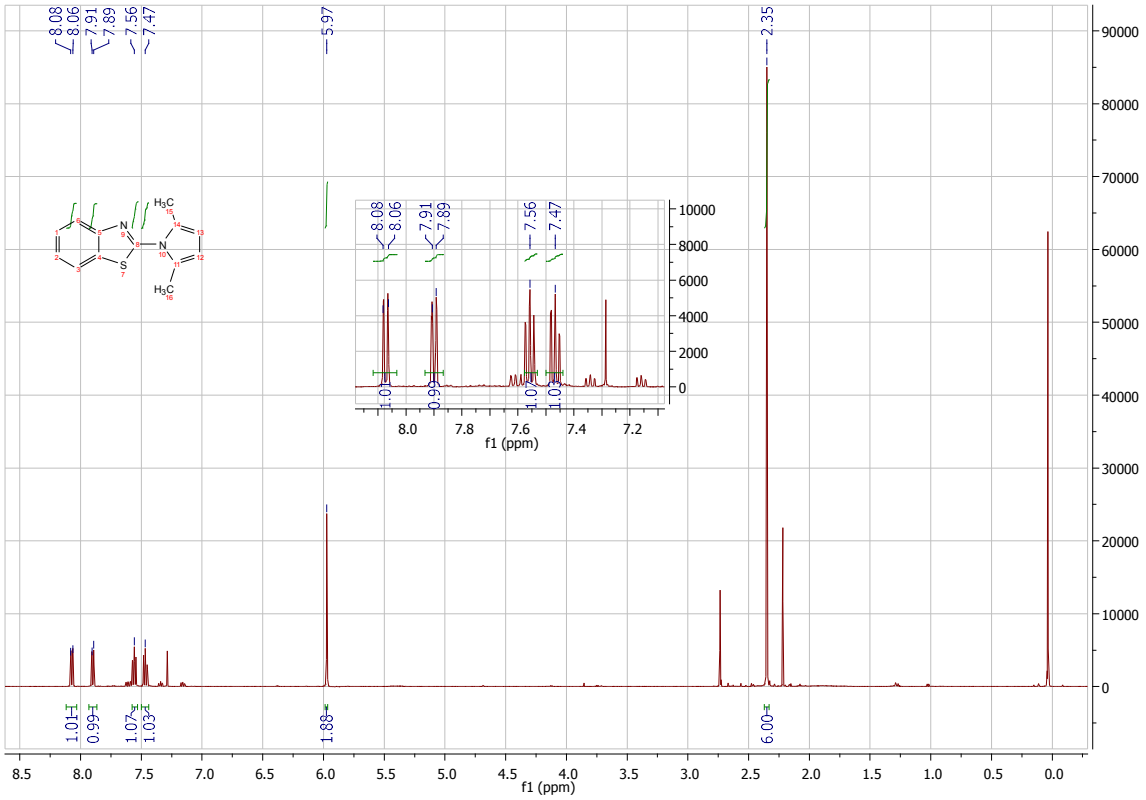
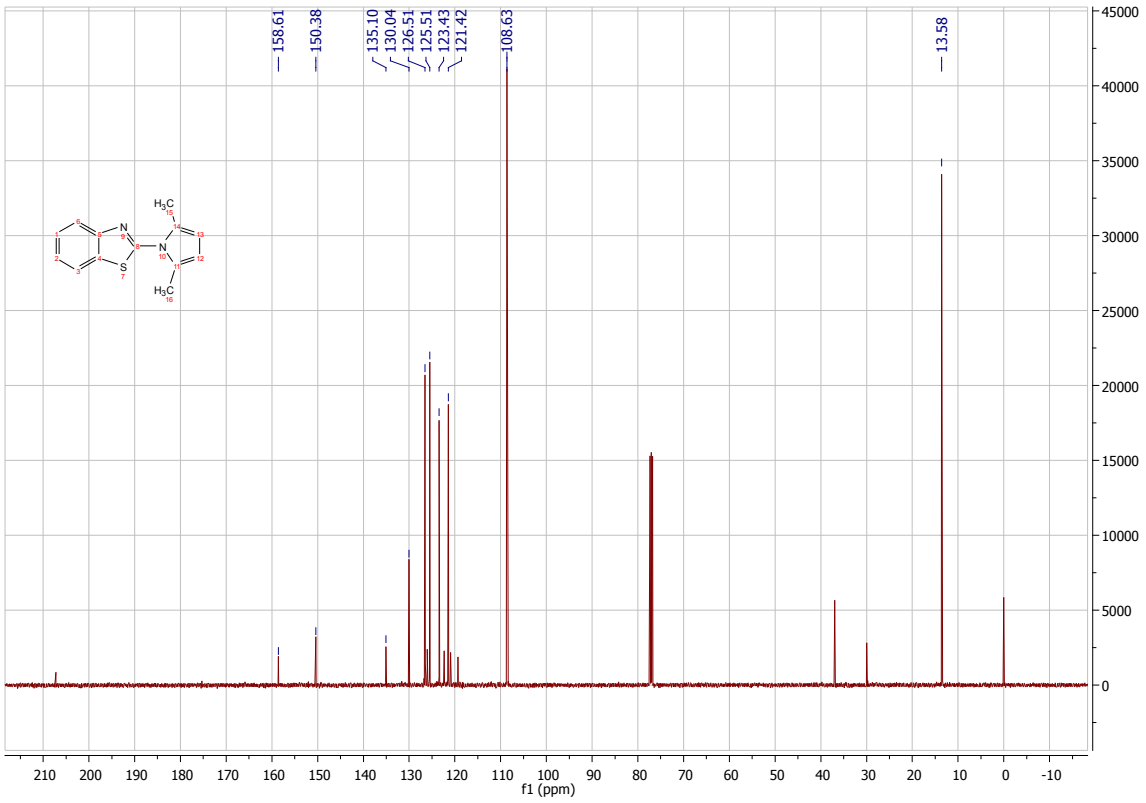
Supplementary Material

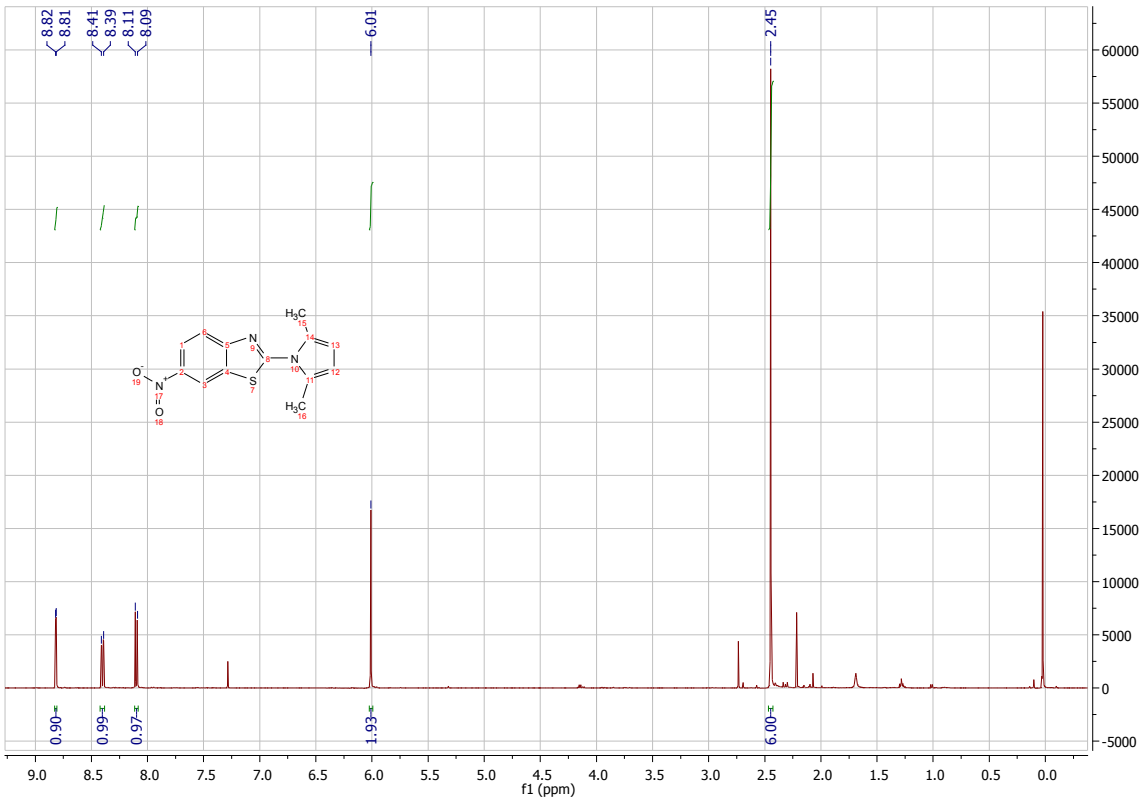
1. ^{1}H ,^{13}C RMN of benzothiazole and chromene pyrrole derivatives

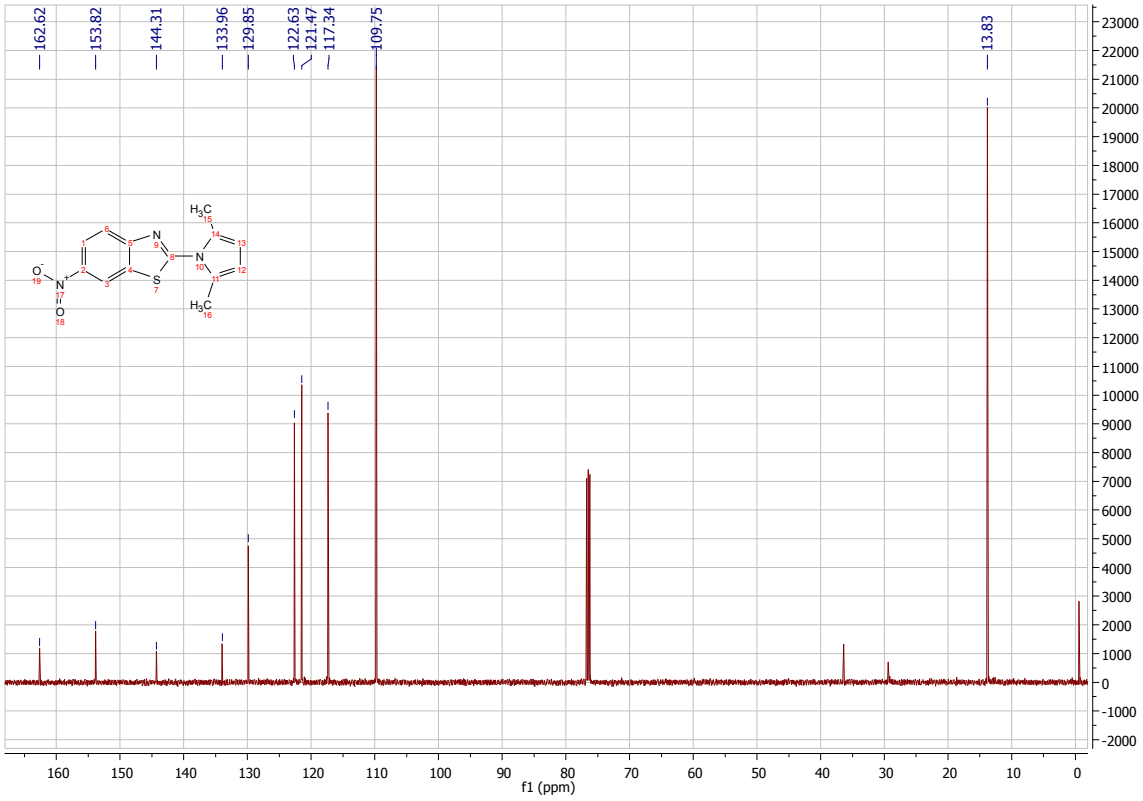
a) 2-(2,5-dimethyl-1H-pyrrol-1-yl)benzo[d]thiazole



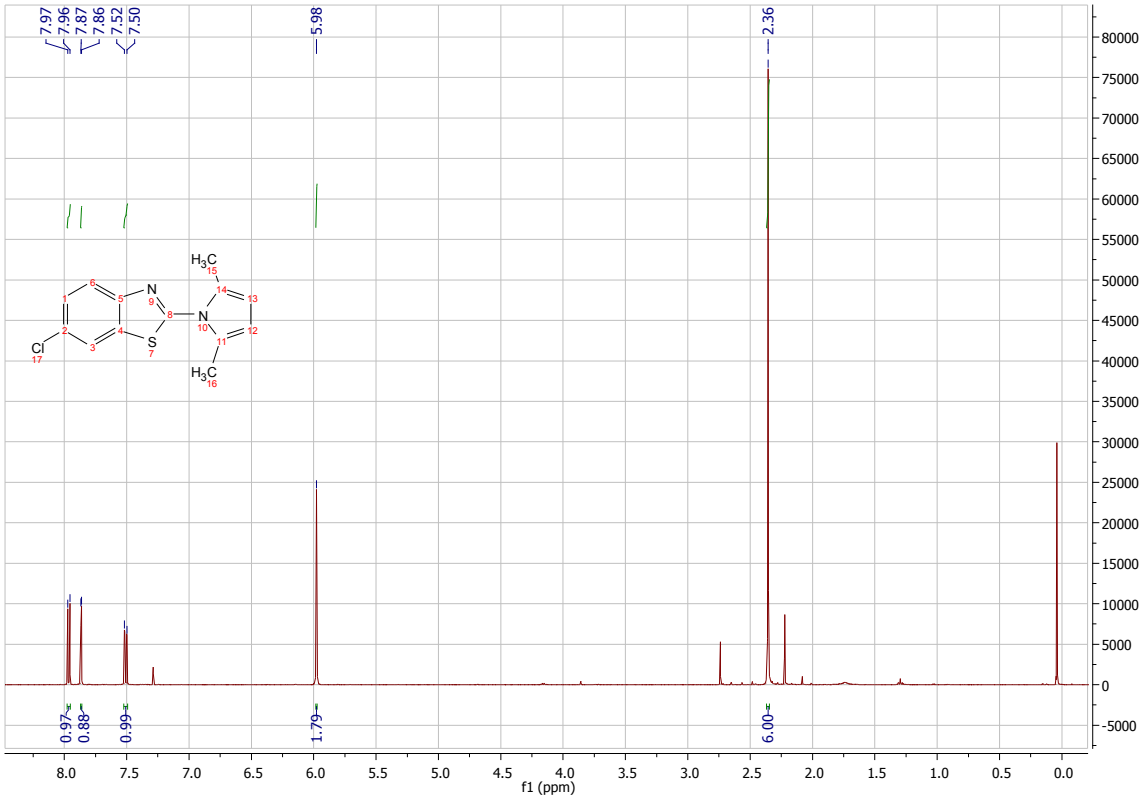


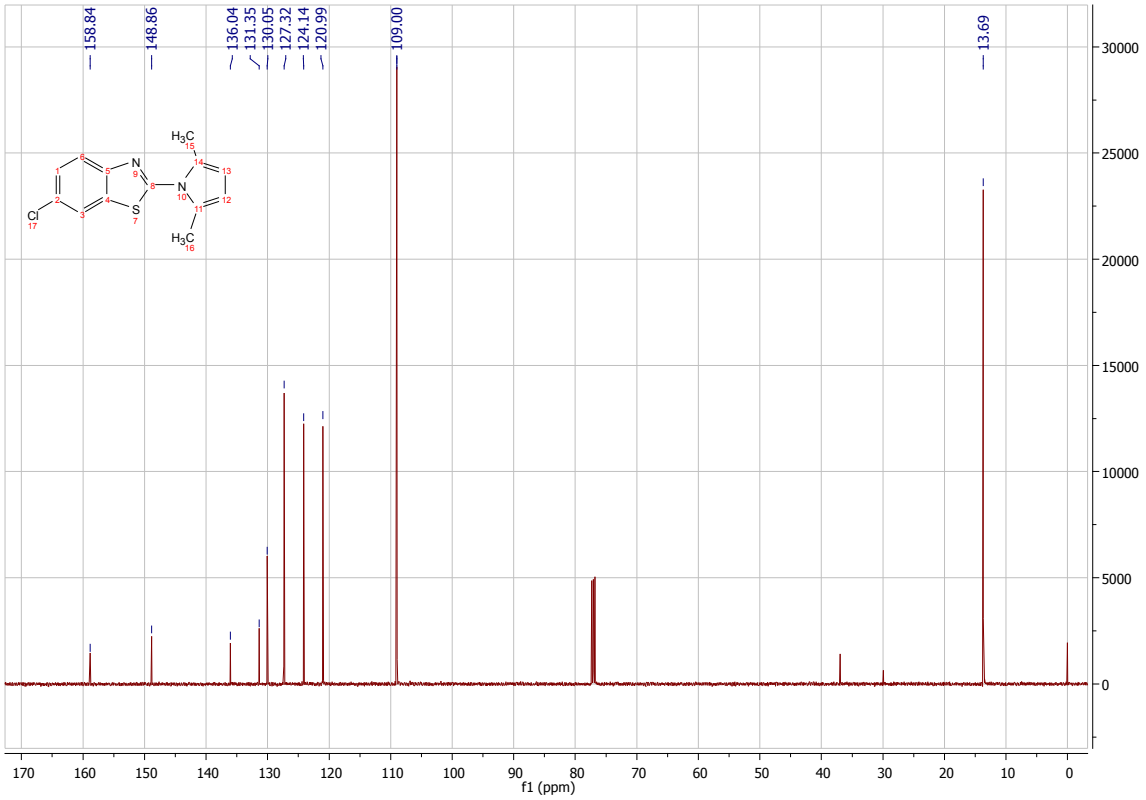
b) 2-(2,5-dimethyl-1H-pyrrol-1-yl)-6-nitrobenzo[d]thiazole



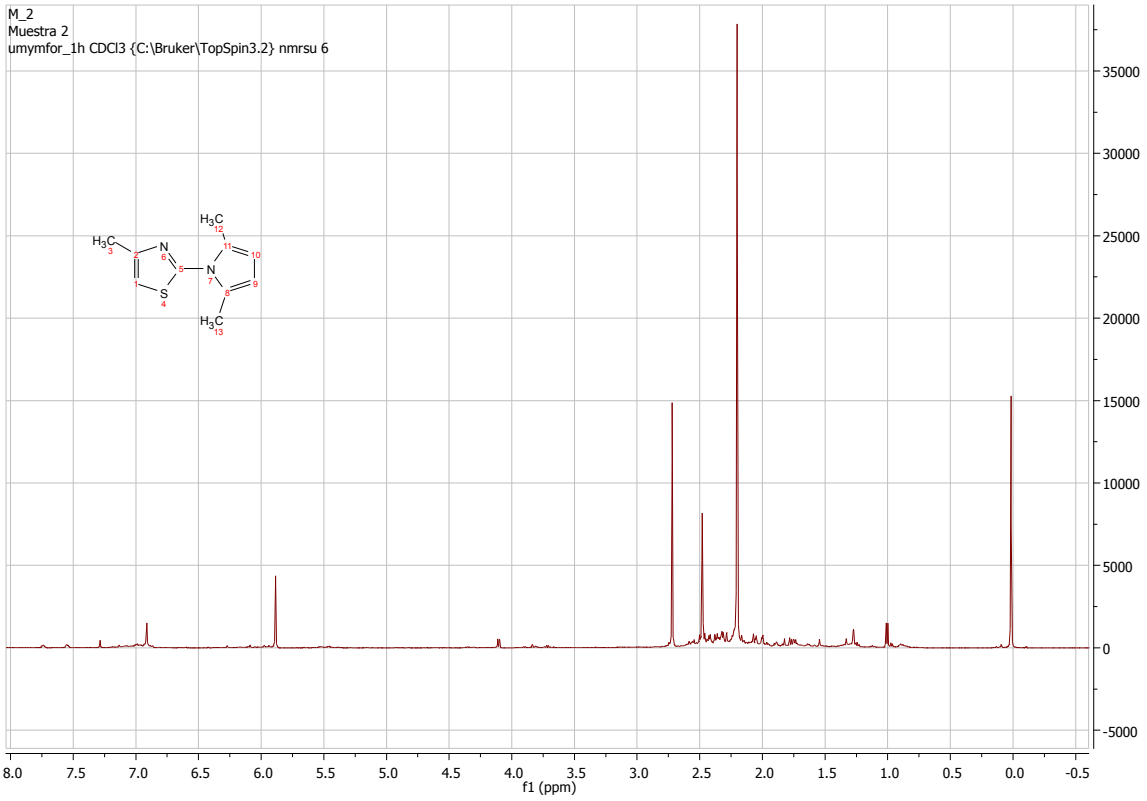


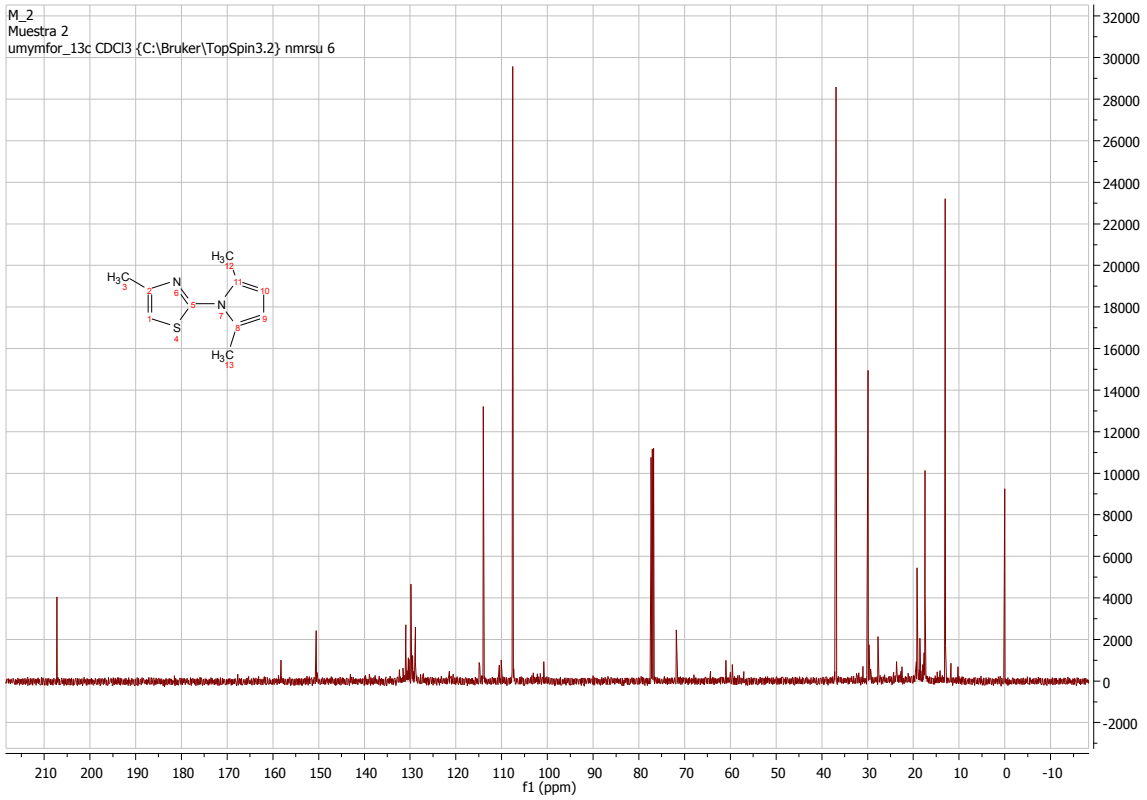
c) 6-chloro-2-(2,5-dimethyl-1H-pyrrol-1-yl)benzo[d]thiazole



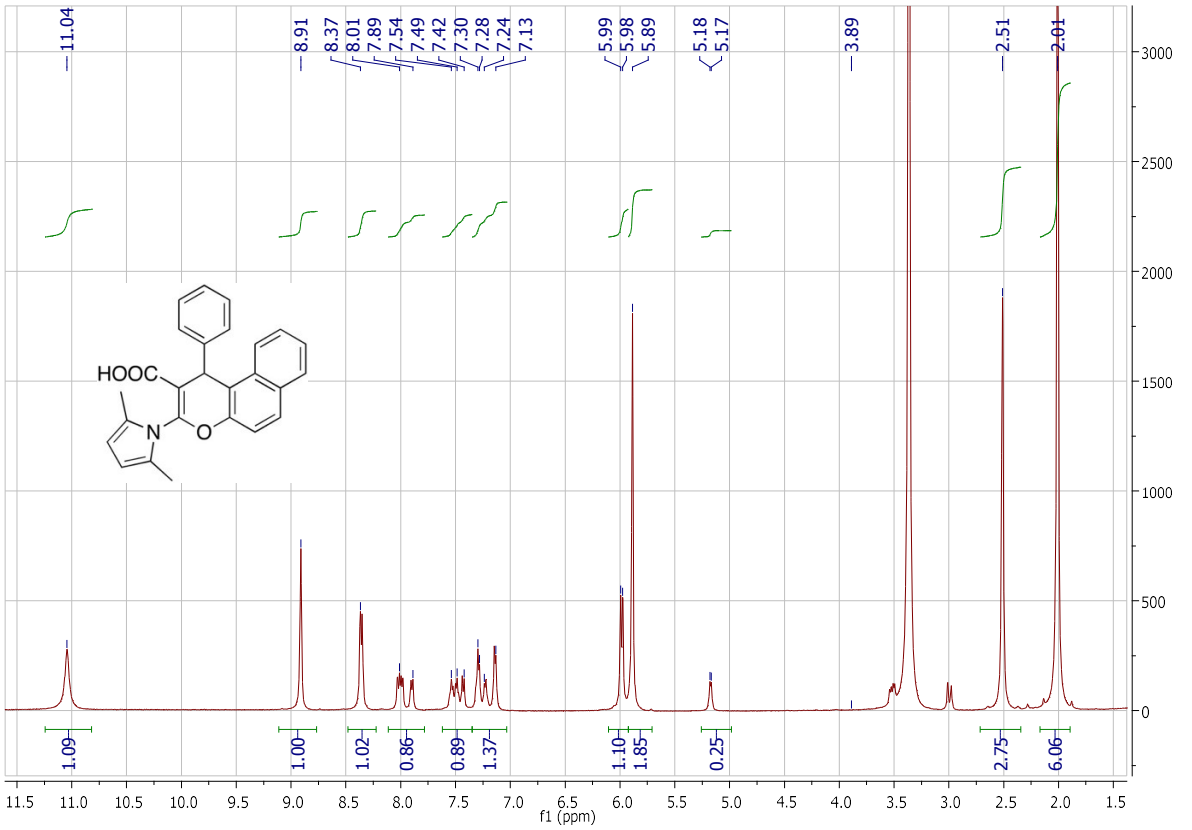


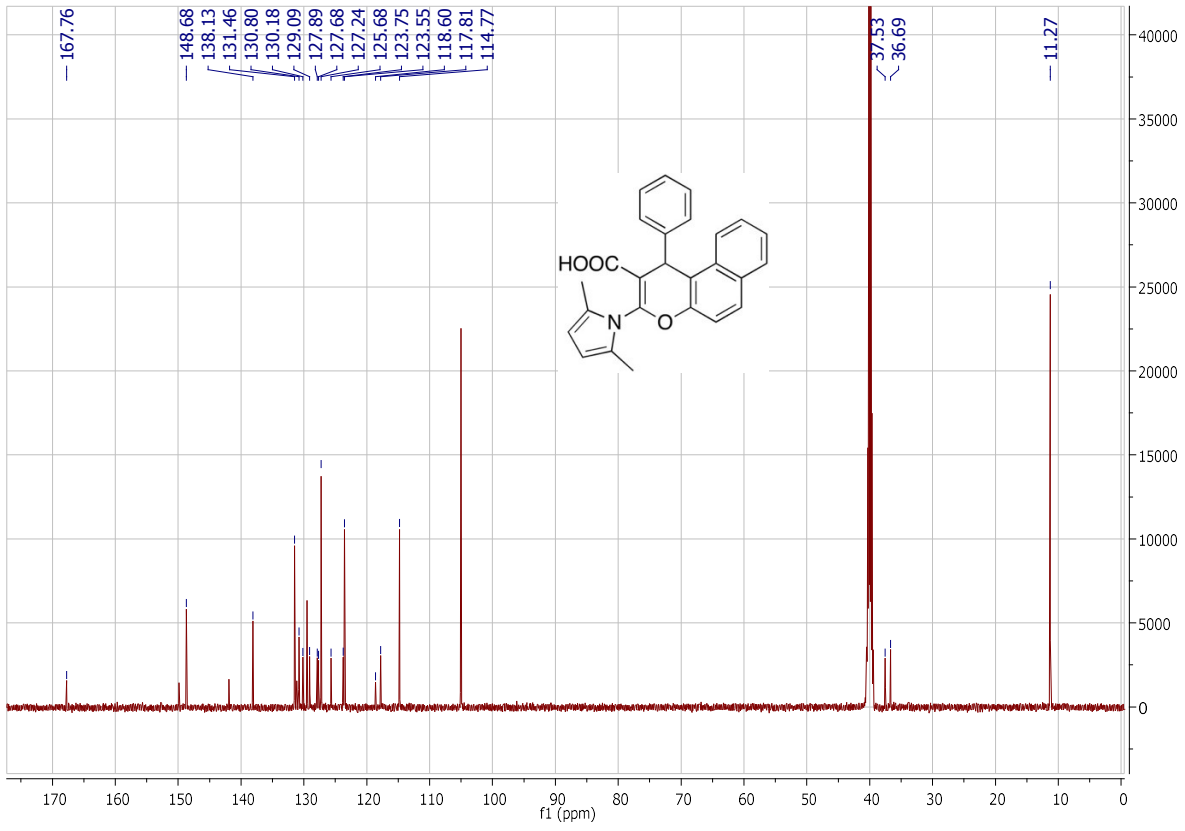
d) 2-(2,5-dimethyl-1H-pyrrol-1-yl)-4-methylthiazole





e) 3-(2,5-dimethyl-1H-pyrrol-1-yl)-1-phenyl-1H-benzo[f]chromene-2-carboxylic acid


11.04
8.91
8.37
8.01
7.89
7.54
7.49
7.42
7.30
7.28
7.24
7.13
5.99
5.98
5.89
5.18
5.17
3.89
2.51
2.01
HOOC
N
O
1.09
1.00
1.02
0.86
0.89
1.37
1.10
1.85
0.25
2.75
6.06
f1 (ppm)


167.76
148.68
138.13
131.46
130.80
130.18
129.09
127.89
127.68
127.24
125.68
123.75
123.55
118.60
117.81
114.77
37.53
36.69
11.27
HOOC
N
O
f1 (ppm)

2. Green metrics[1,2]

Atom Economy

$$\boldsymbol{AE} = \frac{\boldsymbol{MW}\ product}{\sum \boldsymbol{MW}\ reagents}$$

Yield

$$\boldsymbol{Y} = \left(\frac{\boldsymbol{moles}\ product}{\boldsymbol{moles}\ limiting\_reagent}\right)\left(\frac{\boldsymbol{stoich.coeff.}\ limiting\_reagent}{\boldsymbol{stoich.coeff.}\ product}\right)$$

Reaction Mass Efficiency

$$\boldsymbol{RME} = \frac{\sum \boldsymbol{mass}\ reagents}{\boldsymbol{mass}\ product}$$

Stoichiometric Factor

$$\boldsymbol{SF} = 1 + \frac{\sum \boldsymbol{mass}\ excess\ reagents}{\sum \boldsymbol{mass}\ stoichiometric\ reagents}$$

Material Recovery Parameter

$$\boldsymbol{MRP} = \frac{1}{1 + [(\boldsymbol{Y} * \boldsymbol{AE} * \sum \boldsymbol{mass}\ auxiliaries)/(\boldsymbol{SF} * \boldsymbol{mass}\ product)]}$$

Process Mass Intensity

$$\boldsymbol{PMI} = \frac{\sum \boldsymbol{mass}\ imputs}{\boldsymbol{mass}\ product}$$

Turnover Frequency

$$\boldsymbol{TOF} = \frac{\boldsymbol{Mass}\ product}{\boldsymbol{Mass}\ catalyst * \boldsymbol{Reaction\ time}}$$

[1] Andraos, J., Hent, A., 2015. Simplified Application of Material Efficiency Green Metrics to Synthesis Plans: Pedagogical Case Studies Selected from Organic Syntheses. J. Chem. Educ. 92, 1820–1830. https://doi.org/10.1021/acs.jchemed.5b00058

[2] Andraos, J., Sayed, M, 2007. On the Use of "Green" Metrics in the Undergraduate Organic Chemistry Lecture and Lab To Assess the Mass Efficiency of Organic Reactions. J. Chem. Educ. 84, 1004-1010. https://doi.org/10.1021/ed084p1004