molecules

MDPI

Supplementary Materials

Synthesis and In Silico Docking Study towards M-Pro of Novel Heterocyclic Compounds Derived from Pyrazolopyrimidinone as Putative SARS-CoV-2 Inhibitors

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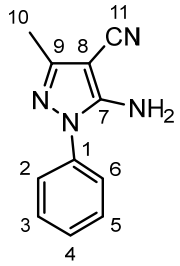
General procedures

TLC was carried out on silica gel (Macherey-Nagel, detection under UV light and with cerium molybdate reagent). The used solvents were dried according to usual procedures. Melting points are uncorrected (Leica hot stage microscope, or BUCHI melting point M-565). IR spectra were recorded on a Perkin Elmer FT-IR spectrometer Spectrum 1000 or on a Perkin-Elmer Spectrum Two (UATR Two Unit). NMR spectra were recorded using the Agilent spectrometers DD2 500 MHz and VNMRS 400 MHz (d given in ppm, J in Hz; typical experiments: APT, H-H-COSY, HMBC, HSQC, NOESY), MS spectra were taken on an Advion Expression CMS instrument, and elemental analyses were conducted on a Foss-Heraeus Vario EL (CHNS) unit.

5-amino-3-methyl-1-phenyl-1H-pyrazole-4-carbonitrile (1)

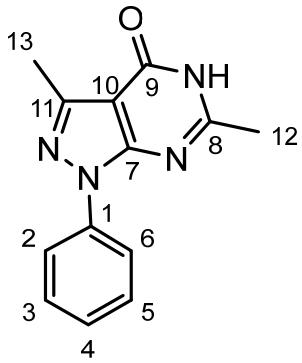


Has already been investigated with reference:

M. Horchani et al., (2021), Int J Mol Sci., 22(19):10258.

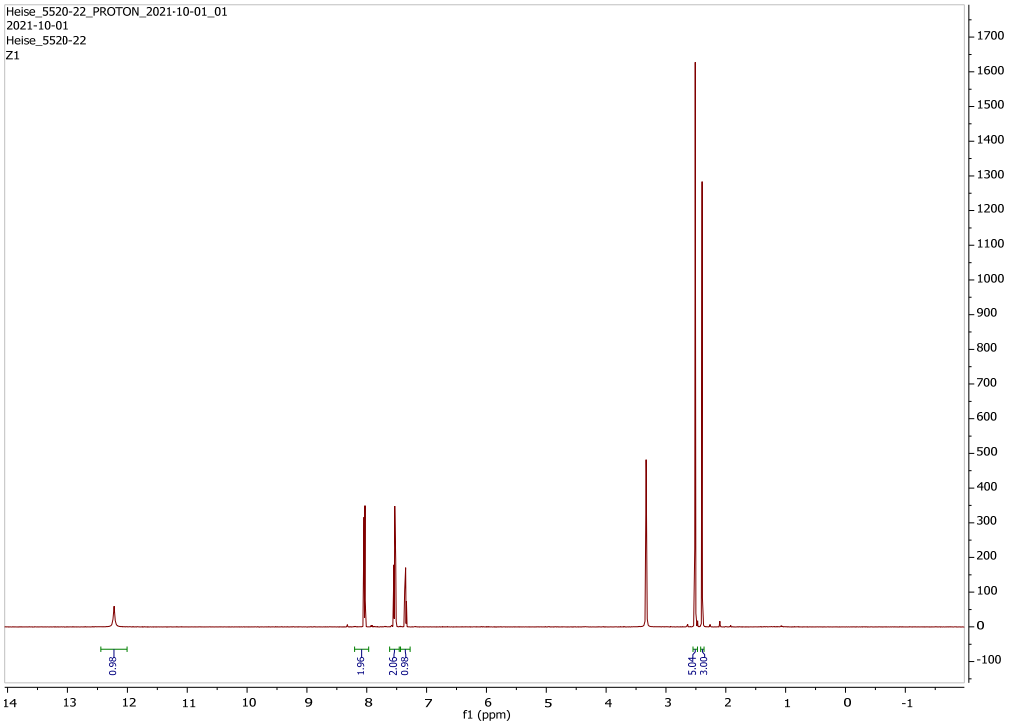
doi: 10.3390/ijms221910258.

Compound (2)

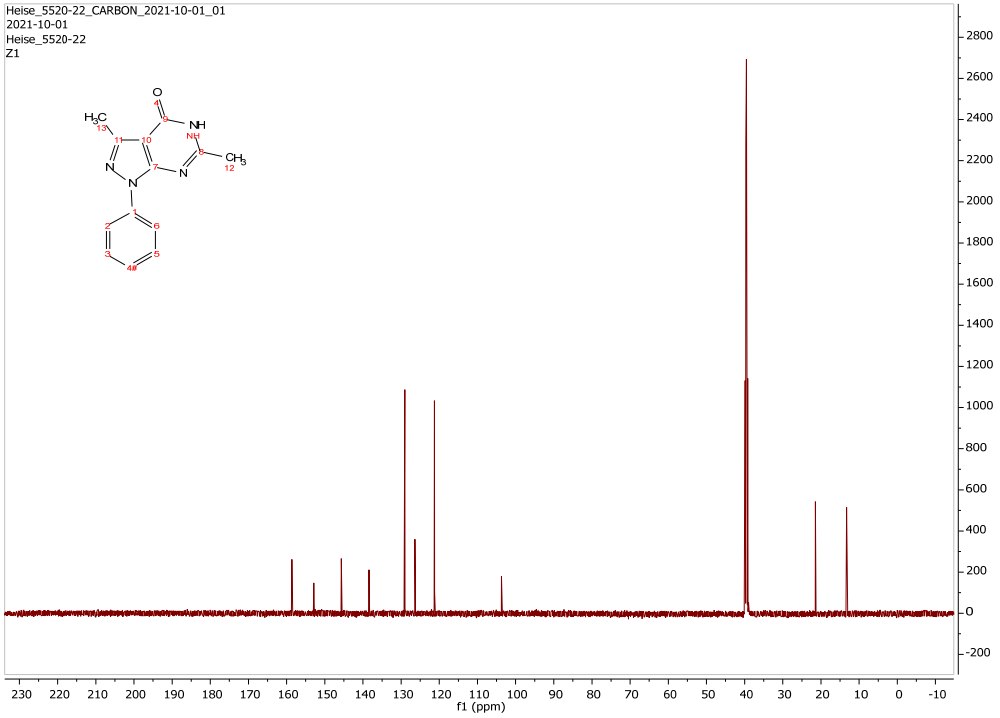


NMR Spectra of **2**

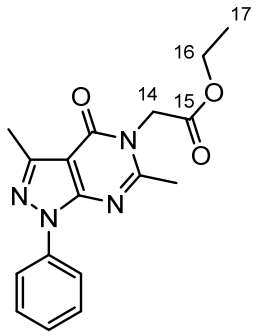
^{1}H-NMR (500 MHz, d-DMSO)



^{13}C-NMR (126 MHz, d-DMSO)



Compound (3)



NMR Spectra of **3**

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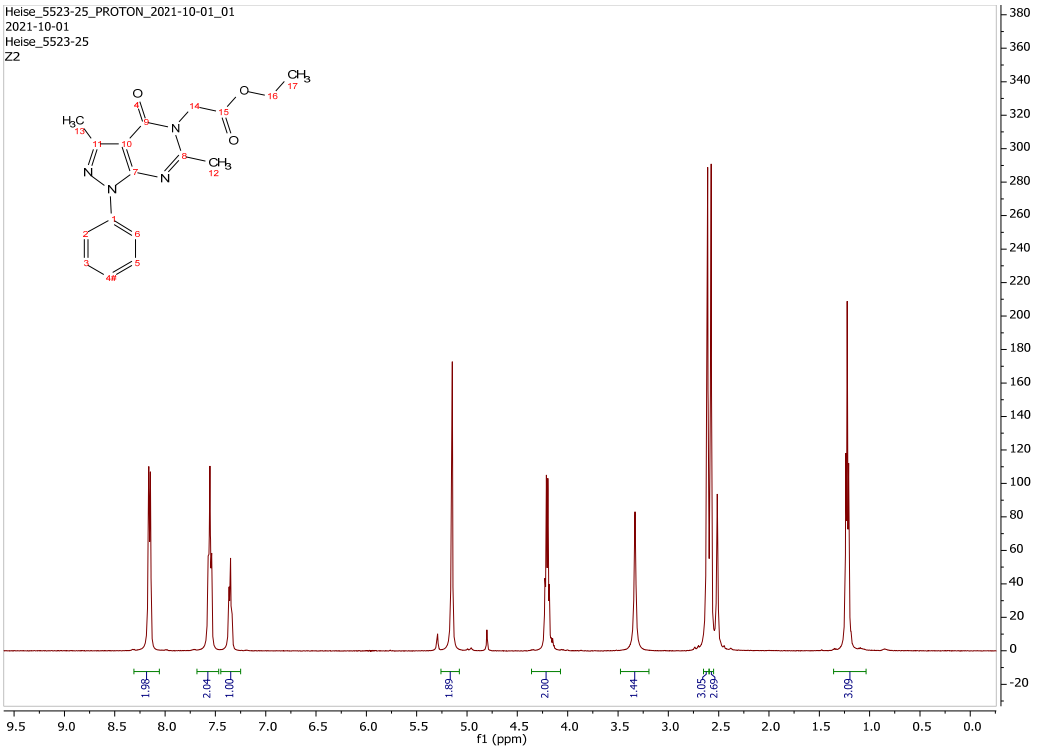
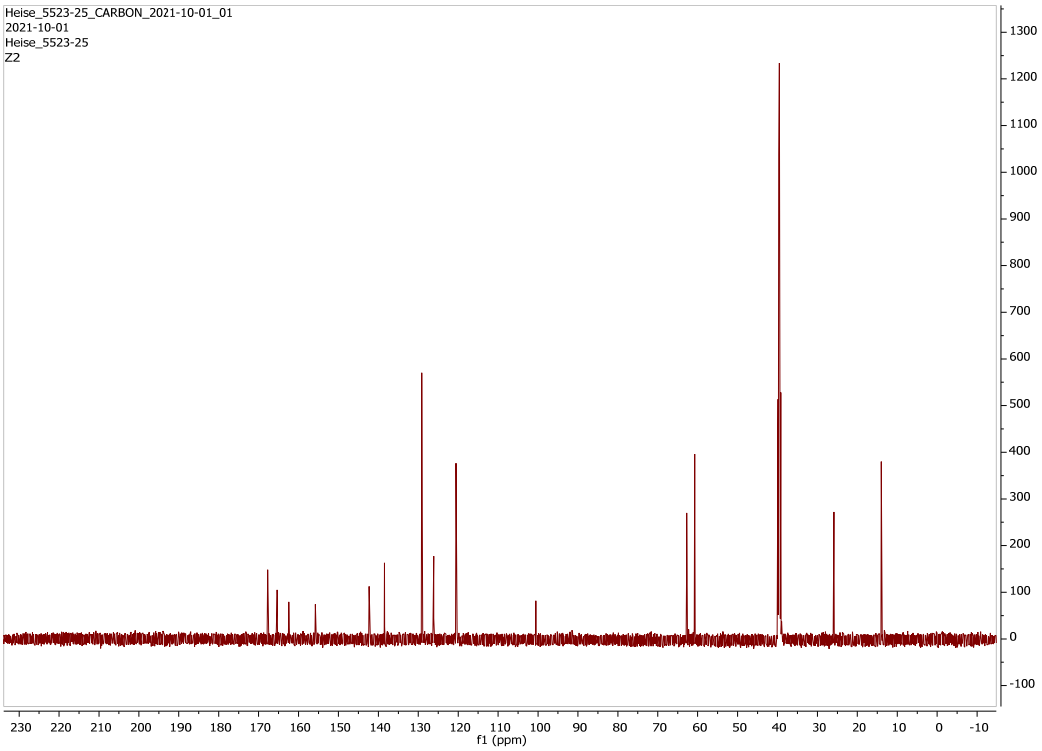
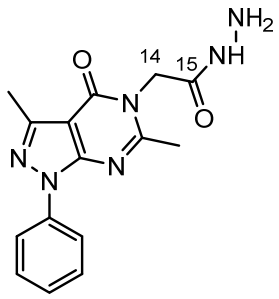


^{13}C-NMR (126 MHz, d-DMSO)



Compound **(4)**



NMR Spectra of **4**

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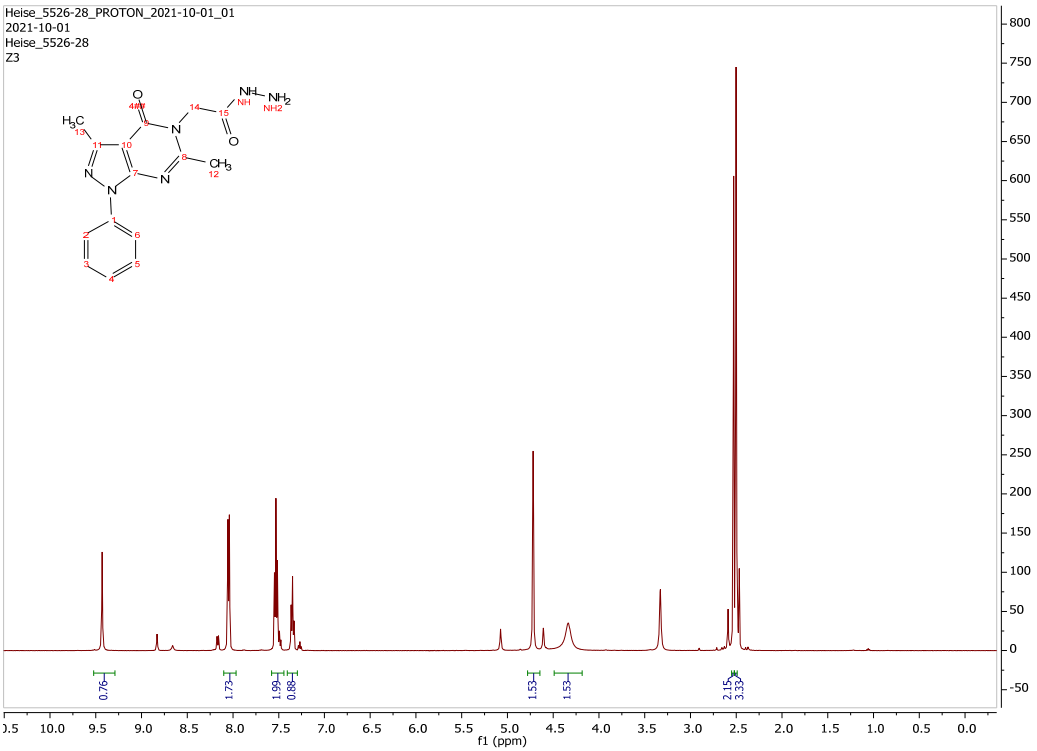
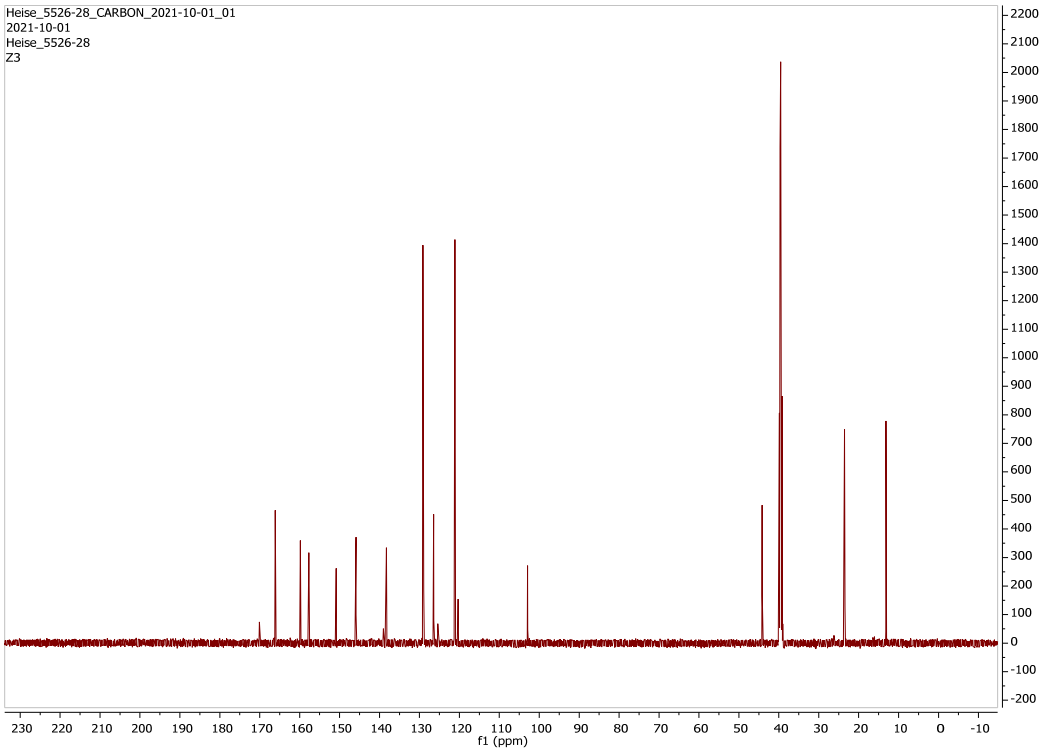
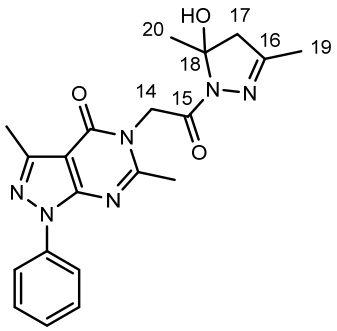


^{13}C-NMR (126 MHz, d-DMSO)

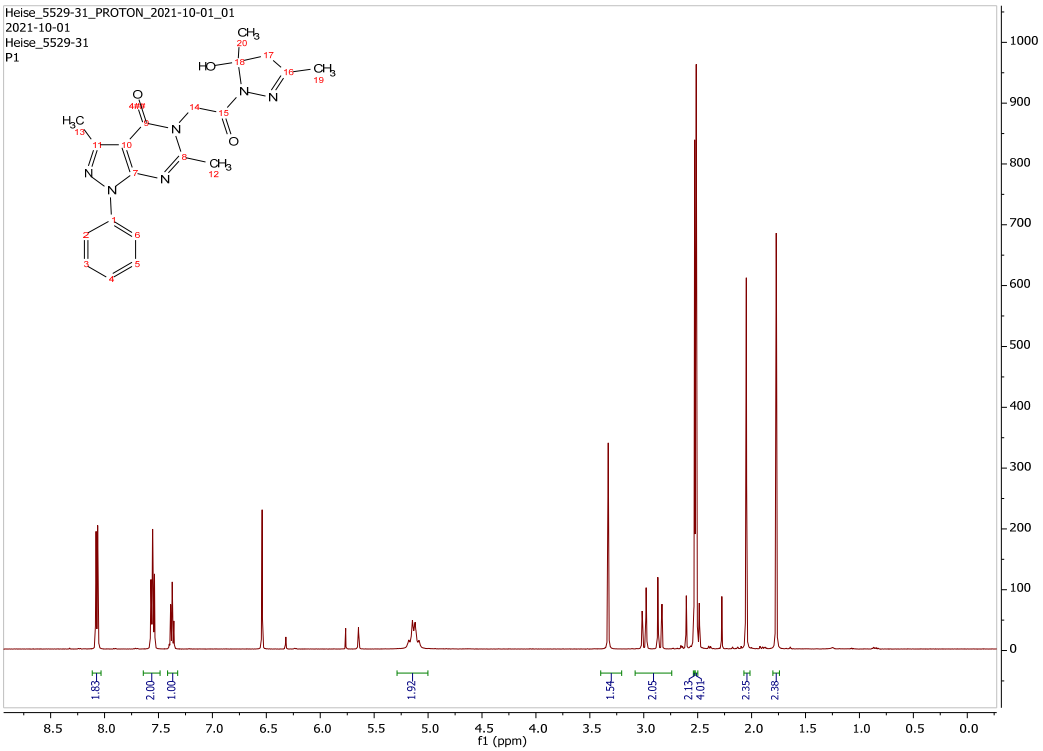


Compound **(5)**

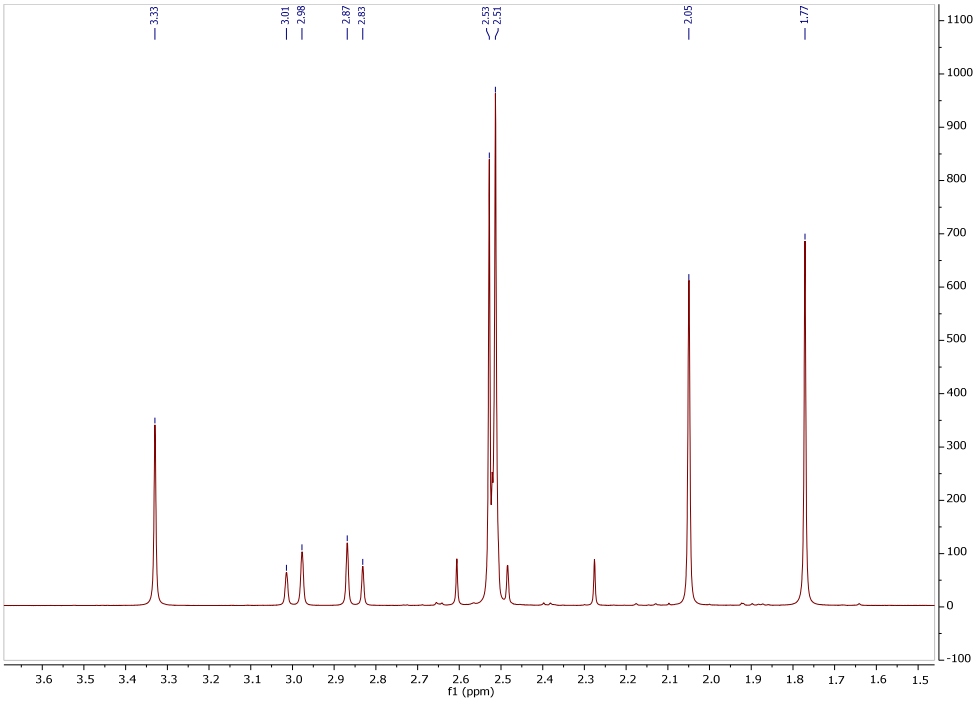


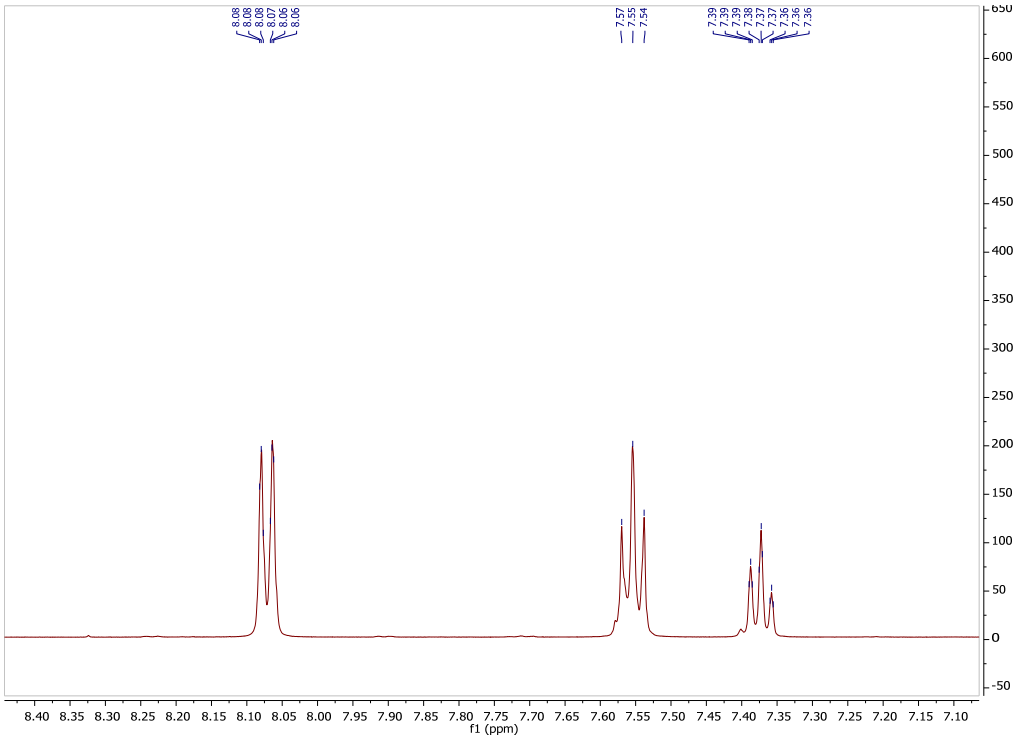
NMR Spectra of **5**

^{1}H-NMR (500 MHz, d-DMSO)



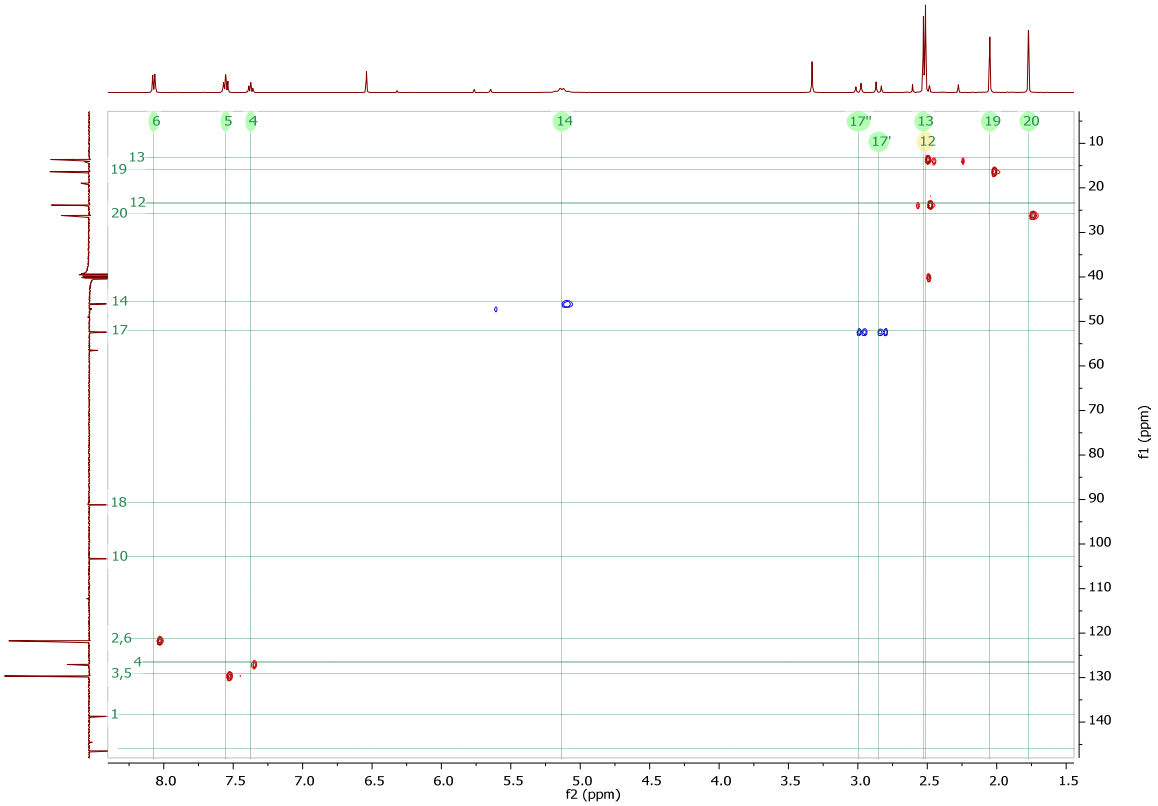
Expansions of the ^{1}H NMR

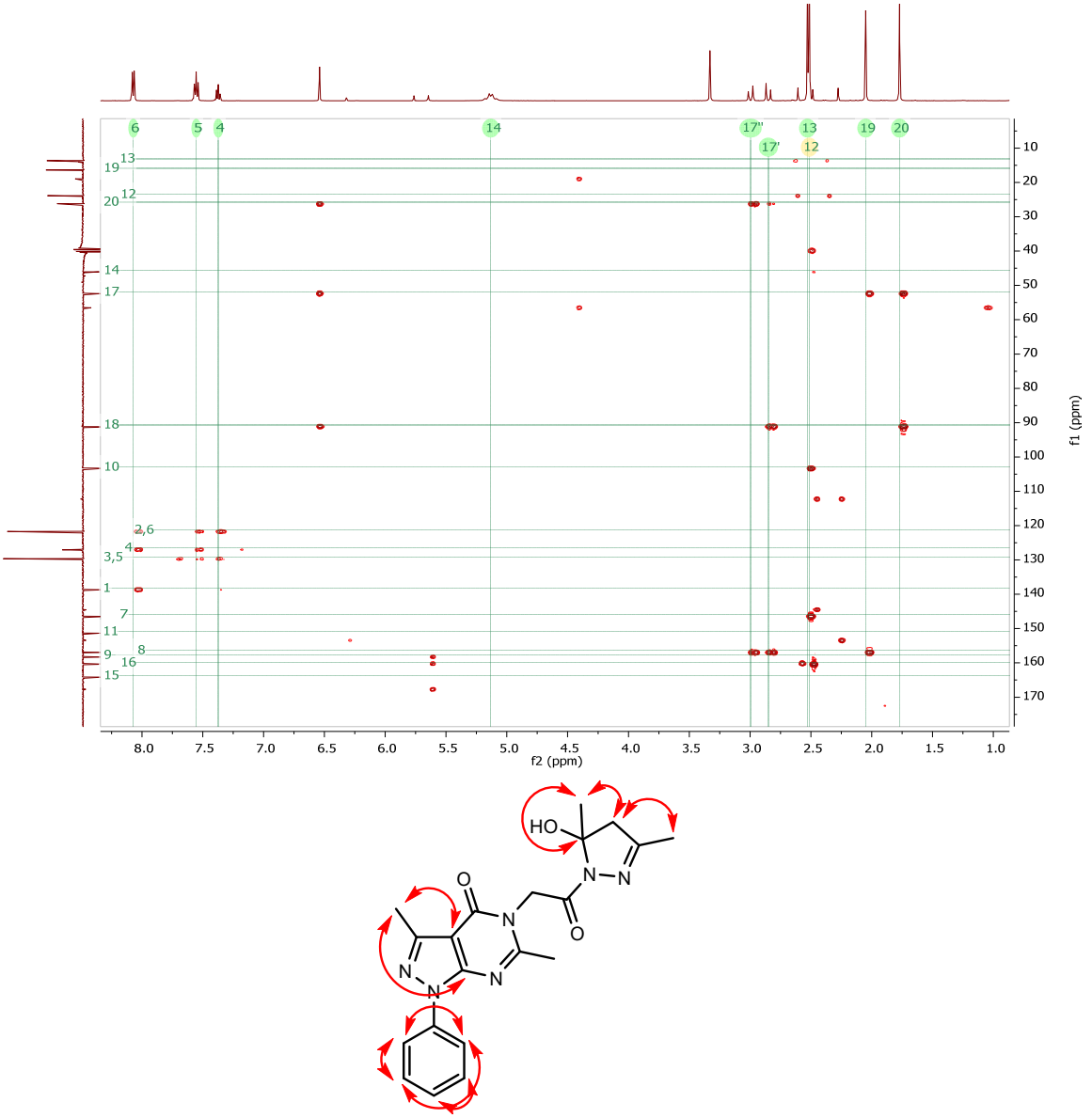




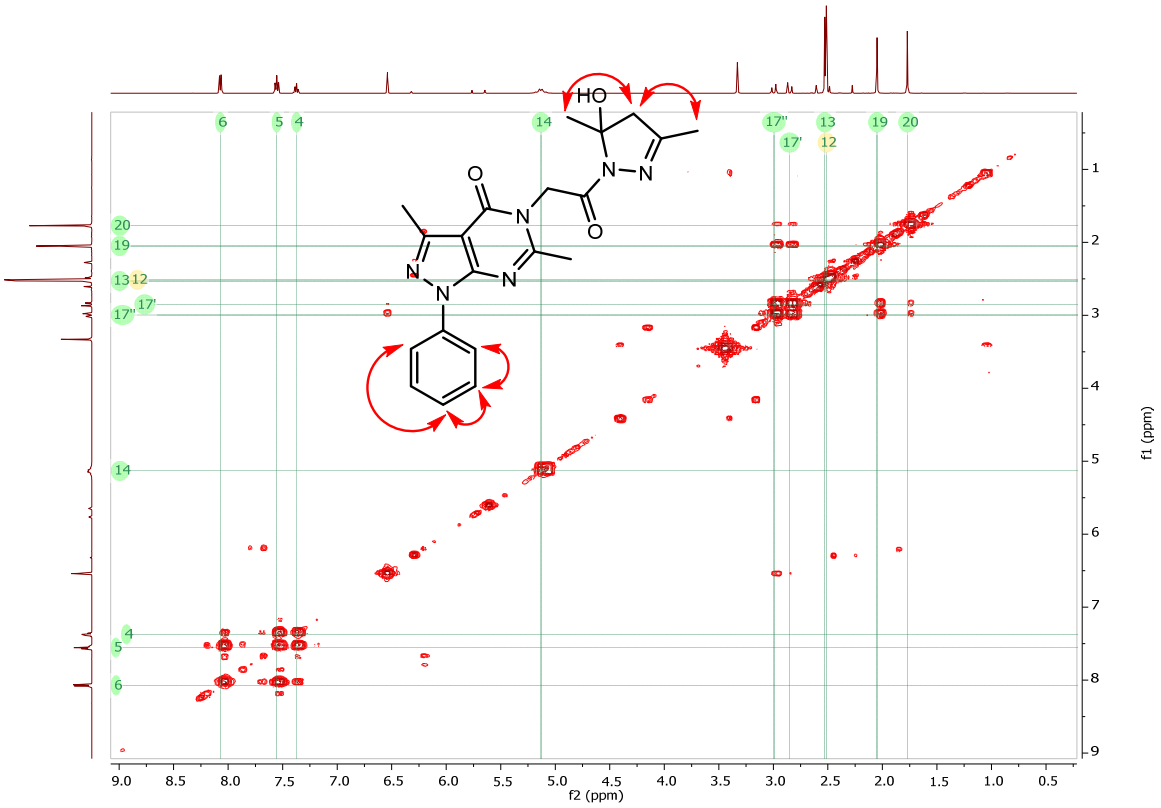
gHSQC-experiment

gHMBC-experiment

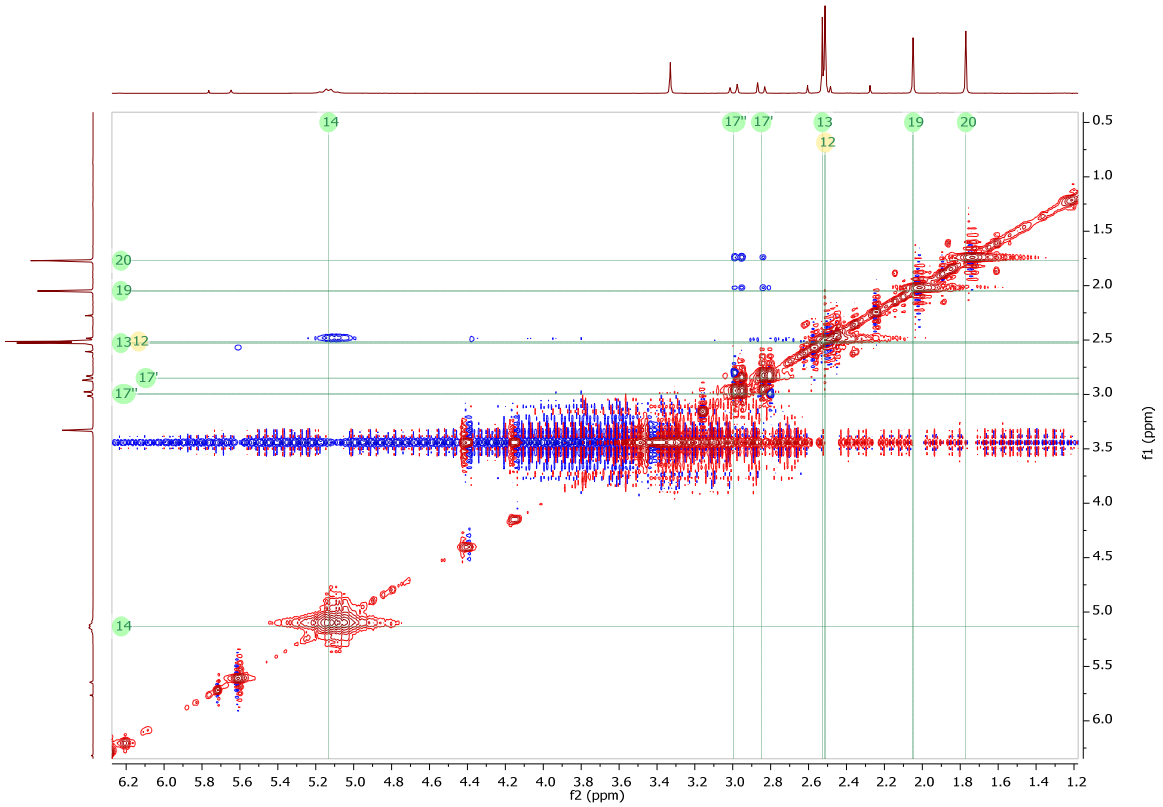



6
5
4
14
17''
17'
13
12
19
20
f2 (ppm)
f1 (ppm)
HO
N
N
O
O
N
N
N
N

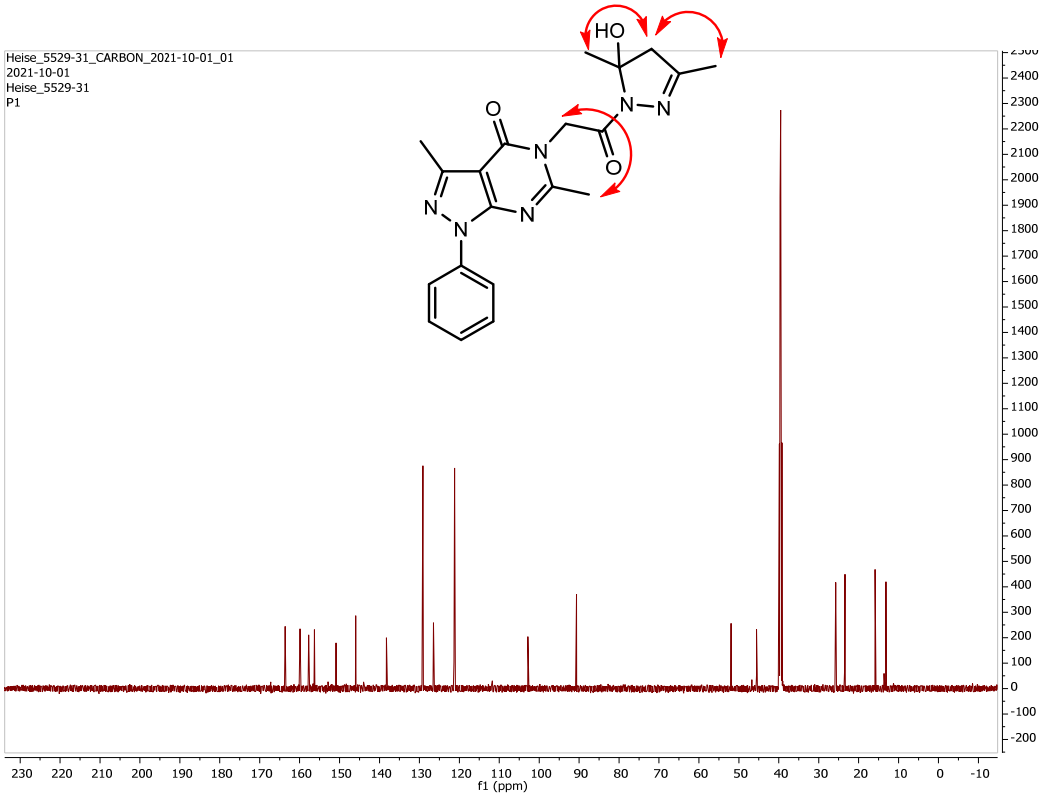
COSY-experiment



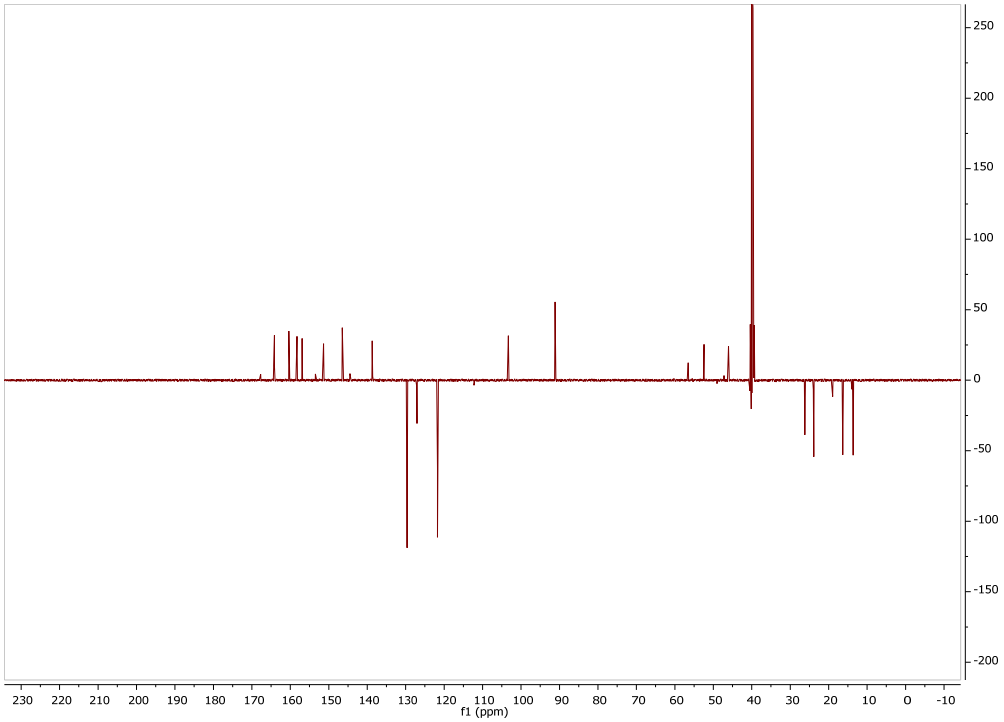
NOESY-experiment



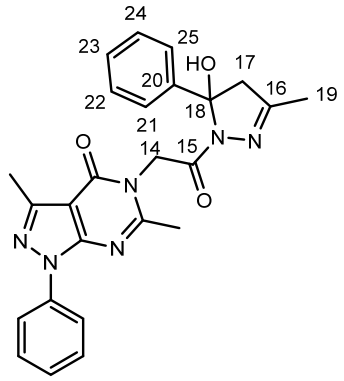
^{13}C-NMR (126 MHz, d-DMSO)



APT- experiment

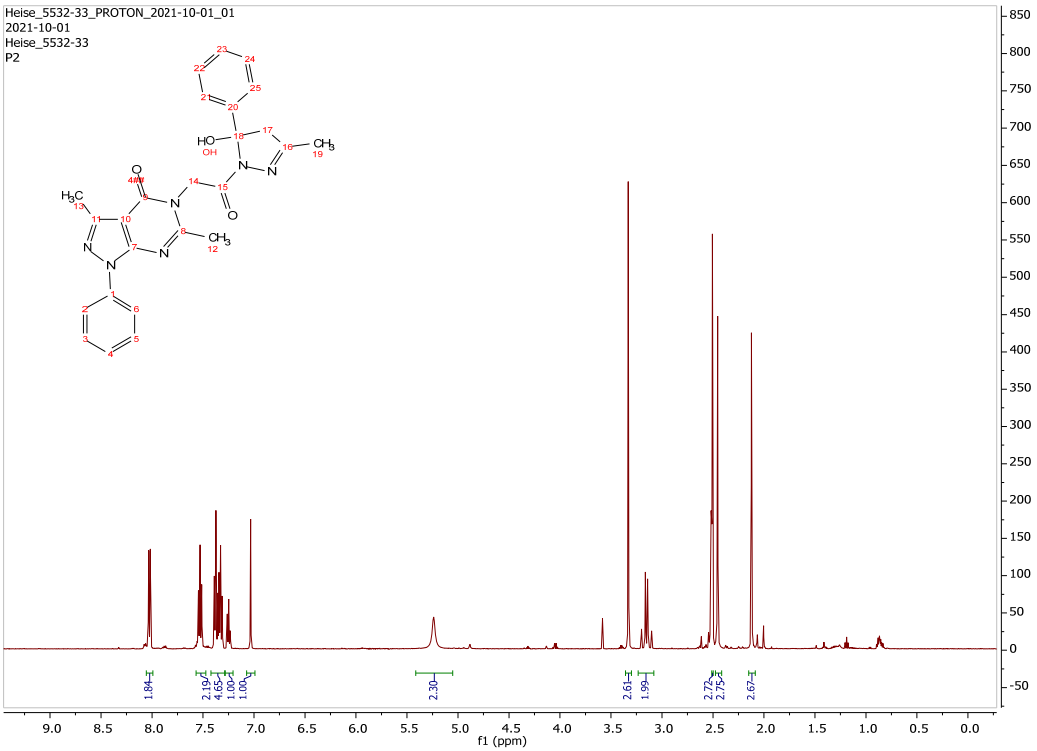


Compound (6)

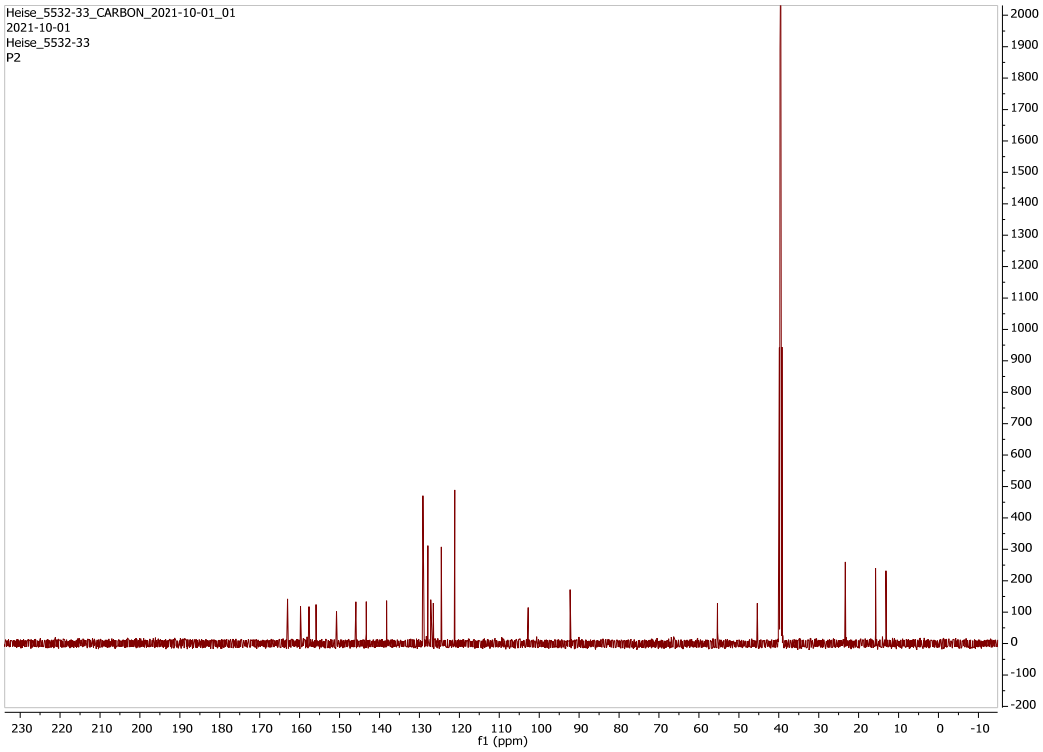


NMR Spectra of **6**

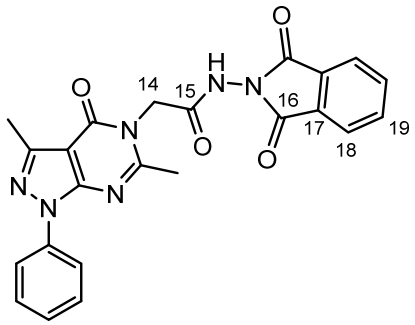
^{1}H-NMR (500 MHz, d-DMSO)



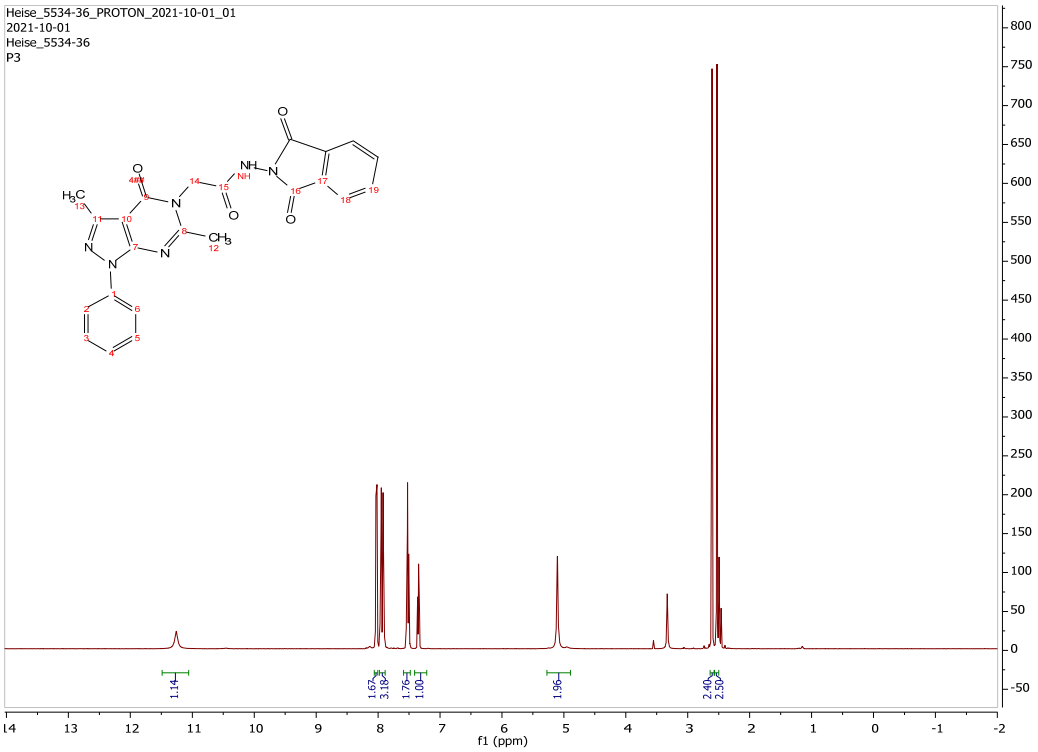
^{13}C-NMR (126 MHz, d-DMSO)



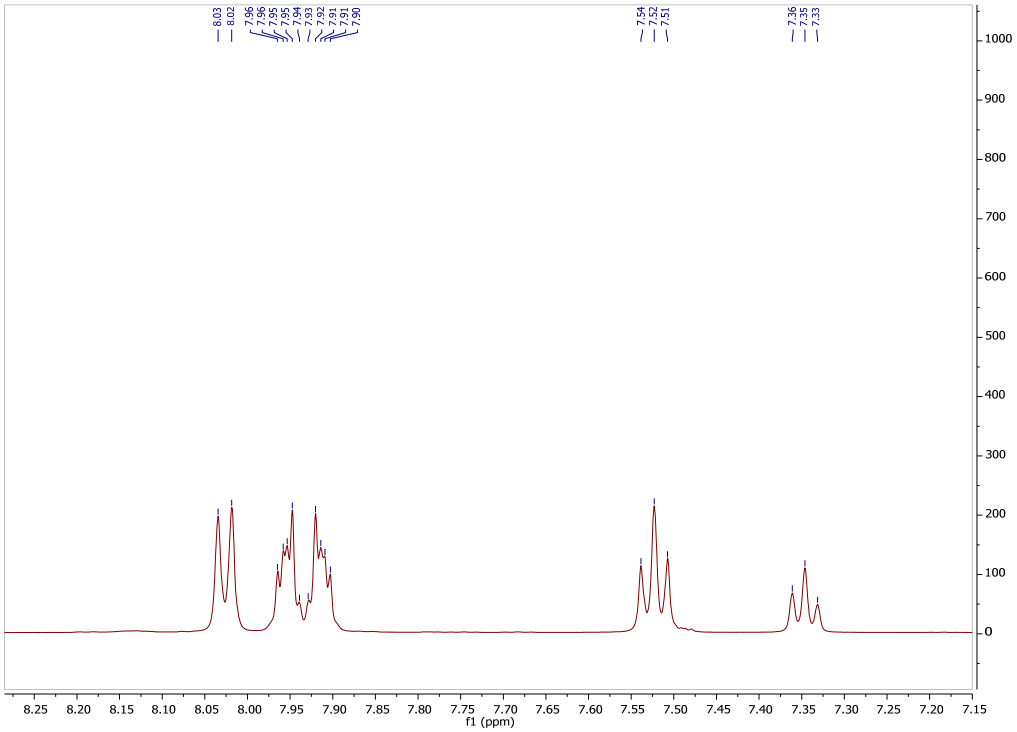
Compound (7)



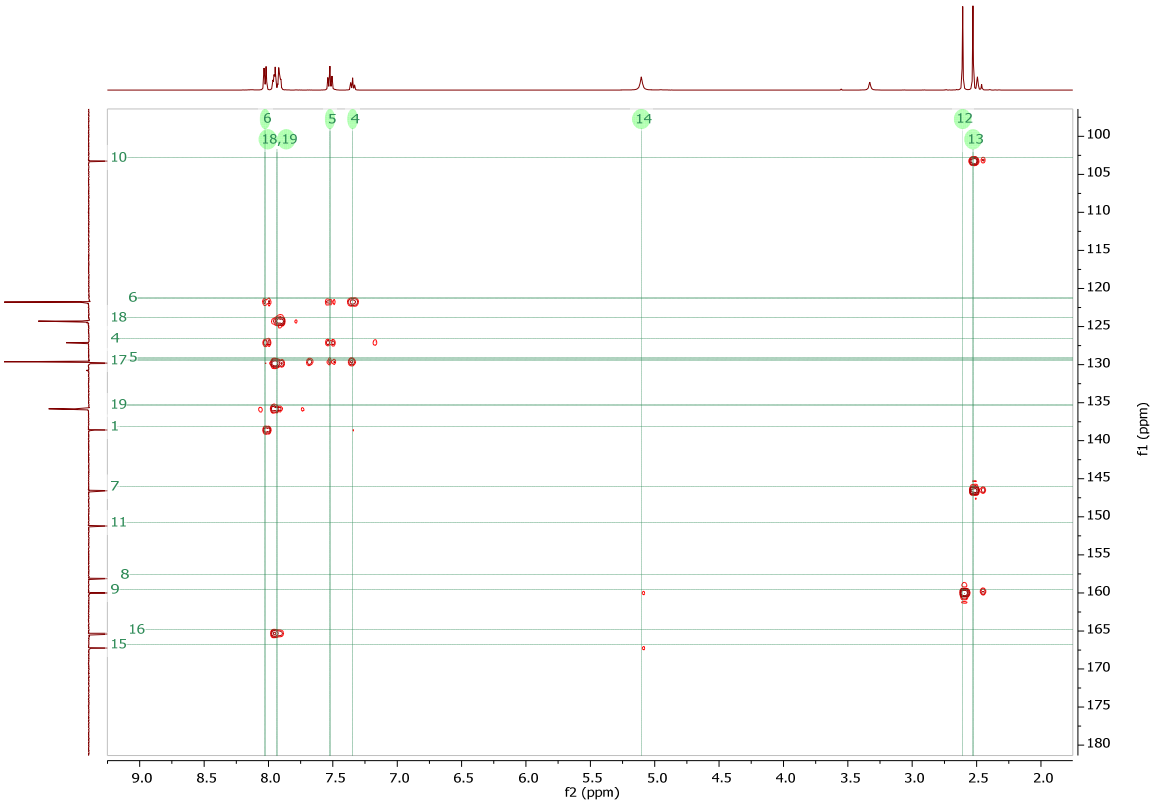
^{1}H-NMR (500 MHz, d-DMSO)



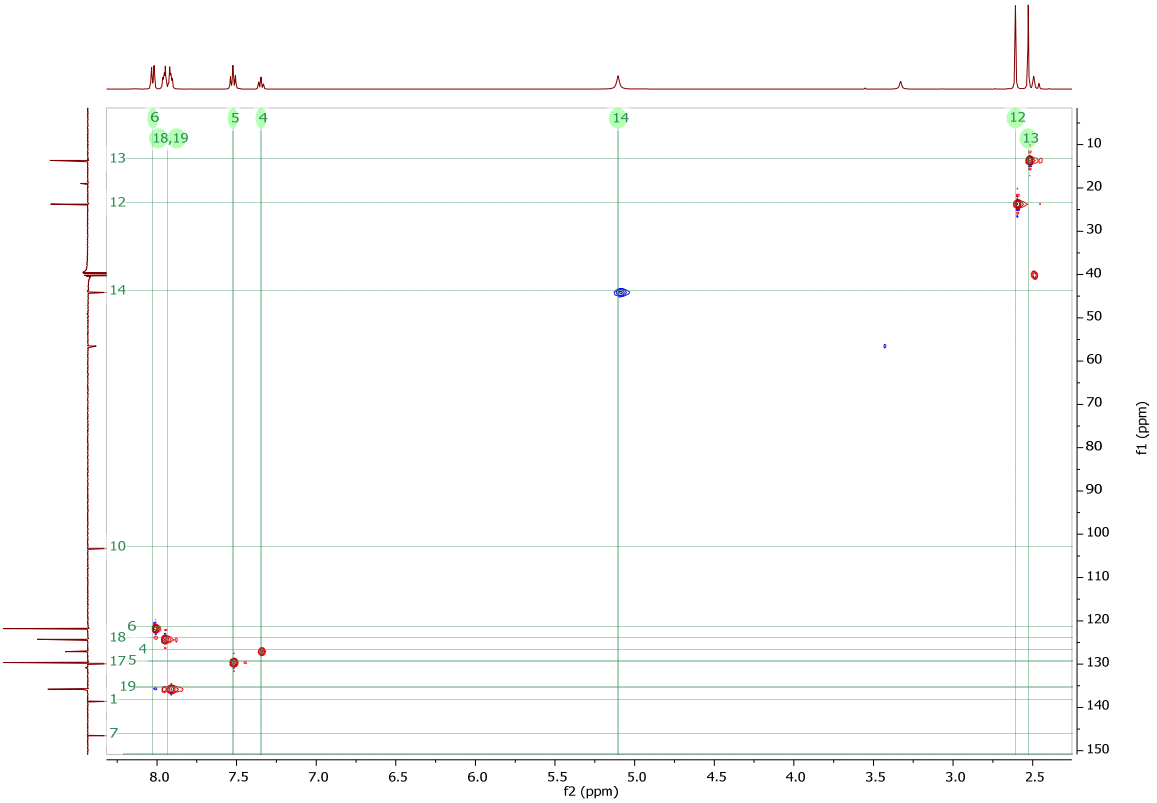
Expansions of the ^{1}H NMR



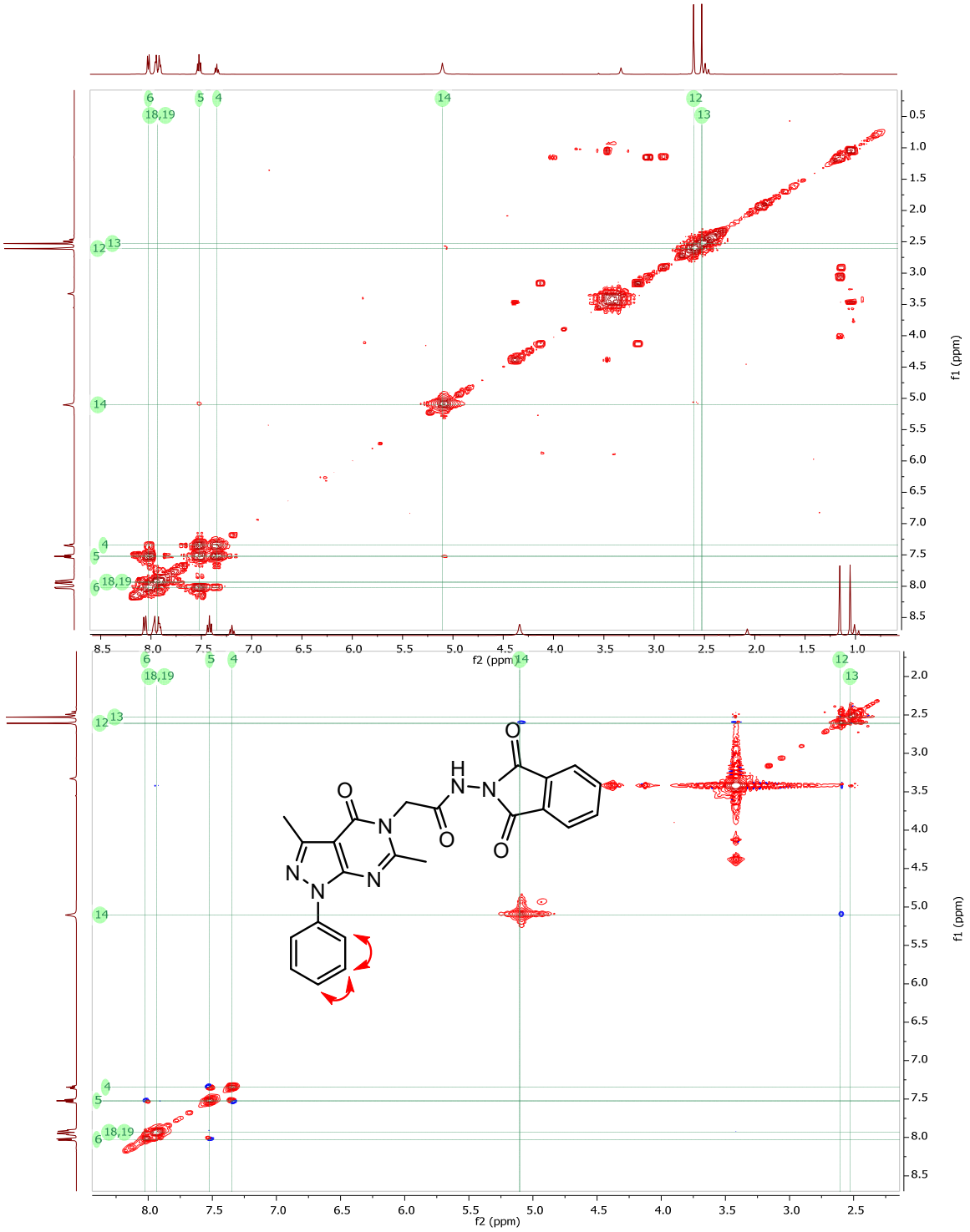
gHSQC-experiment



gHMBC-experiment



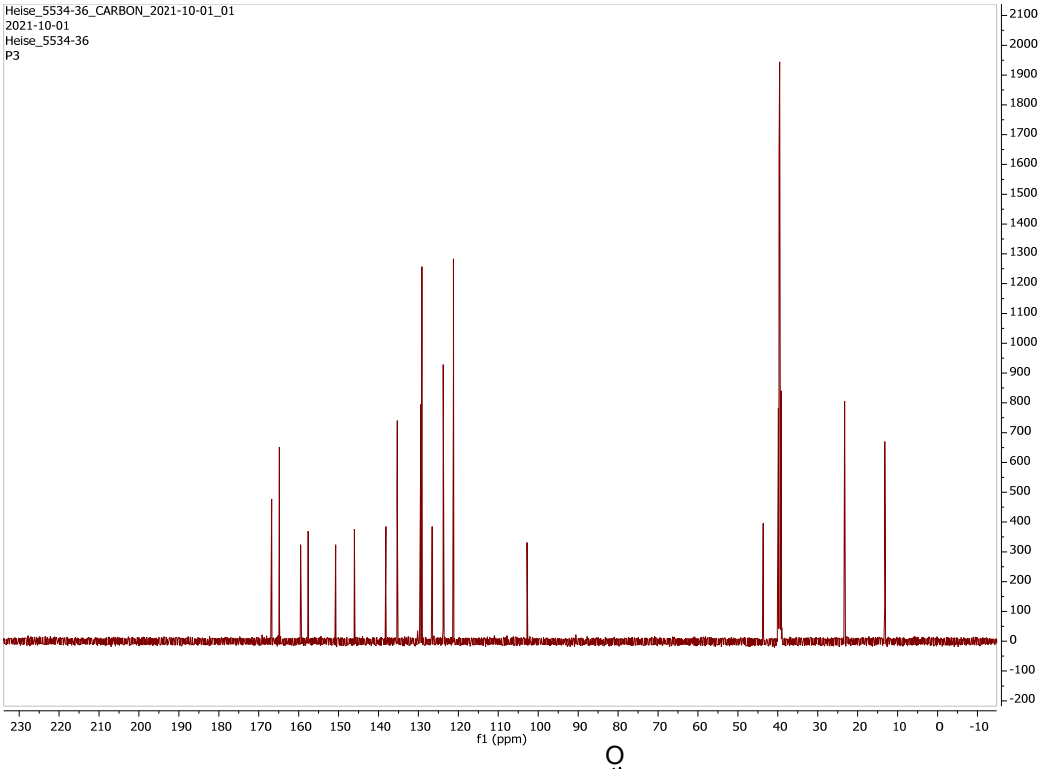
COSY-Experiment



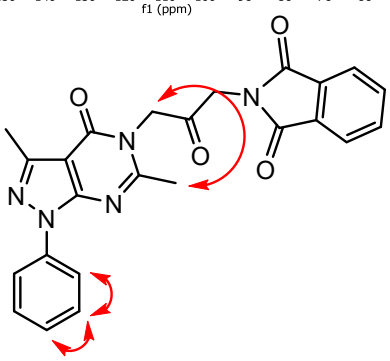
NOESY-

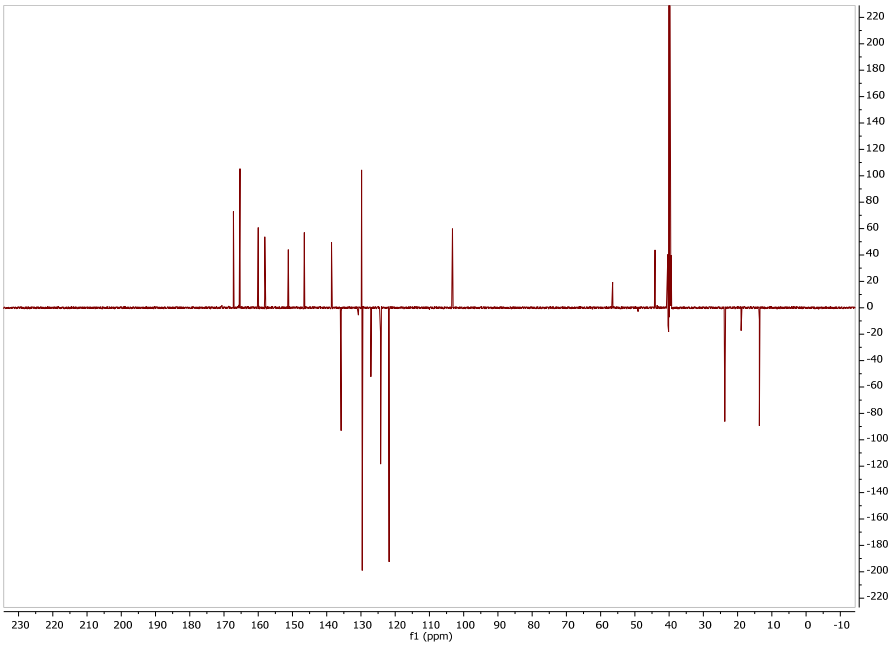
experiment

^{13}C-NMR (126 MHz, d-DMSO)

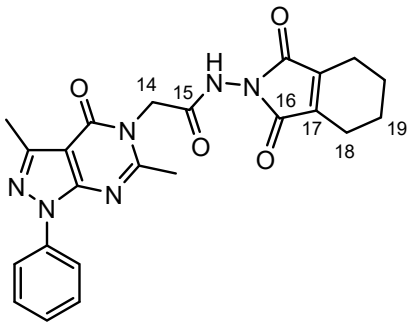


APT-experiment



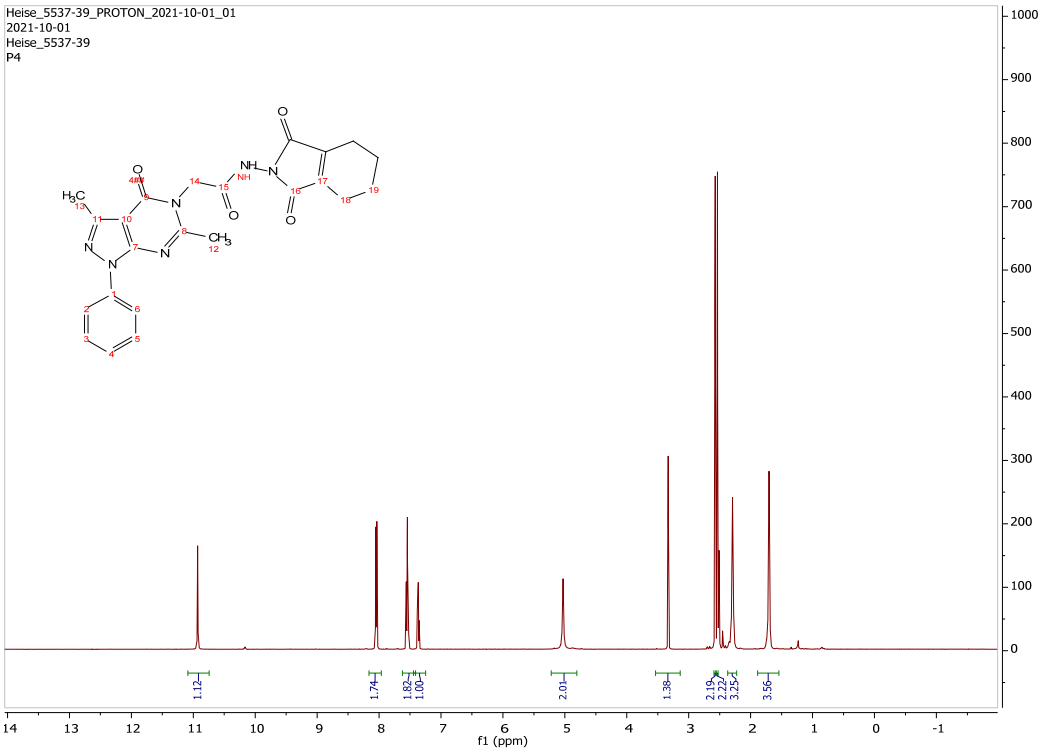

220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Compound (8)

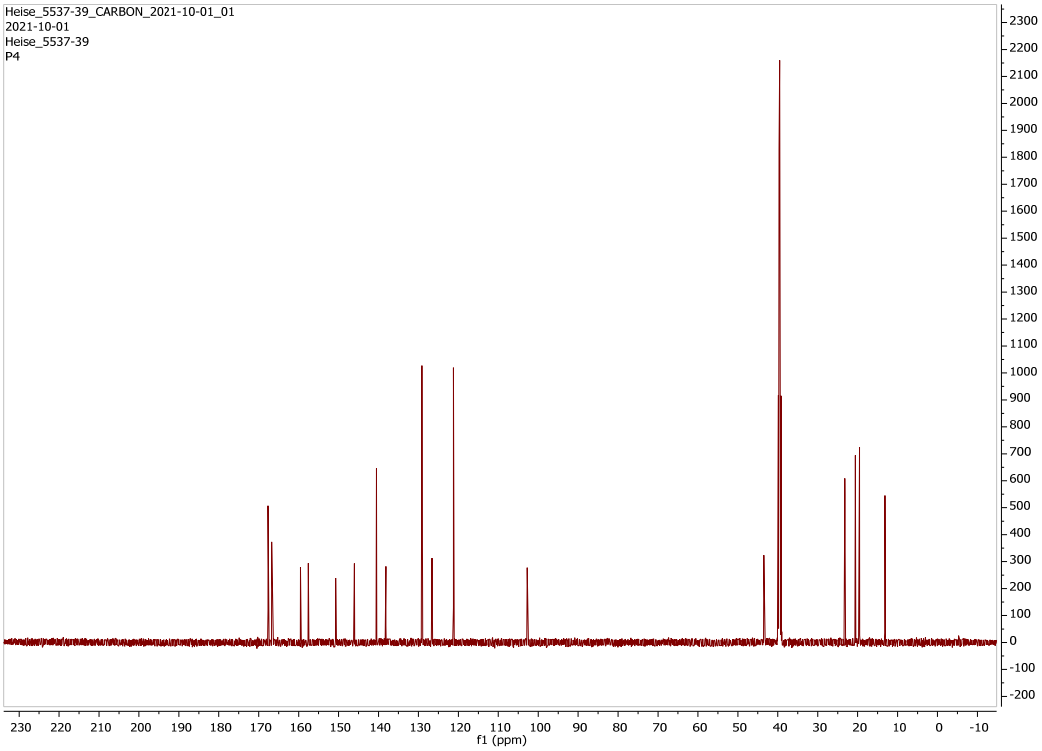

O
H
N
N
O
14
15
16
17
18
19
O
N
N
N
N
O
O

NMR Spectra of **8**

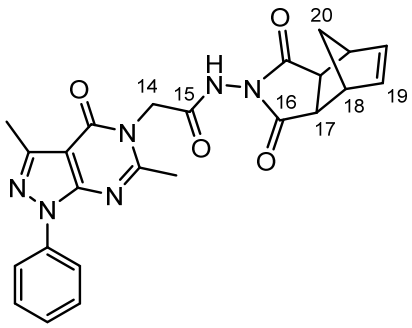
^{1}H-NMR (500 MHz, d-DMSO)



^{13}C-NMR (126 MHz, d-DMSO)

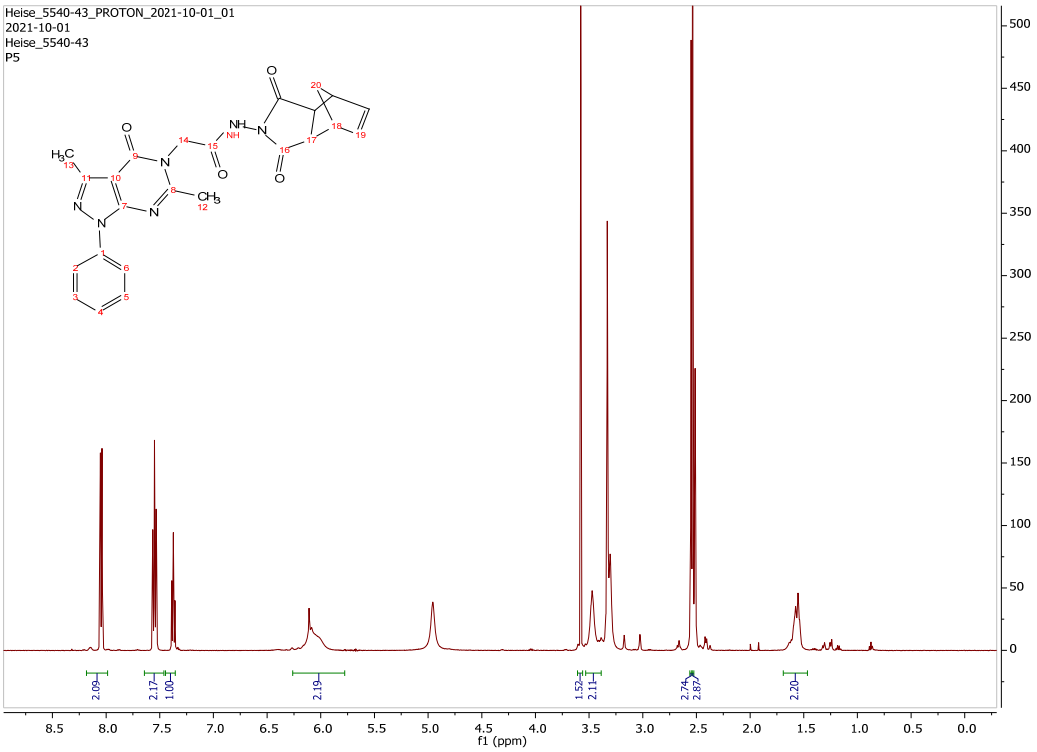


Compound (9)

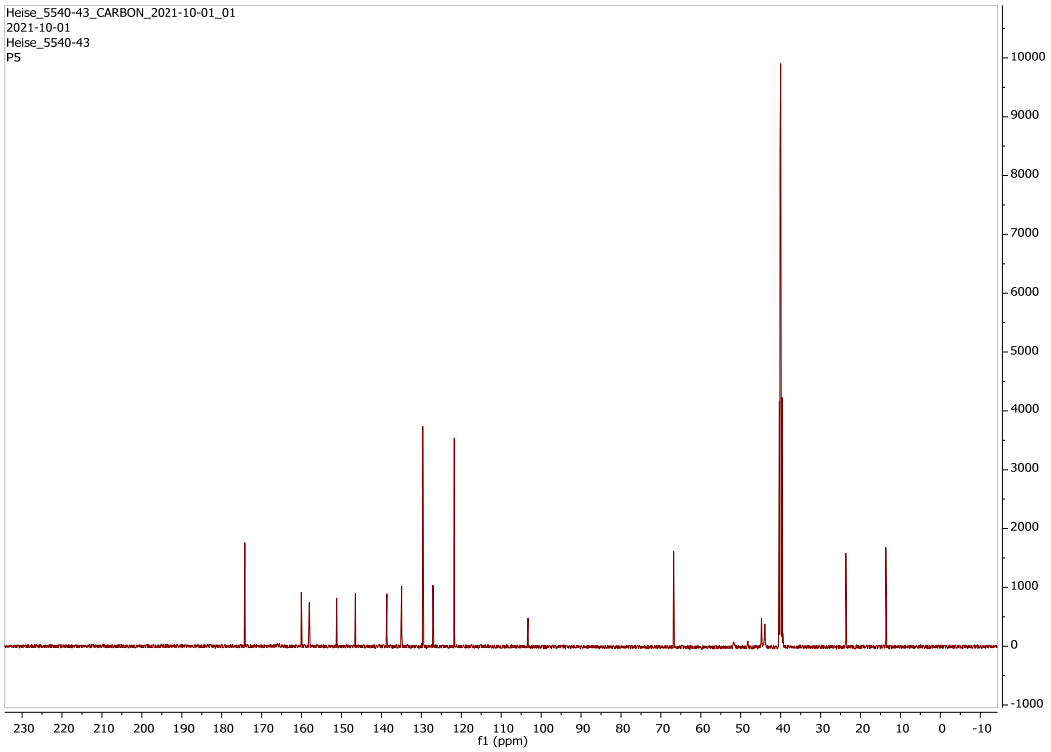


NMR Spectra of **9**

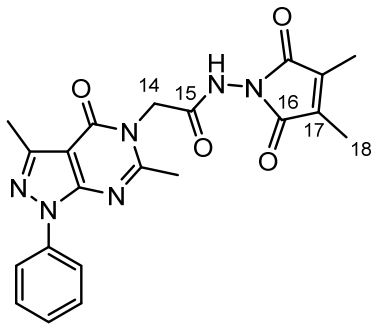
^{1}H-NMR (500 MHz, d-DMSO)



^{13}C-NMR (126 MHz, d-DMSO)

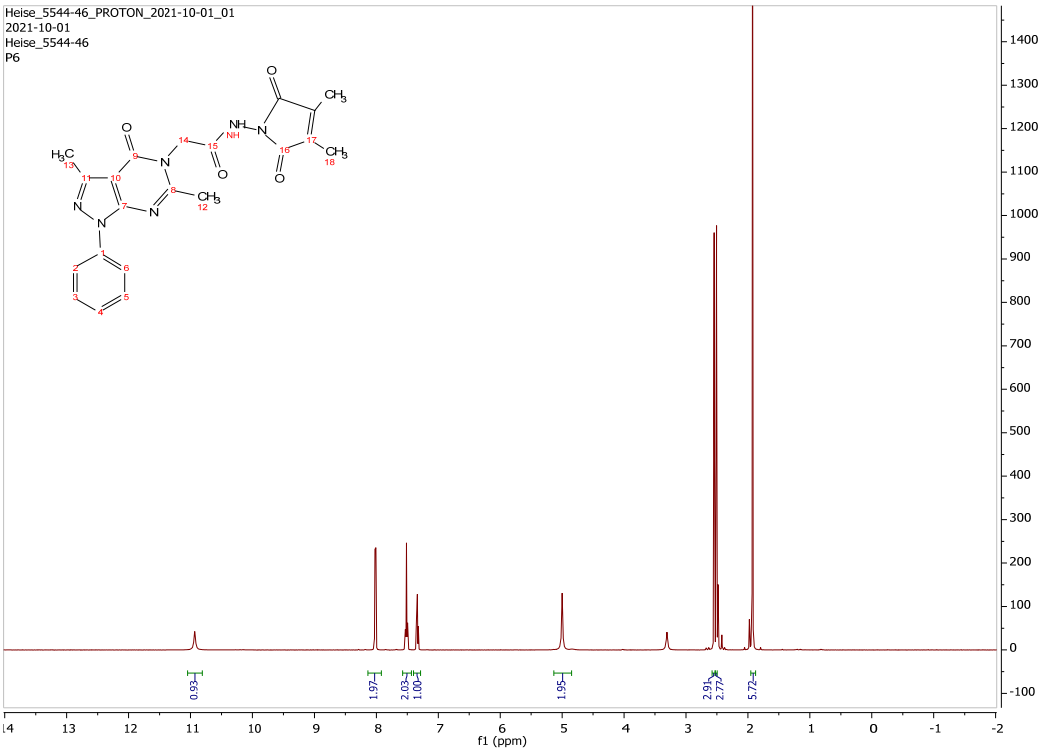


Compound (10)

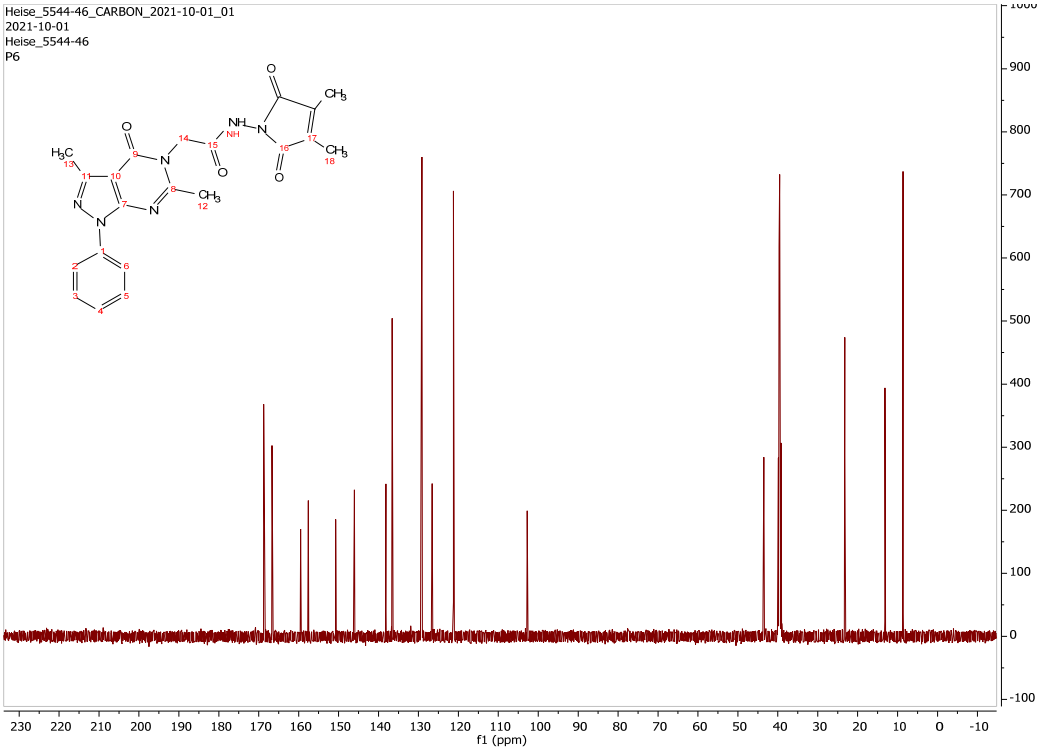


NMR Spectra of **10**

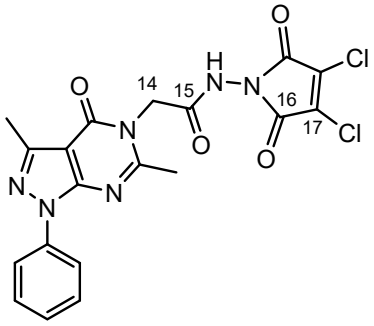
^{1}H-NMR (500 MHz, d-DMSO)



^{13}C-NMR (126 MHz, d-DMSO)

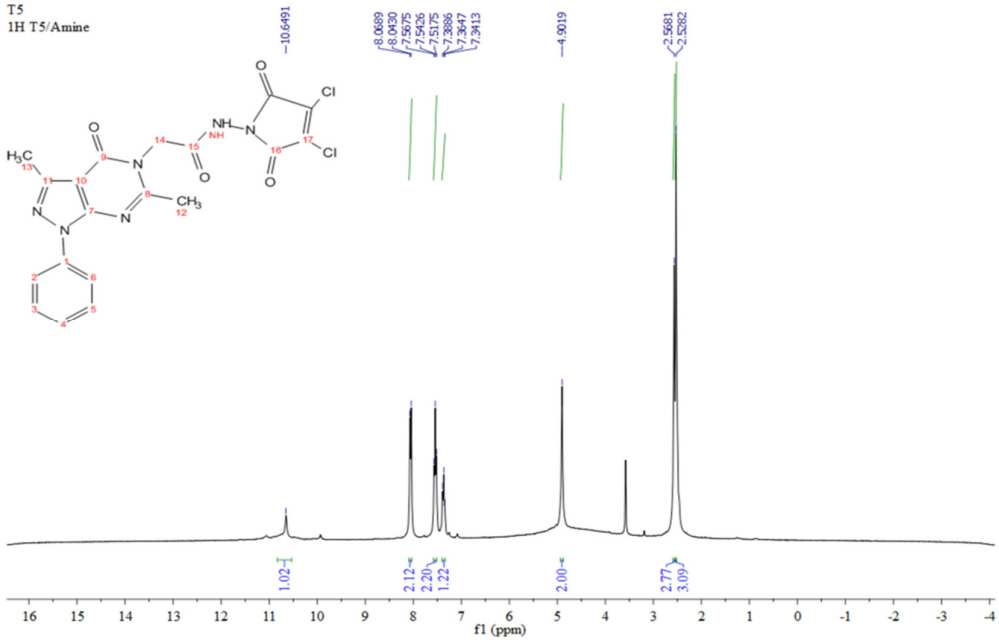


Compound (11)

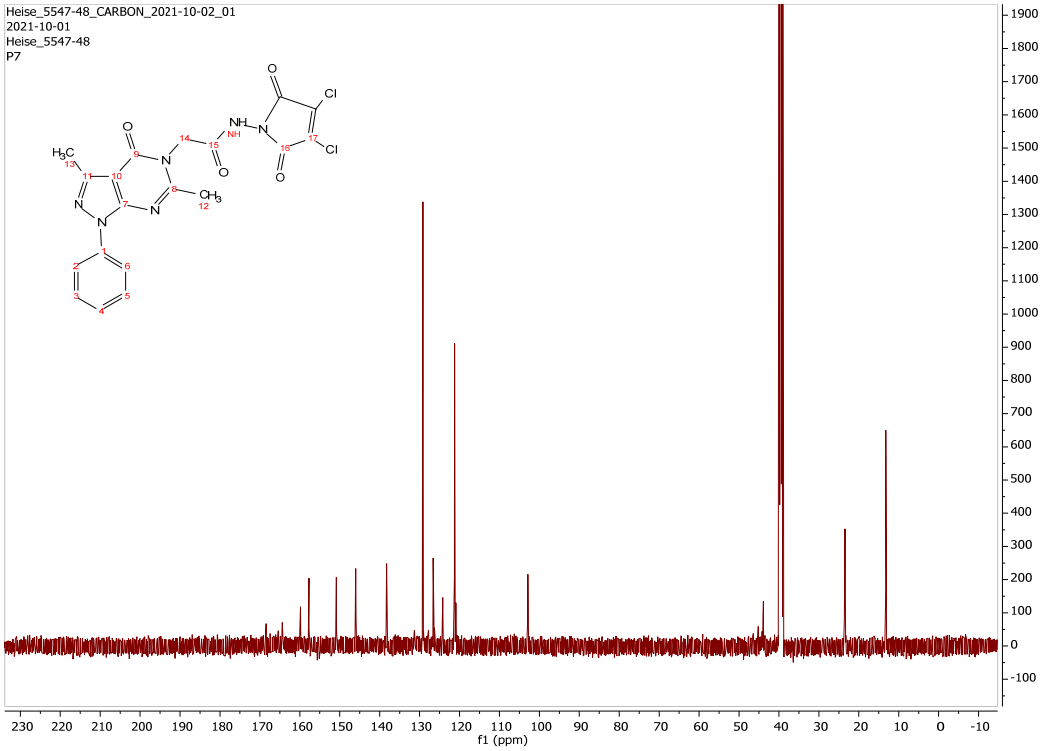


NMR Spectra of **11**

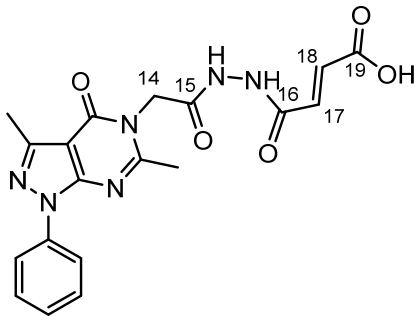
^{1}H-NMR (300 MHz, d-DMSO)



^{13}C-NMR (126 MHz, d-DMSO)

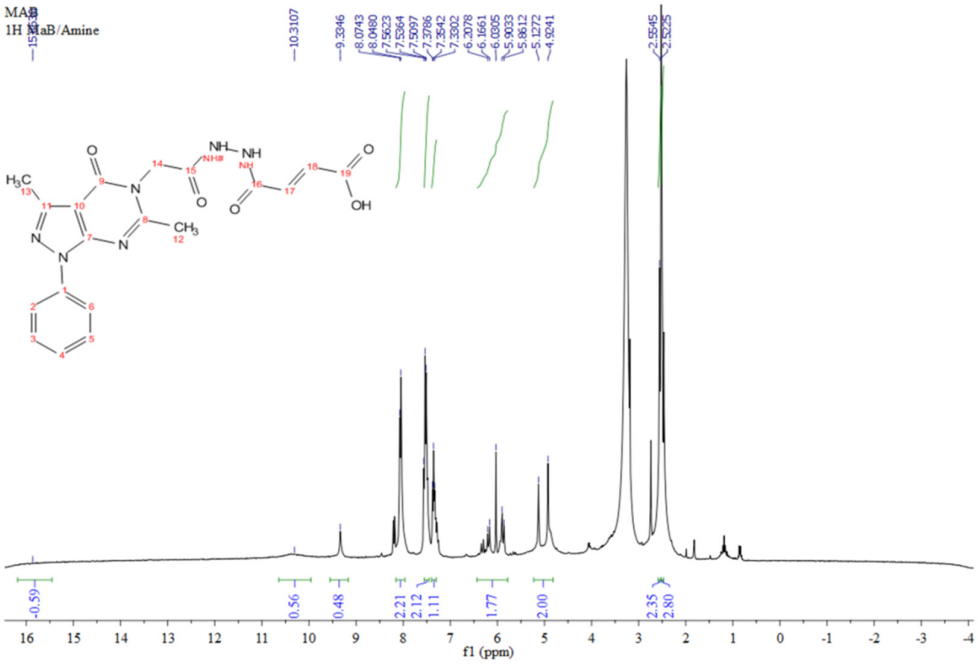


Compound (12)

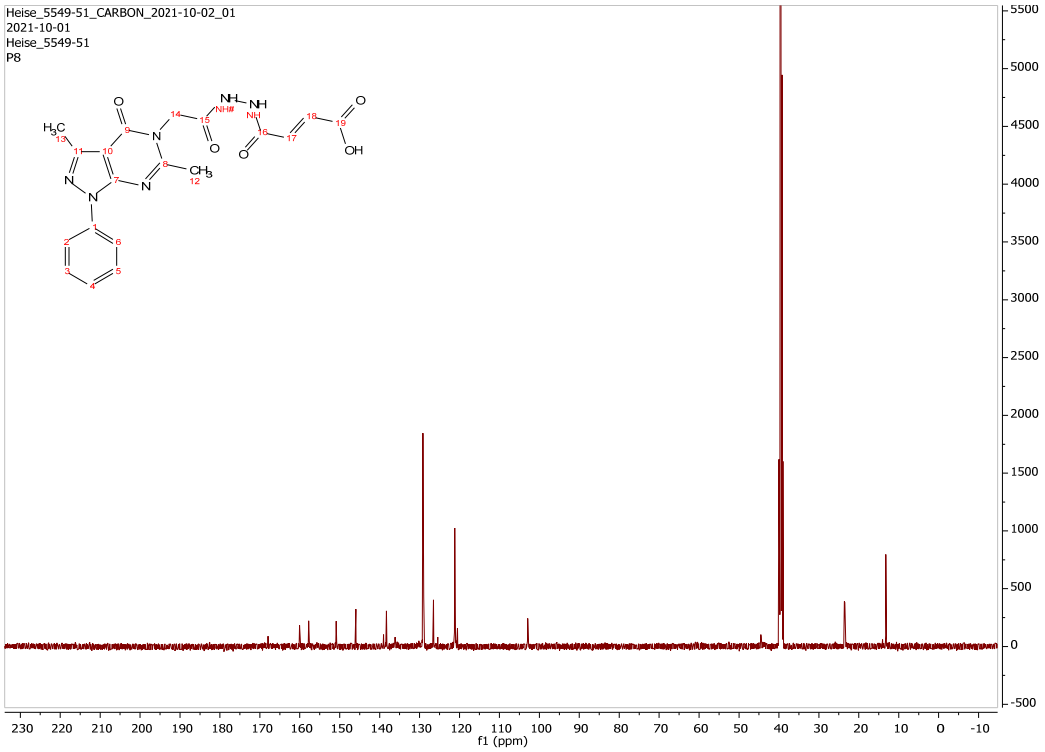


NMR Spectra of **12**

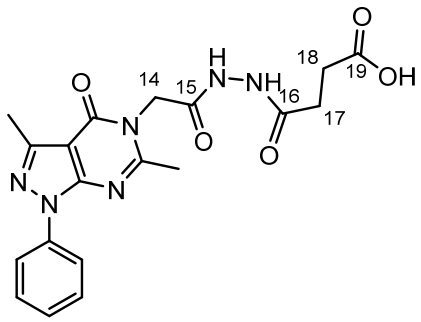
^{1}H-NMR (500 MHz, d-DMSO)



^{13}C-NMR (126 MHz, d-DMSO)

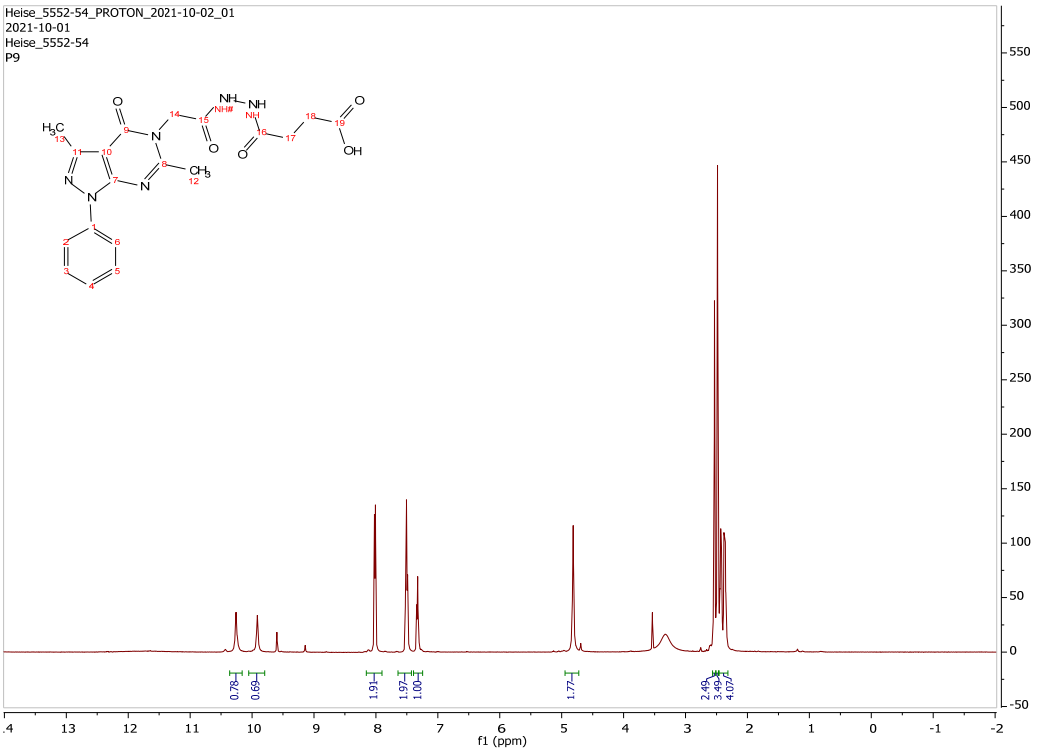


Compound (13)



NMR Spectra of **13**

^{1}H-NMR (500 MHz, d-DMSO)



^{13}C-NMR (126 MHz, d-DMSO)