Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis, investigation of the crystal structure, DFT, and *In silico* medicinal potential of hydrazono- and aminomethylene substituted pyrazolidine-3,5-diones as potential anticancer scaffolds

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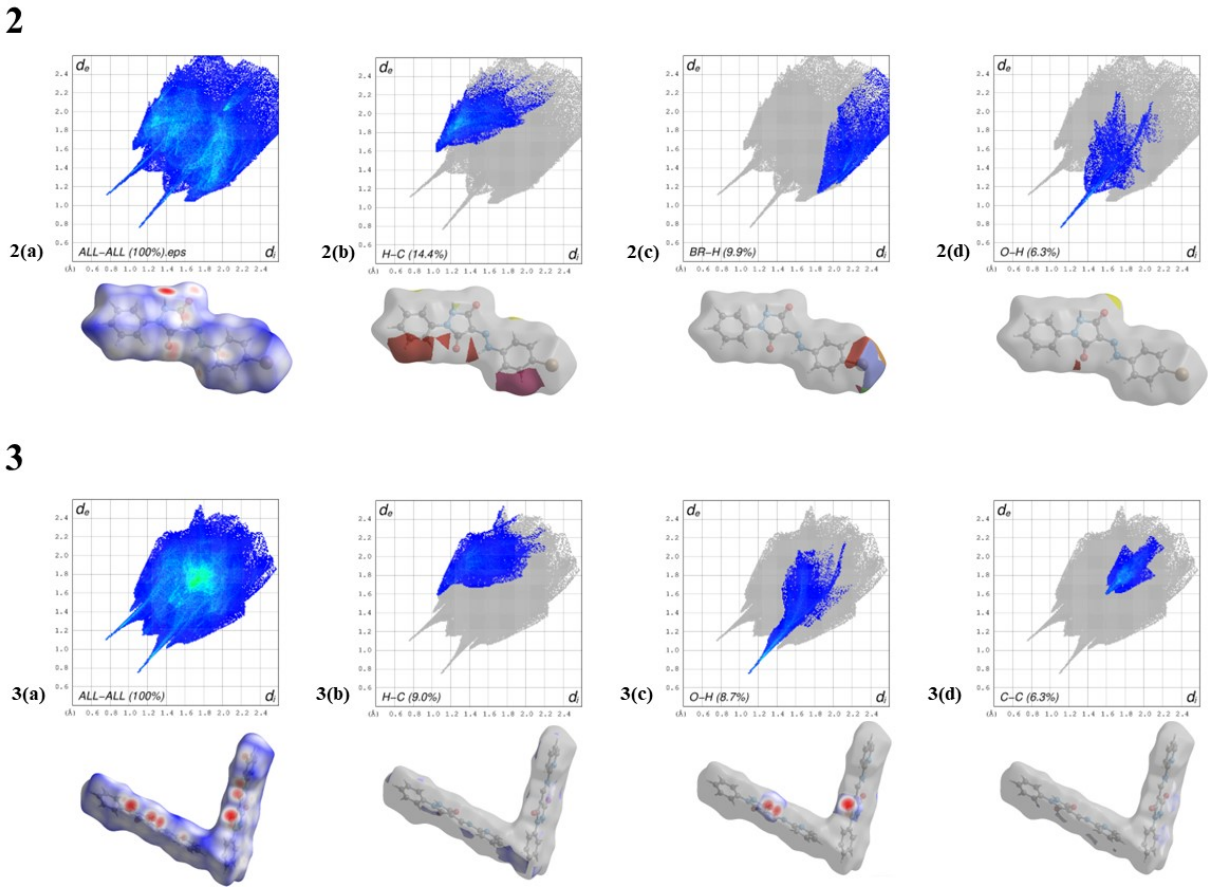

Figure S1. Overall (top left) and delineated two-dimensional fingerprint plots for **2** (2a, 2b, 2c, and 2d) and **3** (3a, 3b, 3c, and 3d).

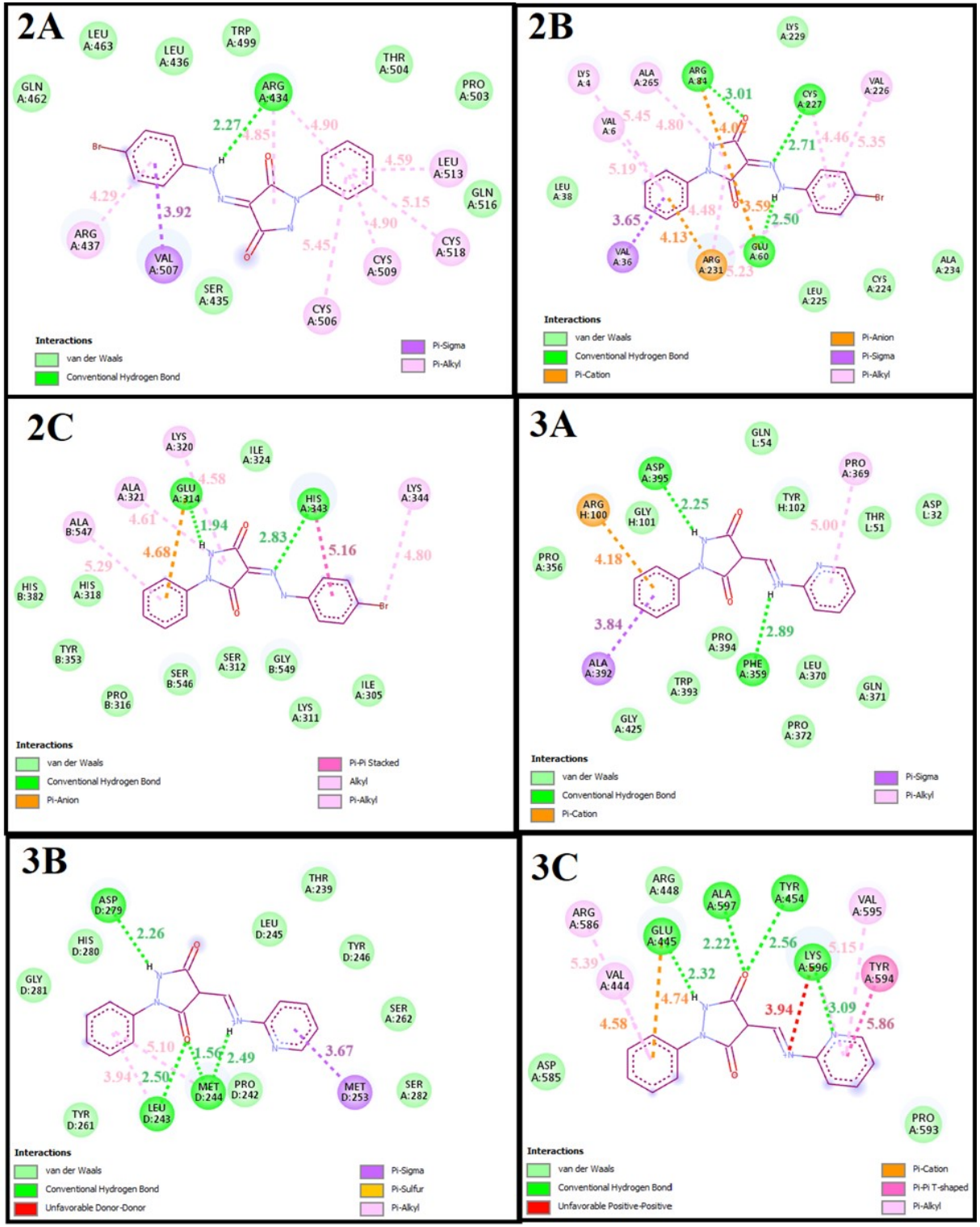
2A
LEU A:463
LEU A:436
TRP A:499
THR A:504
PRO A:503
GLN A:462
ARG A:434
LEU A:513
GLN A:516
CYS A:518
CYS A:509
CYS A:506
SER A:435
ARG A:437
VAL A:507
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Alkyl
2B
LYS A:229
LYS A:4
ALA A:265
ARG A:84
CYS A:227
VAL A:226
VAL A:6
LEU A:38
VAL A:36
ARG A:231
GLU A:60
ALA A:234
CYS A:224
LEU A:225
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Cation
Pi-Anion
Pi-Sigma
Pi-Alkyl
2C
LYS A:320
ILE A:324
ALA A:321
GLU A:314
HIS A:343
LYS A:344
ALA B:547
HIS B:382
HIS A:318
TYR B:353
SER A:312
GLY B:549
SER B:546
PRO B:316
ILE A:305
LYS A:311
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Anion
Pi-Pi Stacked
Alkyl
Pi-Alkyl
3A
GLN L:54
ASP A:395
PRO A:369
ARG H:100
GLY H:101
TYR H:102
THR L:51
ASP L:32
PRO A:356
PRO A:394
PHE A:359
LEU A:370
ALA A:392
TRP A:393
GLN A:371
GLY A:425
PRO A:372
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Cation
Pi-Sigma
Pi-Alkyl
3B
THR A:239
ASP D:279
LEU D:245
HIS D:280
TYR D:246
GLY D:281
SER A:262
MET D:244
PRO D:242
MET D:253
SER A:282
LEU D:243
TYR D:261
Interactions
van der Waals
Conventional Hydrogen Bond
Unfavorable Donor-Donor
Pi-Sigma
Pi-Sulfur
Pi-Alkyl
3C
ARG A:448
ALA A:597
TYR A:454
VAL A:595
ARG A:586
GLU A:445
LYS A:596
TYR A:594
VAL A:444
ASP A:585
PRO A:593
Interactions
van der Waals
Conventional Hydrogen Bond
Unfavorable Positive-Positive
Pi-Cation
Pi-Pi T-shaped
Pi-Alkyl

Figure S2. Two-dimensional representations of the binding pockets and interactions between amino acids and **2** and **3** during the complex formation

Table S1. Crystal and refinement data.

Compound	**2**	3
Chemical formula	$C_{15}H_{11}BrN_4O_2$	$C_{15}H_{12}N_4O_2$
Formula weight (g/mol)	359.19	280.29
Temperature (K)	125(2)	125(2)
Wavelength (Å)	0.71073	
Crystal size (mm)	0.030 x 0.174 0.322	0.058 x 0.187 x 0.270
Crystal system	monoclinic	triclinic
Space group	Pc	P -1
Unit cell dimensions (Å,°)		
a	16.1068(17)	6.1973(8)
b	5.7977(6)	10.2465(13)
c	7.4341(8)	20.461(3)
α	90	102.548(4)
β	94.755(4)	94.531(4)
γ	90	95.302(4)
Volume	691.82(13)	1256.2(3)

Z	2	4
Density (calc., g/cm^3)	1.742	1.482
Abs. Coeff. (mm^{-1})	2.984	0.103
F(000)	360	584
Radiation Source	fine-focus sealed tube (MoKα)	
Theta range (°)	2.54 to 32.13	2.05 to 28.51
Reflections collected	28969	6336
Abs. Corr.	Numerical μ Calculated	Multi-scan
T_{max} and T_{min}	0.616 and 0.447	0.994 and 0.973
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data/Restraints/Parameters	4805 / 4 / 208	6336 / 4 / 392
Final R Indices		
Data ; I>2σ(I)	4278 data; R1 = 0.0419, wR2 = 0.1060	4661 data; R1= 0.0856, wR2 = 0.2151
All data	R1 = 0.0485, wR2 = 0.1092	R1 = 0.1116, wR2 = 0.2266
Goodness-of-fit on F^2	1.094	1.090

Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0640P)^2+$ $0.1076P]^a$	$w=1/[\sigma^2(F_o^2)+(0.0577P)^2+$ $4.9083P]^a$
Largest diff. peak and hole ($eÅ^{-3}$)	1.215 and -0.477	0.356 and -0.355
R.M.S. deviation from mean ($eÅ^{-3}$)	0.110	0.081

$^aP=(F_o^2+2F_c^2)/3$

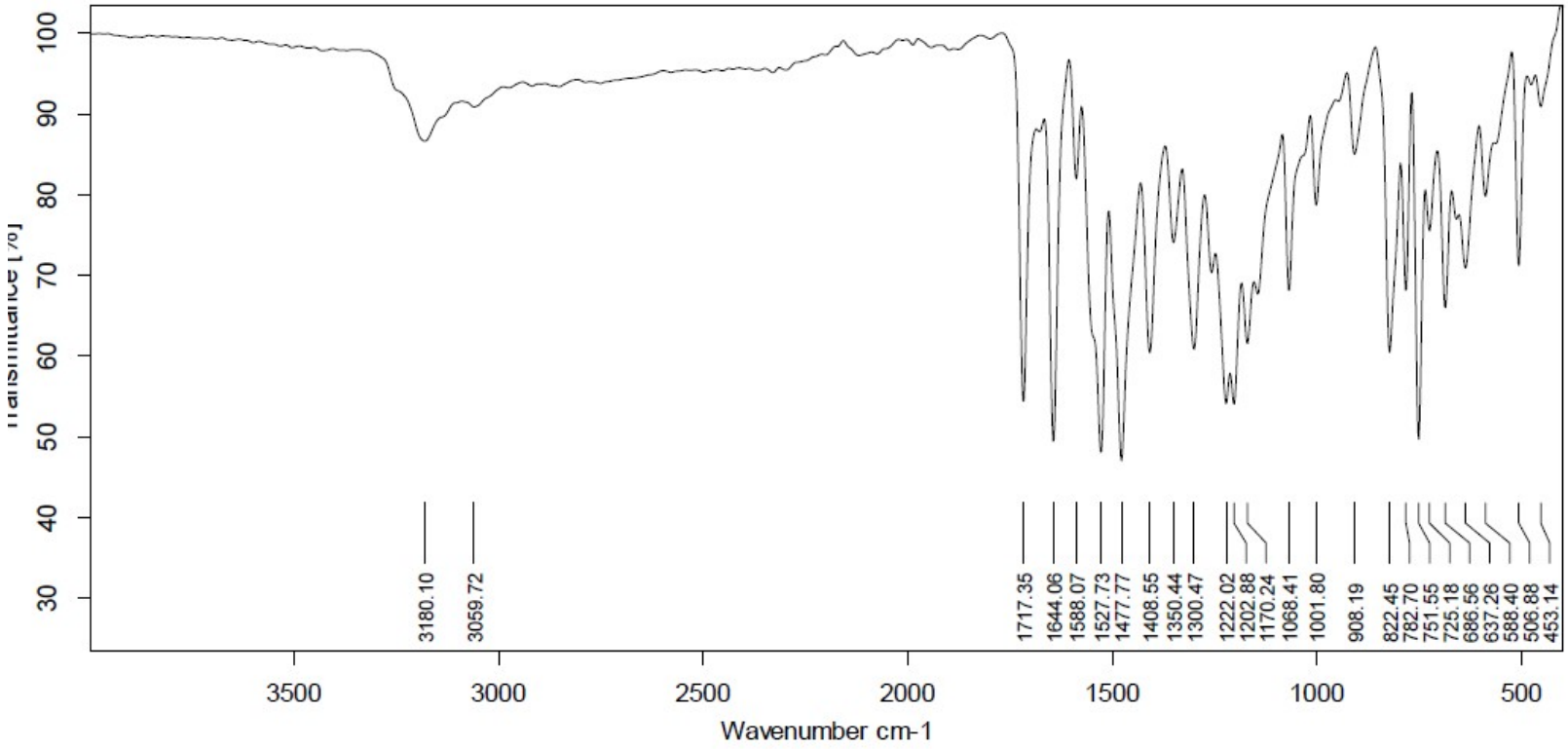

Figure S3. IR spectra of **2**

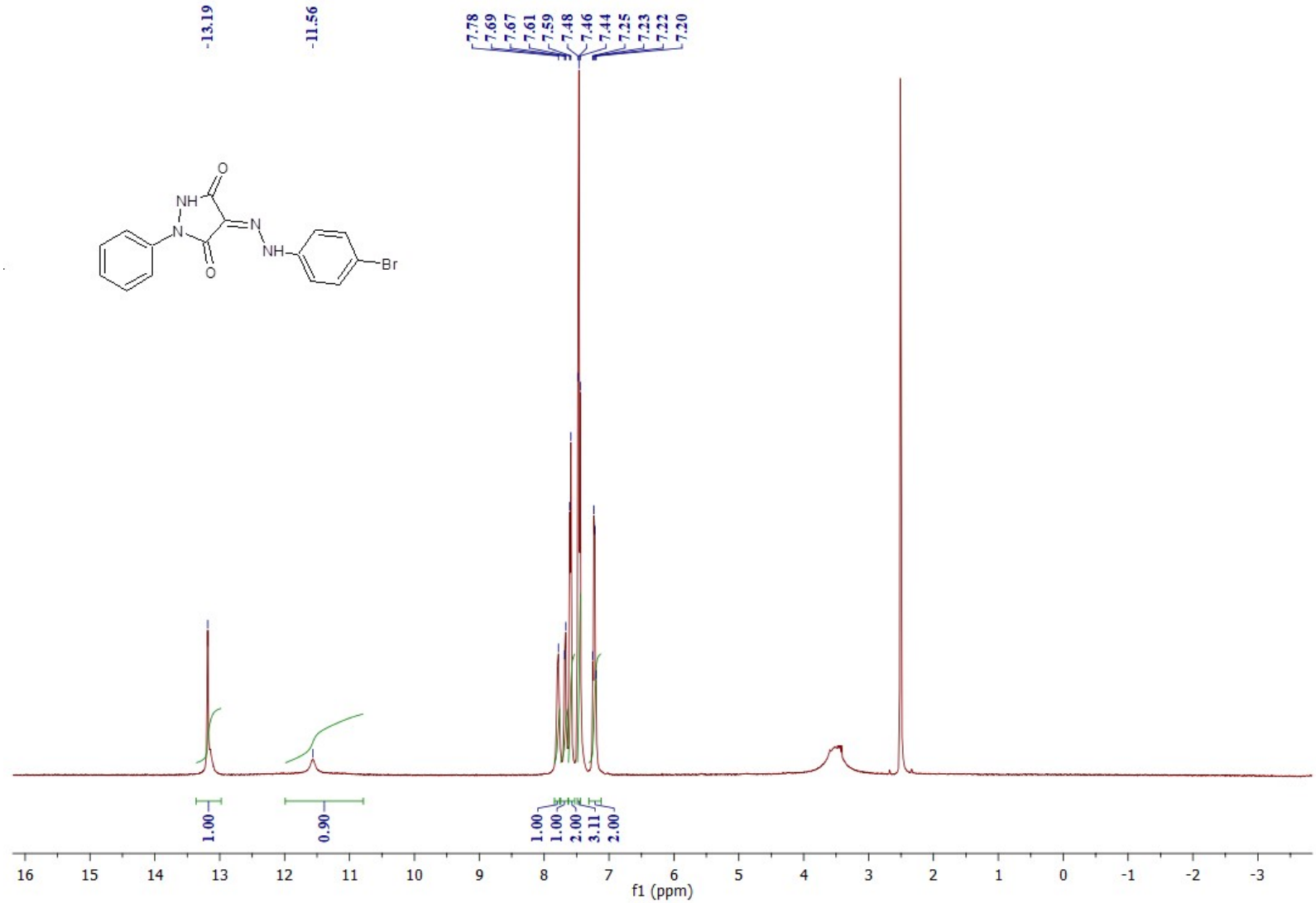

Figure S4. 1H NMR spectrum of **2**

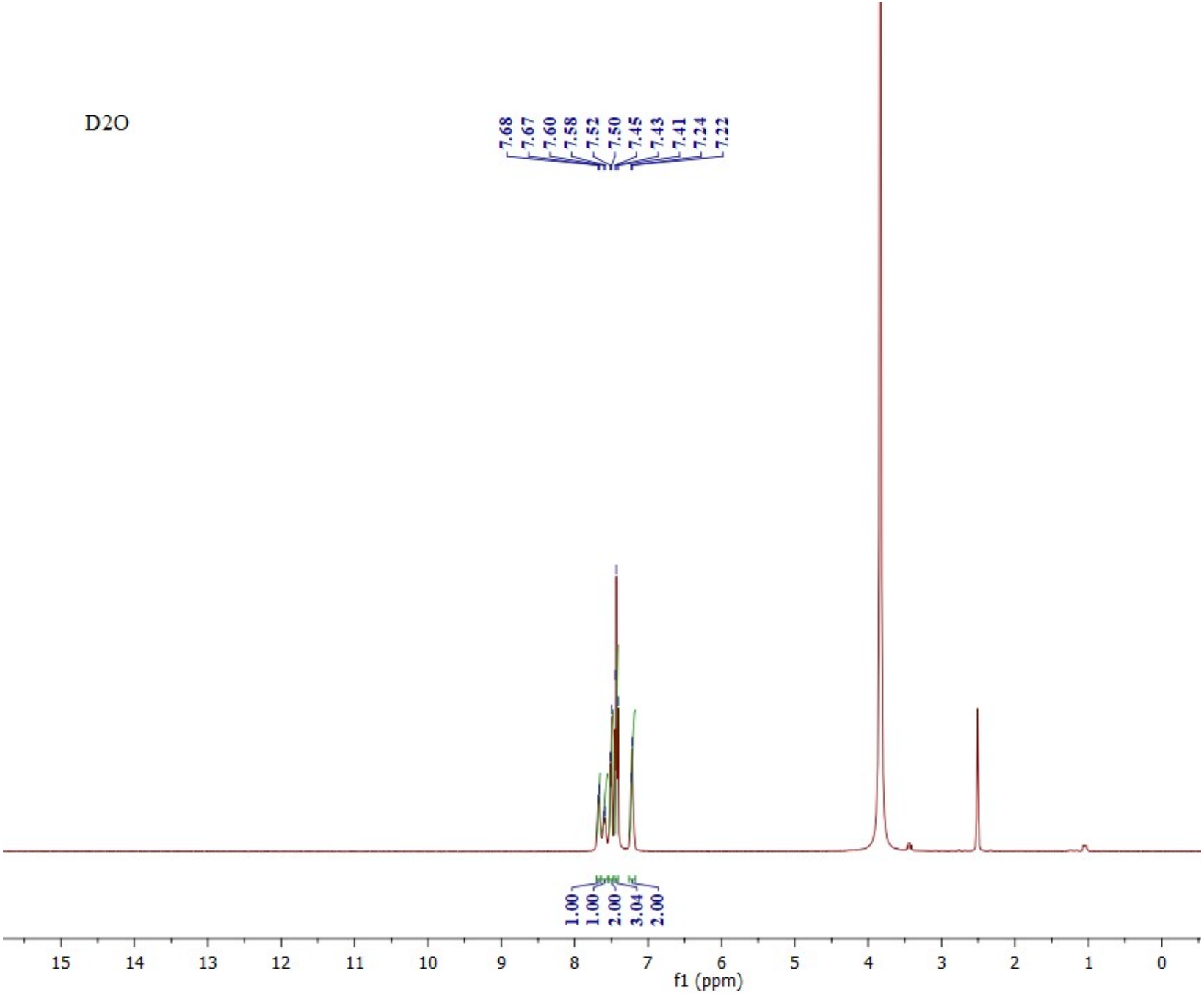

Figure S5. 1H NMR spectrum of **2**

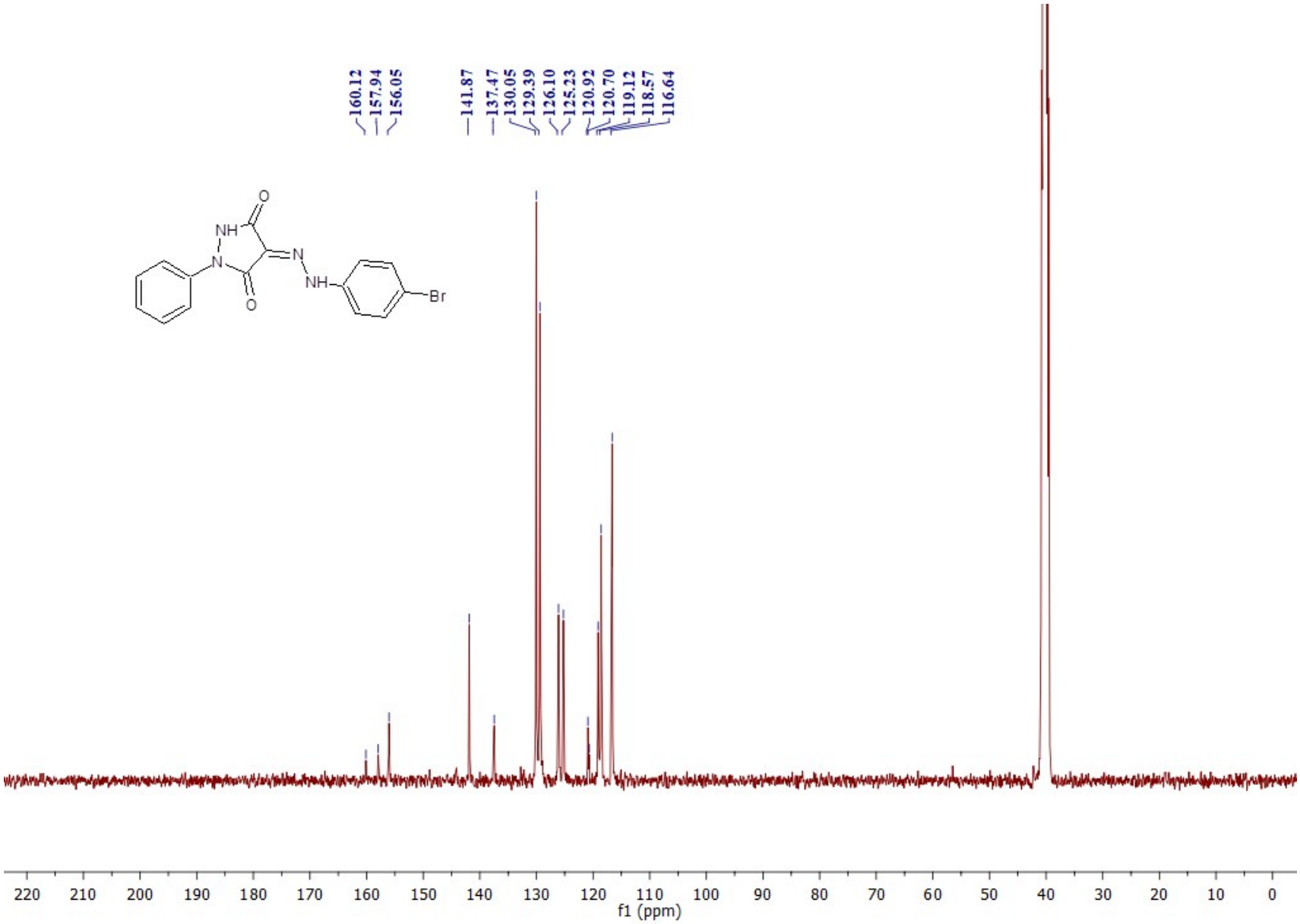

Figure S6. ^{13}C NMR spectrum of **2**

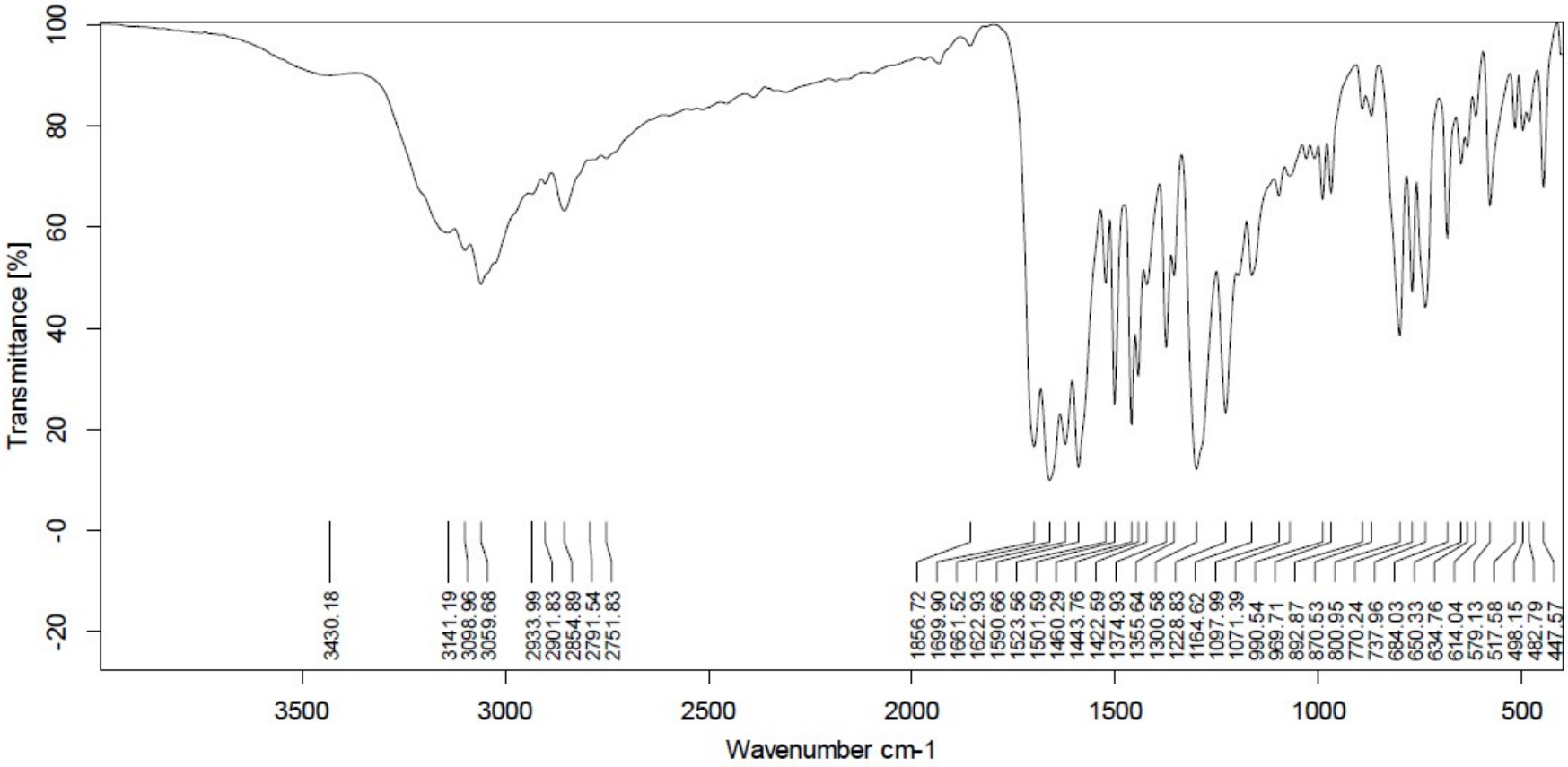

Figure S7. IR spectra of **3**

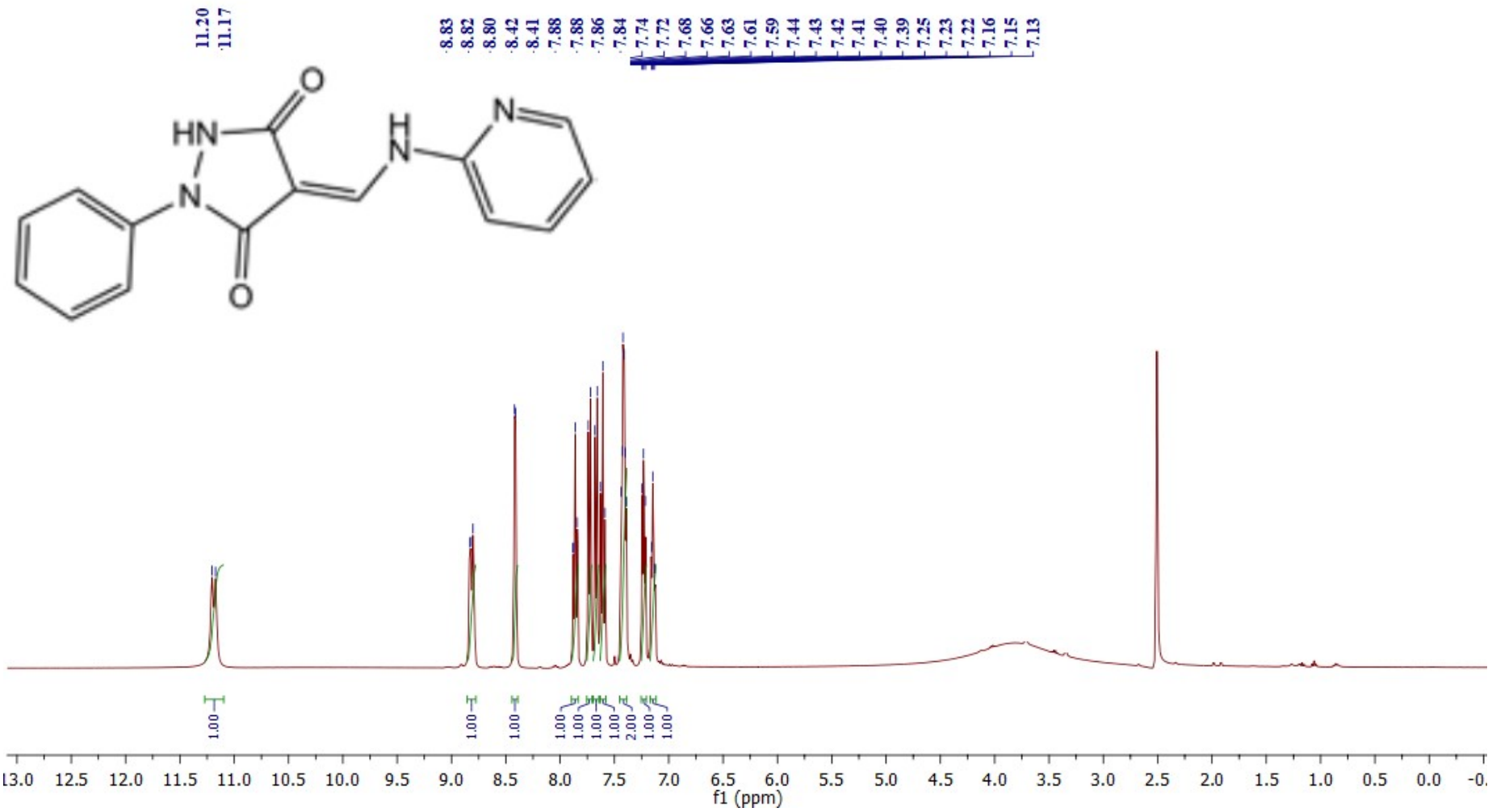

Figure S8. ^{1}H NMR spectrum of **3**