

Supporting Information

Direct Arylation of Sydnone with Aryl Chlorides towards Highly Substituted Pyrazoles

Andrew W. Brown and Joseph P. A. Harrity*

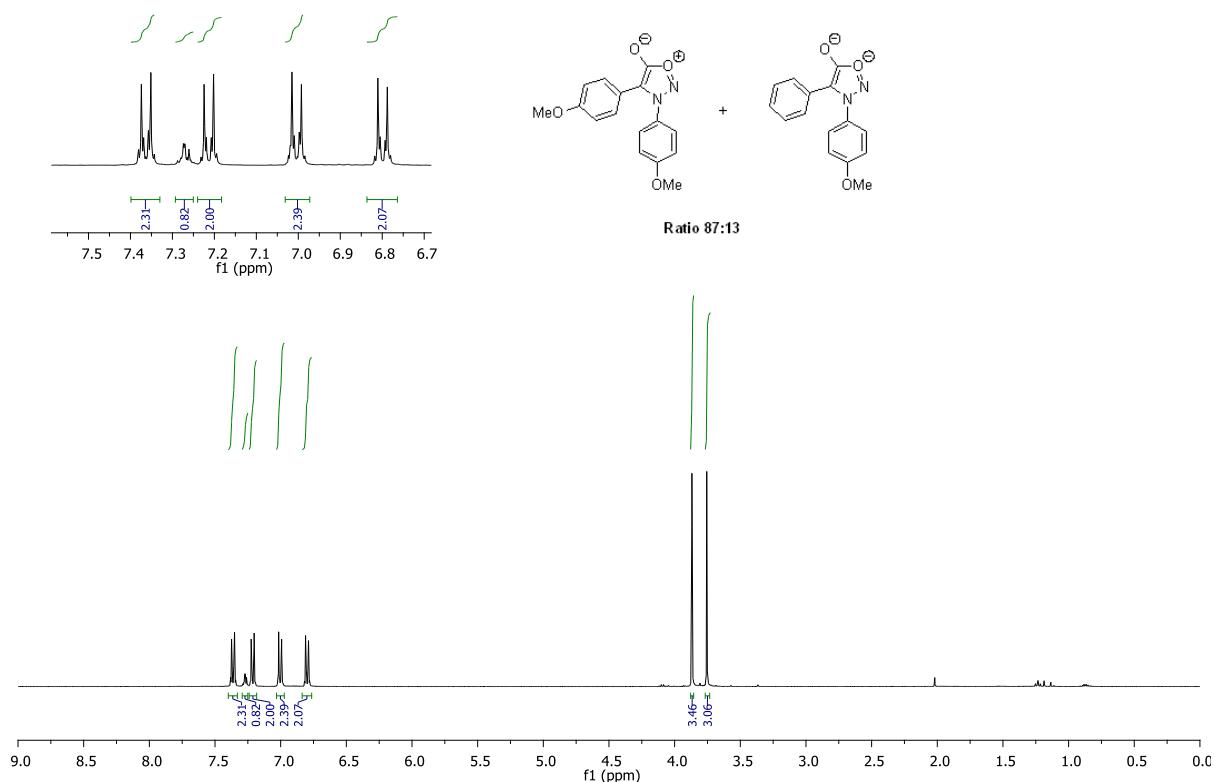
Department of Chemistry, University of Sheffield, Brook Hill, S3 7HF (UK)

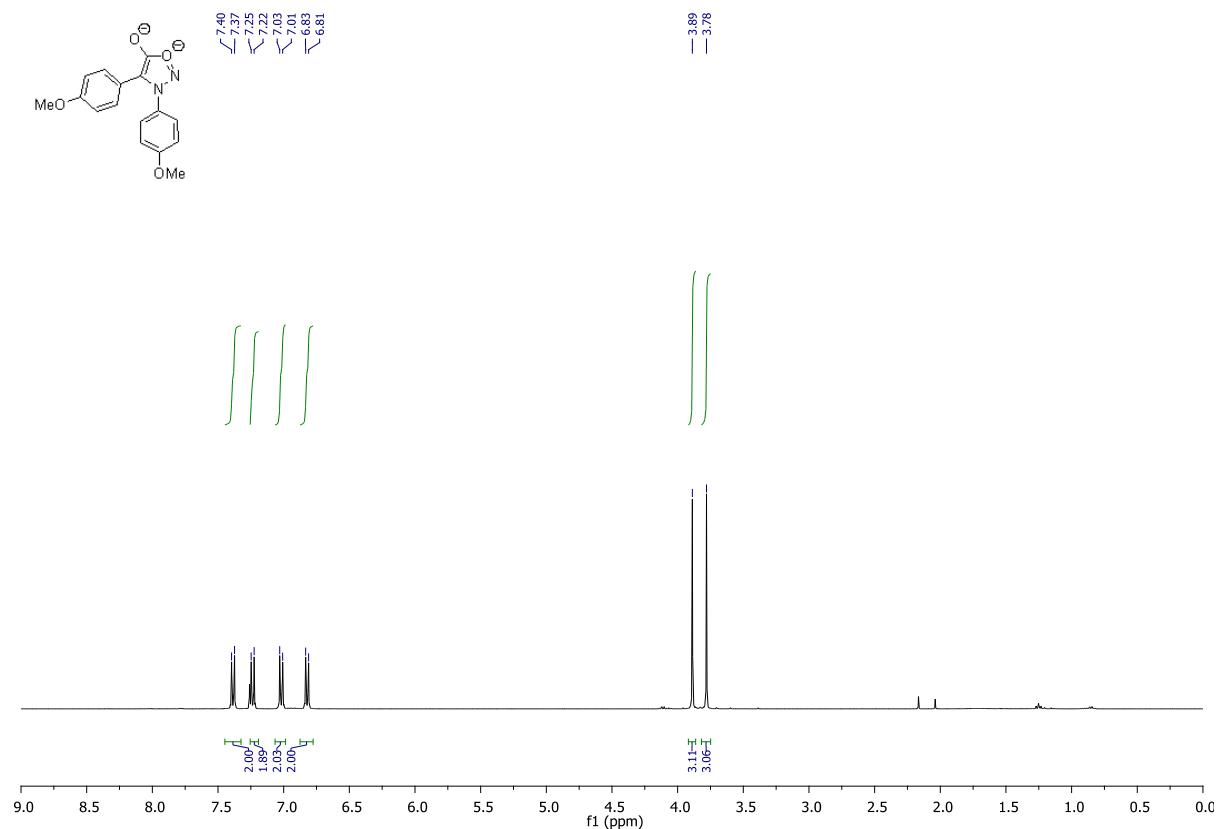
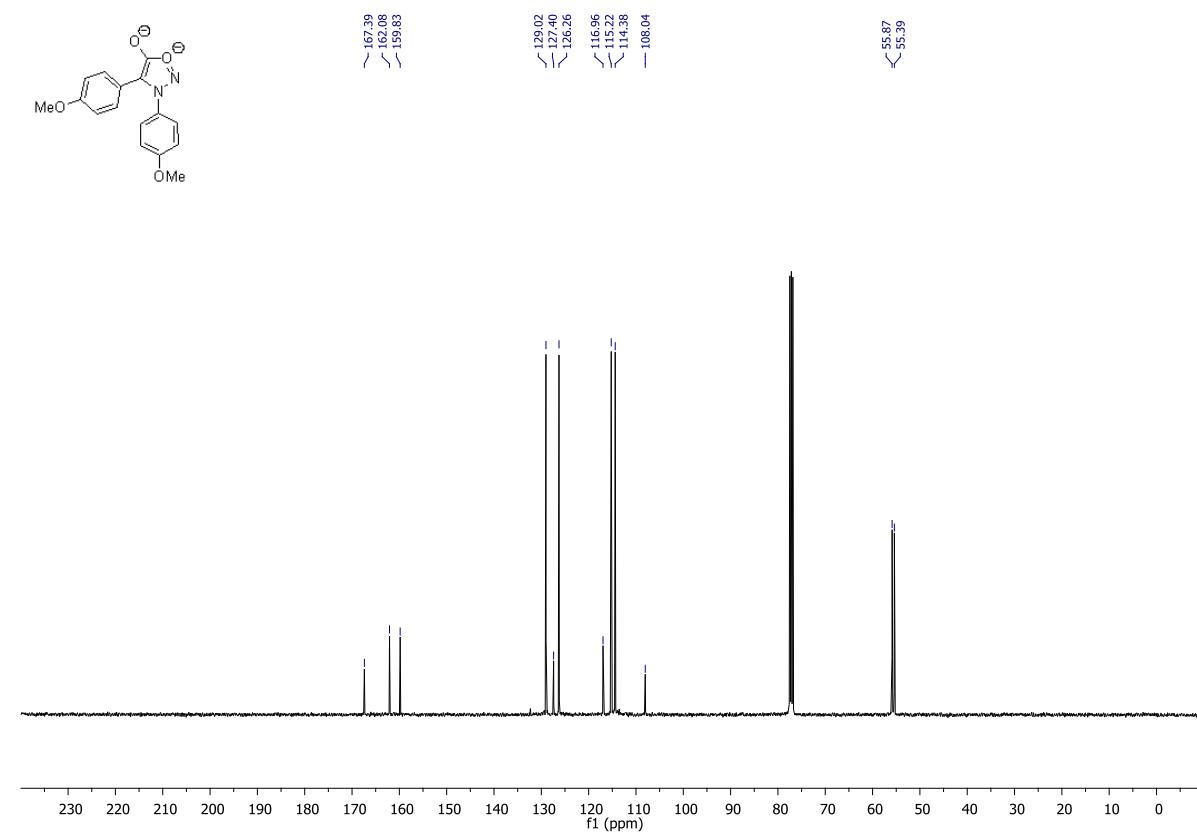
j.harrity@sheffield.ac.uk

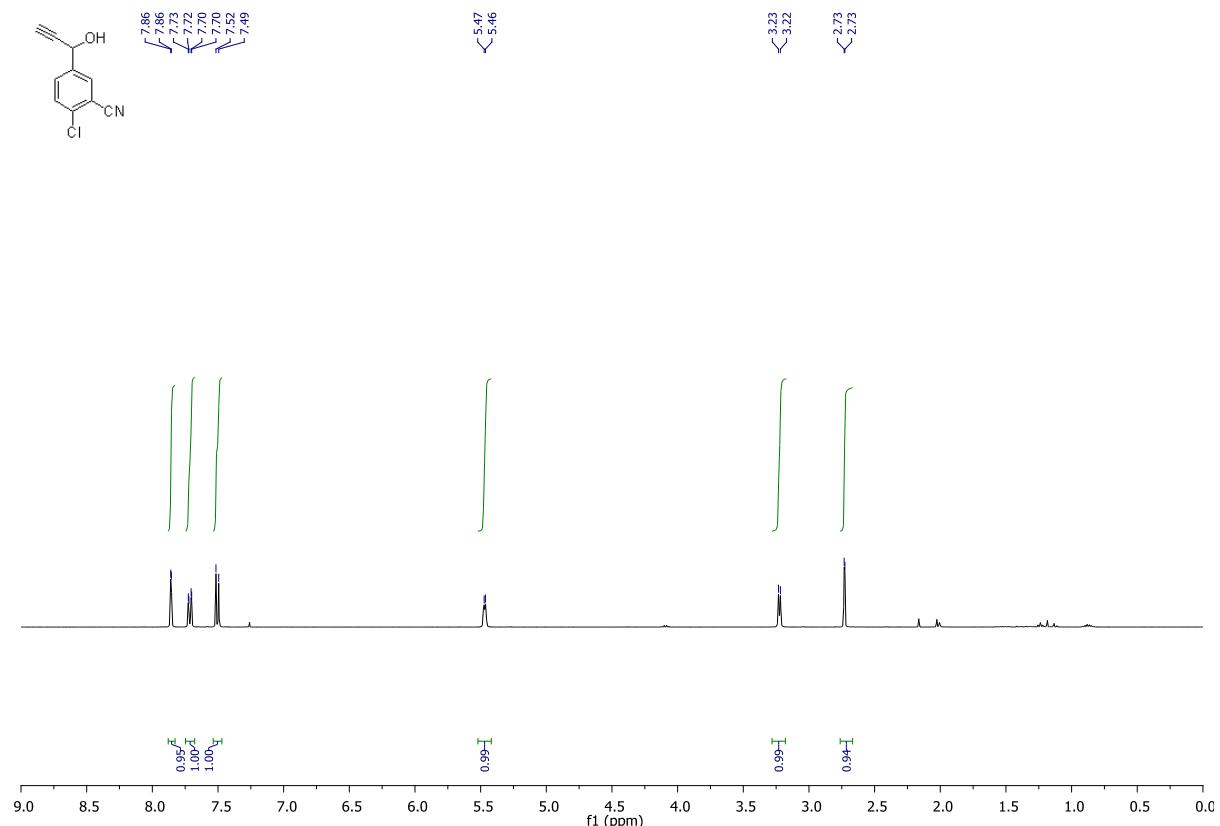
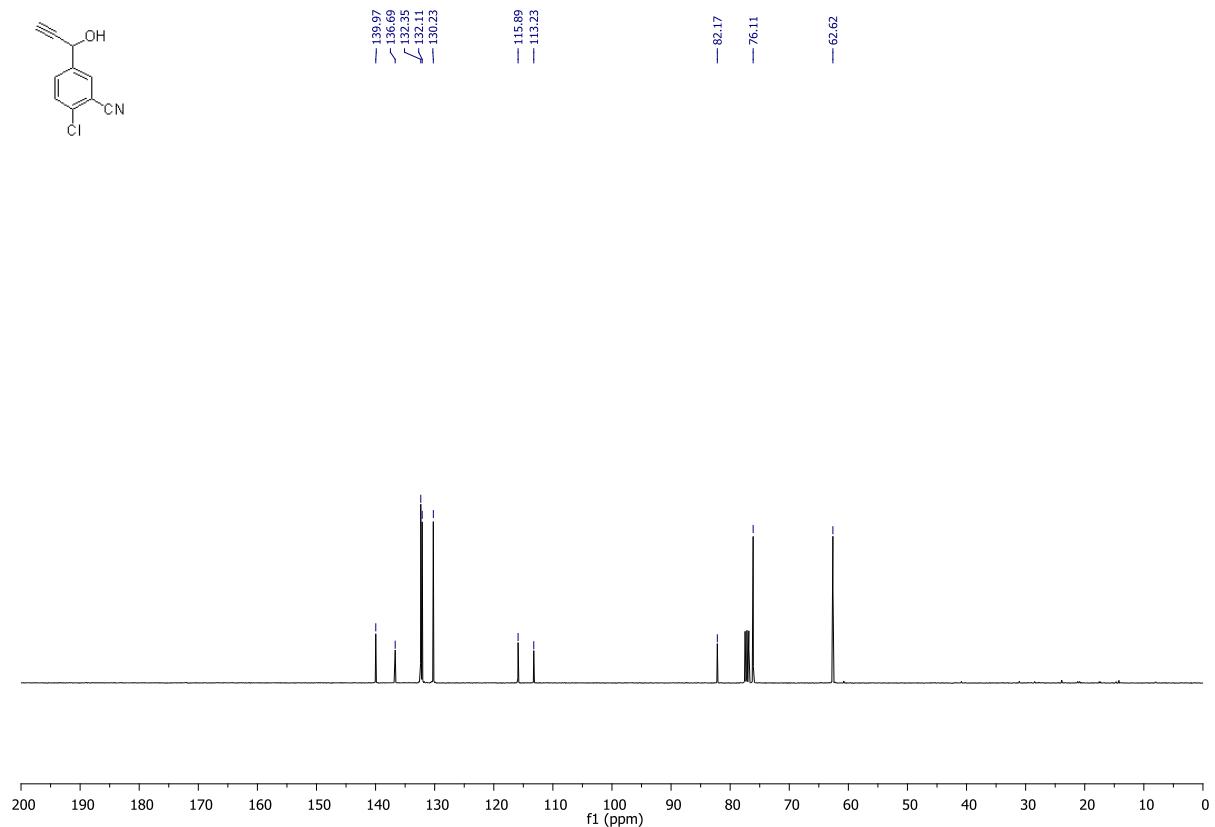
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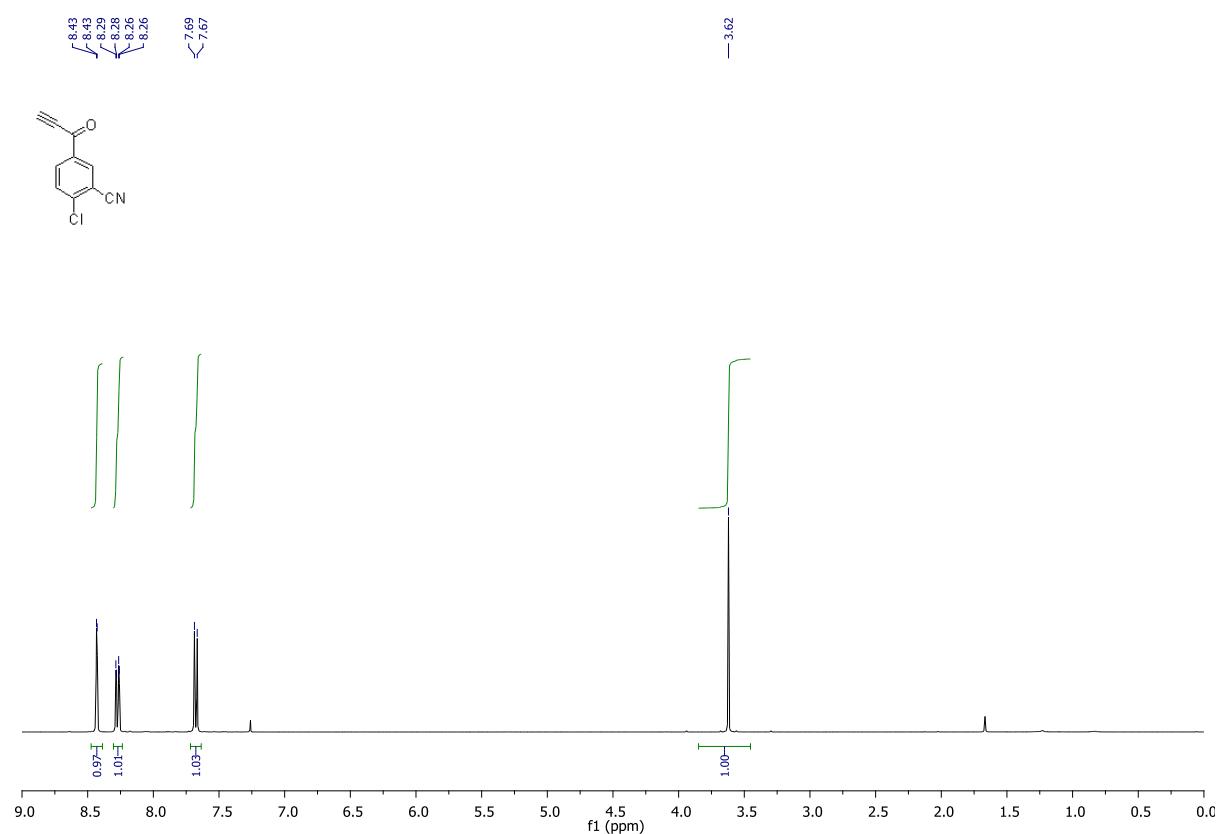
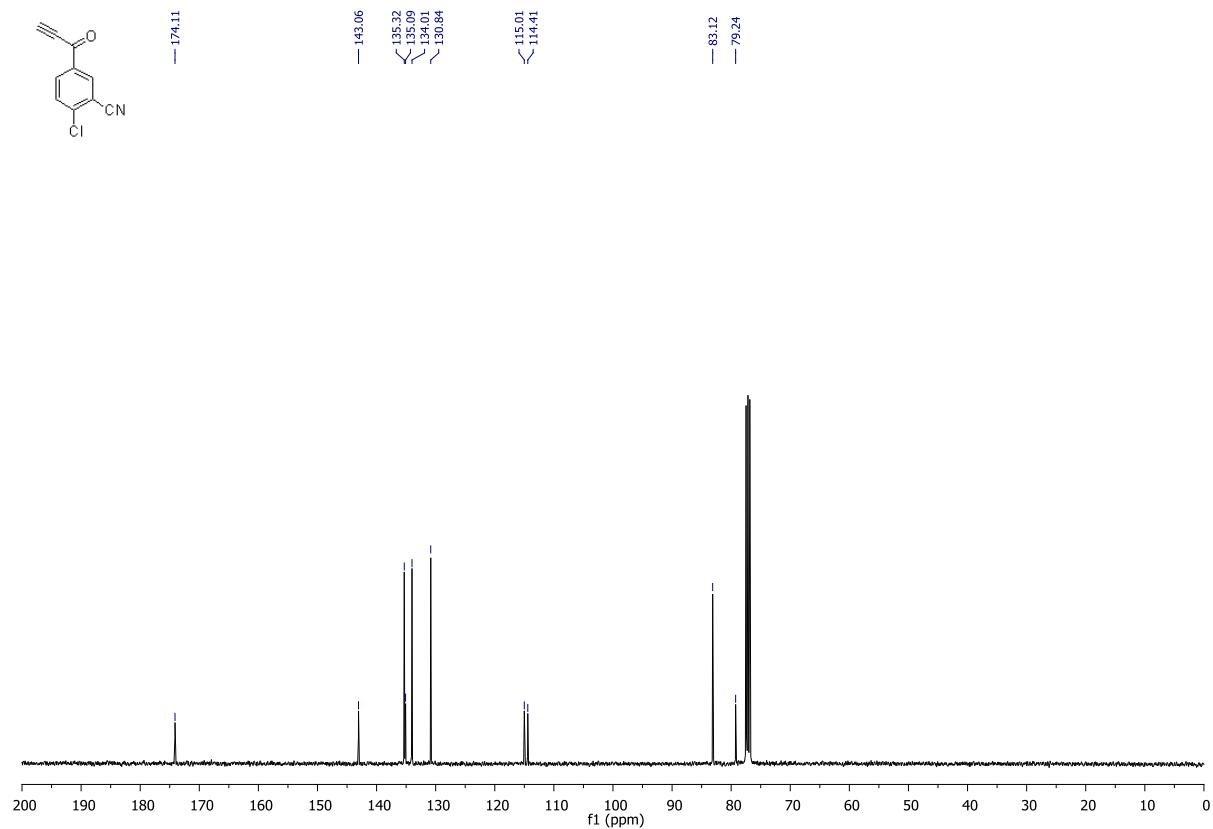
NMR Spectra	Page S2-S34
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¹H NMR of 3,4-Bis(4-methoxyphenyl)sydnone (**2**) and phenyl-N-(4-methoxyphenyl)sydnone (**5**) mixture:

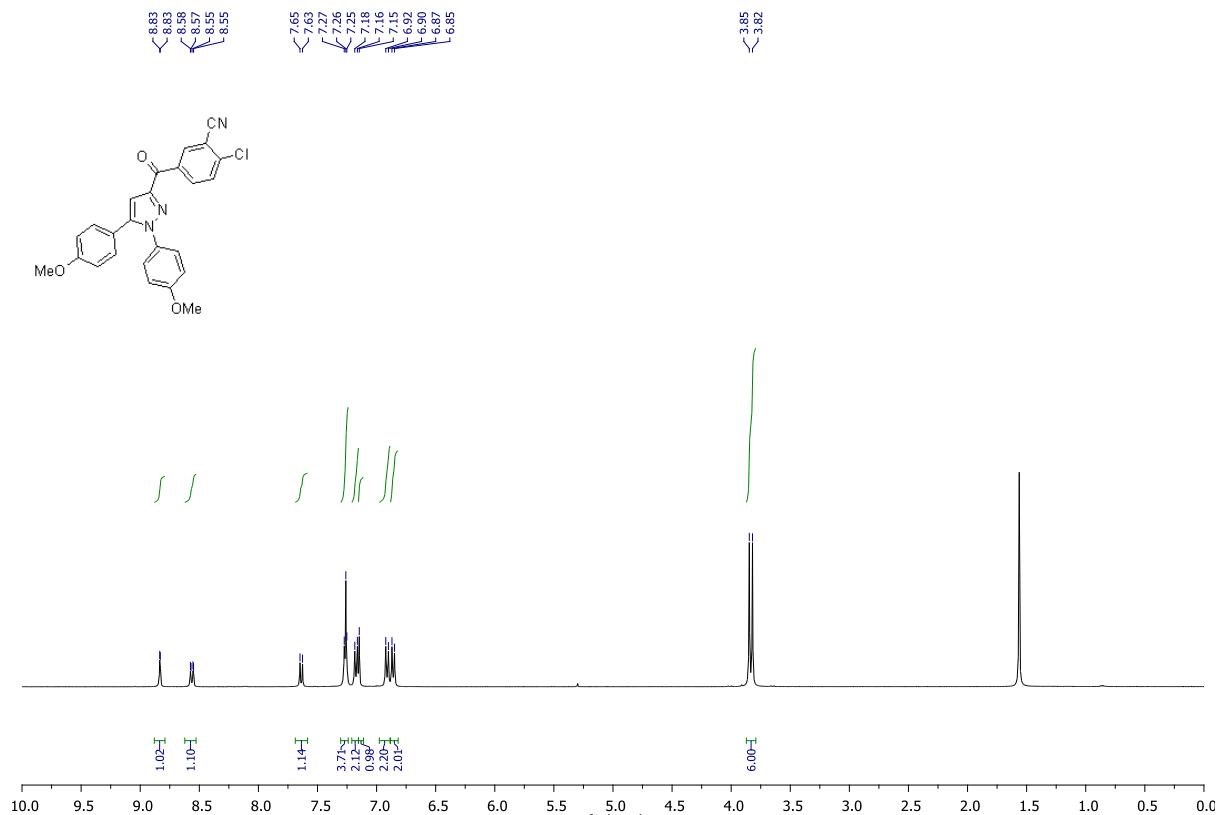


¹H NMR of 3,4-Bis(4-methoxyphenyl)sydnone (**2**):¹³C NMR of 3,4-Bis(4-methoxyphenyl)sydnone (**2**):

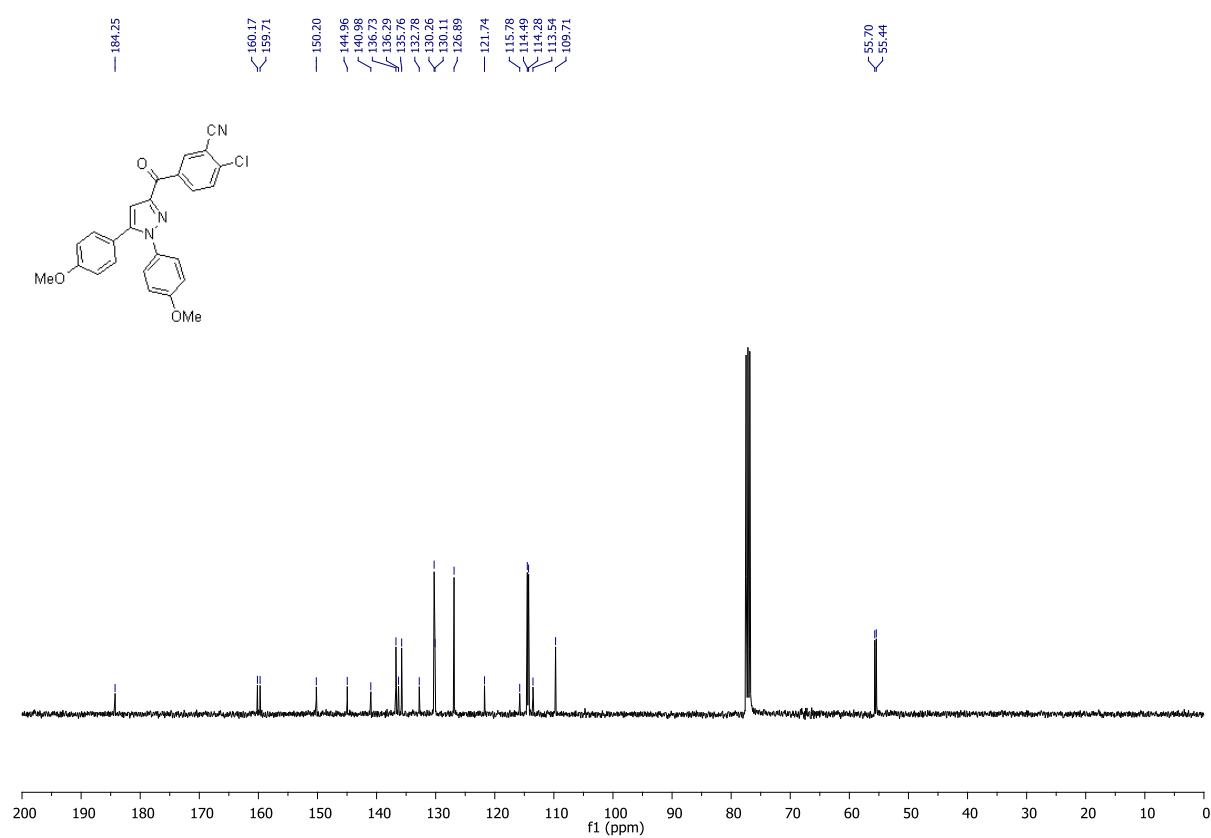
¹H NMR of 3-cyano-4-chloro- α -ethynylbenzenemethanol:¹³C NMR of 3-cyano-4-chloro- α -ethynylbenzenemethanol:

¹H NMR of *1-(3-cyano-4-chlorophenyl)-2-propyn-1-one (3)*:¹³C NMR of *1-(3-cyano-4-chlorophenyl)-2-propyn-1-one (3)*:

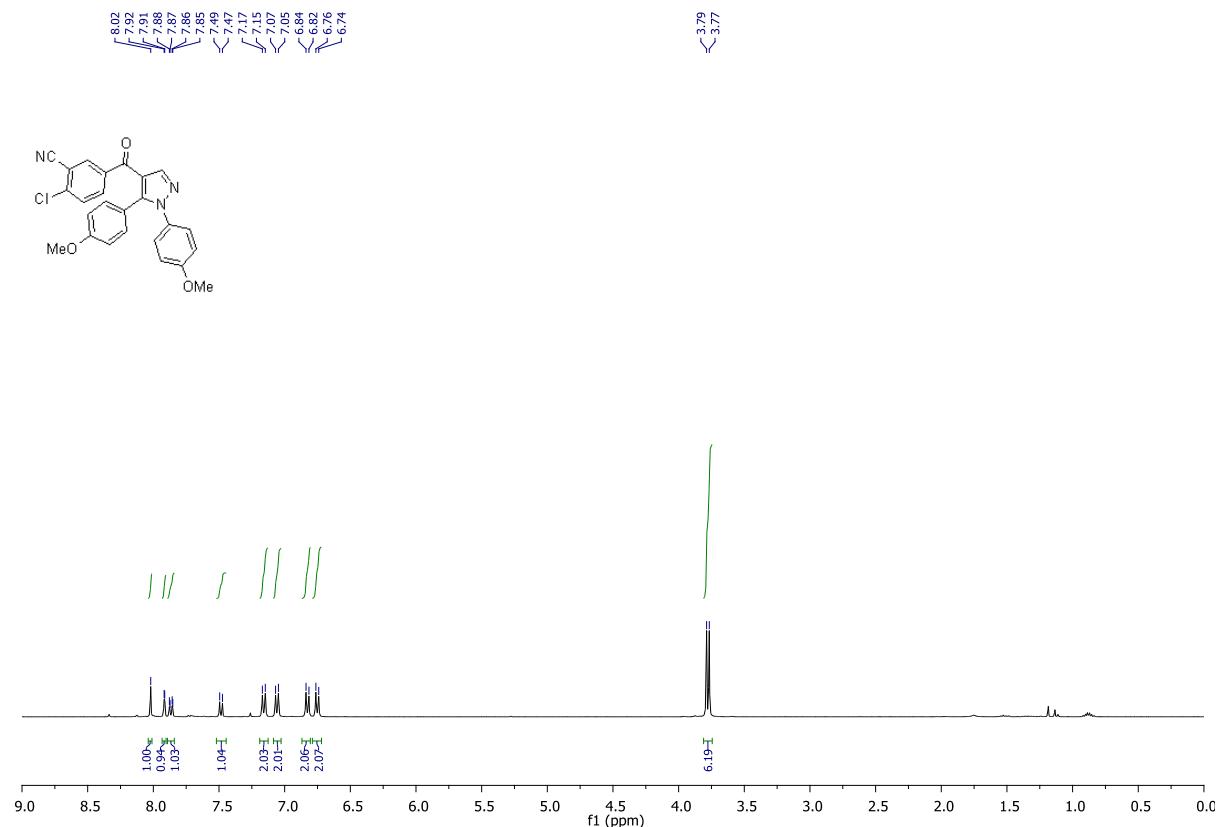
¹H NMR of [1,5-Bis(4-methoxyphenyl)-1*H*-pyrazol-3-yl](3-cyano-4-chlorophenyl)-methanone (**4a**):



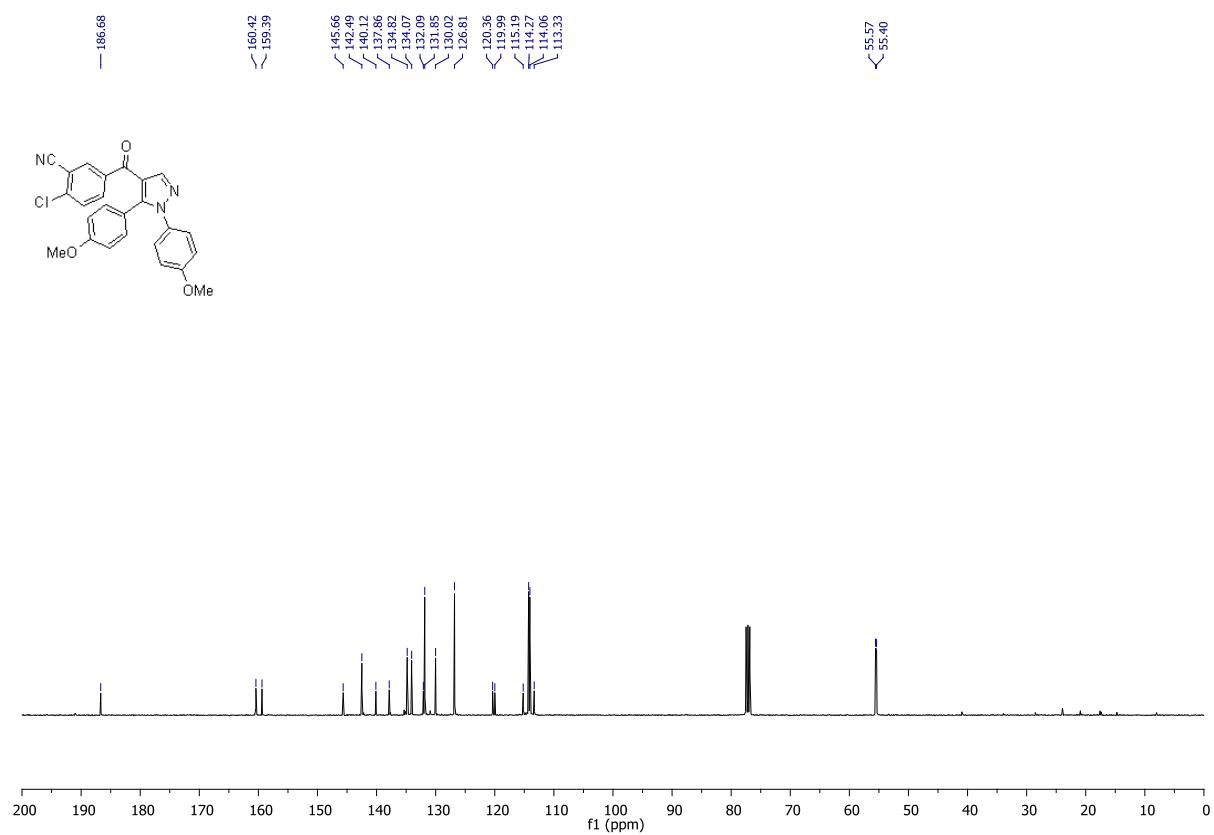
¹³C NMR of [1,5-Bis(4-methoxyphenyl)-1*H*-pyrazol-3-yl](3-cyano-4-chlorophenyl)-methanone (**4a**):

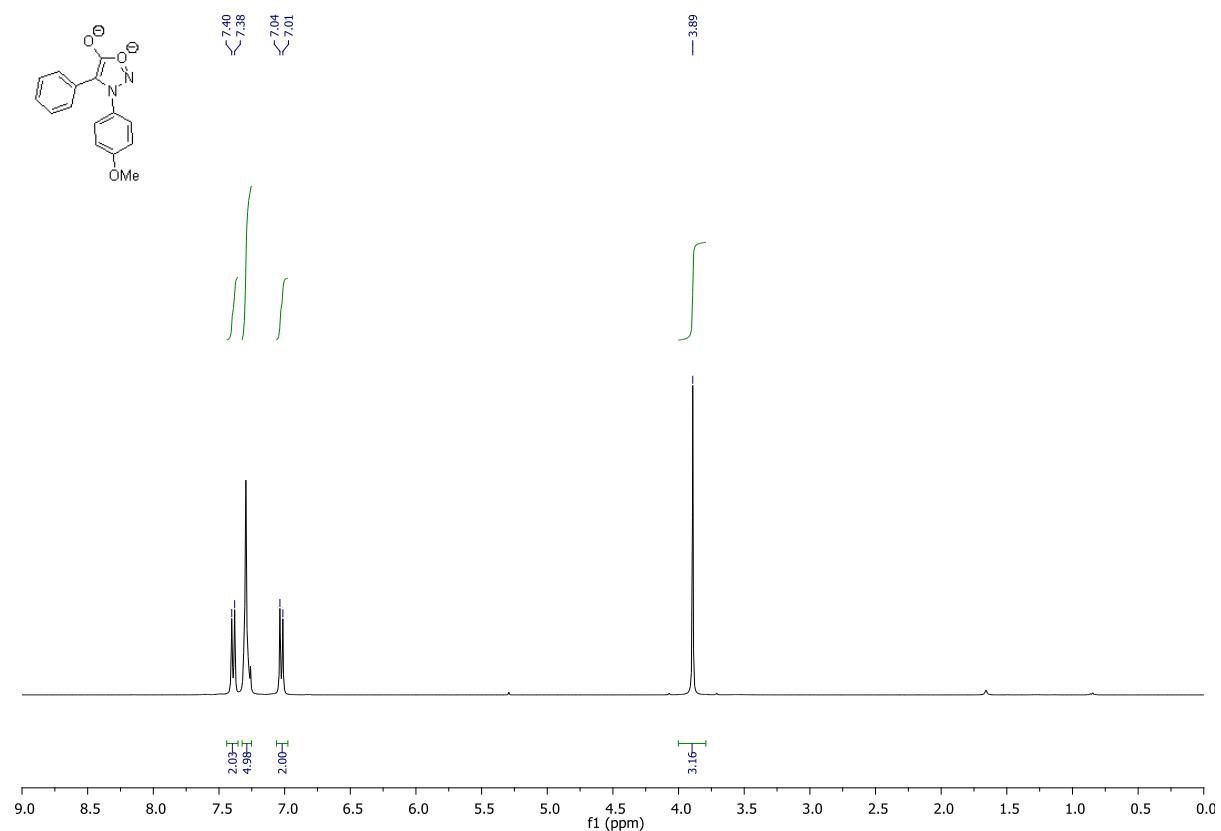
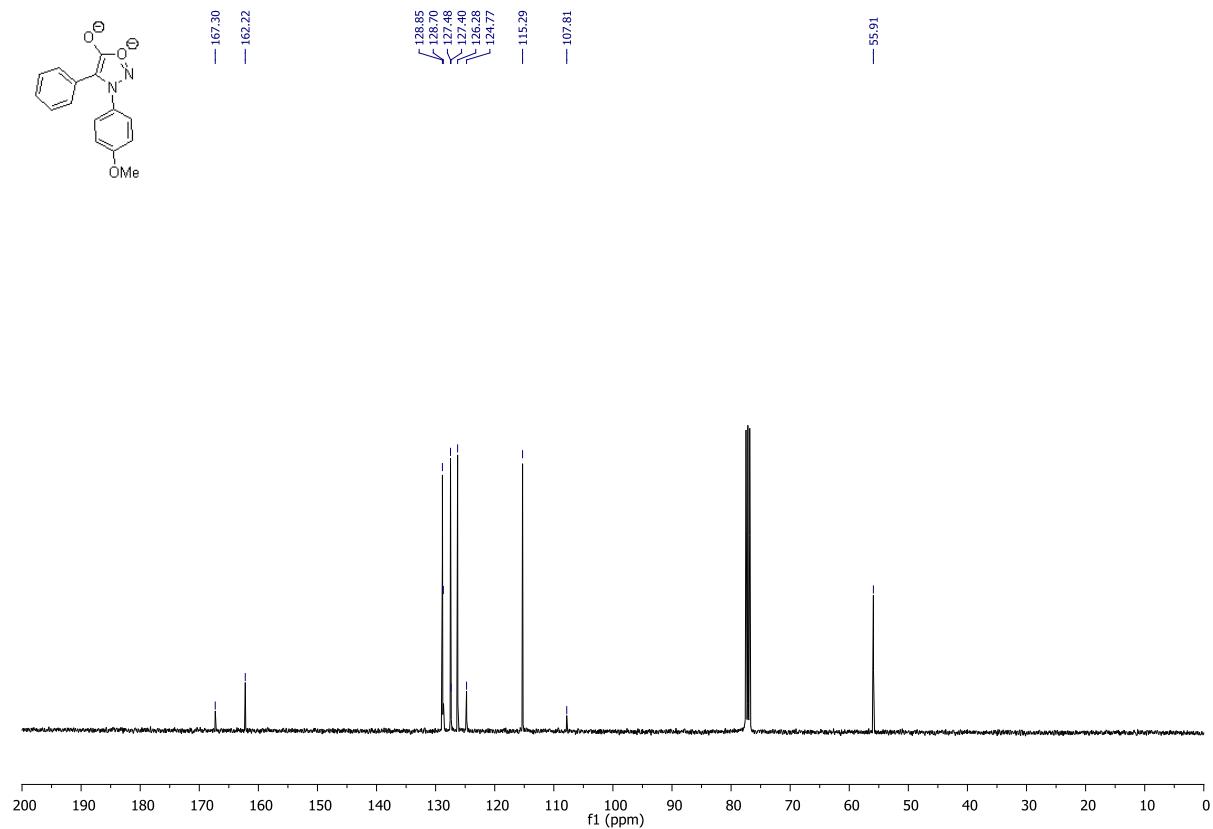


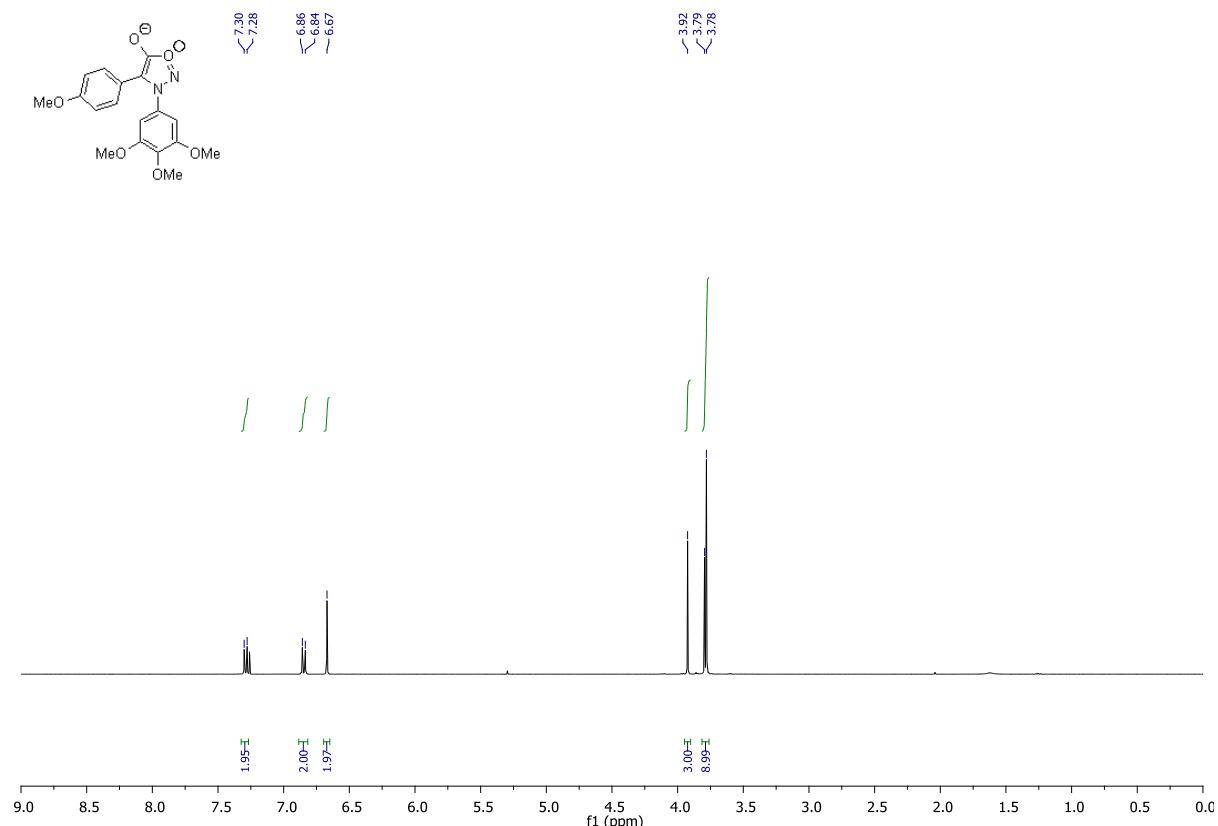
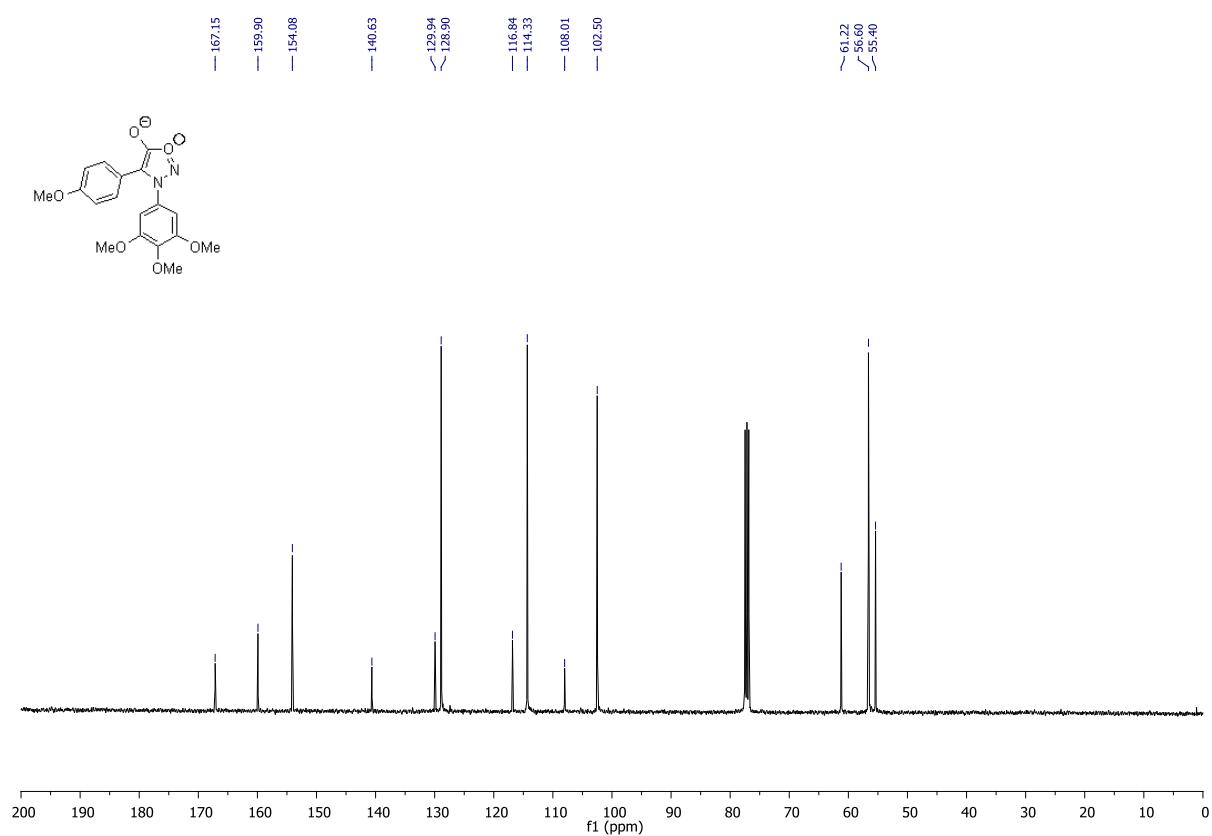
¹H NMR of [1,5-Bis(4-methoxyphenyl)-1*H*-pyrazol-4-yl](3-cyano-4-chlorophenyl)-methanone (**4b**):

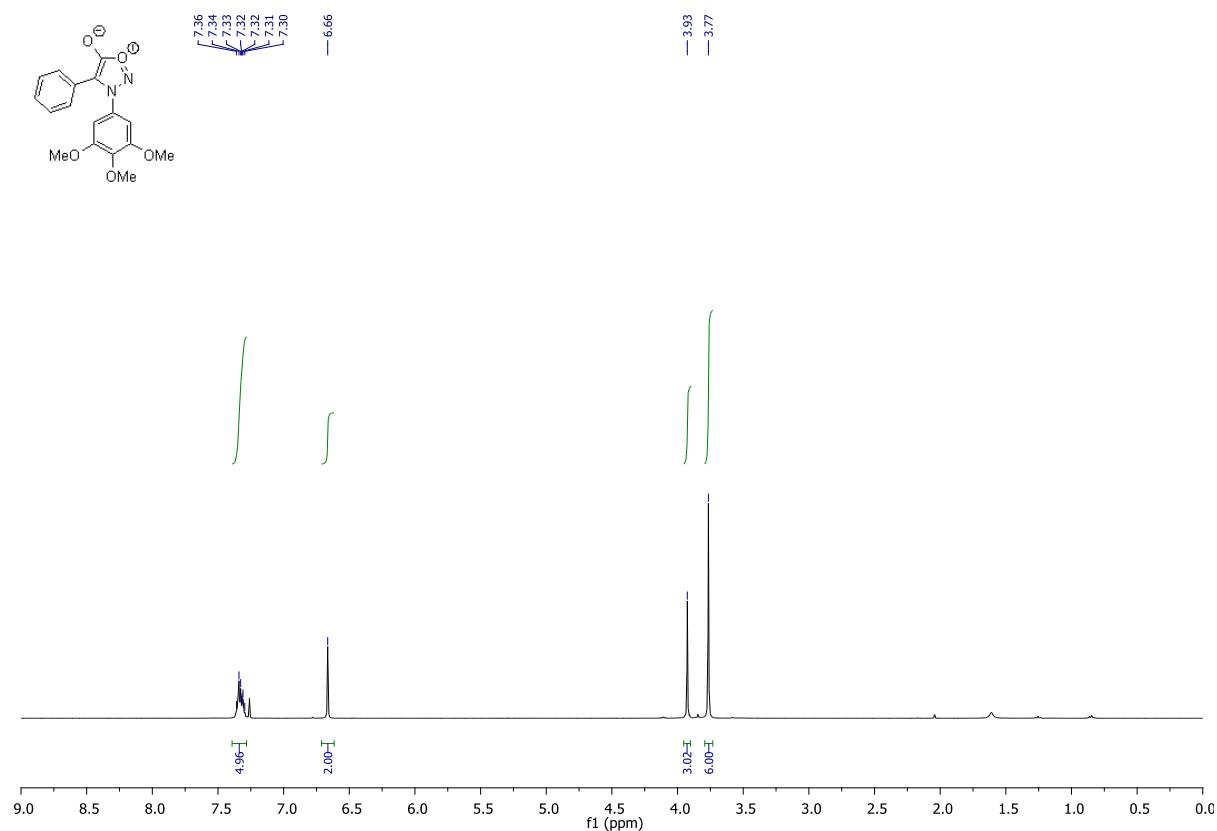
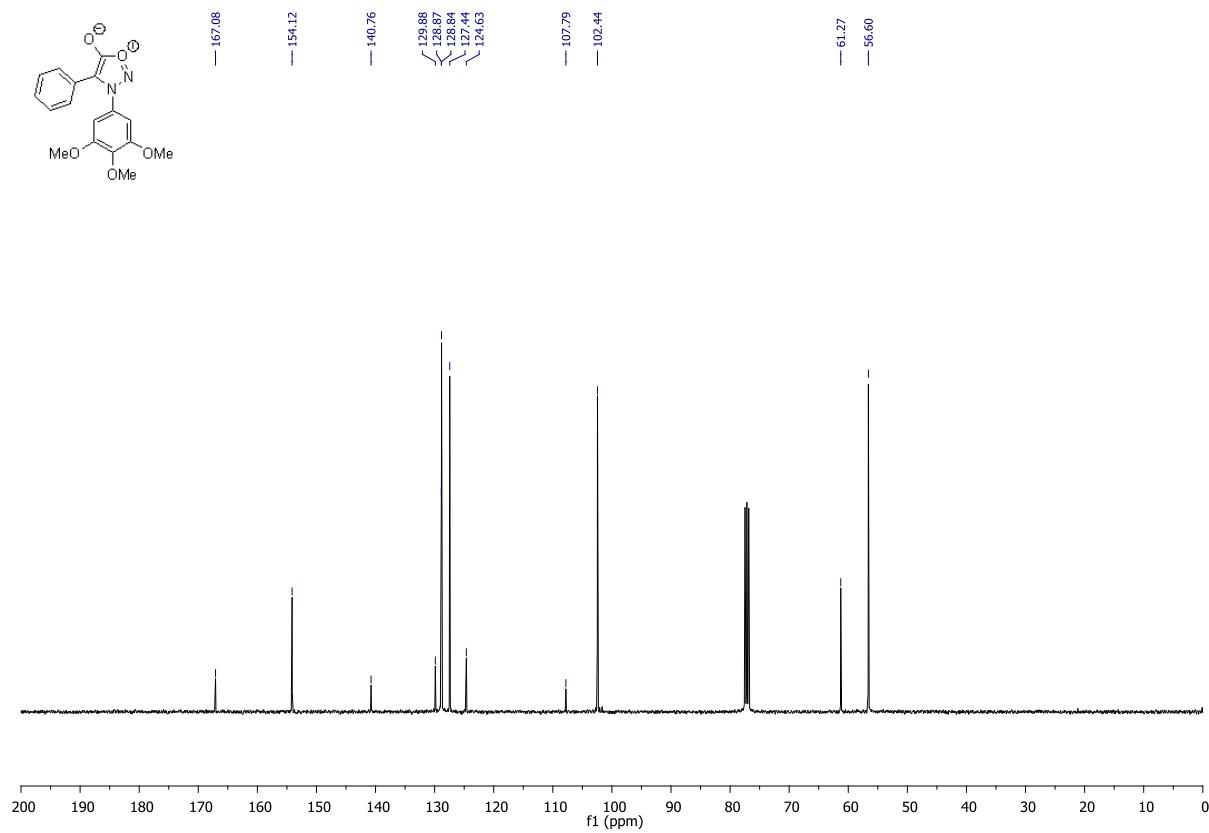


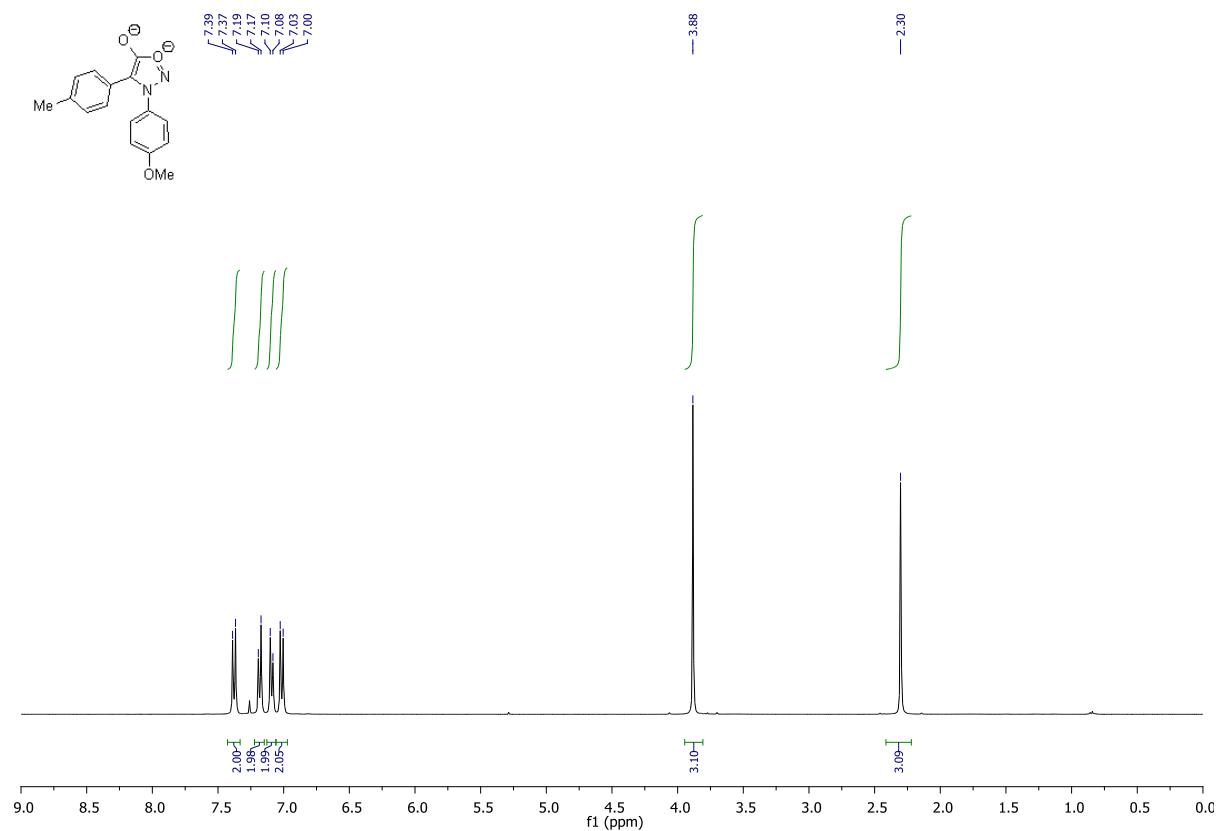
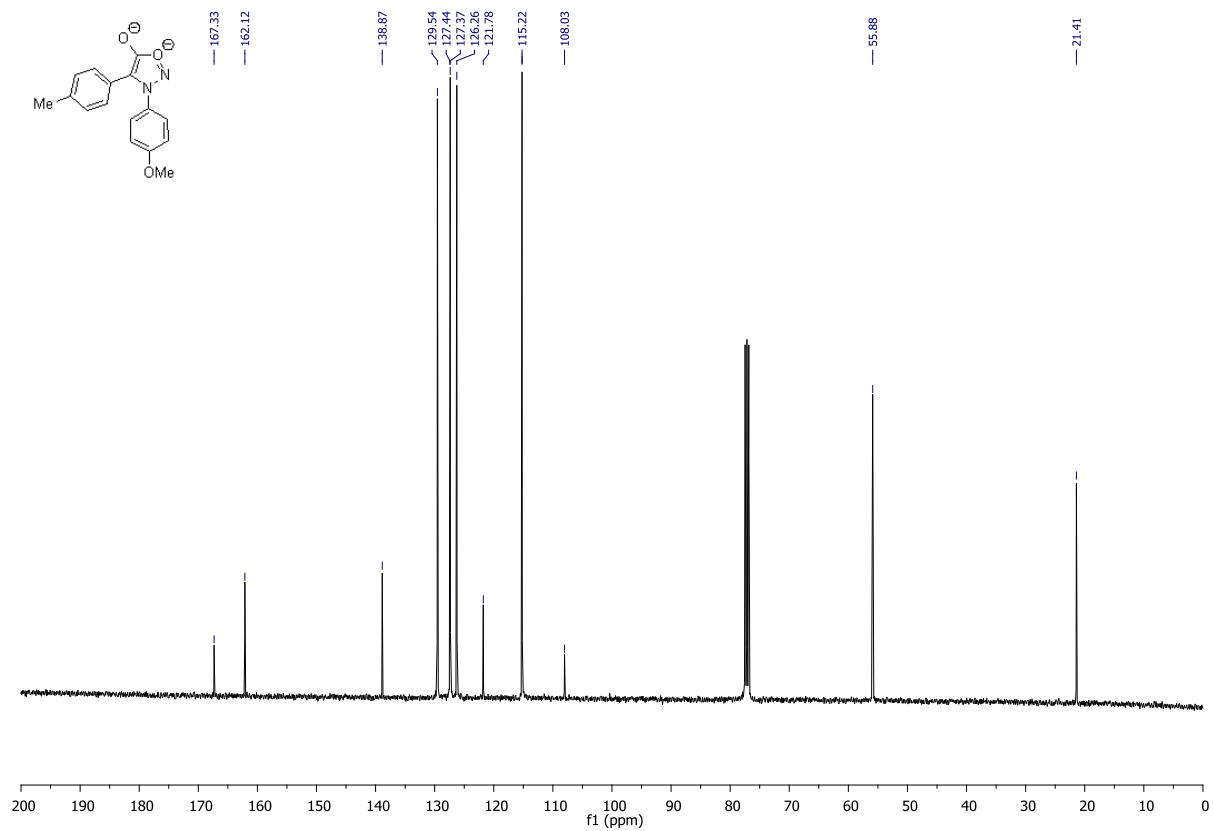
¹³C NMR of [1,5-Bis(4-methoxyphenyl)-1*H*-pyrazol-4-yl](3-cyano-4-chlorophenyl)-methanone (**4b**):

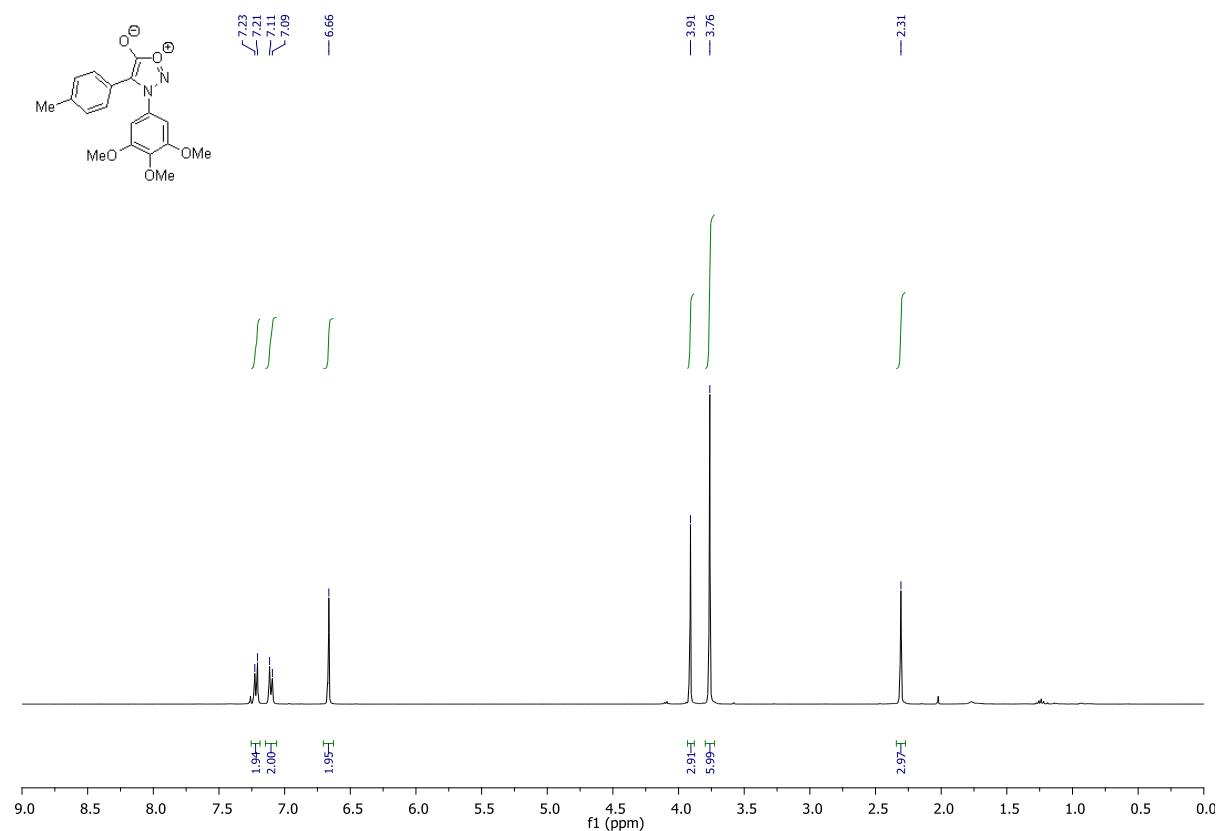
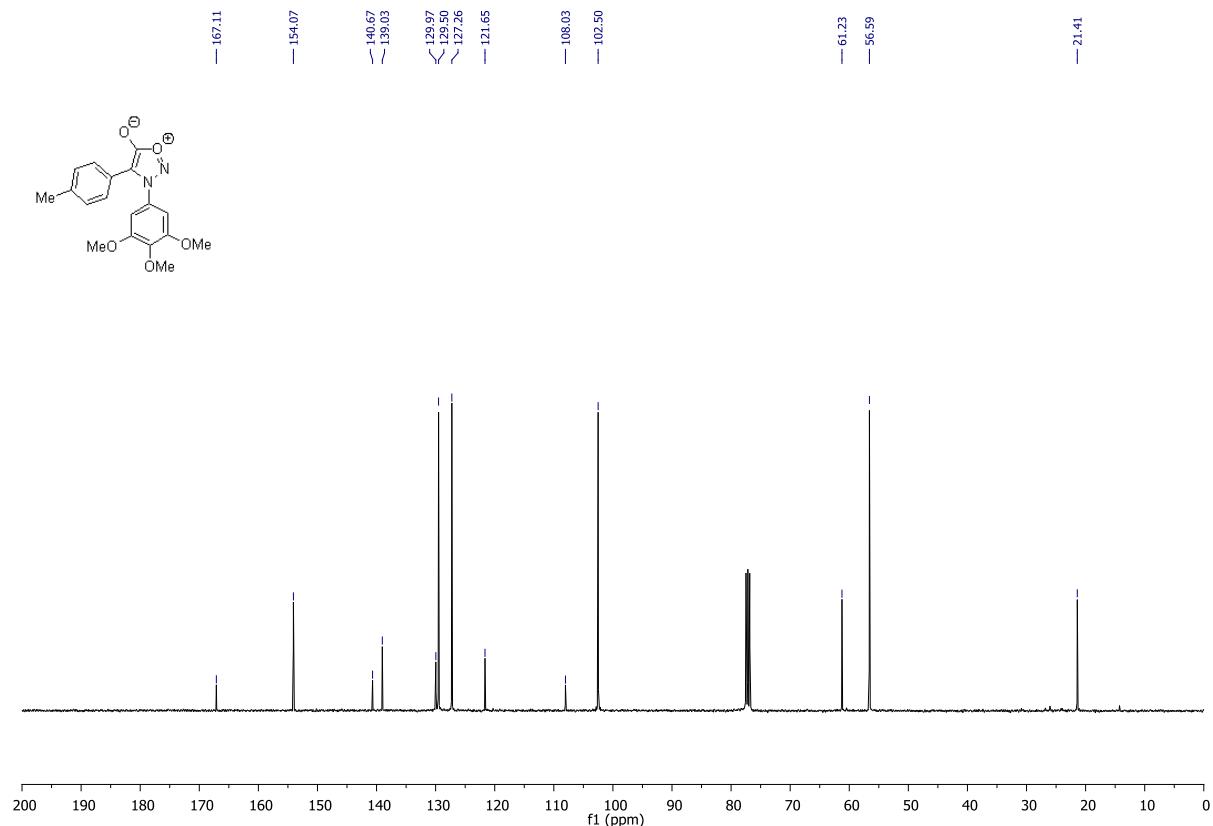


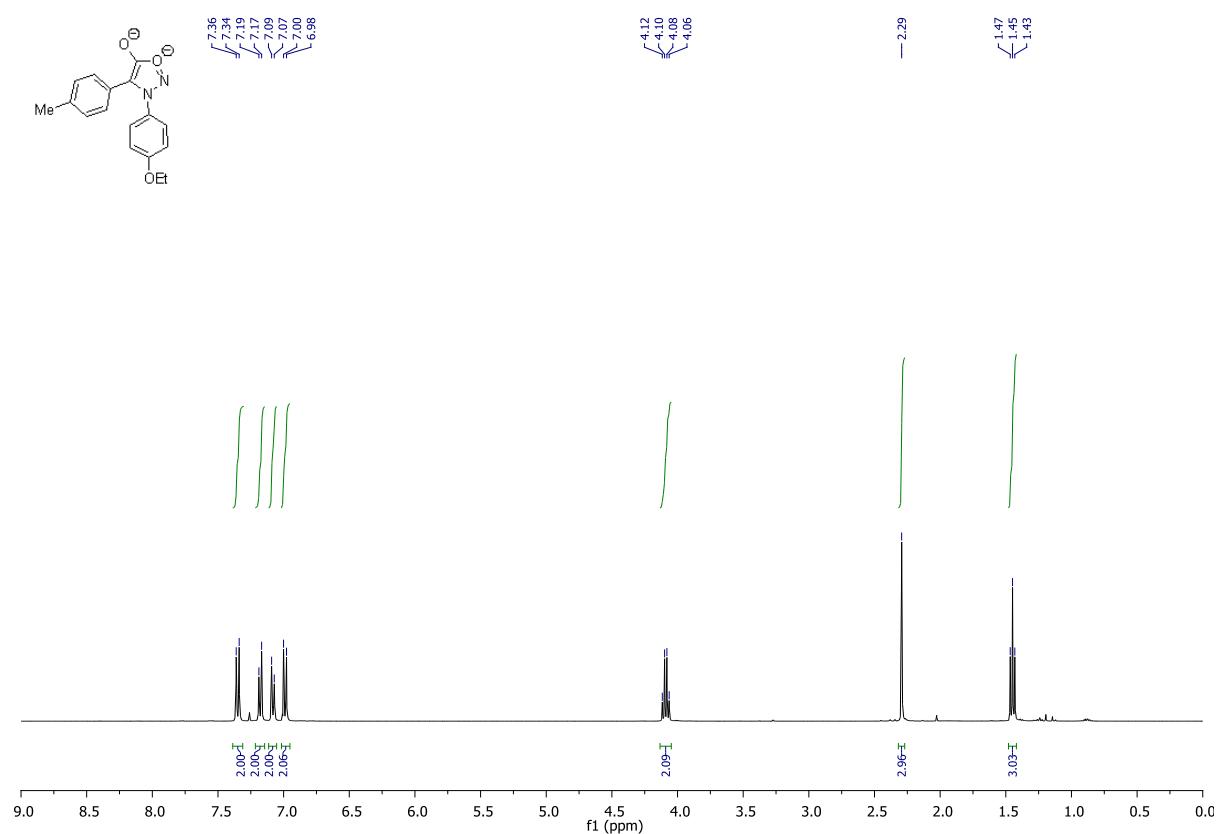
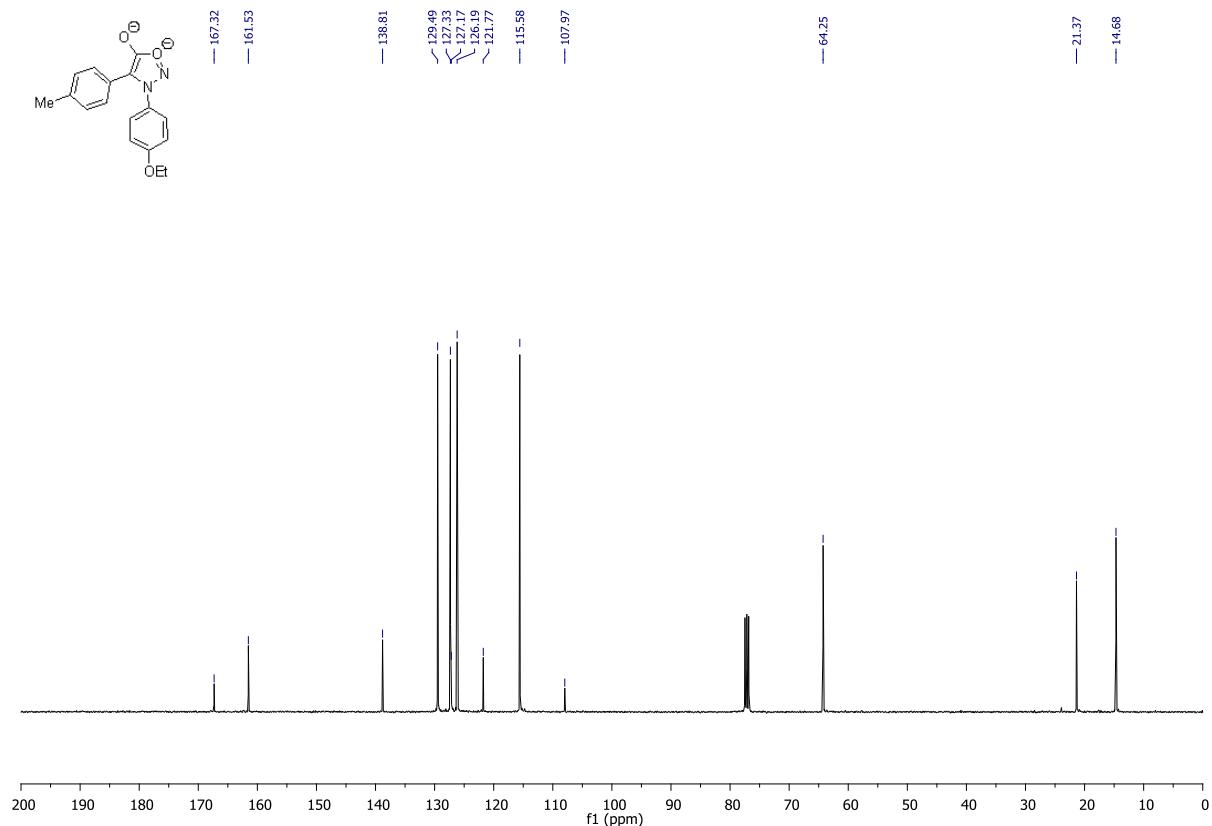
¹H NMR of 4-Phenyl-N-(4-methoxyphenyl)sydnone (**5**):¹³C NMR of 4-Phenyl-N-(4-methoxyphenyl)sydnone (**5**):

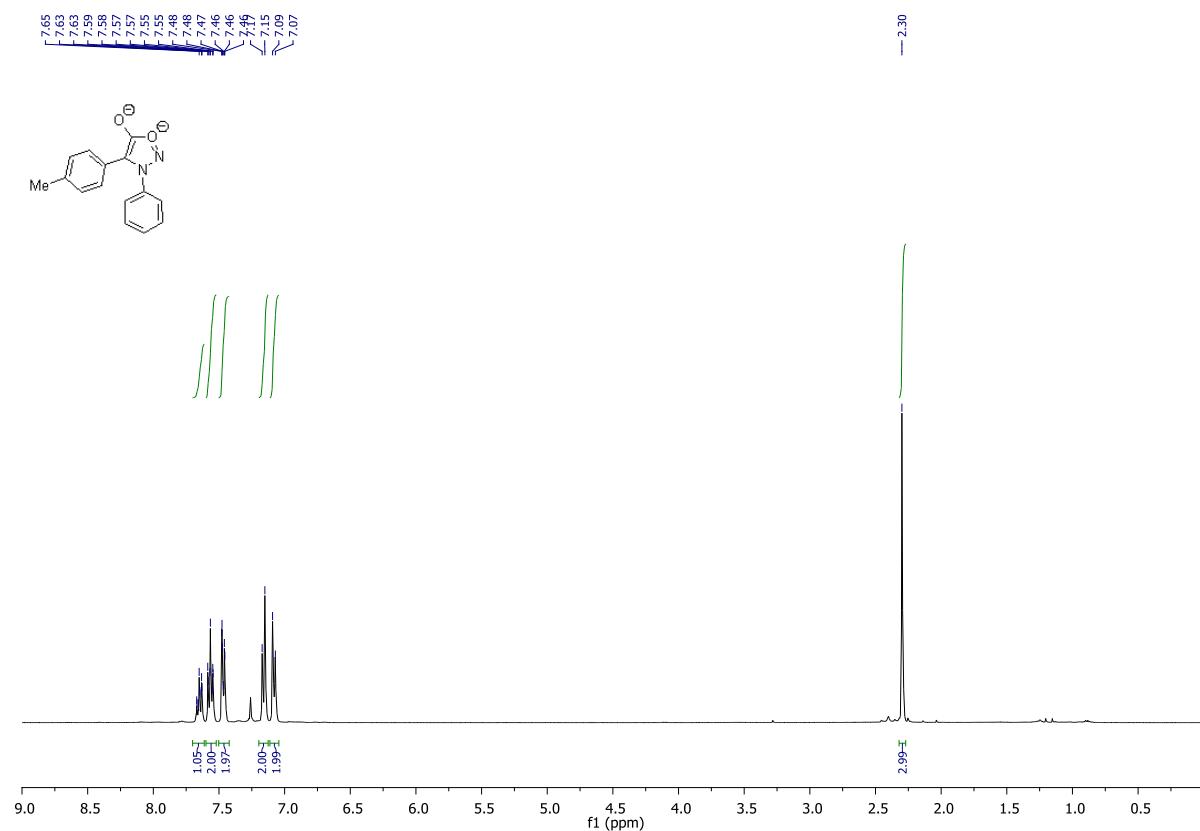
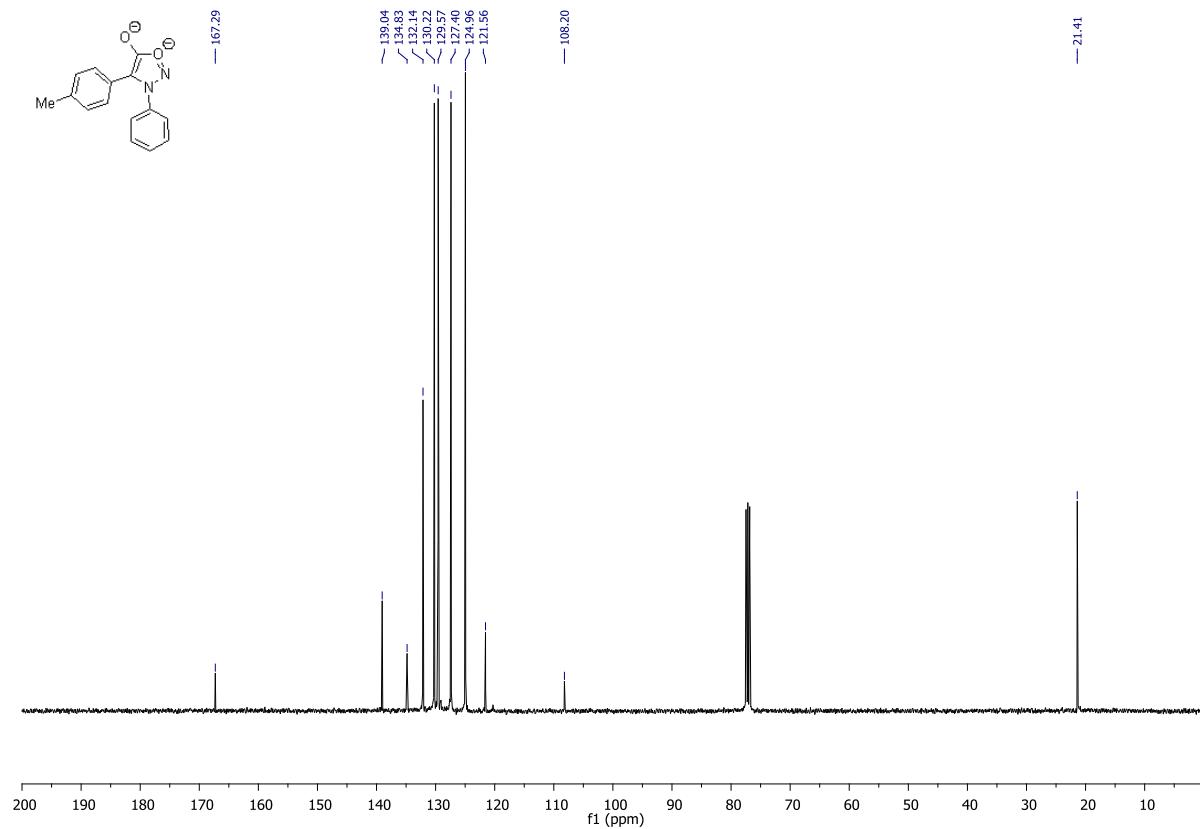
¹H NMR of 4-(4-Methoxyphenyl)-N-(3,4,5-trimethoxyphenyl)sydnone (**6**):¹³C NMR of 4-(4-Methoxyphenyl)-N-(3,4,5-trimethoxyphenyl)sydnone (**6**):

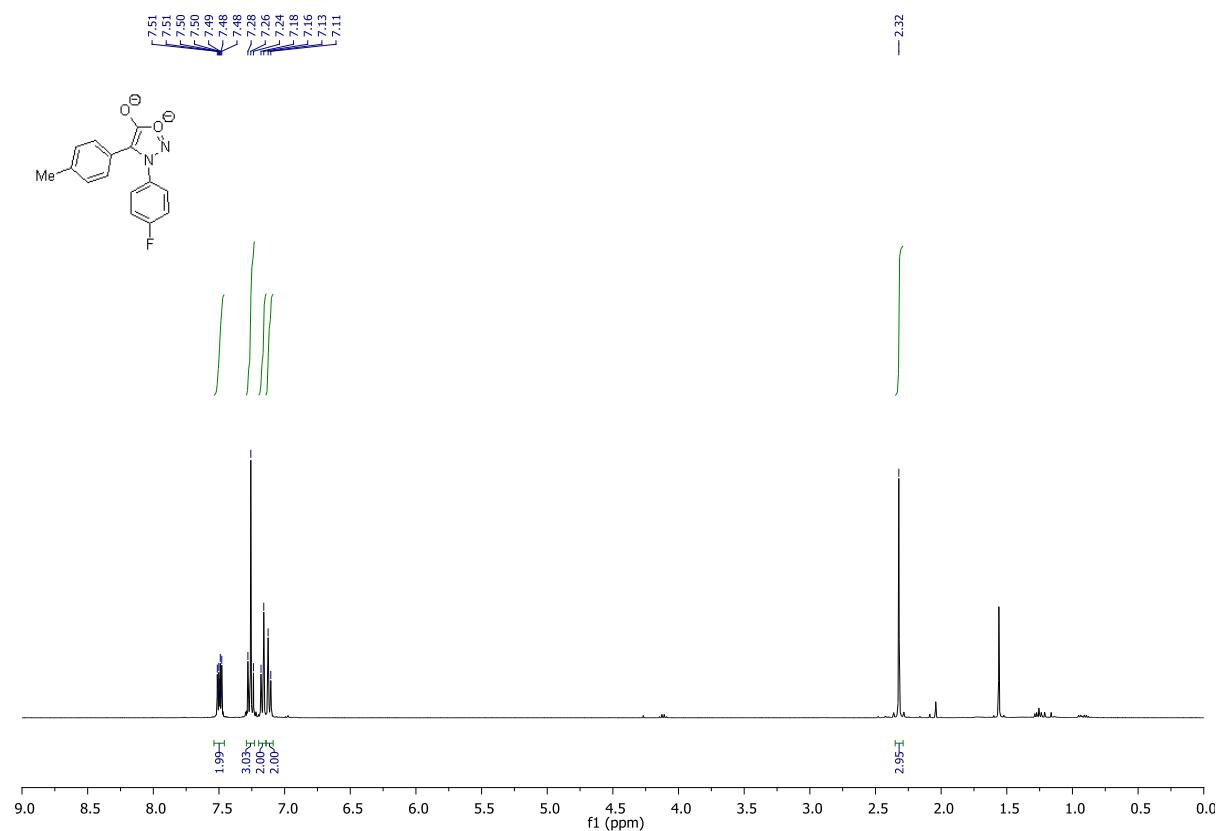
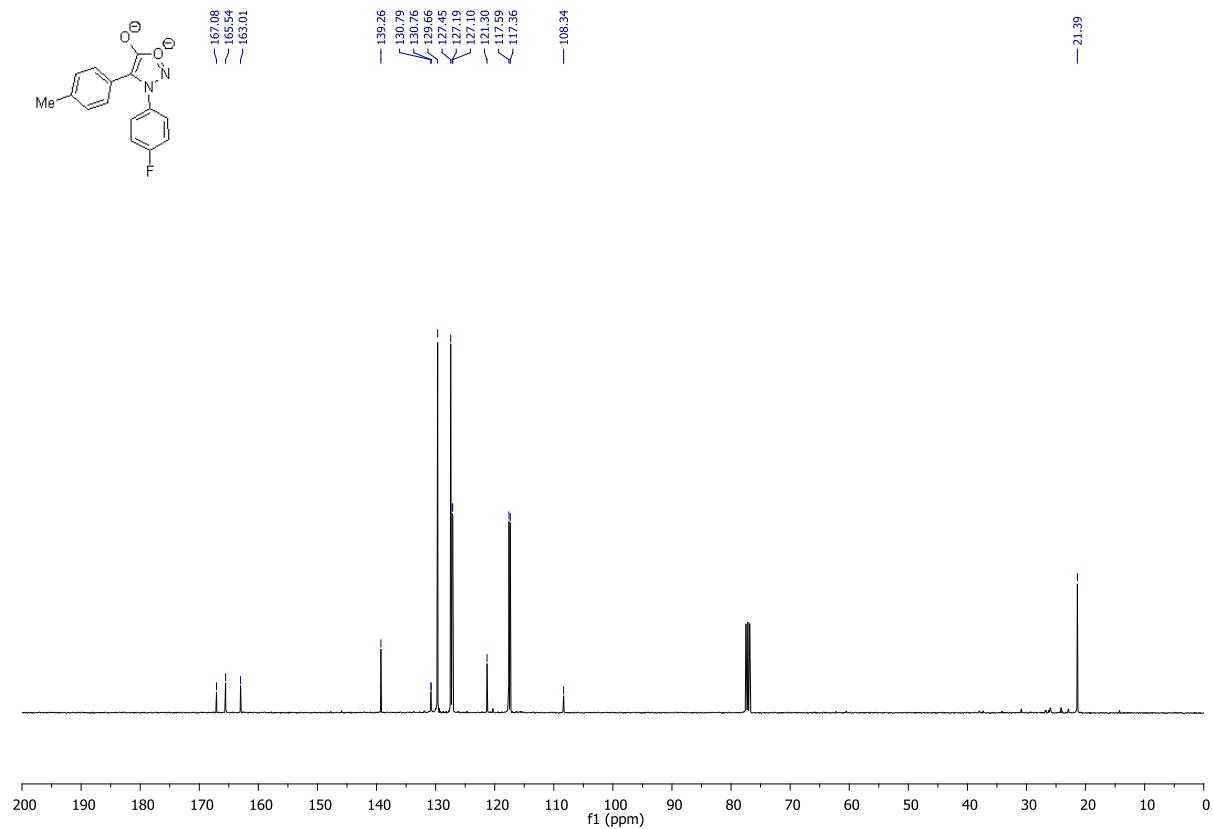
¹H NMR of 4-Phenyl-N-(3,4,5-trimethoxyphenyl)sydnone (**7**):¹³C NMR of 4-Phenyl-N-(3,4,5-trimethoxyphenyl)sydnone (**7**):

¹H NMR of 4-(4-Tolyl)-N-(4-methoxyphenyl)sydnone (**8**):¹³C NMR of 4-(4-Tolyl)-N-(4-methoxyphenyl)sydnone (**8**):

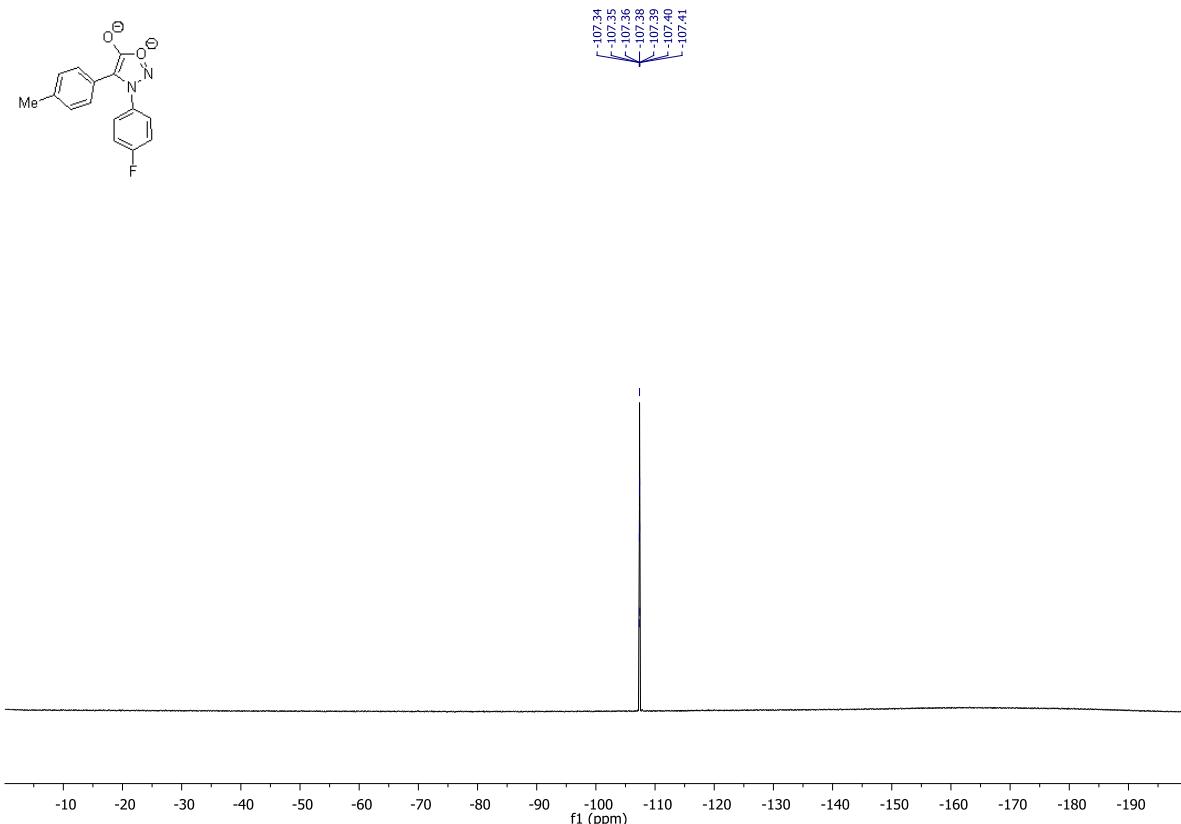
¹H NMR of 4-(4-Tolyl)-N-(3,4,5-trimethoxyphenyl)sydnone (**9**):¹³C NMR of 4-(4-Tolyl)-N-(3,4,5-trimethoxyphenyl)sydnone (**9**):

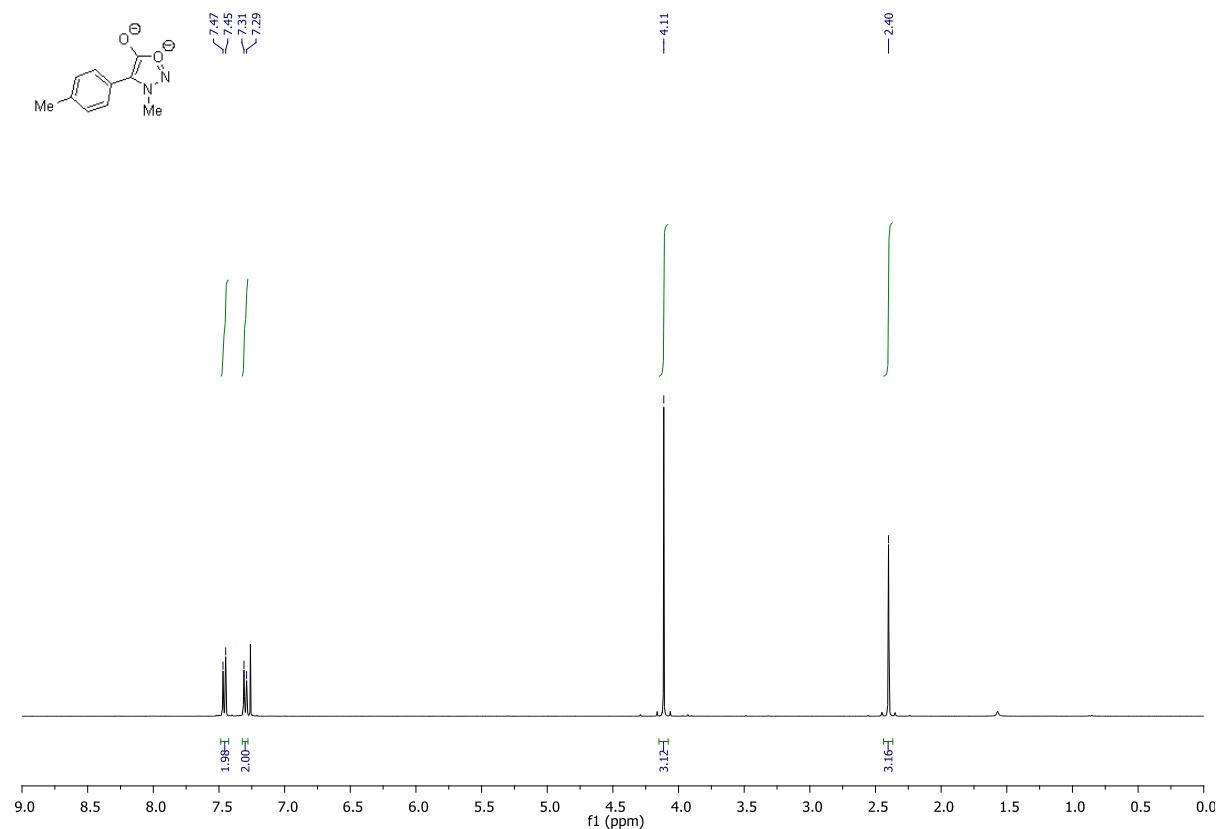
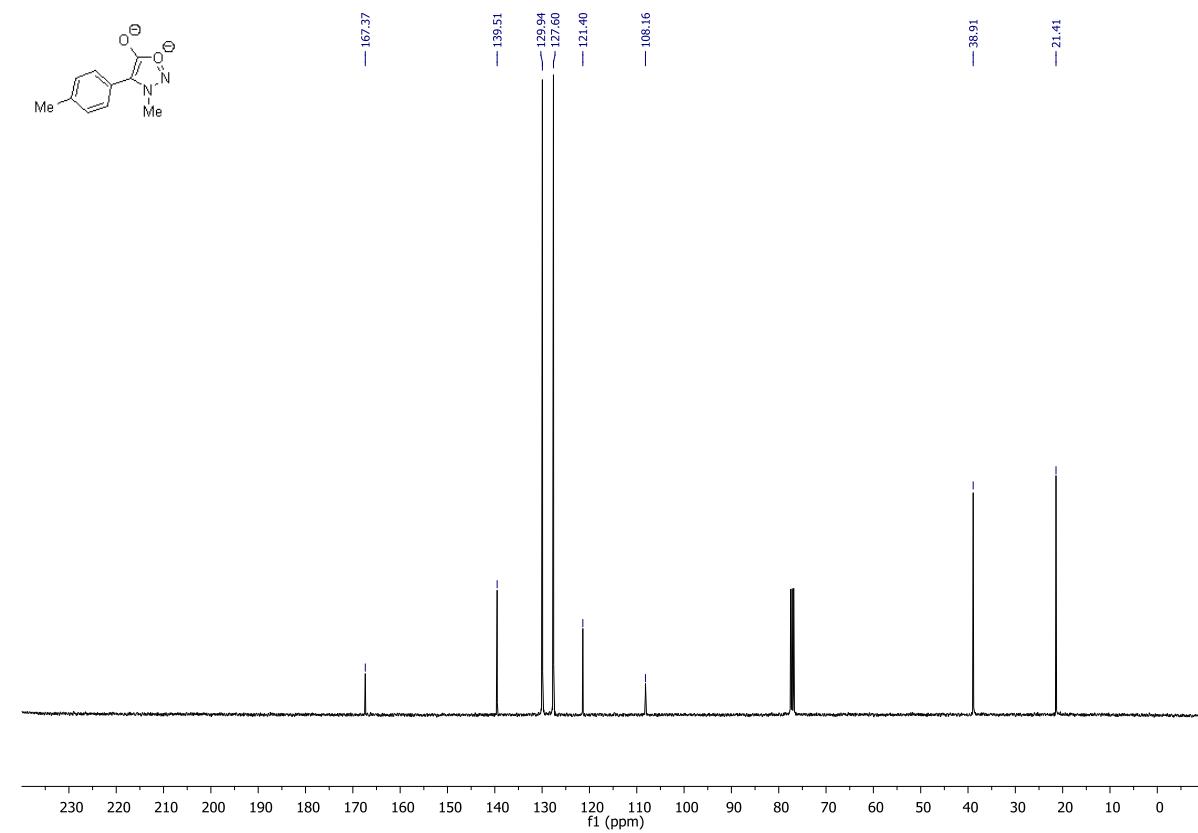
¹H NMR of 4-(*p*-Tolyl)-*N*-(4-ethoxyphenyl)sydnone (**10**):¹³C NMR of 4-(*p*-Tolyl)-*N*-(4-ethoxyphenyl)sydnone (**10**):

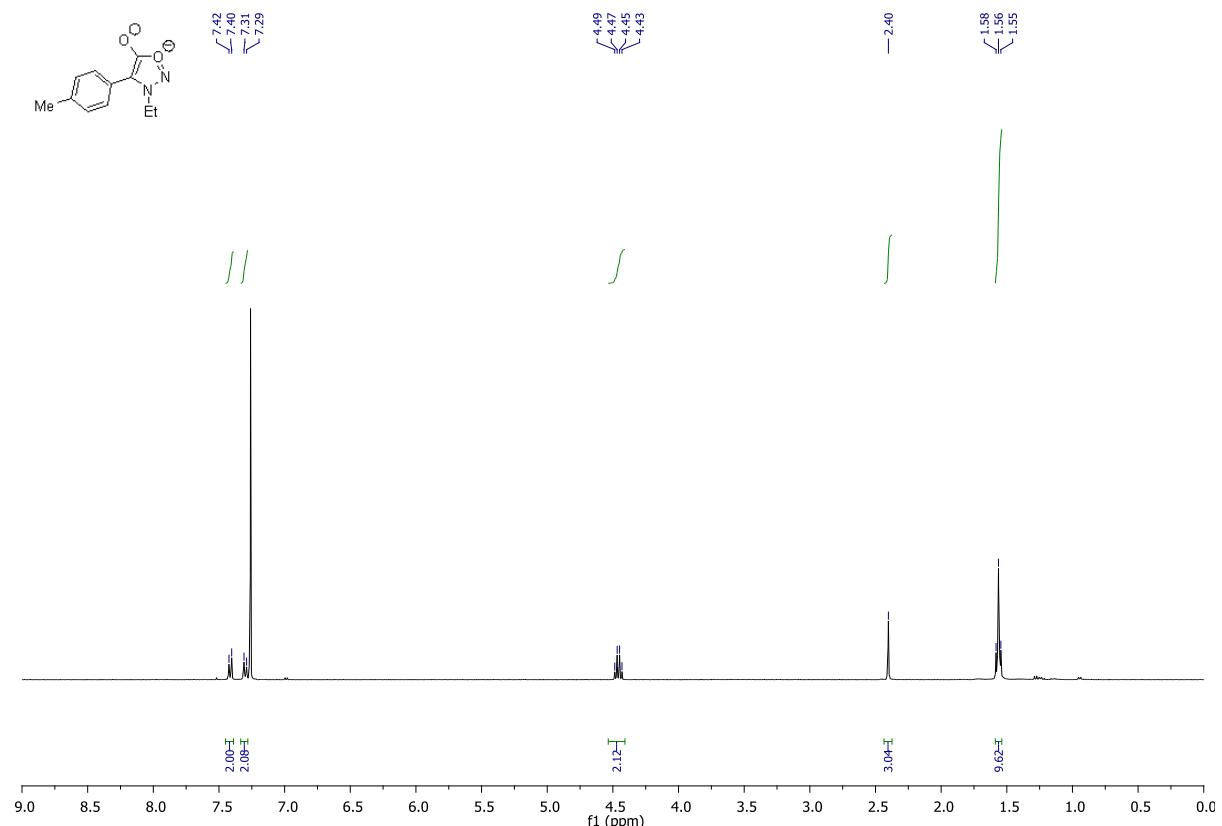
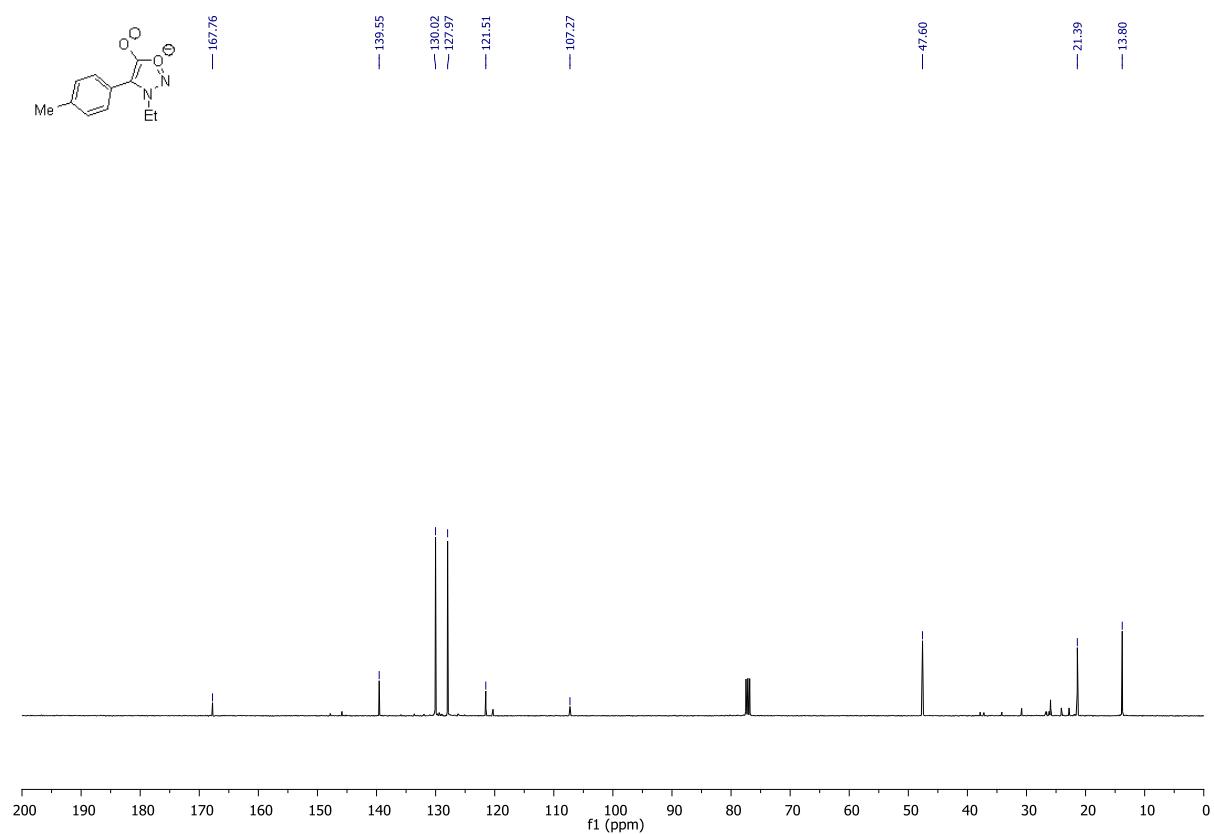
¹H NMR of 4-(*p*-Tolyl)-*N*-phenylsydnone (**11**):¹³C NMR of 4-(*p*-Tolyl)-*N*-phenylsydnone (**11**):

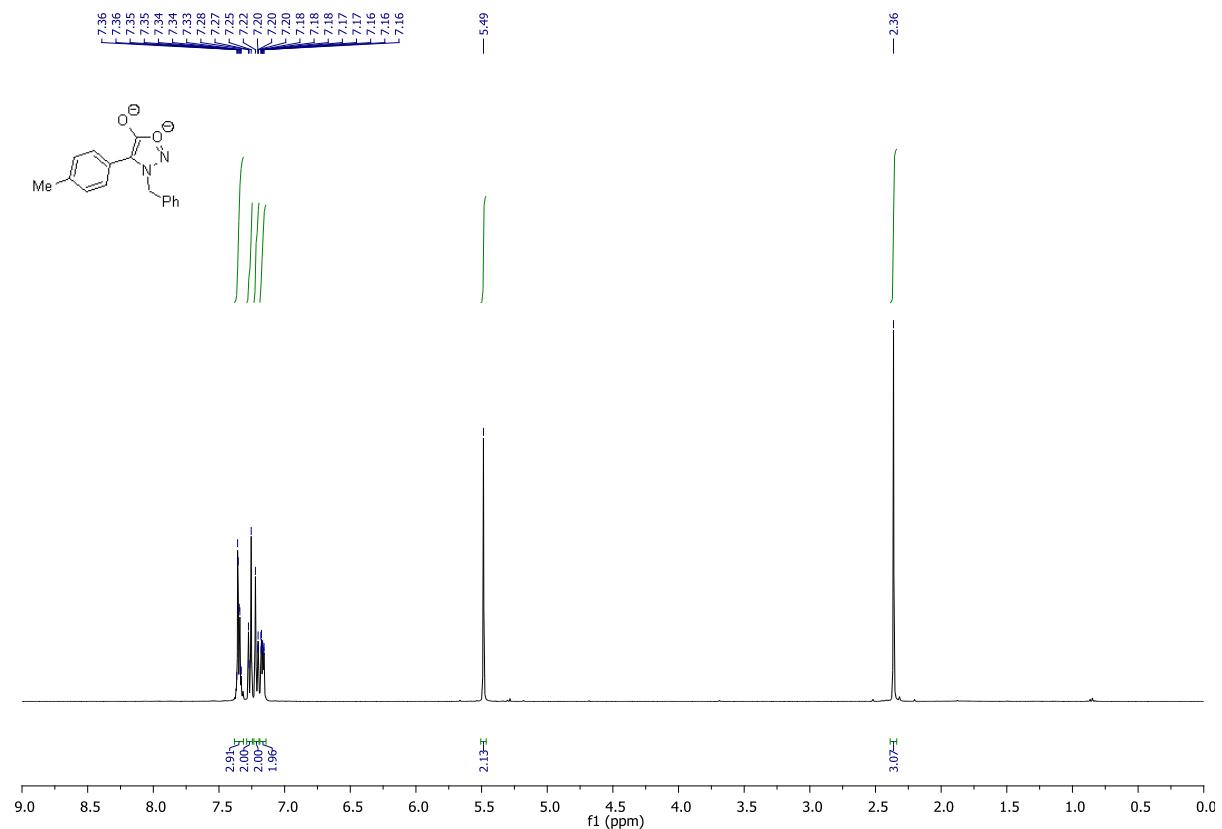
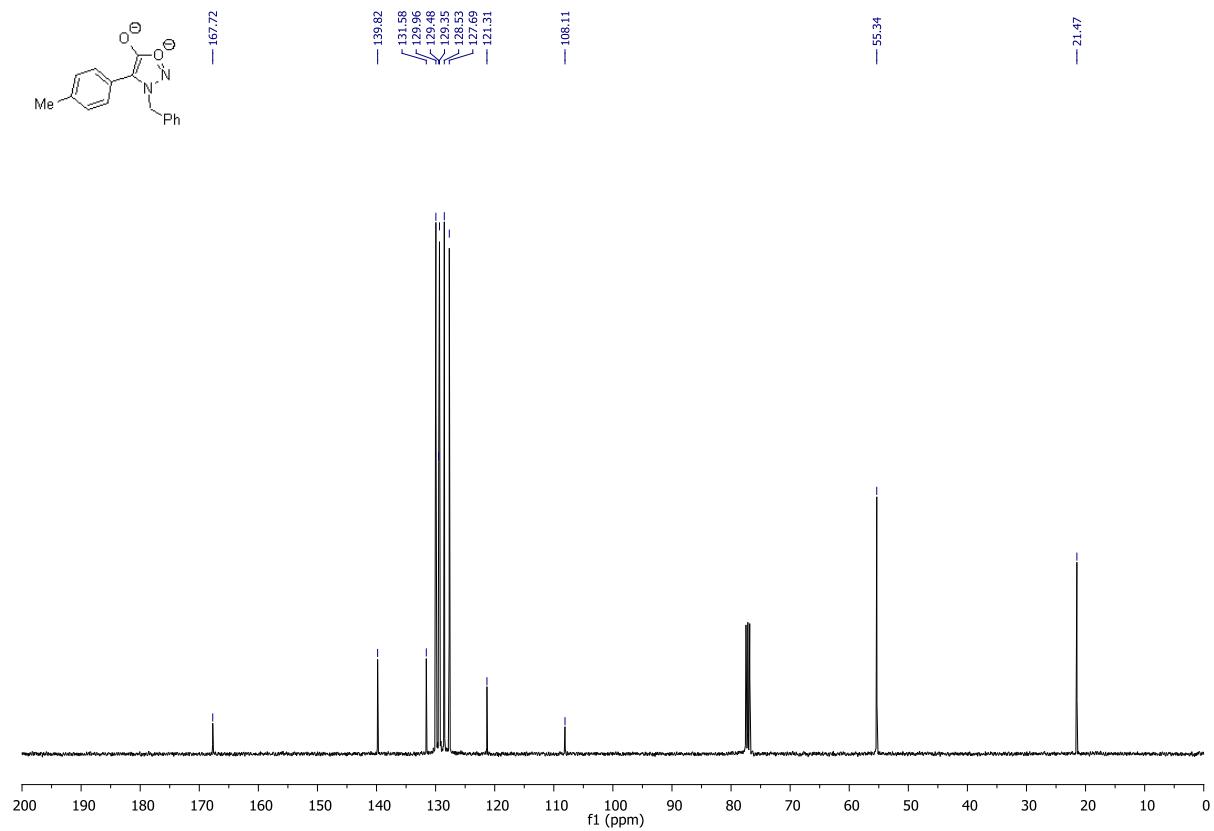
¹H NMR of 4-(*p*-Tolyl)-*N*-(4-fluorophenyl)sydnone (**12**):¹³C NMR of 4-(*p*-Tolyl)-*N*-(4-fluorophenyl)sydnone (**12**):

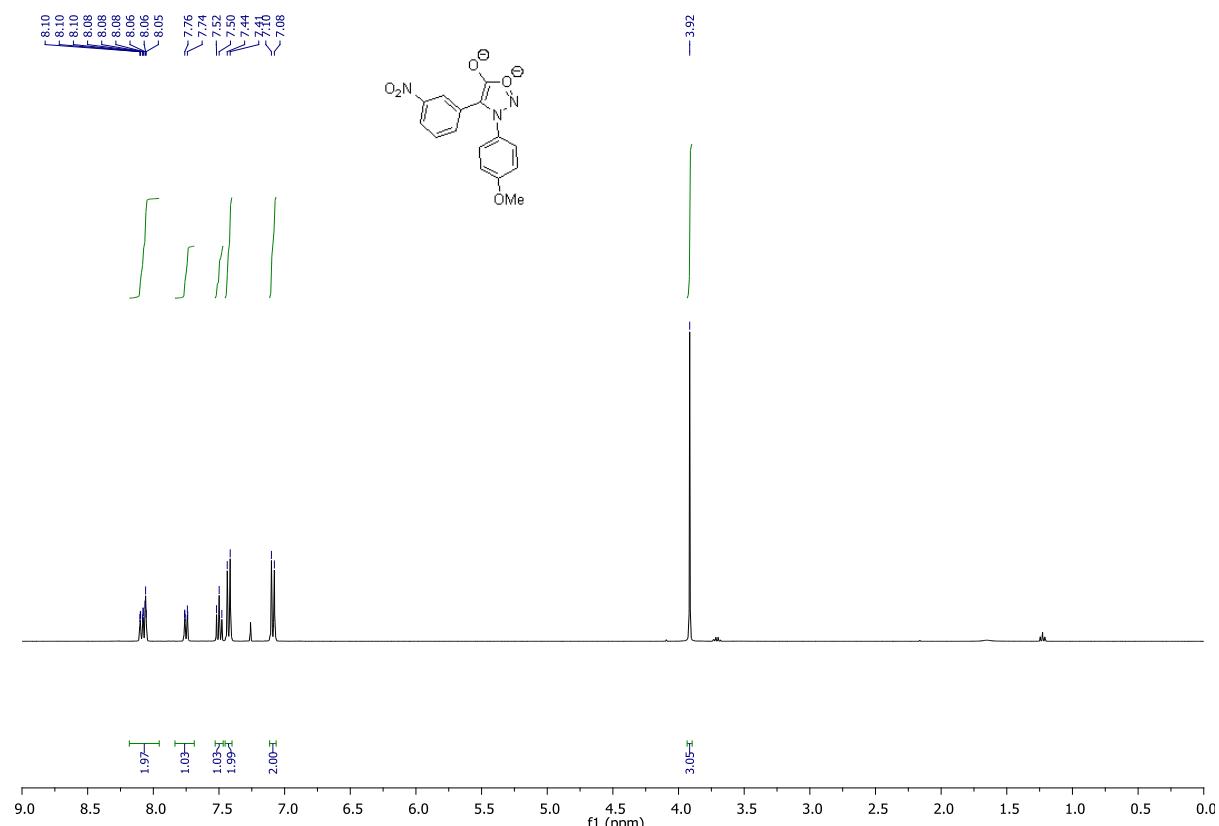
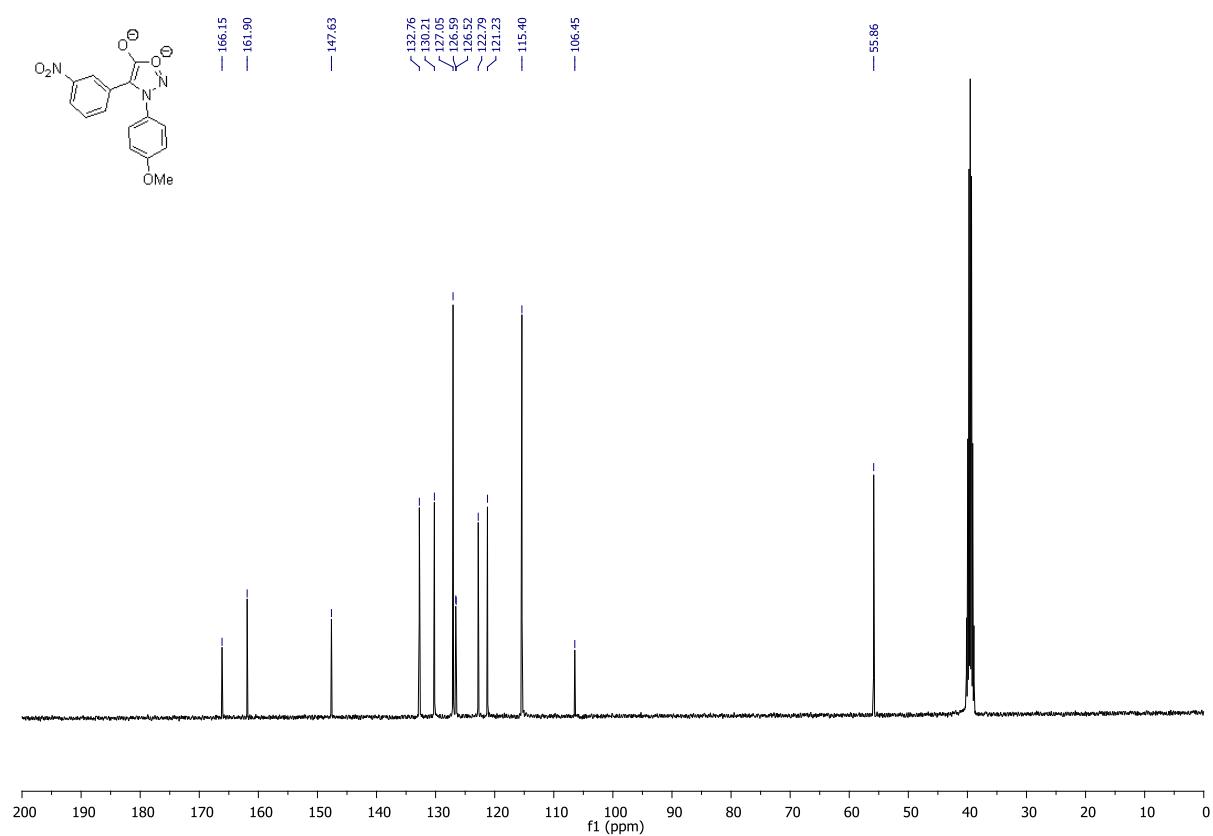
¹⁹F NMR of 4-(*p*-Tolyl)-*N*-(4-fluorophenyl)sydnone (**12**):

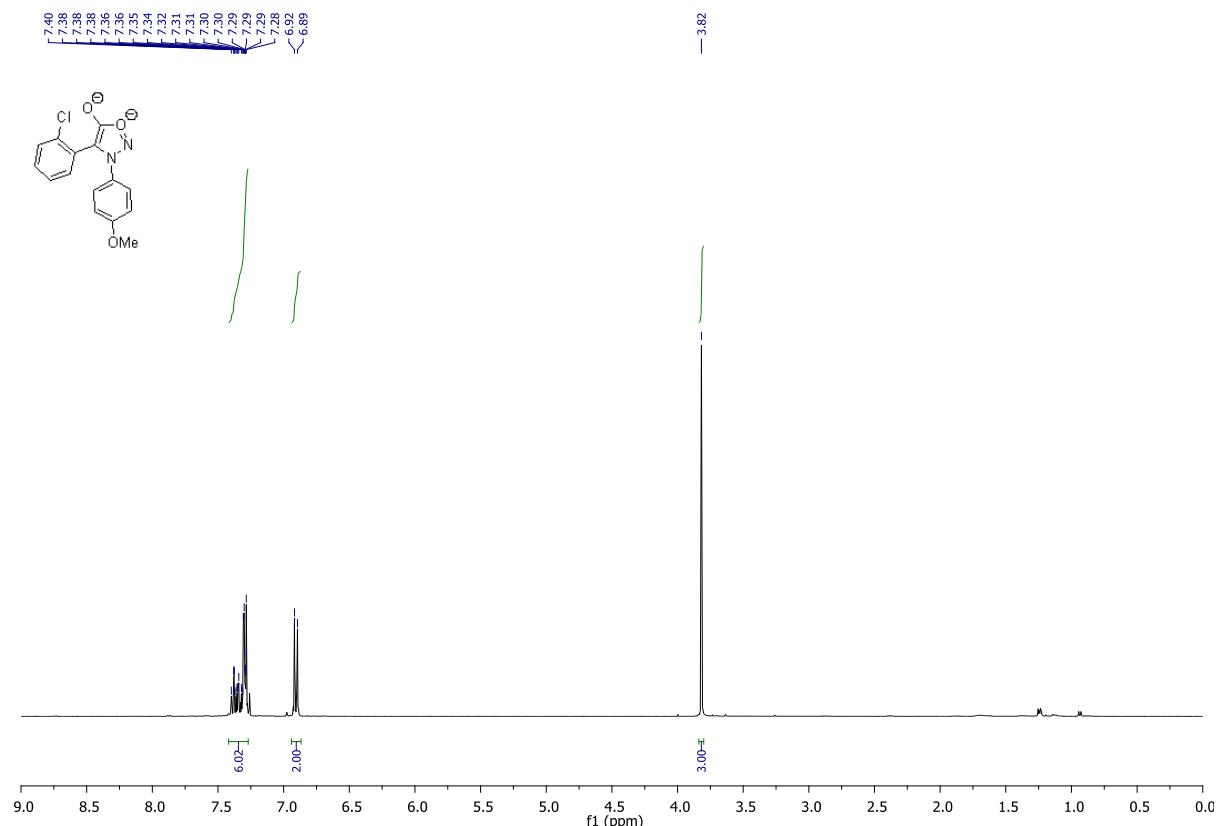
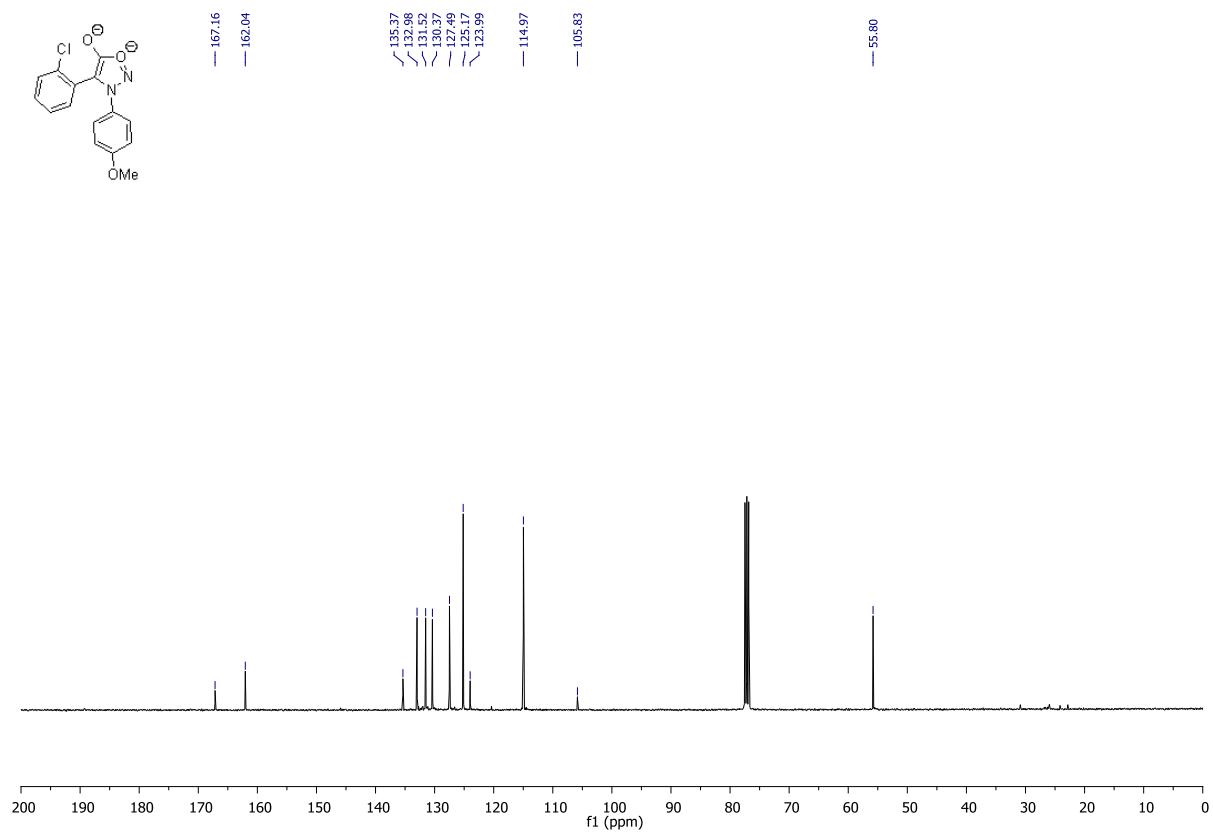


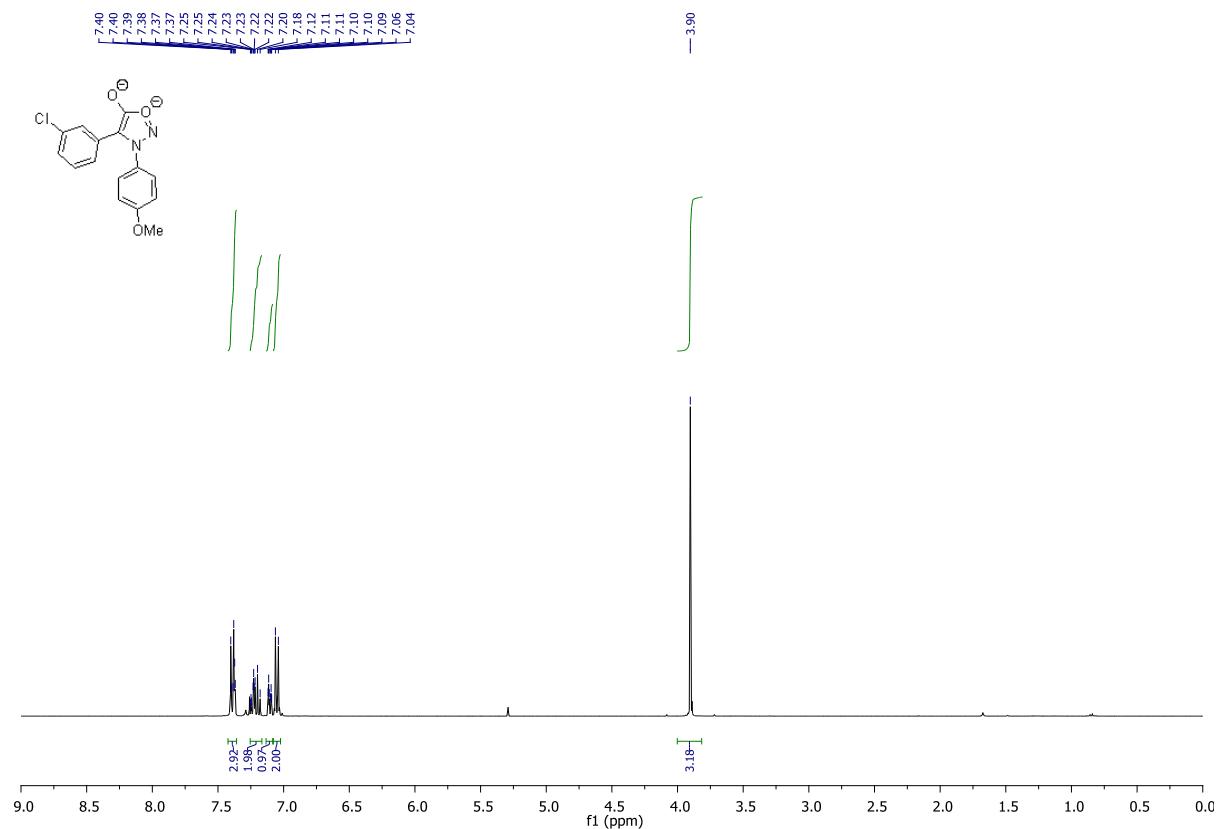
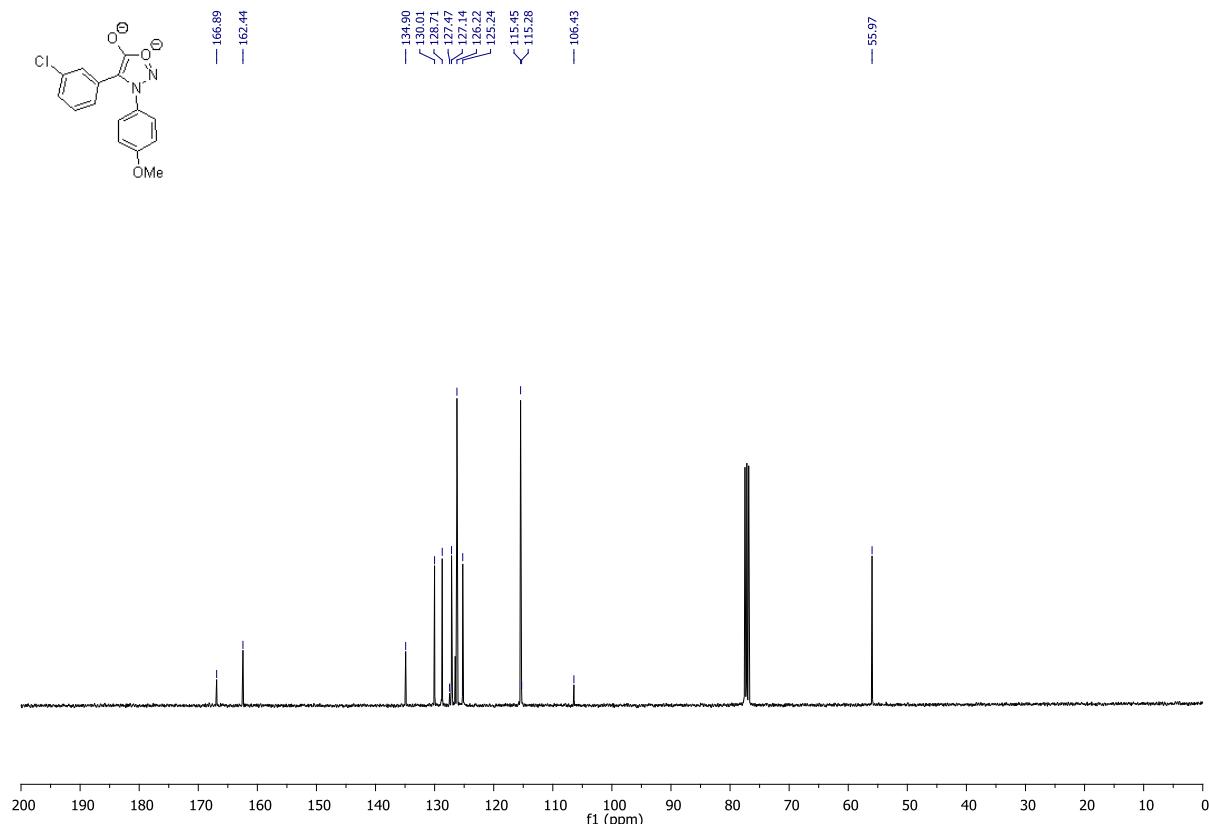
¹H NMR of 4-(*p*-Tolyl)-*N*-(methyl)sydnone (**13**):¹³C NMR of 4-(*p*-Tolyl)-*N*-(methyl)sydnone (**13**):

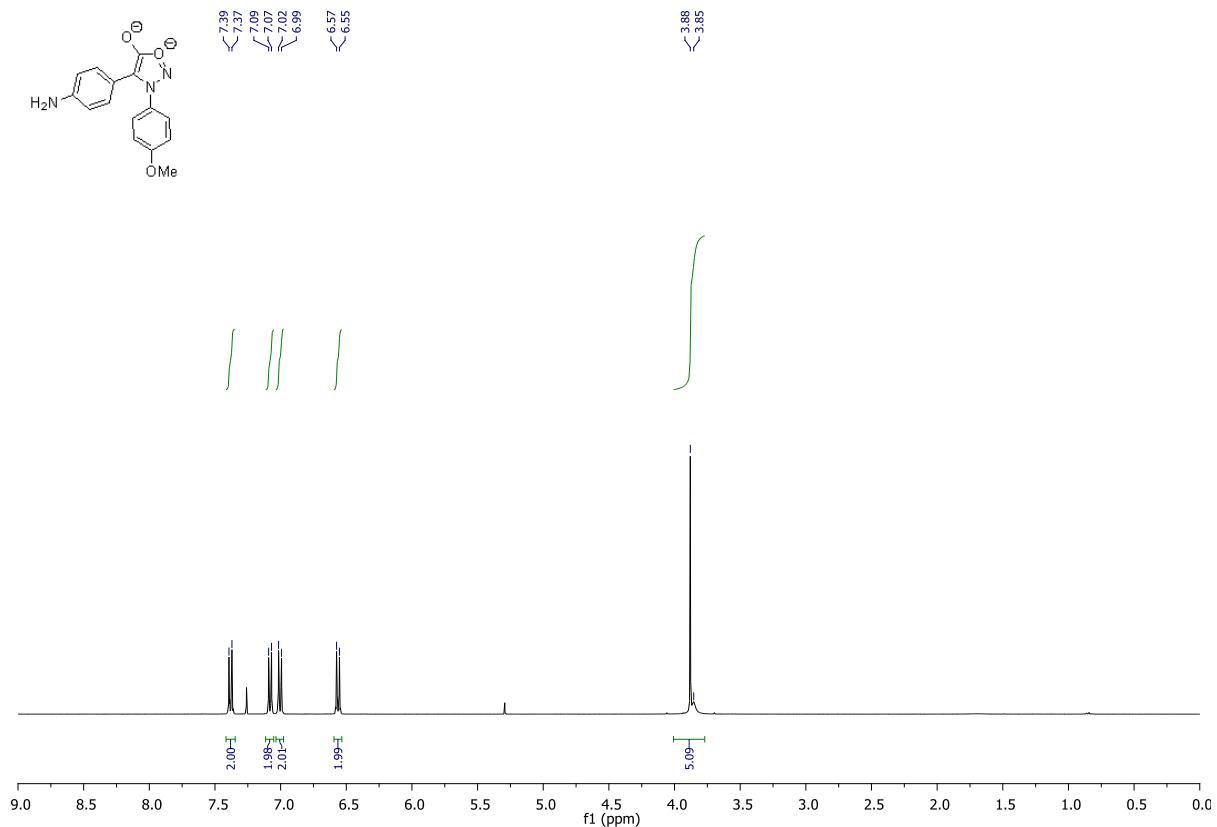
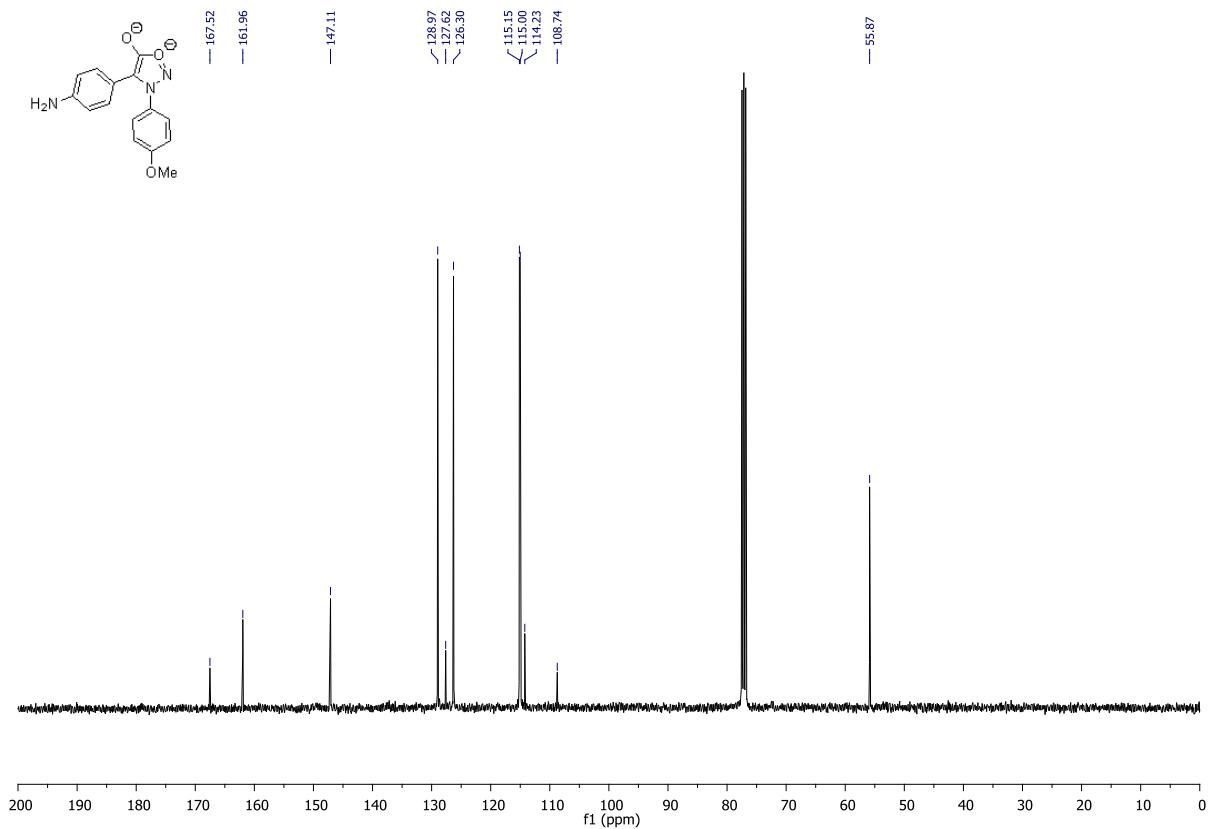
¹H NMR of 4-(*p*-Tolyl)-*N*-(ethyl)sydnone (**14**):¹³C NMR of 4-(*p*-Tolyl)-*N*-(ethyl)sydnone (**14**):

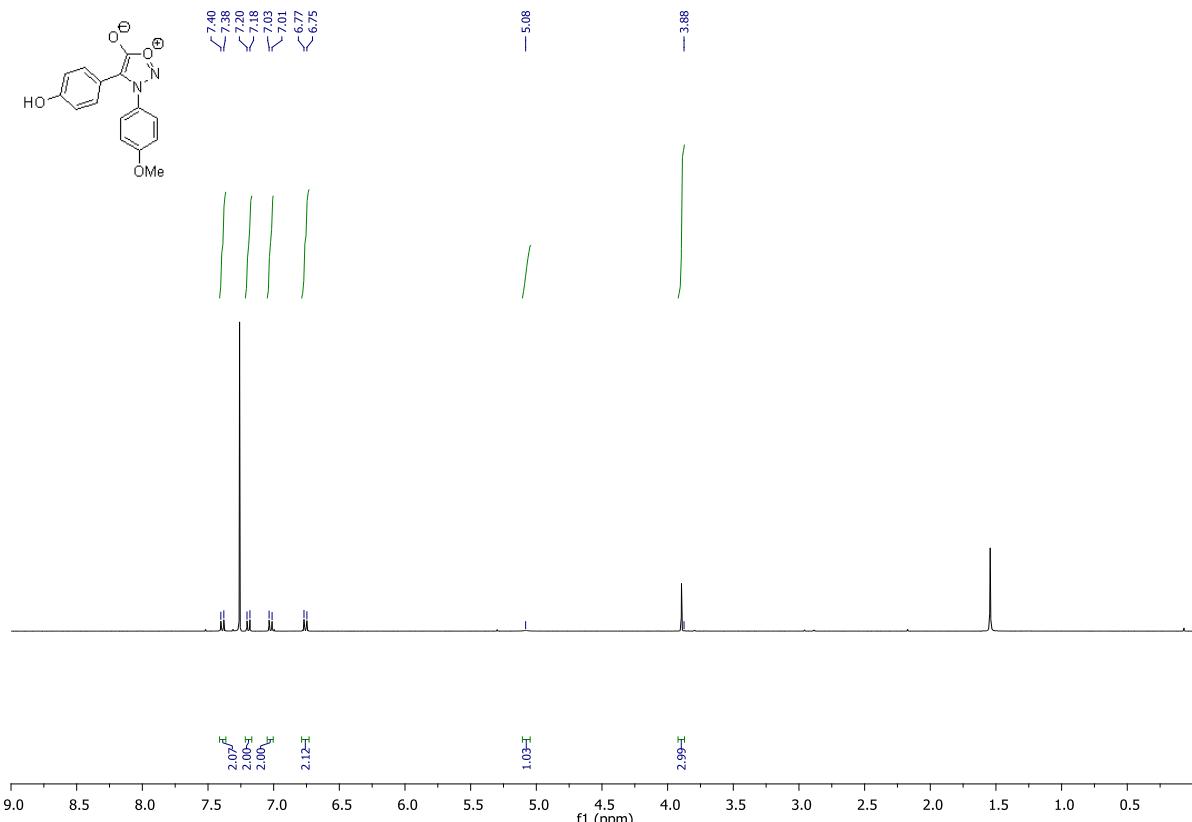
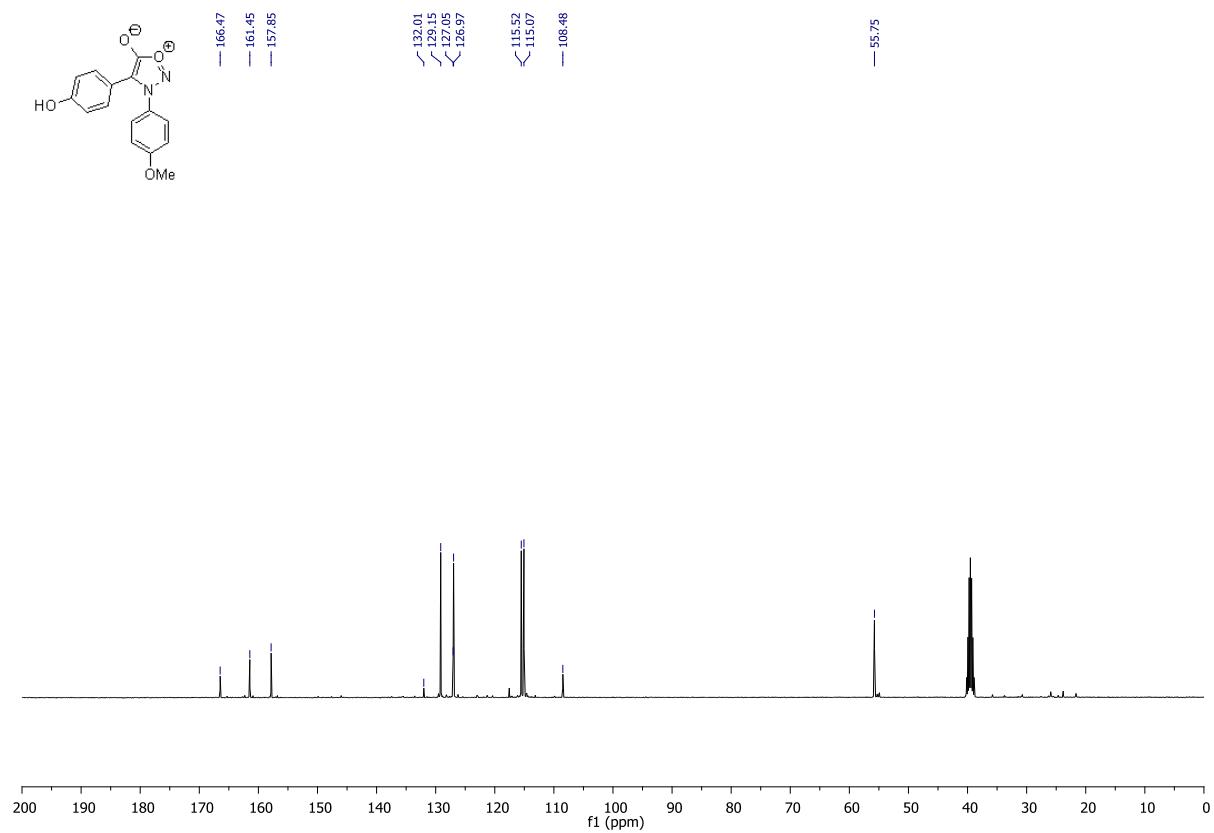
¹H NMR of 4-(*p*-Tolyl)-*N*-(benzyl)sydnone (**15**):¹³C NMR of 4-(*p*-Tolyl)-*N*-(benzyl)sydnone (**15**):

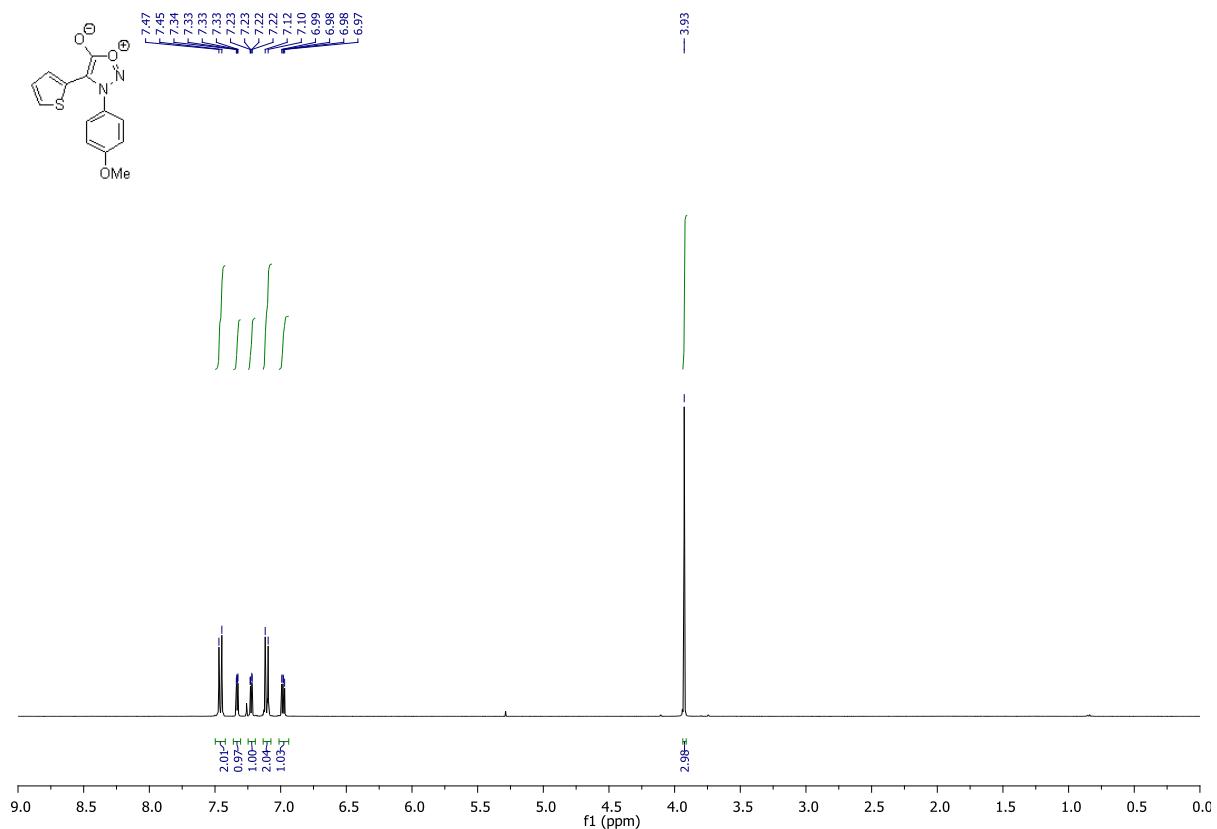
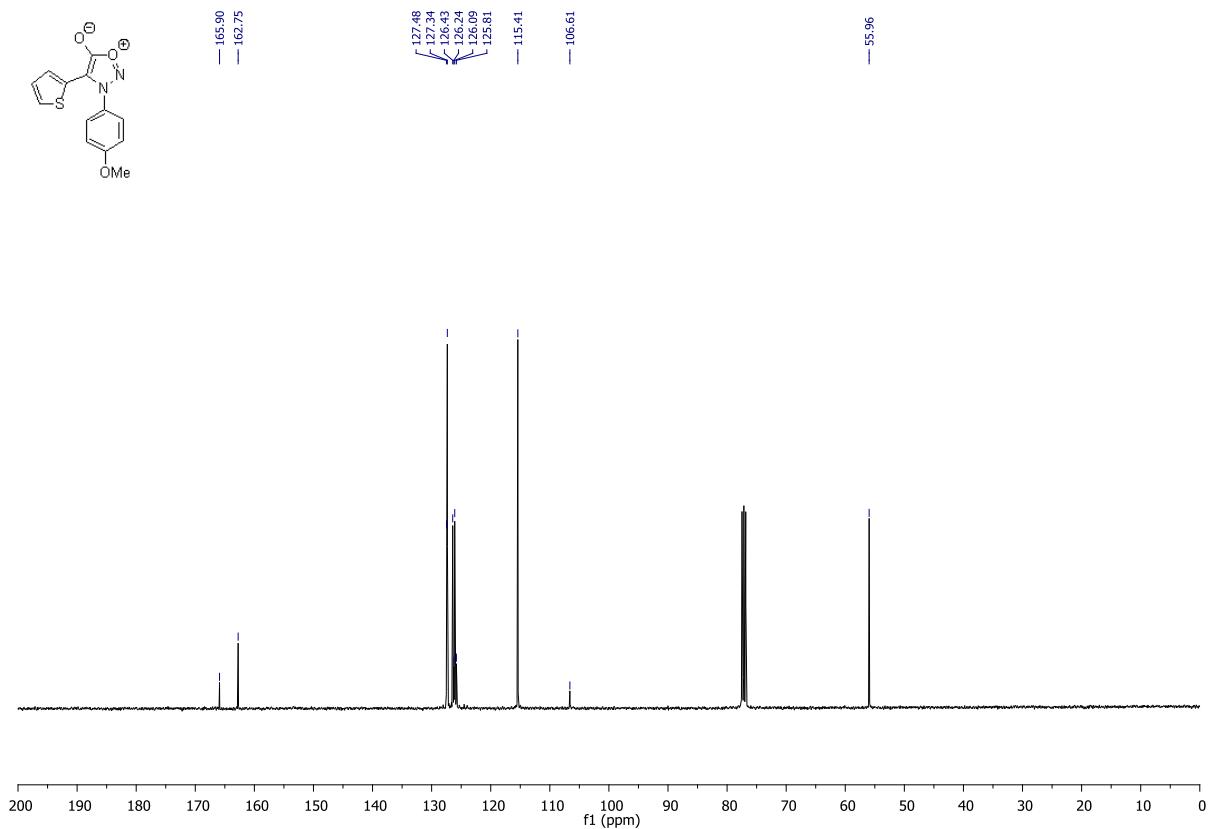
¹H NMR of 4-(3-Nitrophenyl)-N-(4-methoxyphenyl)sydnone (**16**):¹³C NMR of 4-(3-Nitrophenyl)-N-(4-methoxyphenyl)sydnone (**16**):

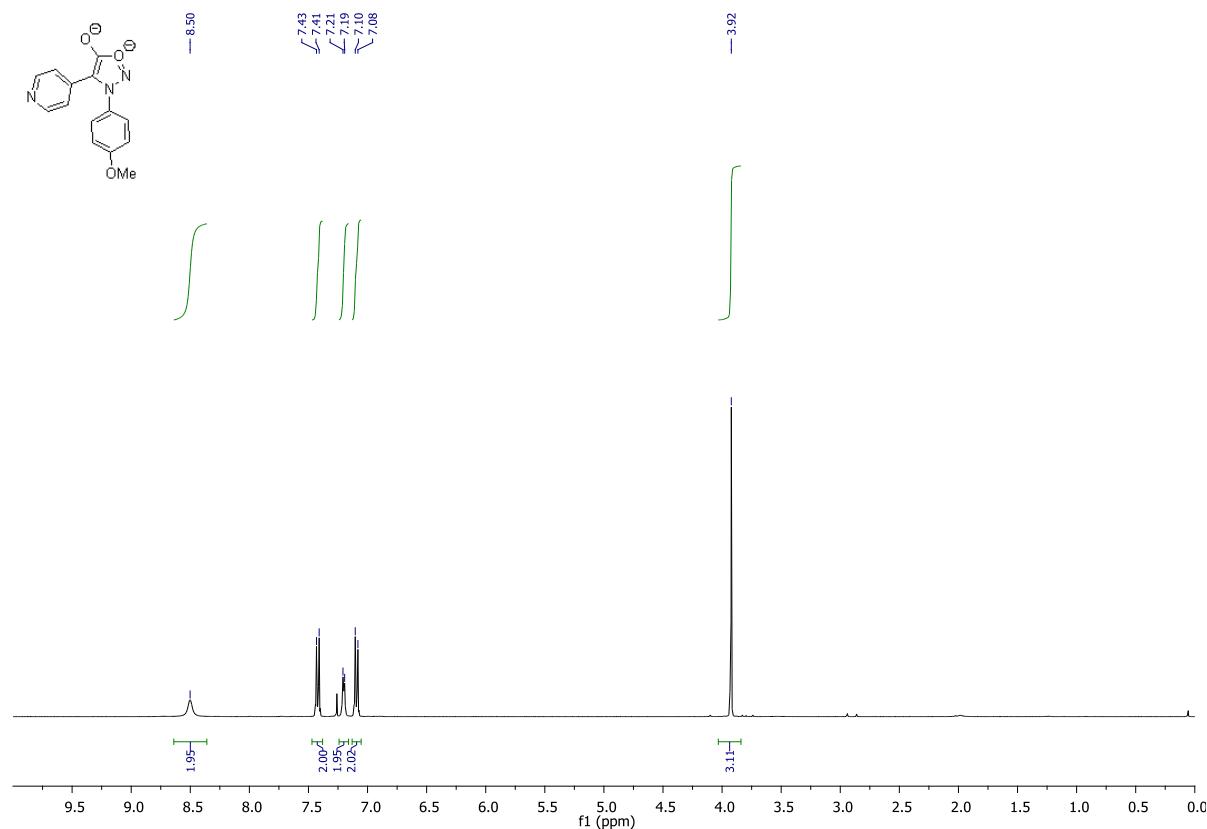
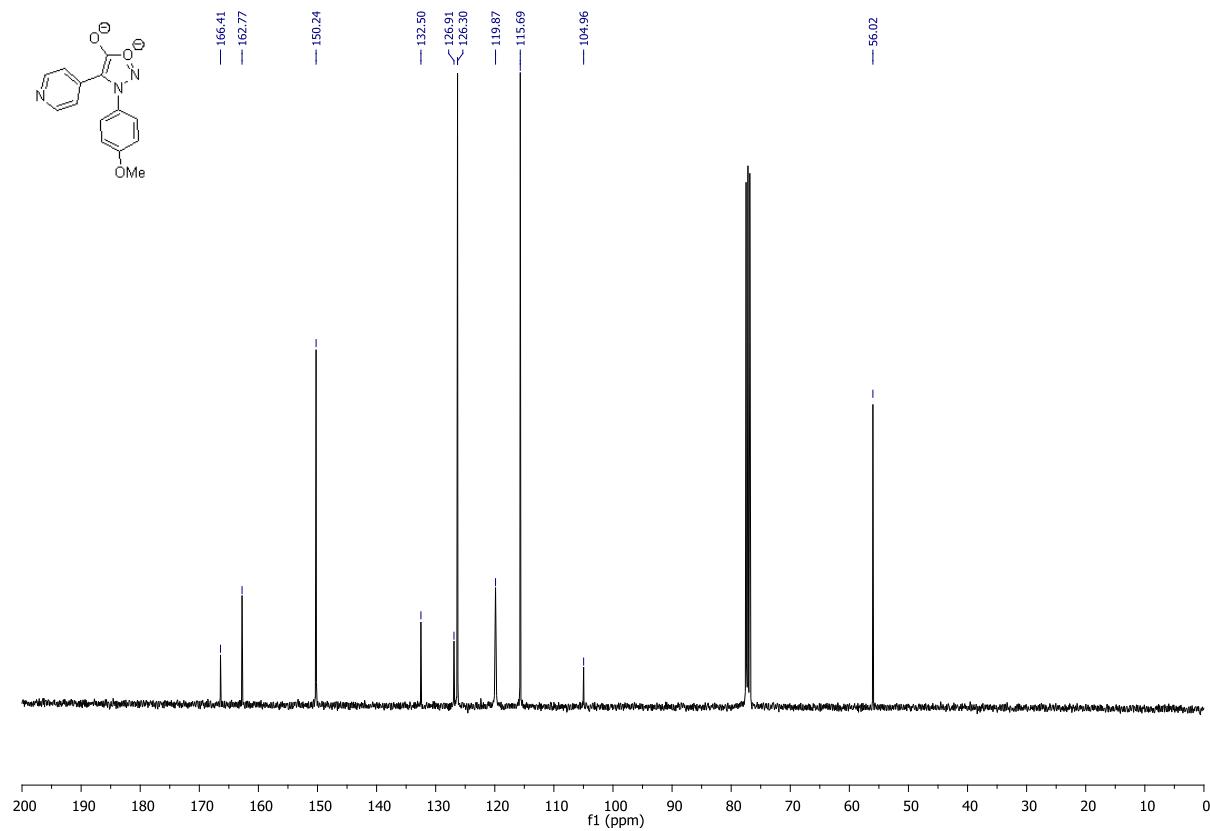
¹H NMR of 4-(2-Chlorophenyl)-N-(4-methoxyphenyl)sydnone (**17**):¹³C NMR of 4-(2-Chlorophenyl)-N-(4-methoxyphenyl)sydnone (**17**):

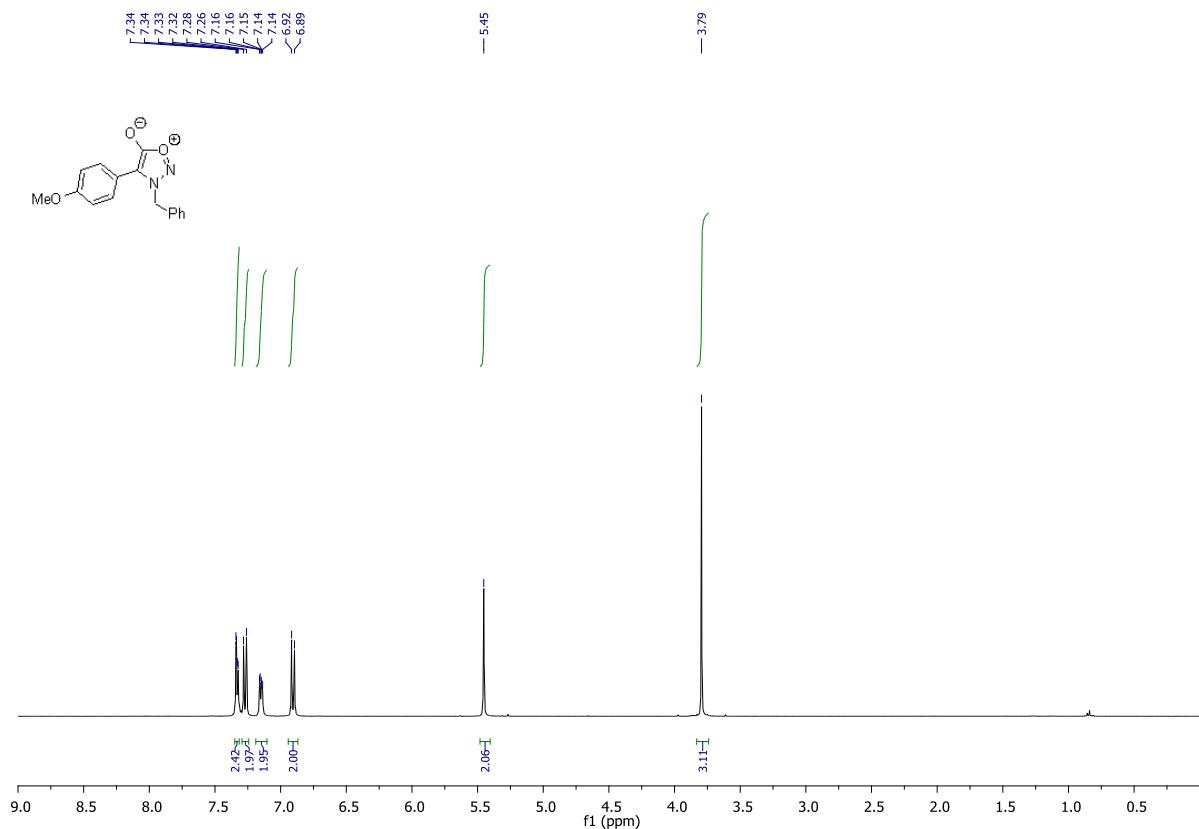
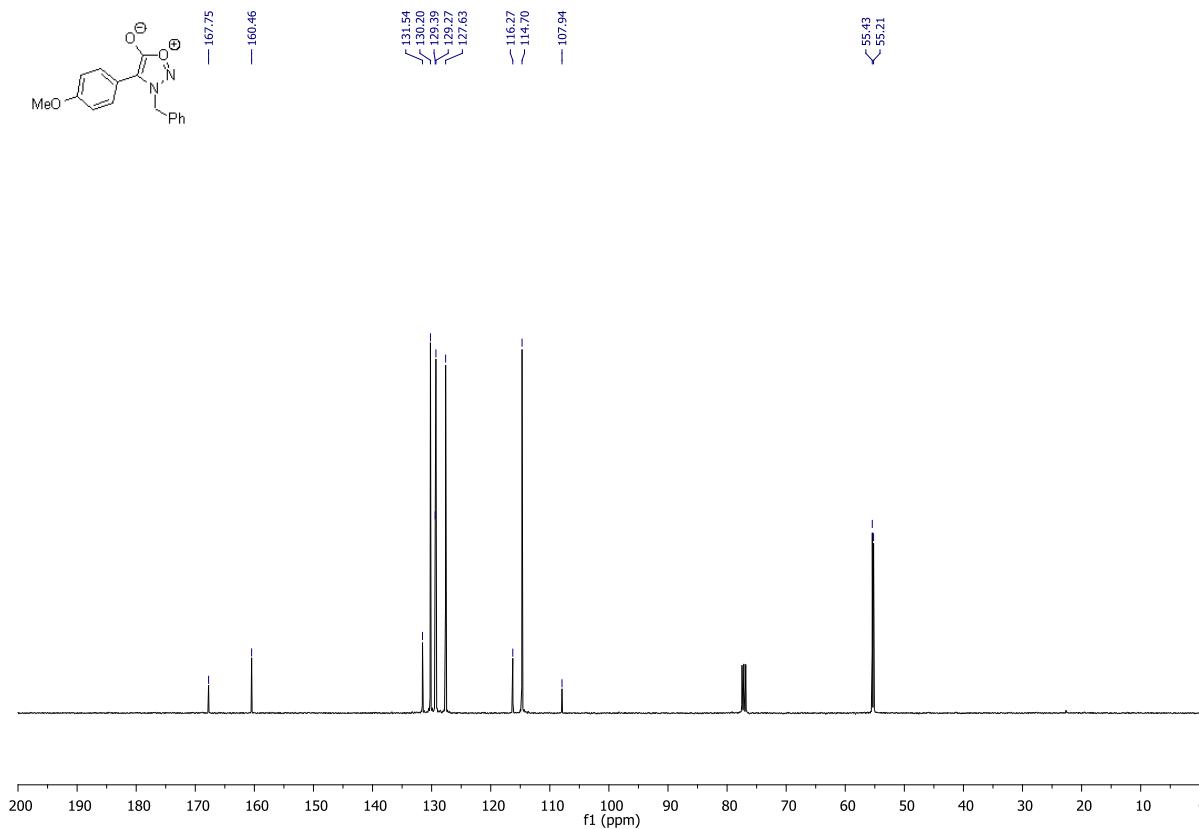
¹H NMR of 4-(3-Chlorophenyl)-N-(4-methoxyphenyl)sydnone (**18**):¹³C NMR of 4-(3-Chlorophenyl)-N-(4-methoxyphenyl)sydnone (**18**):

¹H NMR of 4-(4-Aminophenyl)-N-(4-methoxyphenyl)sydnone (**19**):¹³C NMR of 4-(4-Aminophenyl)-N-(4-methoxyphenyl)sydnone (**19**):

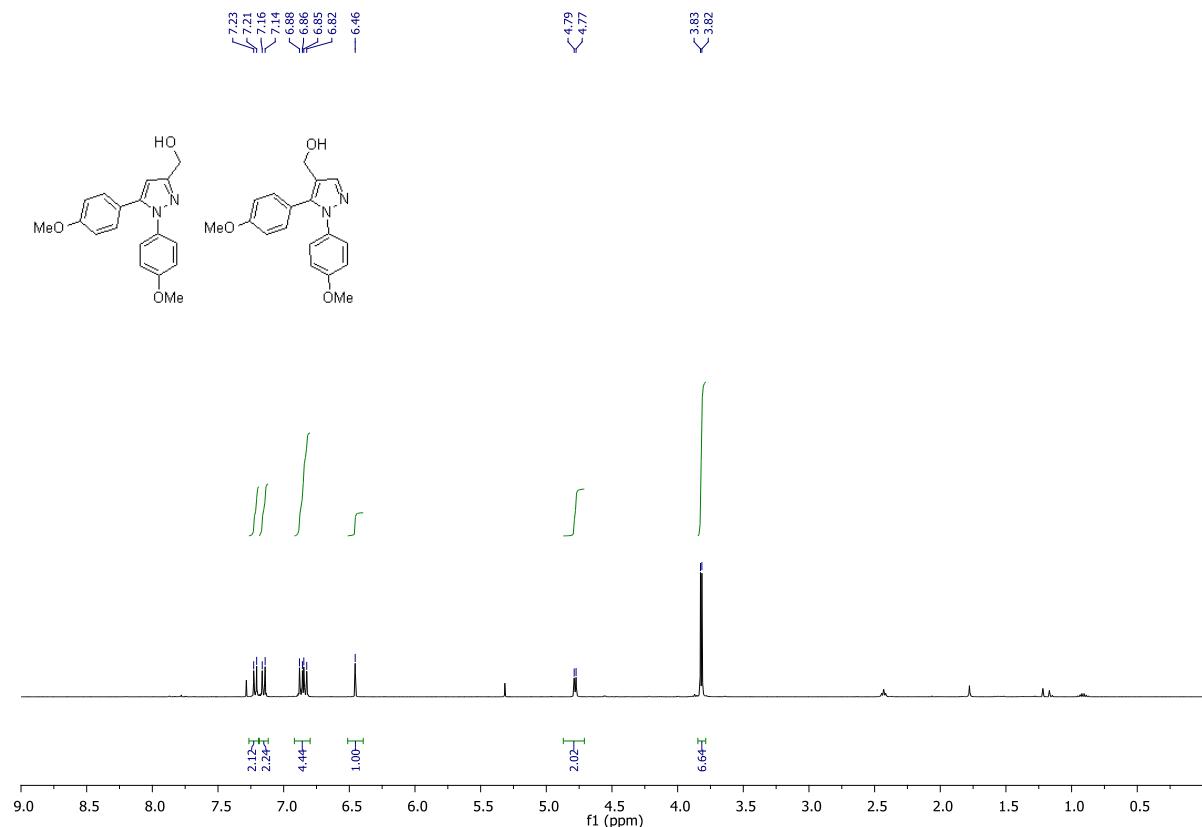
¹H NMR of 4-(4-Hydroxyphenyl)-N-(4-methoxyphenyl)sydnone (**20**):¹³C NMR of 4-(4-Hydroxyphenyl)-N-(4-methoxyphenyl)sydnone (**20**):

¹H NMR of 4-(Thiophen-2-yl)-N-(4-methoxyphenyl)sydnone (**21**):¹³C NMR of 4-(Thiophen-2-yl)-N-(4-methoxyphenyl)sydnone (**21**):

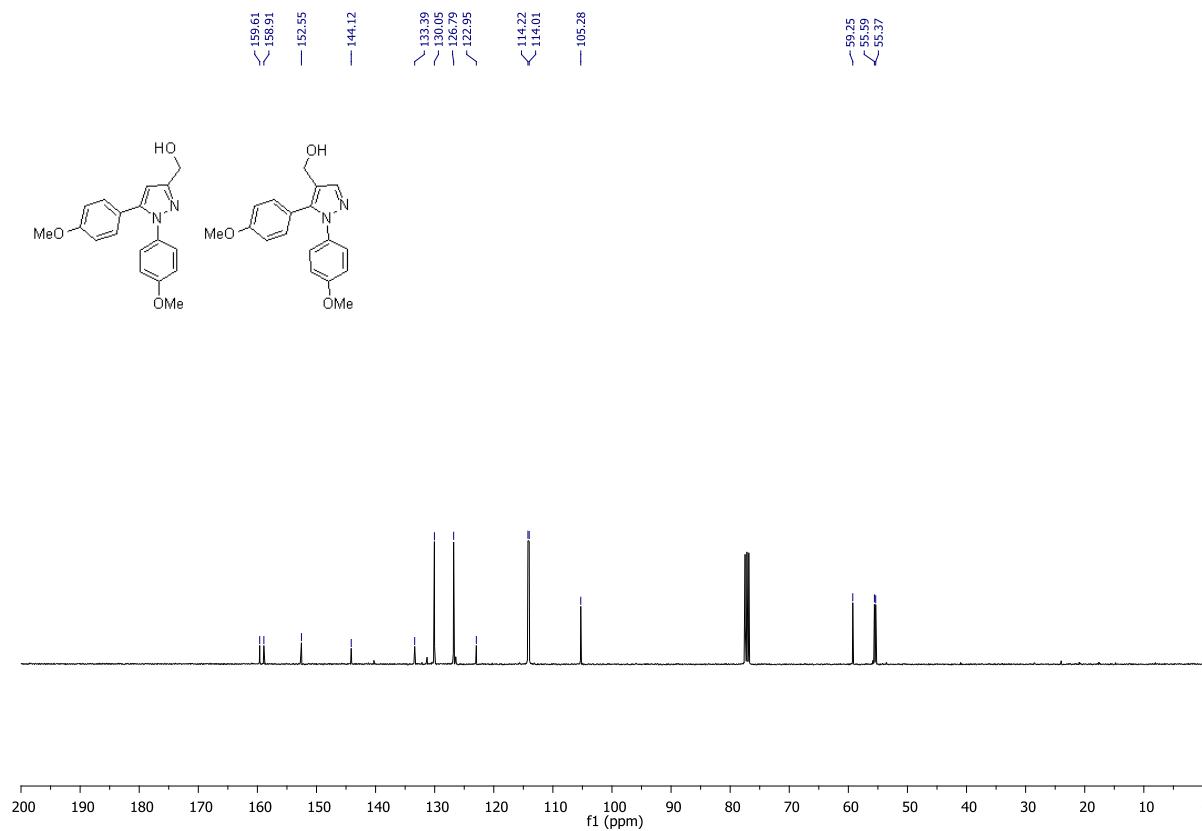
¹H NMR of 4-(4-Pyridyl)-N-(4-methoxyphenyl)sydnone (**22**):¹³C NMR of 4-(4-Pyridyl)-N-(4-methoxyphenyl)sydnone (**22**):

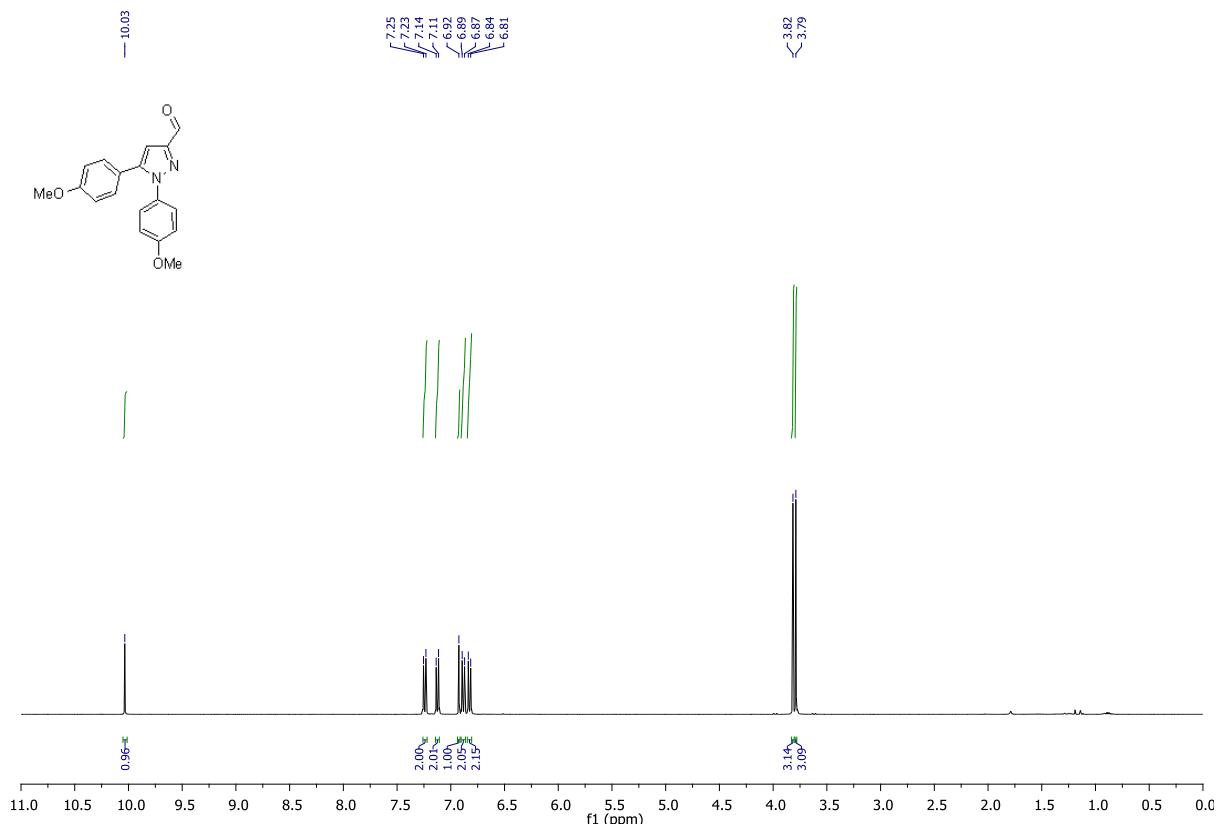
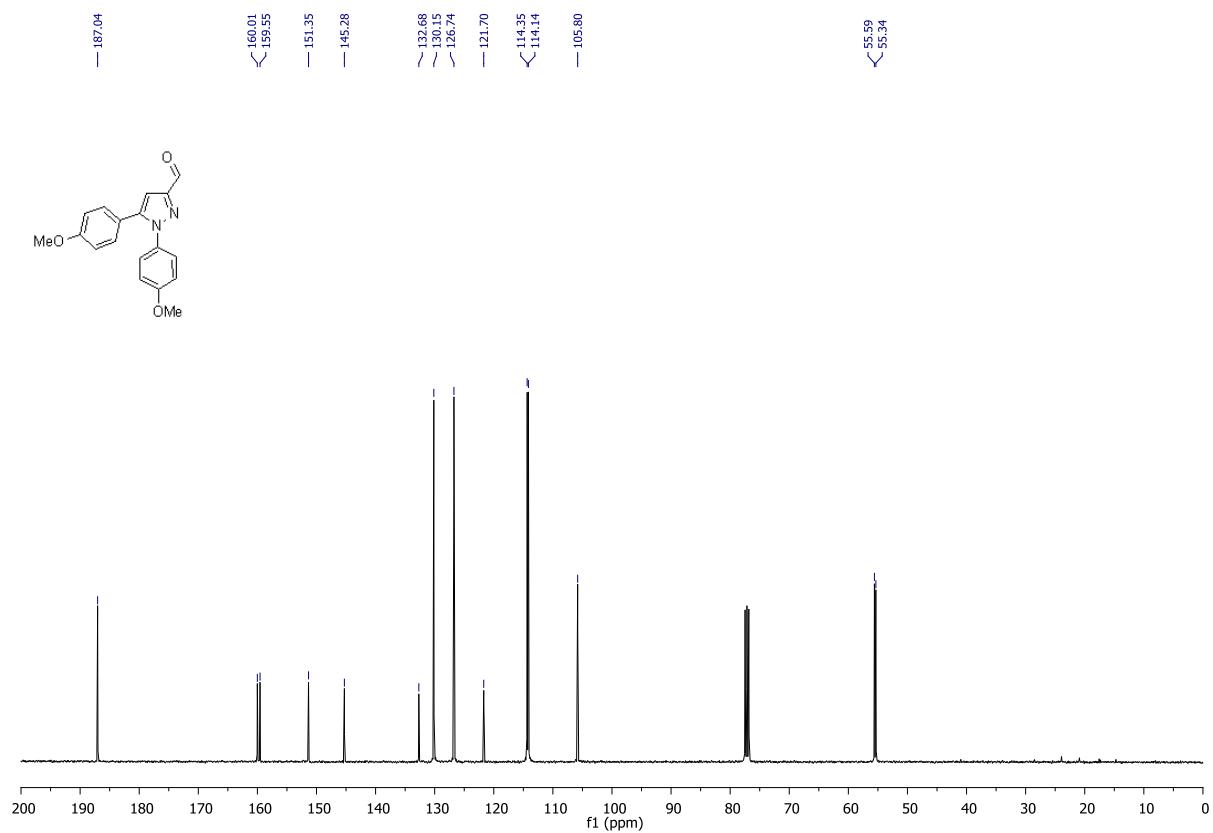
¹H NMR of 4-(4-Methoxyphenyl)-N-benzylsydnone (**23**):¹³C NMR of 4-(4-Methoxyphenyl)-N-benzylsydnone (**23**):

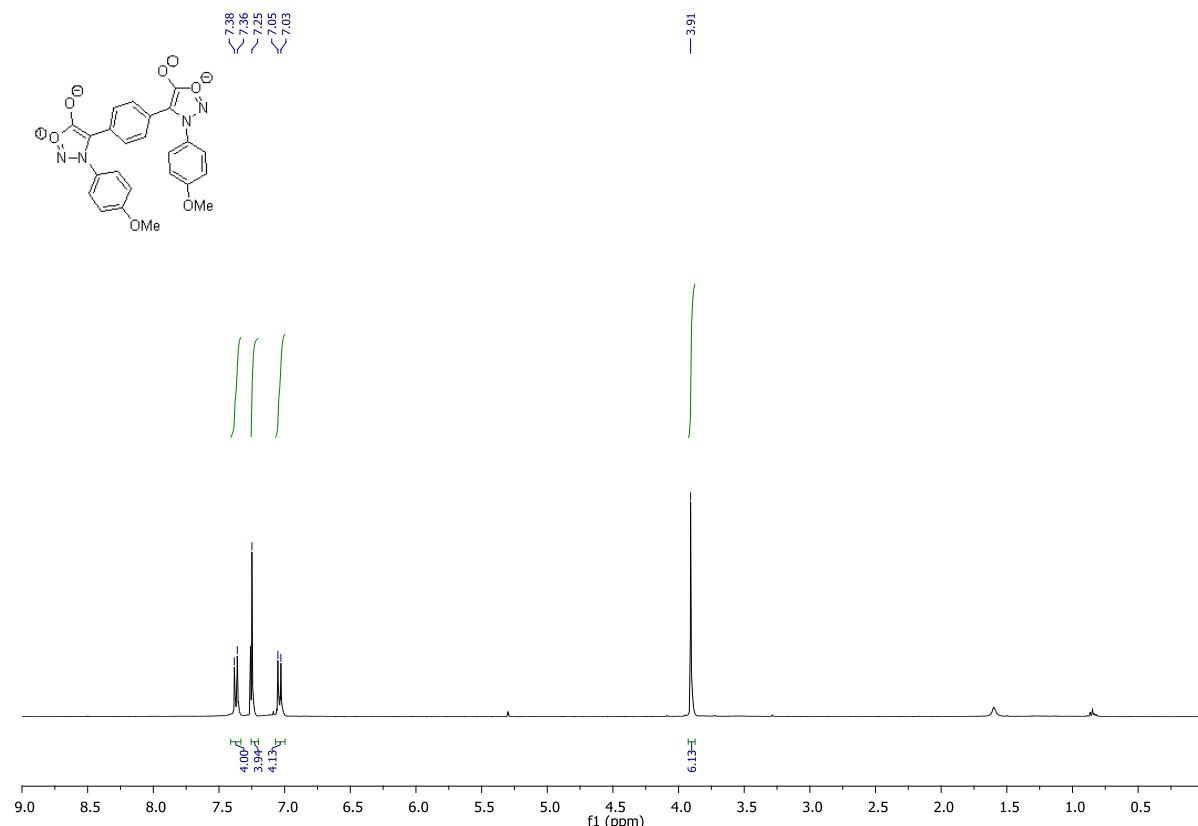
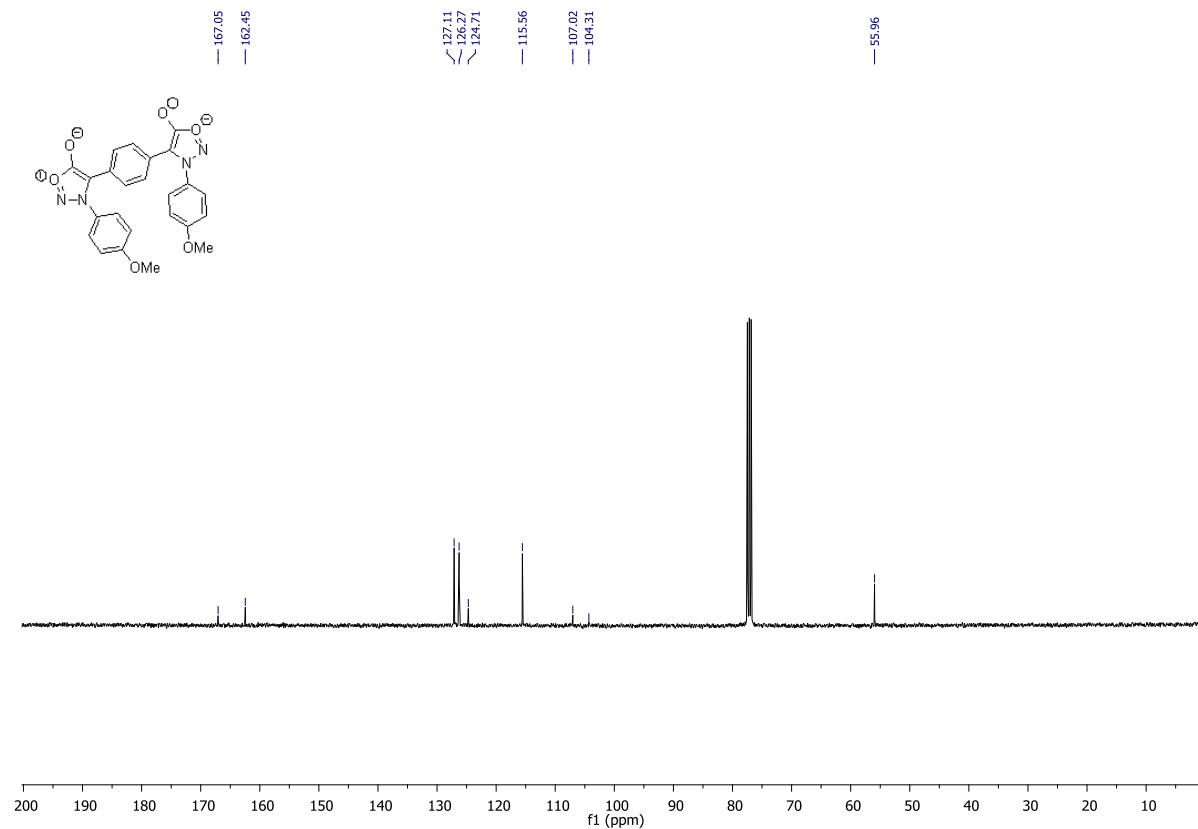
¹H NMR of *1-(4-Methoxyphenyl)-3-(methylalcohol)-5-(4-methoxyphenyl)pyrazole (25a)* and *1-(4-methoxyphenyl)-4-(methylalcohol)-5-(4-methoxyphenyl)pyrazole (25b)*:

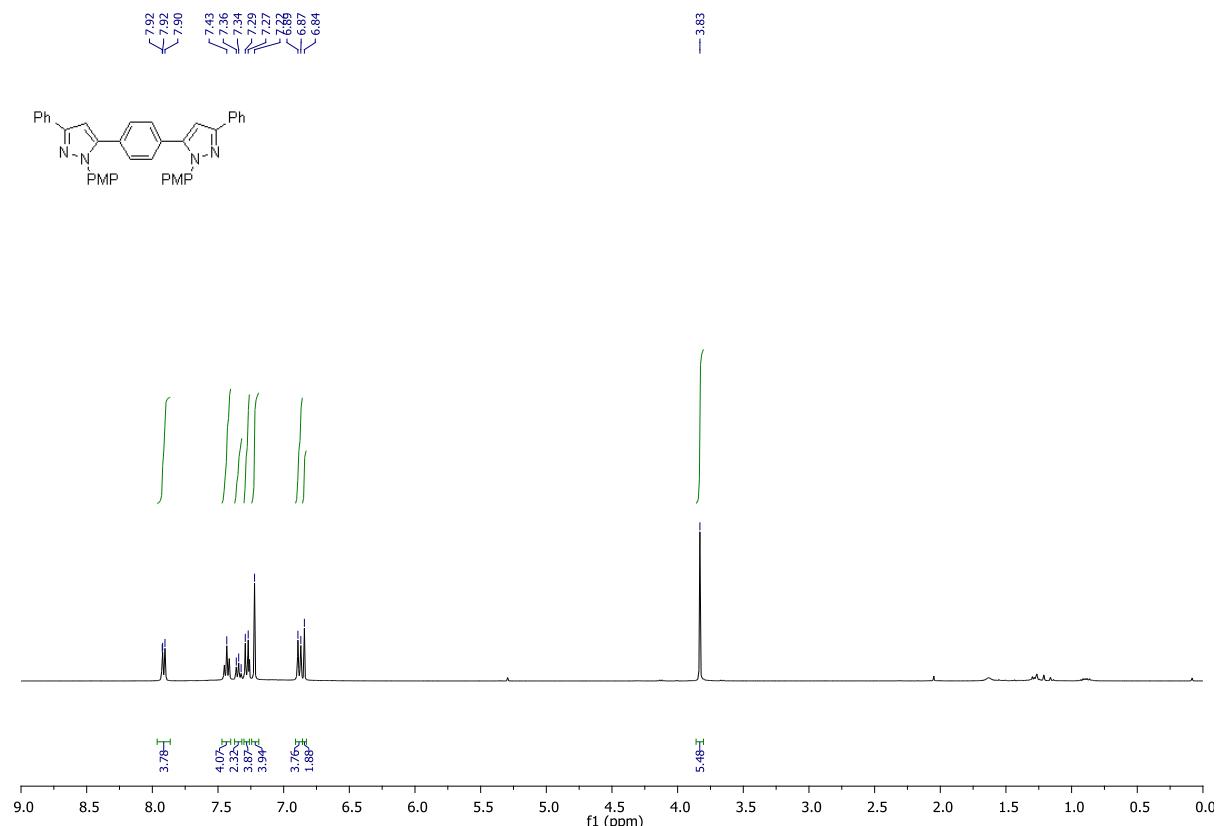
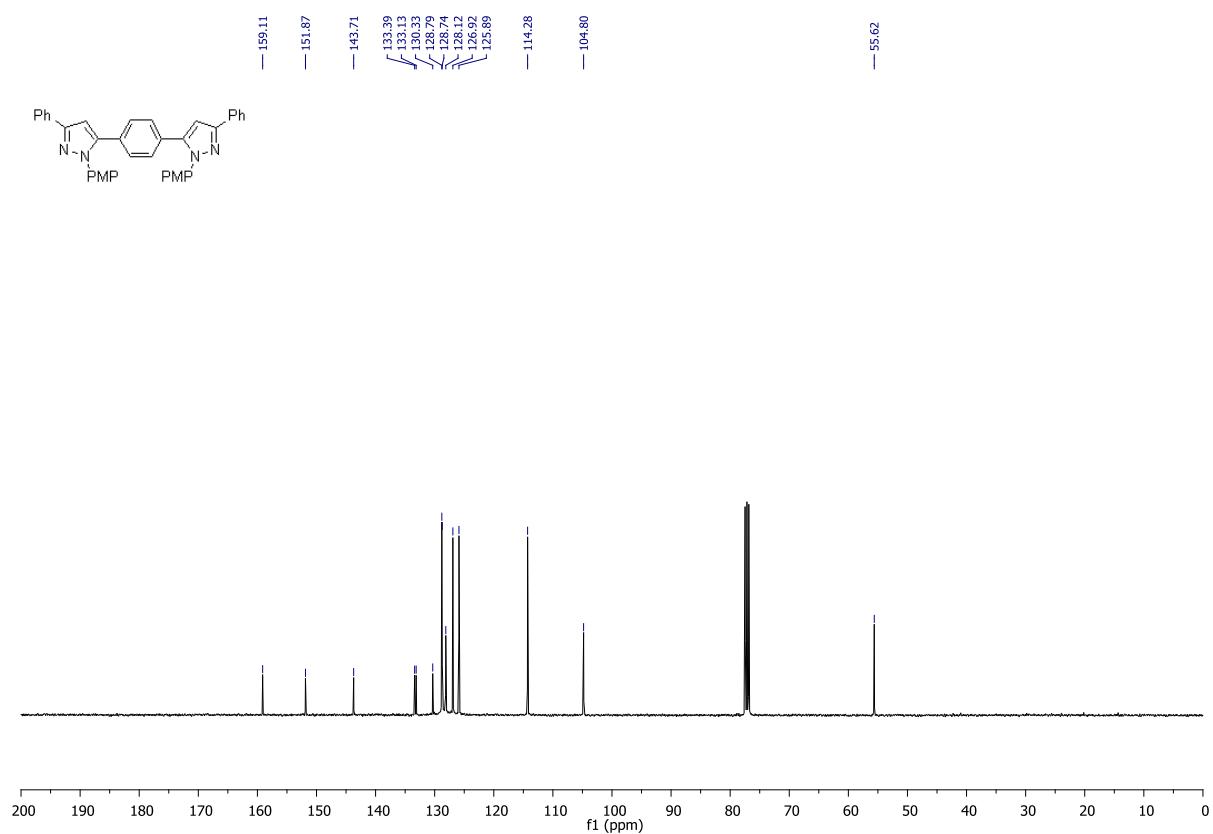


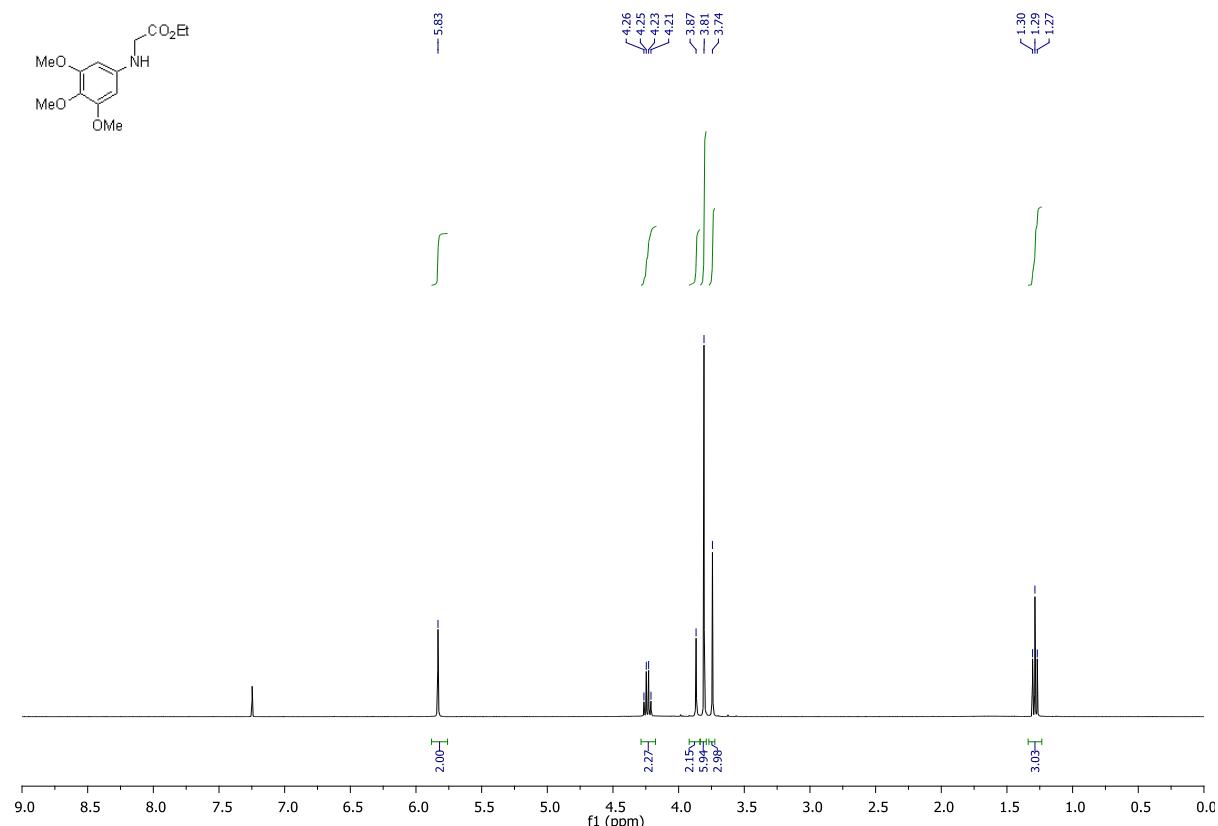
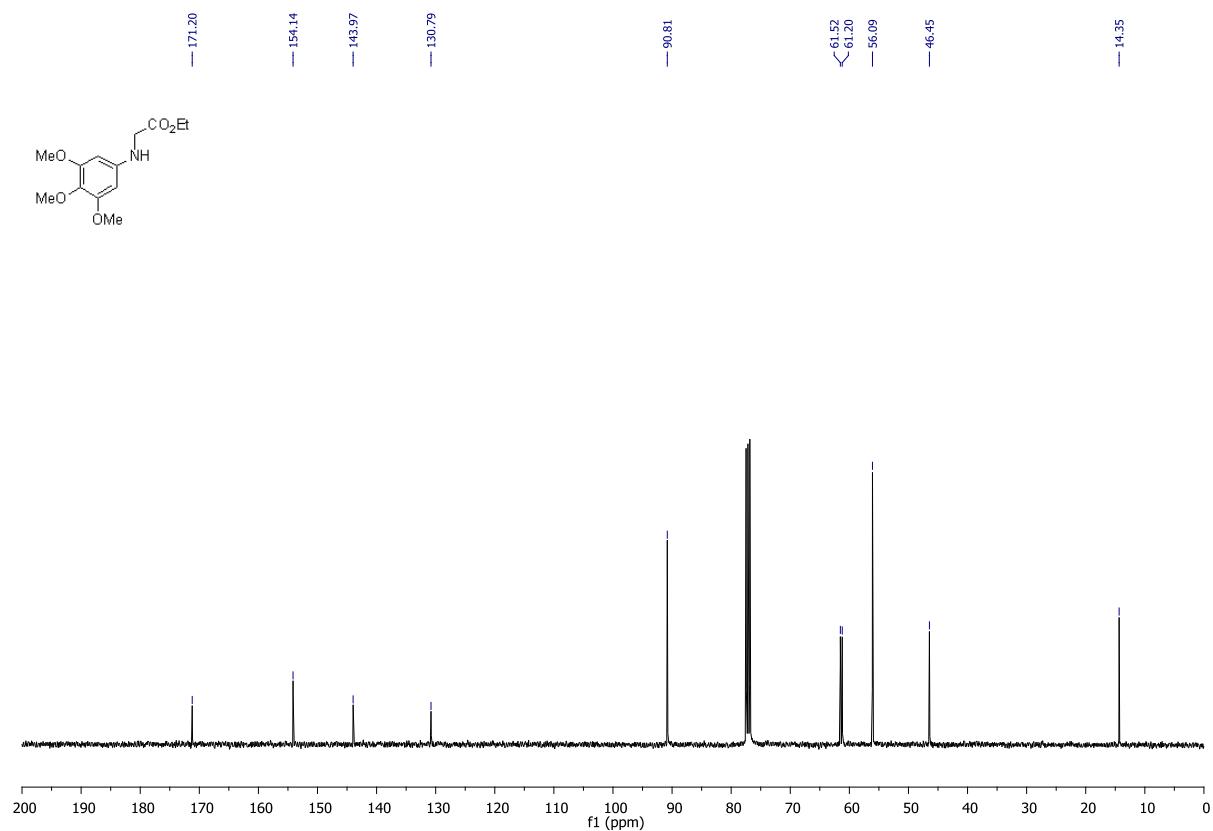
¹³C NMR of *1-(4-Methoxyphenyl)-3-(methylalcohol)-5-(4-methoxyphenyl)pyrazole (25a)* and *1-(4-methoxyphenyl)-4-(methylalcohol)-5-(4-methoxyphenyl)pyrazole (25b)*:

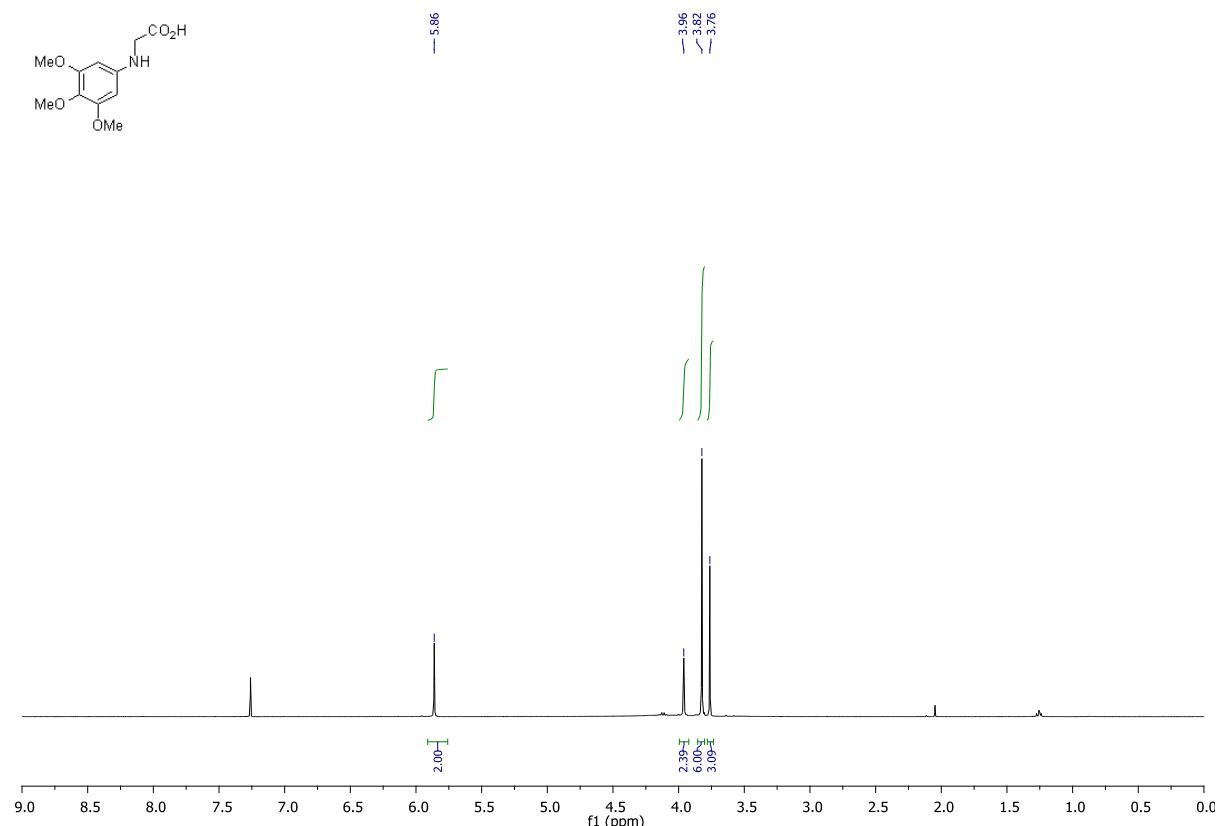
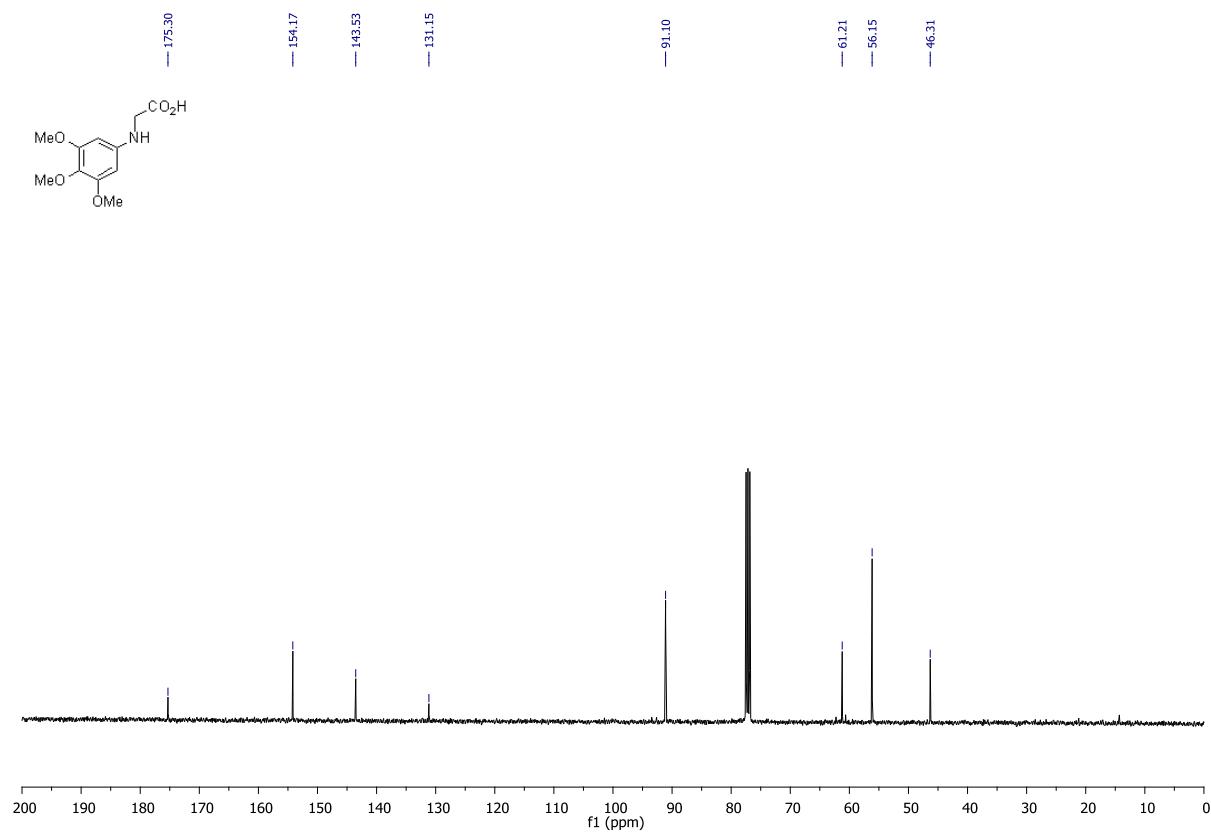


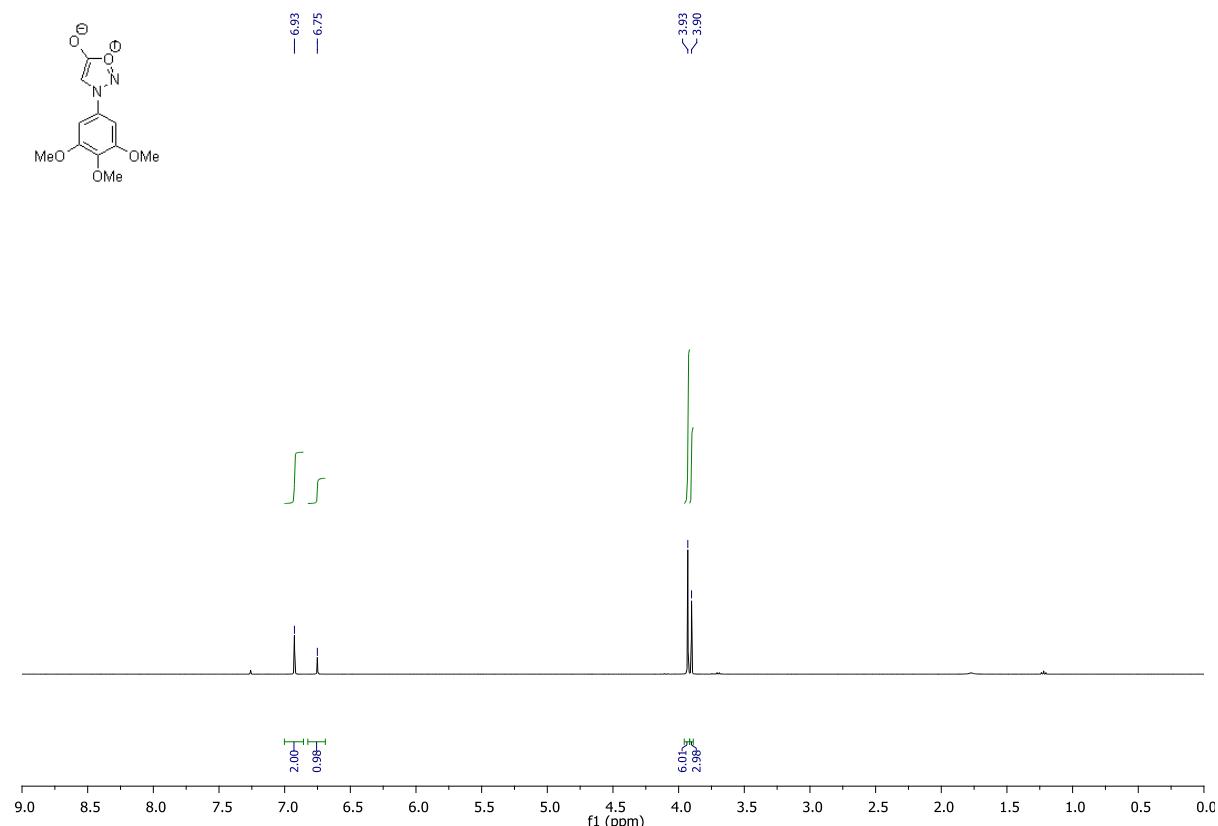
¹H NMR of 1,5-Bis(4-methoxyphenyl)-1*H*-pyrazole-3-carboxaldehyde (**26**):¹³C NMR of 1,5-Bis(4-methoxyphenyl)-1*H*-pyrazole-3-carboxaldehyde (**26**):

¹H NMR of 4,4'-(1,4-phenylene)-bis-N-(4-methoxyphenyl)sydnone (**27**):¹³C NMR of 4,4'-(1,4-phenylene)-bis-N-(4-methoxyphenyl)sydnone (**27**):

¹H NMR of 5,5'-(1,4-phenylene)bis[1-(4-methoxyphenyl)-3-phenyl]-1H-pyrazole (**28**):¹³C NMR of 5,5'-(1,4-phenylene)bis[1-(4-methoxyphenyl)-3-phenyl]-1H-pyrazole (**28**):

¹H NMR of Ethyl 2-((3,4,5-trimethoxyphenyl)amino)acetate:¹³C NMR of Ethyl 2-((3,4,5-trimethoxyphenyl)amino)acetate:

¹H NMR of 2-((3,4,5-trimethoxyphenyl)amino)acetic acid:¹³C NMR of 2-((3,4,5-trimethoxyphenyl)amino)acetic acid:

¹H NMR of *N*-(3,4,5-trimethoxyphenyl)sydnone (**1b**):¹³C NMR of *N*-(3,4,5-trimethoxyphenyl)sydnone (**1b**):