

Supplementary Material

One pot-like regiospecific access to 1-aryl-1*H*-pyrazol-3(2*H*)-one derivatives and evaluation of the anticancer activity

Francesco Mingoia,^{*a} Giovanna Panzeca,^{a,b} Maria Concetta Vitale,^{a,b}
Gabriele La Monica,^b Alessia Bono,^b Antonino Lauria,^b and Annamaria Martorana^b

^a*Istituto per lo Studio dei Materiali Nanostrutturati, Consiglio Nazionale delle Ricerche, (CNR), Palermo, Italy*

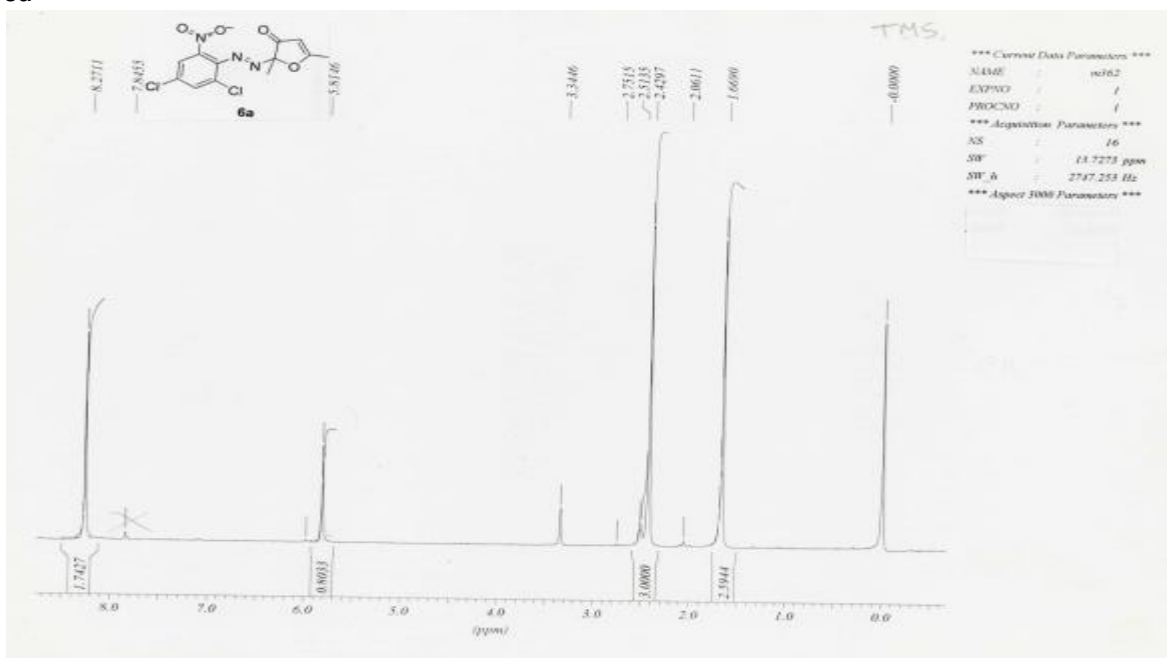
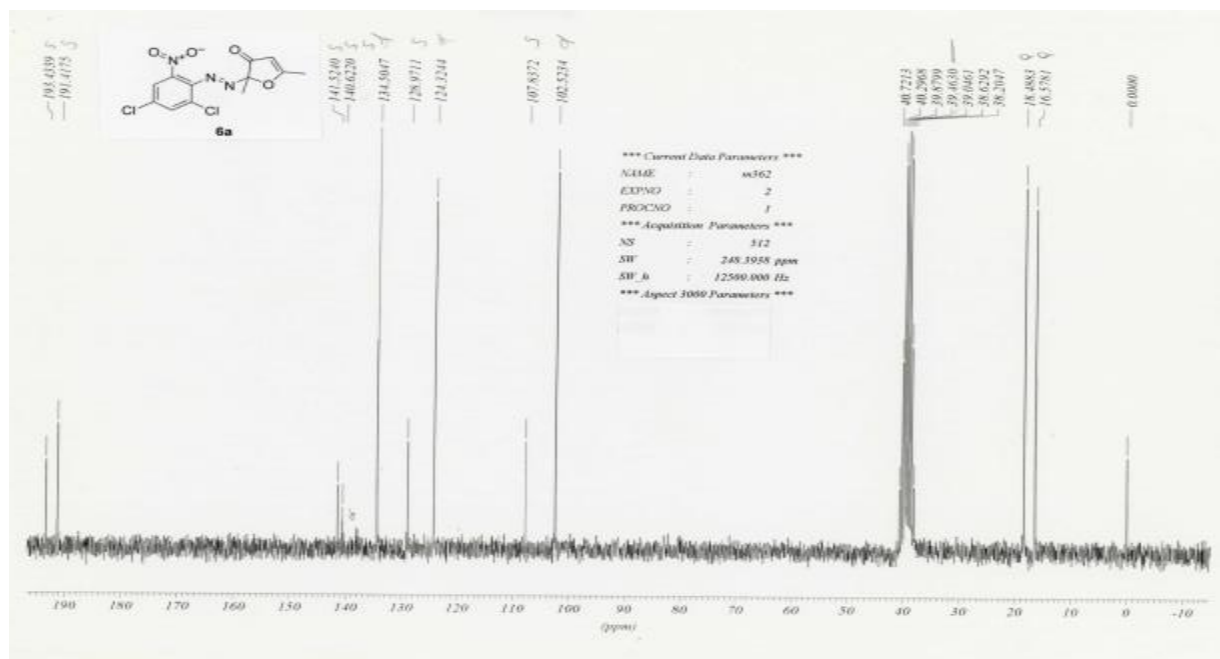
^b*Dipartimento di Scienze e Tecnologie Biologiche Chimiche e Farmaceutiche, Università di Palermo, Italy*

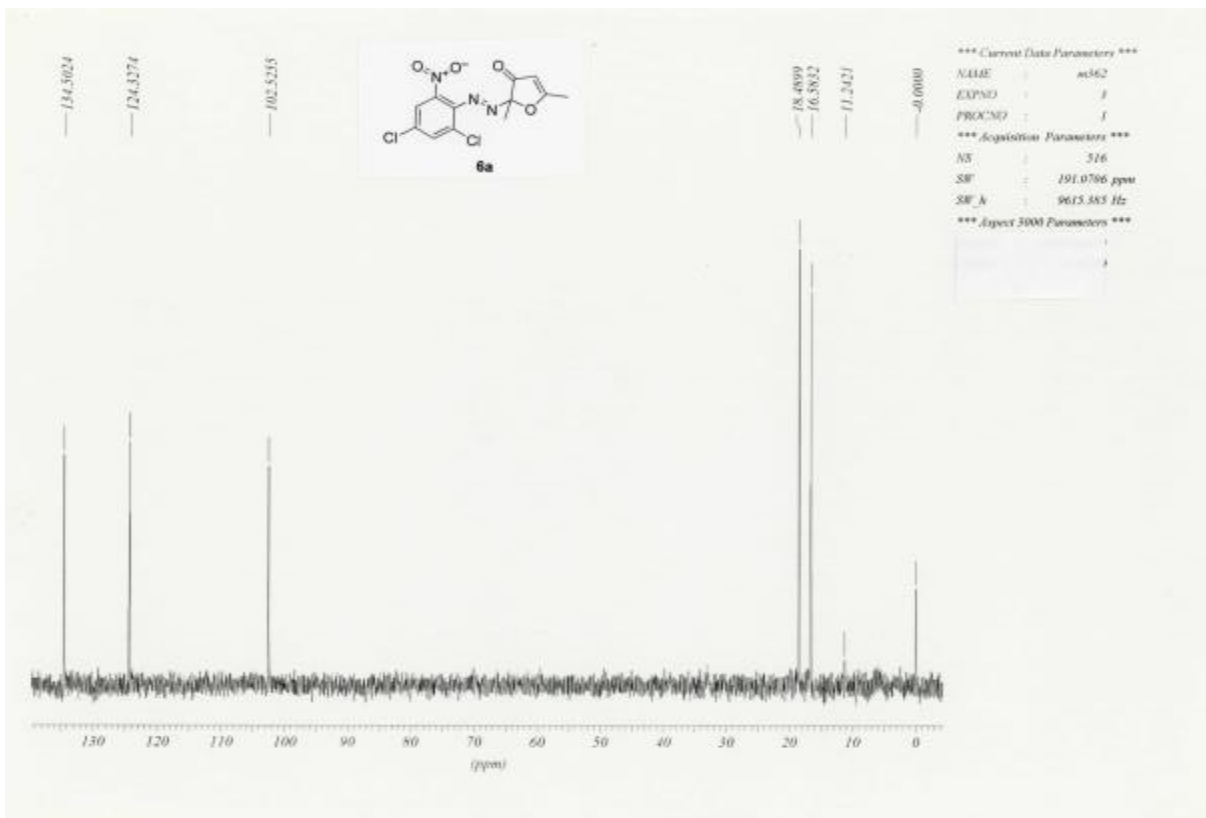
Email: francesco.mingoia@ismn.cnr.it

Table of Contents

¹ H, ¹³ C NMR and FT/IR spectra.....	S2
--	----

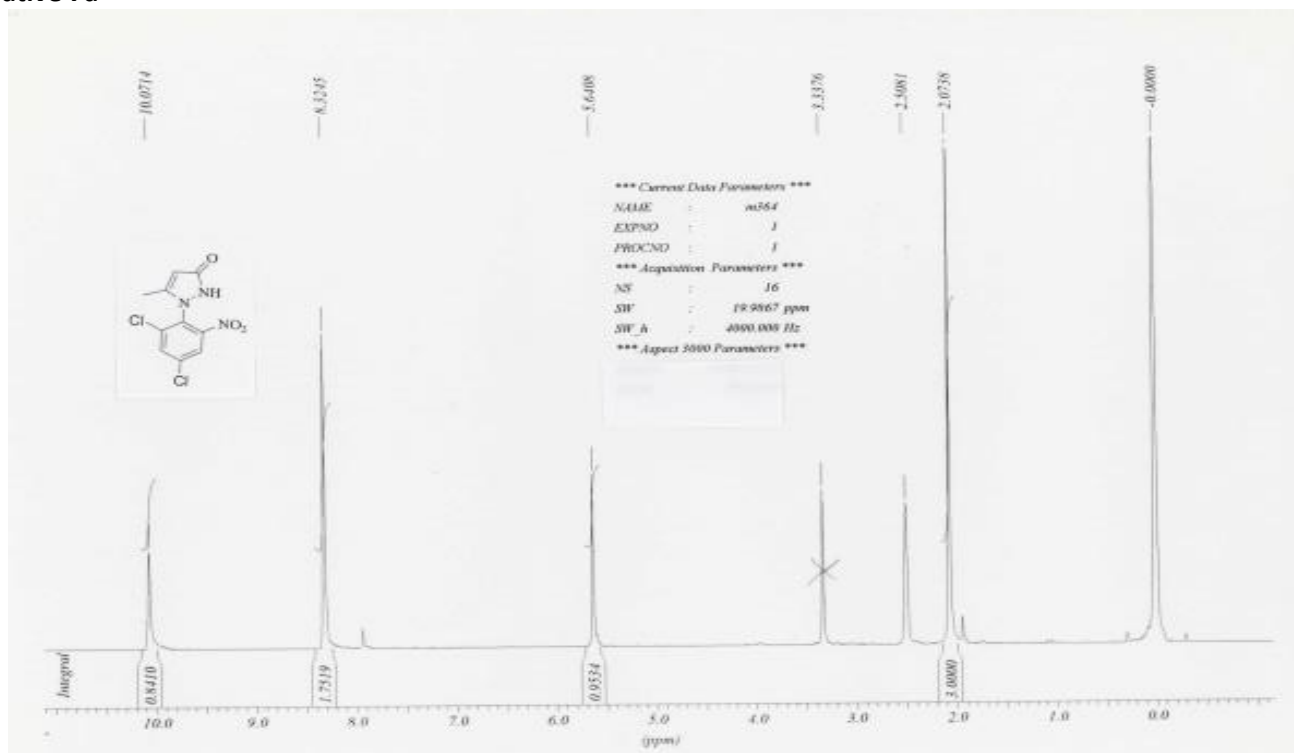
Derivative 6a

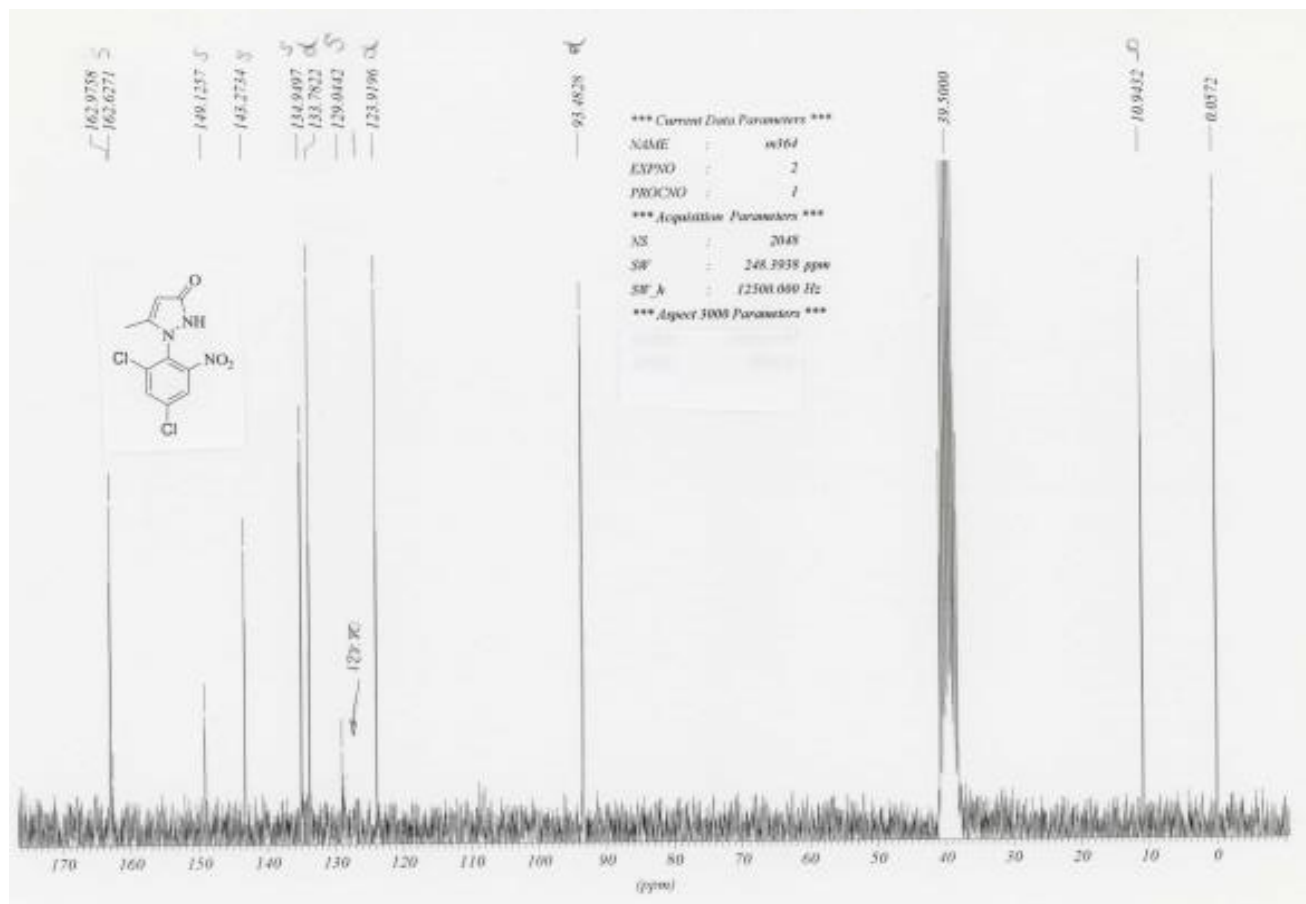
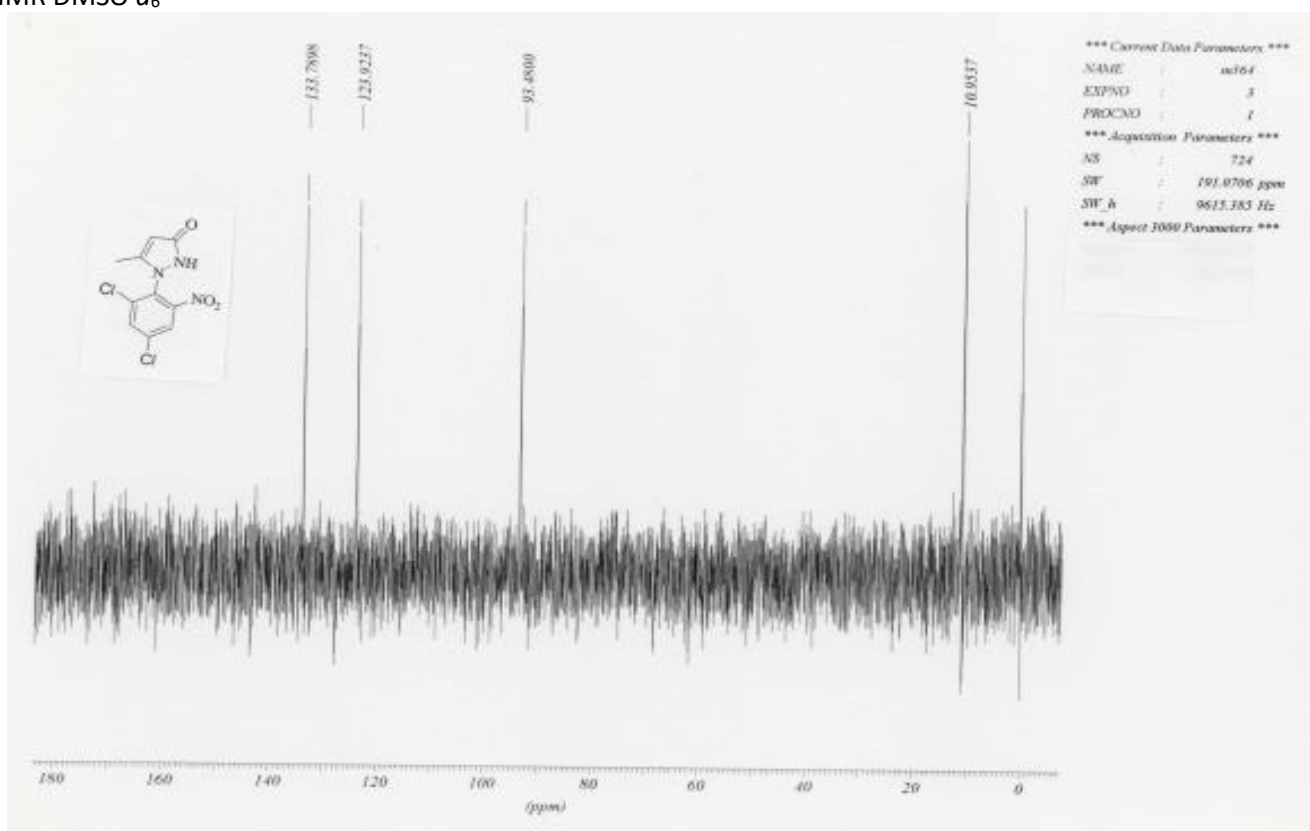
 ^1H NMR (200MHz) $\text{DMSO } d_6$  ^{13}C NMR (51 MHz) $\text{DMSO } d_6$



Dept 135

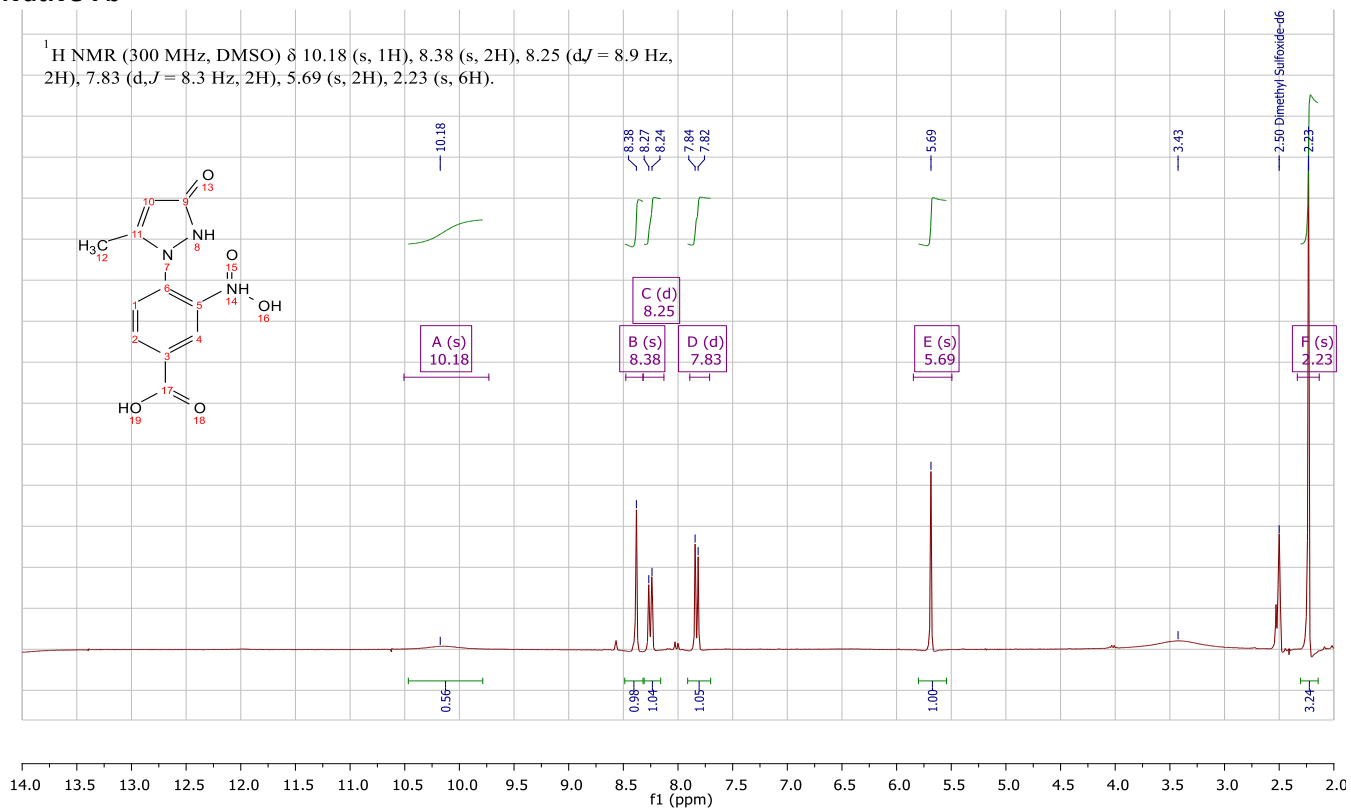
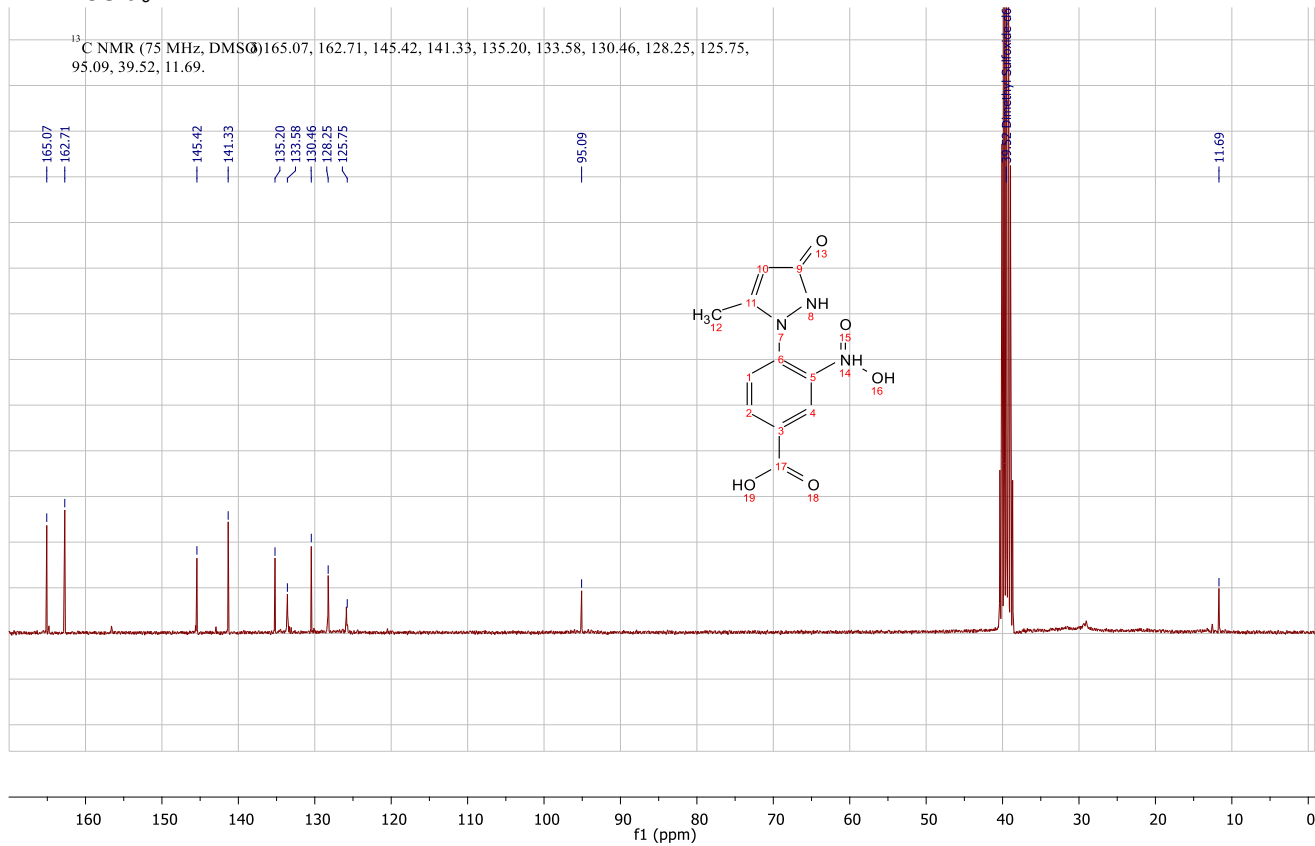
Derivative 7a

¹H NMR DMSO *d*₆

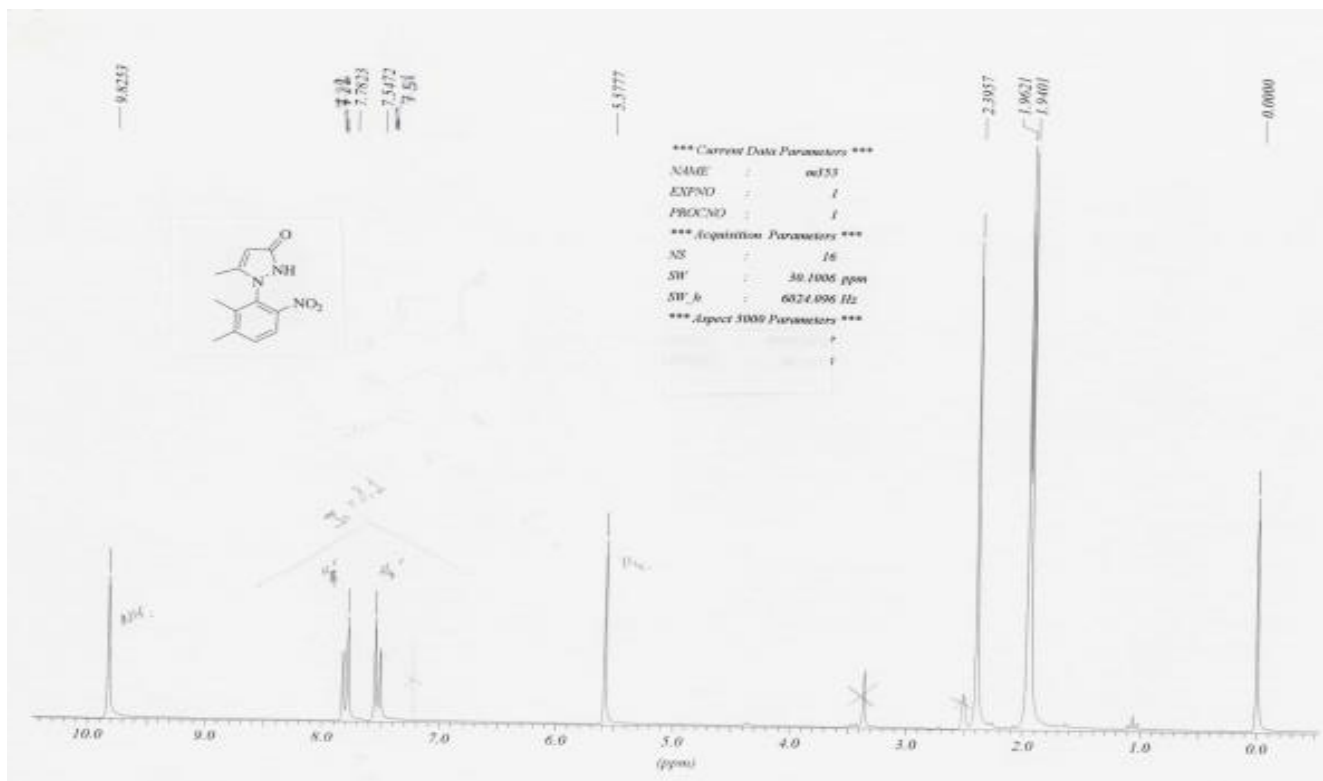
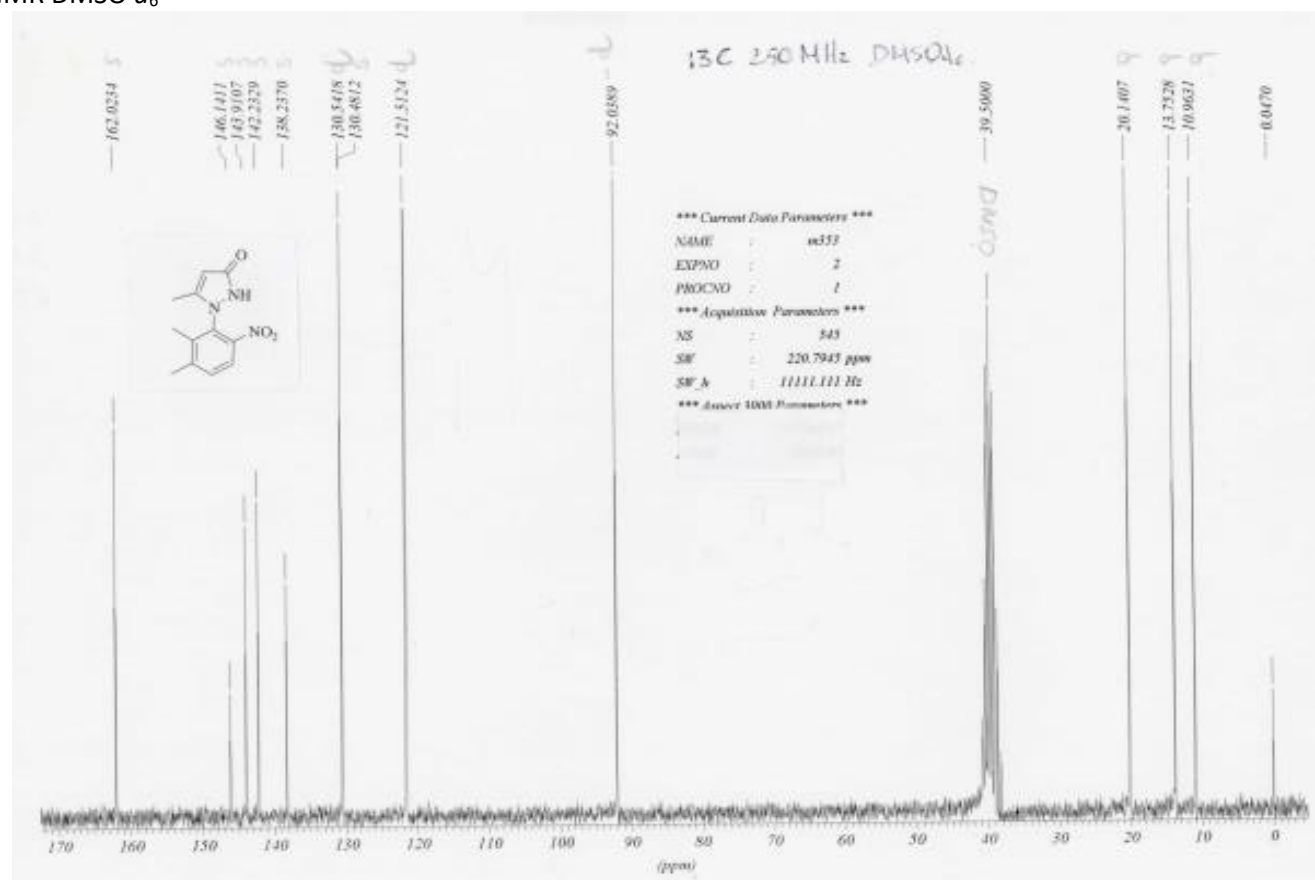
¹³C NMR DMSO *d*₆

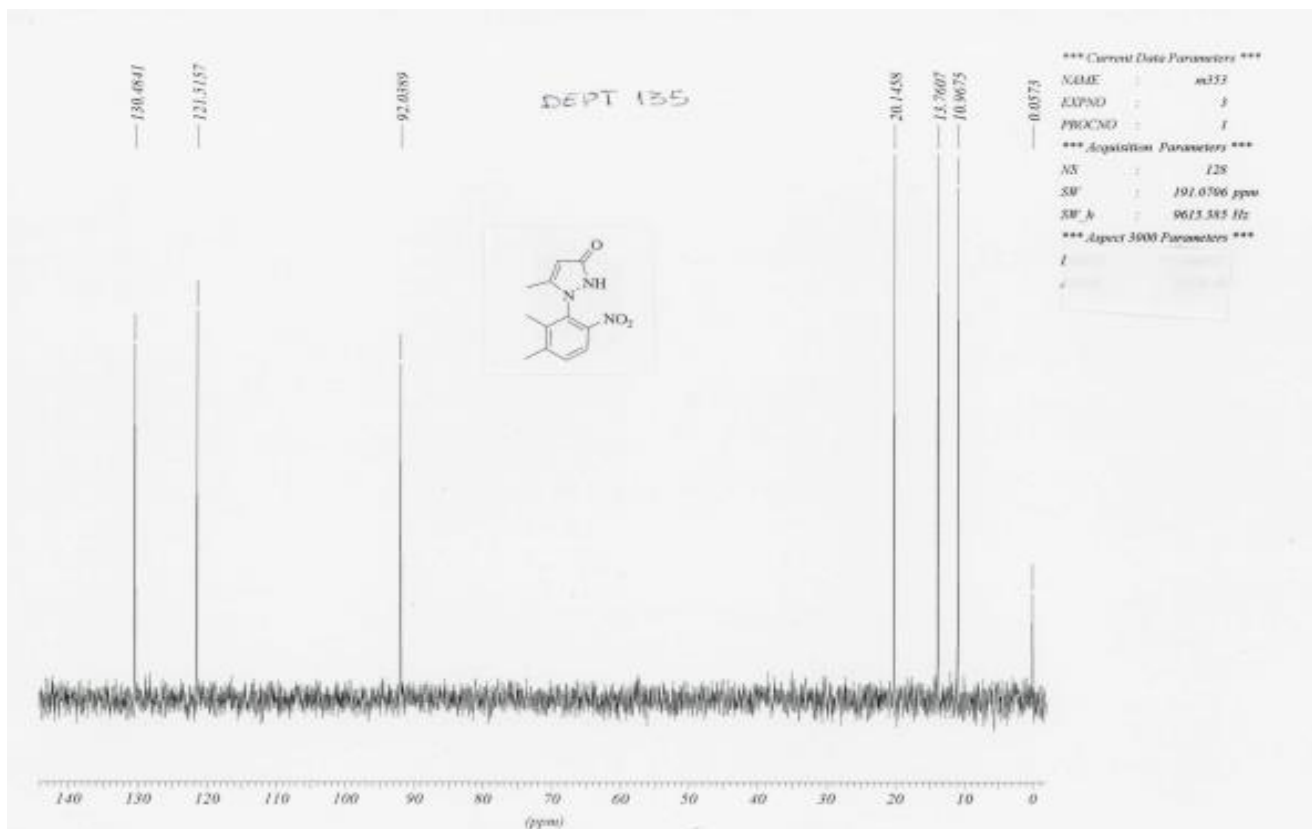
Dept 135

Derivative 7b

¹³C NMR DMSO *d*₆¹³C NMR DMSO *d*₆

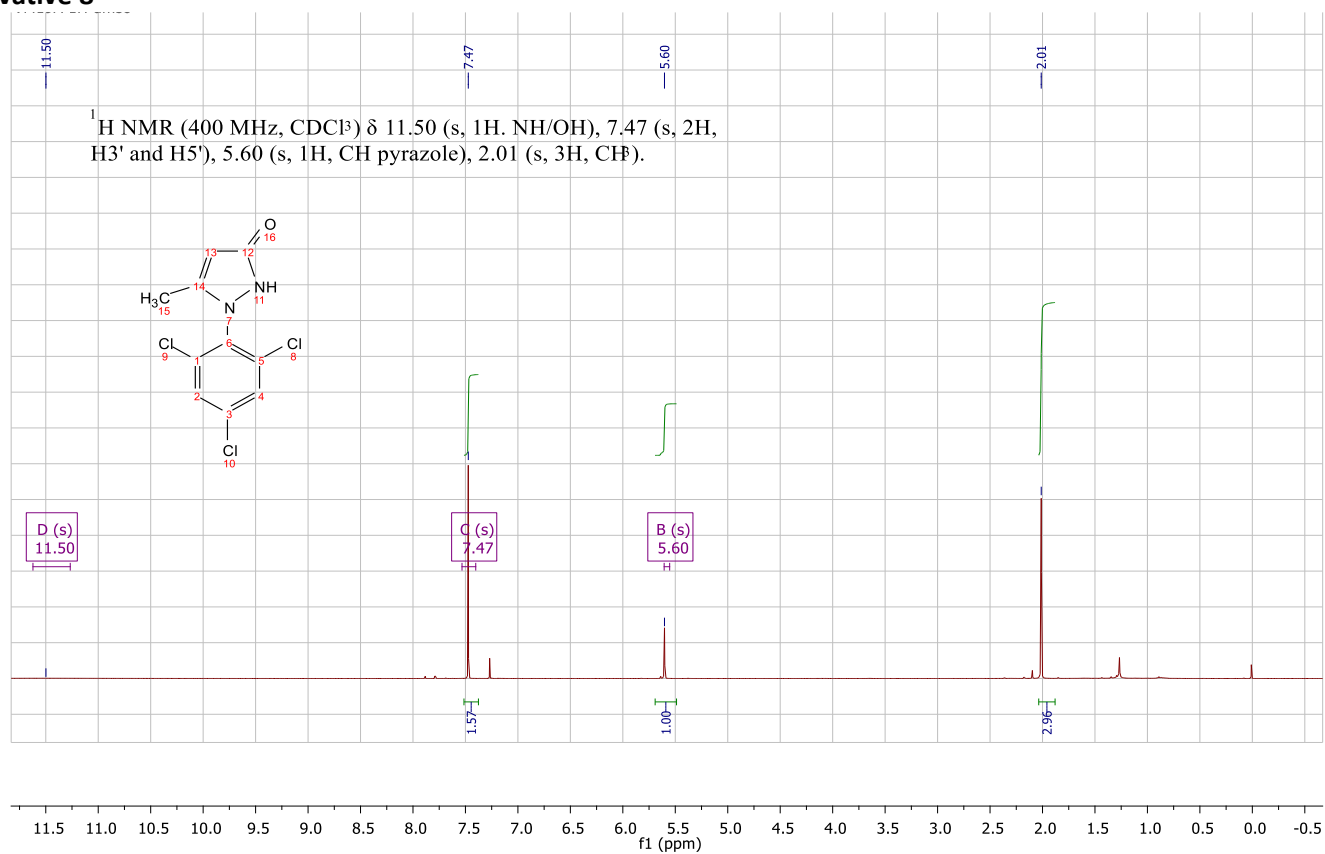
Derivative 7c

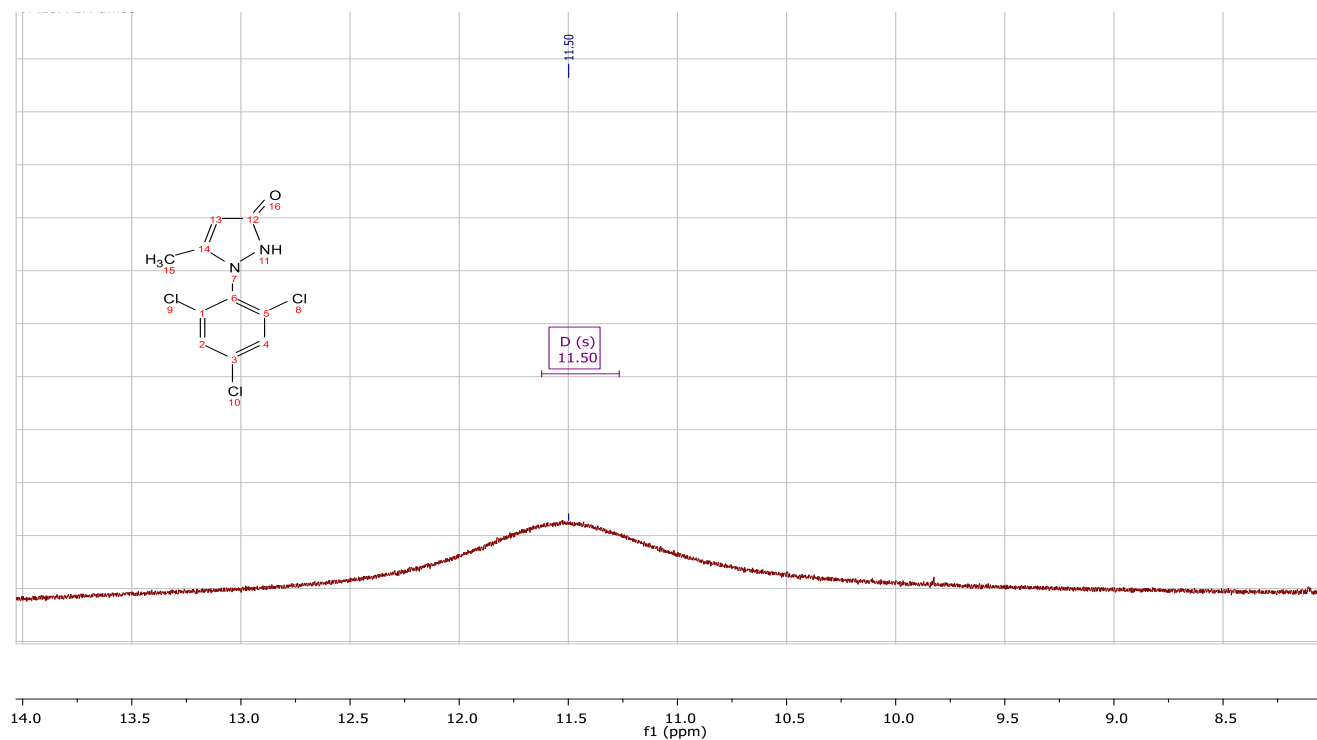
 ^1H NMR DMSO d_6  ^{13}C NMR DMSO d_6



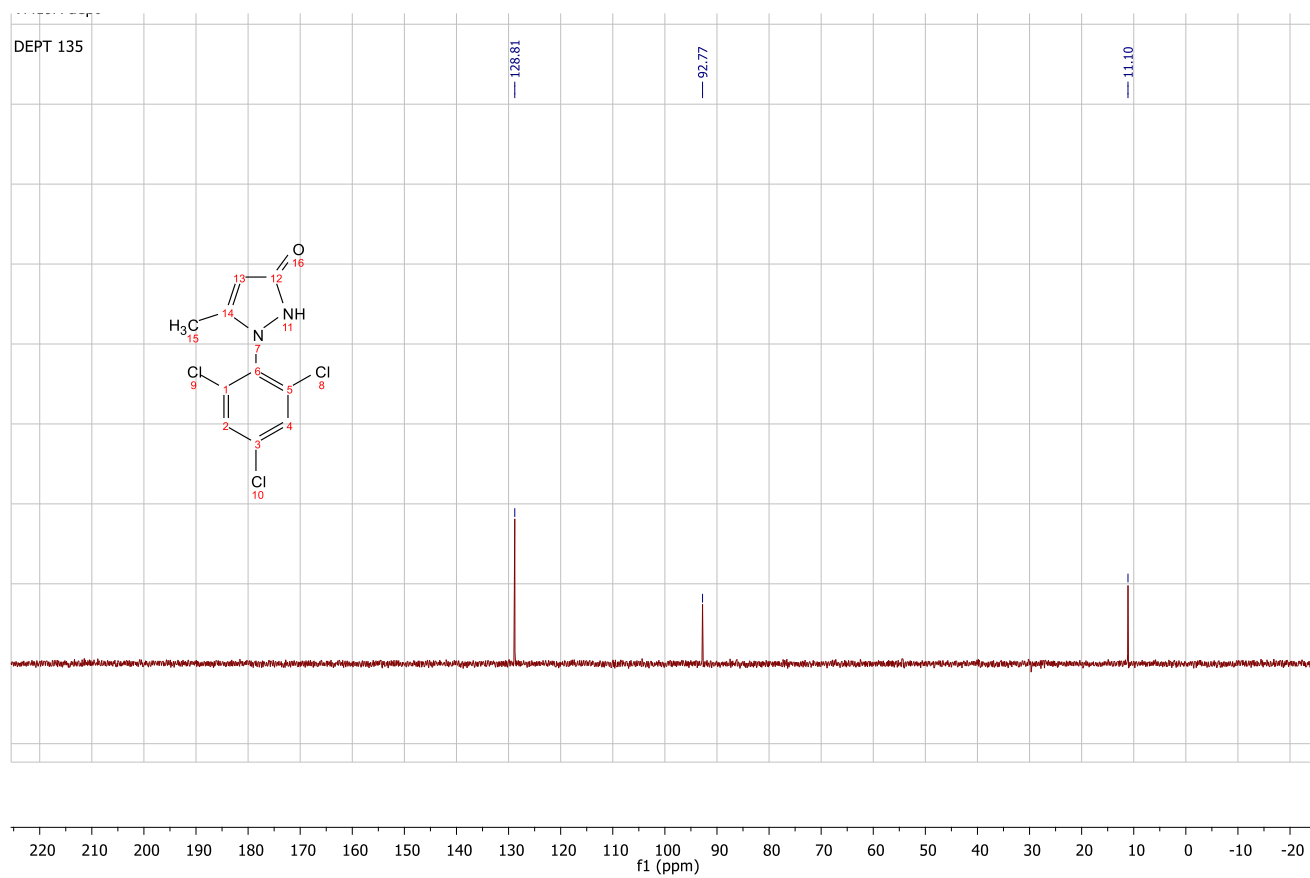
Dept 135

Derivative 8

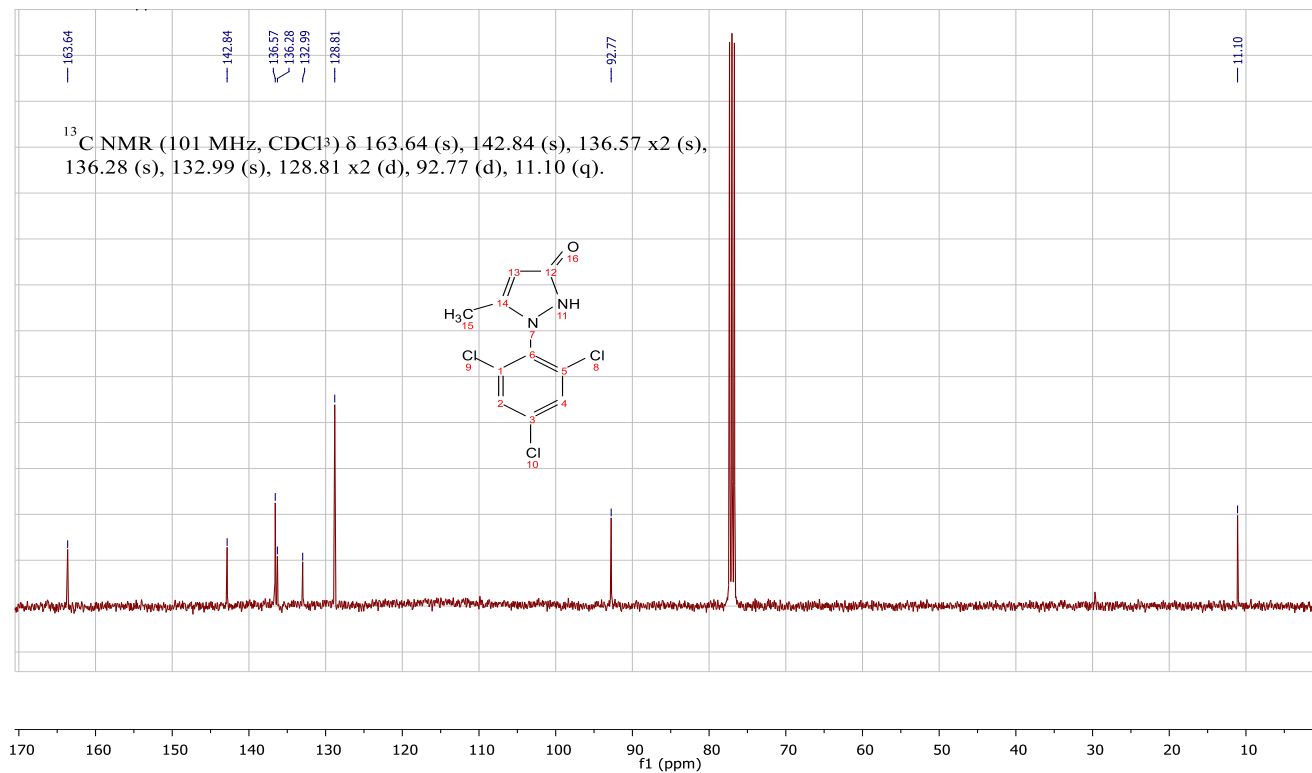
¹H NMR CDCl₃



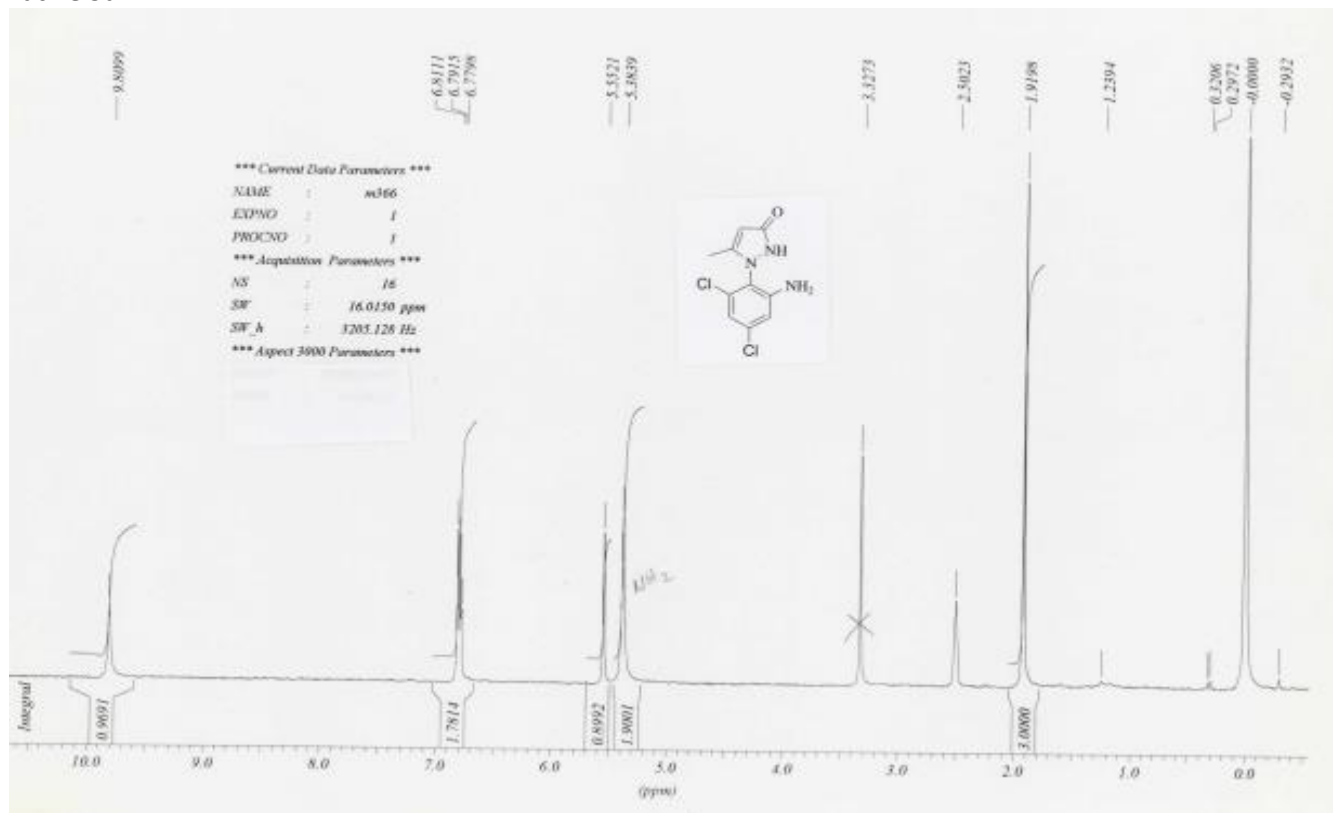
Peak at 11.50 was amplified to better evidence their presence

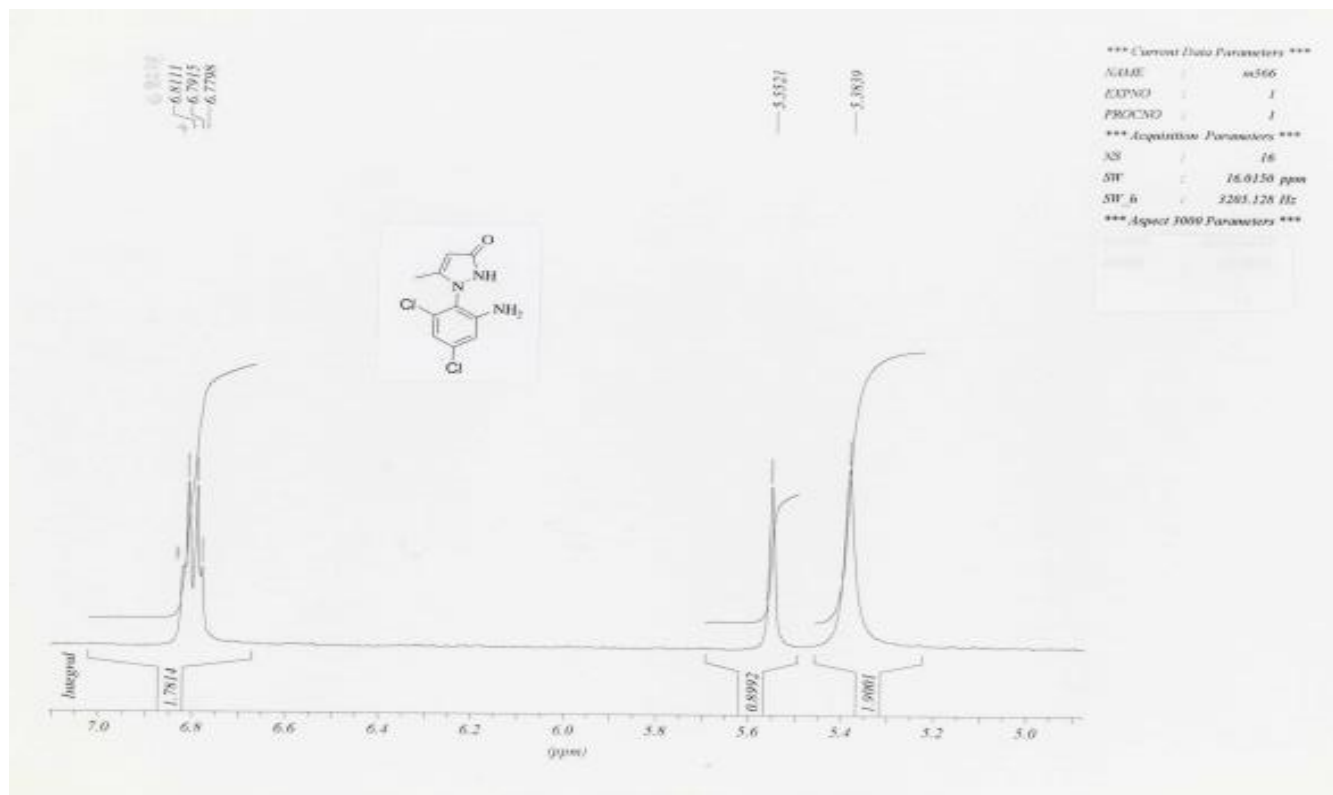
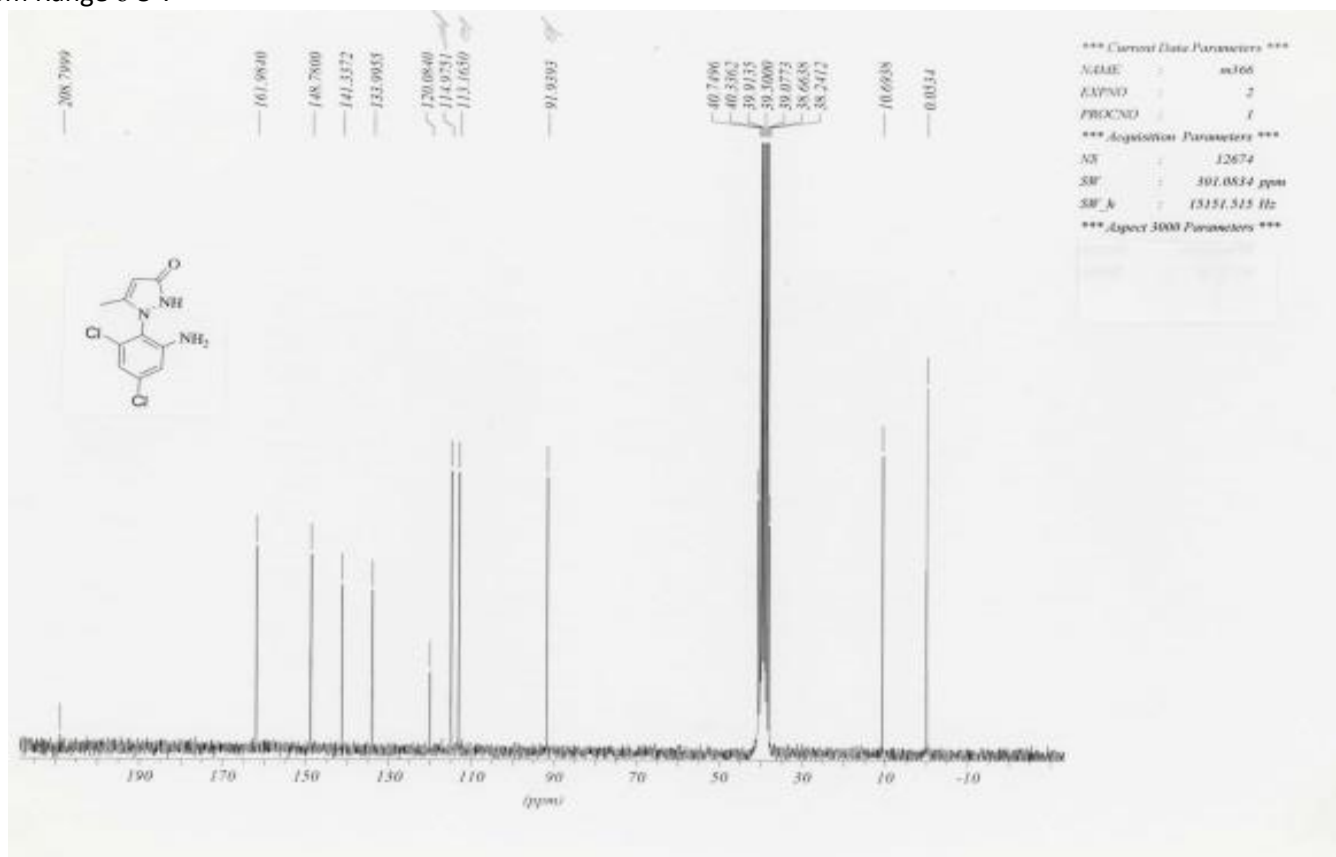


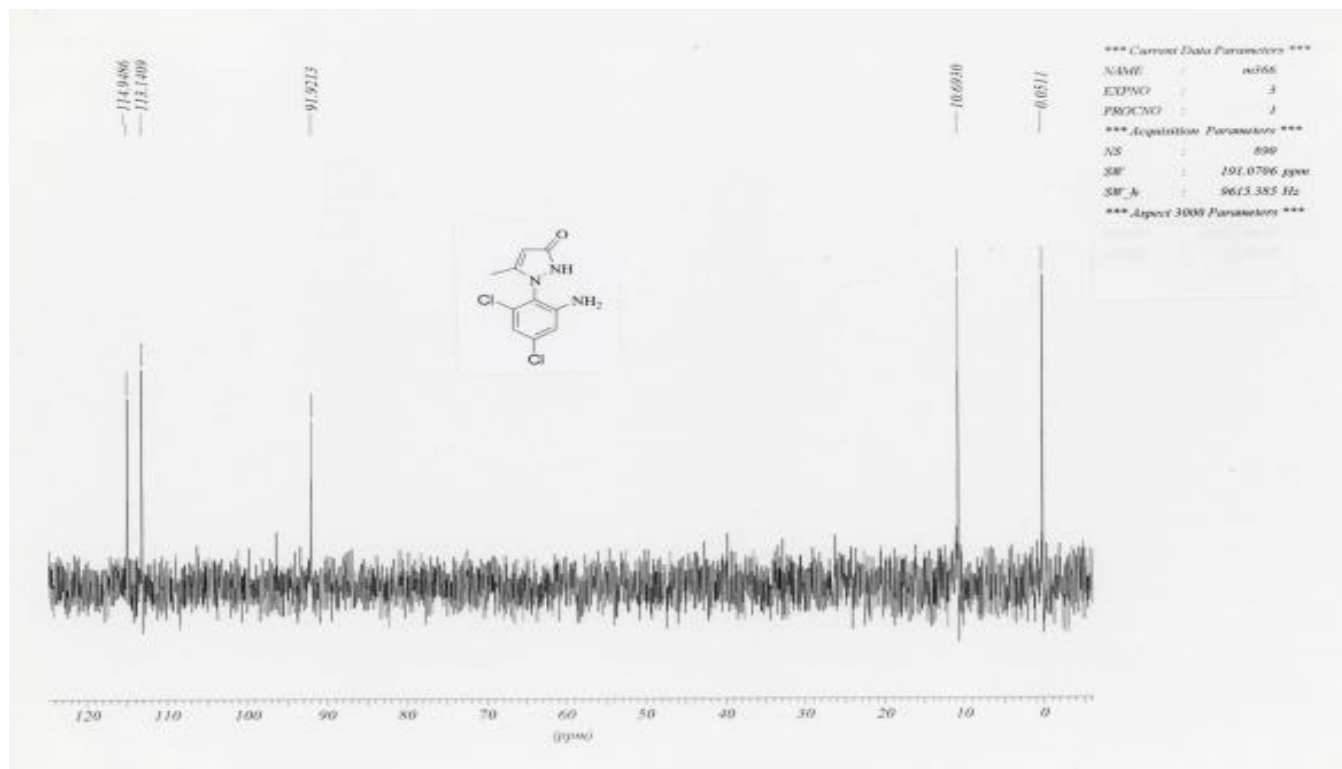
Dept135

 ^{13}C NMR CDCl_3

Derivative 9a

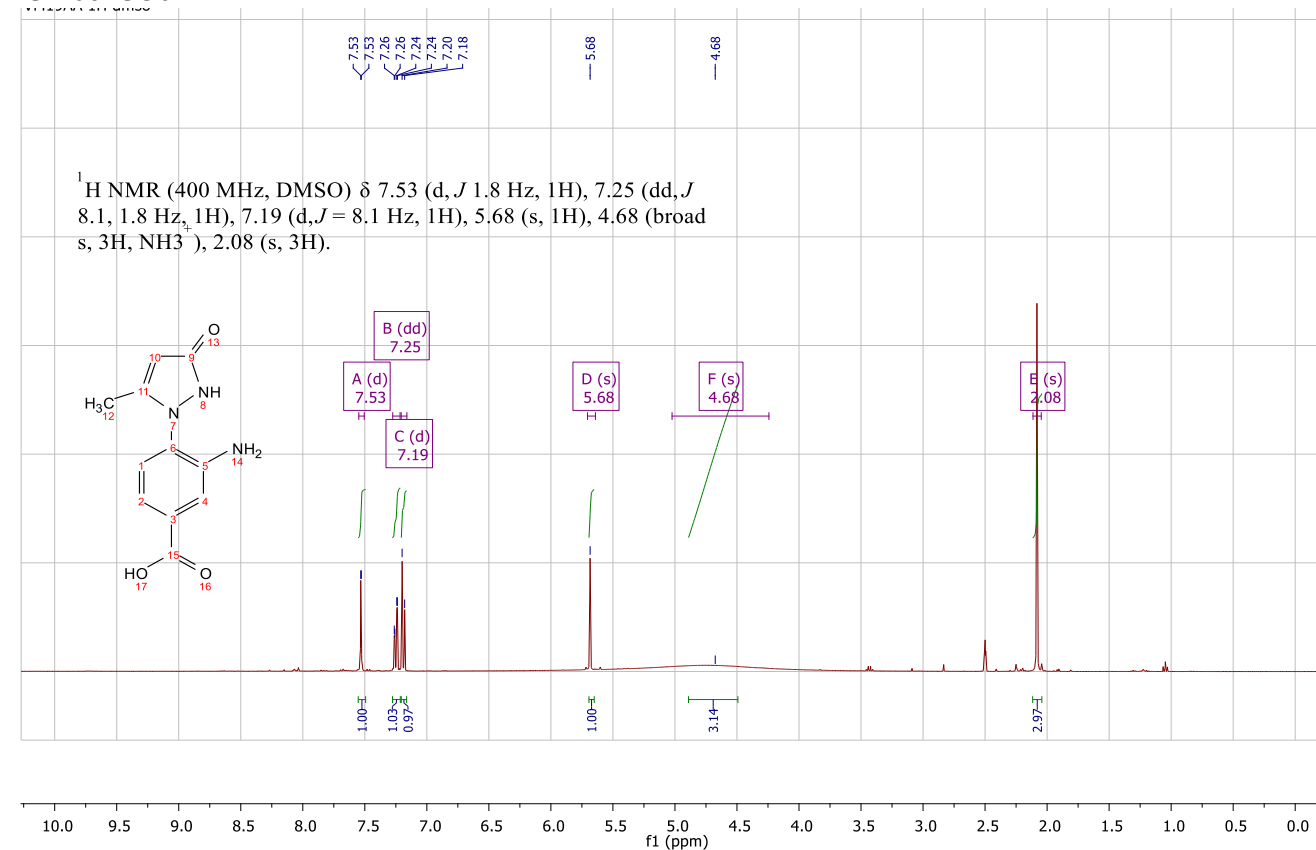
 ^1H NMR $\text{DMSO } d_6$

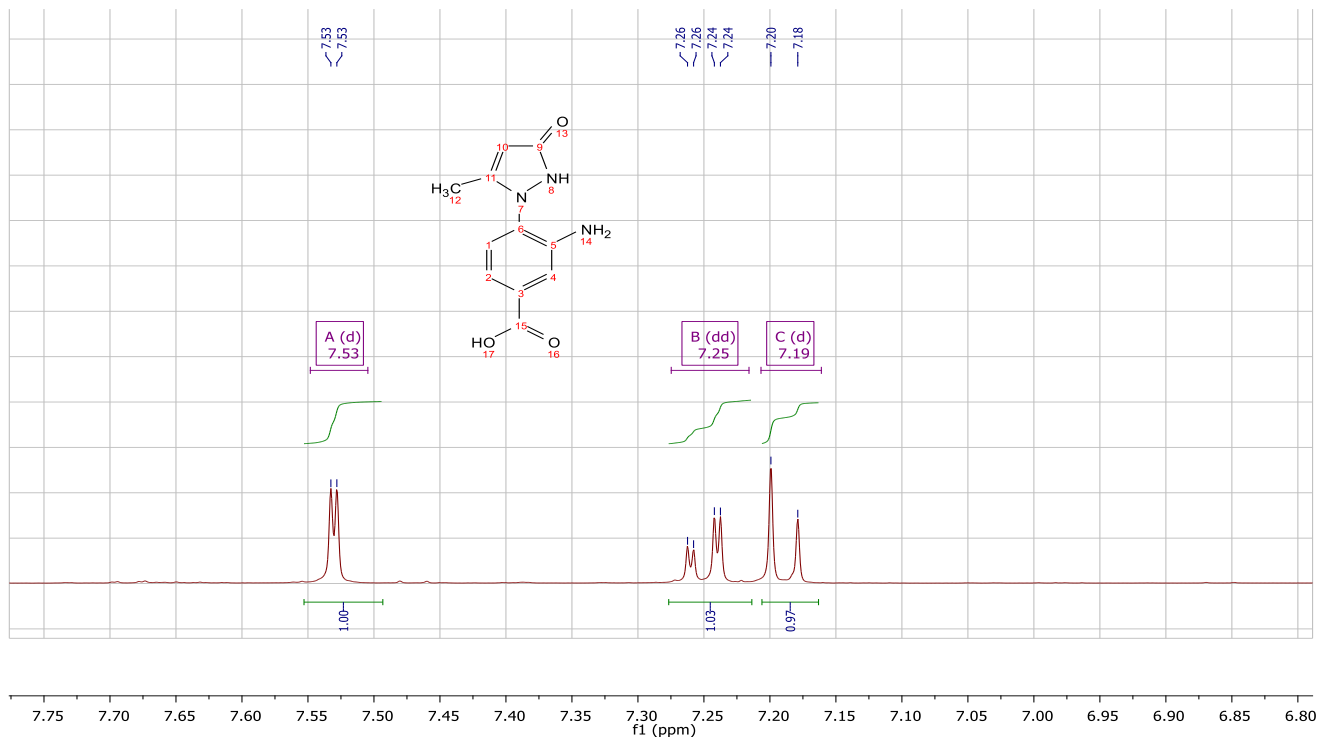
Zoom Range δ 5-7 ^{13}C NMR DMSO d_6



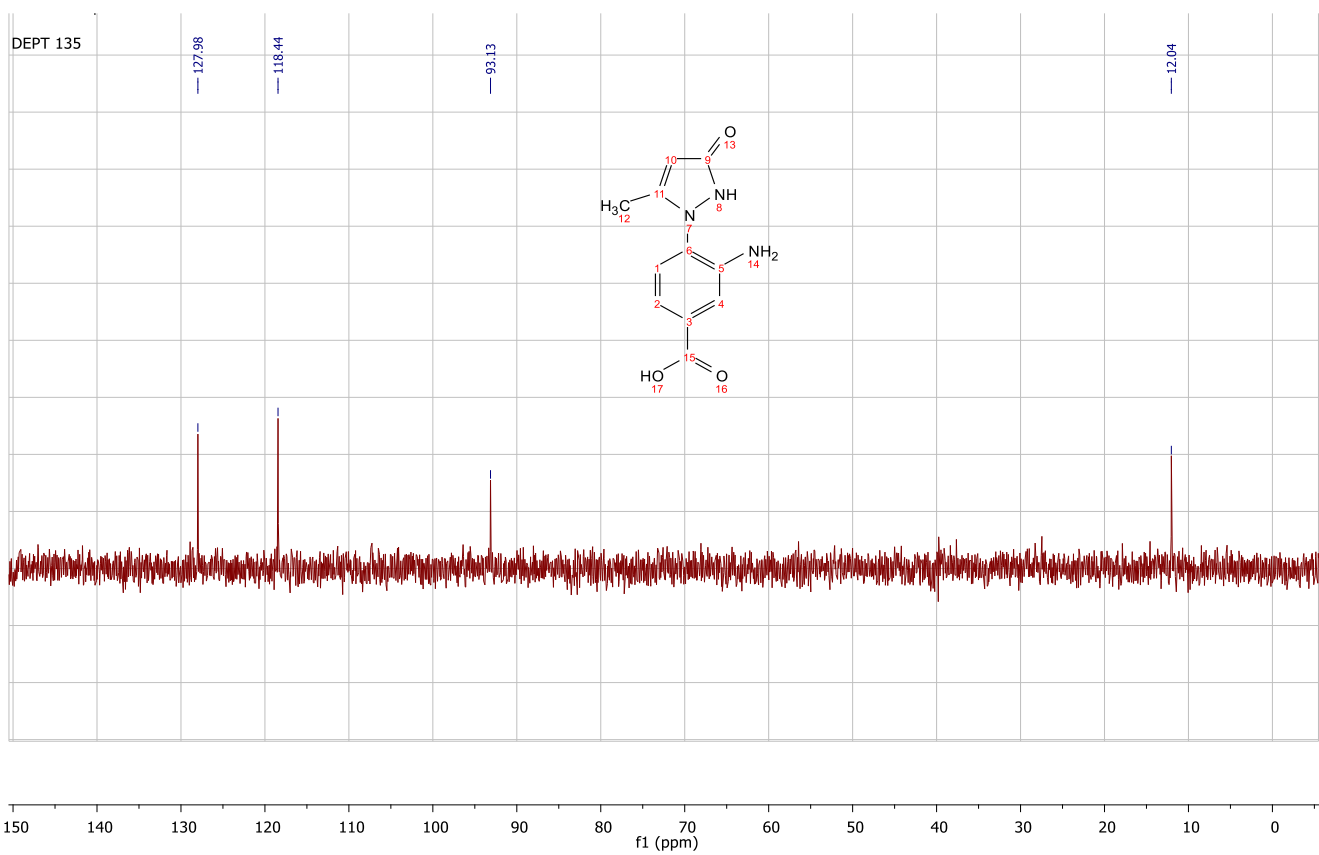
Dept135

Derivative 9b

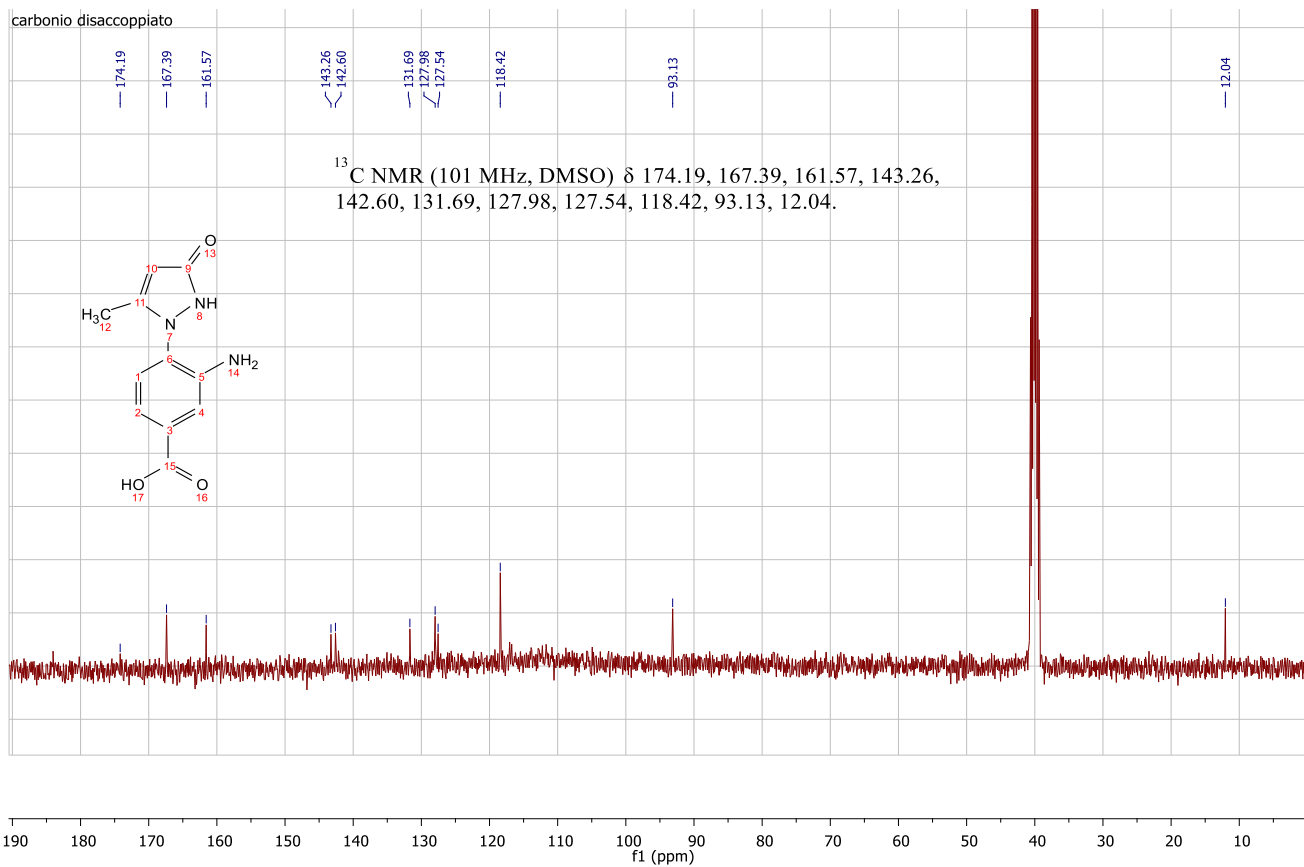
¹H NMR DMSO *d*₆



Aromatic zone

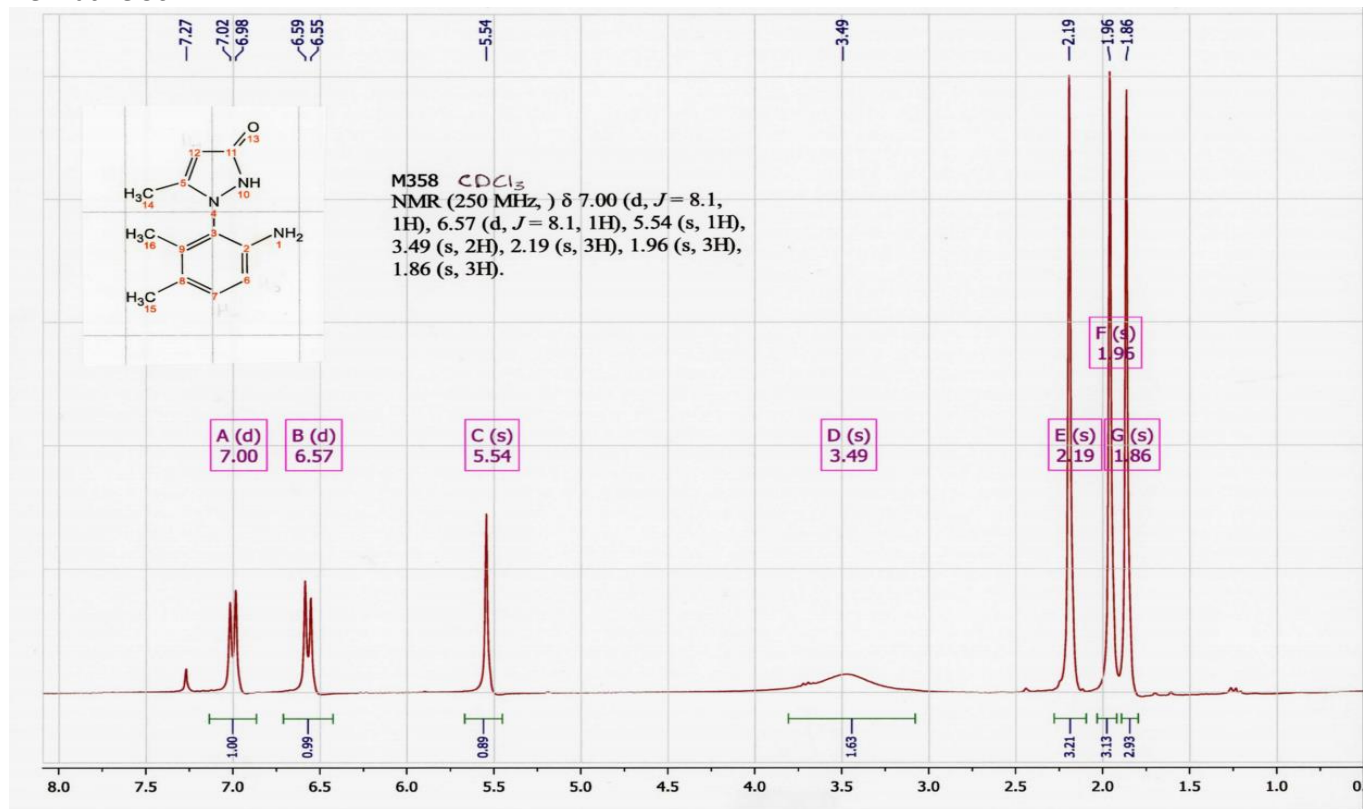


Dept135

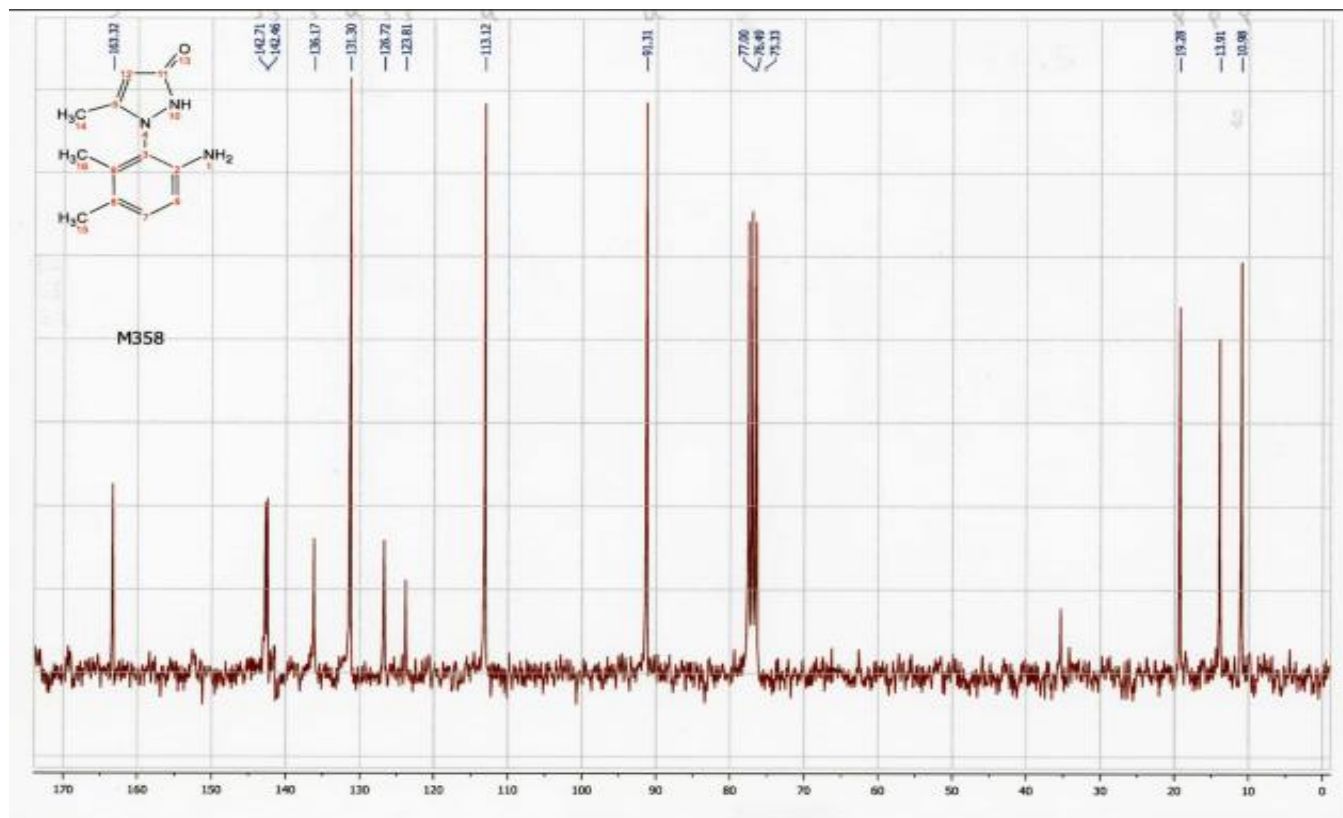


^{13}C NMR DMSO d_6

Derivative 9c

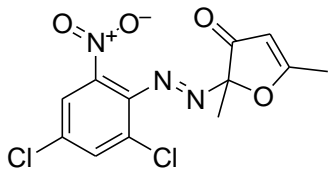


^1H NMR DMSO d_6

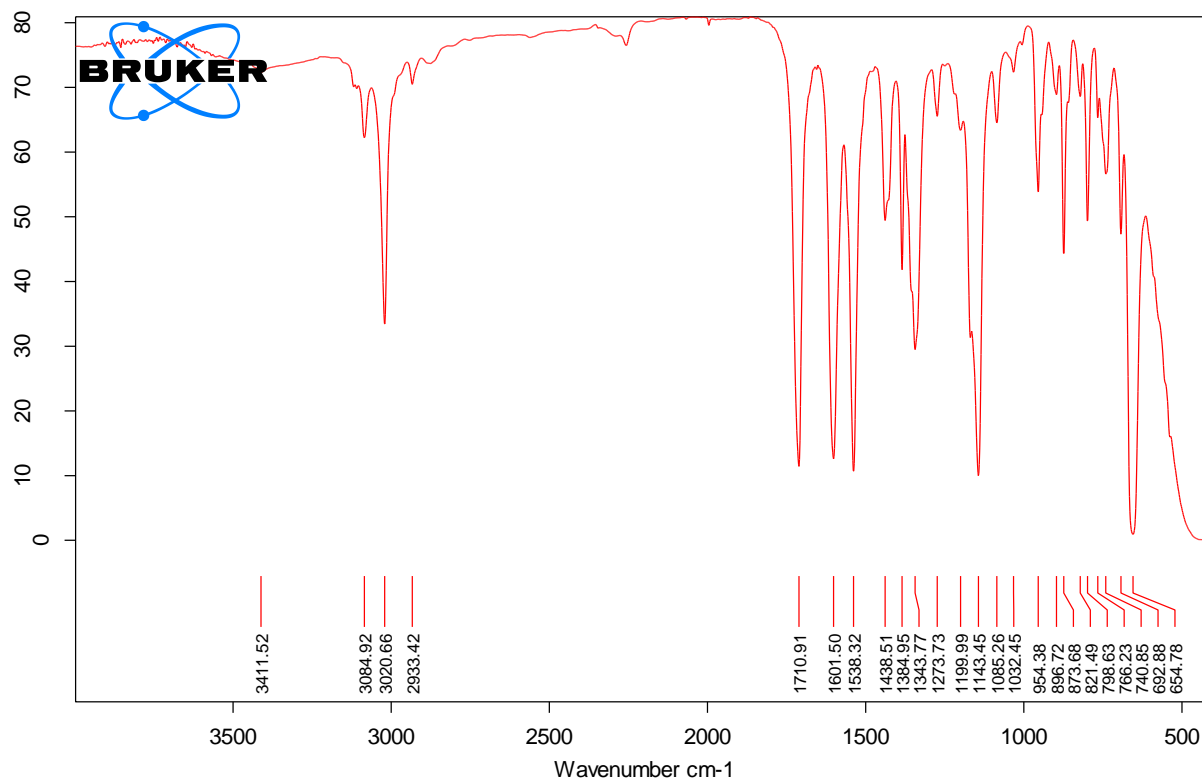
 ^{13}C NMR $\text{DMSO-}d_6$

FT/IR spectra recorded with Bruker Alpha Spectrometer in NaCl window cell in bromoform dispersion or solution.

Derivative 6a



6a

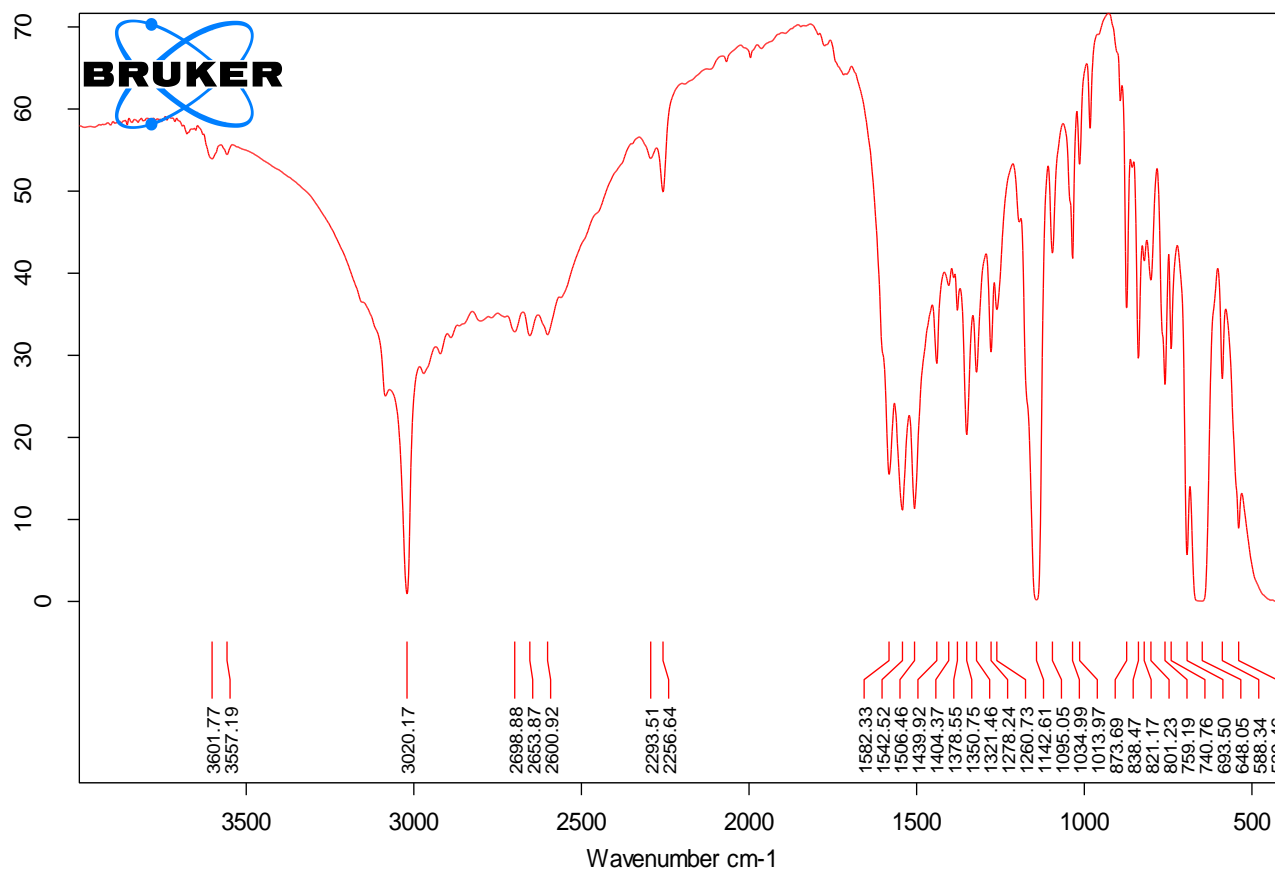
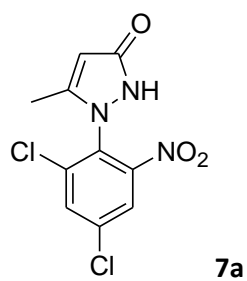


C:\OPUS_7.0.122\MEAS\AzaFuran4,6diClNO2.0

AzaFuran4,6diClNO2

Instrument type and / or accessory

31/01/2022

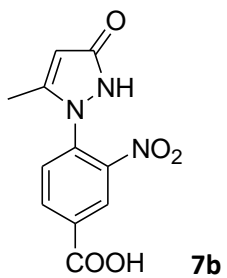


C:\OPUS_7.0.122\MEAS\Nitro-4,6-diCl-pyrzne.0

Nitro-4,6-diCl-pyrzne

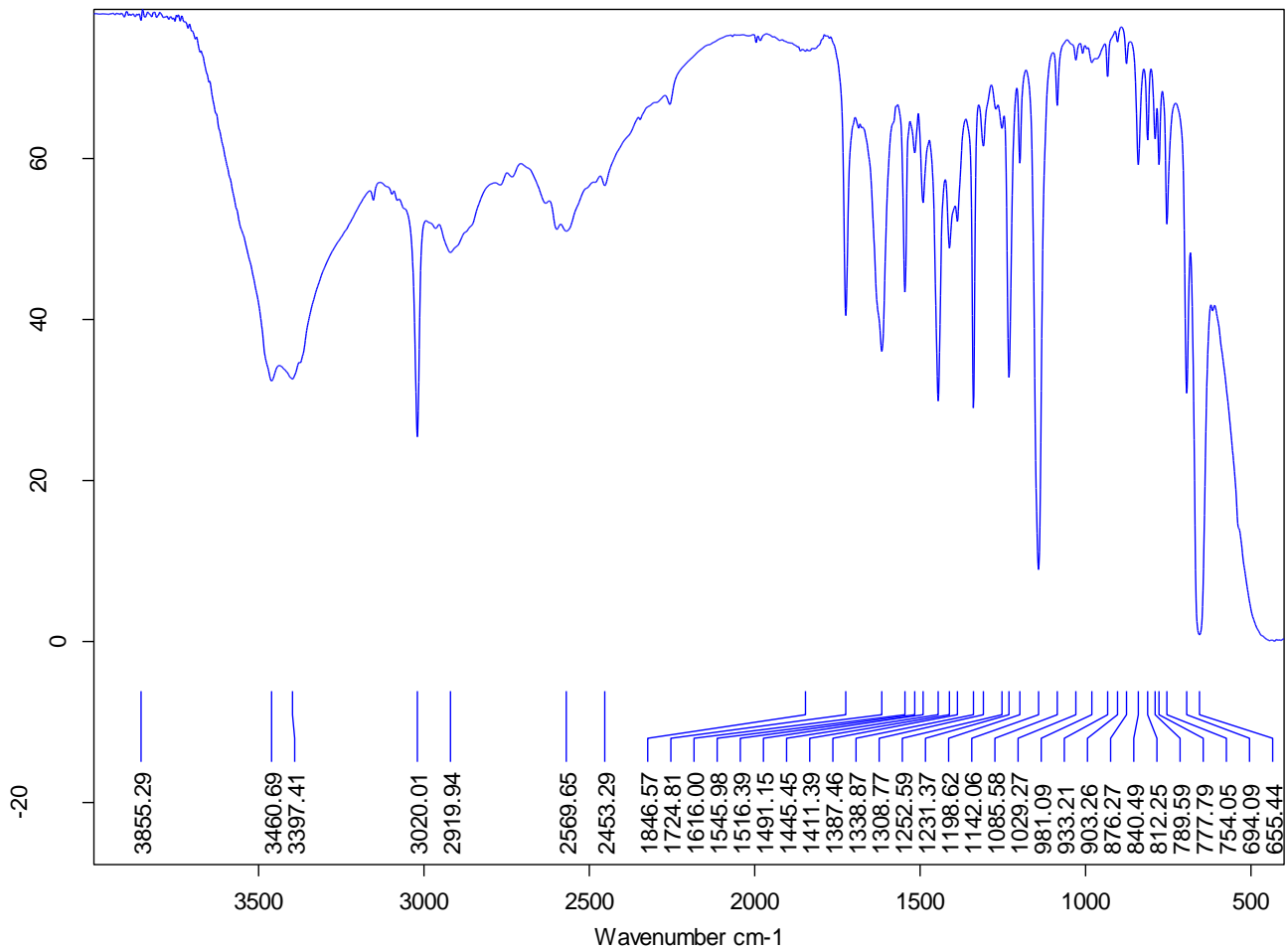
Instrument type and / or accessory

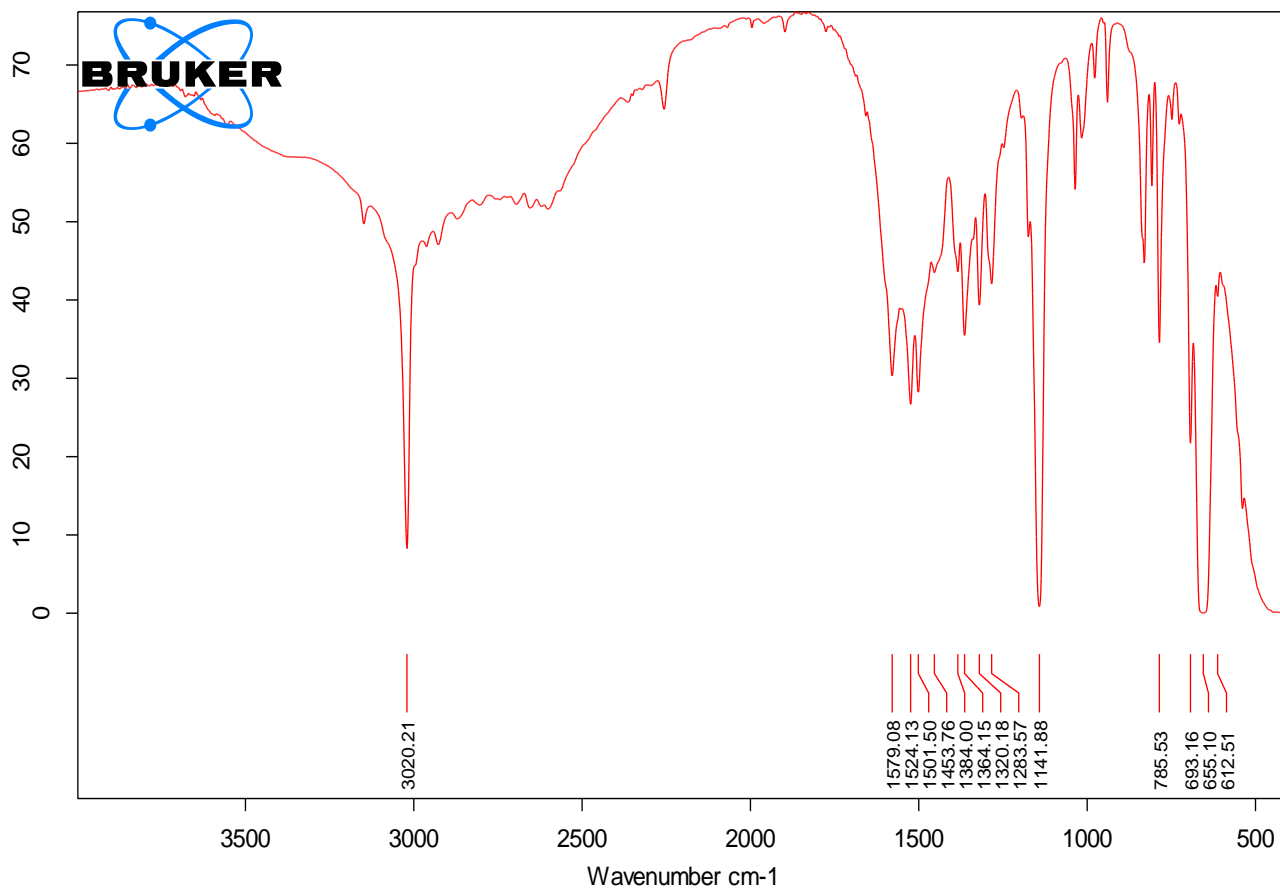
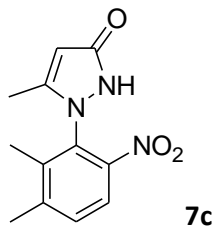
24/01/2022



C:\OPUS_7.0.122\MEAS\Nitro_COOH_dil.0

01/10/2021 11:49:09



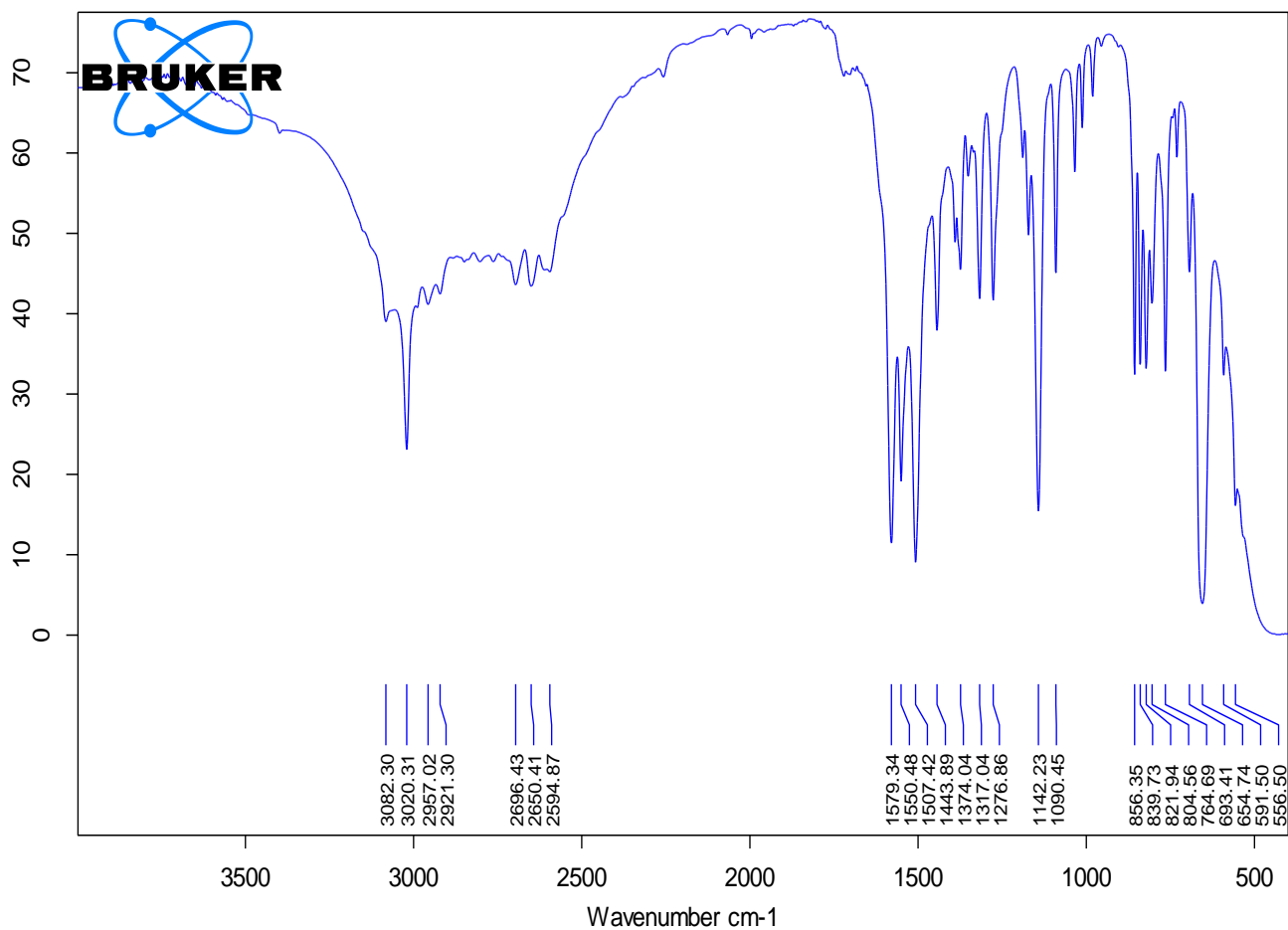
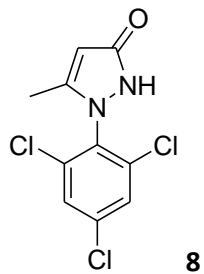


C:\OPUS_7.0.122\MEAS\Nitro56diMe.0

Nitro56diMe

Instrument type and / or accessory

01/10/2021

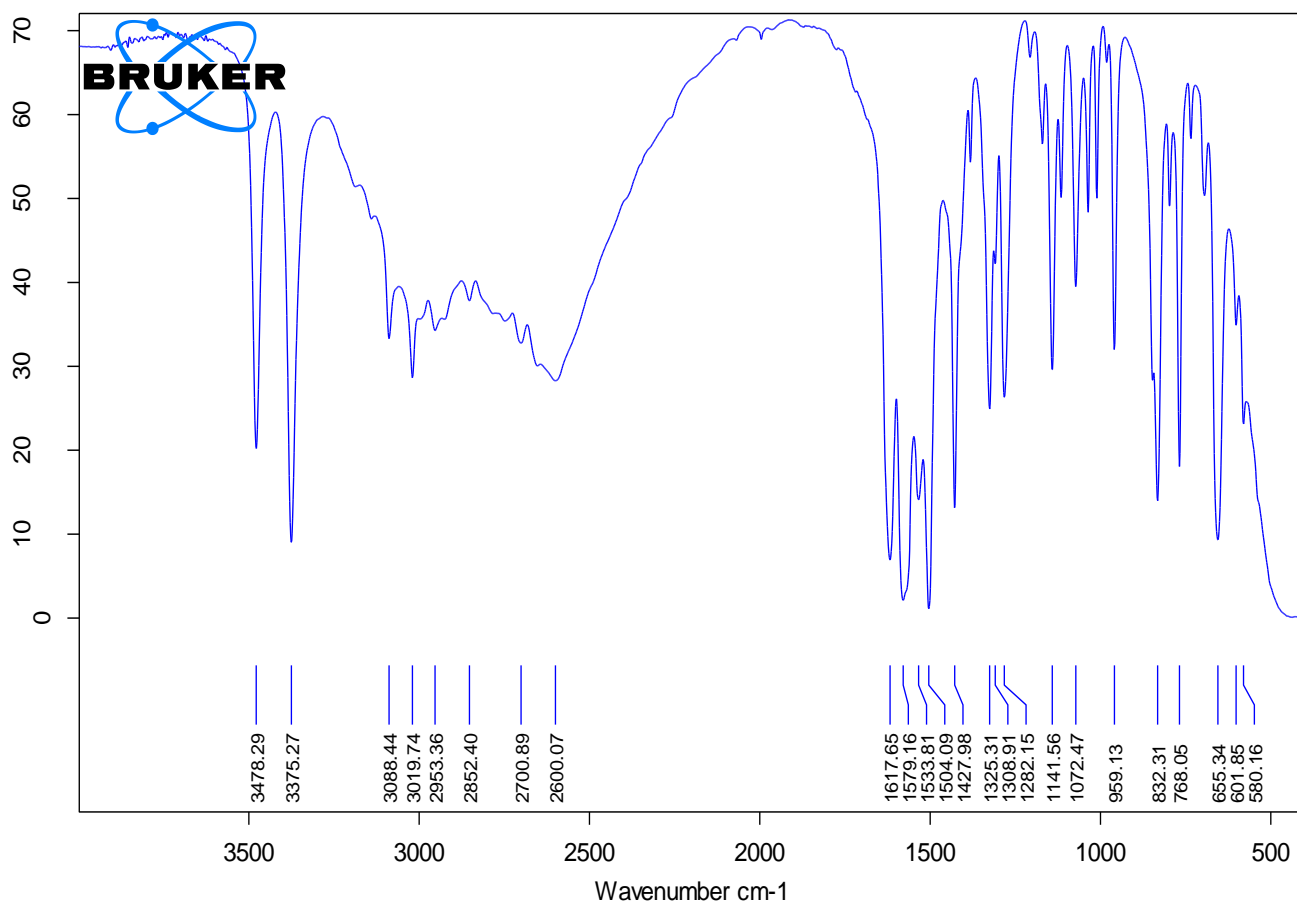
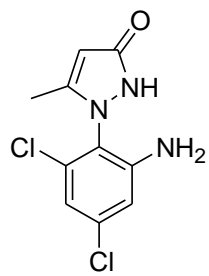


C:\OPUS_7.0.122\MEAS\Pyr_triCl.0

Pyr_triCl

Instrument type and / or accessory

01/10/2021

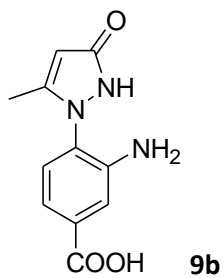


C:\OPUS_7.0.122\MEAS\NH2_46diCl_Pyrzne.1

NH2_46diCl_Pyrzne

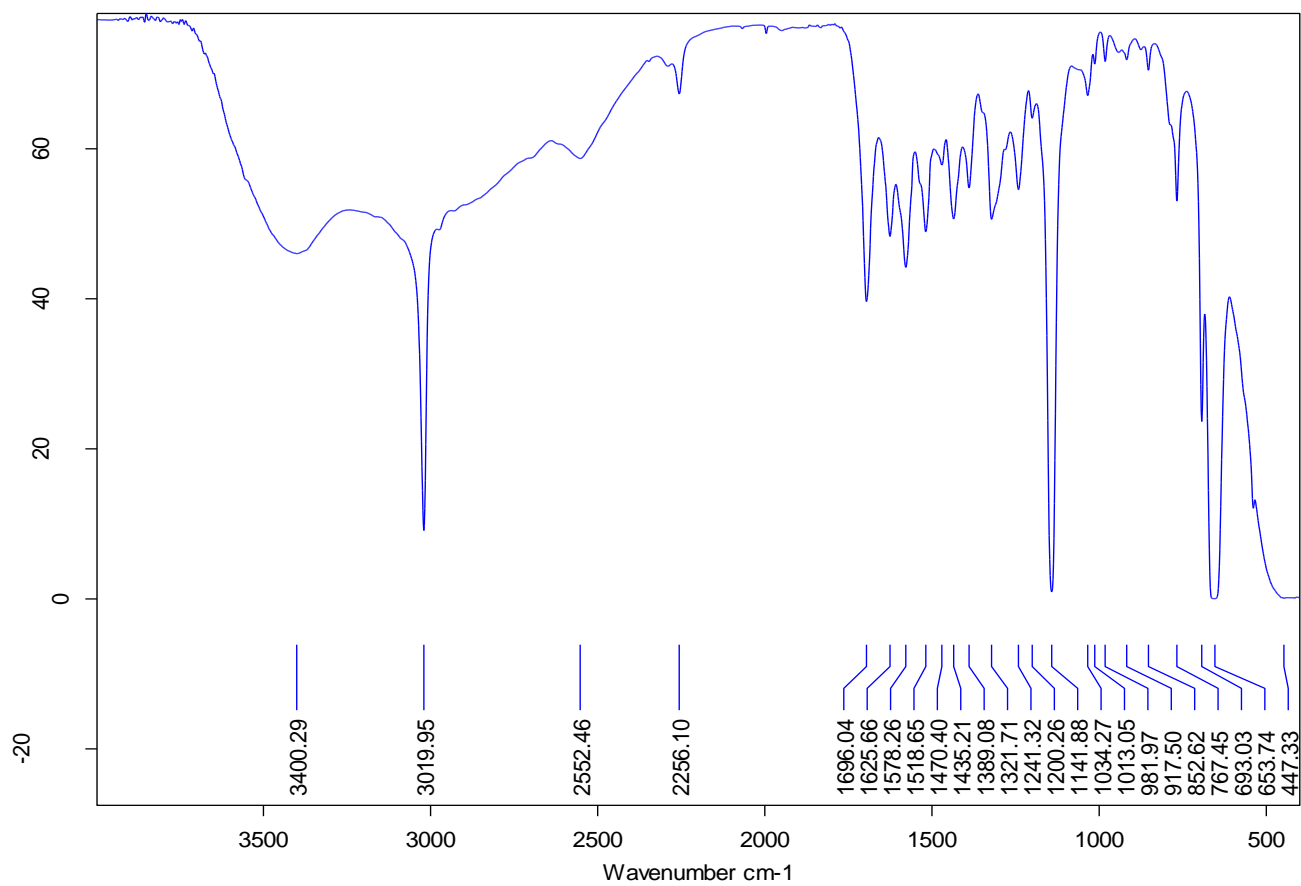
Instrument type and / or accessory

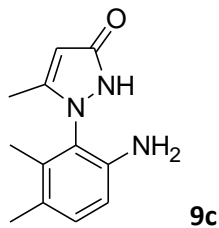
24/01/2022



C:\OPUS_7.0.122\MEAS\NH2_COOH.0

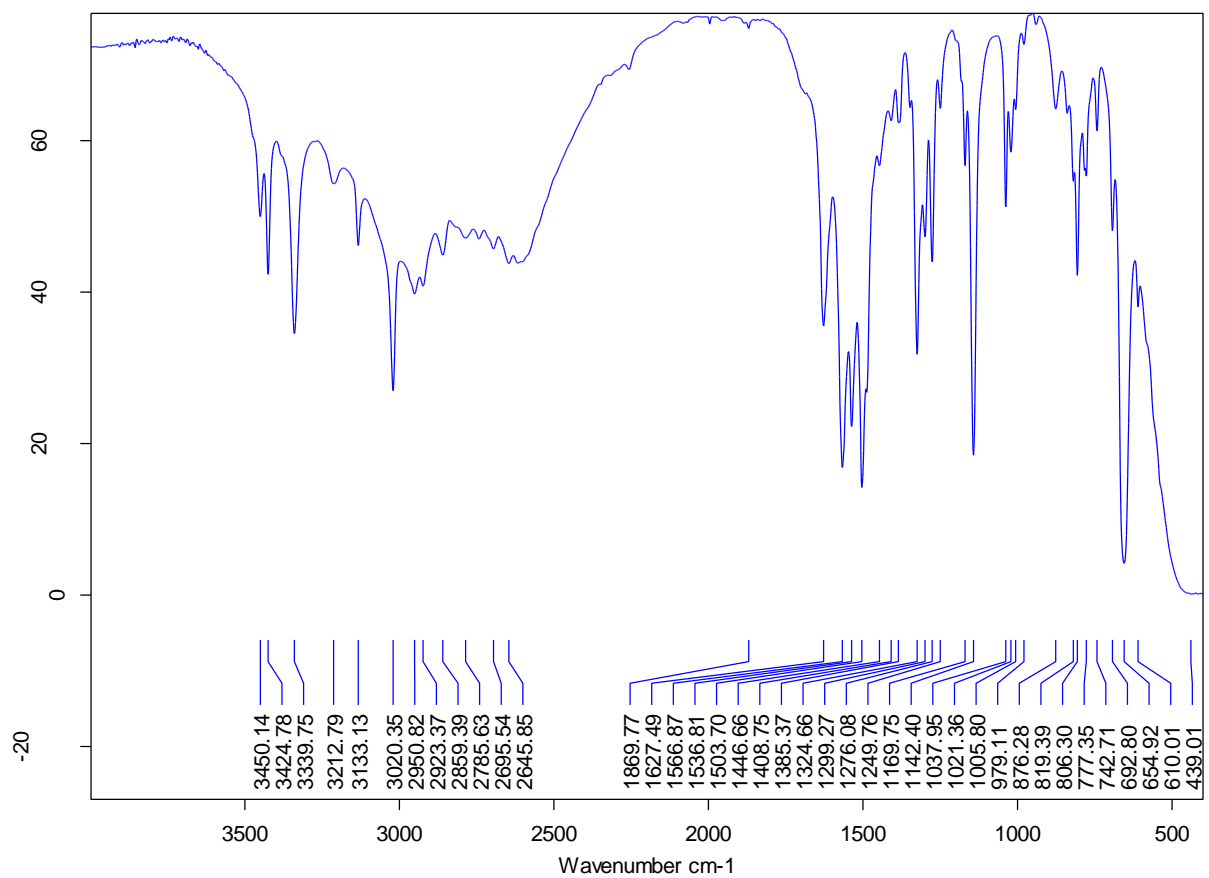
01/10/2021 12:01:48



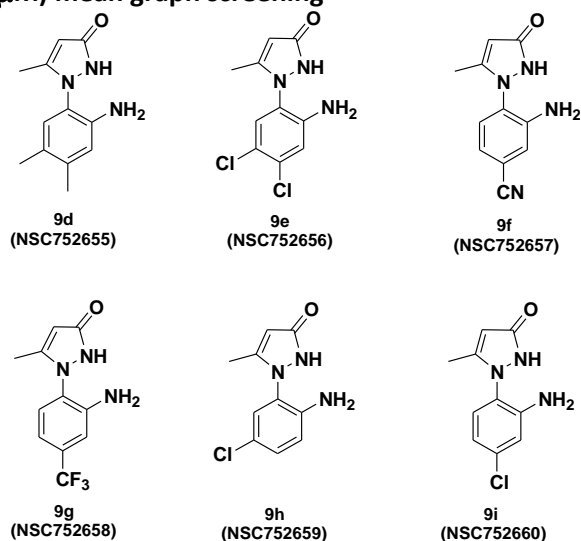


C:\OPUS_7.0.122\MEAS\Amina56diMe_dil.1

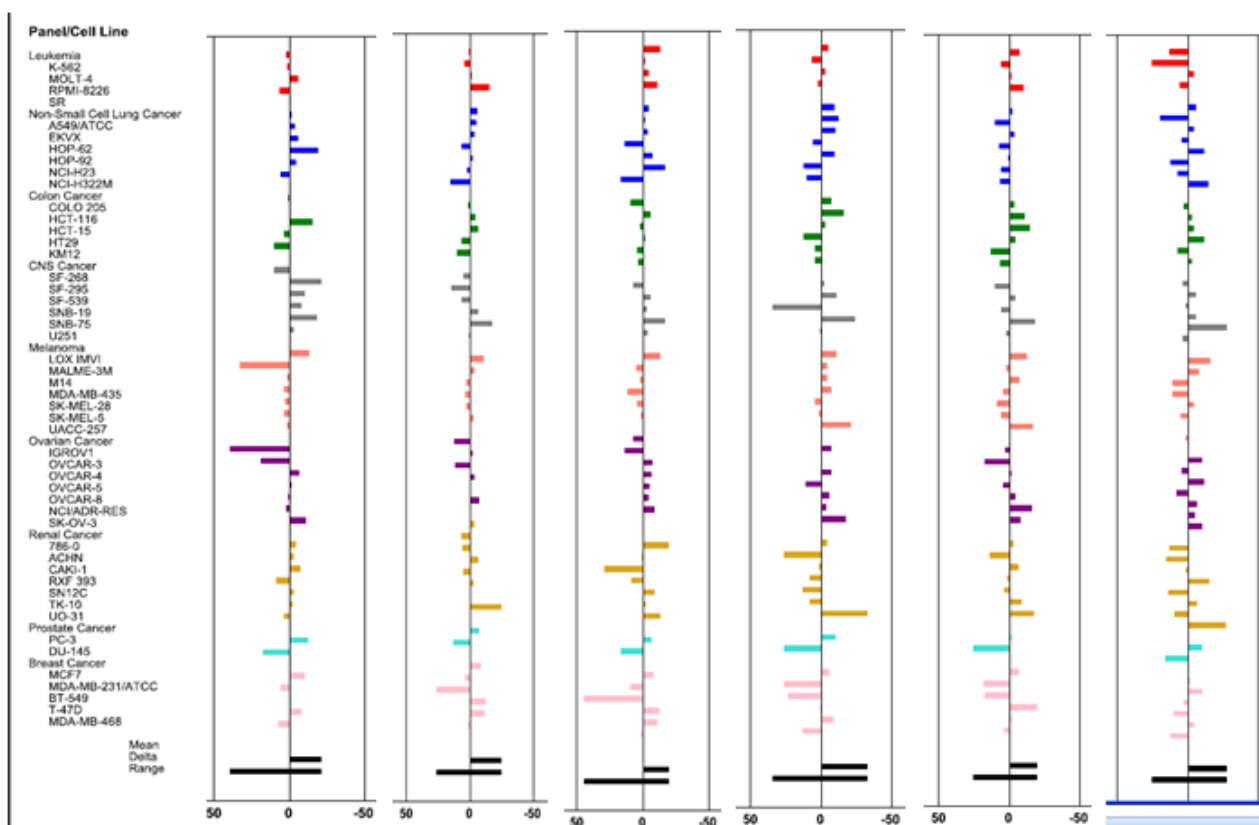
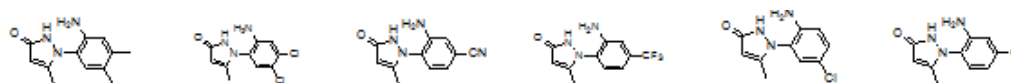
01/10/2021 14:48:32



Page 1 of 1

Antiproliferative NCI one dose (10 μ M) mean graph screening

Pyrazol-3-ones selected by NCI for one dose screening assay.

One dose 10 μ M (SRD) on about 60 tumor cell lines from NATIONAL CANCER INSTITUTE (N.C.I. USA)

The authors thank the National Cancer Institute (Bethesda, MD) team for the antitumor tests reported in this paper.