

# Supporting Information: Structure-Based Optimization of Type III Indoleamine 2,3-Dioxygenase 1 (IDO1) Inhibitors

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<b>Structure</b>	<b>MMG-0472 (Compound 13)</b>
PDB entry	7zv3
<b>Data collection</b>	
Space group	P 21 21 21
Cell dimensions	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	86.65 97.42 132.00
$\alpha$ , $\beta$ , $\gamma$ (°)	90 90 90
Resolution (Å)	48.71 – 2.55 (2.70–2.55)
R-meas (%)	8.2 (76.8)
Mean I/sigma(I)	15.20 (1.89)
Completeness (%)	99.5 (97.1)
<b>Refinement</b>	
Resolution (Å)	48.71 – 2.55 (2.62–2.55)
No. unique reflections	36929 (3506)
R-work/R-free	0.19/0.24
No. non-hydrogen atoms	6109
Protein	5915
Ligand/ion	142
Water	52
Average <i>B</i> -factors	60.76
Protein	60.80
Ligand/ion	60.92
Water	55.60
R.m.s. deviations	
Bond lengths (Å)	0.009
Bond angles (°)	1.05
Ramachandran	
Favored (%)	95.39
Allowed (%)	4.61
Outliers (%)	0.00

Table S1: X-ray data collection and refinement statistics. Statistics for the highest-resolution shell are shown in parentheses.

Compound	Conc. [ $\mu\text{M}$ ]	Inh. [%]	Tox. [%]	IC <sub>50</sub> [ $\mu\text{M}$ ]
<b>9</b>	200	100	4 <sup>1</sup>	0.11 <sup>1</sup>
<b>10</b>				0.023 <sup>2</sup>
<b>11</b>	200	100	0 <sup>1</sup>	0.034 <sup>1</sup>
<b>13</b>	200	76	71 <sup>3</sup>	
<b>19</b>	200	93	3 <sup>1</sup>	8.9 <sup>4</sup>
<b>21</b>				7.0 <sup>4</sup>
<b>22</b>				1.1 <sup>4</sup>
<b>29</b>	200	95	0 <sup>1</sup>	1.7 <sup>4</sup>
<b>30</b>	200	95	0 <sup>1</sup>	0.62 <sup>4</sup>
<b>31</b>	200	100	26 <sup>1</sup>	23 <sup>1</sup>
<b>32</b>				14 <sup>4</sup>
<b>40</b>	200	71	22 <sup>3</sup>	
<b>41</b>	200	32	58 <sup>3</sup>	
<b>42</b>	200	56	5 <sup>3</sup>	110 <sup>3</sup>
<b>46</b>				34 <sup>4</sup>
<b>47</b>				>100 <sup>4</sup>
<b>133</b>	200	0	0 <sup>1</sup>	
<b>136</b>	200	78	0 <sup>1</sup>	
<b>138</b>	200	52	6 <sup>1</sup>	
<b>139</b>	200	100	0 <sup>1</sup>	4.6 <sup>1</sup>

Table S2: Previously determined cellular inhibition and toxicity data shown in Figure 6.

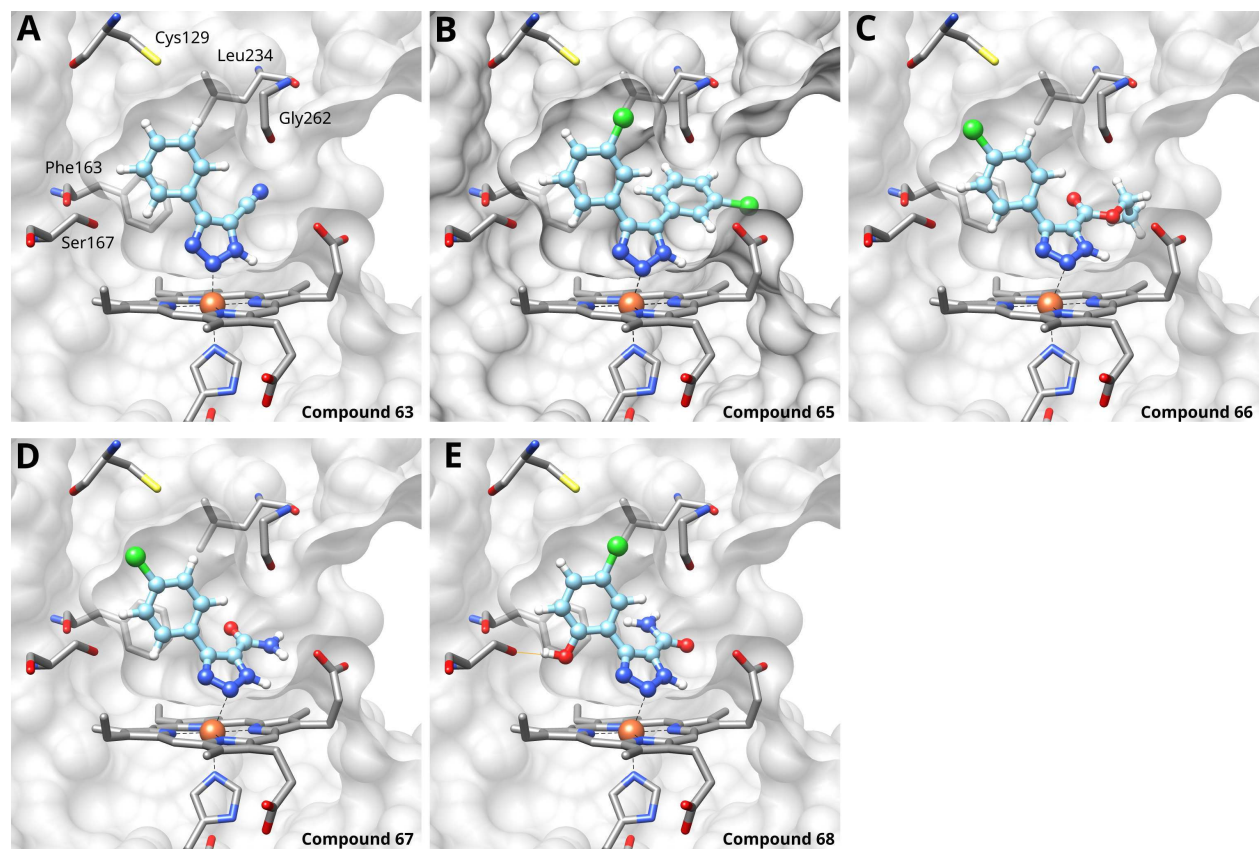


Figure S1: Binding poses predicted by docking for 5-substituted 4-aryl-1,2,3-triazoles. A. Compound **62**; B. Compound **64**; C. Compound **65**; D. Compound **66**; E. Compound **67**. The triazole ring does not assume a binding mode perpendicular to the heme plane.

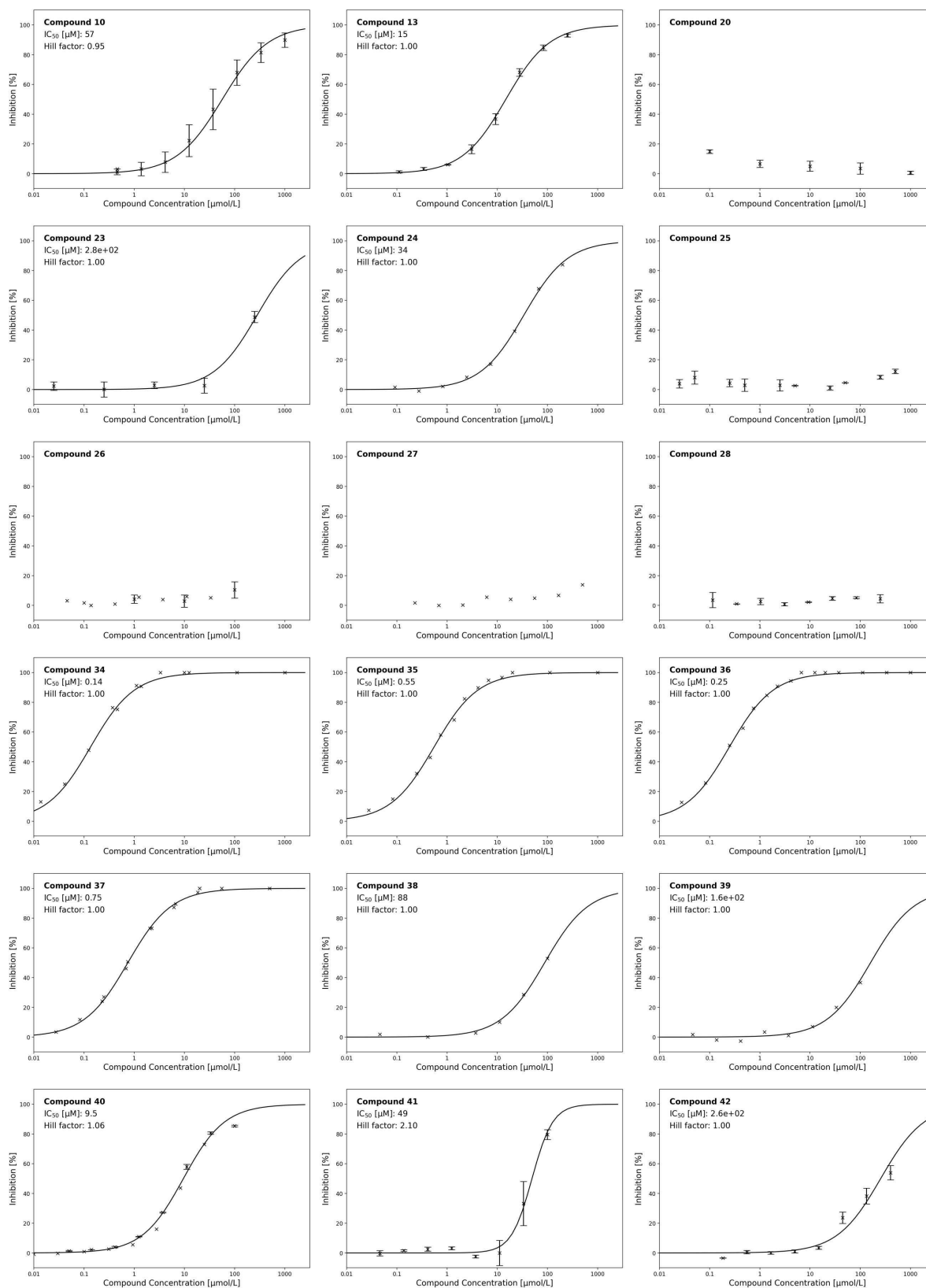
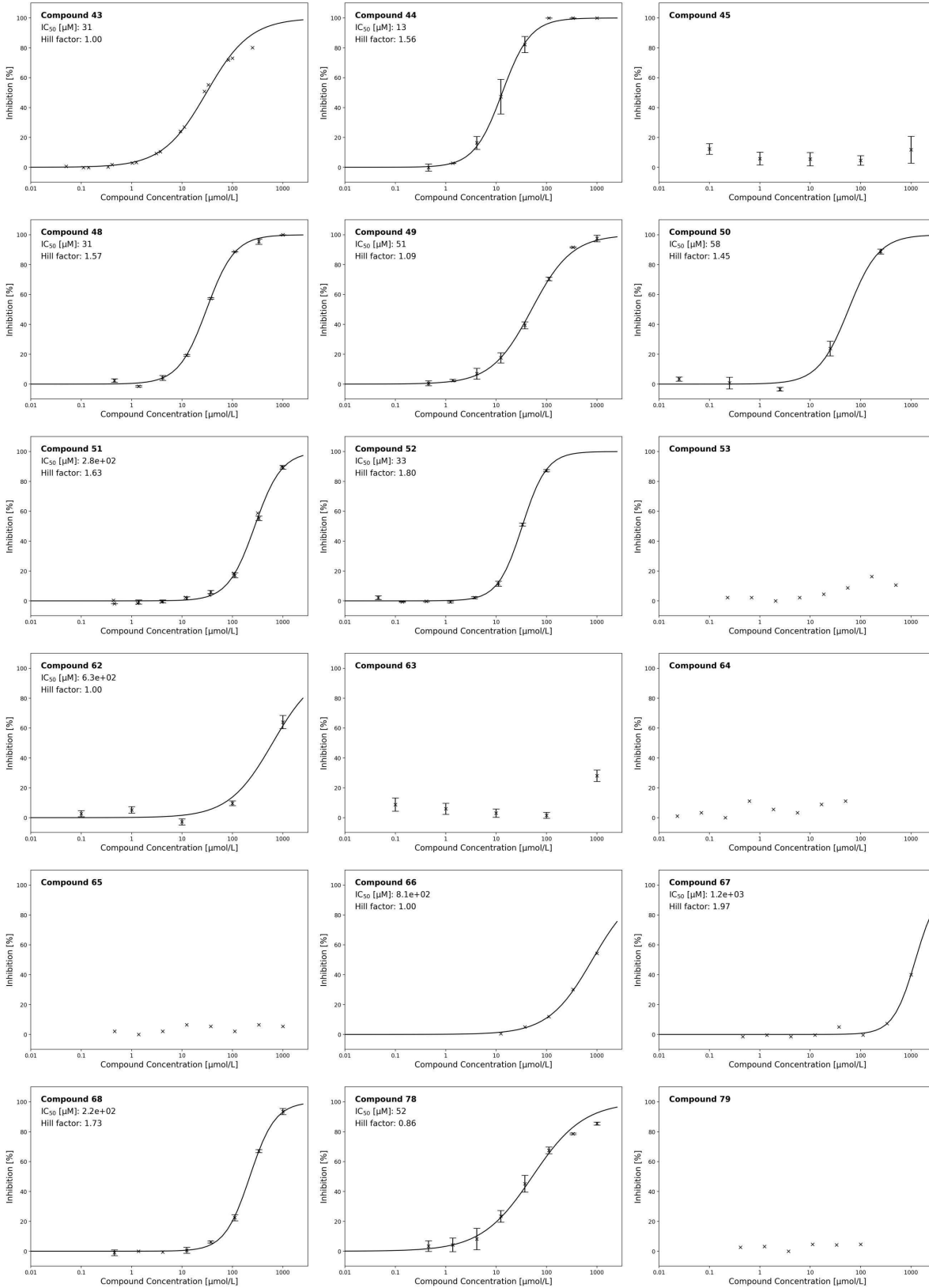
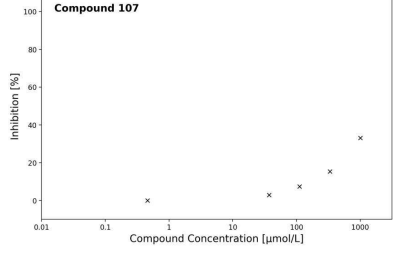
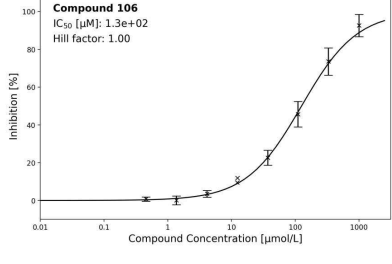
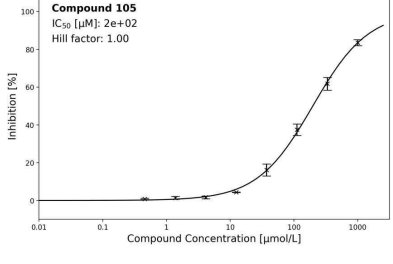
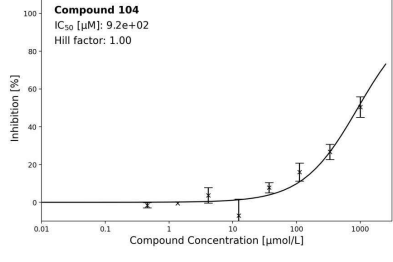
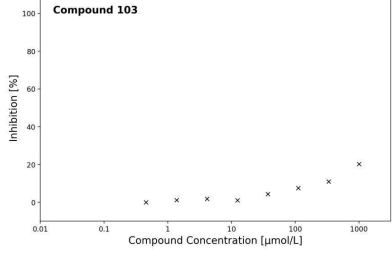
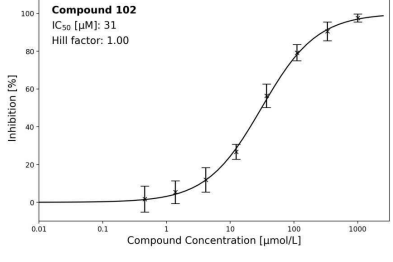
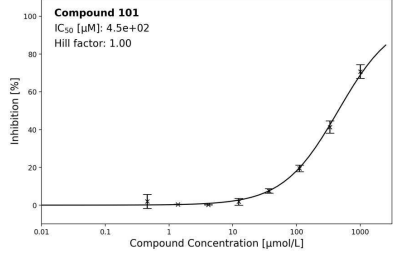
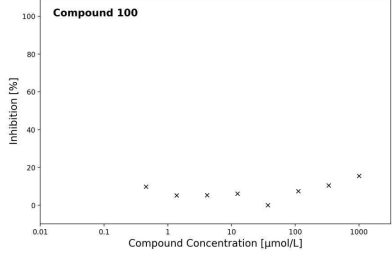
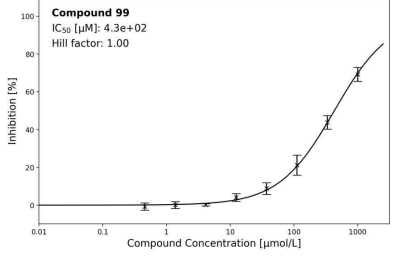
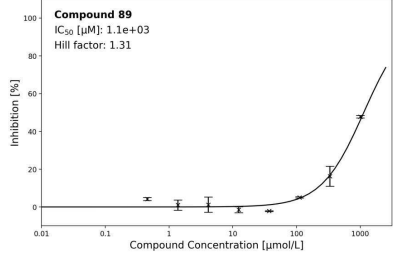
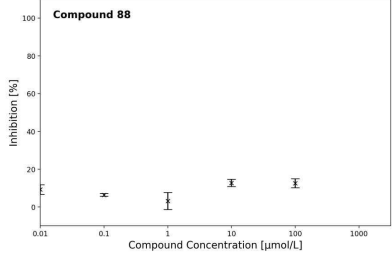
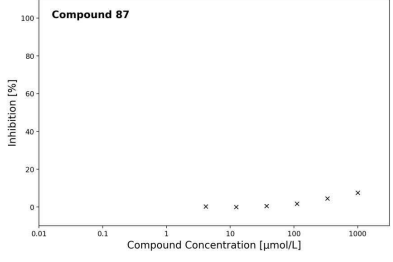
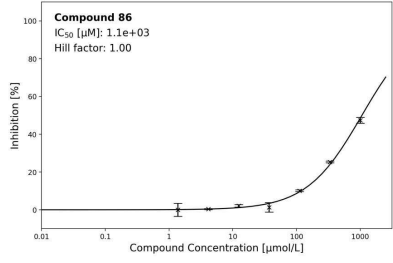
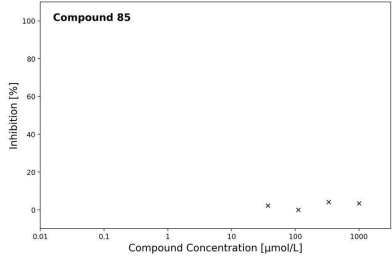
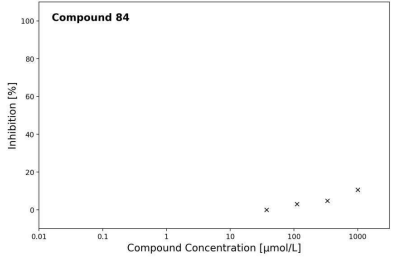
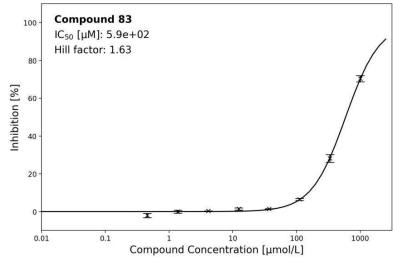
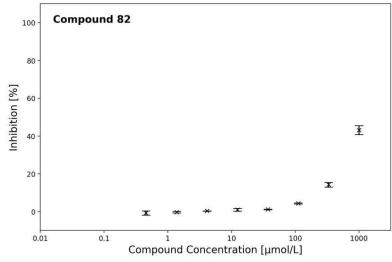
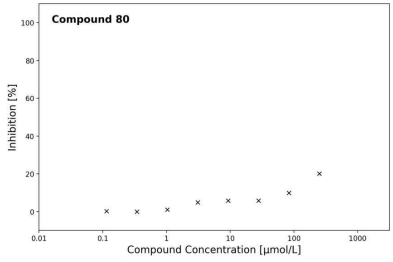
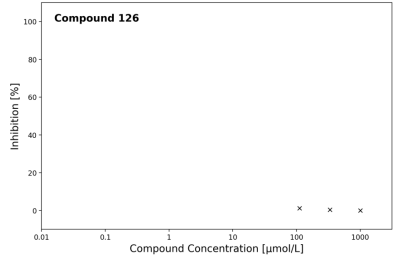
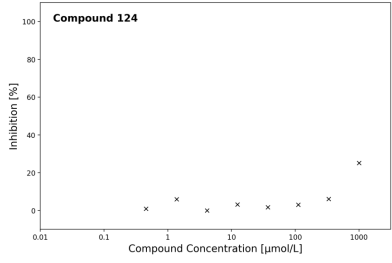
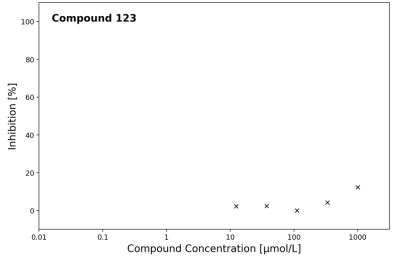
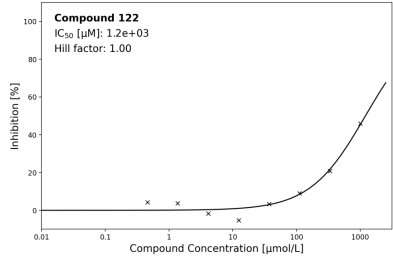
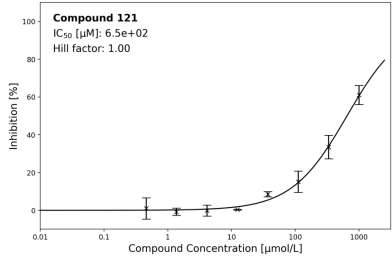
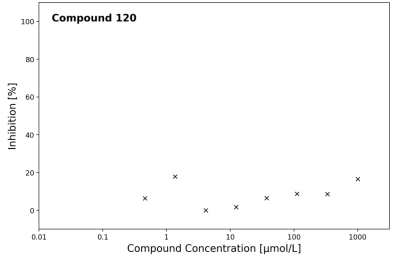
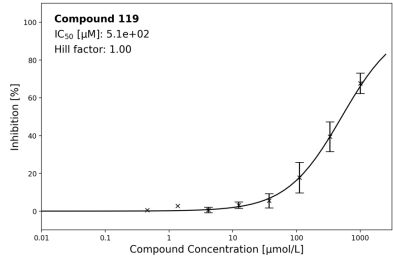
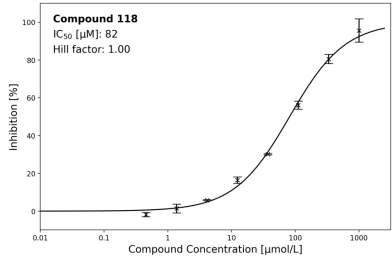
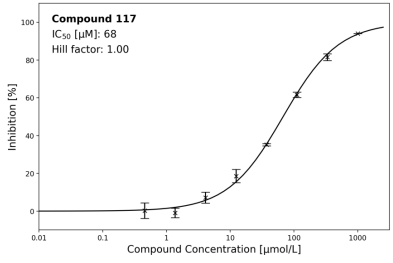
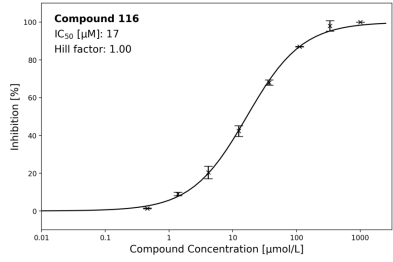
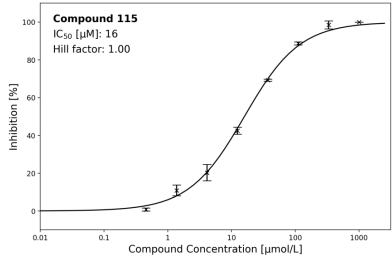
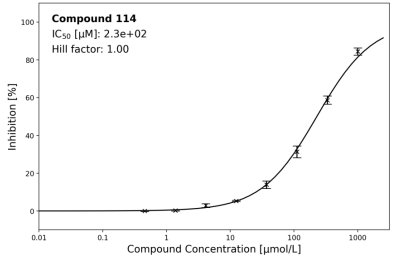
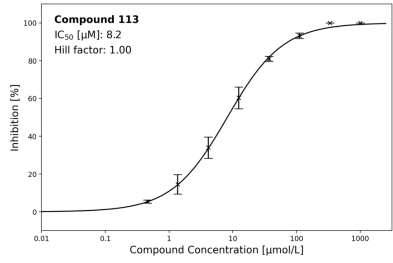
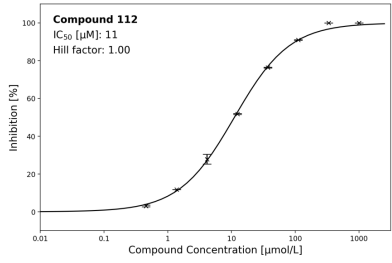
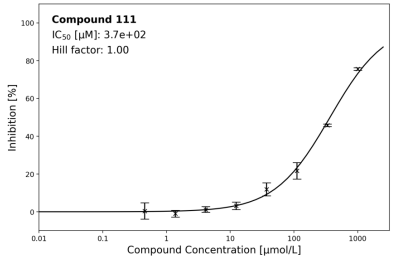
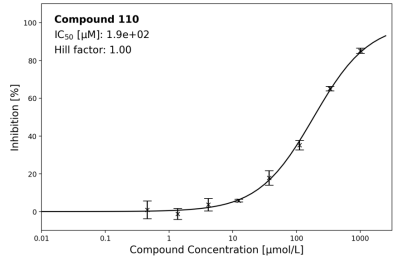
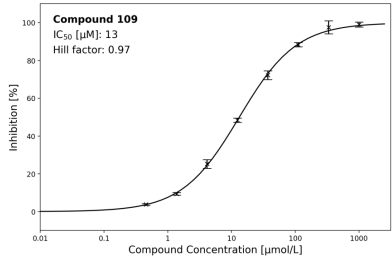
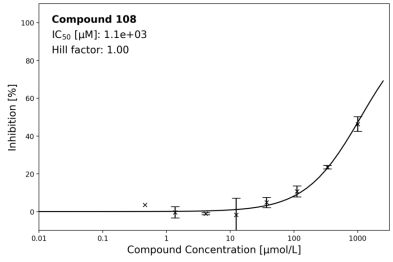


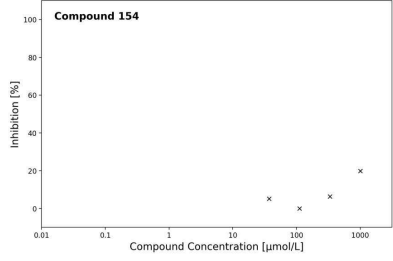
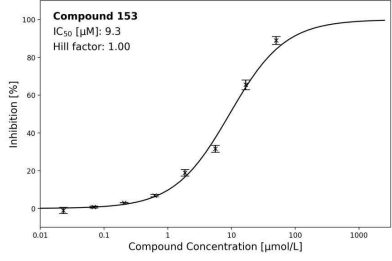
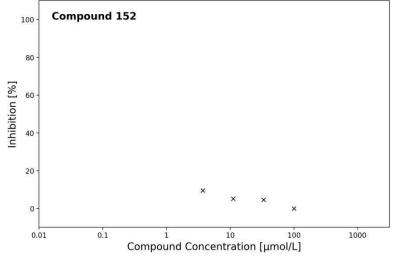
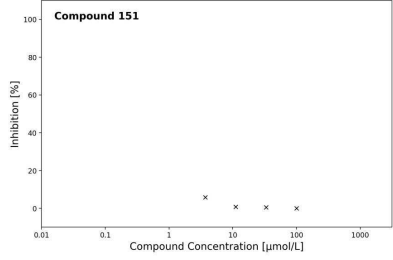
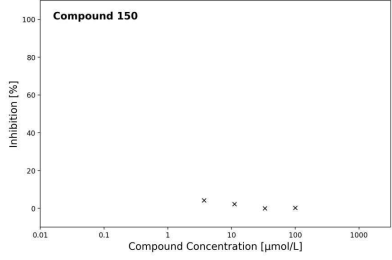
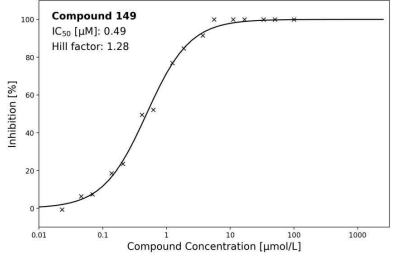
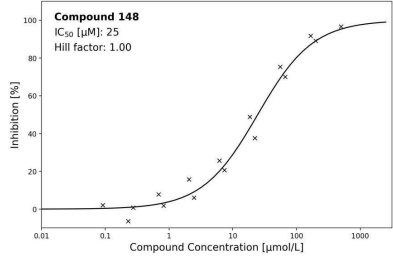
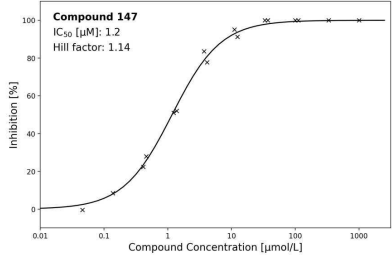
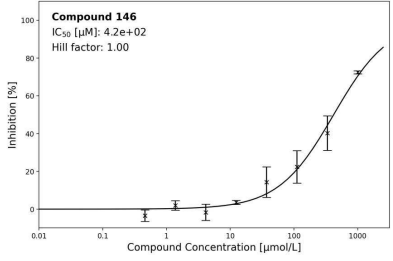
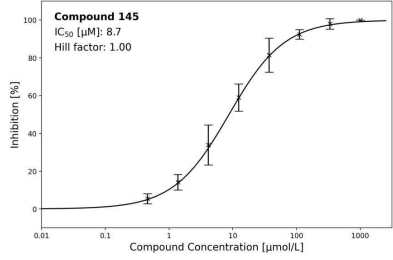
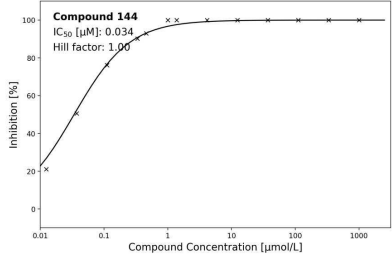
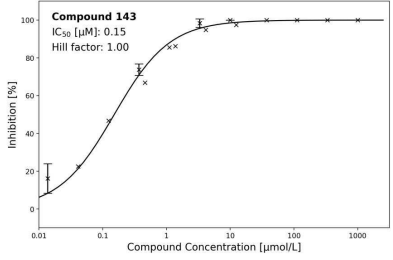
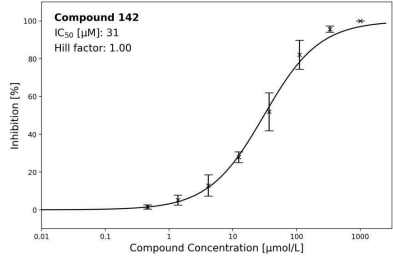
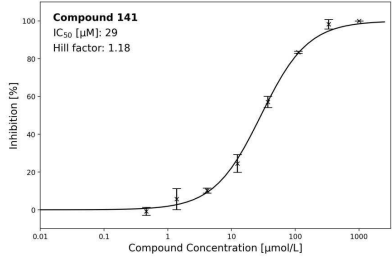
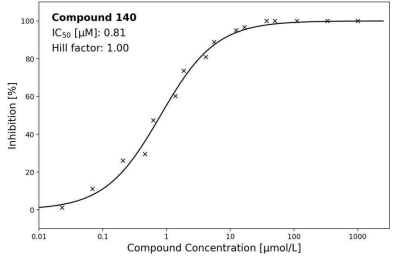
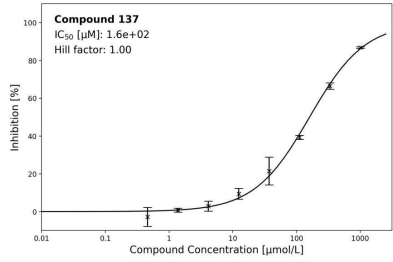
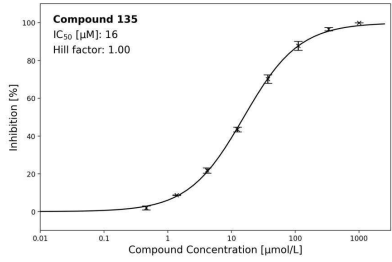
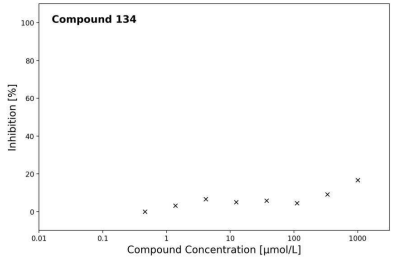
Figure S2: Enzymatic Dose-Response Curves of all Compounds (cont.).

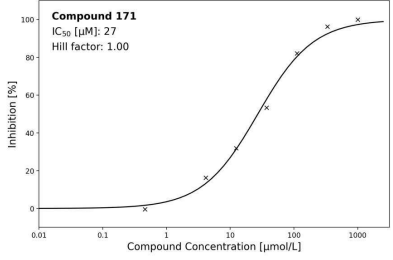
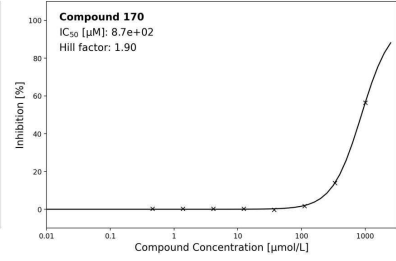
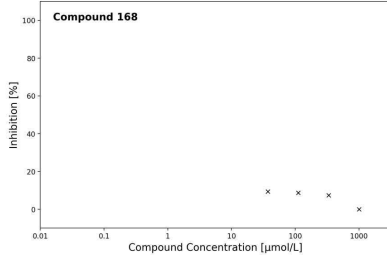
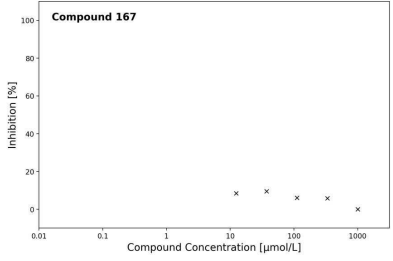
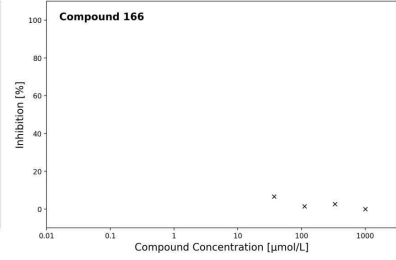
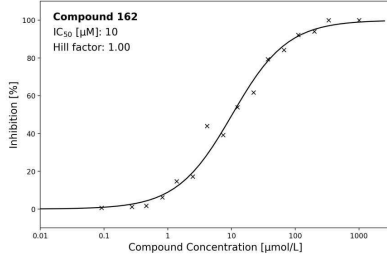
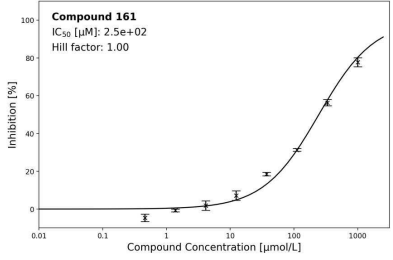
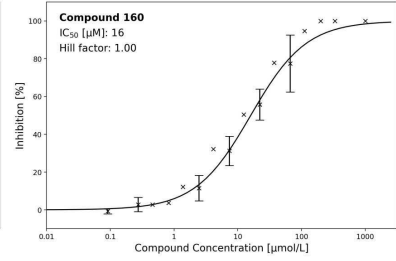
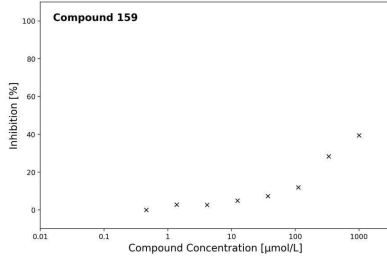
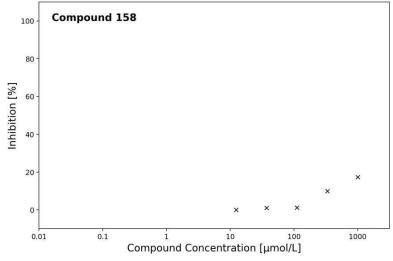
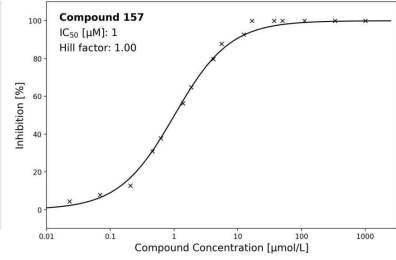
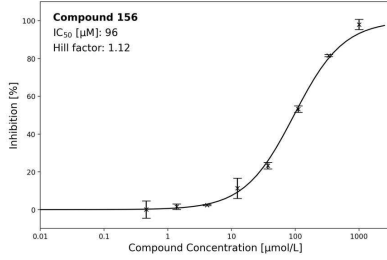
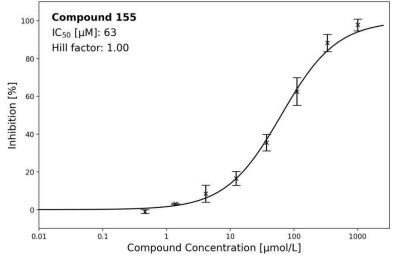


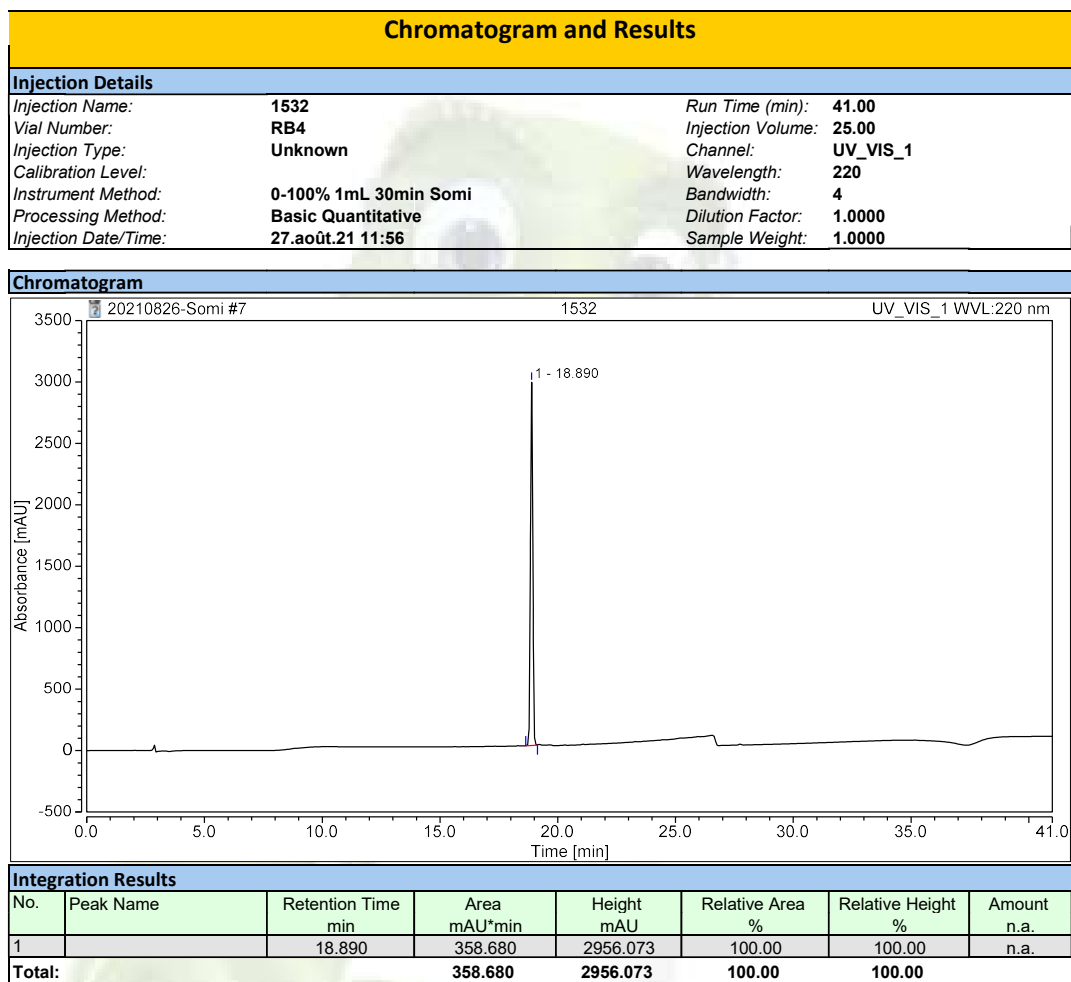


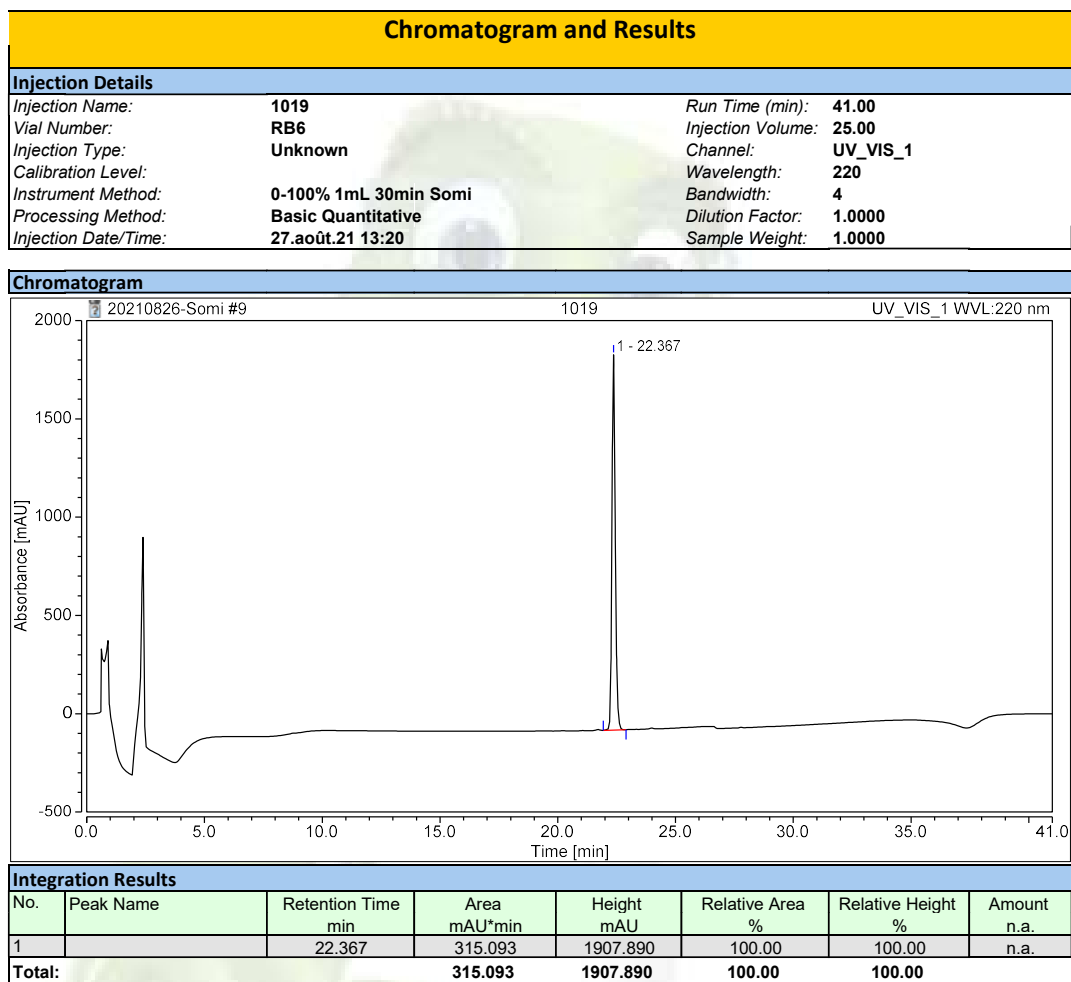








Figure S3: HPLC purity trace of compound **34**.

Figure S4: HPLC purity trace of compound **113**.

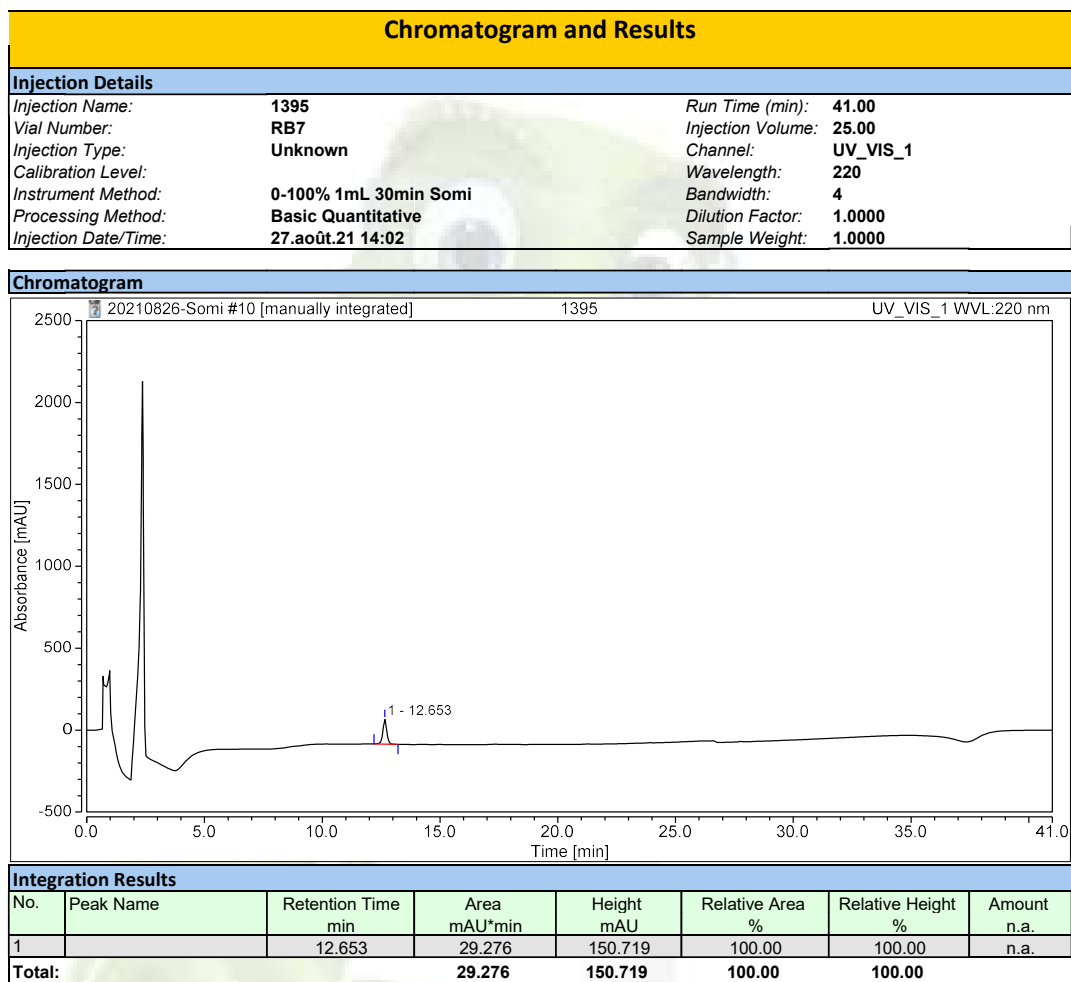


Figure S5: HPLC purity trace of compound 143.

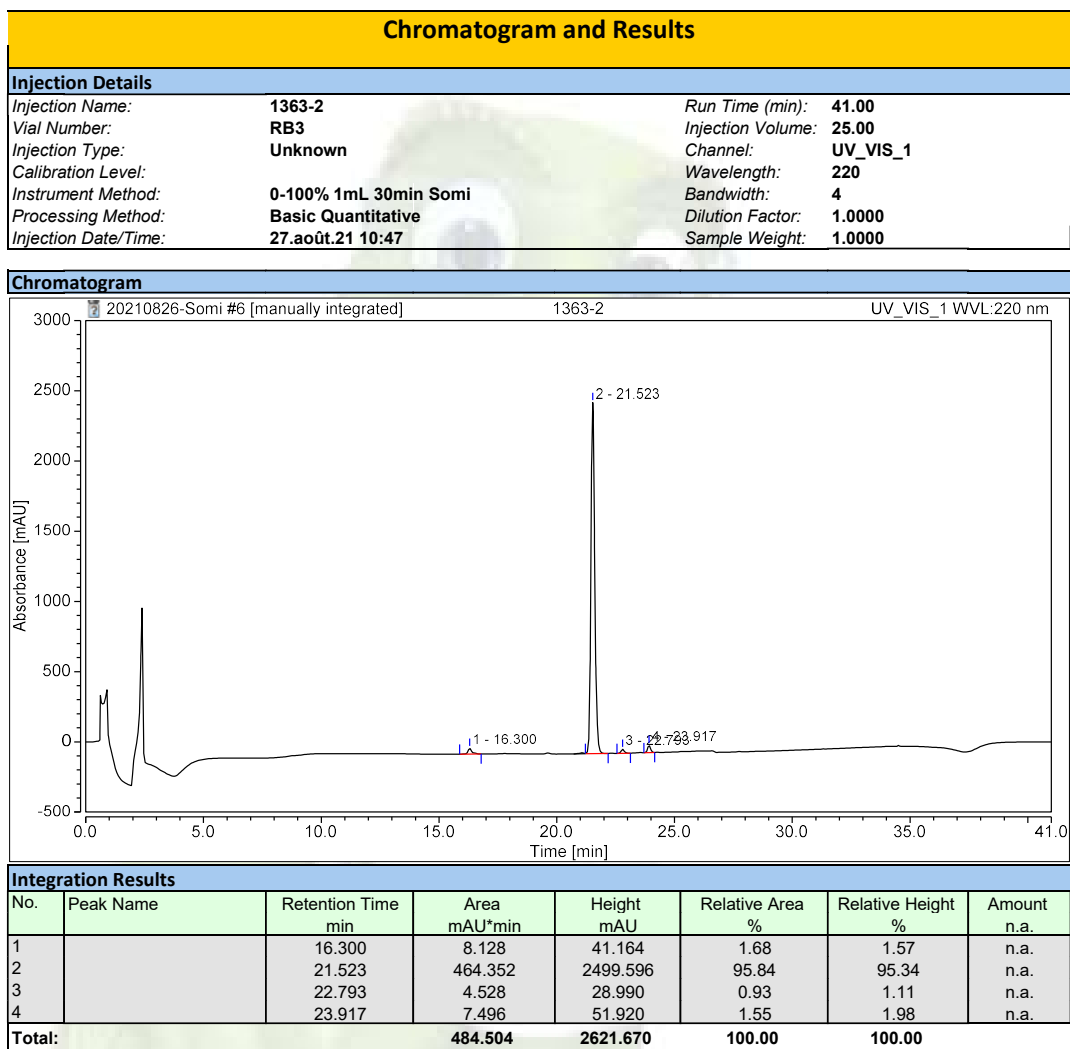
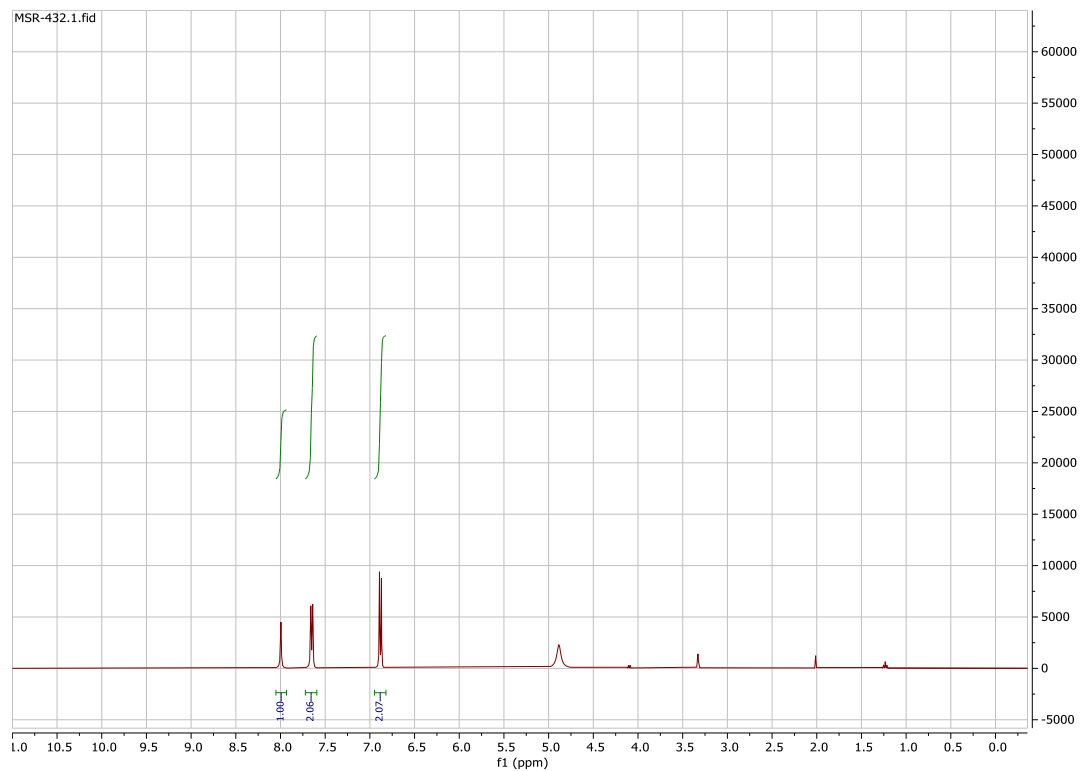
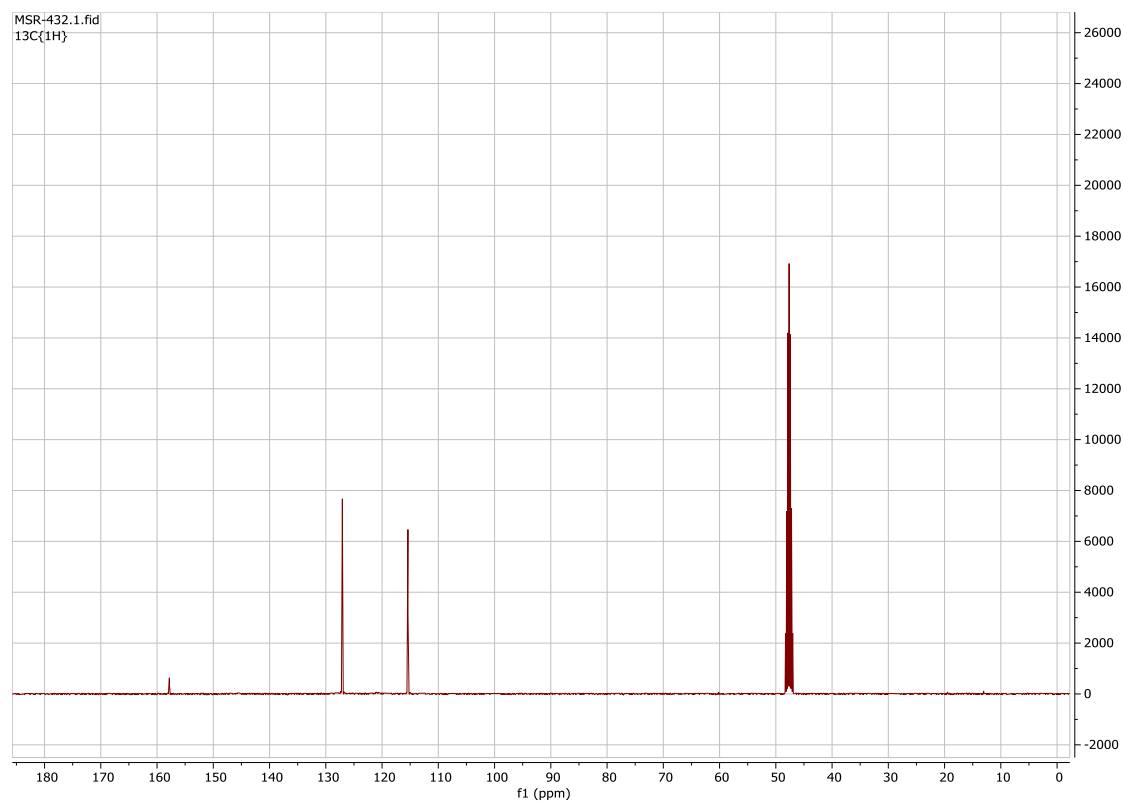


Figure S6: HPLC purity trace of compound 149.

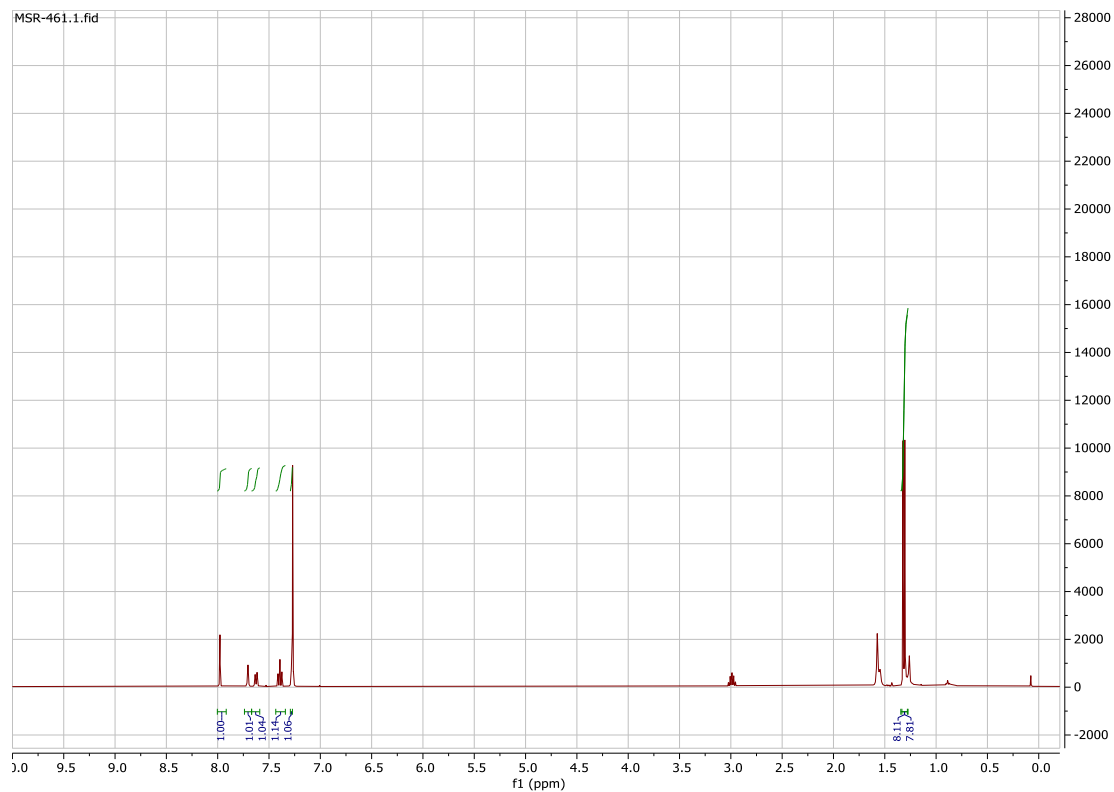
**4-(1,2,3-triazol-4-yl)phenol (20) :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**



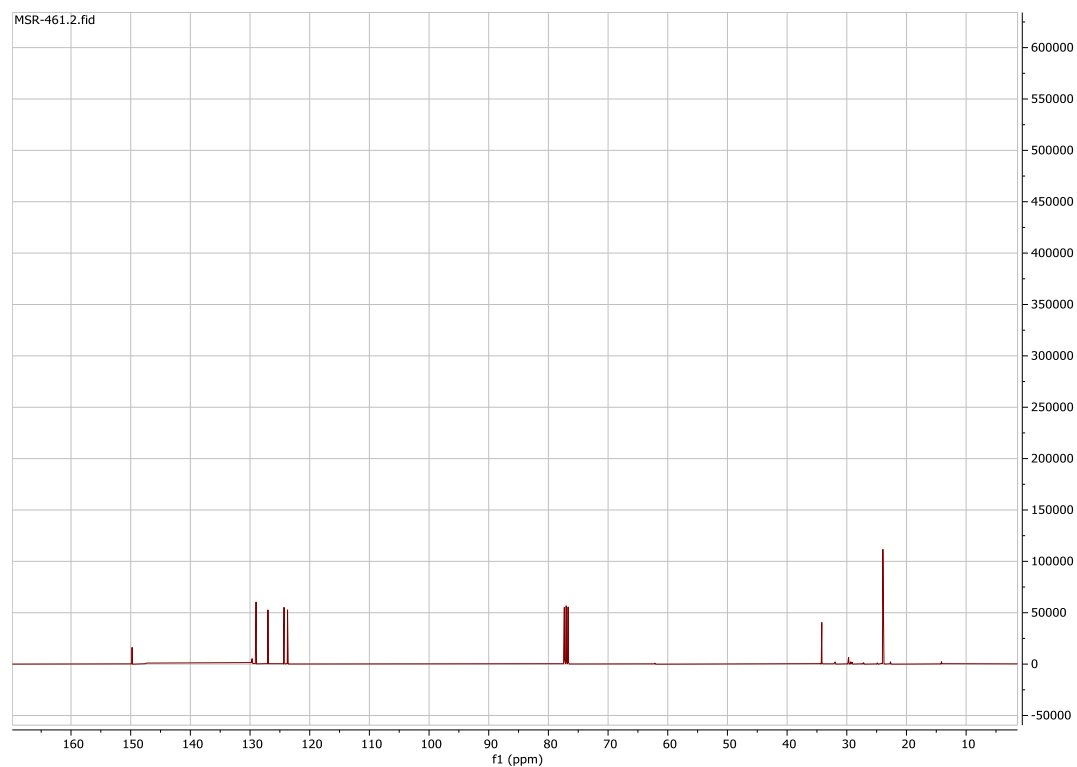
**4-(1,2,3-triazol-4-yl)phenol (20) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**



**4-(3-Isopropylphenyl)-1,2,3-triazole (23) :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**

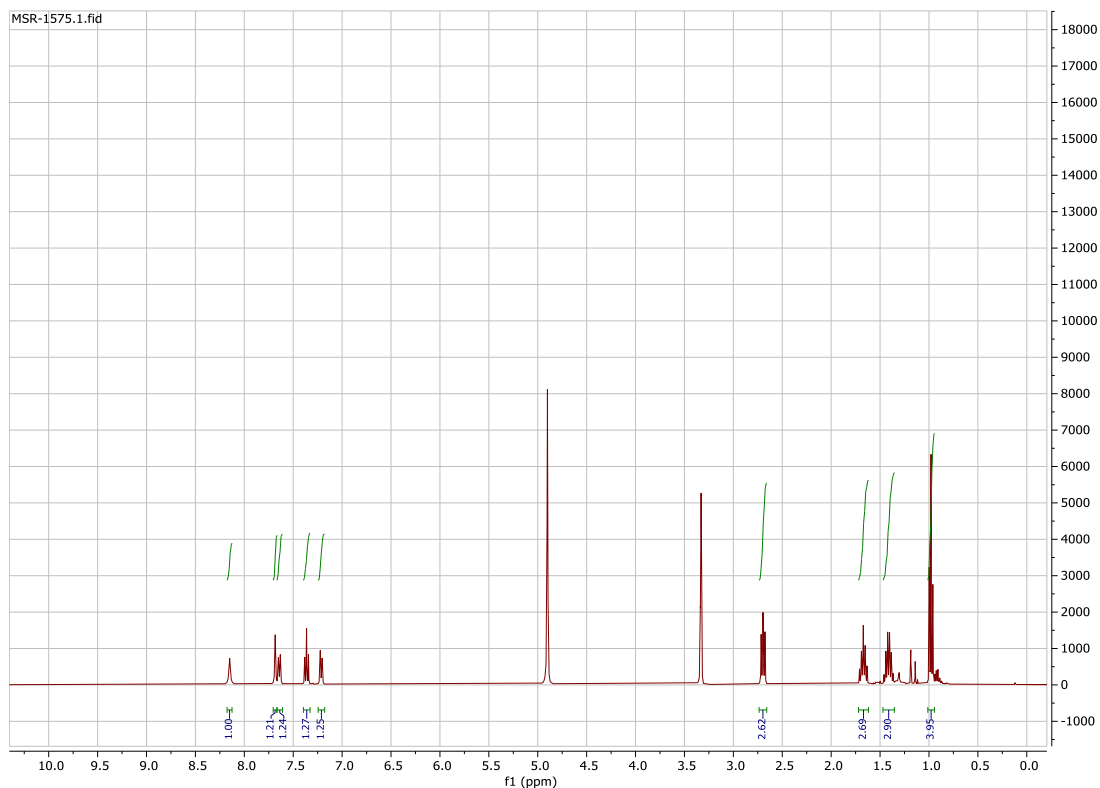


**4-(3-Isopropylphenyl)-1,2,3-triazole (23) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )**

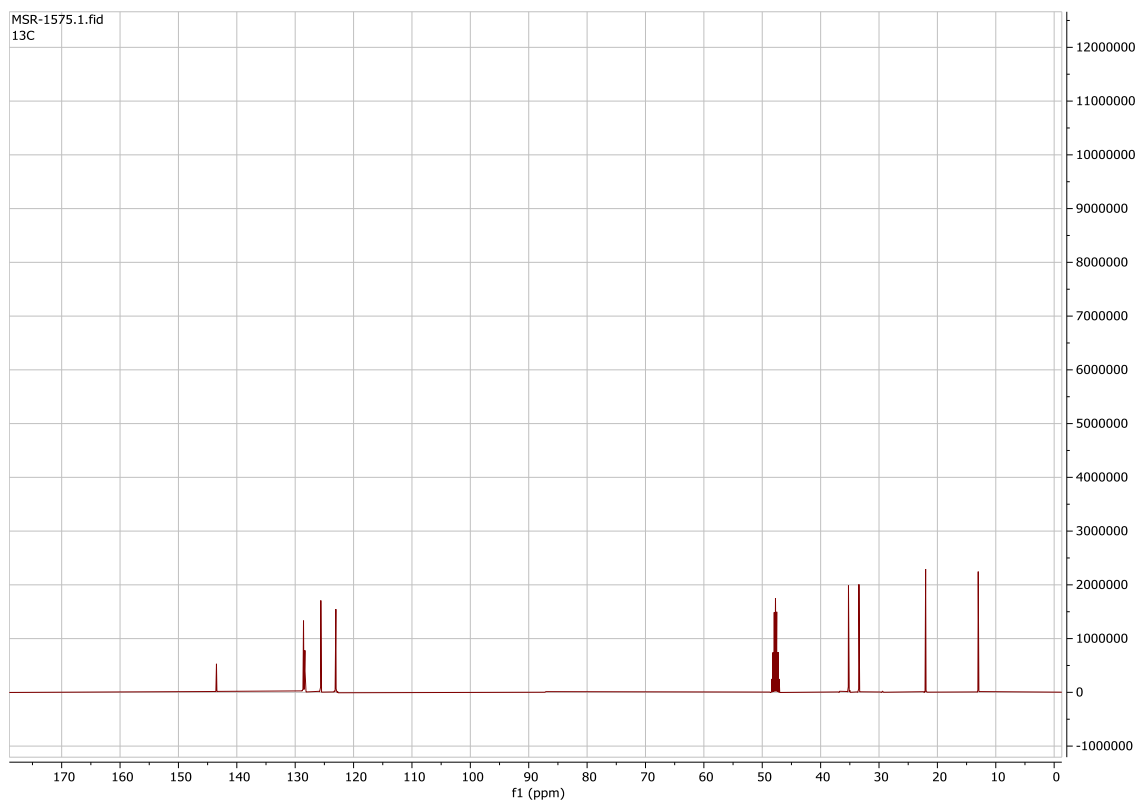




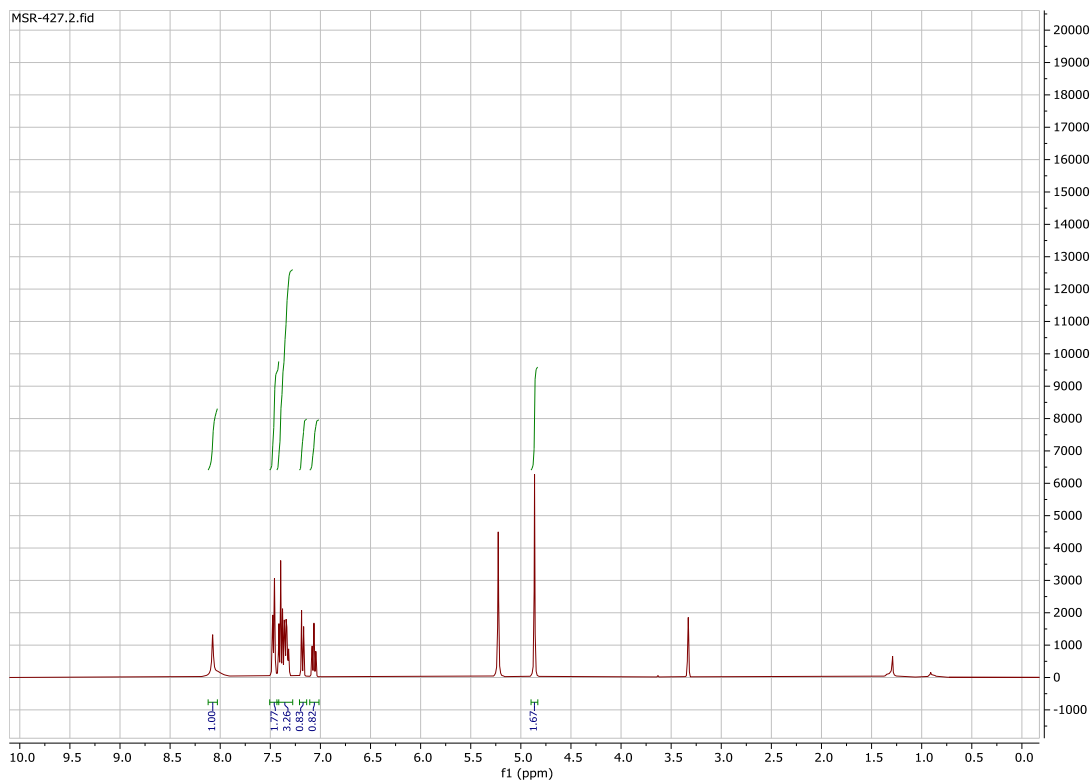
**4-(3-Butylphenyl)-1,2,3-triazole (24):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



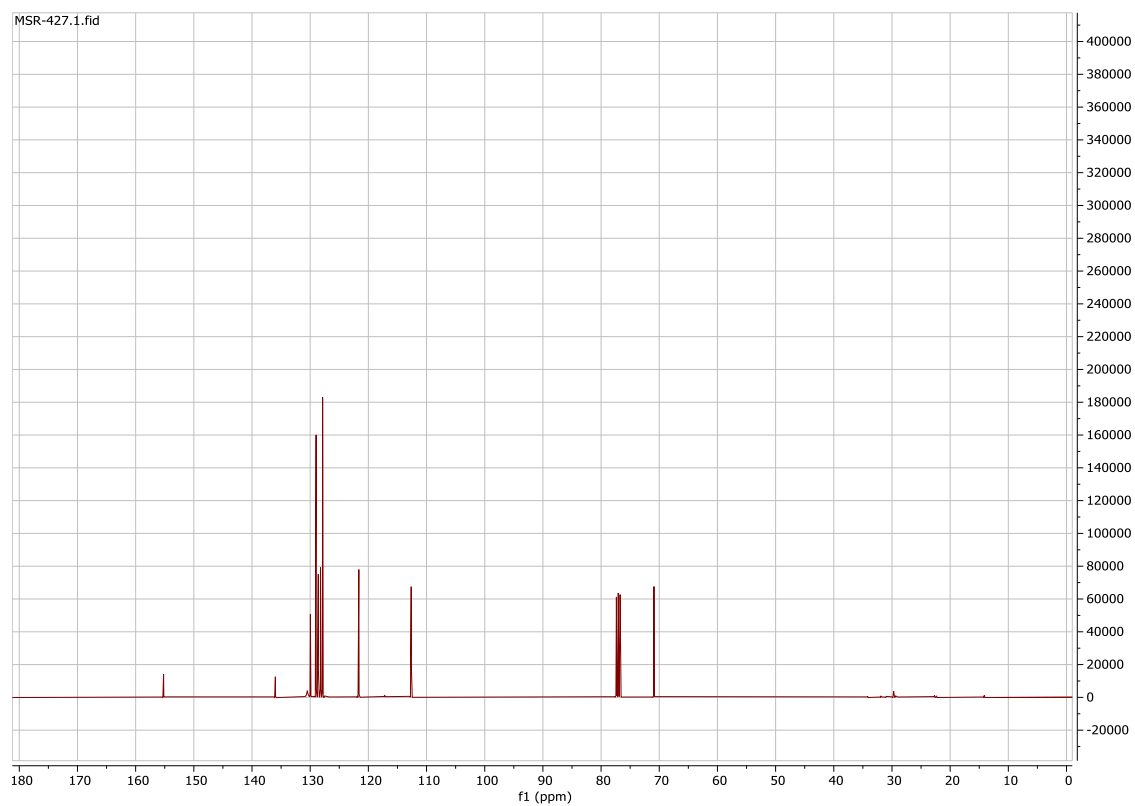
**4-(3-Butylphenyl)-1,2,3-triazole (24):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



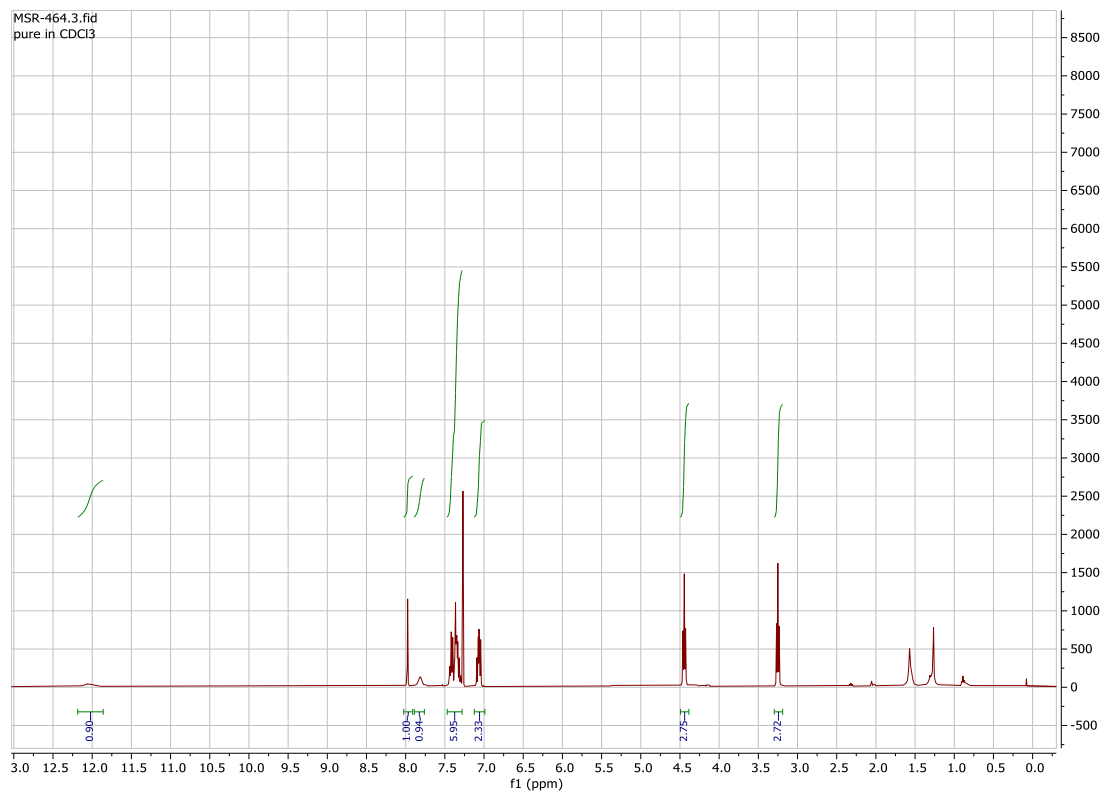
**4-(2-Benzyloxyphenyl)-1,2,3-triazole (25) : <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



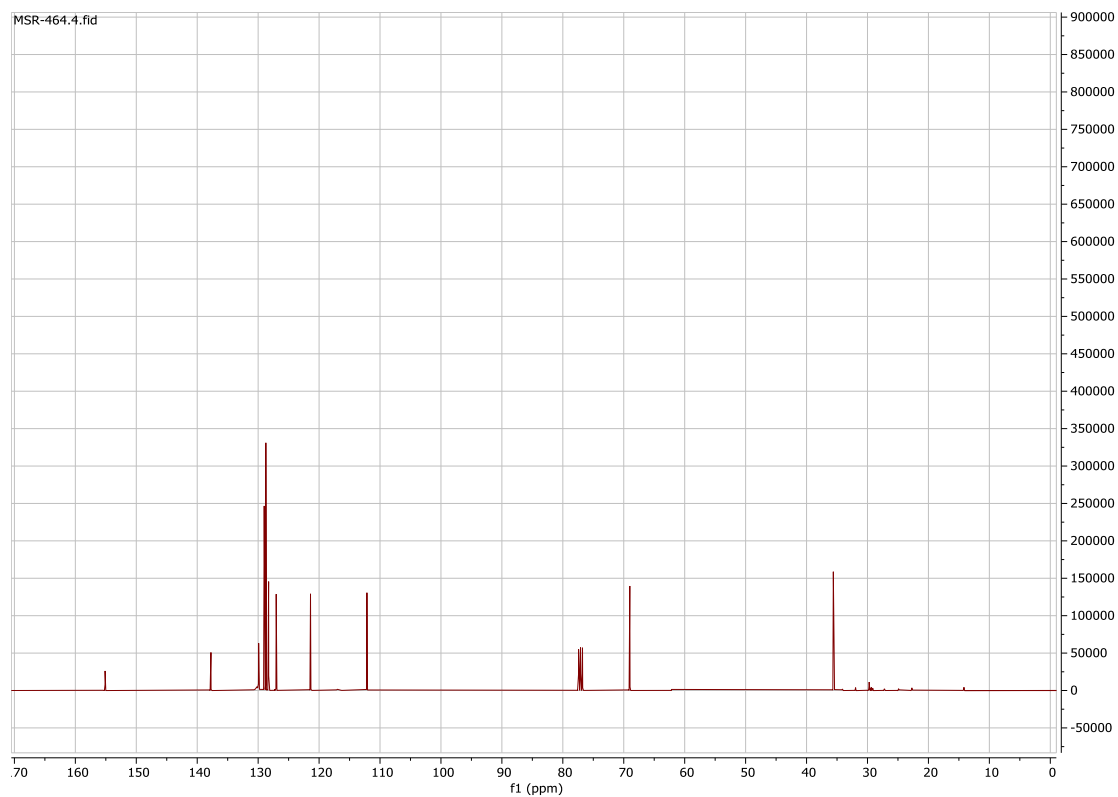
**4-(2-Benzyloxyphenyl)-1,2,3-triazole (25) : <sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



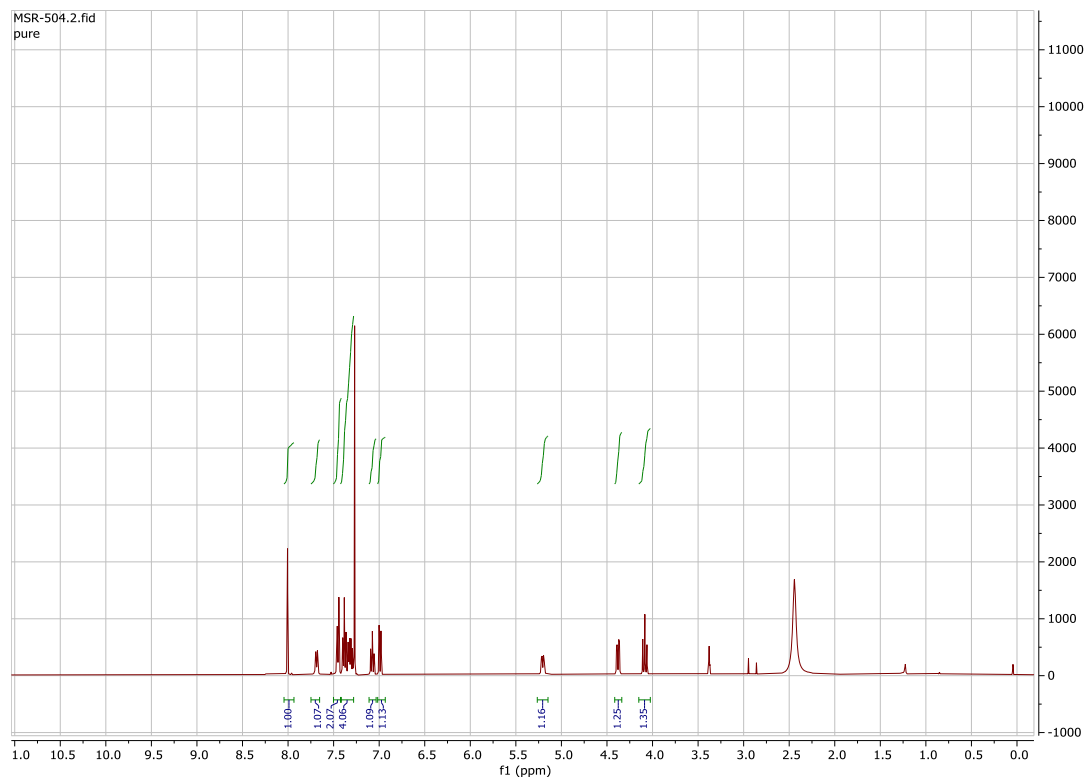
**4-(2-Phenethoxyphenyl)-1,2,3-triazole (26) :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**



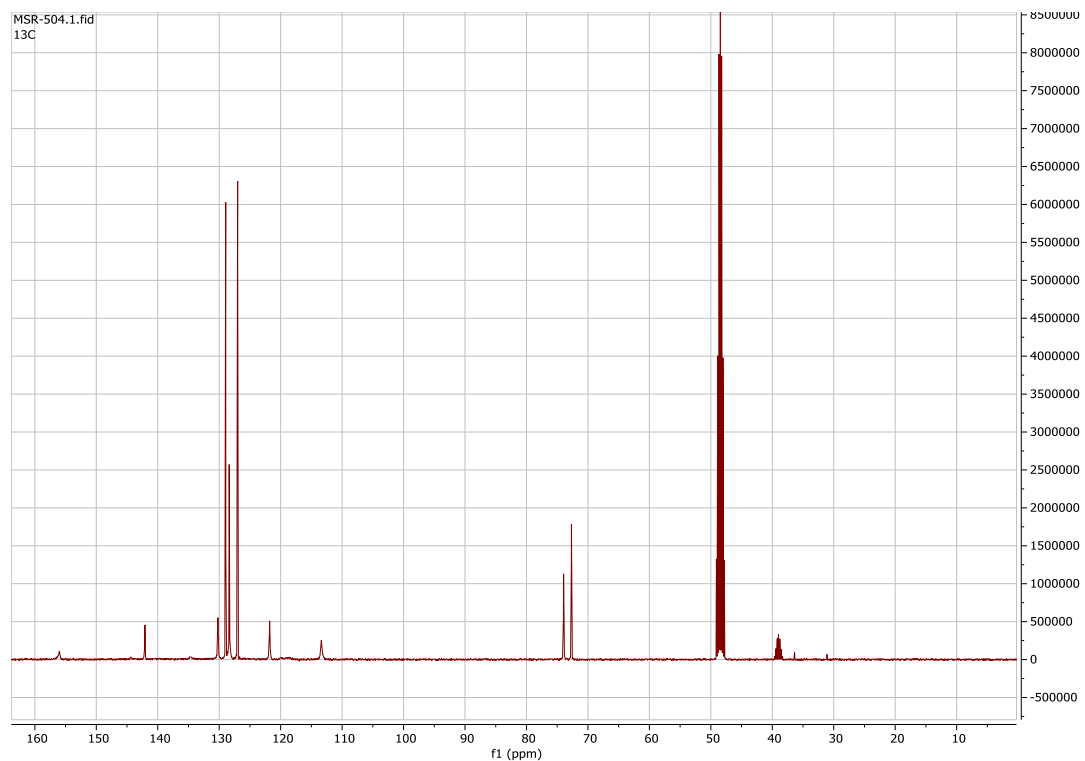
**4-(2-Phenethoxyphenyl)-1,2,3-triazole (26) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )**



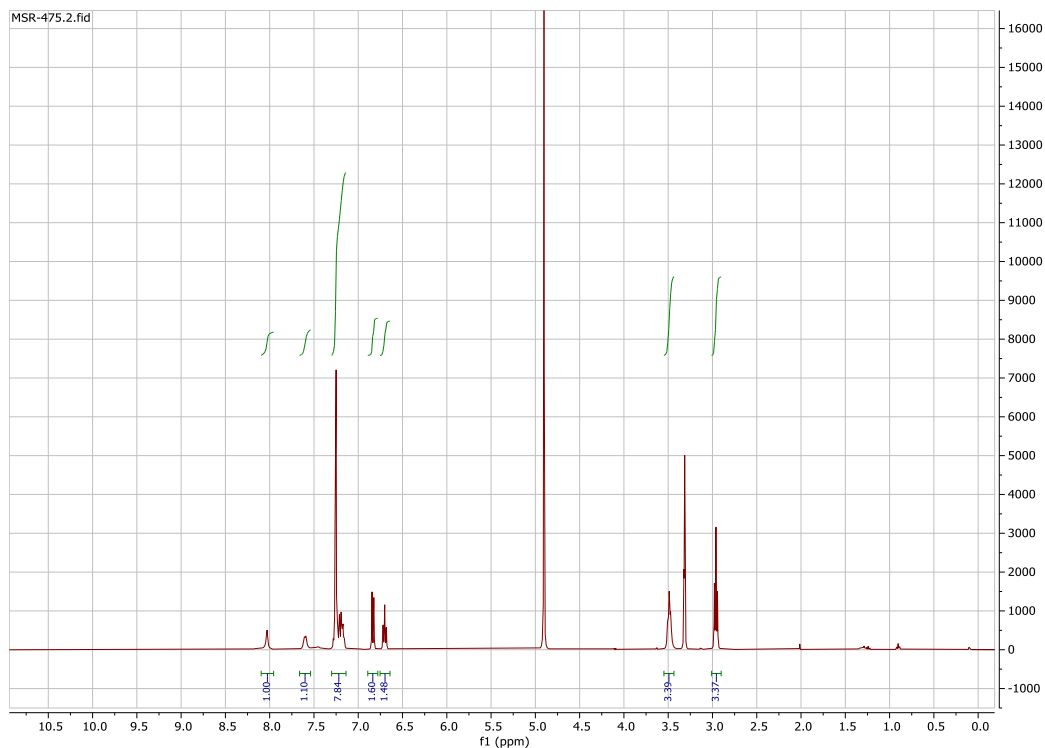
**2-(2-(1H-1,2,3-triazol-5-yl)phenoxy)-1-phenylethan-1-ol (27) : <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



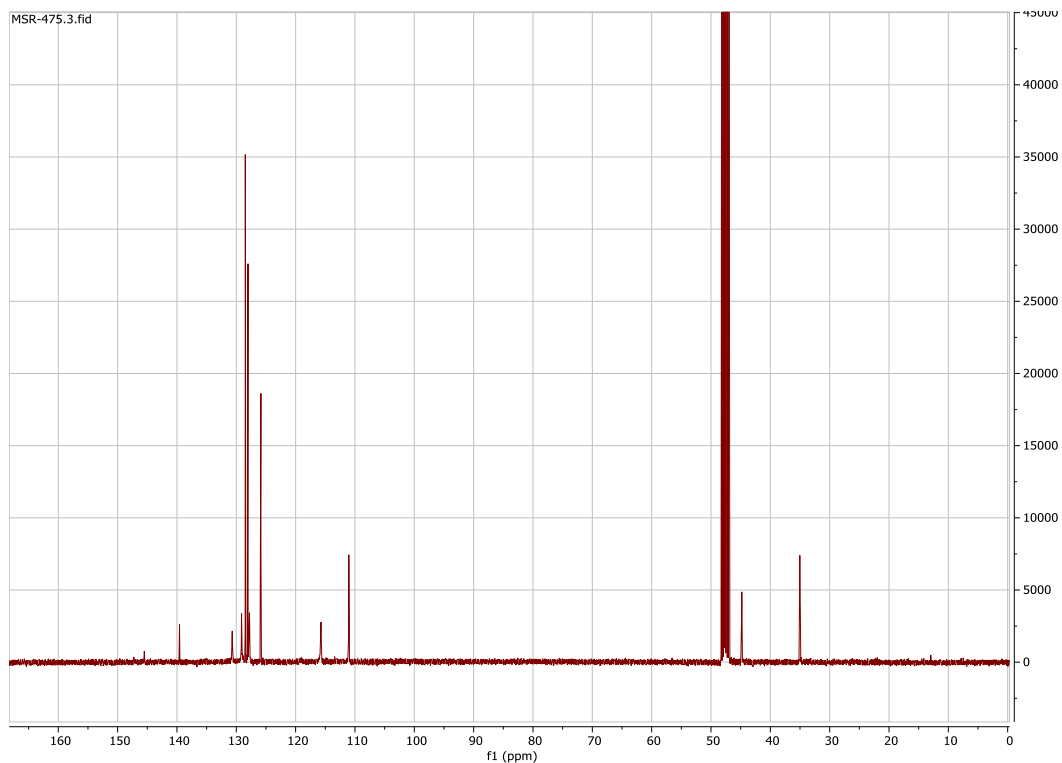
**2-(2-(1H-1,2,3-triazol-5-yl)phenoxy)-1-phenylethan-1-ol (27) : <sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



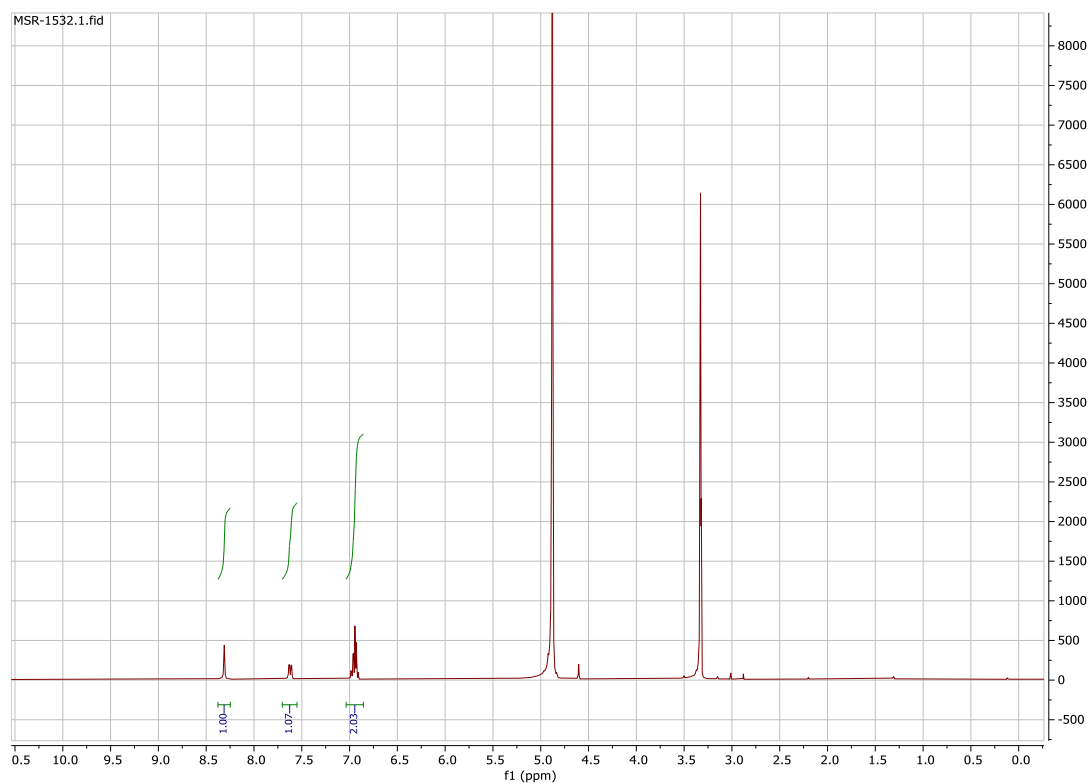
**N-Phenyl-2-(1H-1,2,3-triazol-5-yl)aniline (28) :  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ )**



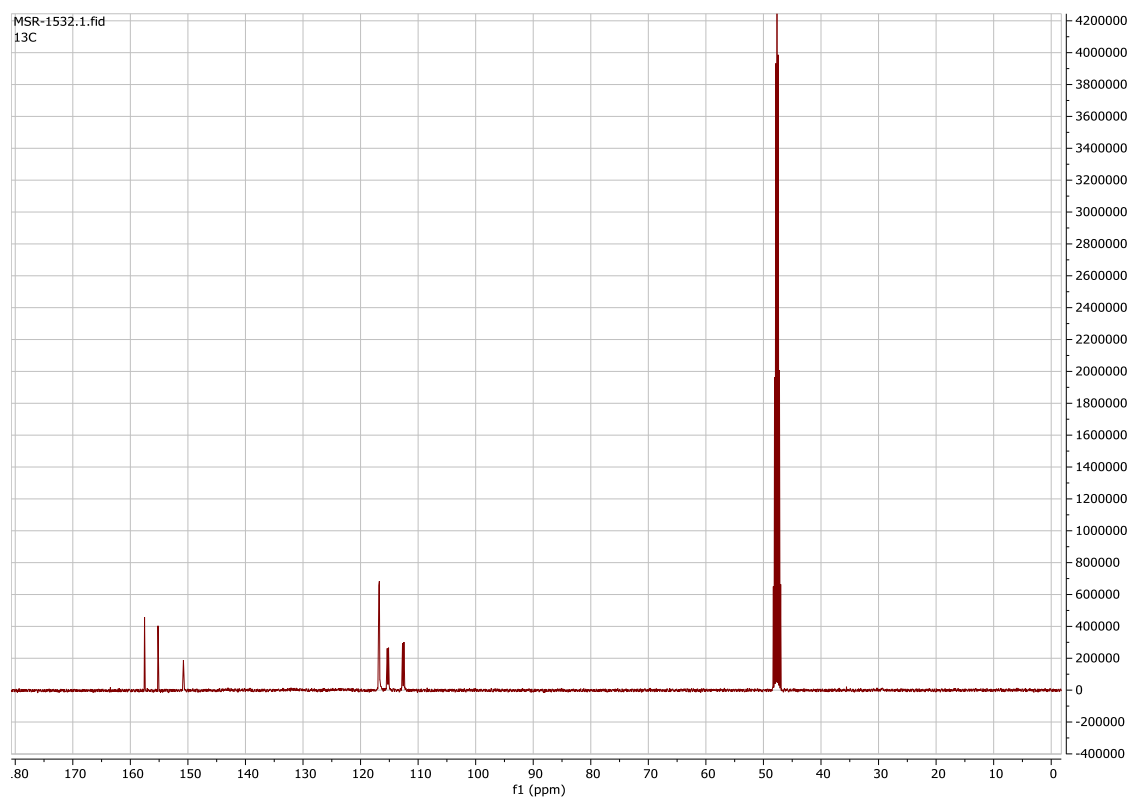
**N-Phenyl-2-(1H-1,2,3-triazol-5-yl)aniline (28) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**



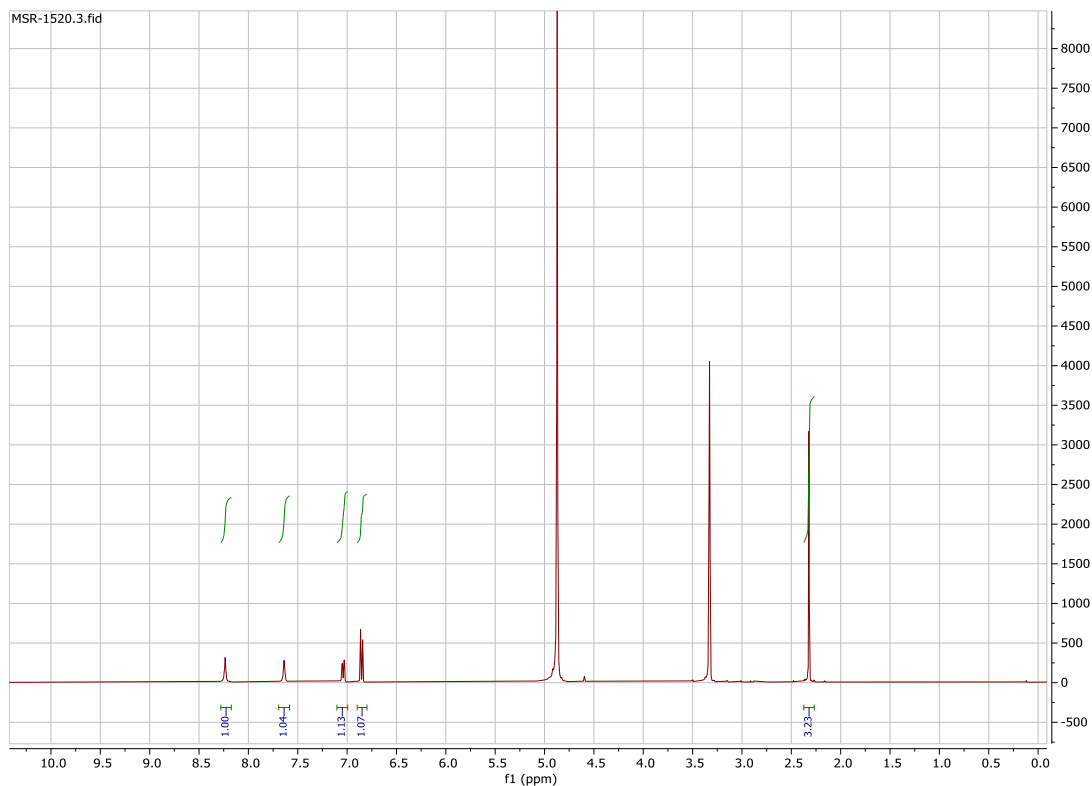
**4-Fluoro-2-(1H-1,2,3-triazol-5-yl)phenol (34):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



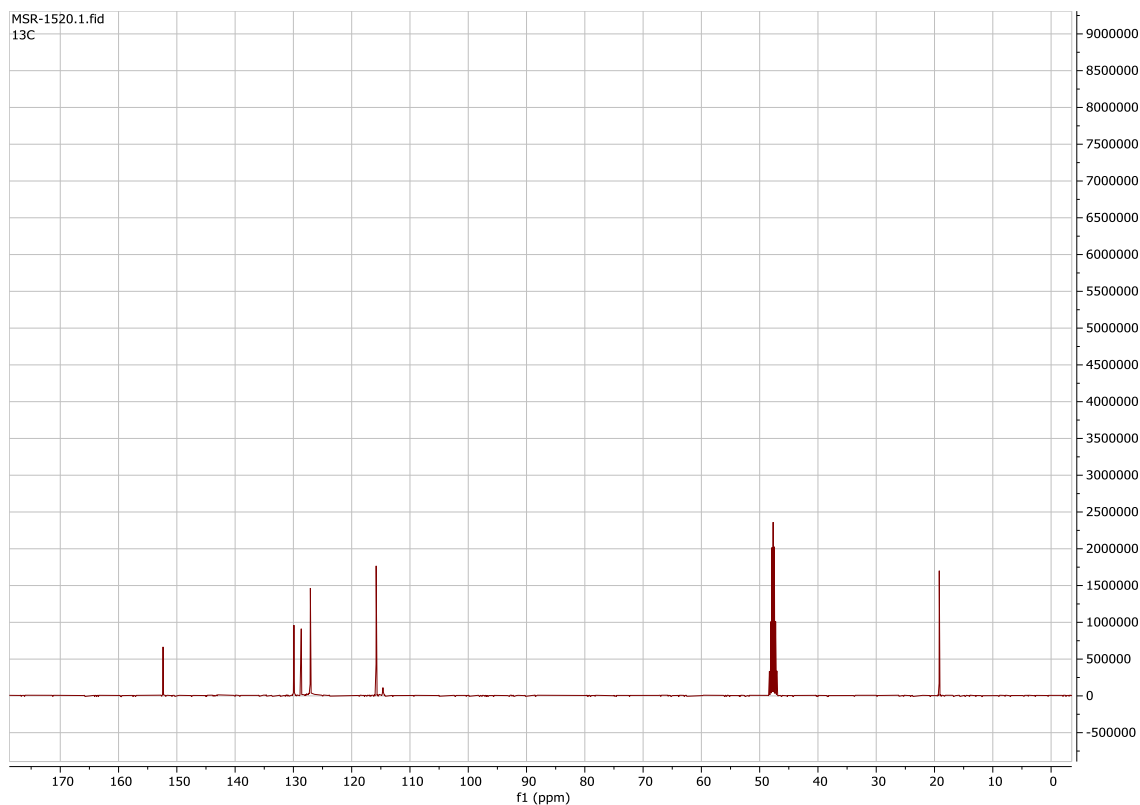
**4-Fluoro-2-(1H-1,2,3-triazol-5-yl)phenol (34):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



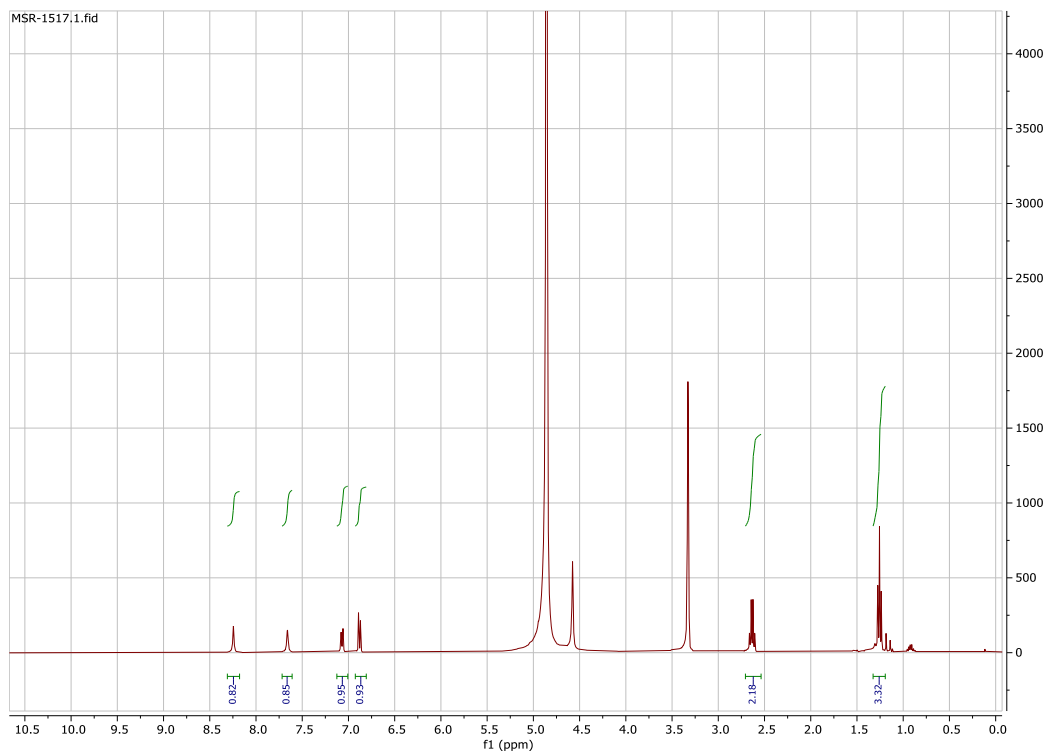
**4-Methyl-2-(1H-1,2,3-triazol-5-yl)phenol (35):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



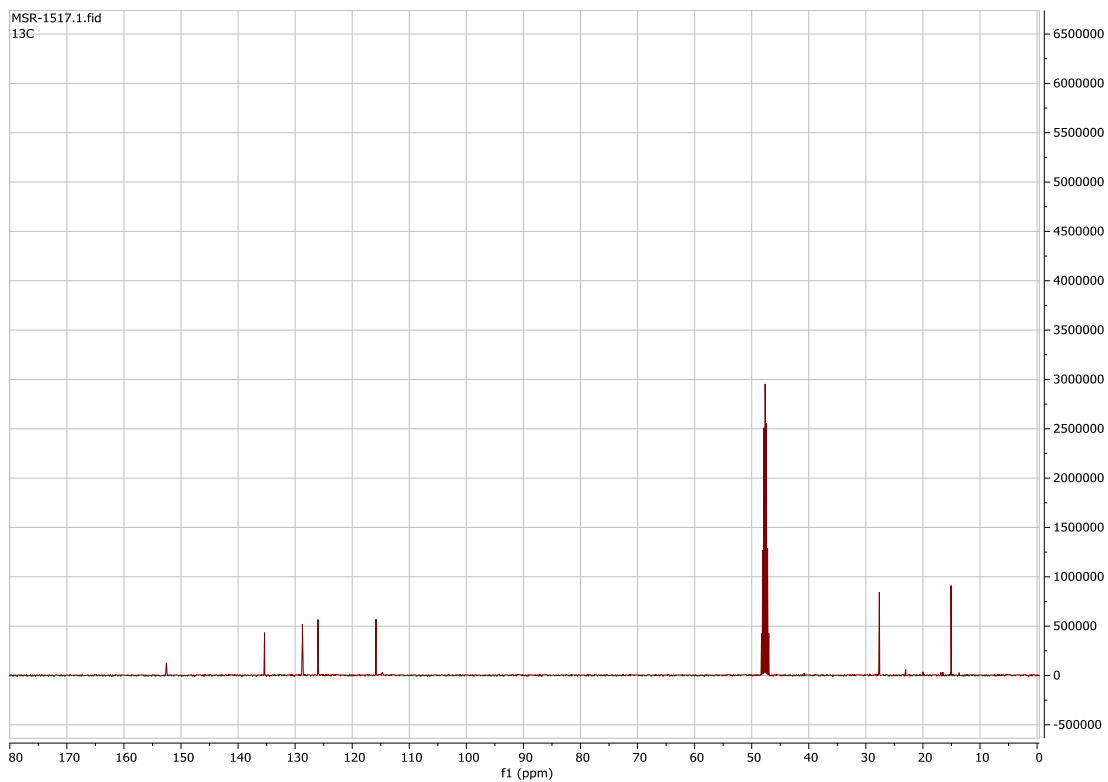
**4-Methyl-2-(1H-1,2,3-triazol-5-yl)phenol (35):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**4-Ethyl-2-(1H-1,2,3-triazol-5-yl)phenol (36):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

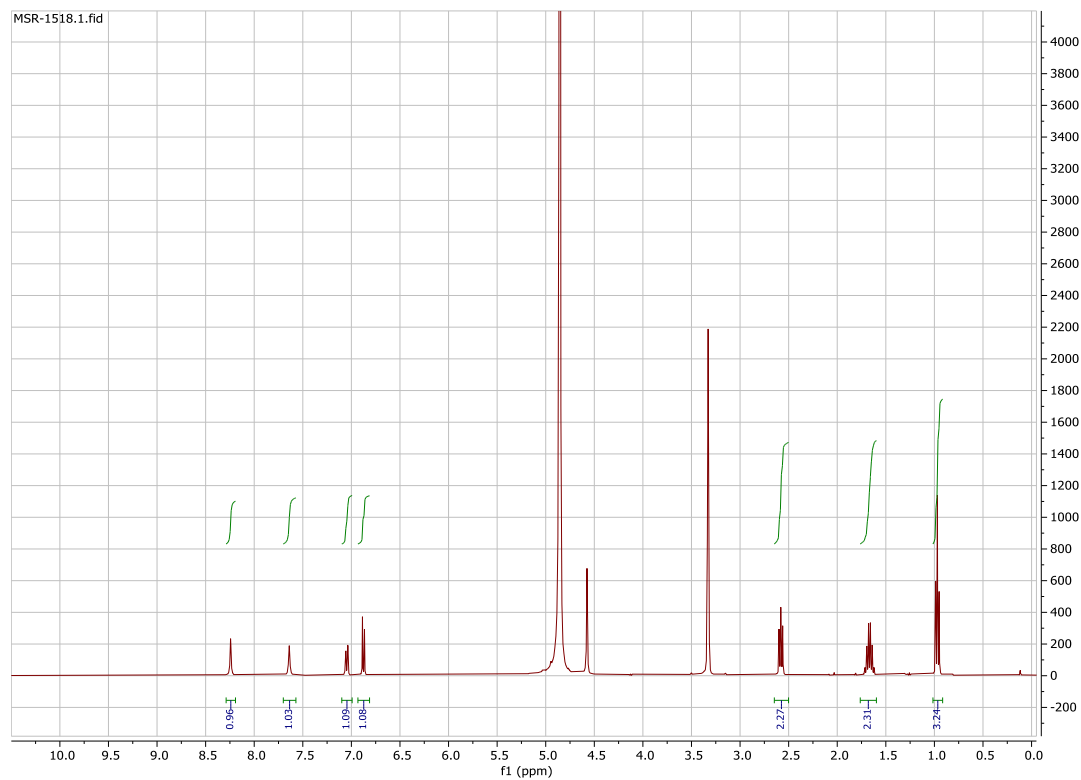


**4-Ethyl-2-(1H-1,2,3-triazol-5-yl)phenol (36):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

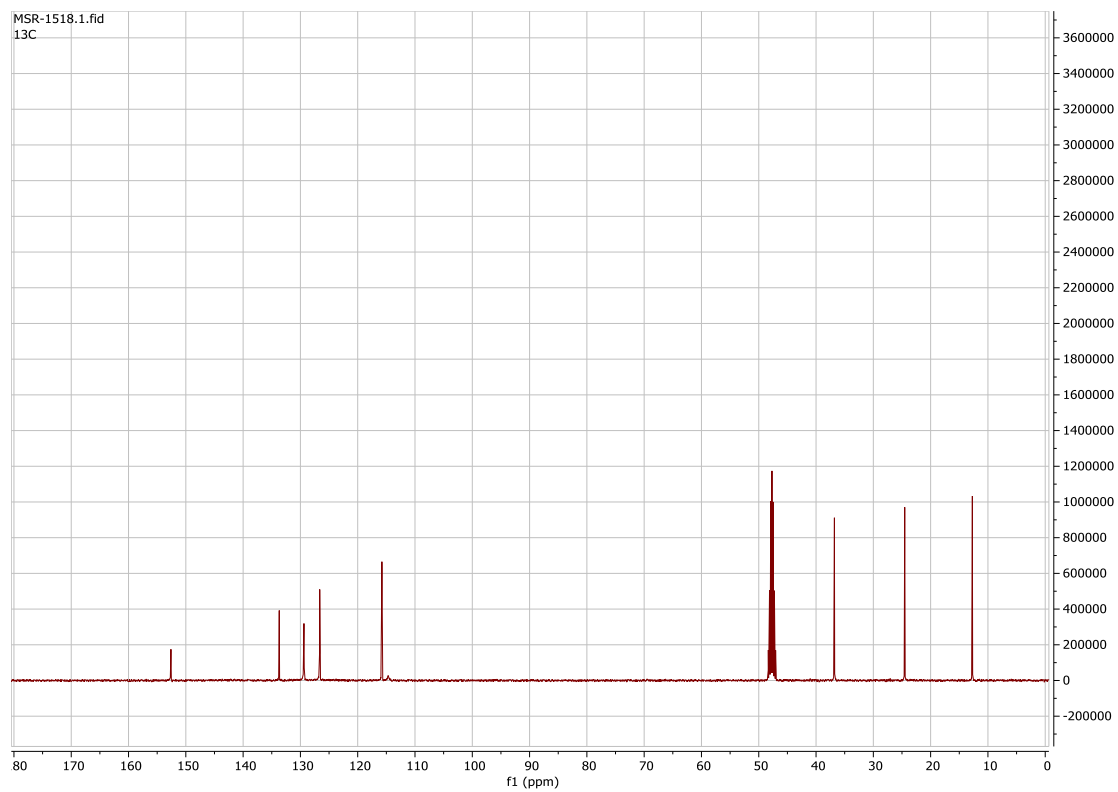




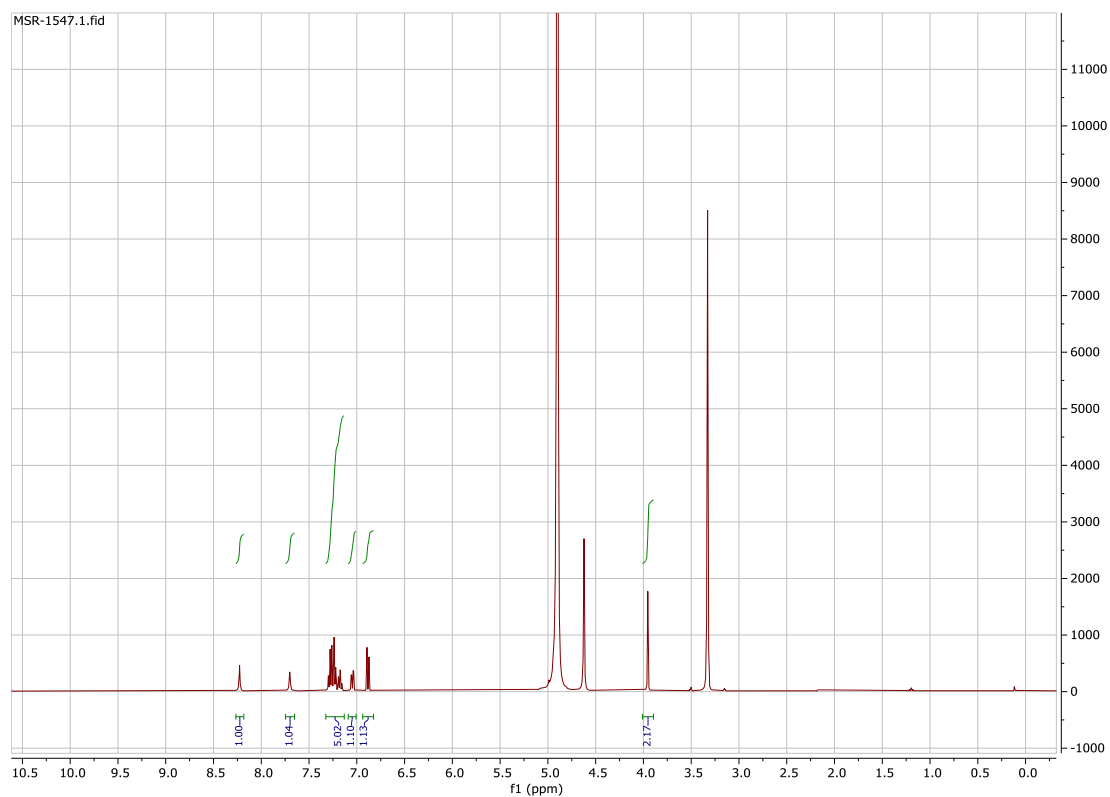
**4-Propyl-2-(1H-1,2,3-triazol-5-yl)phenol (37):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



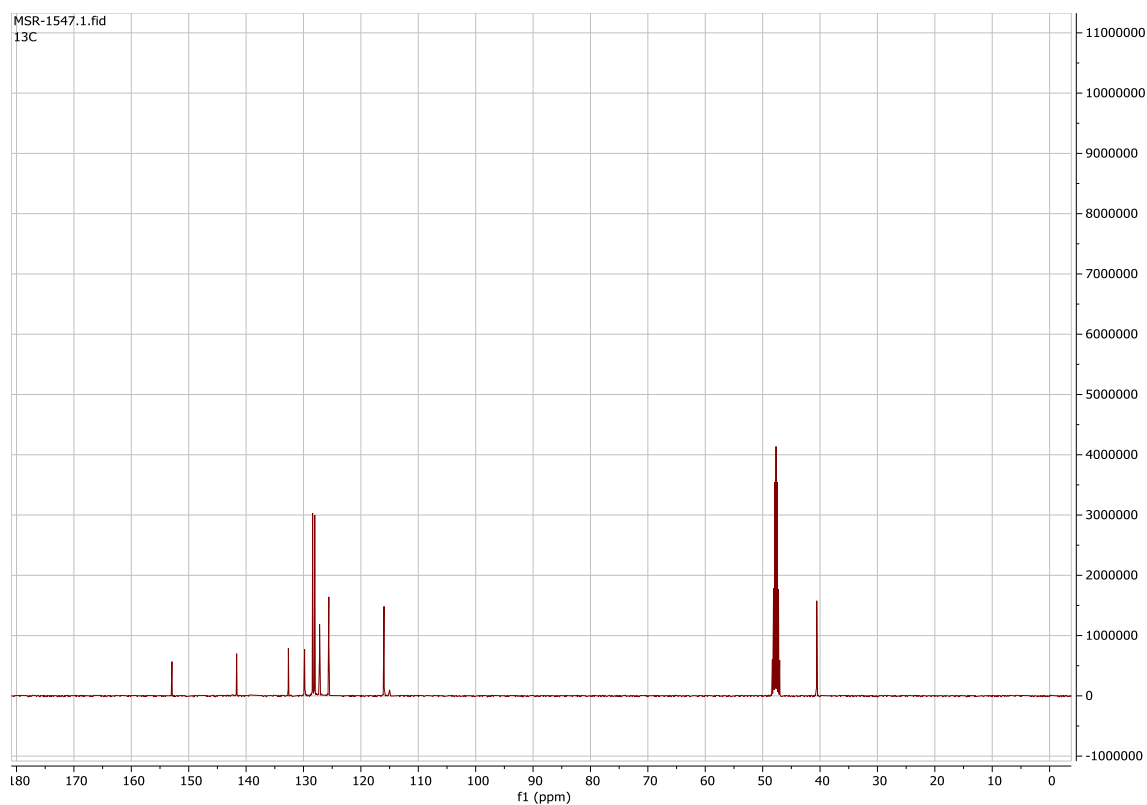
**4-Propyl-2-(1H-1,2,3-triazol-5-yl)phenol (37):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



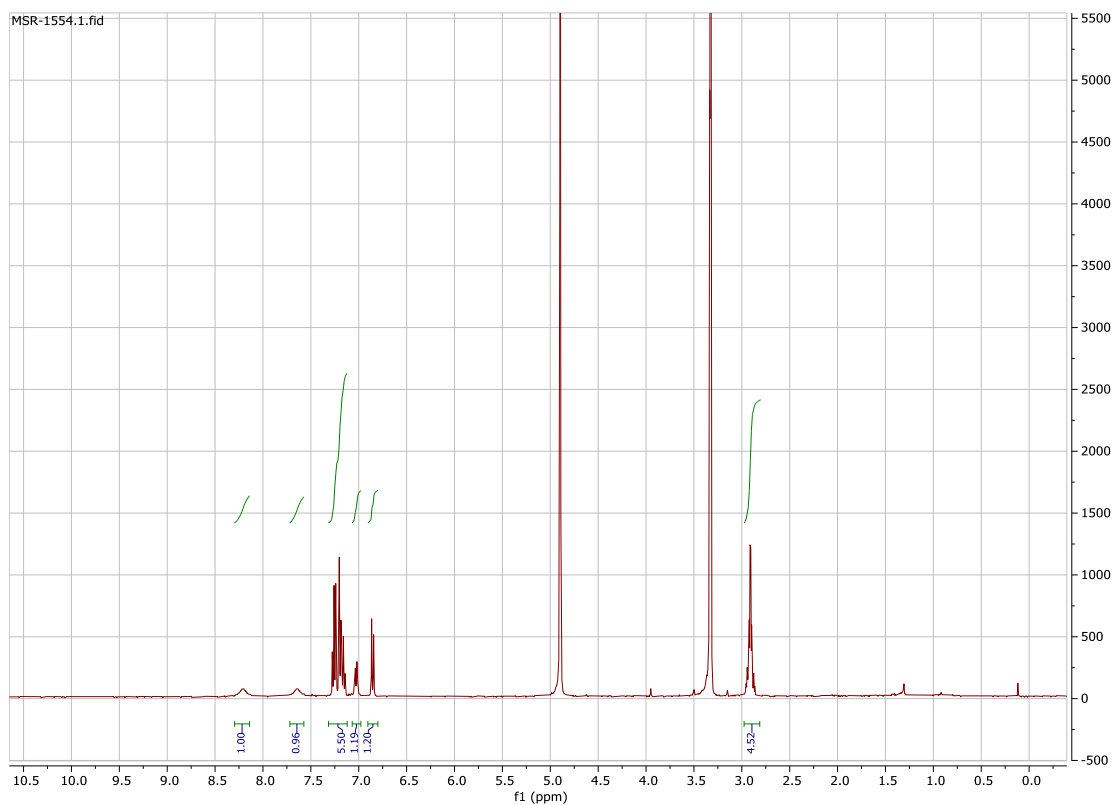
**4-Benzyl-2-(1H-1,2,3-triazol-5-yl)phenol (38):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



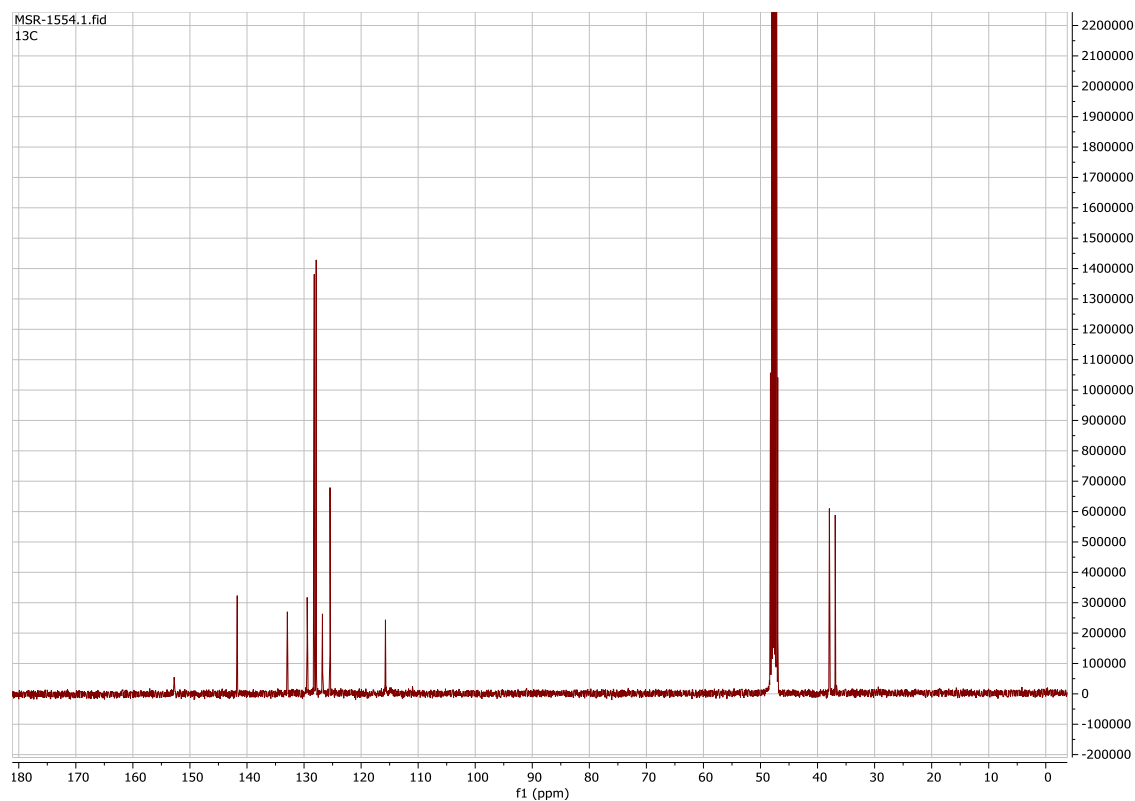
**4-Benzyl-2-(1H-1,2,3-triazol-5-yl)phenol (38):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



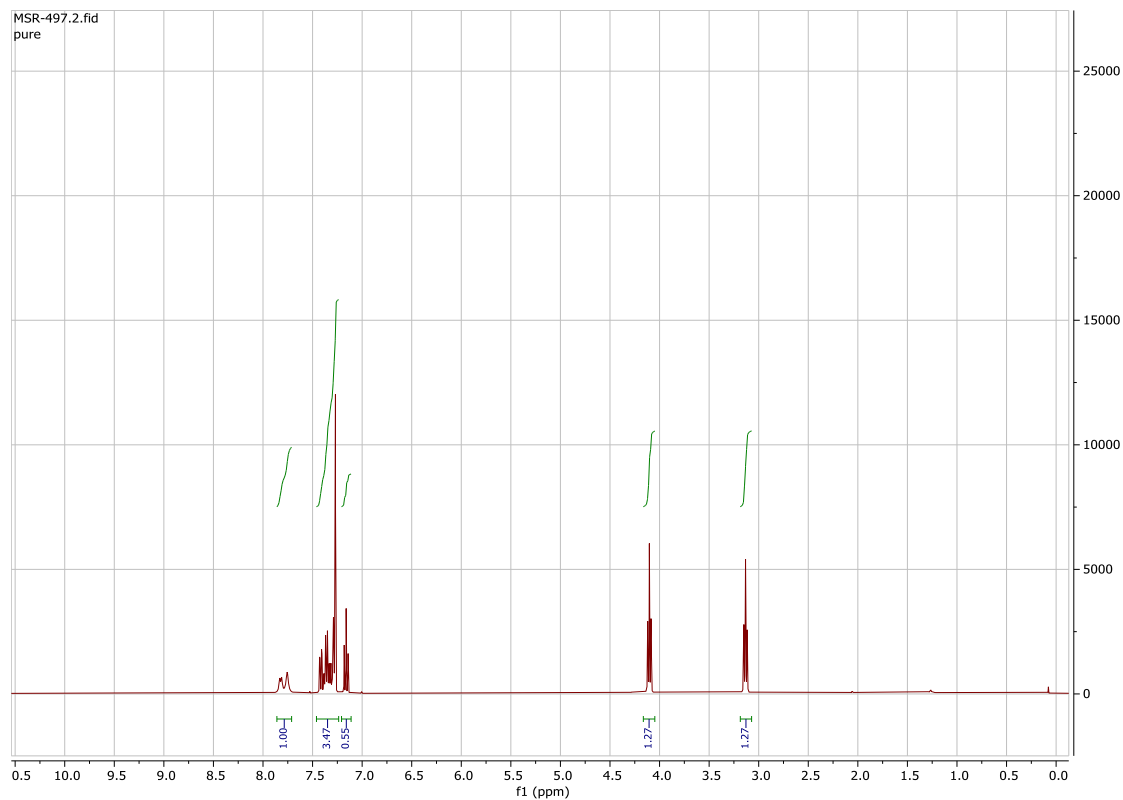
**4-Phenylethyl-2-(1H-1,2,3-triazol-5-yl)phenol (39):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



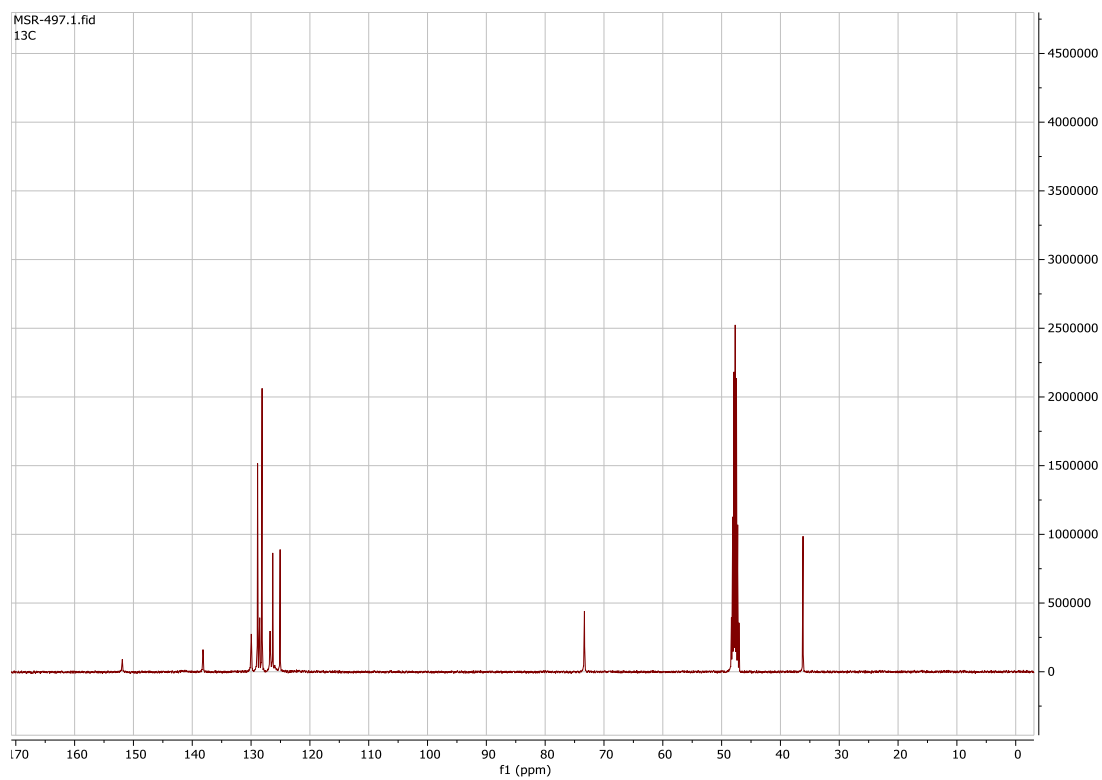
**4-Phenylethyl-2-(1H-1,2,3-triazol-5-yl)phenol (39):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



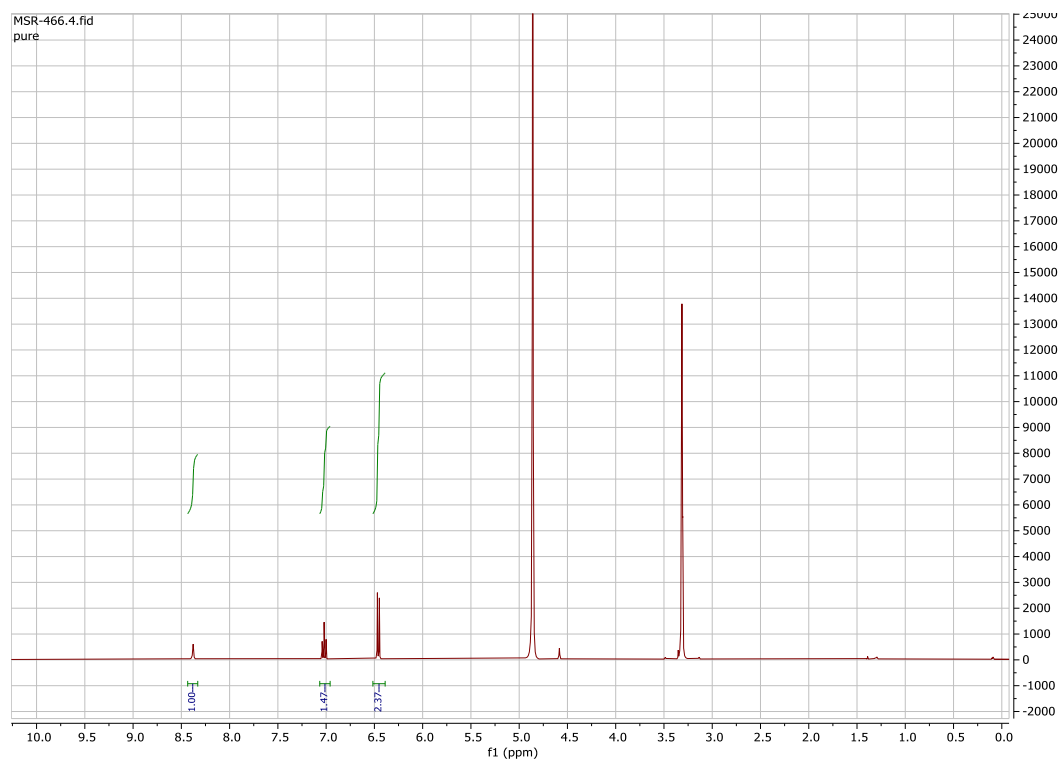
**4-(3-Chloro-2-phenoxyphenyl)-1,2,3-triazole (43) :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**



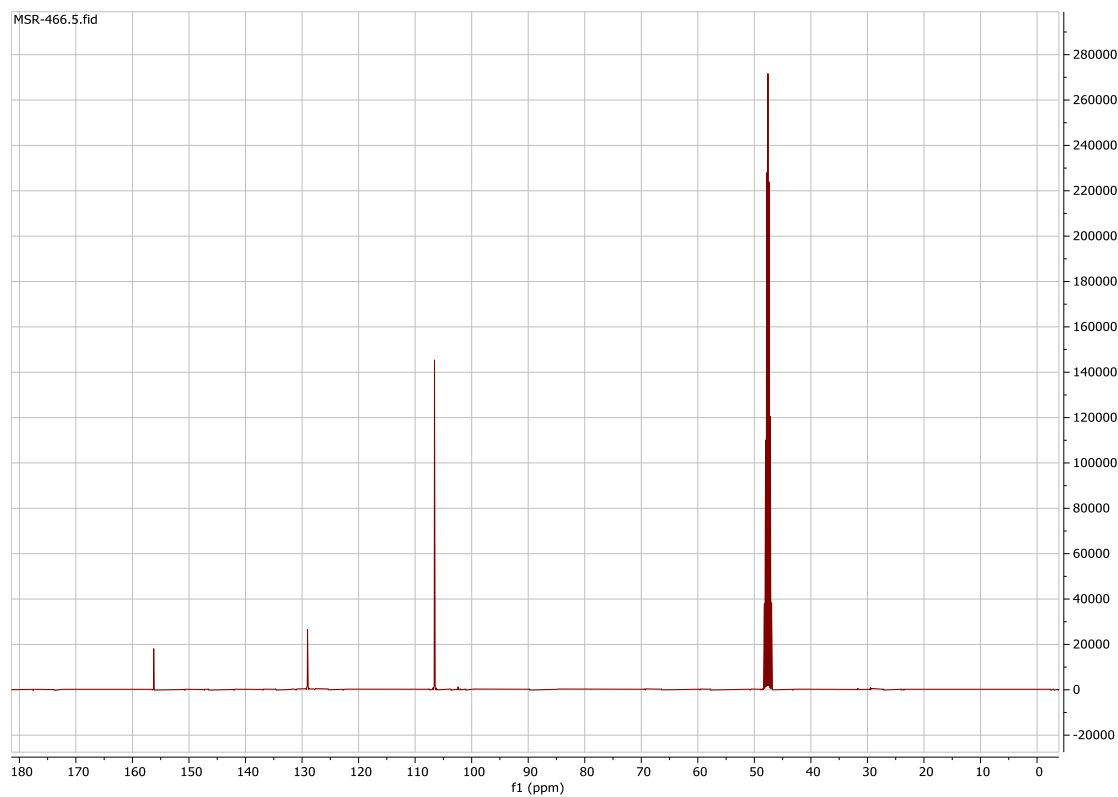
**4-(3-Chloro-2-phenoxyphenyl)-1,2,3-triazole (43) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**



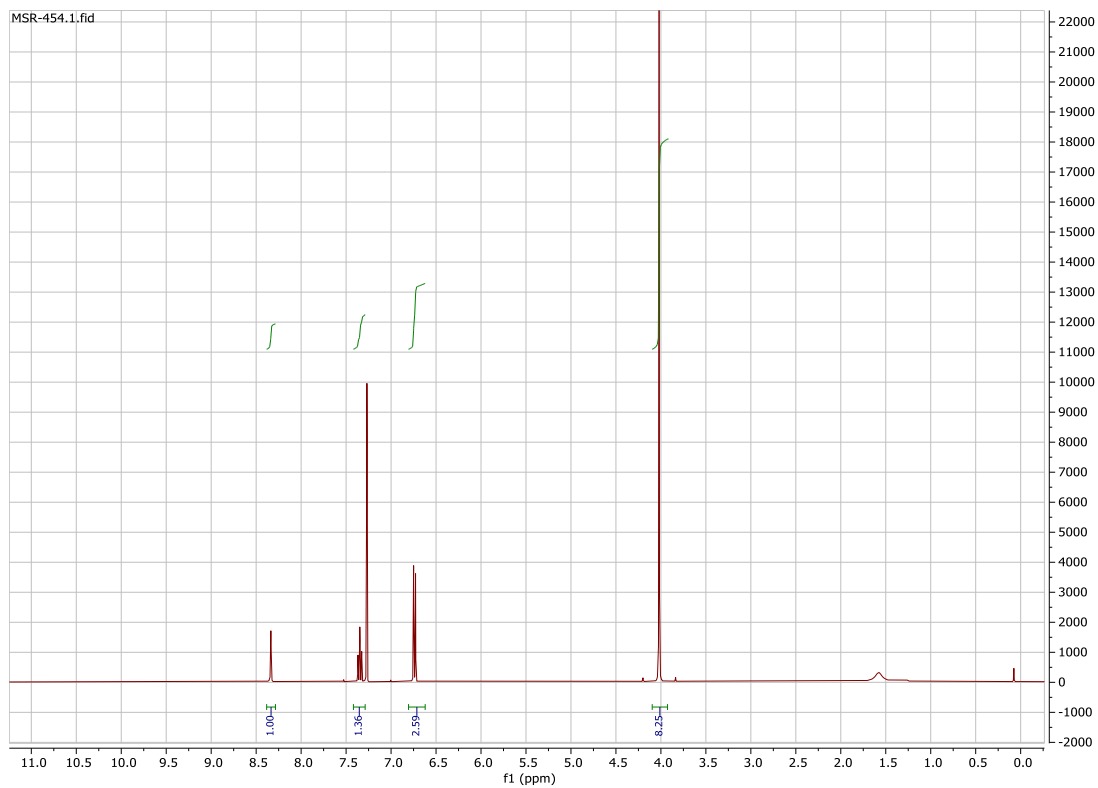
**2-(1H-1,2,3-triazol-5-yl)benzene-1,3-diol (44) :  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ )**



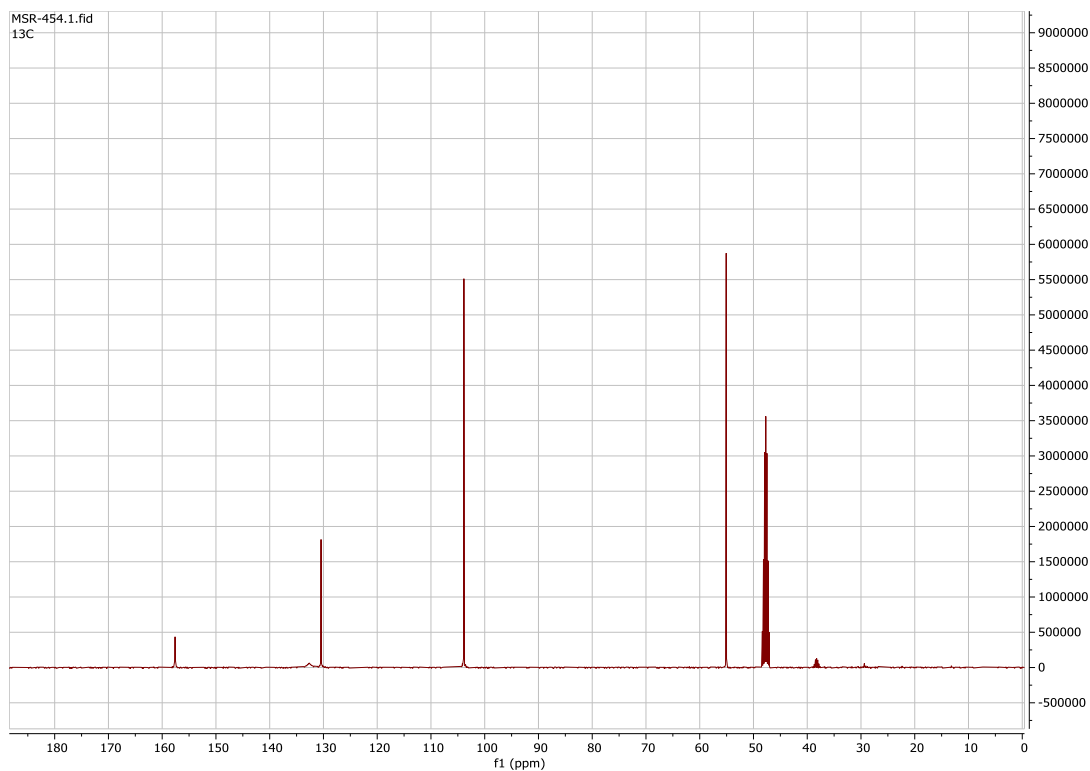
**2-(1H-1,2,3-triazol-5-yl)benzene-1,3-diol (44) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**



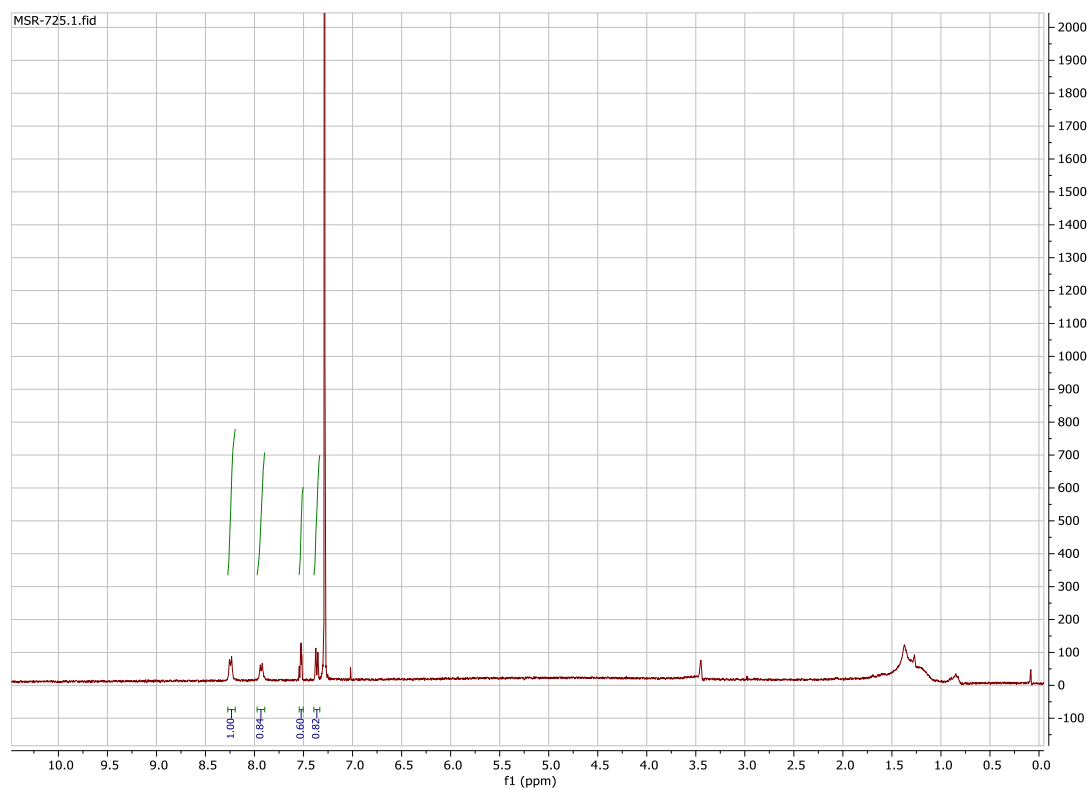
**4-(2,6-Dimethoxyphenyl)-1,2,3-triazole (45) :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**



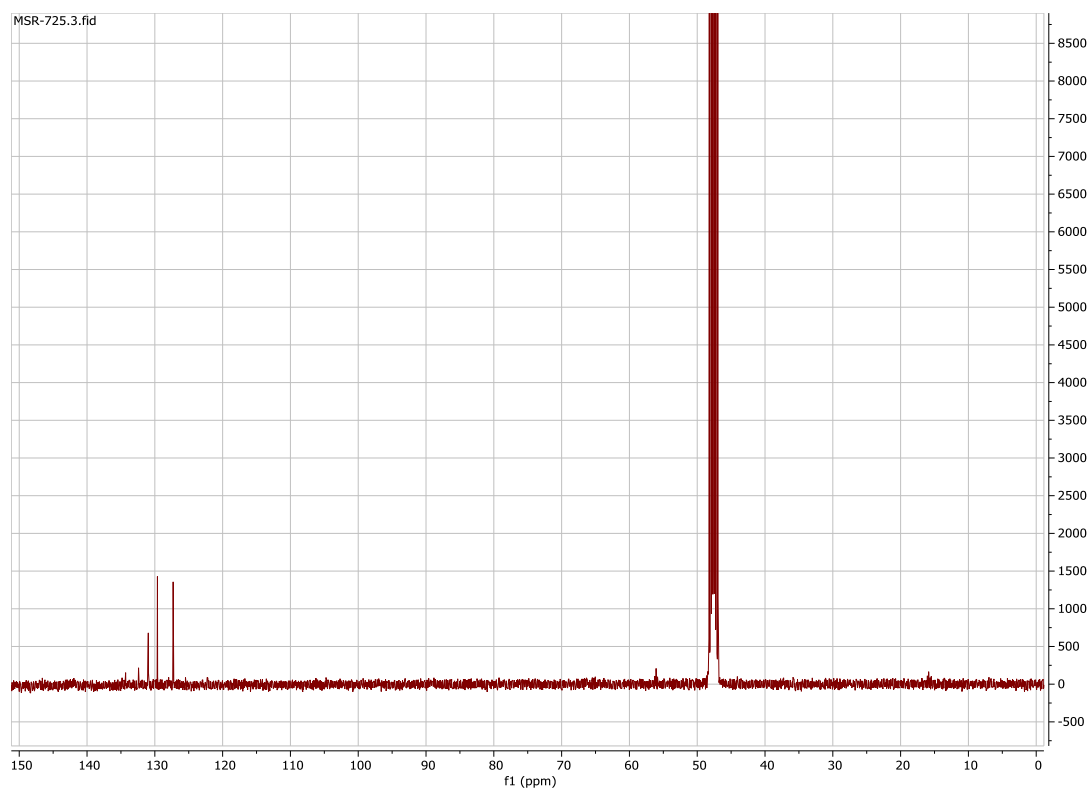
**4-(2,6-Dimethoxyphenyl)-1,2,3-triazole (45) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**



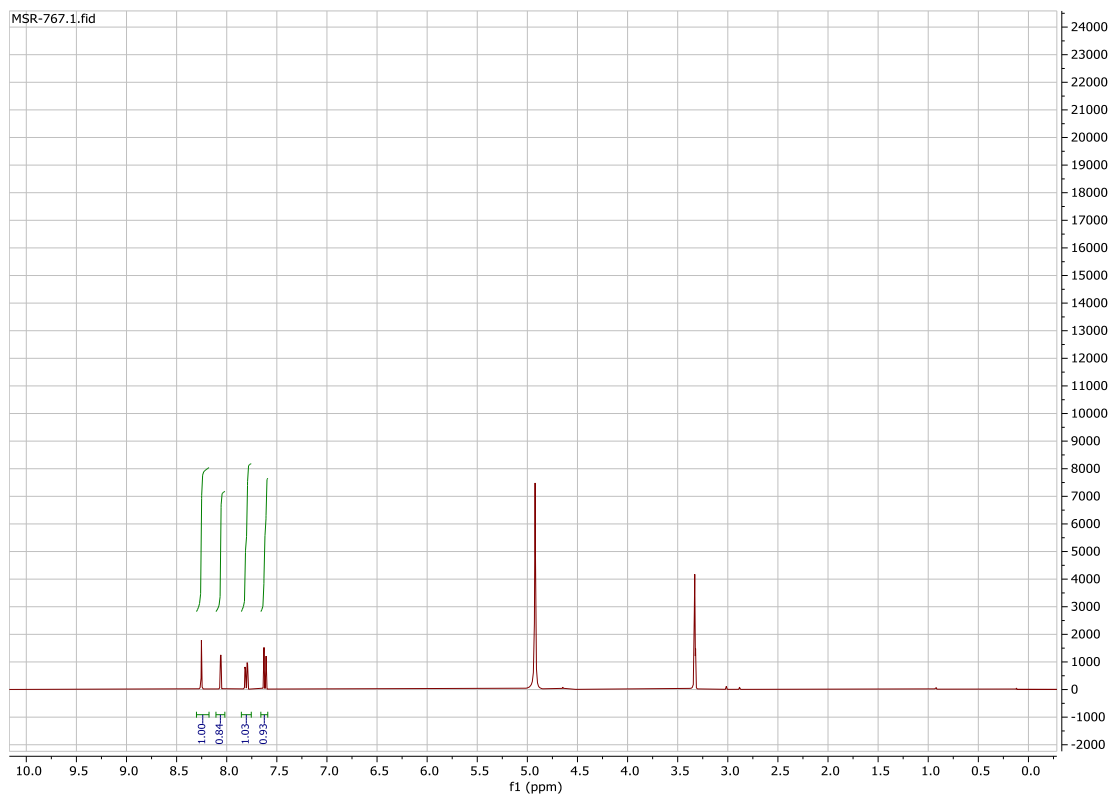
**4-(2,4-Dichlorophenyl)-1,2,3-triazole (48):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



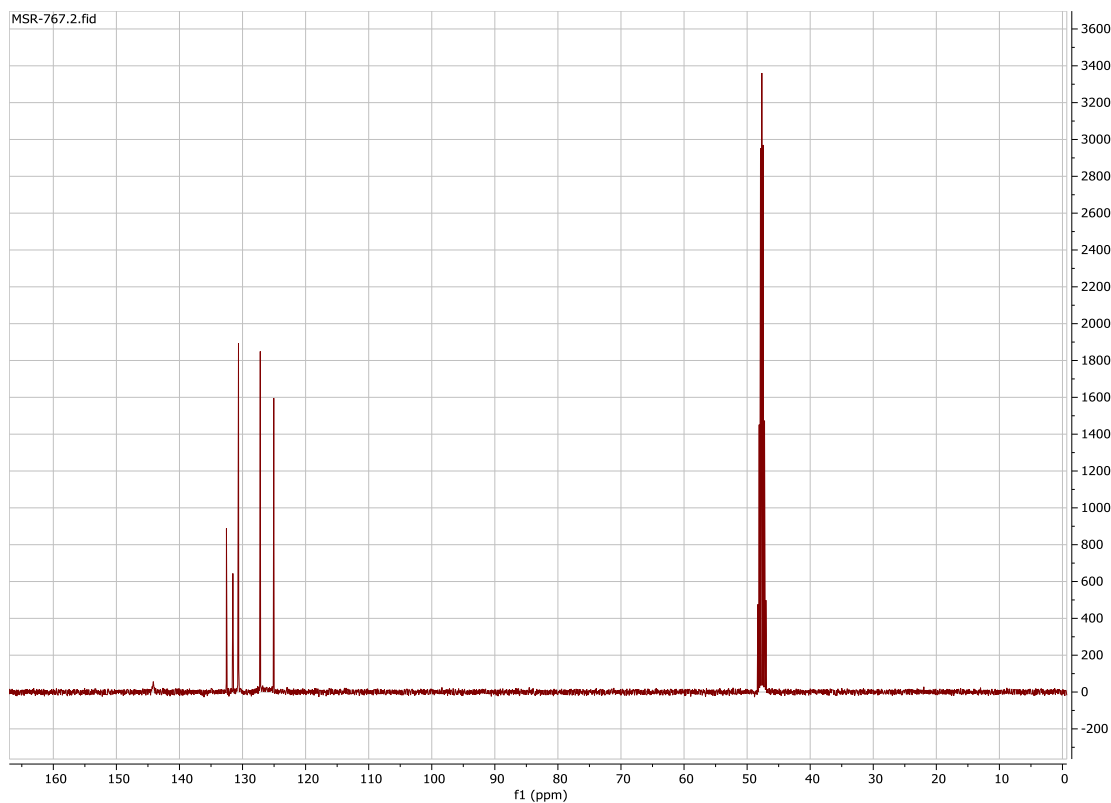
**4-(2,4-Dichlorophenyl)-1,2,3-triazole (48):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**4-(3,4-Dichlorophenyl)-1,2,3-triazole (49):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

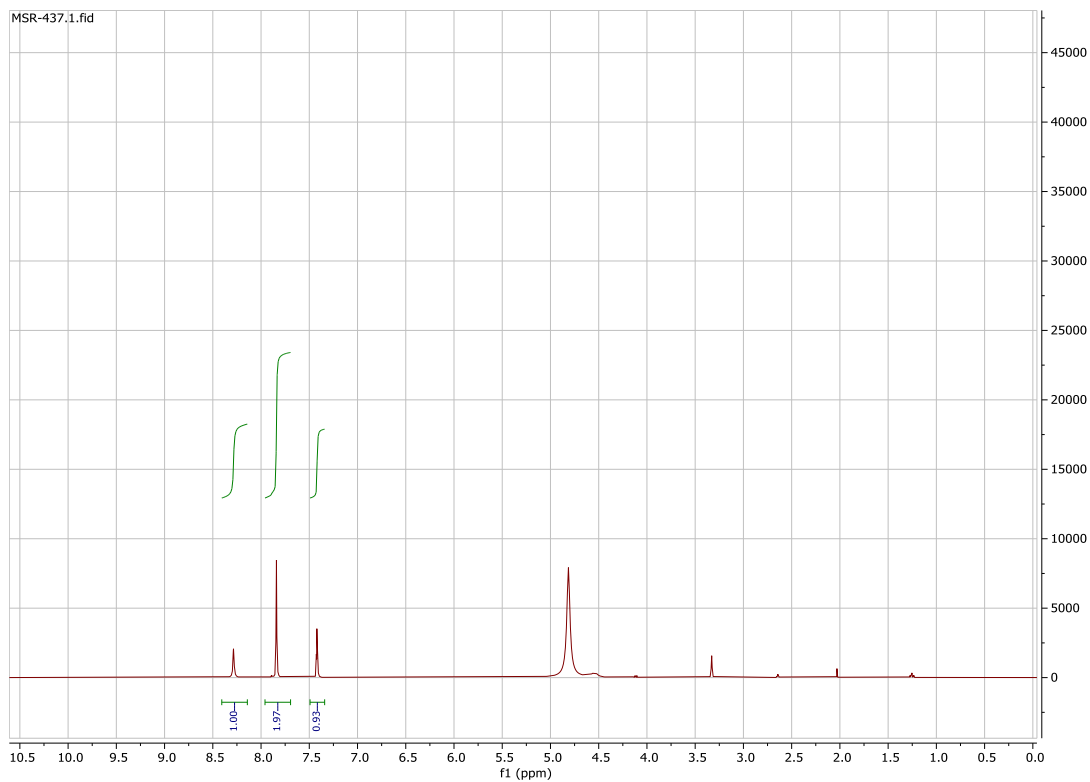


**4-(3,4-Dichlorophenyl)-1,2,3-triazole (49):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

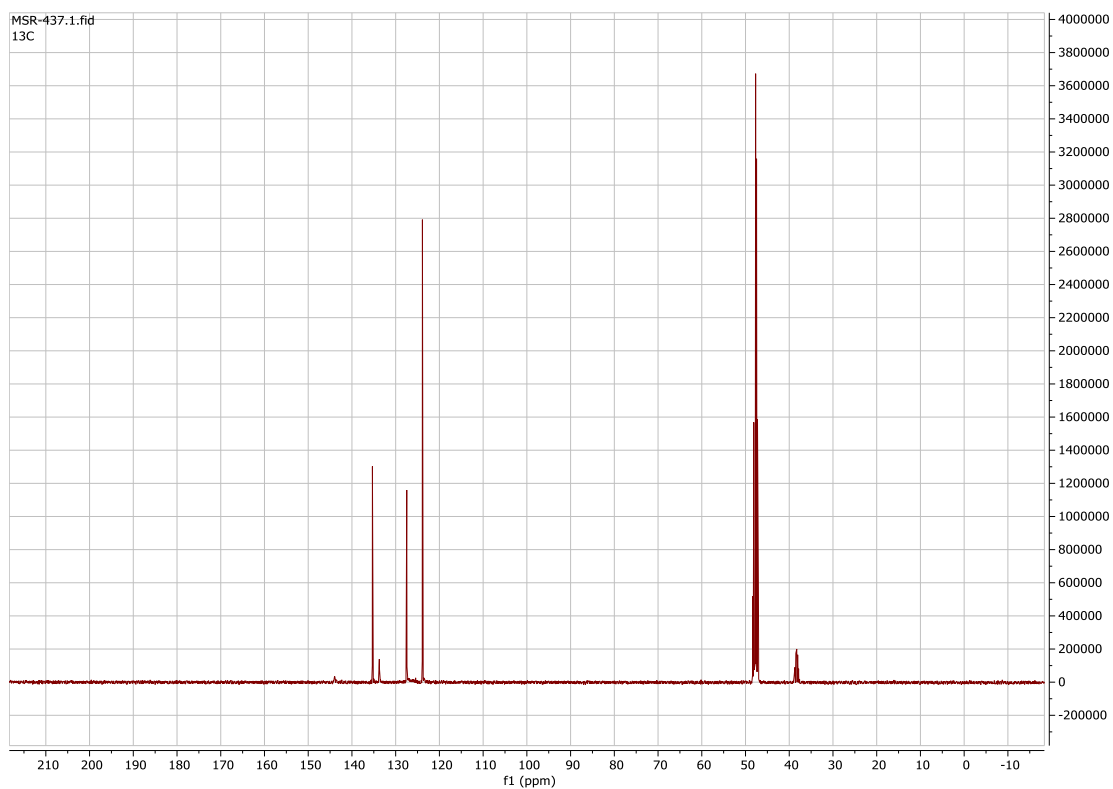




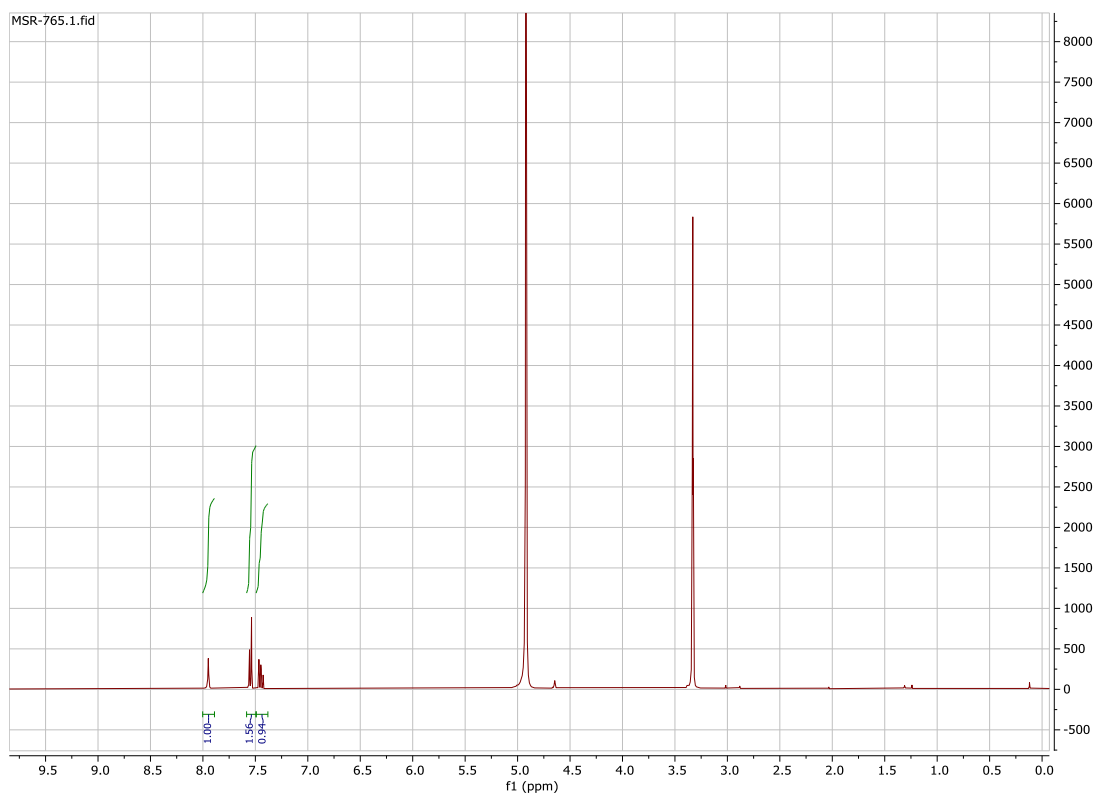
**4-(3,5-Dichlorophenyl)-1,2,3-triazole (50) :  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ )**



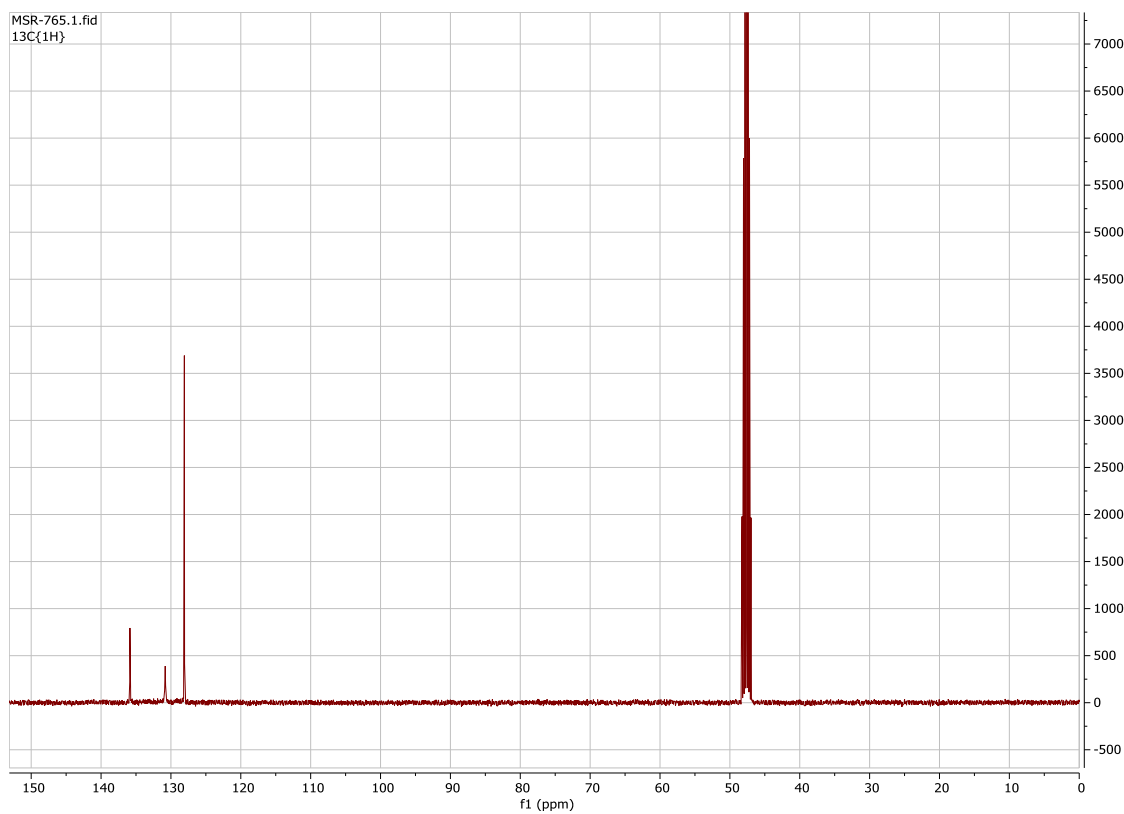
**4-(3,5-Dichlorophenyl)-1,2,3-triazole (50) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**



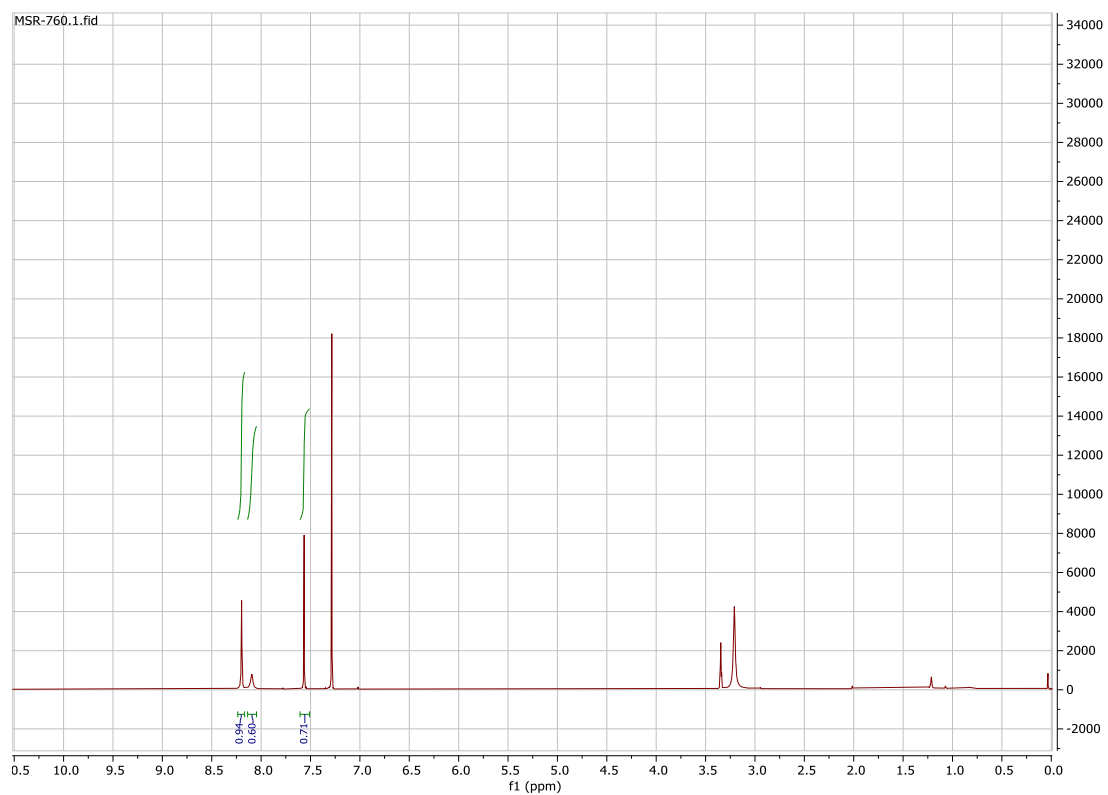
**4-(2,6-Dichlorophenyl)-1,2,3-triazole (51):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



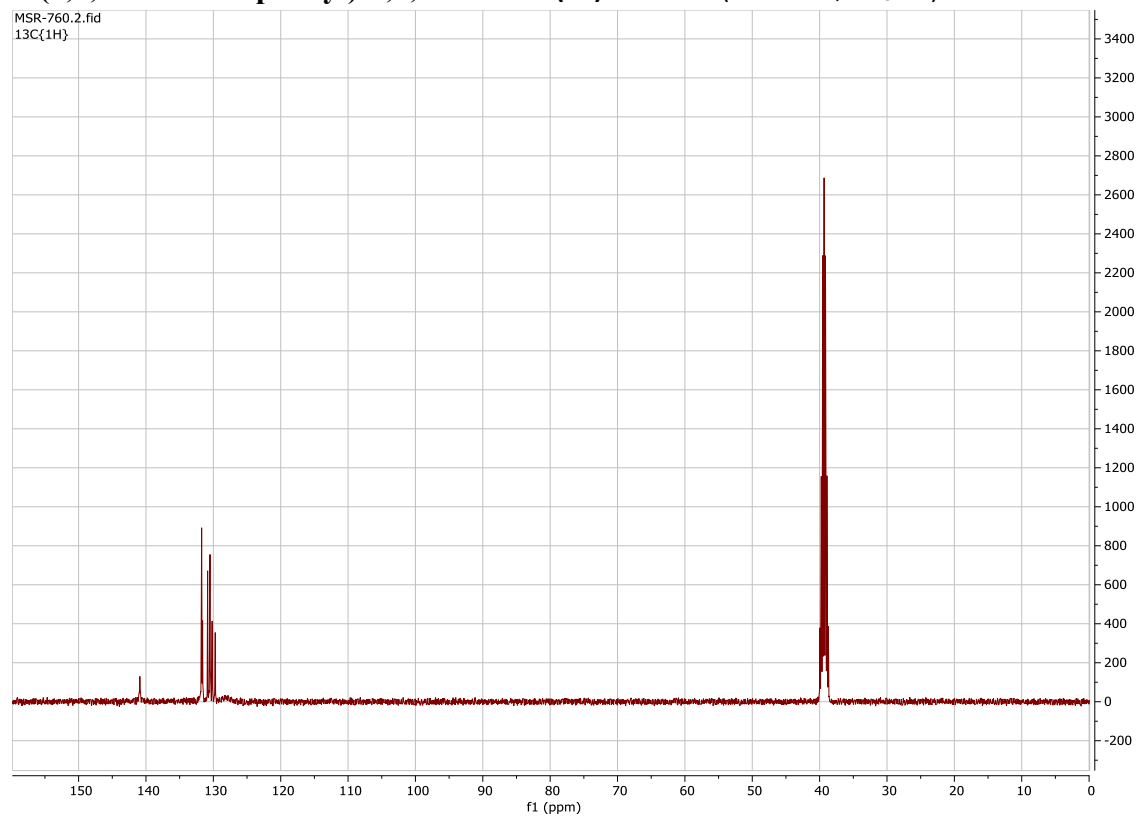
**4-(2,6-Dichlorophenyl)-1,2,3-triazole (51):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



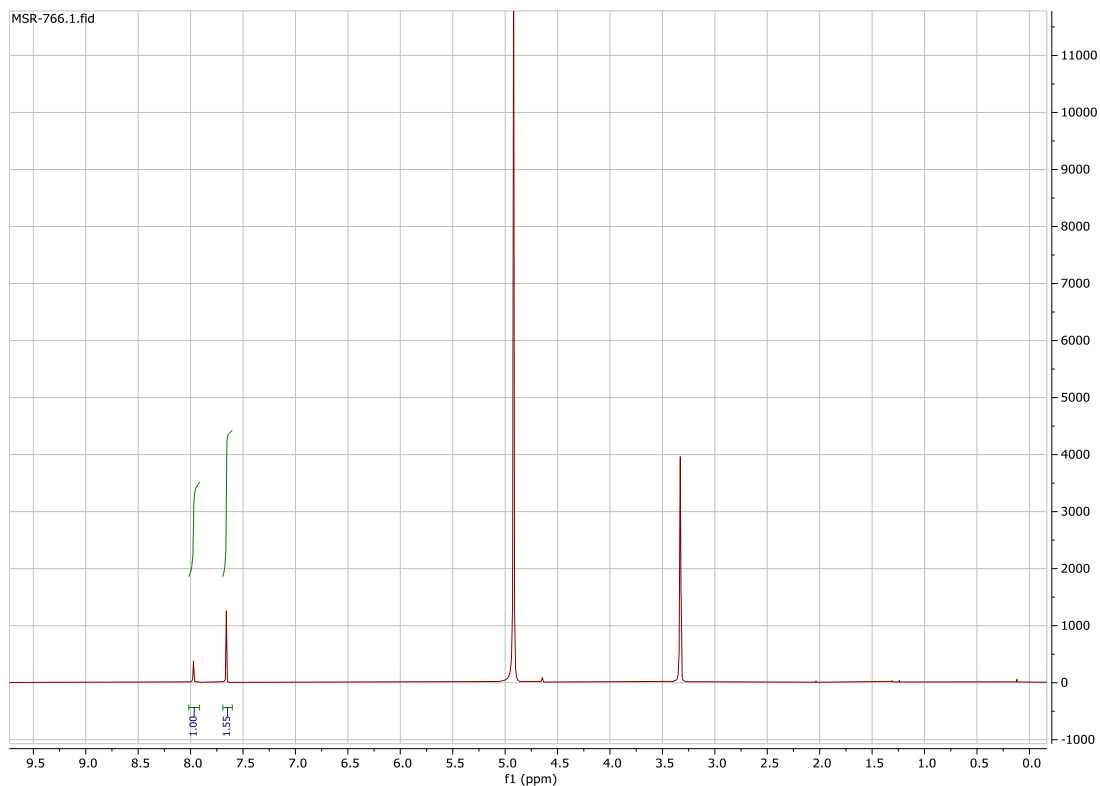
**4-(2,4,5-Trichlorophenyl)-1,2,3-triazole (52):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



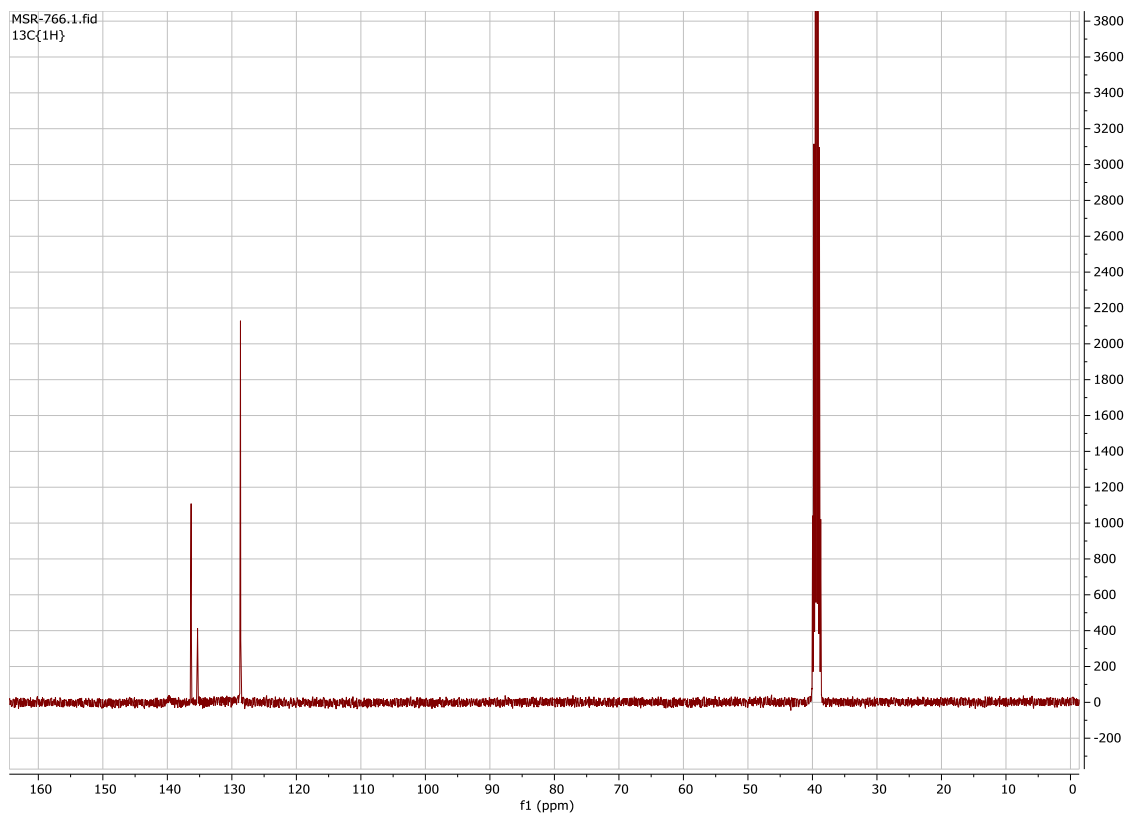
**4-(2,4,5-Trichlorophenyl)-1,2,3-triazole (52):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



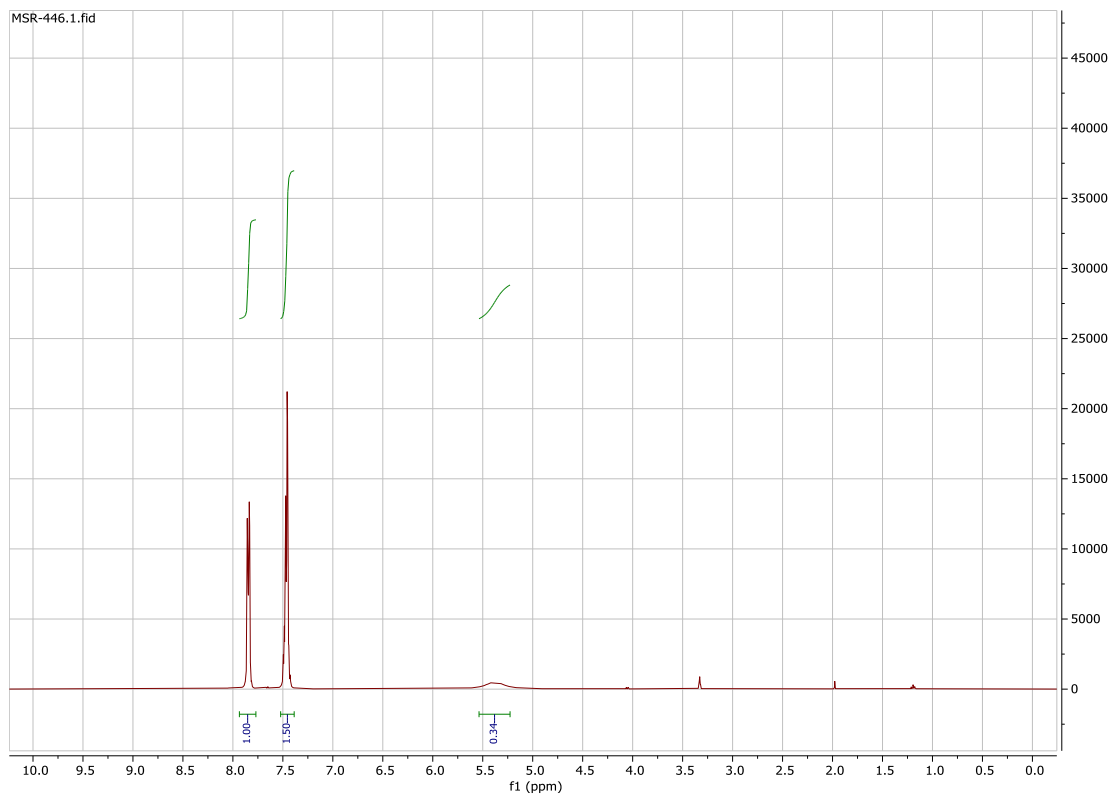
**4-(2,4,6-Trichlorophenyl)-1,2,3-triazole (53):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



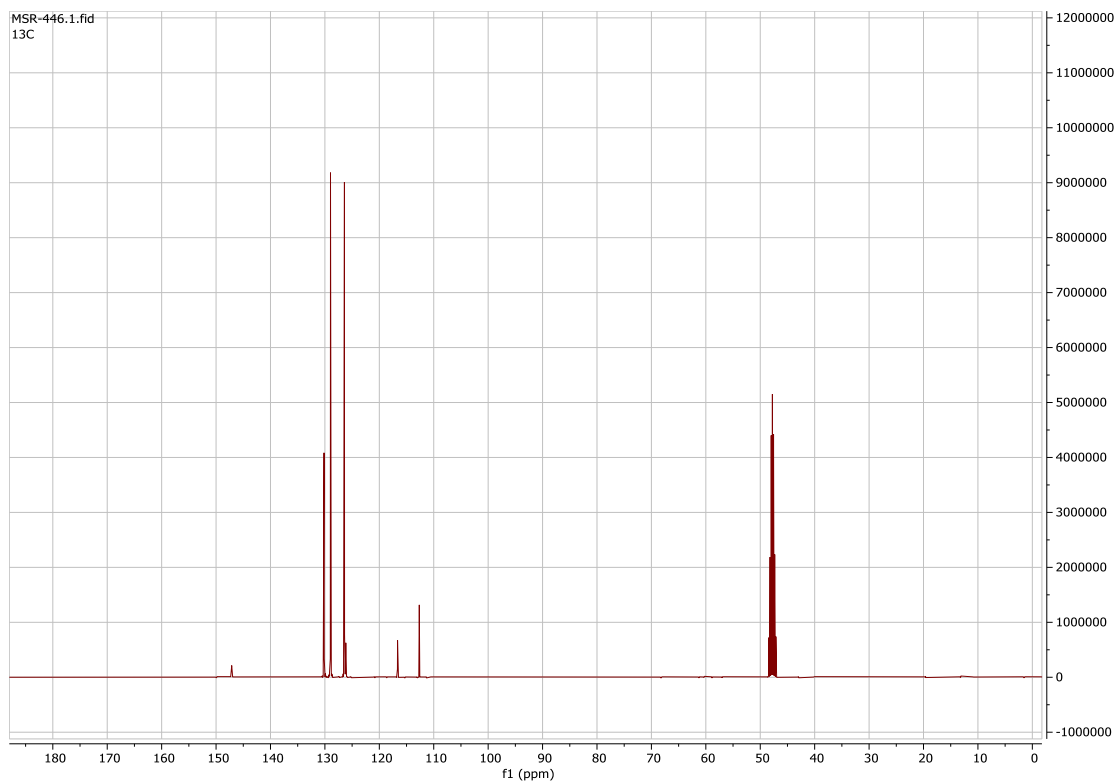
**4-(2,4,6-Trichlorophenyl)-1,2,3-triazole (53):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



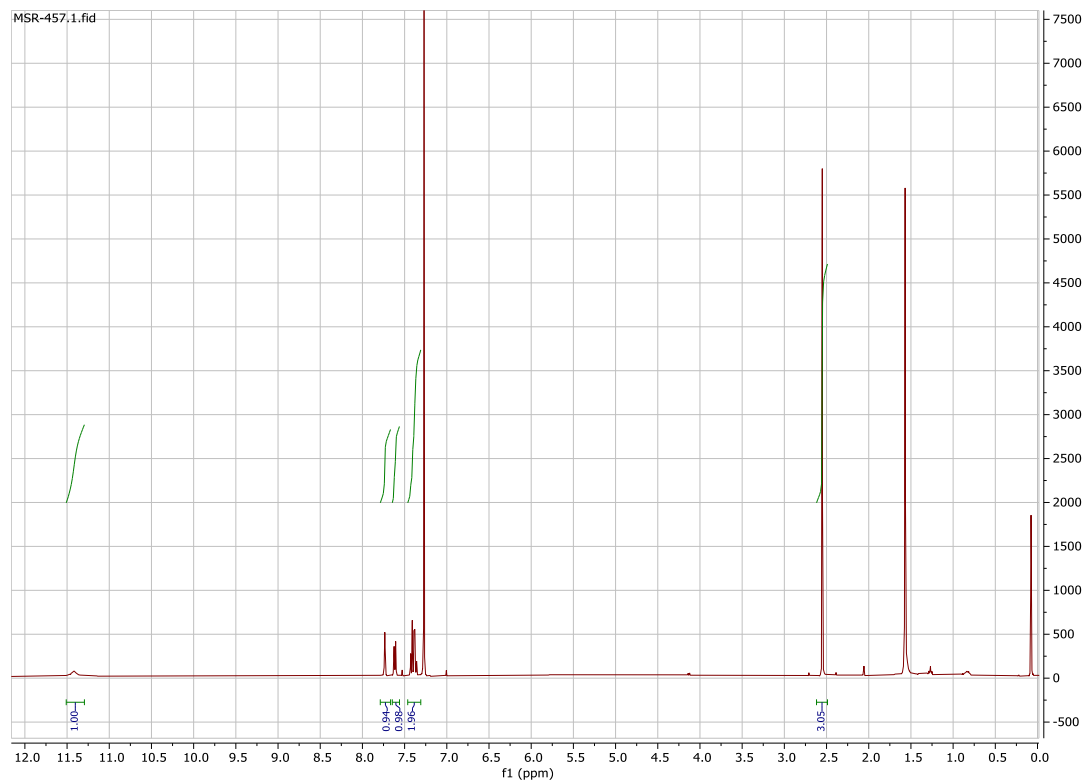
**4-Phenyl-1H-1,2,3-triazole-5-carbonitrile (62) : <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



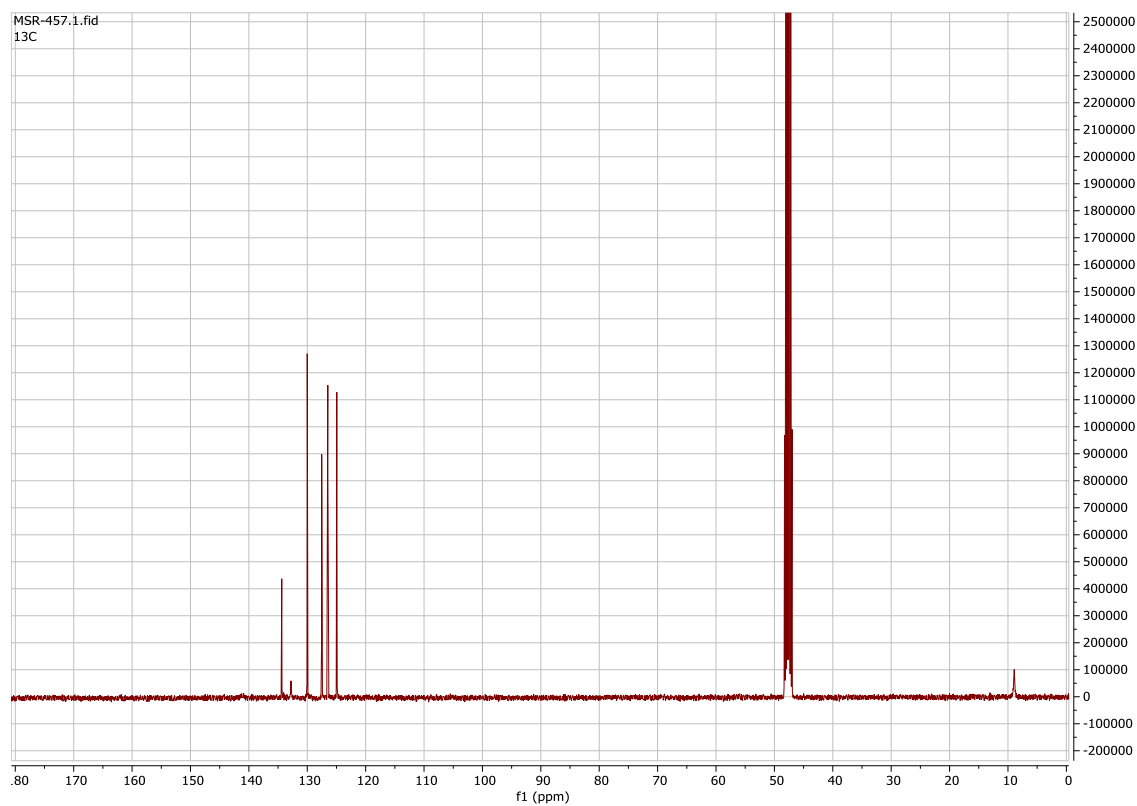
**4-Phenyl-1H-1,2,3-triazole-5-carbonitrile (62) : <sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



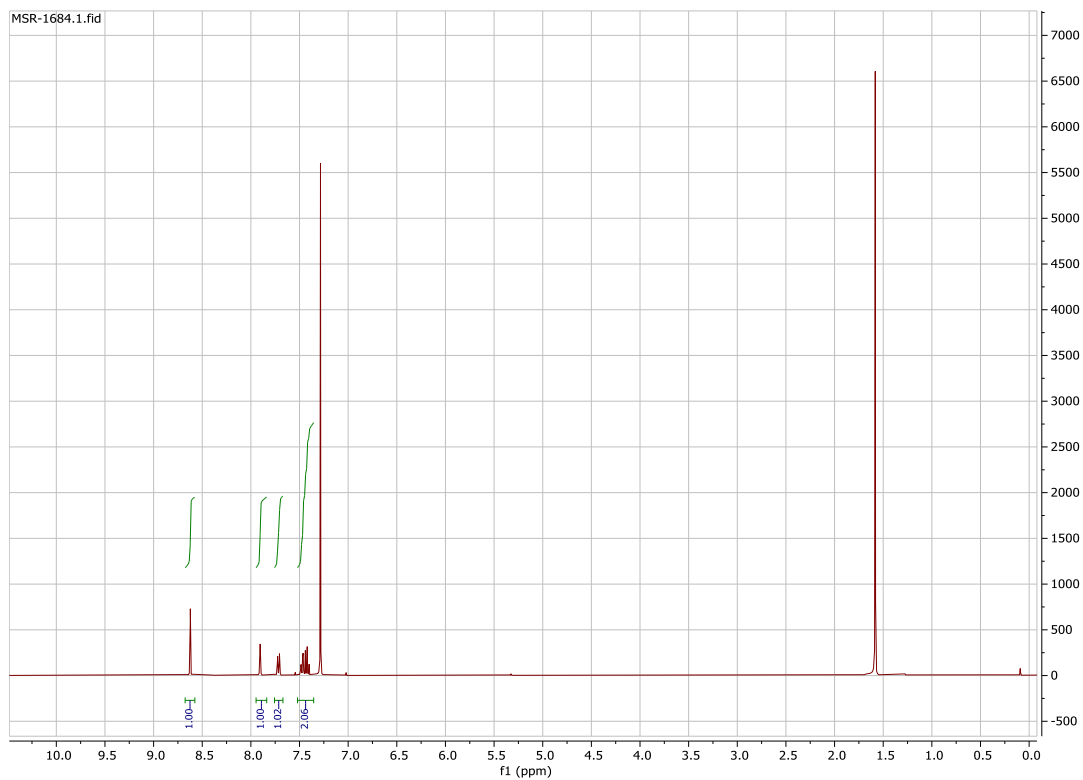
4-(3-Chlorophenyl)-5-methyl-1,2,3-triazole (63) :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



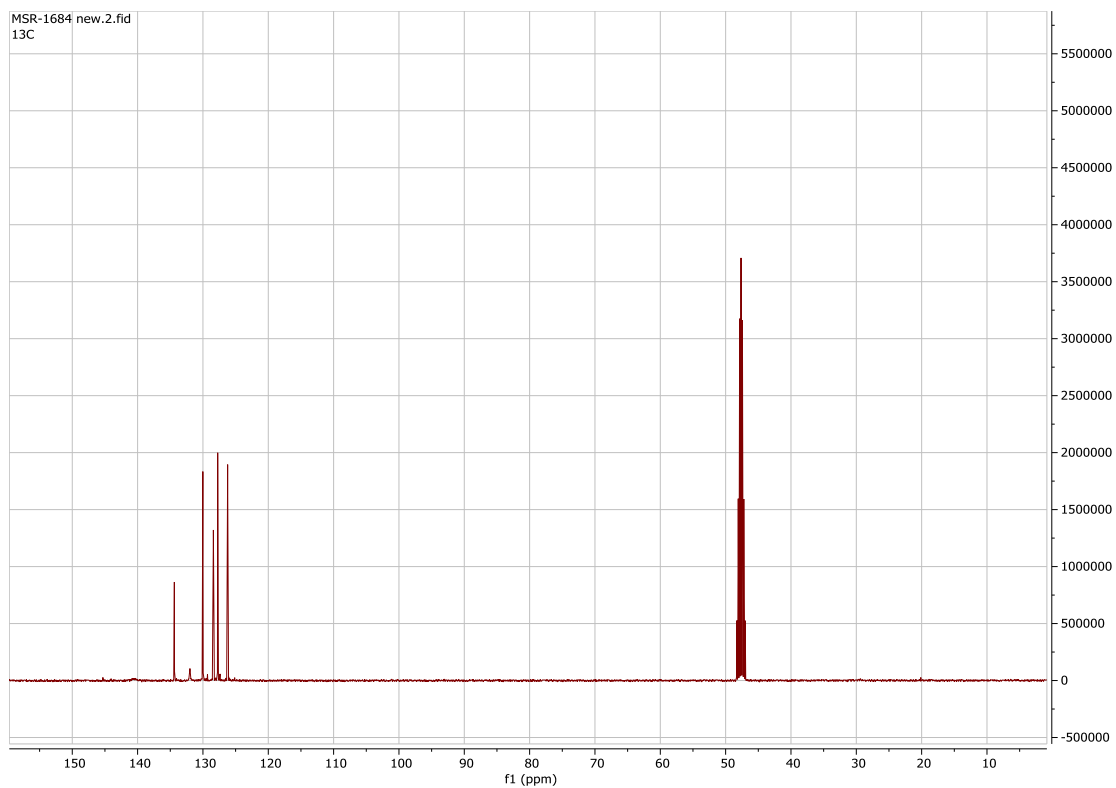
4-(3-Chlorophenyl)-5-methyl-1,2,3-triazole (63) :  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )



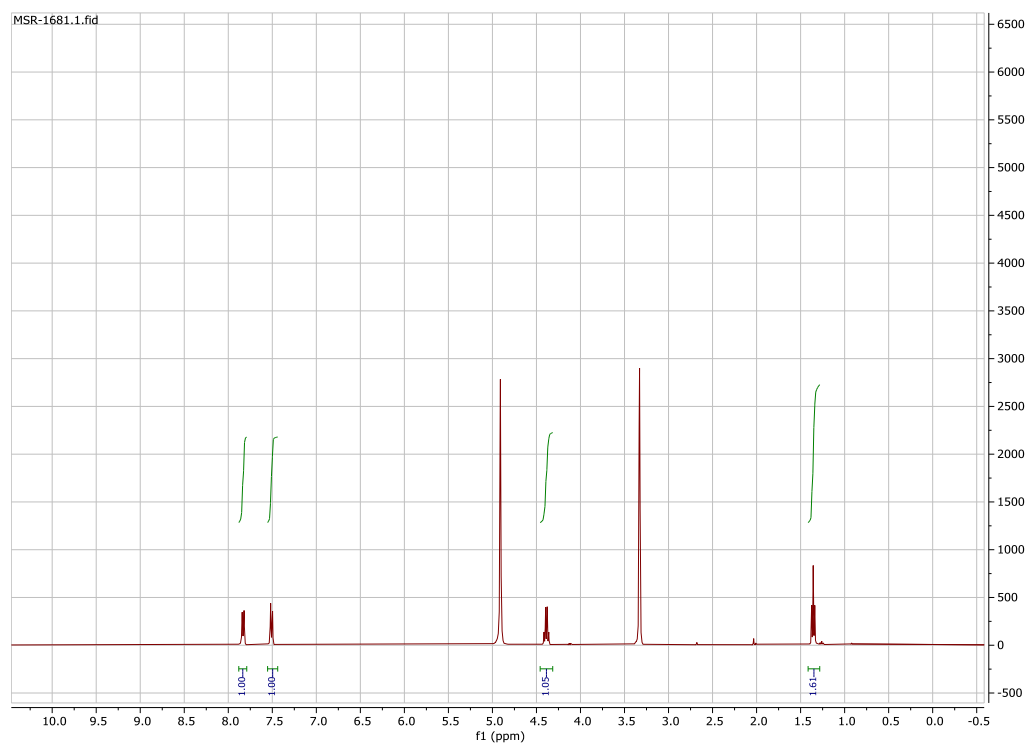
**4,5-Bis(3-chlorophenyl)-1,2,3-triazole (64):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



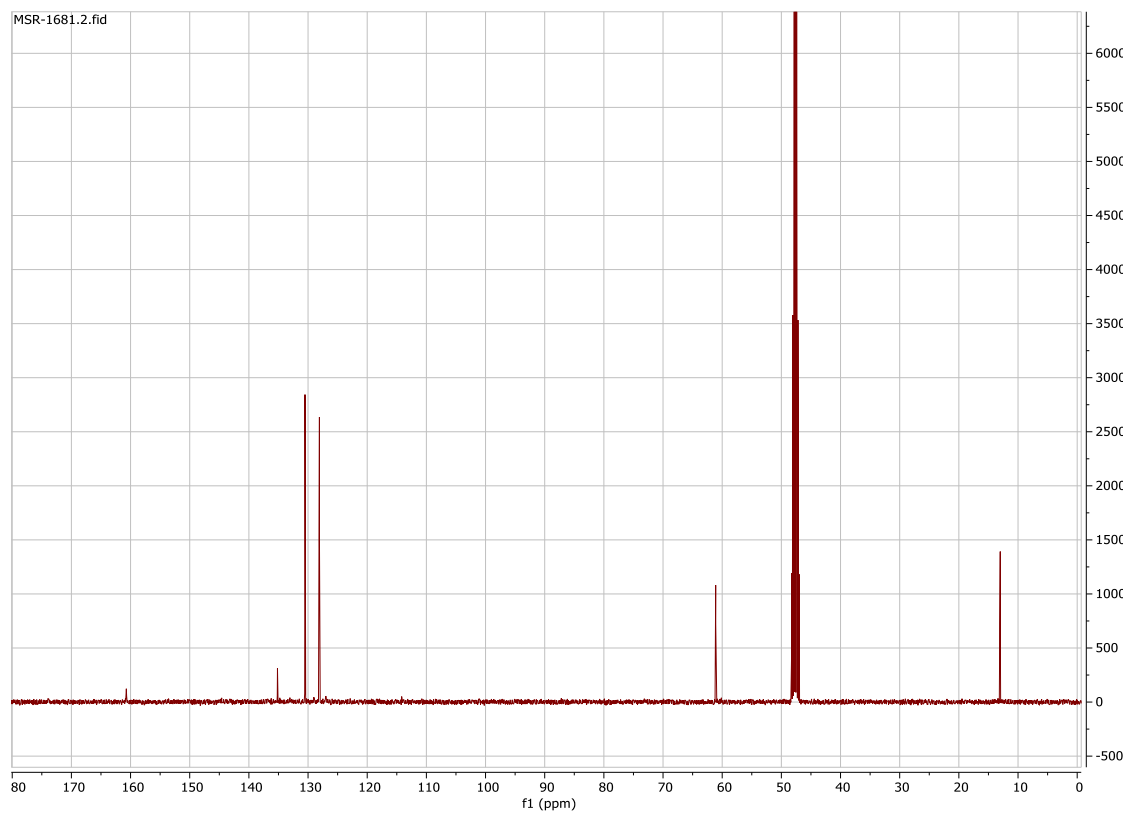
**4,5-Bis(3-chlorophenyl)-1,2,3-triazole (64):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**Ethyl 4-(3-chlorophenyl)-1*H*-1,2,3-triazole-5-carboxylate (65):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

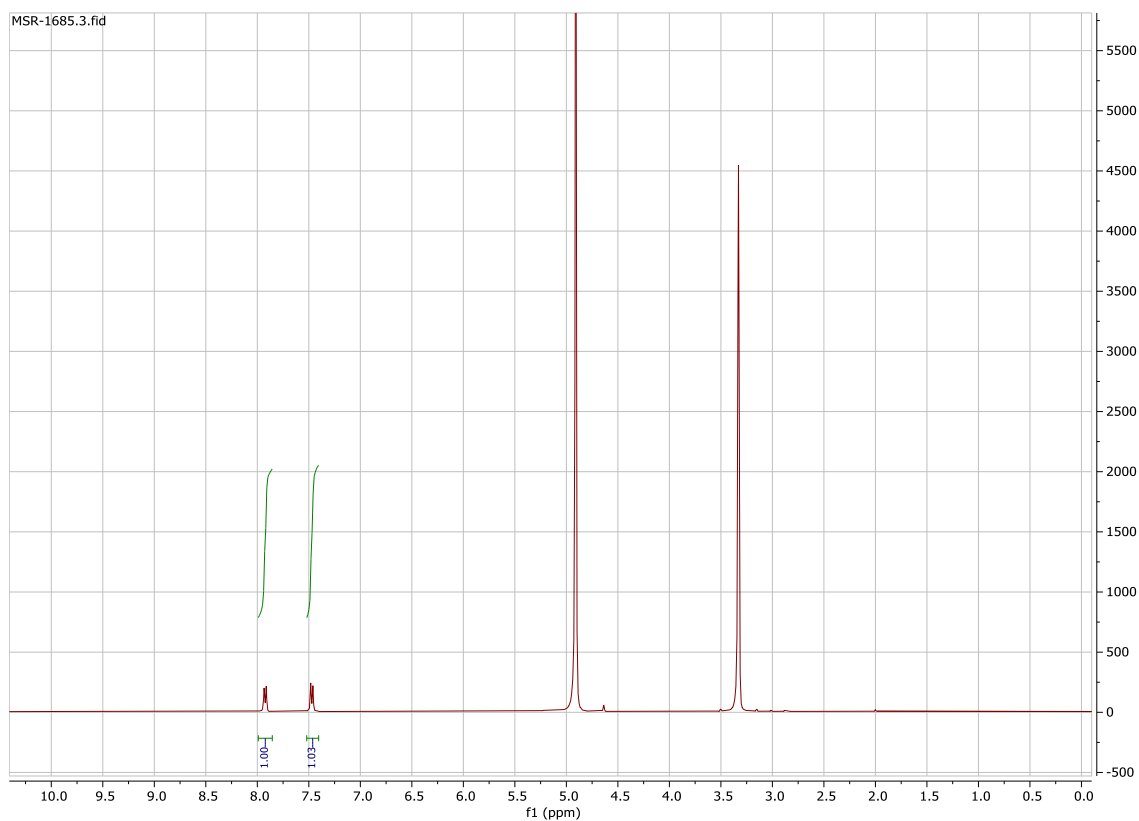


**Ethyl 4-(3-chlorophenyl)-1*H*-1,2,3-triazole-5-carboxylate (65):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

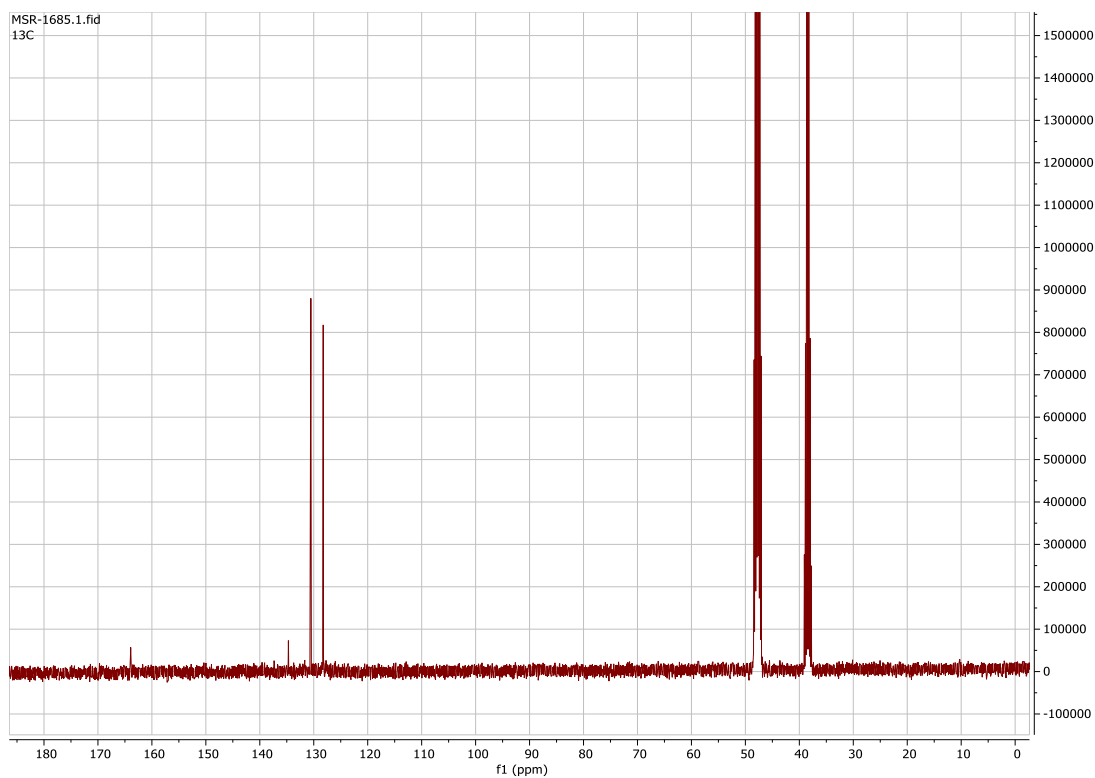




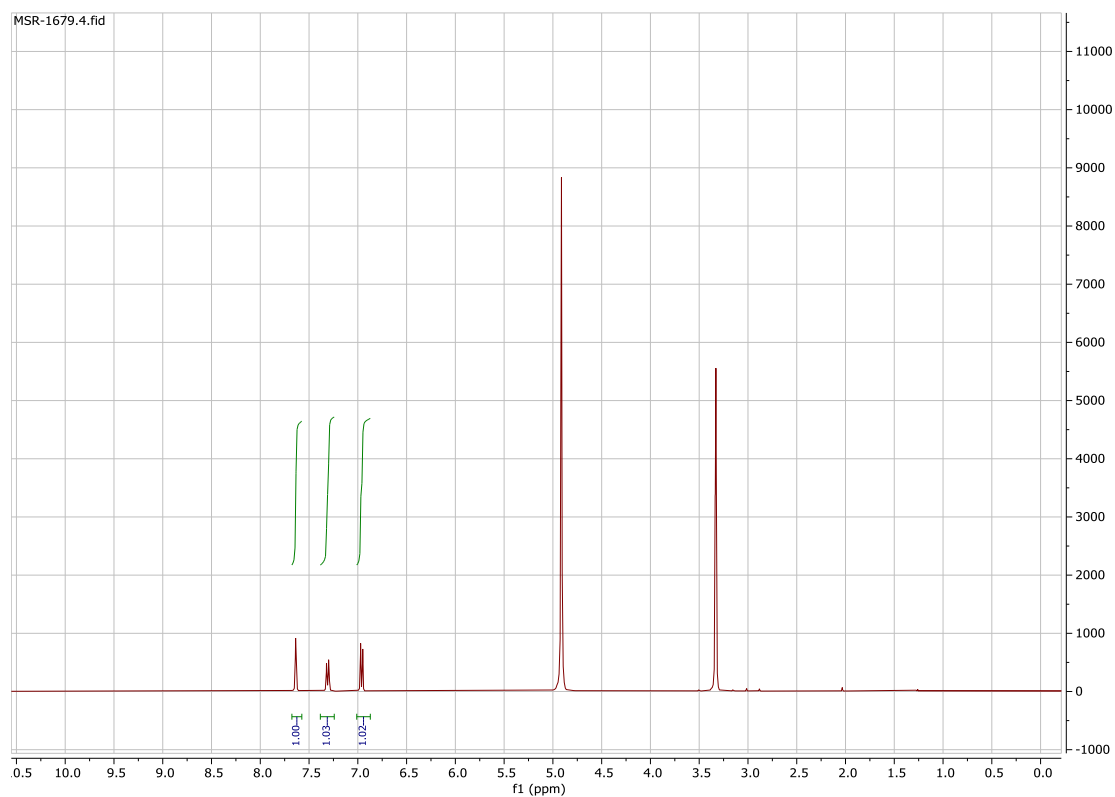
**4-(4-Chlorophenyl)-1*H*-1,2,3-triazole-5-carboxamide (66):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



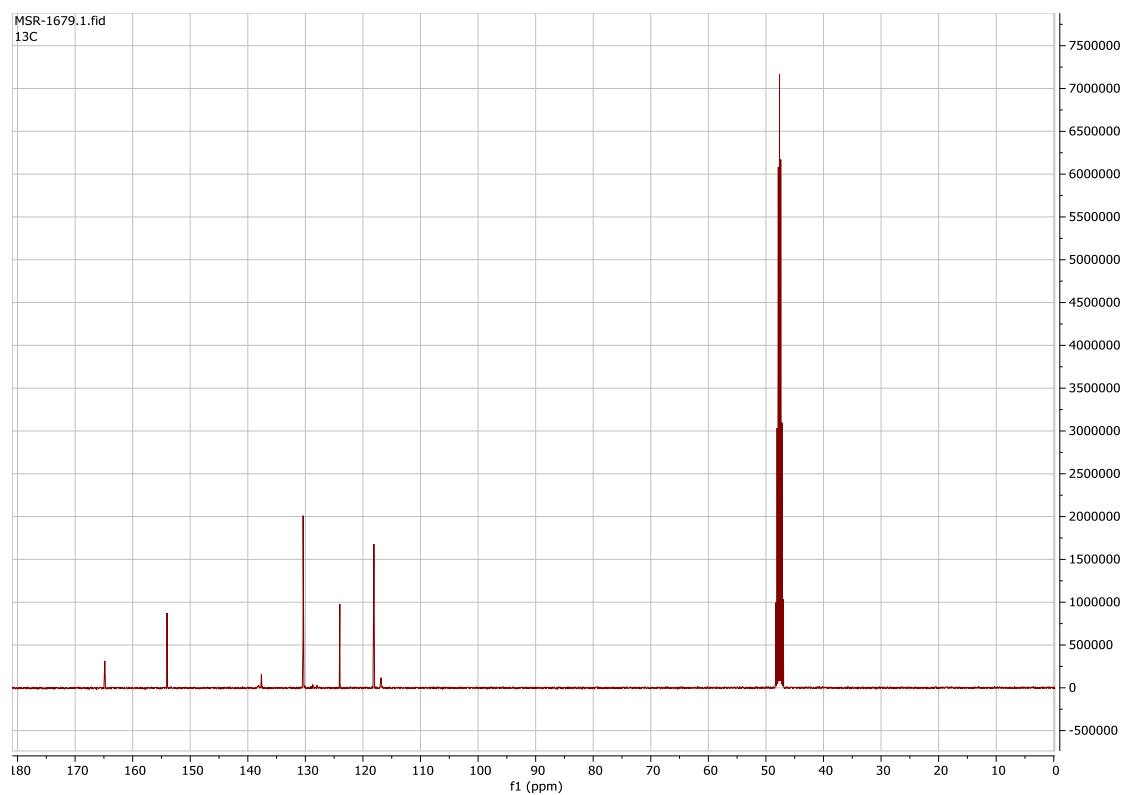
**4-(4-Chlorophenyl)-1*H*-1,2,3-triazole-5-carboxamide (66):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



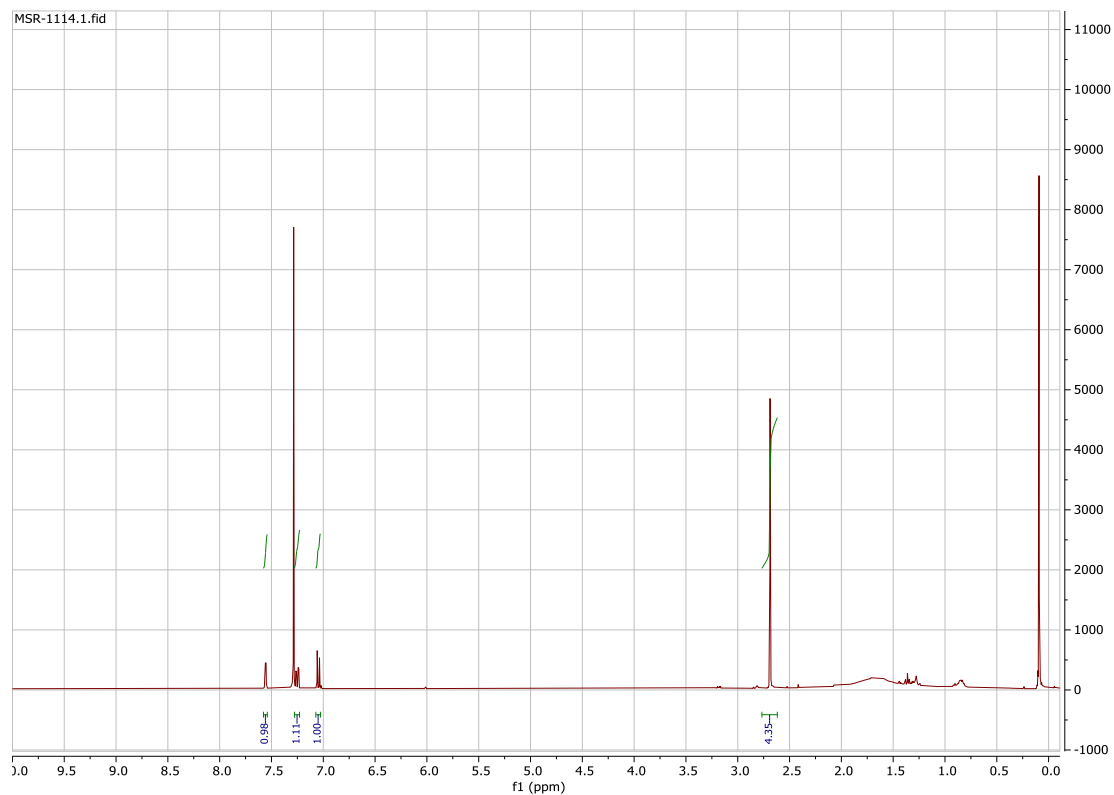
**4-(4-Chloro-2-hydroxyphenyl)-1H-1,2,3-triazole-5-carboxamide (67):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



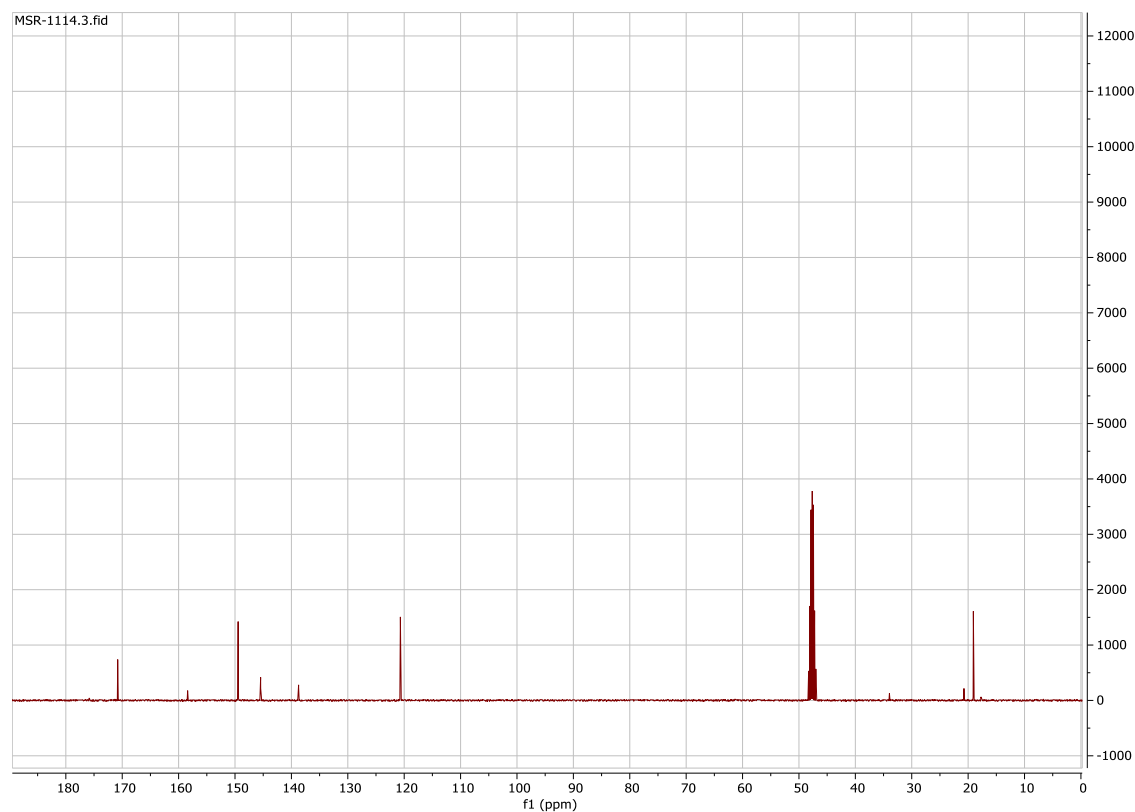
**4-(4-Chloro-2-hydroxyphenyl)-1H-1,2,3-triazole-5-carboxamide (67):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



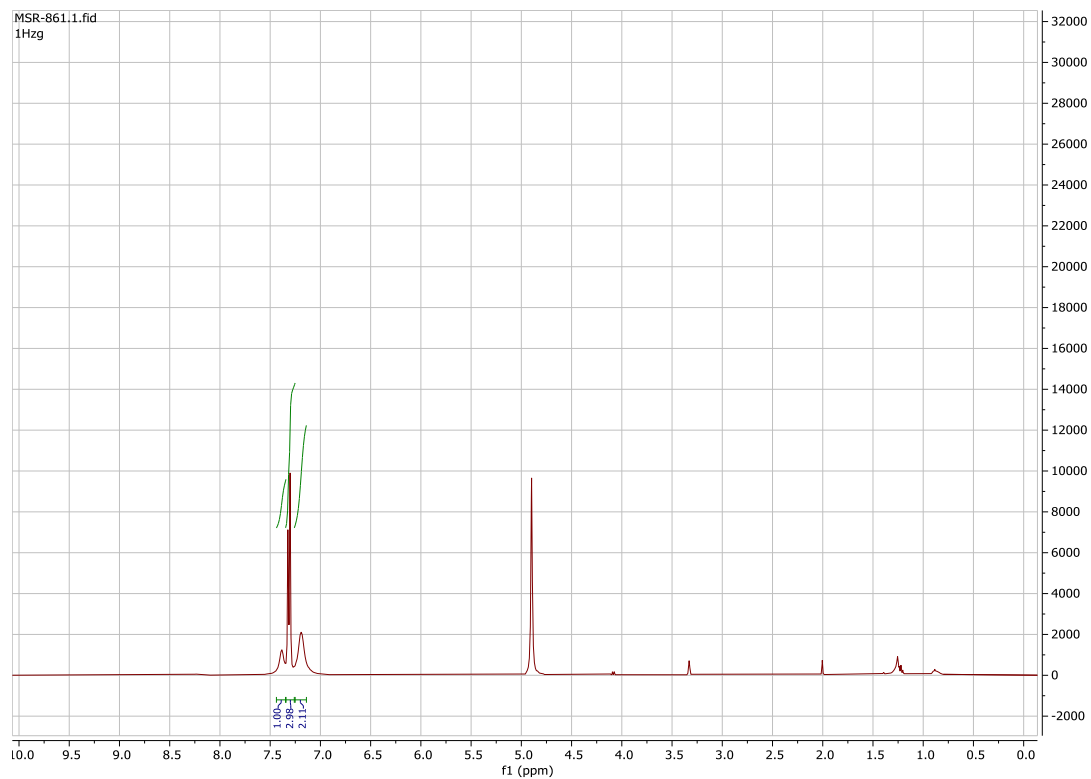
**4-Chloro-2-(5-methyl-1,2,3-triazol-4-yl)phenol (68):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**



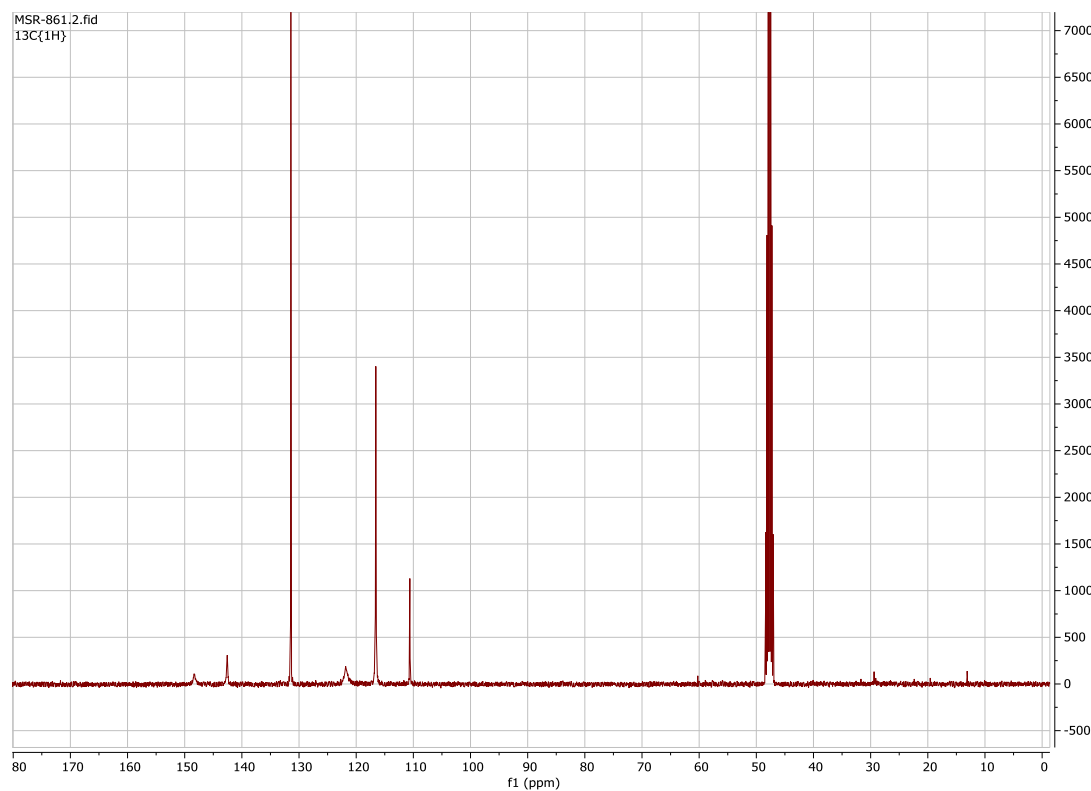
**4-Chloro-2-(5-methyl-1,2,3-triazol-4-yl)phenol (68):  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**



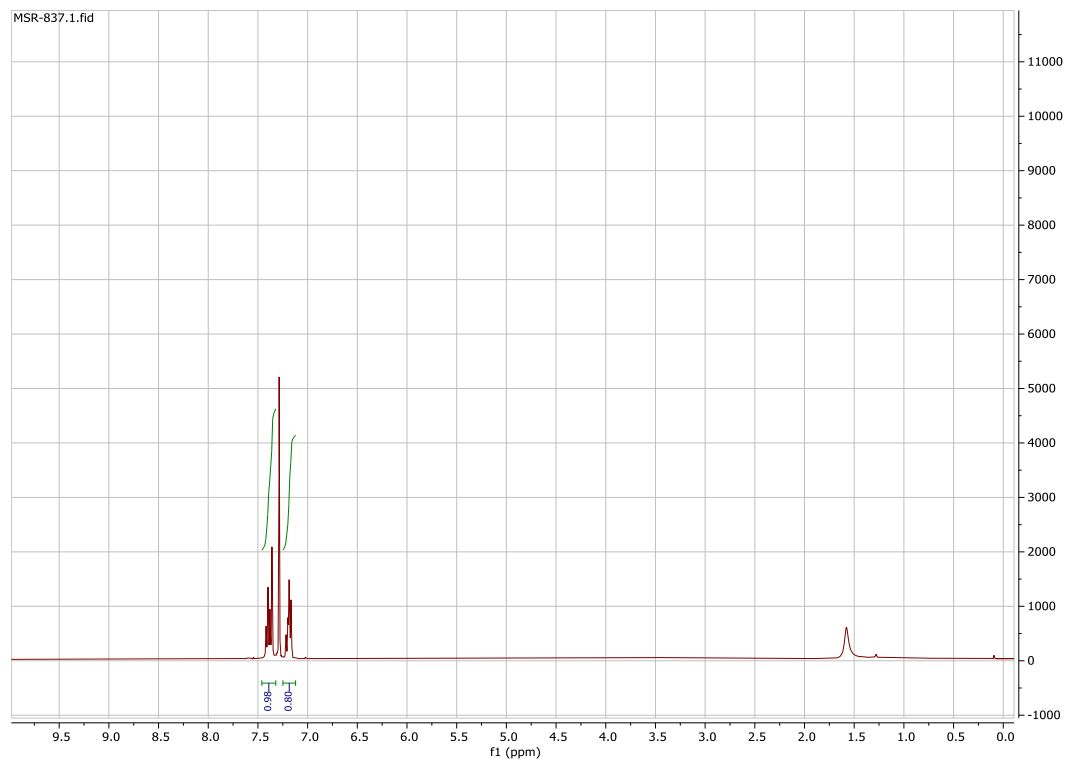
***N*-(4-Bromophenyl)-1,2,3-triazol-4-amine (78):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



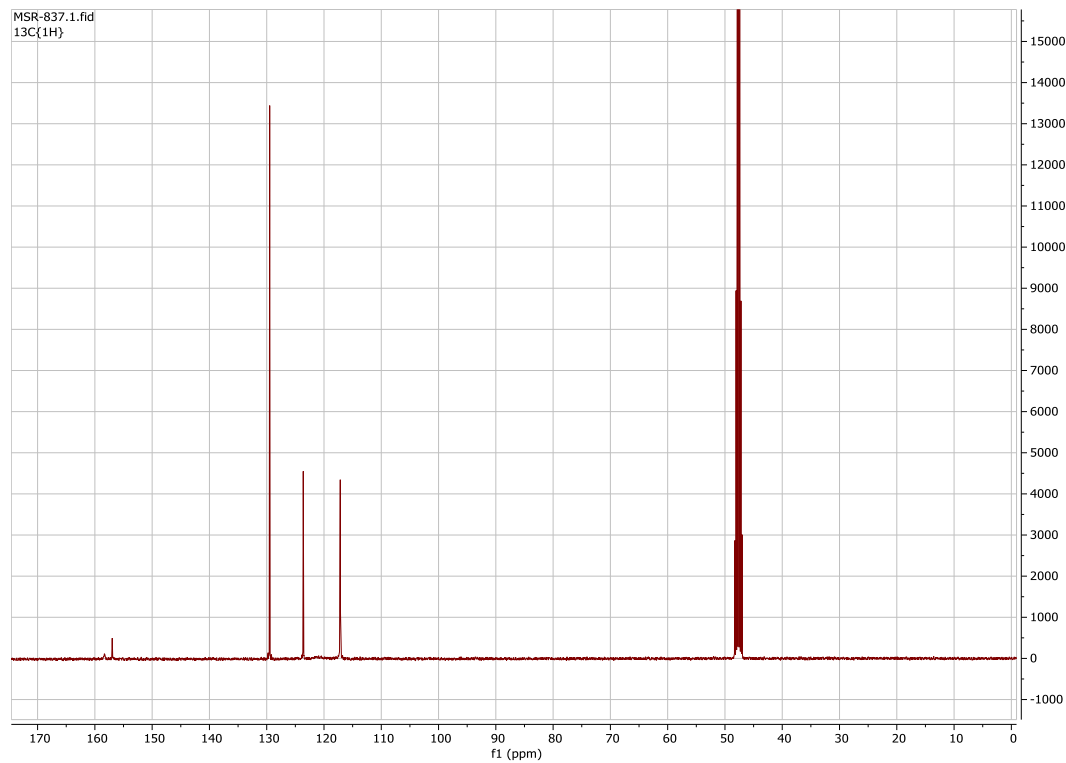
***N*-(4-Bromophenyl)-1,2,3-triazol-4-amine (78):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



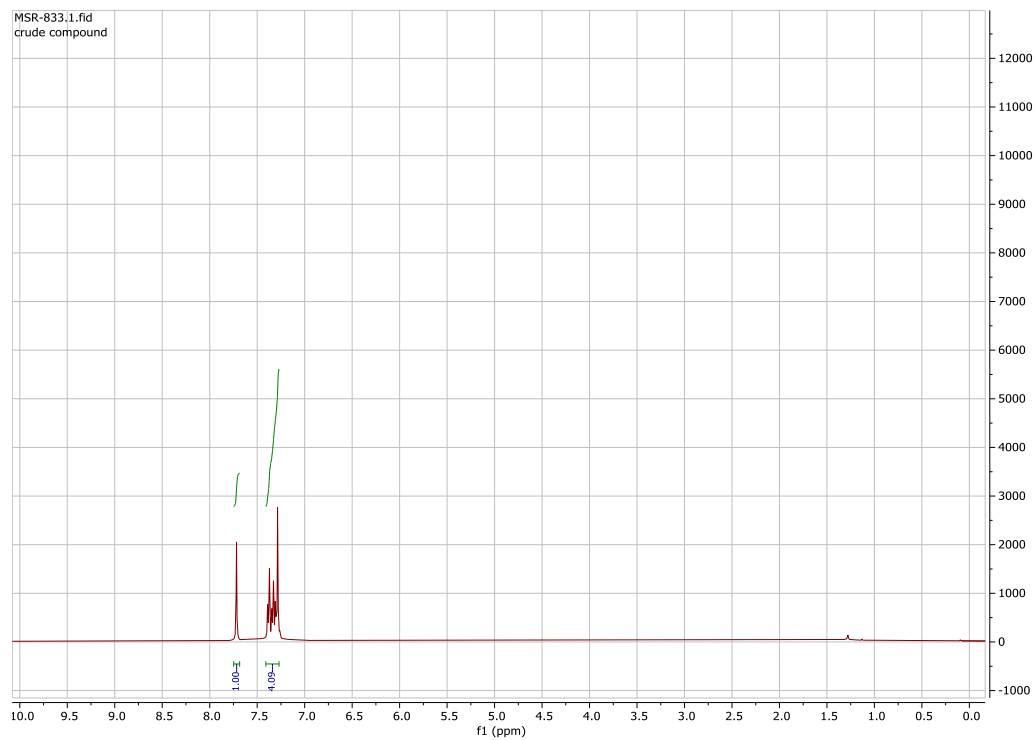
**4-(Phenoxy)-1,2,3-triazole (82):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



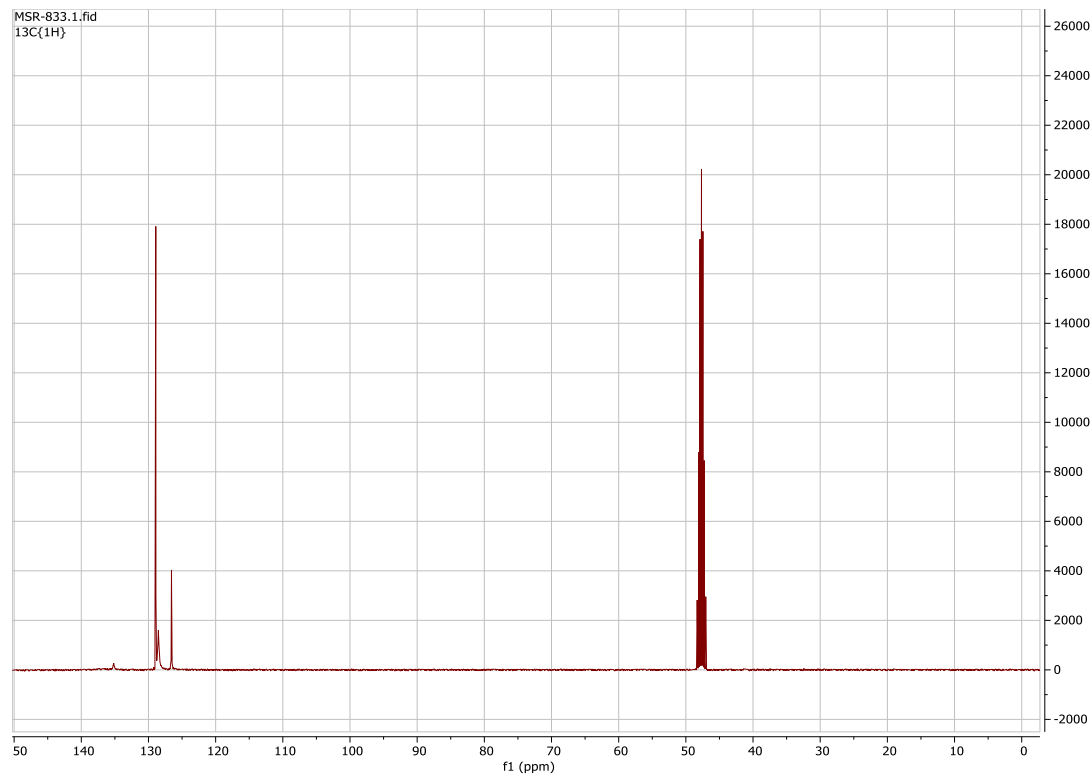
**4-(Phenoxy)-1,2,3-triazole (82):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



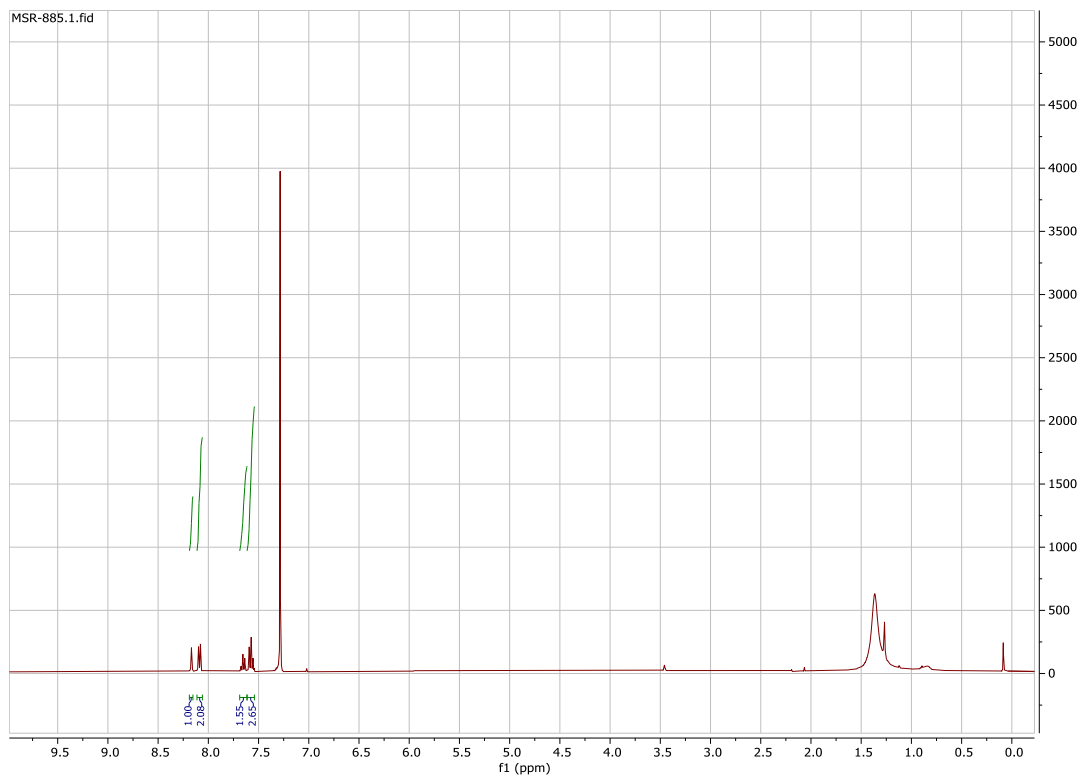
**4-(Phenylthio)-1,2,3-triazole (83):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



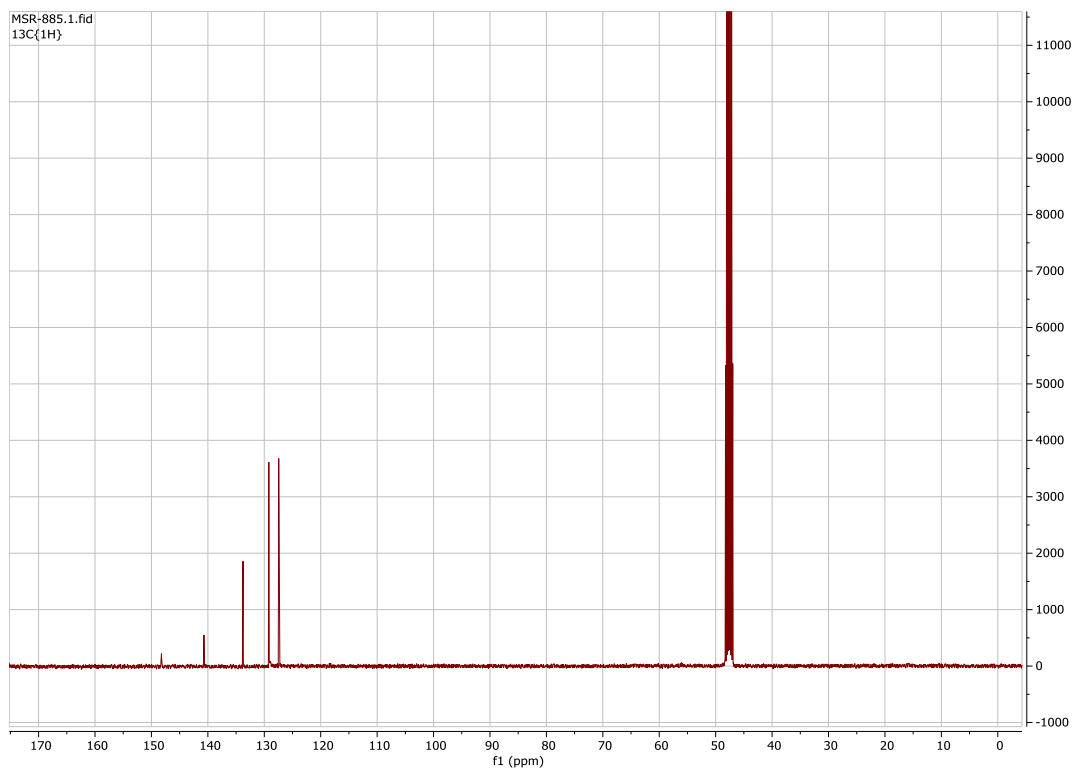
**4-(Phenylthio)-1,2,3-triazole (83):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



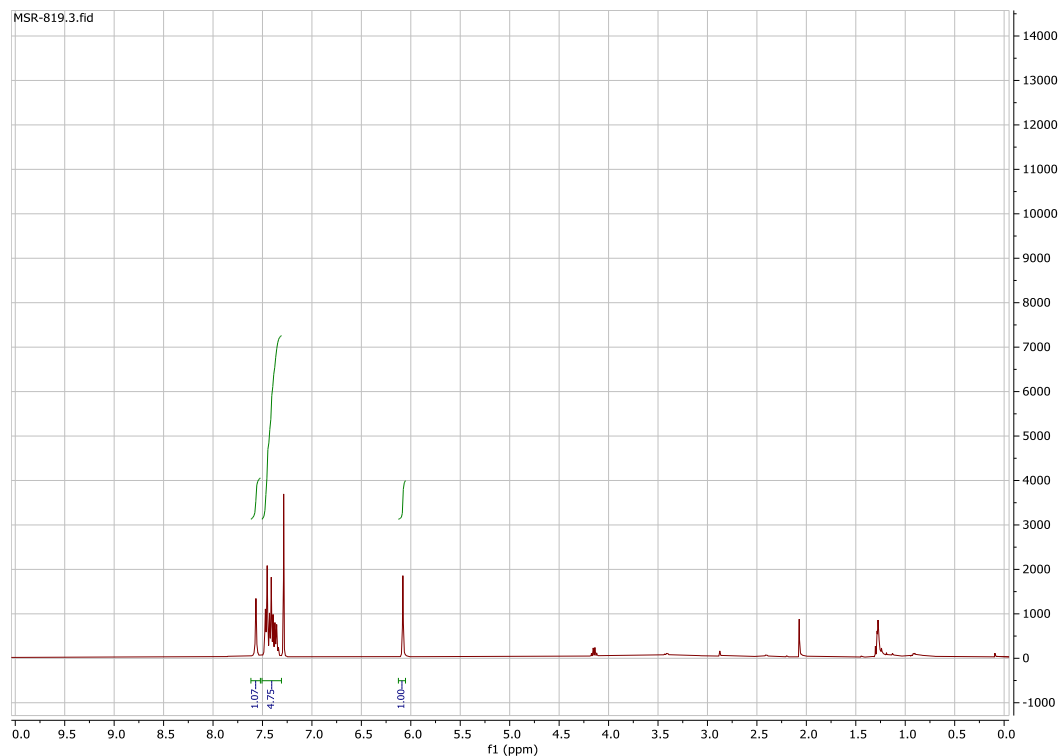
**4-(Phenylsulfonyl)-1*H*-1,2,3-triazole (84):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



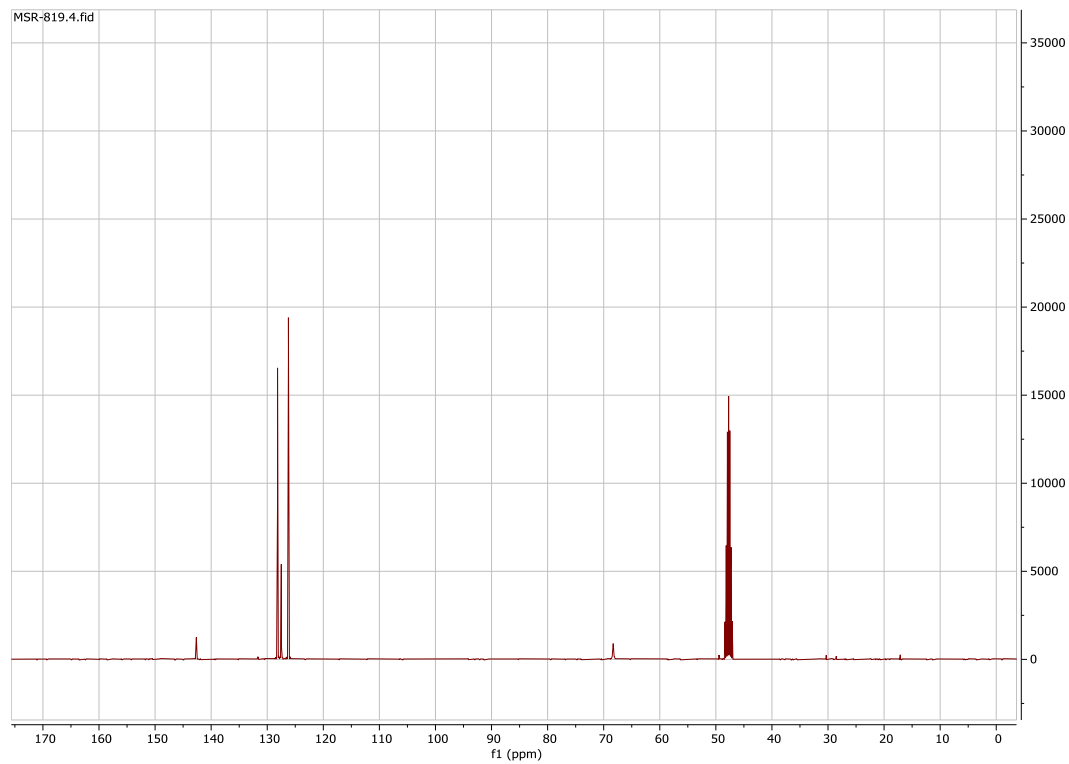
**4-(Phenylsulfonyl)-1*H*-1,2,3-triazole (84):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**Phenyl(1,2,3-triazol-4-yl)methanol (85):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )**

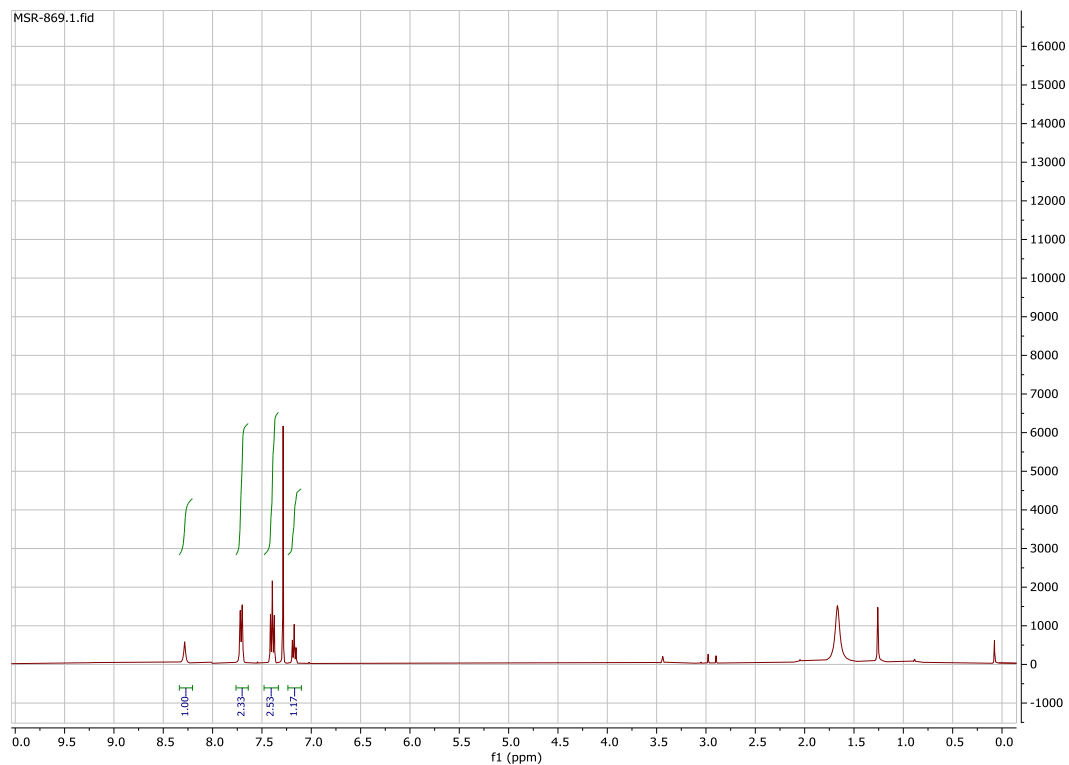


**Phenyl(1,2,3-triazol-4-yl)methanol (85):  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )**

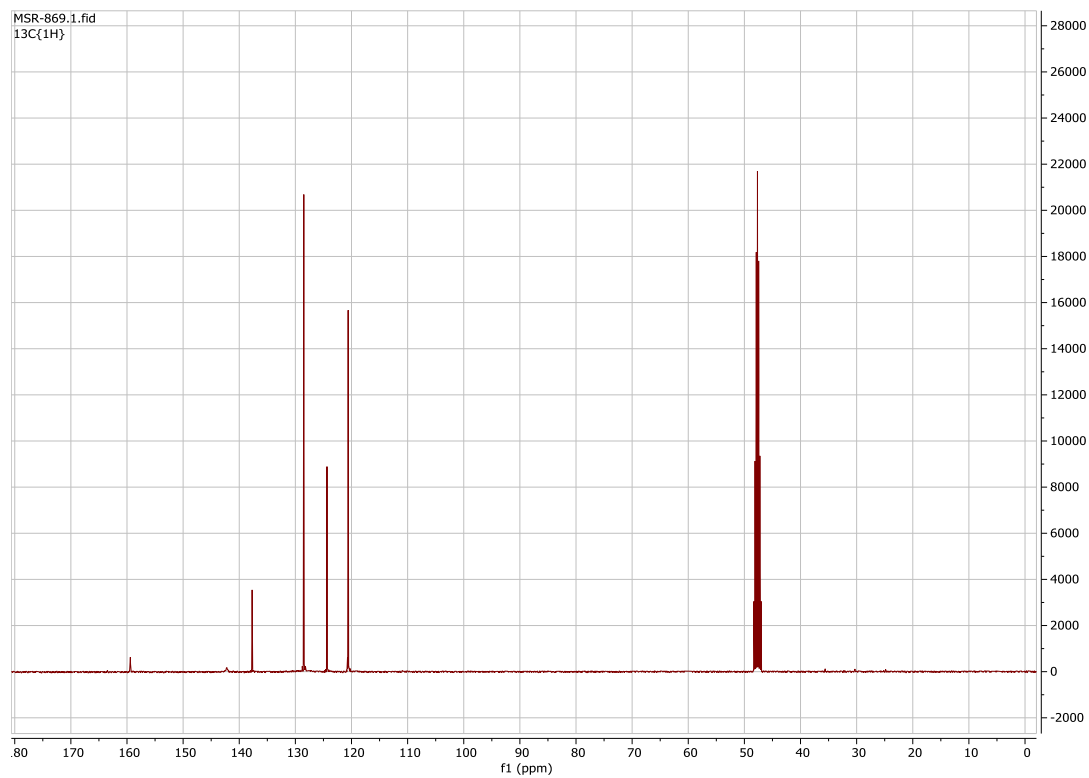




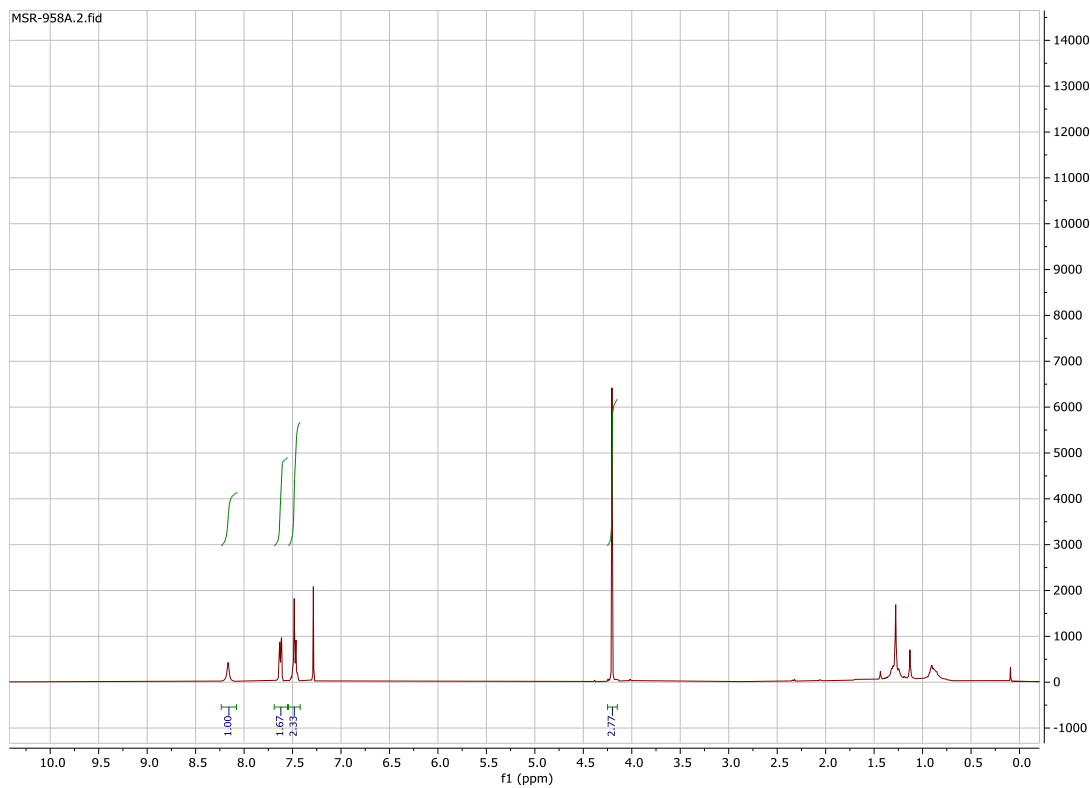
***N*-Phenyl-1*H*-1,2,3-triazole-4-carboxamide (86):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



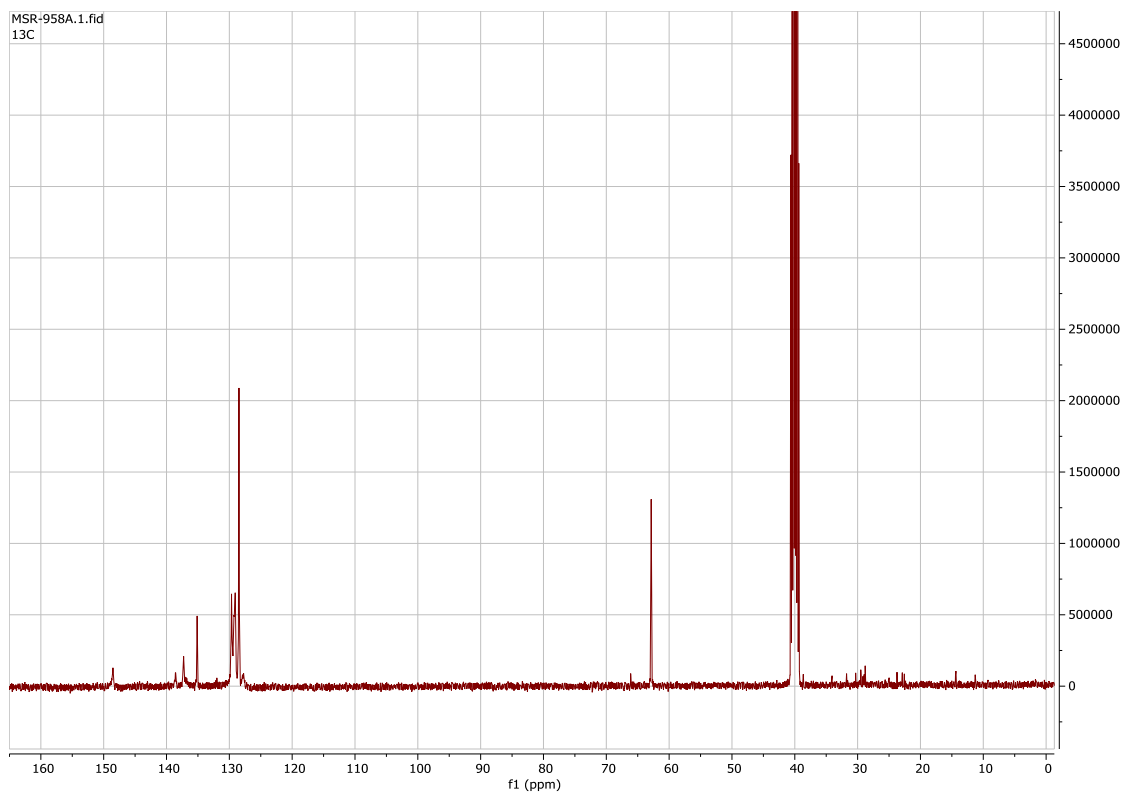
***N*-Phenyl-1*H*-1,2,3-triazole-4-carboxamide (86):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



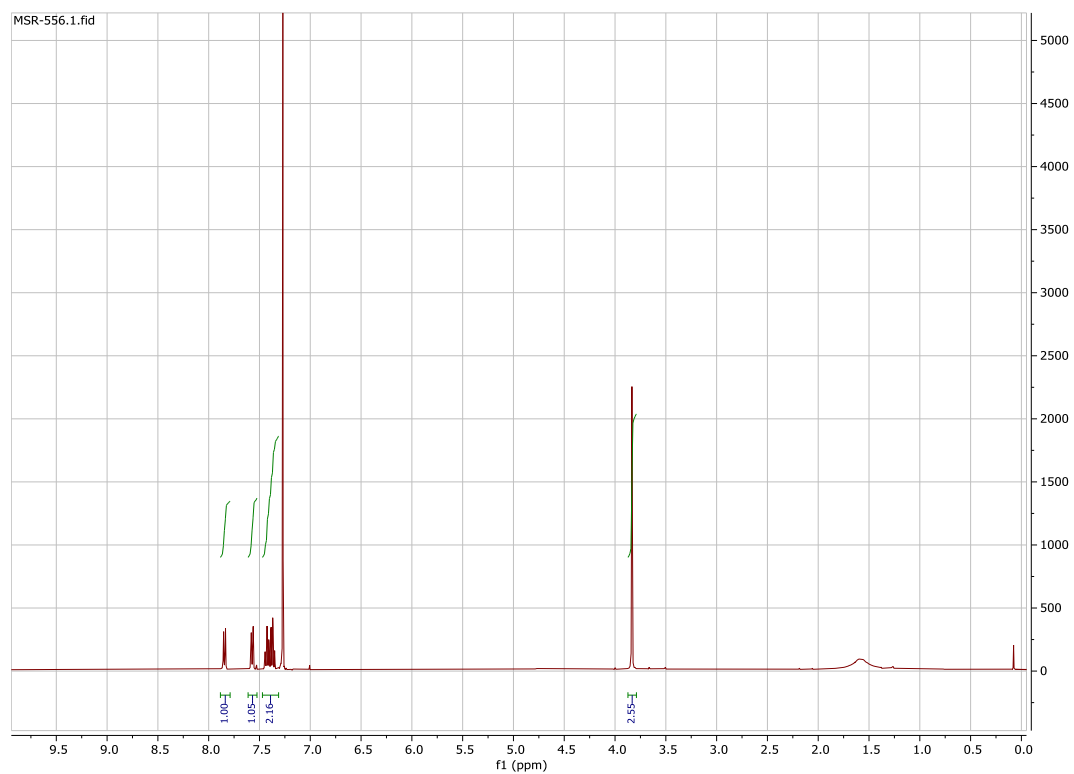
**Phenyl(1*H*-1,2,3-triazol-4-yl)methanone O-methyl oxime (87):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



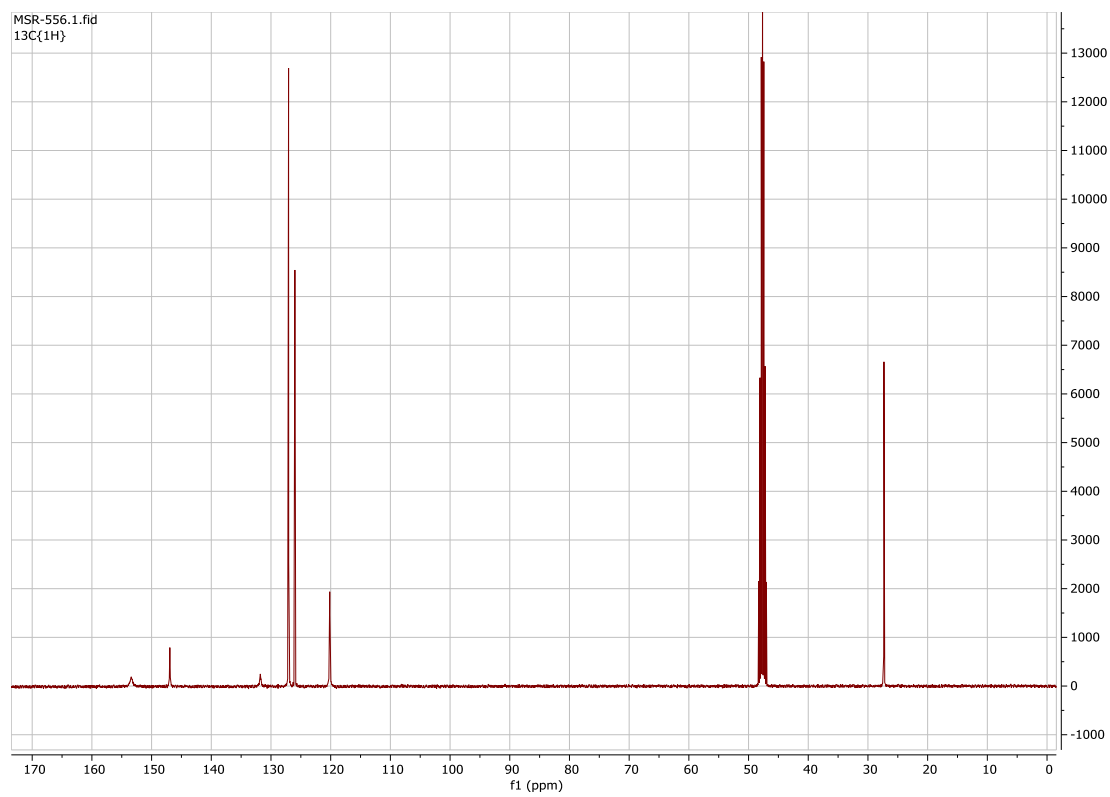
**Phenyl(1*H*-1,2,3-triazol-4-yl)methanone O-methyl oxime (87):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



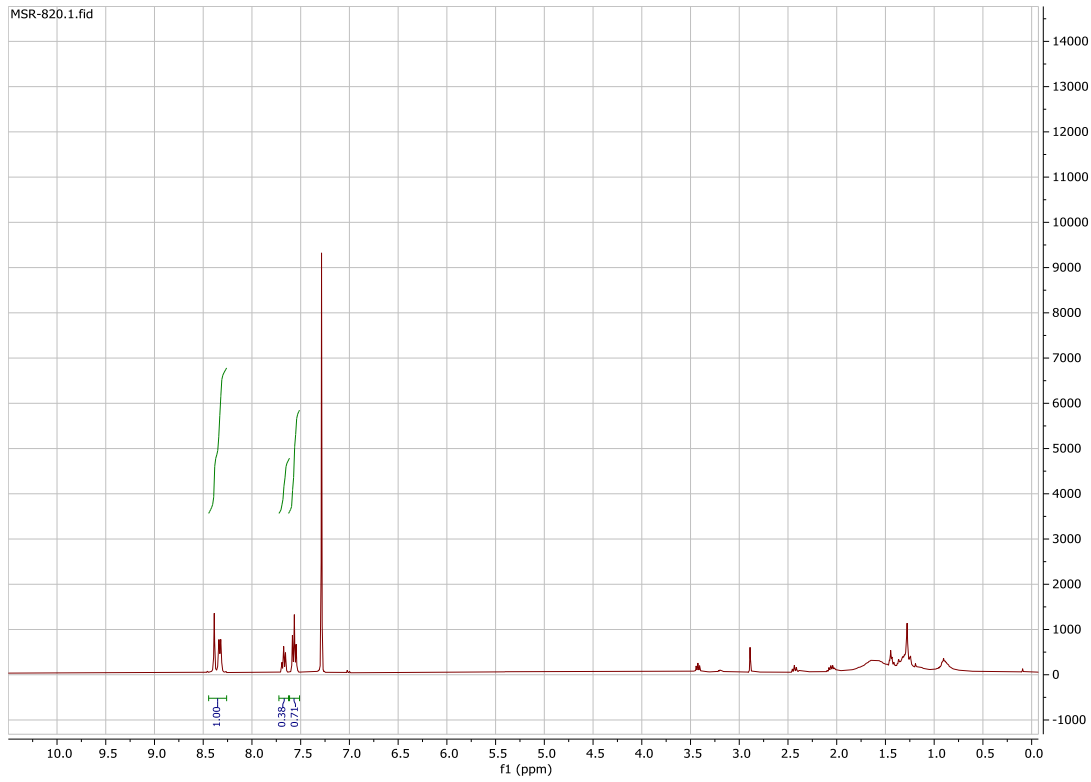
**3,8-Dihydroindeno[1,2-*d*][1,2,3]triazole (89):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



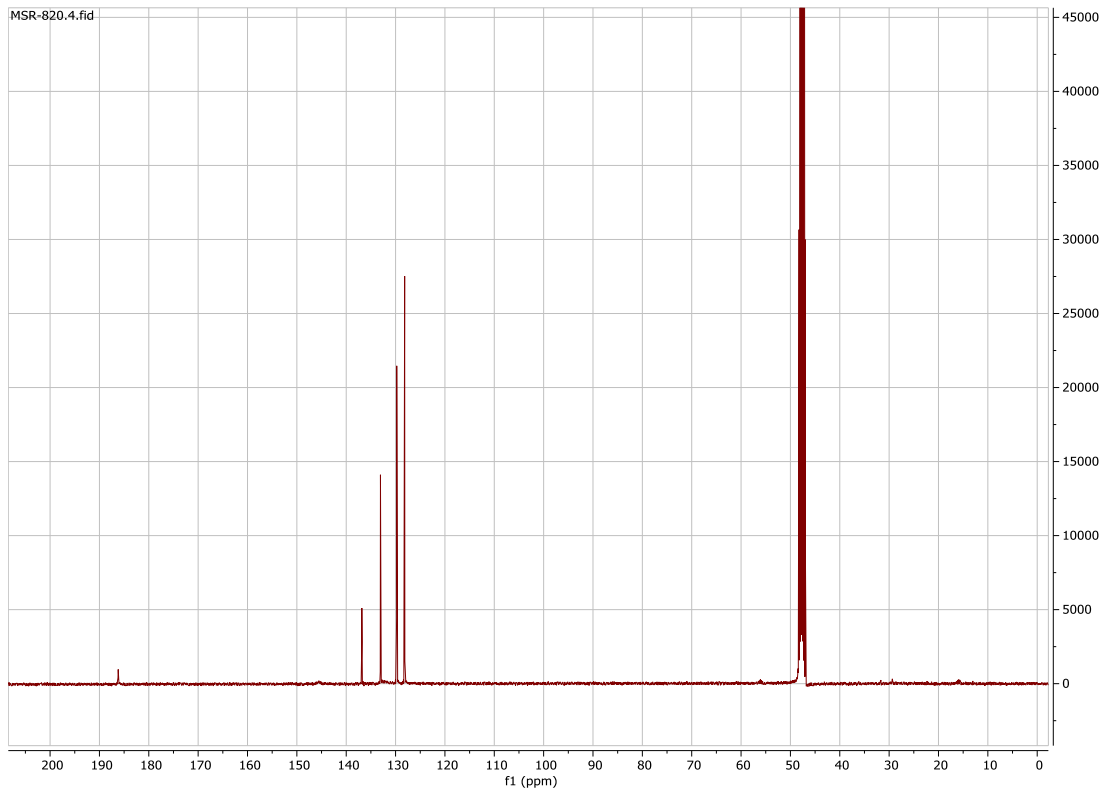
**3,8-Dihydroindeno[1,2-*d*][1,2,3]triazole (89):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



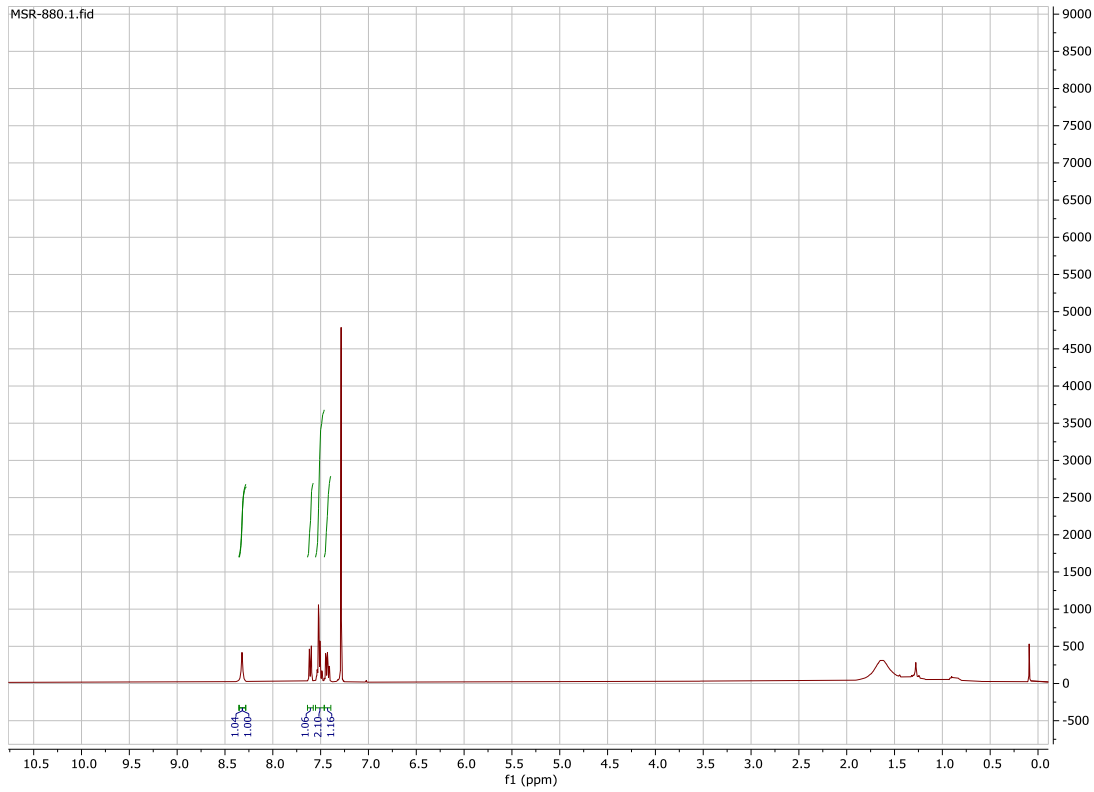
Phenyl(1*H*-1,2,3-triazol-5-yl)methanone (99): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



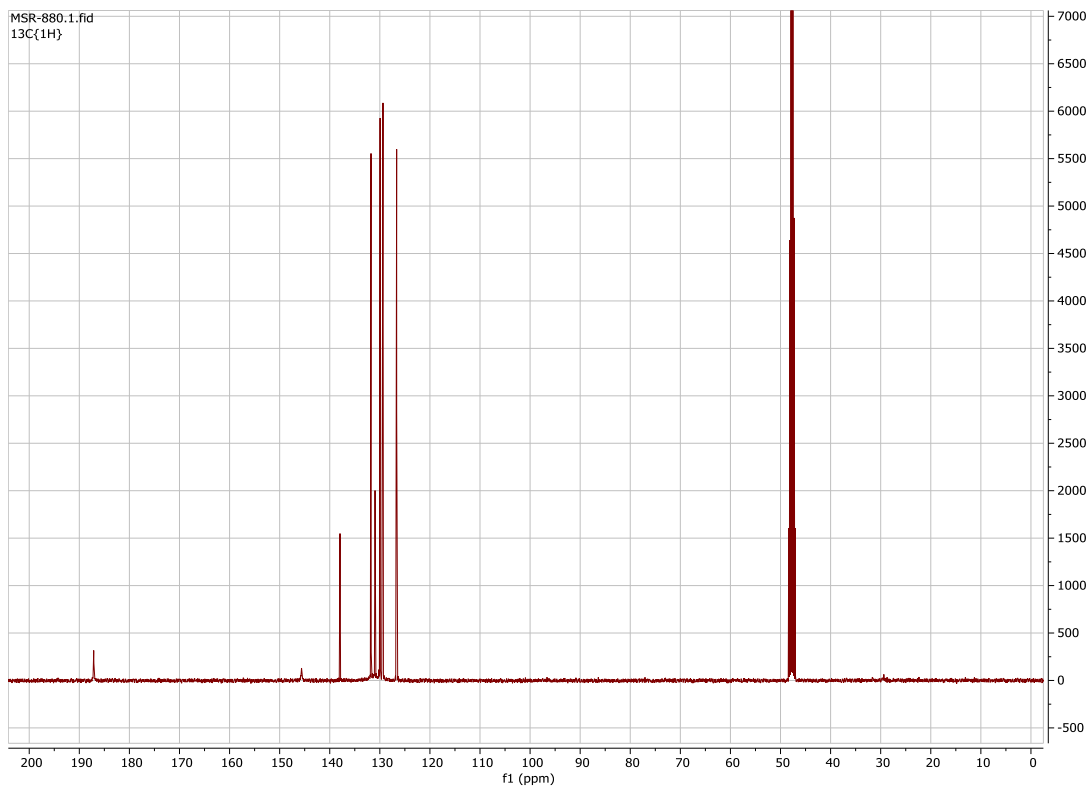
Phenyl(1*H*-1,2,3-triazol-5-yl)methanone (99): <sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)



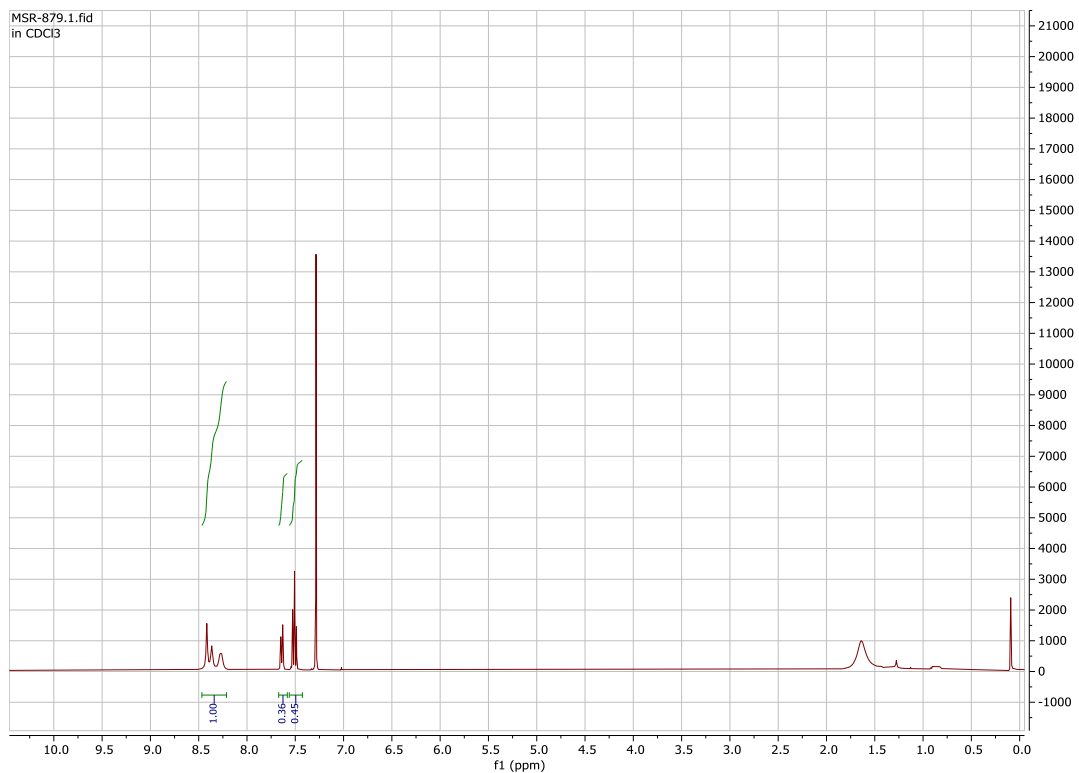
**(2-Chlorophenyl)(1H-1,2,3-triazol-5-yl)methanone (100):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



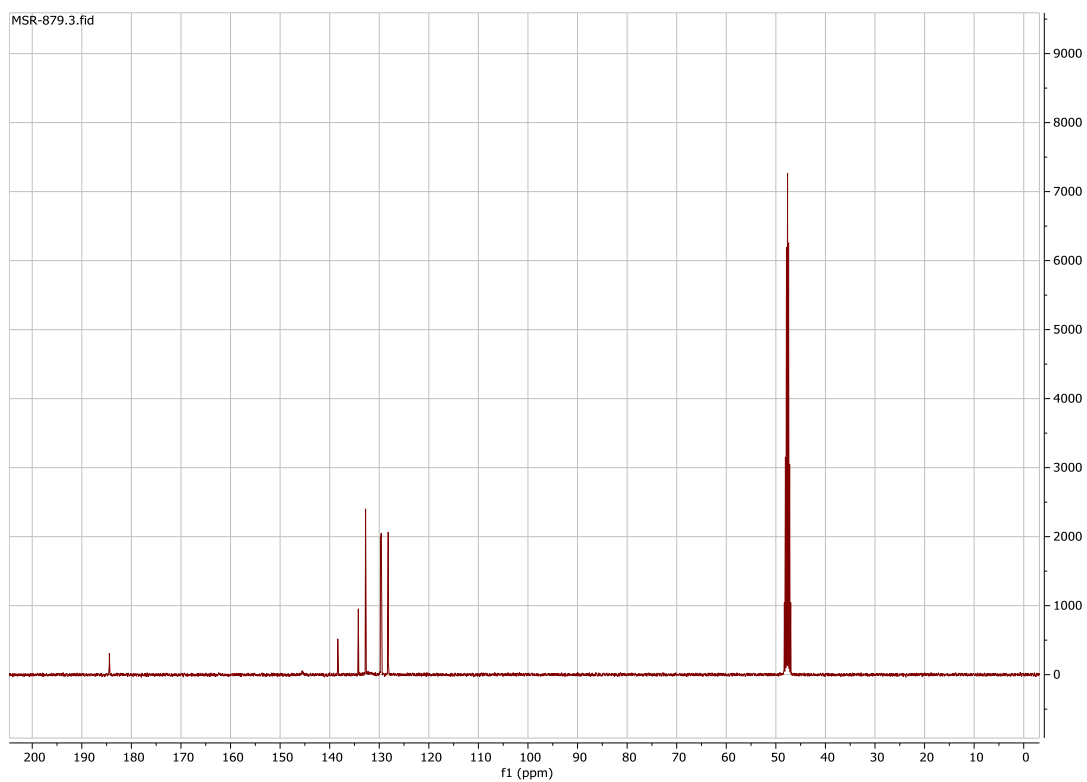
**(2-Chlorophenyl)(1H-1,2,3-triazol-5-yl)methanone (100):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



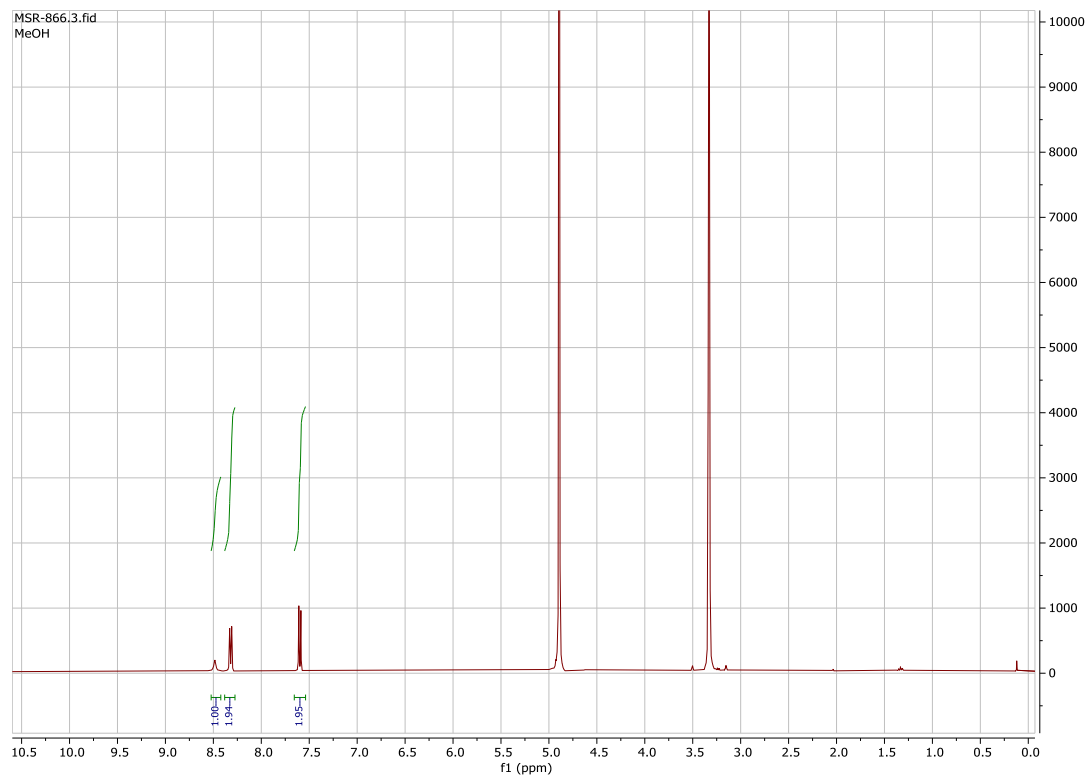
**(3-Chlorophenyl)(1H-1,2,3-triazol-5-yl)methanone (101):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



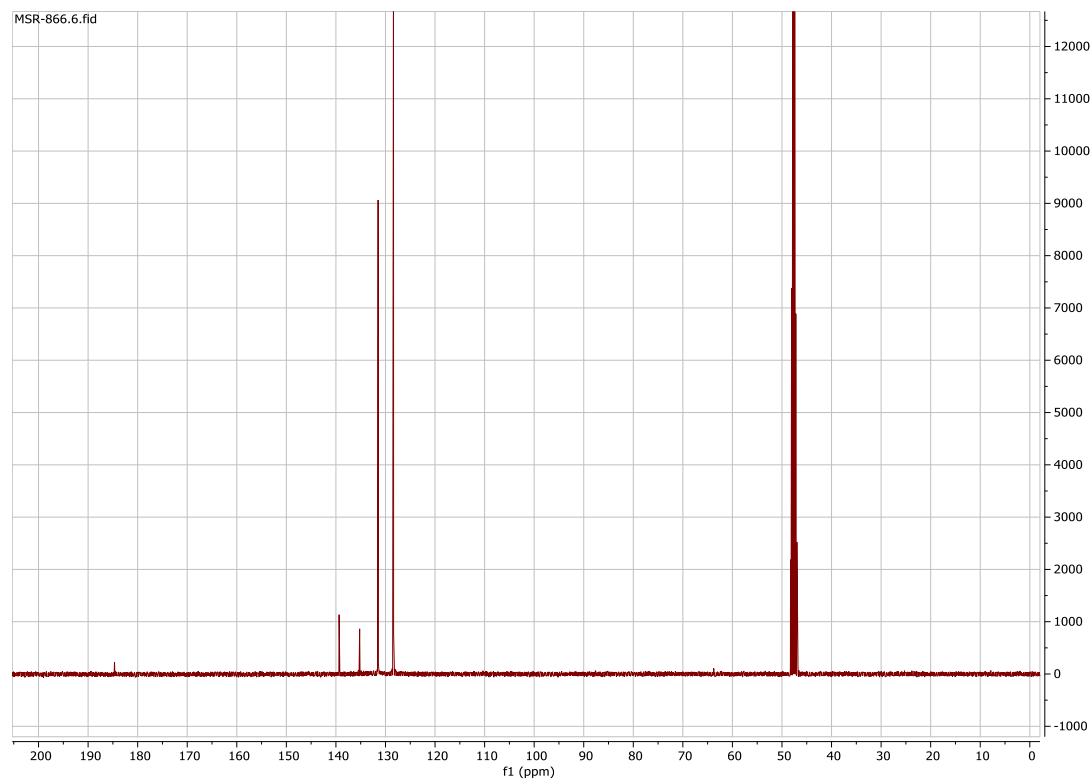
**(3-Chlorophenyl)(1H-1,2,3-triazol-5-yl)methanone (101):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



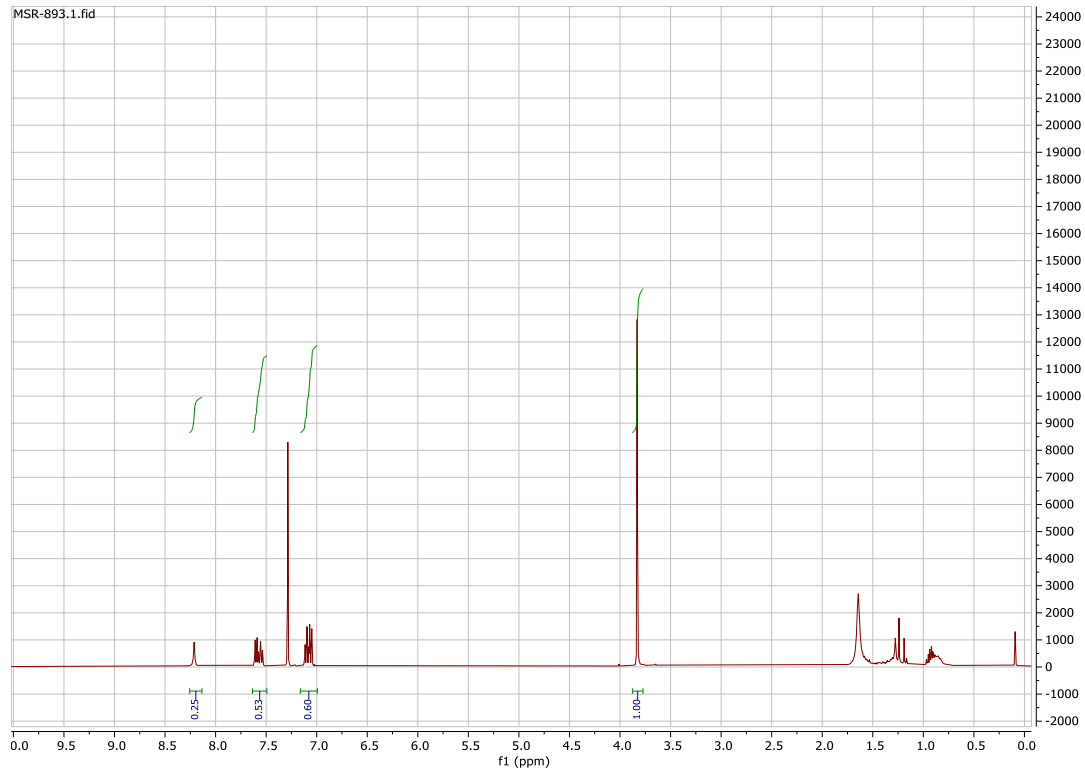
**(4-Chlorophenyl)(1H-1,2,3-triazol-5-yl)methanone (102):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



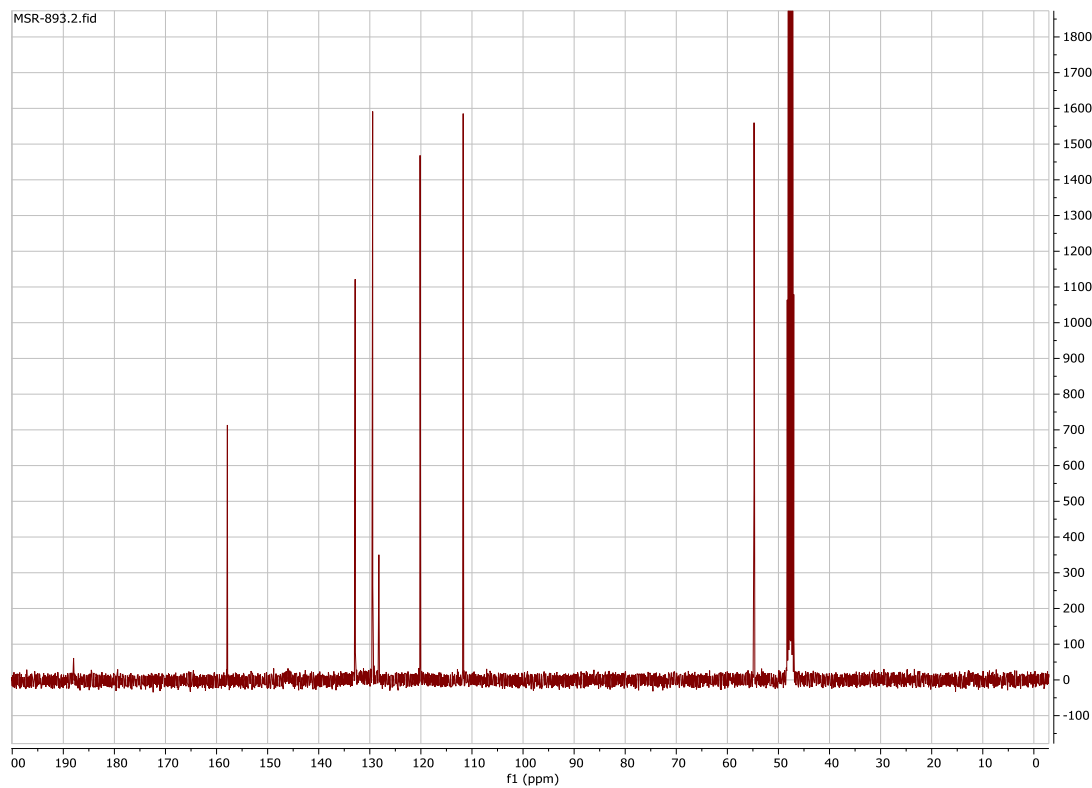
**(4-Chlorophenyl)(1H-1,2,3-triazol-5-yl)methanone (102):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**(2-Methoxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (103):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**

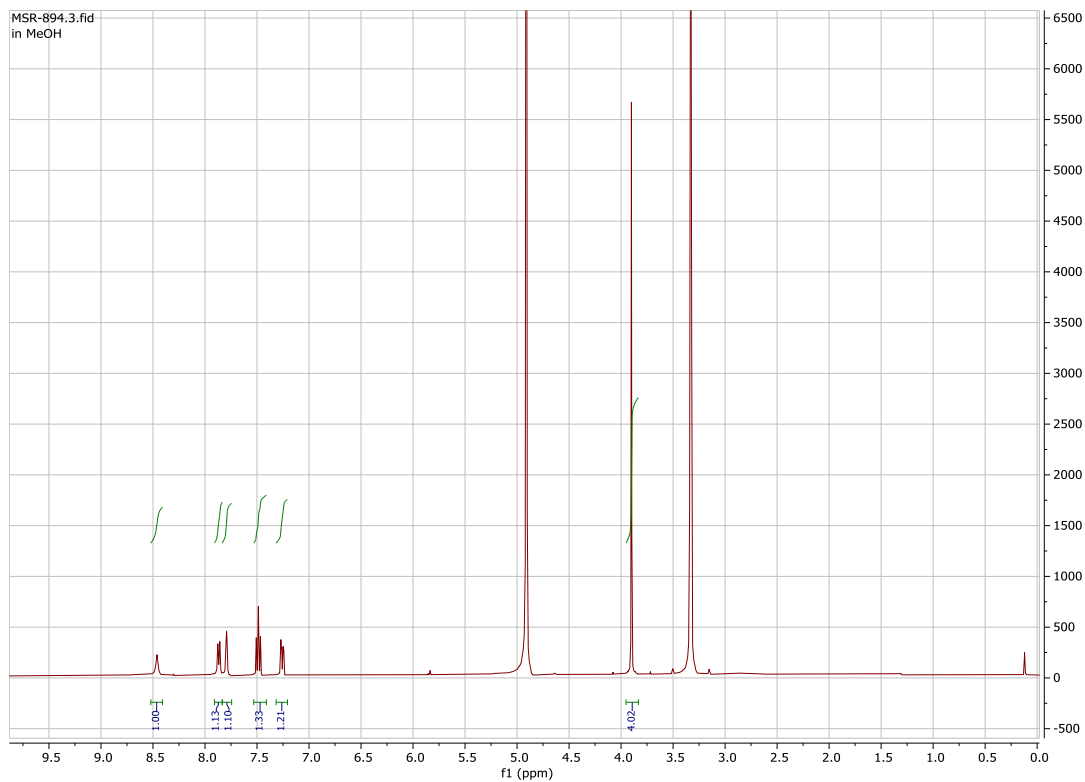


**(2-Methoxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (103):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

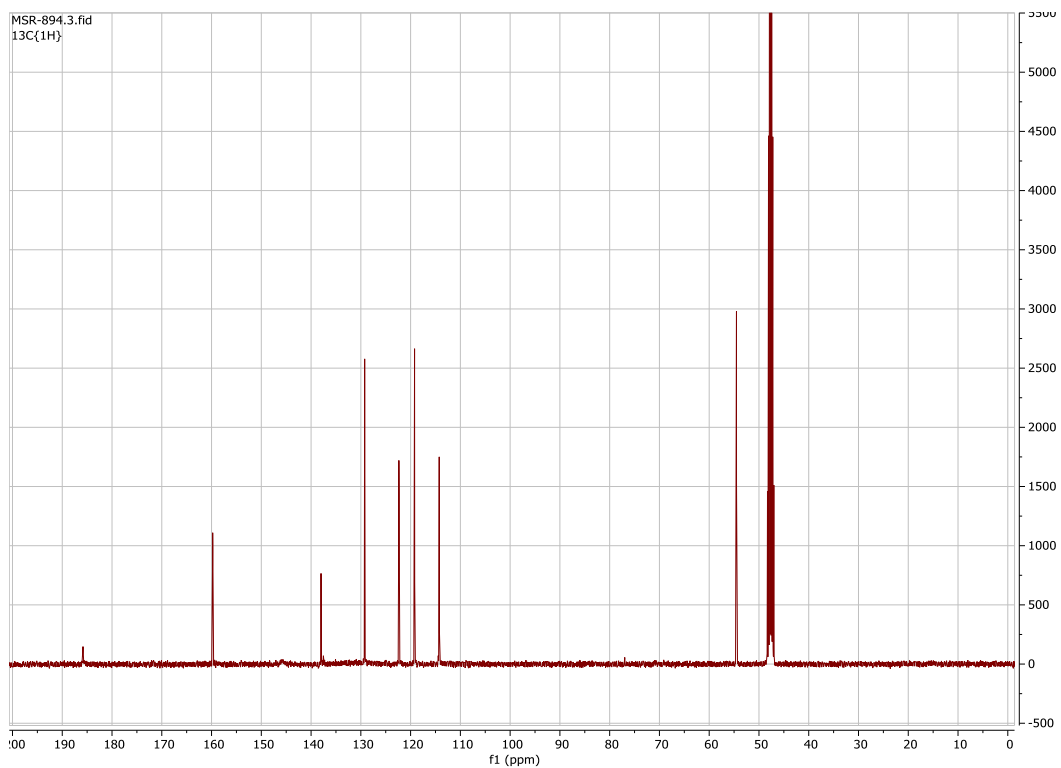




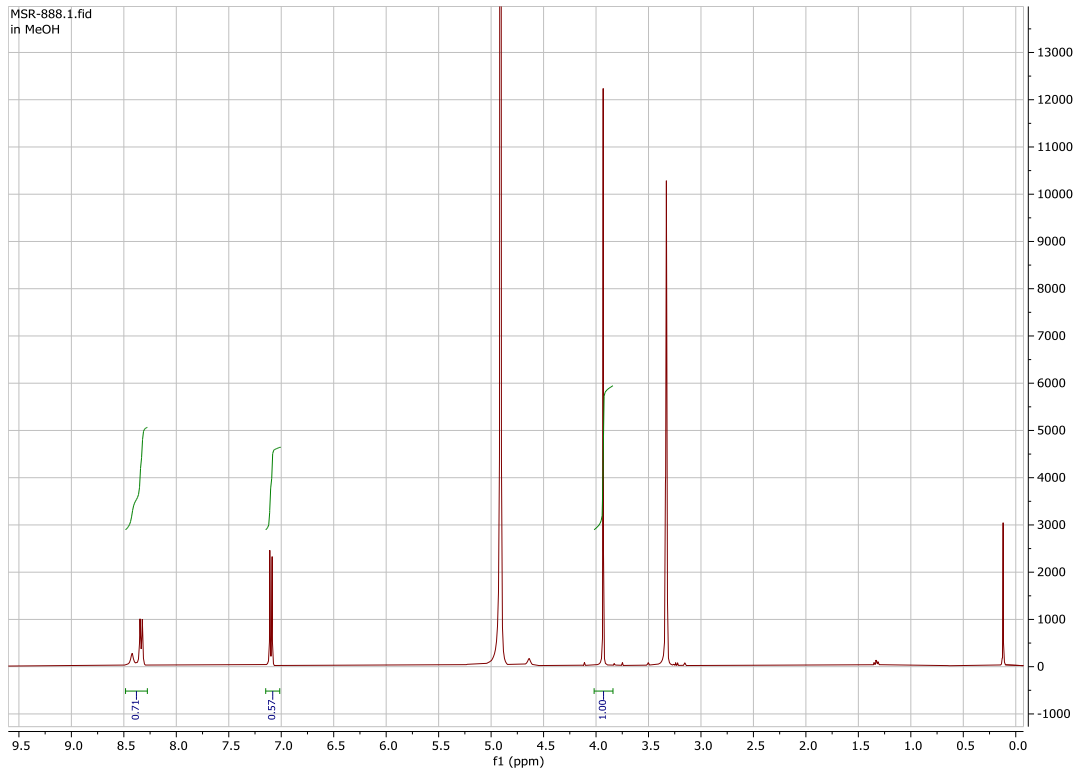
**(3-Methoxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (104):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



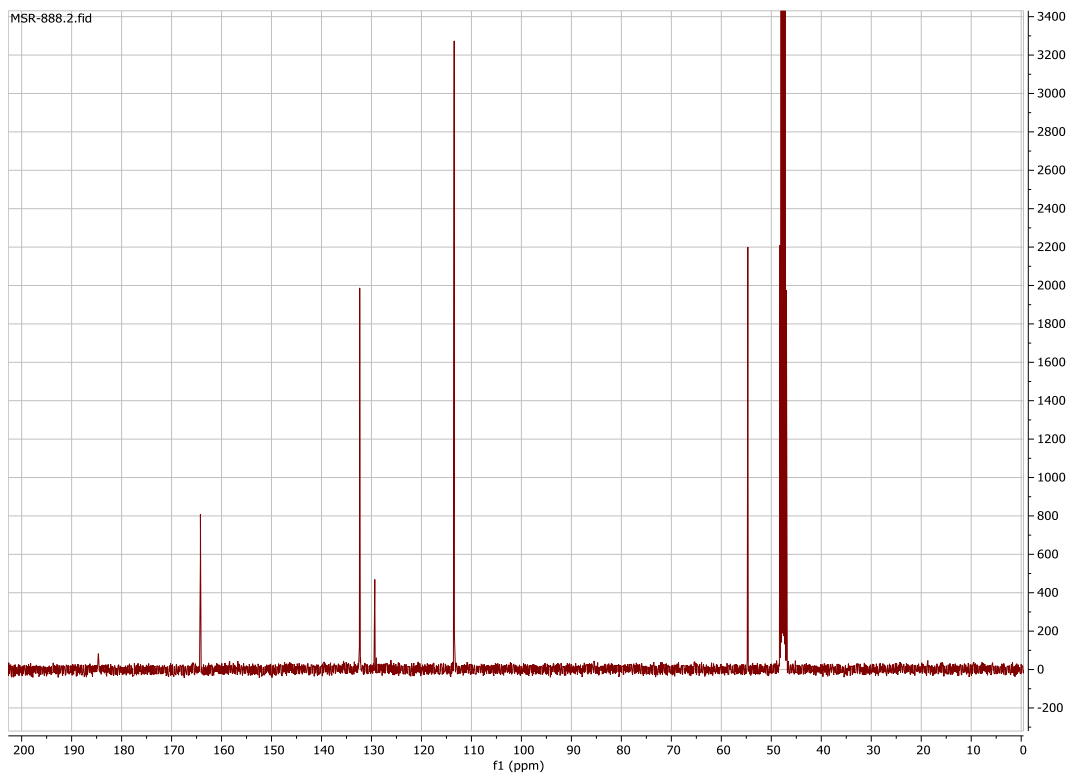
**(3-Methoxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (104):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



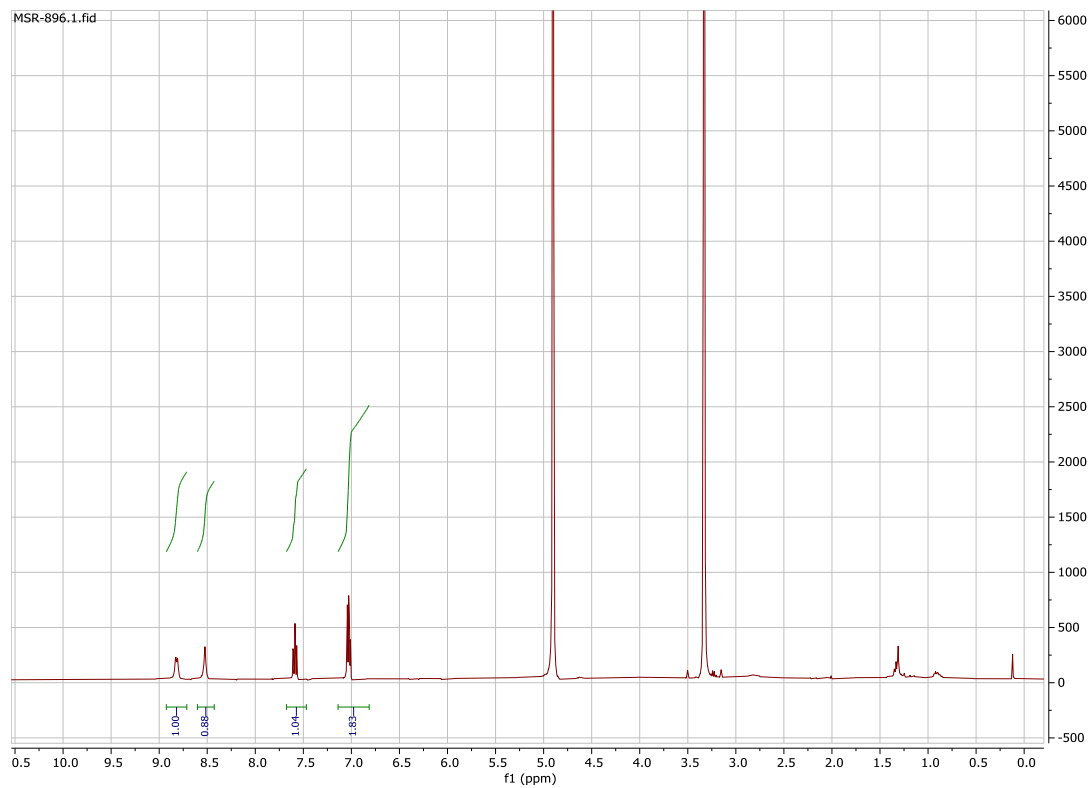
**(4-Methoxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (105):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



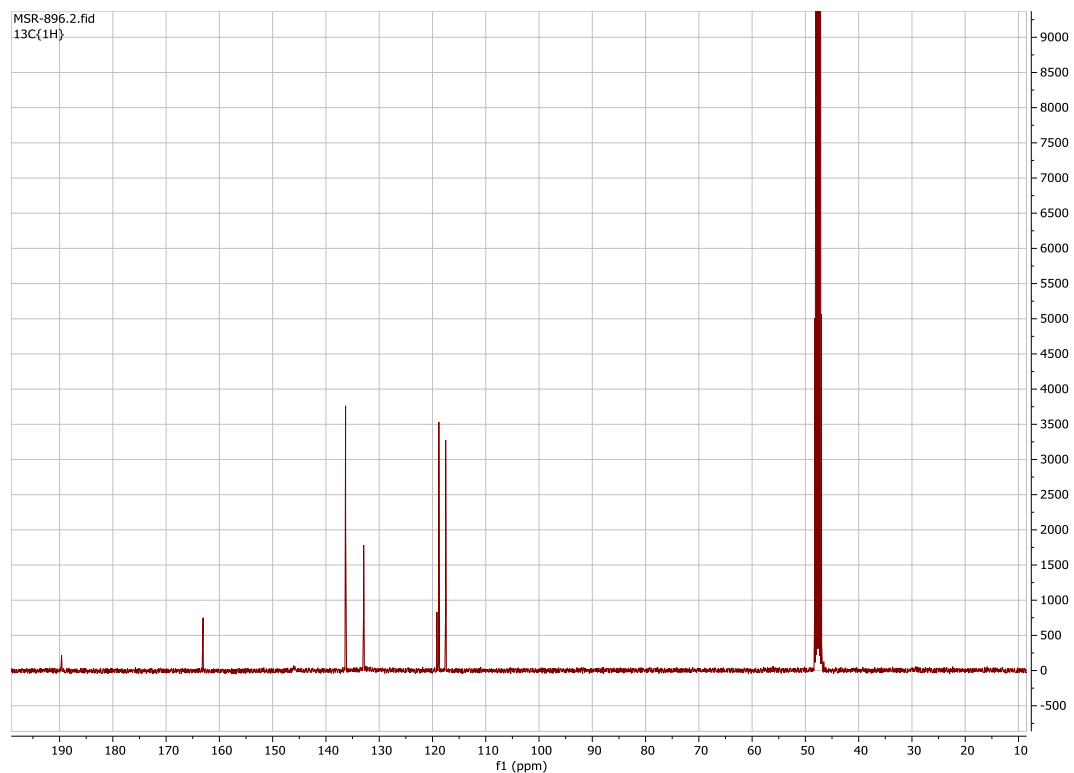
**(4-Methoxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (105):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



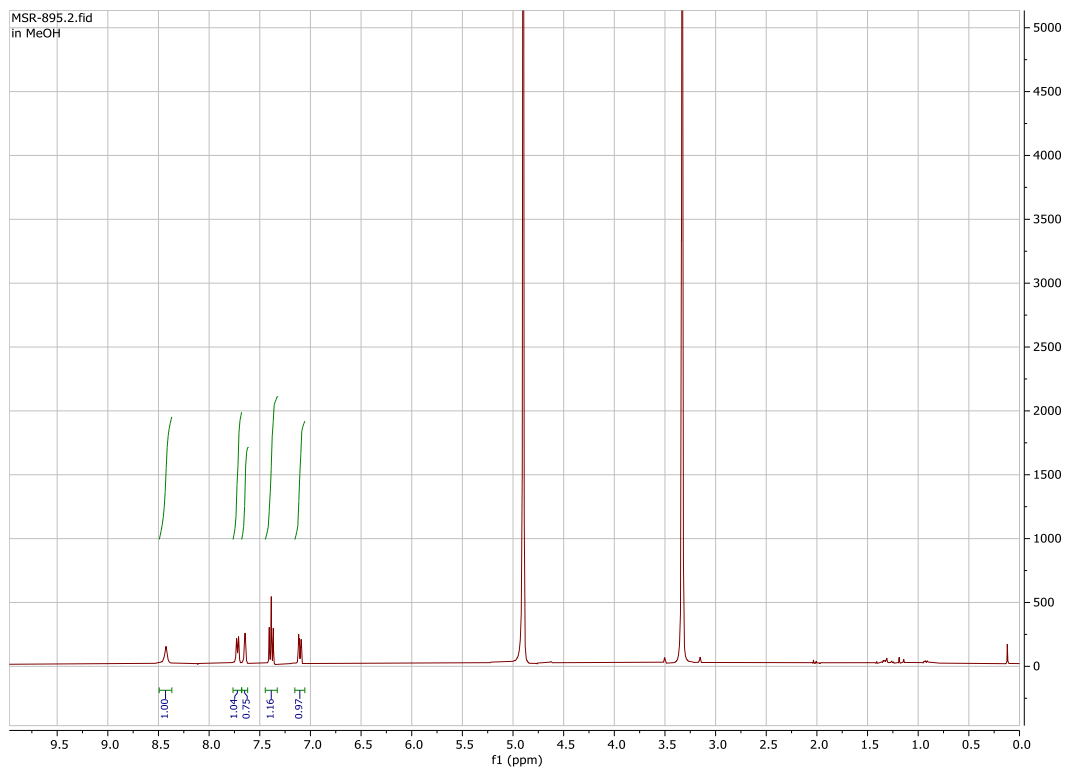
**(2-Hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (106):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



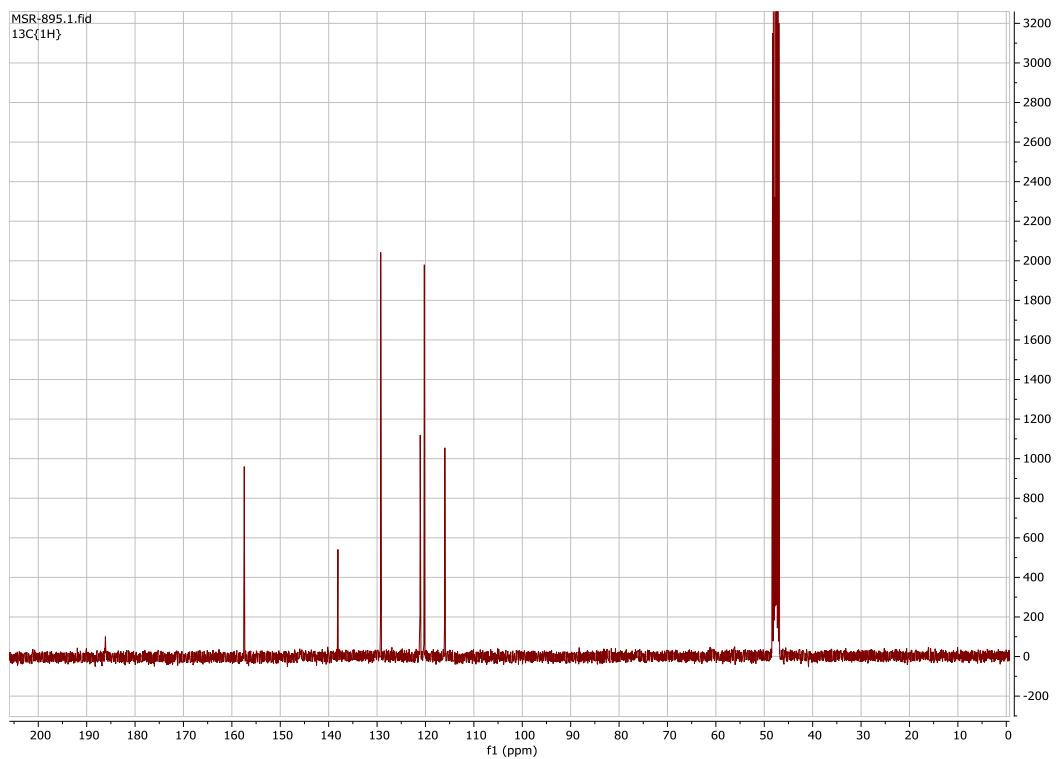
**(2-Hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (106):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



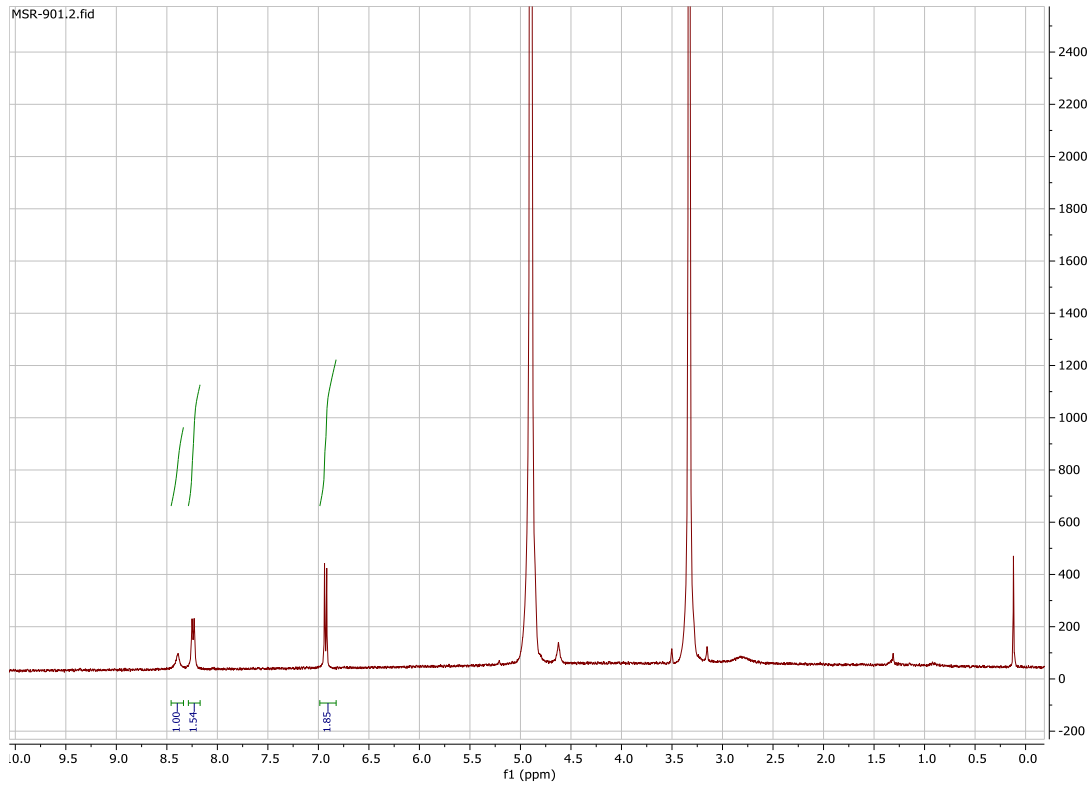
**(3-Hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (107):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



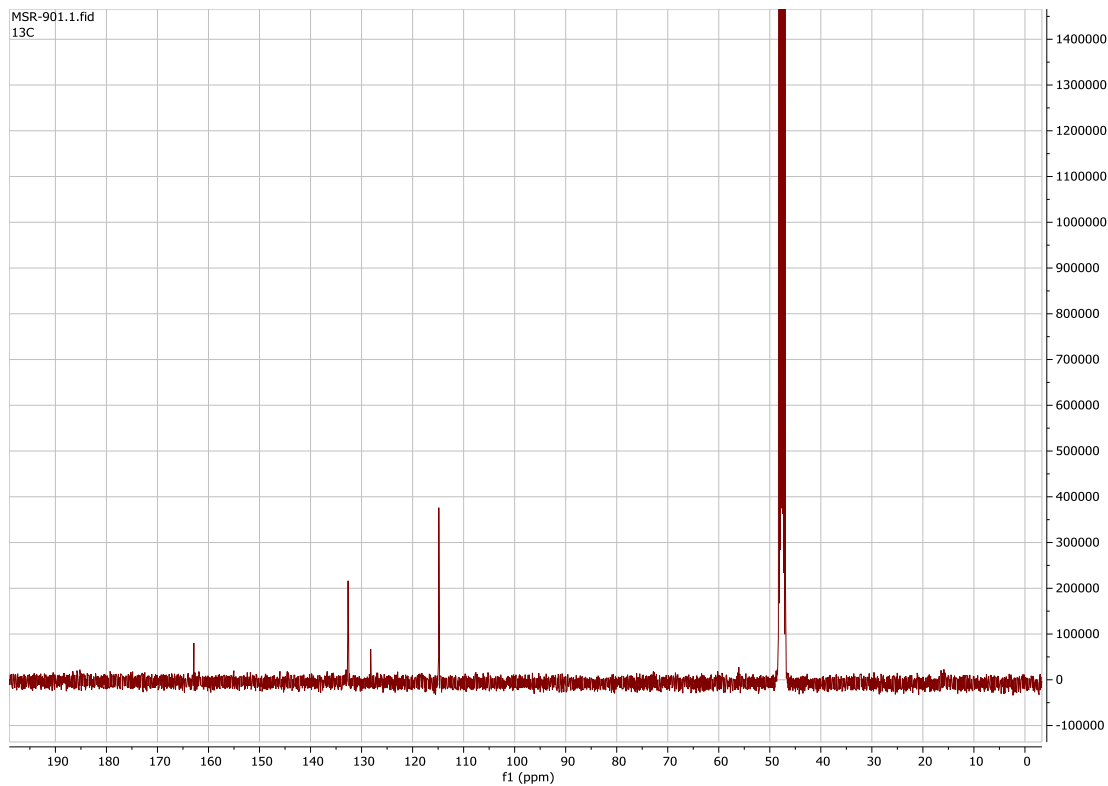
**(3-Hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (107):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



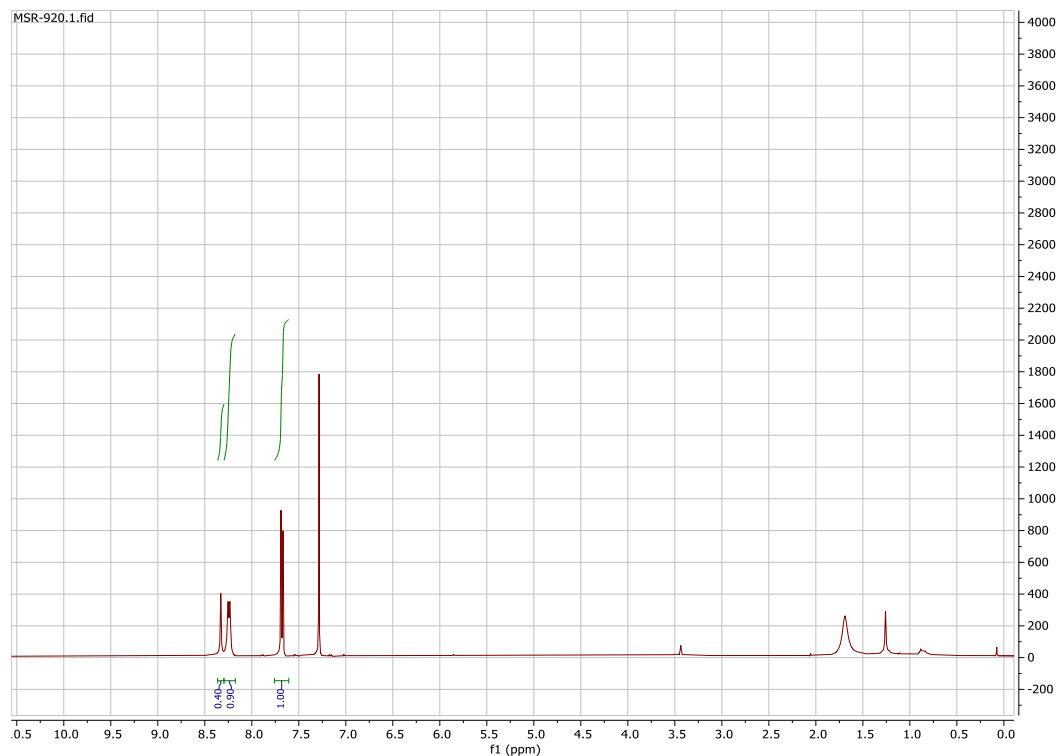
**(4-Hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (108):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



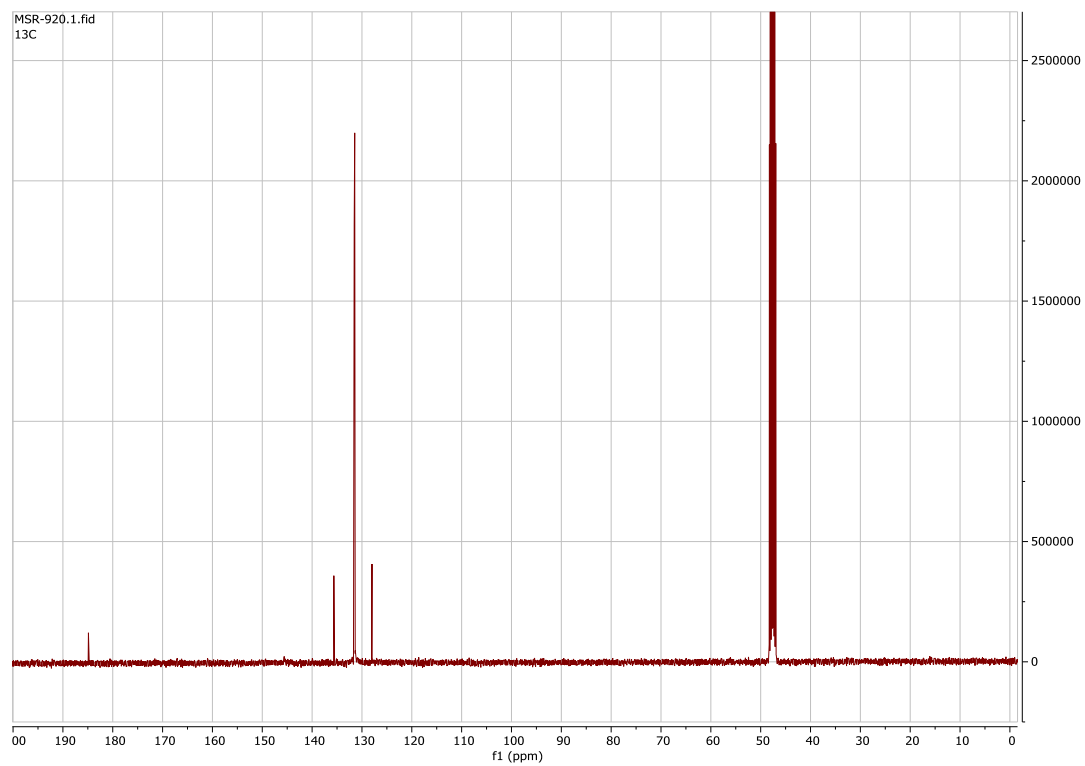
**(4-Hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (108):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



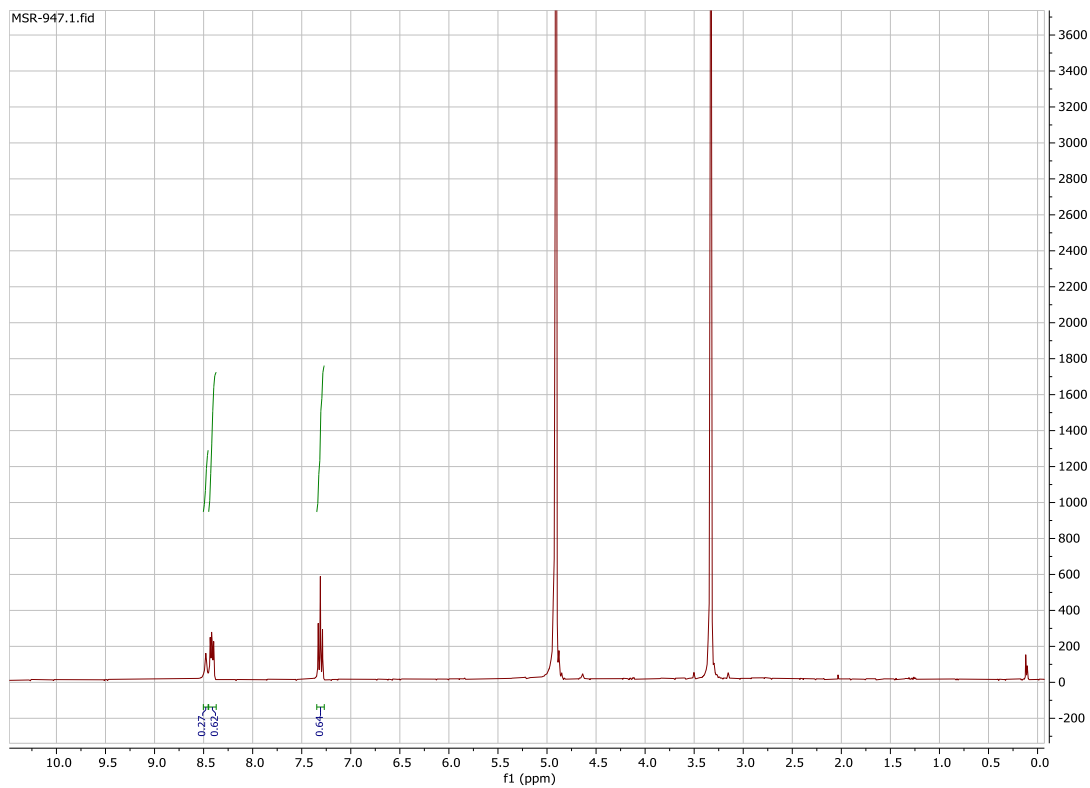
**(4-Bromophenyl)(1H-1,2,3-triazol-5-yl)methanone (109):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



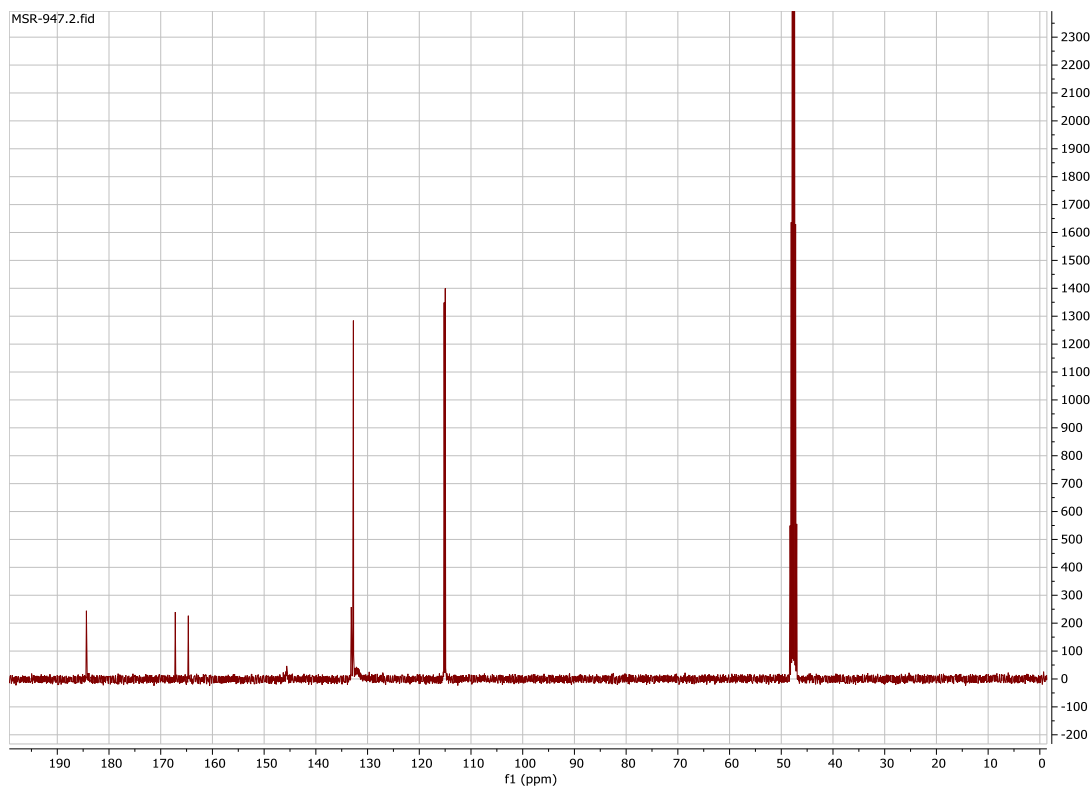
**(4-Bromophenyl)(1H-1,2,3-triazol-5-yl)methanone (109):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



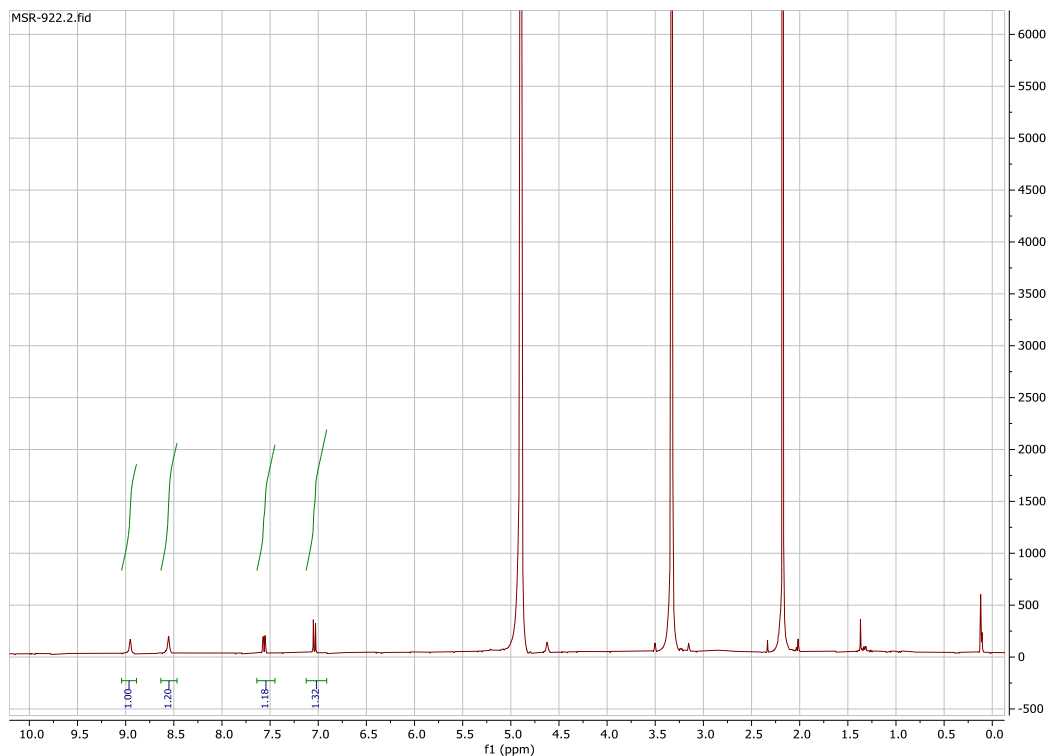
**(4-Fluorophenyl)(1H-1,2,3-triazol-5-yl)methanone (110):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



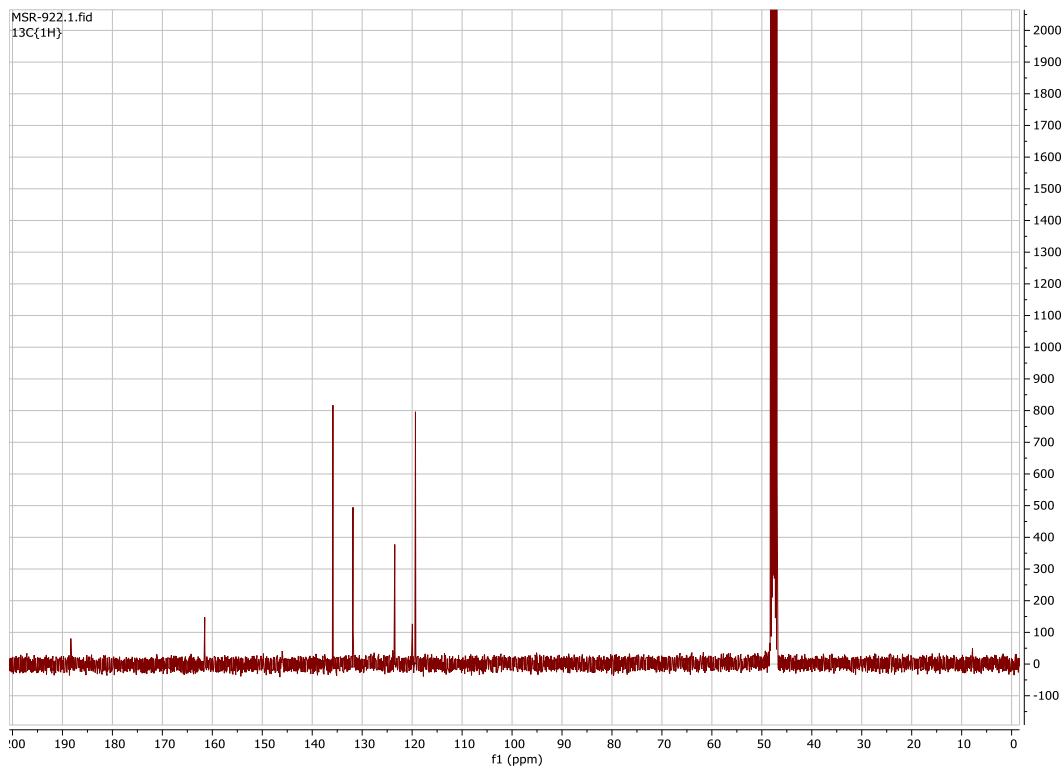
**(4-Fluorophenyl)(1H-1,2,3-triazol-5-yl)methanone (110):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**(5-Chloro-2-hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (111):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

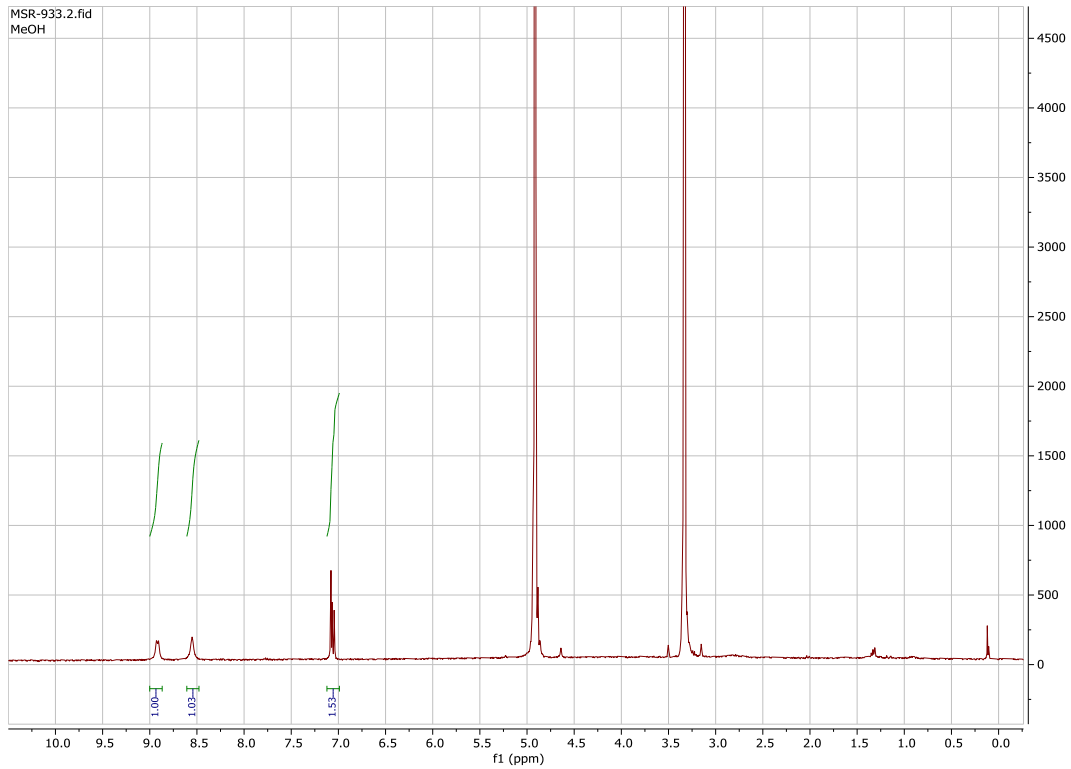


**(5-Chloro-2-hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (111):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

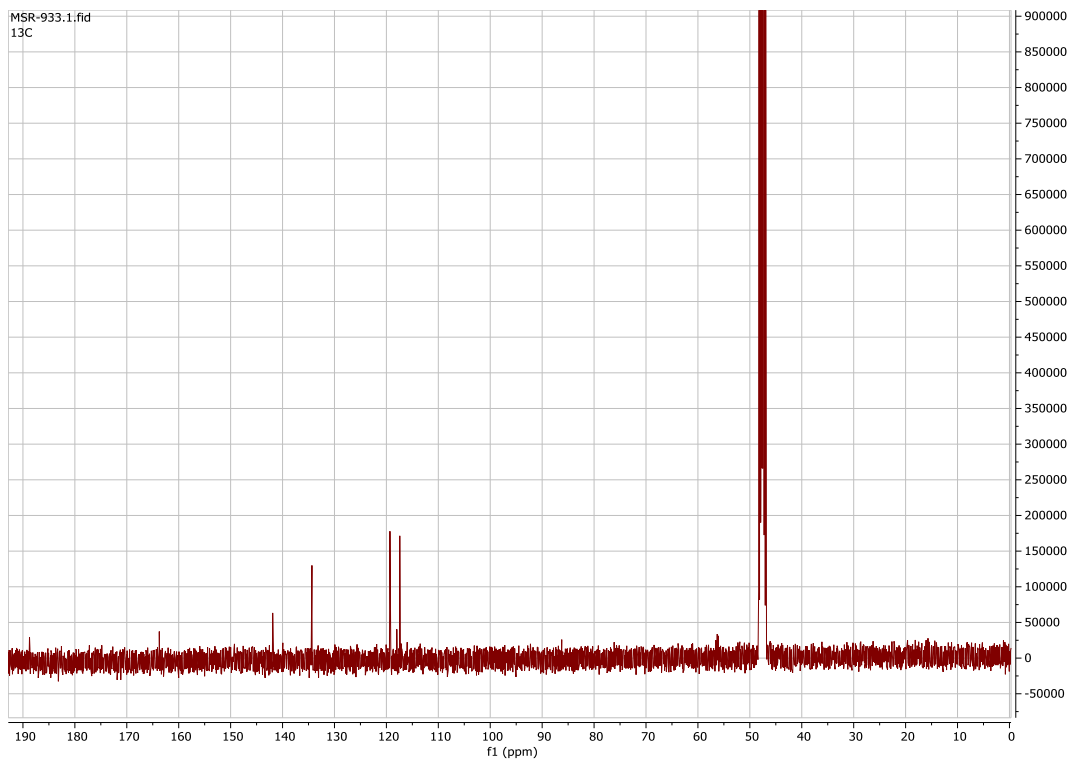




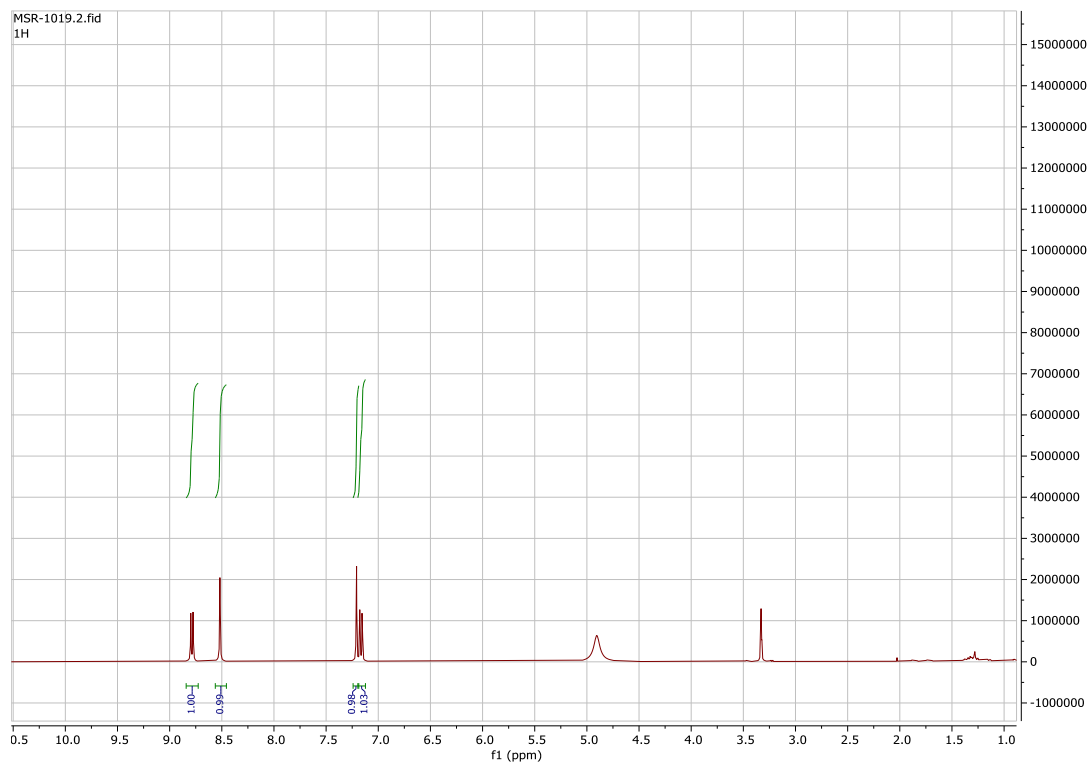
**(4-Chloro-2-hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (112):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



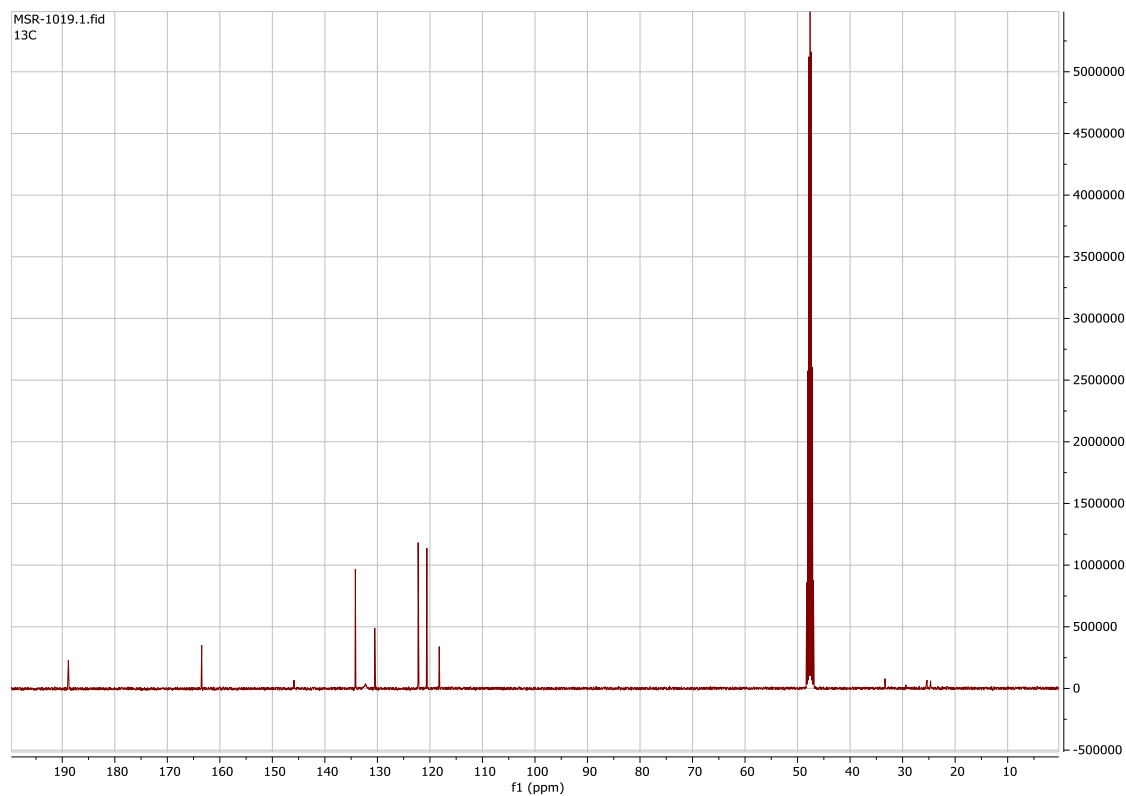
**(4-Chloro-2-hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (112):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



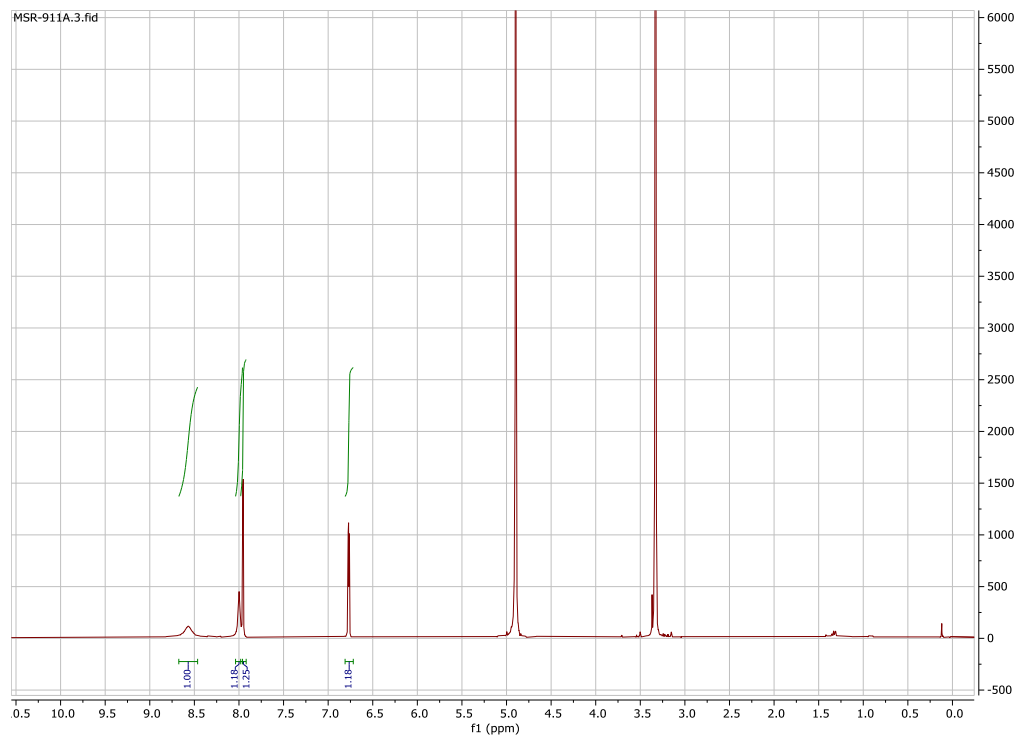
**(4-Bromo-2-hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (113):**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ )



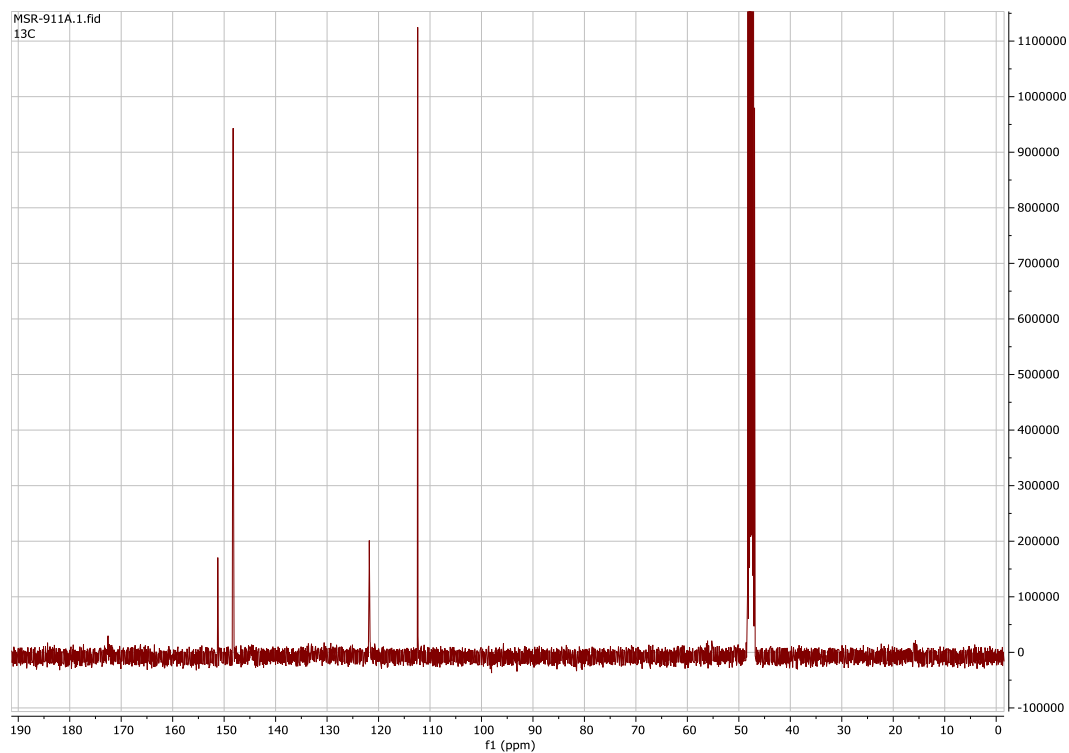
**(4-Bromo-2-hydroxyphenyl)(1H-1,2,3-triazol-5-yl)methanone (113):**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )



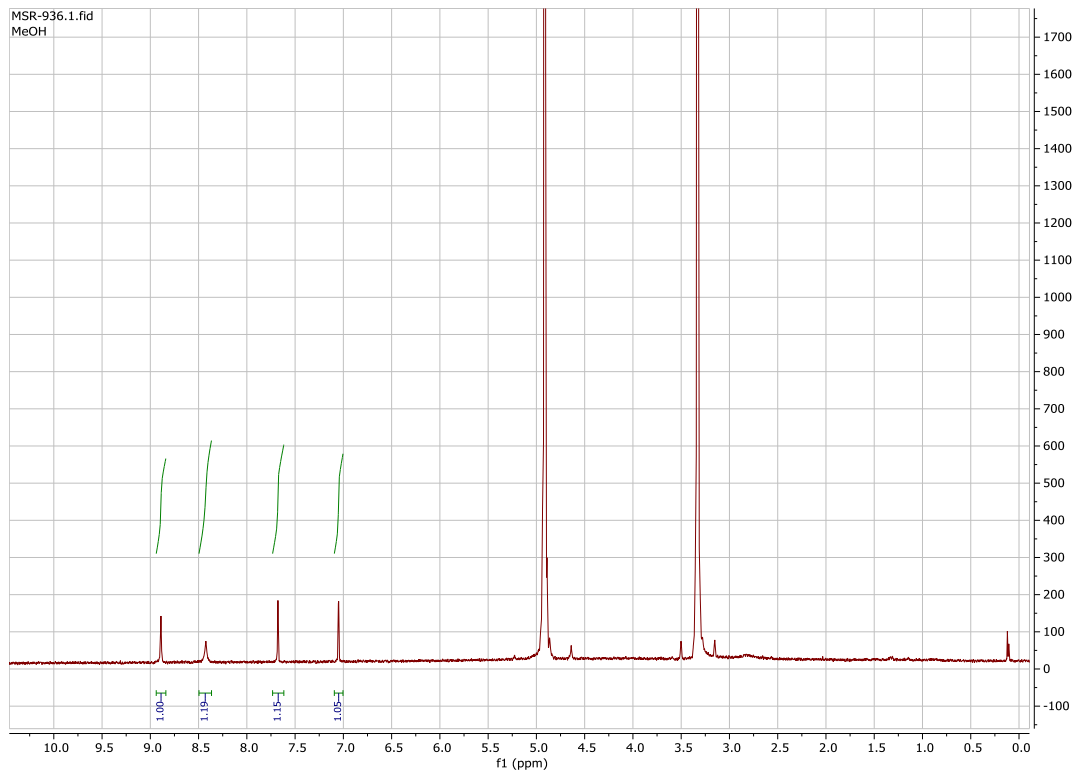
**Furan-2-yl(1H-1,2,3-triazol-5-yl)methanone (114):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



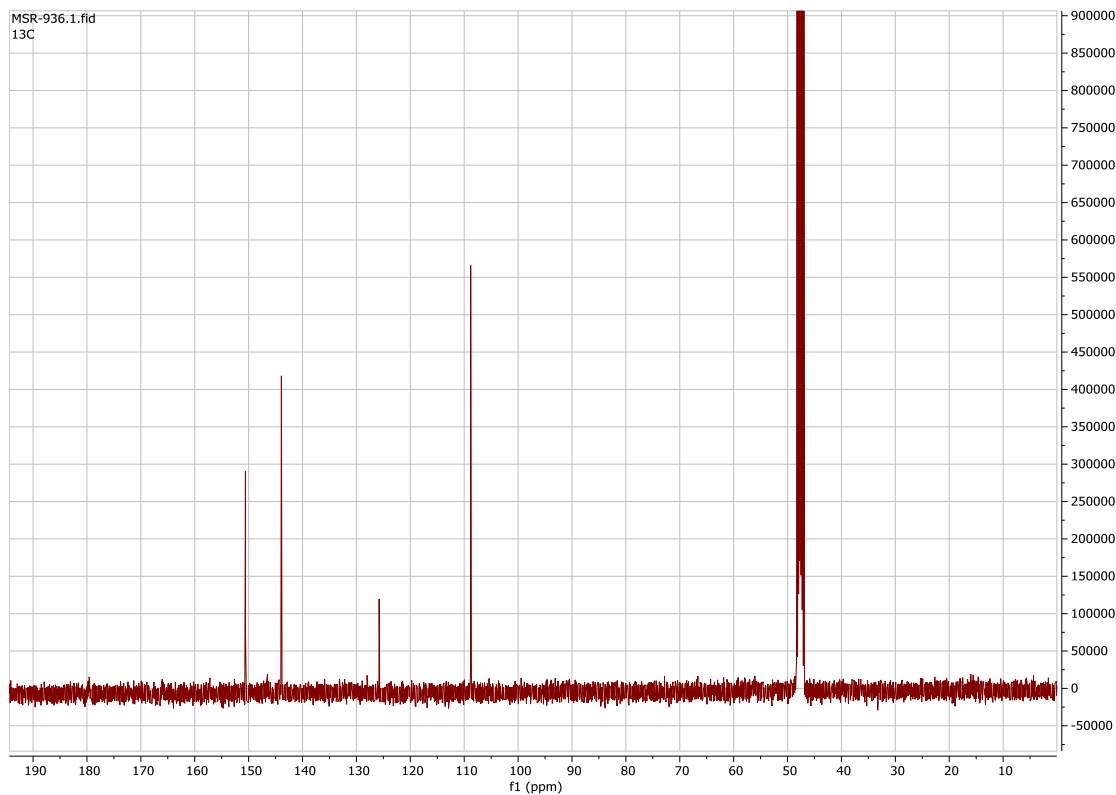
**Furan-2-yl(1H-1,2,3-triazol-5-yl)methanone (114):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



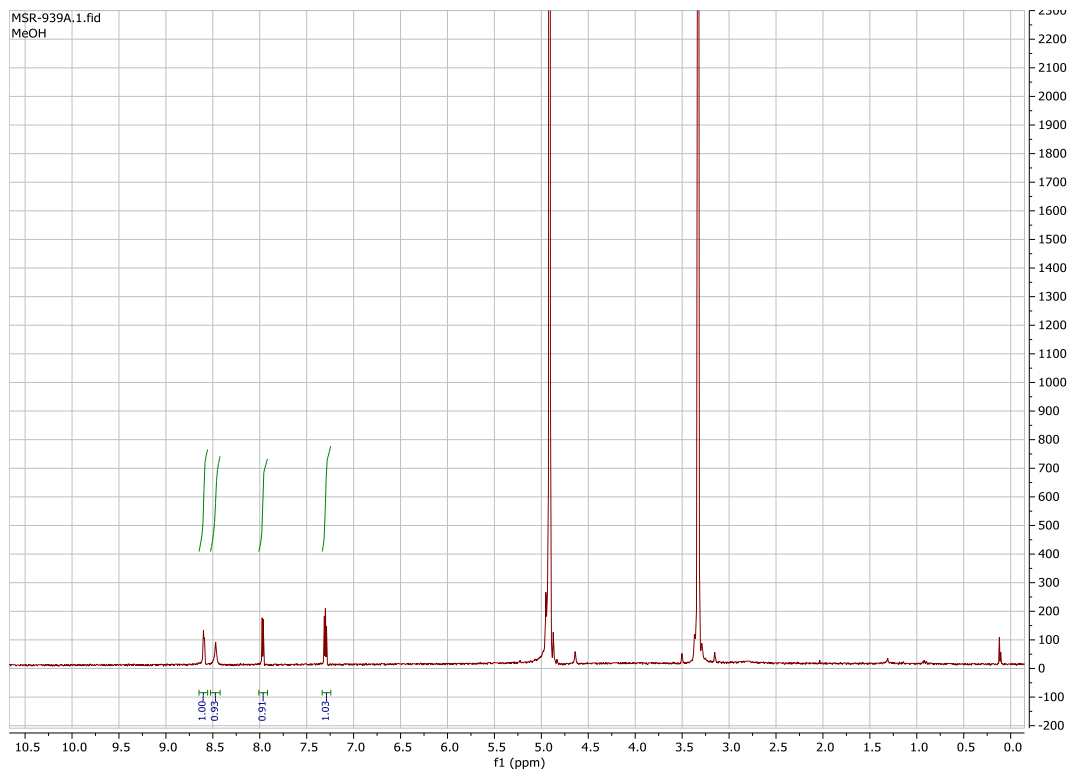
Furan-3-yl(1H-1,2,3-triazol-5-yl)methanone (115):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)



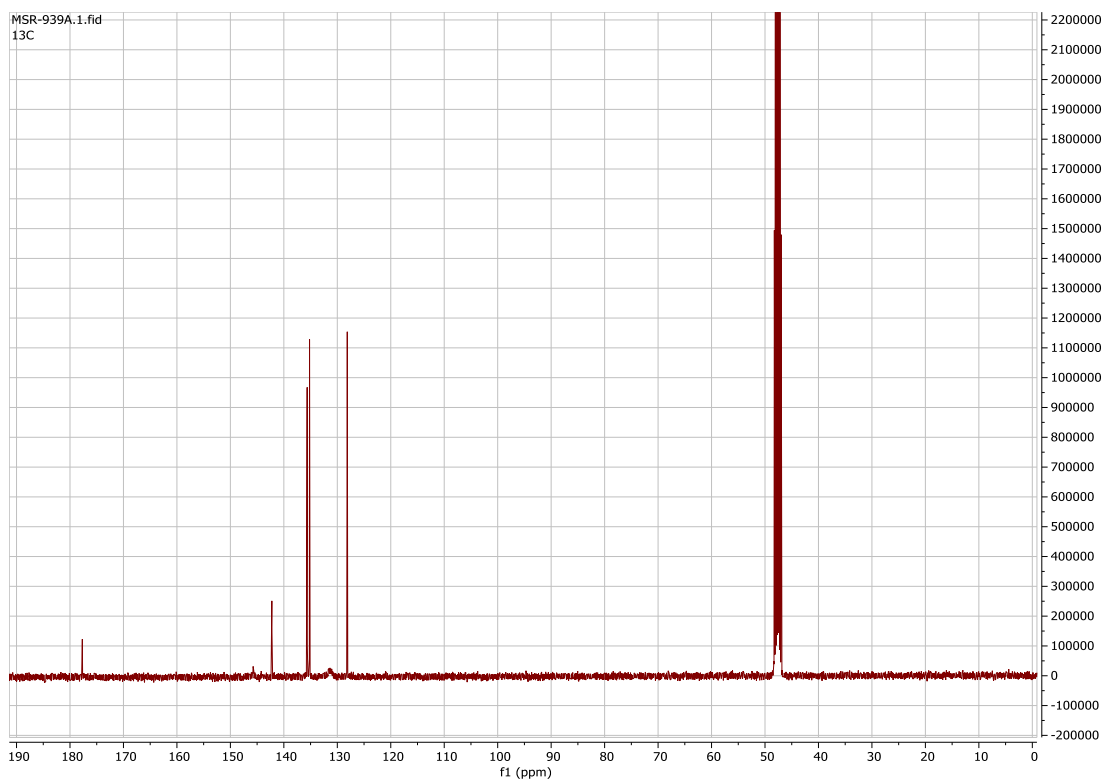
Furan-3-yl(1H-1,2,3-triazol-5-yl)methanone (115):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)



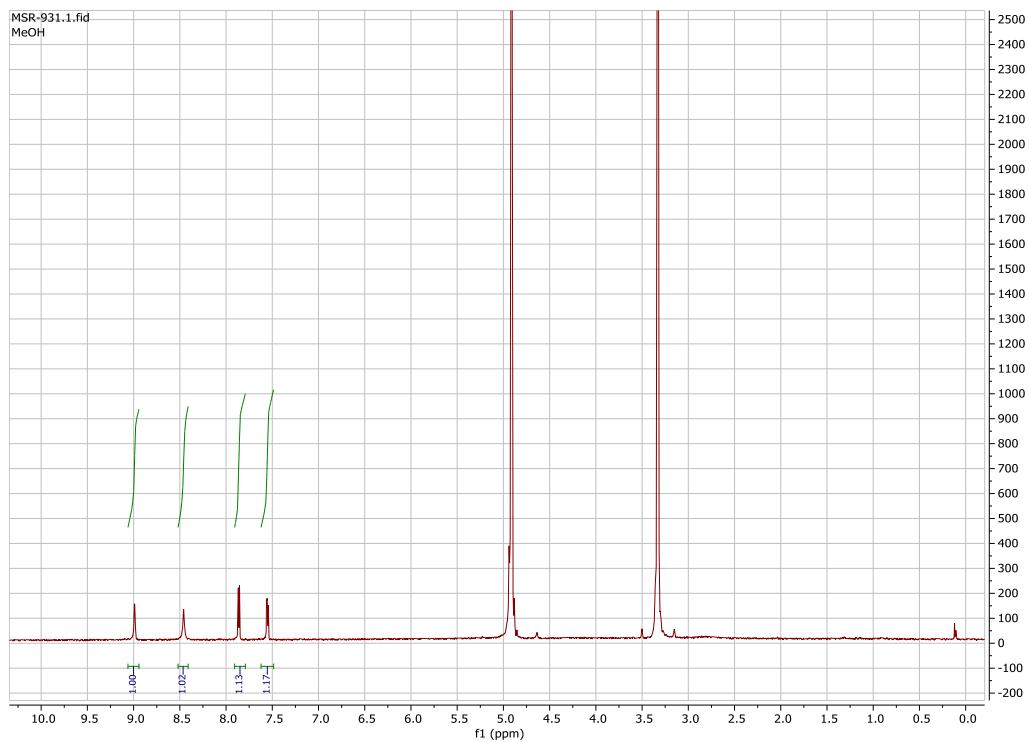
Thiophen-2-yl(1H-1,2,3-triazol-5-yl)methanone (116):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)



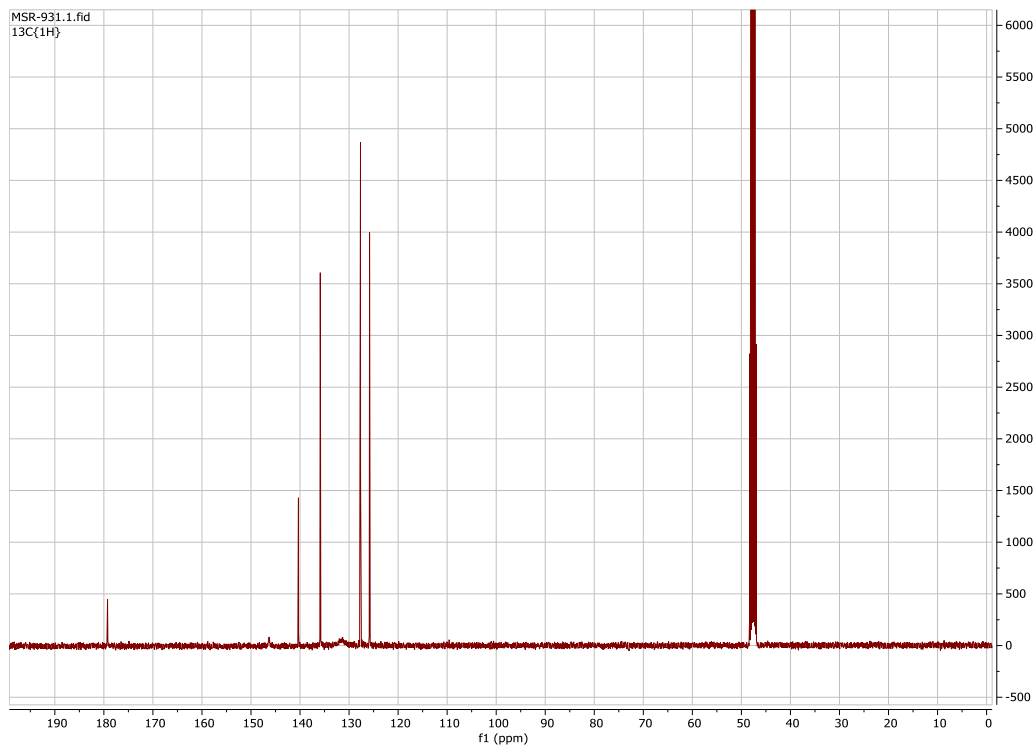
Thiophen-2-yl(1H-1,2,3-triazol-5-yl)methanone (116):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)



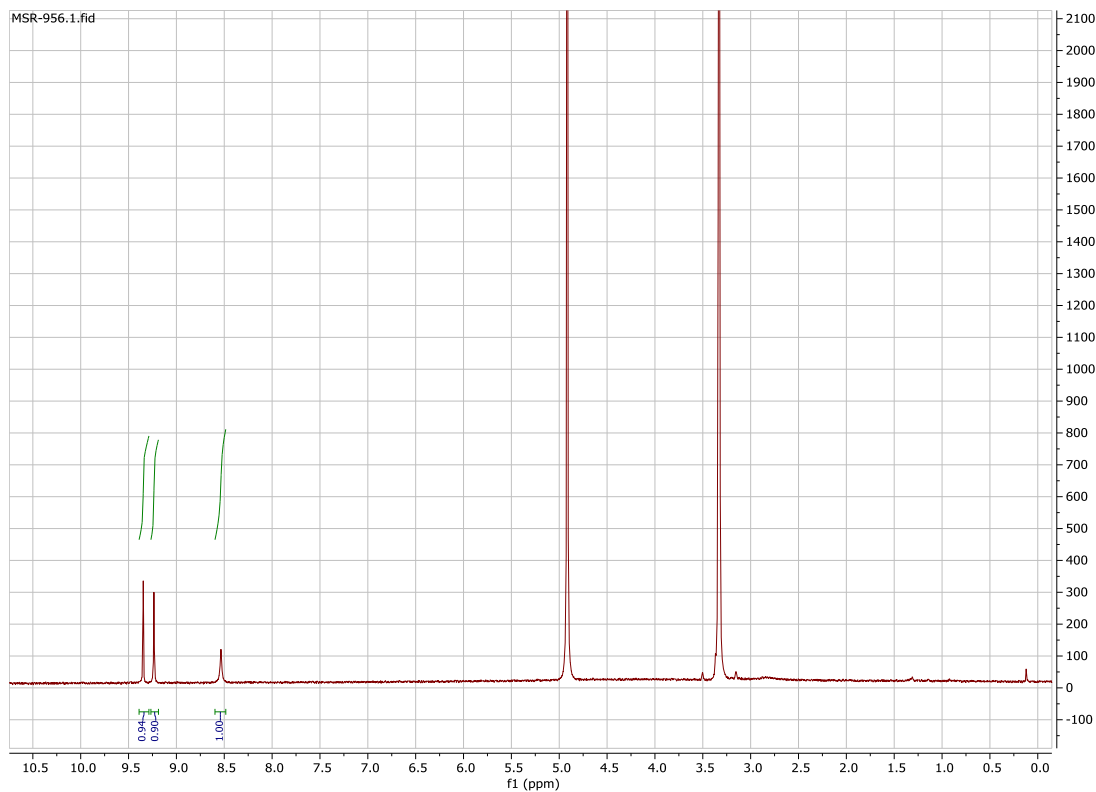
**Thiophen-3-yl(1H-1,2,3-triazol-5-yl)methanone (117):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



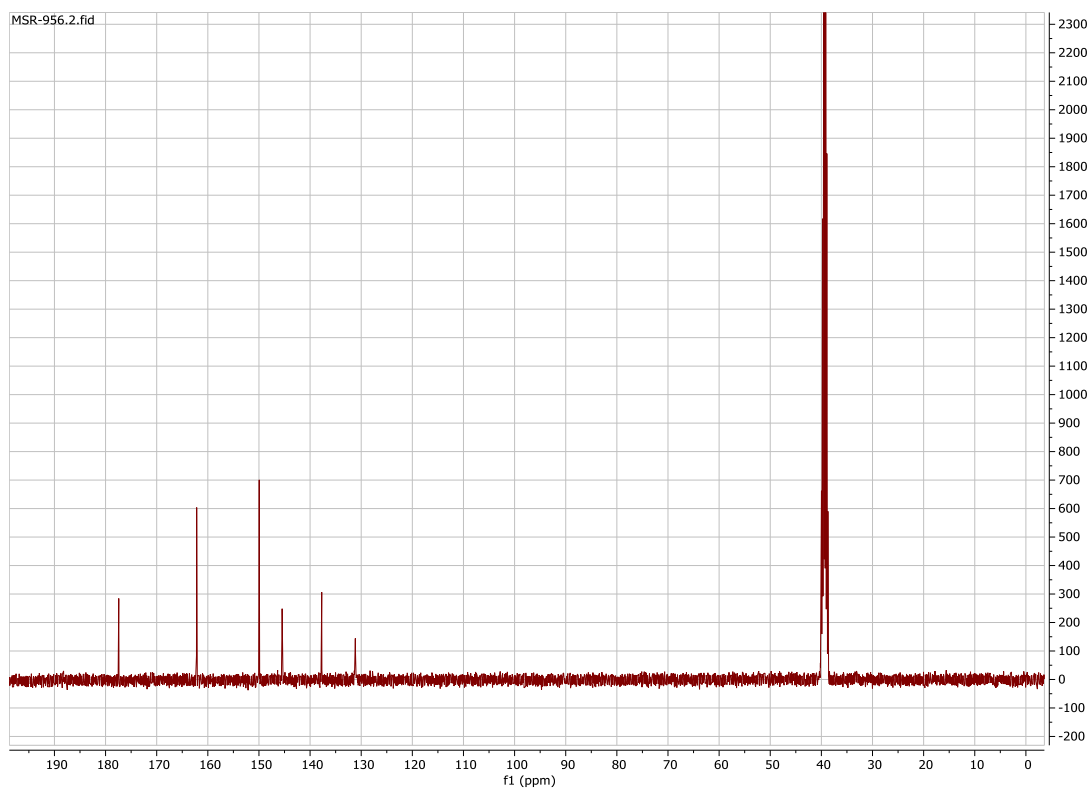
**Thiophen-3-yl(1H-1,2,3-triazol-5-yl)methanone (117):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



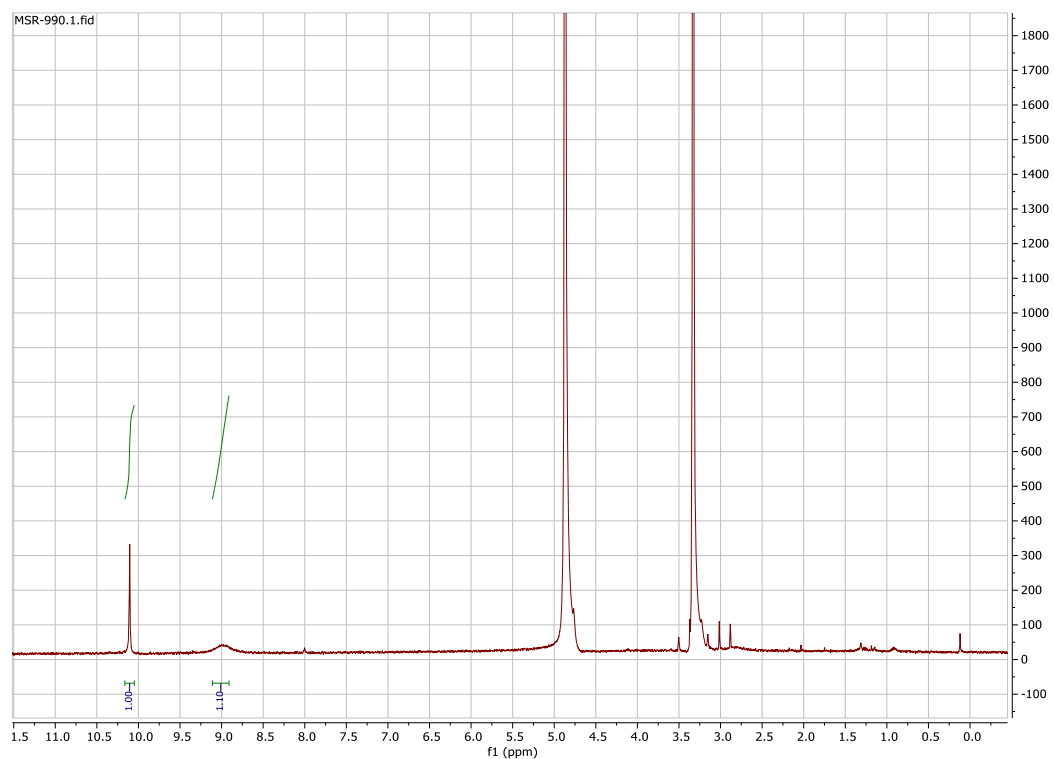
Thiazol-4-yl(1*H*-1,2,3-triazol-5-yl)methanone (118):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)



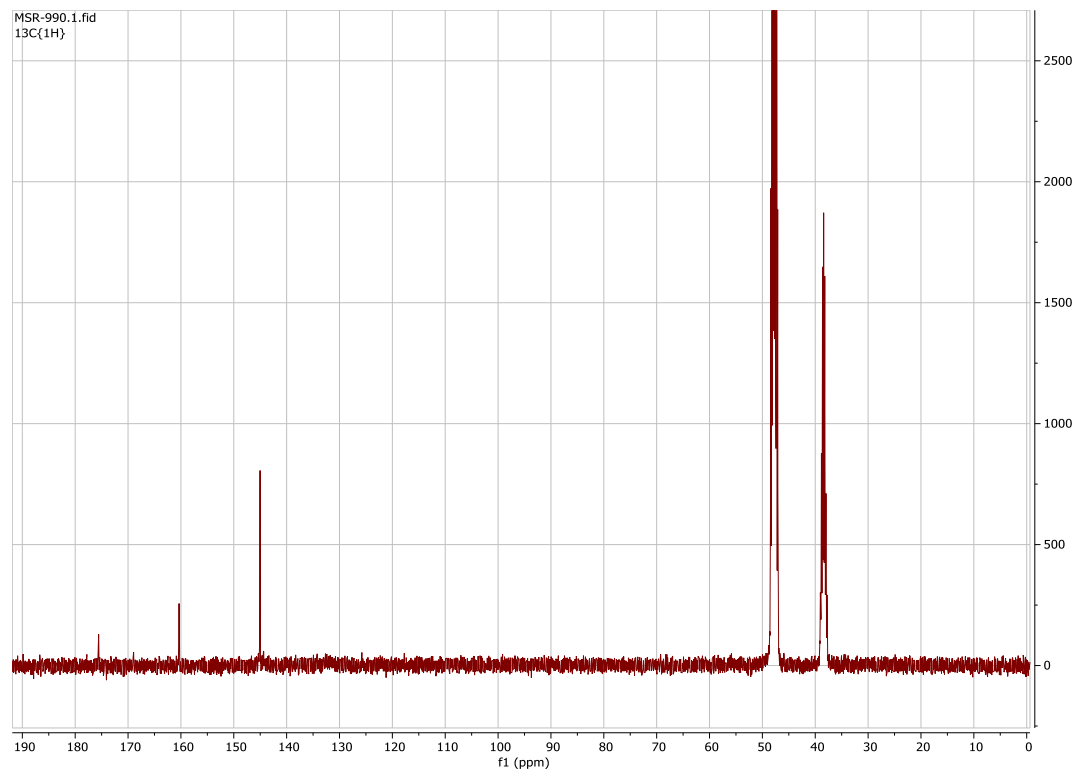
Thiazol-4-yl(1*H*-1,2,3-triazol-5-yl)methanone (118):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)



**(1,2,3-Thiadiazol-4-yl)(1H-1,2,3-triazol-5-yl)methanone (119):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

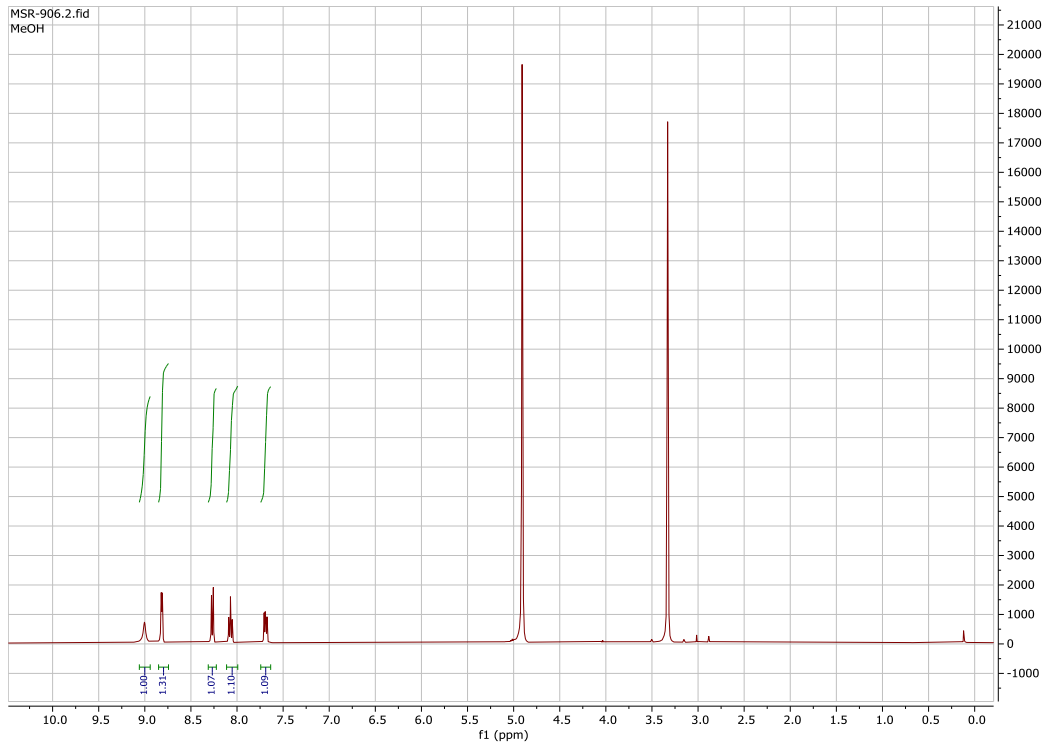


**(1,2,3-Thiadiazol-4-yl)(1H-1,2,3-triazol-5-yl)methanone (119):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

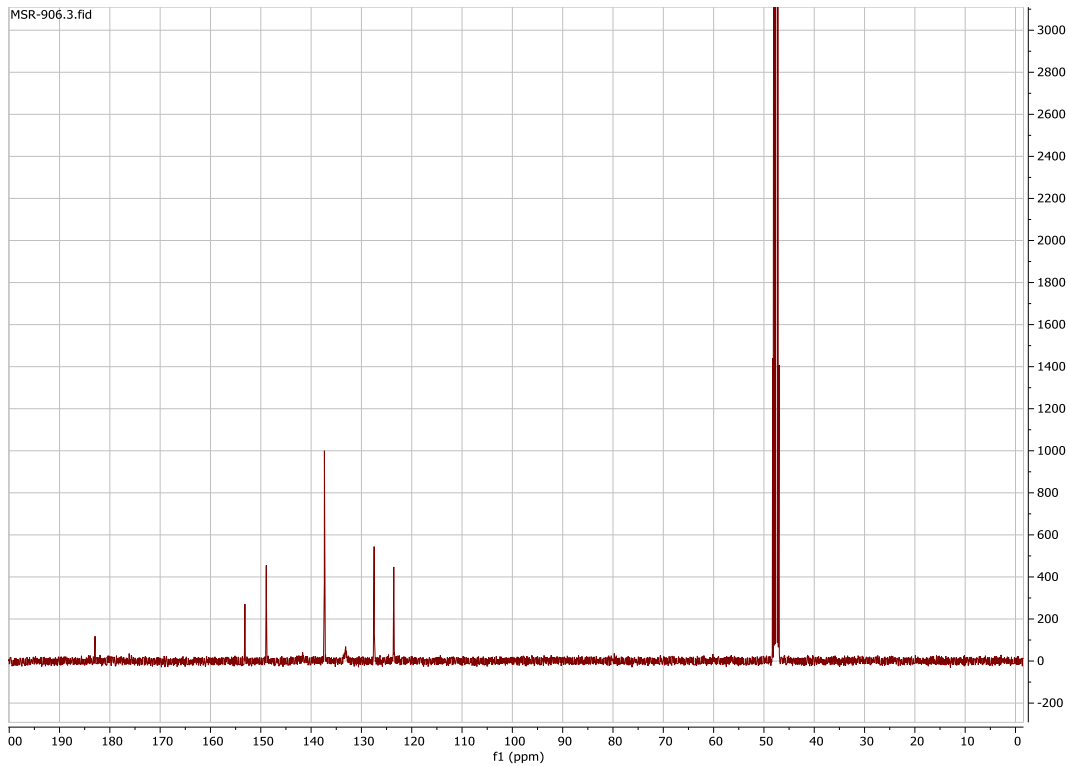




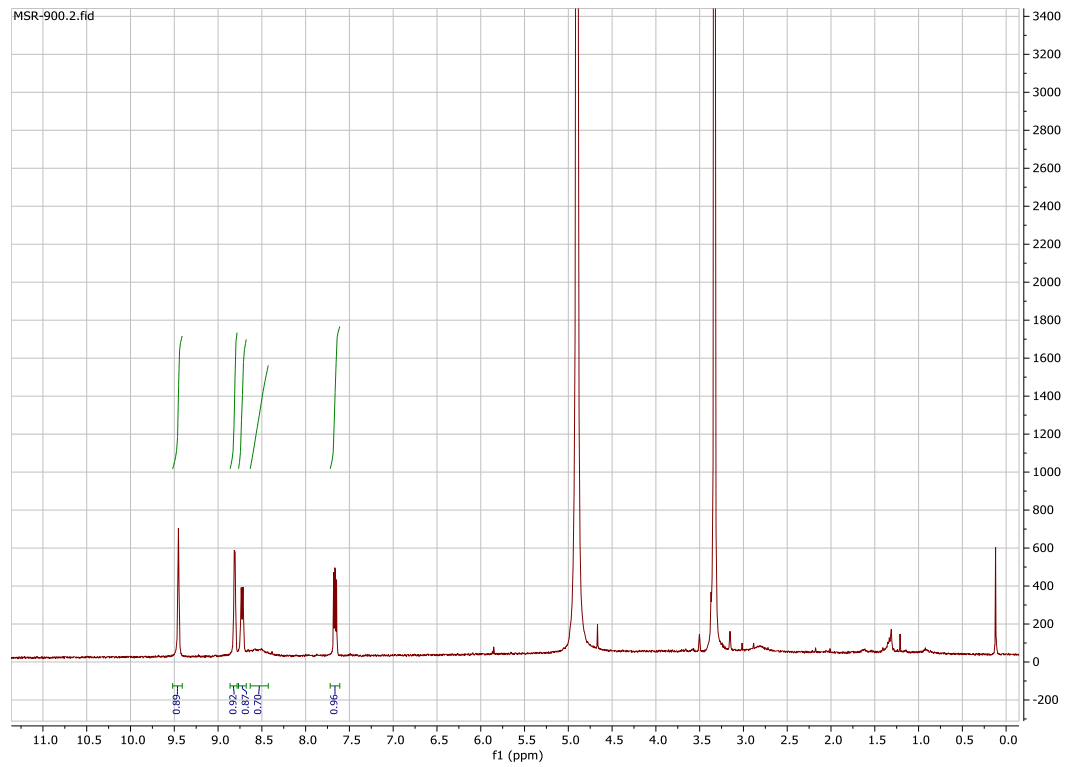
**Pyridin-2-yl(1H-1,2,3-triazol-5-yl)methanone (120):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



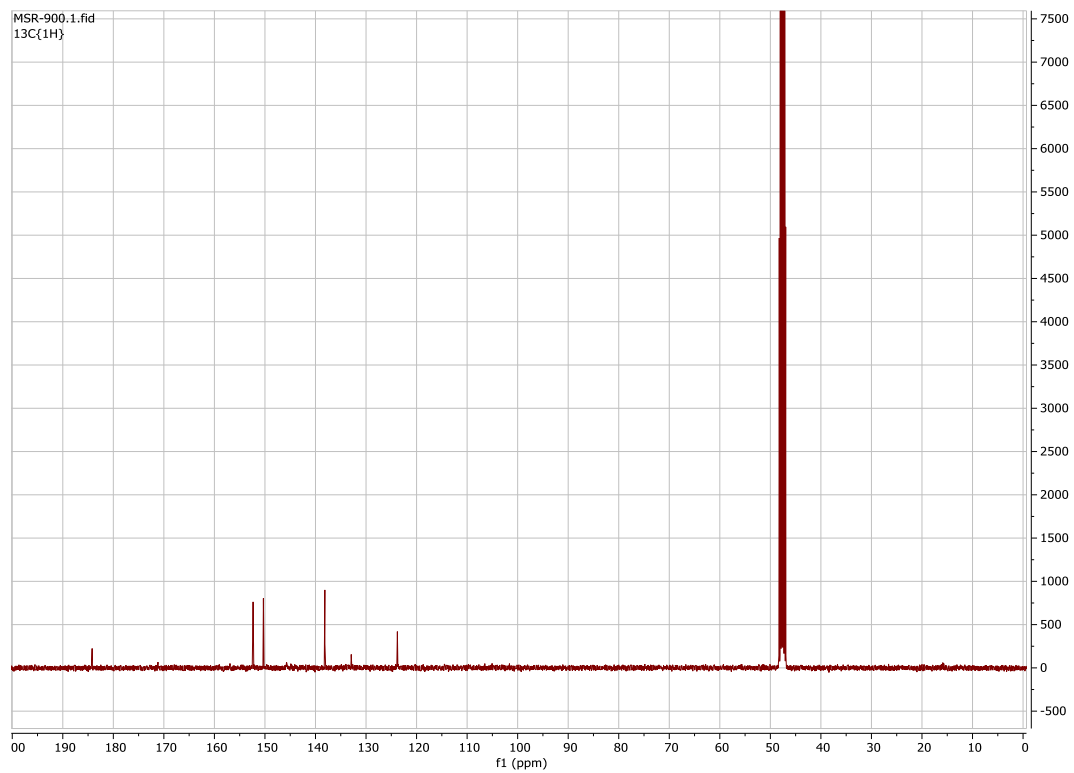
**Pyridin-2-yl(1H-1,2,3-triazol-5-yl)methanone (120):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



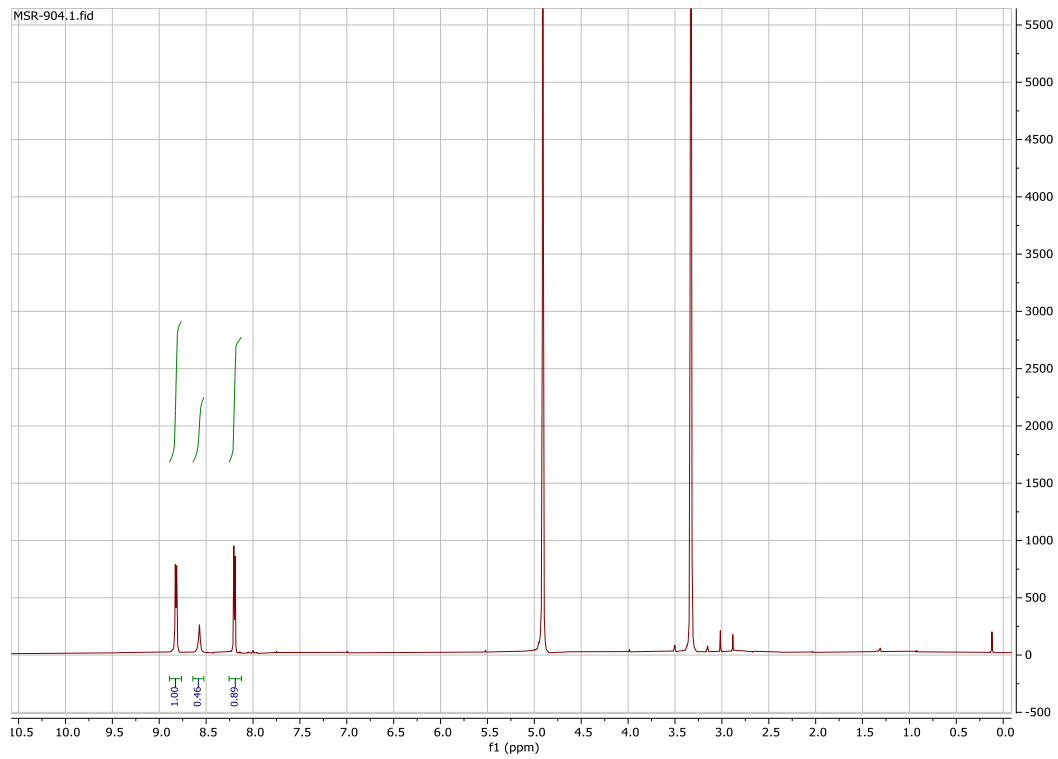
**Pyridin-3-yl(1H-1,2,3-triazol-5-yl)methanone (121):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



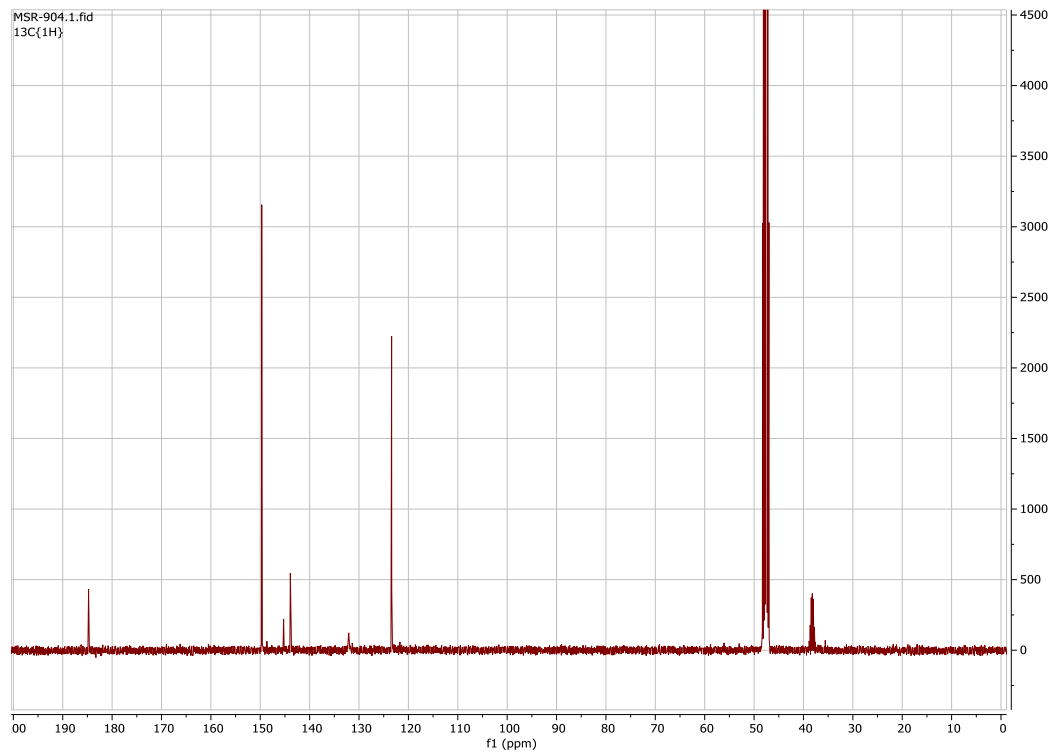
**Pyridin-3-yl(1H-1,2,3-triazol-5-yl)methanone (121):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



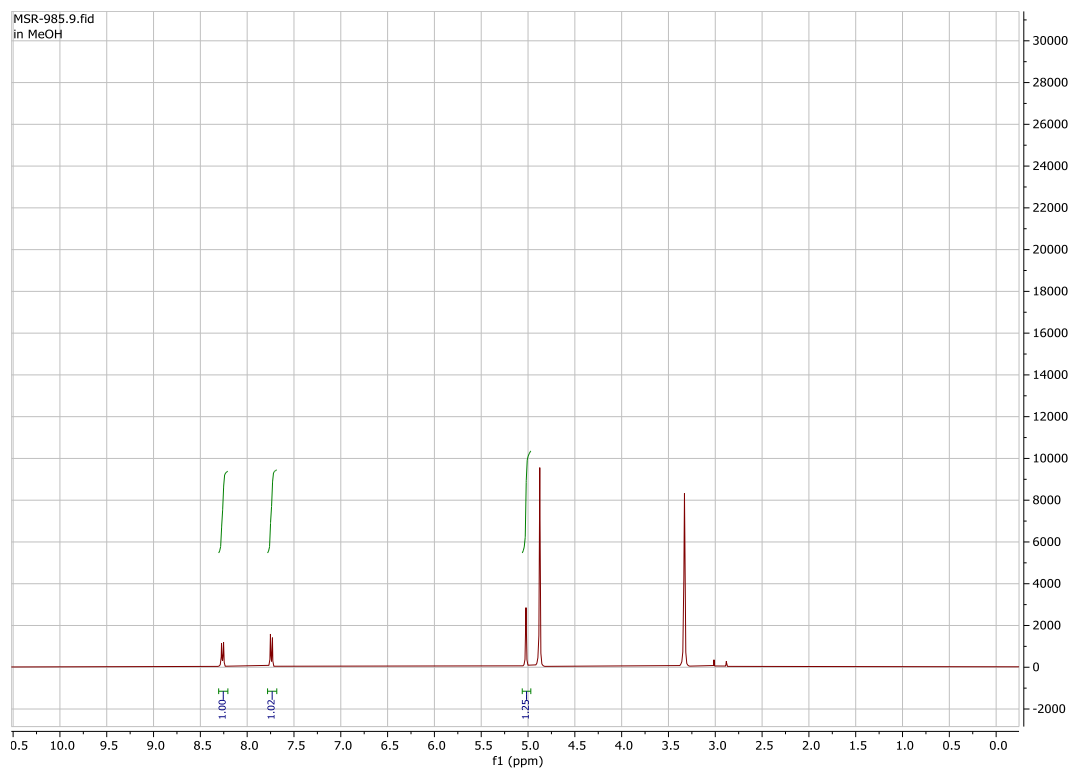
**Pyridin-4-yl(1H-1,2,3-triazol-5-yl)methanone (122):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



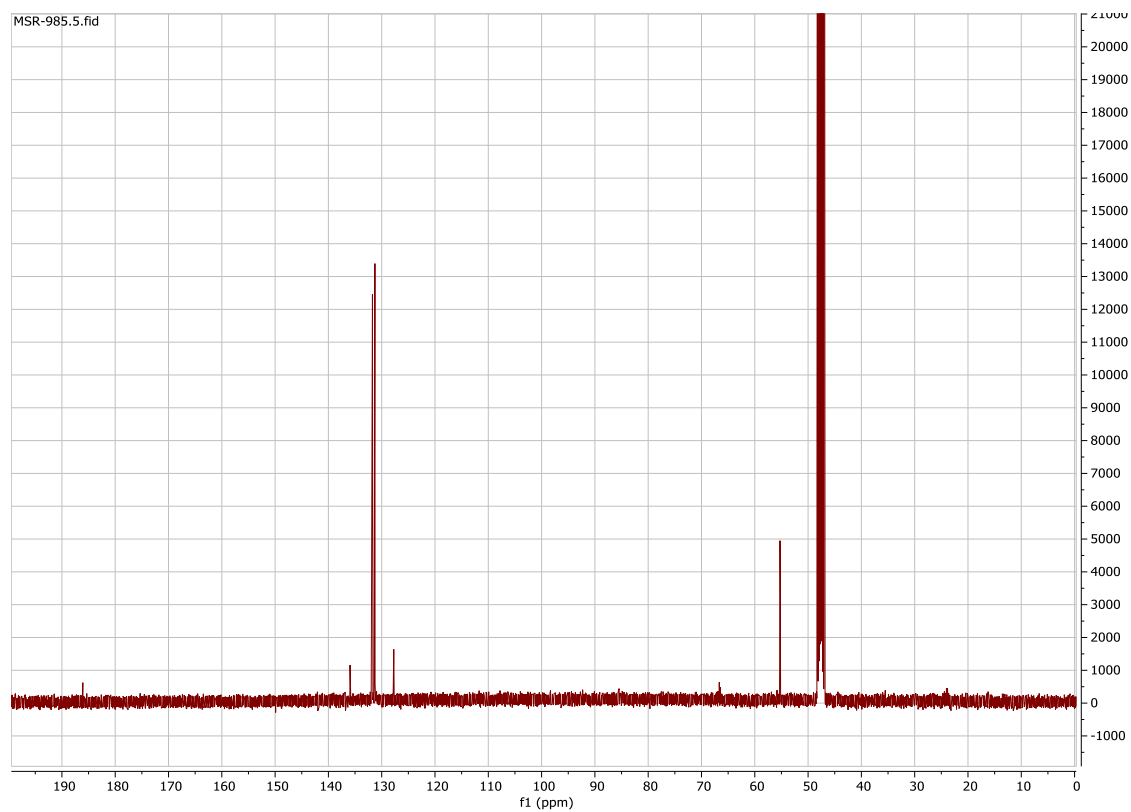
**Pyridin-4-yl(1H-1,2,3-triazol-5-yl)methanone (122):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



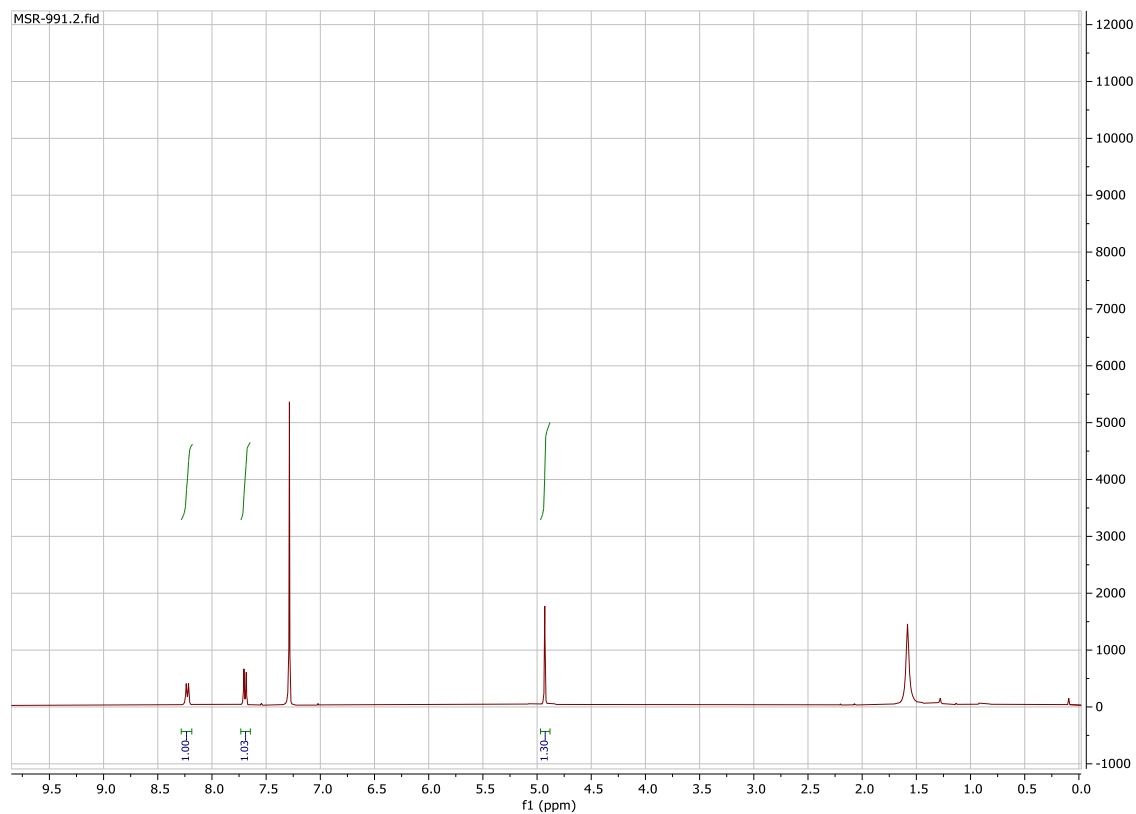
**(4-Bromophenyl)(4-(hydroxymethyl)-1H-1,2,3-triazol-5-yl)methanone (123):**  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_3\text{OD}$ )



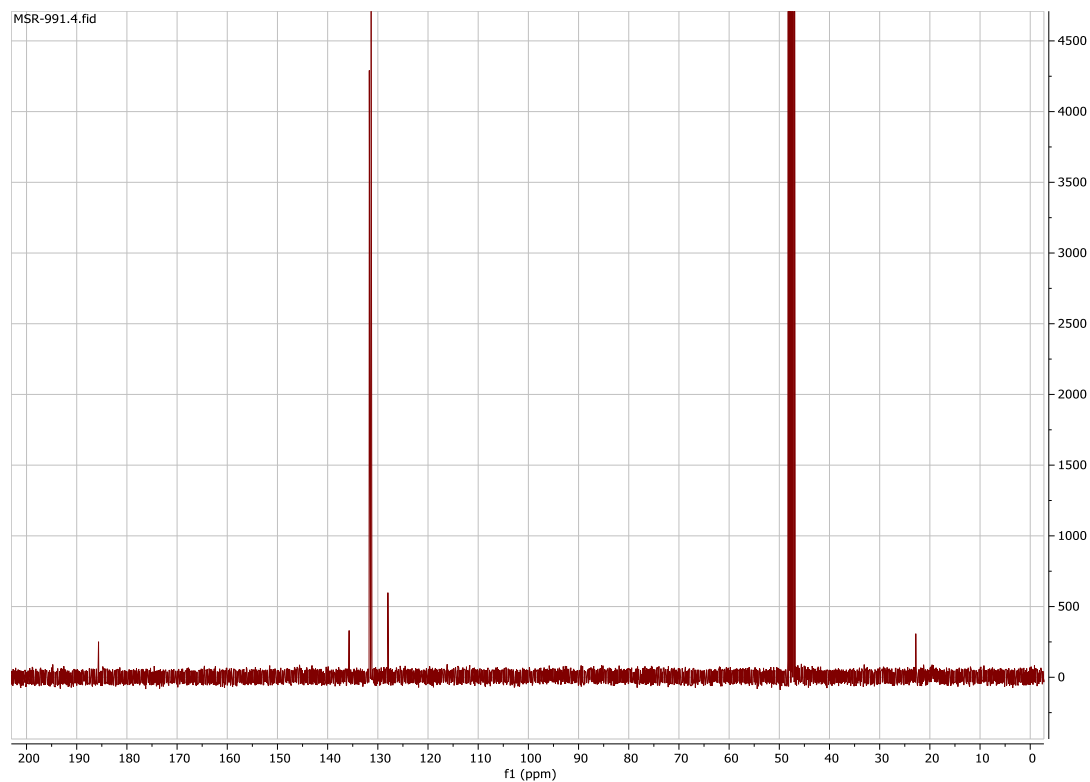
**(4-Bromophenyl)(4-(hydroxymethyl)-1H-1,2,3-triazol-5-yl)methanone (123):**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )



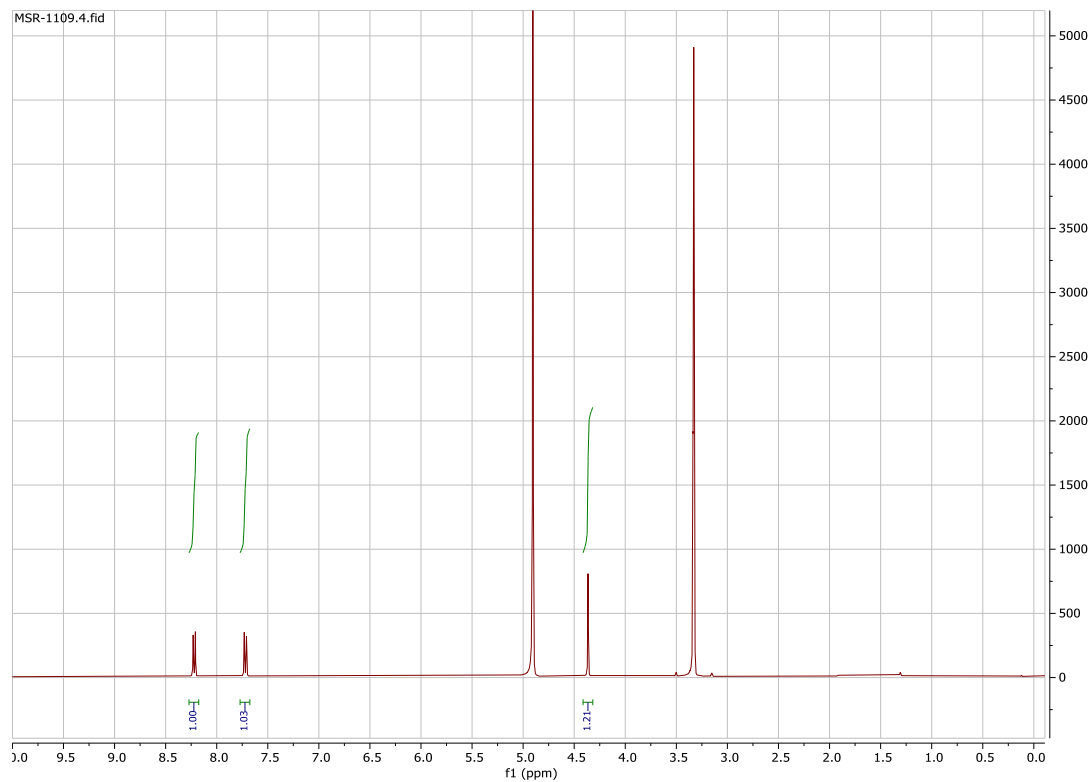
**(4-(Bromomethyl)-1H-1,2,3-triazol-5-yl)(4-bromophenyl)methanone (124):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



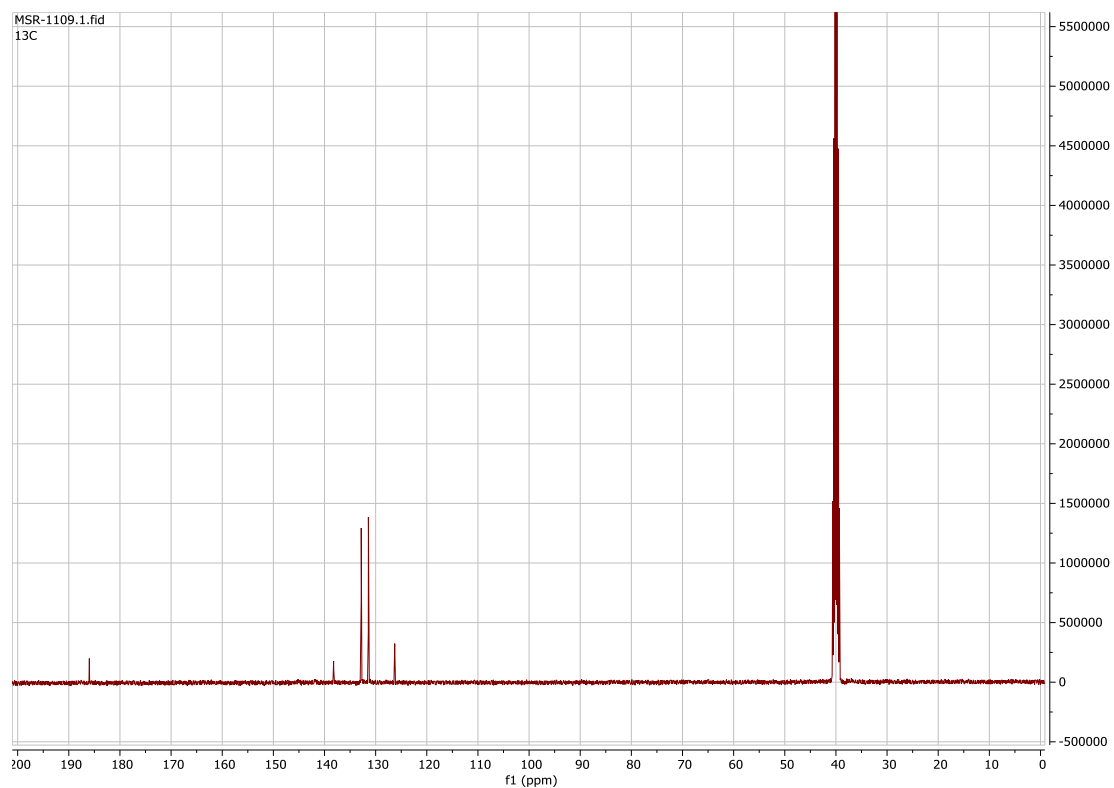
**(4-(Bromomethyl)-1H-1,2,3-triazol-5-yl)(4-bromophenyl)methanone (124):**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ )



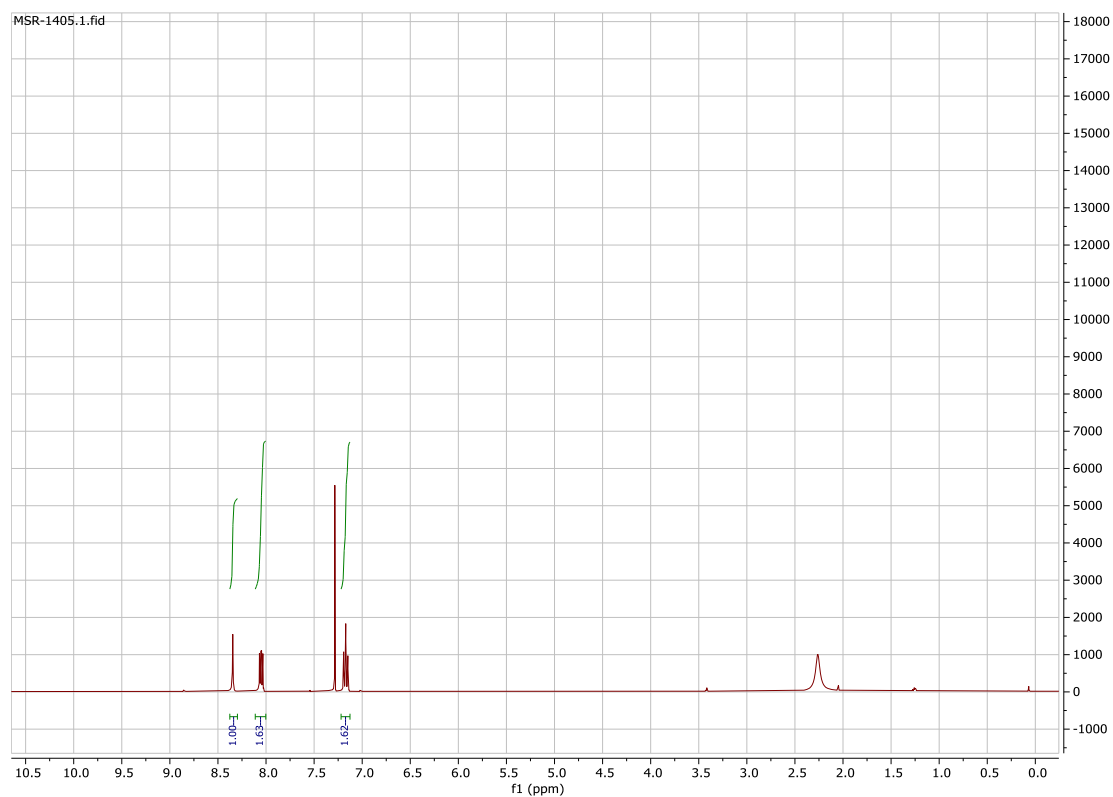
**(4-(aminomethyl)-1H-1,2,3-triazol-5-yl)(4-bromophenyl)methanone (126):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



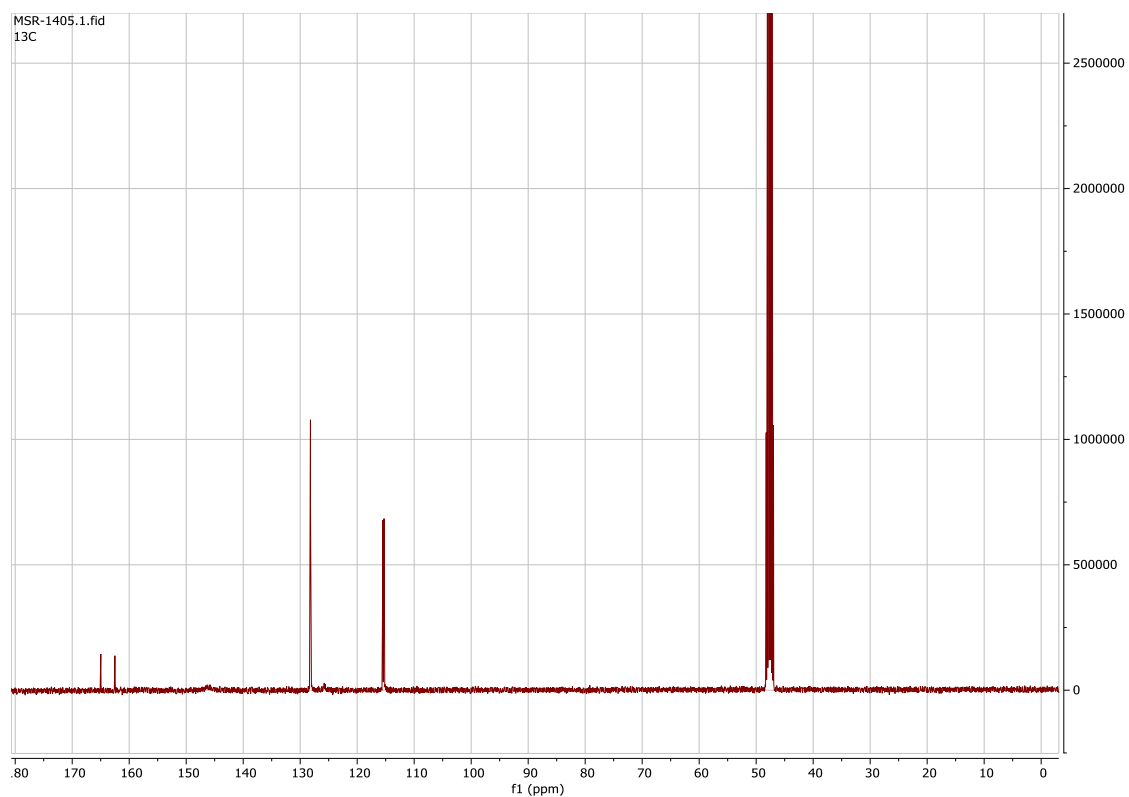
**(4-(aminomethyl)-1H-1,2,3-triazol-5-yl)(4-bromophenyl)methanone (126):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



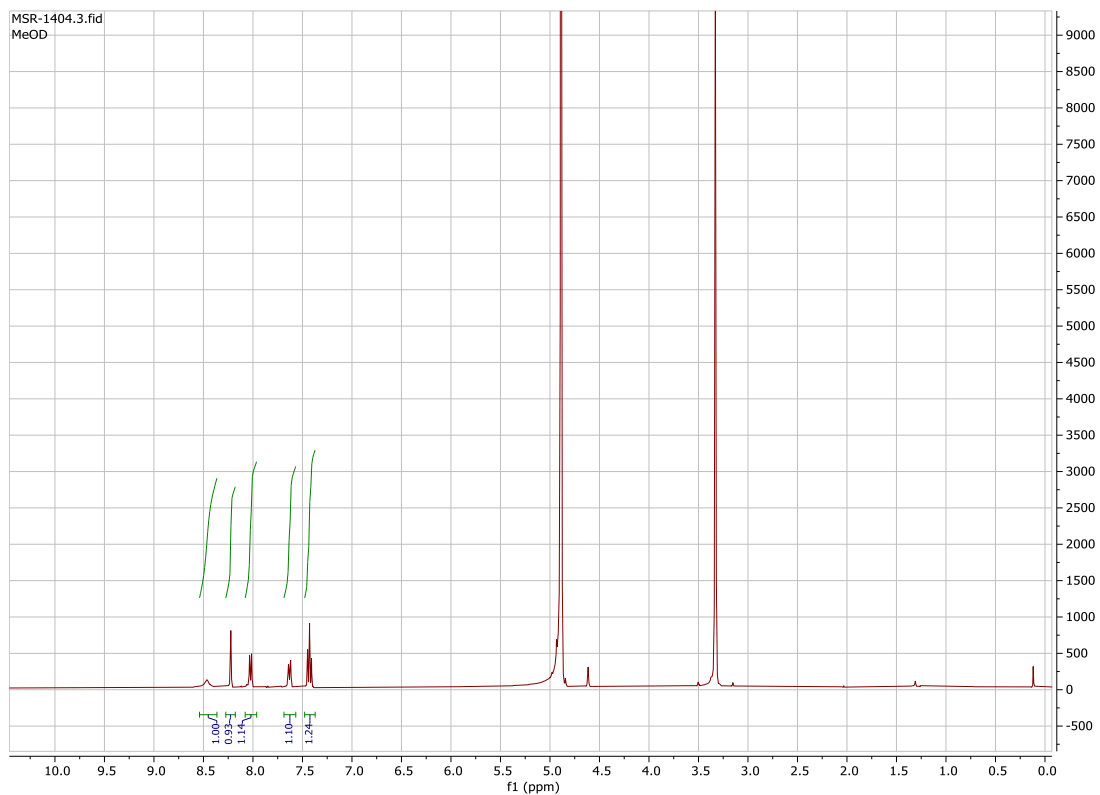
**3-(4-Fluorophenyl)-1H-1,2,4-triazole (134):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



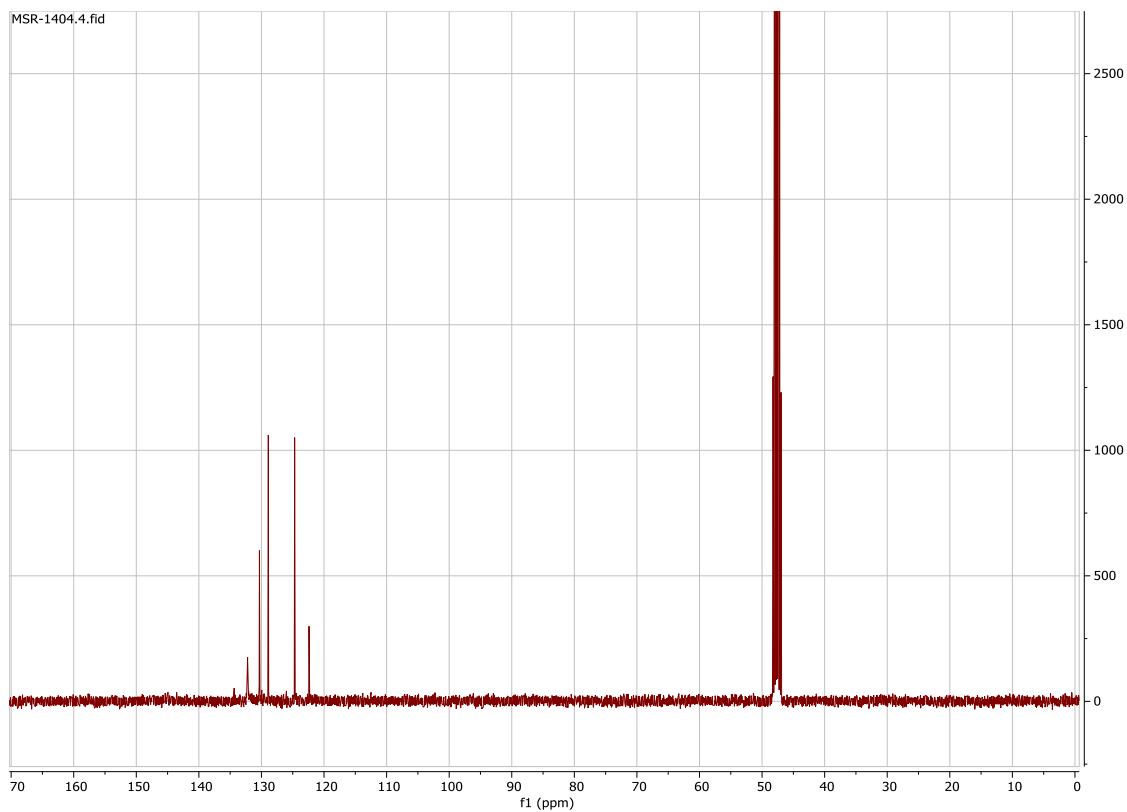
**3-(4-Fluorophenyl)-1H-1,2,4-triazole (134):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**3-(3-Bromophenyl)-1*H*-1,2,4-triazole (135):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

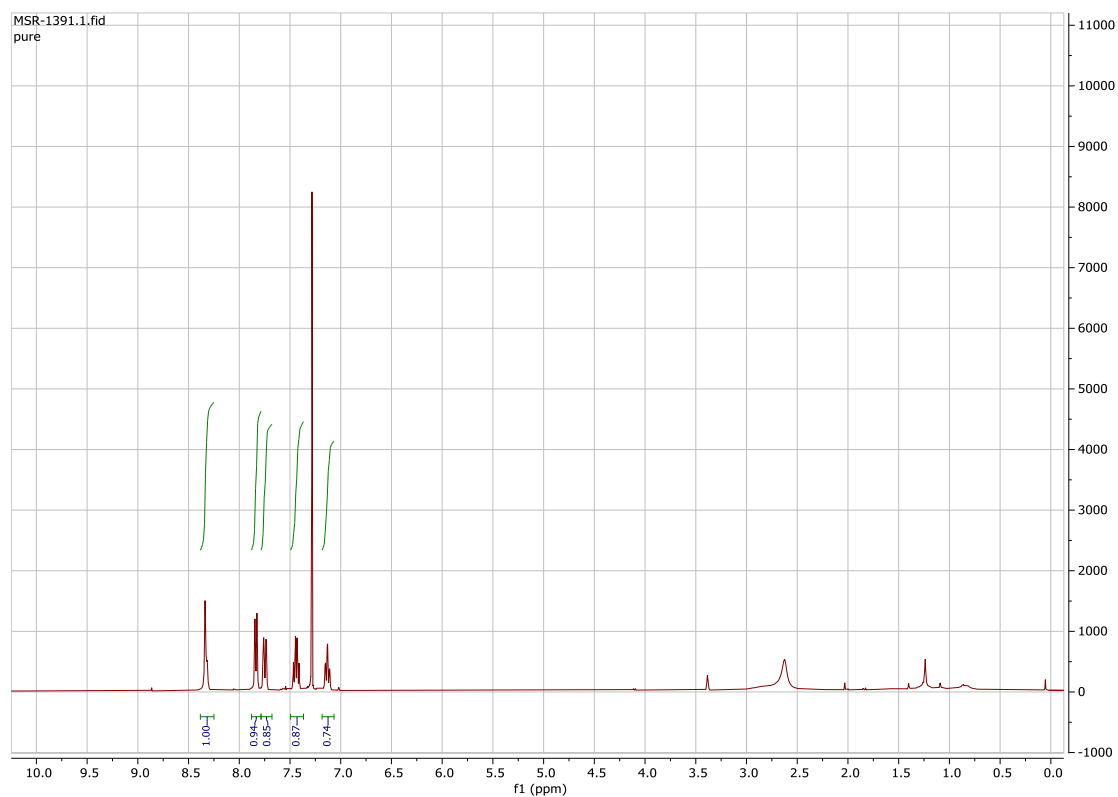


**3-(3-Bromophenyl)-1*H*-1,2,4-triazole (135):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

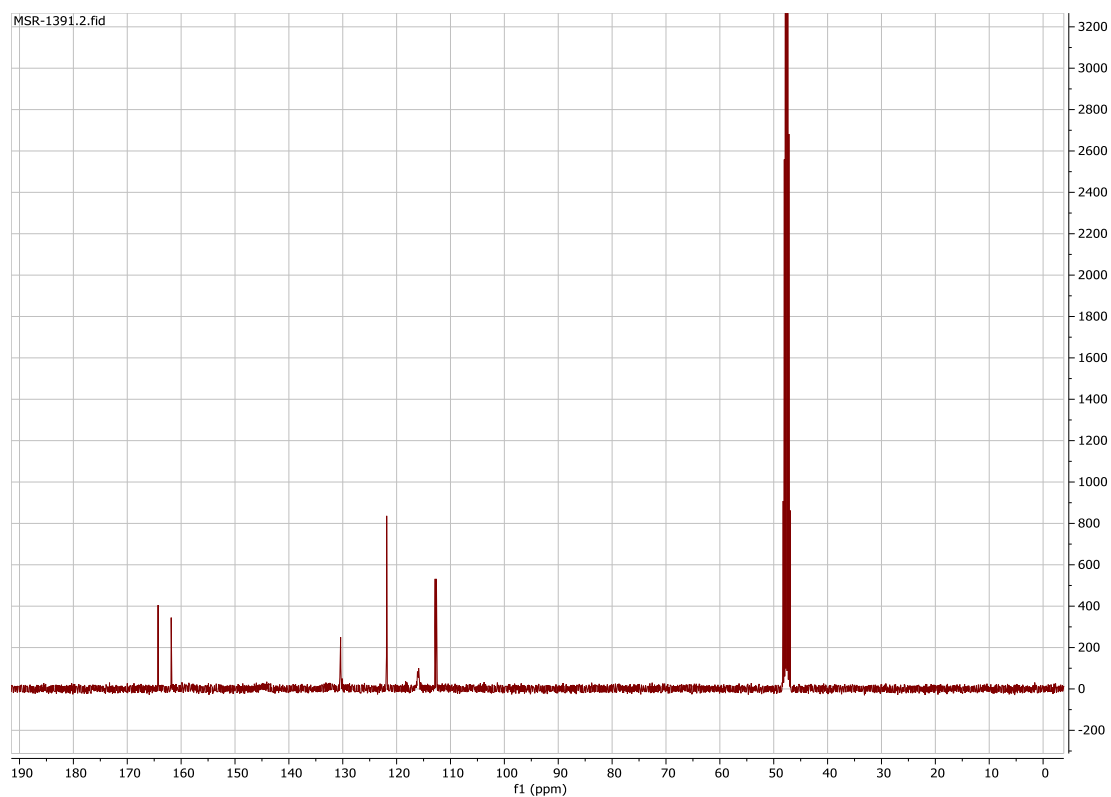




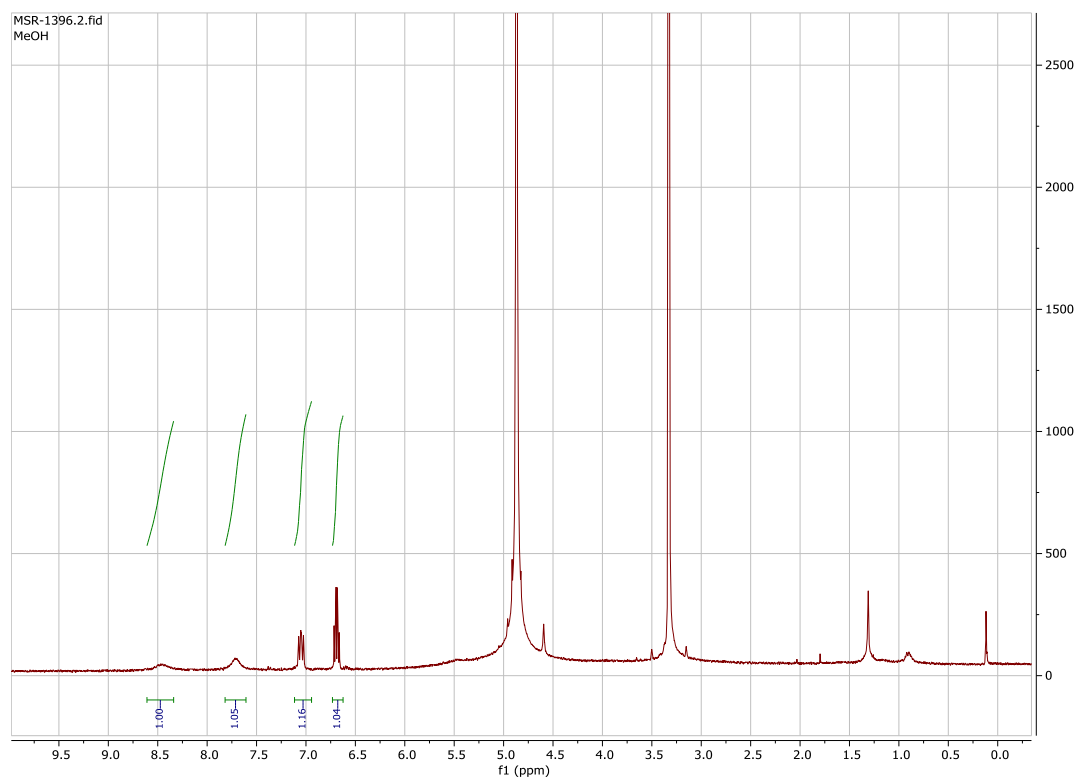
**3-(3-Fluorophenyl)-1H-1,2,4-triazole (137):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



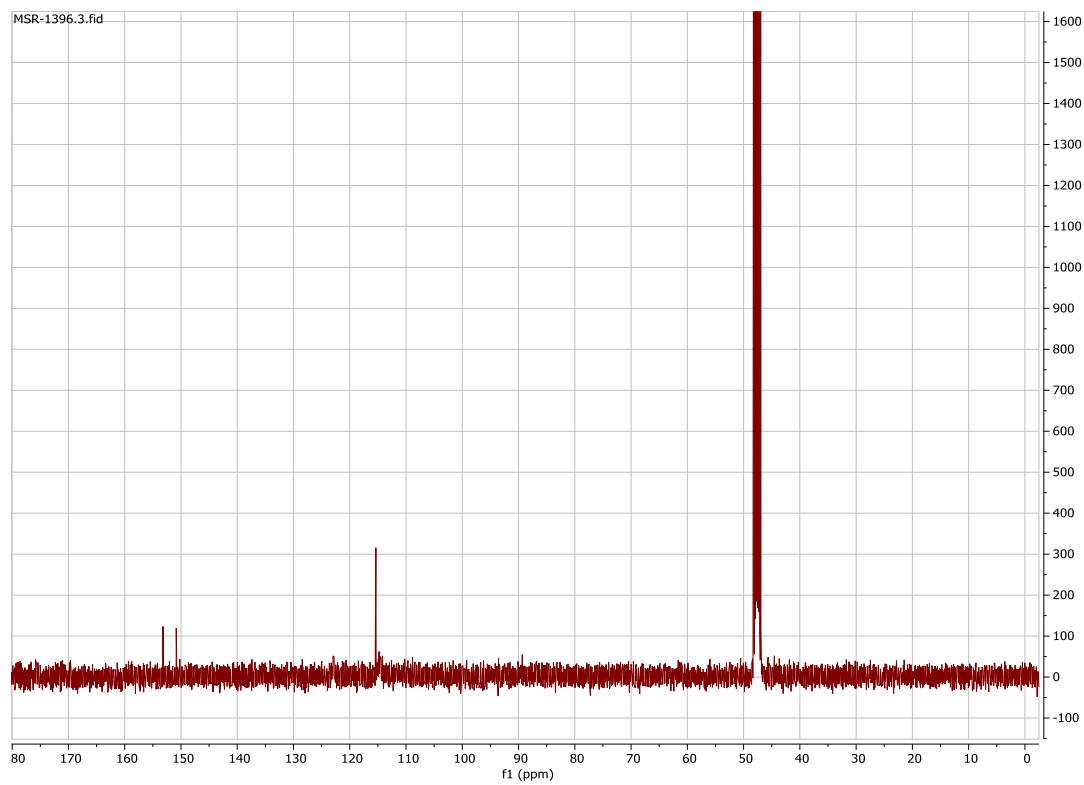
**3-(3-Fluorophenyl)-1H-1,2,4-triazole (137):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



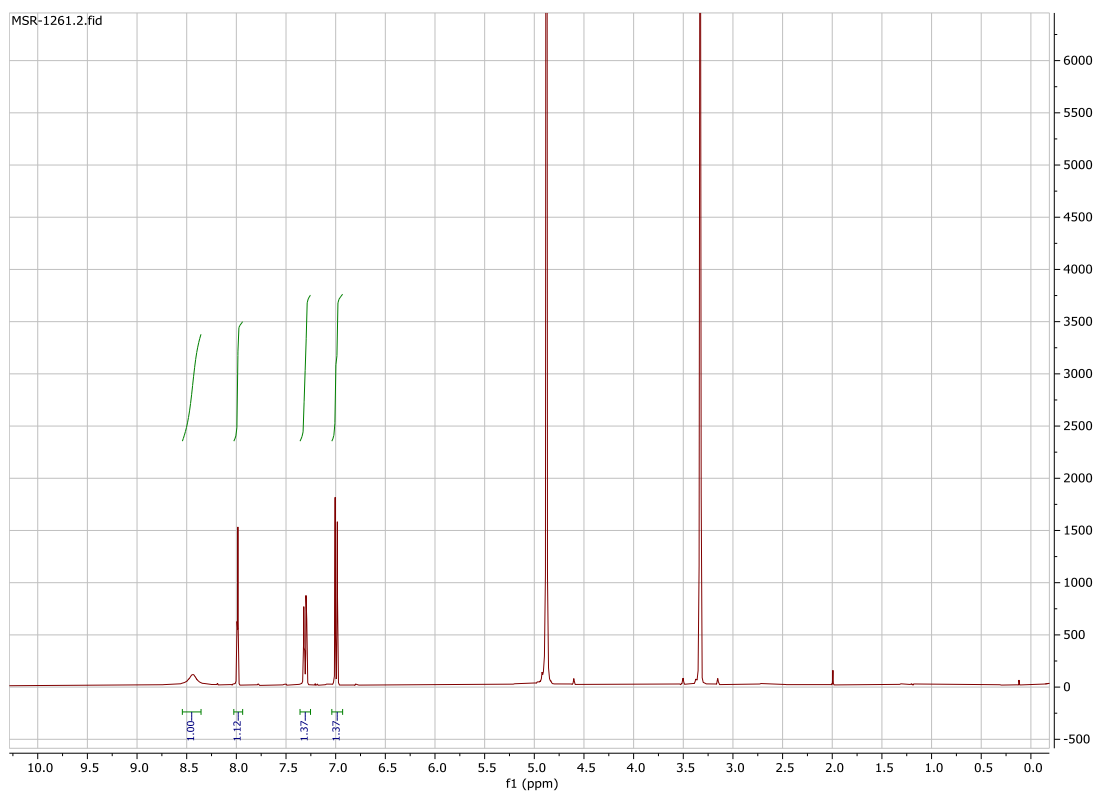
**2-Fluoro-6-(1H-1,2,4-triazol-3-yl)aniline (140):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



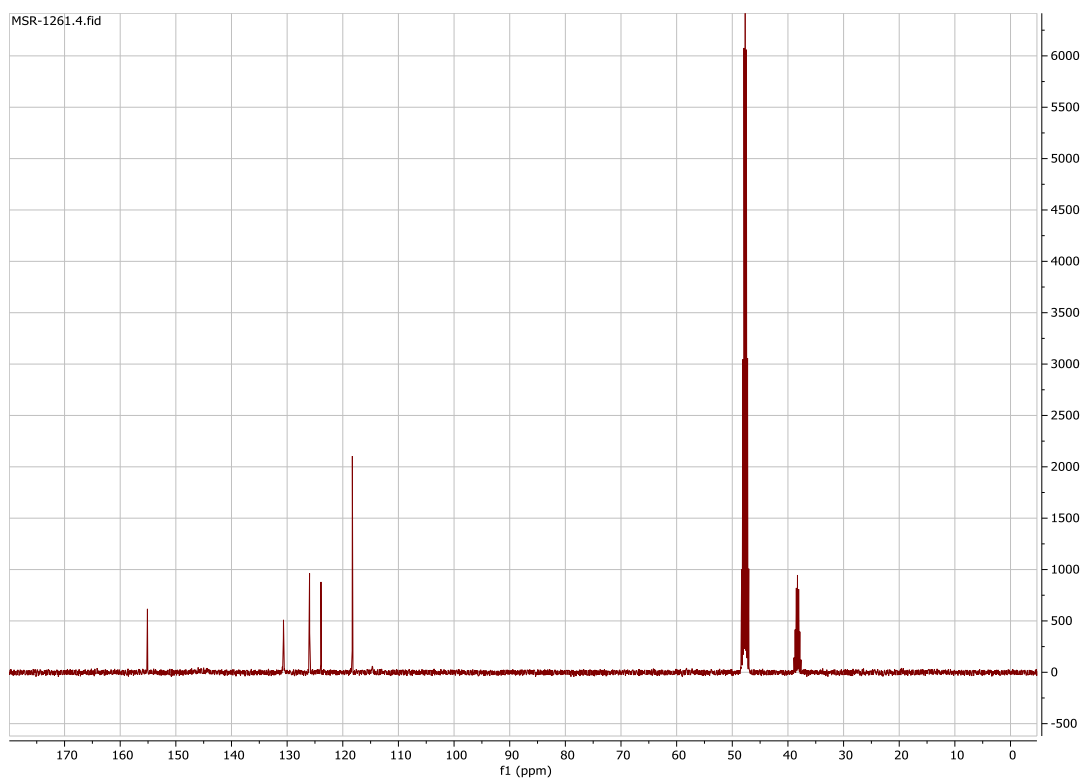
**2-Fluoro-6-(1H-1,2,4-triazol-3-yl)aniline (140):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



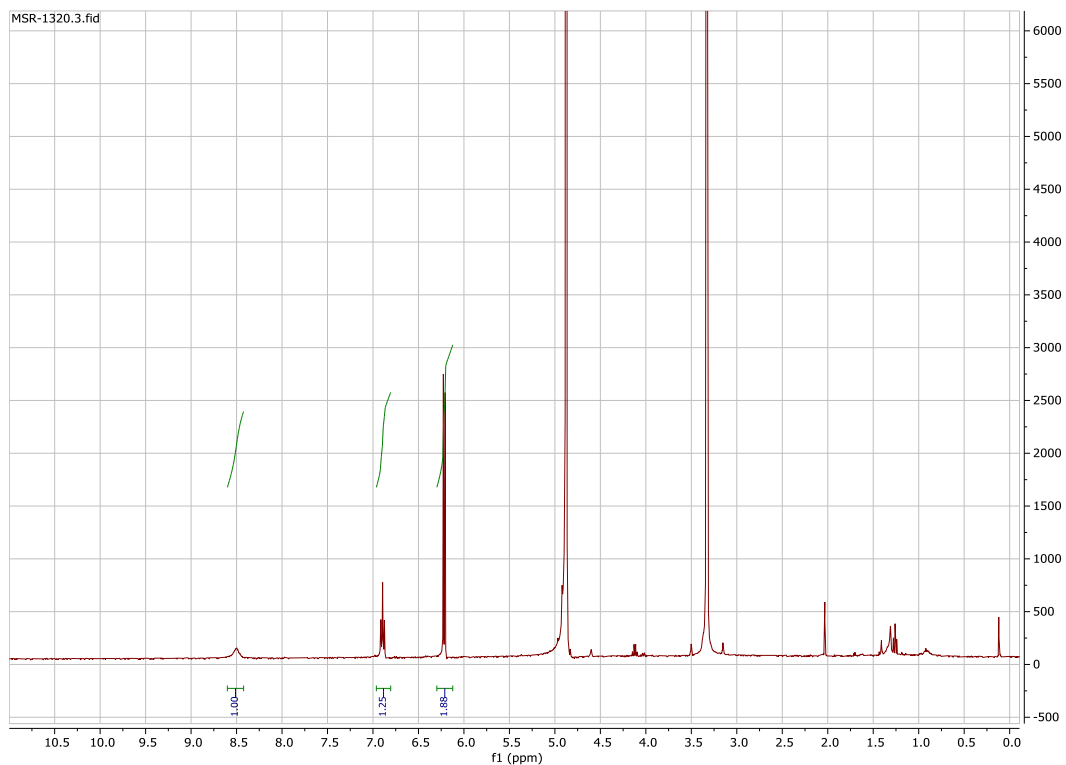
**2-Chloro-6-(1H-1,2,4-triazol-3-yl)aniline (141):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



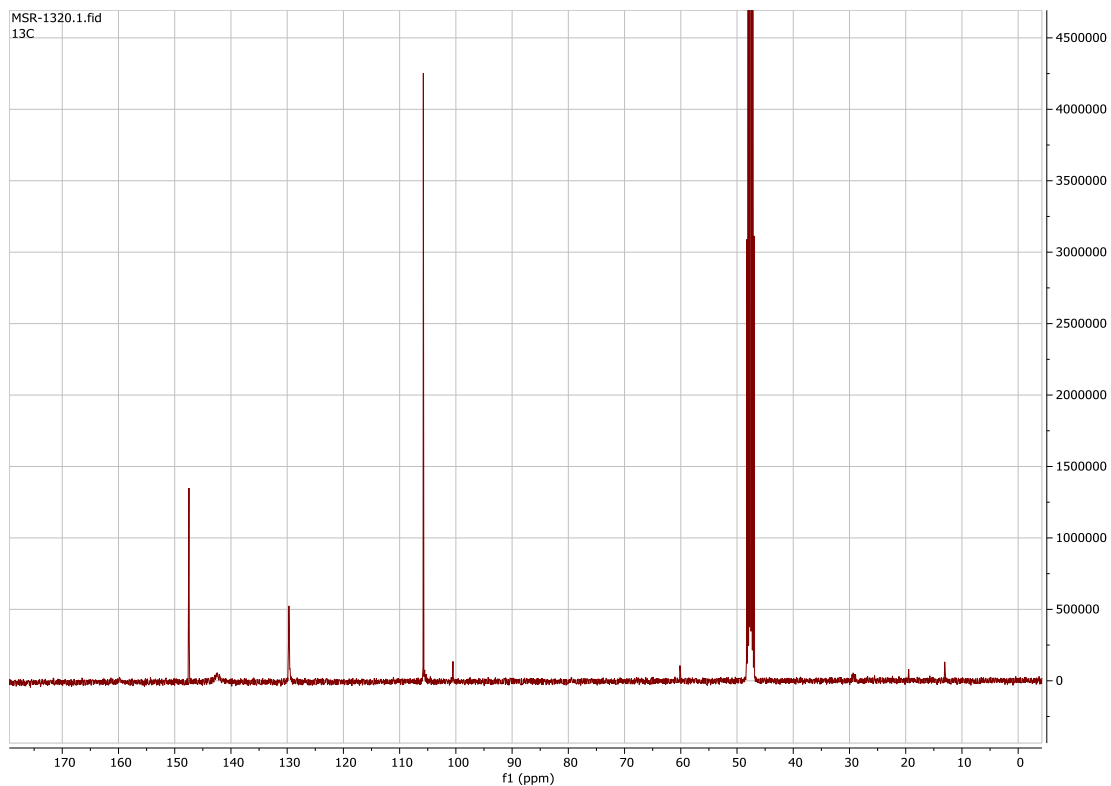
**2-Chloro-6-(1H-1,2,4-triazol-3-yl)aniline (141):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



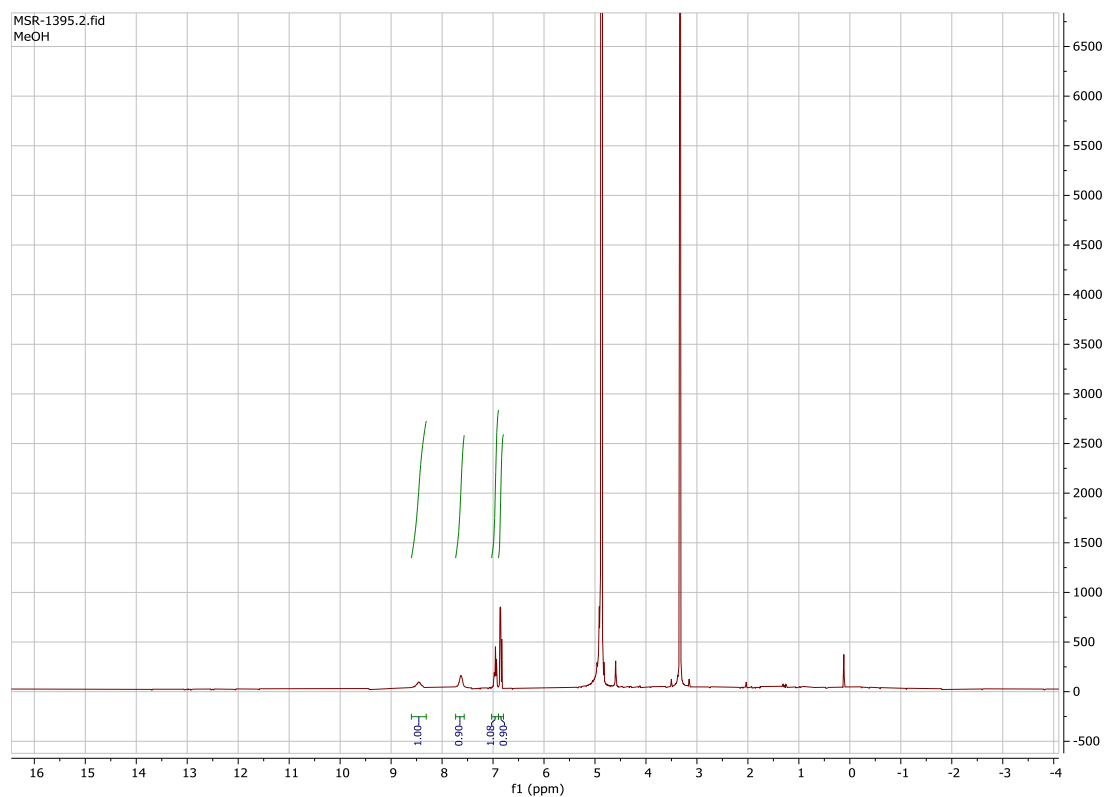
**2-(1*H*-1,2,4-Triazol-3-yl)benzene-1,3-diamine (142):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



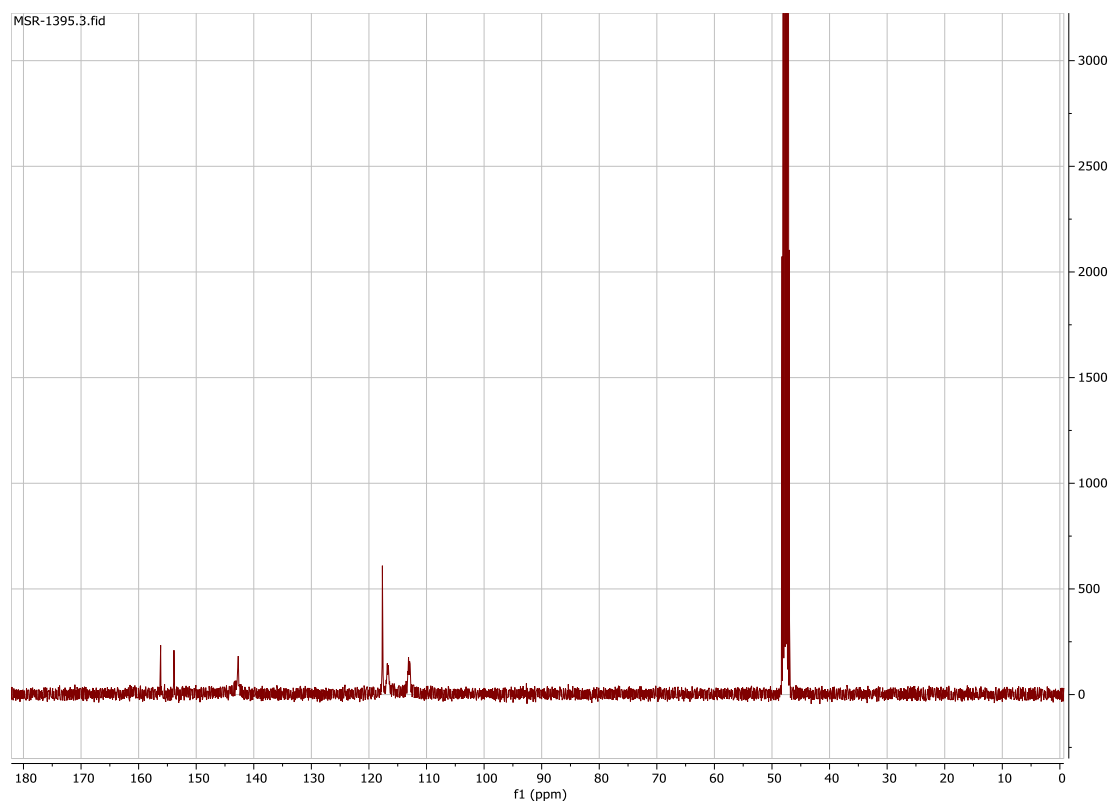
**2-(1*H*-1,2,4-Triazol-3-yl)benzene-1,3-diamine (142):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



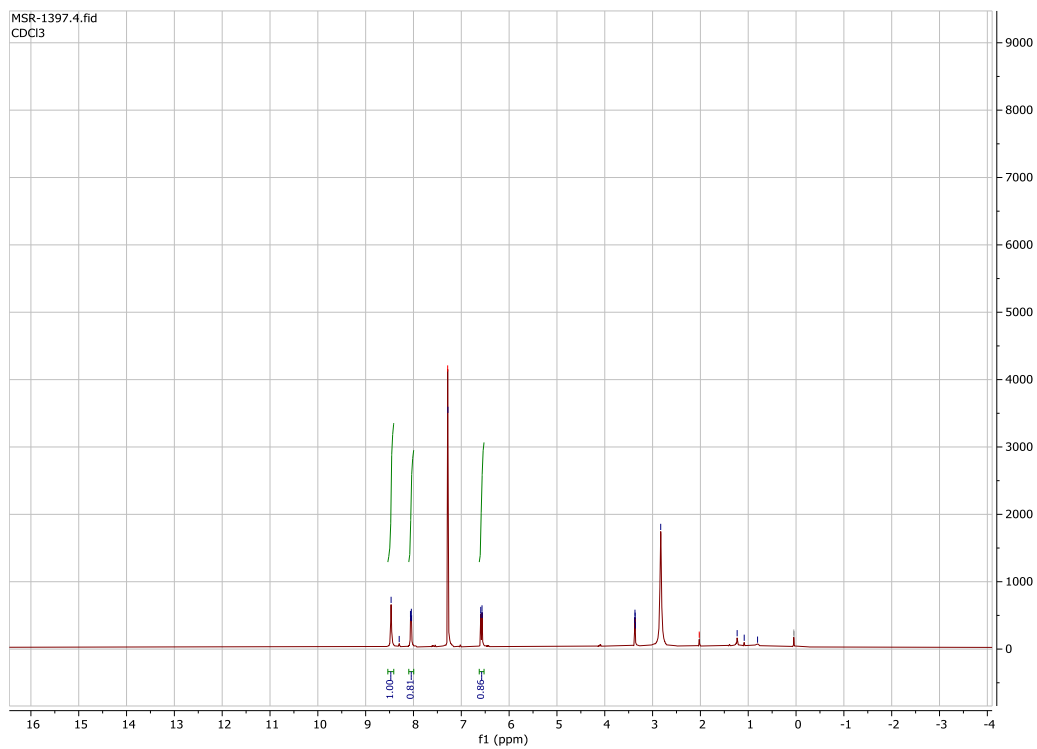
**4-Fluoro-2-(1H-1,2,4-triazol-3-yl)aniline (143):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



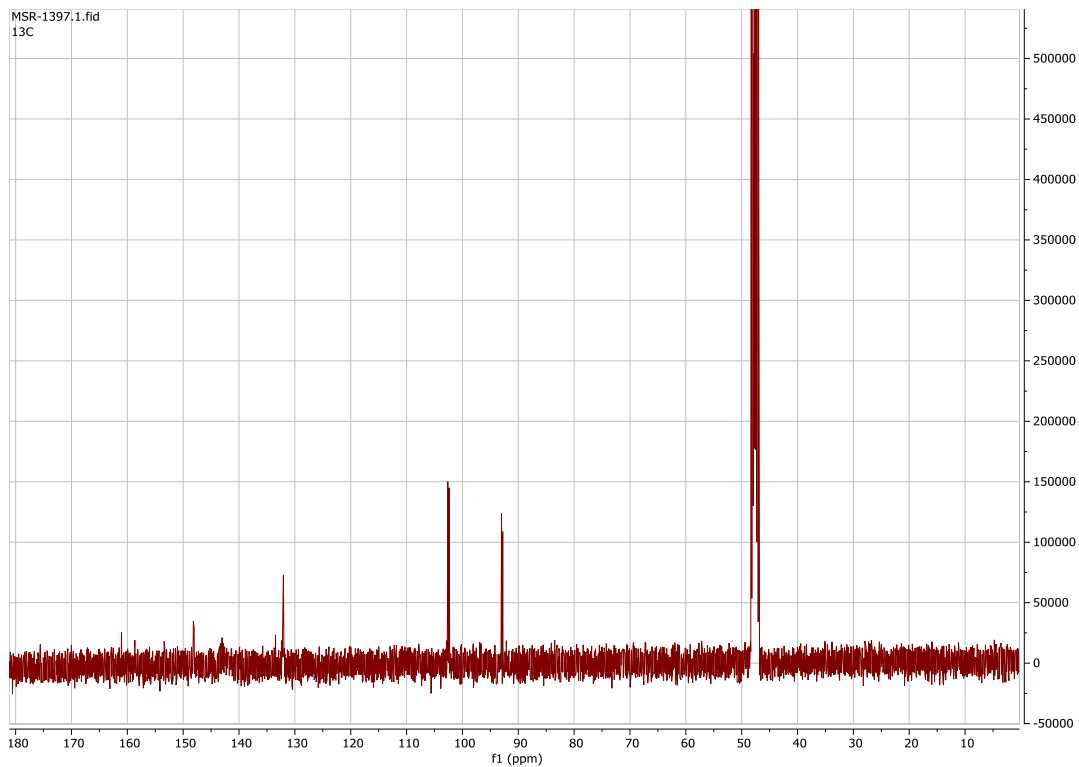
**4-Fluoro-2-(1H-1,2,4-triazol-3-yl)aniline (143):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



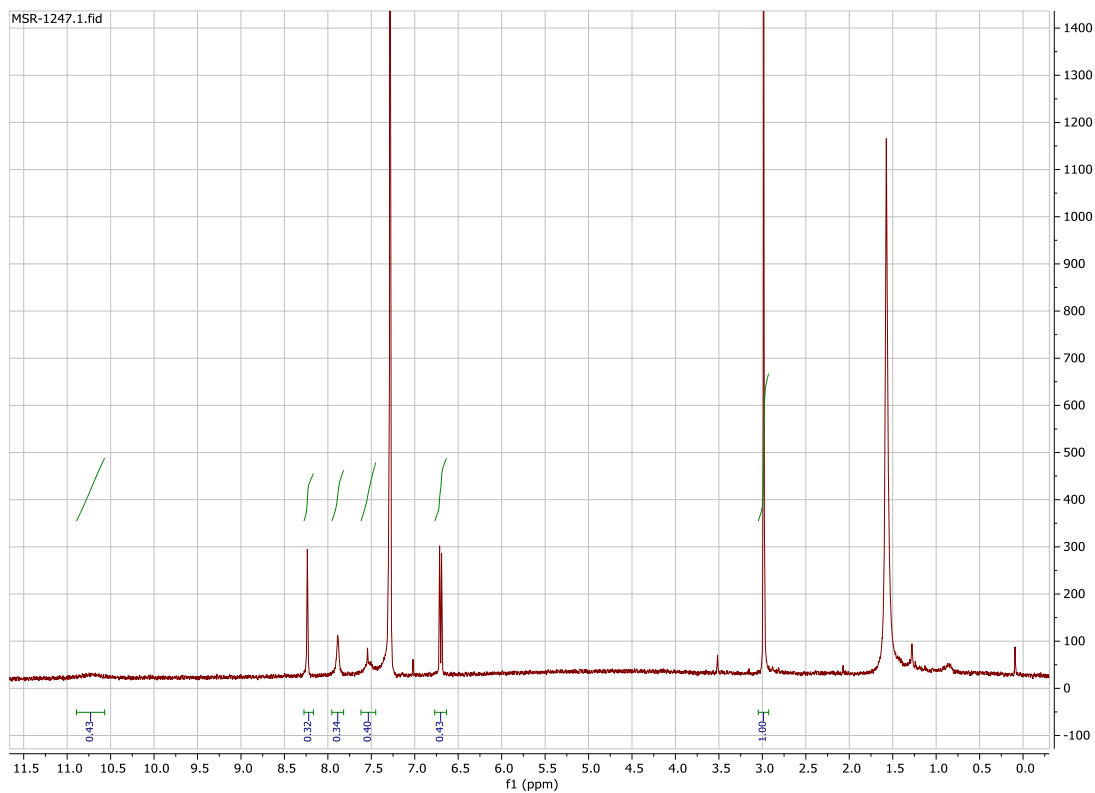
**4-Bromo-5-fluoro-2-(1H-1,2,4-triazol-3-yl)aniline (144):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



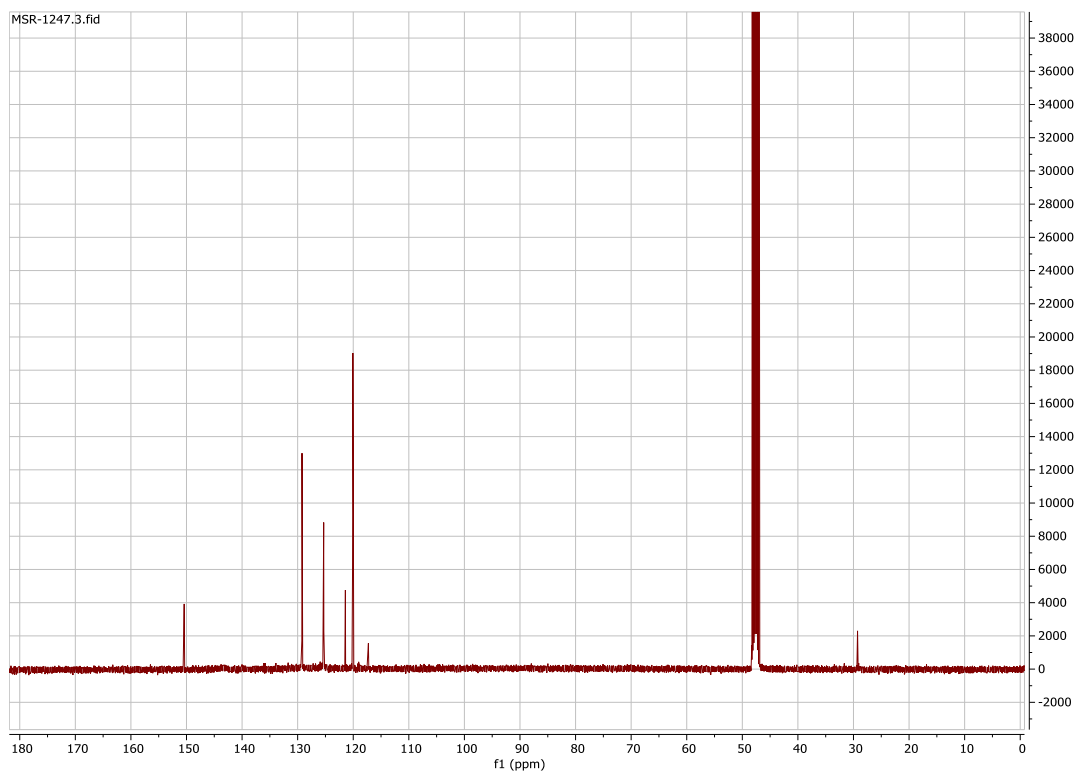
**4-Bromo-5-fluoro-2-(1H-1,2,4-triazol-3-yl)aniline (144):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



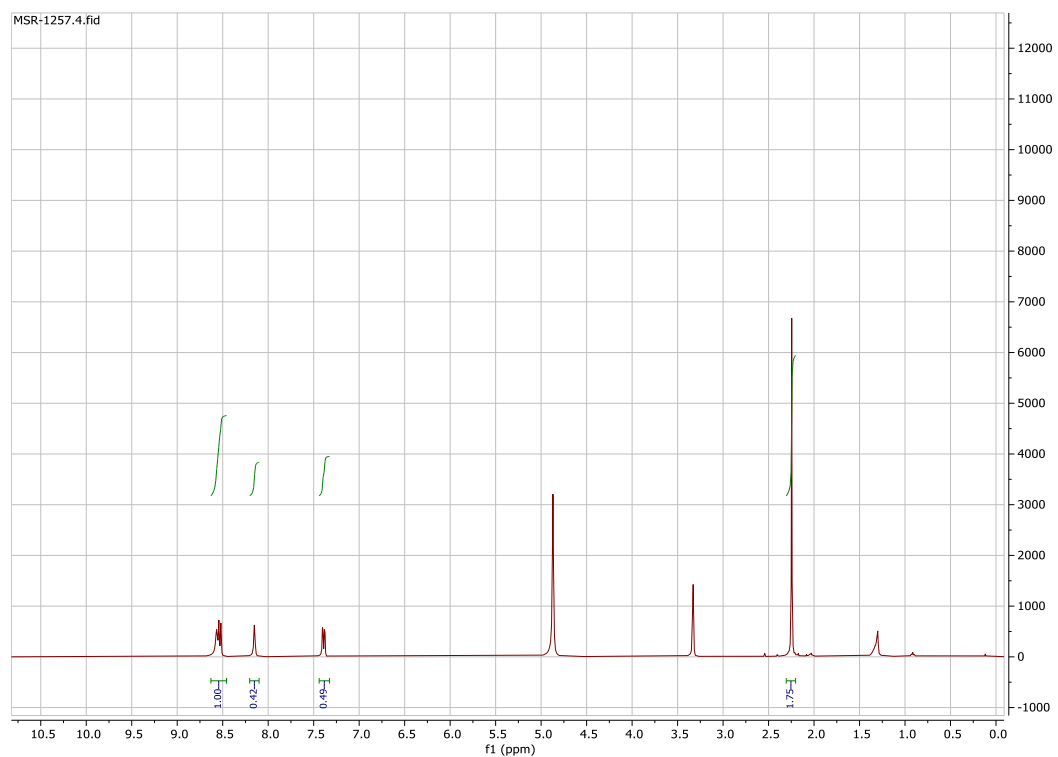
**4-Chloro-*N*-methyl-2-(1*H*-1,2,4-triazol-3-yl)aniline (145): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



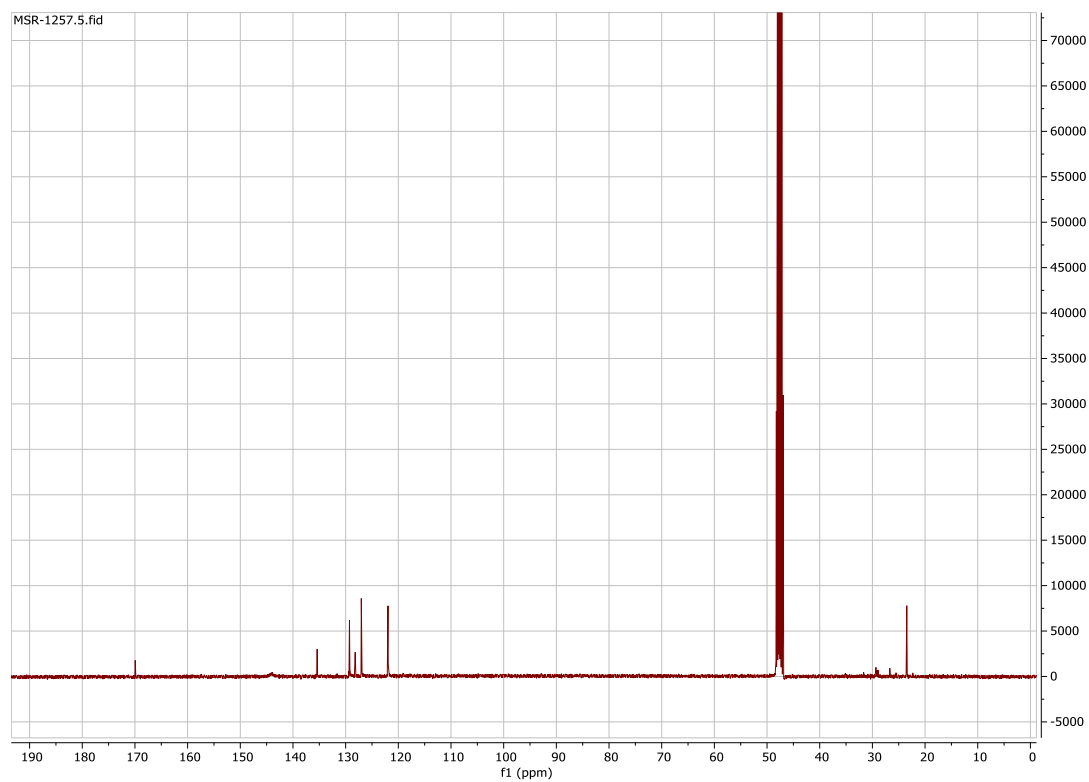
**4-Chloro-*N*-methyl-2-(1*H*-1,2,4-triazol-3-yl)aniline (145): <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>:CD<sub>3</sub>OD)**



***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)acetamide (146):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

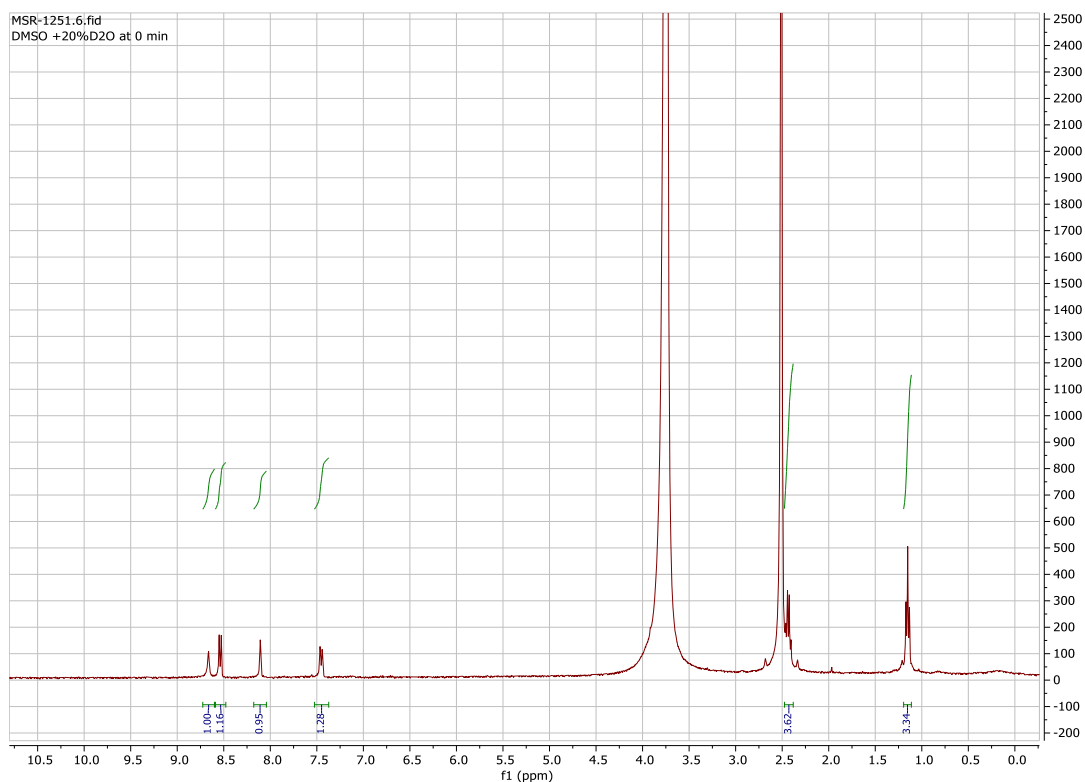


***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)acetamide (146):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

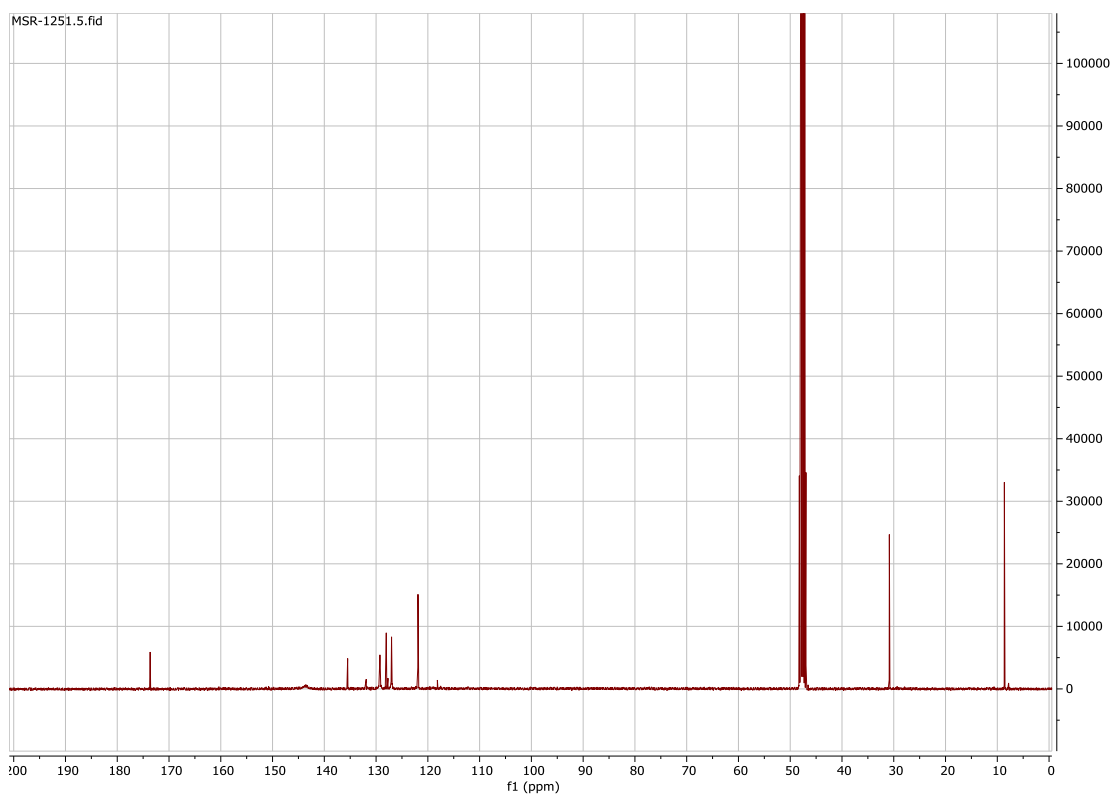




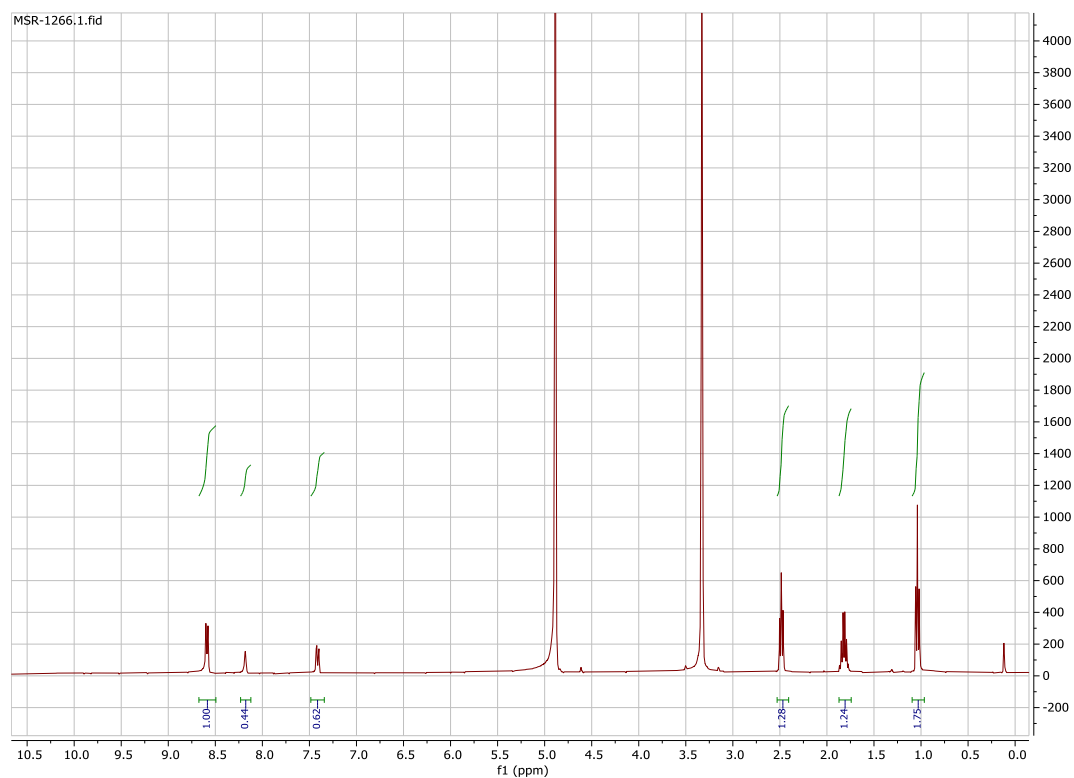
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)propionamide (147):<sup>1</sup>H NMR (400 MHz, DMSO+D<sub>2</sub>O)**



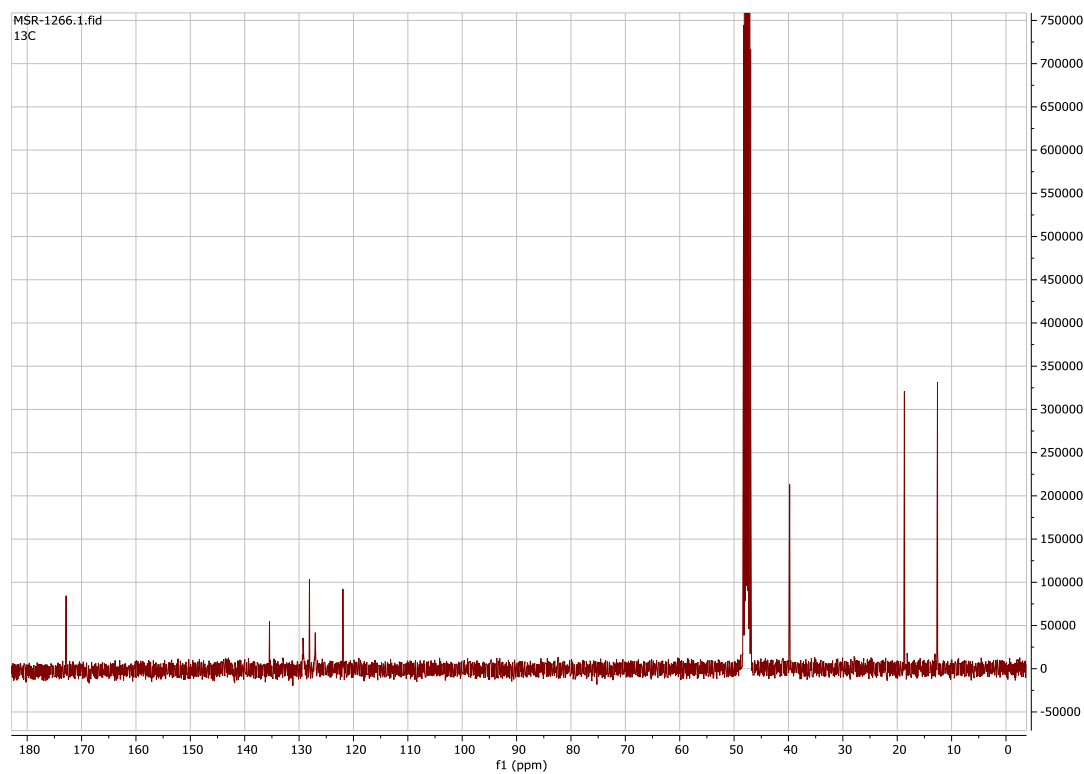
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)propionamide (147):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



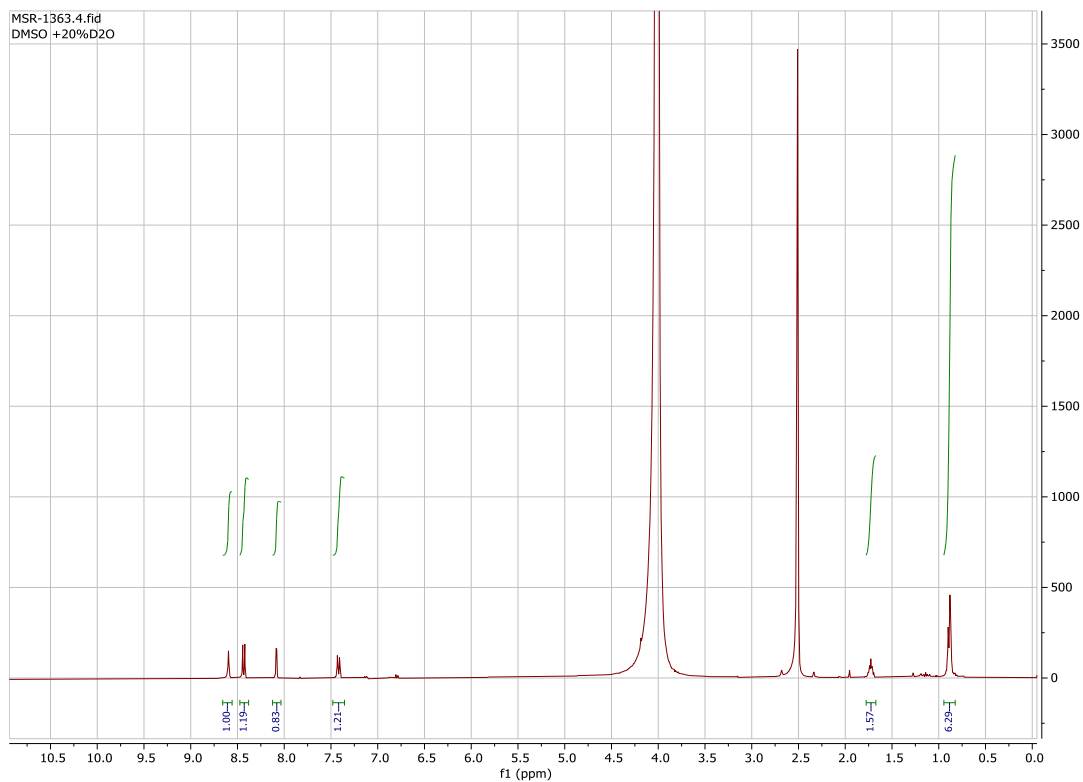
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)butyramide (148):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



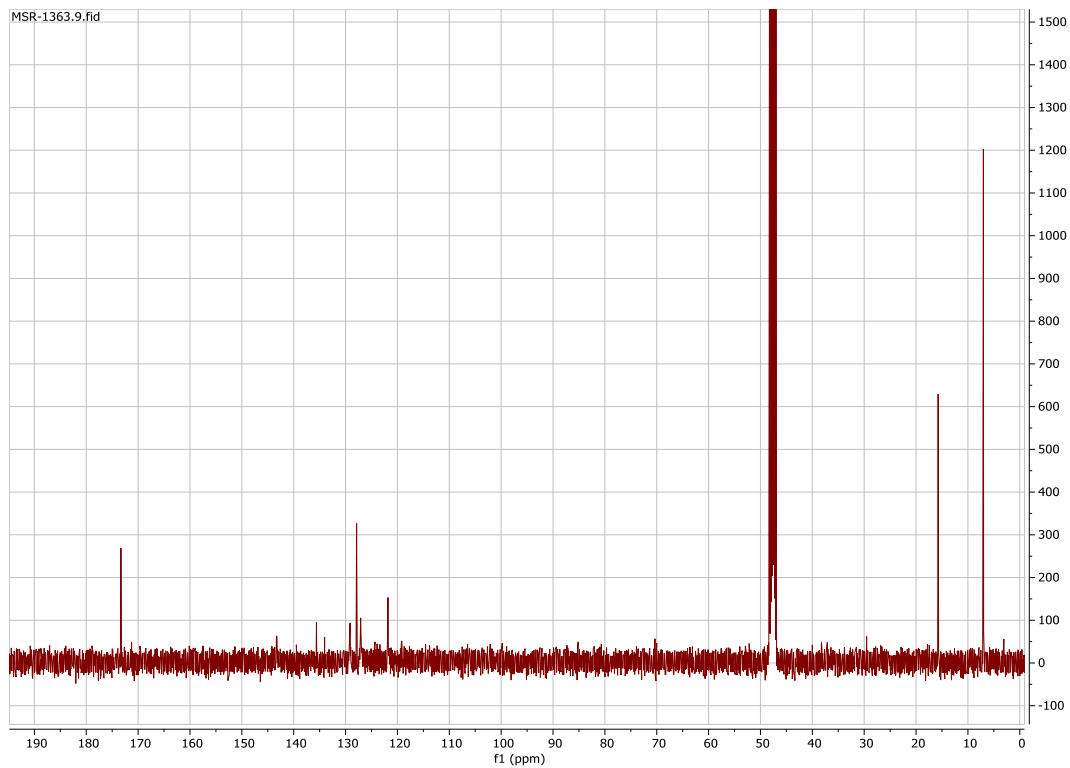
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)butyramide (148):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



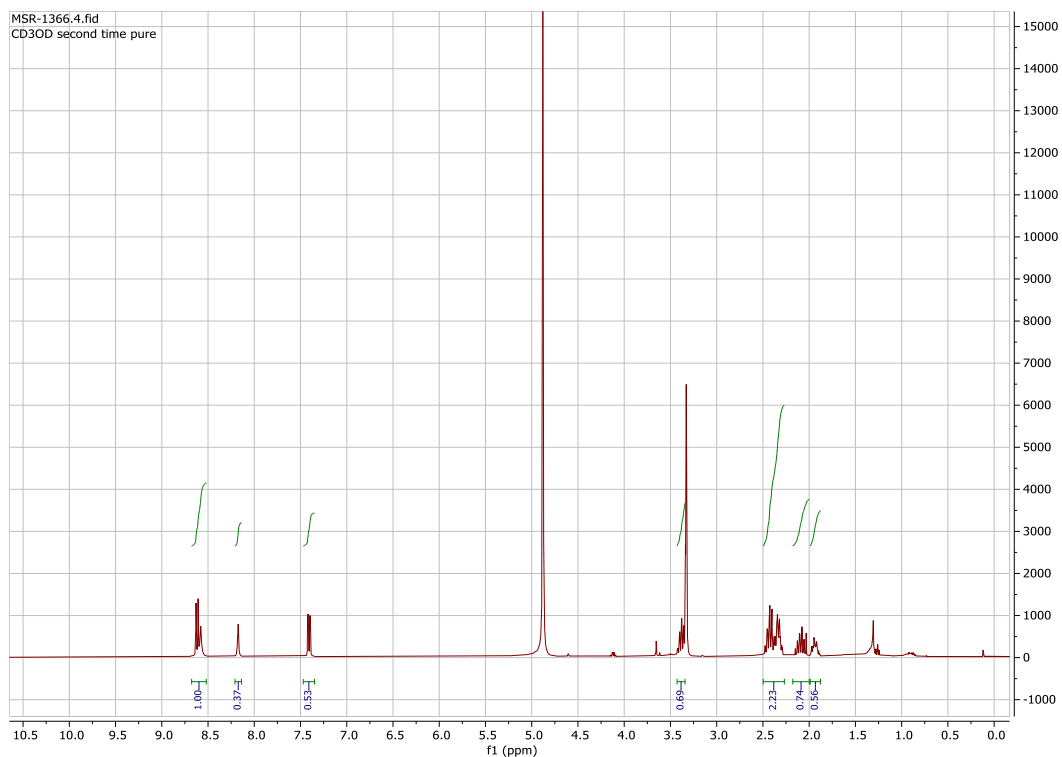
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)cyclopropanecarboxamide (149):<sup>1</sup>H NMR (400 MHz, DMSO+D<sub>2</sub>O)**



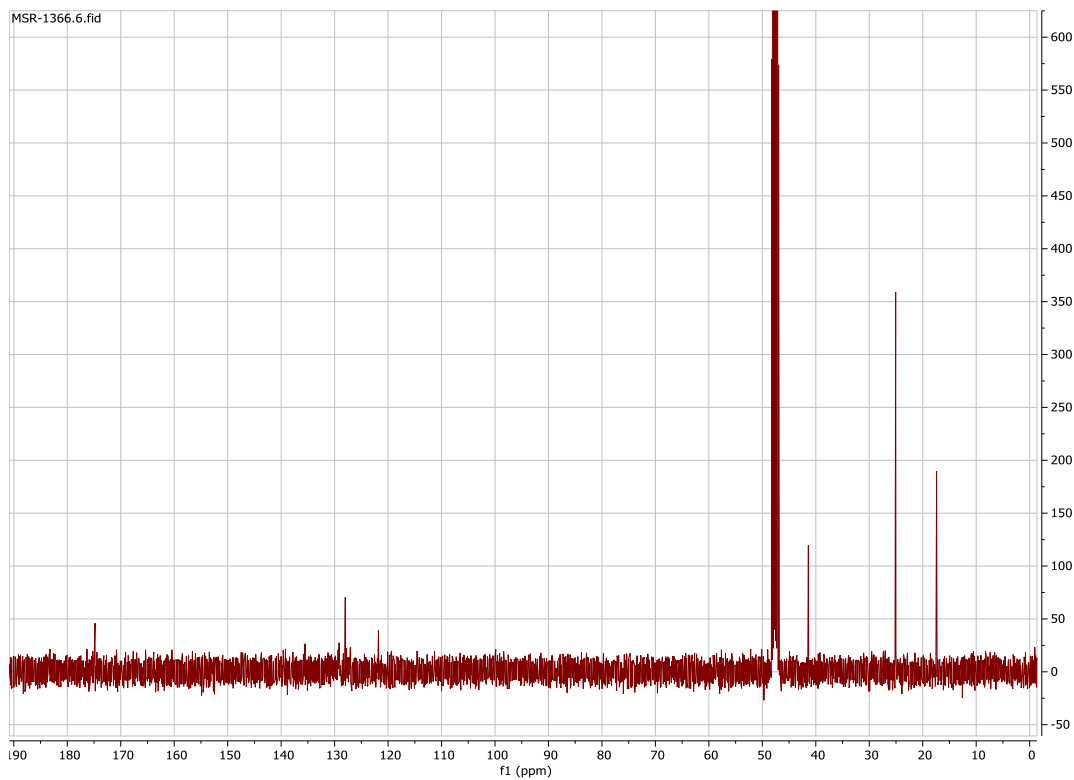
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)cyclopropanecarboxamide (149):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



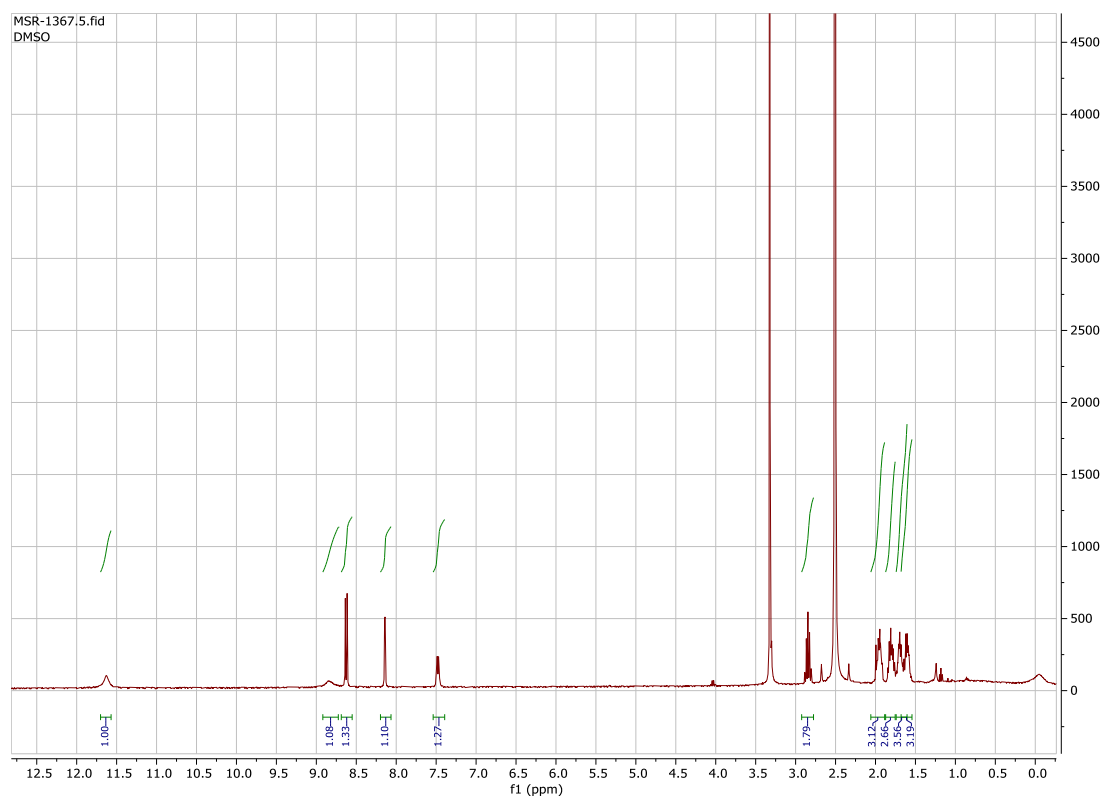
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)cyclobutanecarboxamide (150):<sup>1</sup>H NMR (400 MHz, DMSO)**



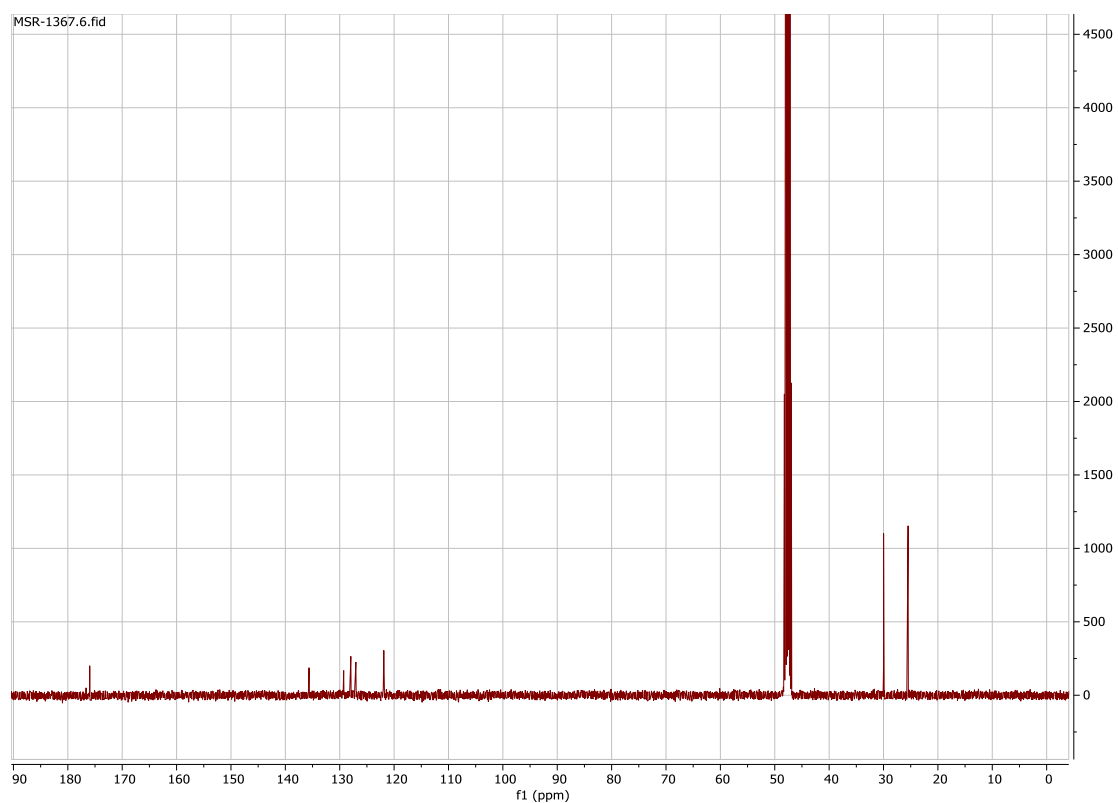
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)cyclobutanecarboxamide (150):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



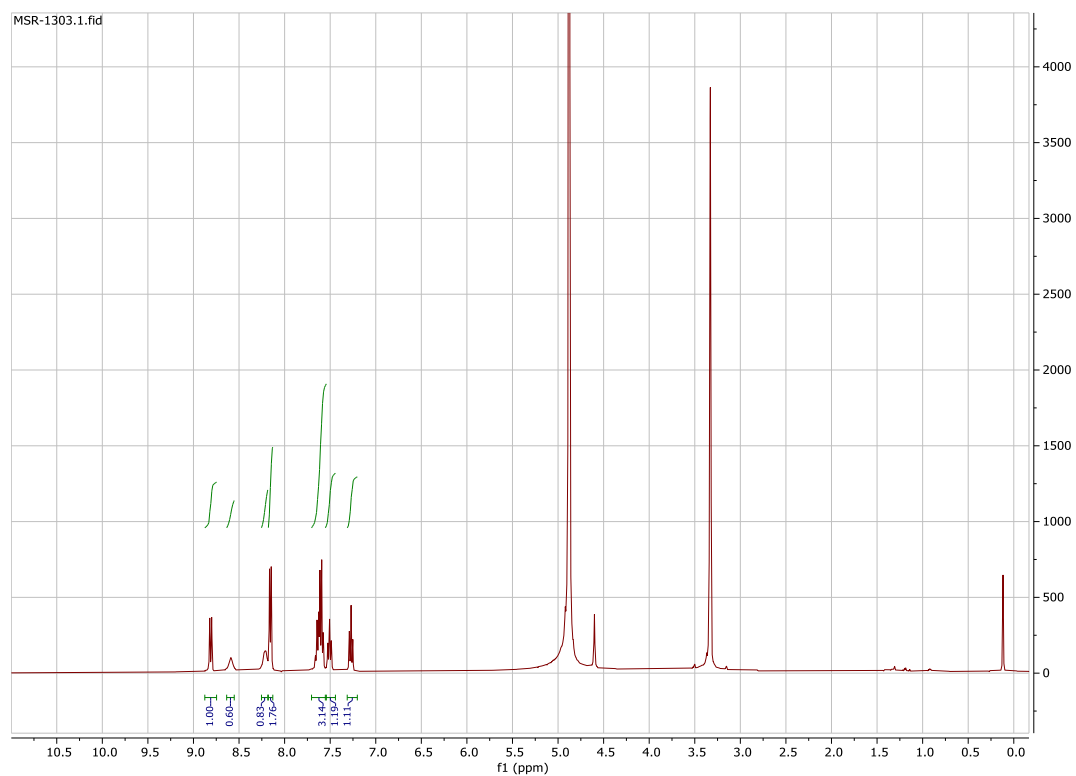
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)cyclopentanecarboxamide (151):<sup>1</sup>H NMR (400 MHz, DMSO)**



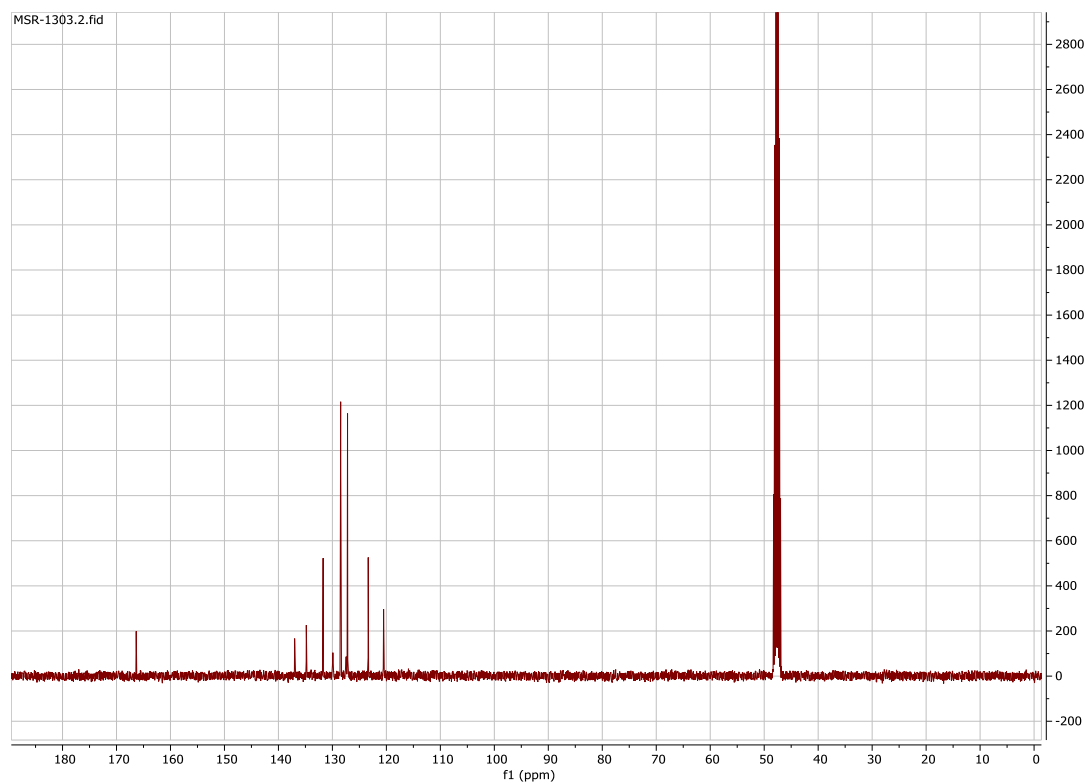
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)cyclopentanecarboxamide (151):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



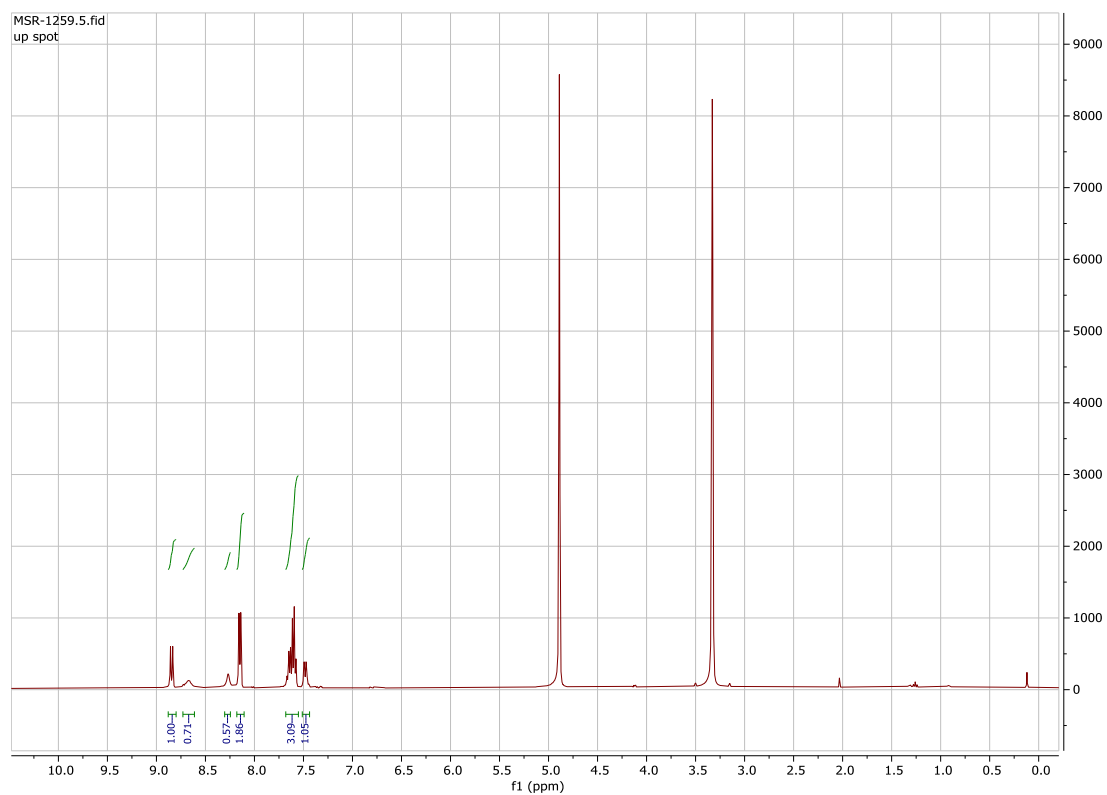
***N*-(2-(1*H*-1,2,4-Triazol-3-yl)phenyl)benzamide (152):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



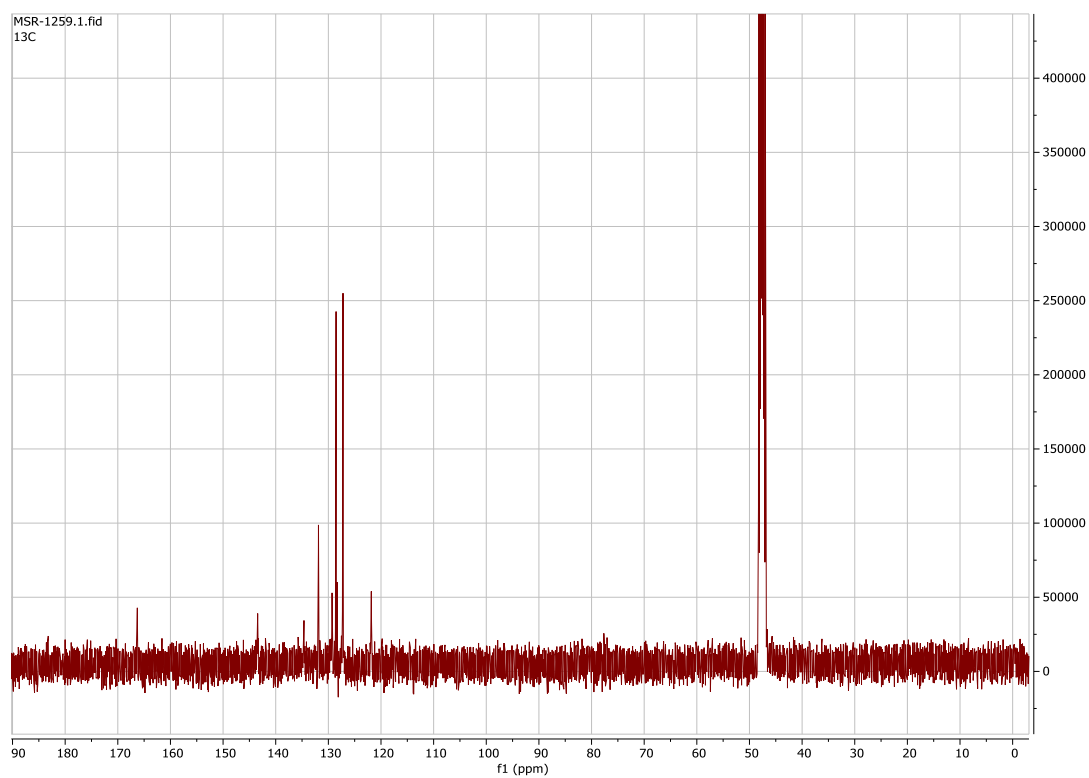
***N*-(2-(1*H*-1,2,4-Triazol-3-yl)phenyl)benzamide (152):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



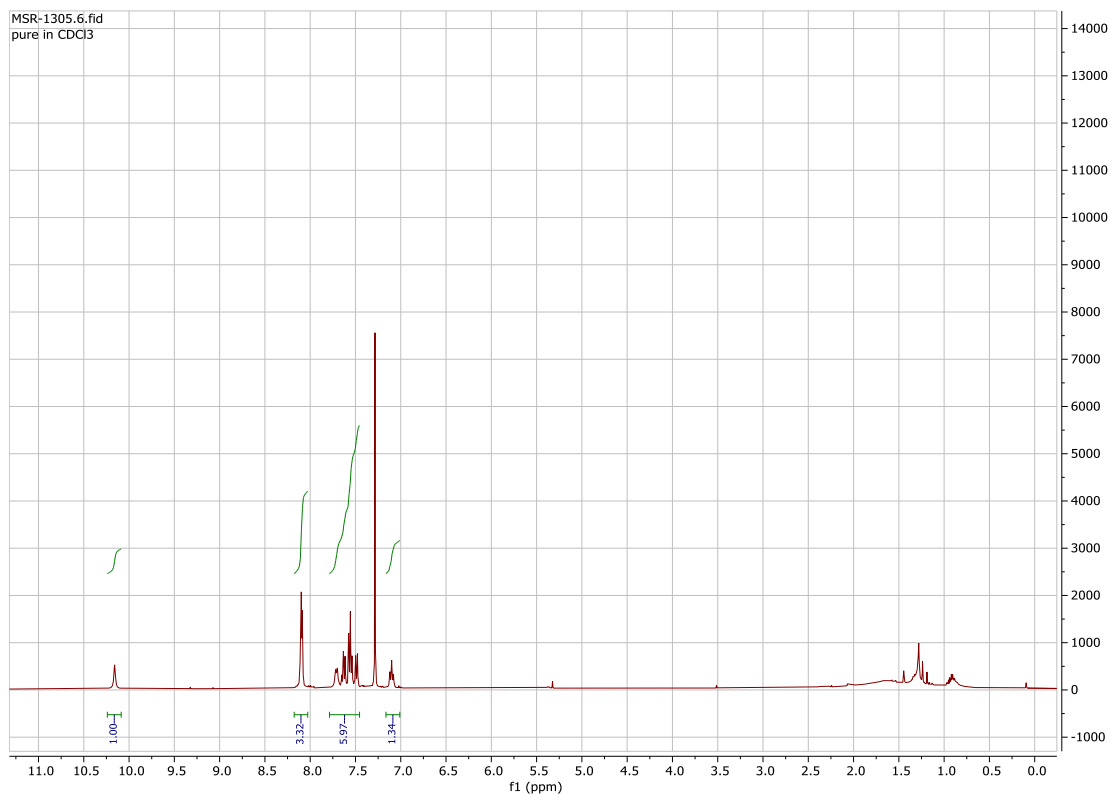
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)benzamide (153):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



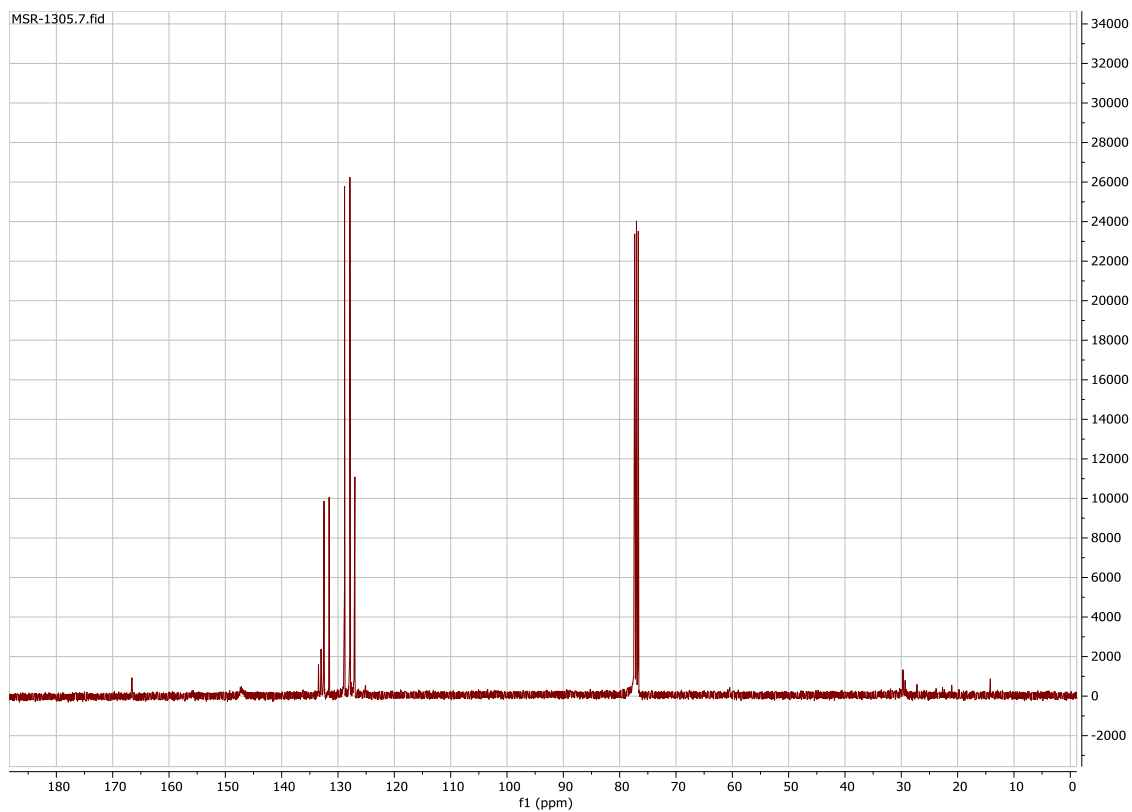
***N*-(4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)phenyl)benzamide (153):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



***N*-(2-Chloro-6-(1*H*-1,2,4-triazol-3-yl)phenyl)benzamide (154):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**

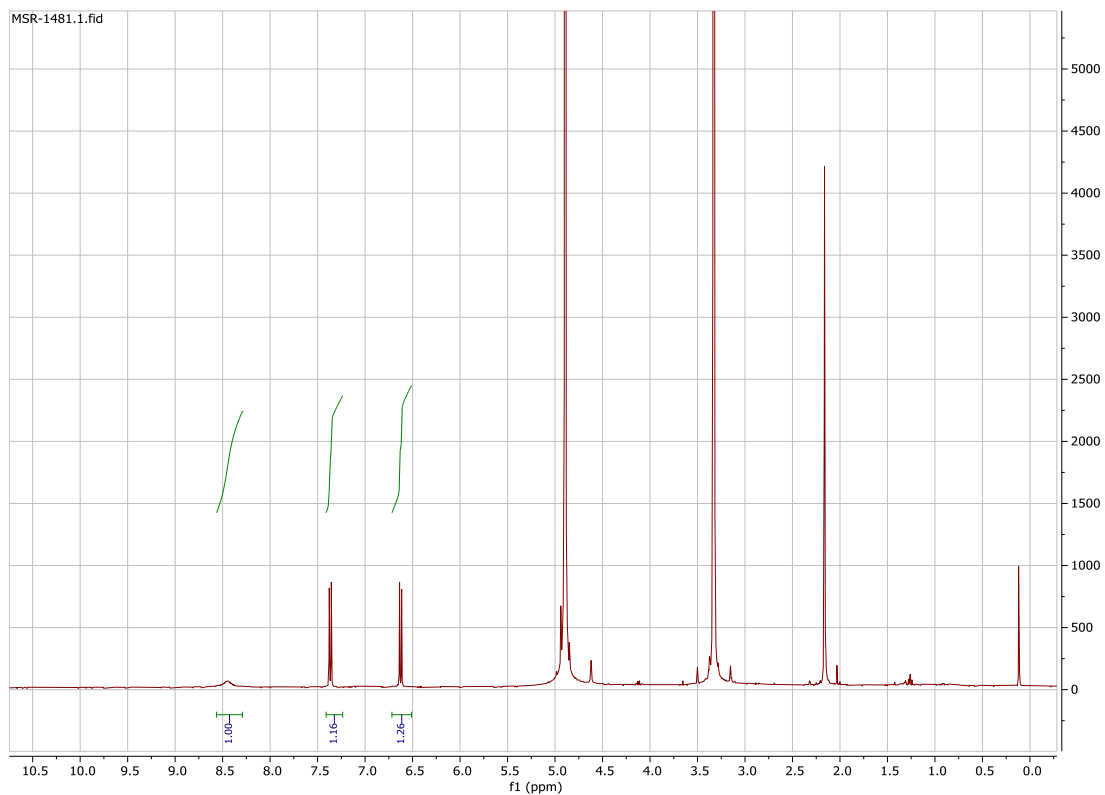


***N*-(2-Chloro-6-(1*H*-1,2,4-triazol-3-yl)phenyl)benzamide (154):<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)**

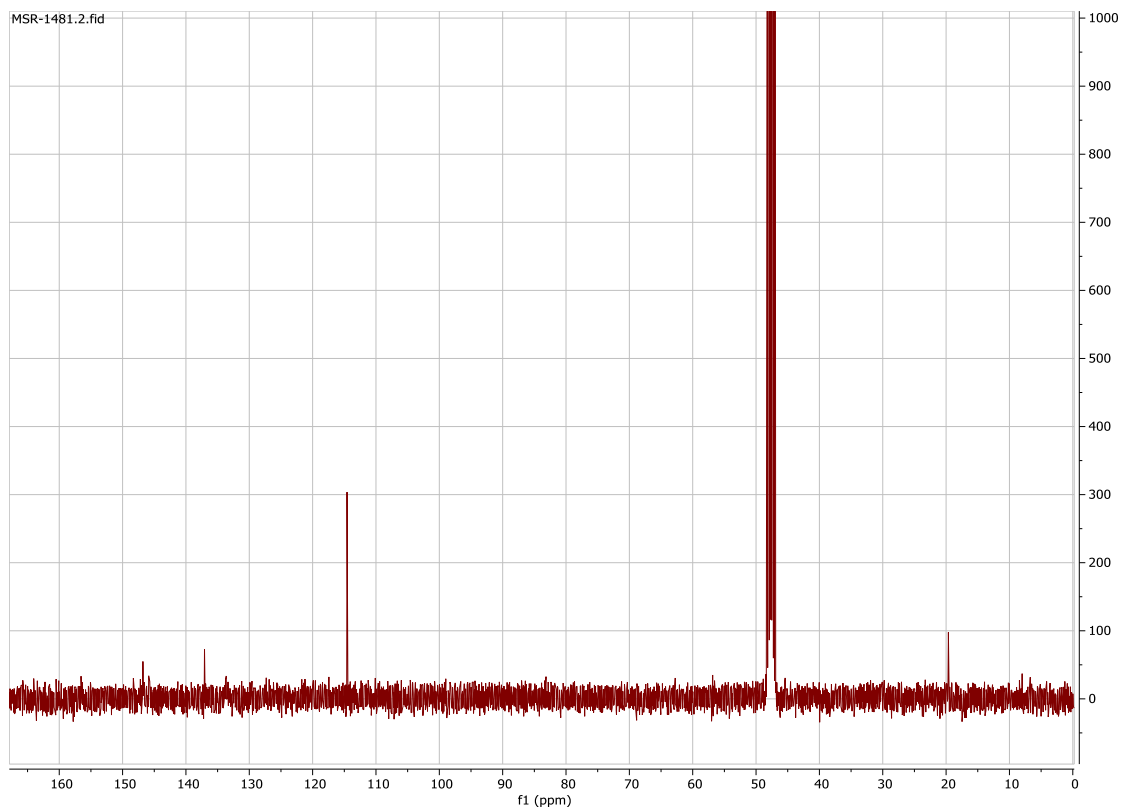




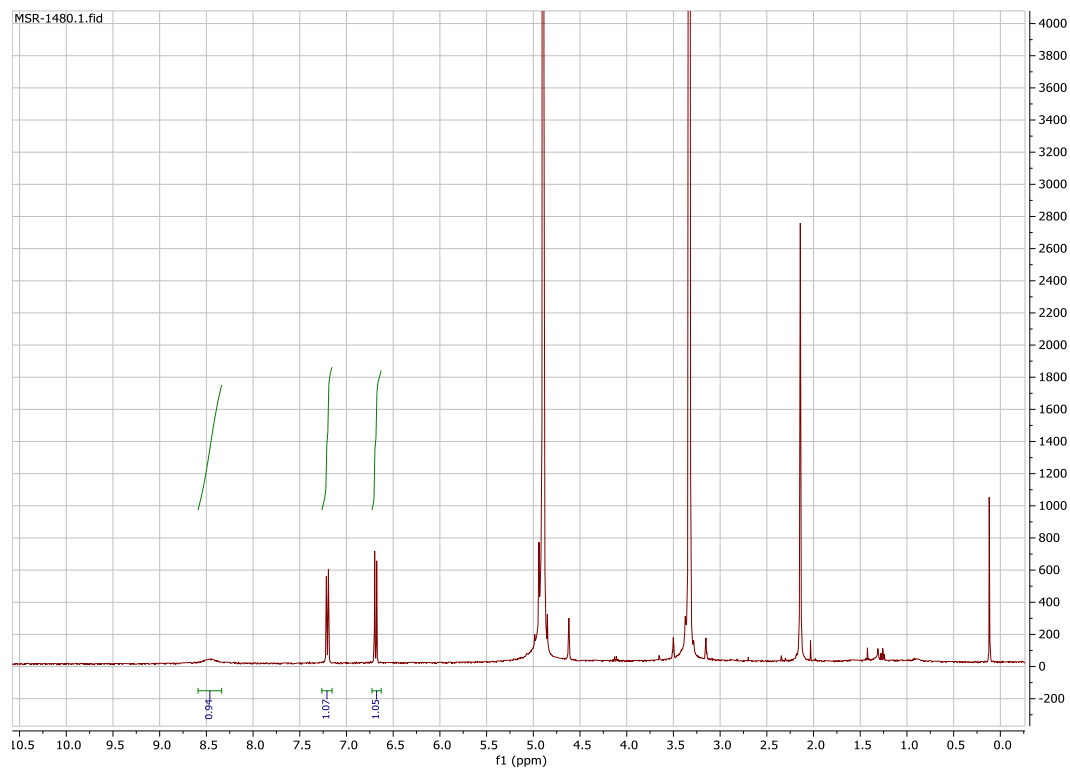
**4-Bromo-3-methyl-2-(1H-1,2,4-triazol-3-yl)aniline (155):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



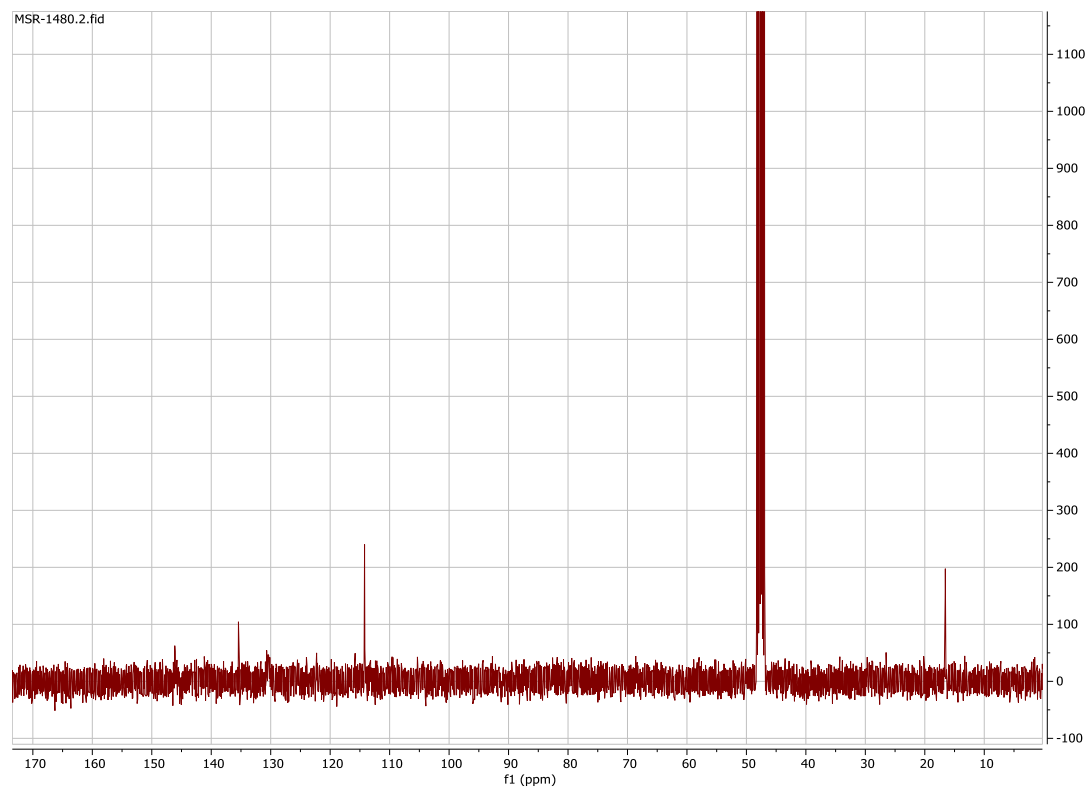
**4-Bromo-3-methyl-2-(1H-1,2,4-triazol-3-yl)aniline (155):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



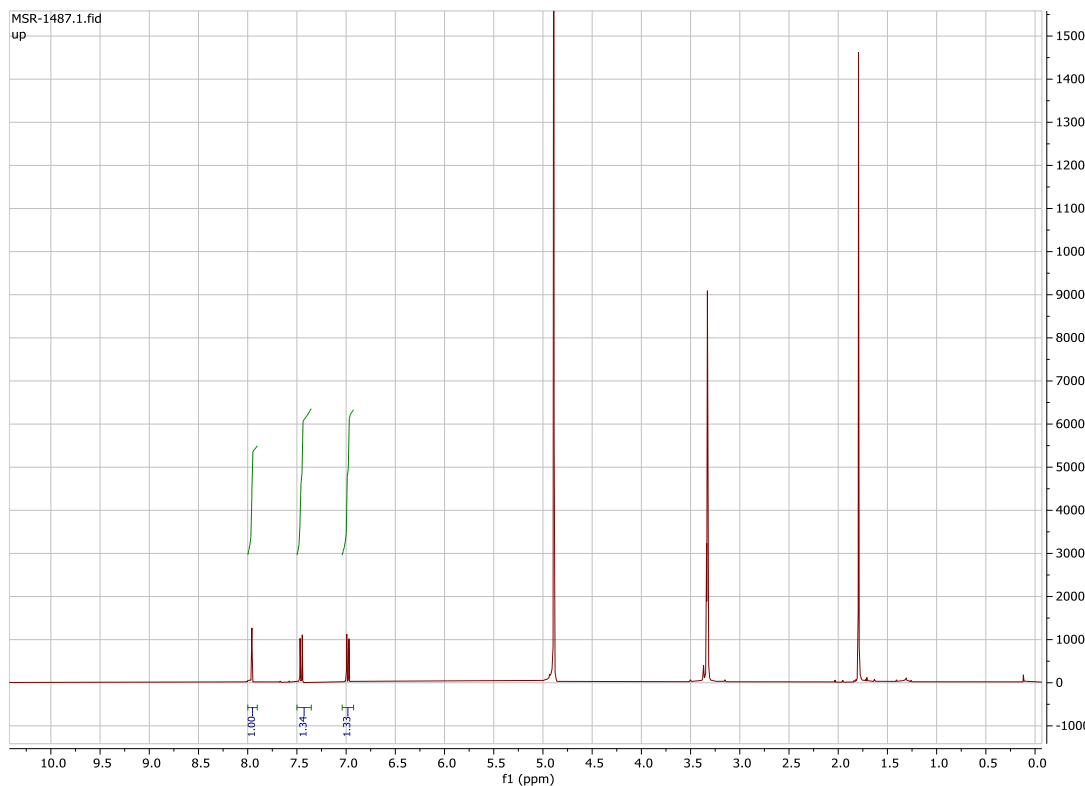
**4-Chloro-3-methyl-2-(1*H*-1,2,4-triazol-3-yl)aniline (156):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



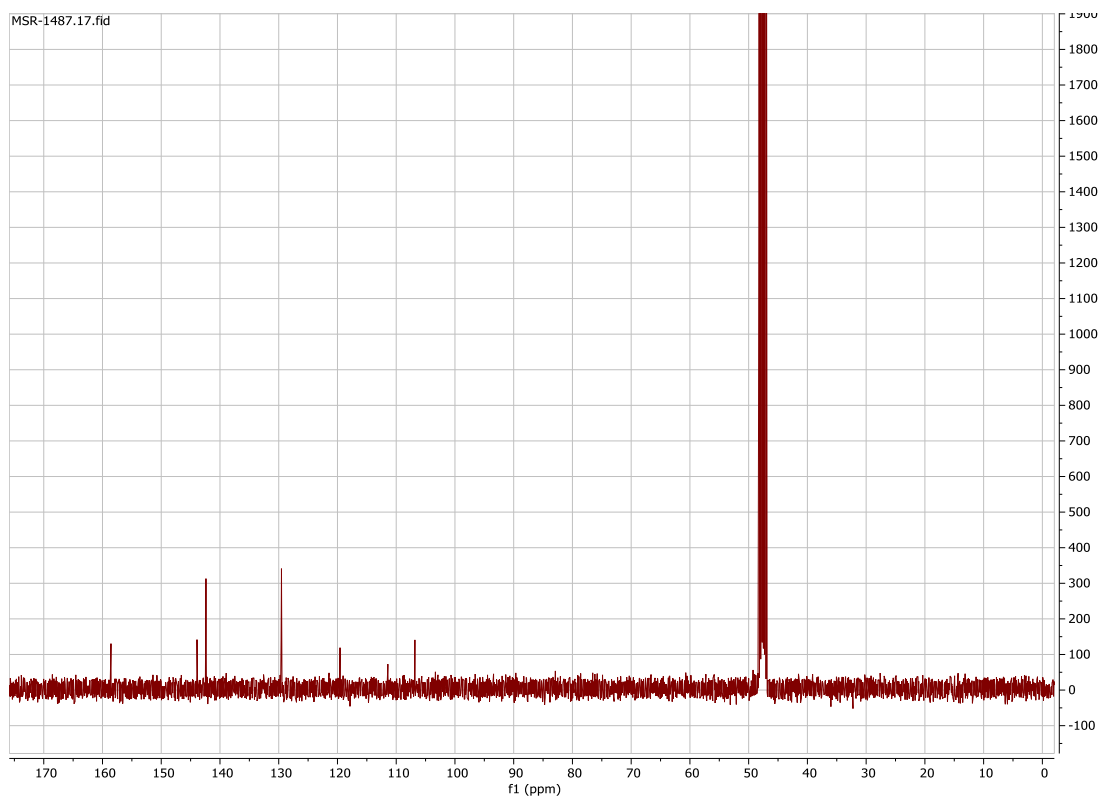
**4-Chloro-3-methyl-2-(1*H*-1,2,4-triazol-3-yl)aniline (156):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



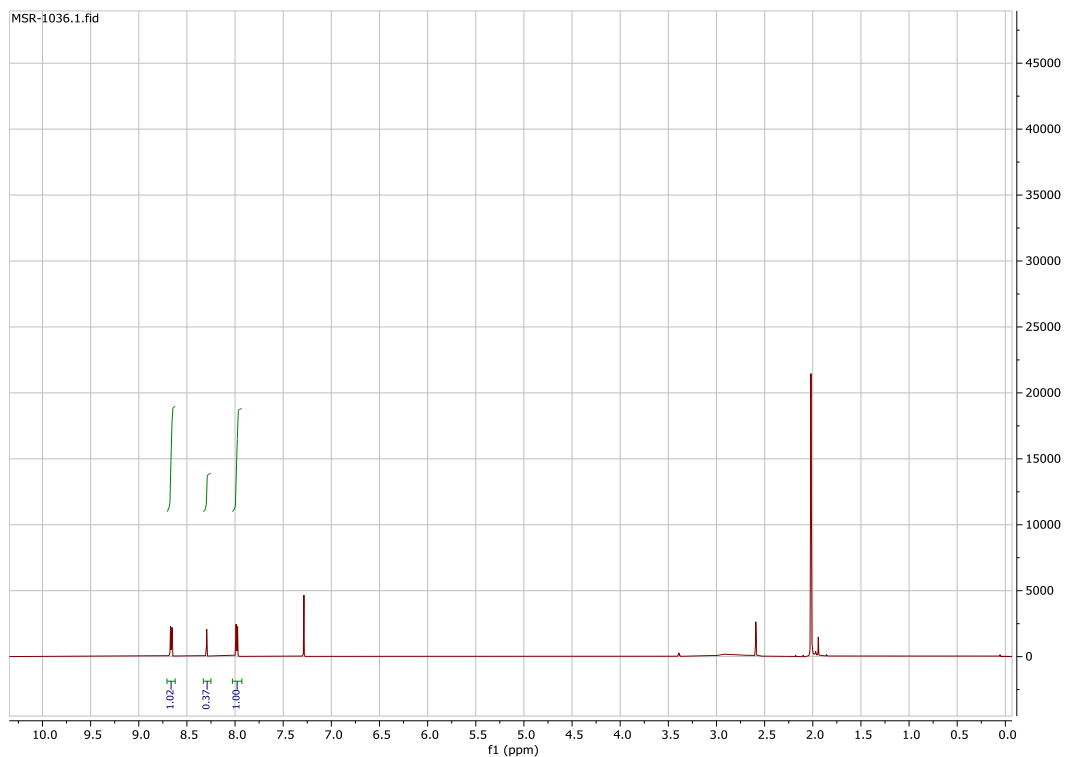
**4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)benzene-1,3-diamine (157):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



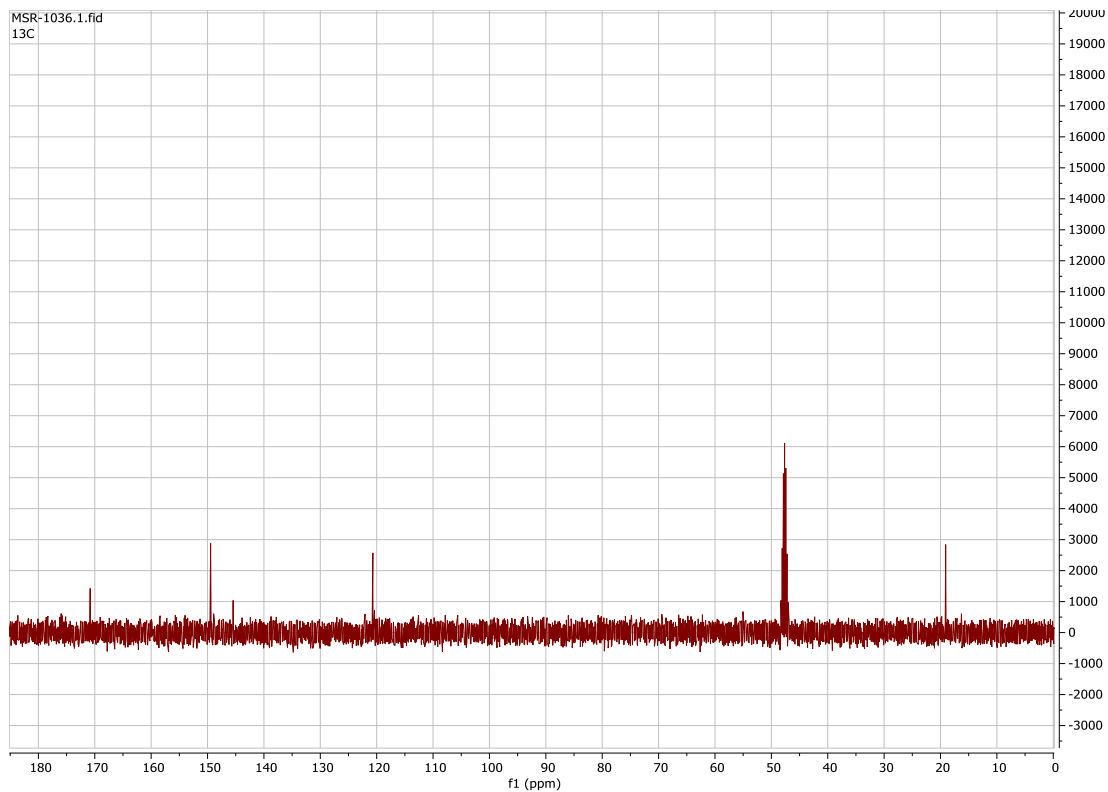
**4-Chloro-2-(1*H*-1,2,4-triazol-3-yl)benzene-1,3-diamine (157):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



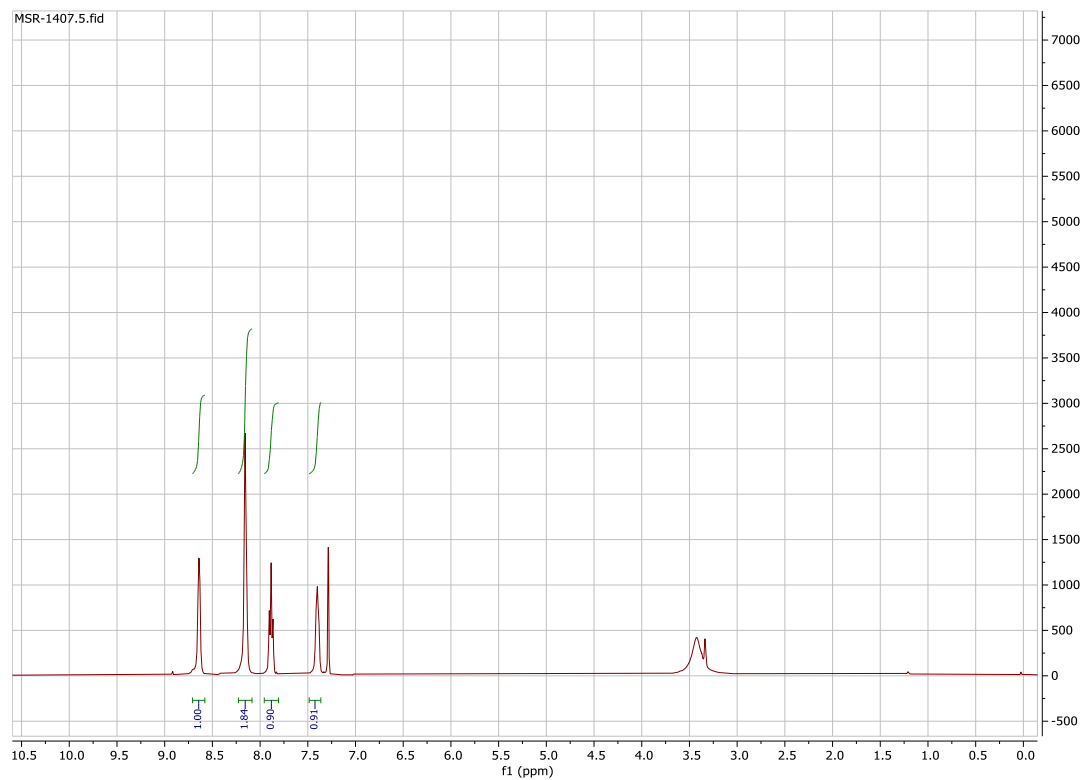
**4-(1*H*-1,2,4-Triazol-3-yl)pyridine (158):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



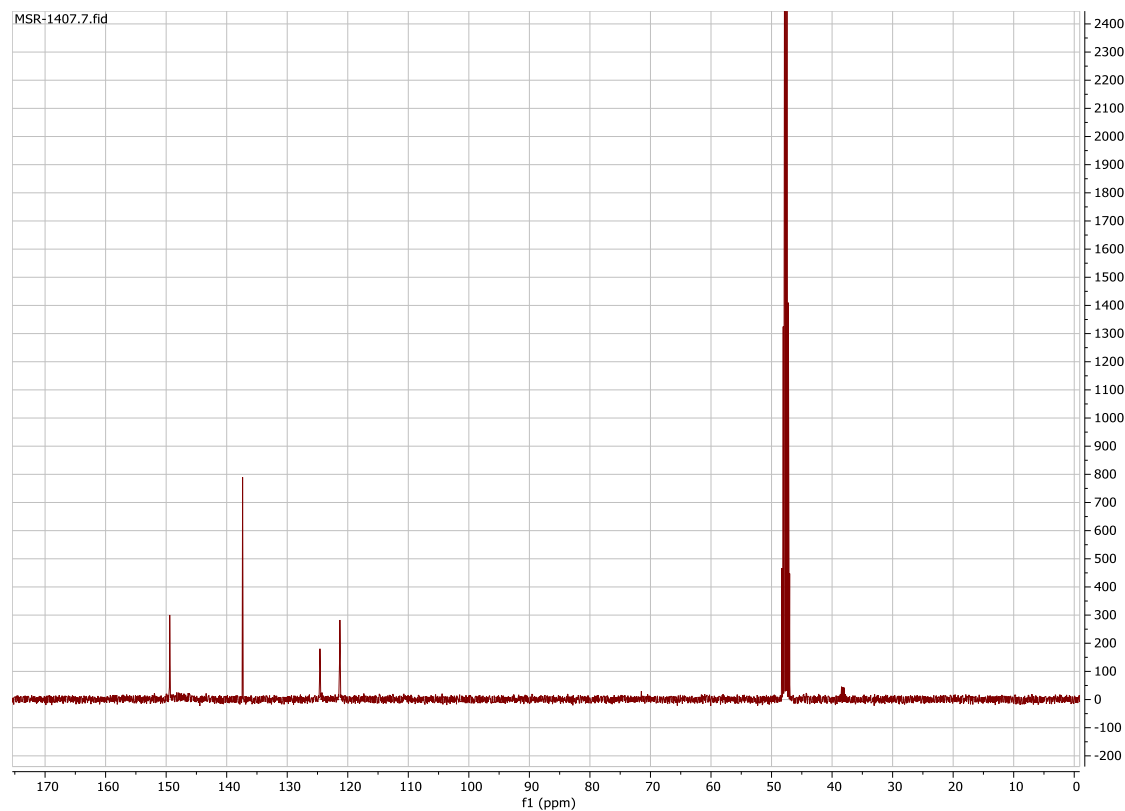
**4-(1*H*-1,2,4-Triazol-3-yl)pyridine (158):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



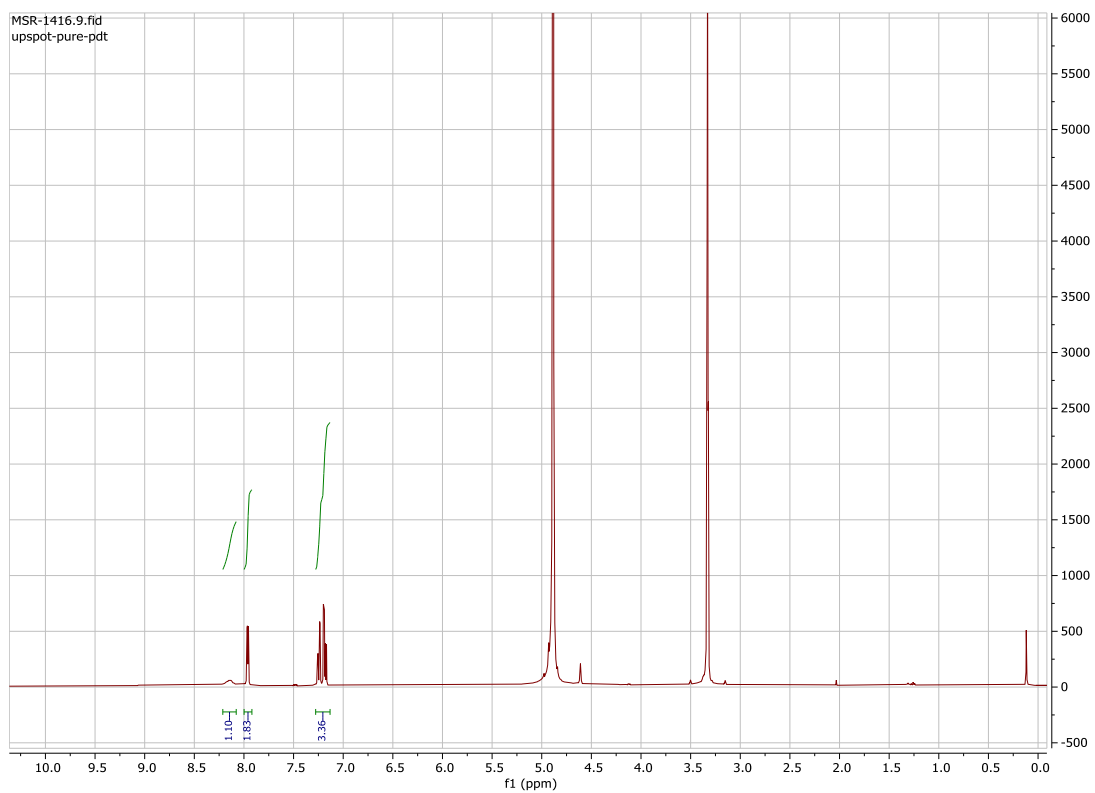
**2-(1H-1,2,4-Triazol-3-yl)pyridine (159):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



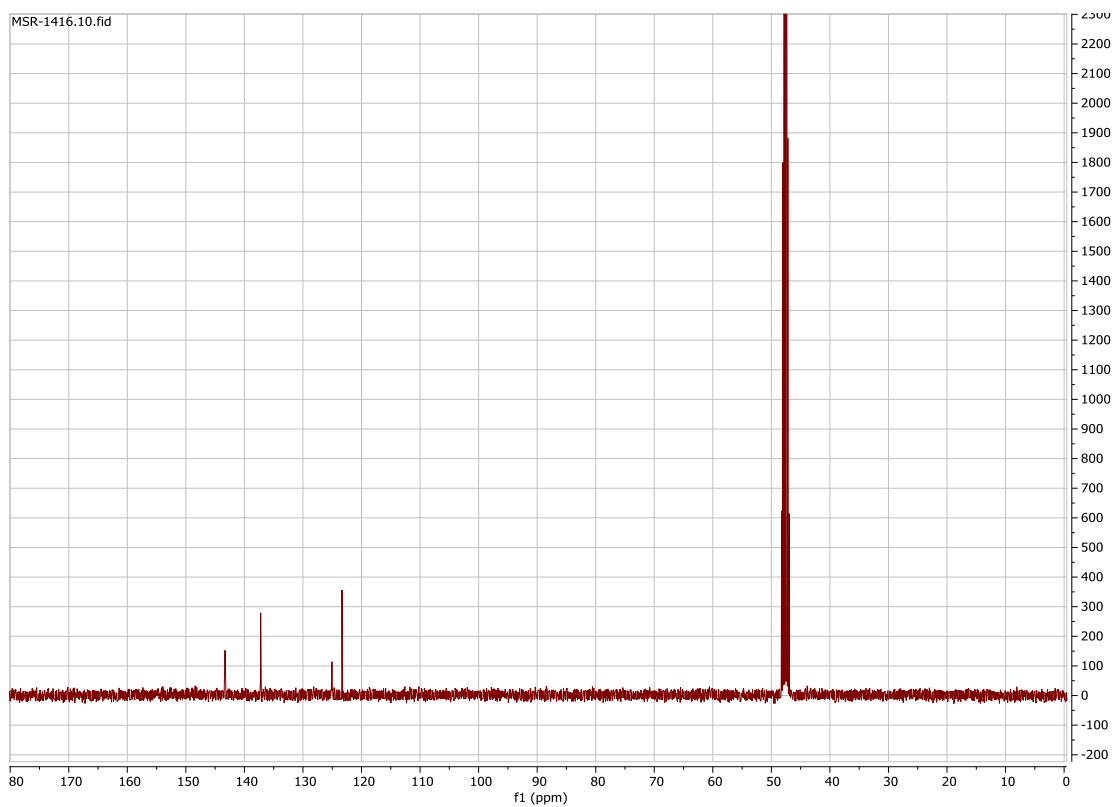
**2-(1H-1,2,4-Triazol-3-yl)pyridine (159):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



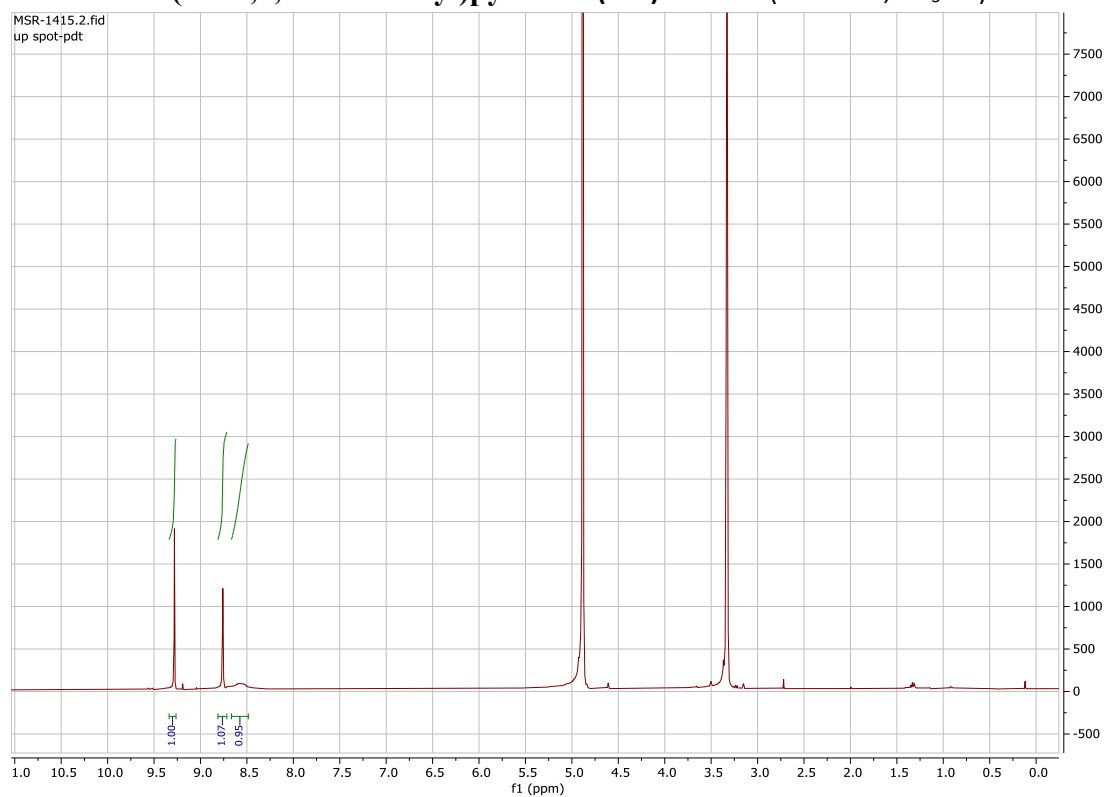
**2-(1H-1,2,4-Triazol-3-yl)pyridine-3-amine (160):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



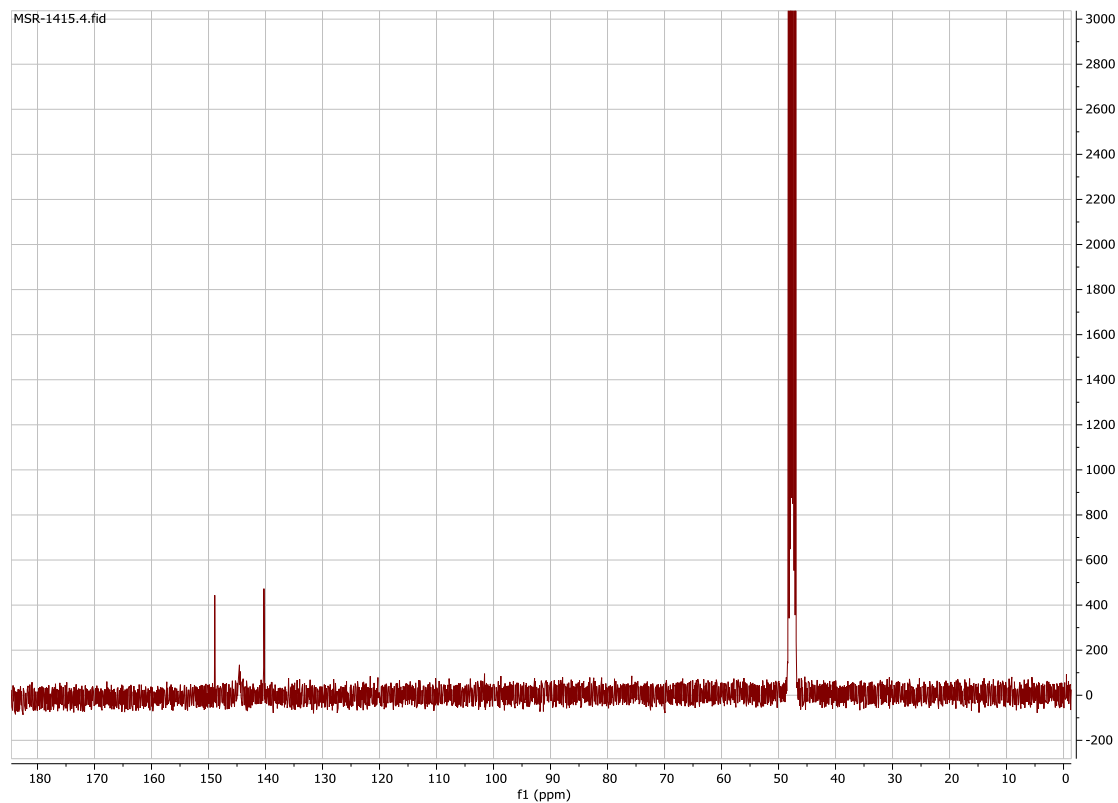
**2-(1H-1,2,4-Triazol-3-yl)pyridine-3-amine (160):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



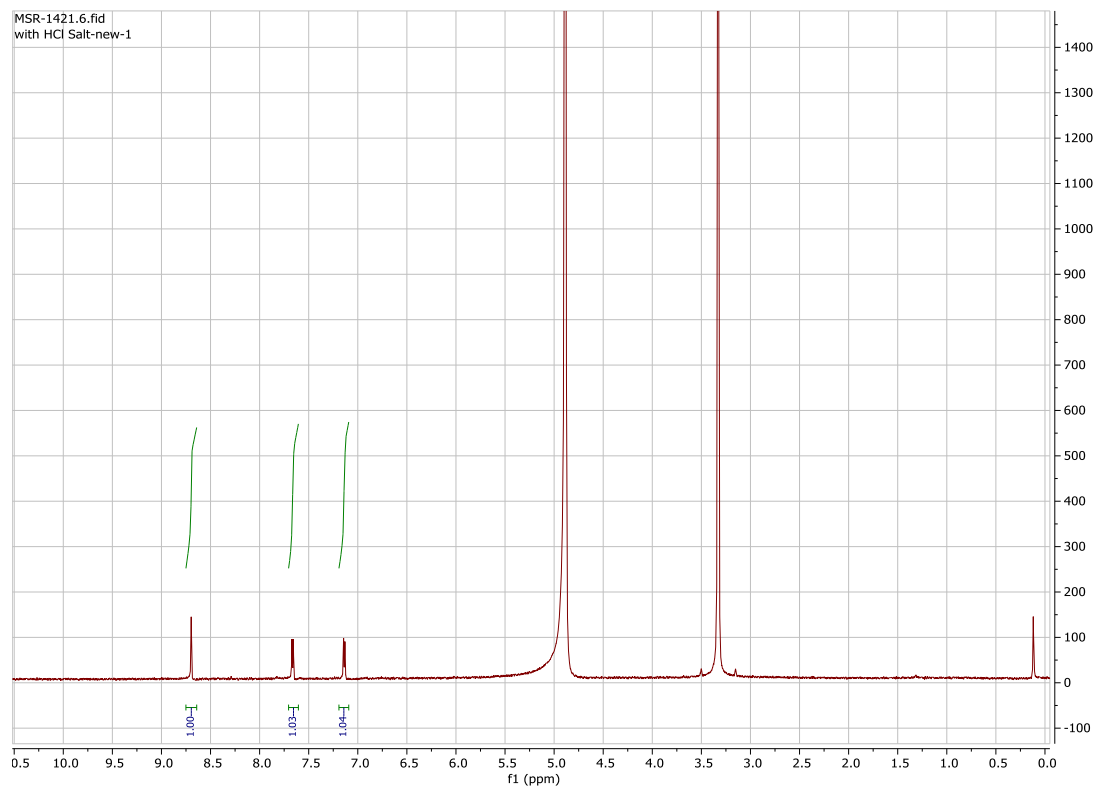
**2-Chloro-6-(1H-1,2,4-triazol-3-yl)pyrazine (161):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**



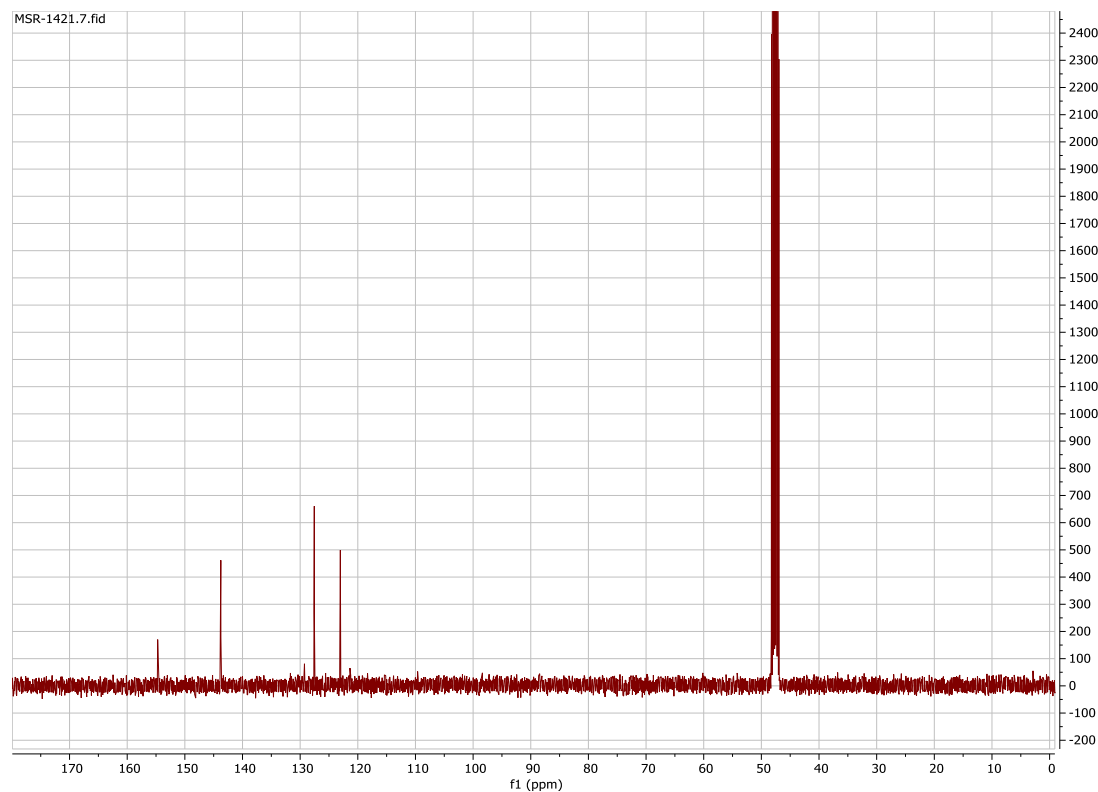
**2-Chloro-6-(1H-1,2,4-triazol-3-yl)pyrazine (161):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



**2-(1*H*-1,2,4-Triazol-3-yl)thiophen-3-amine (162):<sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)**

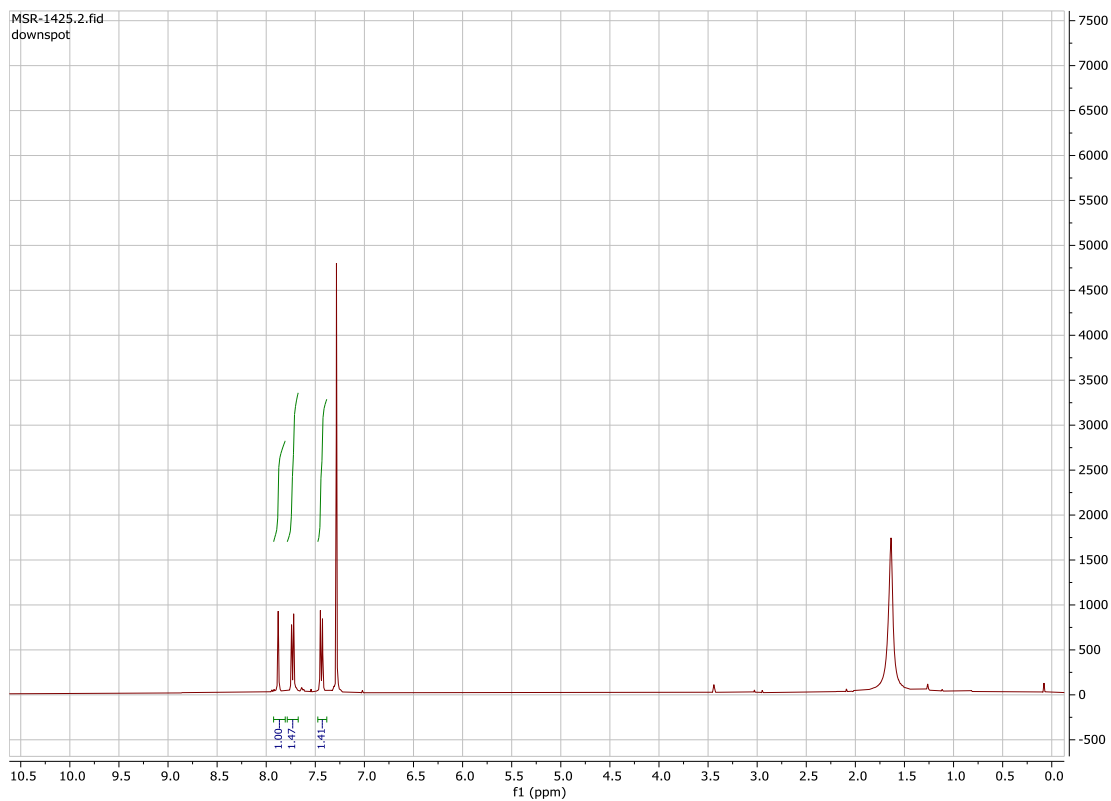


**2-(1*H*-1,2,4-Triazol-3-yl)thiophen-3-amine (162):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**

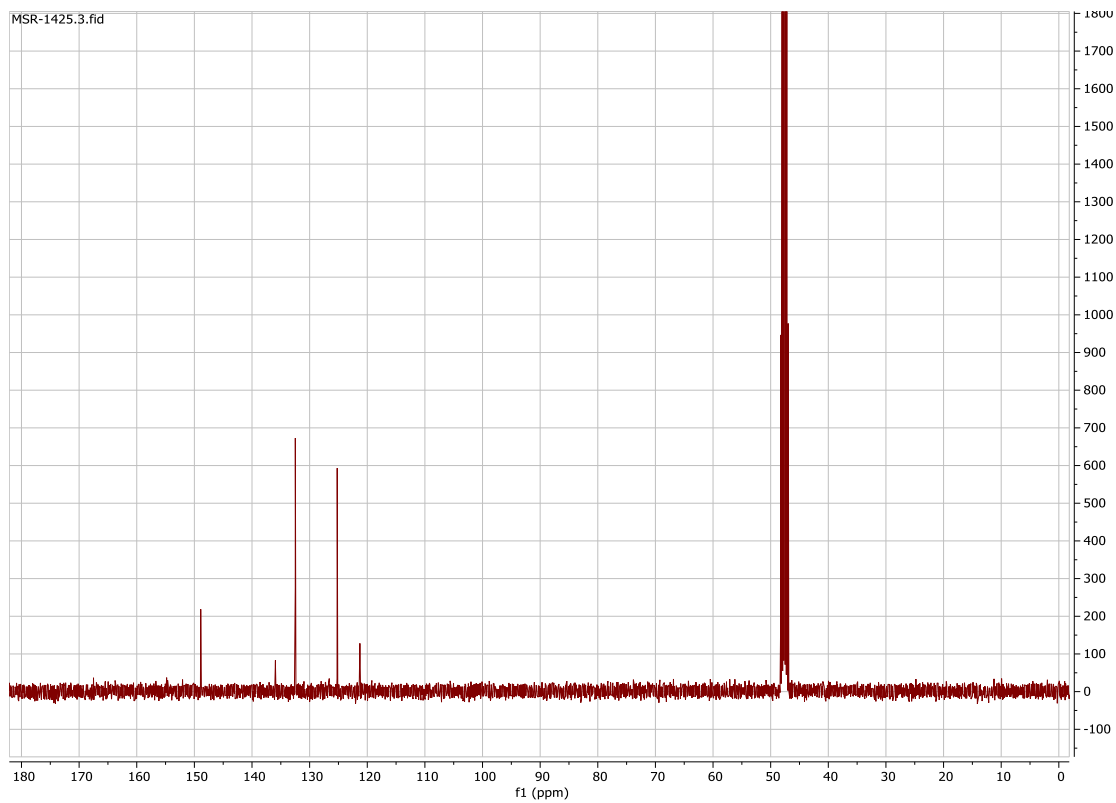




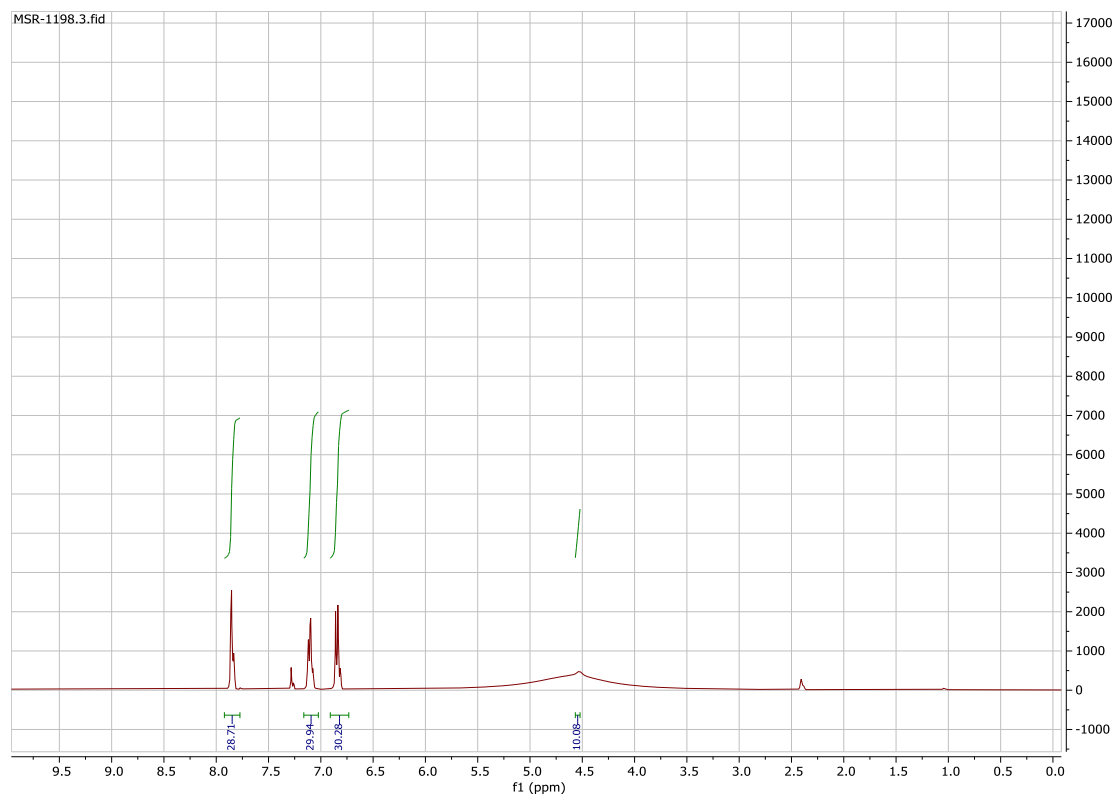
***N*-(4-Bromophenyl)-4*H*-1,2,4-triazol-3-amine (166):<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)**



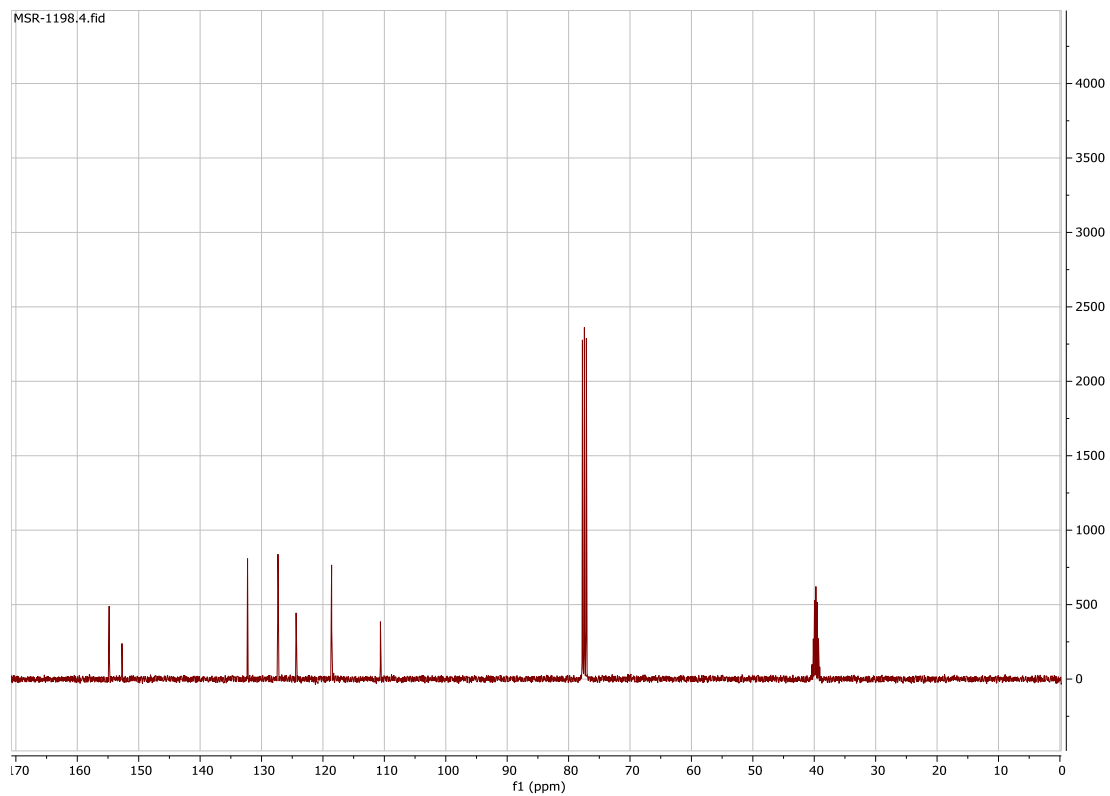
***N*-(4-Bromophenyl)-4*H*-1,2,4-triazol-3-amine (166):<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD)**



2-((1,9a-dihydrobenzo[4,5]thiazolo[2,3-c][1,2,4]triazol-3-yl)thio)acetamide (168):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



2-((1,9a-dihydrobenzo[4,5]thiazolo[2,3-c][1,2,4]triazol-3-yl)thio)acetamide (168):  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3:\text{CD}_3\text{OD}$ )



## References

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- (3) Röhrig, U. F.; Majjigapu, S. R.; Caldelari, D.; Dilek, N.; Reichenbach, P.; Ascencao, K.; Irving, M.; Coukos, G.; Vogel, P.; Zoete, V.; Michielin, O. 1,2,3-Triazoles as inhibitors of indoleamine 2,3-dioxygenase 2 (IDO2). *Bioorg. Med. Chem. Lett.* **2016**, *26*, 4330–3.
- (4) Röhrig, U. F.; Majjigapu, S. R.; Grosdidier, A.; Bron, S.; Stroobant, V.; Pilotte, L.; Colau, D.; Vogel, P.; Van den Eynde, B. J.; Zoete, V.; Michielin, O. Rational design of 4-aryl-1,2,3-triazoles for indoleamine 2,3-dioxygenase 1 inhibition. *J. Med. Chem.* **2012**, *55*, 5270–5290.