Supporting Information

Iodine/DMSO mediated one pot access of 1-aryl-2-(pyrazol-5-yl)ethane-1,2-diones via domino reaction from functionalized pent-2-ene-1,5-diones

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X-ray Crystallographic Data for compound 3m

Crystallization procedure (solvent evaporation method): Slow evaporation of a saturated solution of 2m in chloroform at room temperature produced red colored cube shaped crystals suitable for X-ray analysis. Single crystal diffraction data for 2m were collected at room temperature with an Oxford XCalibur CCD diffractometer equipped with a graphite monochromatic Mo-Kα radiation (λ = 0.71073 Å).[1] Data reduction was performed with the CrysAllis-PRO.[1] The experimental data was processed and analysed using the software package Olex2.[2] The structure was solved with the olex,[2] solve program,[3] and by employing the charge flipping algorithm. The refined structure was obtained using the olex 2 where refine refinement package,[4] utilizes Gauss-Newton minimization.

The ORTEP diagram shows the compound crystallizes in a triclinic system having four molecules in the unit cell and shows one 2-methoxyphenyl ring planer with pyrazole and other is perpendicular to pyrazole. The C=O group and NH of the pyrazole ring forms an intermolecular hydrogen bonding (**Figure 1**). The hydrogen atoms were placed at the calculated positions and included in the last cycles of the refinement. Crystallographic data collection and structure solution parameters are summarized in **Table 1.**

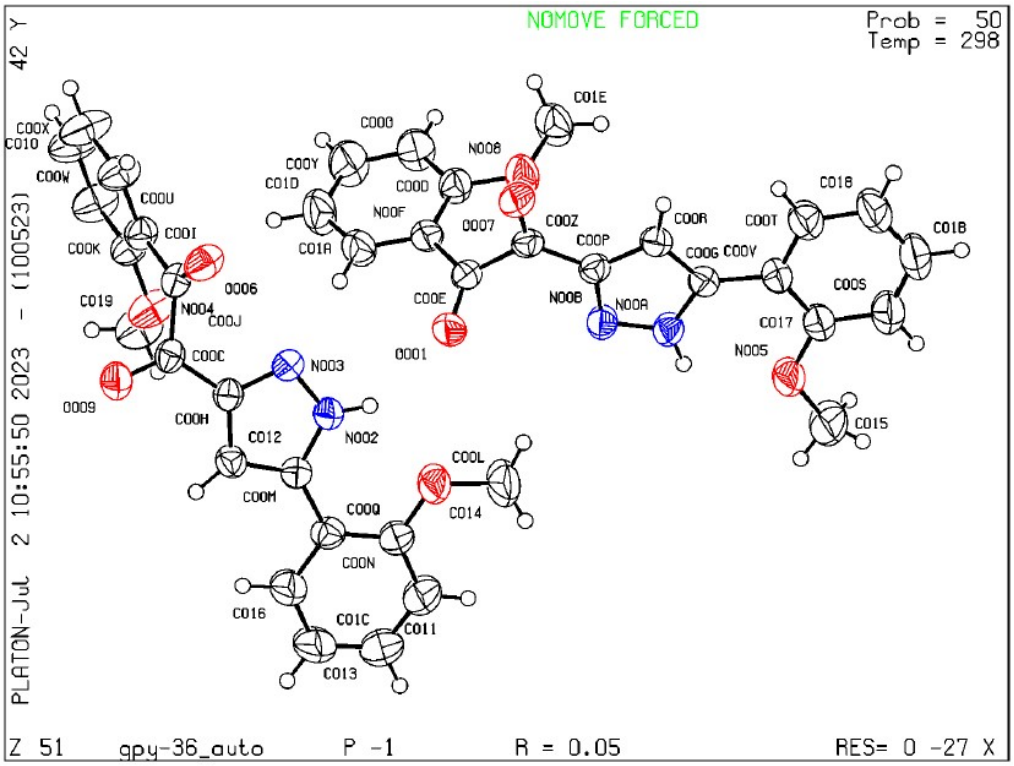


Figure 1. ORTEP diagram of **3m**; thermal ellipsoids are drawn at the 50% probability level.

Table 1. Crystal data and structure refinement for 3m

Empirical formula	$C_{19}H_{16}N_2O_4$
CCDC	2278961
Formula weight	336.34
Temperature/K	298
Crystal system	triclinic
Space group	P-1
a/Å	8.3993(5)
b/Å	19.2977(9)
c/Å	11.0438(6)
α/°	90
β/°	107.107(6)
γ/°	90
Volume/Å^3	1710.86(17)
Z	4
ρ_{calc}g/cm^3	1.306
μ/mm^{-1}	0.093
F(000)	704.0
Crystal size/mm^3	0.3 × 0.2 × 0.2
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.602 to 62.242
Index ranges	-10 ≤ h ≤ 11, -27 ≤ k ≤ 25, -14 ≤ l ≤ 15
Reflections collected	20045
Independent reflections	8249 [Rint = 0.0375, Rsigma = 0.0538]
Data/restraints/parameters	8249/0/459
Goodness-of-fit on F^2	1.039
`Final R indexes [I>=2σ (I)]	R1 = 0.0492, wR2 = 0.1181
Final R indexes [all data]	R1 = 0.0958, wR2 = 0.1348

Largest diff. peak/hole / e $Å^{-3}$	0.16/-0.19

References

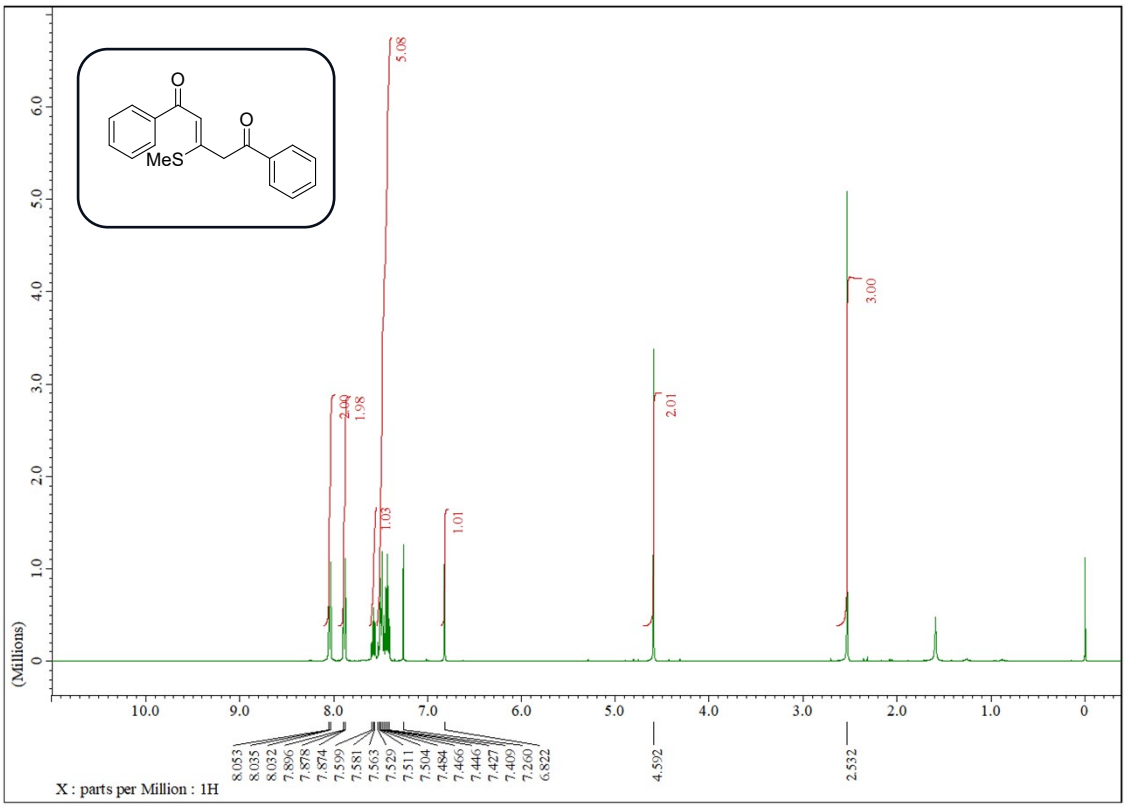
1. Oxford Diffraction Ltd. CrysAlisPro, v. 1.171.33.49b, 2009.

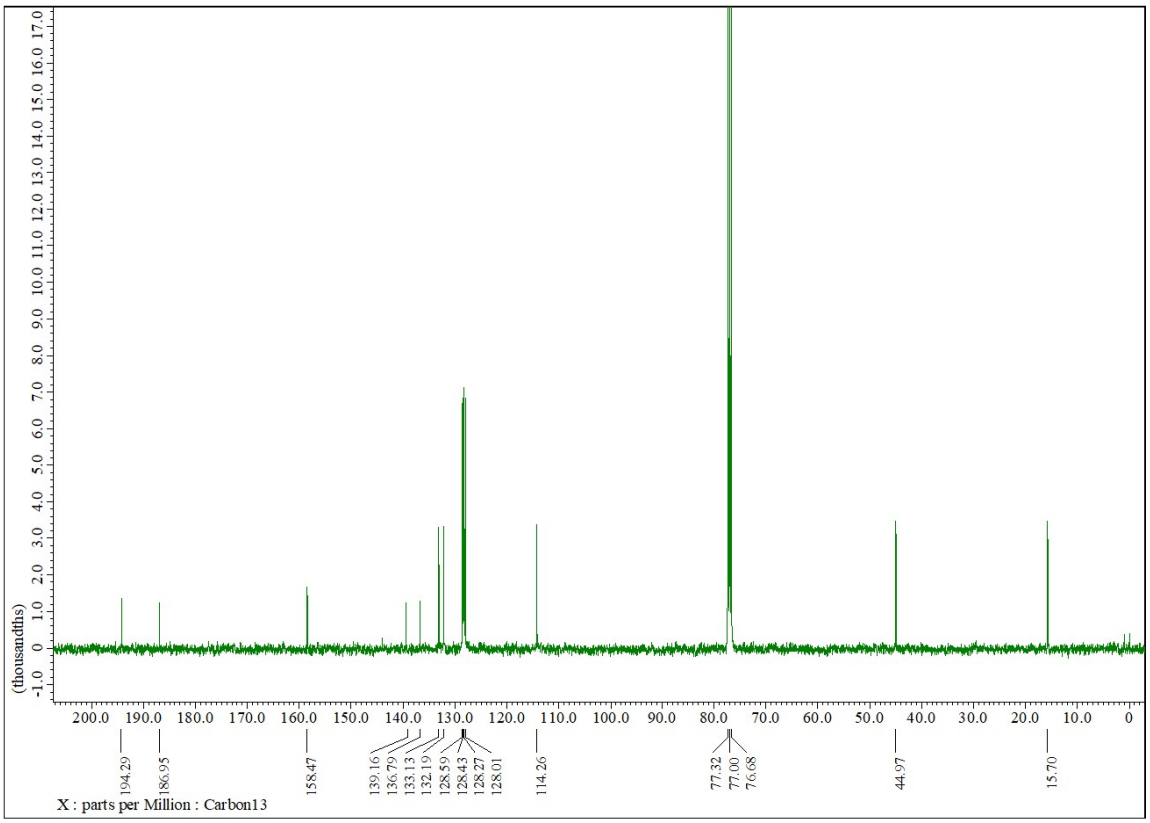
2. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

3. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.

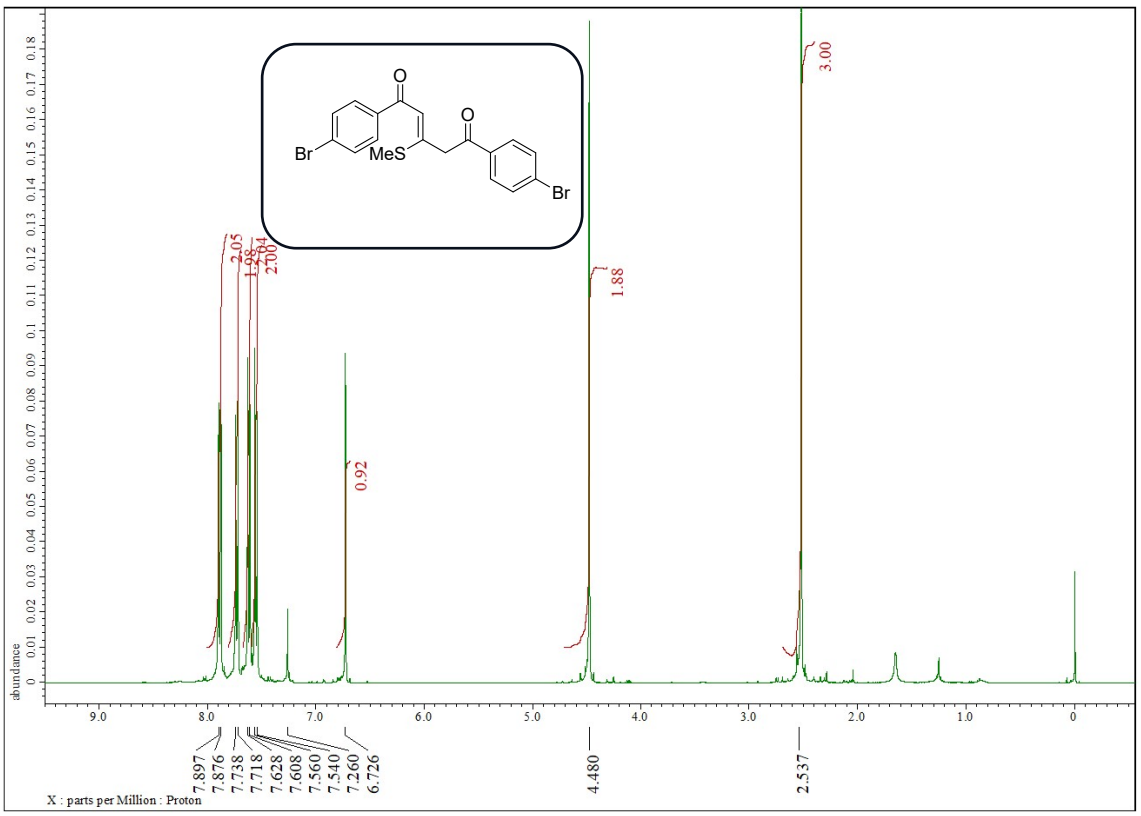
4. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

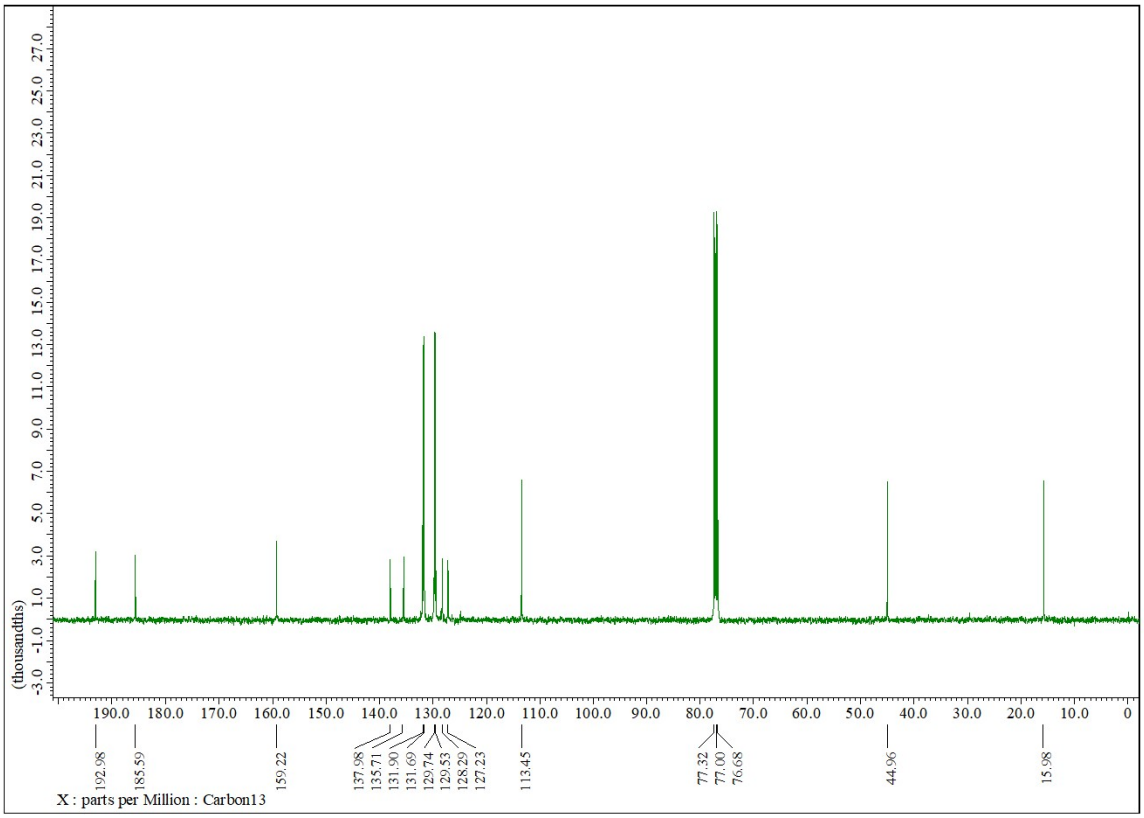
^{1}H NMR and ^{13}C NMR spectra of (Z)-3-(methylthio)-1,5-diphenylpent-2-ene-1,5-dione (1a)



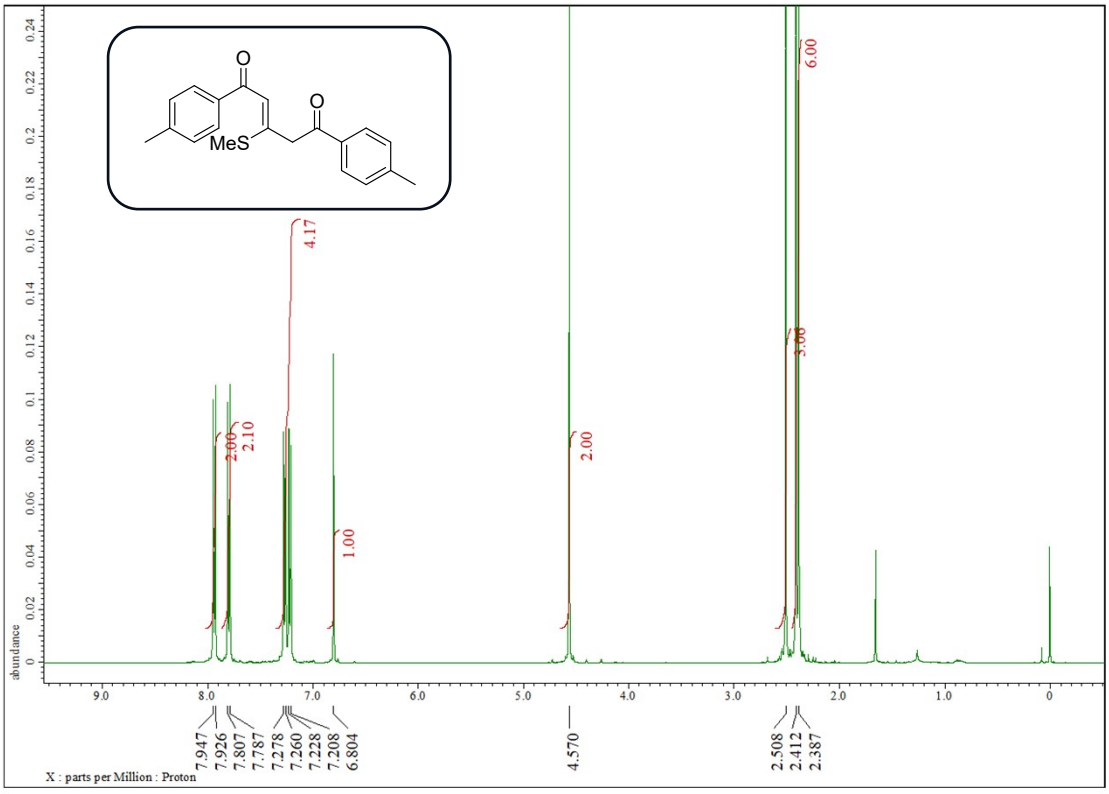


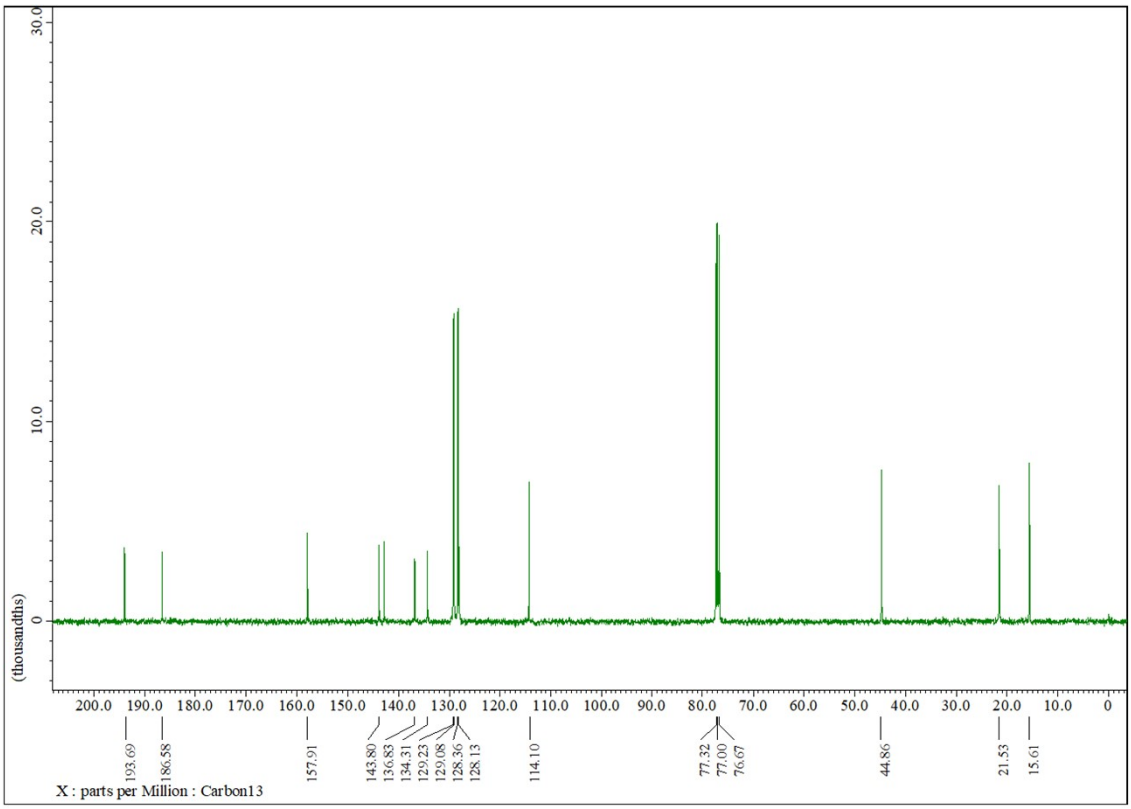
^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-bis(4-bromophenyl)-3-(methylthio)pent-2-ene-1,5-dione (1b)



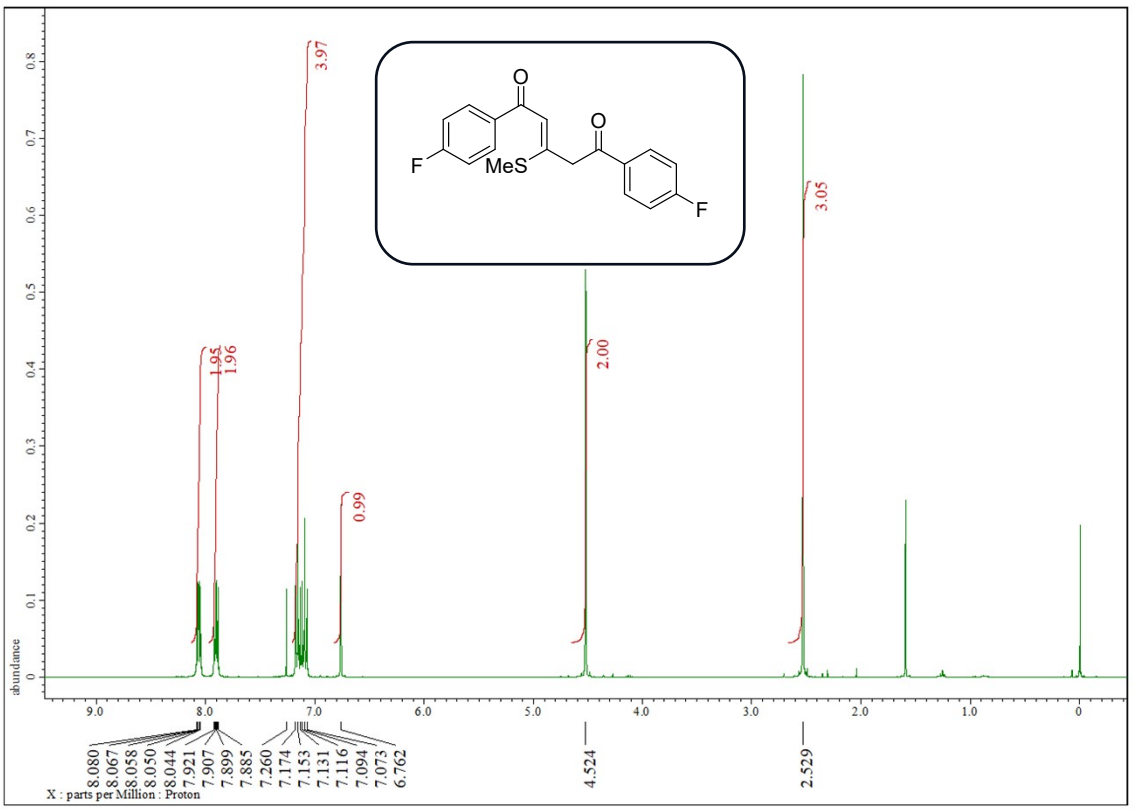


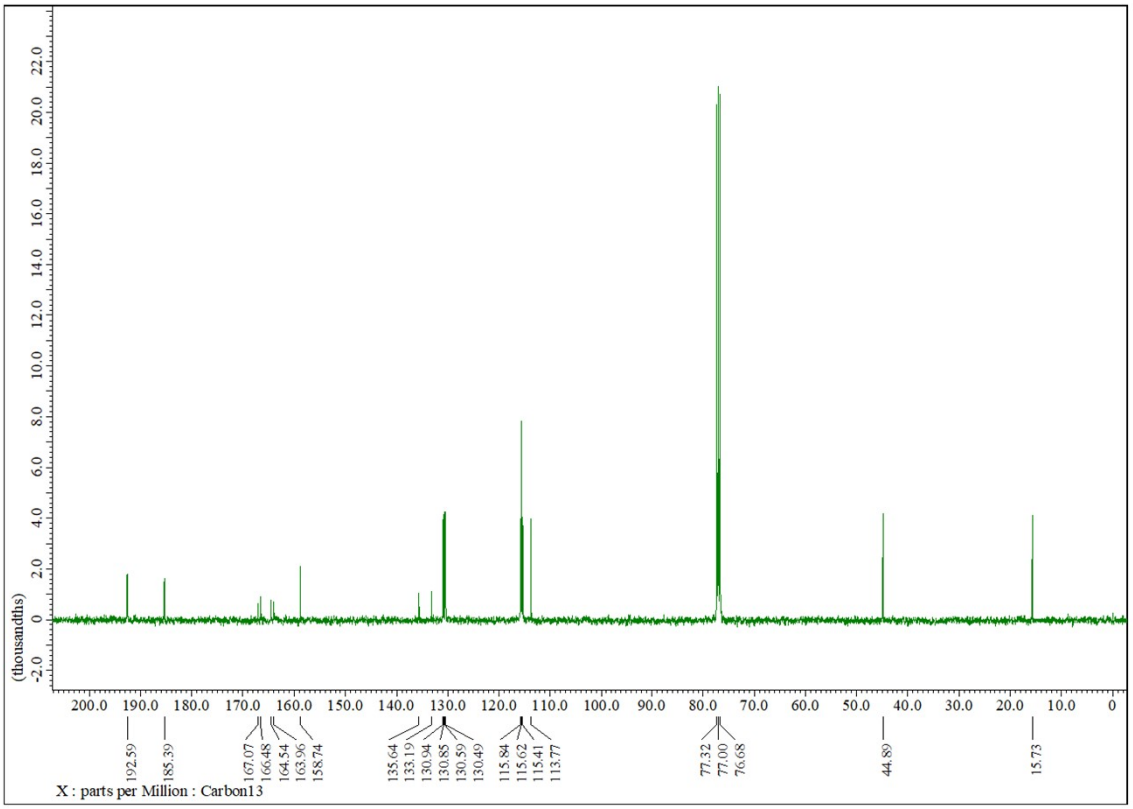
^{1}H NMR and ^{13}C NMR spectra of (Z)-3-(methylthio)-1,5-di-p-tolylpent-2-ene-1,5-dione (1c)





^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-bis(4-flurophenyl)-3-(methylthio)pent-2-ene-1,5-dione (1d)





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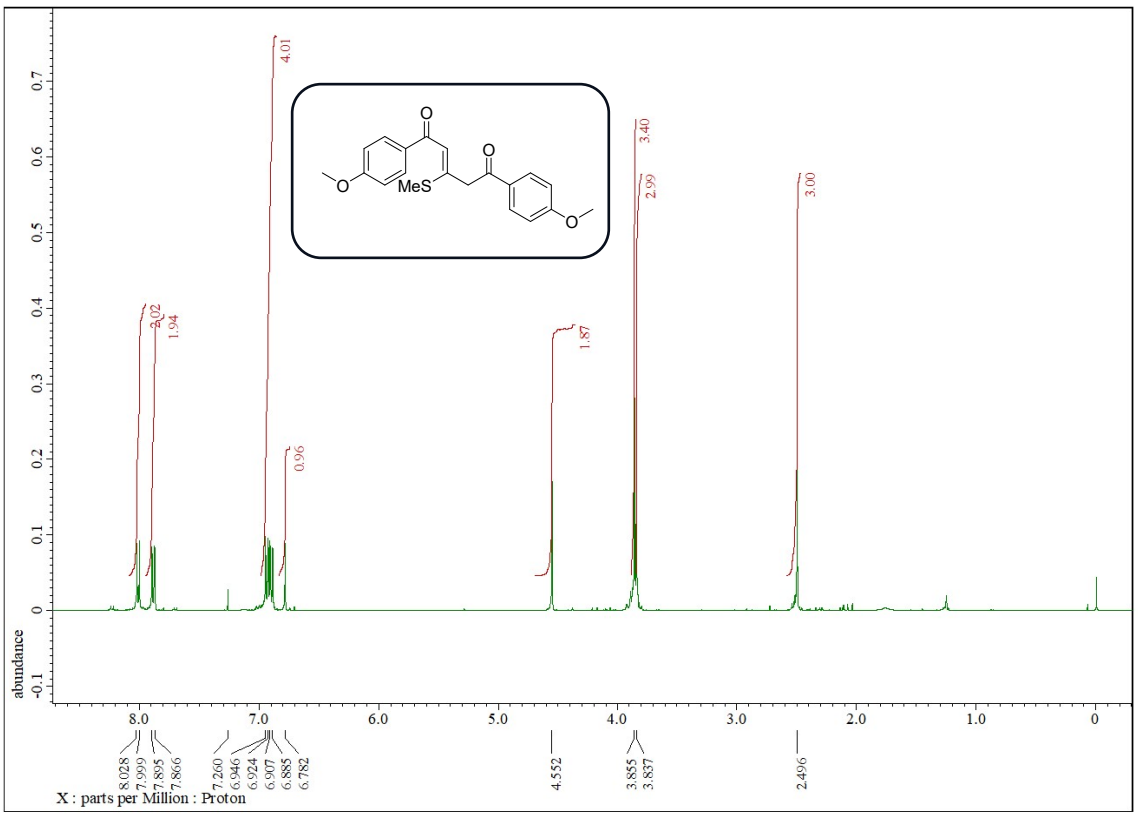
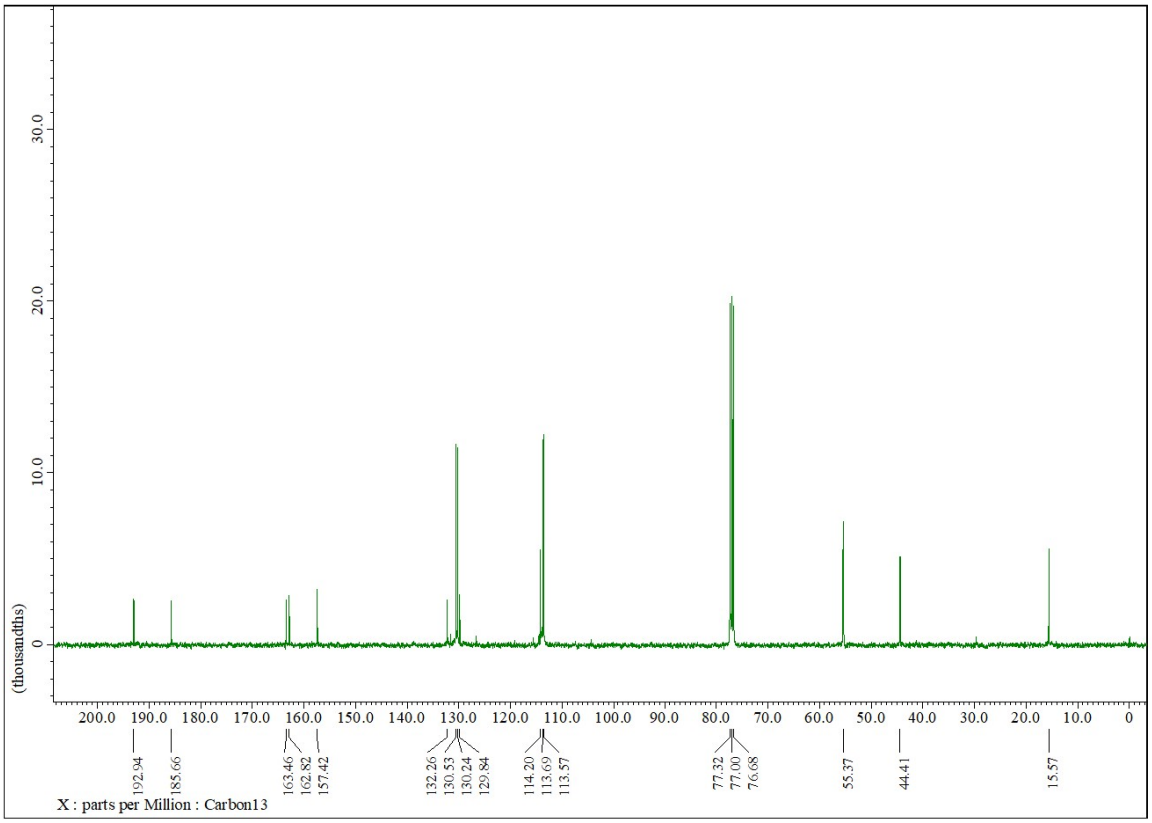
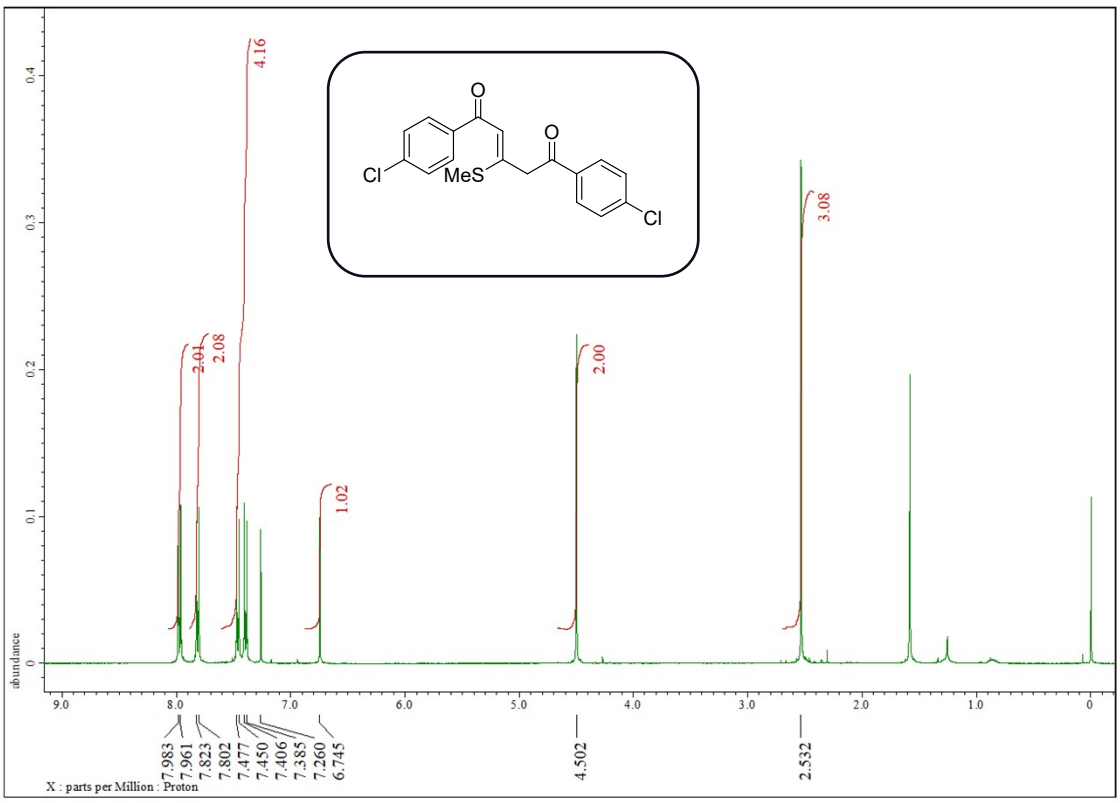
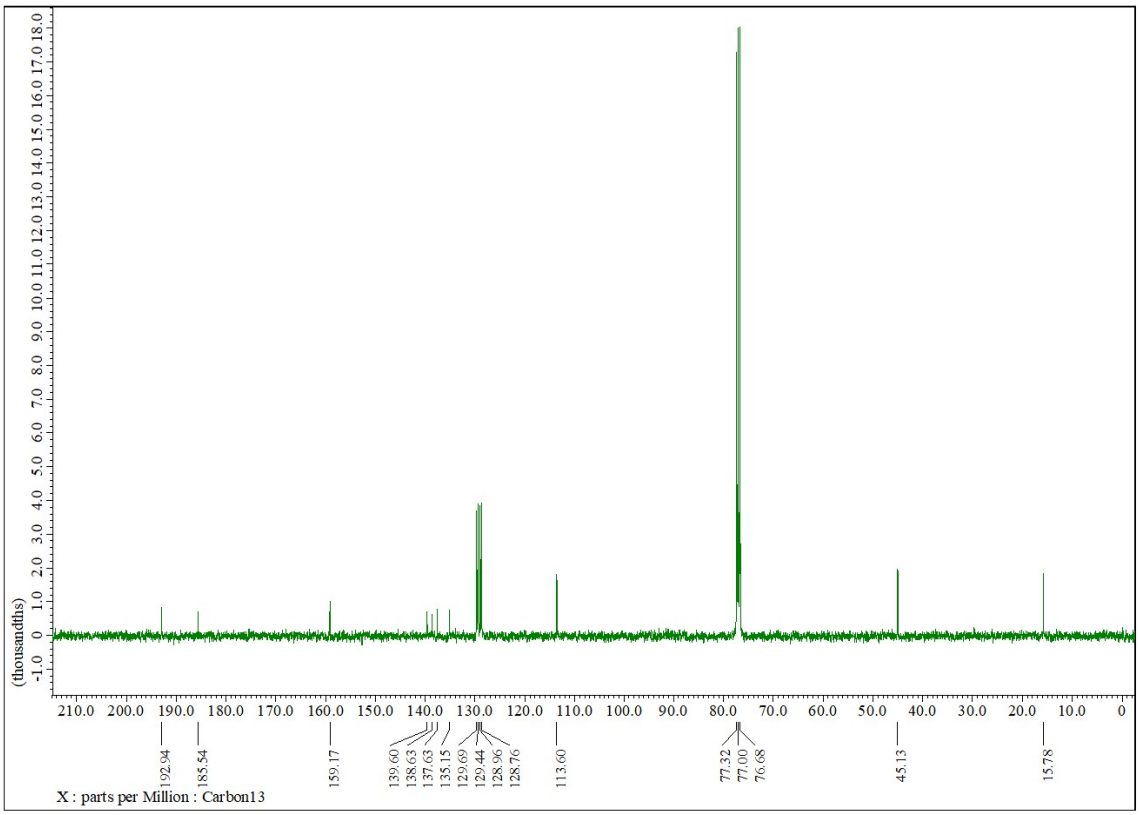


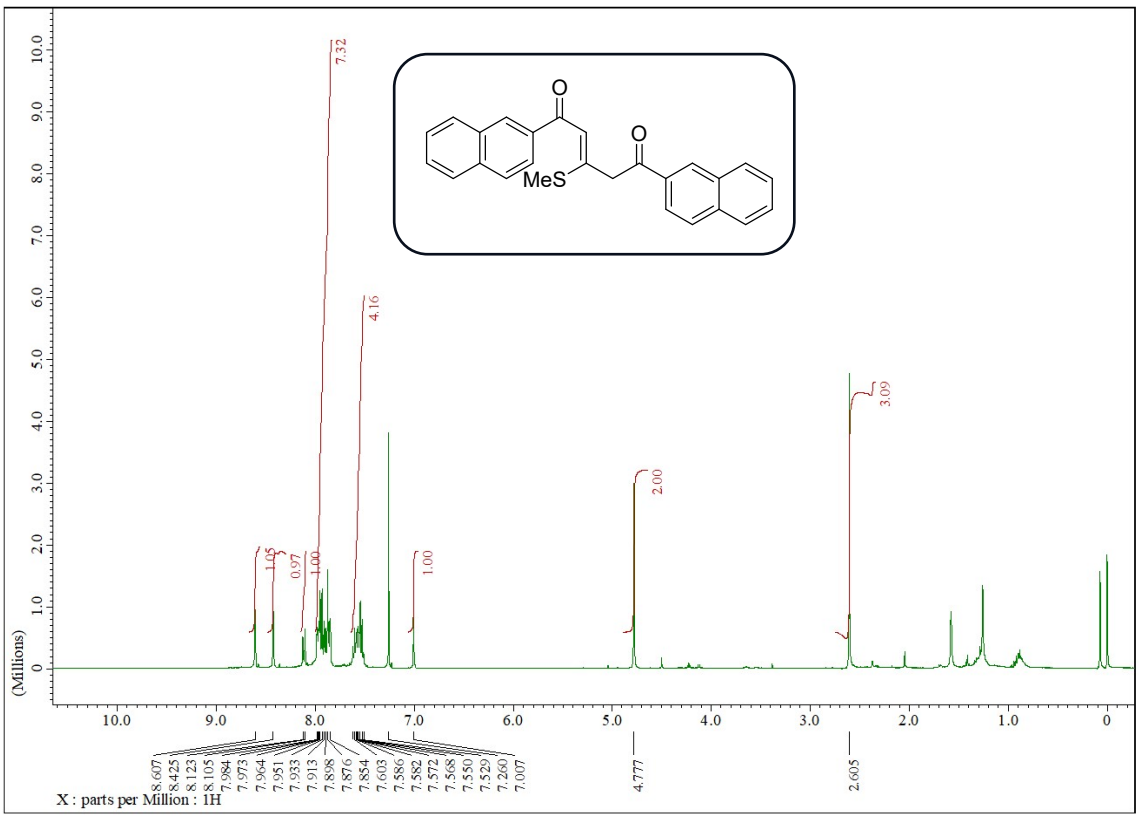


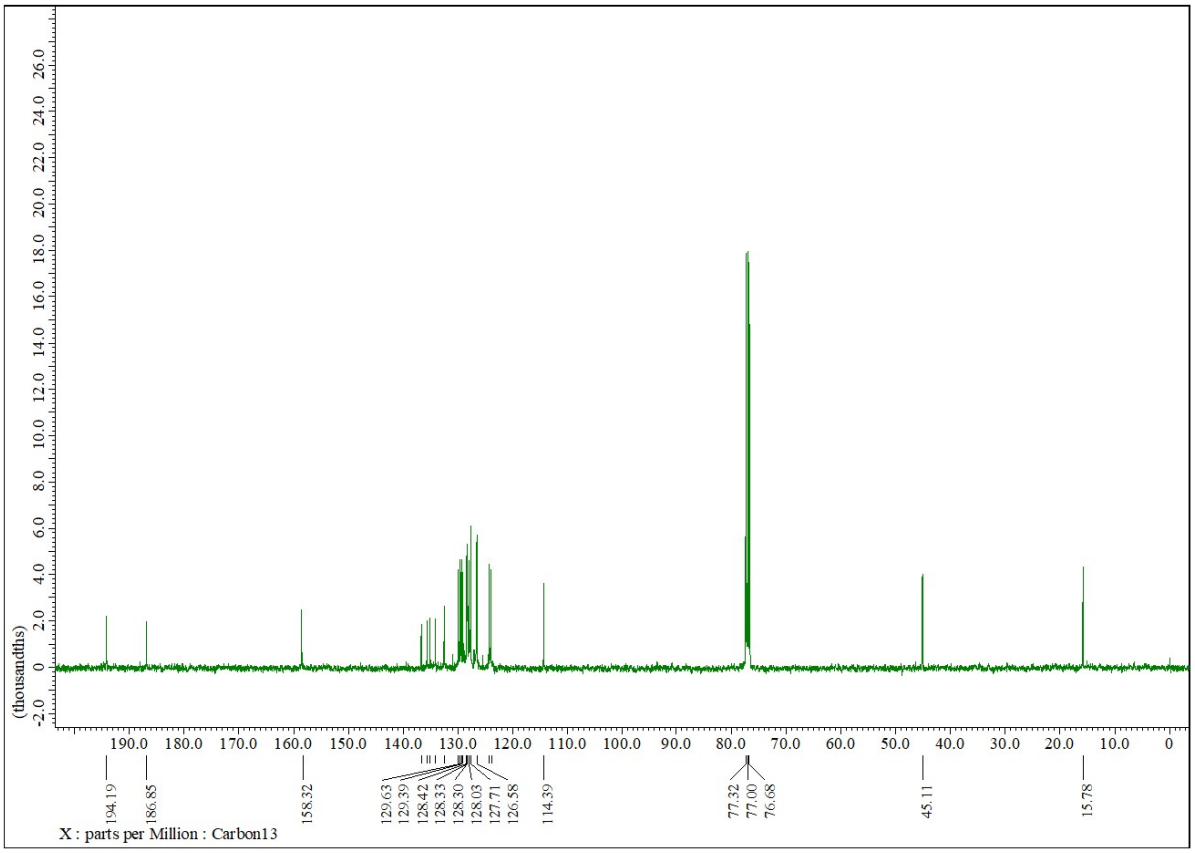
^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-bis(4-chlorophenyl)-3-(methylthio)pent-2-ene-1,5-dione (1f)



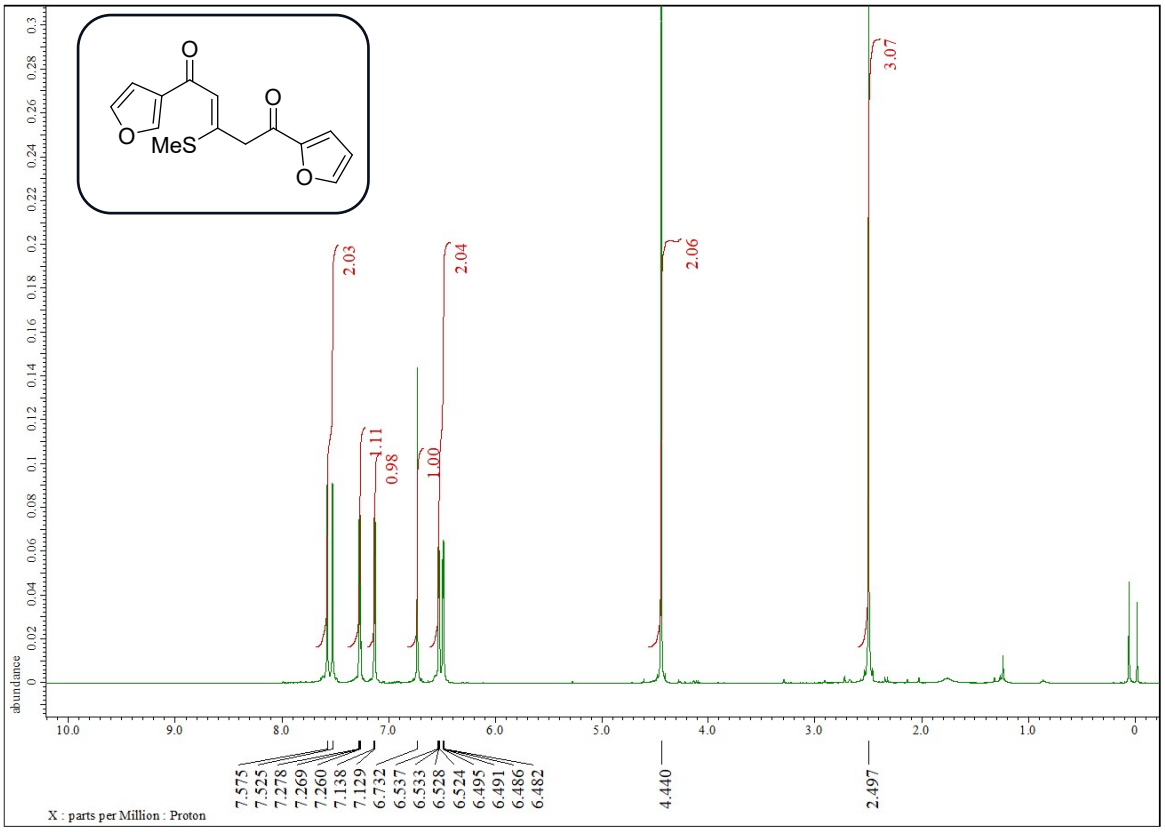


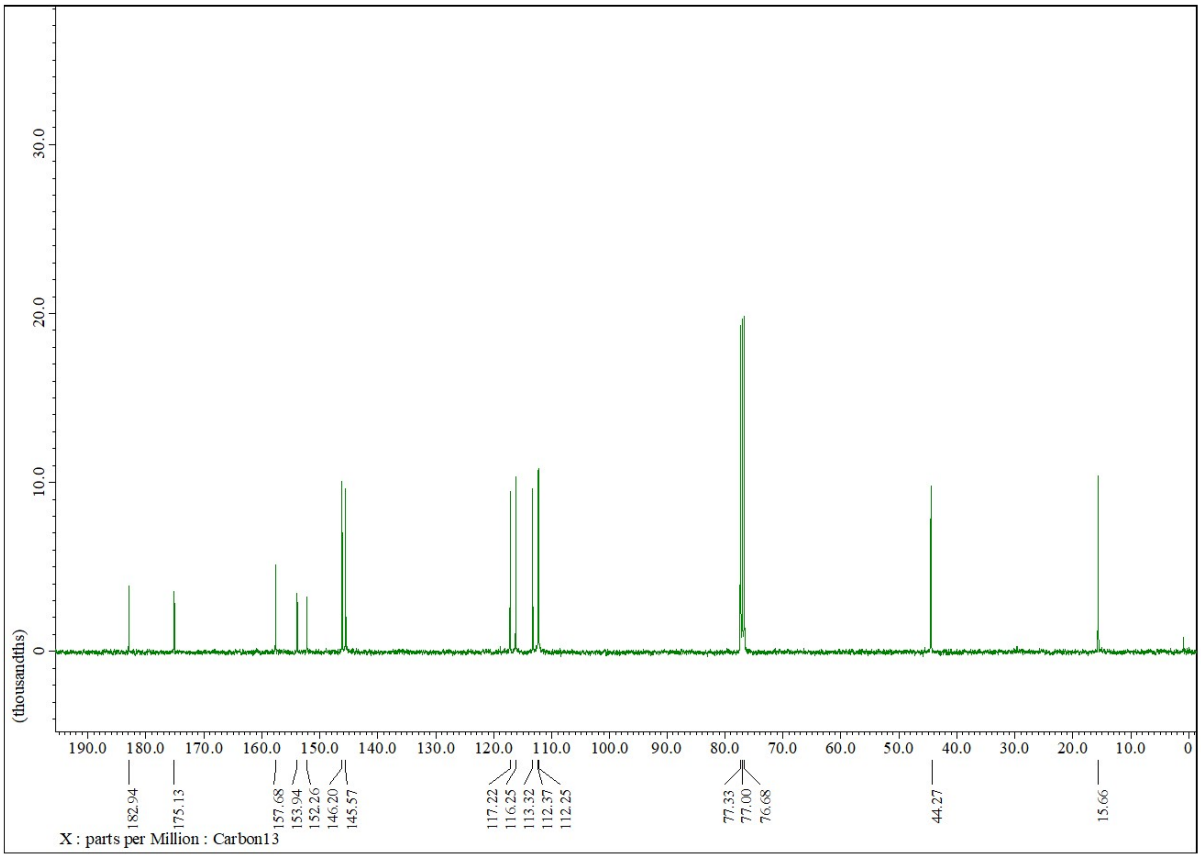
^{1}H NMR and ^{13}C NMR spectra of (Z)-3-(methylthio)-1,5-di(naphthalene-2-yl)-pent-2-ene-1,5-dione (1g)



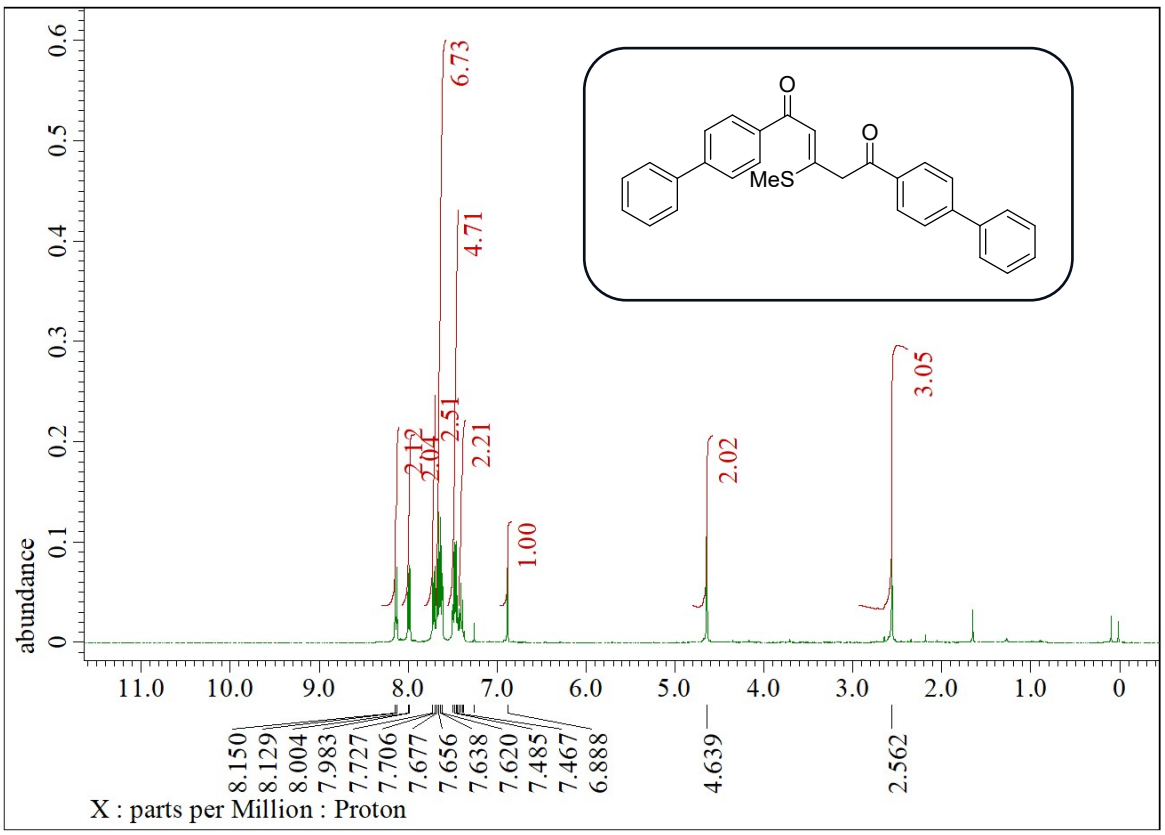


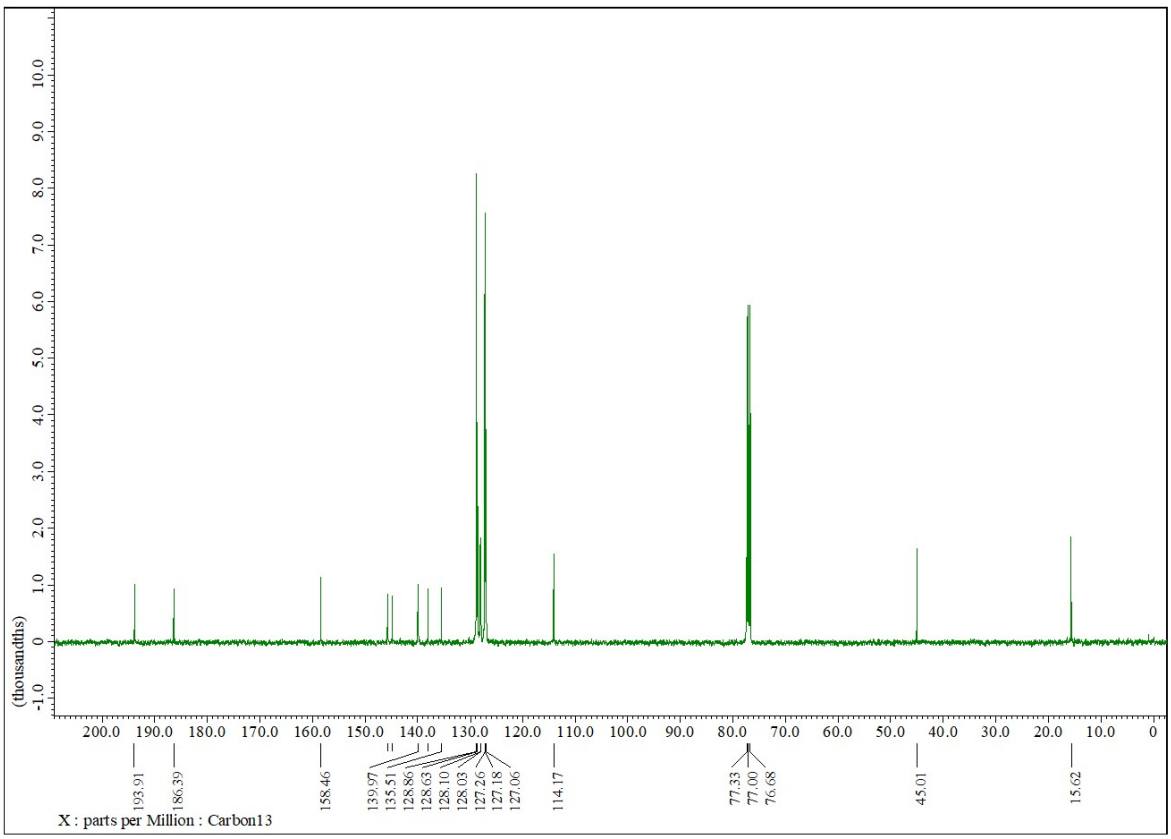
^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-di(furan-3-yl)-3-(methylthio)pent-2-ene-1,5-dione (1h)



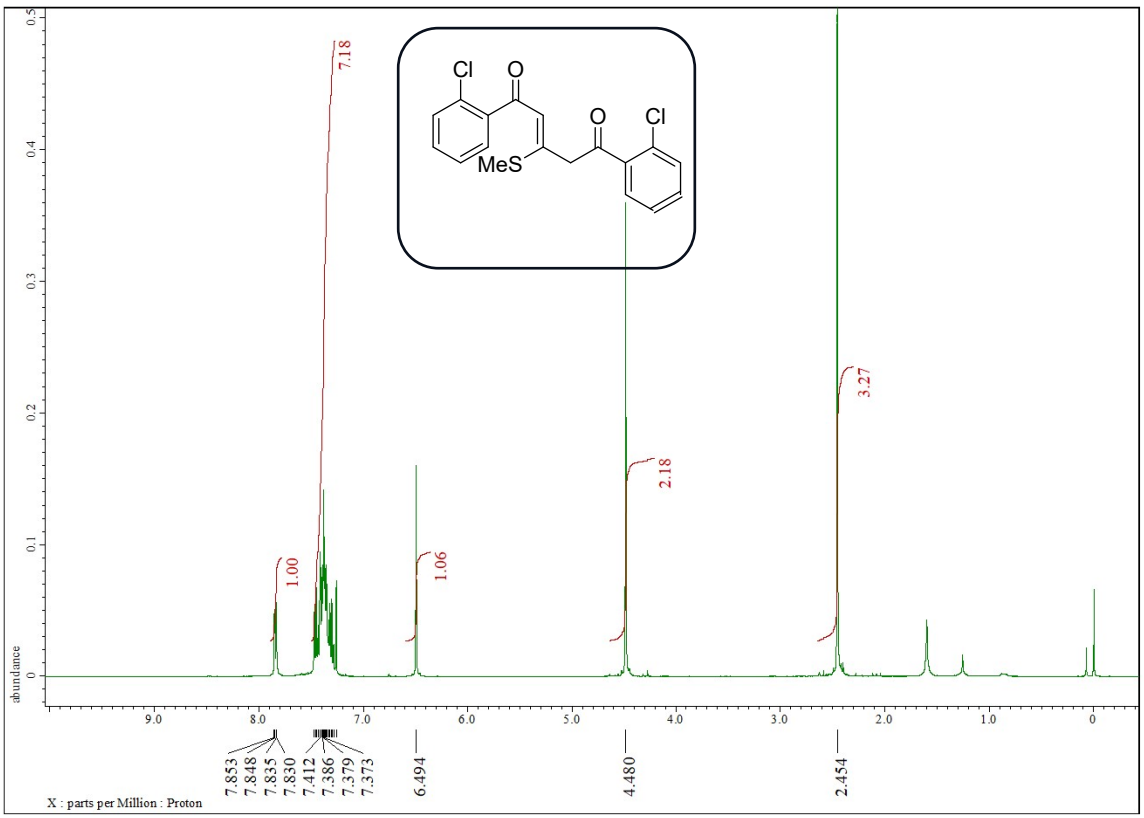


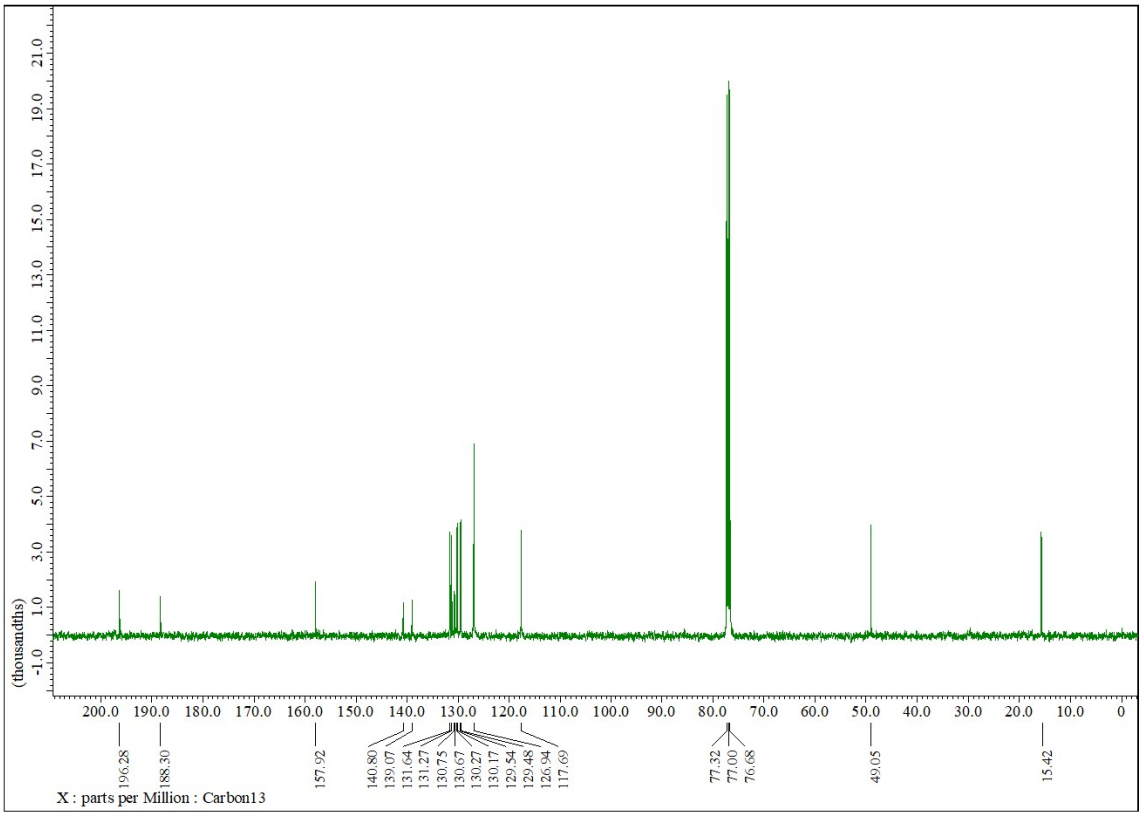
^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-di([1,1'-biphenyl]-4-yl)-3-(methylthio)- pent-2-ene-1,5-dione (1i)



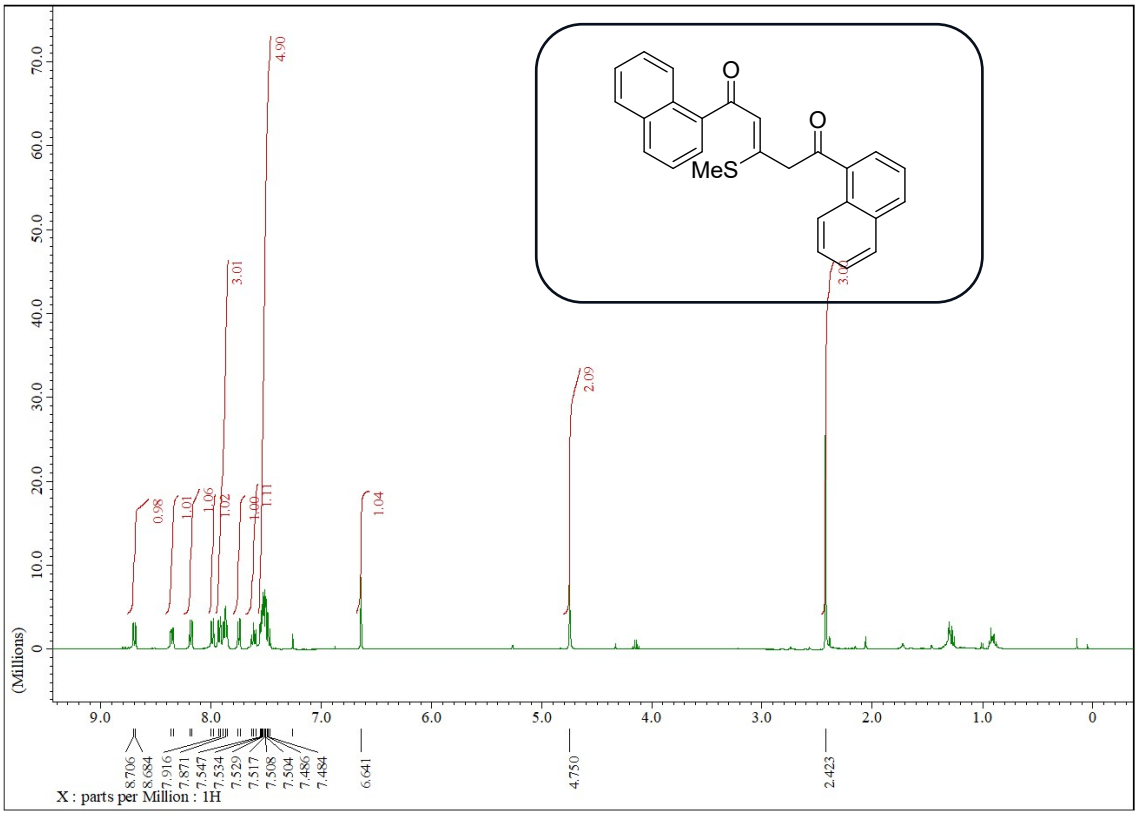


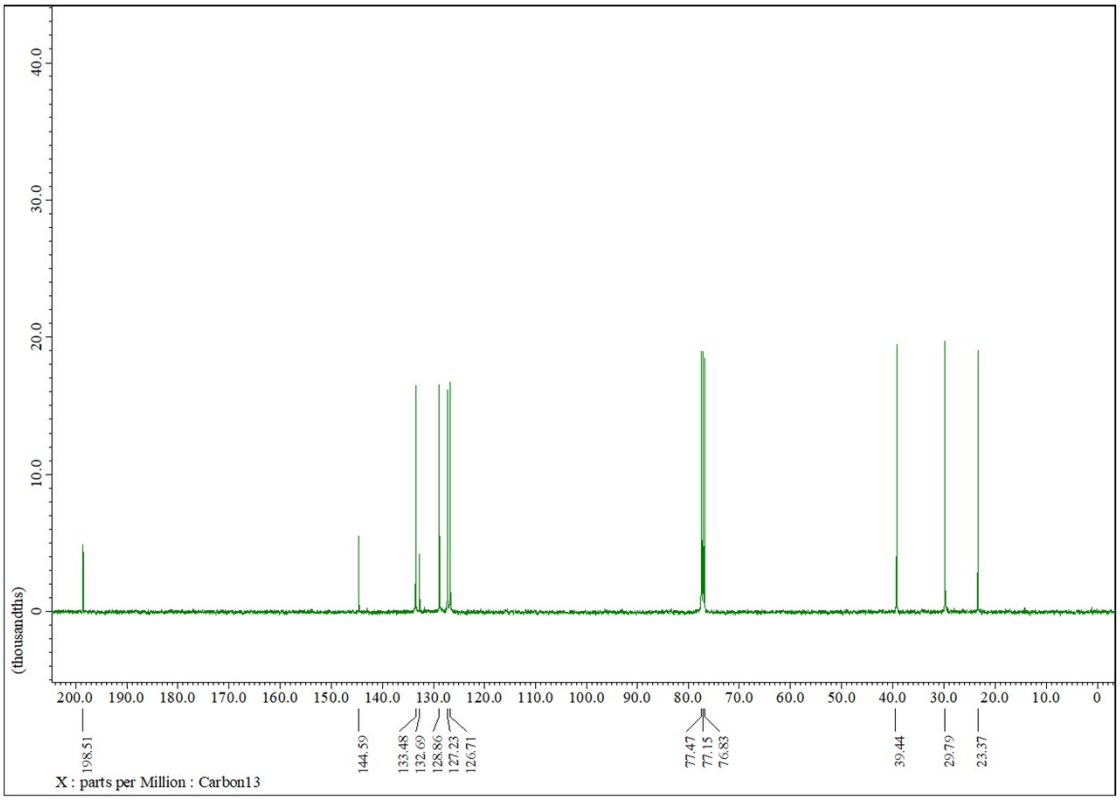
^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-bis(2-chlorophenyl)-3-(methylthio)pent-2-ene-1,5-dione (1j)



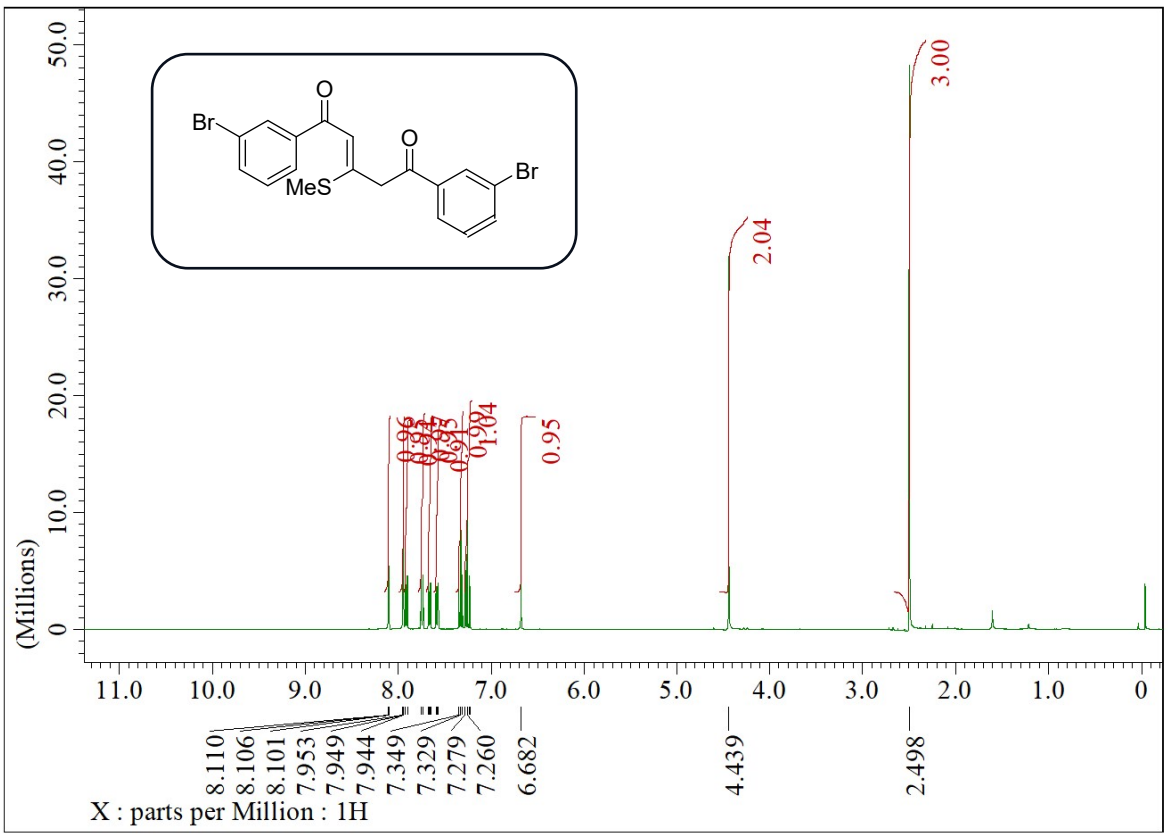


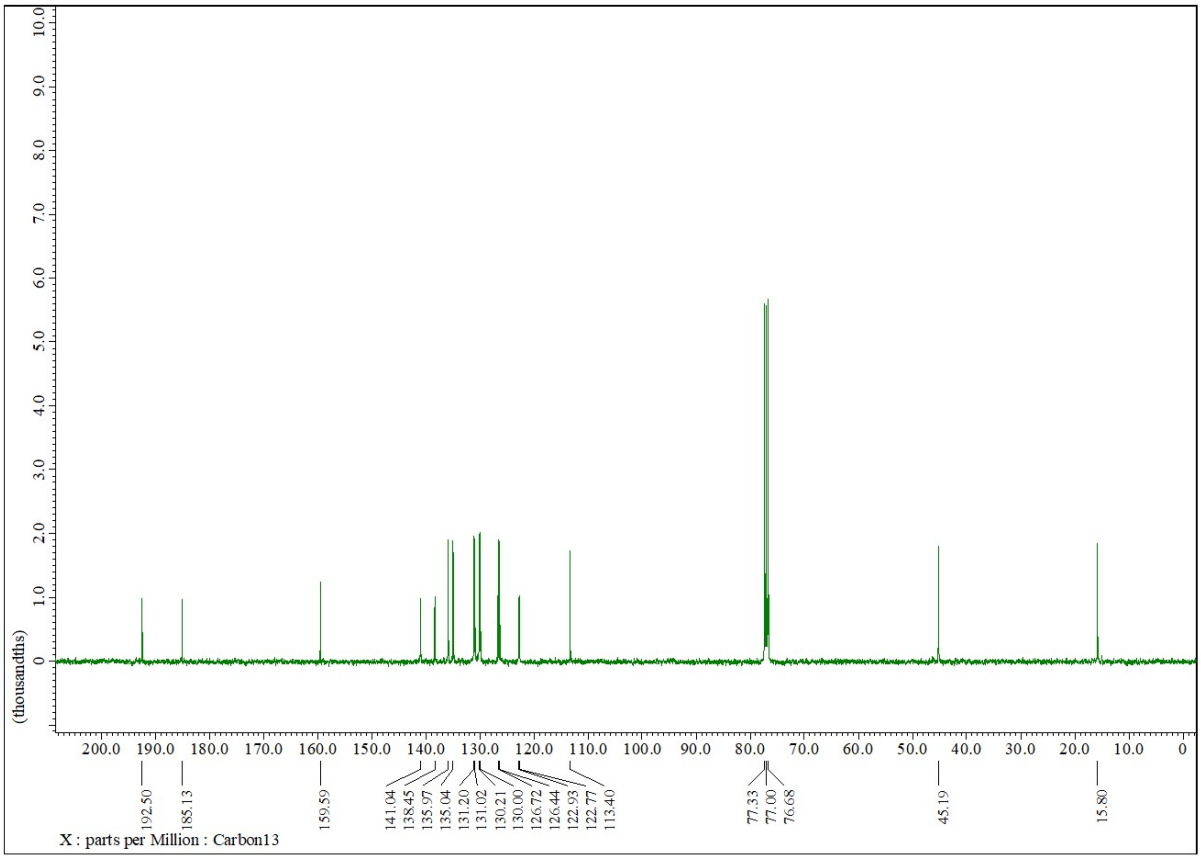
^{1}H NMR and ^{13}C NMR spectra of (Z)-3-(methylthio)-1,5-di(naphthalene-1-yl)-pent-2-ene-1,5-dione (1k)



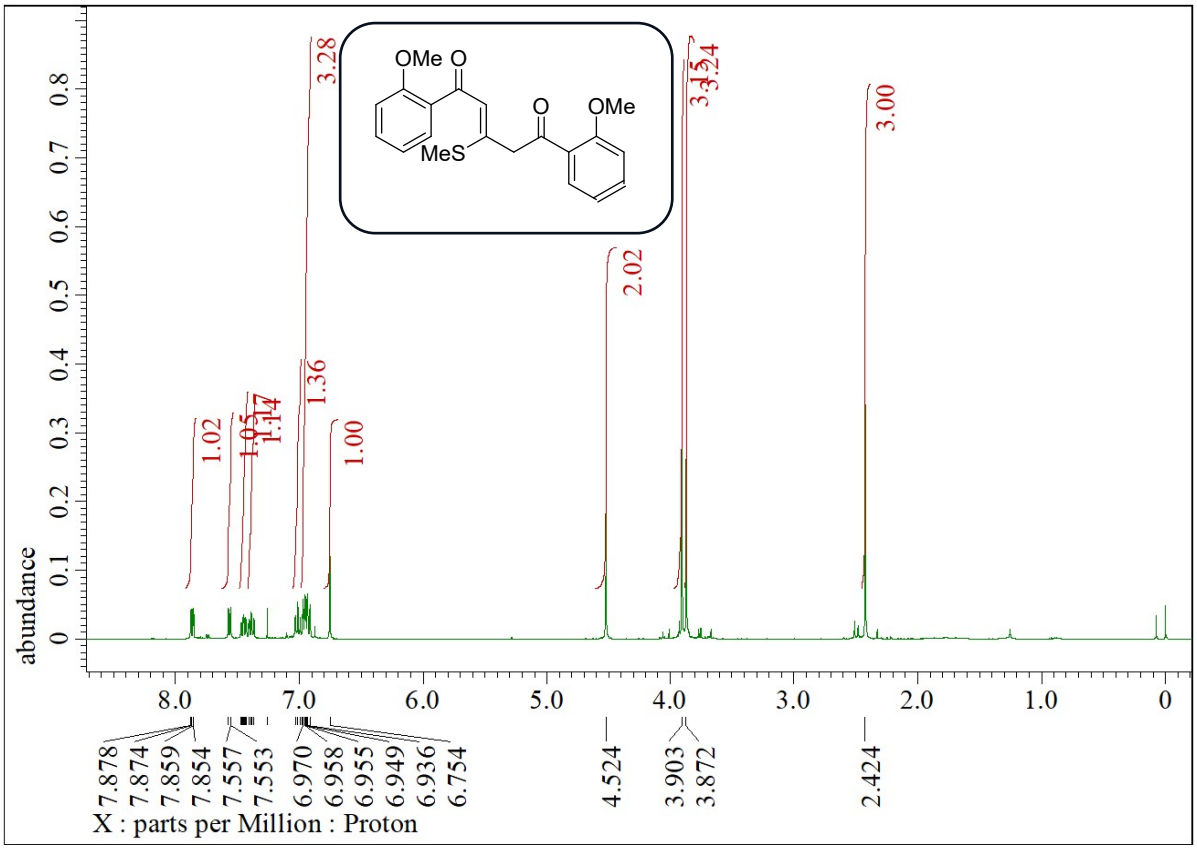


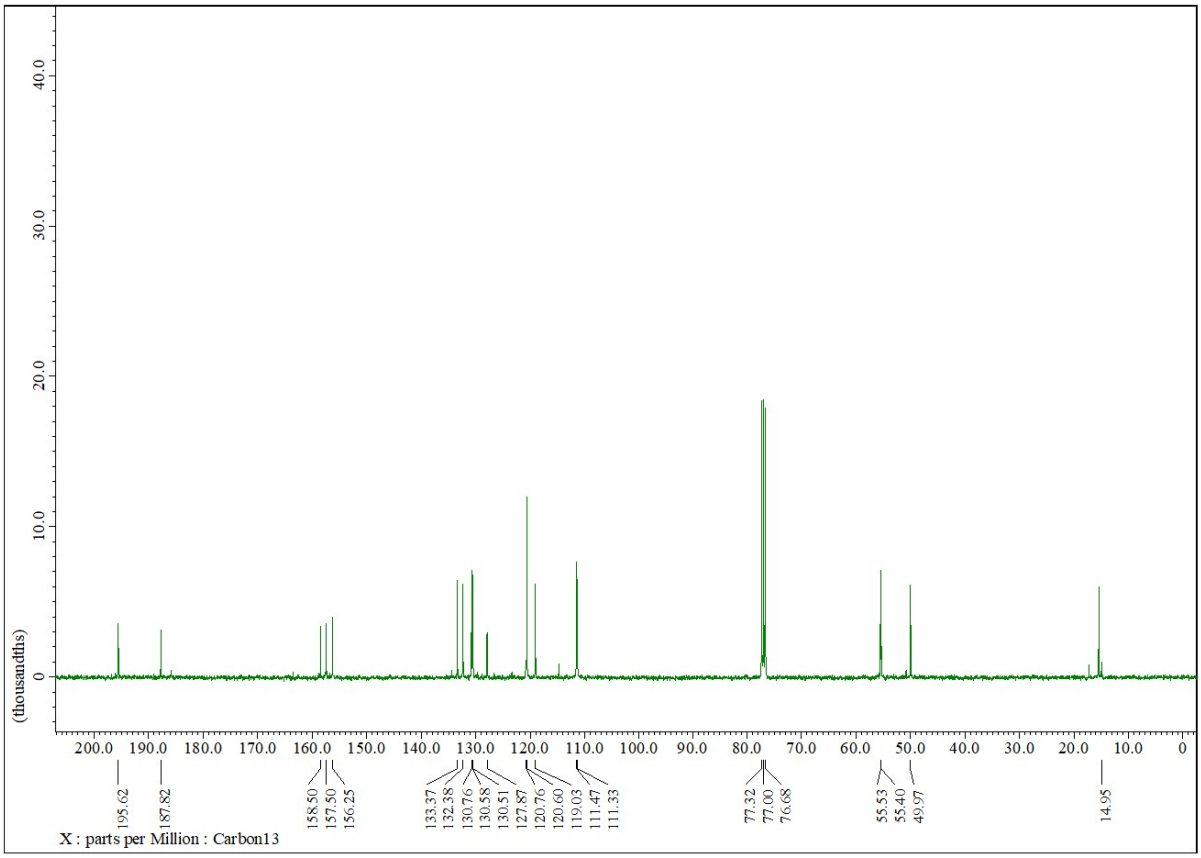
^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-bis(3-bromophenyl)-3-(methylthio)pent-2-ene-1,5-dione (1l)





^{1}H NMR and ^{13}C NMR spectra of (Z)-1,5-bis(2-methoxyphenyl)-3-(methylthio)pent-2-ene-1,5-dione (1m)





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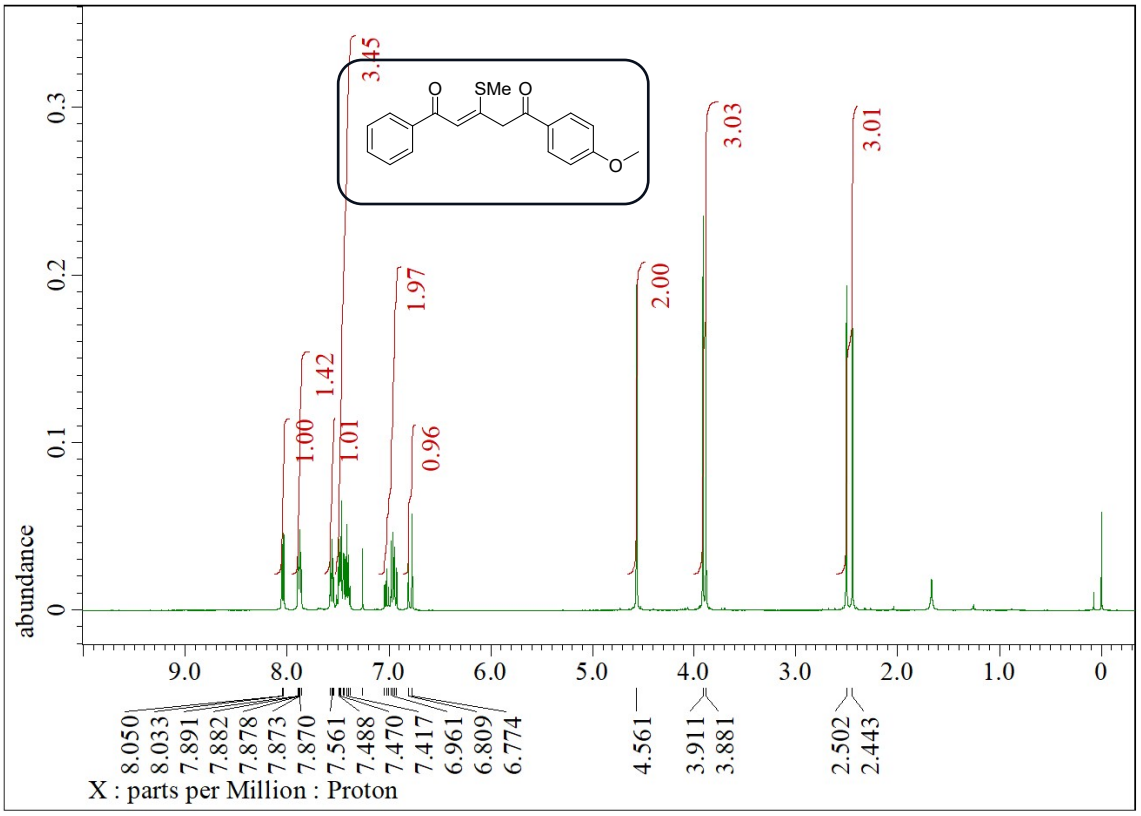
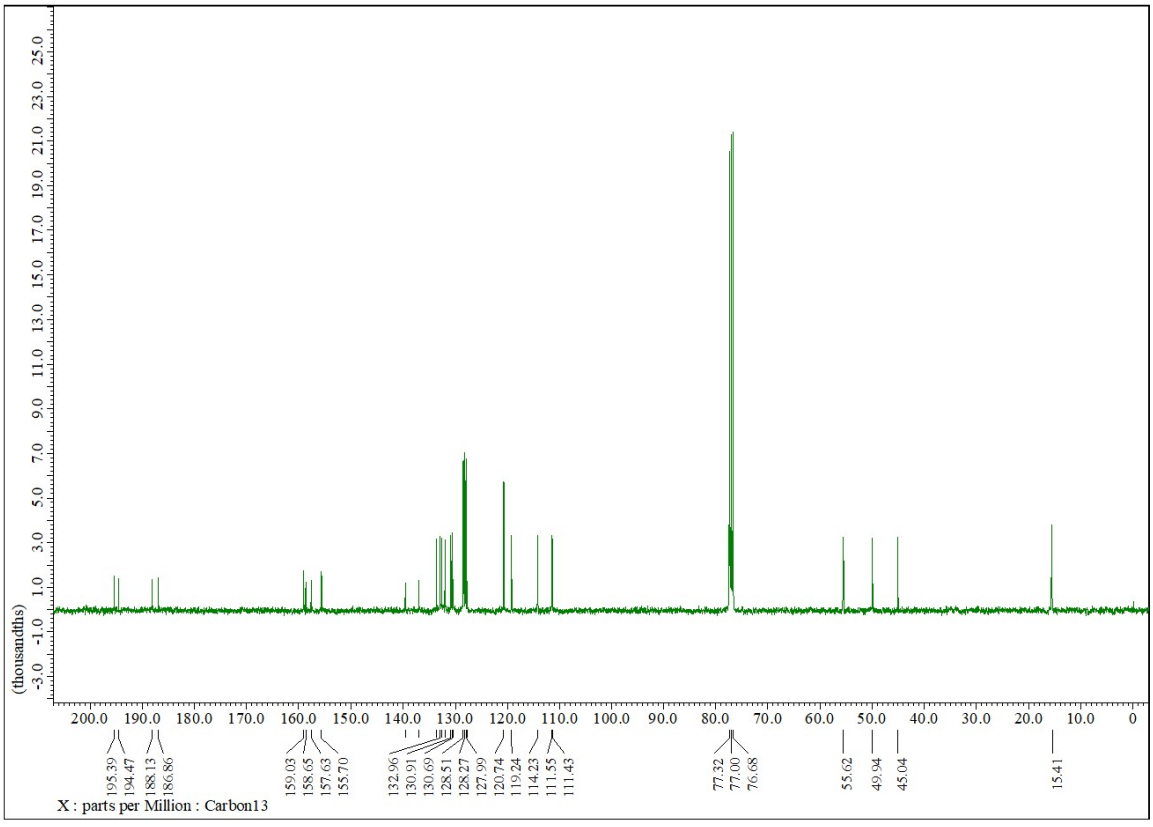
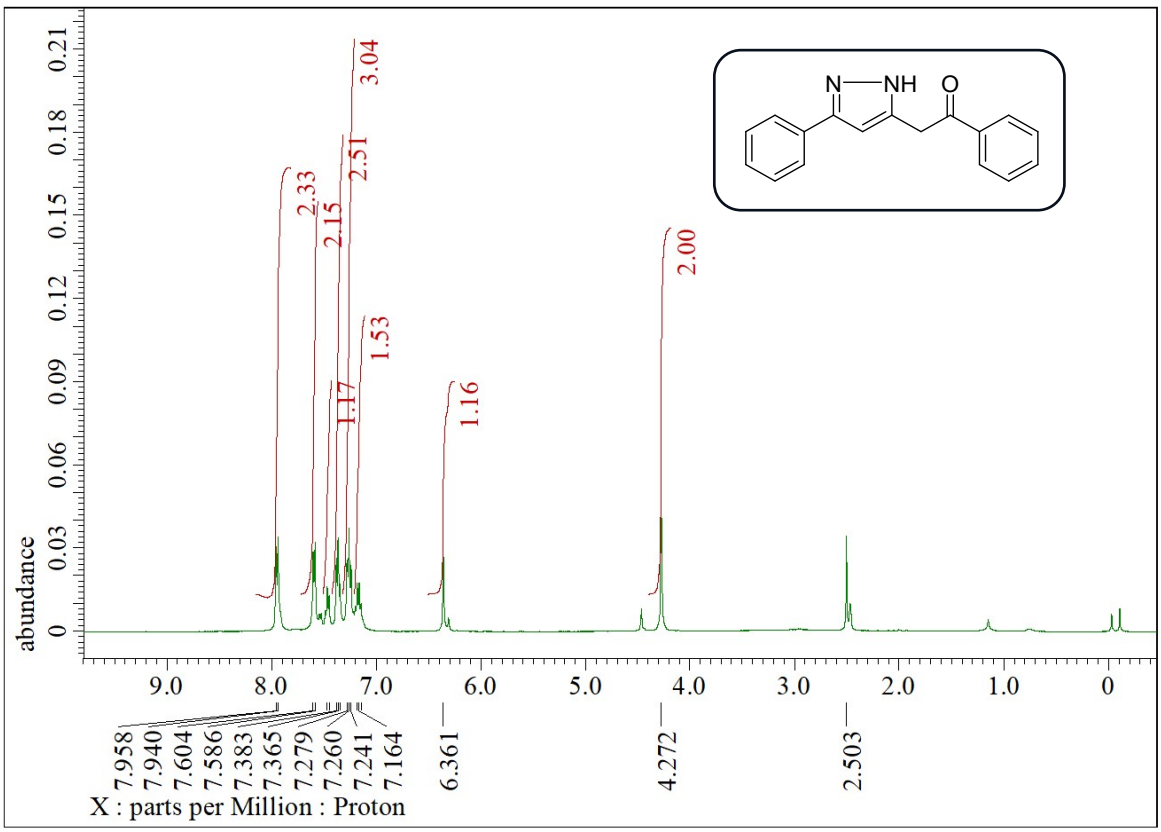
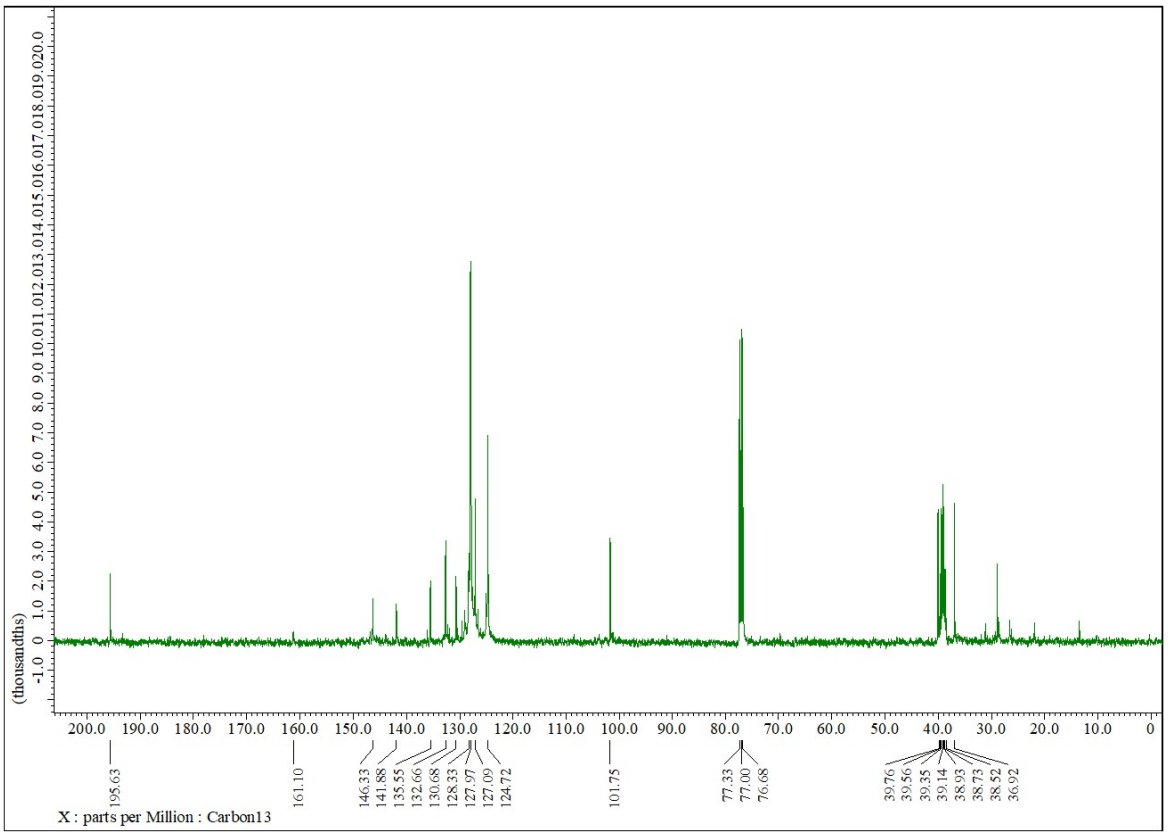


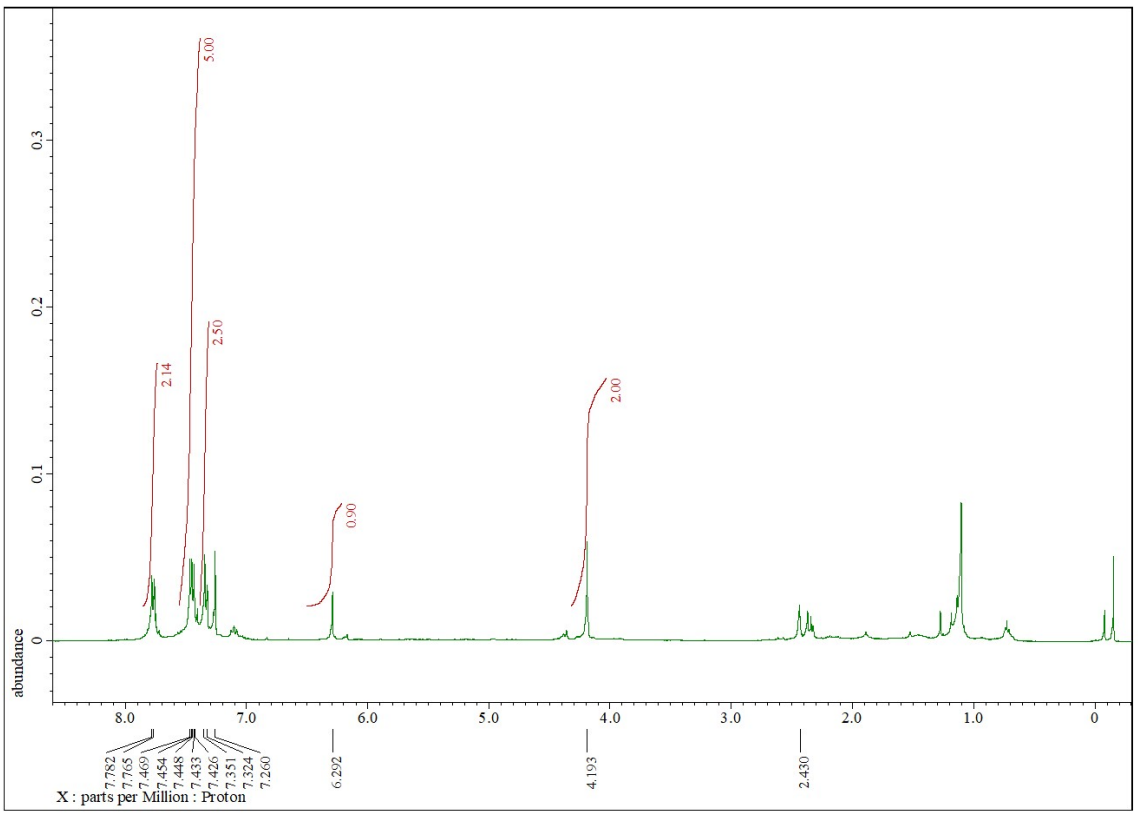


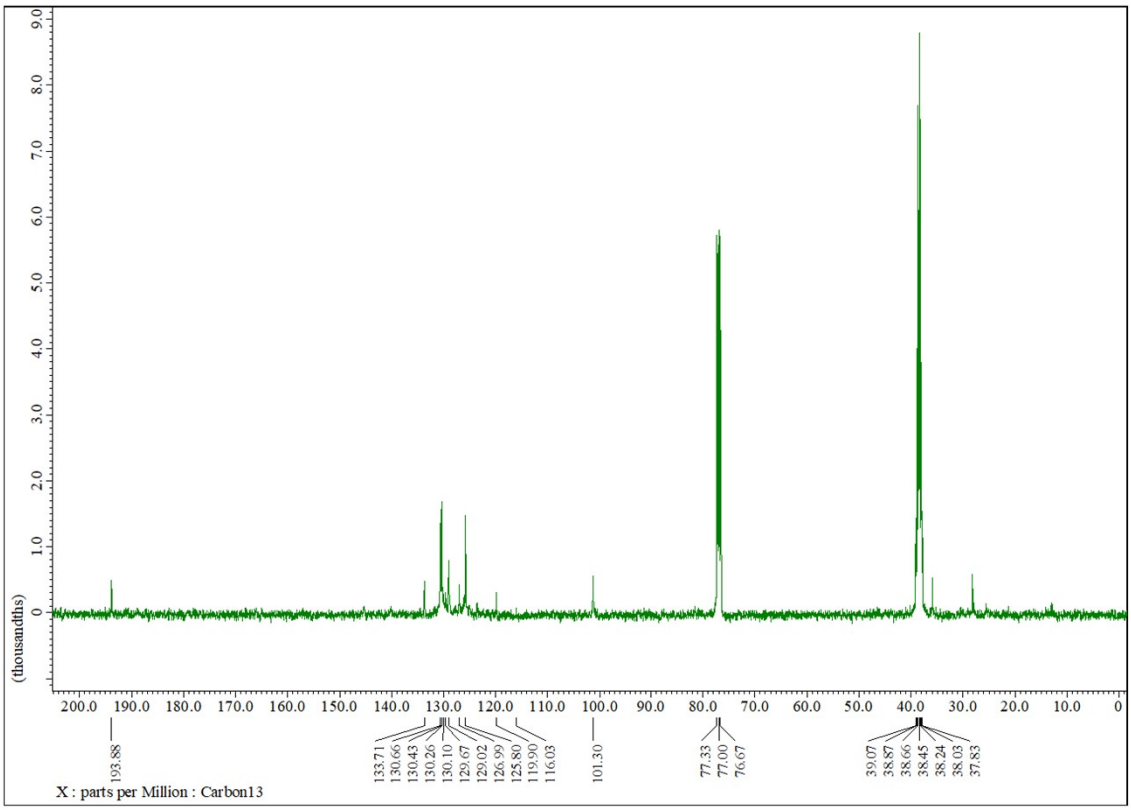
^{1}H NMR and ^{13}C NMR spectra of 1-(phenyl)-2-(3-(phenyl-1*H*-pyrazol-5-yl) ethan-1-one (2a)



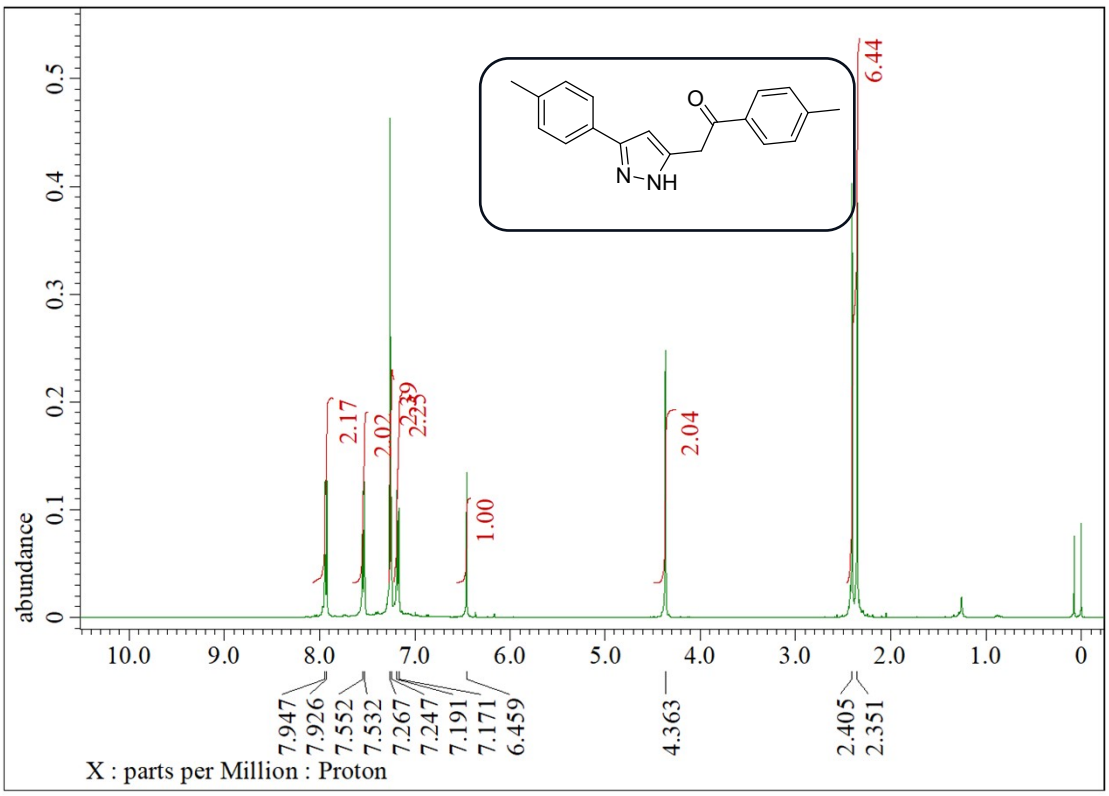


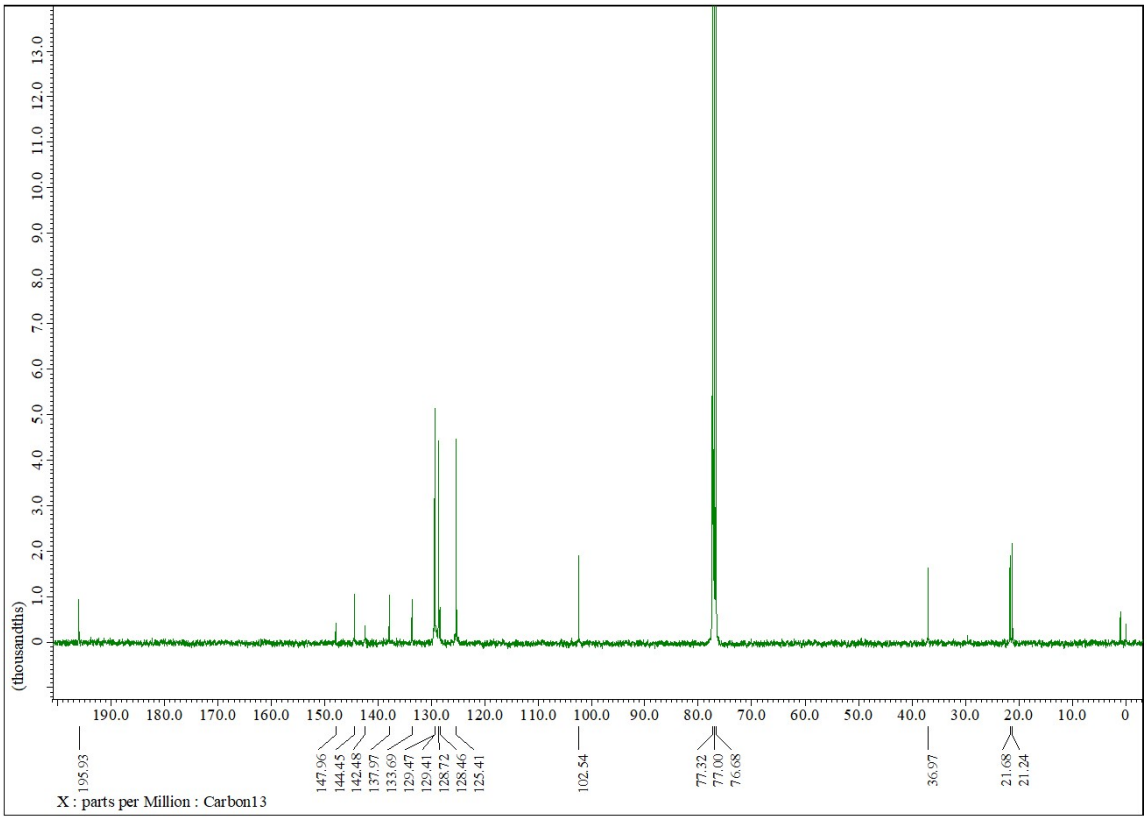
^{1}H NMR and ^{13}C NMR spectra of 1-(4-bromophenyl)-2-(3-4-bromophenyl)-1*H*-pyrazol-5-yl) ethan-1-one (2b)



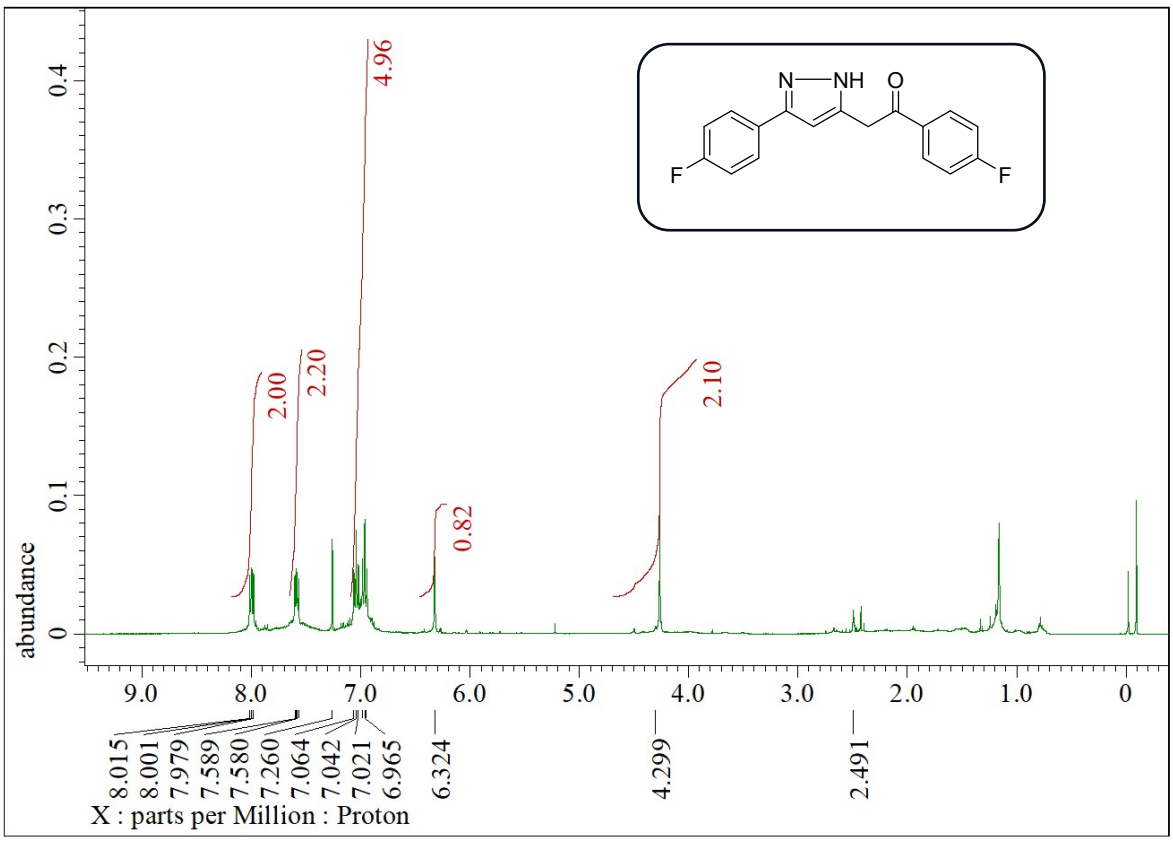


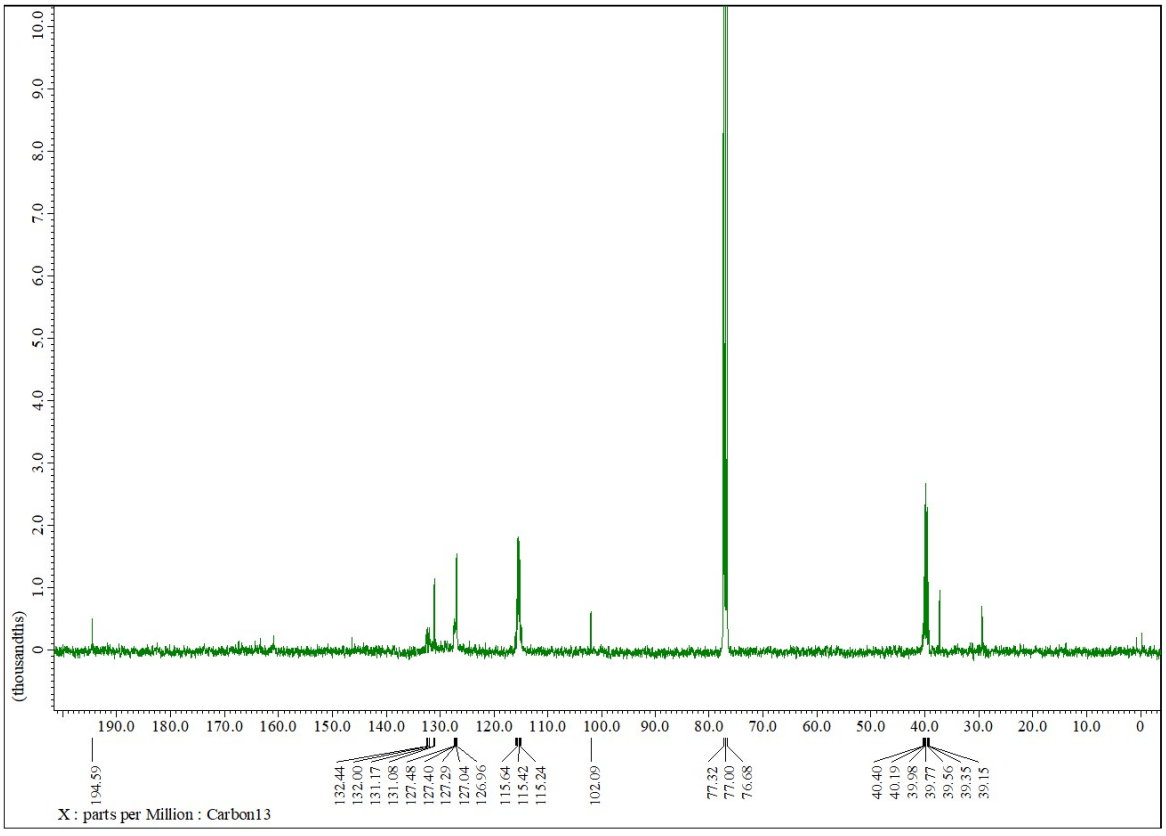
^{1}H NMR and ^{13}C NMR spectra of 1-(*p*-tolyl)-2-(3-(*p*-tolyl)-1*H*-pyrazol-5-yl) ethan-1-one (2c)



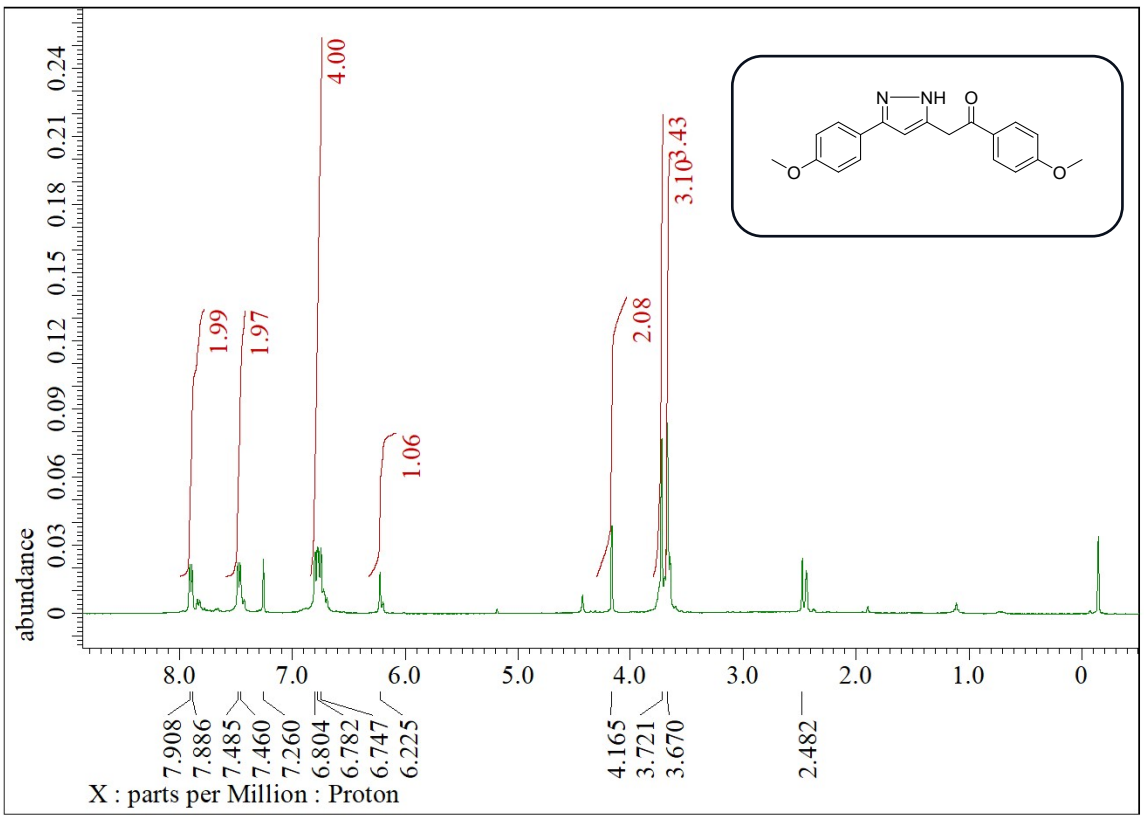


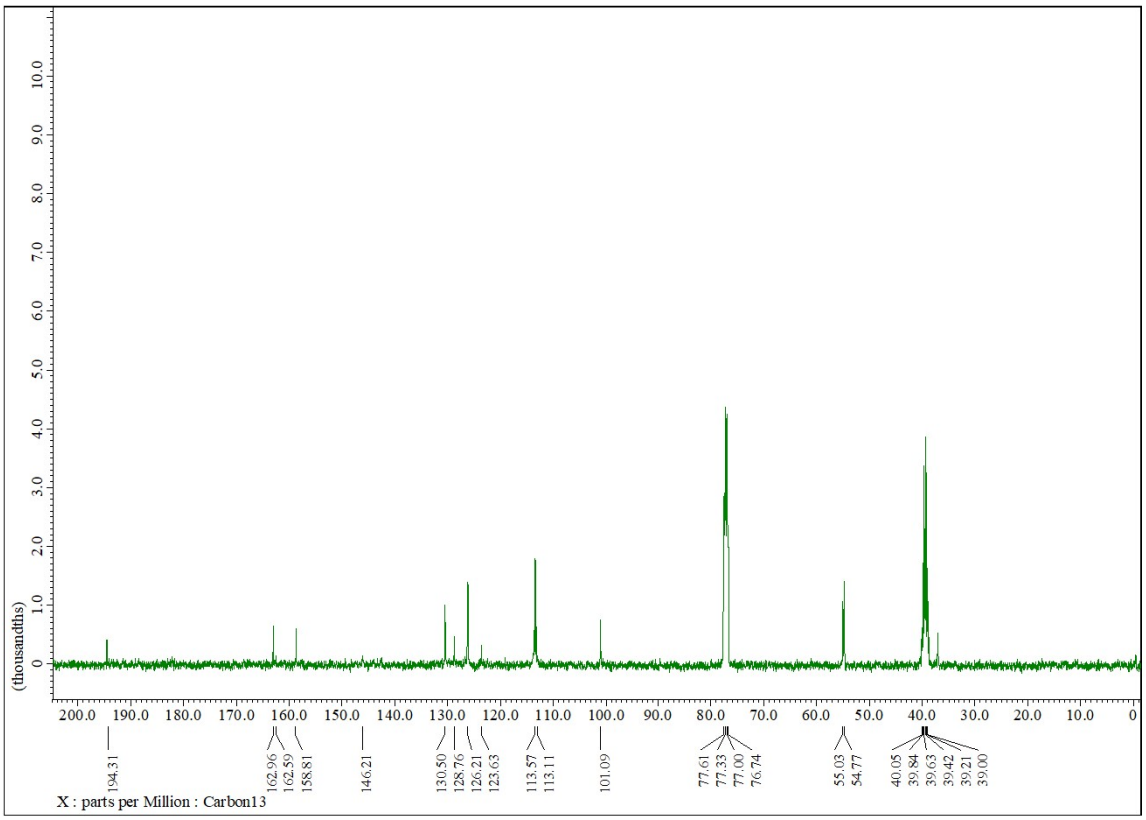
^{1}H NMR and ^{13}C NMR spectra of 1-(4-flurophenyl)-2-(3-4-flurophenyl)-1*H*-pyrazol-5-yl) ethan-1-one (2d)



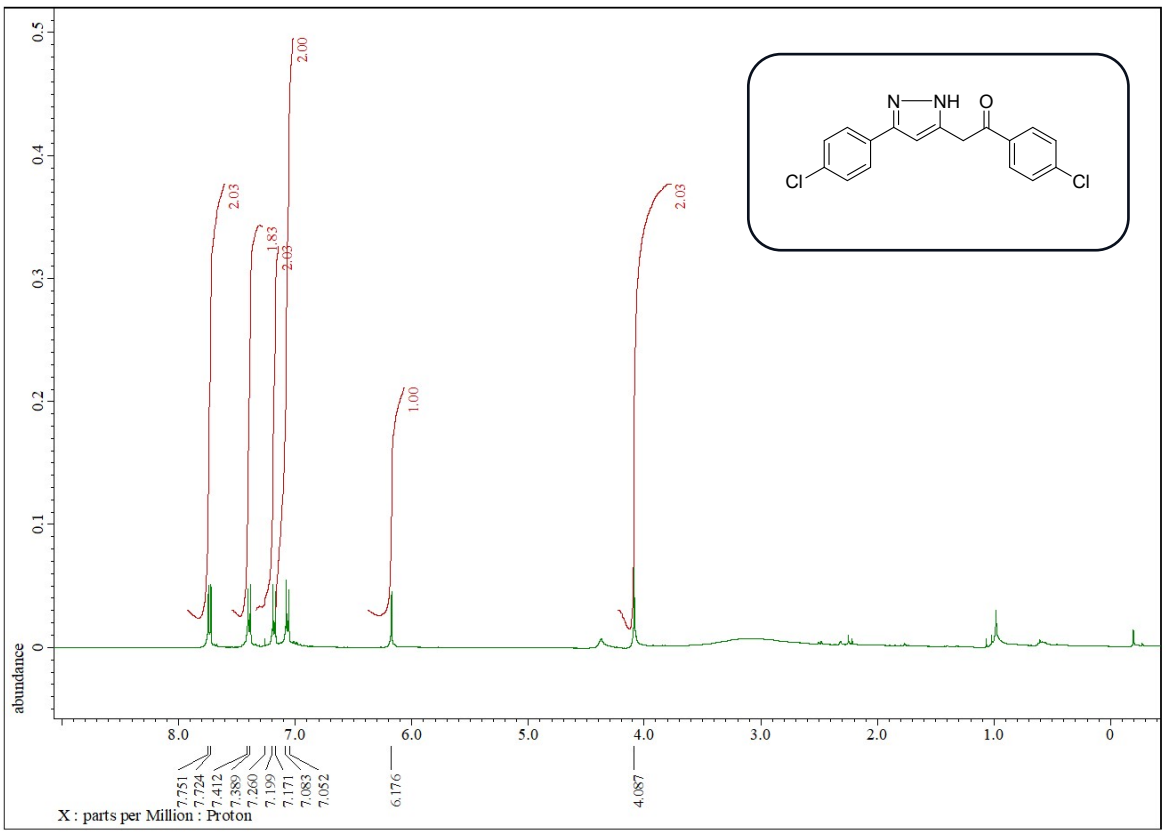


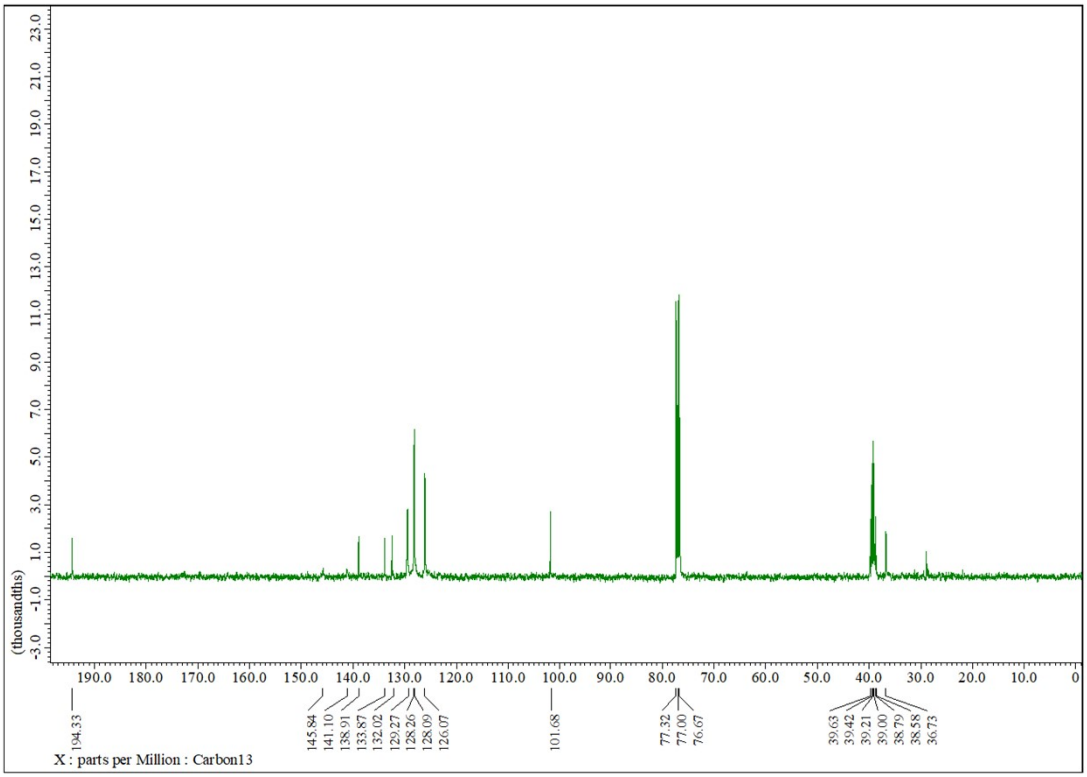
^{1}H NMR and ^{13}C NMR spectra of 1-(4-methoxyhenyl)-2-(3-4-methoxyphenyl)-1*H*-pyrazol-5-yl) ethan-1-one (2e)



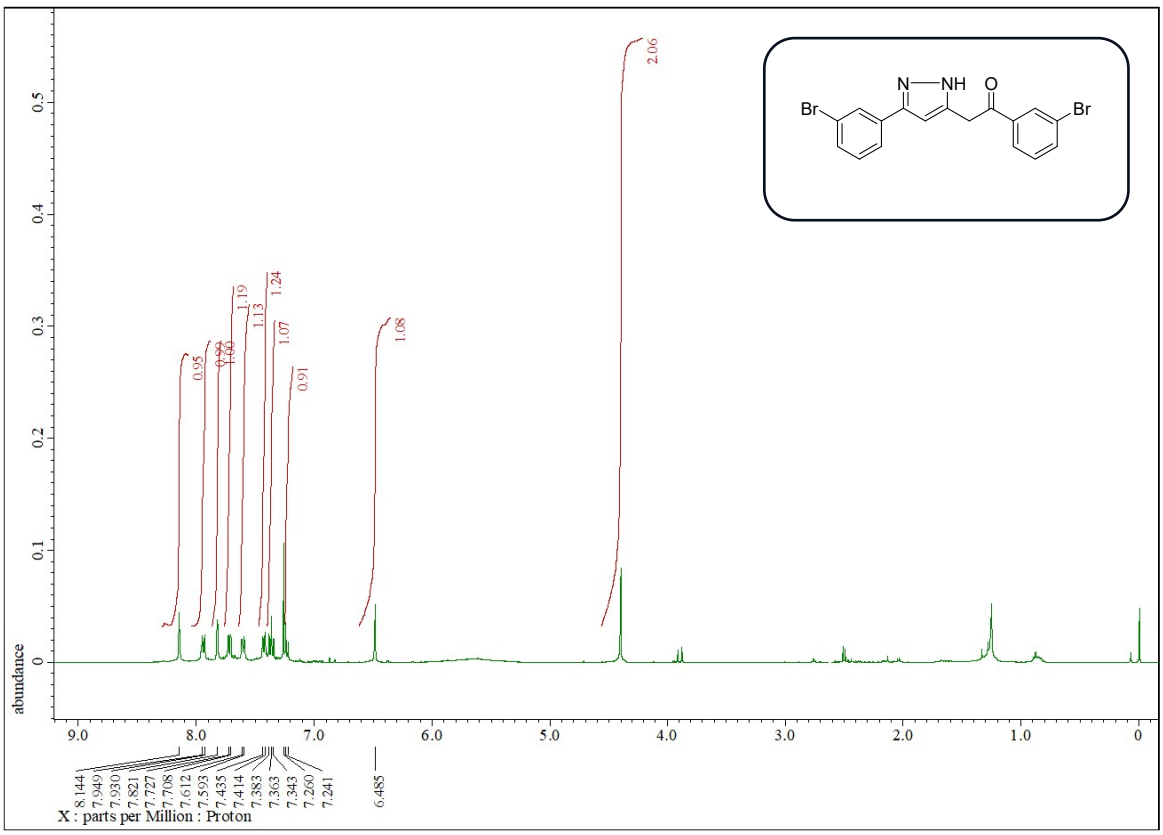


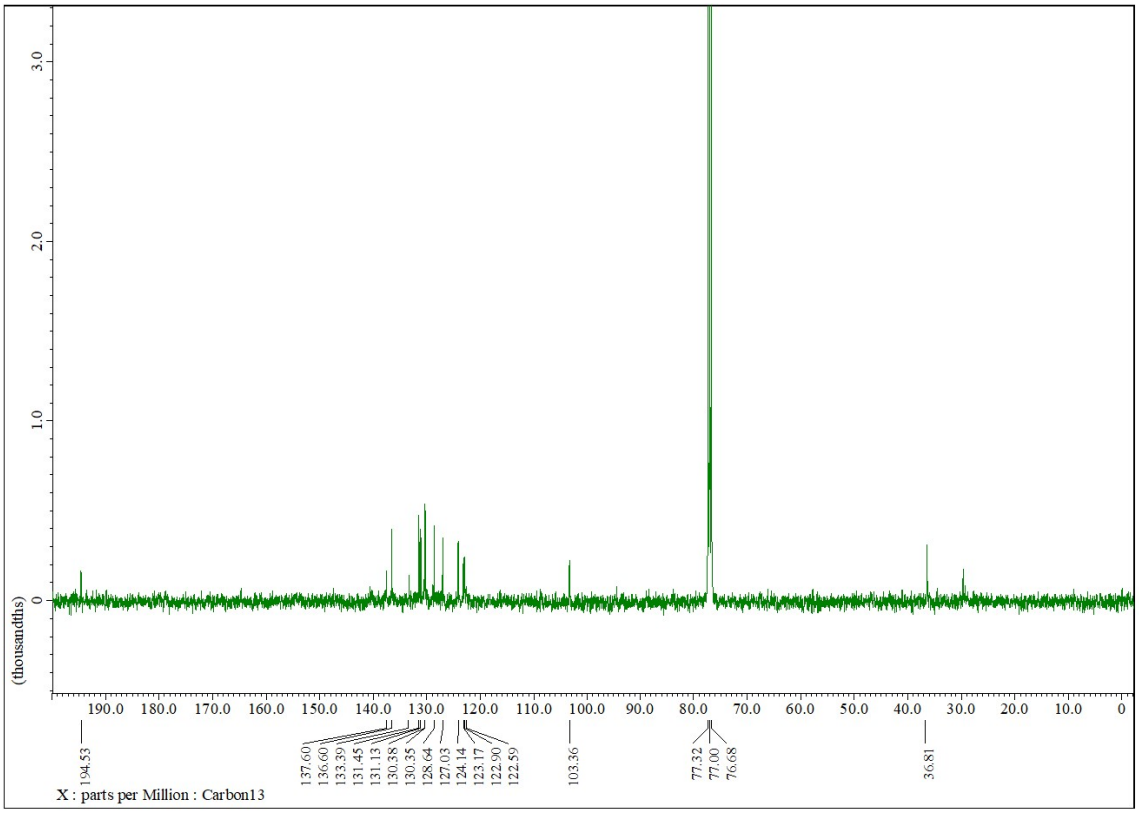
^{1}H NMR and ^{13}C NMR spectra of 1-(4-chlorohenyl)-2-(3-4-chlorophenyl)-1*H*-pyrazol-5-yl) ethan-1-one (2f)



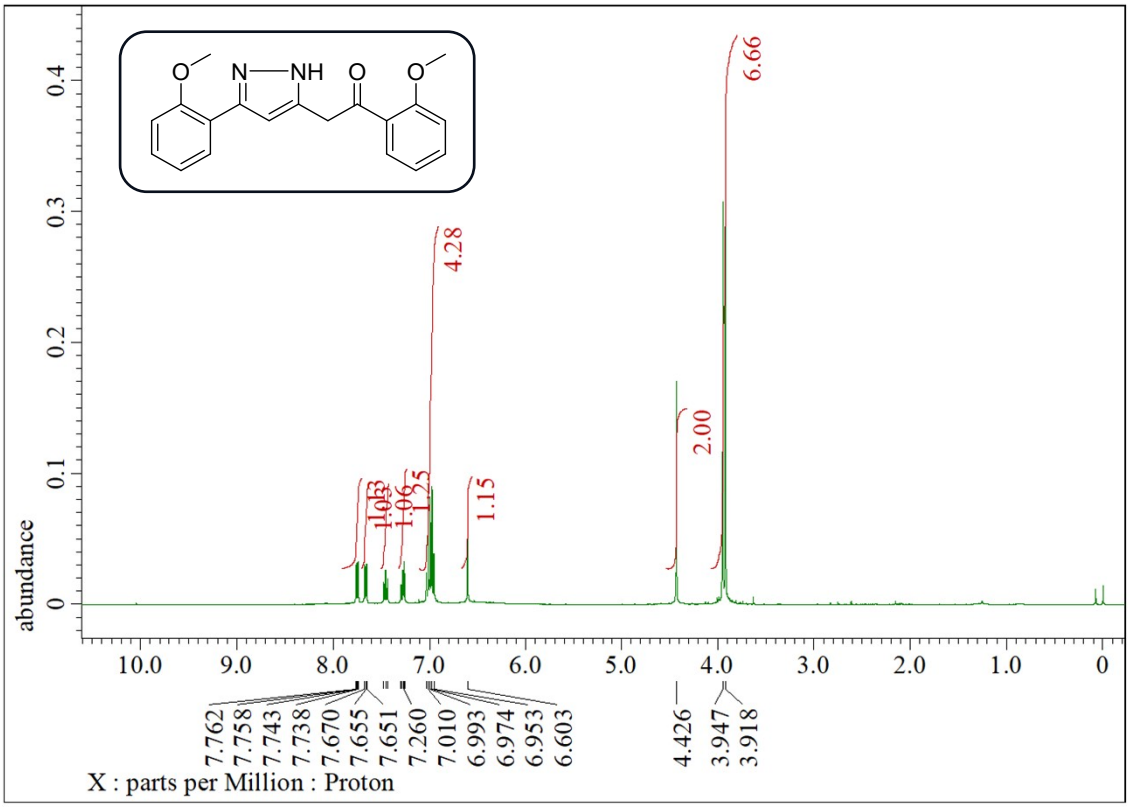


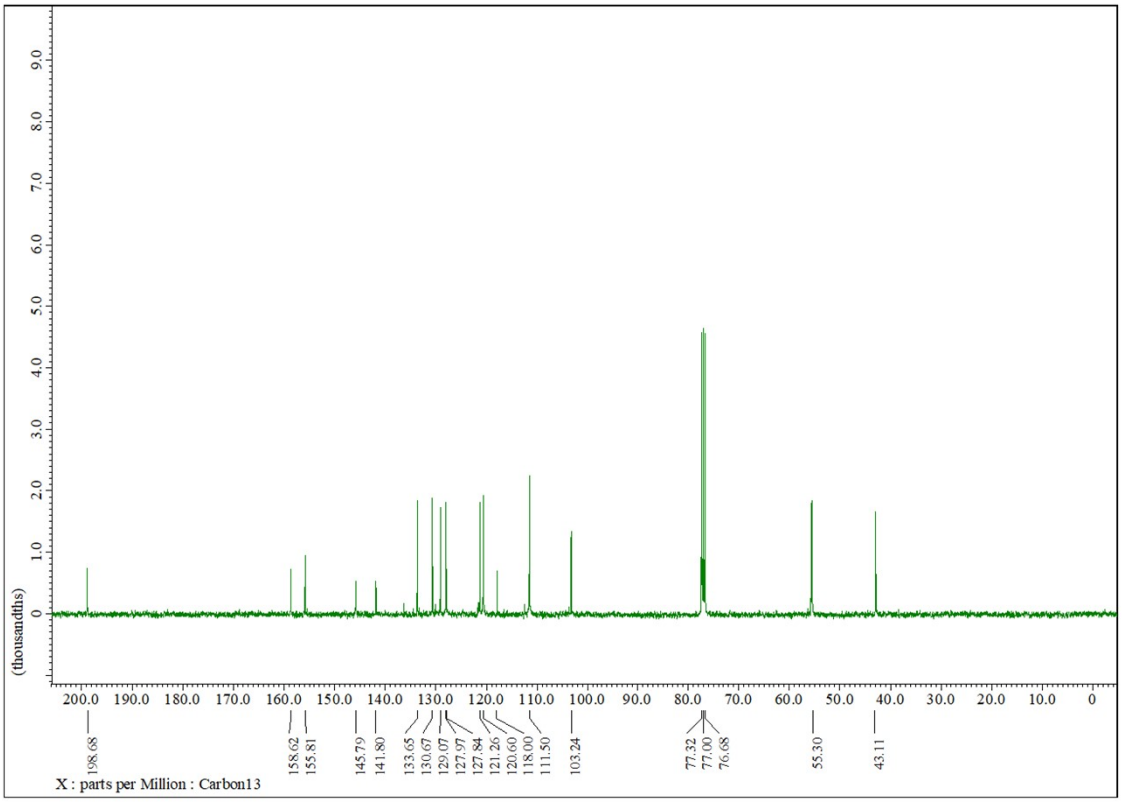
^{1}H NMR and ^{13}C NMR spectra of 1-(3-bromophenyl)-2-(3-3-bromophenyl)-1*H*-pyrazol-5-yl) ethan-1-one (2g)



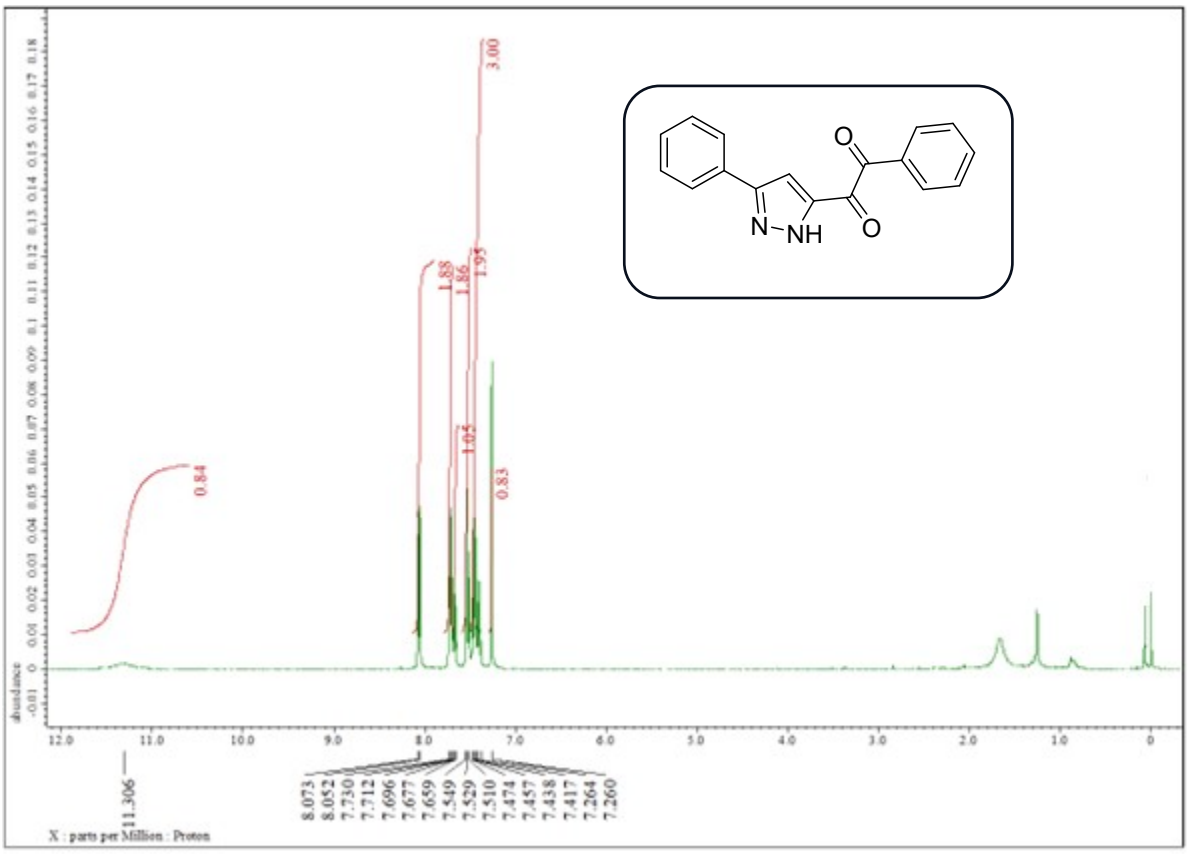


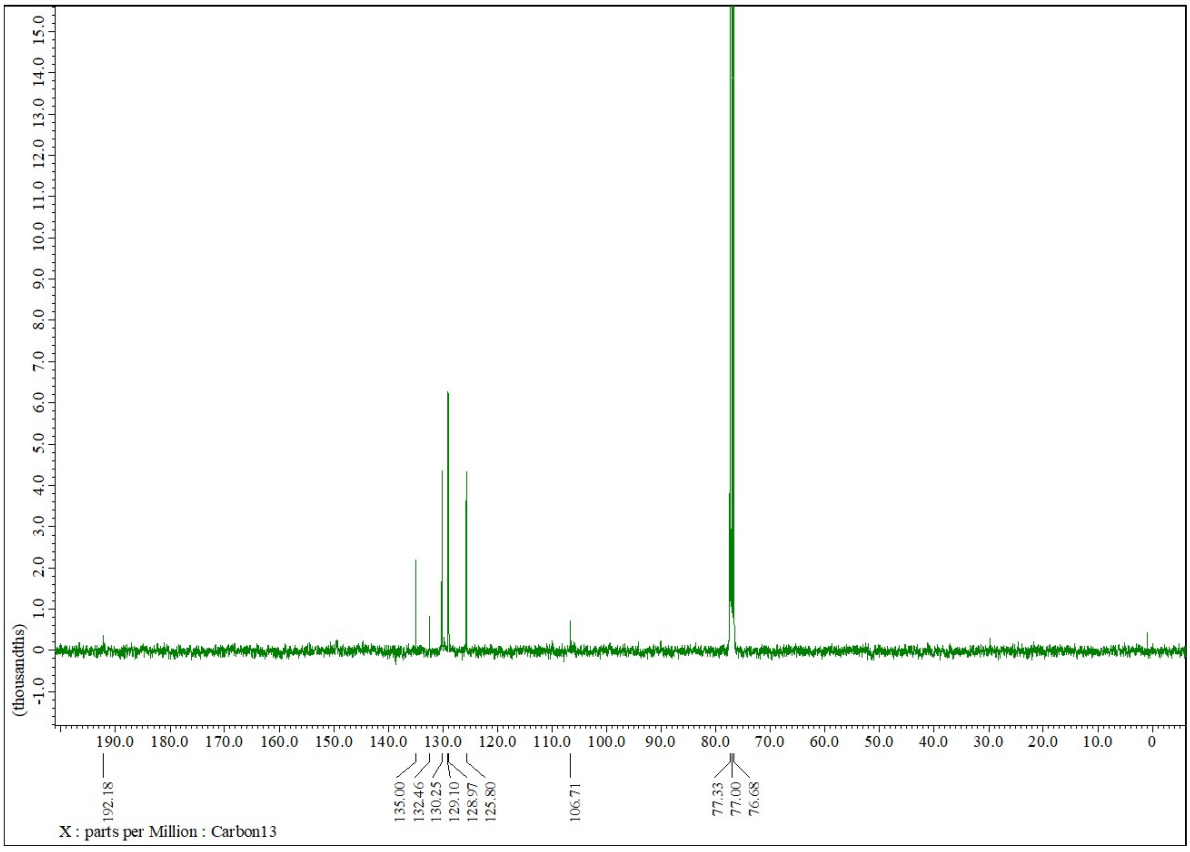
^{1}H NMR and ^{13}C NMR spectra of 1-(2-methoxyhenyl)-2-(3-2-methoxyphenyl)-1*H*-pyrazol-5-yl) ethan-1-one (2h)



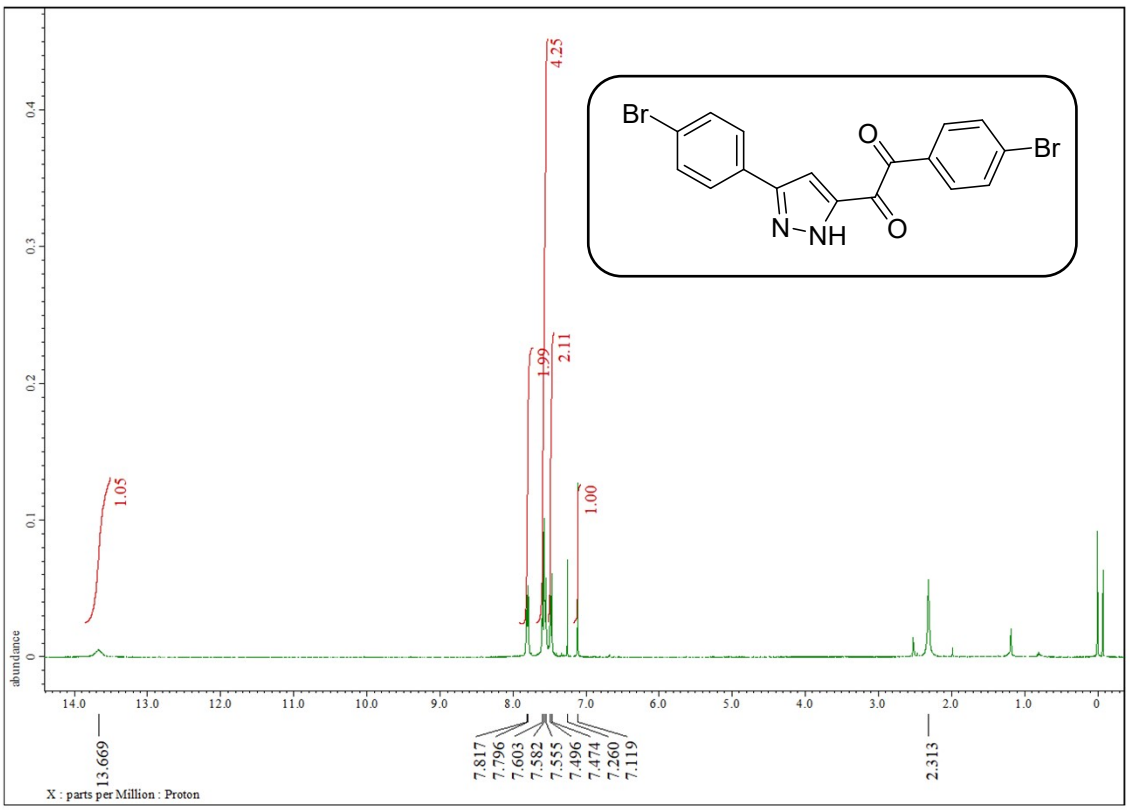


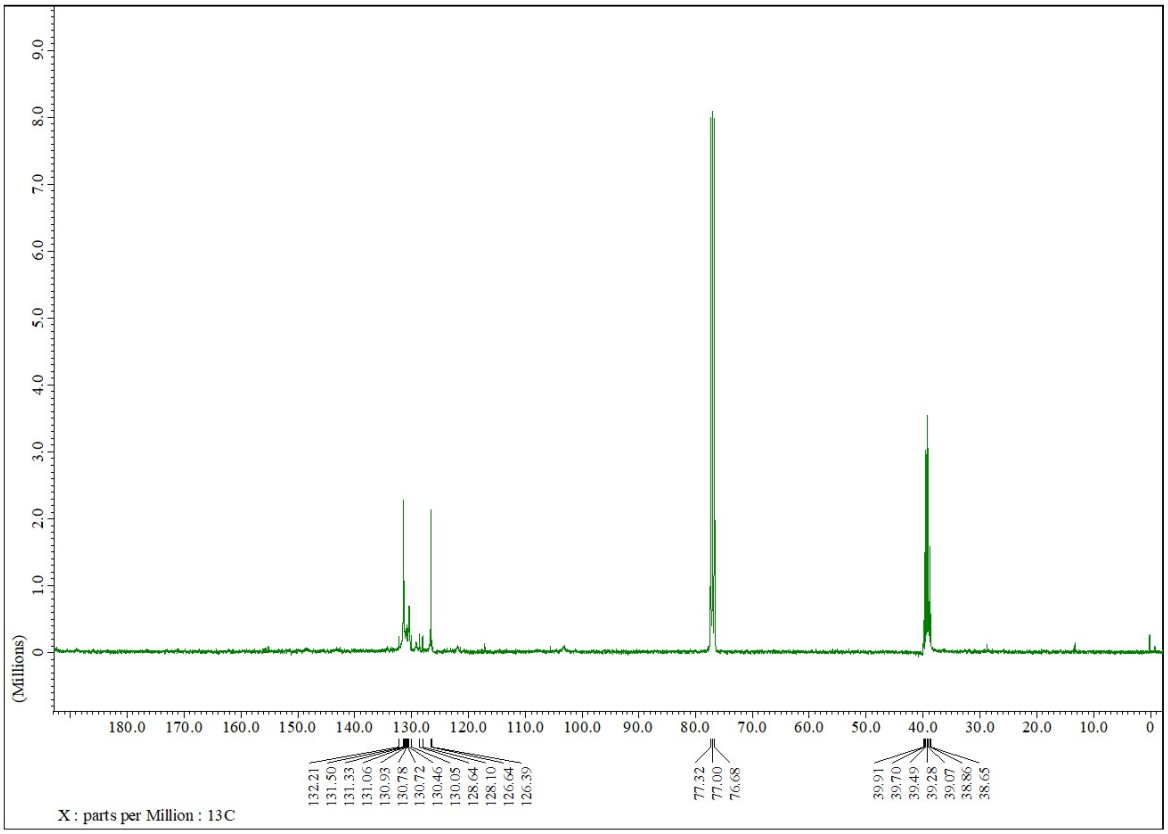
^{1}H NMR and ^{13}C NMR spectra of 1-phenyl-2-(3-phenyl-1*H*-pyrazol-5-yl)ethane-1,2-dione (3a)



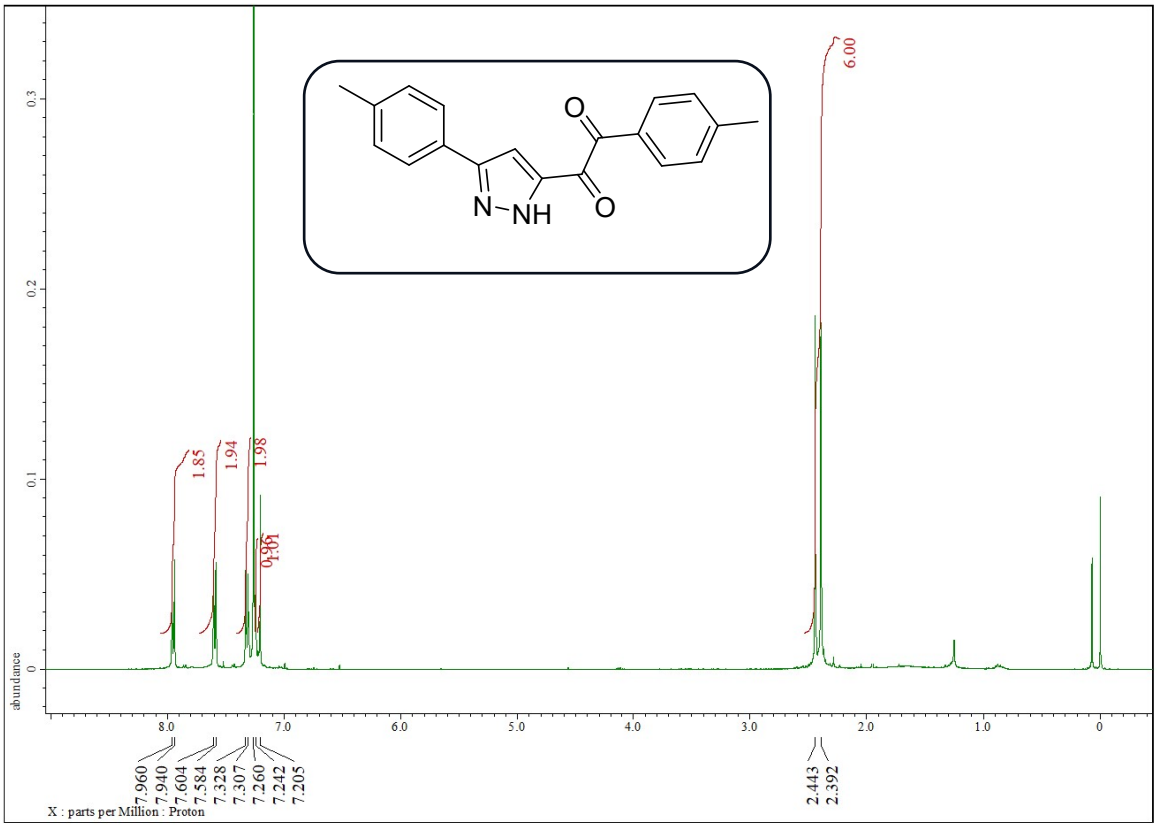


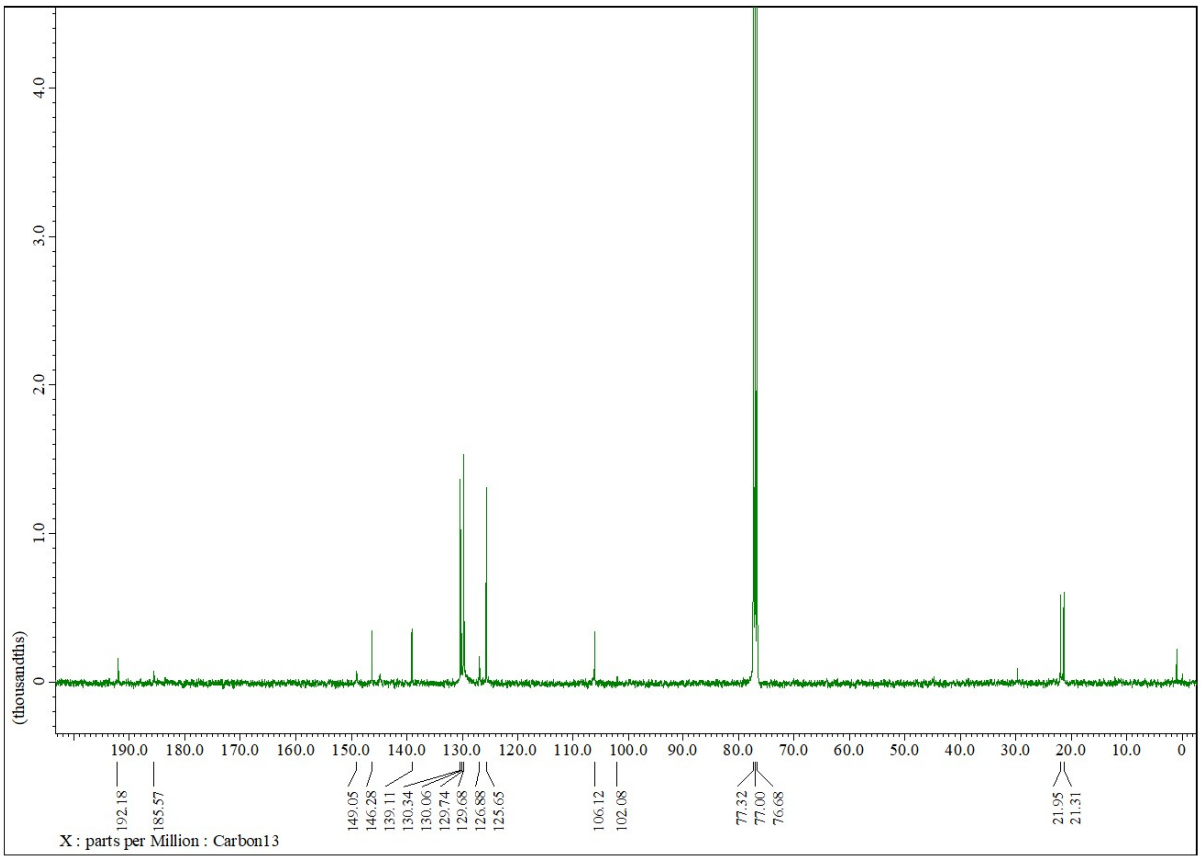
^{1}H NMR and ^{13}C NMR spectra of 1-(4-bromophenyl)-2-(3-(4-bromophenyl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3b)



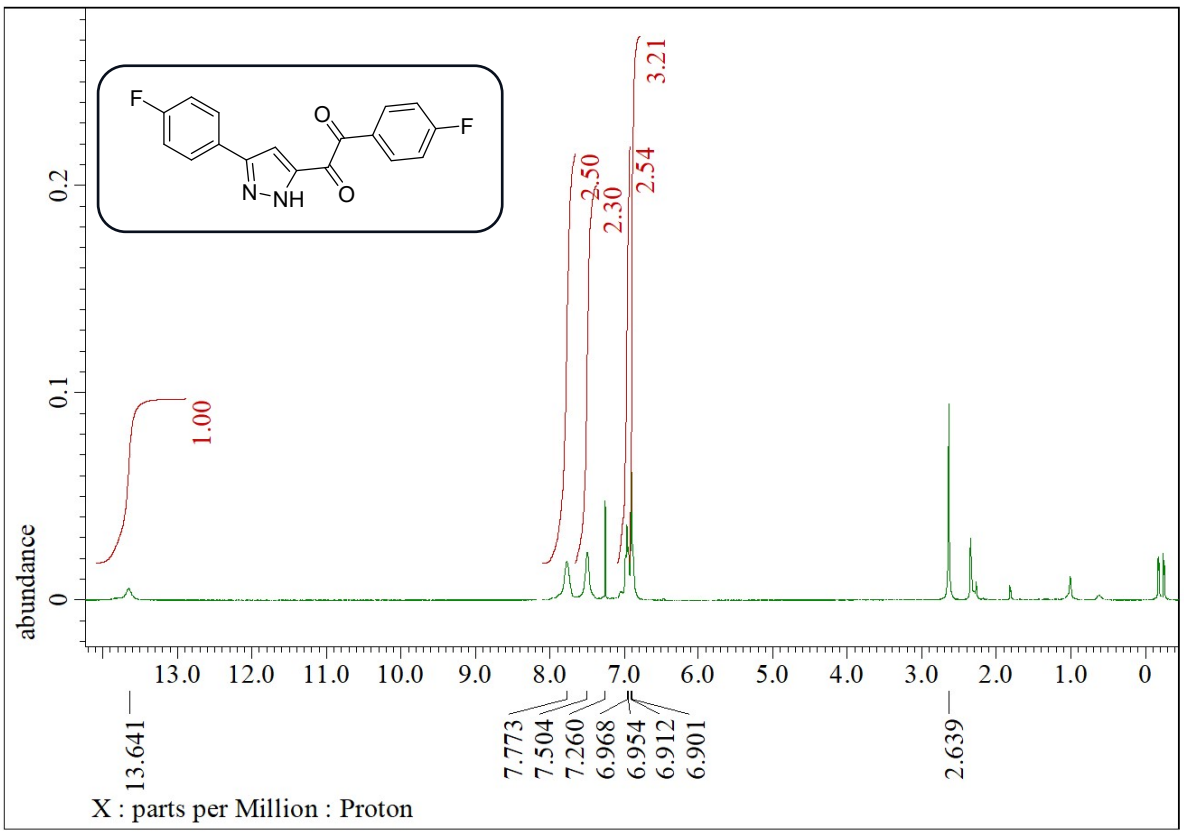


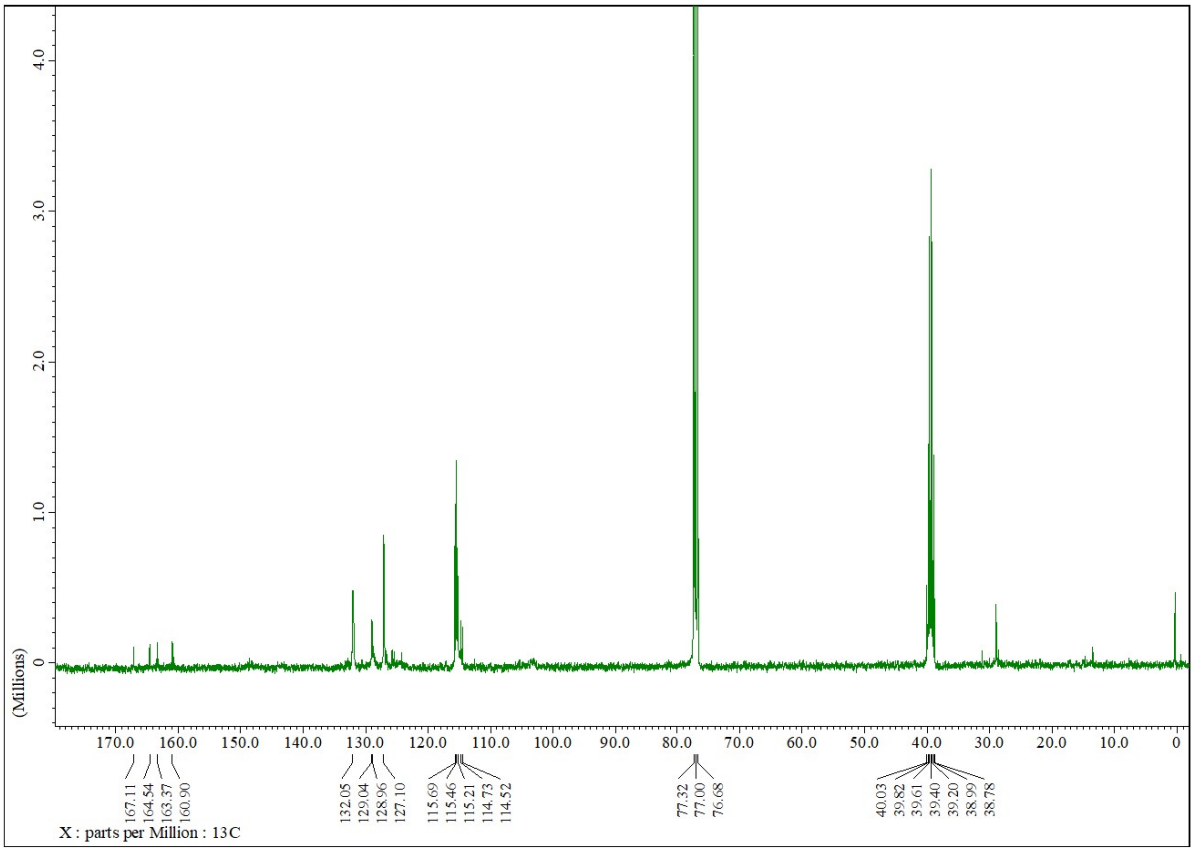
^{1}H NMR and ^{13}C NMR spectra of 1-(*p*-tolyl)-2-(3-(*p*-tolyl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3c)



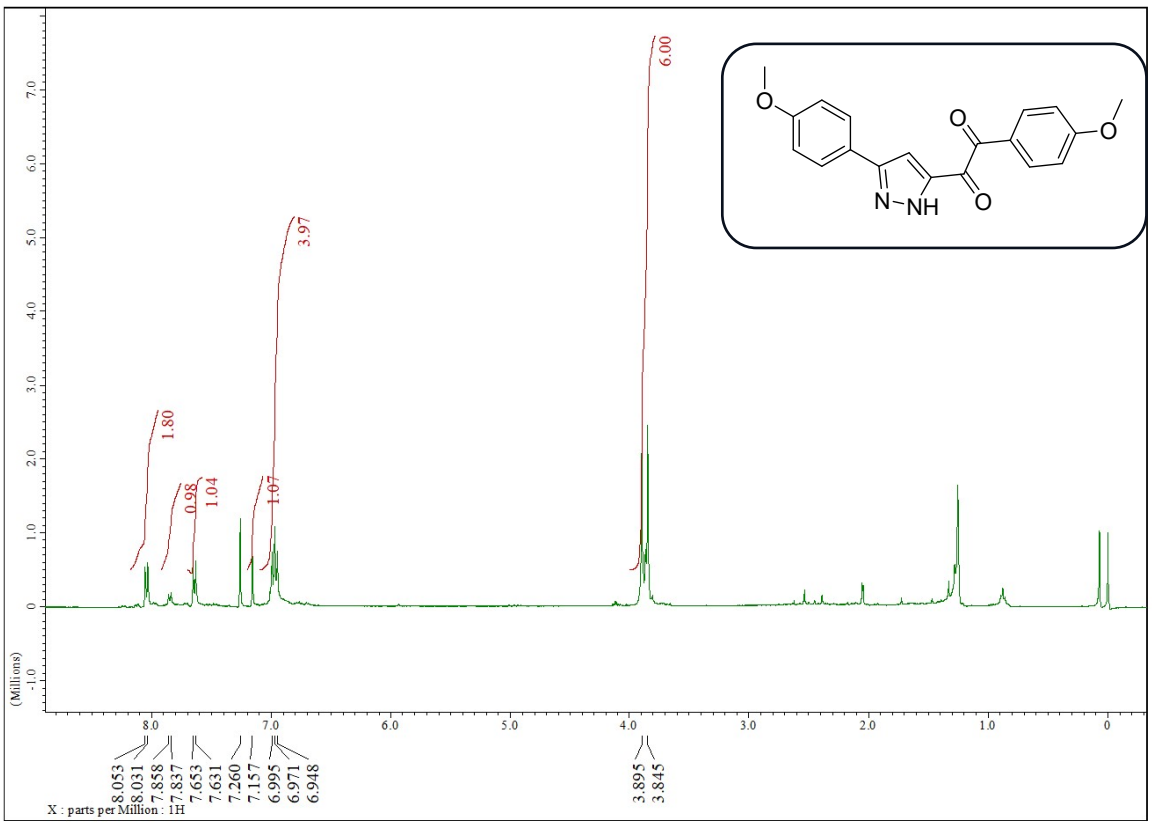


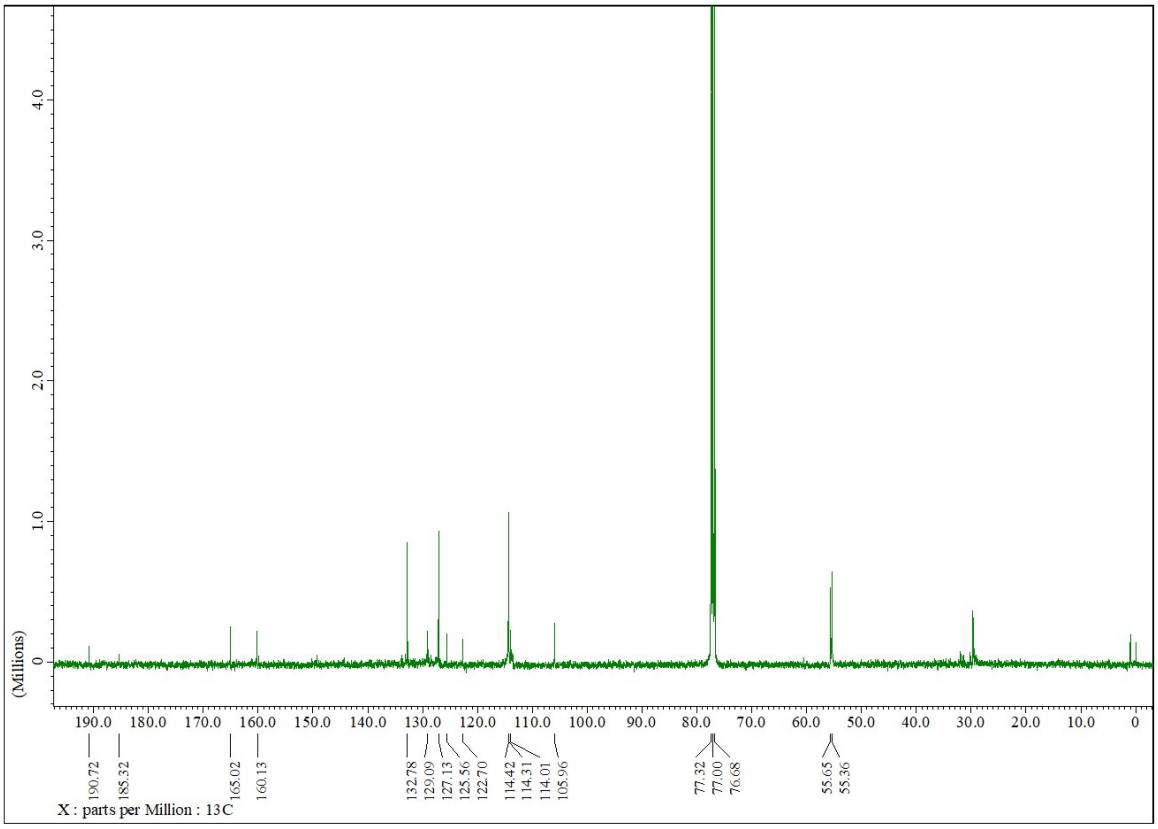
^{1}H NMR and ^{13}C NMR spectra of 1-(4-flurophenyl)-2-(3-(4-flurophenyl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3d)



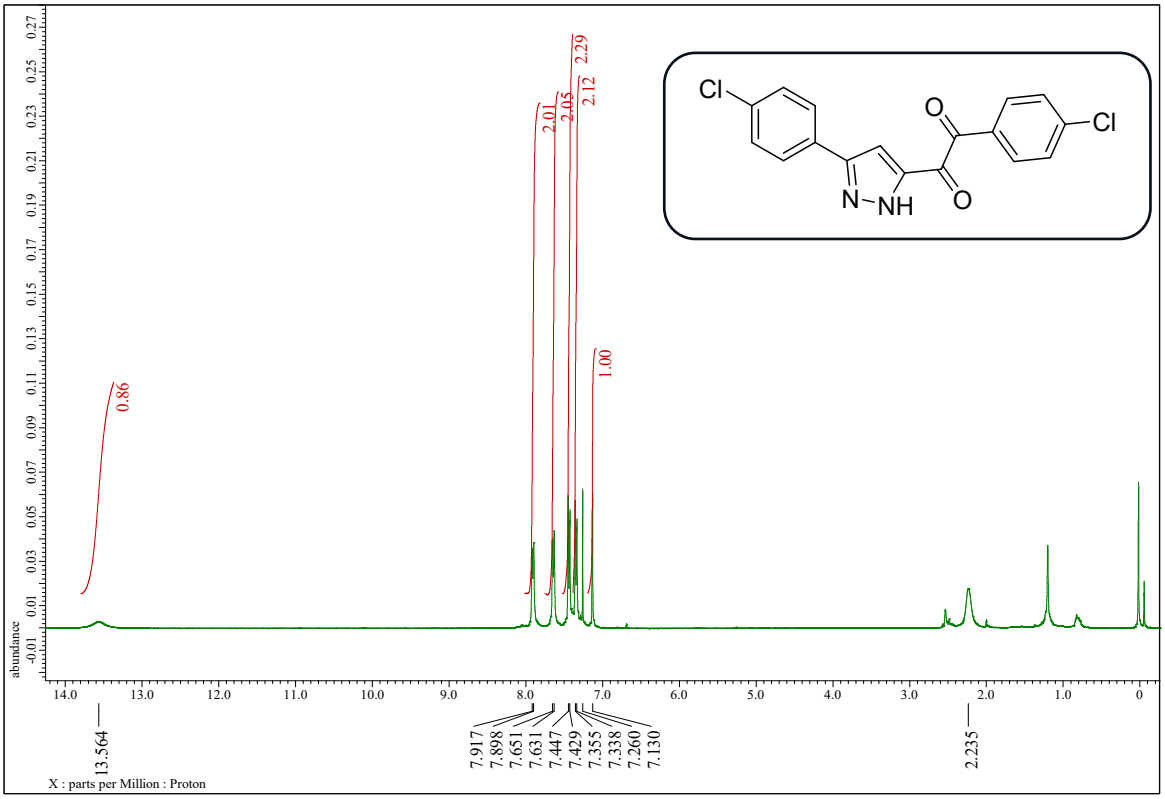


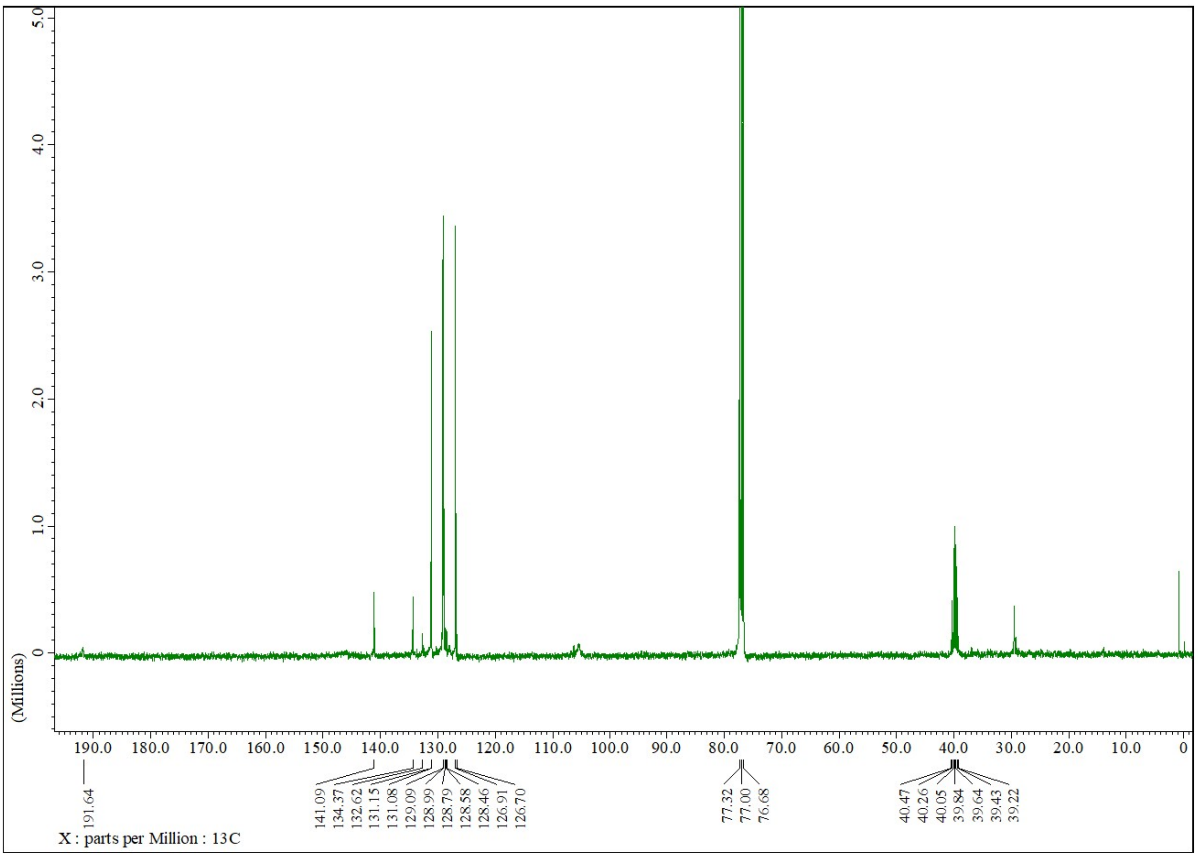
^{1}H NMR and ^{13}C NMR spectra of 1-(4-methoxyphenyl)-2-(3-(4-methoxyphenyl)-1*H*-pyrazol-5-yl) ethane-1,2-dione (3e)



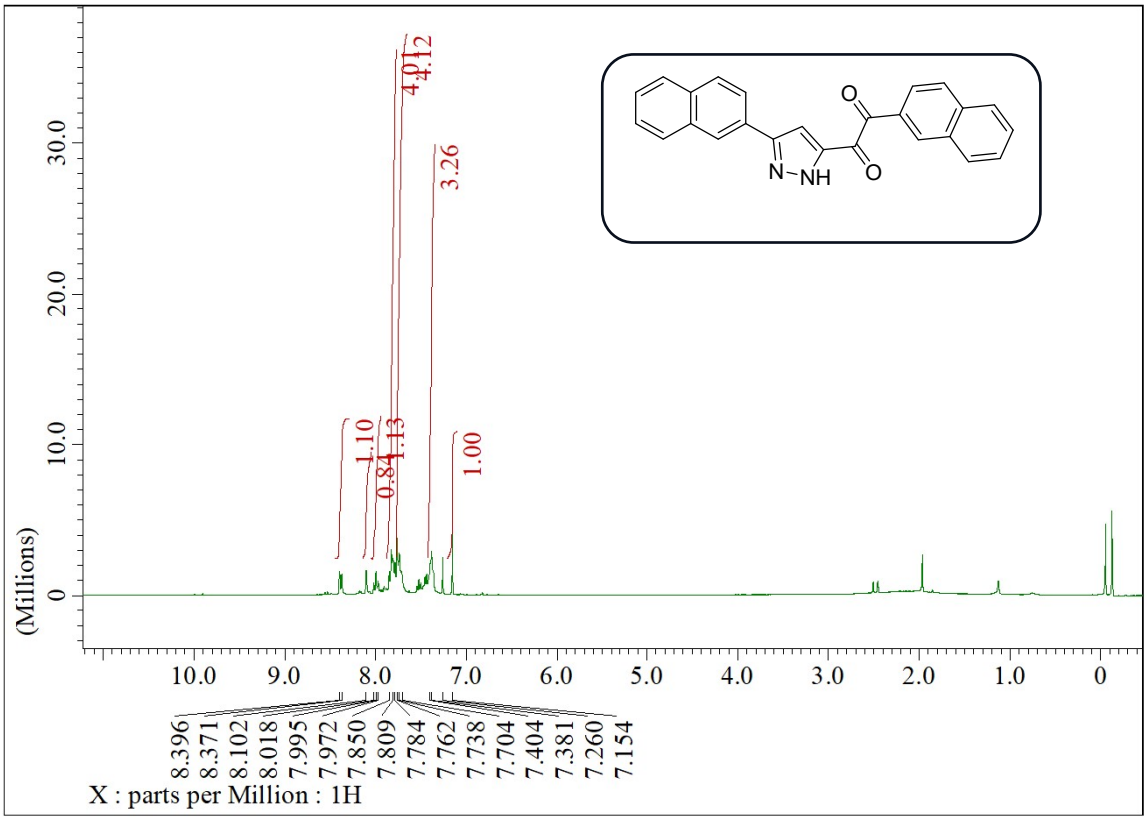


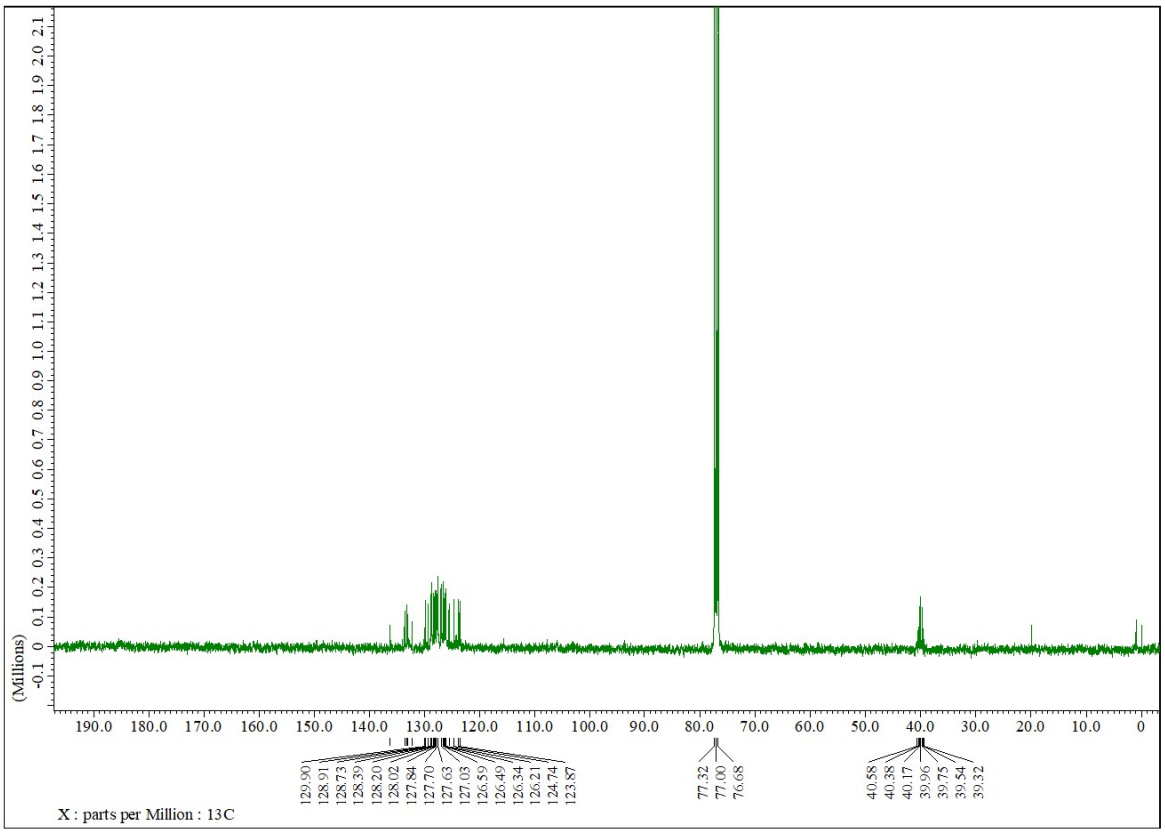
^{1}H NMR and ^{13}C NMR spectra of 1-(4-chlorophenyl)-2-(3-(4-chlorophenyl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3f)



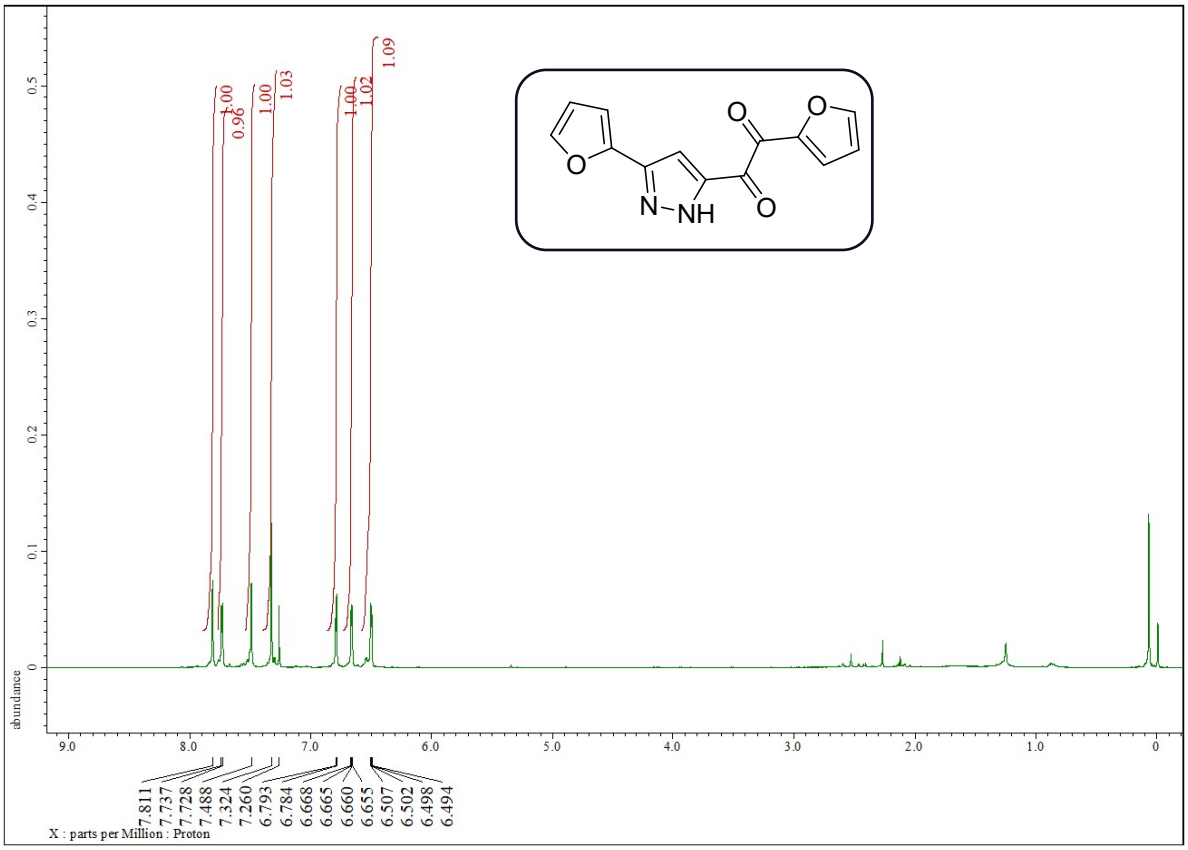


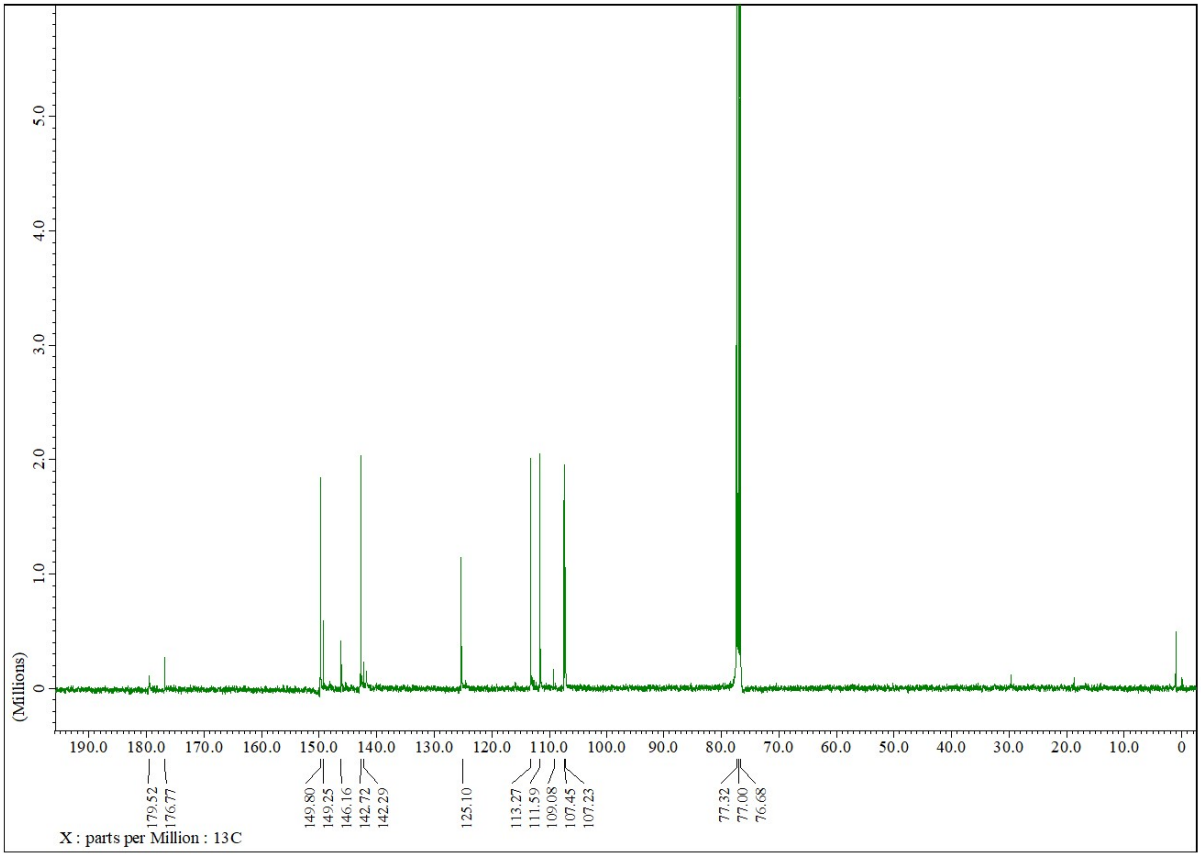
^{1}H NMR and ^{13}C NMR spectra of 1-(naphthalene-2-yl)-2-(3-(napthalen-2-yl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3g)



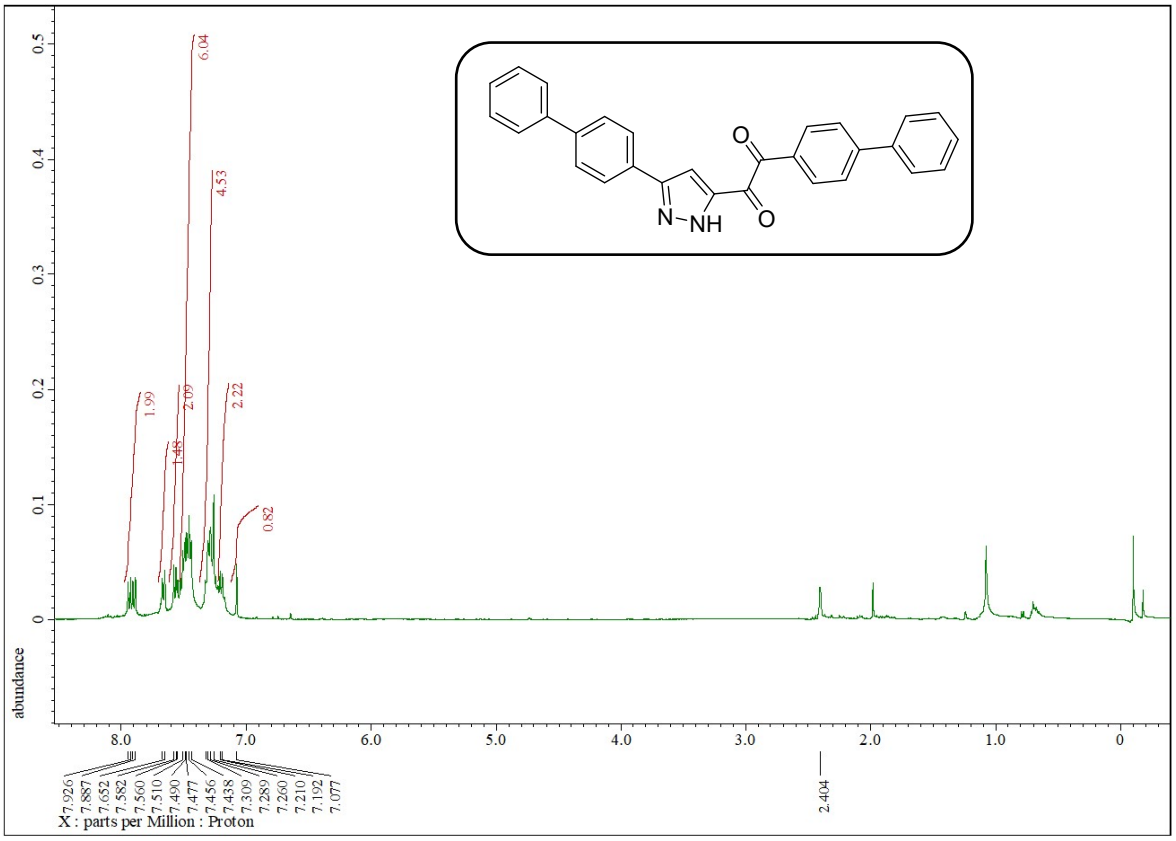


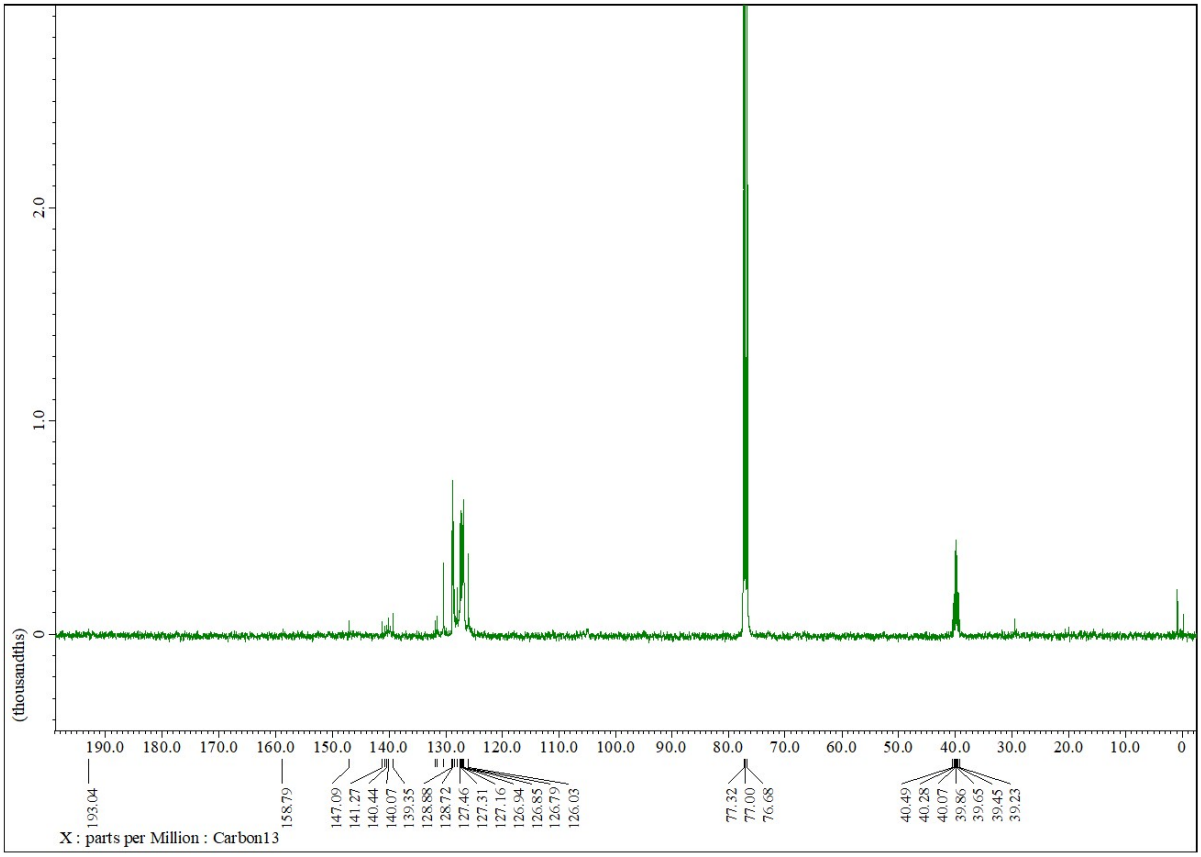
^{1}H NMR and ^{13}C NMR spectra of 1-(furan-2-yl)-2-(3-(furan-2-yl)-1H-pyrazol-5-yl) ethane-1,2-dione (3h)



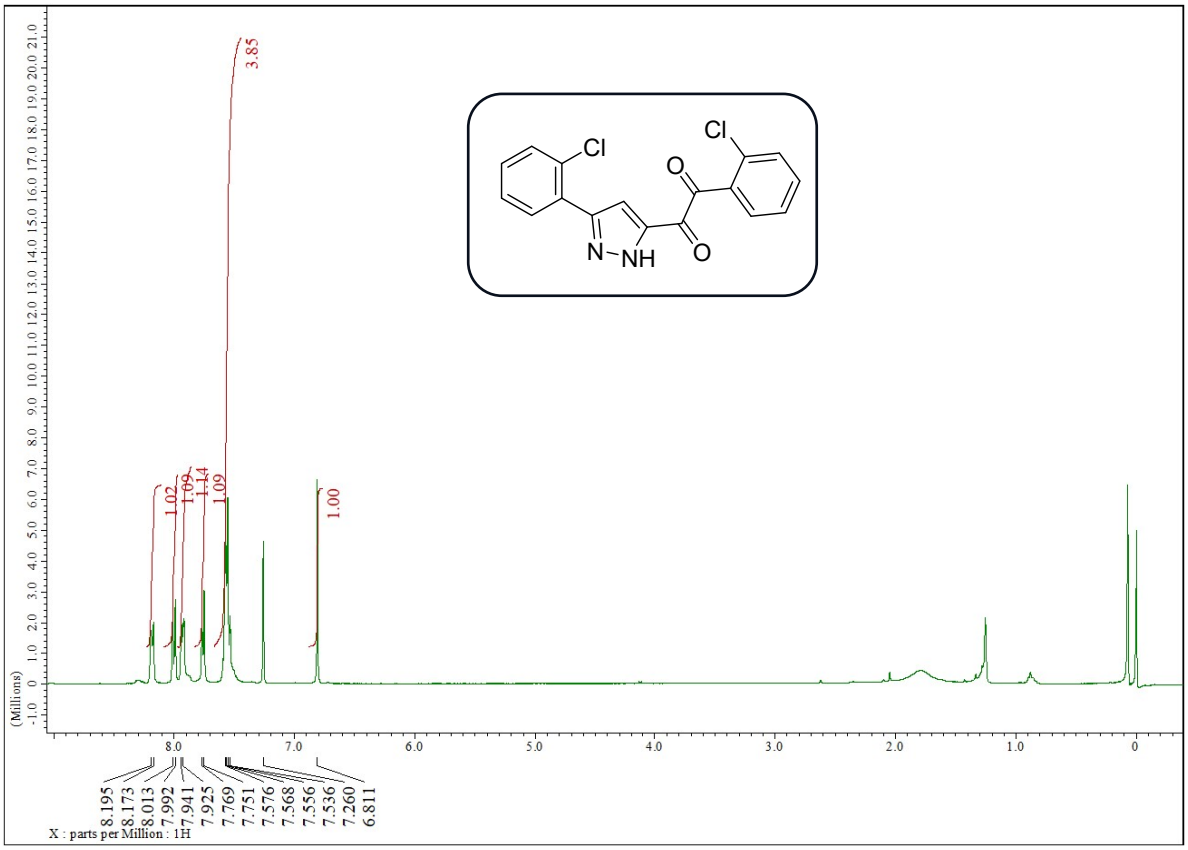


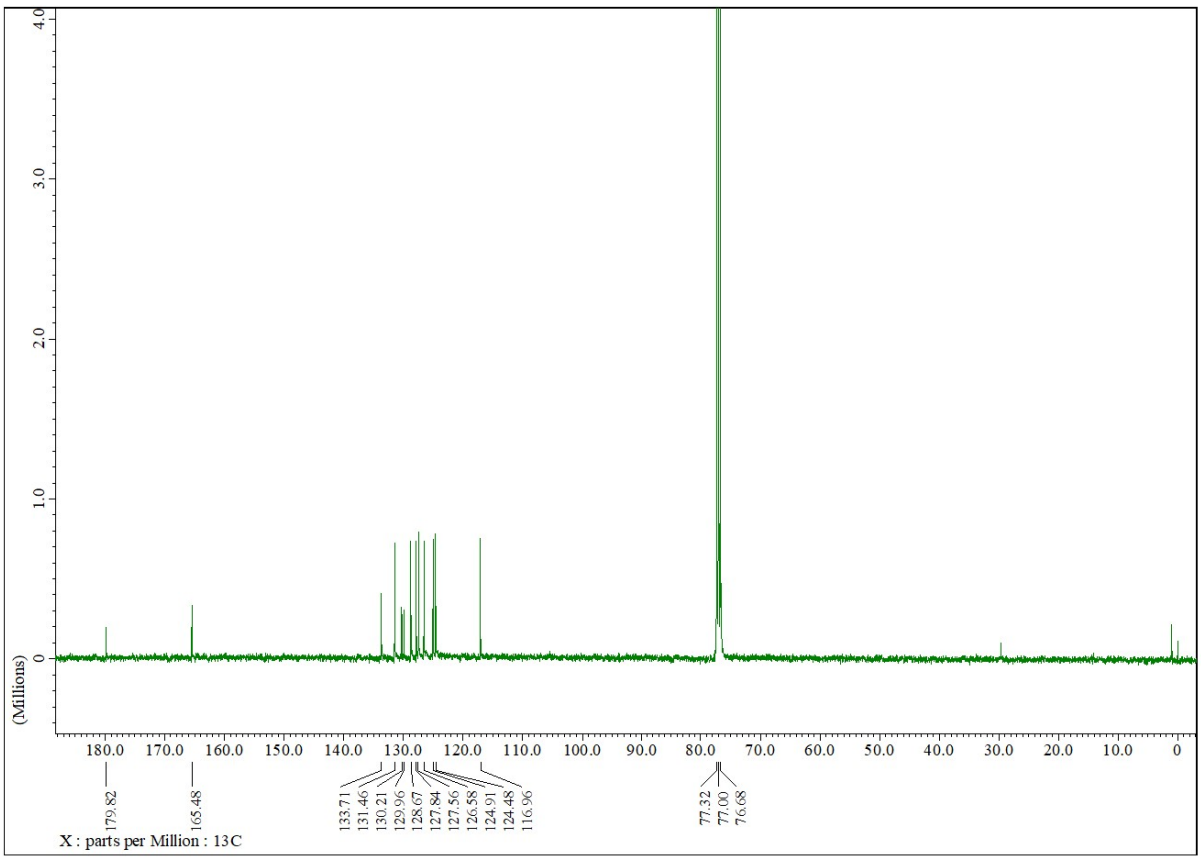
^{1}H NMR and ^{13}C NMR spectra of 1-([1,1-biphenyl]-4-yl)-2-(3-([1,1-biphenyl]-4-yl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3i)



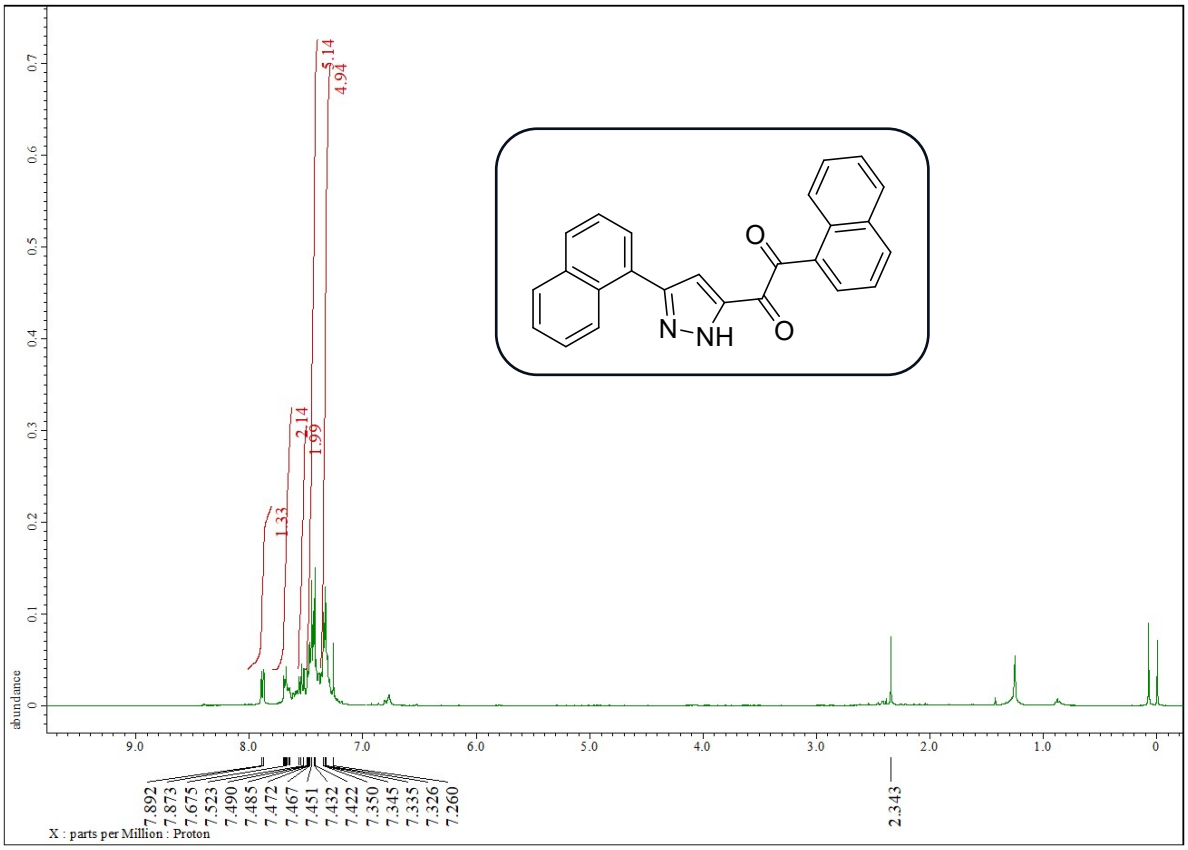


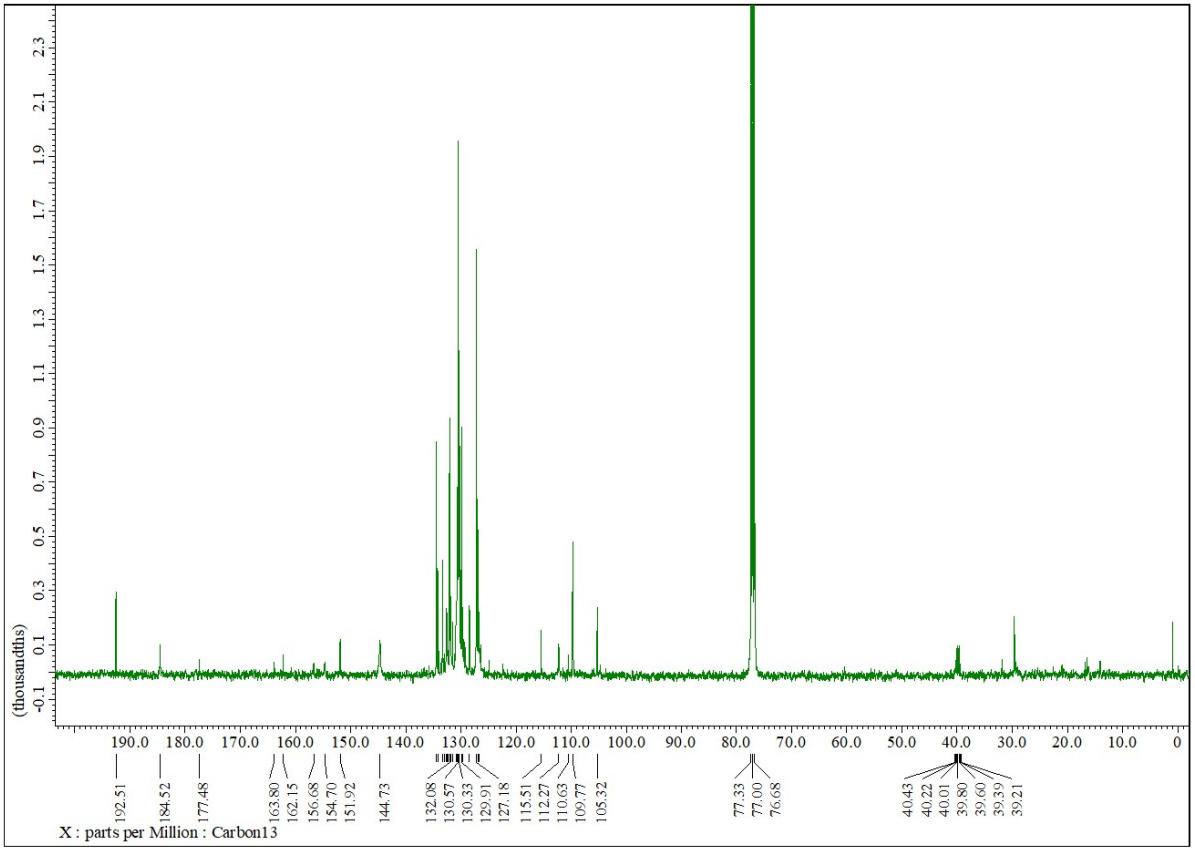
^{1}H NMR and ^{13}C NMR spectra of 1-(2-chlorophenyl)-2-(3-(2-chlorophenyl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3j)



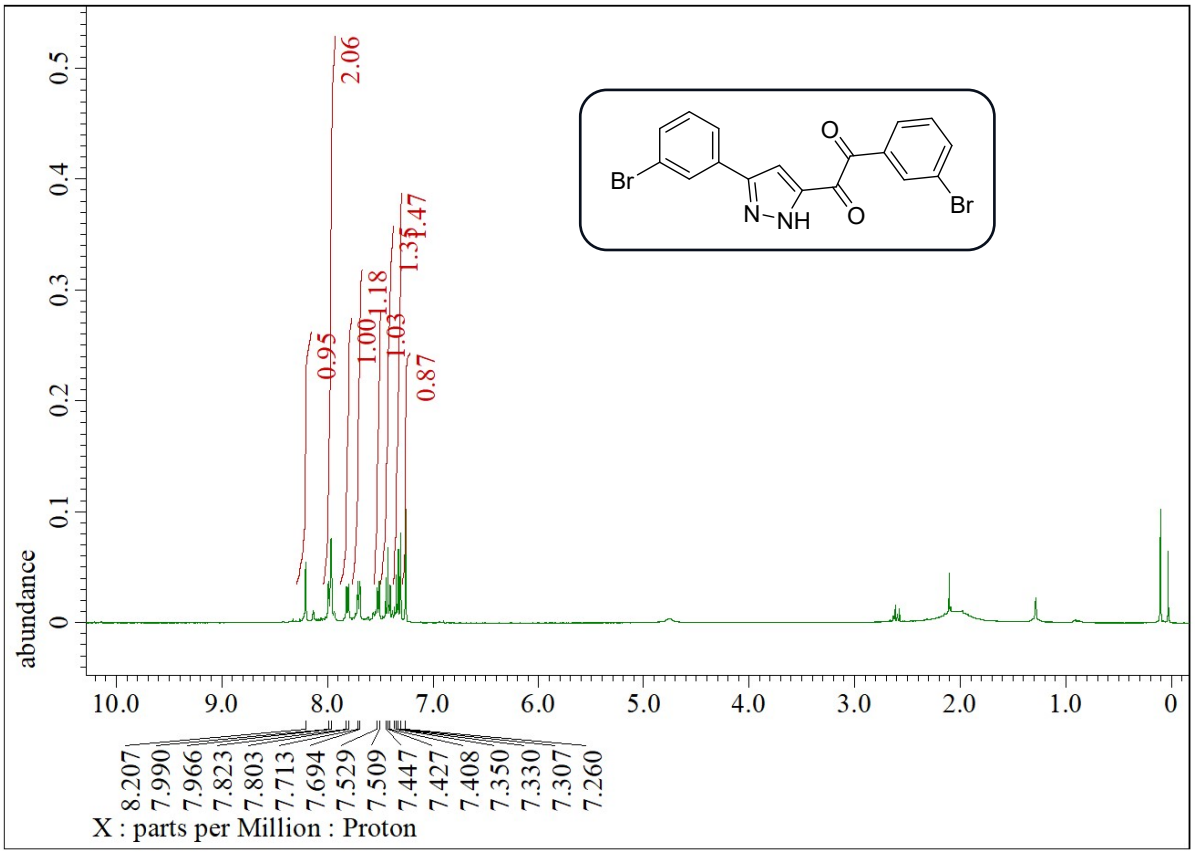


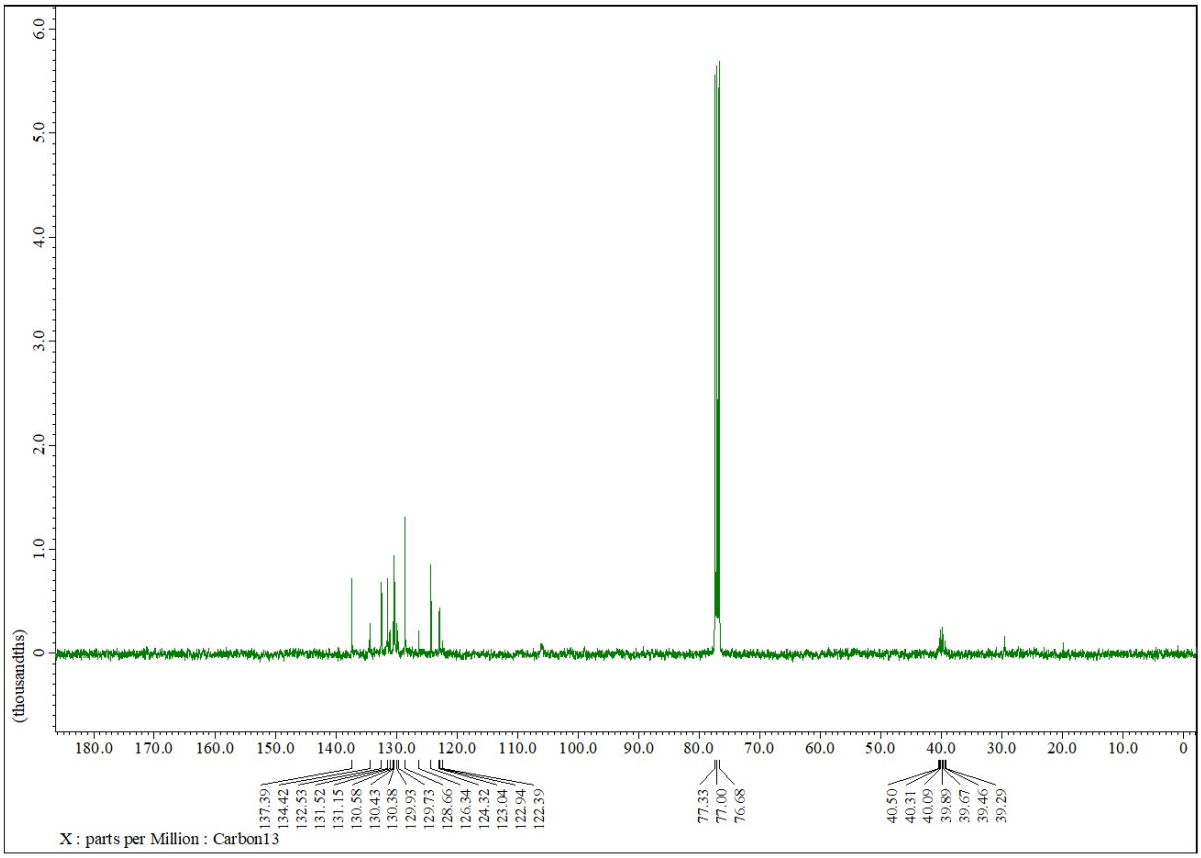
^{1}H NMR and ^{13}C NMR spectra of 1-(naphthalene-1-yl)-2-(3-(napthalen-1-yl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3k)



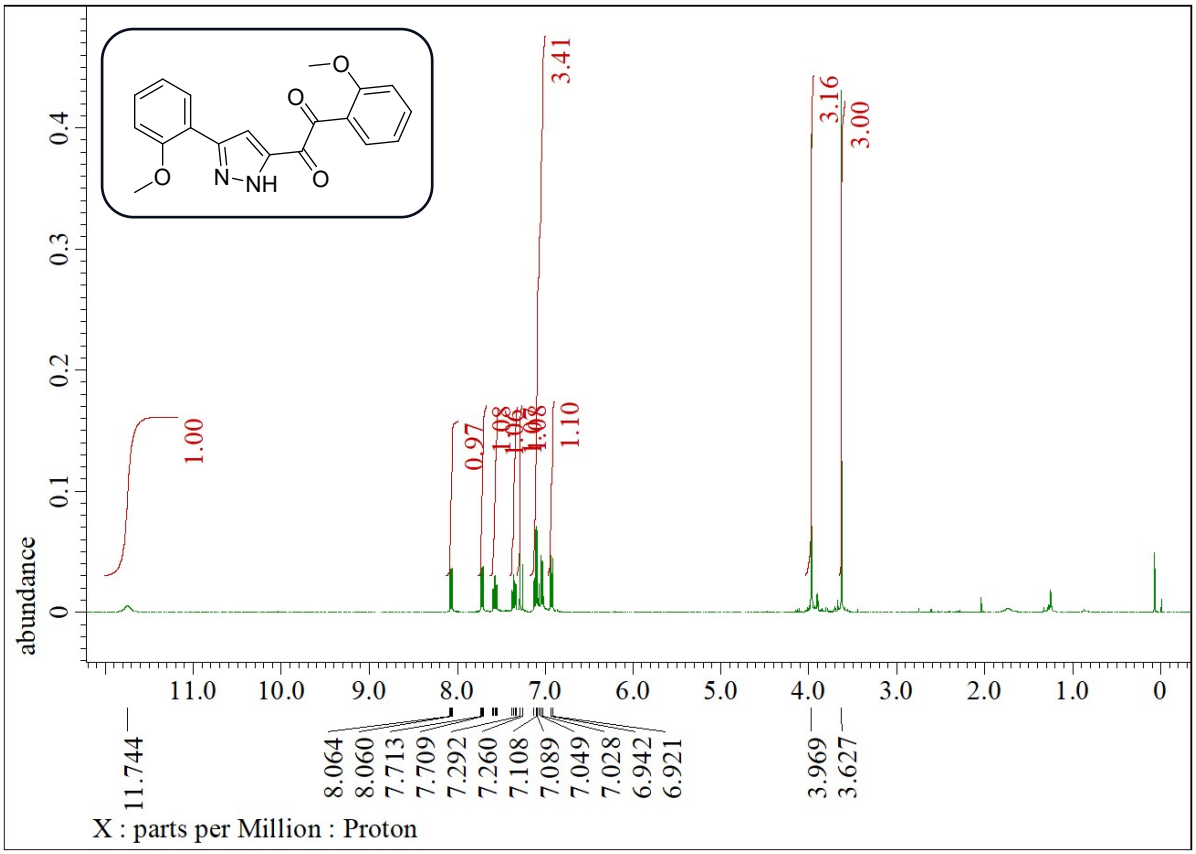


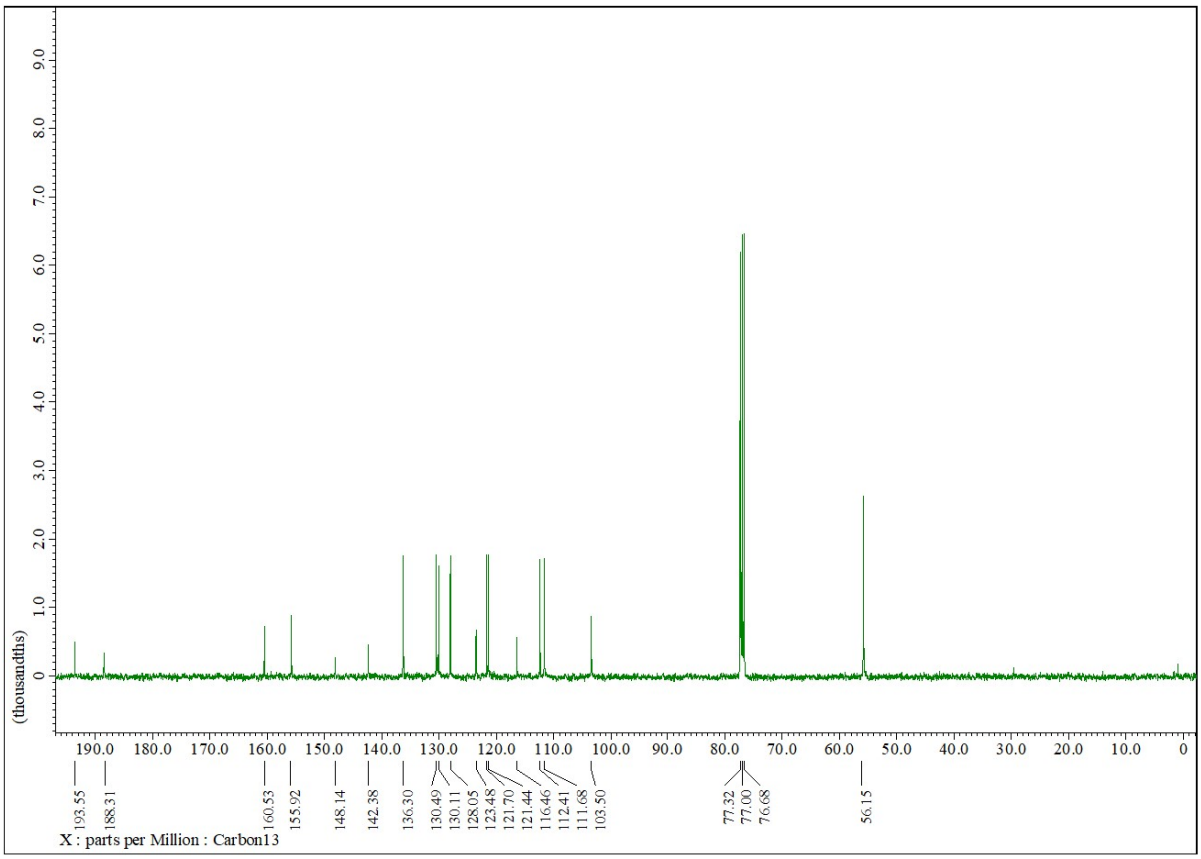
^{1}H NMR and ^{13}C NMR spectra of 1-(3-bromophenyl)-2-(3-(3-bromophenyl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3l)



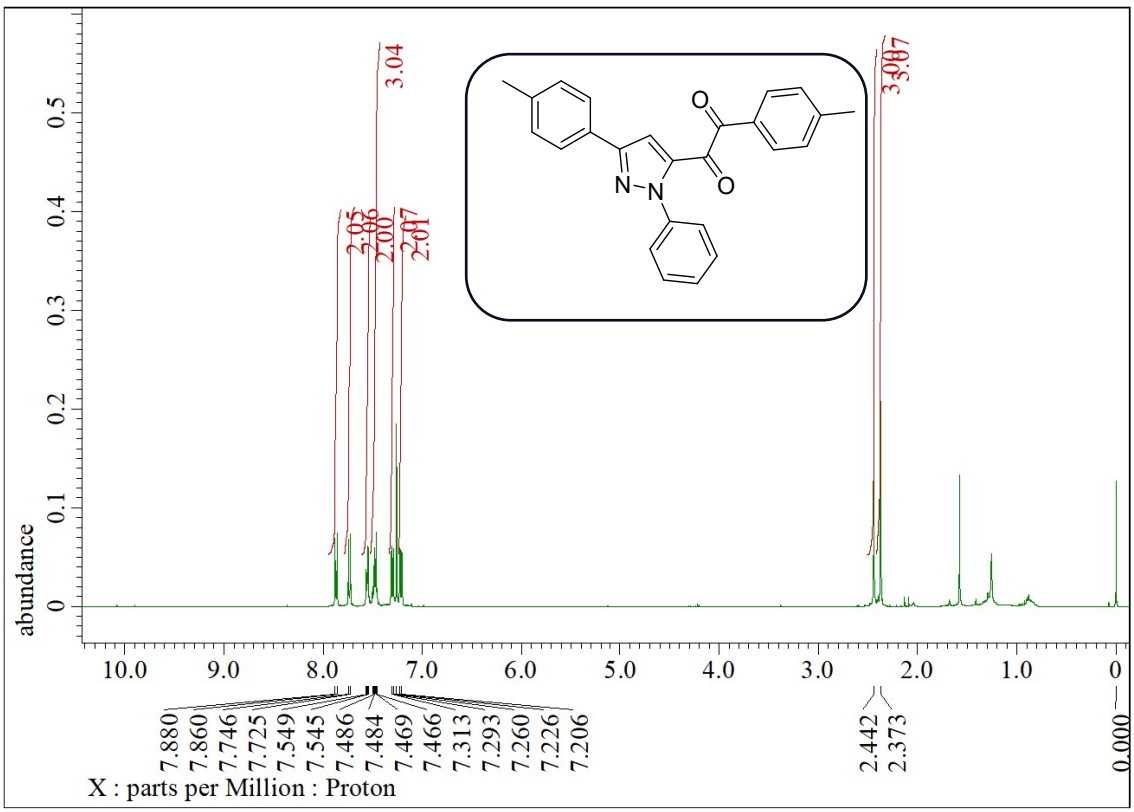


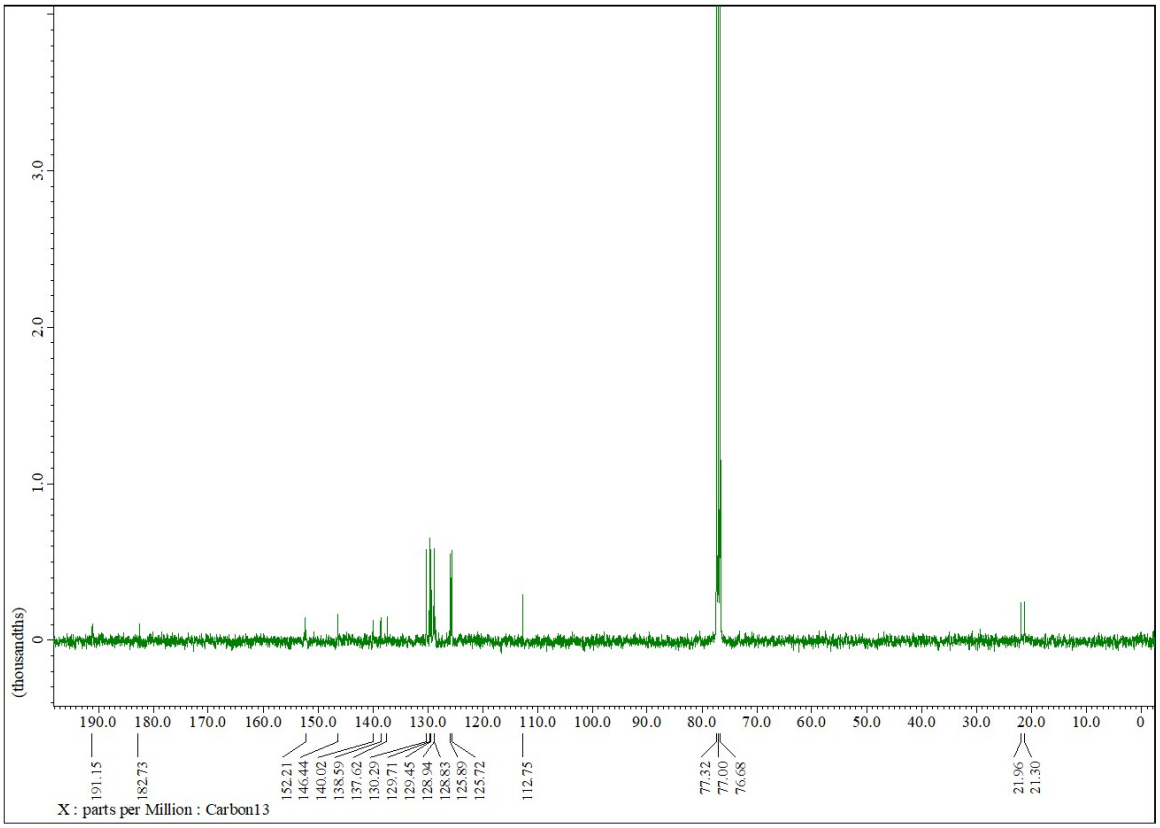
^{1}H NMR and ^{13}C NMR spectra of 1-(2-methoxyphenyl)-2-(3-(2-methoxyphenyl)-1*H*-pyrazol-5-yl)ethane-1,2-dione (3m)



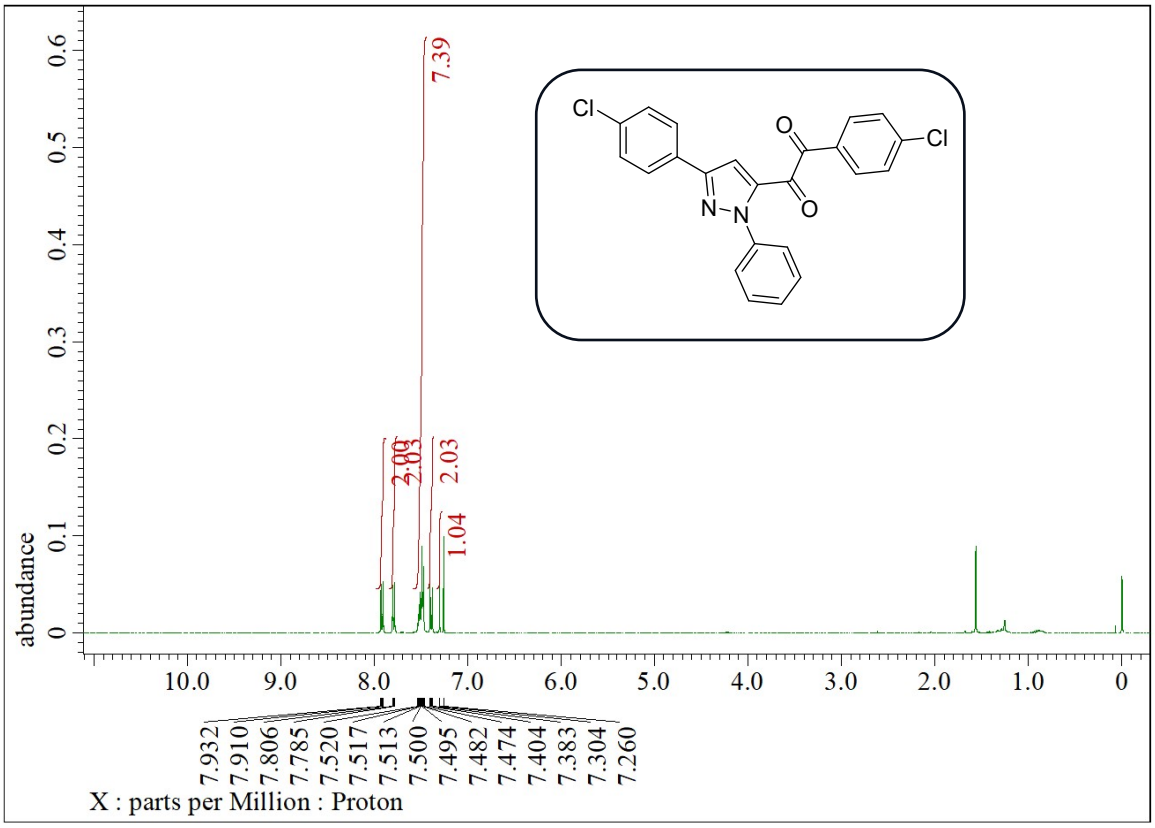


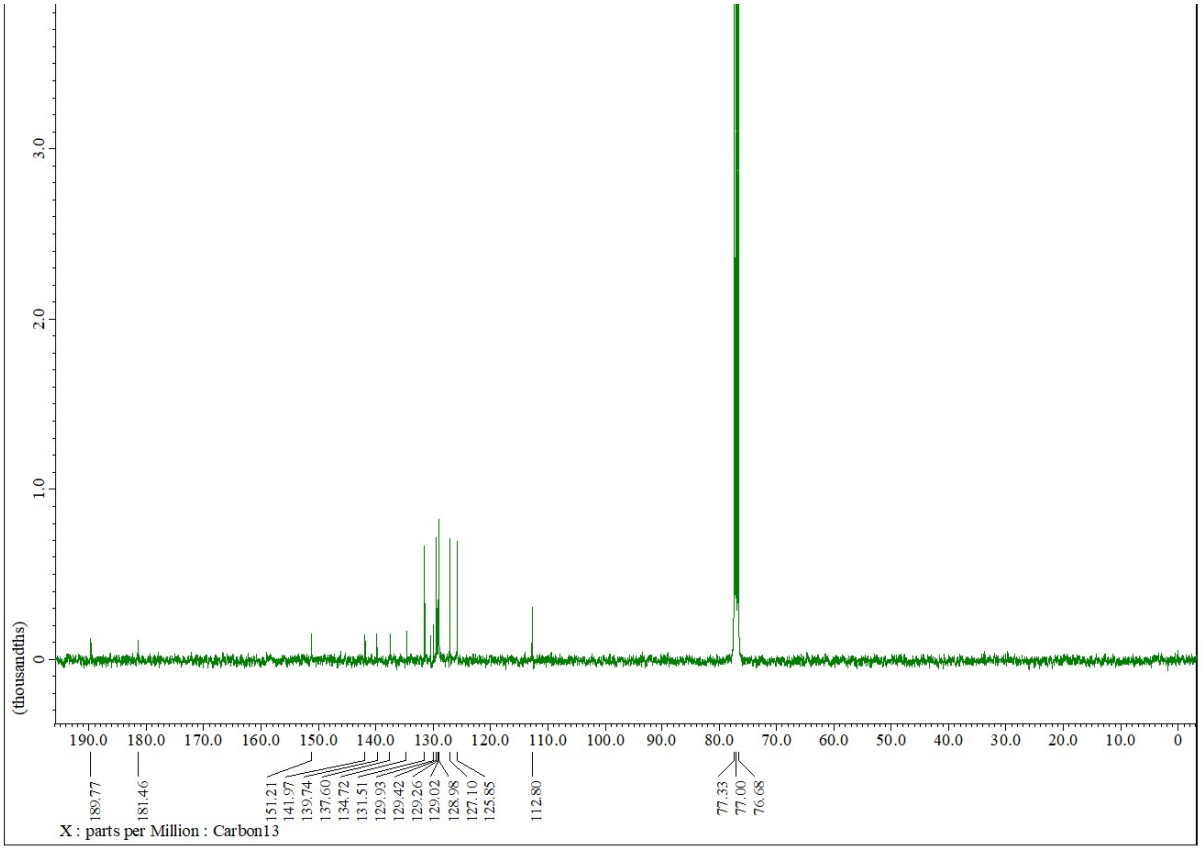
^{1}H NMR and ^{13}C NMR spectra of 1-(1-phenyl-3-(*p*-tolyl)-1*H*-pyrazol-5-yl)-2-(*p*-tolyl)ethane-1,2-dione (4a)



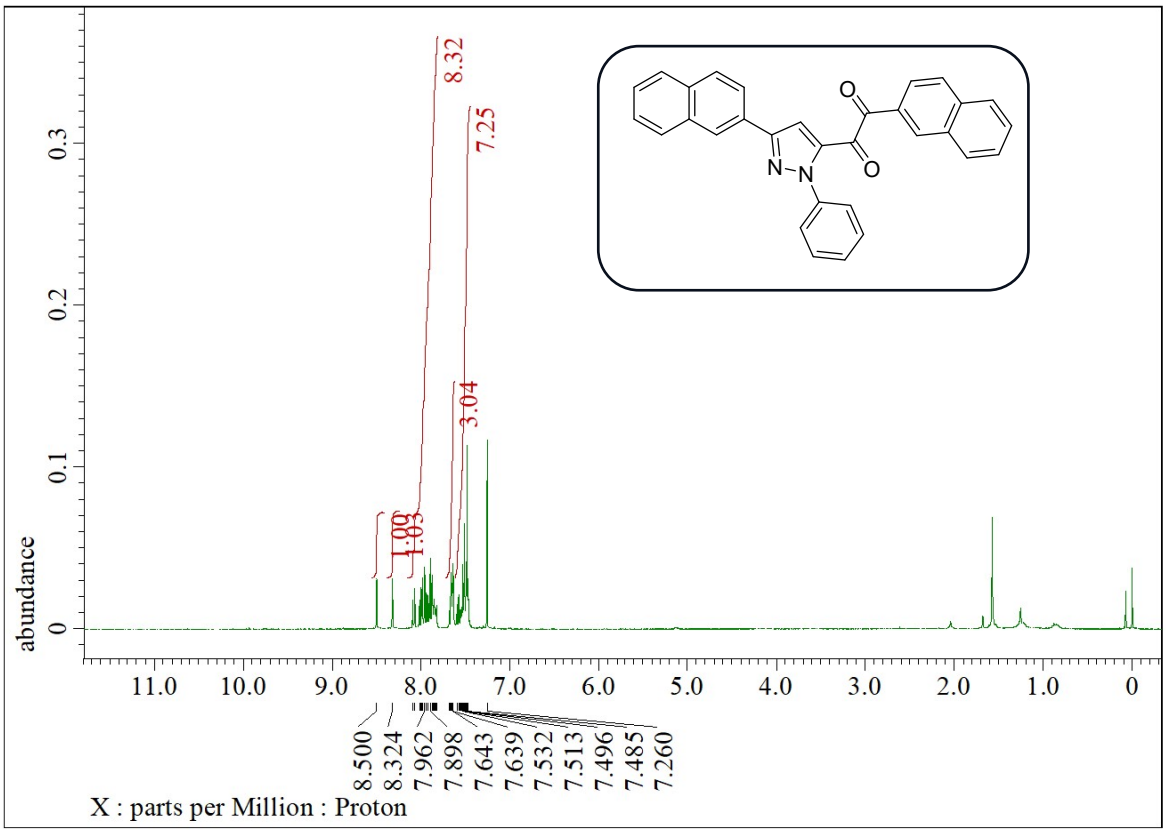


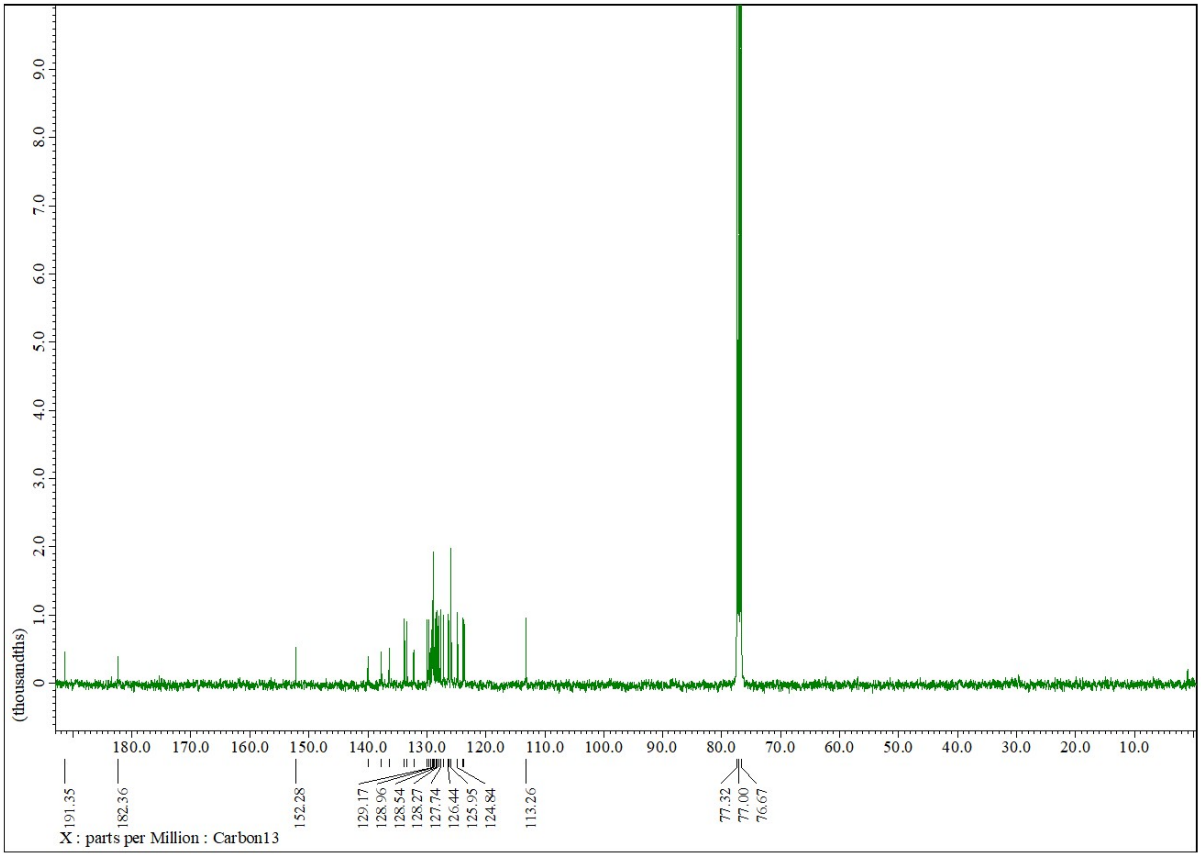
^{1}H NMR and ^{13}C NMR spectra of 1-(1-phenyl-3-(*p*-chlorophenyl)-1*H*-pyrazol-5-yl)-2-(*p*-chlorophenyl)ethane-1,2-dione (4b)



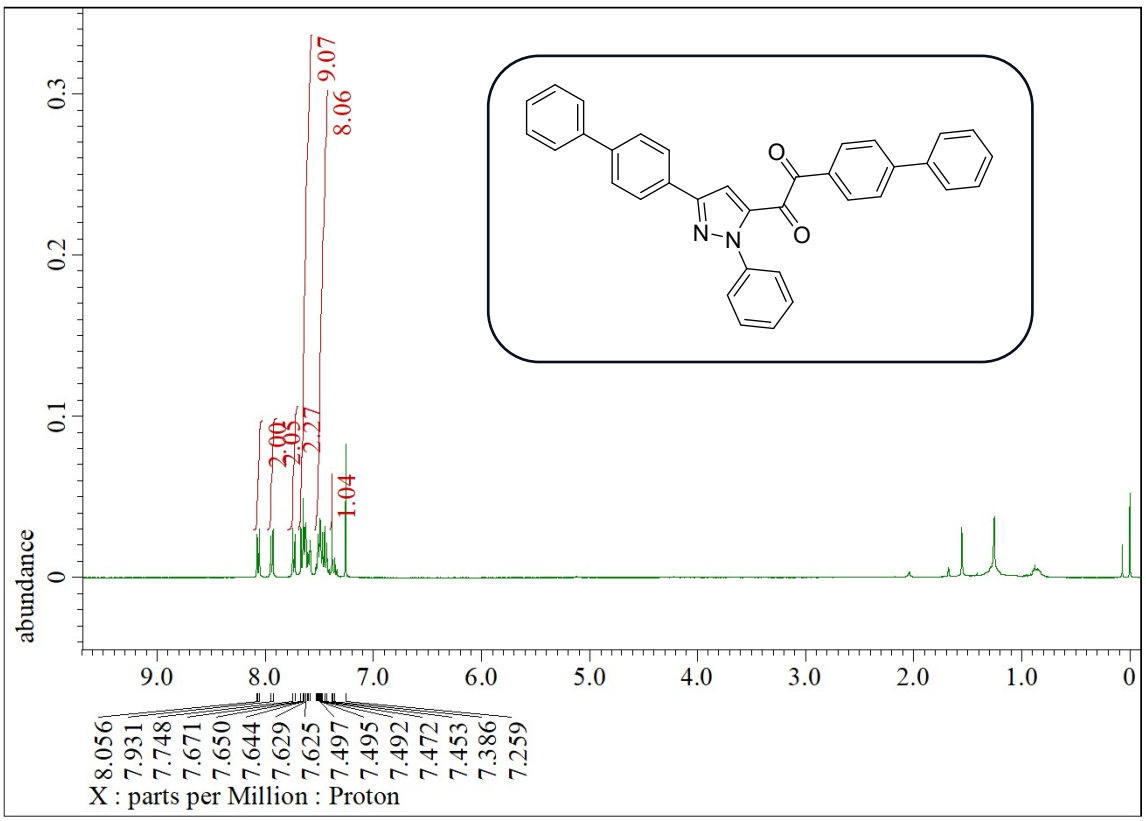


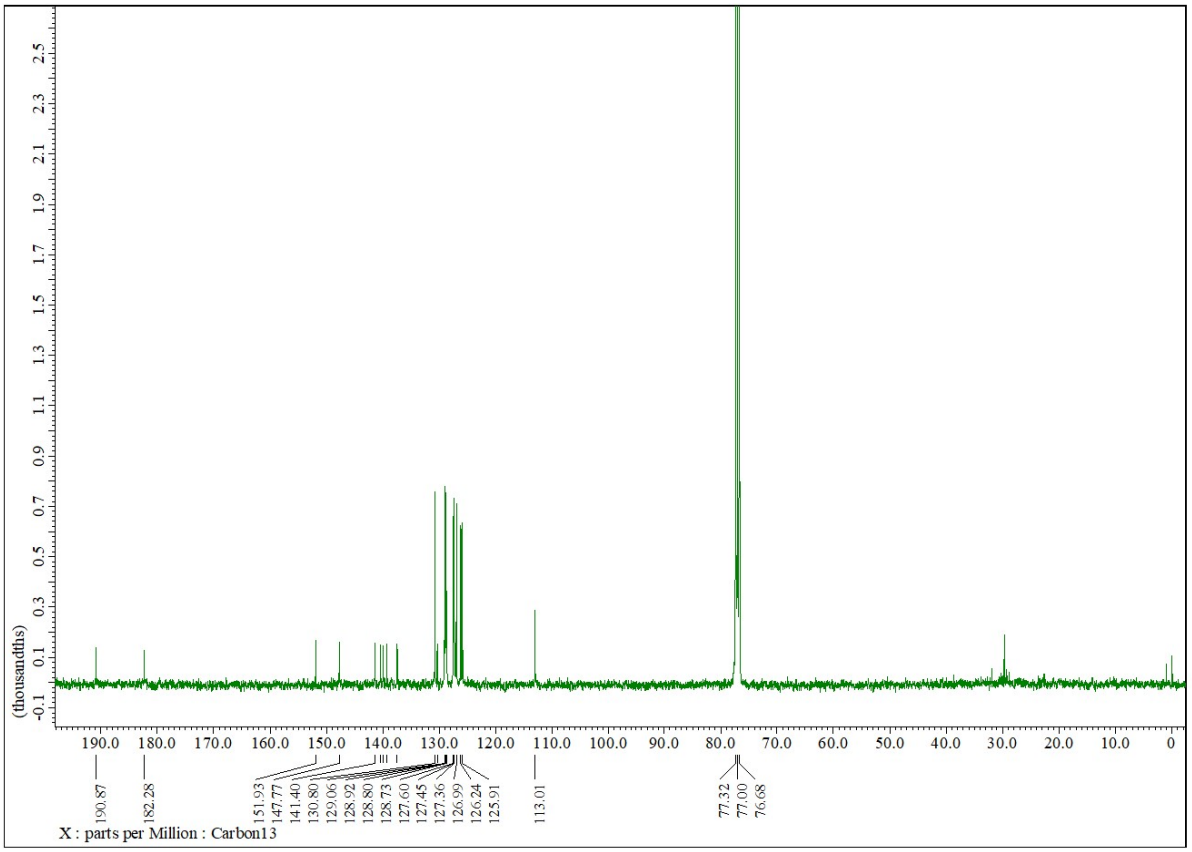
^{1}H NMR and ^{13}C NMR spectra of 1-(napthalen-2-yl)-2-(3-napthalen-2-yl)-1-phenyl-1*H*-pyrazol-5-yl)ethane-1,2-dione(4c)



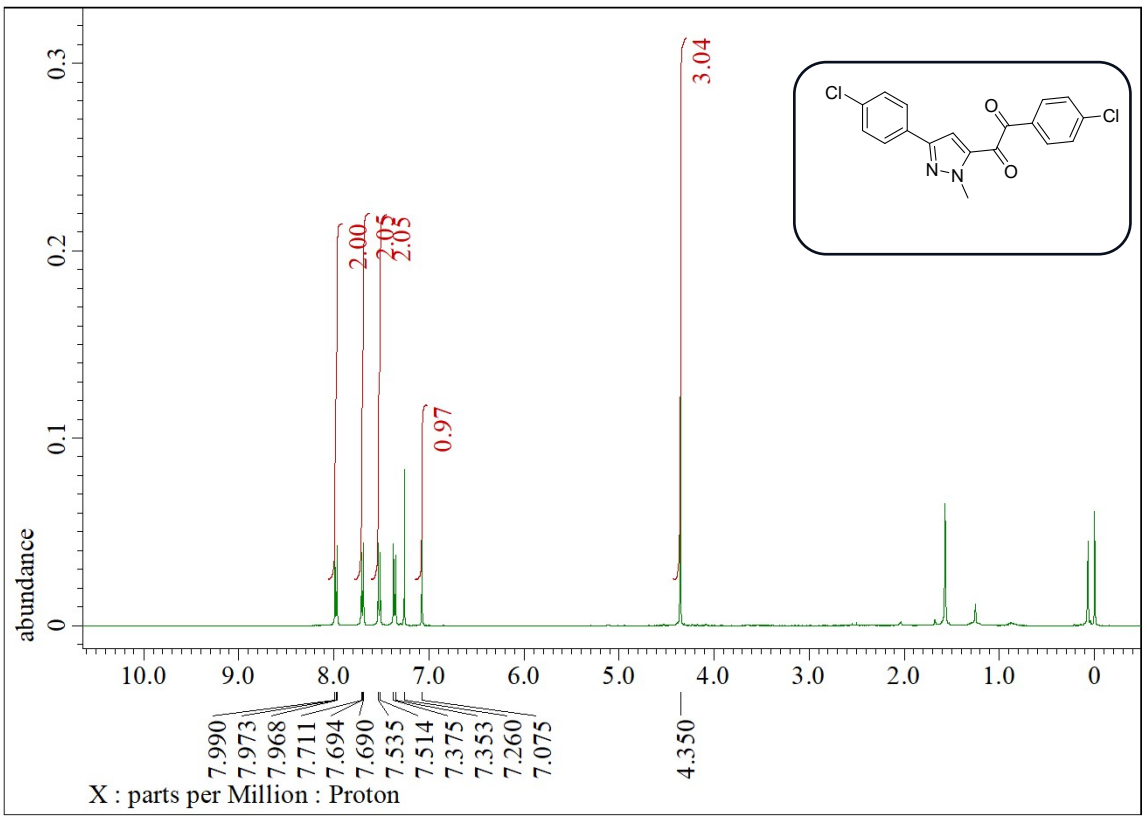


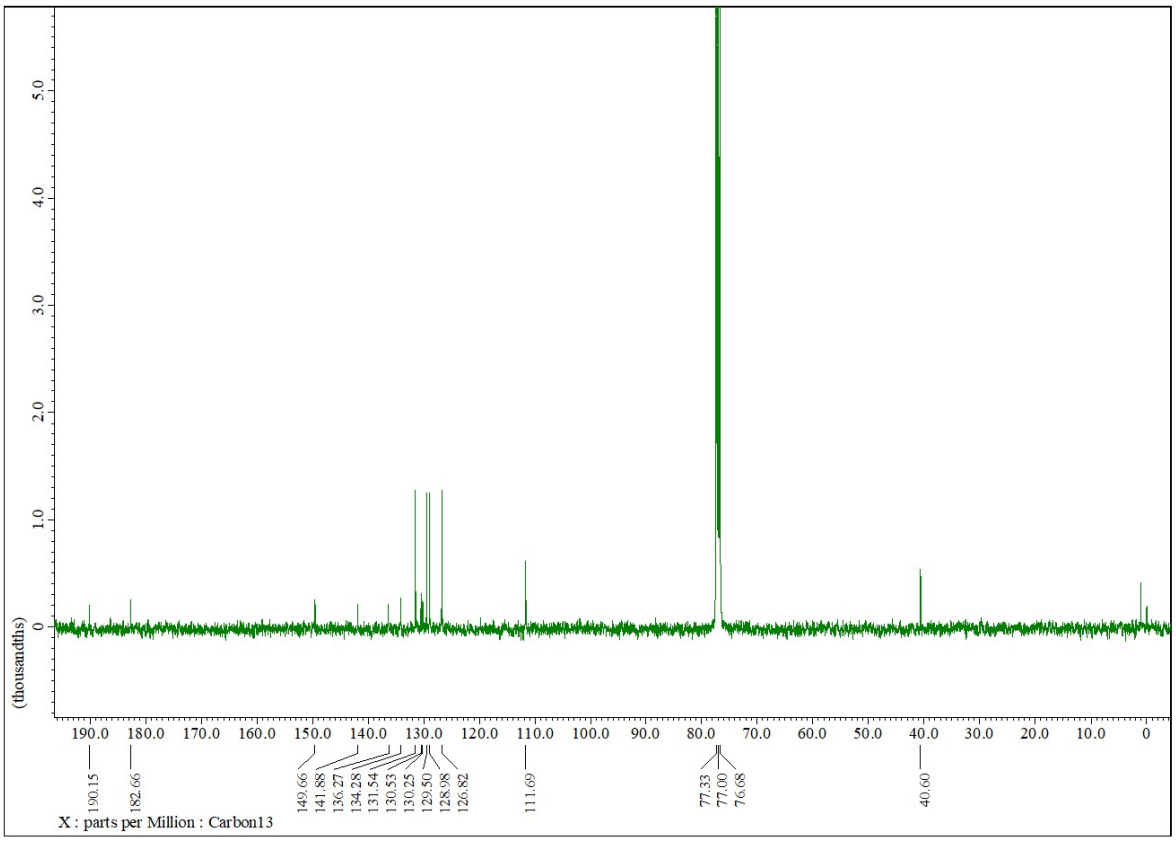
^{1}H NMR and ^{13}C NMR spectra of 1-([1,1-biphenyl]-4-yl)-2-(3-([1,1-biphenyl]-4-yl)-1-phenyl-1*H*-pyrazol-5-yl)ethane-1,2-dione (4d)



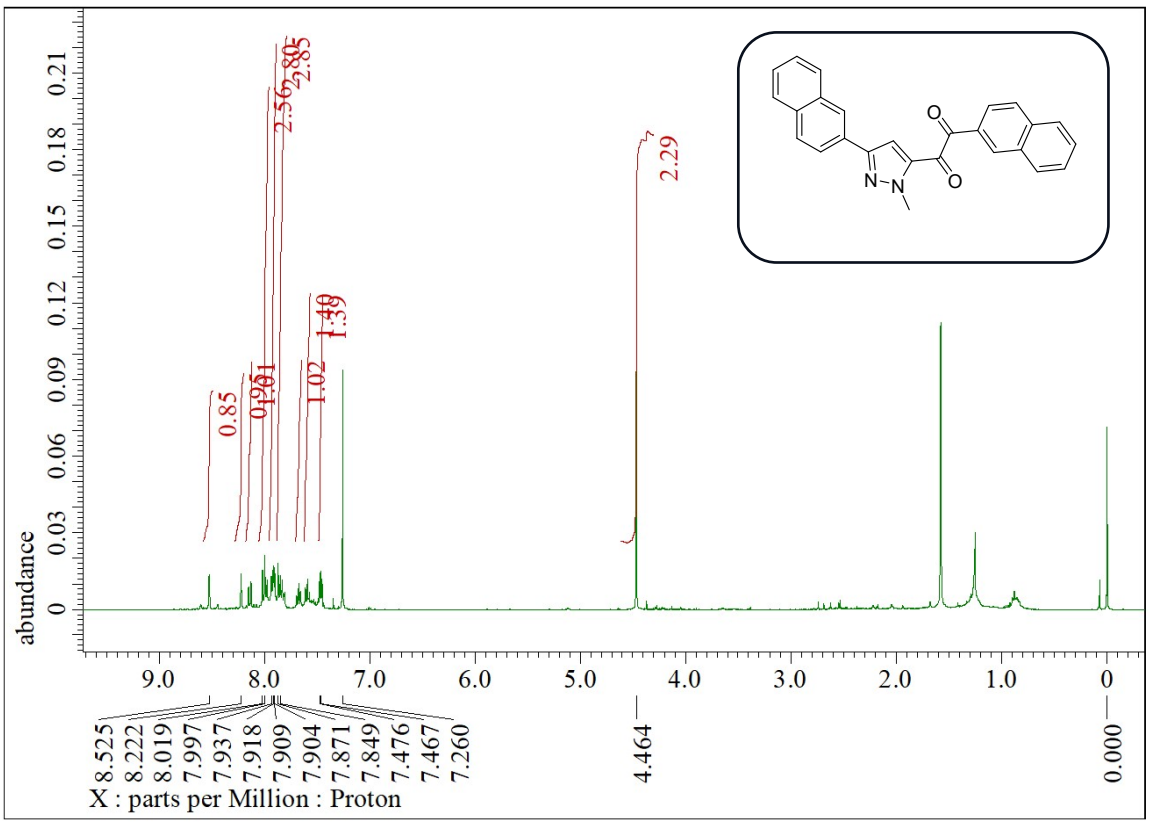


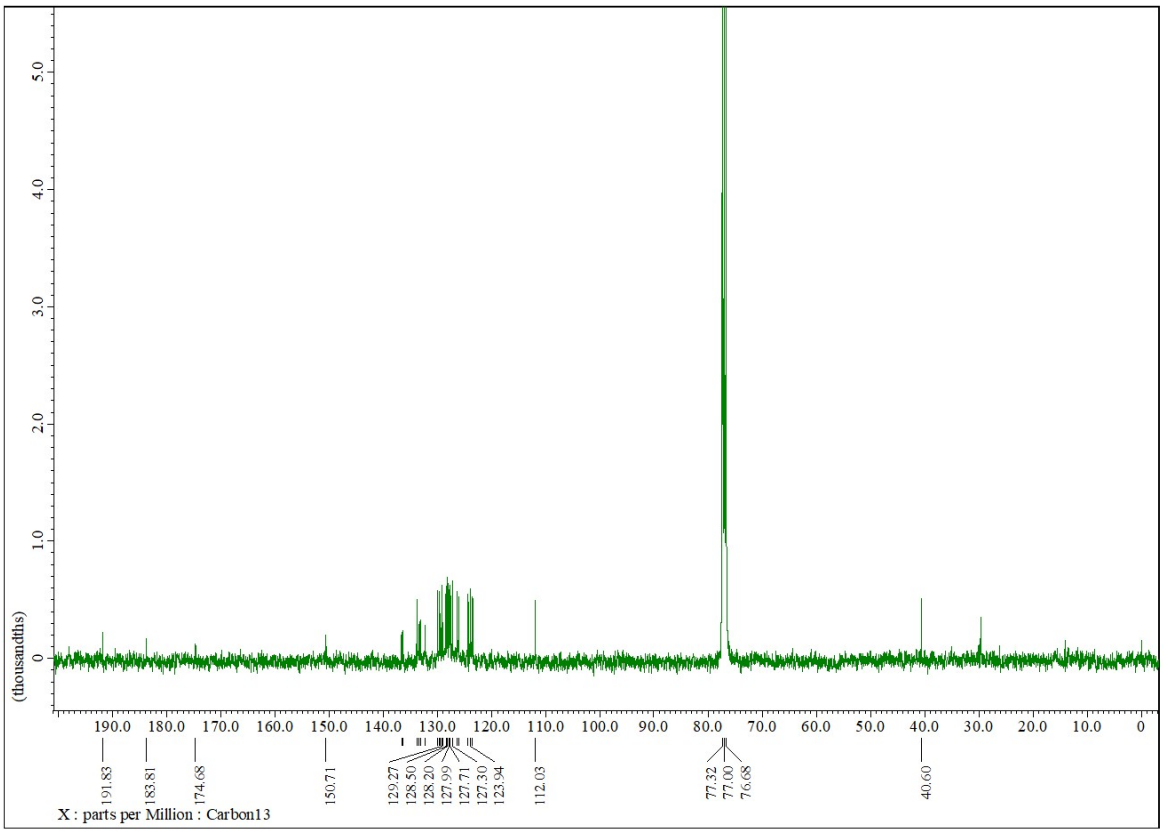
^{1}H NMR and ^{13}C NMR spectra of 1-(4-chlorophenyl)-2-(3-(4-chlorophenyl)-1-methyl-1*H*-pyrazol-5-yl)ethane-1,2-dione (4e)



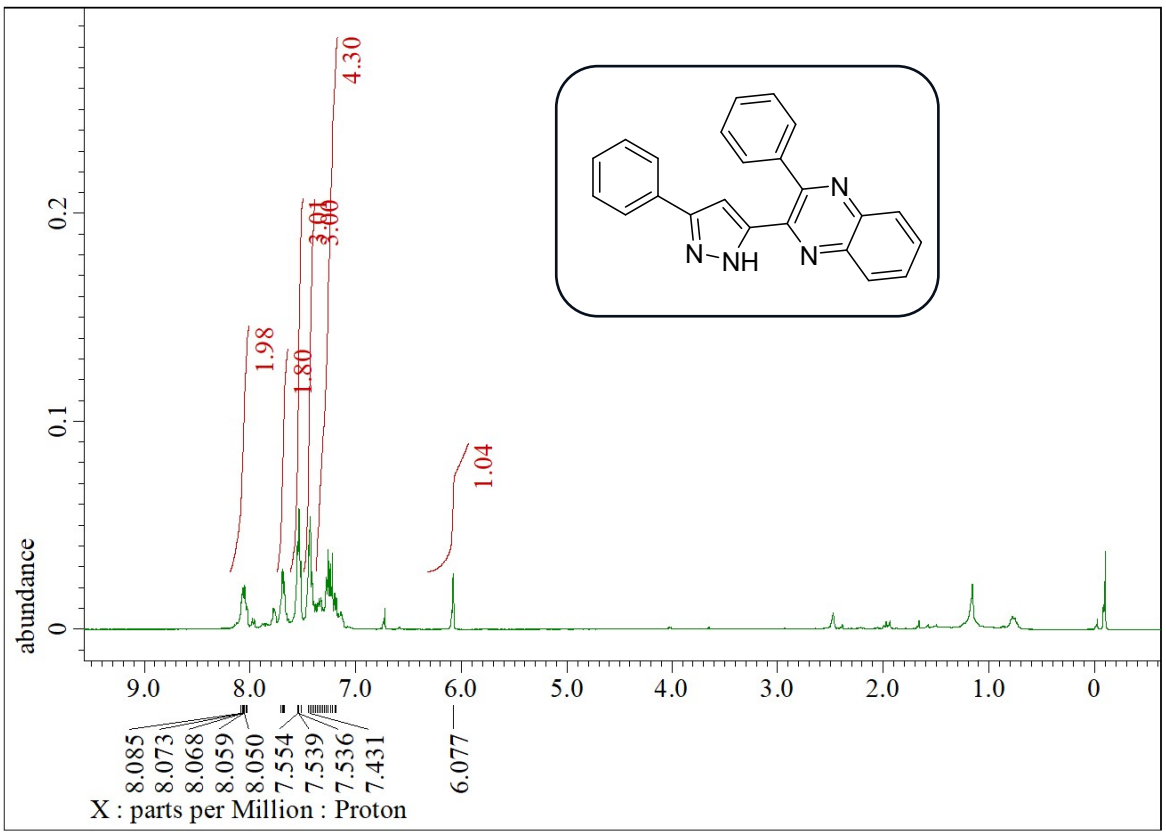


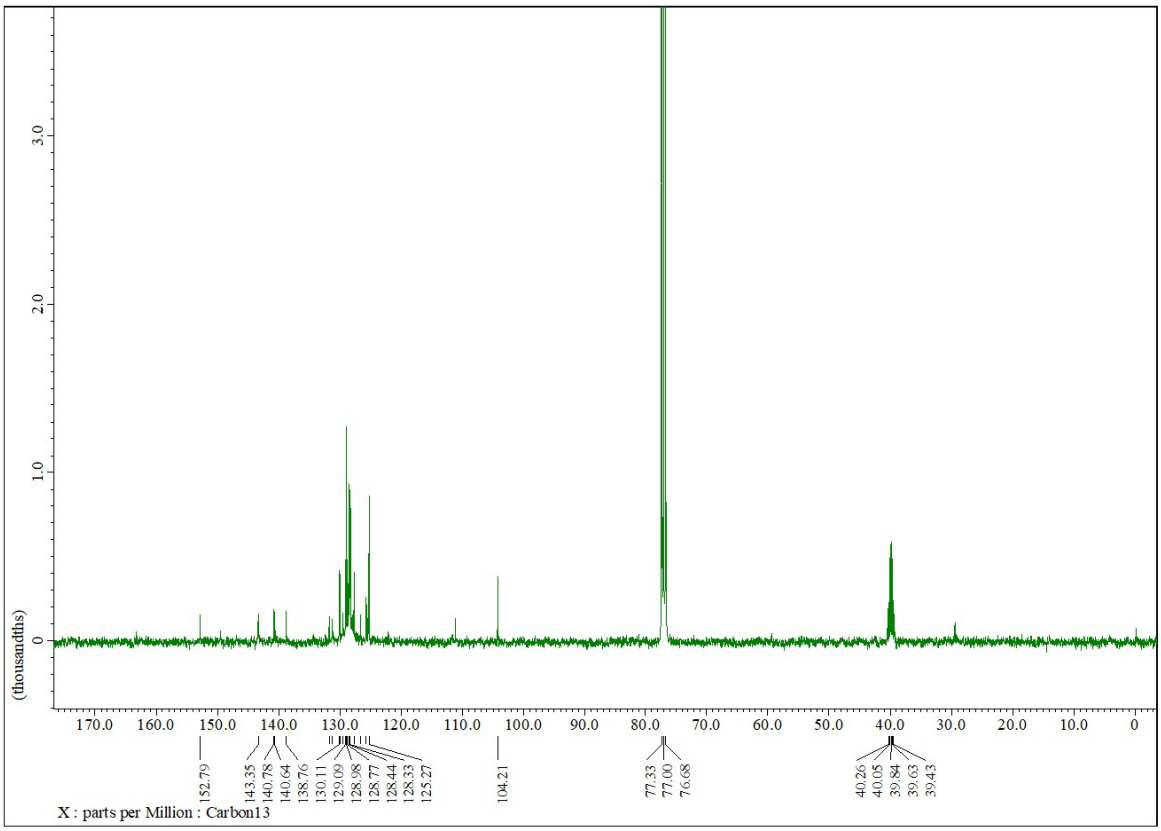
^{1}H NMR and ^{13}C NMR spectra of 1-(1-methyl-3-(napthalen-2-yl)-1*H*-pyrazol-5yl)-2-(napthalen-2-yl)ethane-1,2-dione (4f)



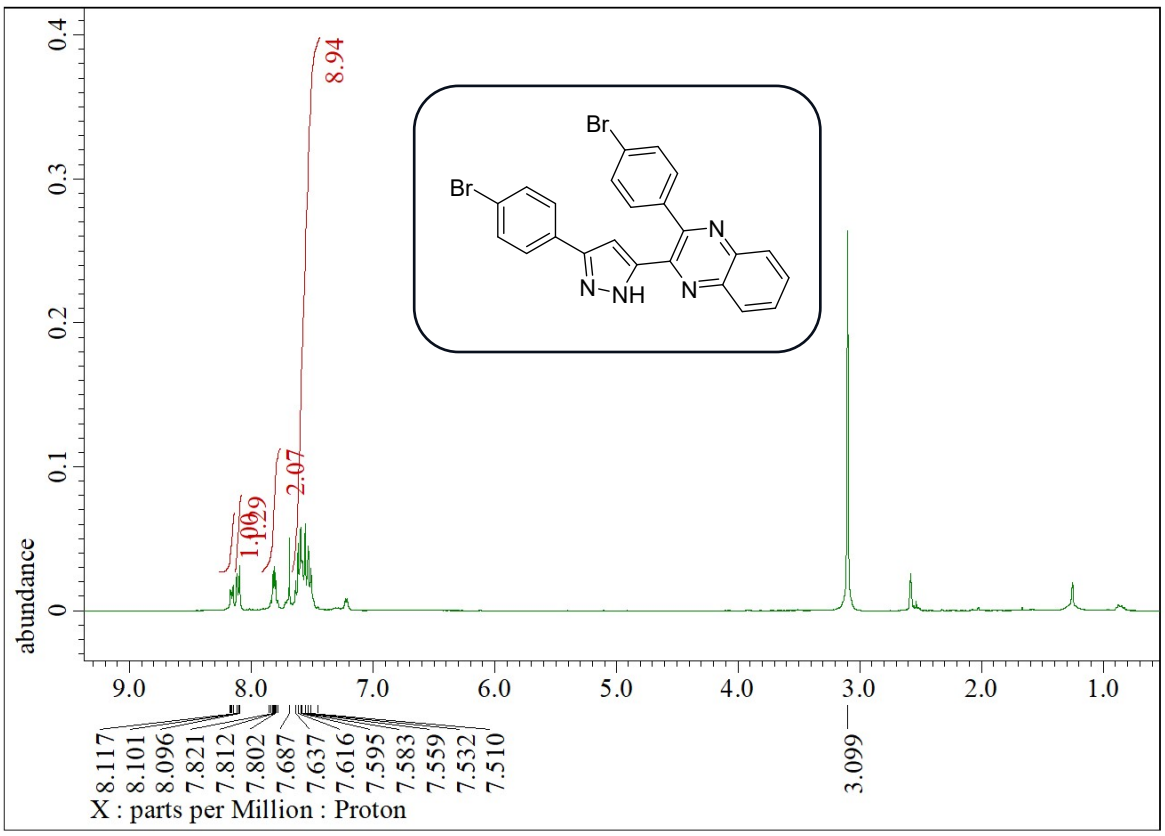


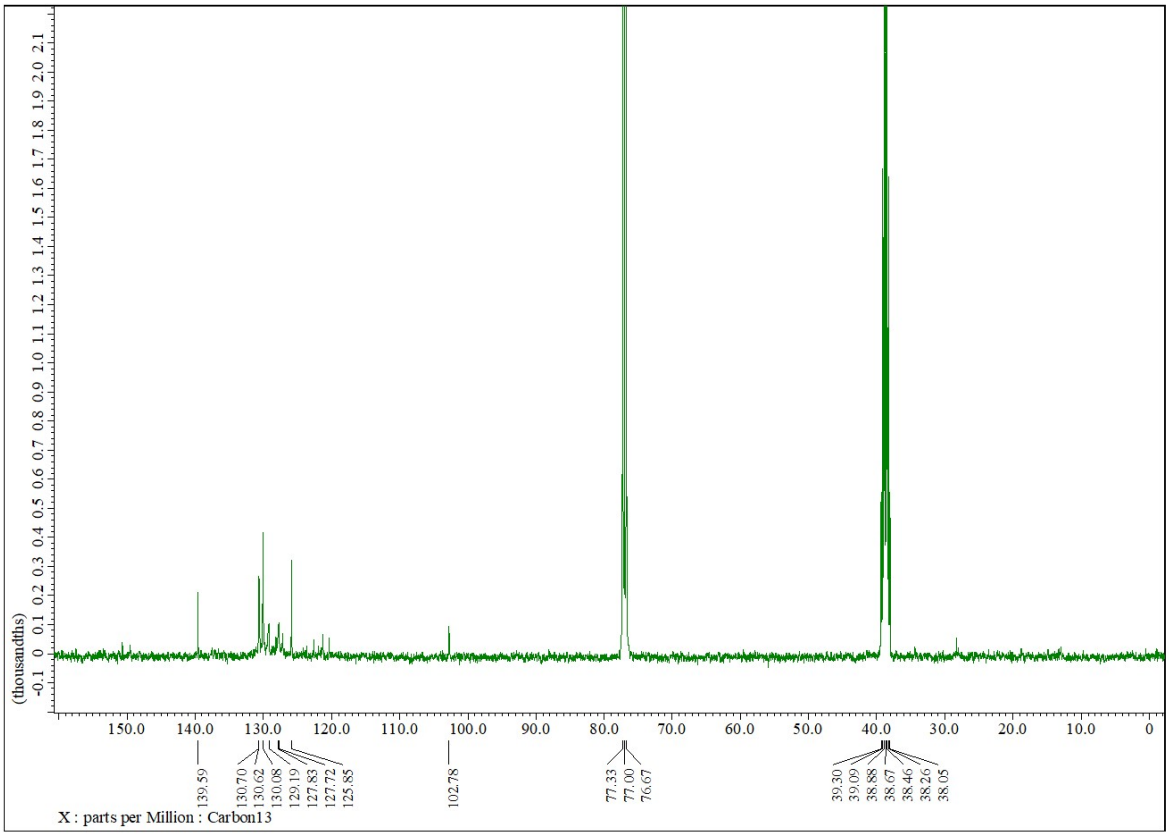
^{1}H NMR and ^{13}C NMR spectra of 2-phenyl-3-(3-phenyl-1*H*-pyrazol-5-yl) quinoxaline (5a)



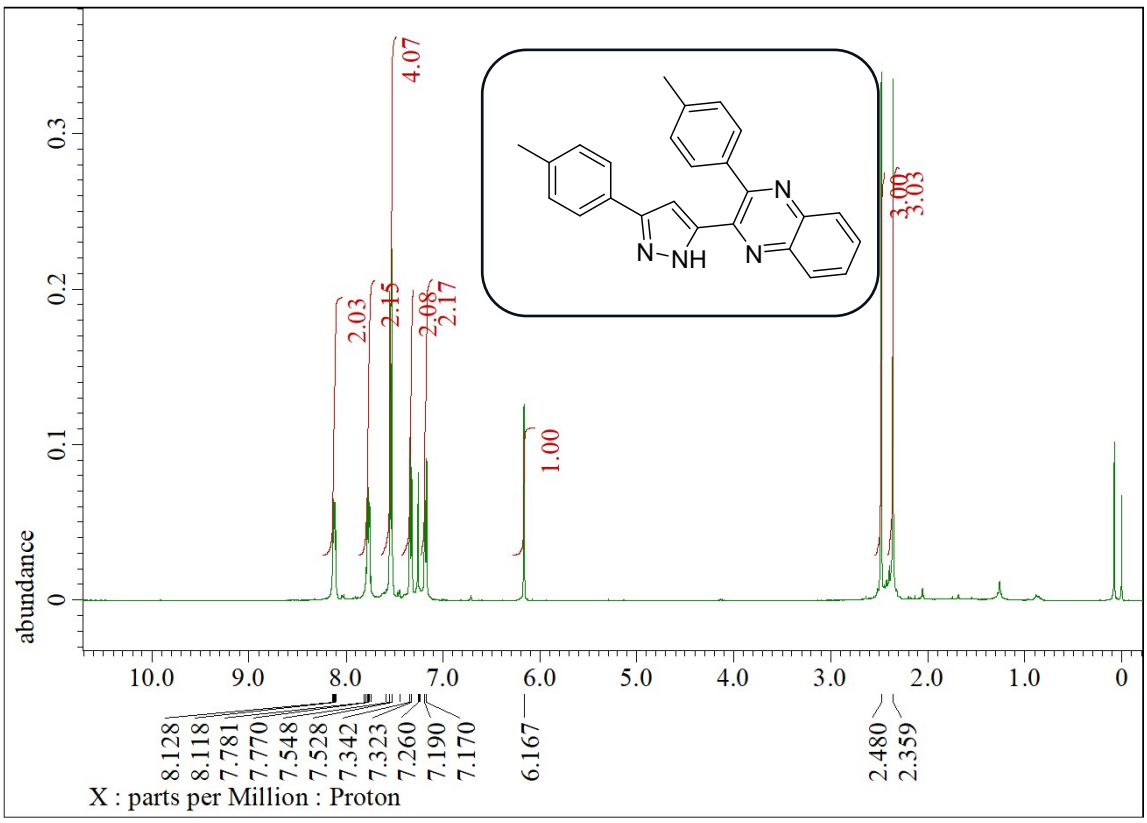


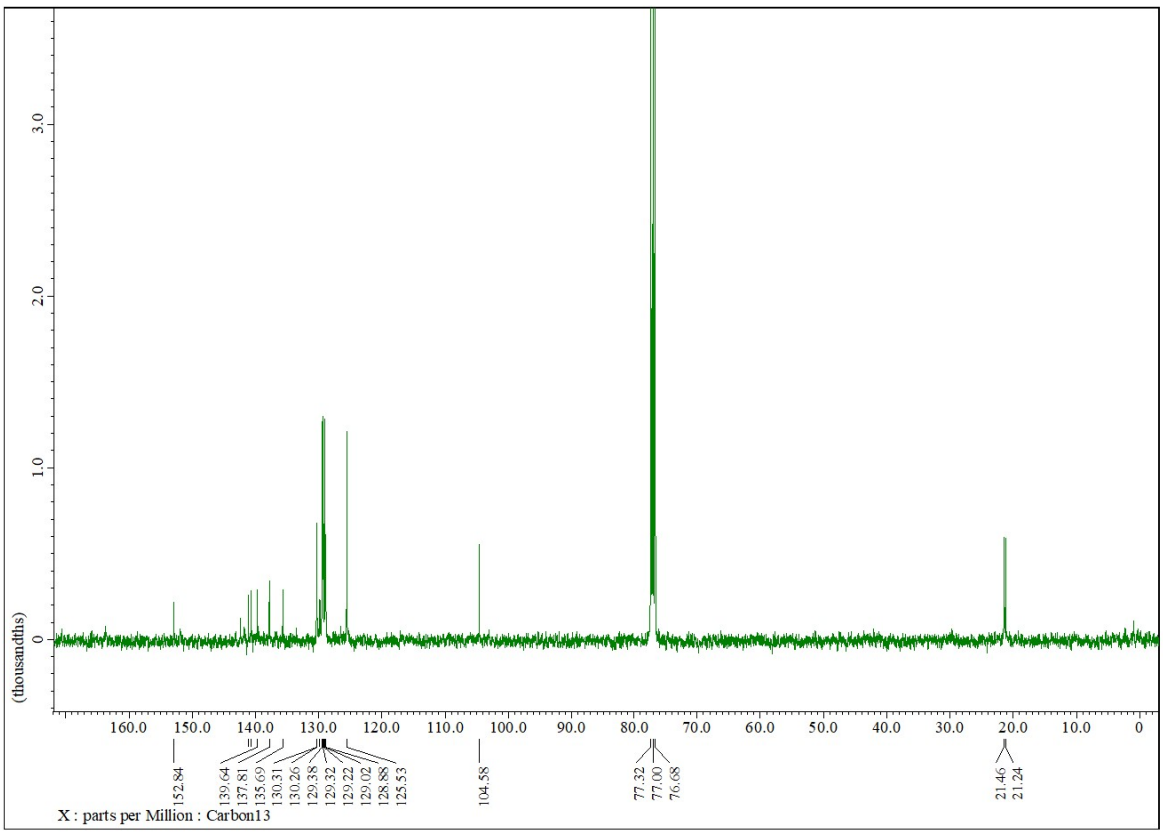
^{1}H NMR and ^{13}C NMR spectra of 2-(4-bromophenyl)-3-(3-(4-bromophenyl)-1*H*-pyrazol-5-yl)quinoxaline (5b)



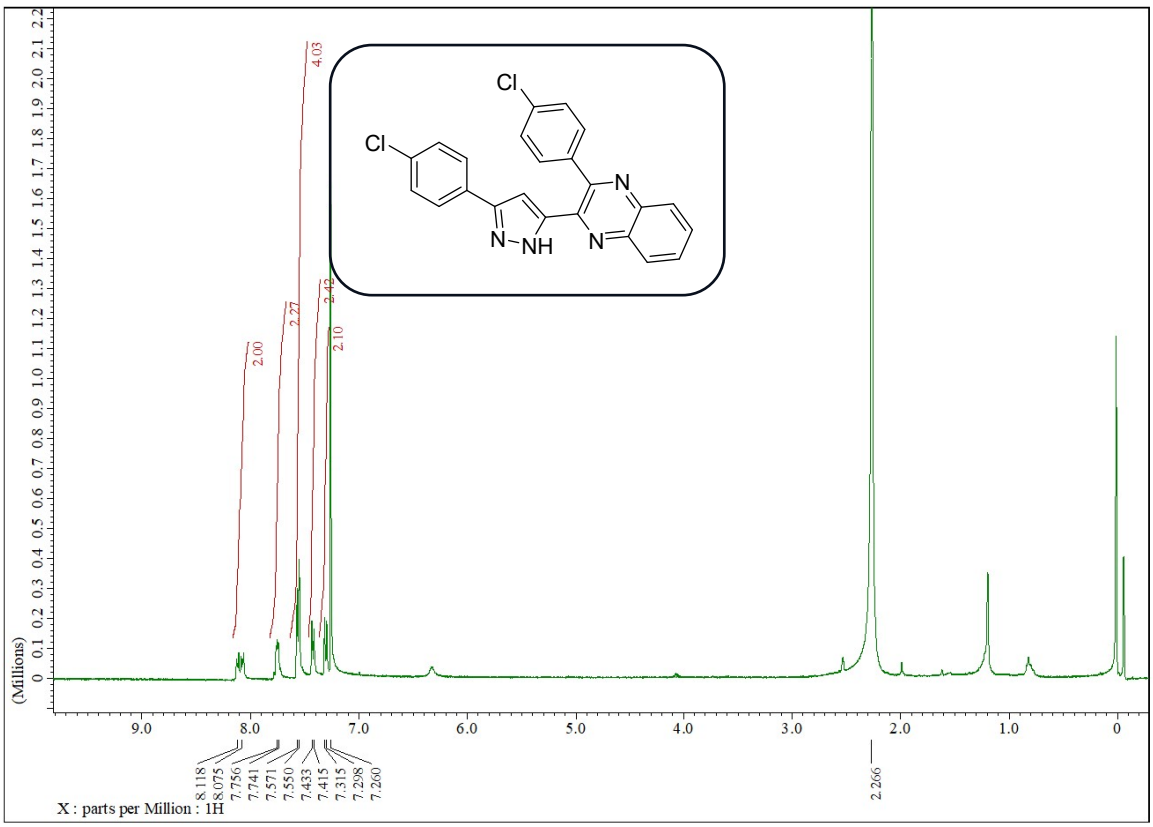


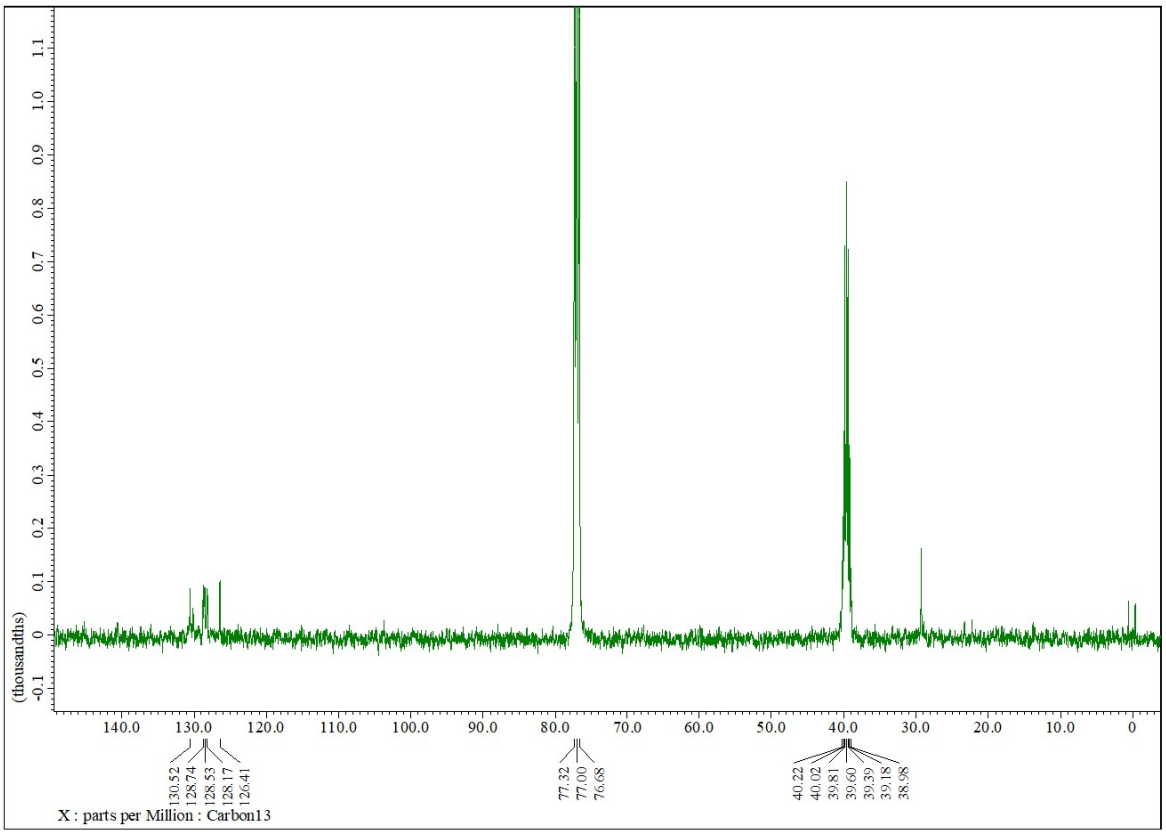
^{1}H NMR and ^{13}C NMR spectra of 2-(p-tolyl)-3-(3-(p-tolyl)-1*H*-pyrazol-5-yl)quinoxaline (5c)



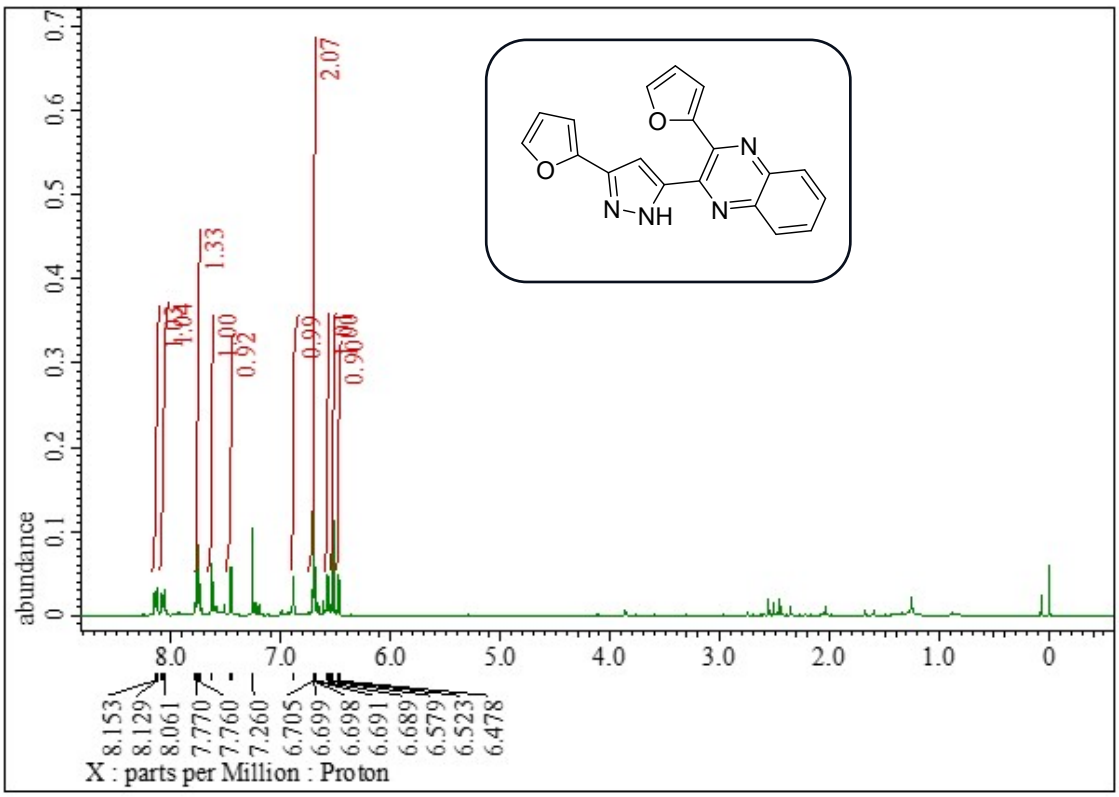


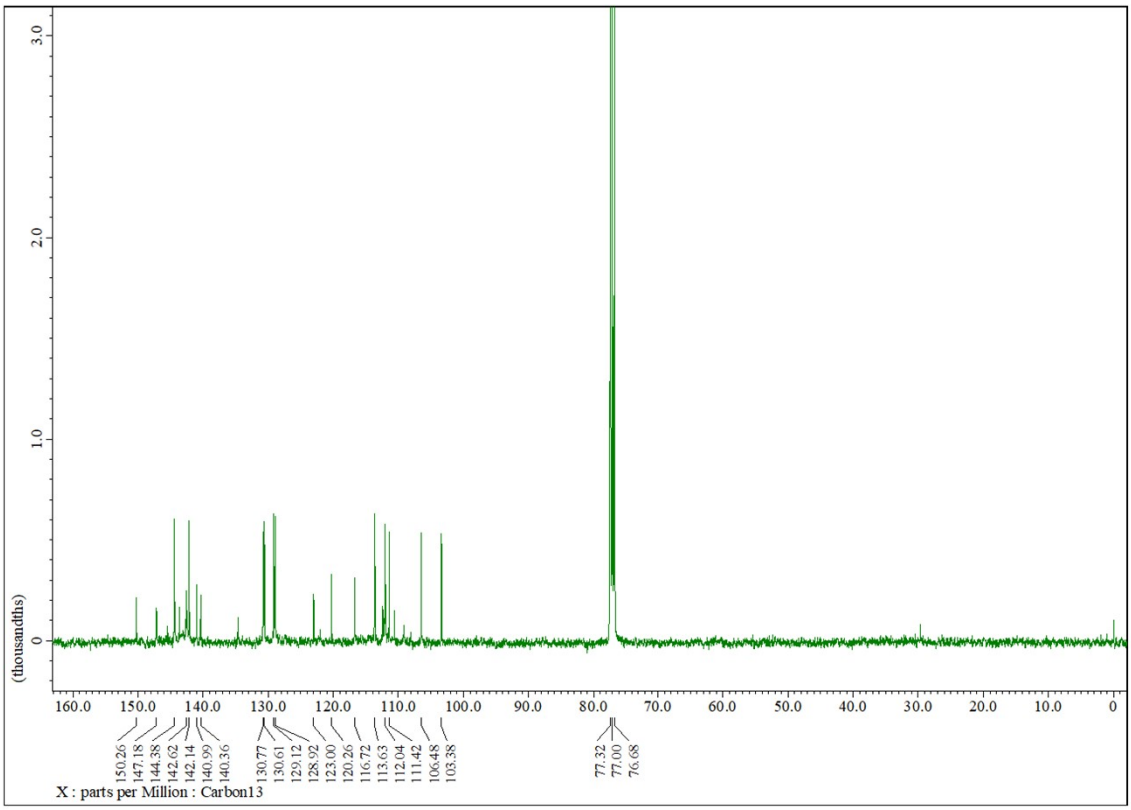
^{1}H NMR and ^{13}C NMR spectra of 2-(4-chlorophenyl)-3-(3-(4-chlorophenyl)-1*H*-pyrazol-5-yl)quinoxaline (5d)





^{1}H NMR and ^{13}C NMR spectra of 2-(furan-2-yl)-3-(3-(furan-2-yl)-1*H*-pyrazol-5-yl)quinoxaline (5e)





^{1}H NMR and ^{13}C NMR spectra of 2-(3-bromophenyl)-3-(3-(3-bromophenyl)-1*H*-pyrazol-5-yl)quinoxaline (5f)