

Supplementary Material

An efficient and convenient approach for the synthesis of novel pyrazolo[1,2-*a*]triazole-triones and evaluation of their antimicrobial activities

Pooja Saluja,^A Jitender M. Khurana,^{A,C} Chetan Sharma^B and Kamal R. Aneja^B

^ADepartment of Chemistry, University of Delhi, Delhi 110007, India

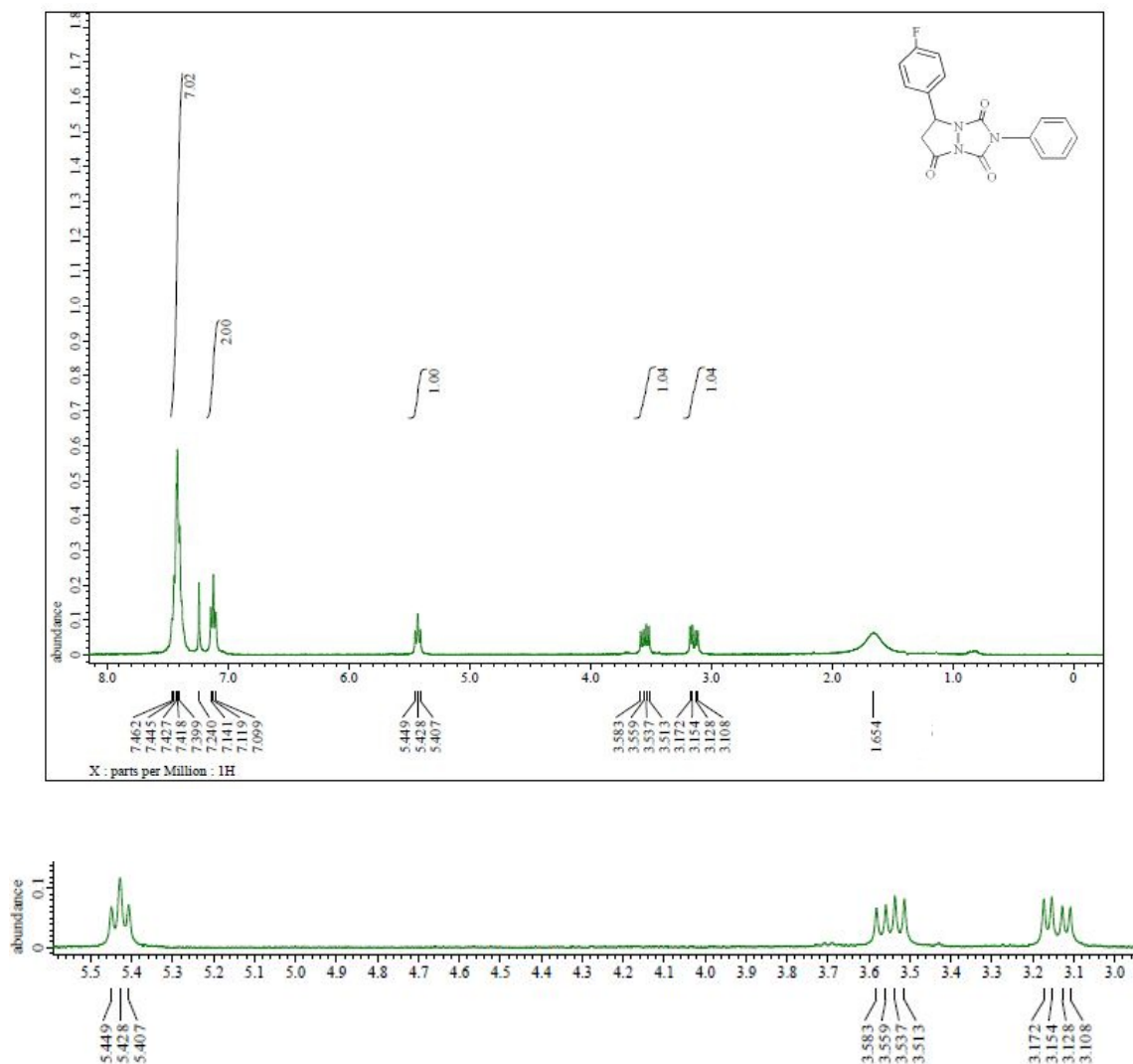
^BDepartment of Microbiology, Kurukshetra University, Kurukshetra 136119, Haryana, India

^CCorresponding author. Tel.: +91 11 27667725-1384; E-mail: jmkhurana1@yahoo.co.in

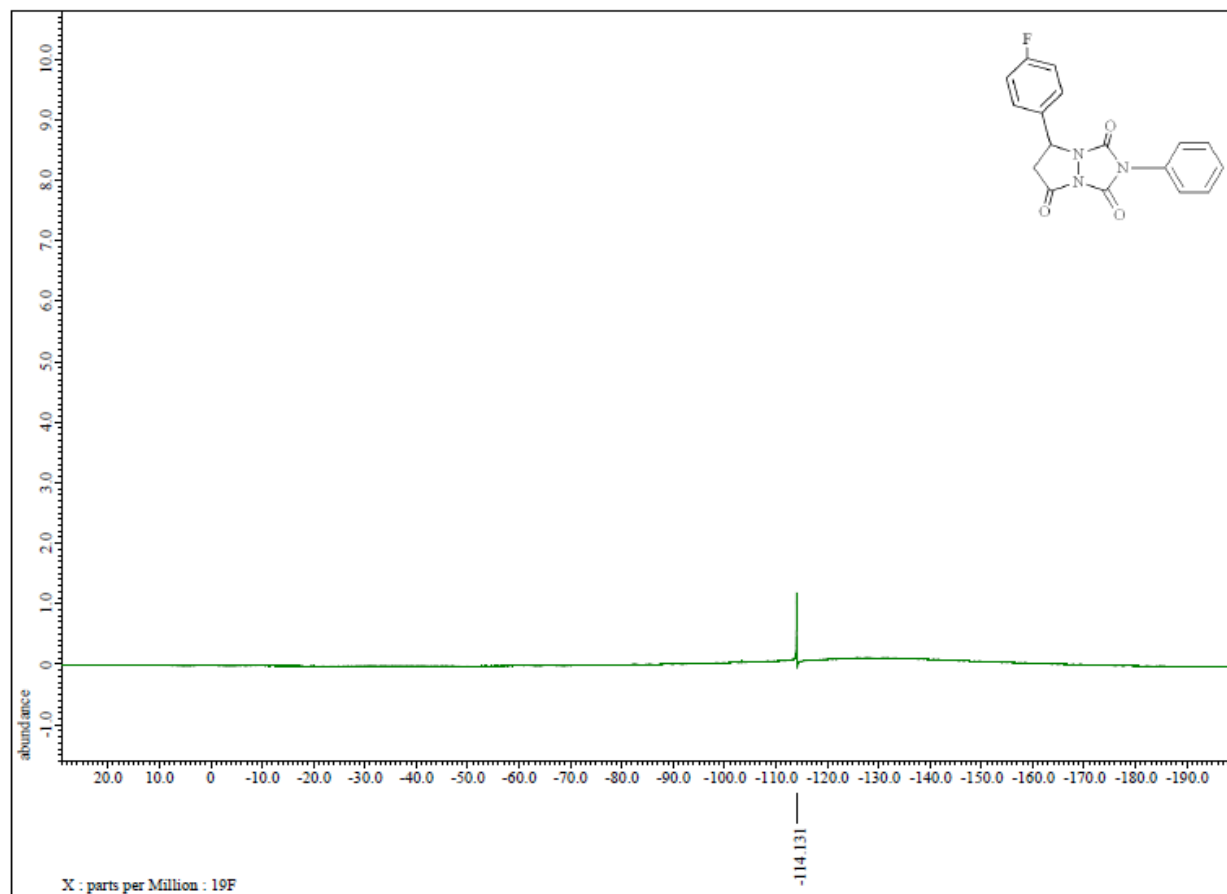
Spectral data:

7-(4-fluorophenyl)-2-phenyldihydropyrazolo[1,2-*a*][1,2,4]triazole-1,3,5(2*H*)-trione (*IIa*)

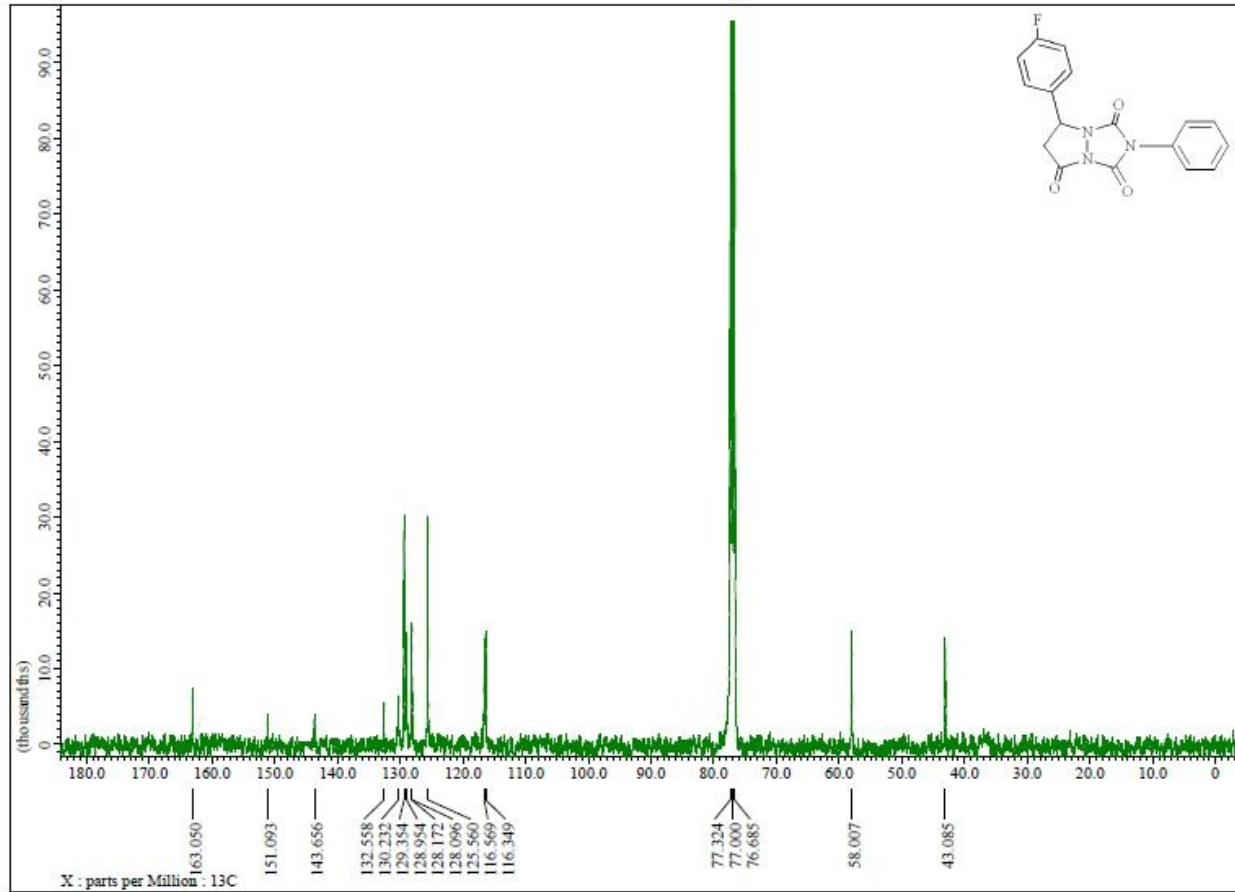
¹H NMR of *IIa* in Chloroform-*d*



^{19}F NMR of IIa in DMSO-d_6

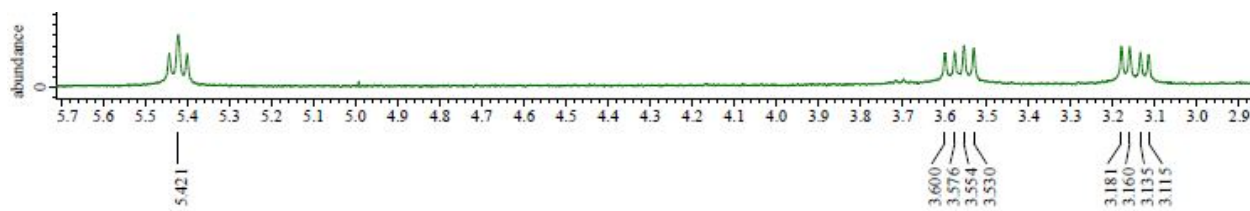
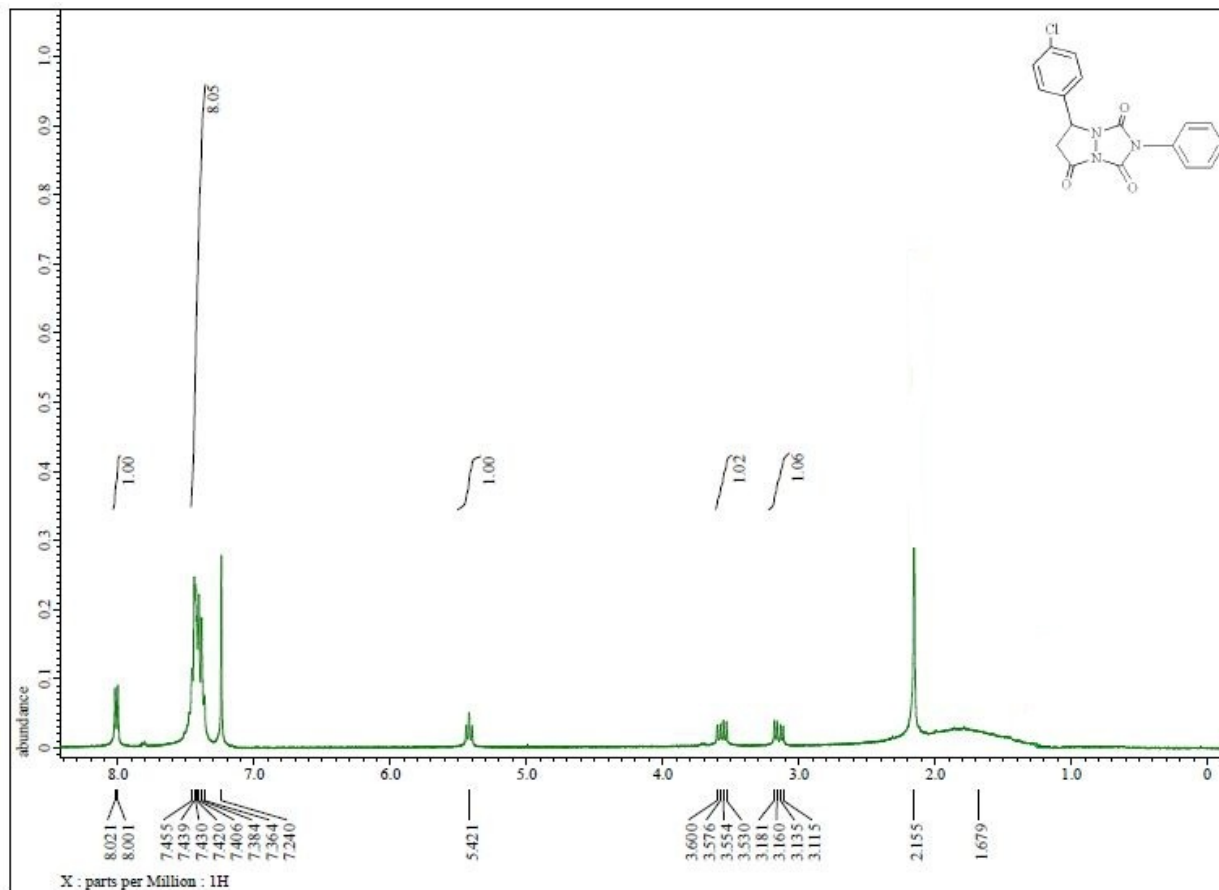


¹³C NMR of IIa in Chloroform-d

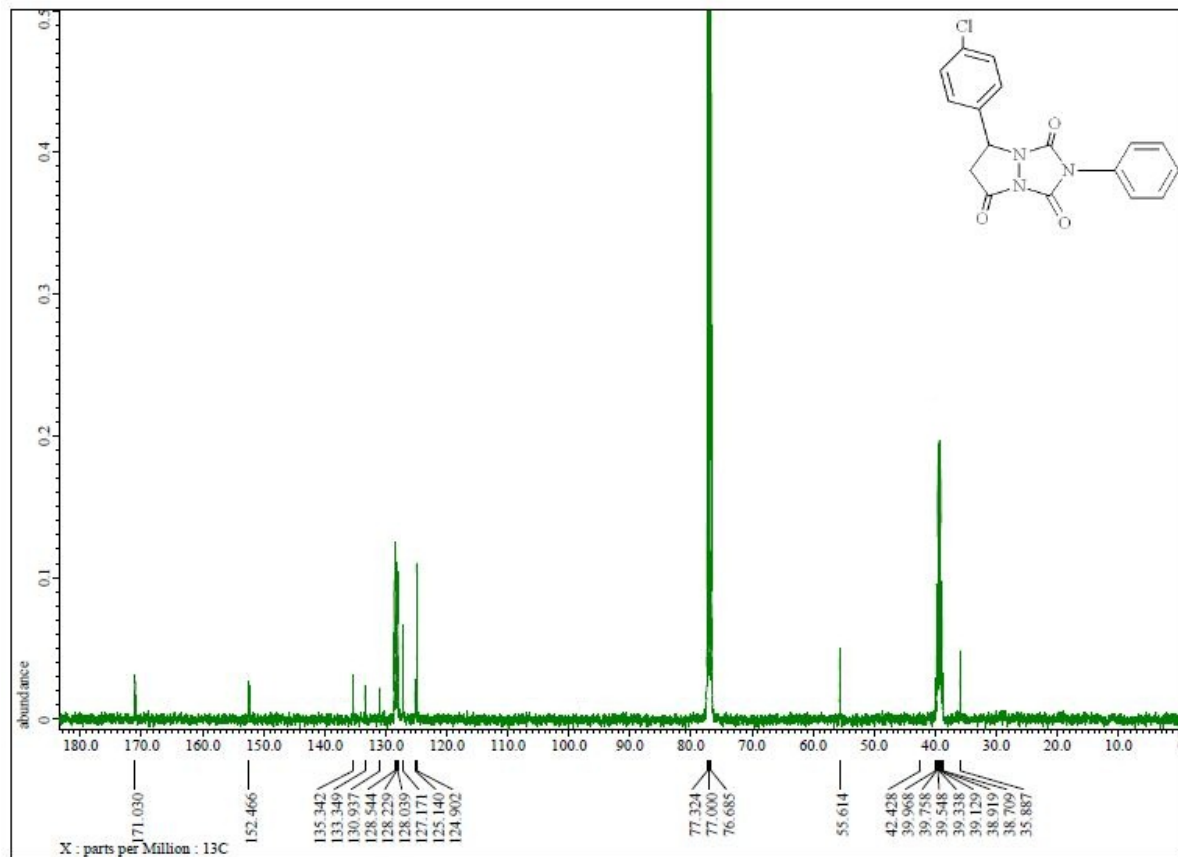


7-(4-chlorophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (Iib)

¹H NMR of Iib in Chloroform-d



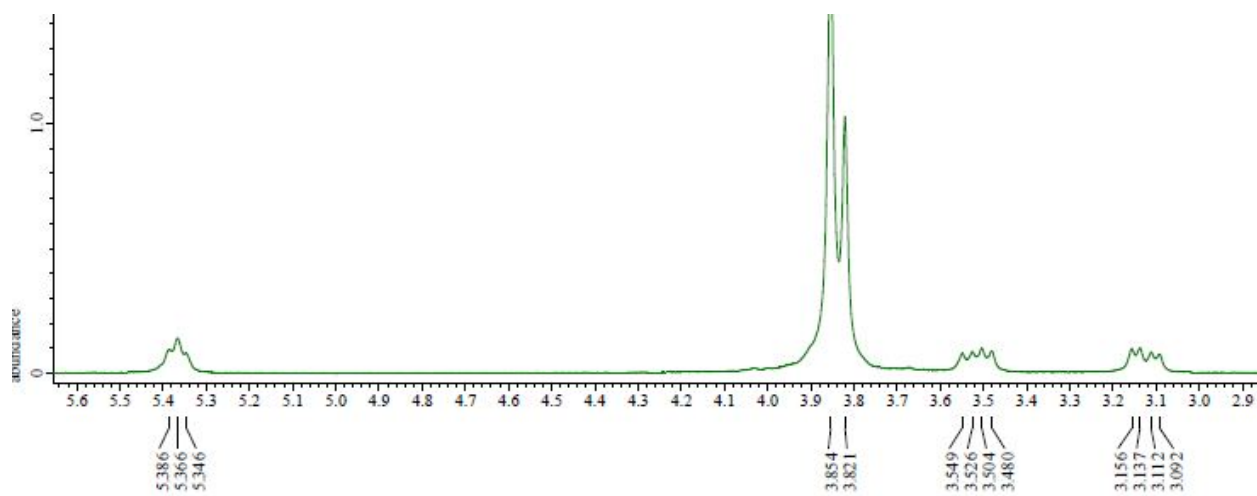
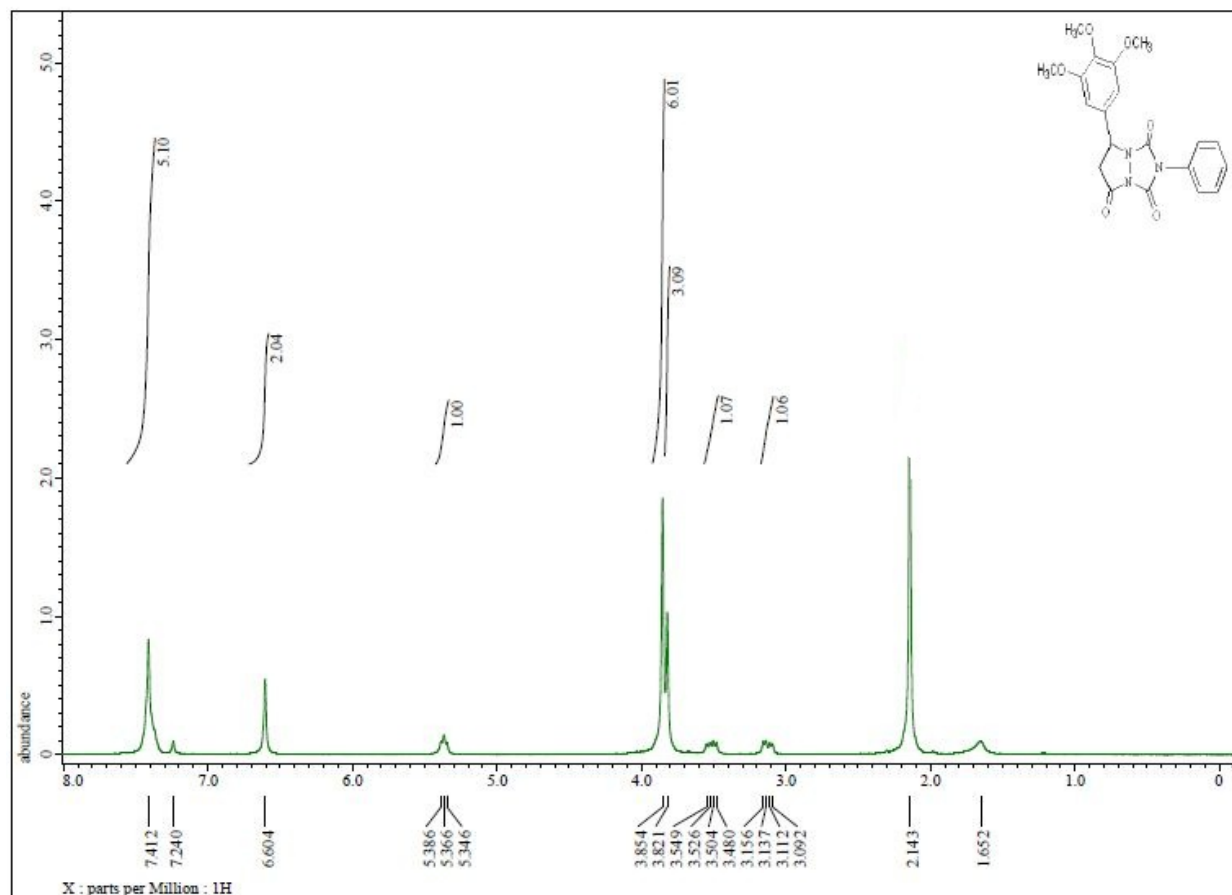
¹³C NMR of IIb in Chloroform-d + DMSO-d₆



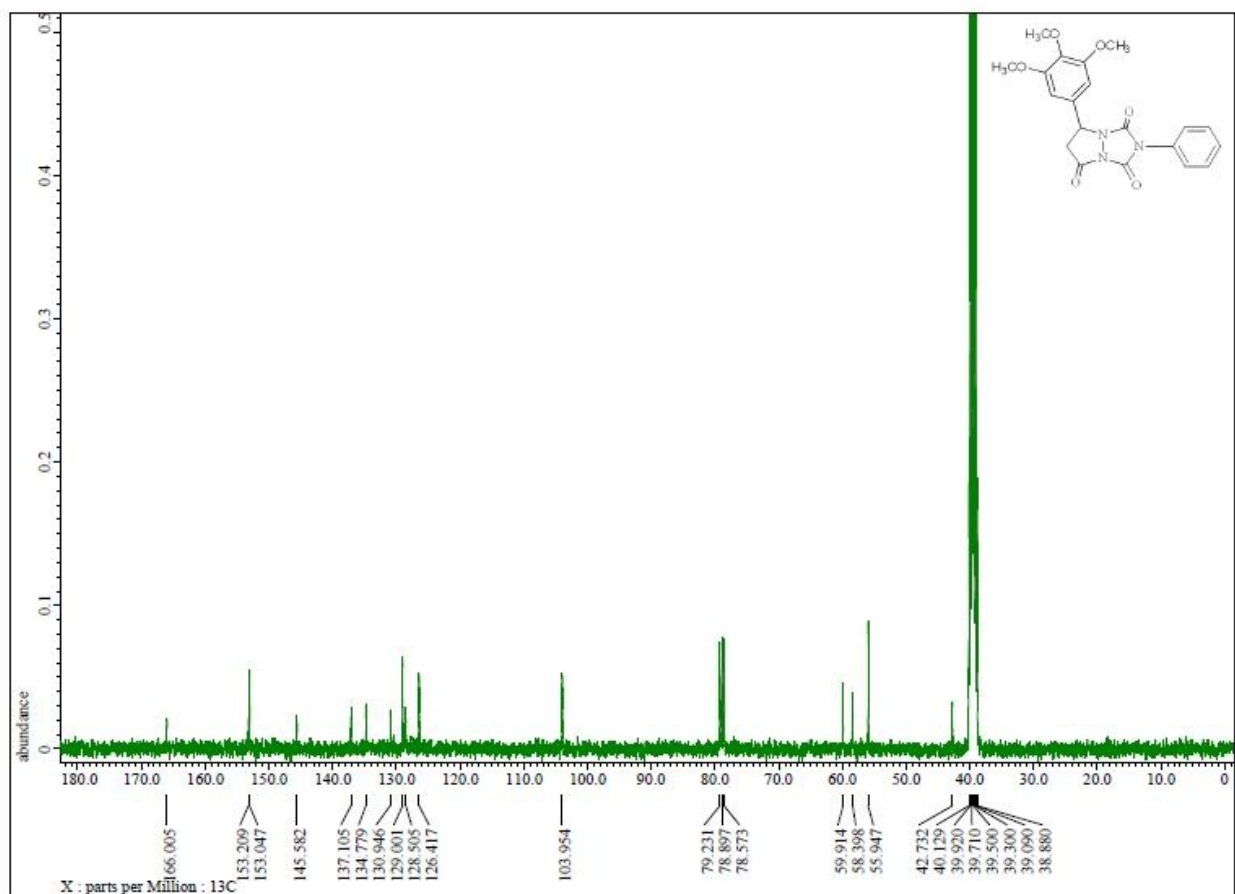
2-phenyl-7-(3,4,5-trimethoxyphenyl)dihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione

(IIc)

¹H NMR of IIc in Chloroform-d

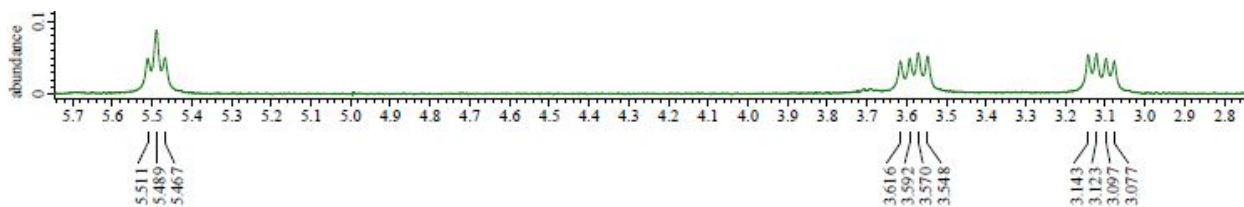
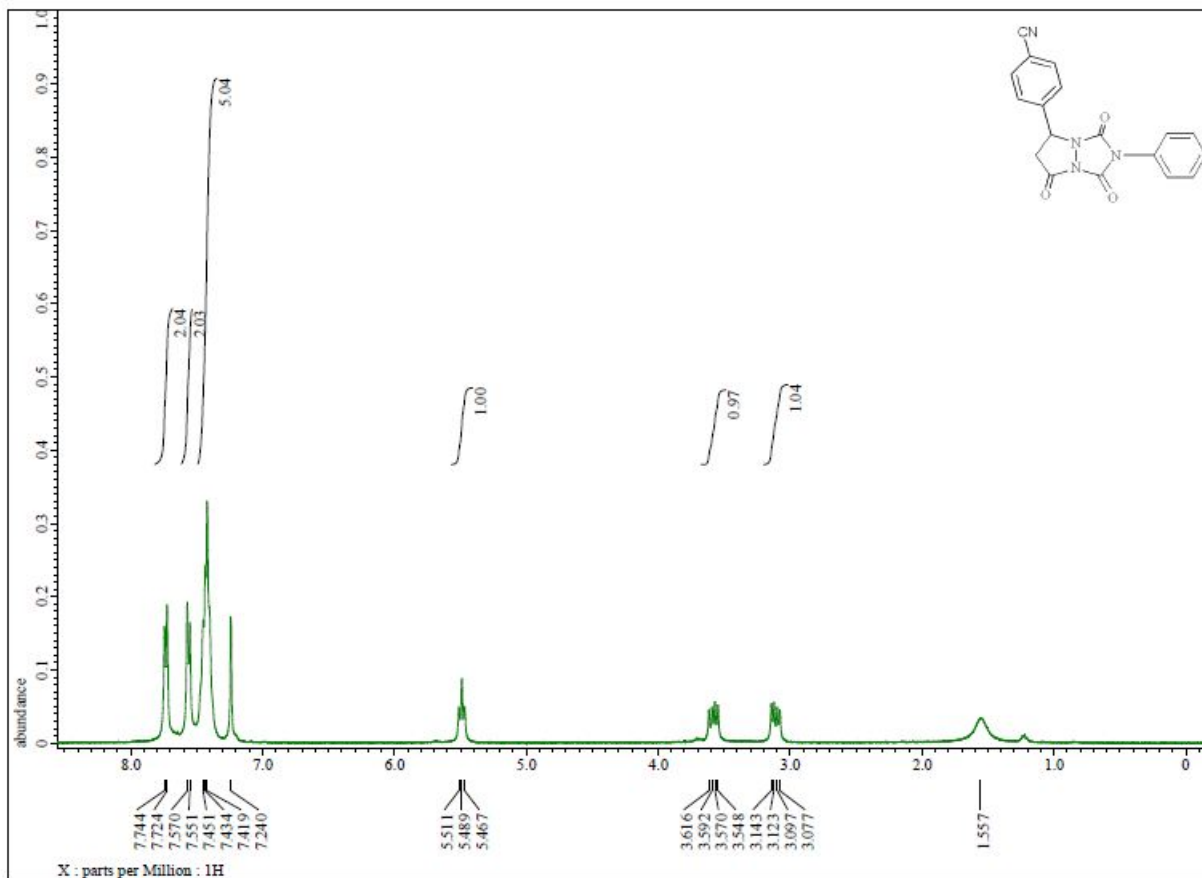


^{13}C NMR of IIc in Chloroform- d_3 + DMSO- d_6

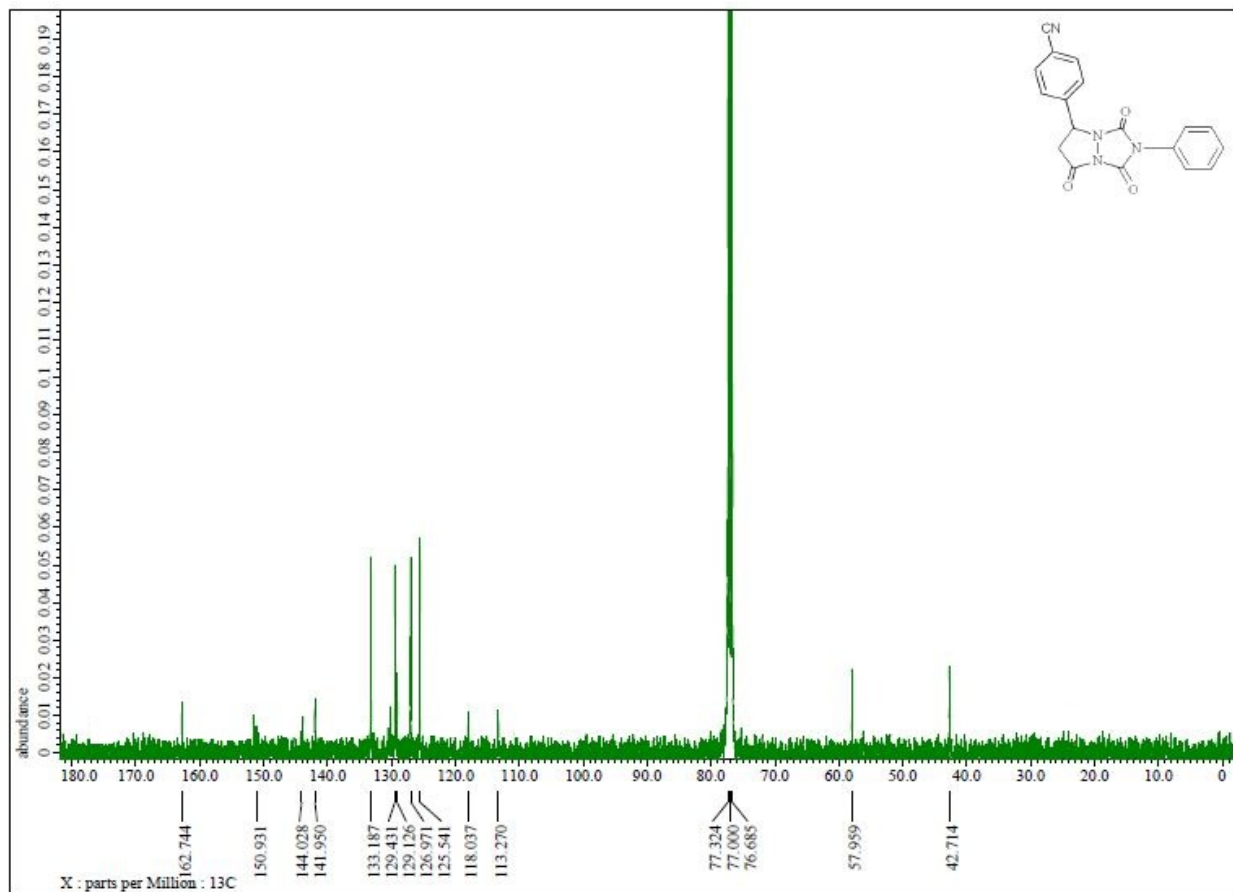


4-(1,3,7-trioxo-2-phenylhexahydropyrazolo[1,2-a][1,2,4]triazol-5-yl)benzonitrile (IId)

¹H NMR of IId in Chloroform-d

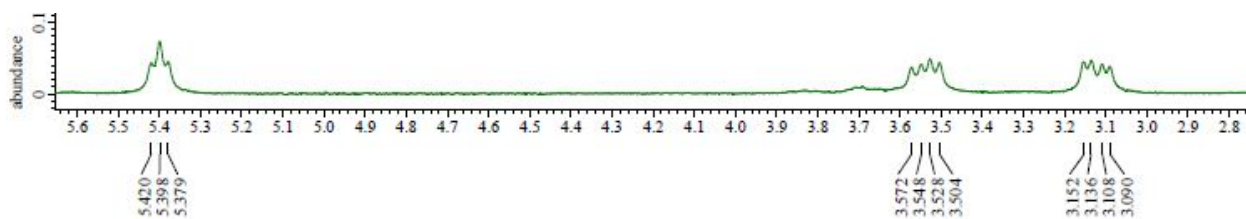
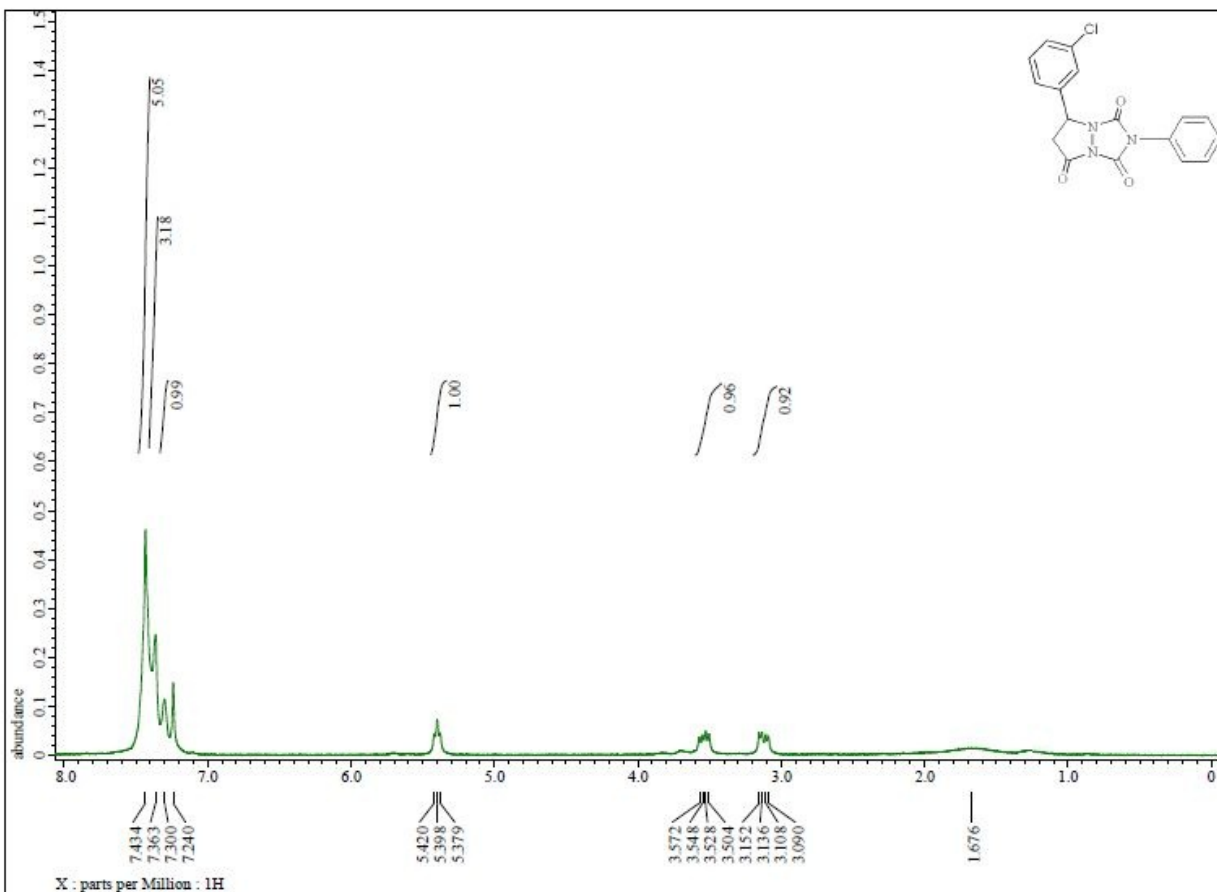


¹³C NMR of IId in Chloroform-d

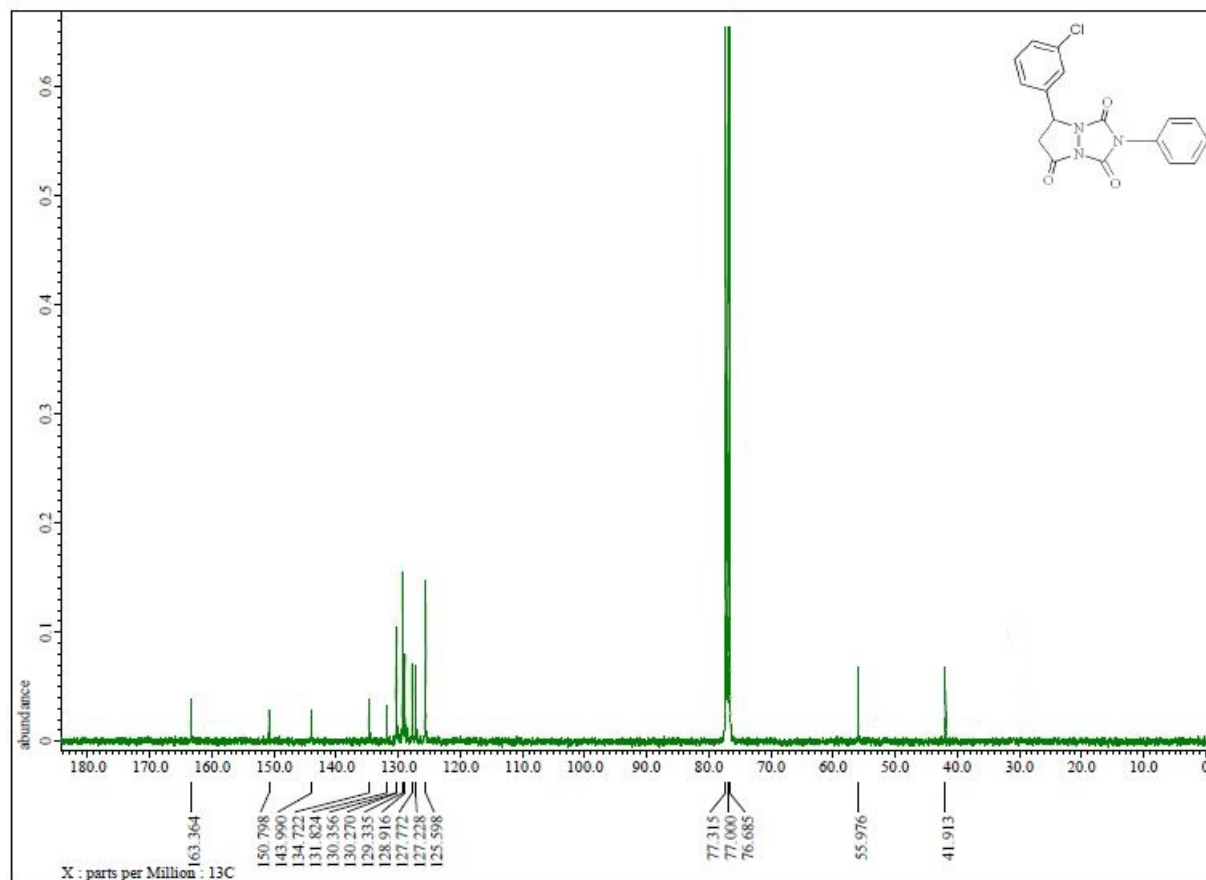


7-(3-chlorophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIe)

¹H NMR of IIe in Chloroform-d

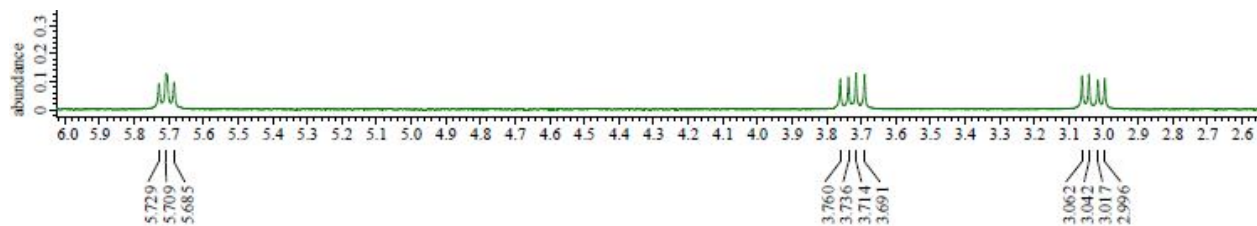
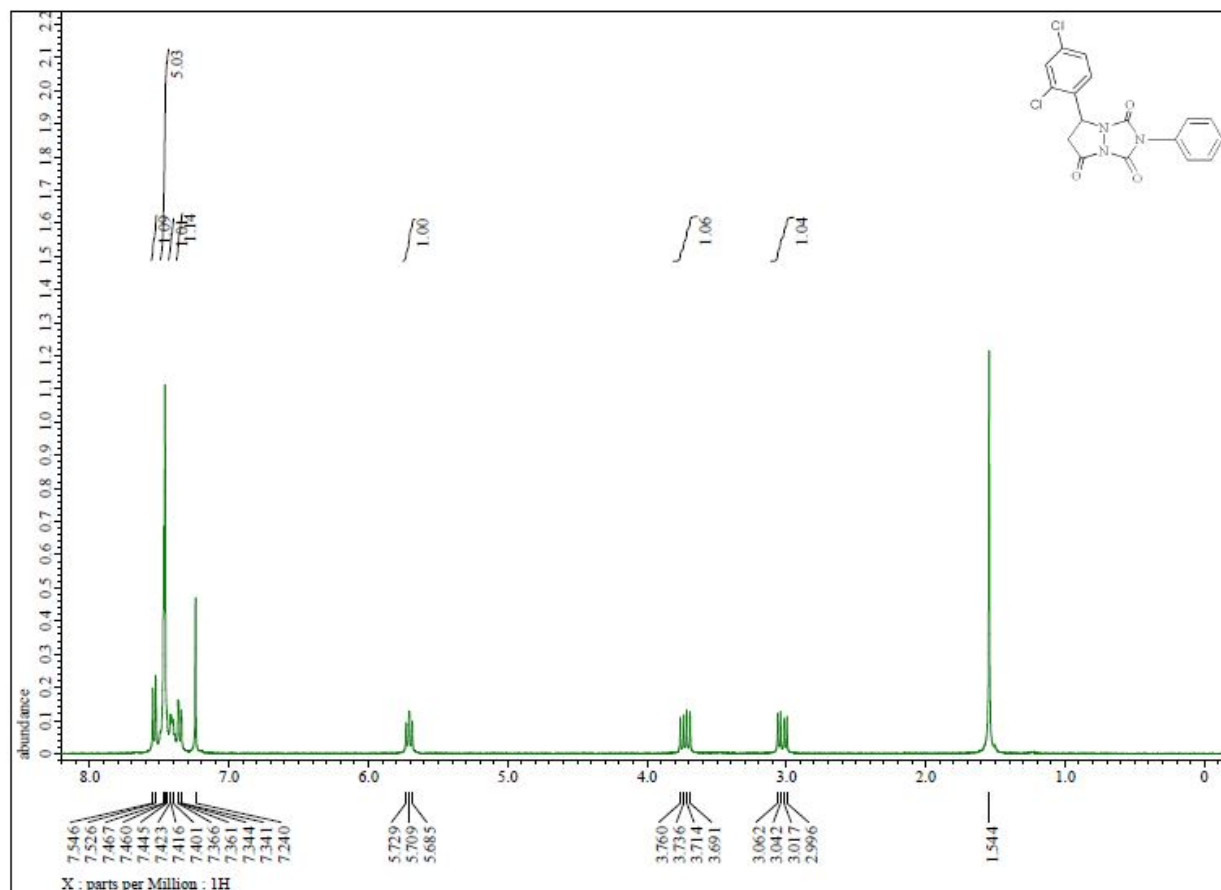


¹³C NMR of IIe in Chloroform-d

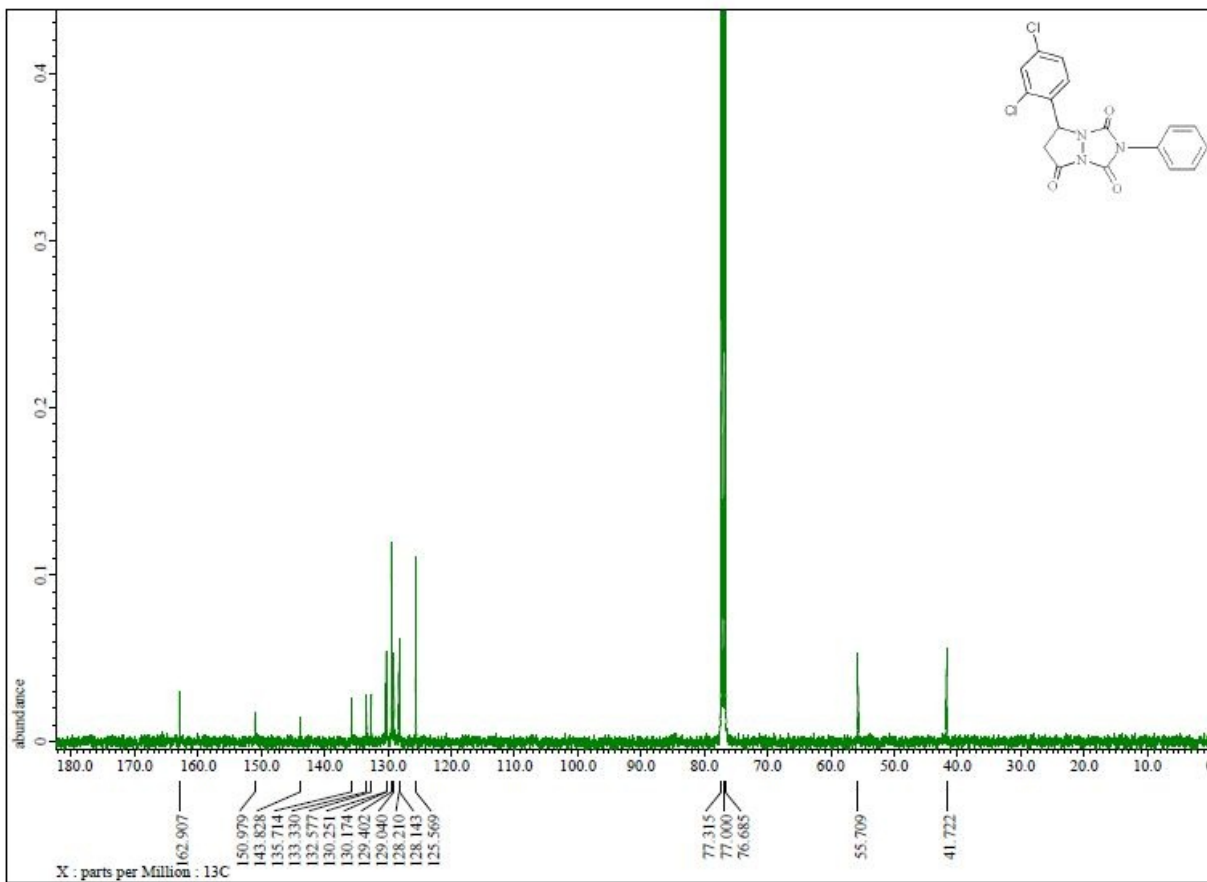


7-(2,4-dichlorophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIf)

¹H NMR of IIf in Chloroform-d

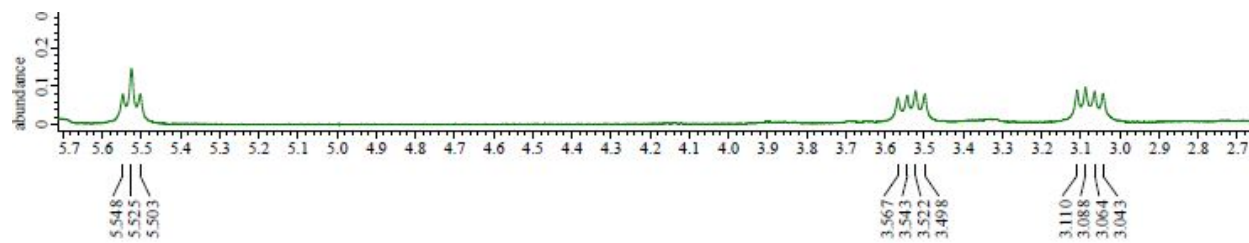
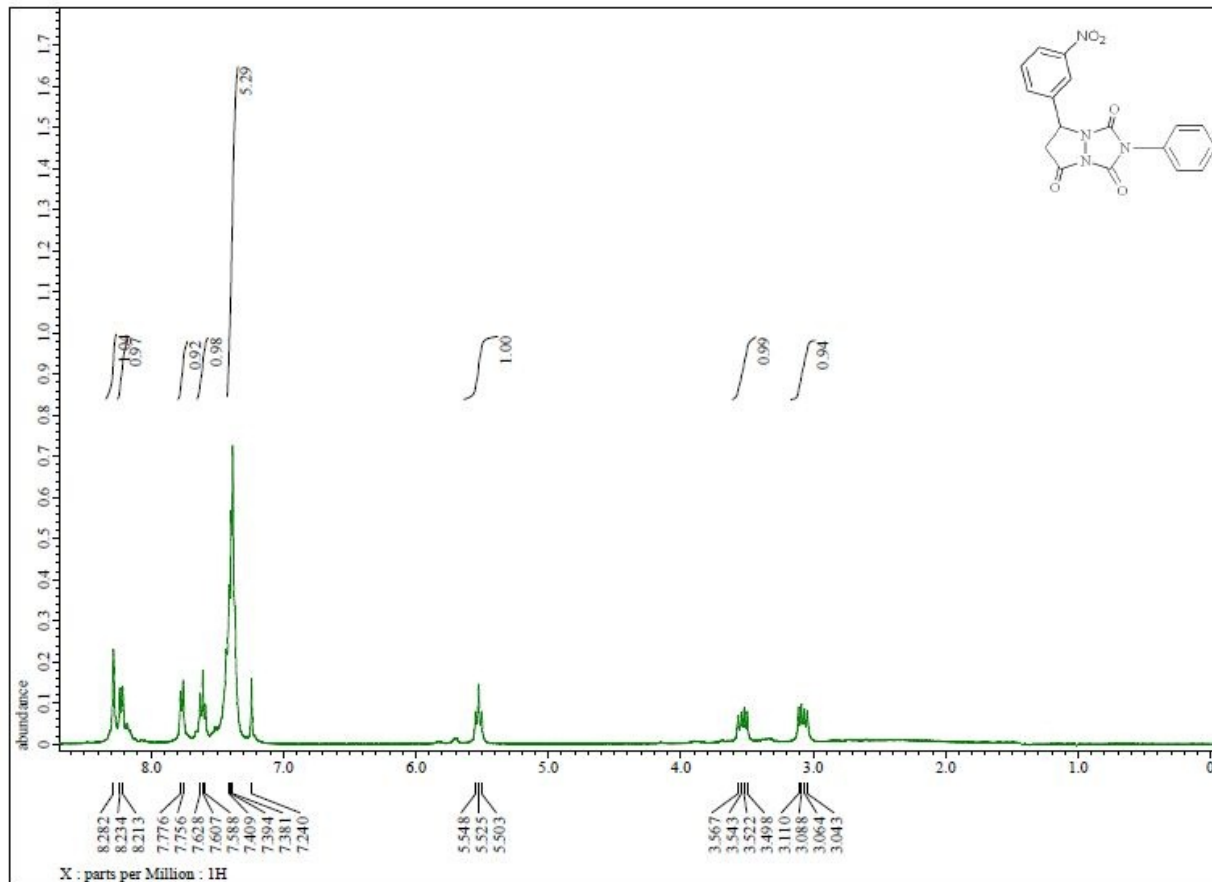


¹³C NMR of IIf in Chloroform-d

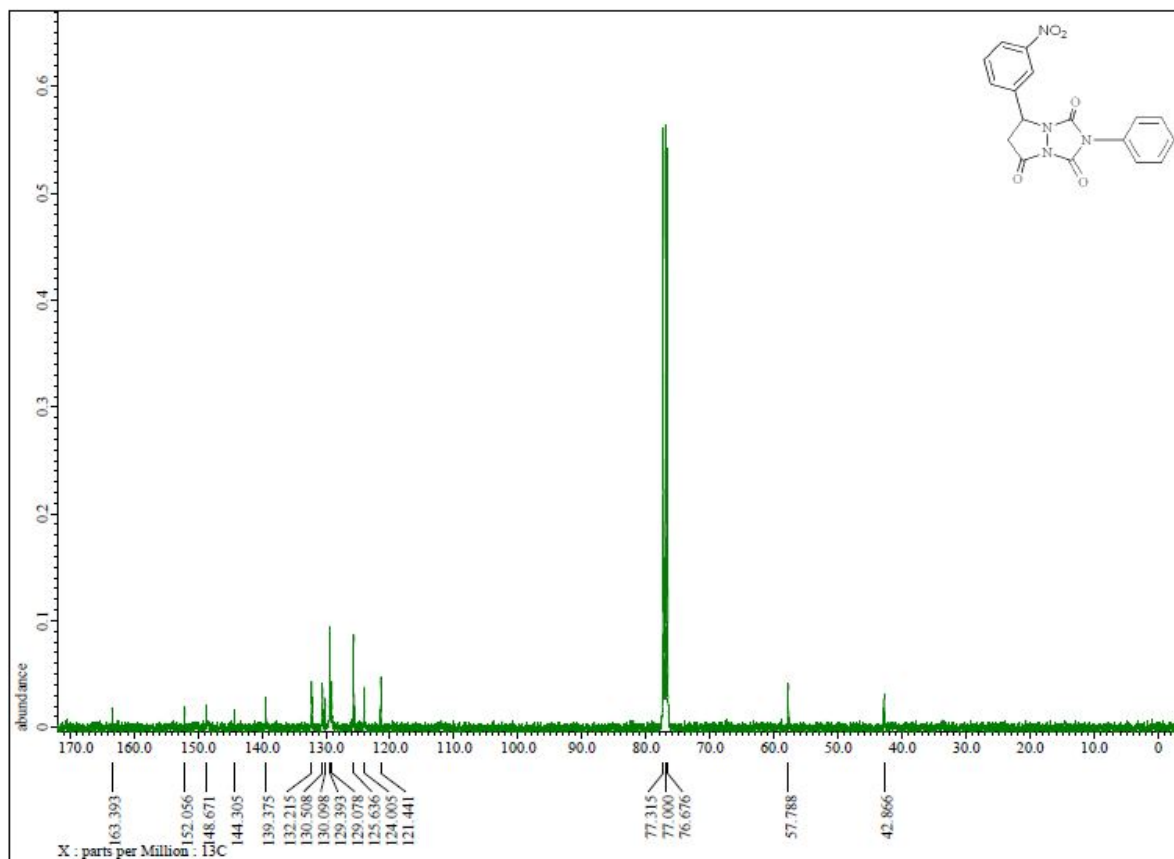


7-(3-nitrophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIg)

¹H NMR of IIg in Chloroform-d

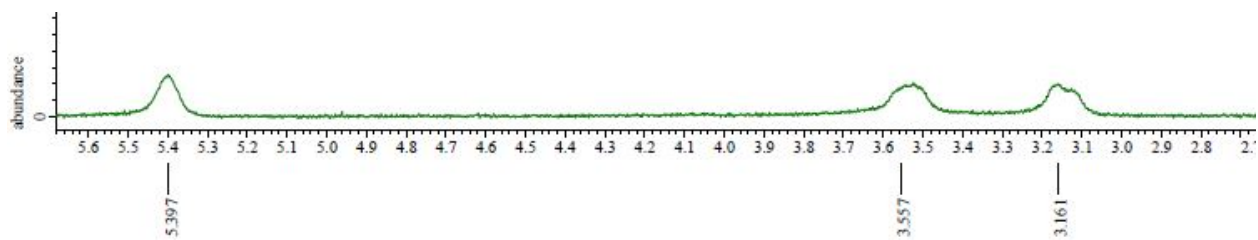
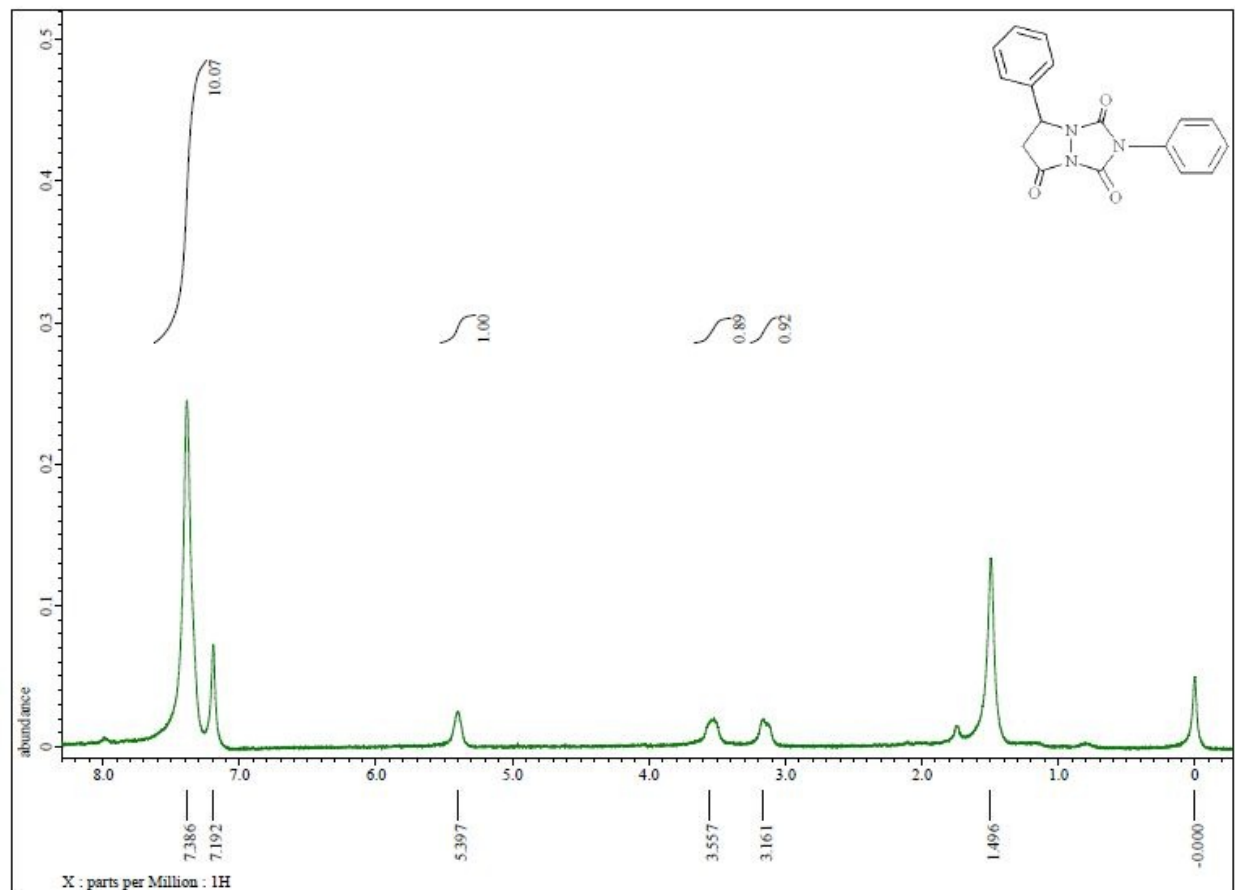


¹³C NMR of IIg in Chloroform-d

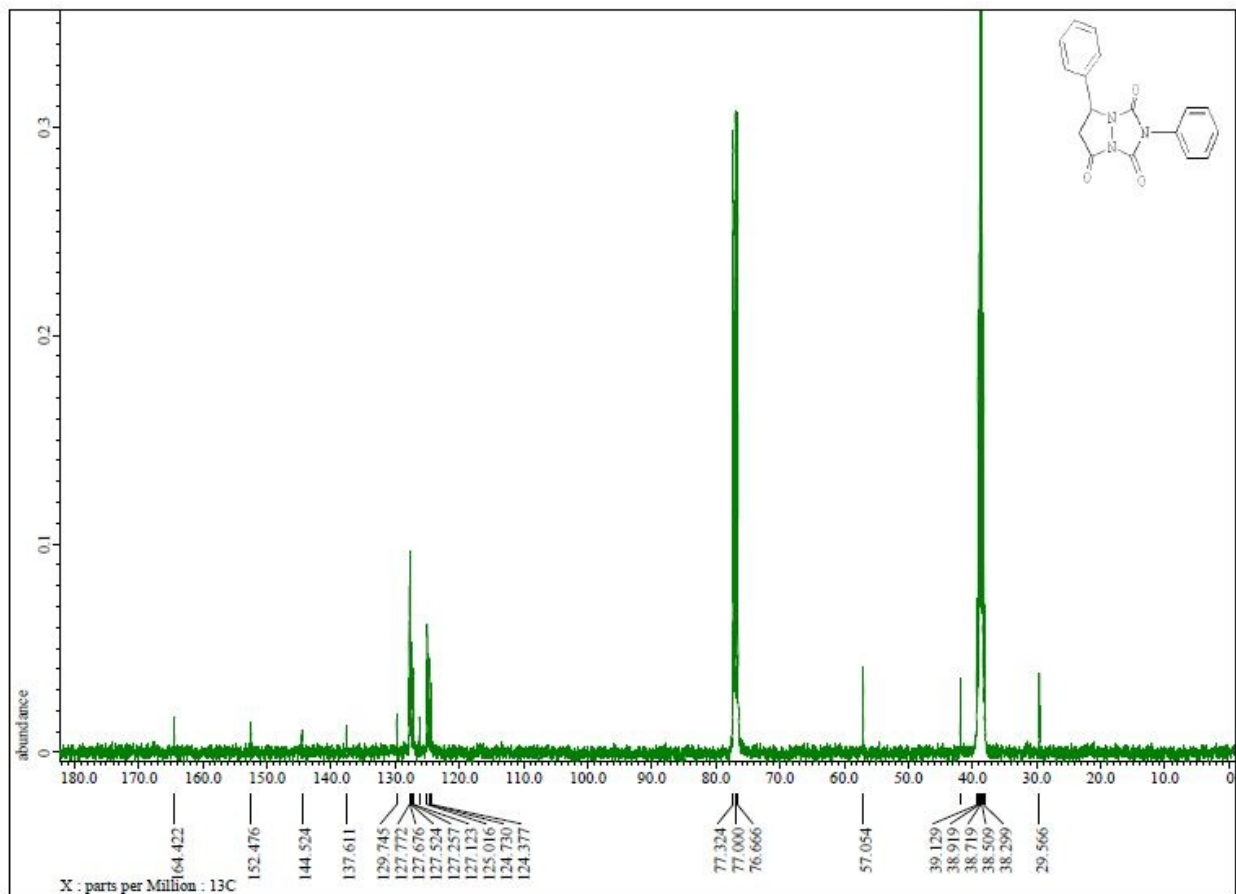


2,7-diphenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIh)

¹H NMR of IIh in Chloroform-d

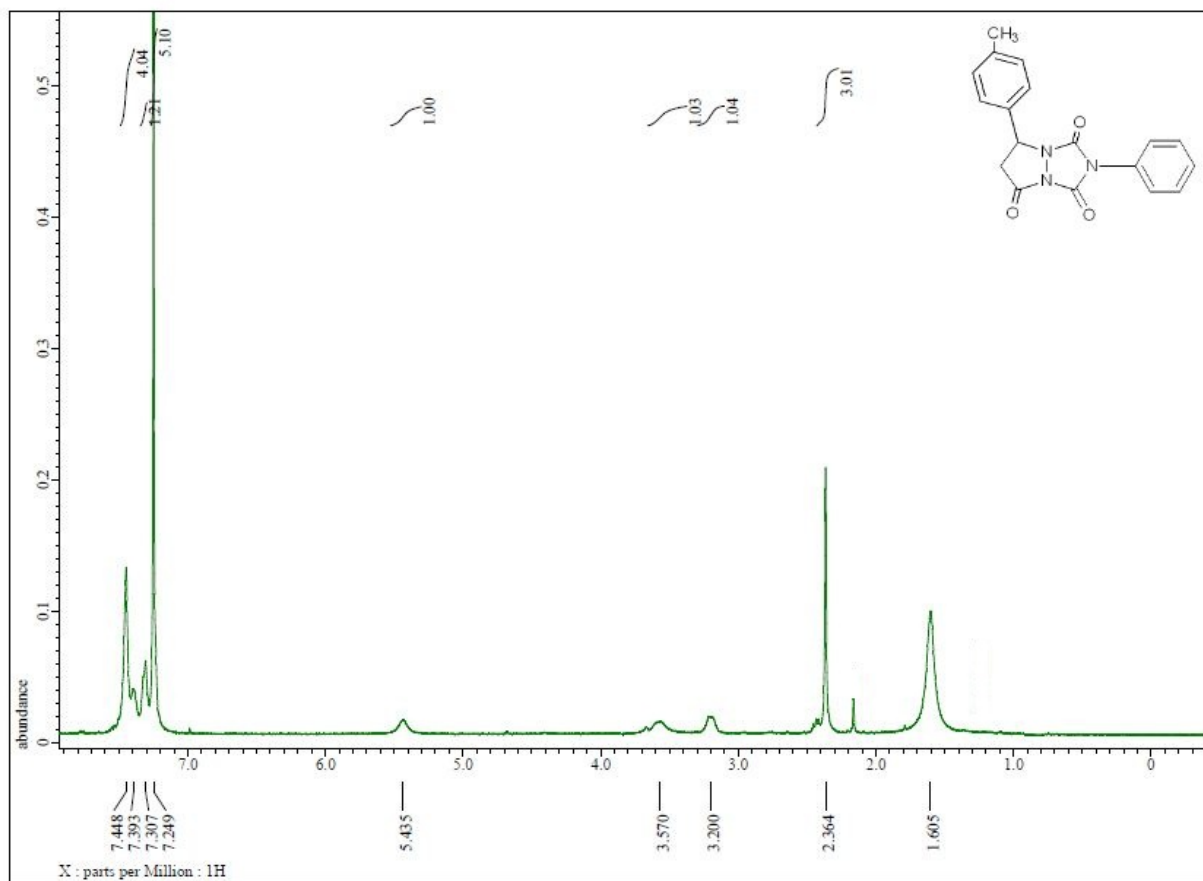


¹³C NMR of IIh in Chloroform-d₃+ DMSO-d₆

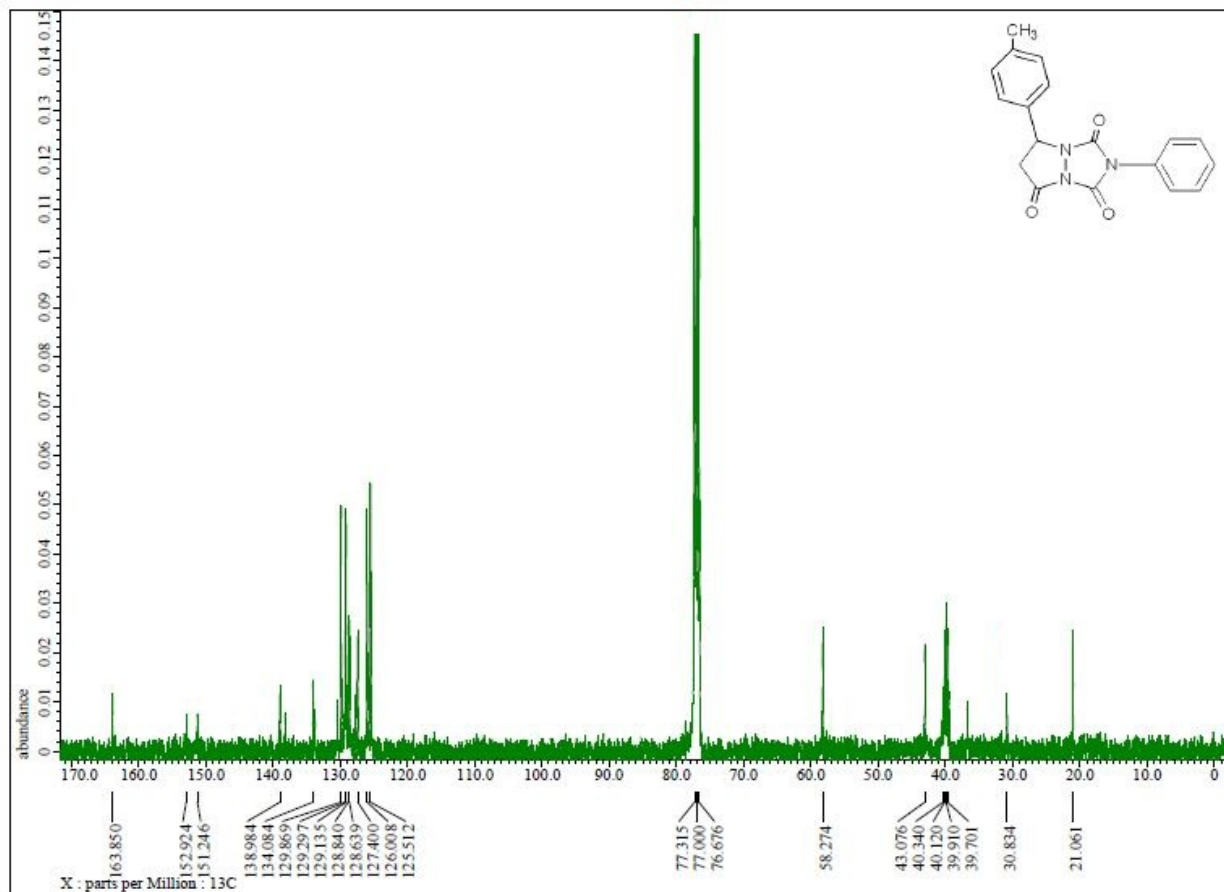


2-phenyl-7-(4-methylphenyl)dihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (III)

¹H NMR of III in Chloroform-d

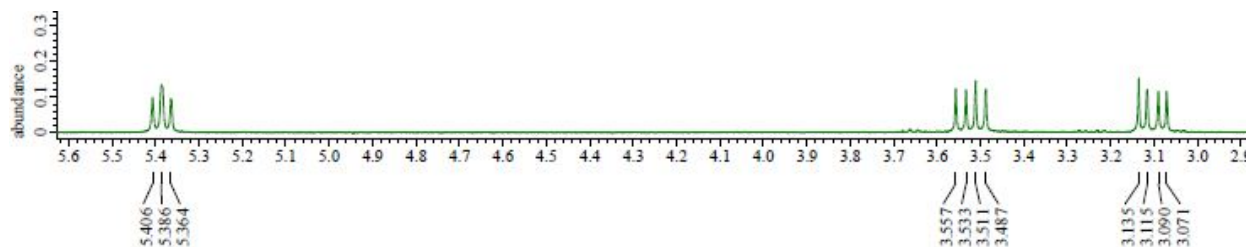
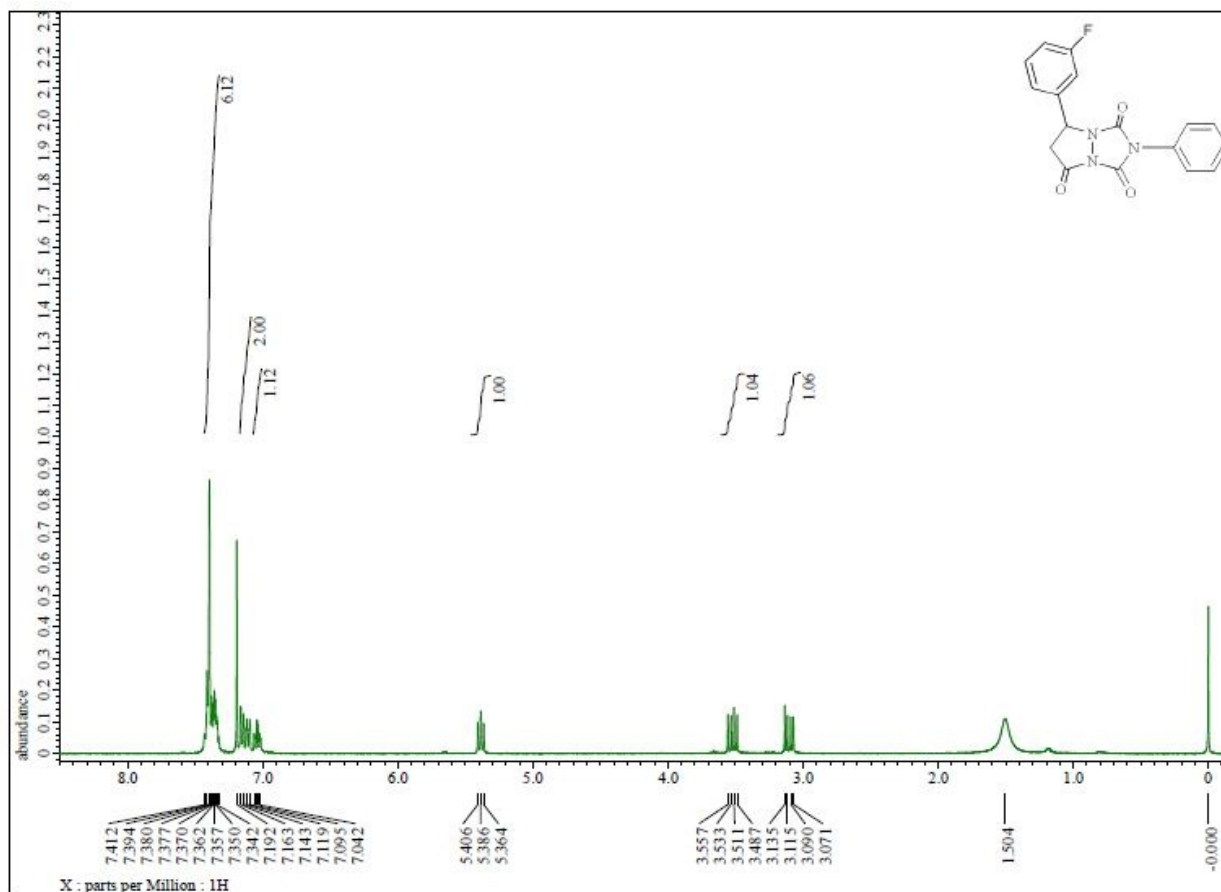


^{13}C NMR of III in Chloroform-d + DMSO-d₆

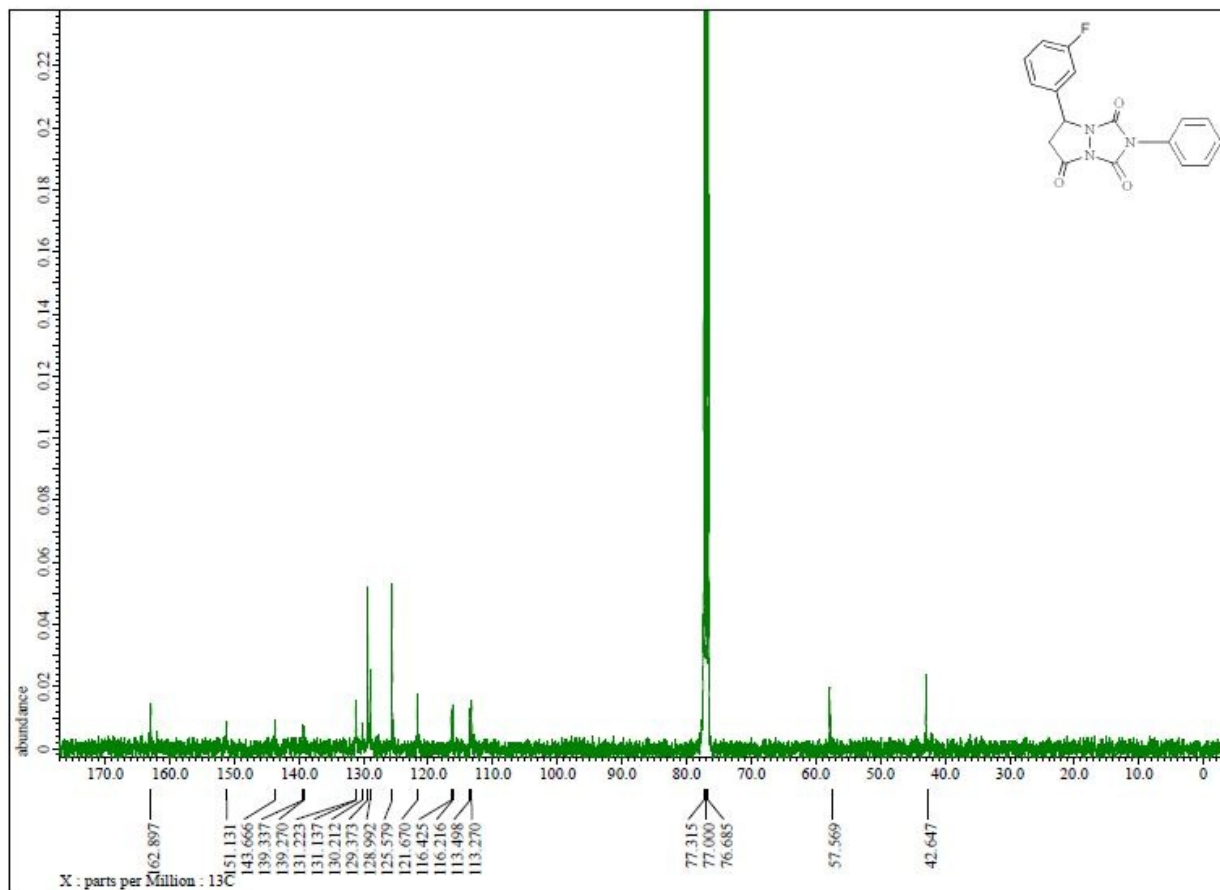


7-(3-fluorophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIj)

¹H NMR of IIj in Chloroform-d

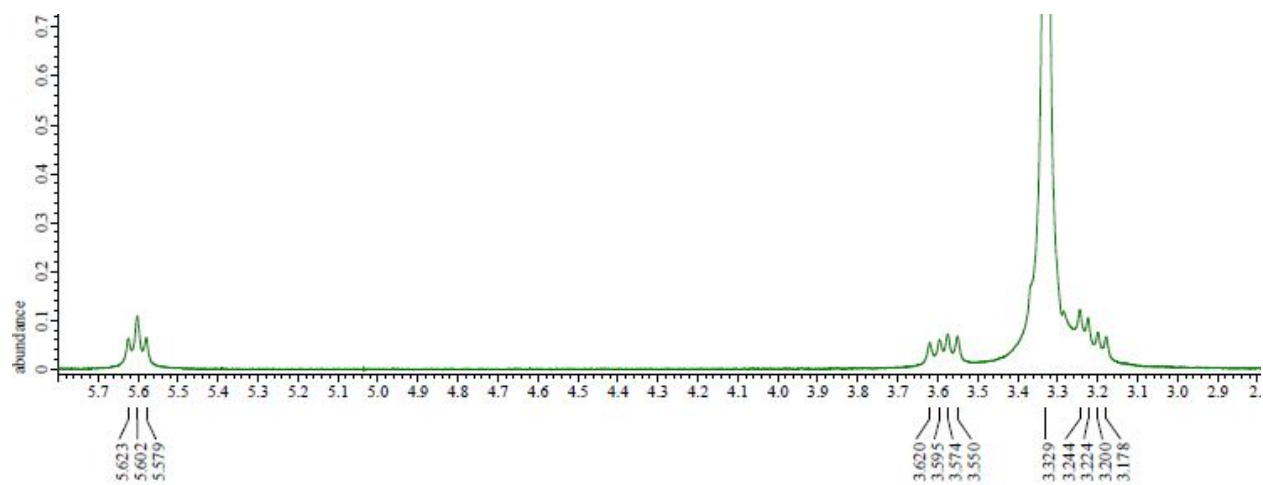
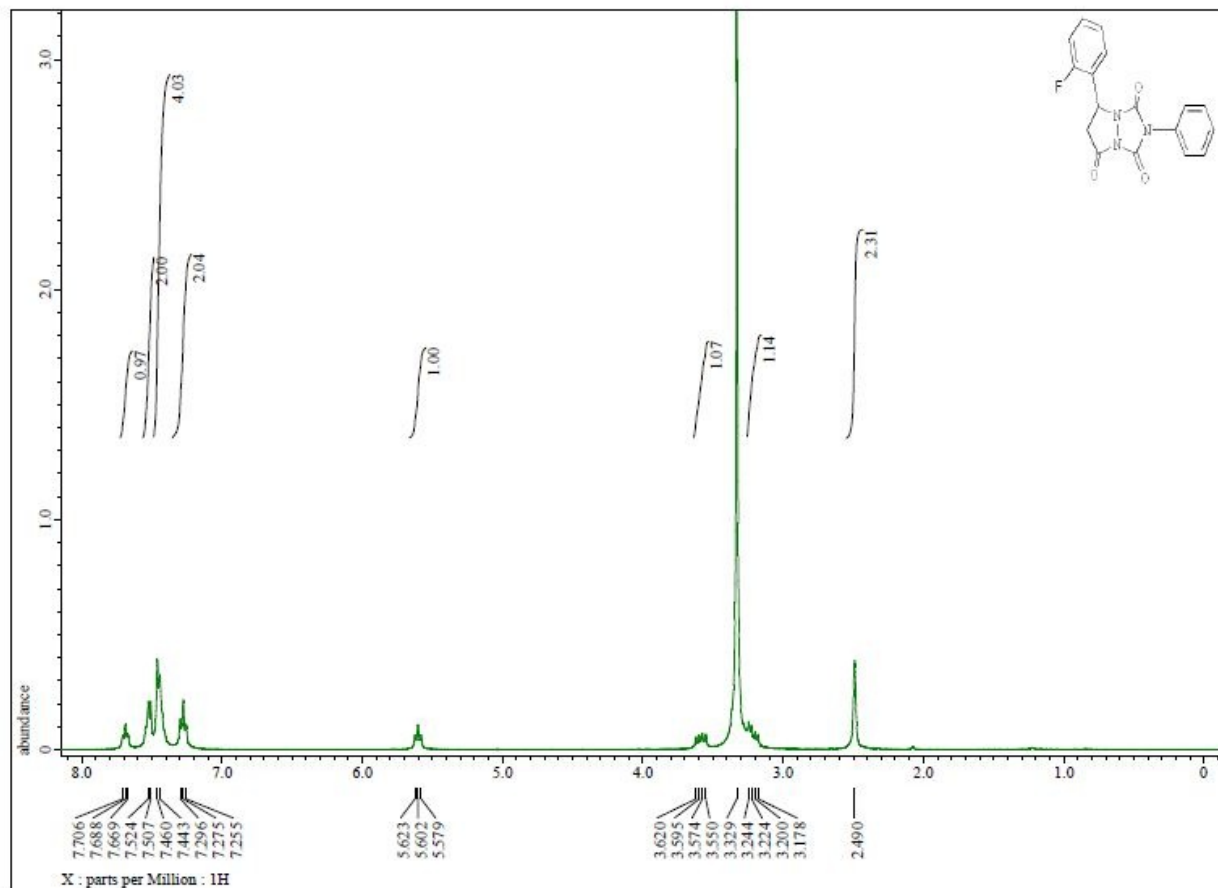


¹³C NMR of IIj in Chloroform-d

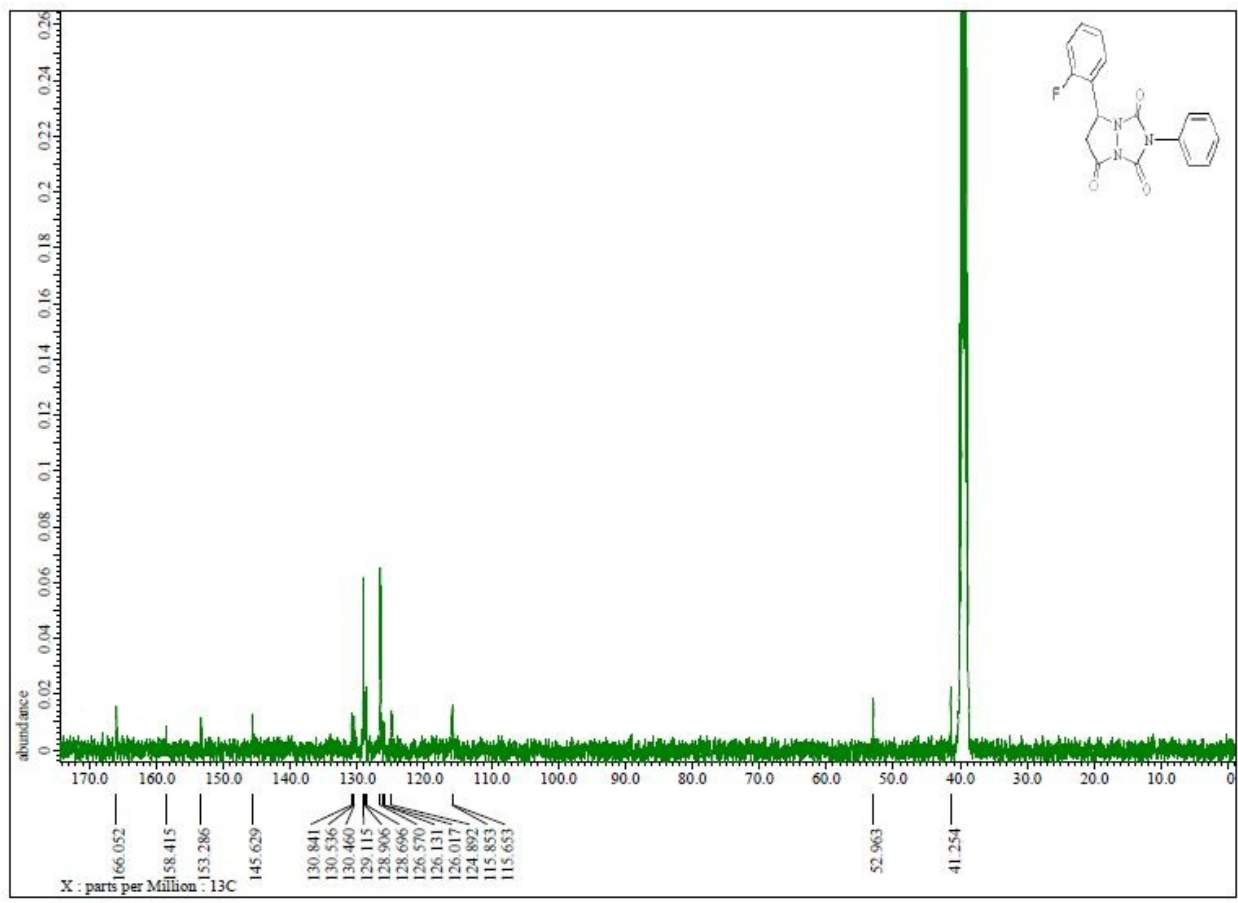


7-(2-fluorophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIIk)

¹H NMR of IIIk in Chloroform-d

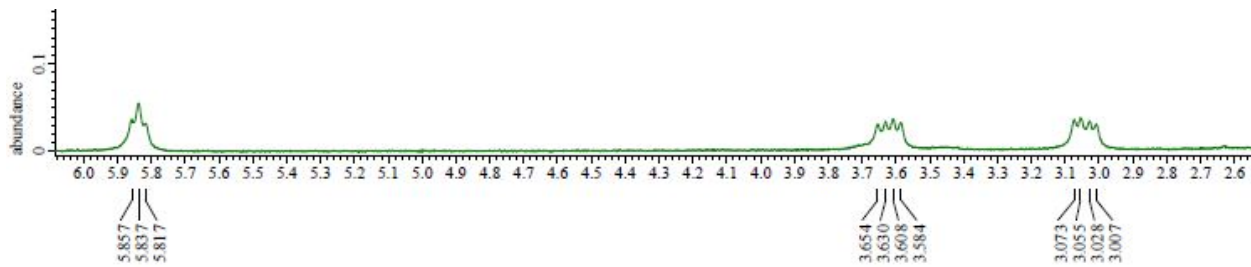
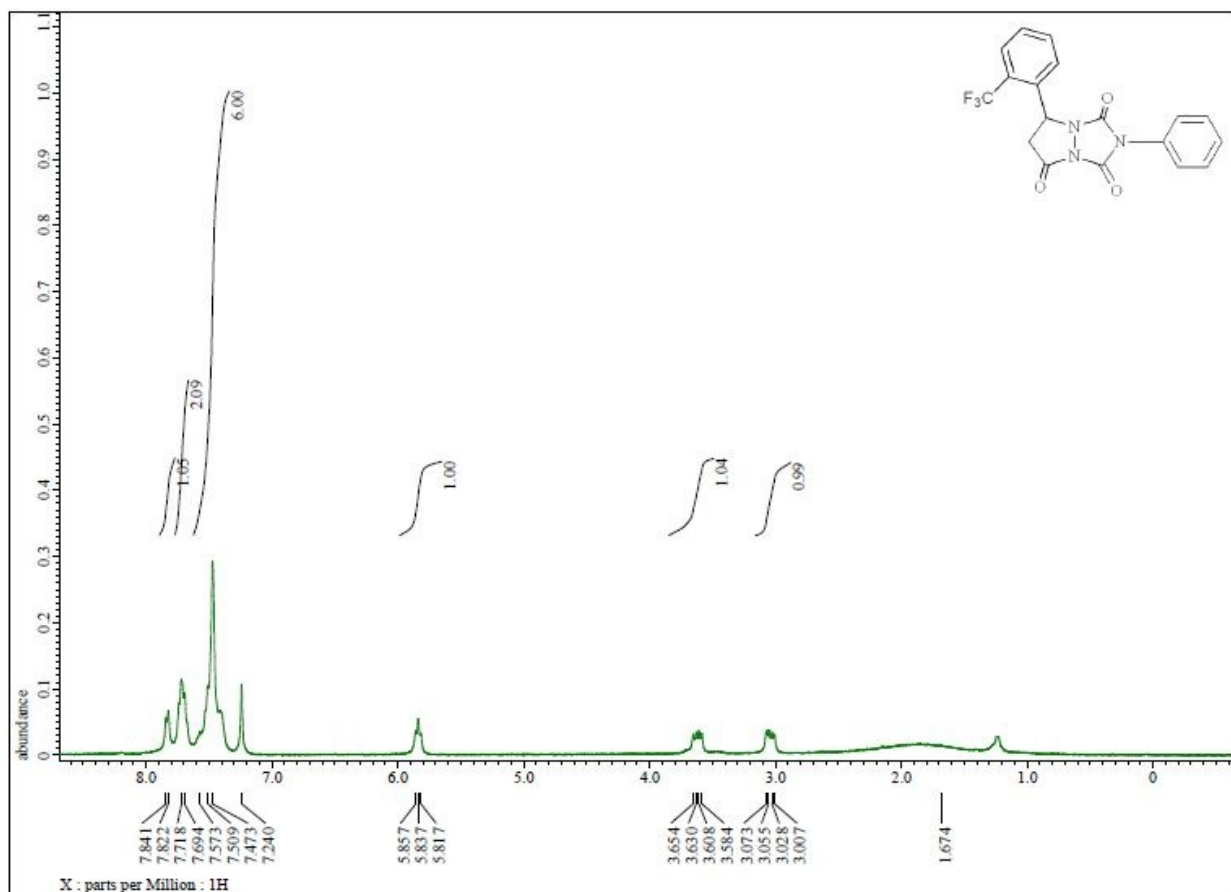


¹³C NMR of IIk in Chloroform-d + DMSO-d₆

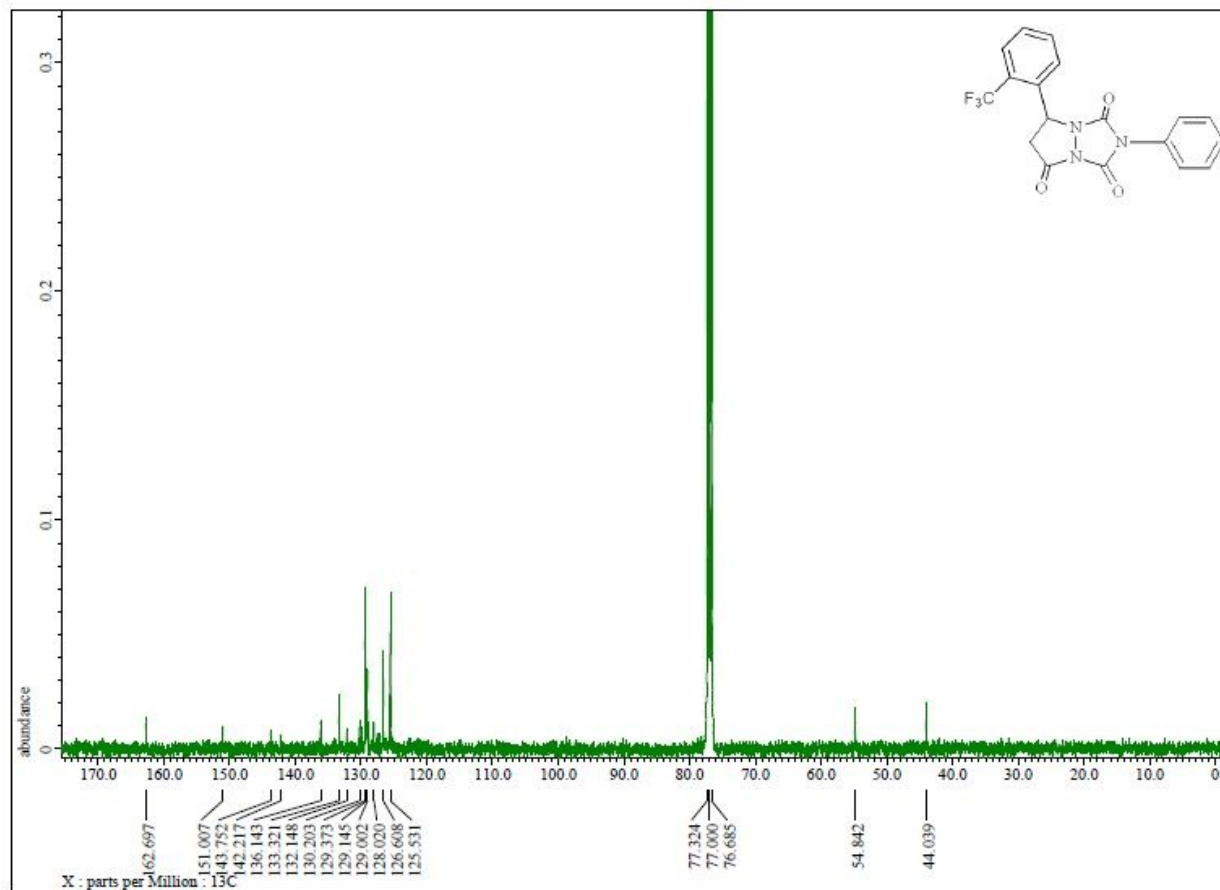


2-phenyl-7-(2-(trifluoromethyl)phenyl)dihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione
(III)

¹H NMR of III in Chloroform-d

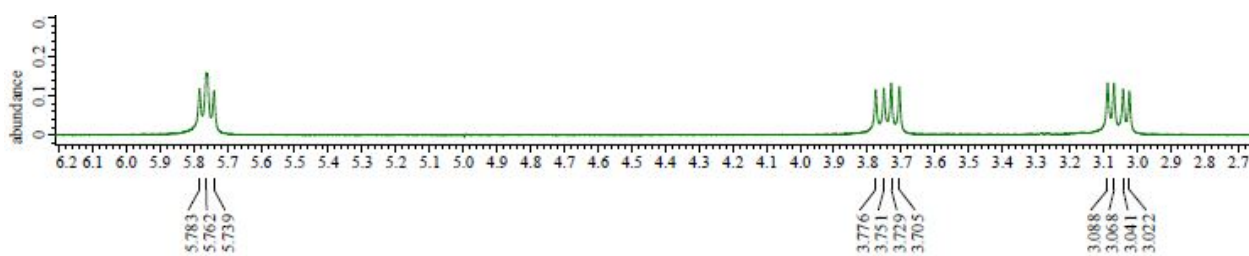
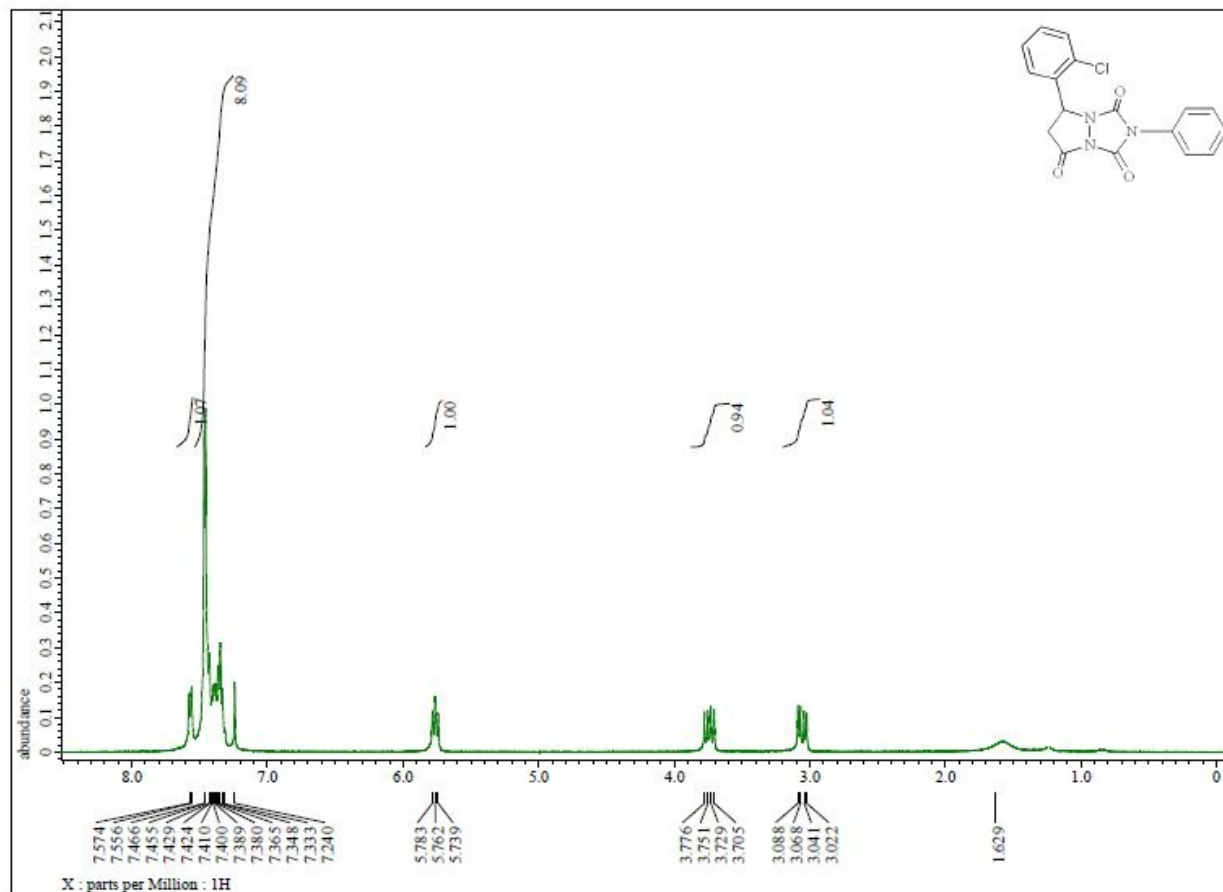


¹³C NMR of III in Chloroform-d

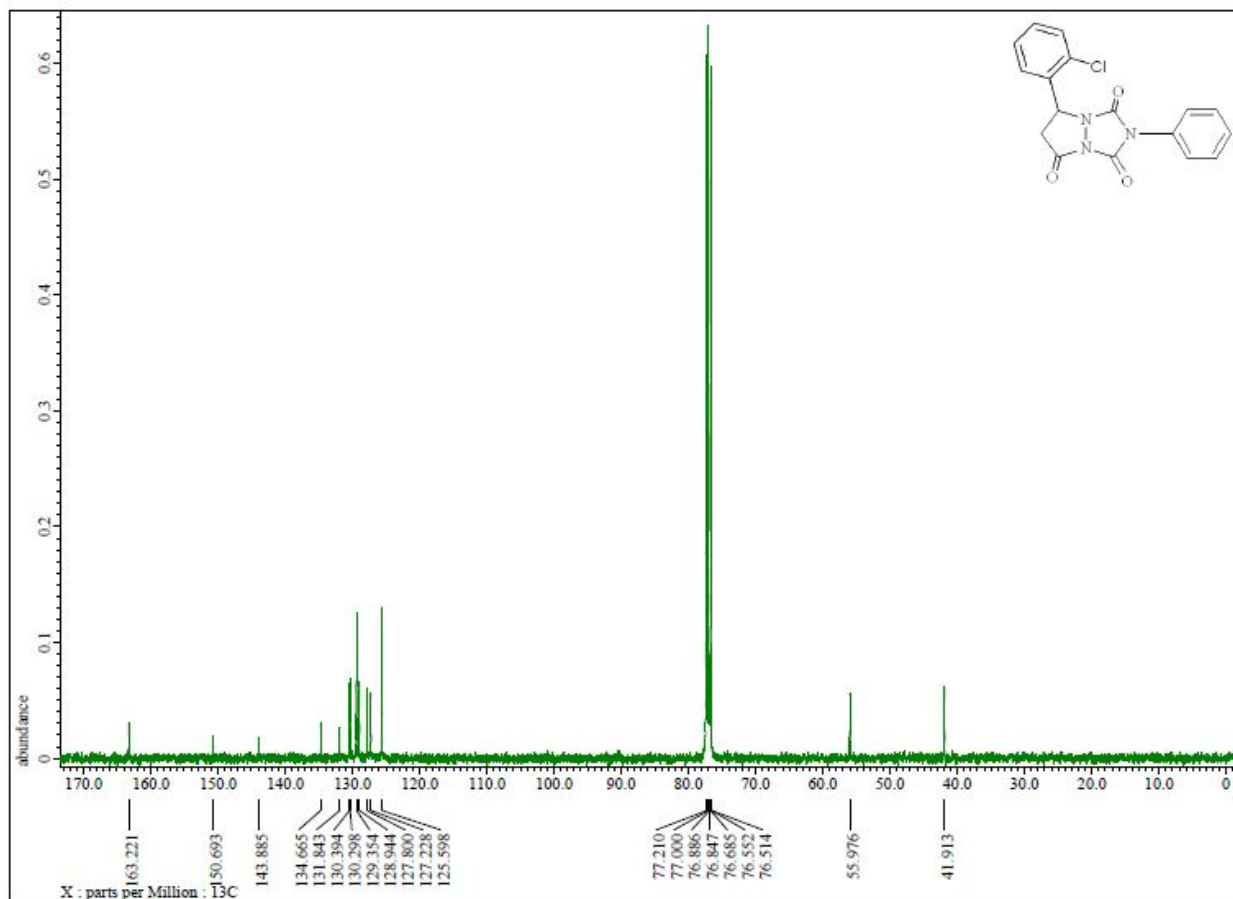


7-(2-chlorophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIm)

¹H NMR of IIm in Chloroform-d

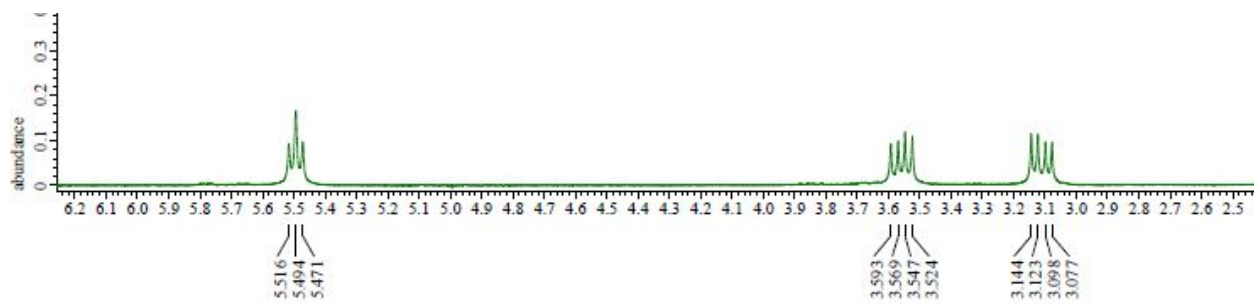
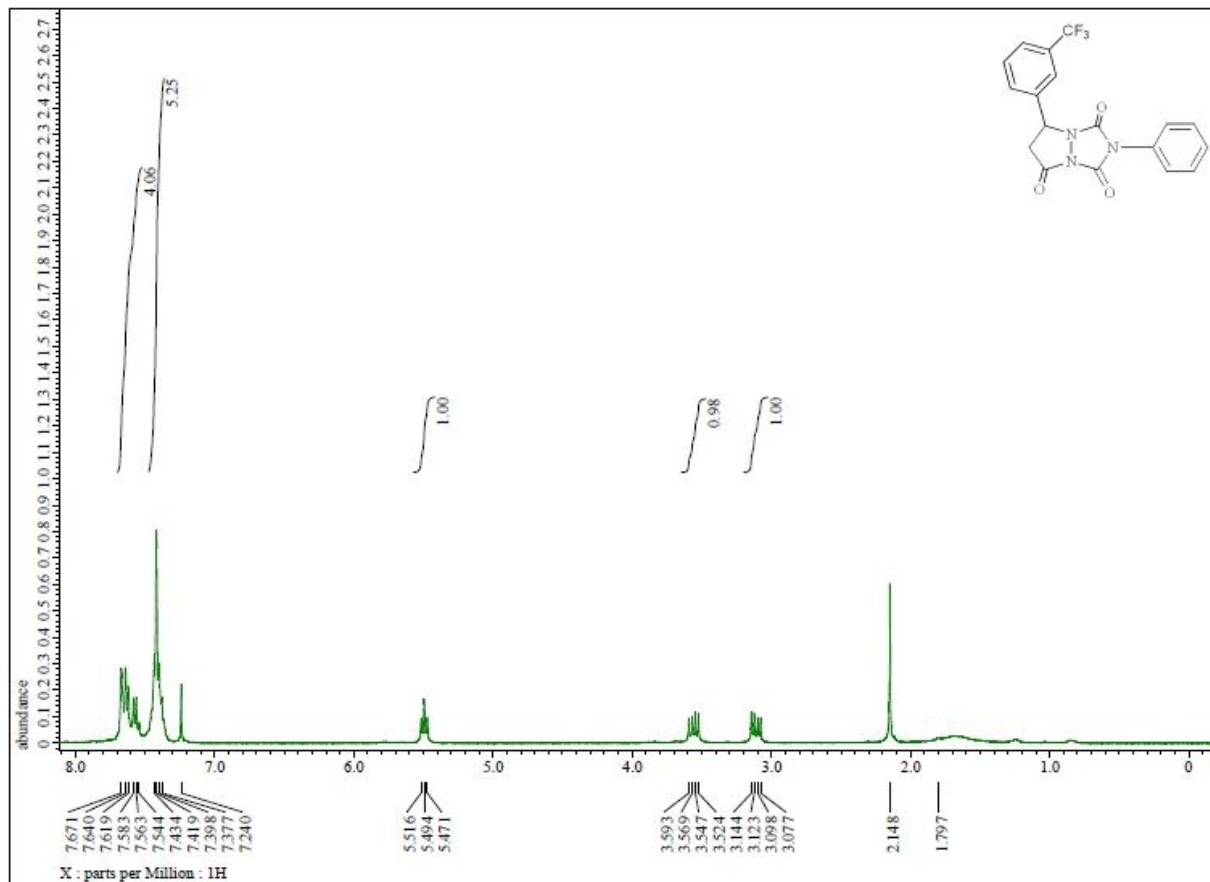


¹³C NMR of IIm in Chloroform-d

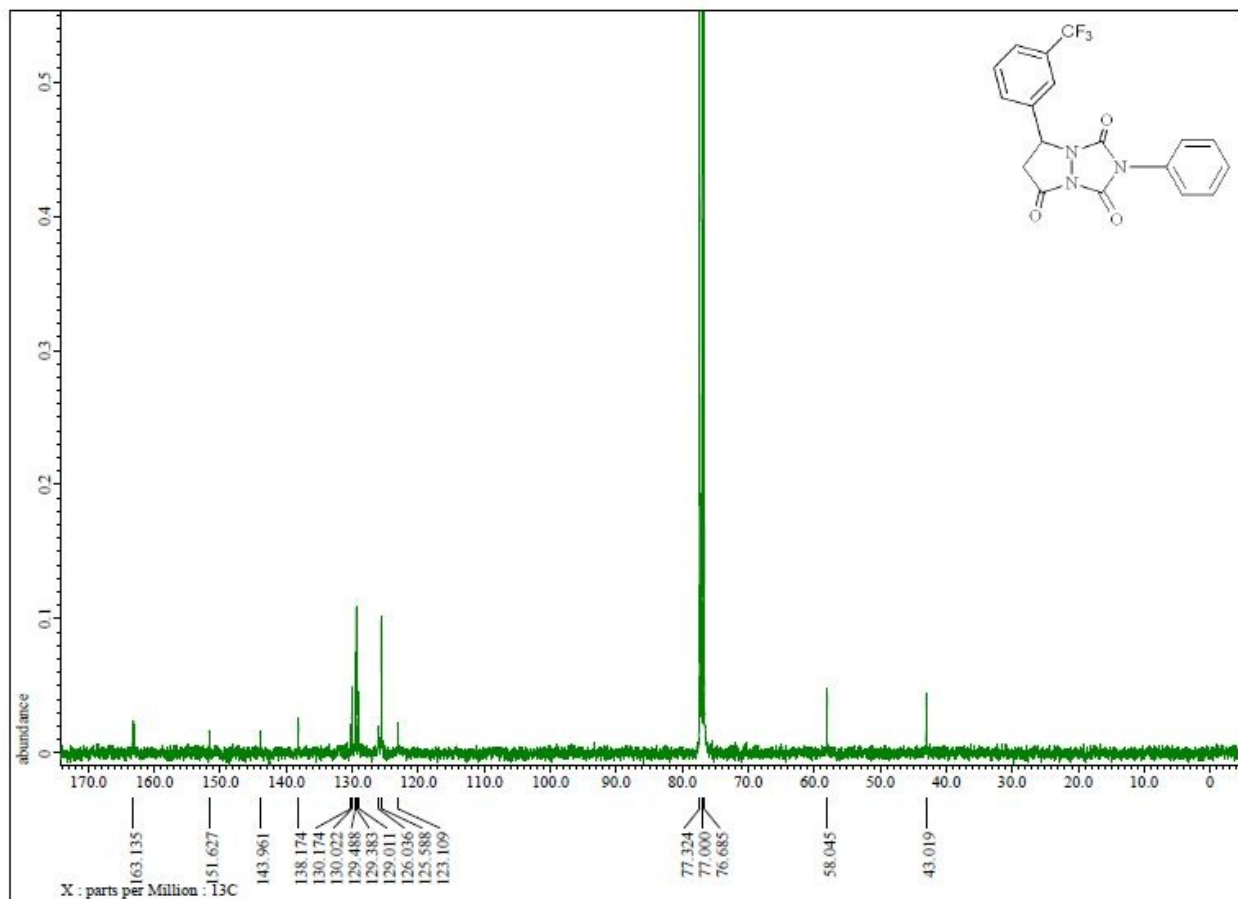


2-phenyl-7-(3-(trifluoromethyl)phenyl)dihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione
(II_n)

¹H NMR of II_n in Chloroform-d

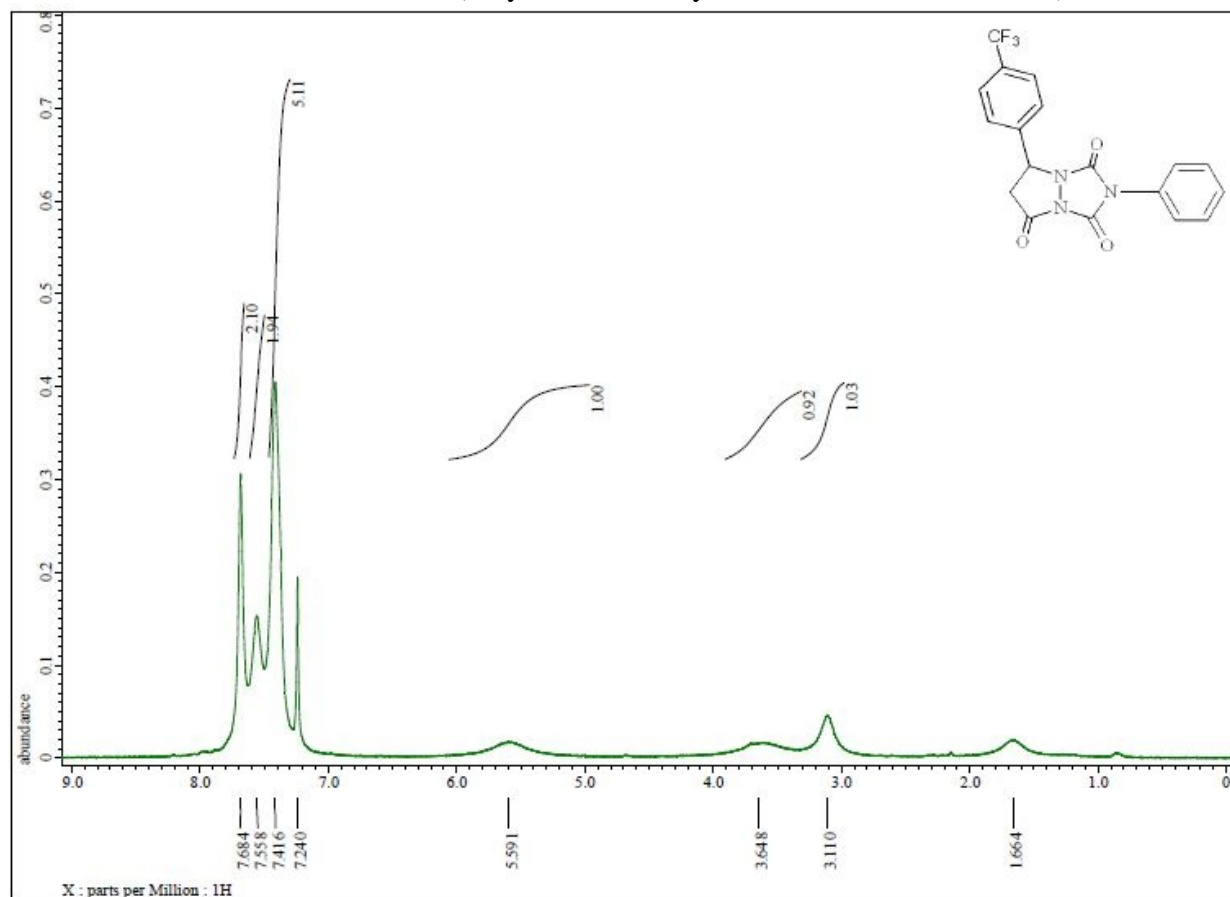


¹³C NMR of IIa in Chloroform-d

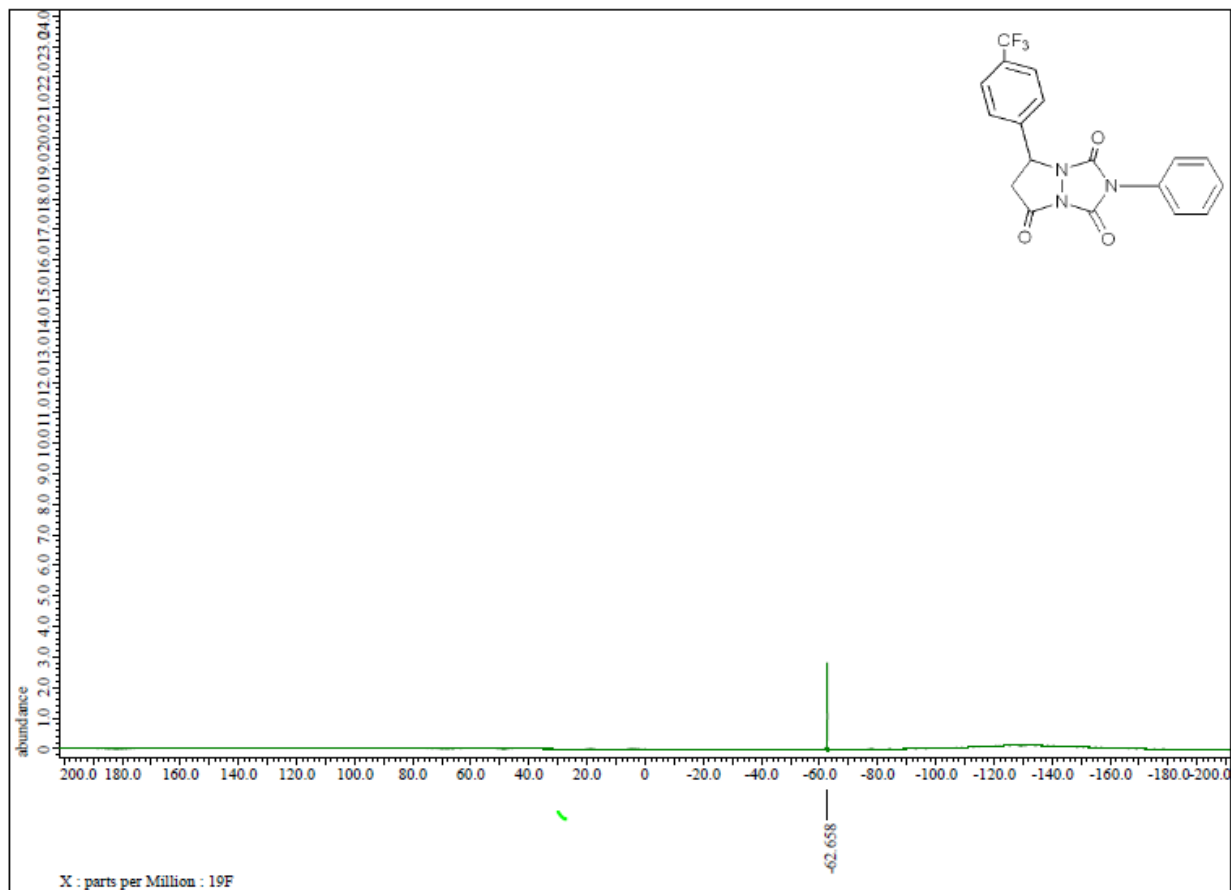


2-phenyl-7-(4-(trifluoromethyl)phenyl)dihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione
(IIo)

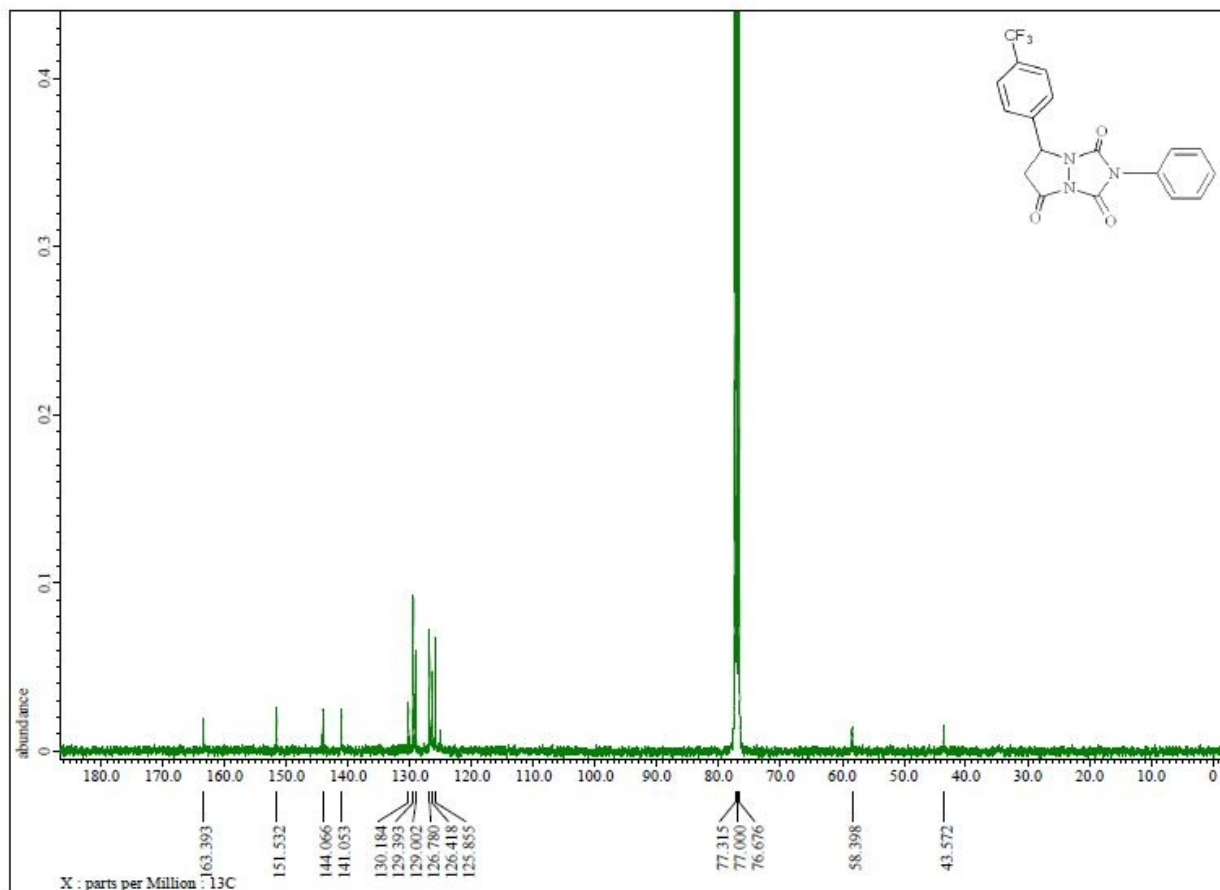
¹H NMR of IIo in Chloroform-d (very less solubility in both CDCl₃ and DMSO).



¹⁹F NMR of IIo in Chloroform-d

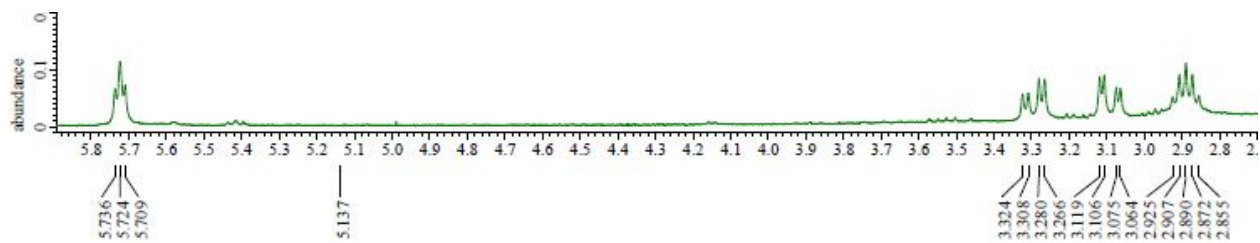
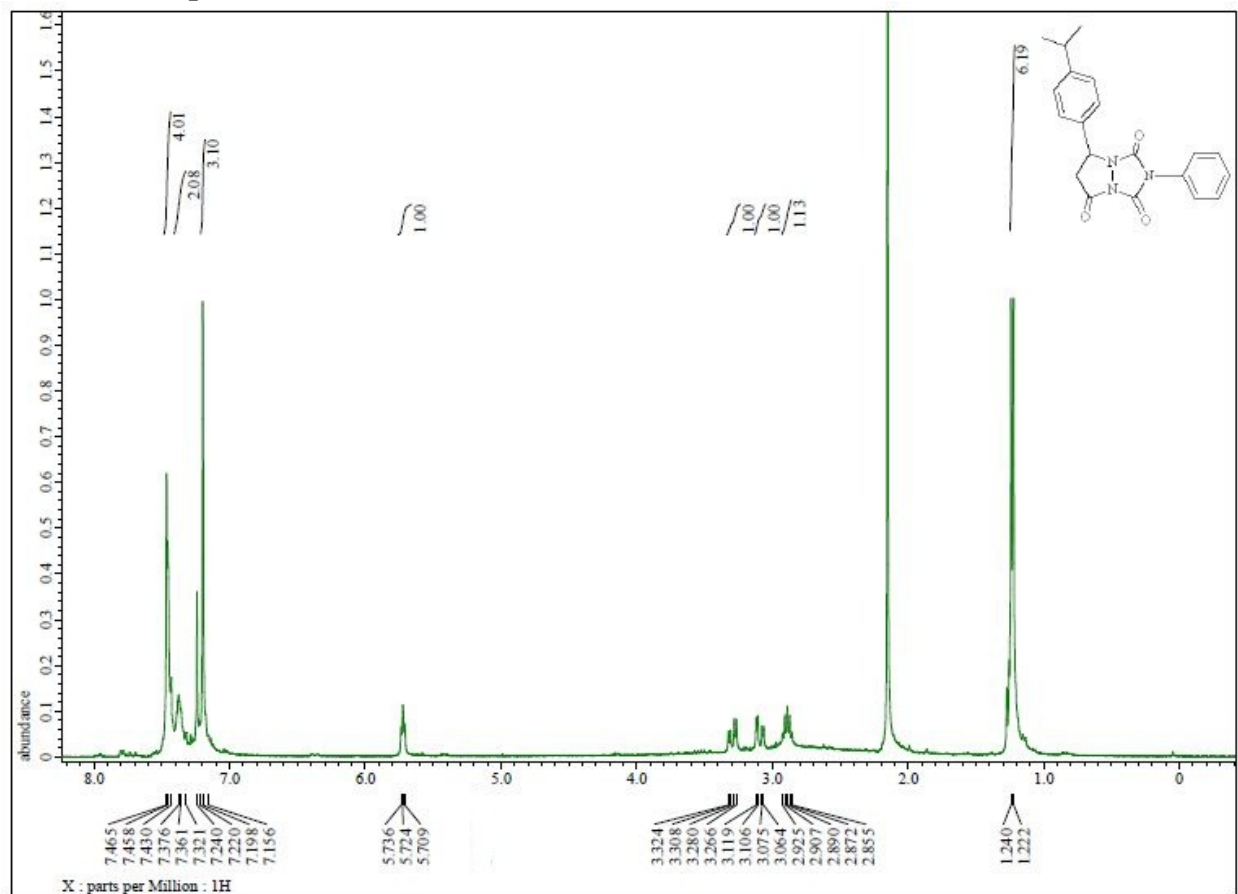


¹³C NMR of IIo in Chloroform-d

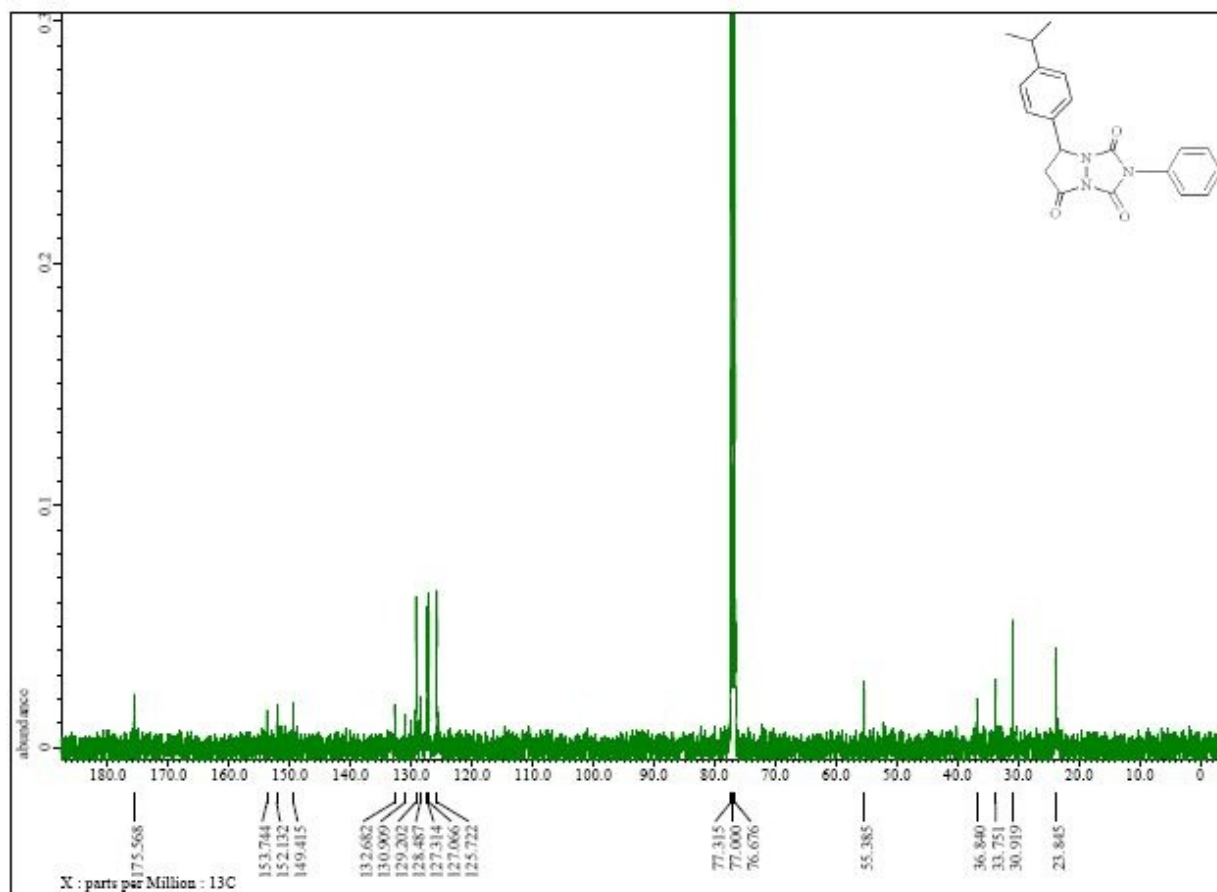


7-(4-isopropylphenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione (IIp)

¹H NMR of IIp in Chloroform-d

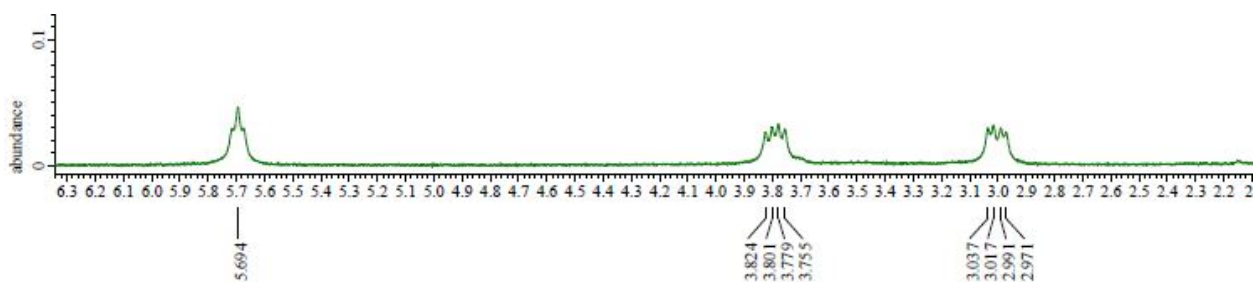
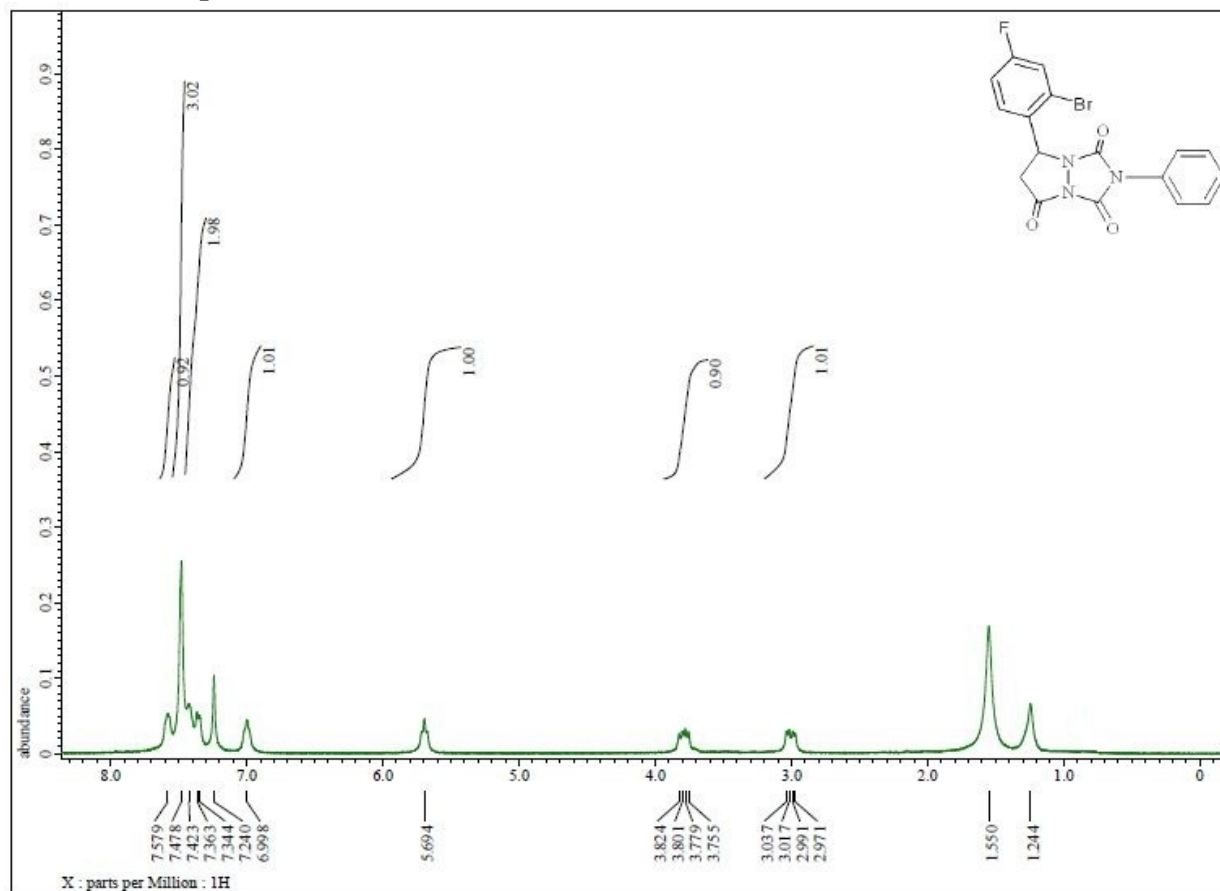


¹³C NMR of Iip in Chloroform-d

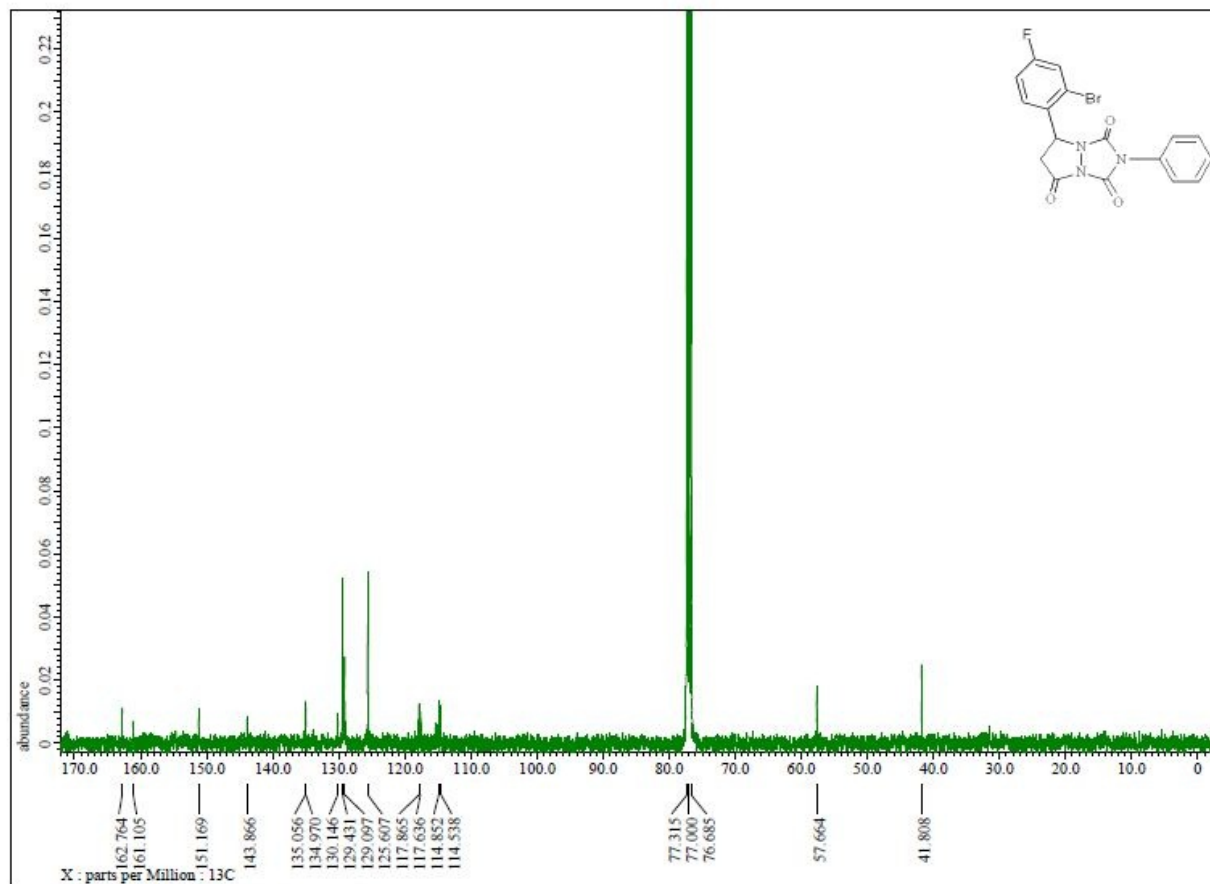


7-(2-bromo-4-fluorophenyl)-2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione
(IIq)

¹H NMR of IIq in Chloroform-d

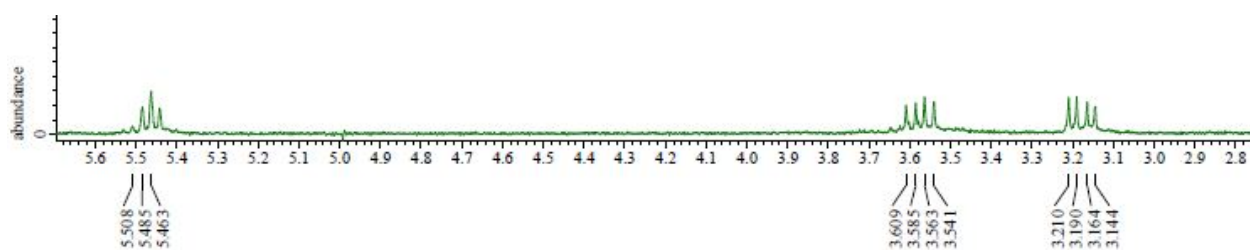
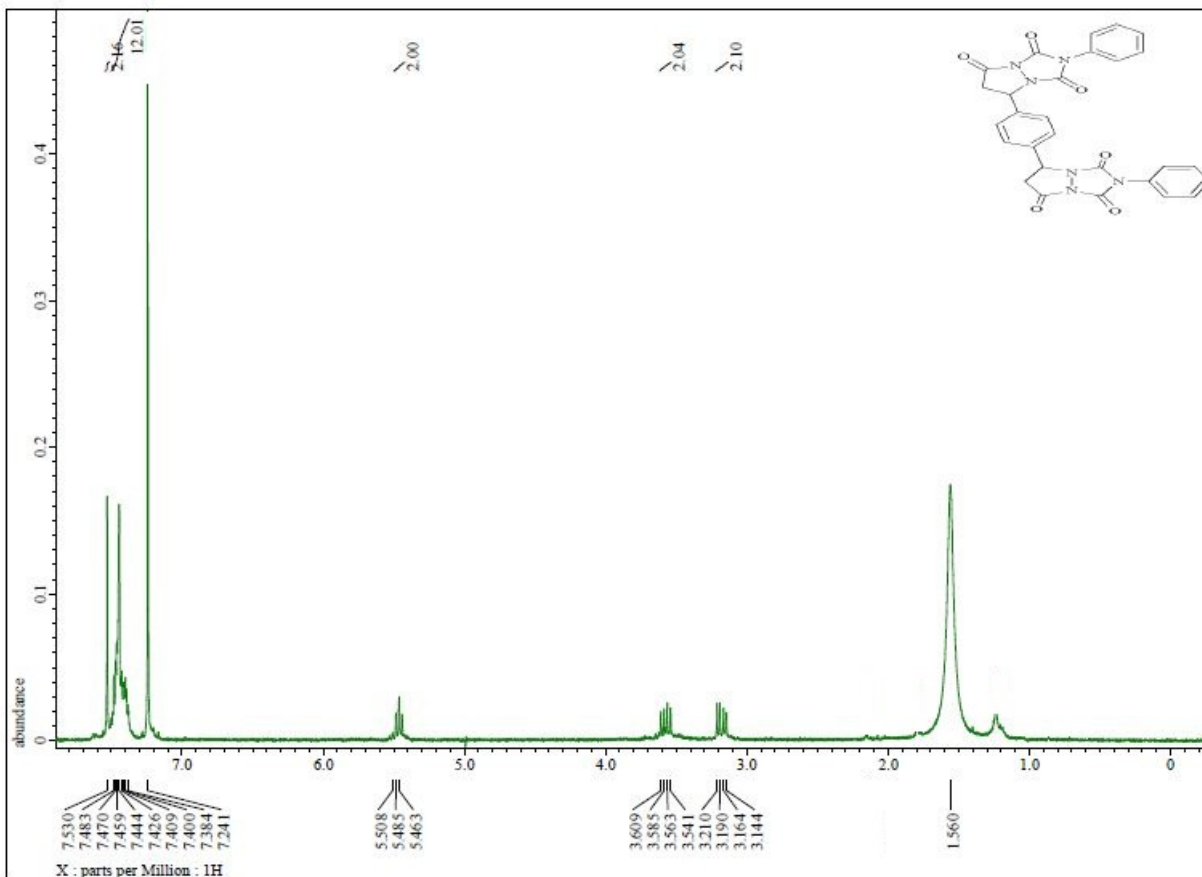


¹³C NMR of IIq in Chloroform-d



7,7'-(1,4-phenylene)bis(2-phenyldihydropyrazolo[1,2-a][1,2,4]triazole-1,3,5(2H)-trione) (IIr)

¹H NMR of IIr in Chloroform-d



¹³C NMR of IIr in Chloroform-d + DMSO-d₆

