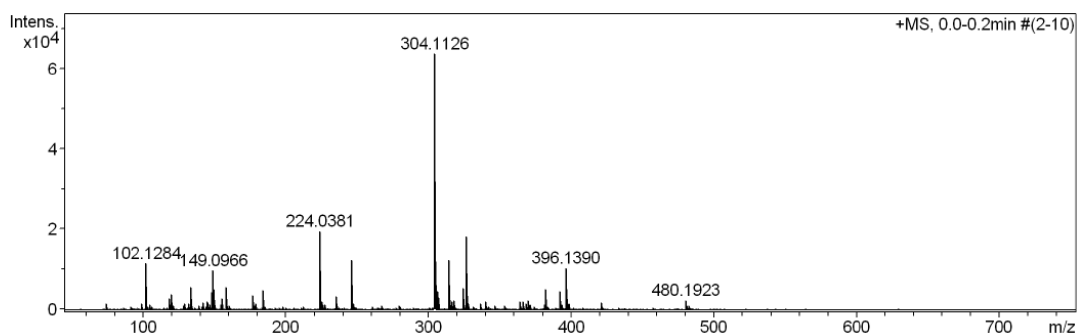
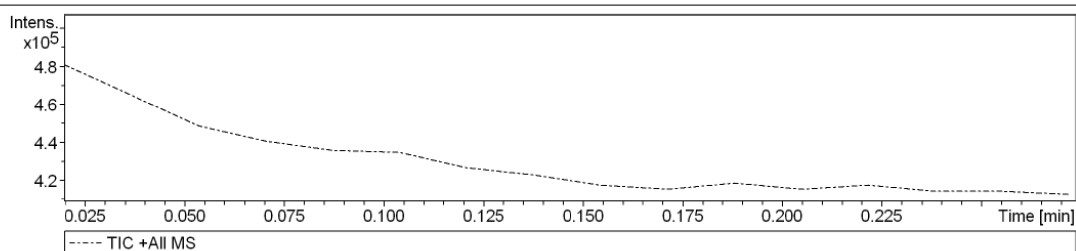
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 Method Pos\_tune\_low.m  
 Sample Name Tmix-131118  
 Comment

Acquisition Date 12/29/2020 10:50:50 PM

Operator Amit S.Sahu  
 Instrument micrOTOF-Q II 10337

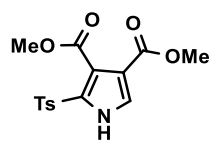
### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

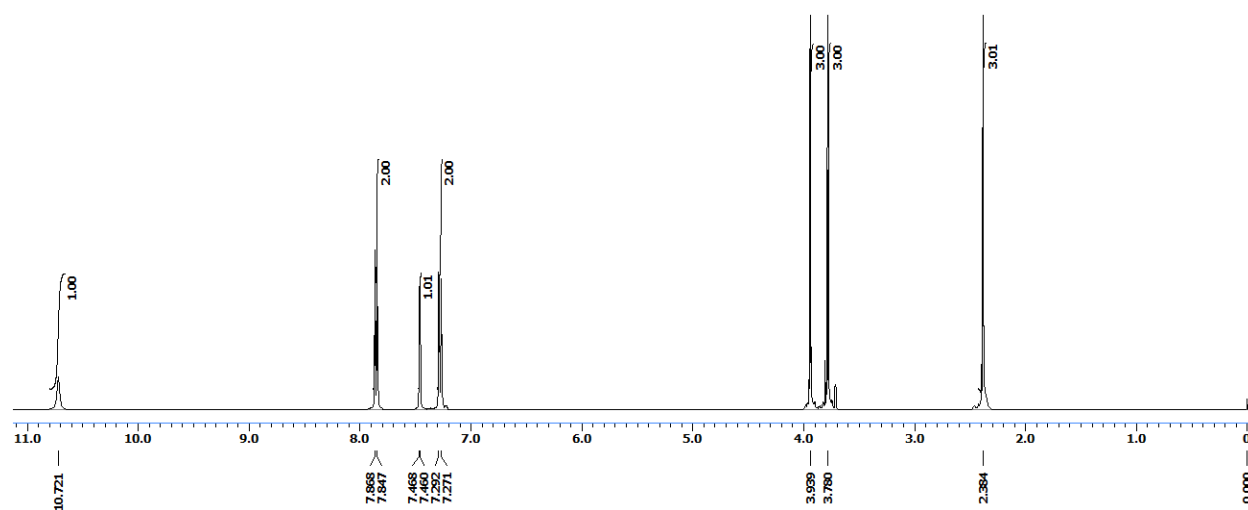
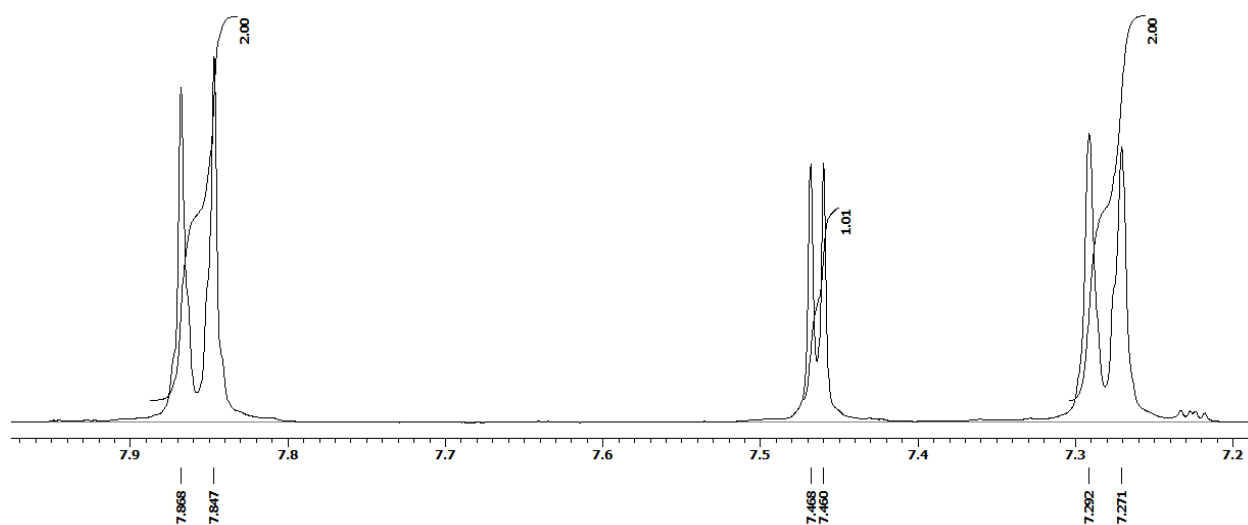




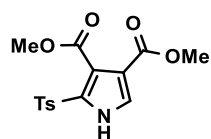
<sup>1</sup>H NMR



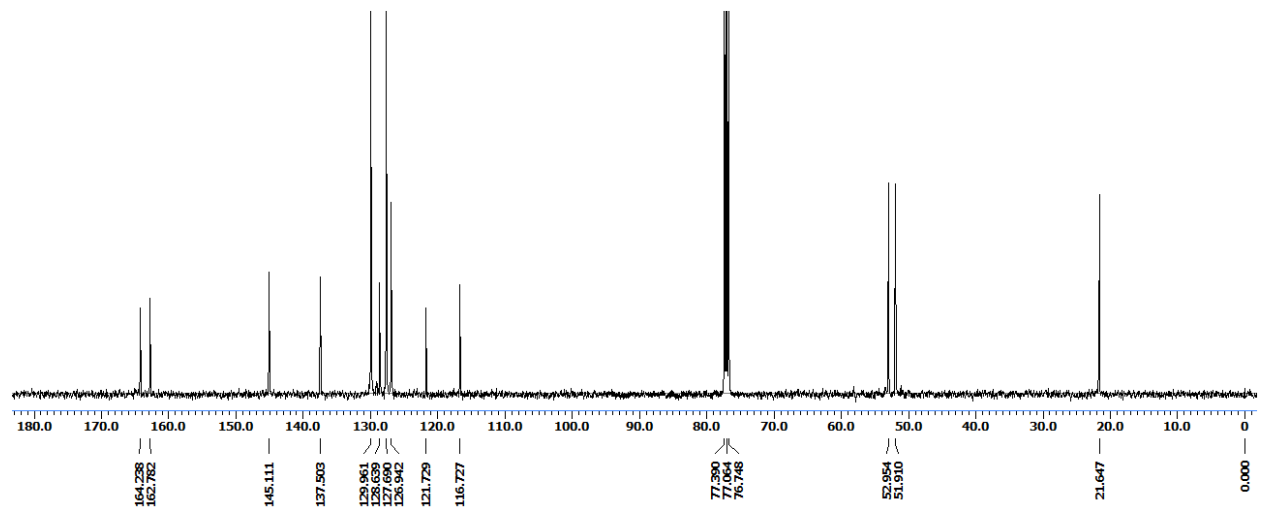
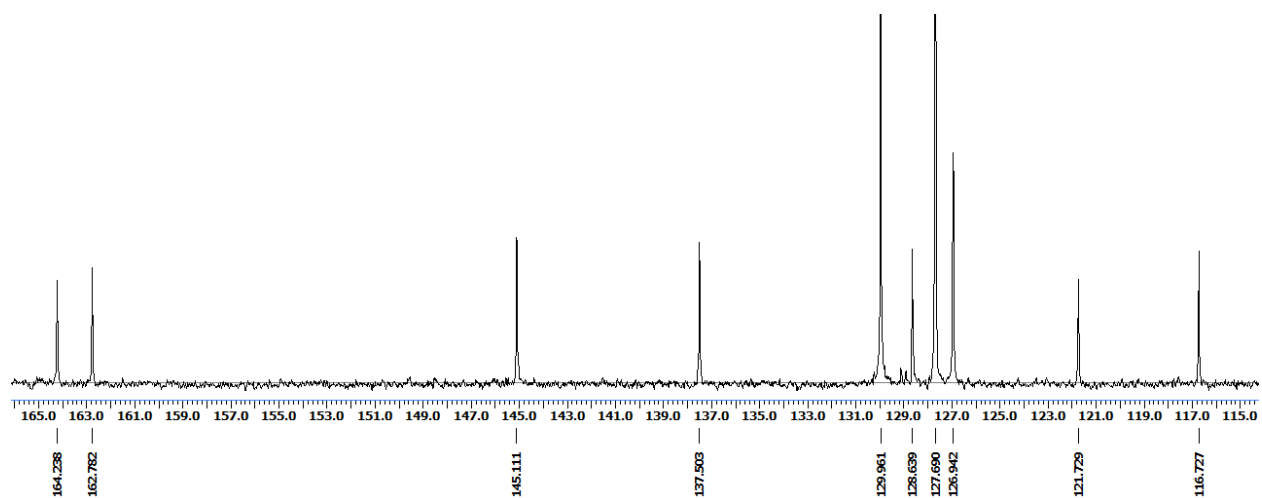
Dimethyl 2-tosyl-1H-pyrrole-3,4-dicarboxylate (5b)



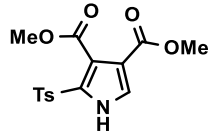
<sup>13</sup>C NMR



Dimethyl 2-tosyl-1H-pyrrole-3,4-dicarboxylate (5b)



# HRMS



## Dimethyl 2-tosyl-1H-pyrrole-3,4-dicarboxylate (5b)

### Analysis Info

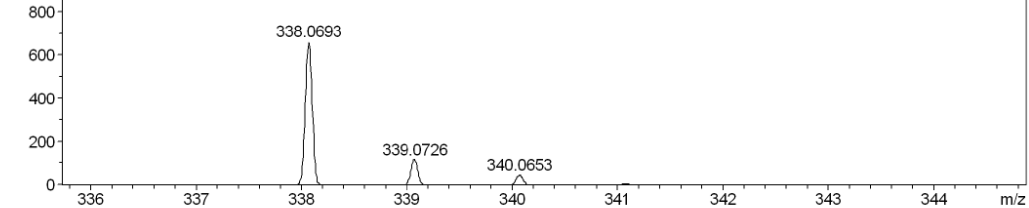
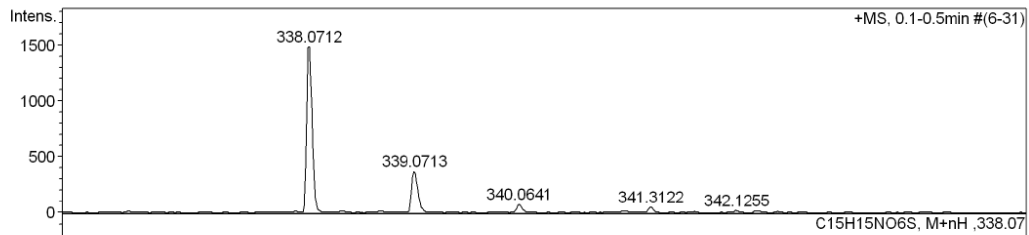
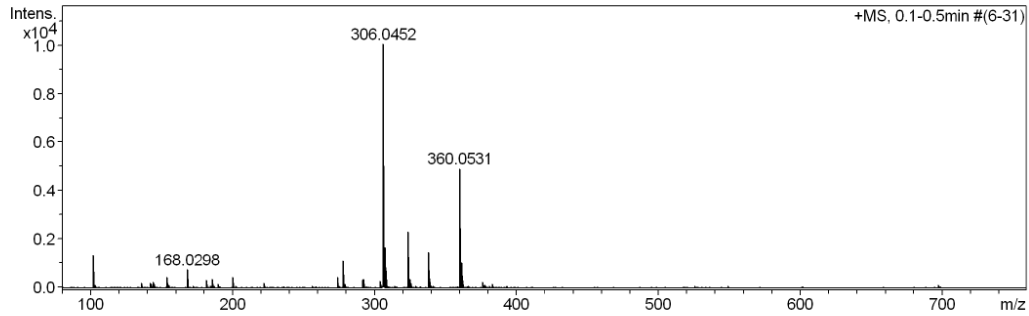
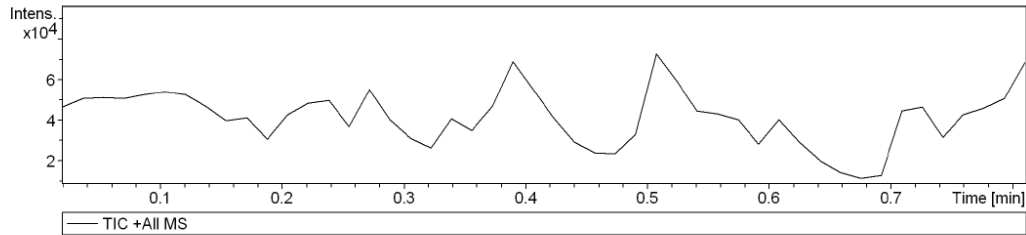
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Sample Name Tmix-131118  
Comment

Acquisition Date 12/30/2020 12:02:07 AM

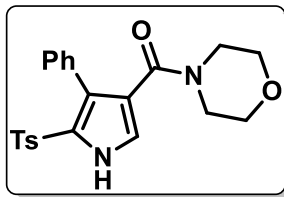
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

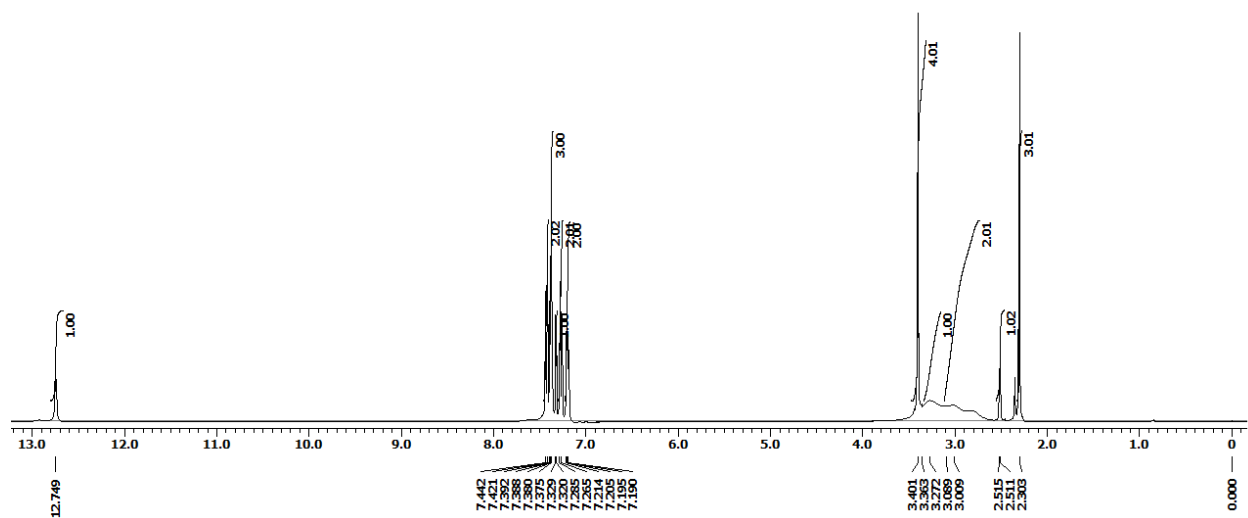
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



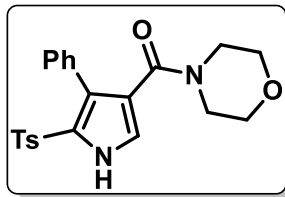
<sup>1</sup>H NMR



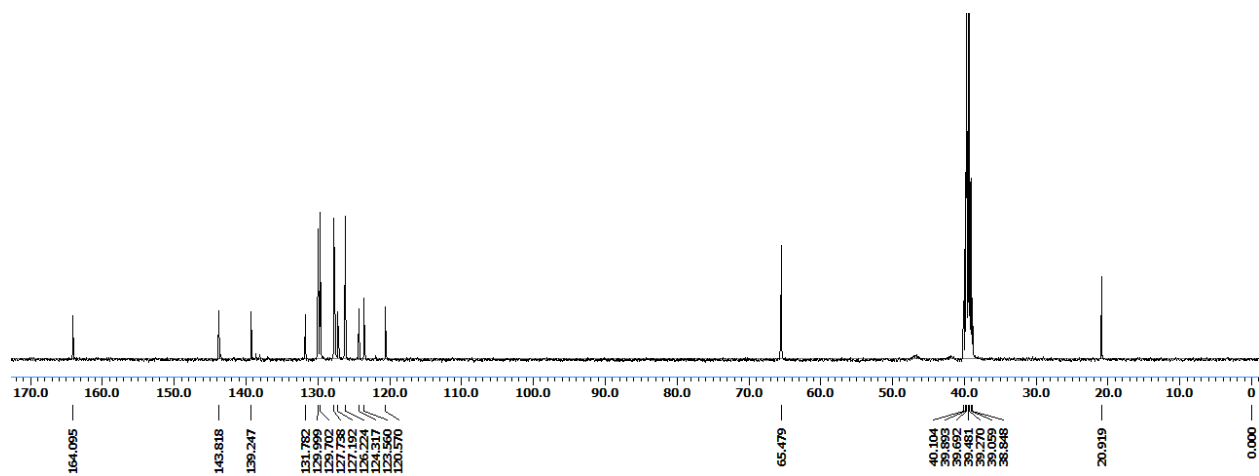
Morpholino(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (5c)



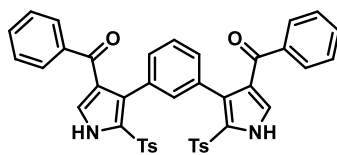
<sup>13</sup>C NMR



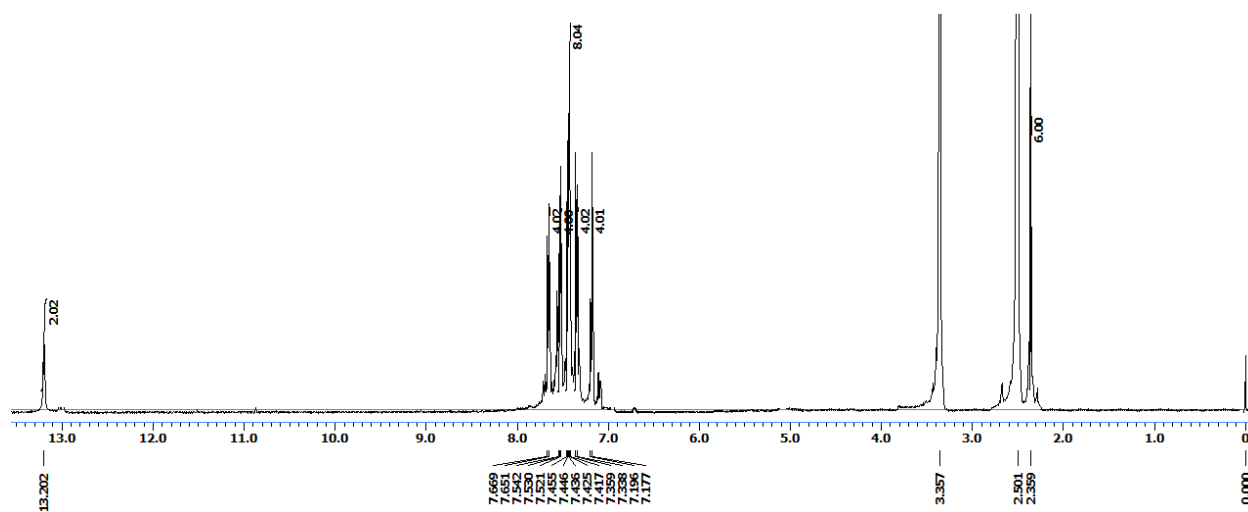
Morpholino(4-phenyl-5-tosyl-1H-pyrrol-3-yl)methanone (5c)



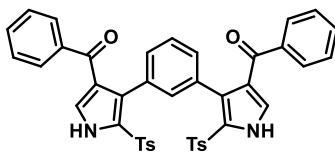
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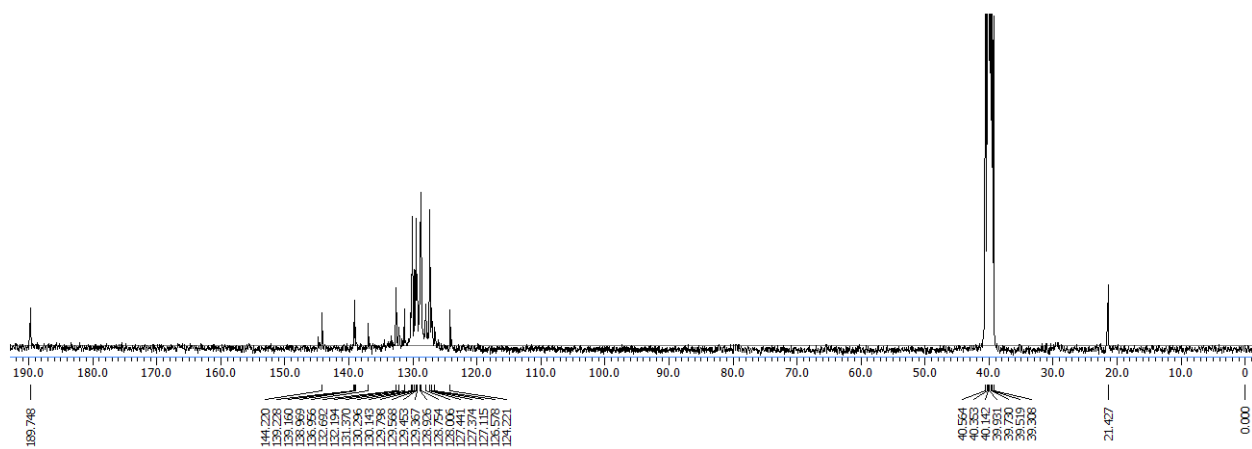
(6a)



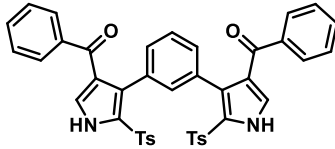
<sup>13</sup>C NMR



(6a)



# HRMS



(6a)

## Analysis Info

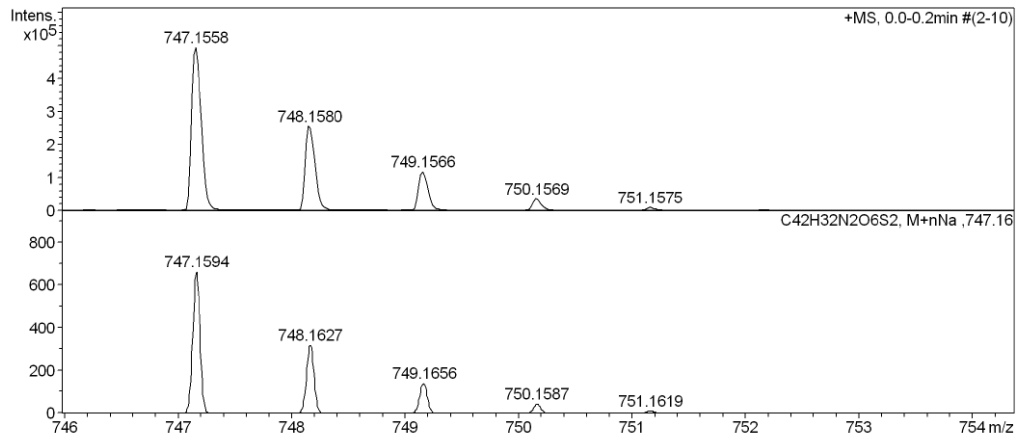
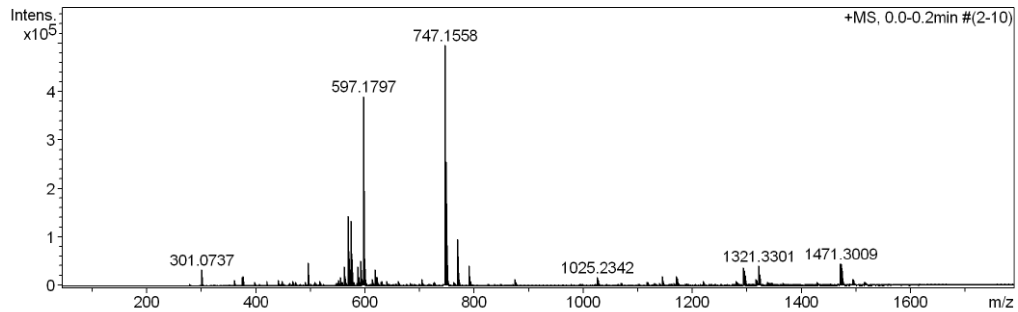
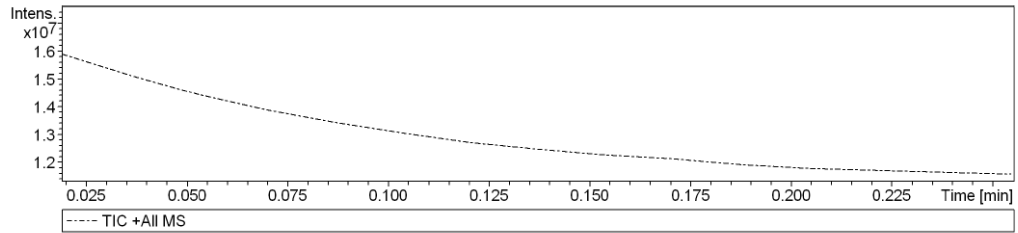
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Method pos tune\_wide\_030118.m  
Sample Name Tmix-131118  
Comment

Acquisition Date 12/30/2020 2:12:19 PM

Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

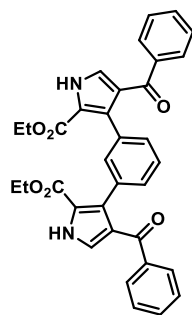
## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste

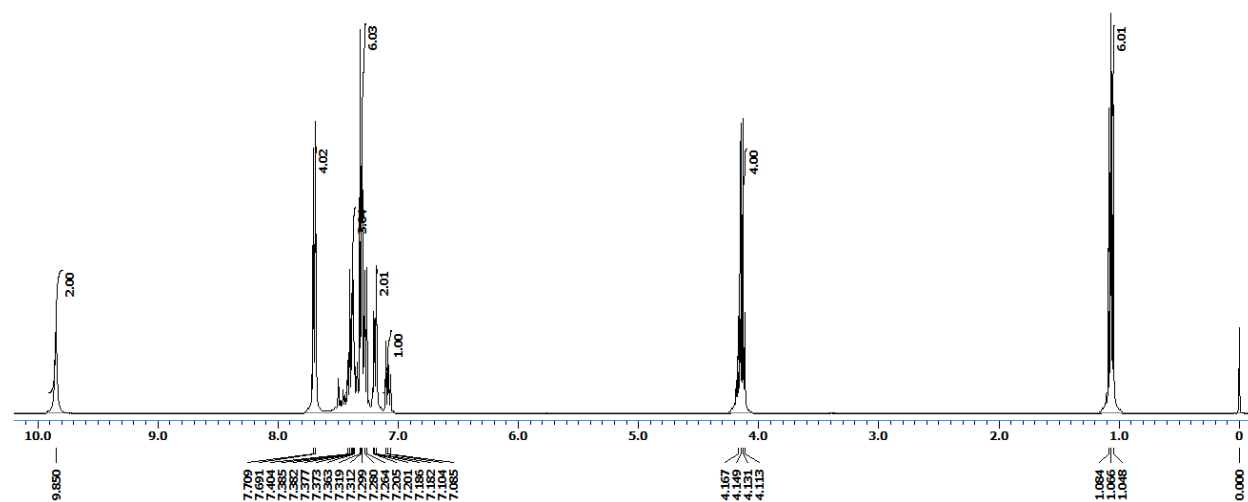
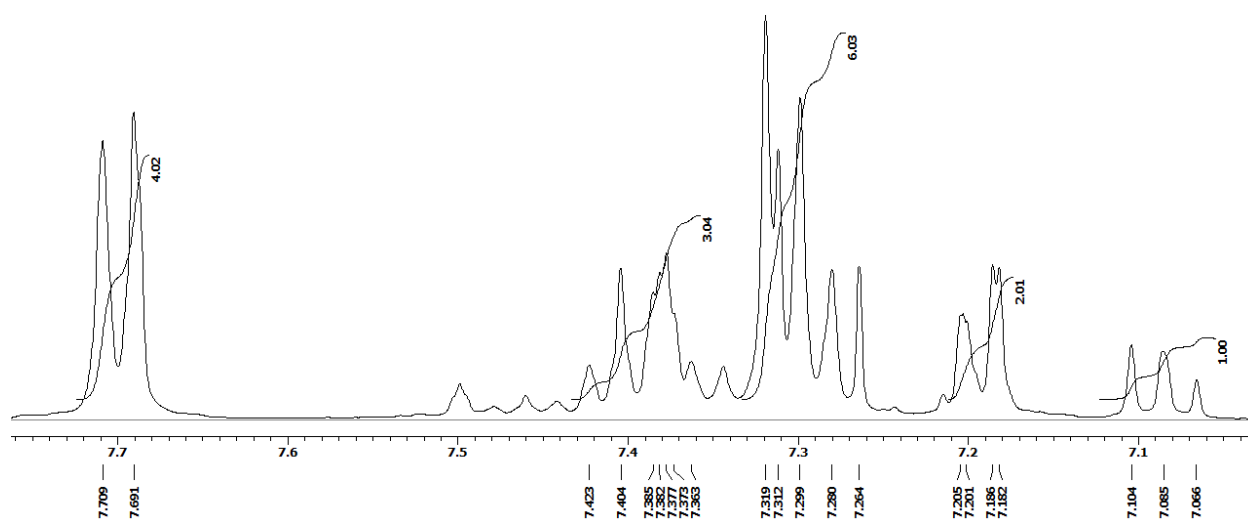




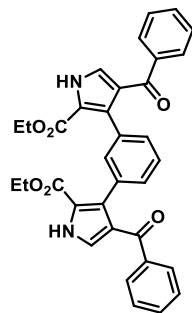
# <sup>1</sup>H NMR



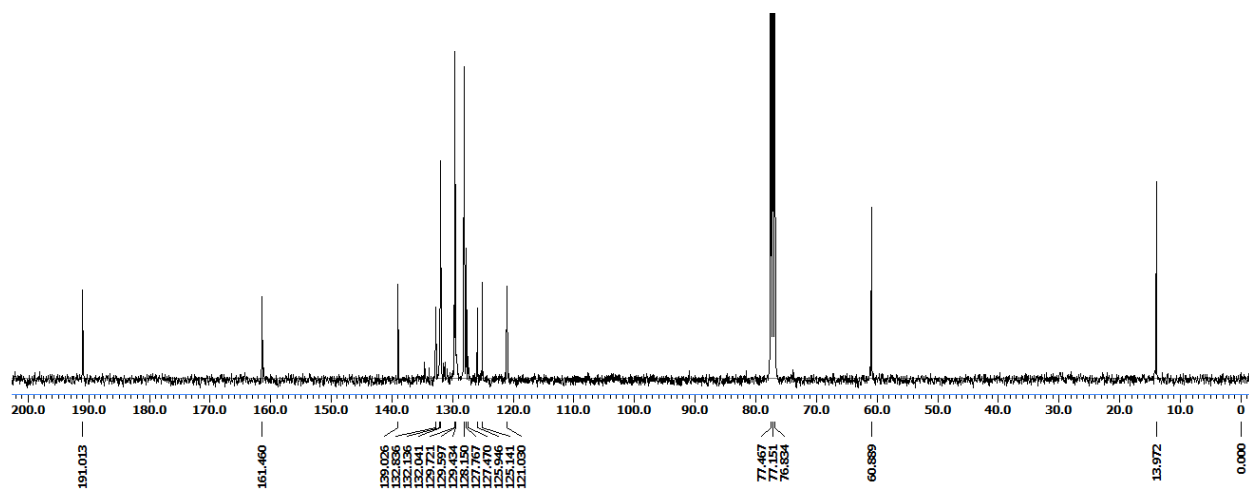
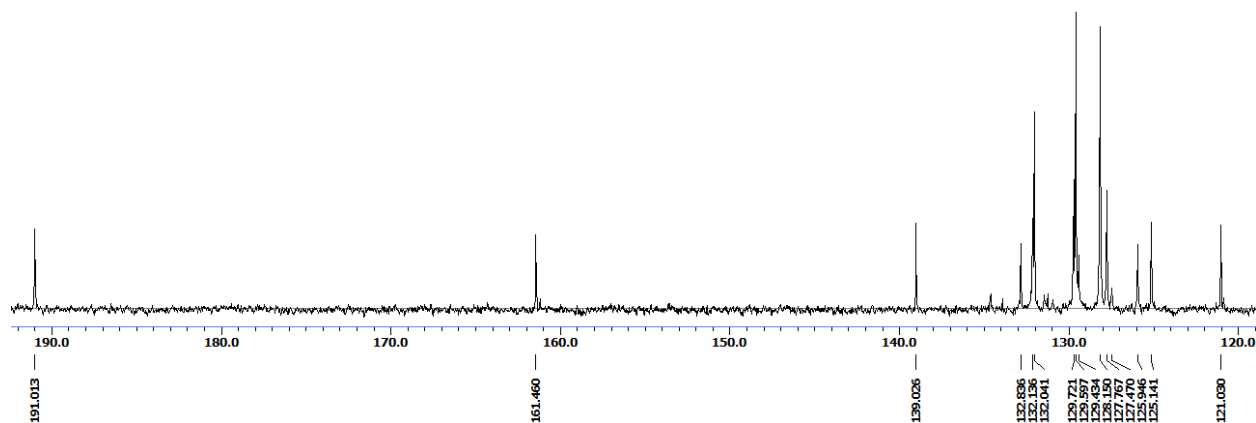
Diethyl 3,3'-(1,3-phenylene)bis(4-benzoyl-1H-pyrrole-2-carboxylate) (6b)



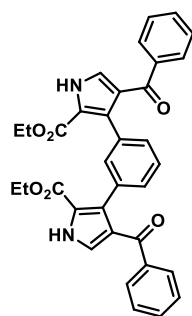
<sup>13</sup>C NMR



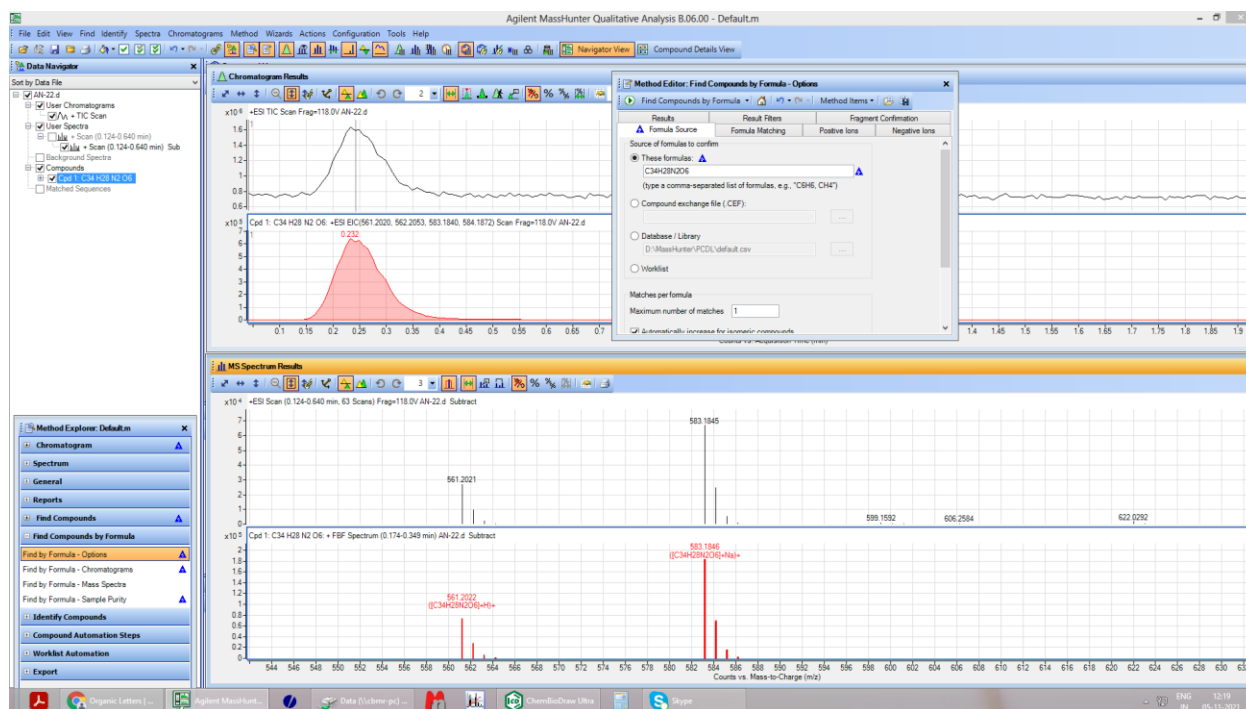
Diethyl 3,3'-(1,3-phenylene)bis(4-benzoyl-1H-pyrrole-2-carboxylate) (6b)



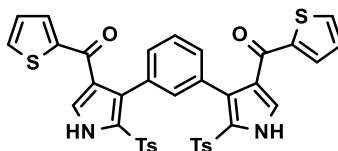
## HRMS



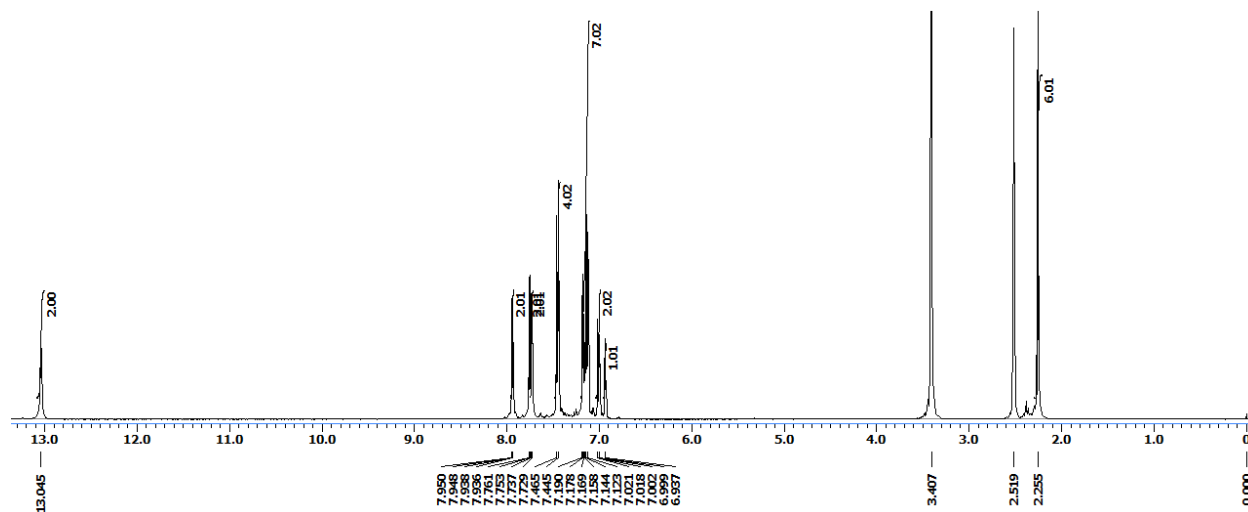
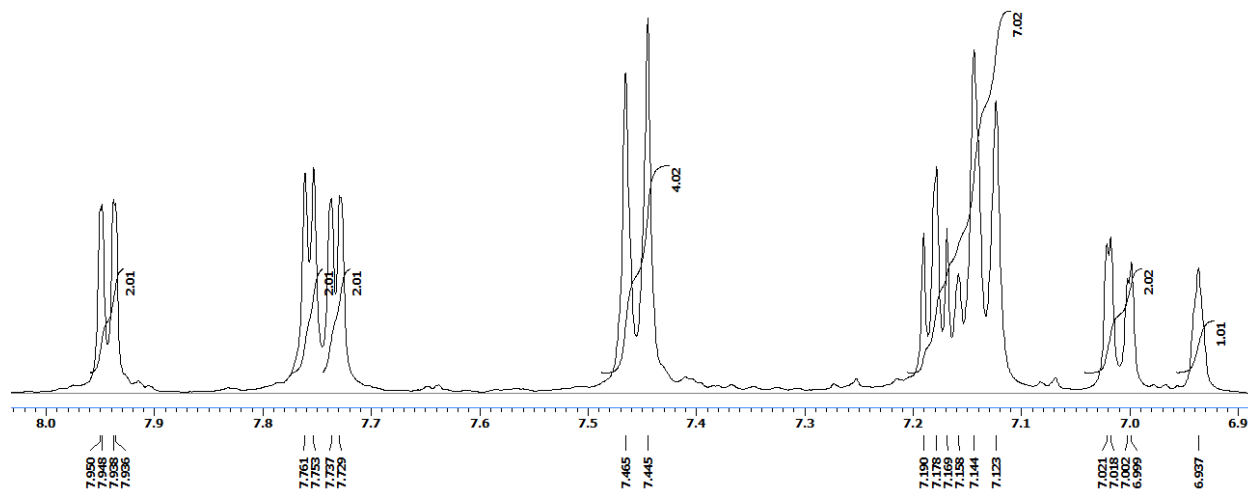
Diethyl 3,3'-(1,3-phenylene)bis(4-benzoyl-1*H*-pyrrole-2-carboxylate) (6b)



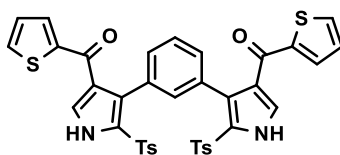
<sup>1</sup>H NMR



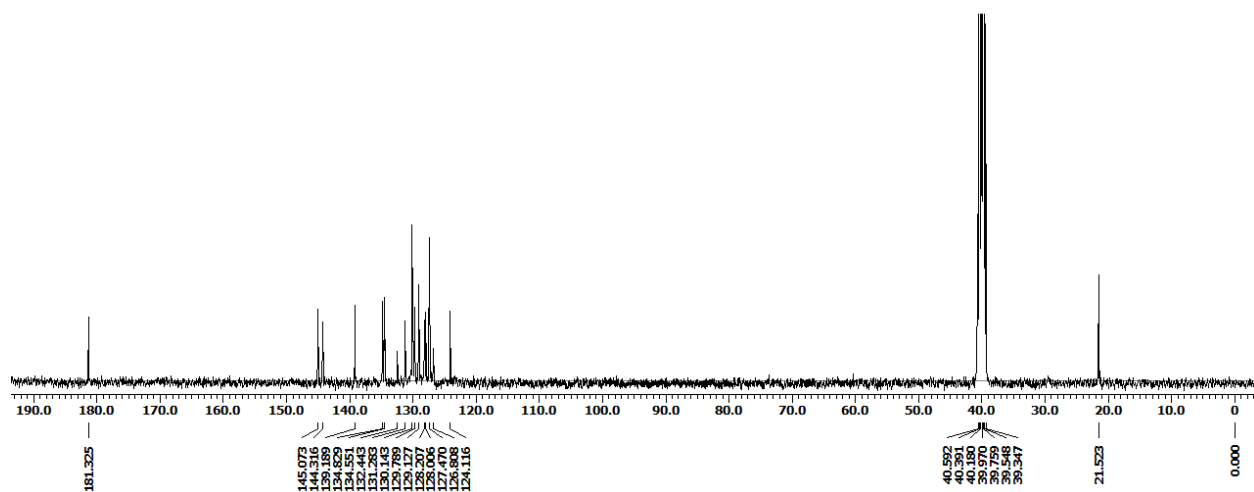
Thiophen-2-yl(4-(3-(4-(thiophene-2-carbonyl)-2-tosyl-1H-pyrrol-3-yl)phenyl)-5-tosyl-1H-pyrrol-3-yl)methanone (6c)



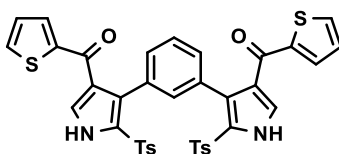
<sup>13</sup>C NMR



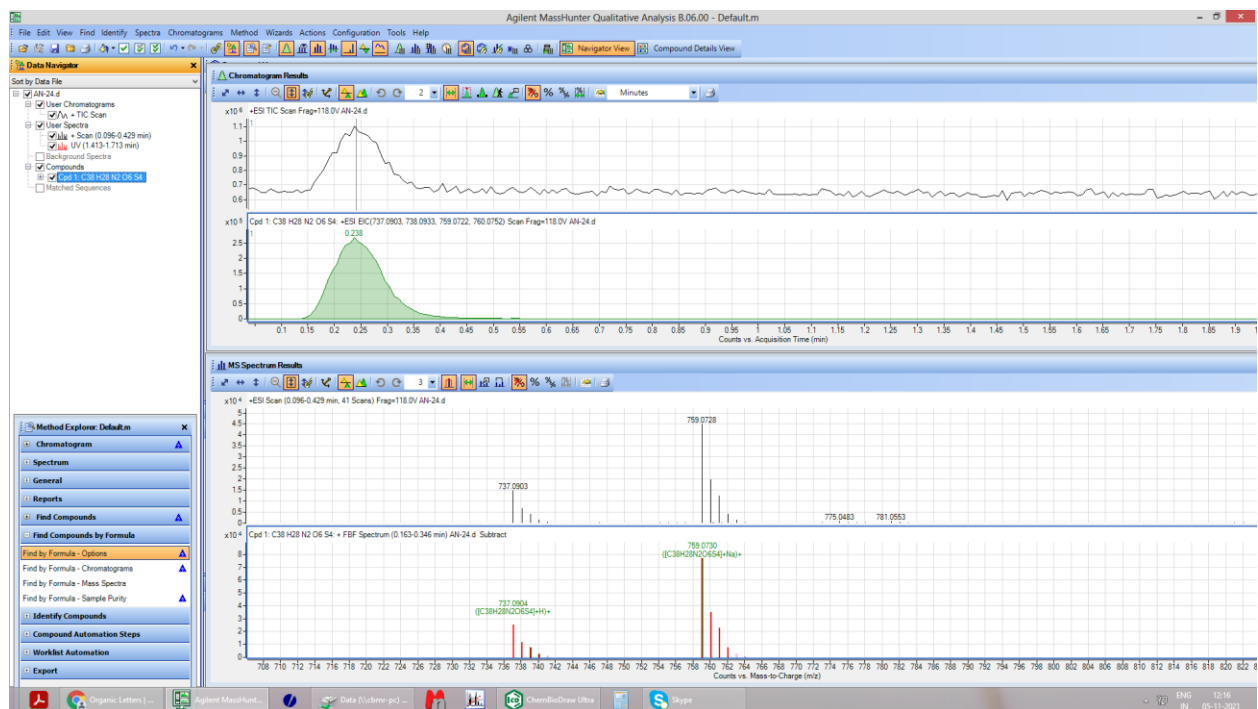
Thiophen-2-yl(4-(3-(4-(thiophene-2-carbonyl)-2-tosyl-1H-pyrrol-3-yl)phenyl)-5-tosyl-1H-pyrrol-3-yl)methanone (6c)



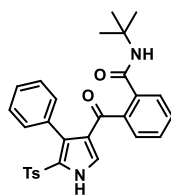
## HRMS



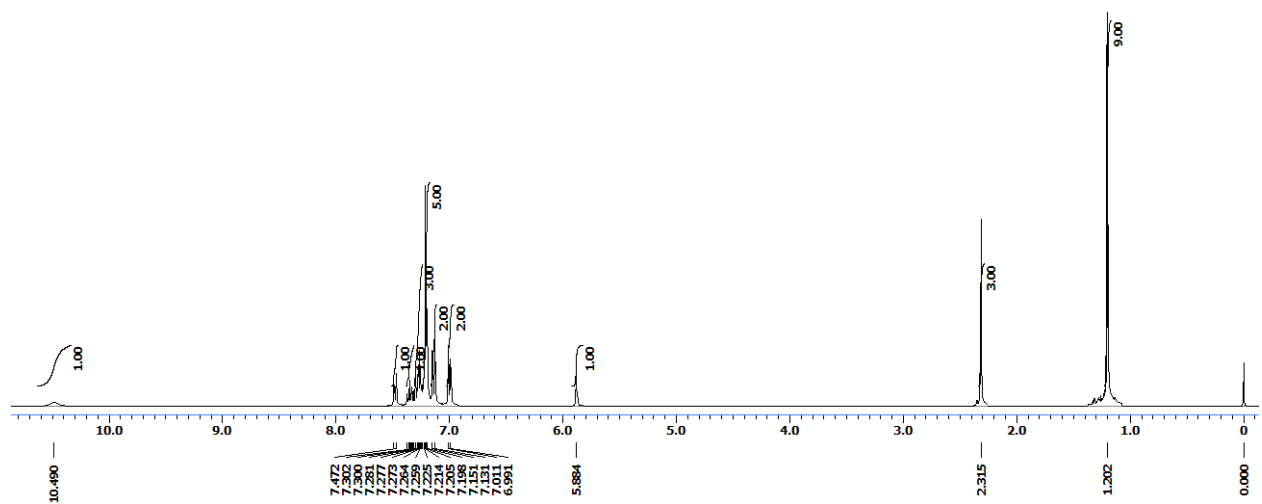
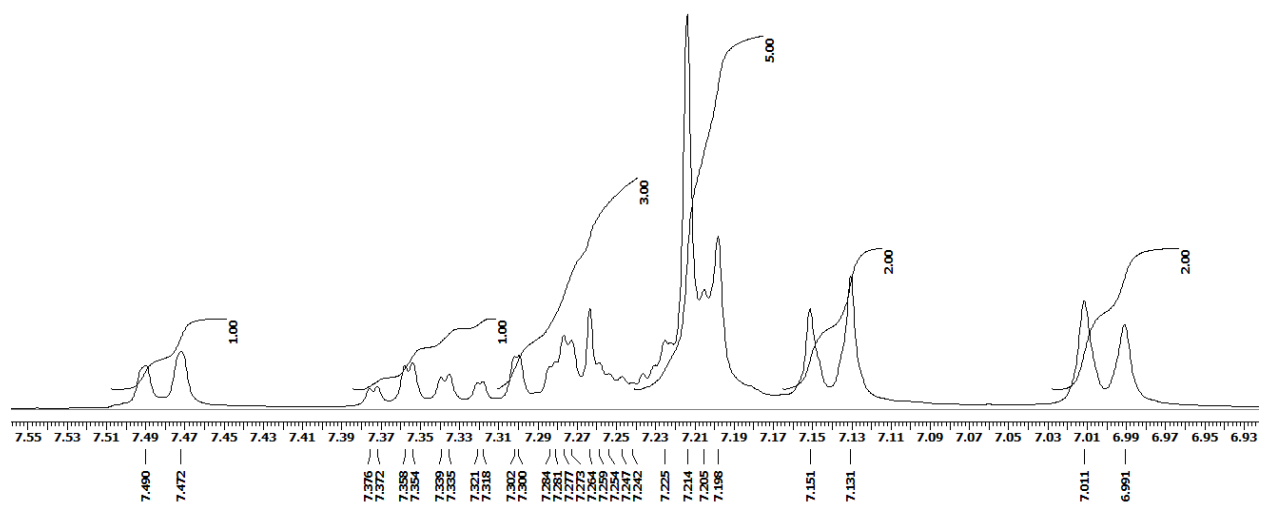
**Thiophen-2-yl(4-(3-(4-(thiophene-2-carbonyl)-2-tosyl-1H-pyrrol-3-yl)phenyl)-5-tosyl-1H-pyrrol-3-yl)methanone (6c)**



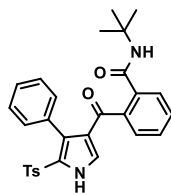
# <sup>1</sup>H NMR



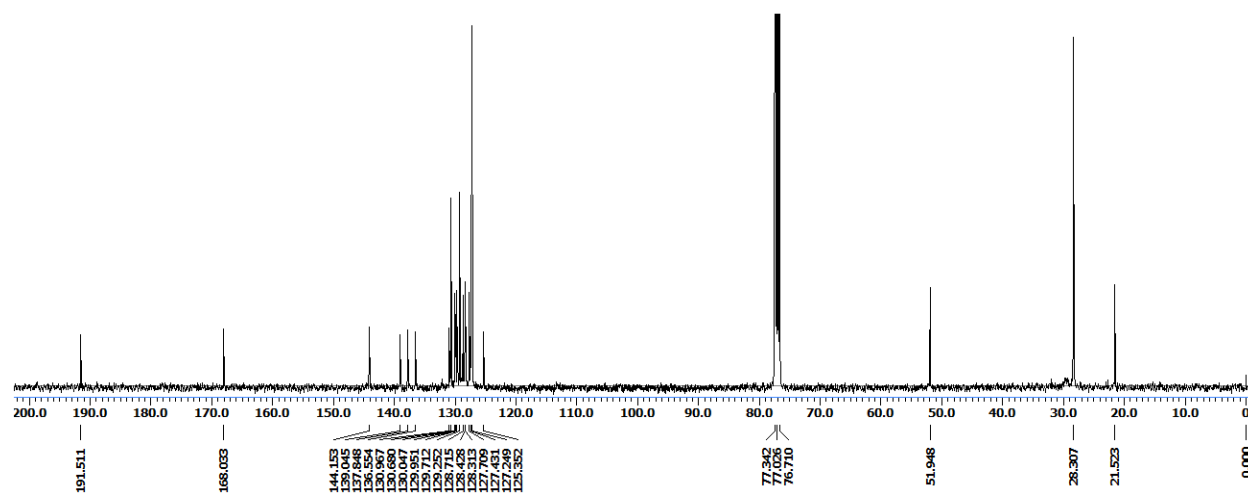
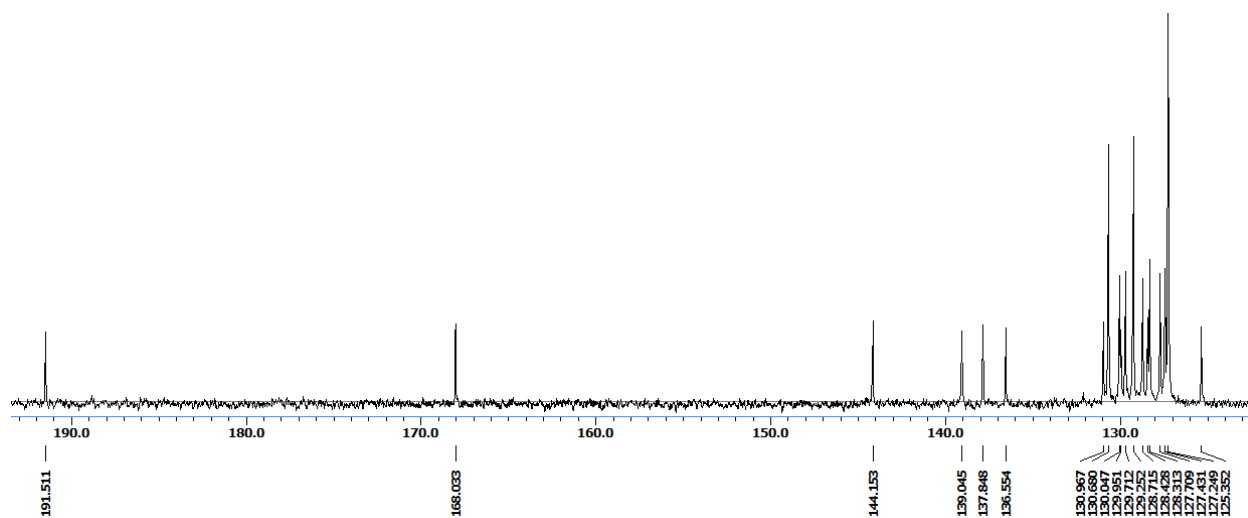
N-(*tert*-butyl)-2-(4-phenyl-5-tosyl-1H-pyrrole-3-carbonyl)benzamide (8a)



<sup>13</sup>C NMR

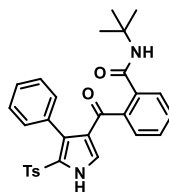


N-(*tert*-butyl)-2-(4-phenyl-5-tosyl-1*H*-pyrrole-3-carbonyl)benzamide (8a)





# HRMS



## N-(tert-butyl)-2-(4-phenyl-5-tosyl-1H-pyrrole-3-carbonyl)benzamide (8a)

### Analysis Info

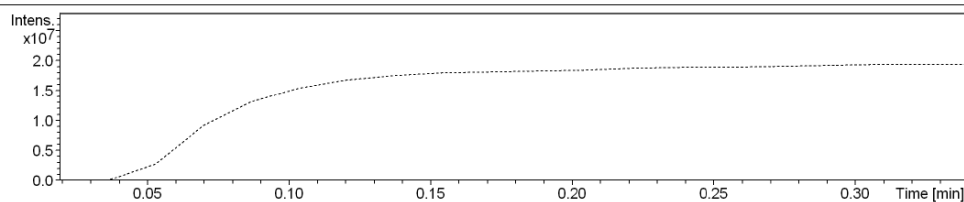
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 Sample Name Tmix-131118  
 Comment

Acquisition Date 12/30/2020 2:15:02 PM

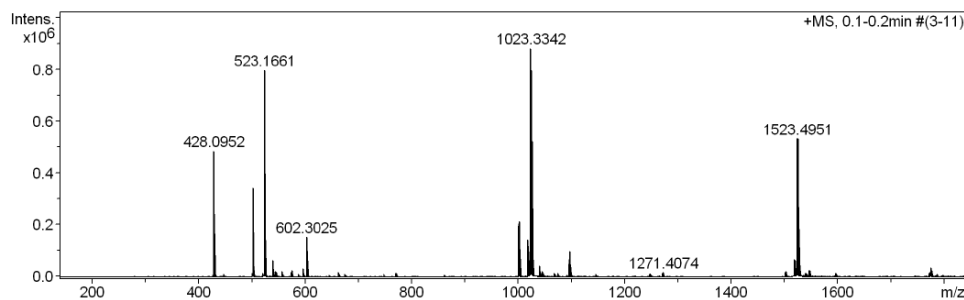
Operator Amit S.Sahu  
 Instrument micrOTOF-Q II 10337

### Acquisition Parameter

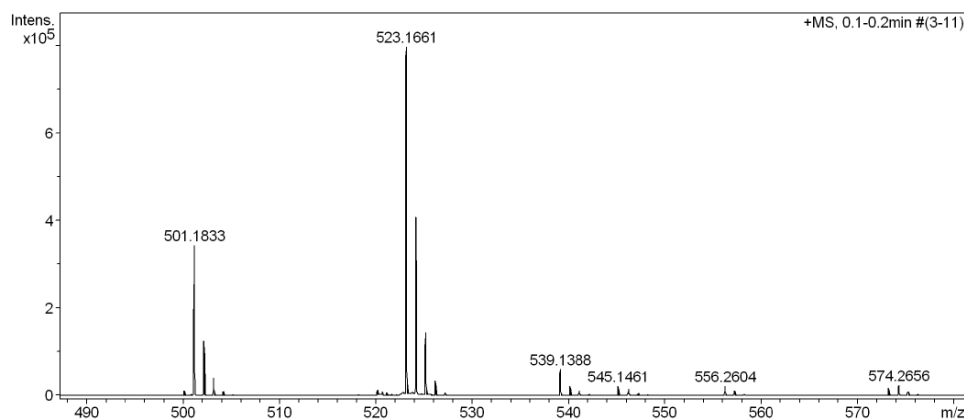
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



----- TIC +All MS

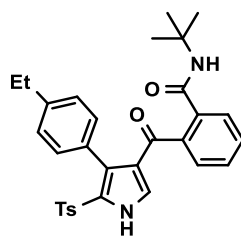


+MS, 0.1-0.2min #(3-11)

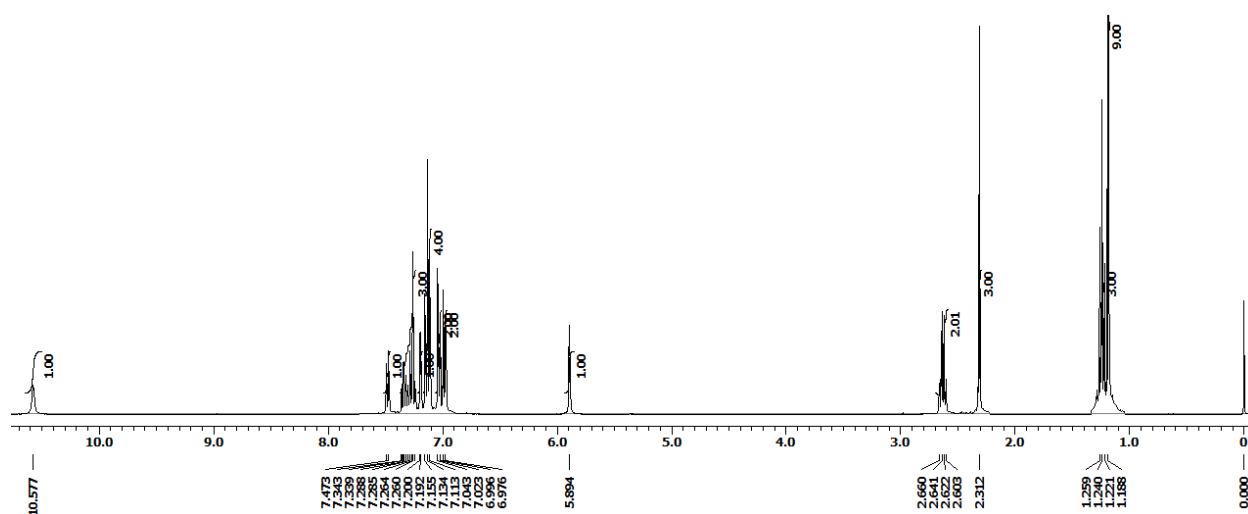
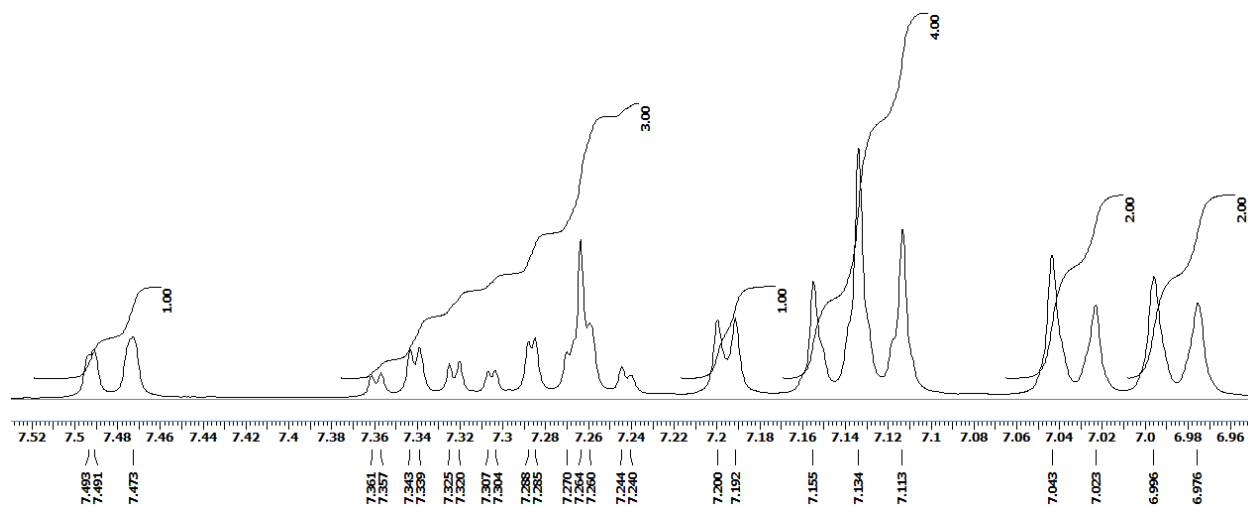


+MS, 0.1-0.2min #(3-11)

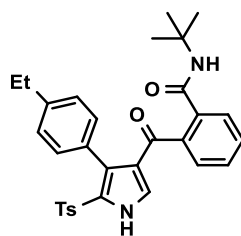
# <sup>1</sup>H NMR



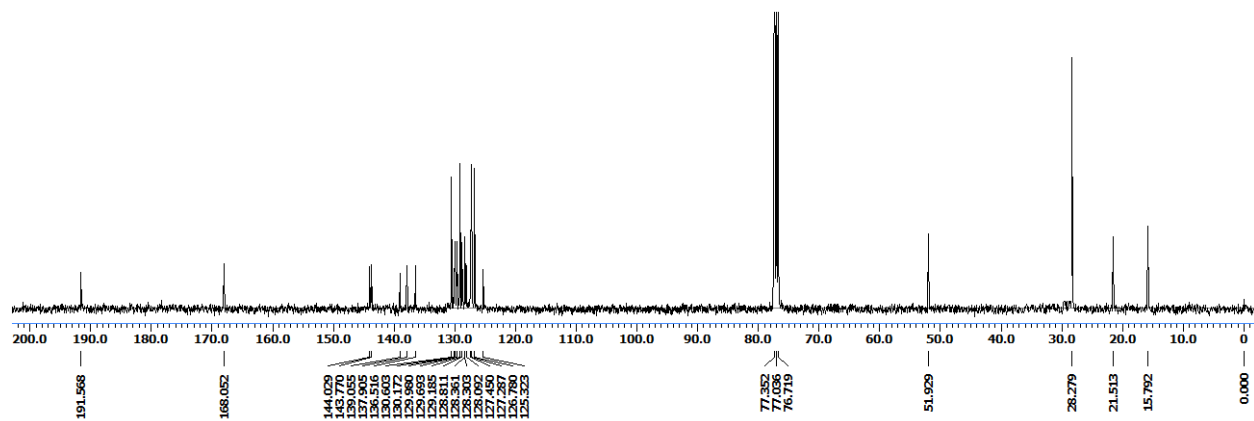
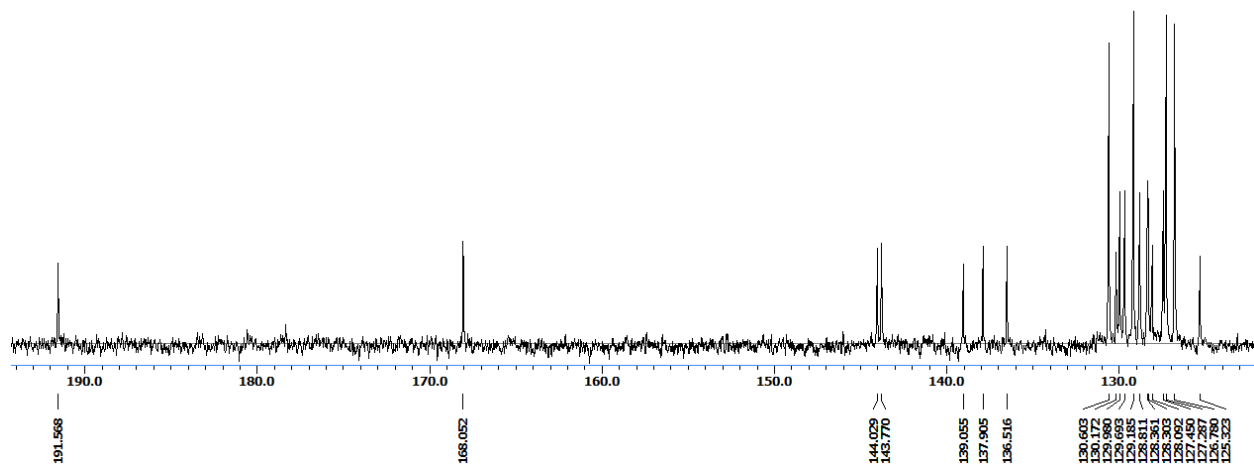
**N-(tert-butyl)-2-(4-(4-ethylphenyl)-5-tosyl-1H-pyrrole-3-carbonyl)benzamide (8b)**



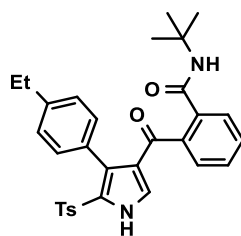
<sup>13</sup>C NMR



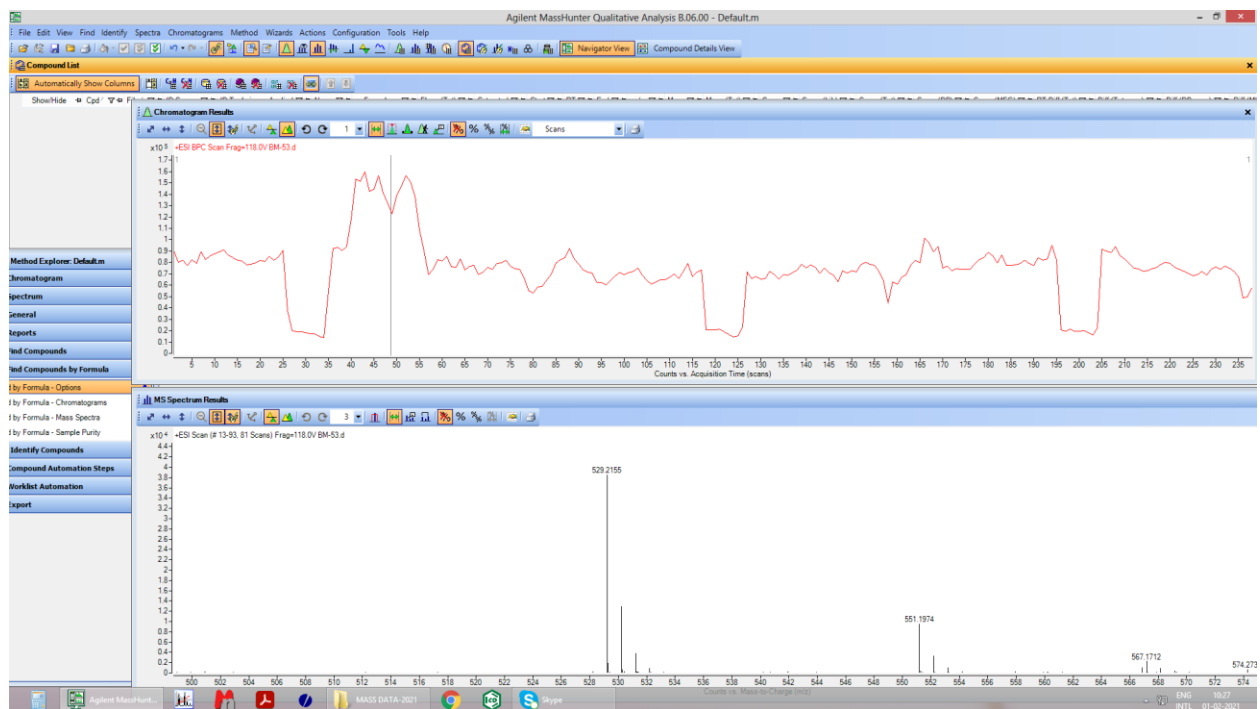
**N-(tert-butyl)-2-(4-(4-ethylphenyl)-5-tosyl-1H-pyrrole-3-carbonyl)benzamide (8b)**



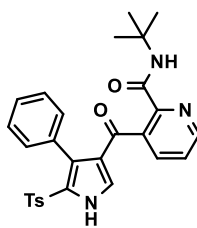
## HRMS



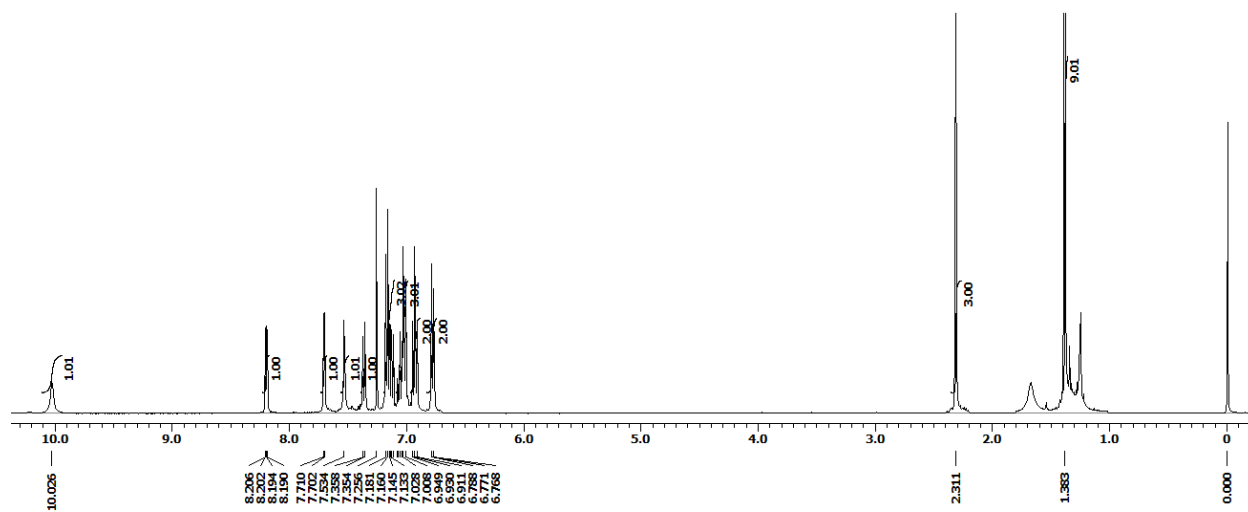
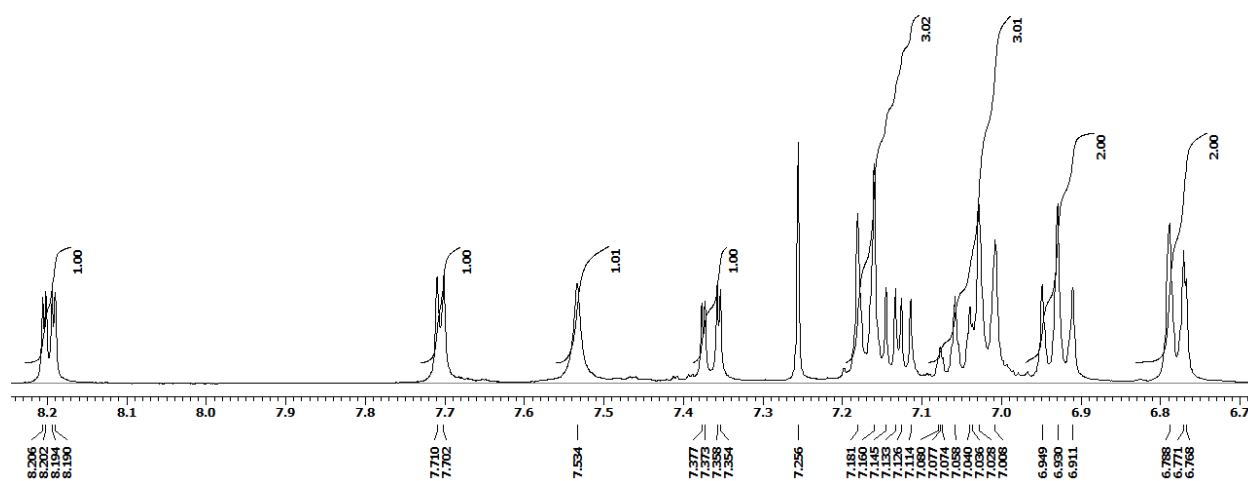
**N-(tert-butyl)-2-(4-(4-ethylphenyl)-5-tosyl-1H-pyrrole-3-carbonyl)benzamide (8b)**



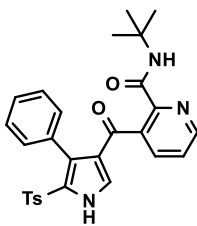
# <sup>1</sup>H NMR



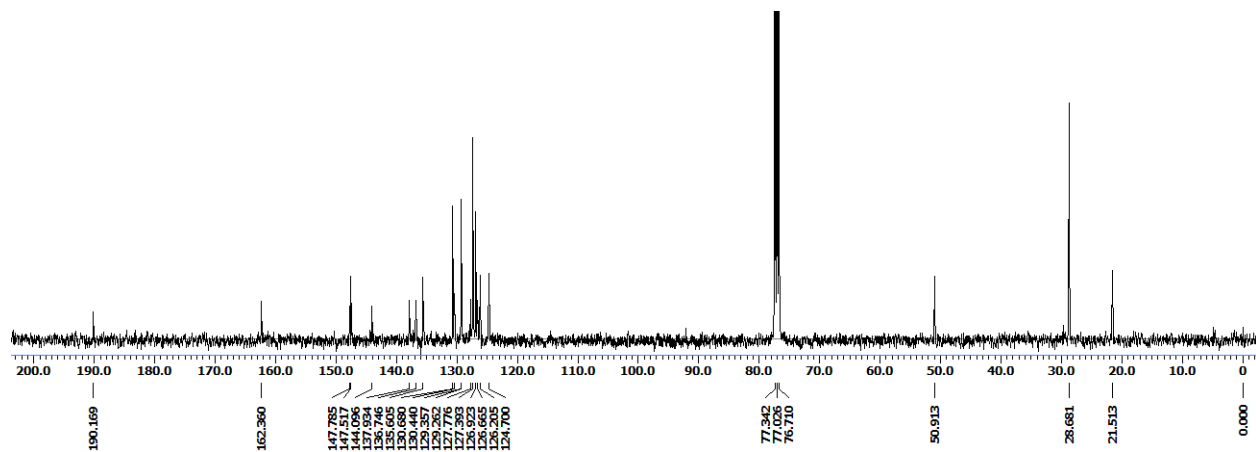
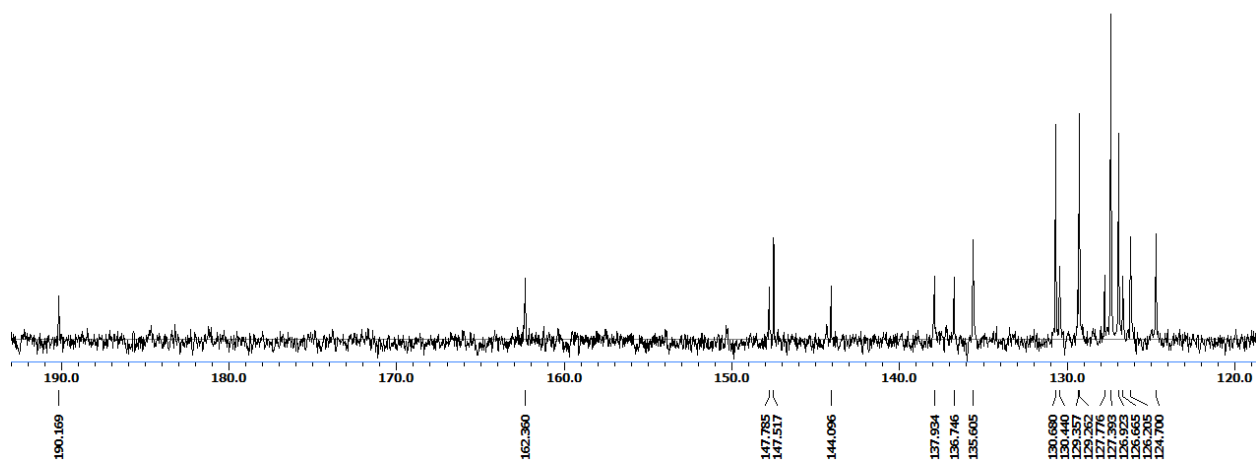
N-(*tert*-butyl)-3-(4-phenyl-5-tosyl-1*H*-pyrrole-3-carbonyl)picolinamide (8c)



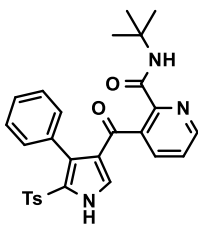
<sup>13</sup>C NMR



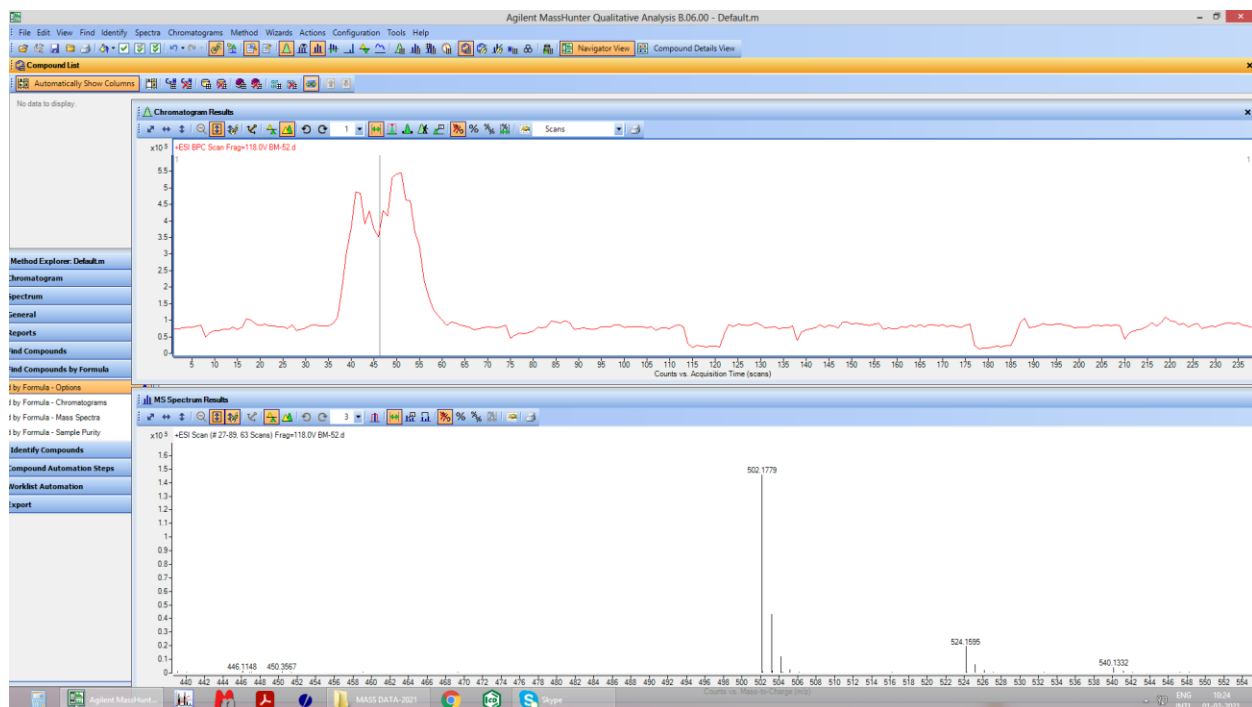
N-(*tert*-butyl)-3-(4-phenyl-5-tosyl-1*H*-pyrrole-3-carbonyl)picolinamide (8c)



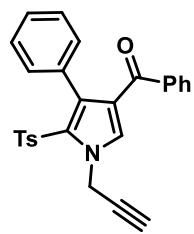
# HRMS



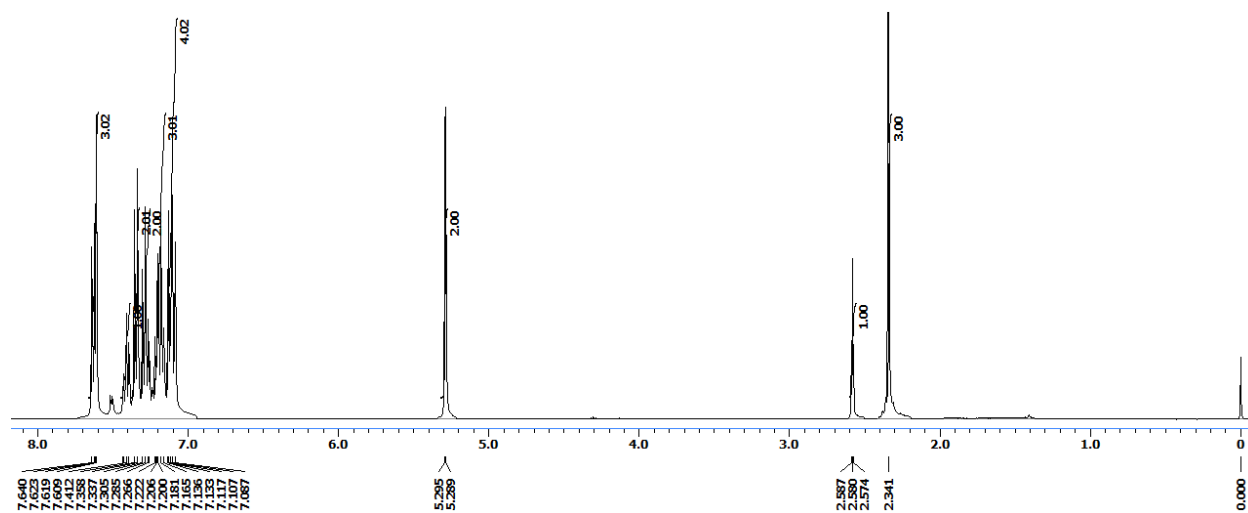
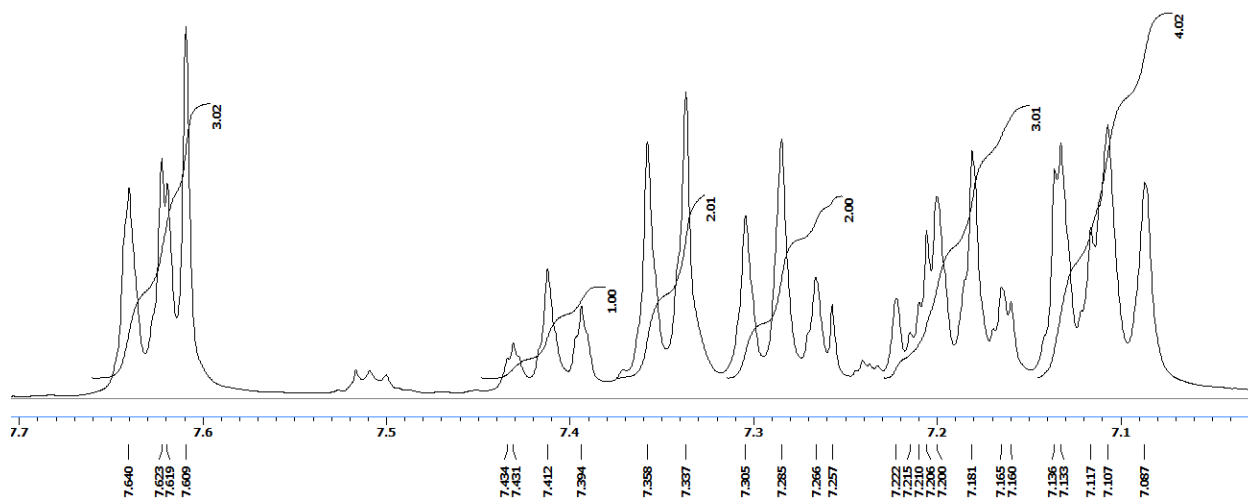
**N-(*tert*-butyl)-3-(4-phenyl-5-tosyl-1*H*-pyrrole-3-carbonyl)picolinamide (8c)**



# <sup>1</sup>H NMR

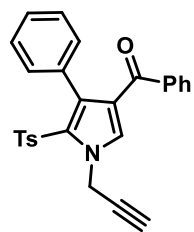


Phenyl(4-phenyl-1-(prop-2-yn-1-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (10)

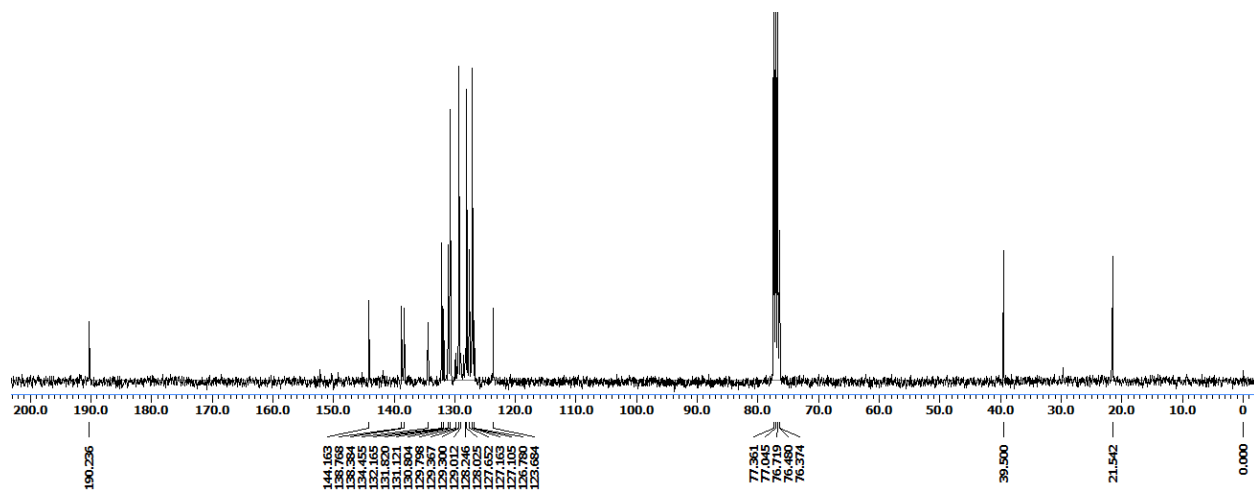
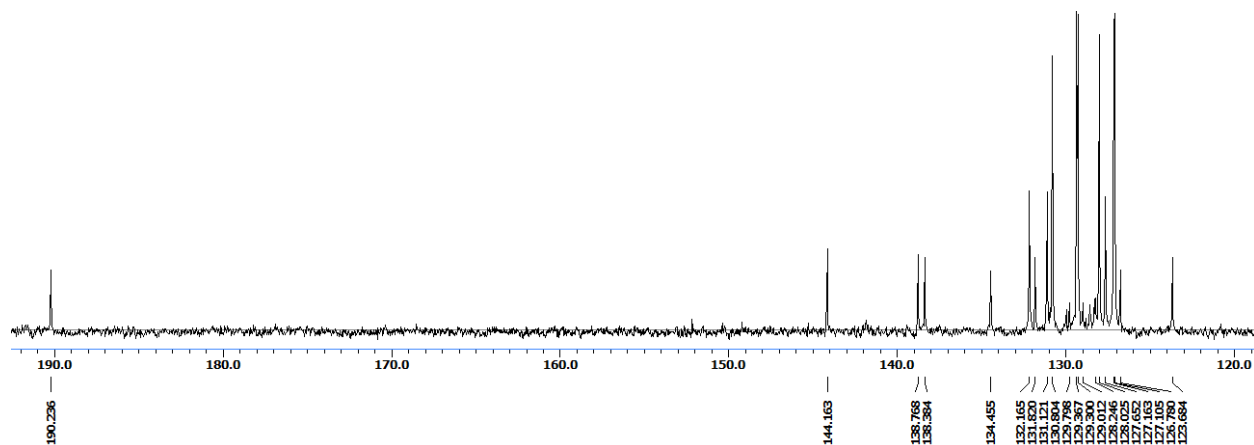




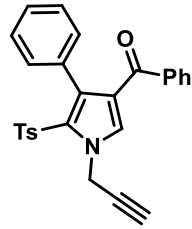
<sup>13</sup>C NMR



Phenyl(4-phenyl-1-(prop-2-yn-1-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (10)



# HRMS



## Phenyl(4-phenyl-1-(prop-2-yn-1-yl)-5-tosyl-1H-pyrrol-3-yl)methanone (10)

### Analysis Info

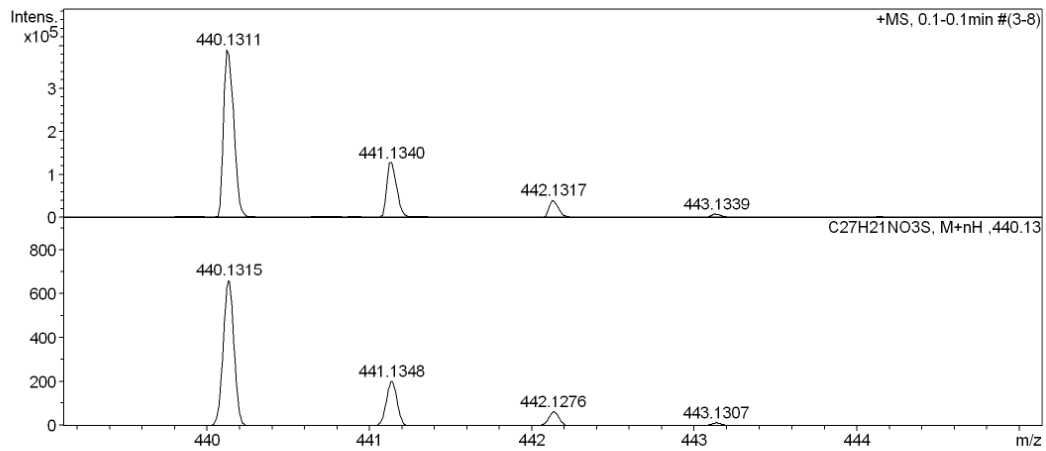
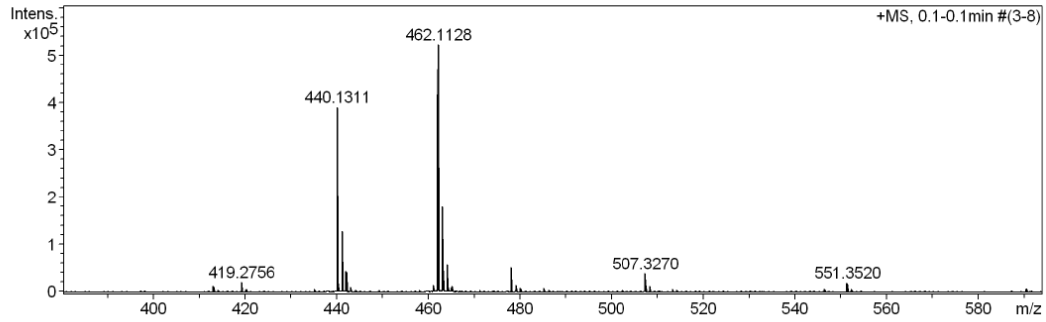
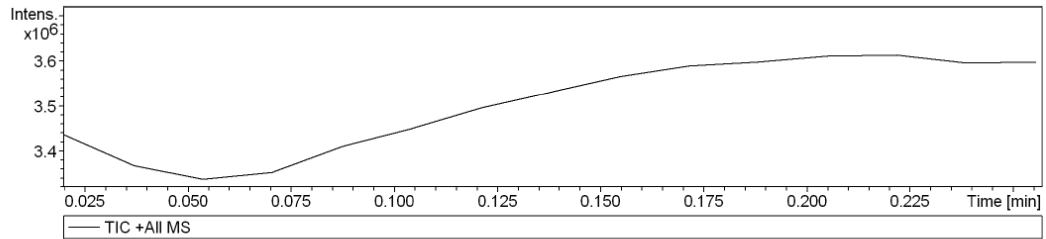
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Sample Name Tmix-131118  
Comment

Acquisition Date 12/29/2020 10:33:12 PM

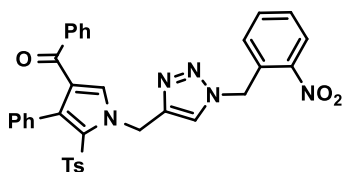
Operator Amit S.Sahu  
Instrument micrOTOF-Q II 10337

### Acquisition Parameter

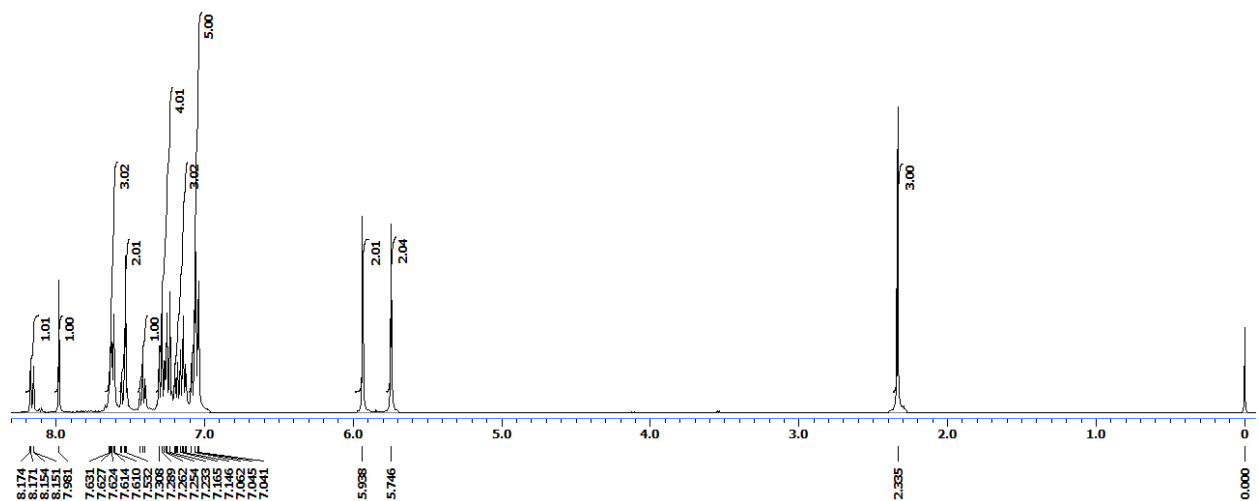
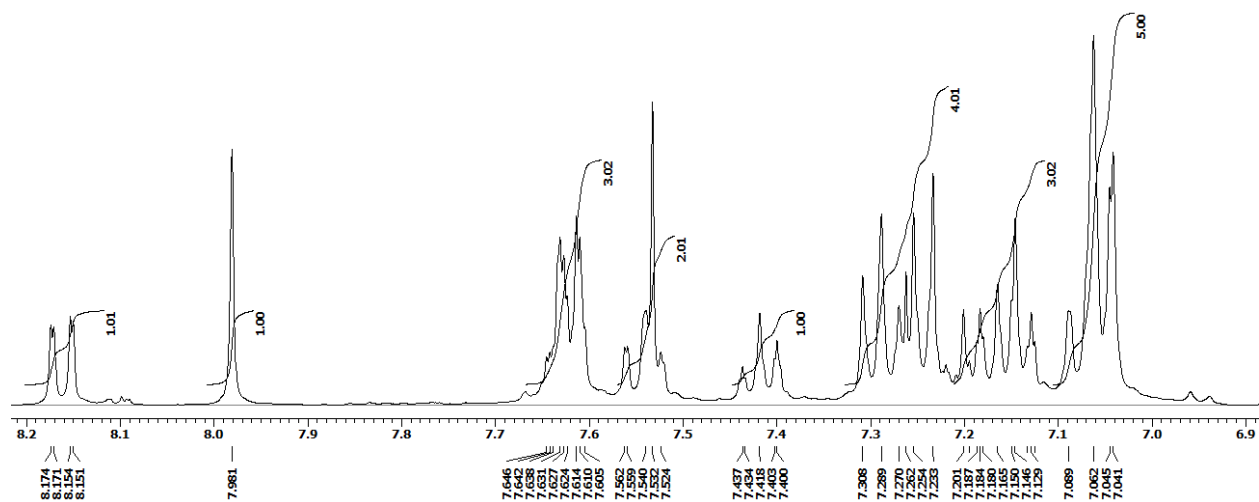
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



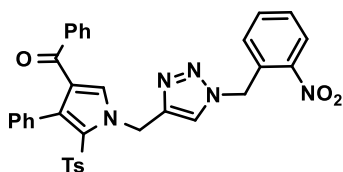
# <sup>1</sup>H NMR



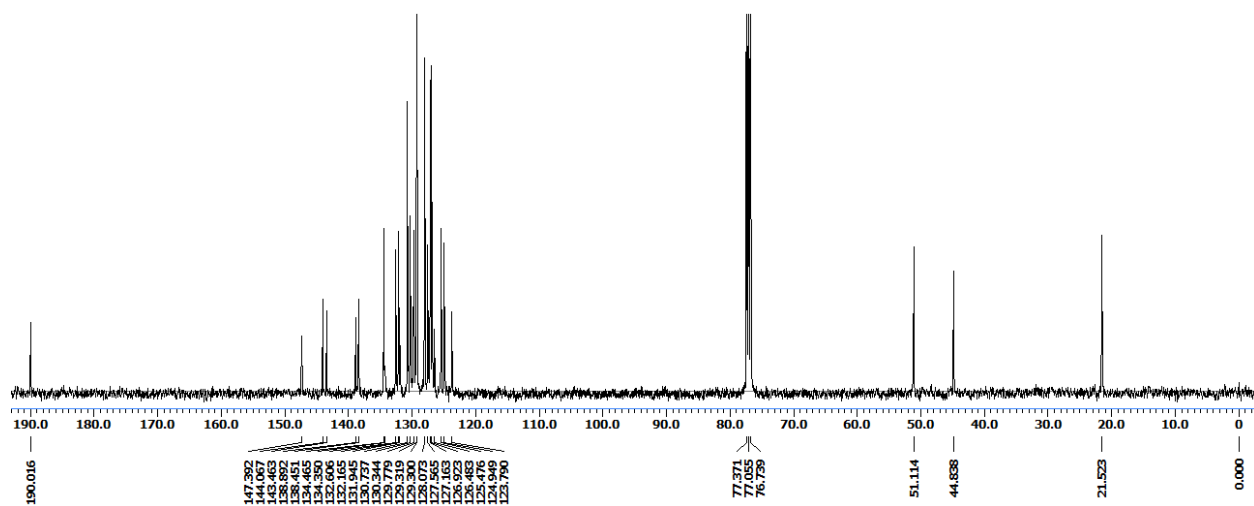
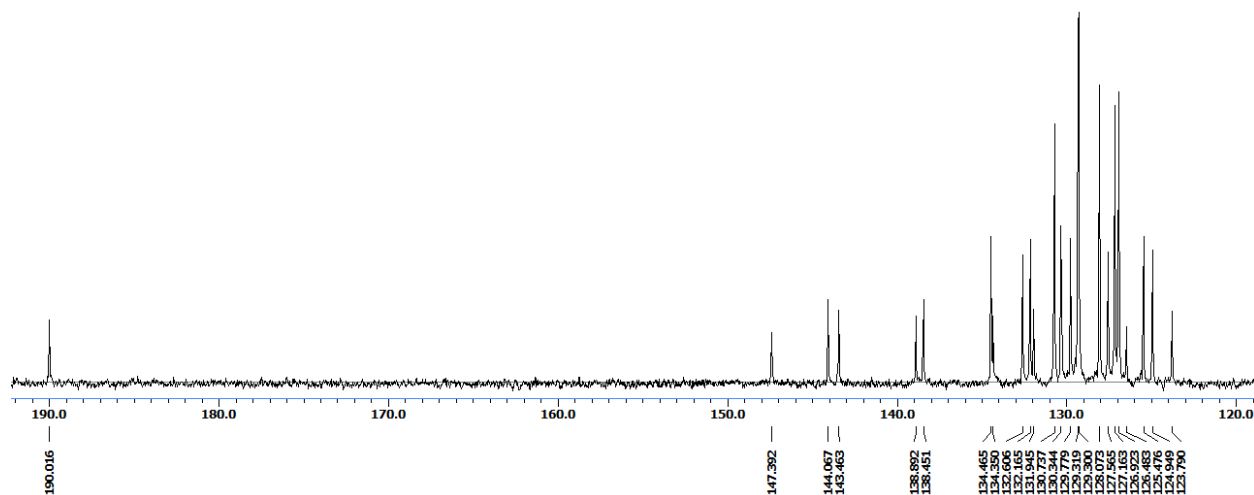
(1-((1-(2-Nitrobenzyl)-1H-1,2,3-triazol-4-yl)methyl)-4-phenyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (12)



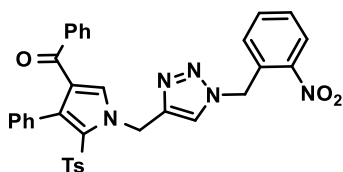
<sup>13</sup>C NMR



(1-((1-(2-Nitrobenzyl)-1H-1,2,3-triazol-4-yl)methyl)-4-phenyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (12)



# HRMS

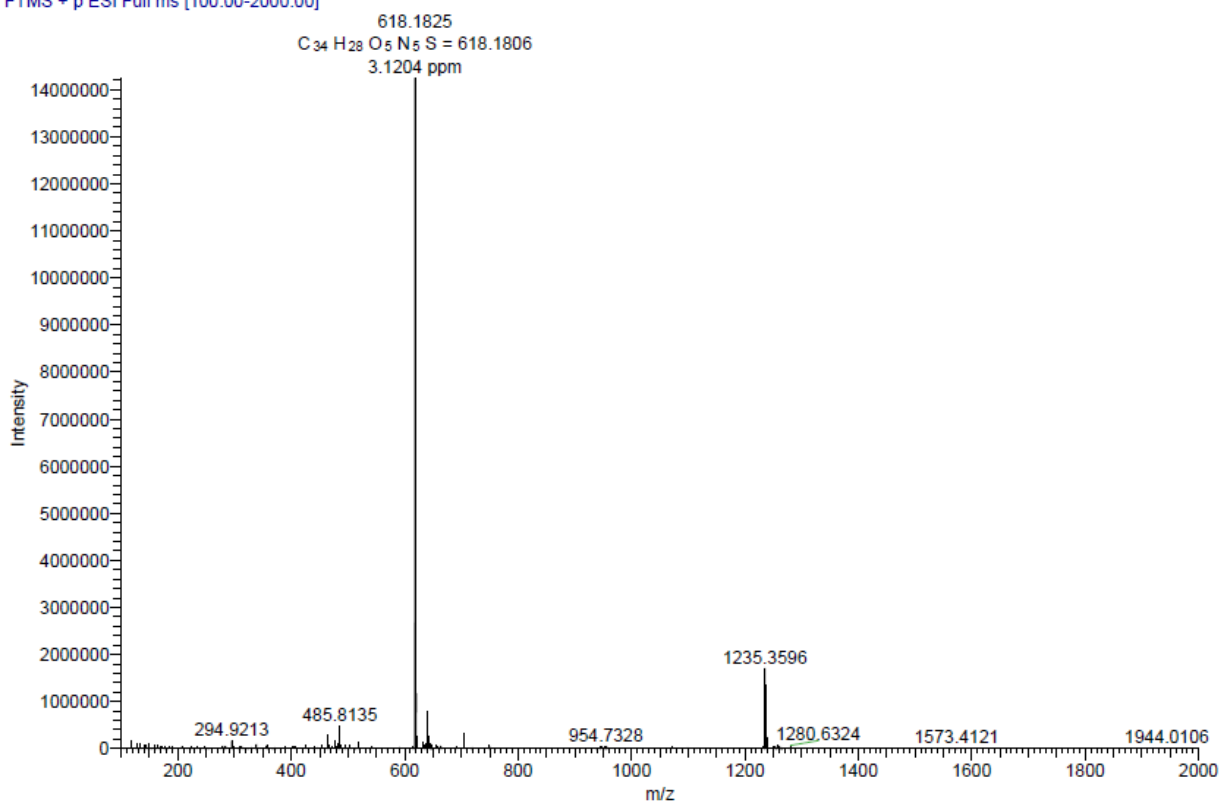


(1-((1-(2-Nitrobenzyl)-1H-1,2,3-triazol-4-yl)methyl)-4-phenyl-5-tosyl-1H-pyrrol-3-yl)(phenyl)methanone (12)

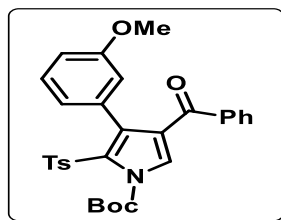
Y:\Internal\12022021\AN-43

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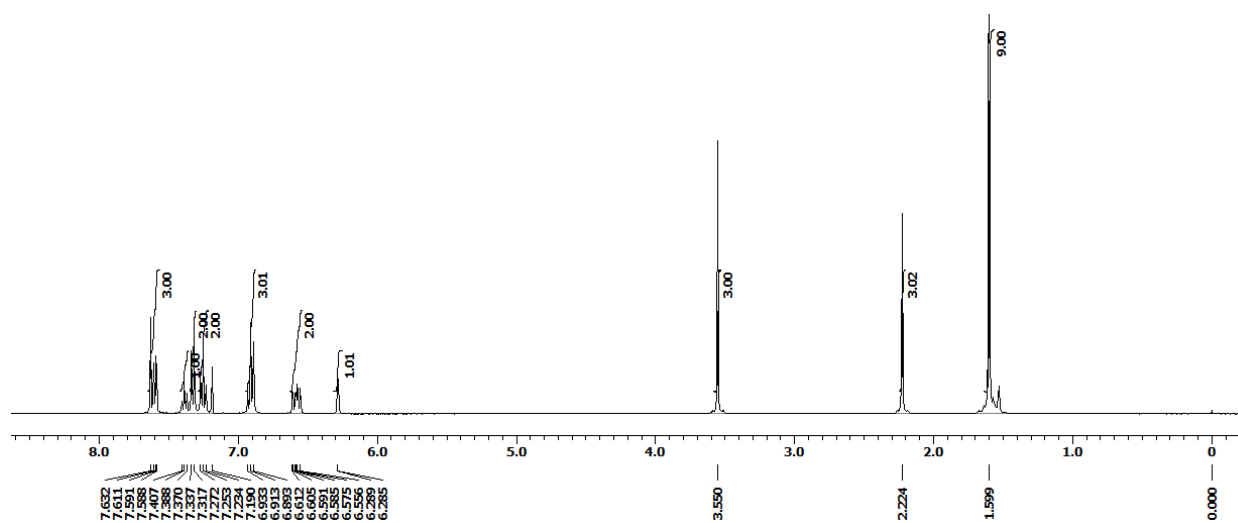
AN-43 #121 RT: 0.61 AV: 1 NL: 1.42E7  
T: FTMS + p ESI Full ms [100.00-2000.00]



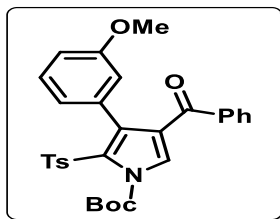
# <sup>1</sup>H NMR



*tert*-butyl 4-benzoyl-3-(3-methoxyphenyl)-2-tosyl-1*H*-pyrrole-1-carboxylate (14)



<sup>13</sup>C NMR



*tert*-butyl 4-benzoyl-3-(3-methoxyphenyl)-2-tosyl-1*H*-pyrrole-1-carboxylate (14)

