

## Supporting Information

### **Dihydropyrrole-3-thiones: one-pot synthesis from propargylamines, acyl chlorides and sodium sulfide**

Pavel A. Volkov, Kseniya O. Khrapova, Ekaterina M. Vyi, Anton A. Telezhkin,  
Ivan A. Bidusenko, Alexander I. Albanov, Elena Yu. Schmidt, Boris A. Trofimov\*

*A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of  
Sciences, 1 Favorsky St., Irkutsk 664033, Russian Federation*

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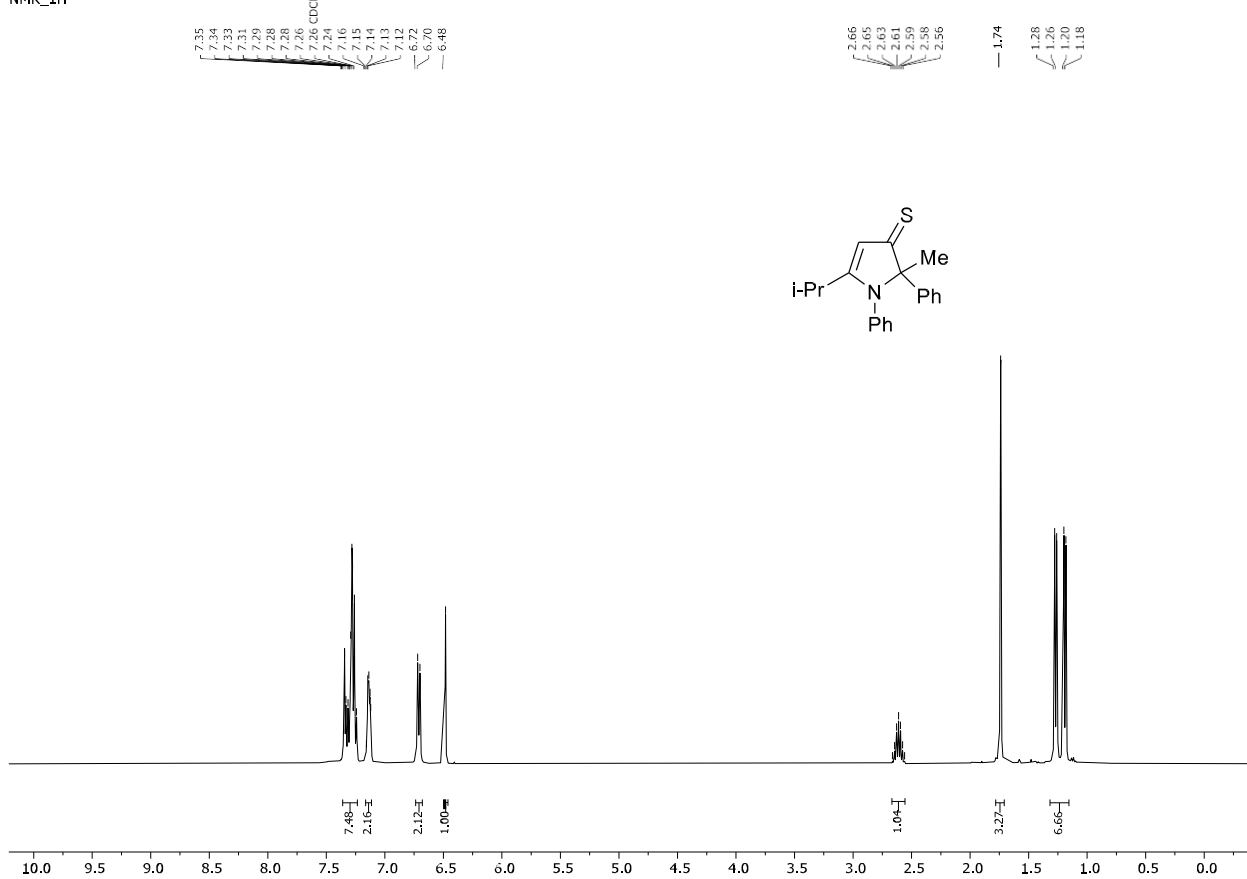
**1. NMR Spectra**

**S2**

# 1. NMR Spectra

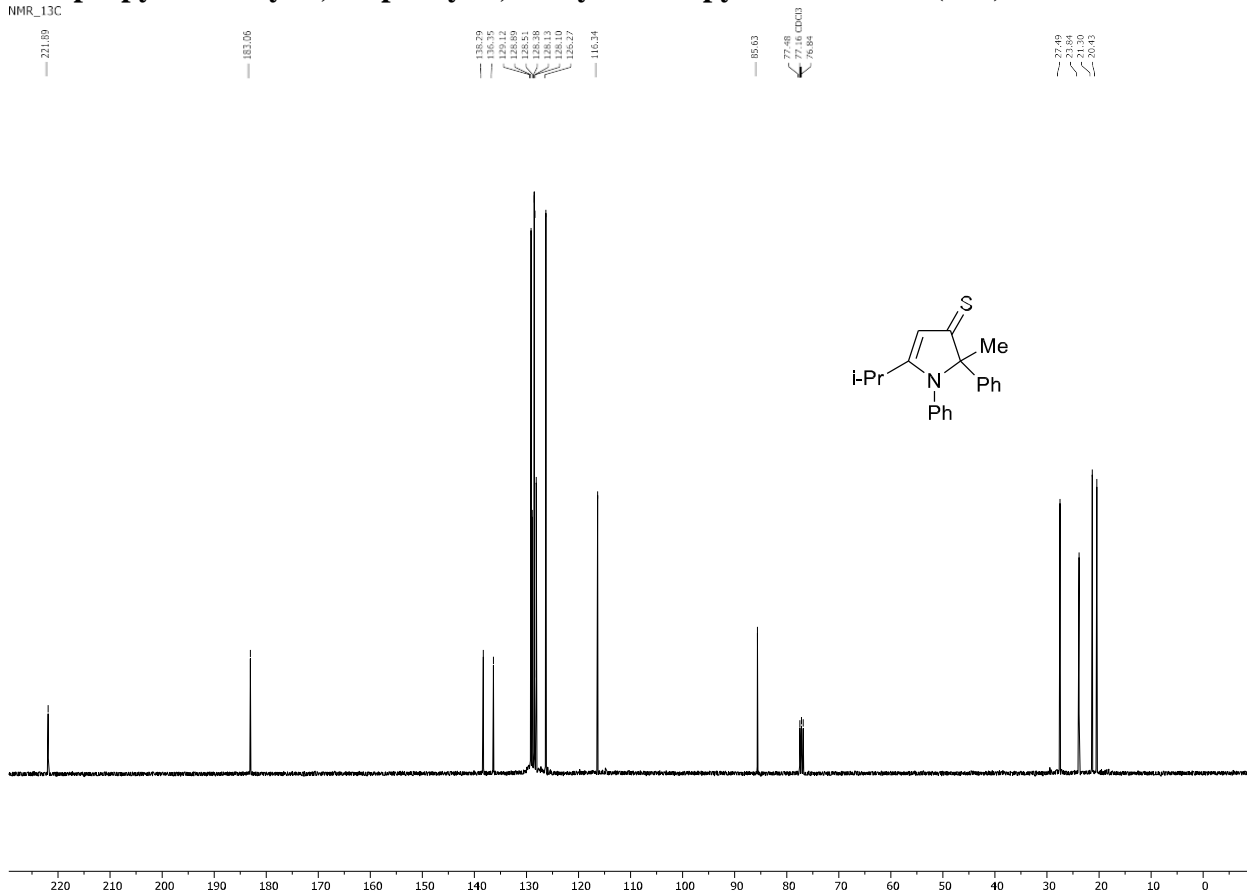
## 5-Isopropyl-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ab)

NMR\_1H



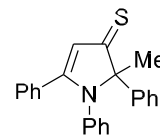
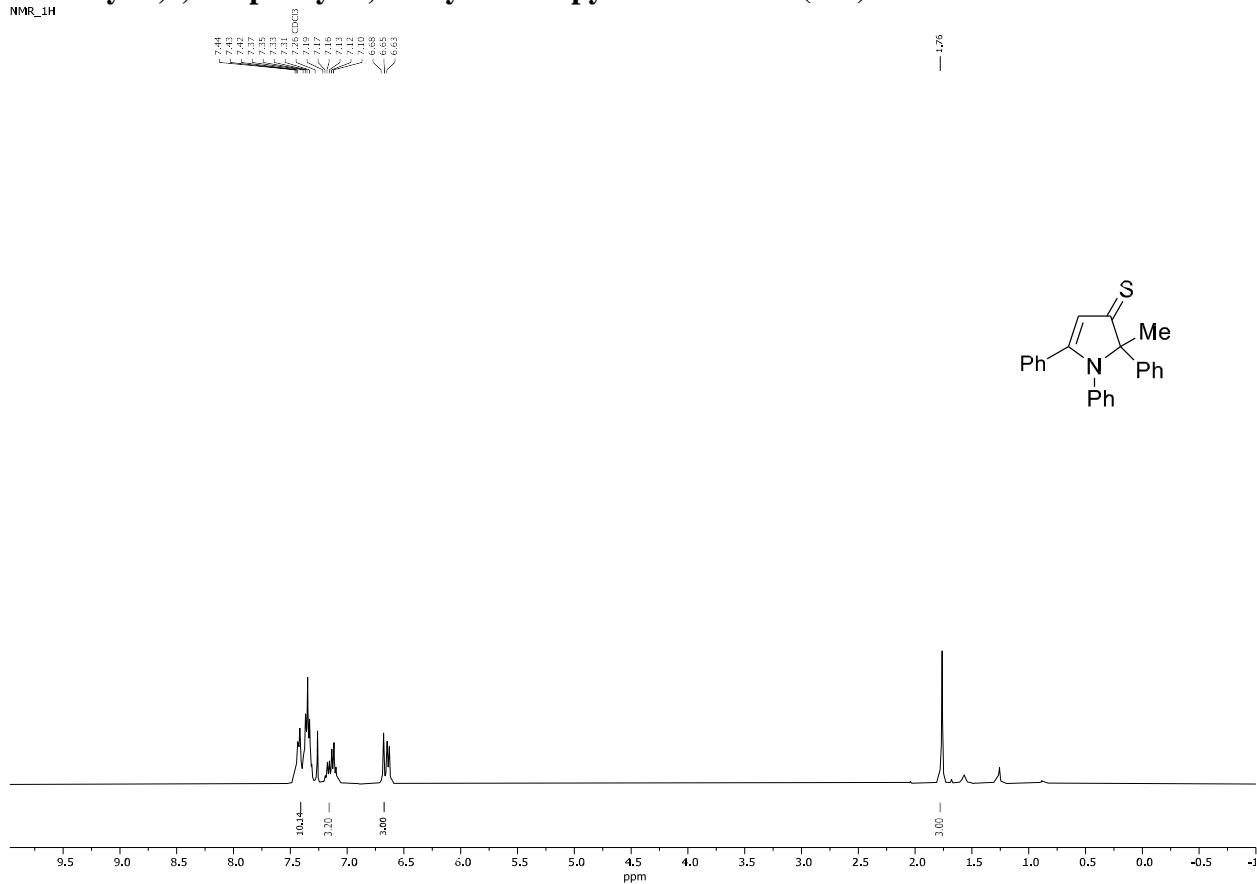
## 5-Isopropyl-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ab)

NMR\_13C



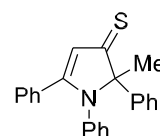
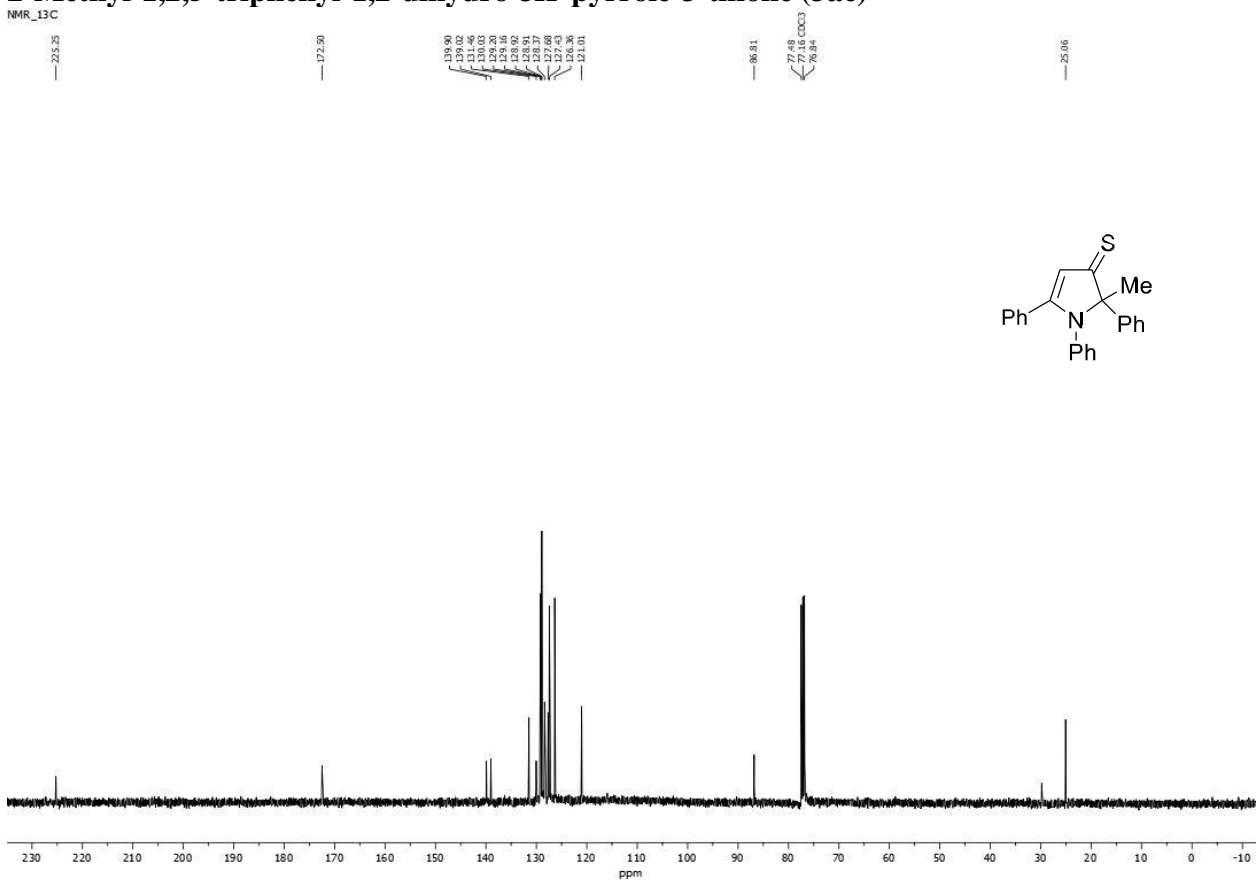
## 2-Methyl-1,2,5-triphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ac)

NMR\_1H



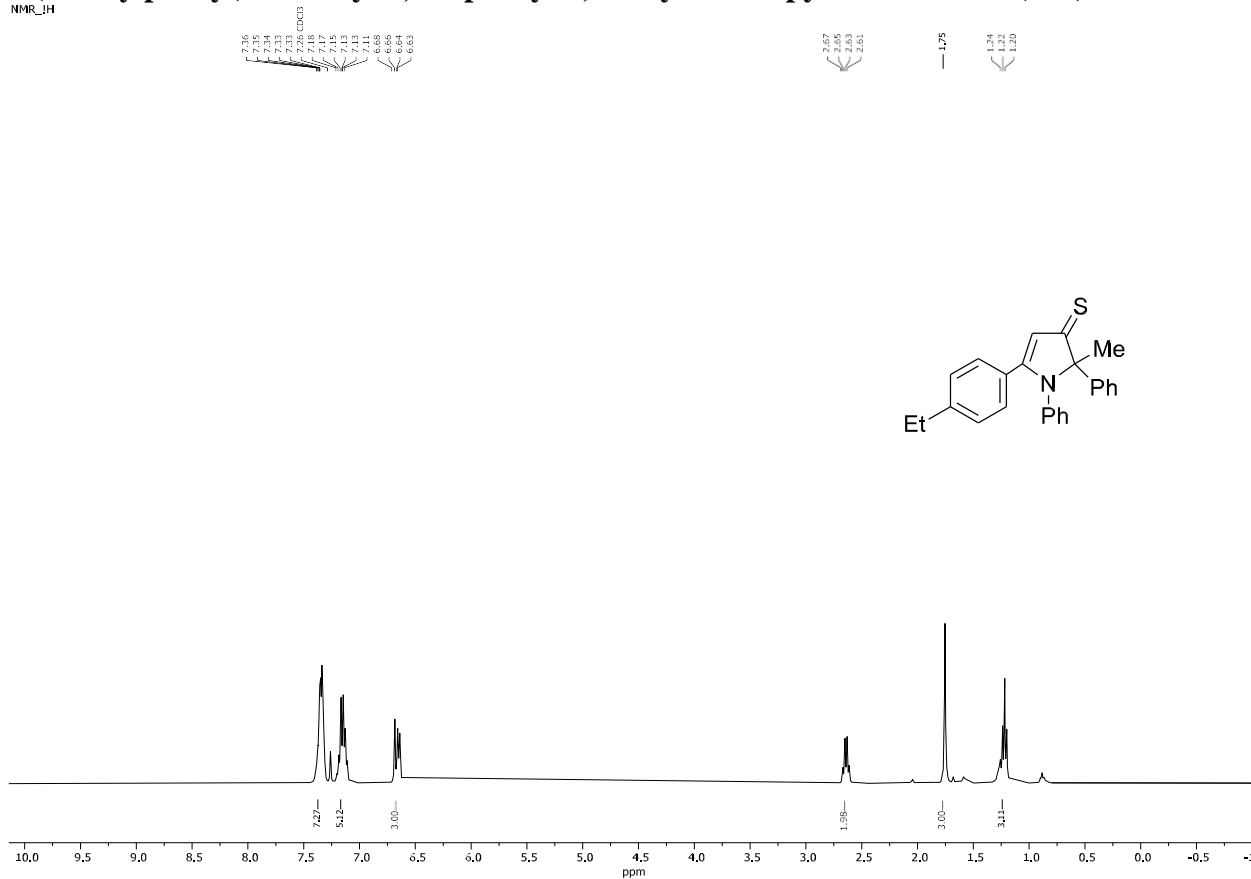
## 2-Methyl-1,2,5-triphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ac)

NMR\_13C



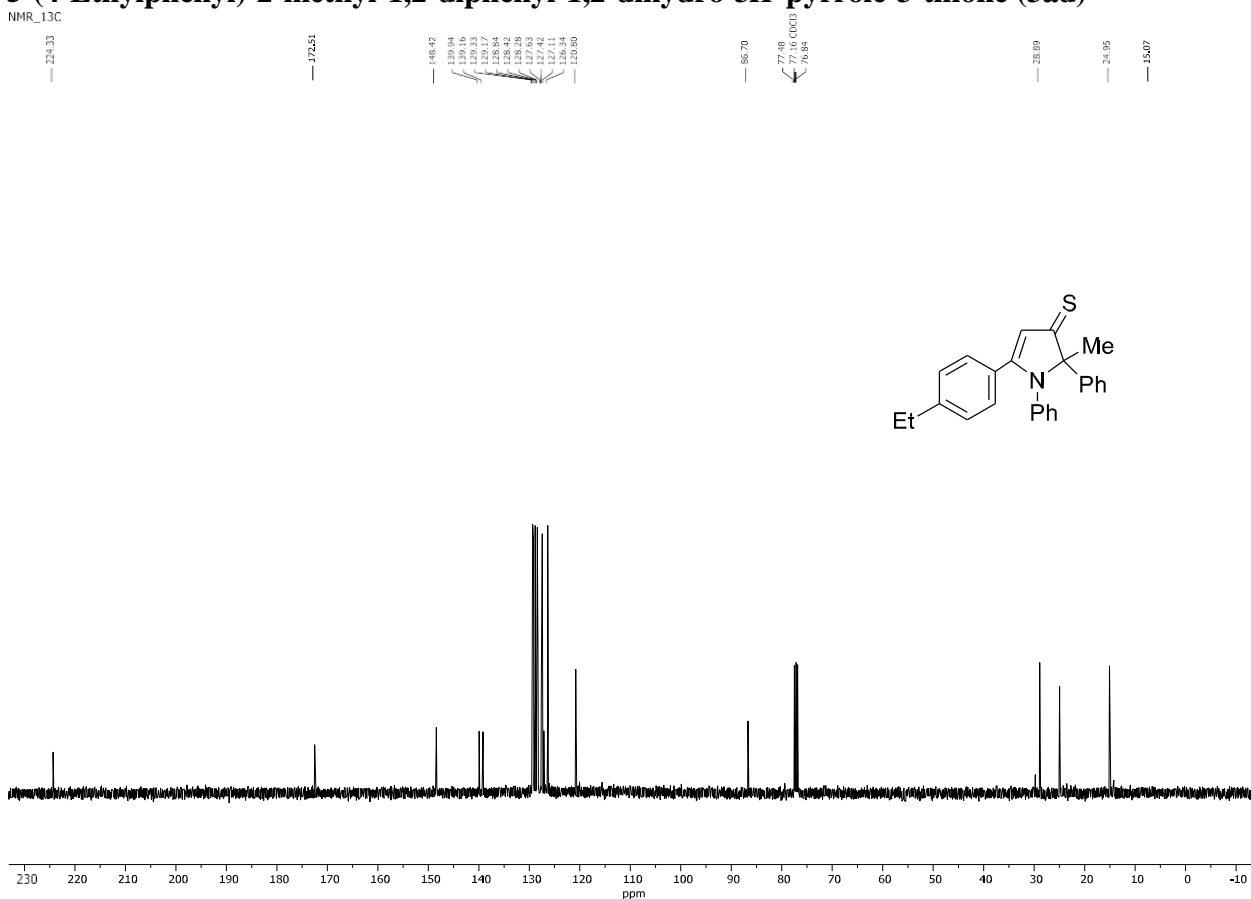
### 5-(4-Ethylphenyl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ad)

NMR\_1H



### 5-(4-Ethylphenyl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ad)

NMR\_13C

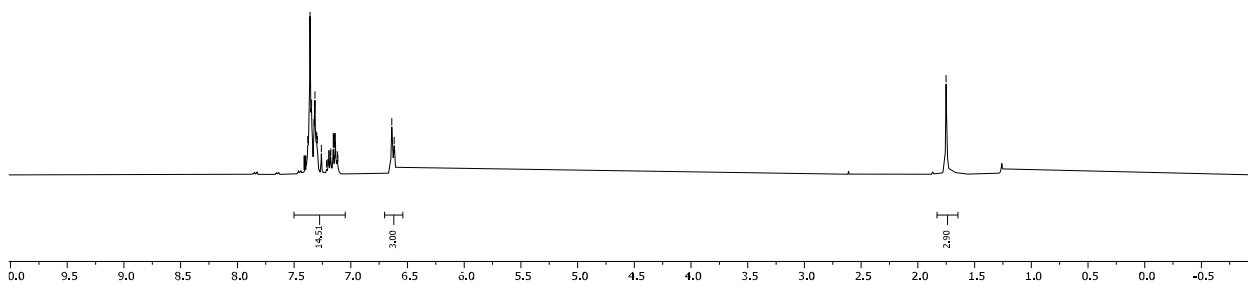
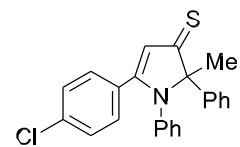


### 5-(4-Chlorophenyl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ae)

NMR\_1H



1.75



### 5-(4-Chlorophenyl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ae)

NMR\_13C

225.83

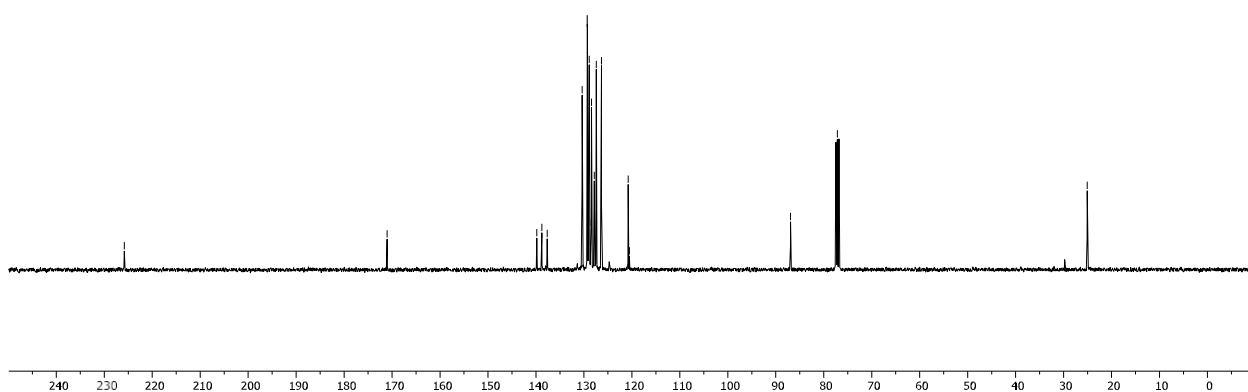
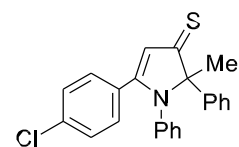
171.03

139.82  
138.78  
138.77  
130.37  
129.33  
128.89  
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128.44  
127.43  
126.35  
120.54

86.92

77.16 CDCl3

25.07

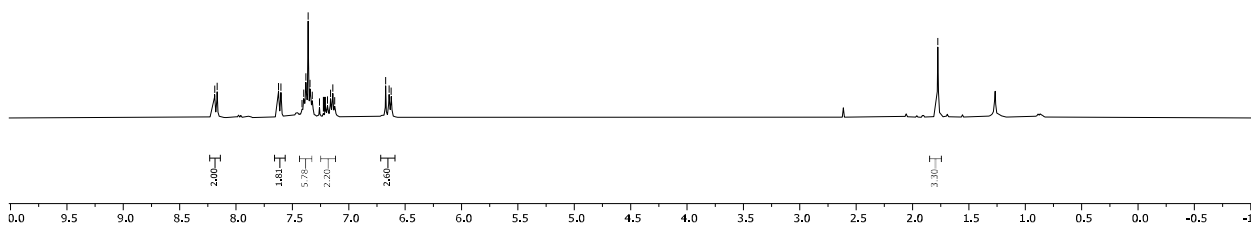
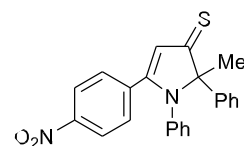


## 2-Methyl-5-(4-nitrophenyl)-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3af)

NMR\_1H



1.28



## 2-Methyl-5-(4-nitrophenyl)-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3af)

NMR\_13C

227.74

168.44

148.90

139.66

138.39

136.50

129.91

128.97

128.36

128.08

127.33

126.32

124.04

121.32

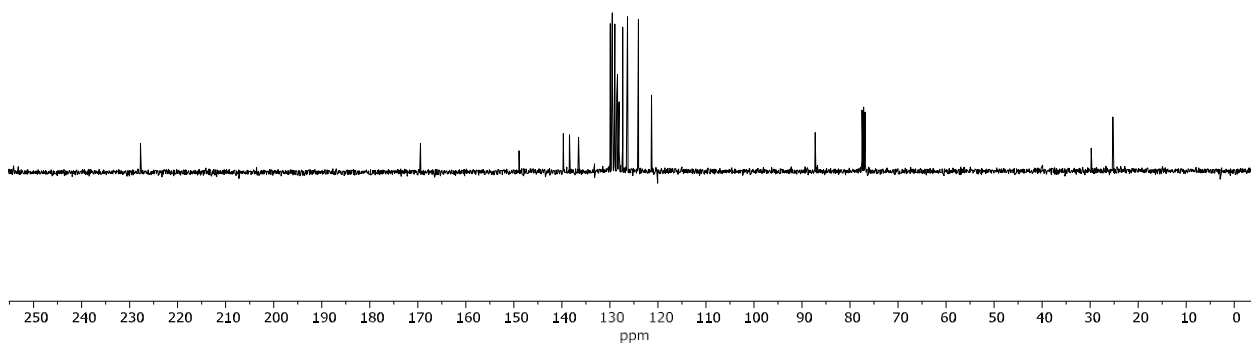
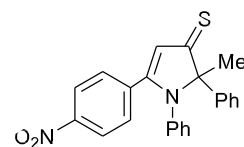
87.25

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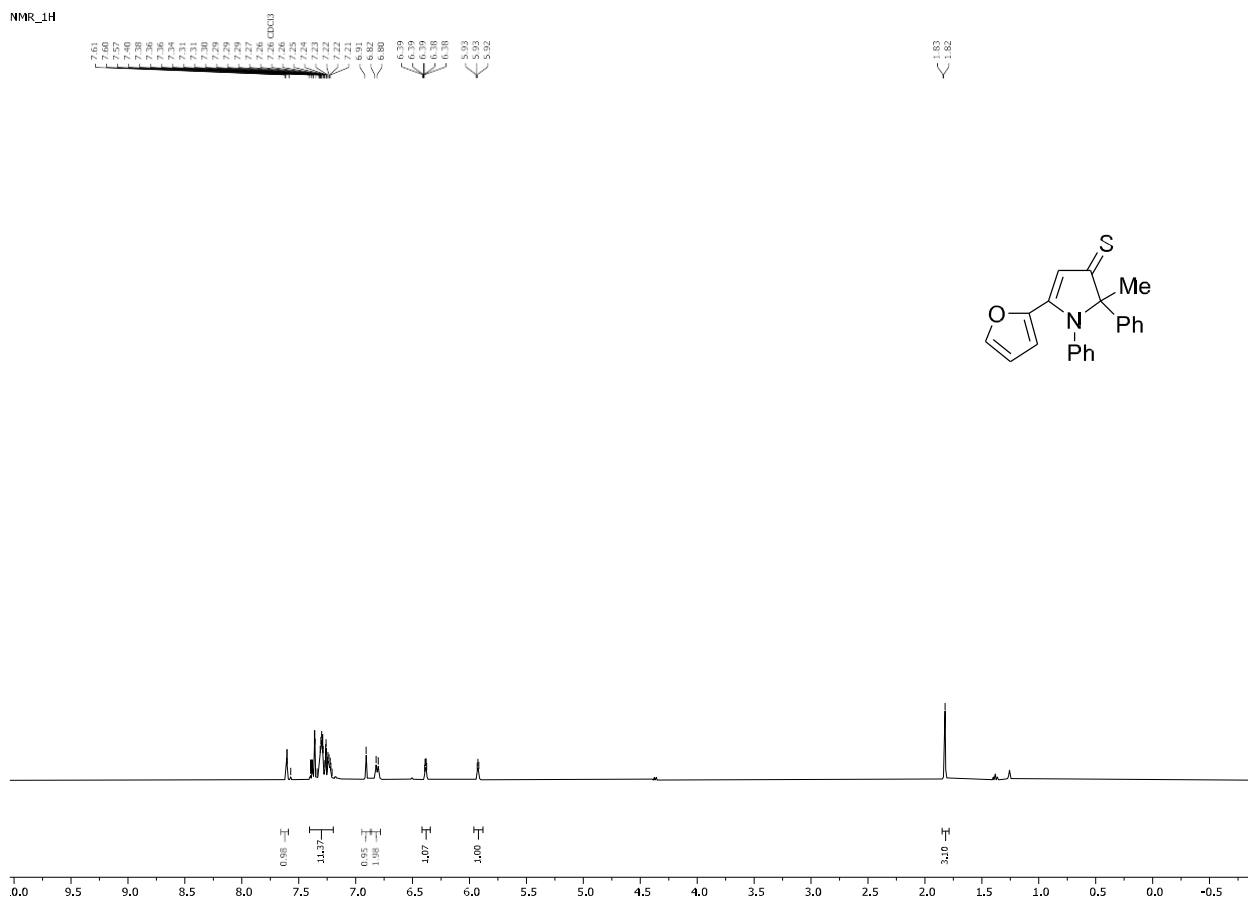
77.00 CDCl<sub>3</sub>

76.84

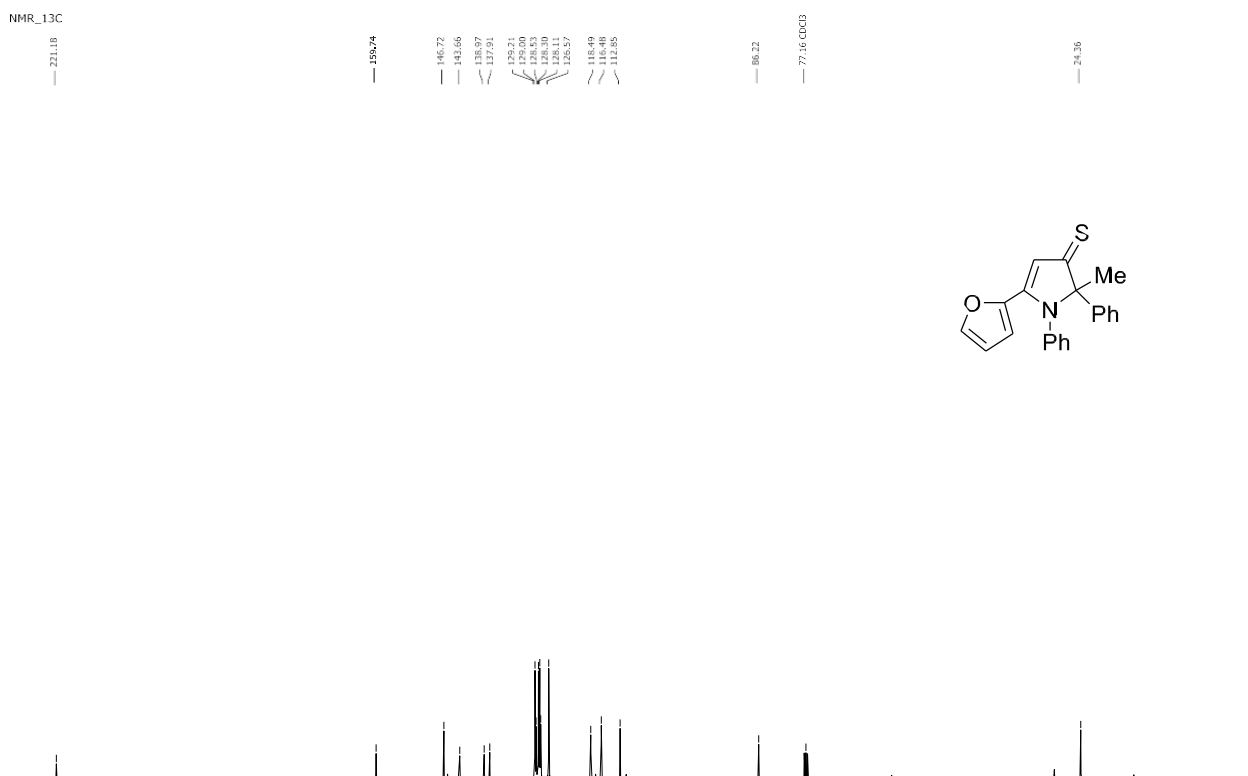
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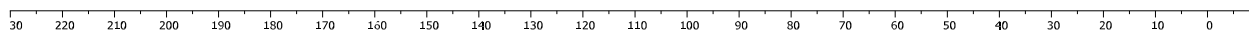
### 5-(Furan-2-yl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ag)



### 5-(Furan-2-yl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ag)



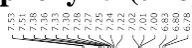
**5-(Furan-2-yl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ag)**





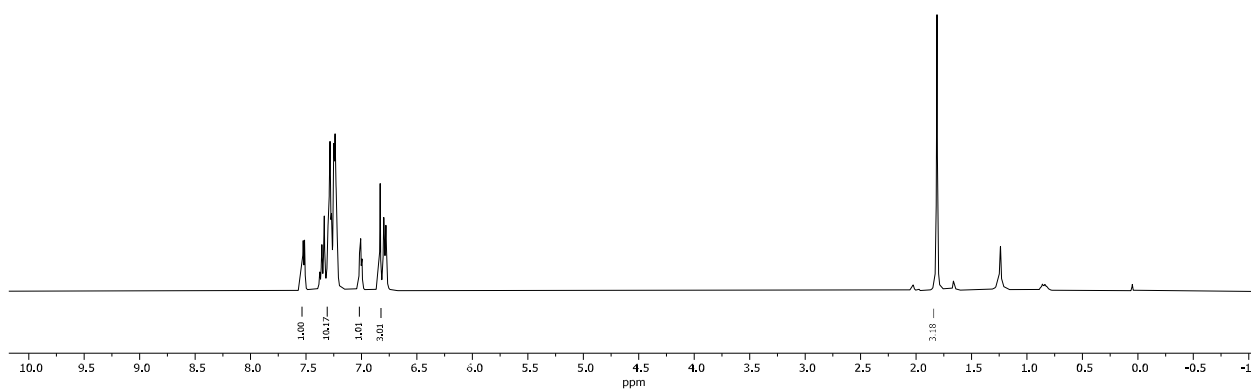
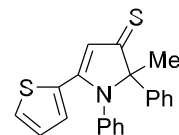
### 2-Methyl-1,2-diphenyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3ah)

NMR\_1H



1.81

0.05



### 2-Methyl-1,2-diphenyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3ah)

NMR\_13C

21.05

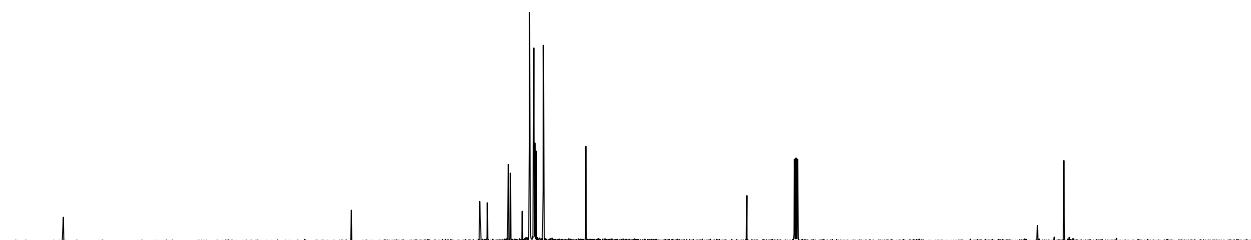
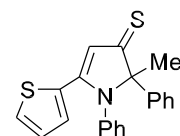
164.48

139.77  
137.79  
133.64  
133.62  
130.52  
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128.29  
118.42

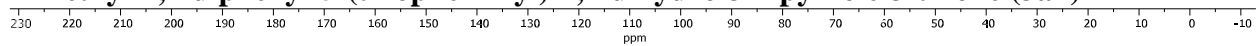
86.80

77.45  
77.16 CDCl3  
76.84

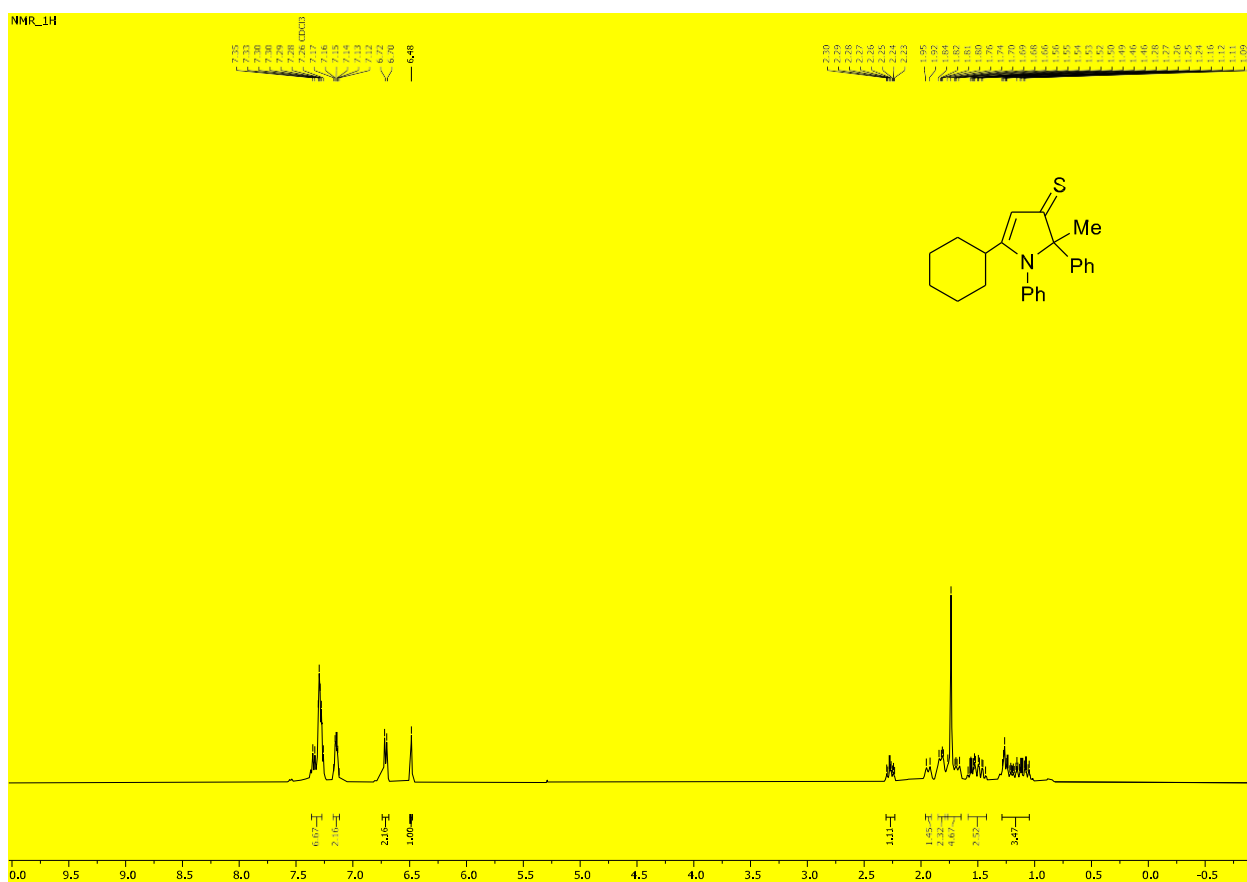
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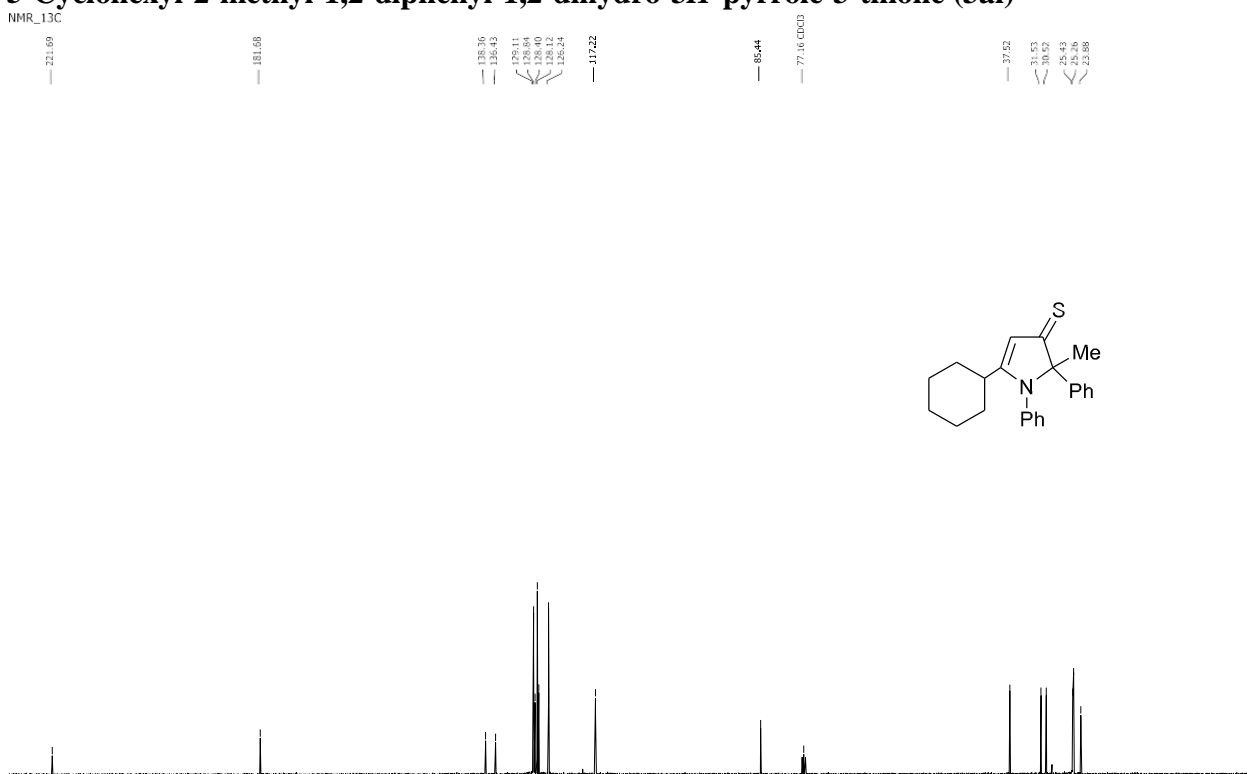
**2-Methyl-1,2-diphenyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3ah)**



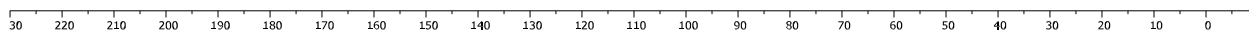
### 5-Cyclohexyl-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ai)



### 5-Cyclohexyl-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ai)

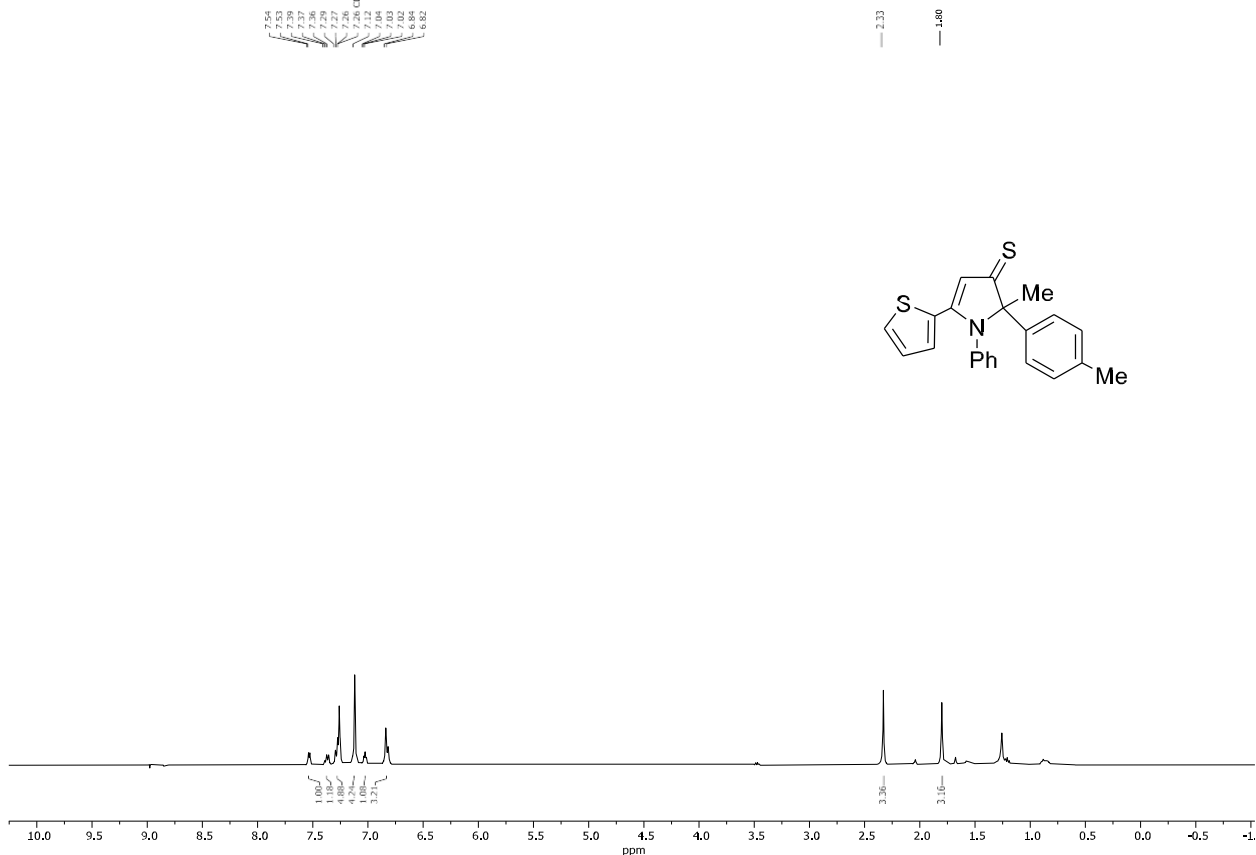


**5-Cyclohexyl-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3ai)**



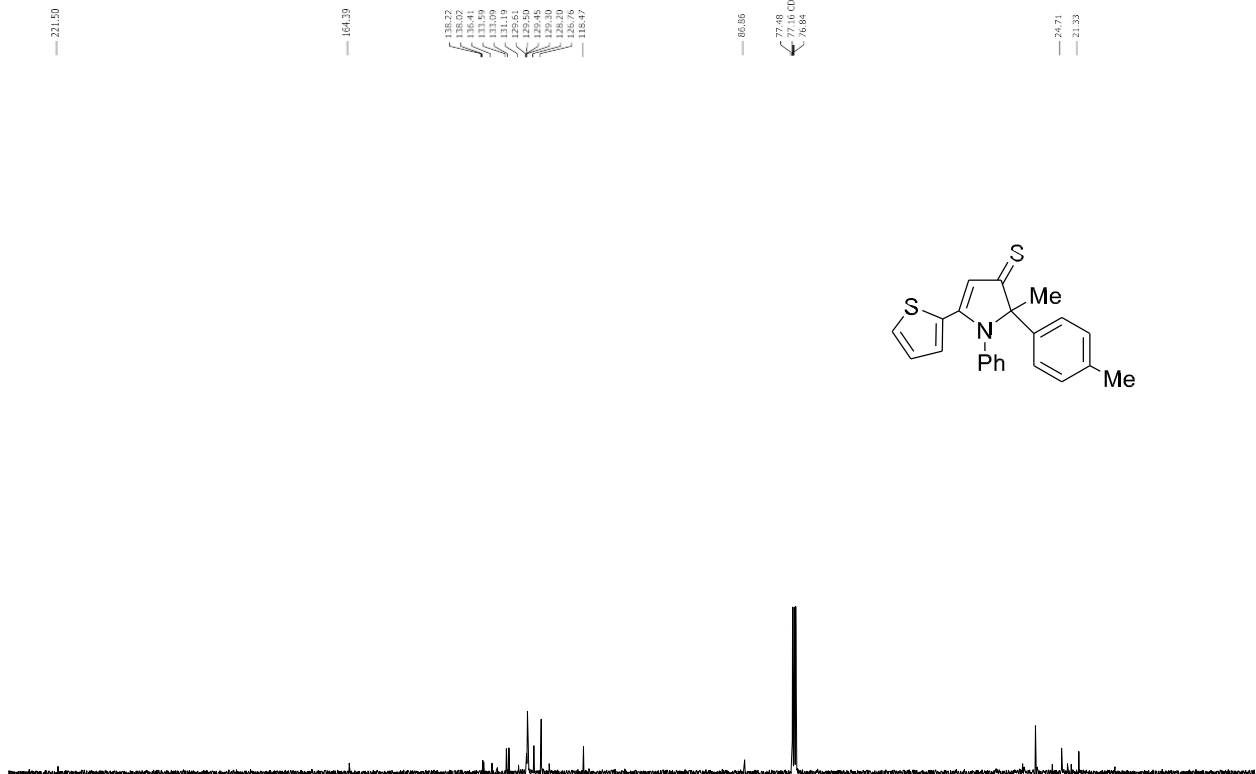
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NMR\_1H

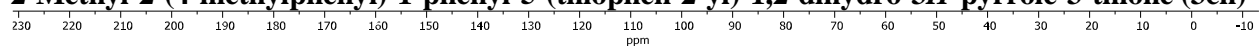


### 2-Methyl-2-(4-methylphenyl)-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3ch)

NMR\_13C



**2-Methyl-2-(4-methylphenyl)-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3ch)**

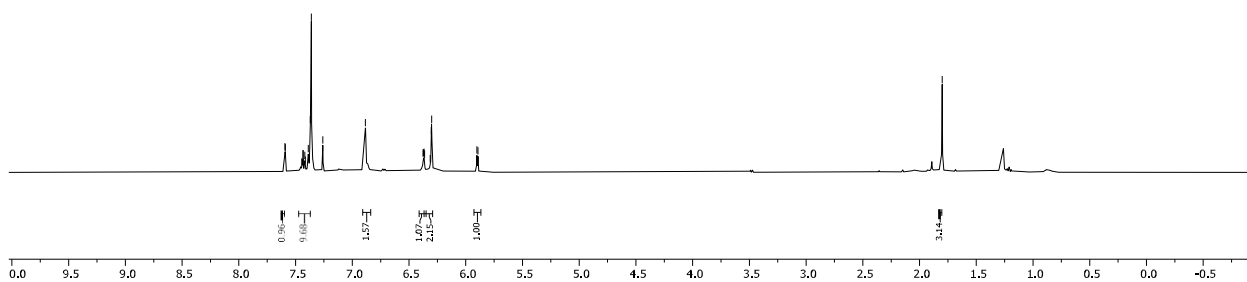
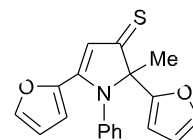


### 2,5-Di(furan-2-yl)-2-methyl-1-phenyl-1,2-dihydro-3H-pyrrole-3-thione (3eg)

NMR\_1H

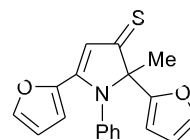


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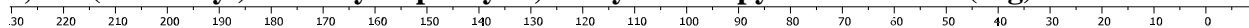


### 2,5-Di(furan-2-yl)-2-methyl-1-phenyl-1,2-dihydro-3H-pyrrole-3-thione (3eg)

NMR\_13C



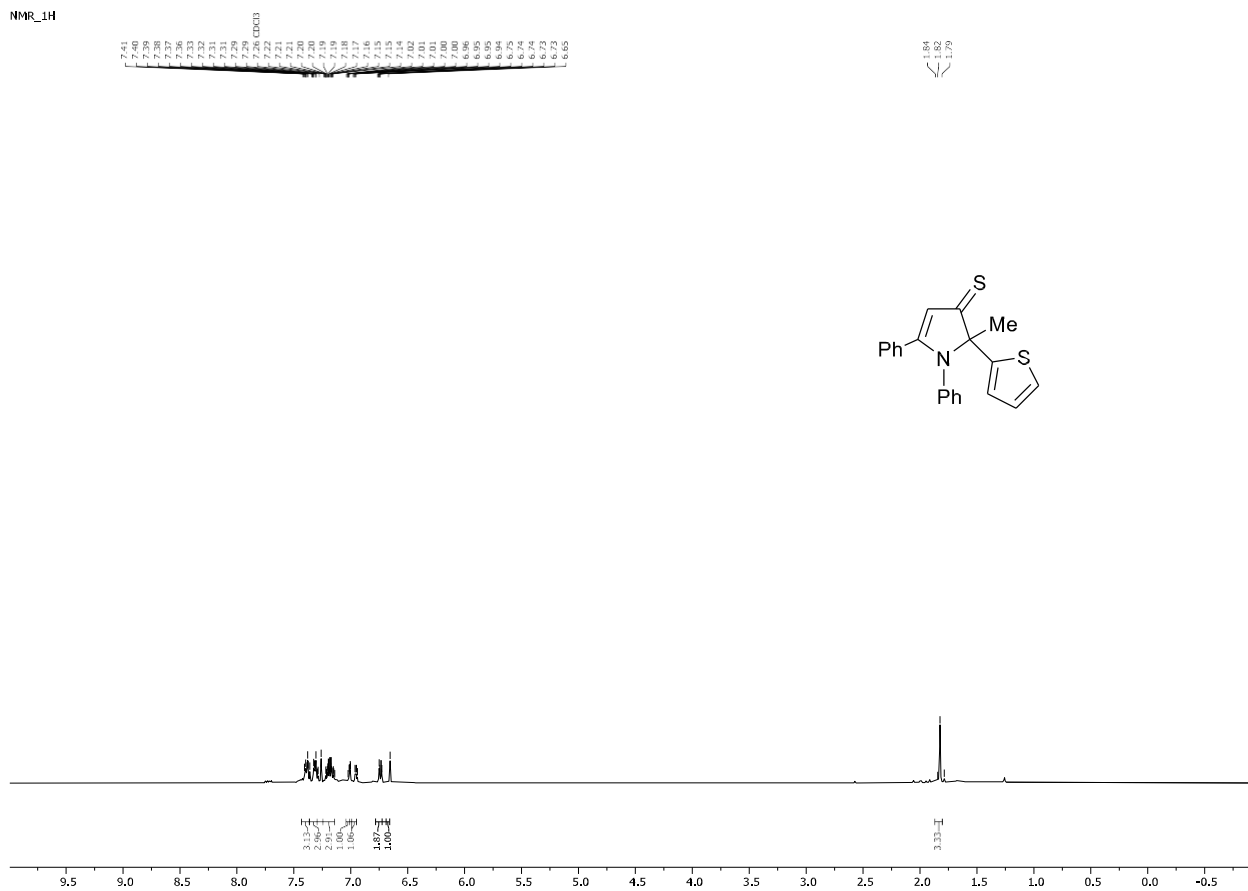
**2,5-Di(furan-2-yl)-2-methyl-1-phenyl-1,2-dihydro-3H-pyrrole-3-thione (3eg)**





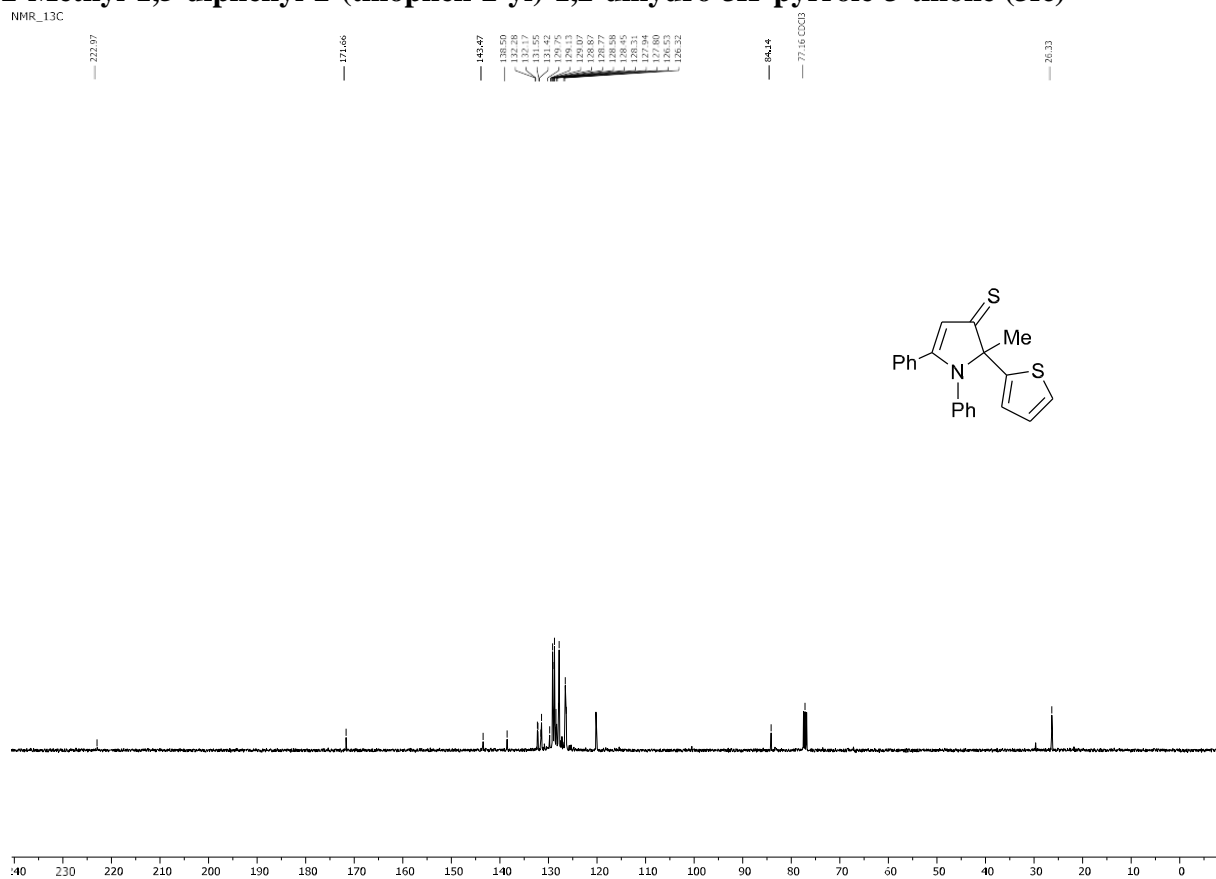
## 2-Methyl-1,5-diphenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fc)

NMR\_1H



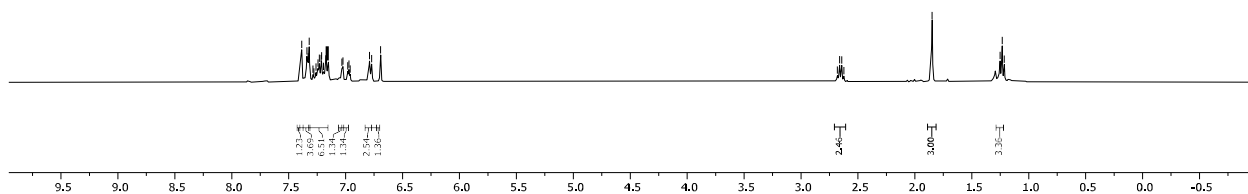
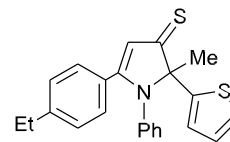
## 2-Methyl-1,5-diphenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fc)

NMR\_13C



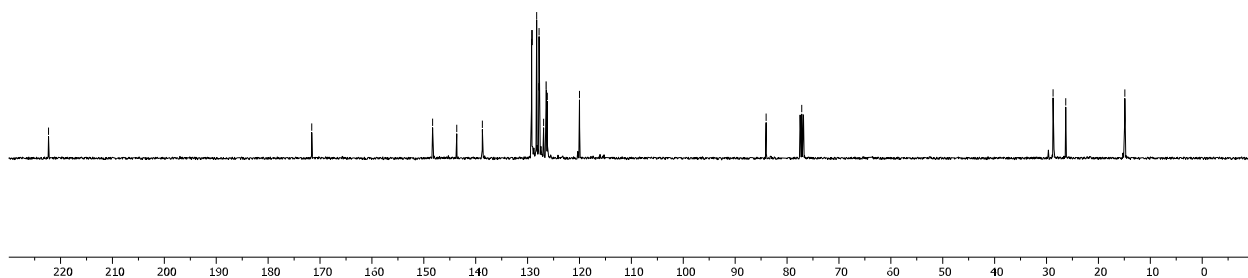
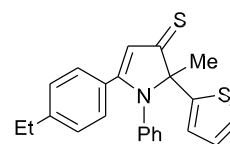
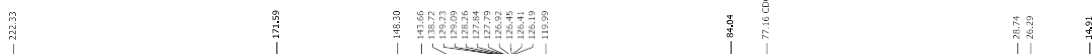
### 5-(4-Ethylphenyl)-2-methyl-1-phenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fd)

NMR\_1H



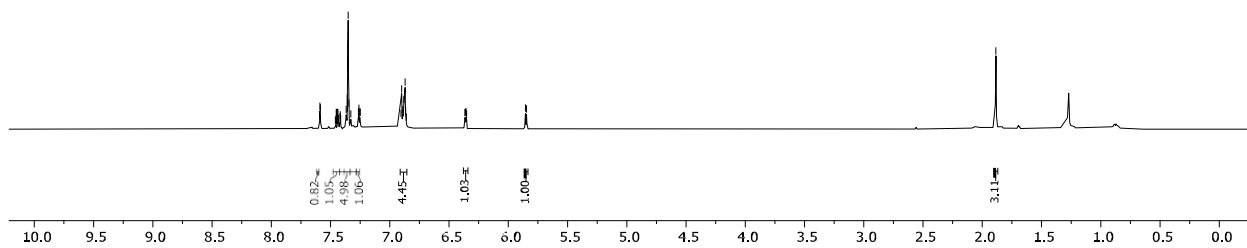
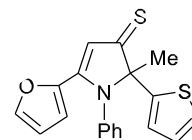
### 5-(4-Ethylphenyl)-2-methyl-1-phenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fd)

NMR\_13C



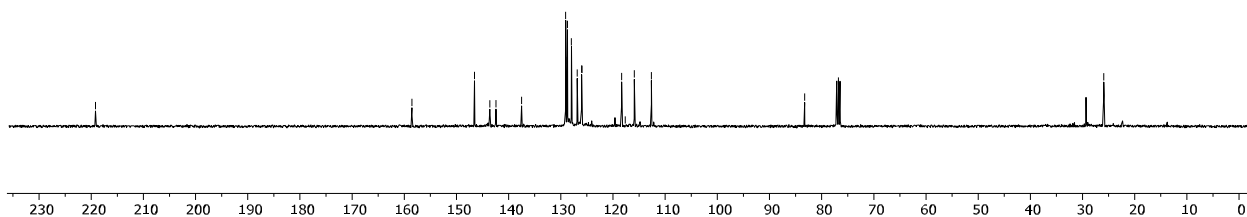
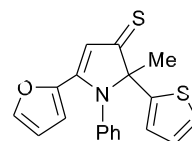
### 5-(Furan-2-yl)-2-methyl-1-phenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fg)

NMR\_1H



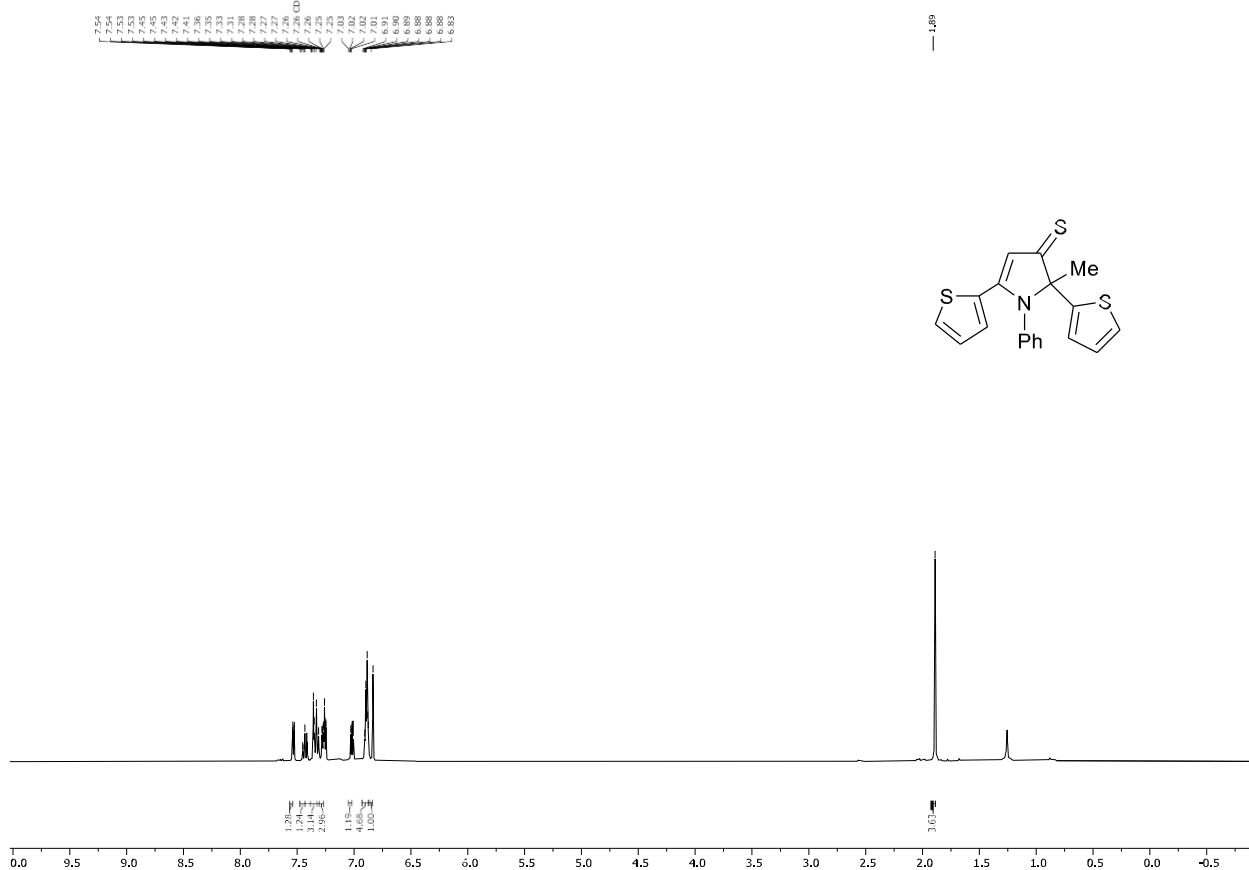
### 5-(Furan-2-yl)-2-methyl-1-phenyl-2-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fg)

NMR\_13C



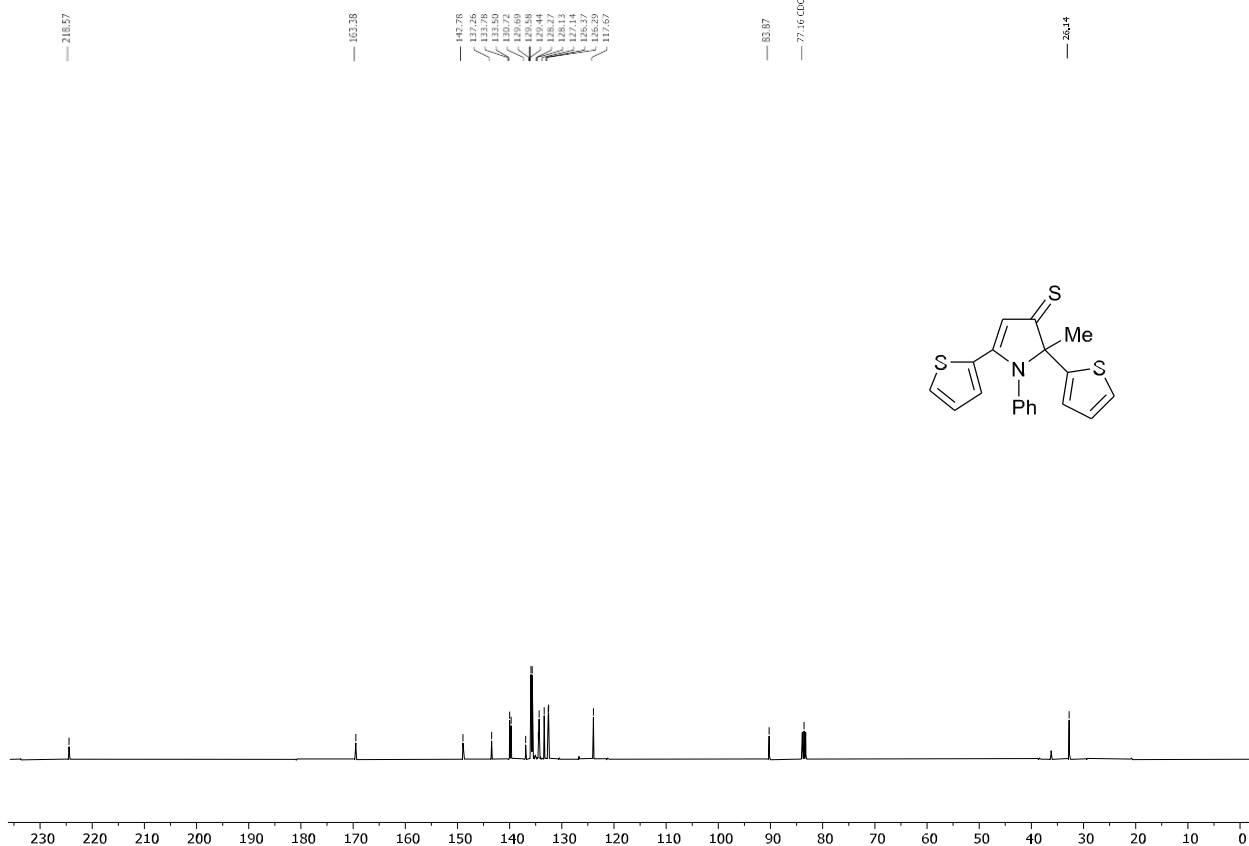
## 2-Methyl-1-phenyl-2,5-di(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fh)

NMR\_1H

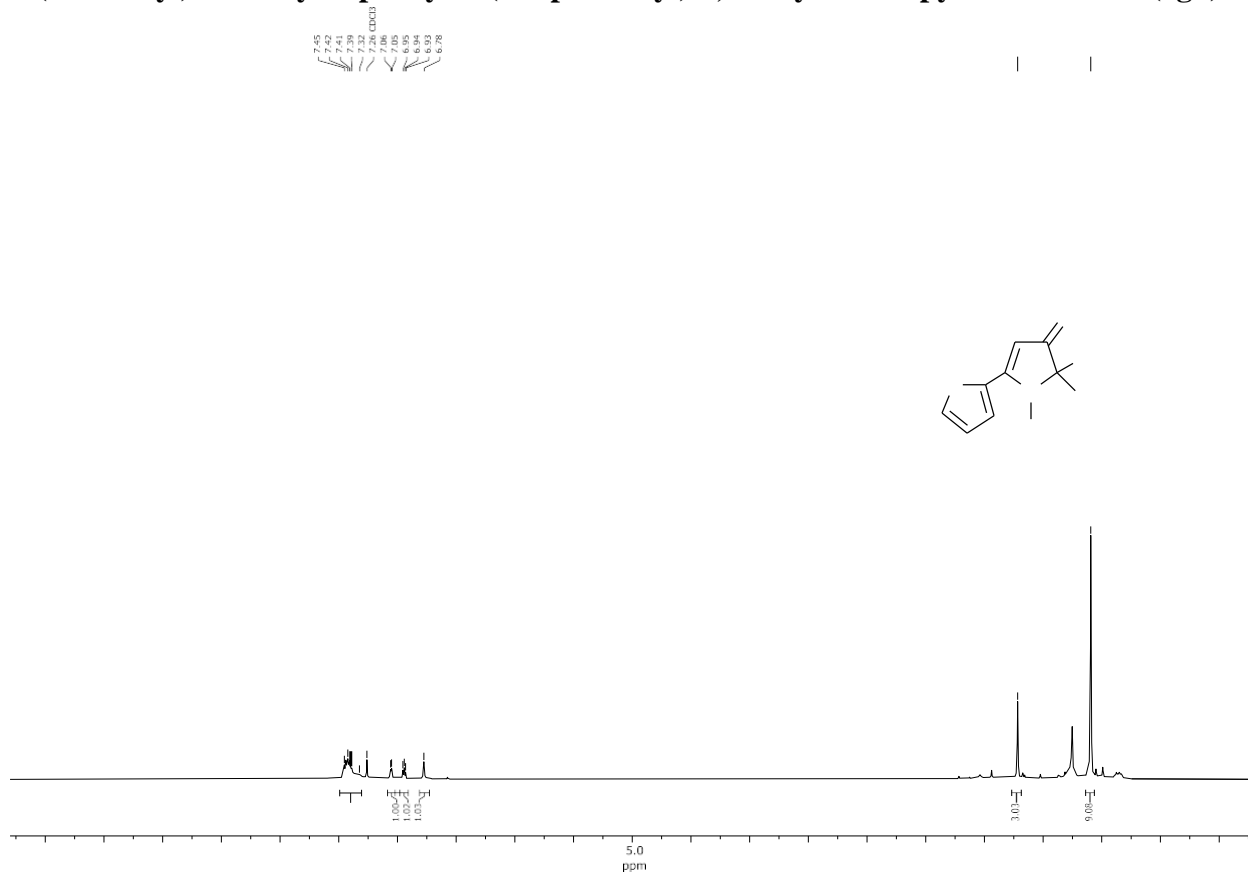


## 2-Methyl-1-phenyl-2,5-di(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3fh)

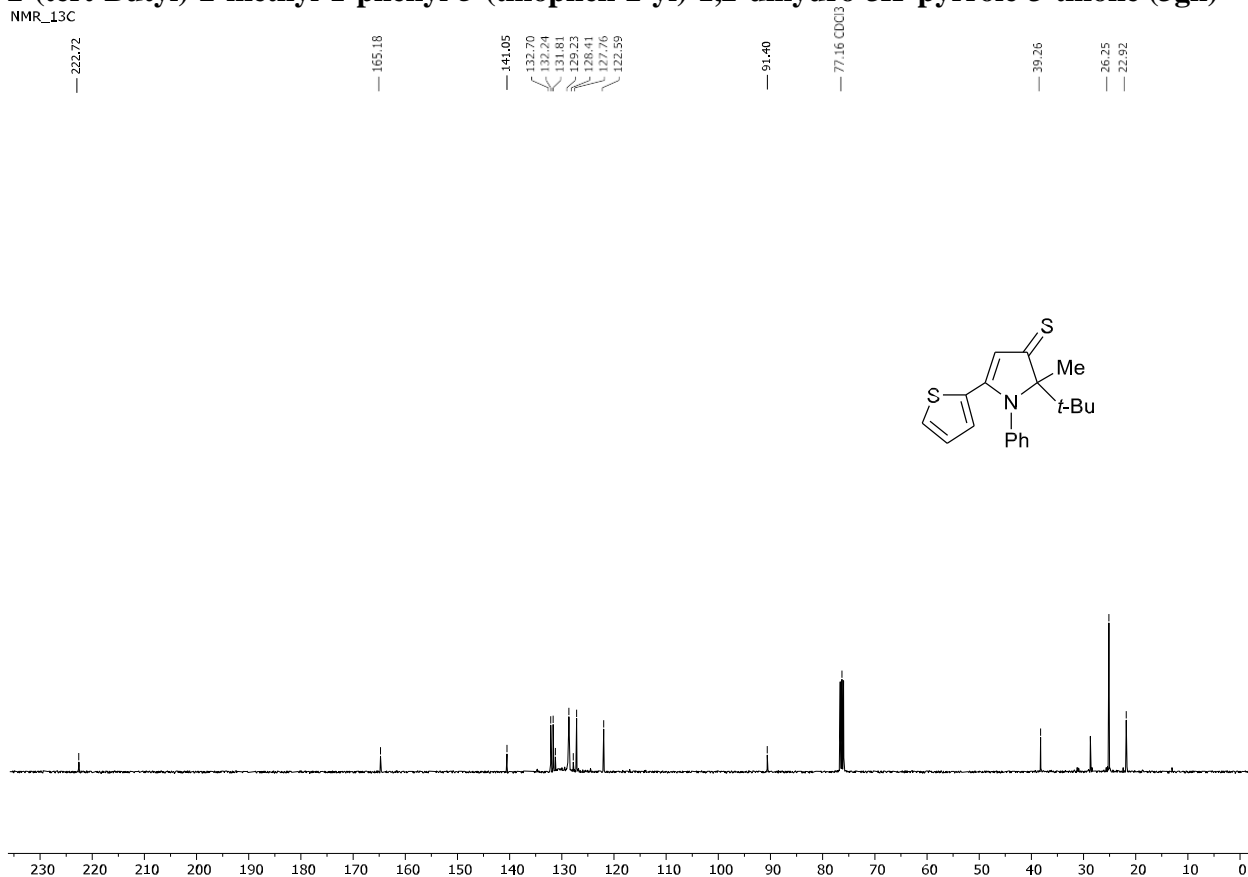
NMR\_13C



**2-(tert-Butyl)-2-methyl-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3gh)**

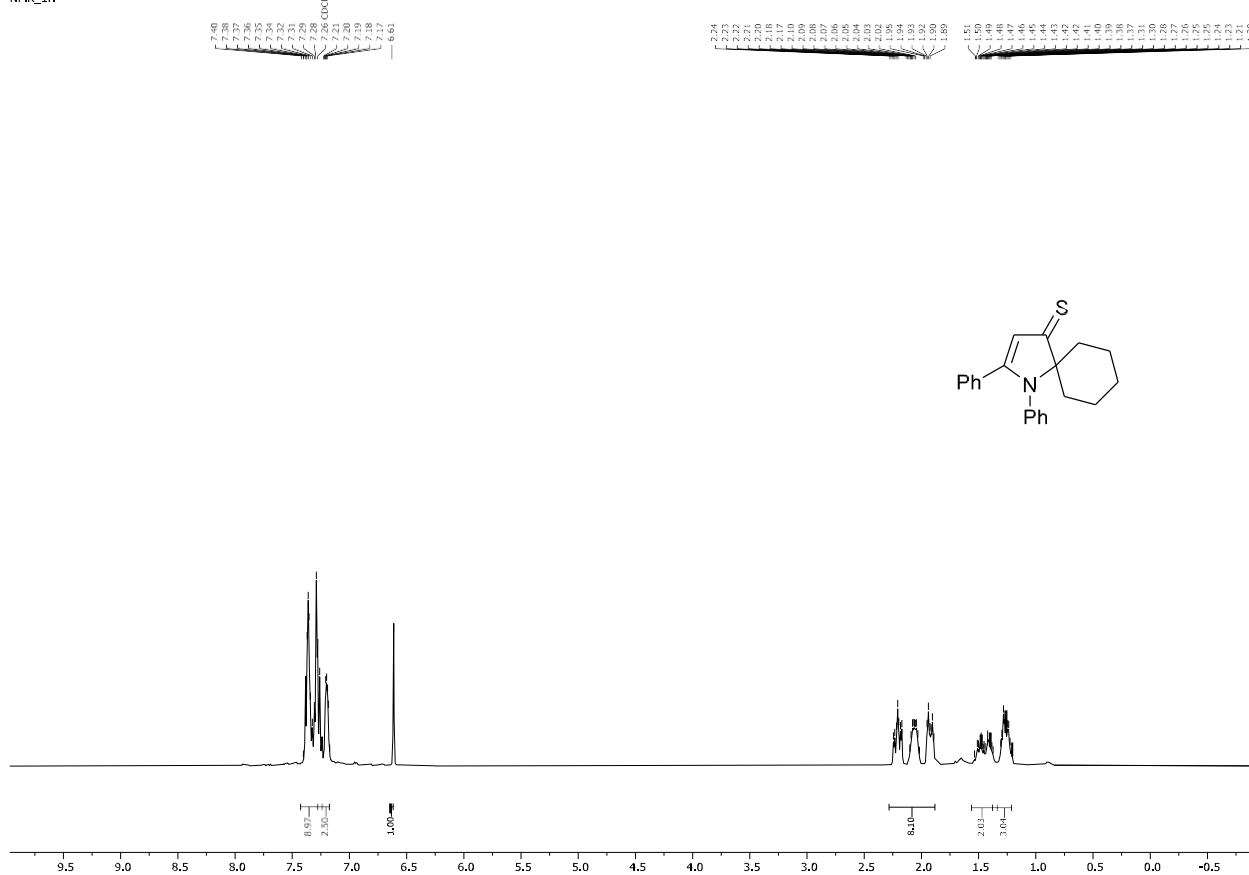


**2-(tert-Butyl)-2-methyl-1-phenyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3gh)**



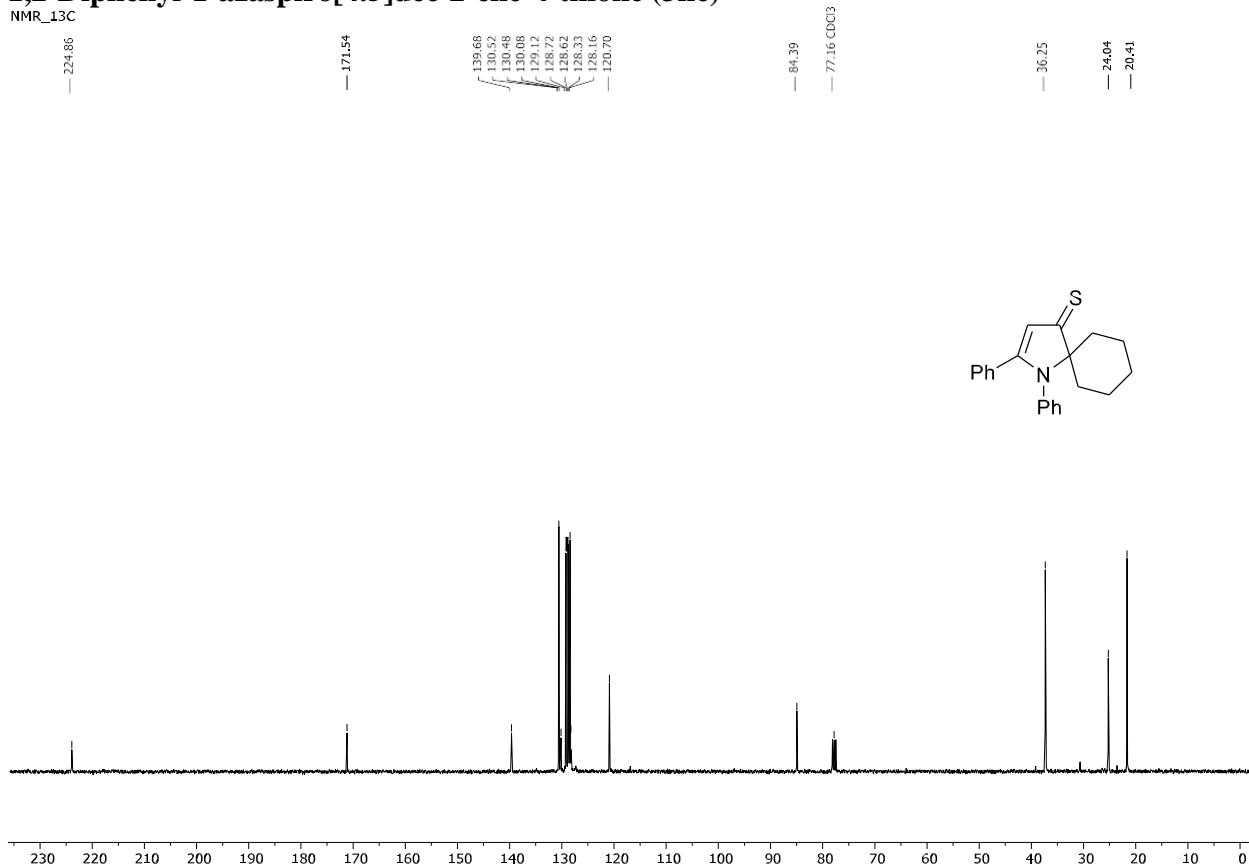
# 1,2-Diphenyl-1-azaspiro[4.5]dec-2-ene-4-thione (3hc)

NMR\_1H



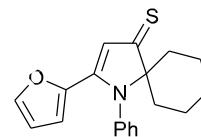
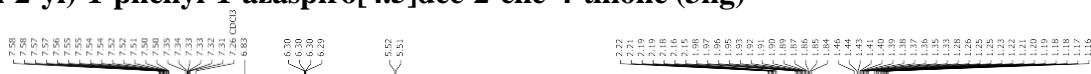
# 1,2-Diphenyl-1-azaspiro[4.5]dec-2-ene-4-thione (3hc)

NMR\_13C



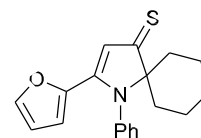
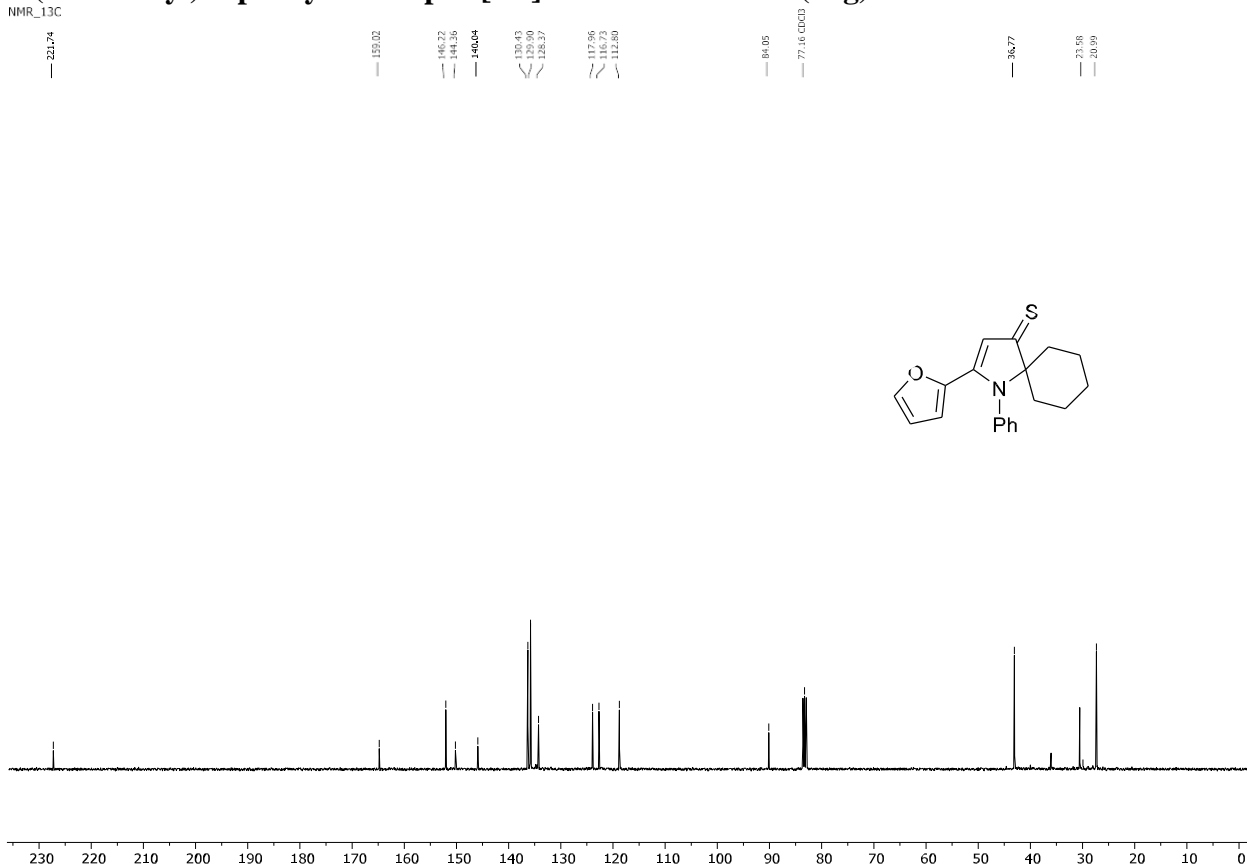
### 2-(Furan-2-yl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-thione (3hg)

NMR\_1H



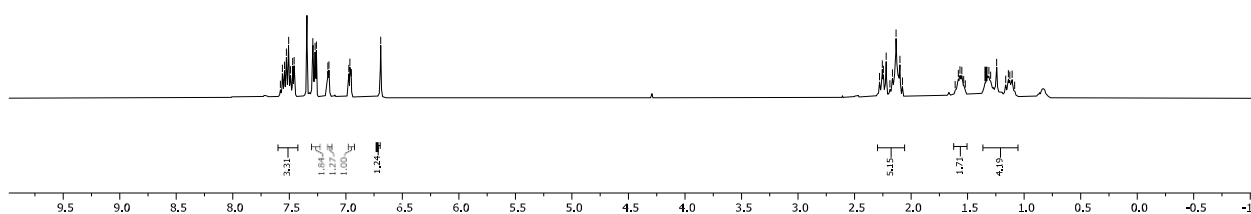
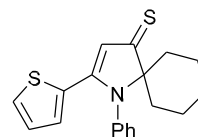
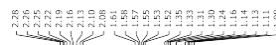
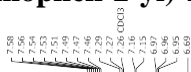
### 2-(Furan-2-yl)-1-phenyl-1-azaspiro[4.5]dec-2-ene-4-thione (3hg)

NMR\_13C



# 1-Phenyl-2-(thiophen-2-yl)-1-azaspiro[4.5]dec-2-ene-4-thione (3hh)

NMR\_1H



# 1-Phenyl-2-(thiophen-2-yl)-1-azaspiro[4.5]dec-2-ene-4-thione (3hh)

NMR\_13C

222.21

162.87

138.19

133.39

131.00

131.22

131.10

130.09

129.98

128.42

127.89

117.50

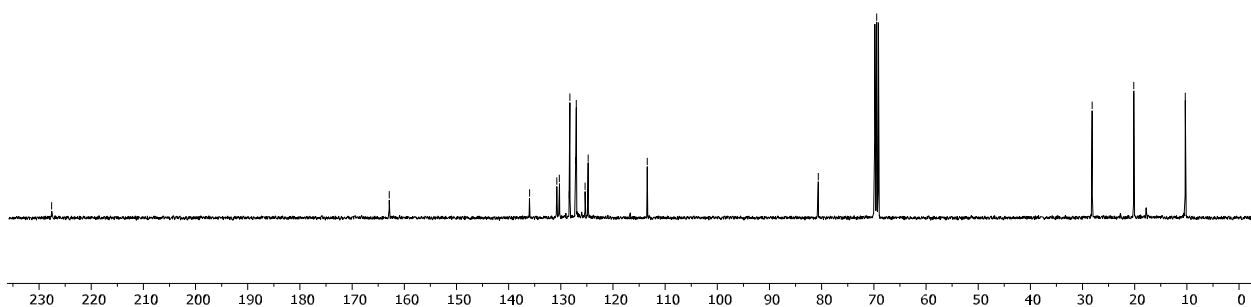
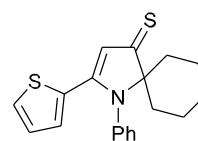
87.42

77.16 CDCl3

39.27

31.94

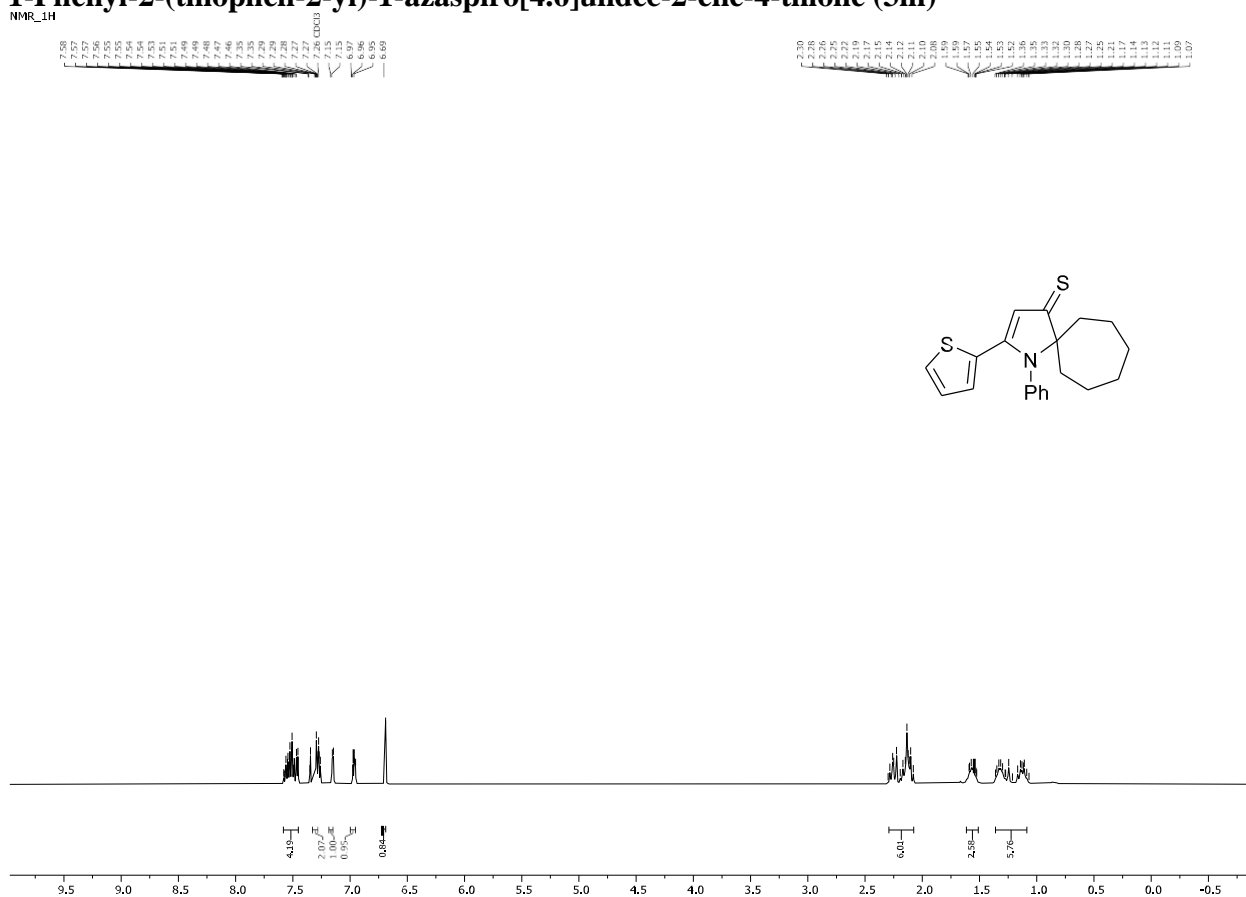
22.90





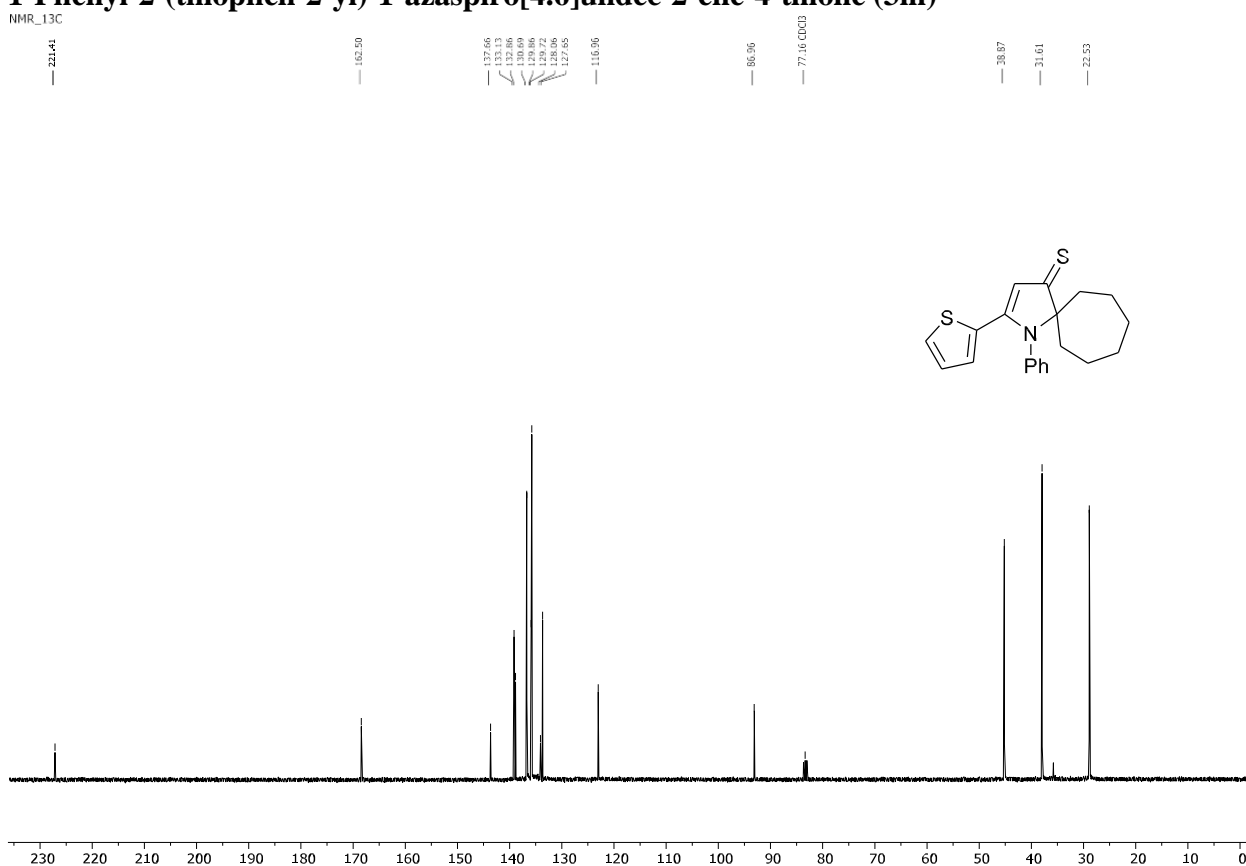
# 1-Phenyl-2-(thiophen-2-yl)-1-azaspiro[4.6]undec-2-ene-4-thione (3ih)

NMR\_1H



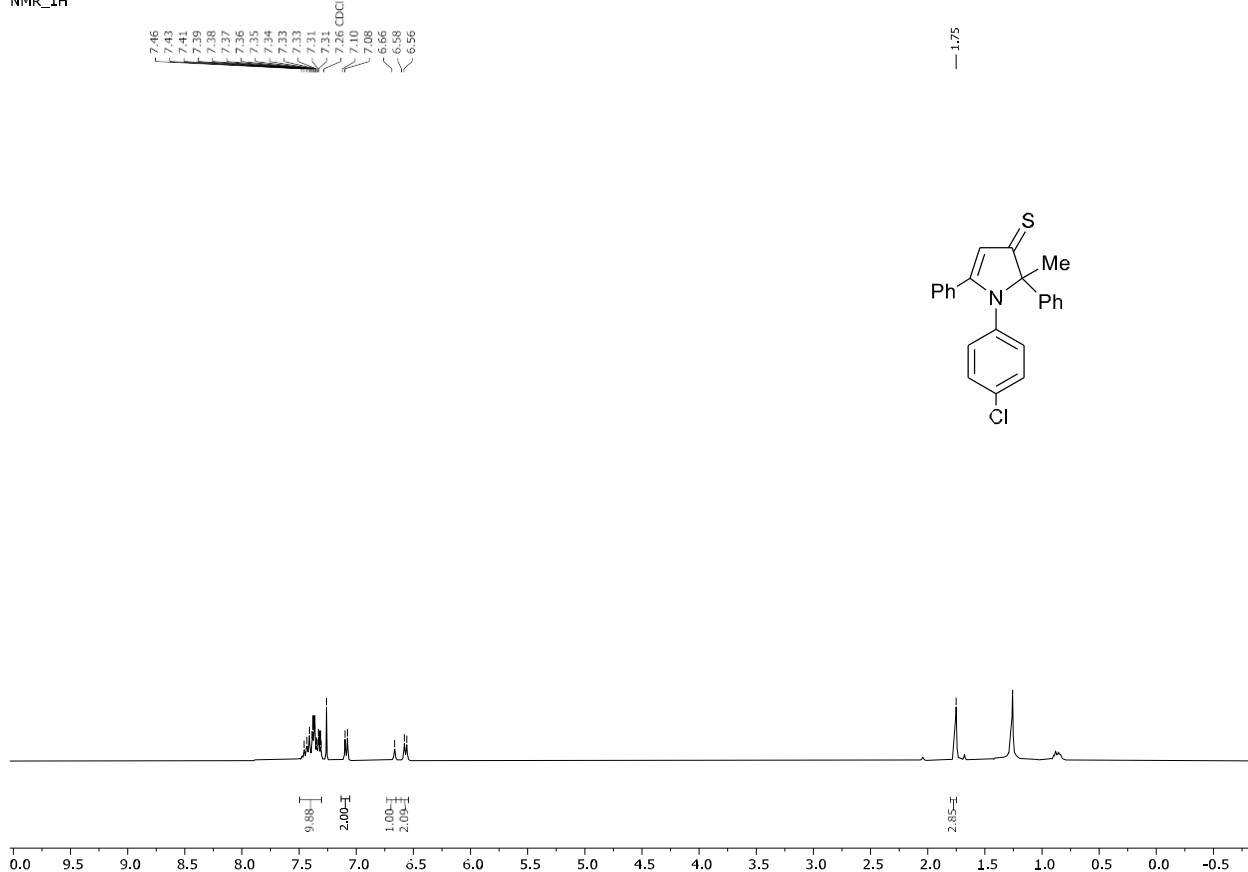
# 1-Phenyl-2-(thiophen-2-yl)-1-azaspiro[4.6]undec-2-ene-4-thione (3ih)

NMR\_13C



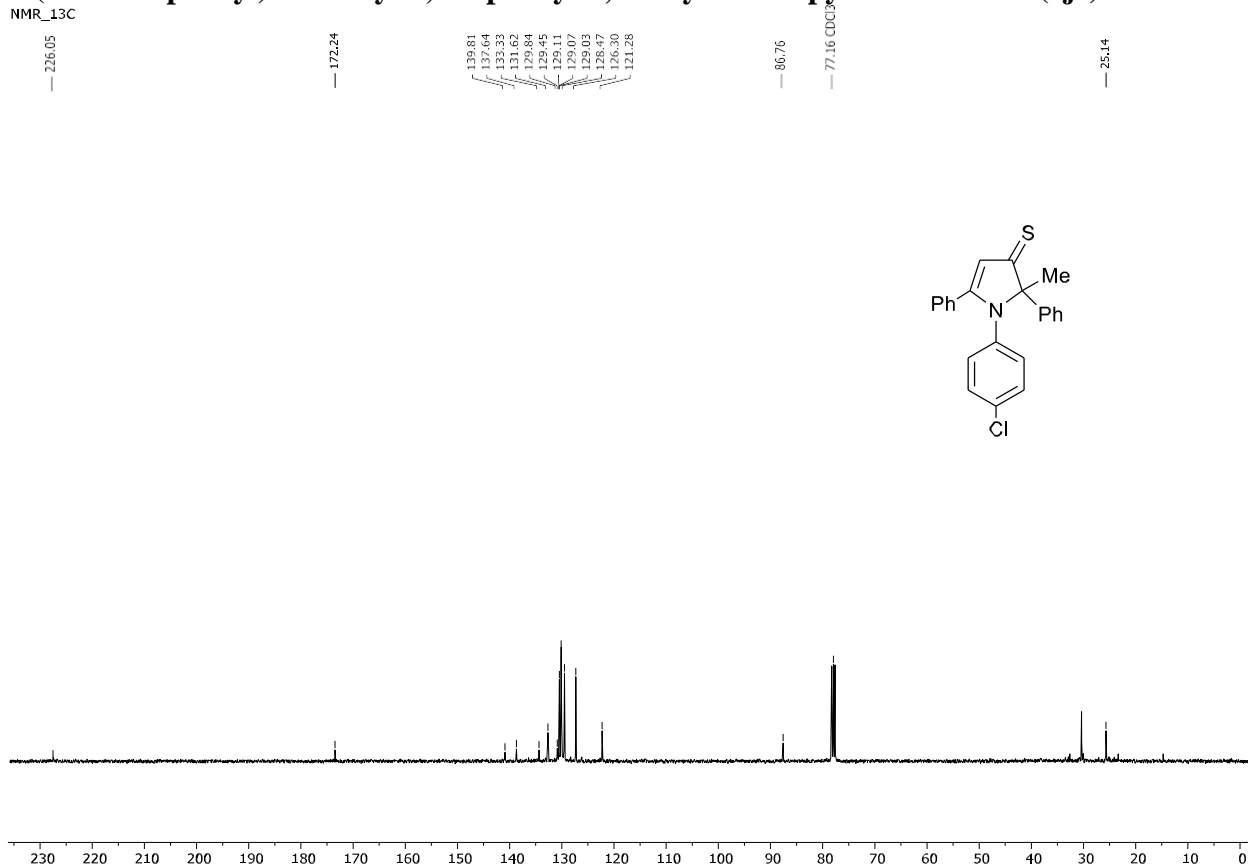
# 1-(4-Chlorophenyl)-2-methyl-2,5-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3jc)

NMR\_1H



# 1-(4-Chlorophenyl)-2-methyl-2,5-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (3jc)

NMR\_13C

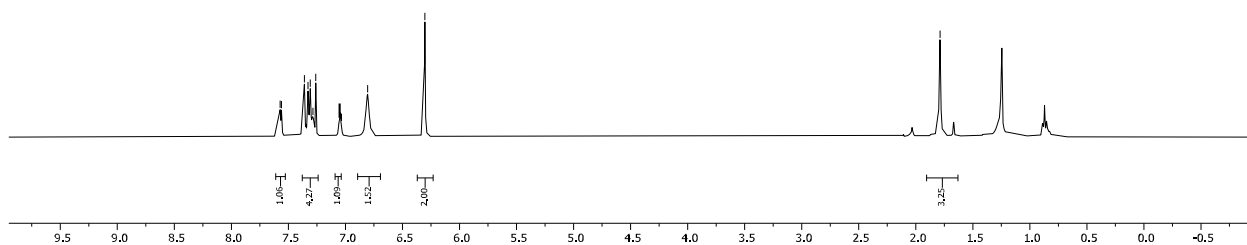
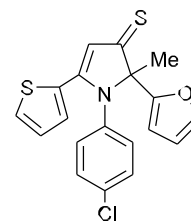


### 1-(4-Chlorophenyl)-2-(furan-2-yl)-2-methyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3kh)

NMR\_1H

7.57  
7.56  
7.55  
7.31  
7.31  
7.31  
7.26 CDCl<sub>3</sub>  
7.05  
7.05  
6.81  
6.81  
6.30

1.79



### 1-(4-Chlorophenyl)-2-(furan-2-yl)-2-methyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3kh)

NMR\_13C

216.56

164.13

150.76

142.58

135.77

135.40

133.72

130.67

130.28

128.58

117.81

110.50

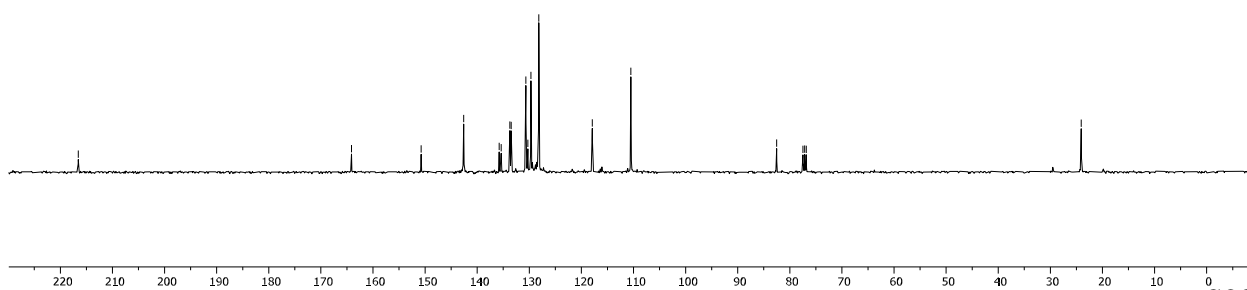
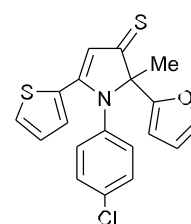
82.53

77.48 CDCl<sub>3</sub>

77.16 CDCl<sub>3</sub>

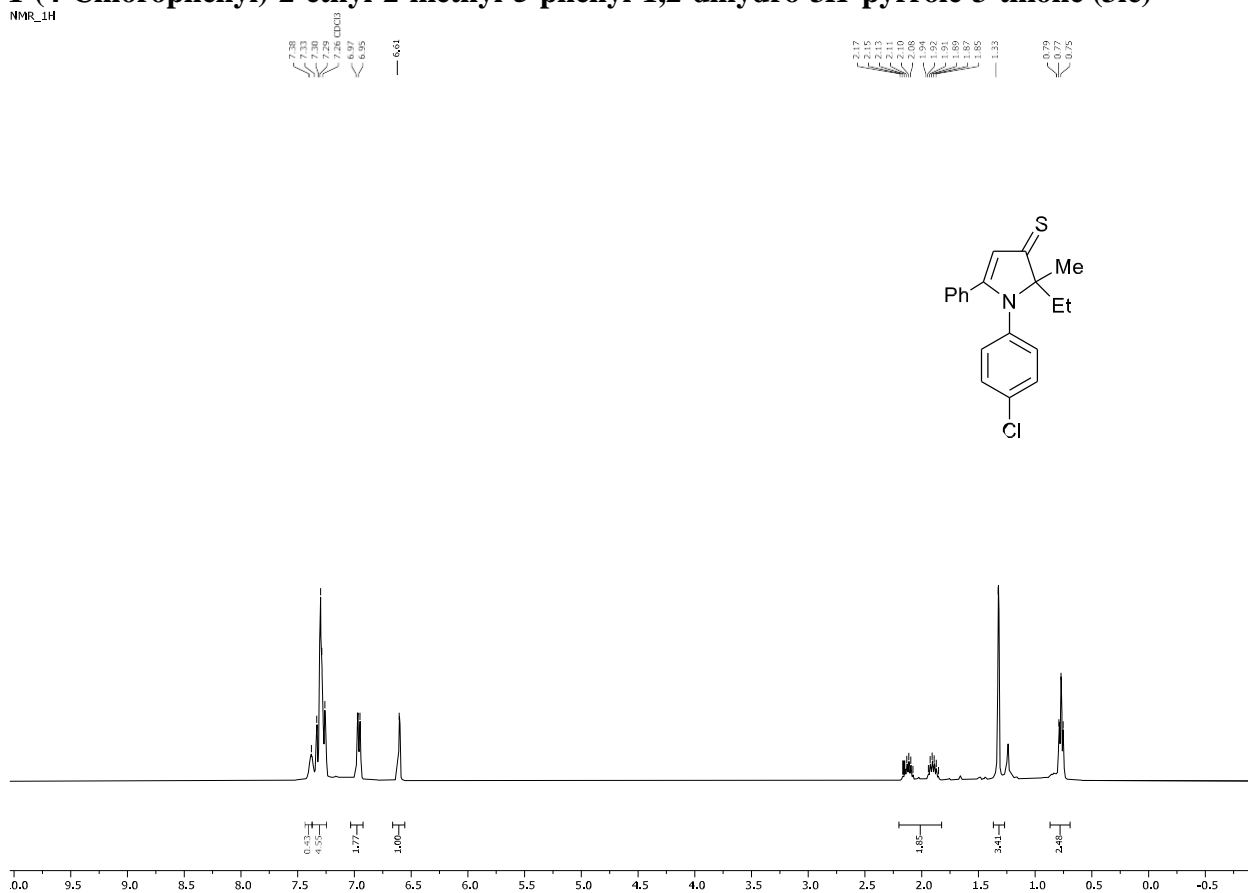
76.84

21.08



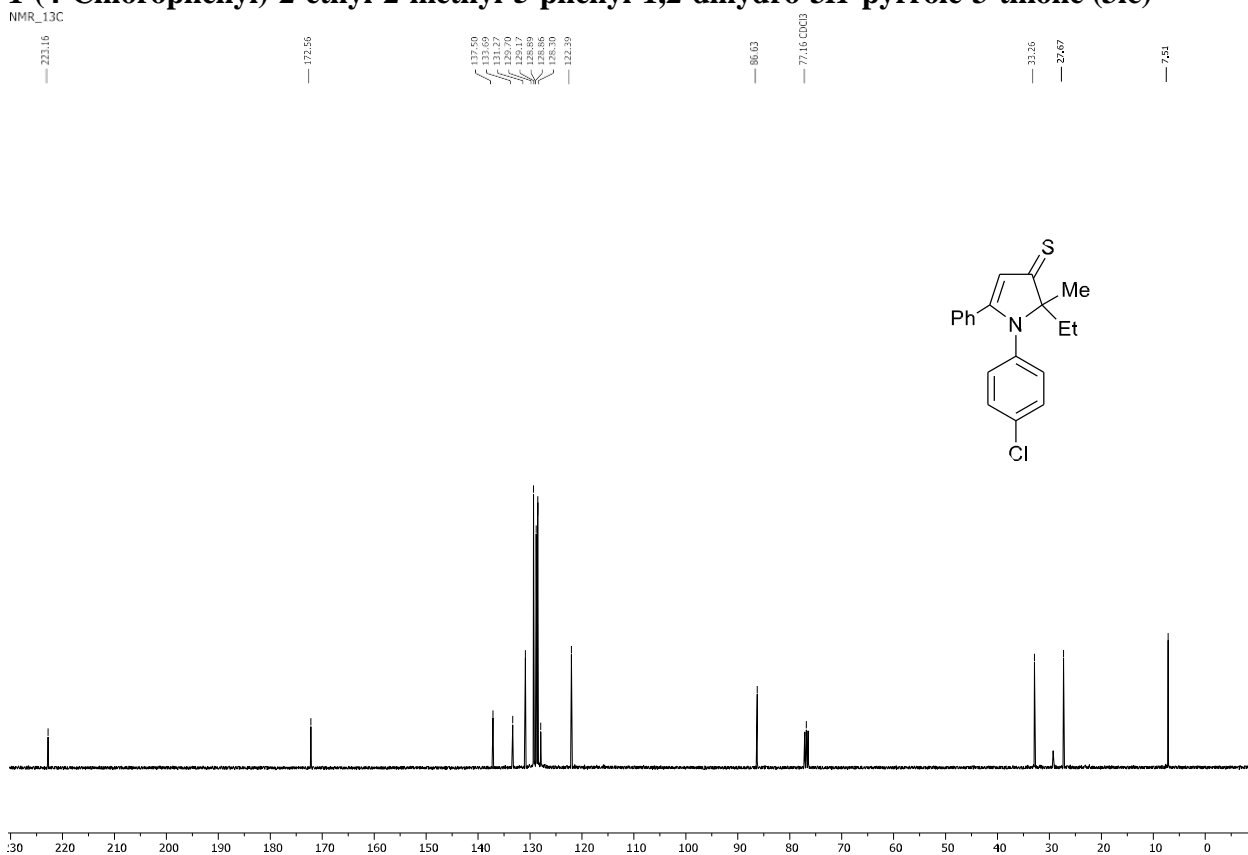
# 1-(4-Chlorophenyl)-2-ethyl-2-methyl-5-phenyl-1,2-dihydro-3H-pyrrole-3-thione (3lc)

NMR\_1H



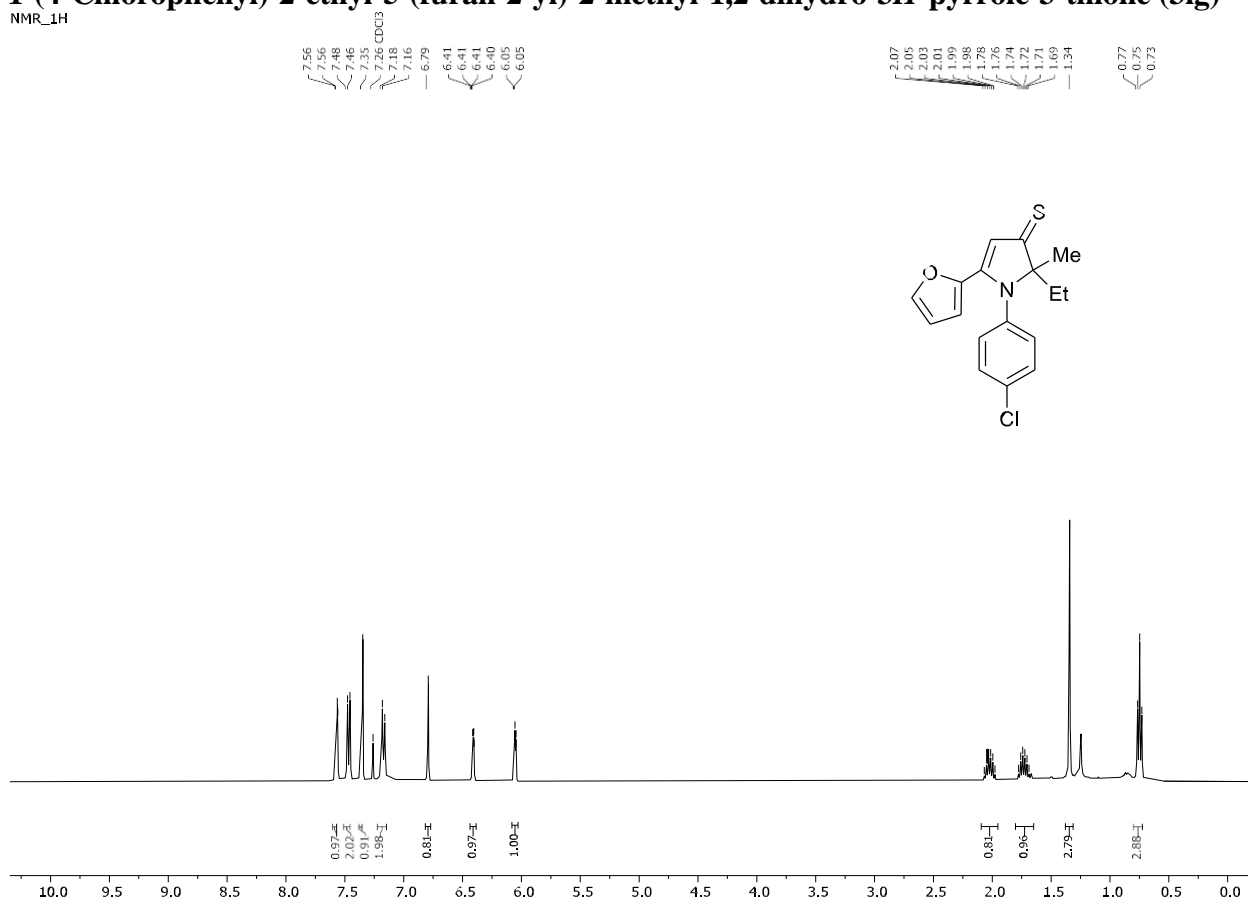
# 1-(4-Chlorophenyl)-2-ethyl-2-methyl-5-phenyl-1,2-dihydro-3H-pyrrole-3-thione (3lc)

NMR\_13C



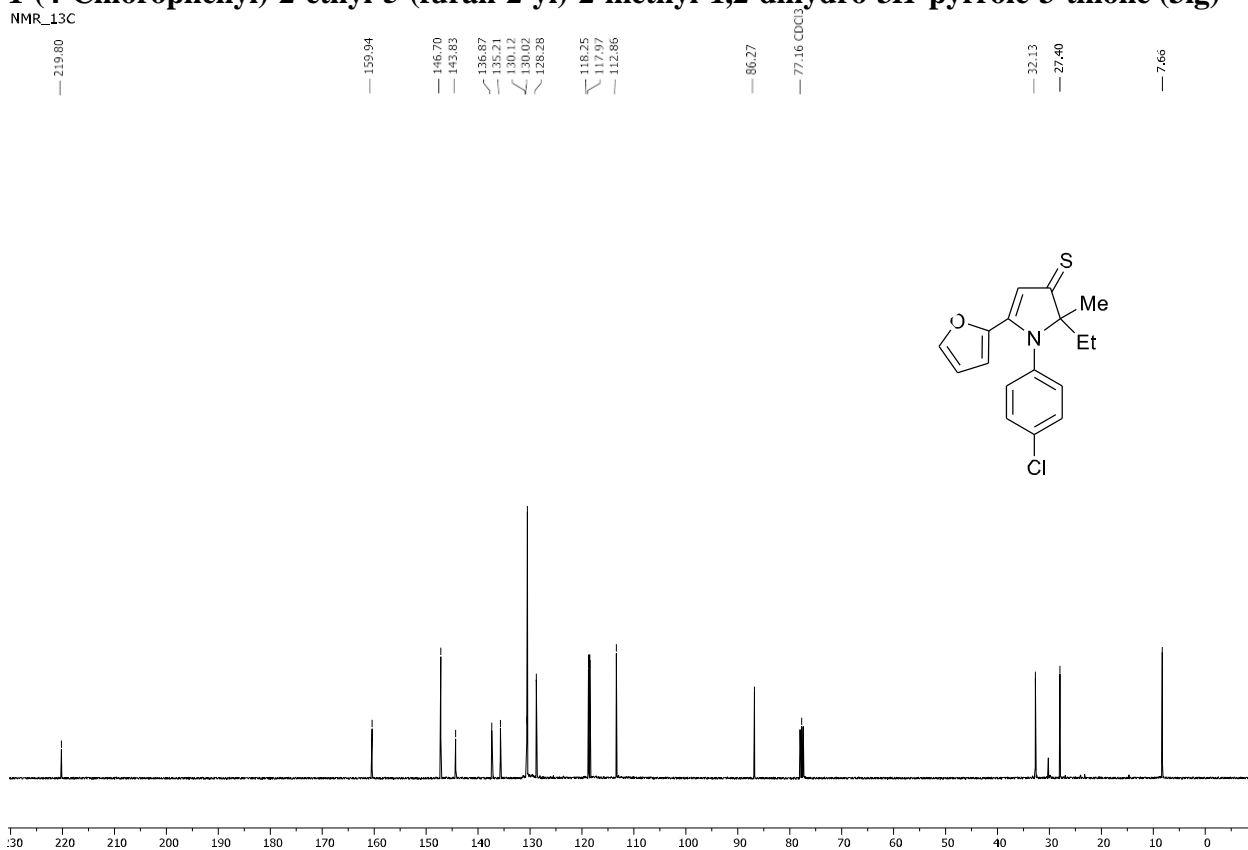
### 1-(4-Chlorophenyl)-2-ethyl-5-(furan-2-yl)-2-methyl-1,2-dihydro-3H-pyrrole-3-thione (3lg)

NMR\_1H

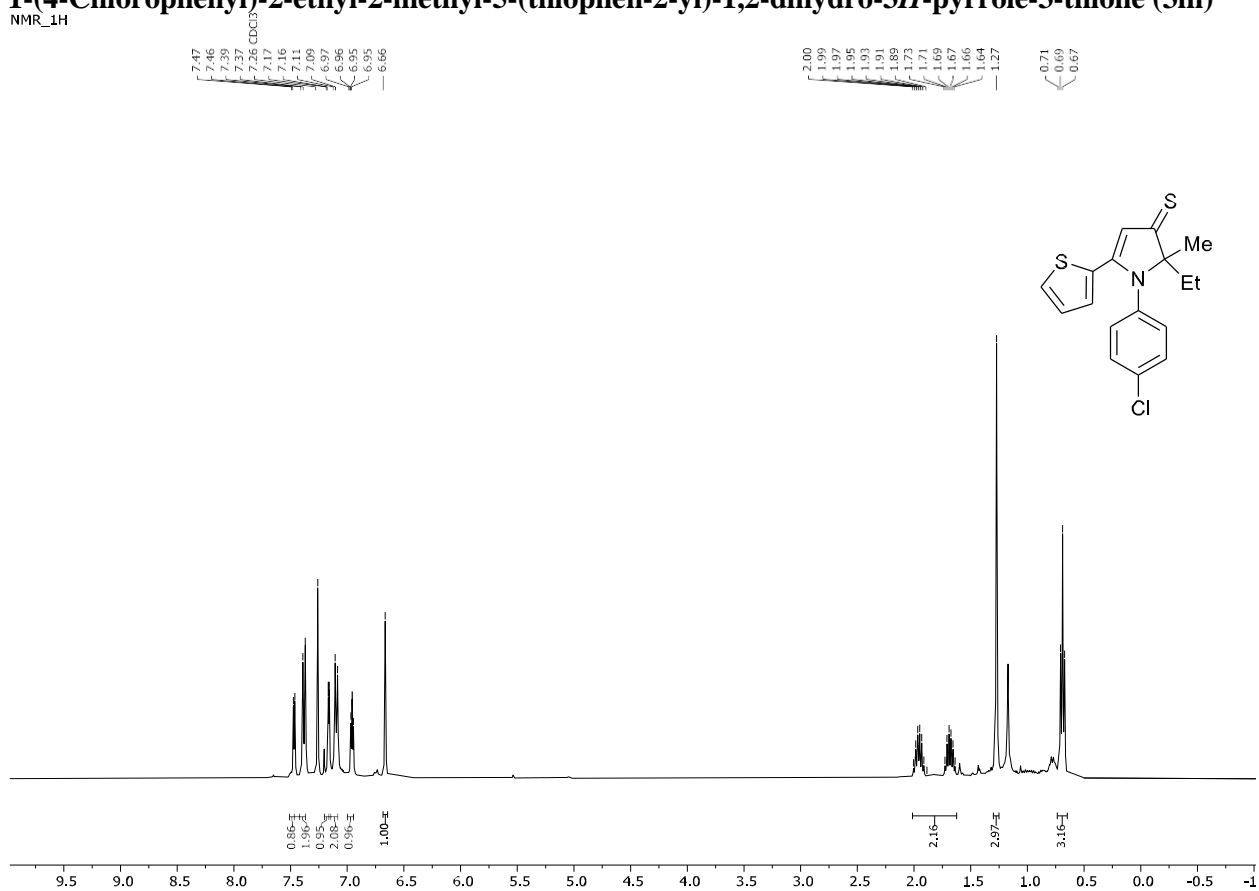


### 1-(4-Chlorophenyl)-2-ethyl-5-(furan-2-yl)-2-methyl-1,2-dihydro-3H-pyrrole-3-thione (3lg)

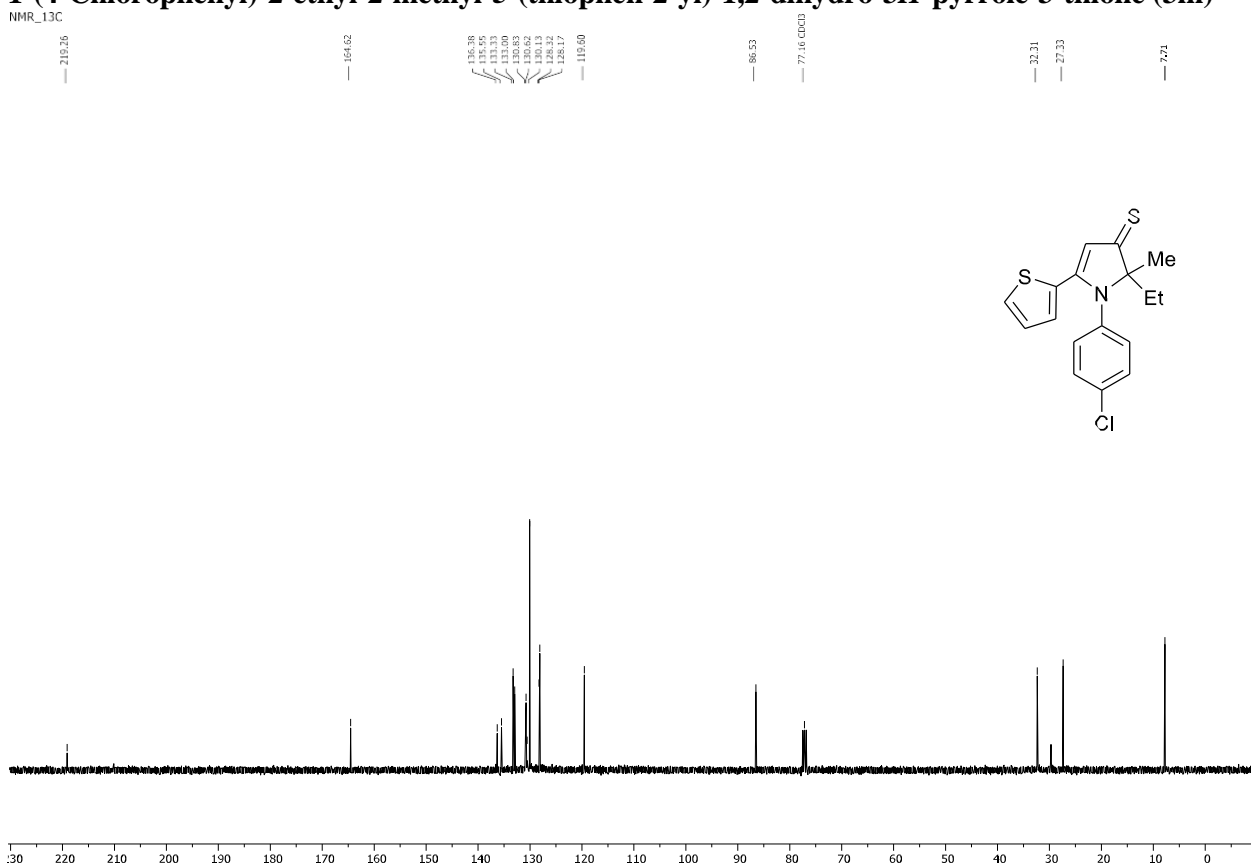
NMR\_13C



**1-(4-Chlorophenyl)-2-ethyl-2-methyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3lh)**

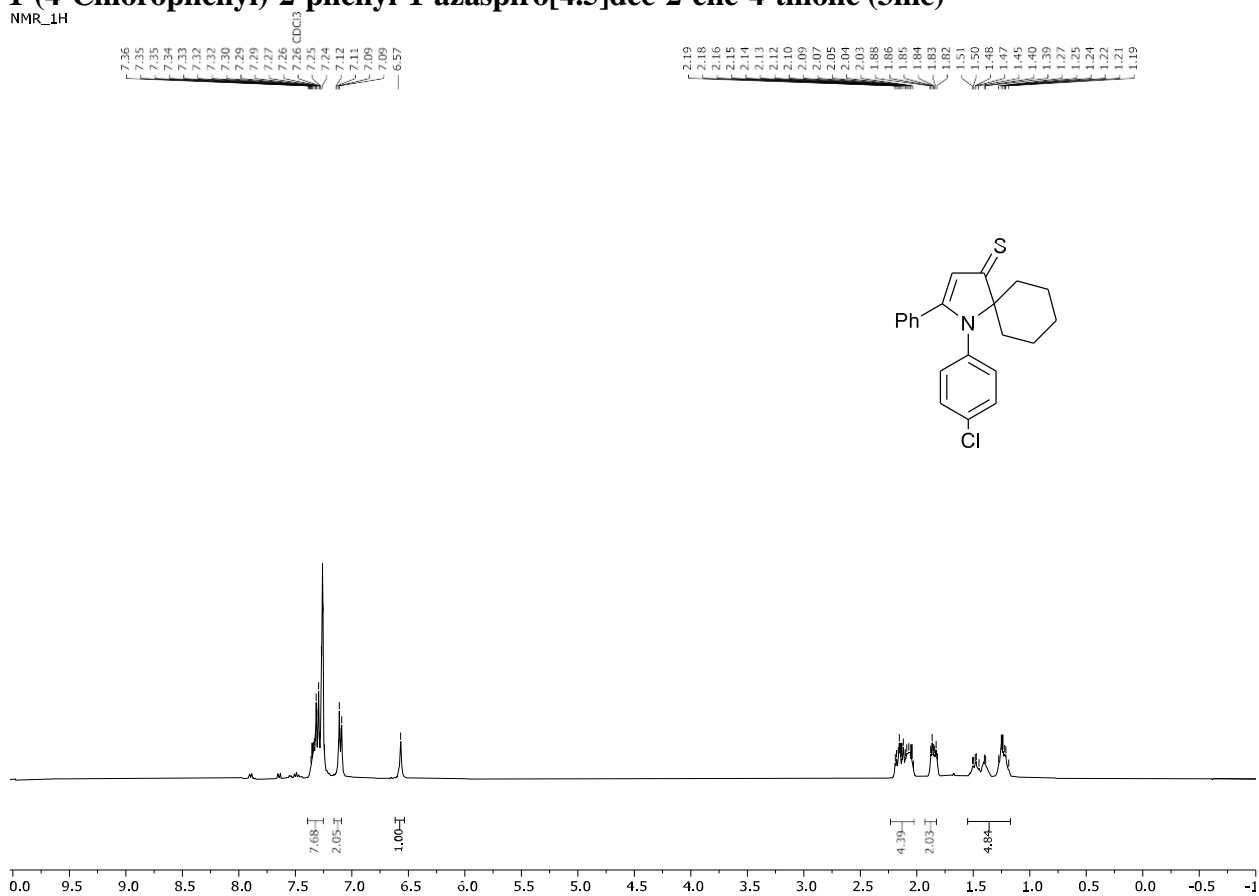


**1-(4-Chlorophenyl)-2-ethyl-2-methyl-5-(thiophen-2-yl)-1,2-dihydro-3H-pyrrole-3-thione (3lh)**



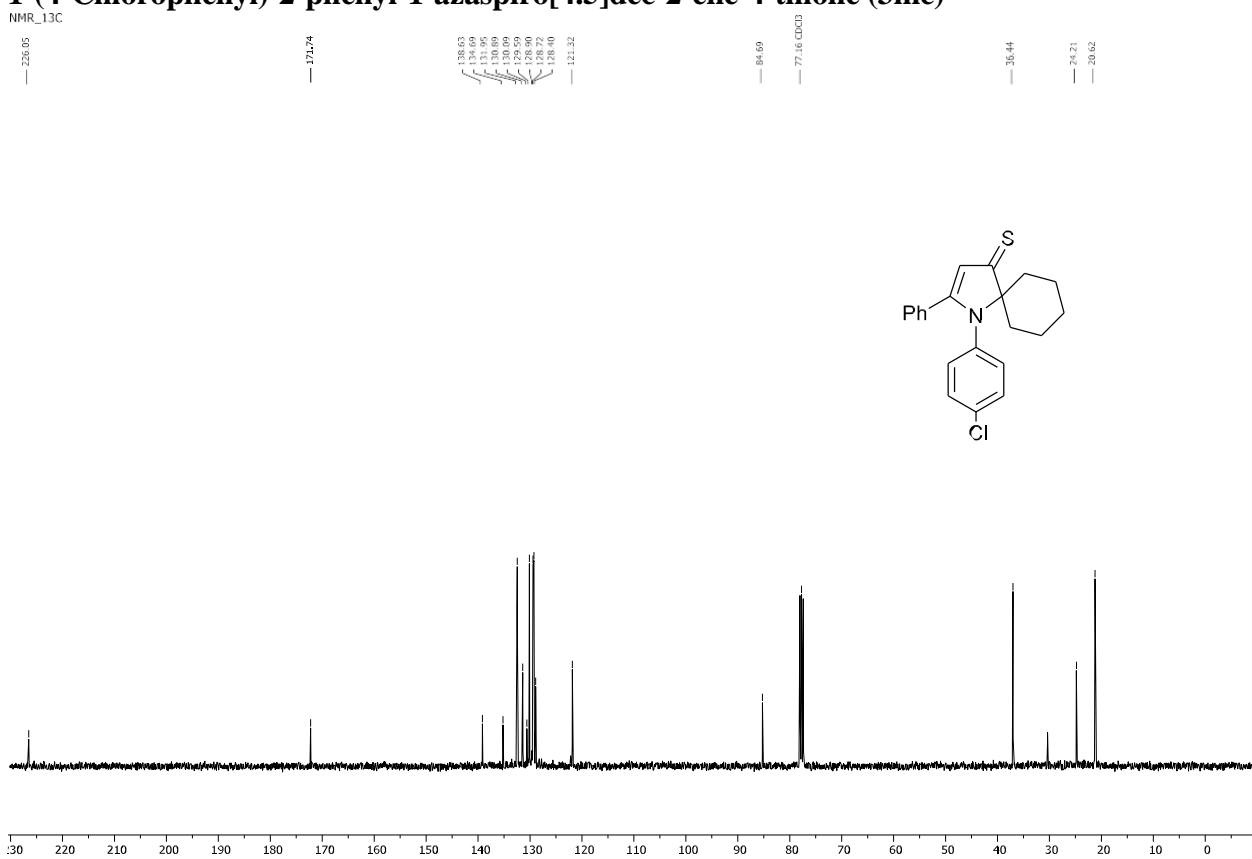
# 1-(4-Chlorophenyl)-2-phenyl-1-azaspiro[4.5]dec-2-ene-4-thione (3mc)

NMR\_1H



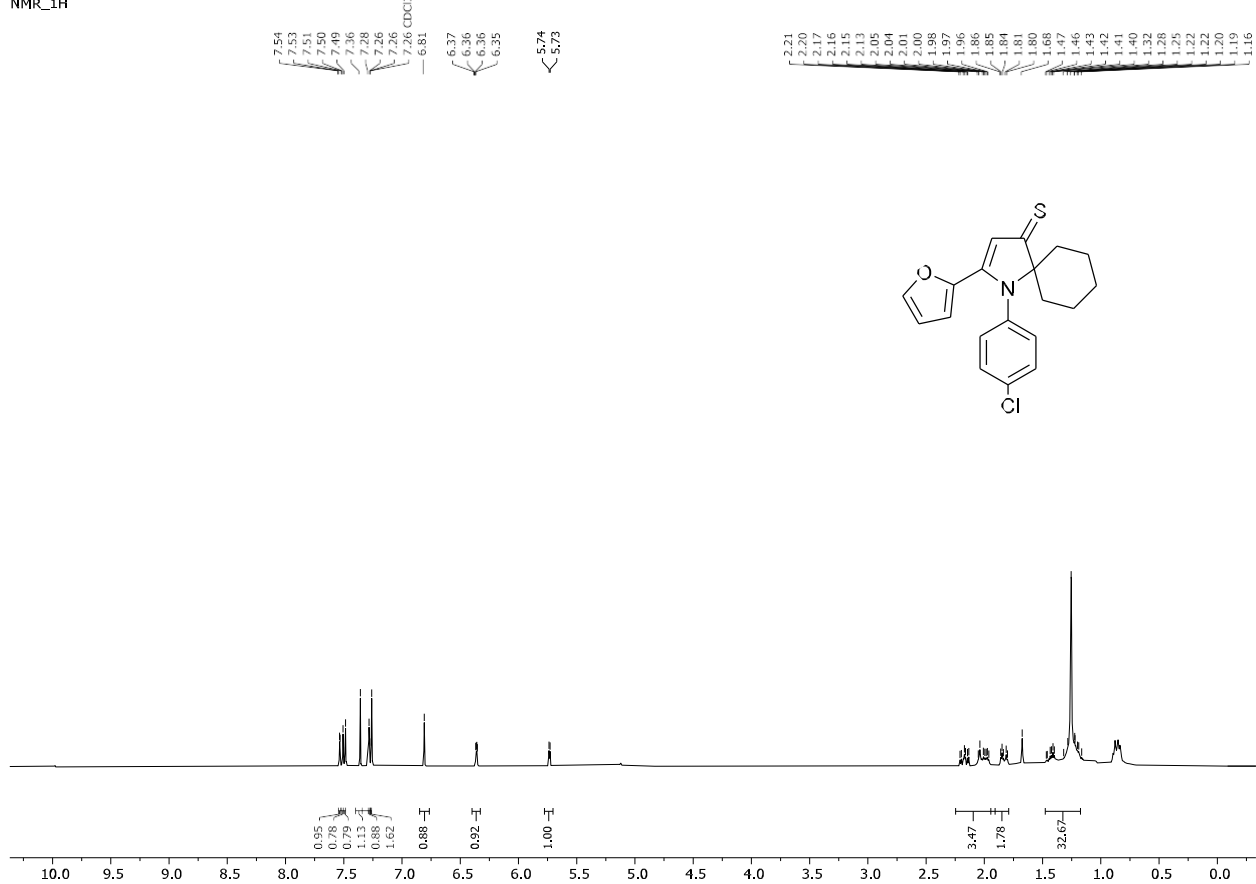
# 1-(4-Chlorophenyl)-2-phenyl-1-azaspiro[4.5]dec-2-ene-4-thione (3mc)

NMR\_13C



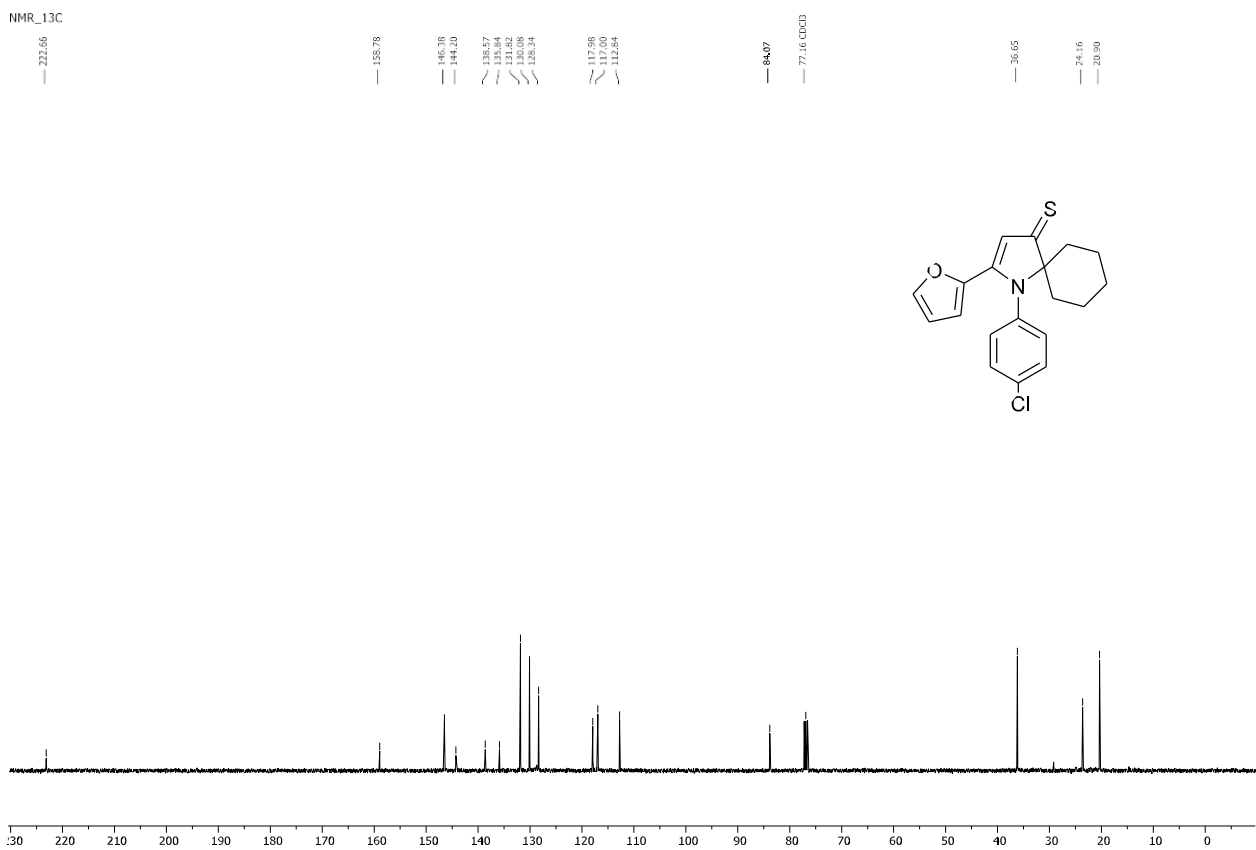
# 1-(4-Chlorophenyl)-2-(furan-2-yl)-1-azaspiro[4.5]dec-2-ene-4-thione (3mg)

NMR\_1H



# 1-(4-Chlorophenyl)-2-(furan-2-yl)-1-azaspiro[4.5]dec-2-ene-4-thione (3mg)

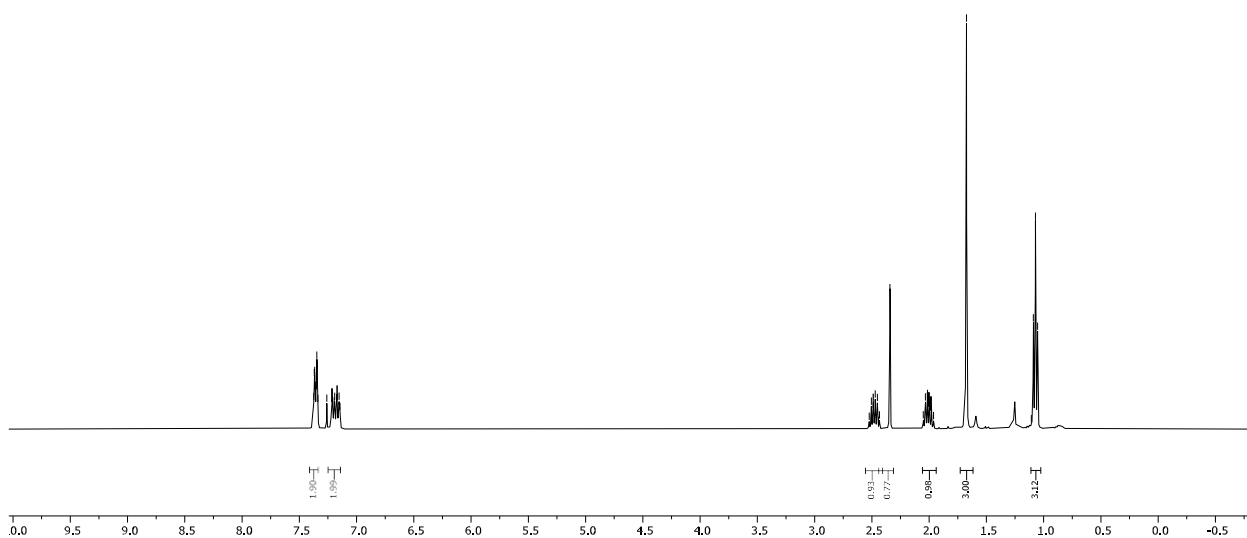
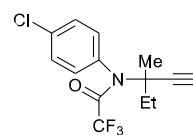
NMR\_13C





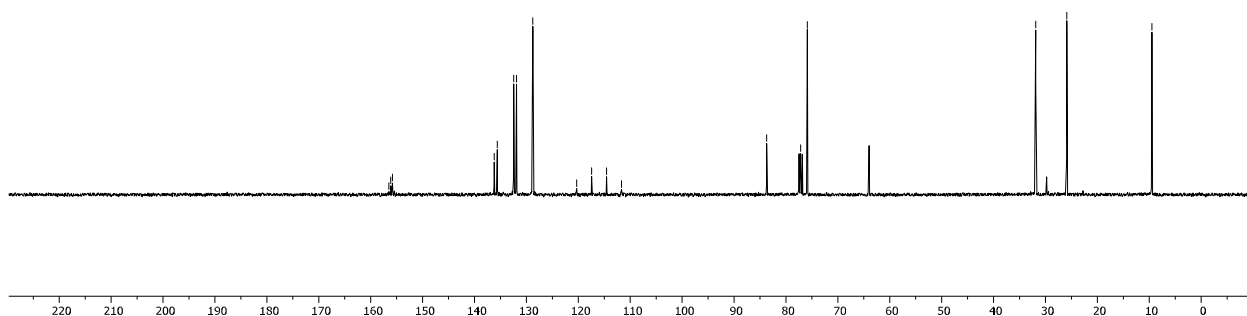
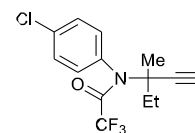
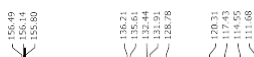
***N*-(4-Chlorophenyl)-2,2,2-trifluoro-*N*-(3-methylpent-1-yn-3-yl)acetamide**

NMR\_1H



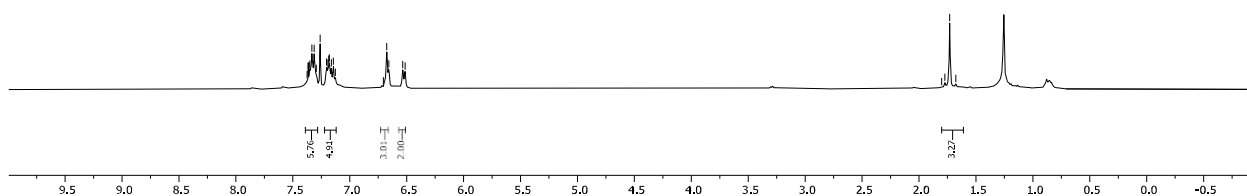
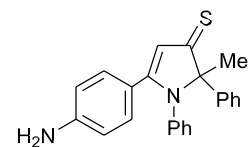
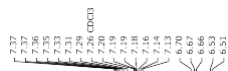
***N*-(4-Chlorophenyl)-2,2,2-trifluoro-*N*-(3-methylpent-1-yn-3-yl)acetamide**

NMR\_13C



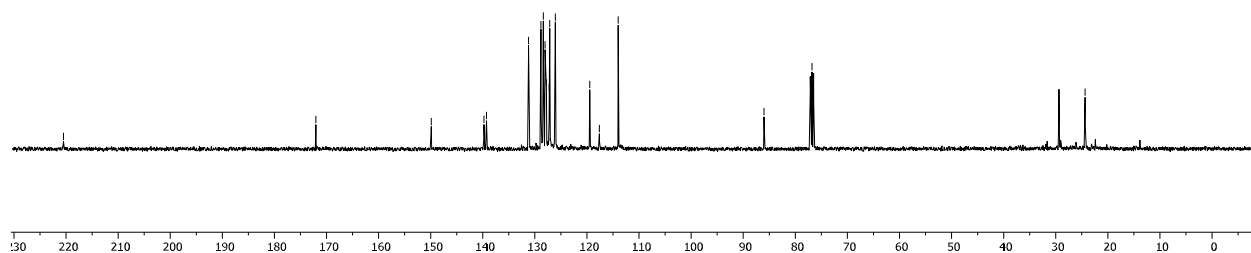
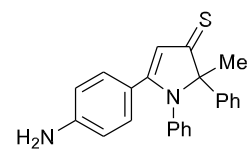
# 5-(4-Aminophenyl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (5)

NMR\_1H



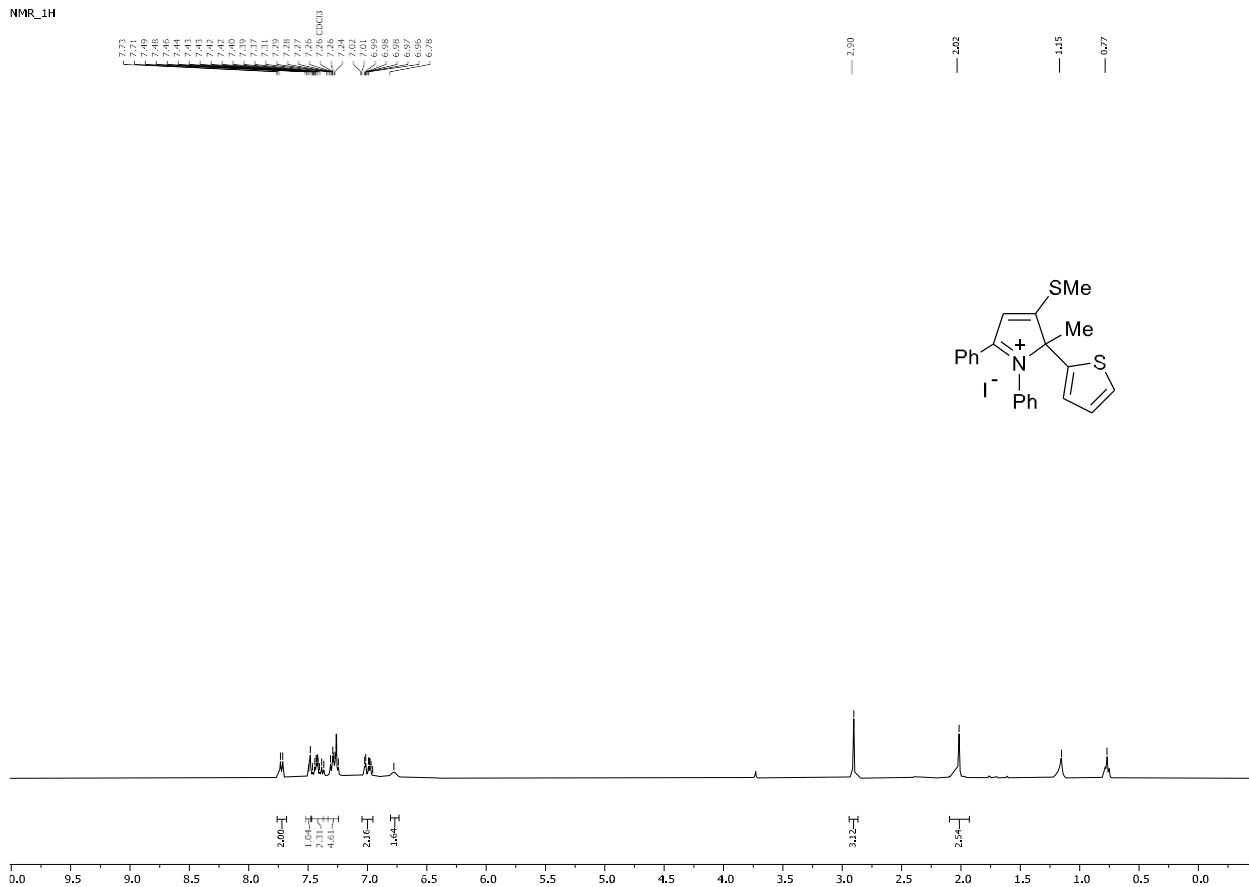
# 5-(4-Aminophenyl)-2-methyl-1,2-diphenyl-1,2-dihydro-3H-pyrrole-3-thione (5)

NMR\_13C



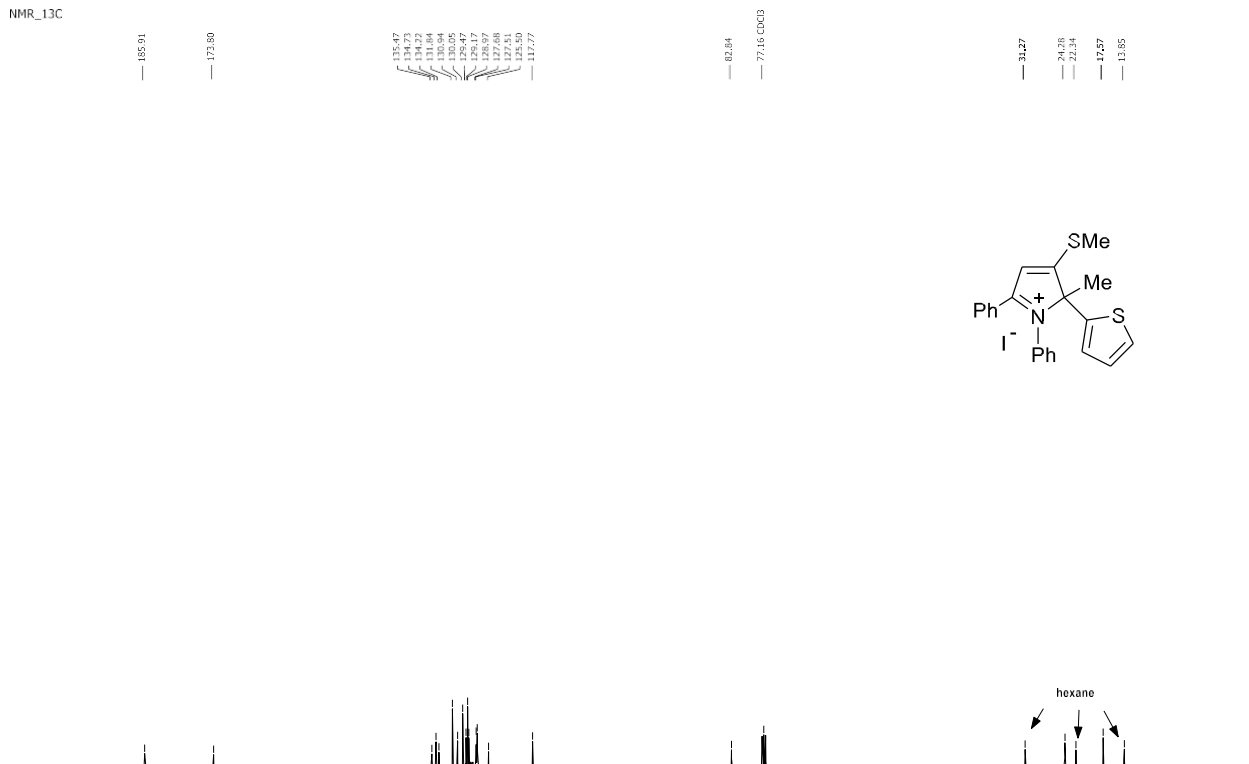
## 2-Methyl-3-(methylthio)-1,5-diphenyl-2-(thiophen-2-yl)-2H-pyrrol-1-ium iodide (9)

NMR\_1H



## 2-Methyl-3-(methylthio)-1,5-diphenyl-2-(thiophen-2-yl)-2H-pyrrol-1-ium iodide (9)

NMR\_13C



**2-Methyl-3-(methylthio)-1,5-diphenyl-2-(thiophen-2-yl)-2H-pyrrol-1-ium iodide (9)**

