Electronic Supplementary Information

Ni(II) complex with bishydrazone ligand: synthesis, characterization, DNA binding studies and pro–apoptotic and pro–differentiation induction in human cancerous cell lines

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Content

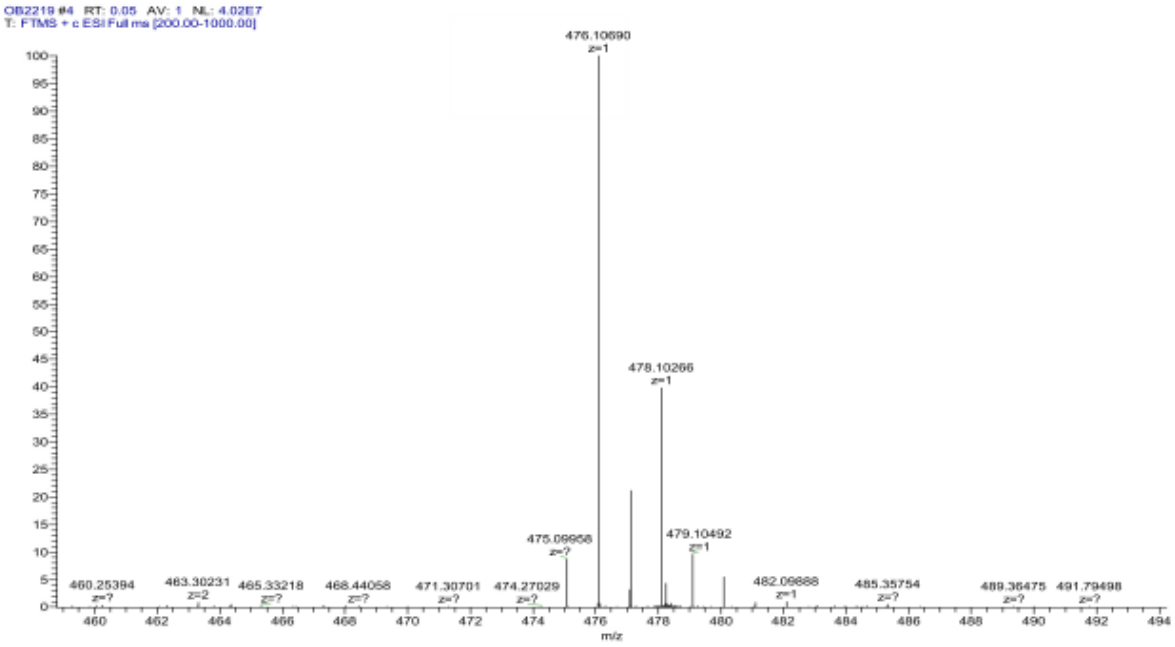

Figure S1. Mass spectrum of **1** in acetonitrile.

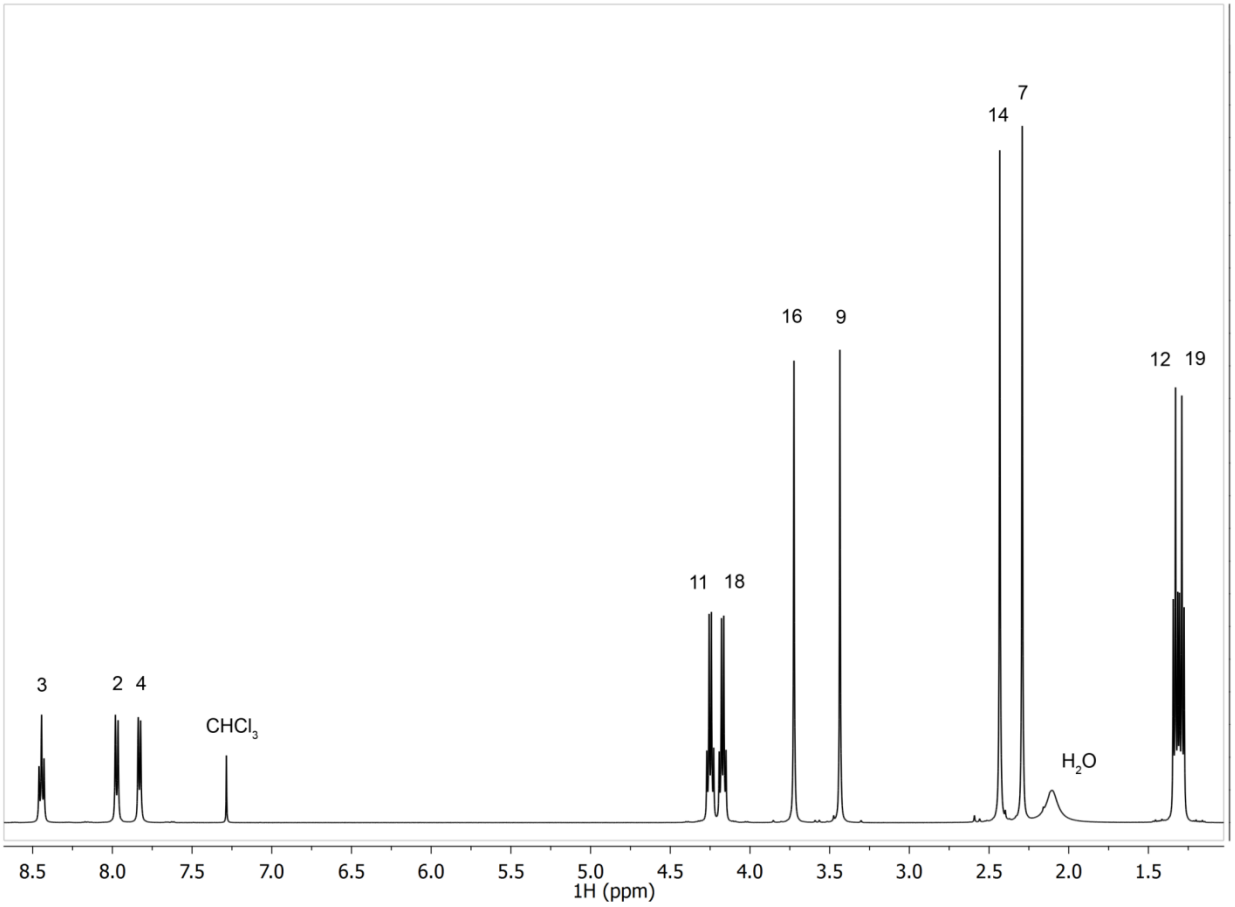

Figure S2. ^{1}H NMR spectrum of **1** in $CDCl_3$.

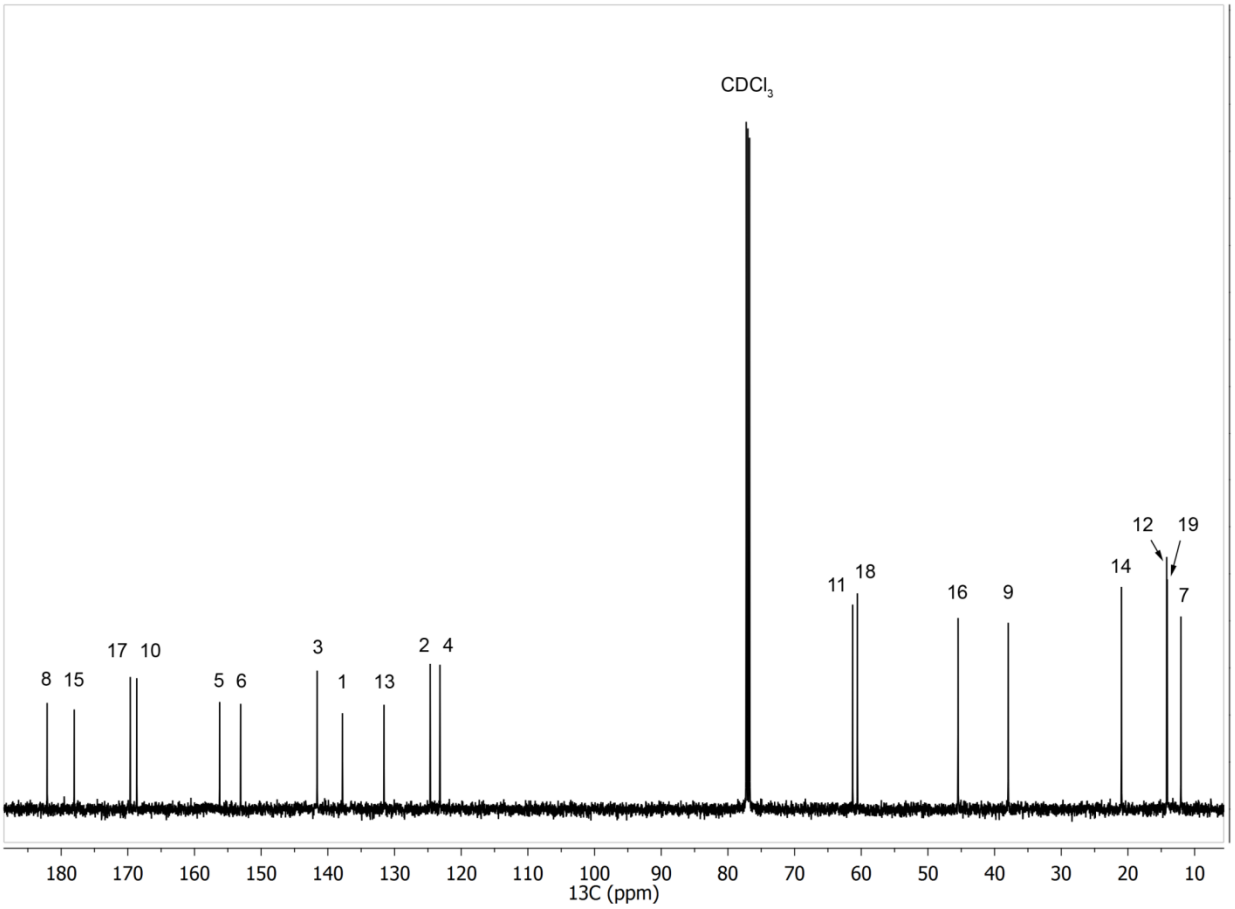

Figure S3. ^{13}C NMR spectrum of **1** in $CDCl_3$.

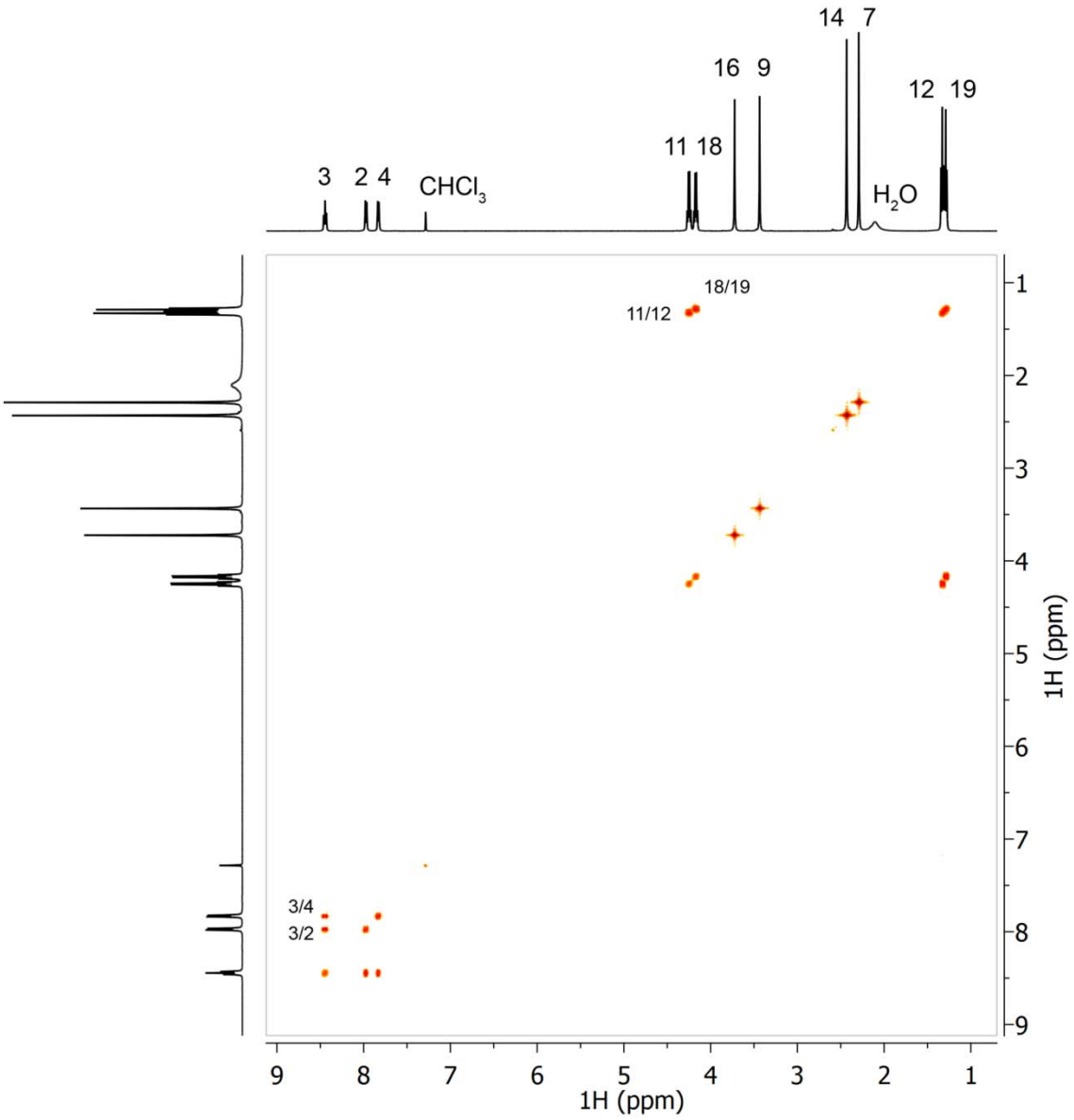

Figure S4. COSY spectrum of **1** in $CDCl_3$.

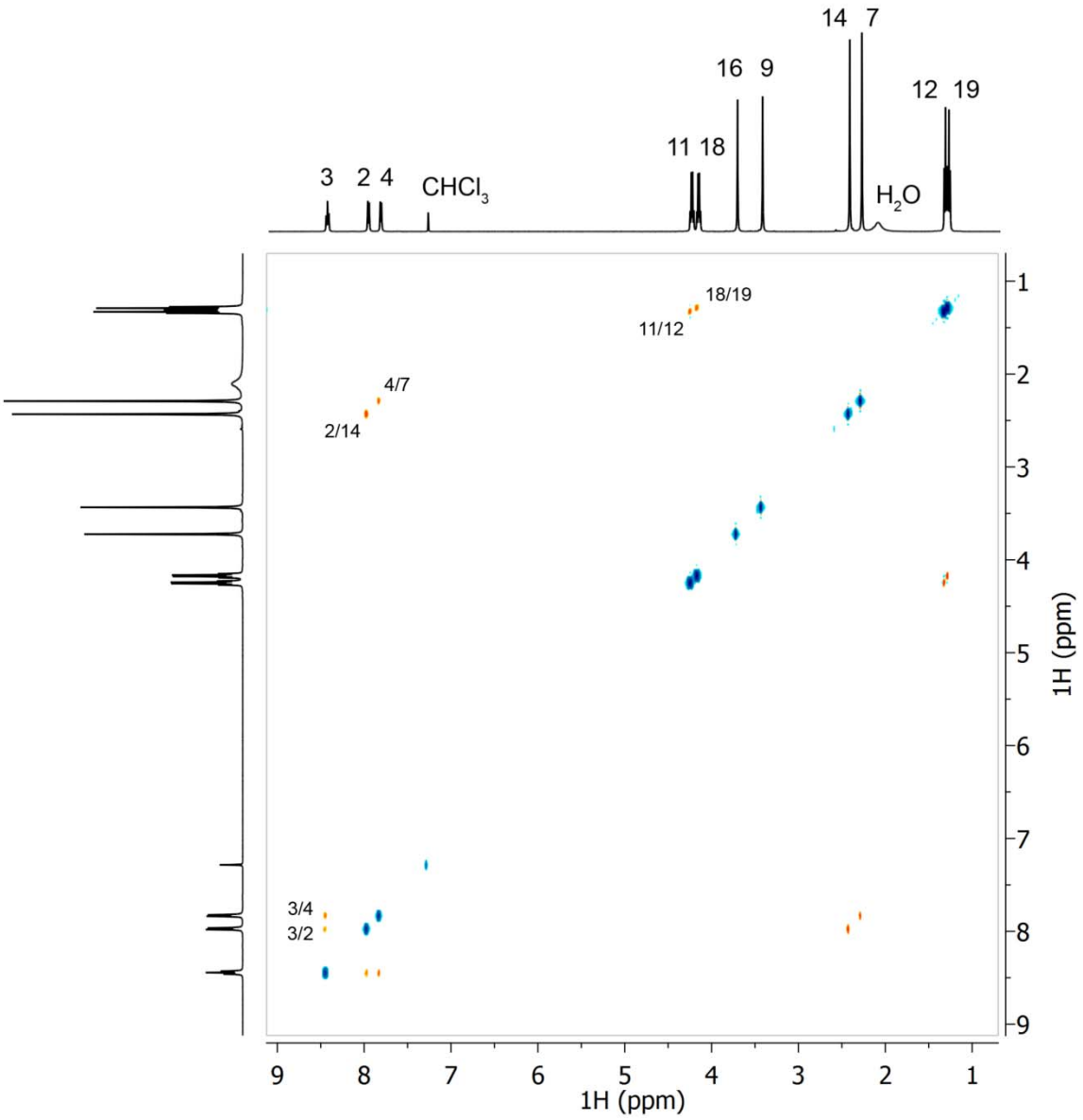

Figure S5. NOESY spectrum of **1** in $CDCl_3$.

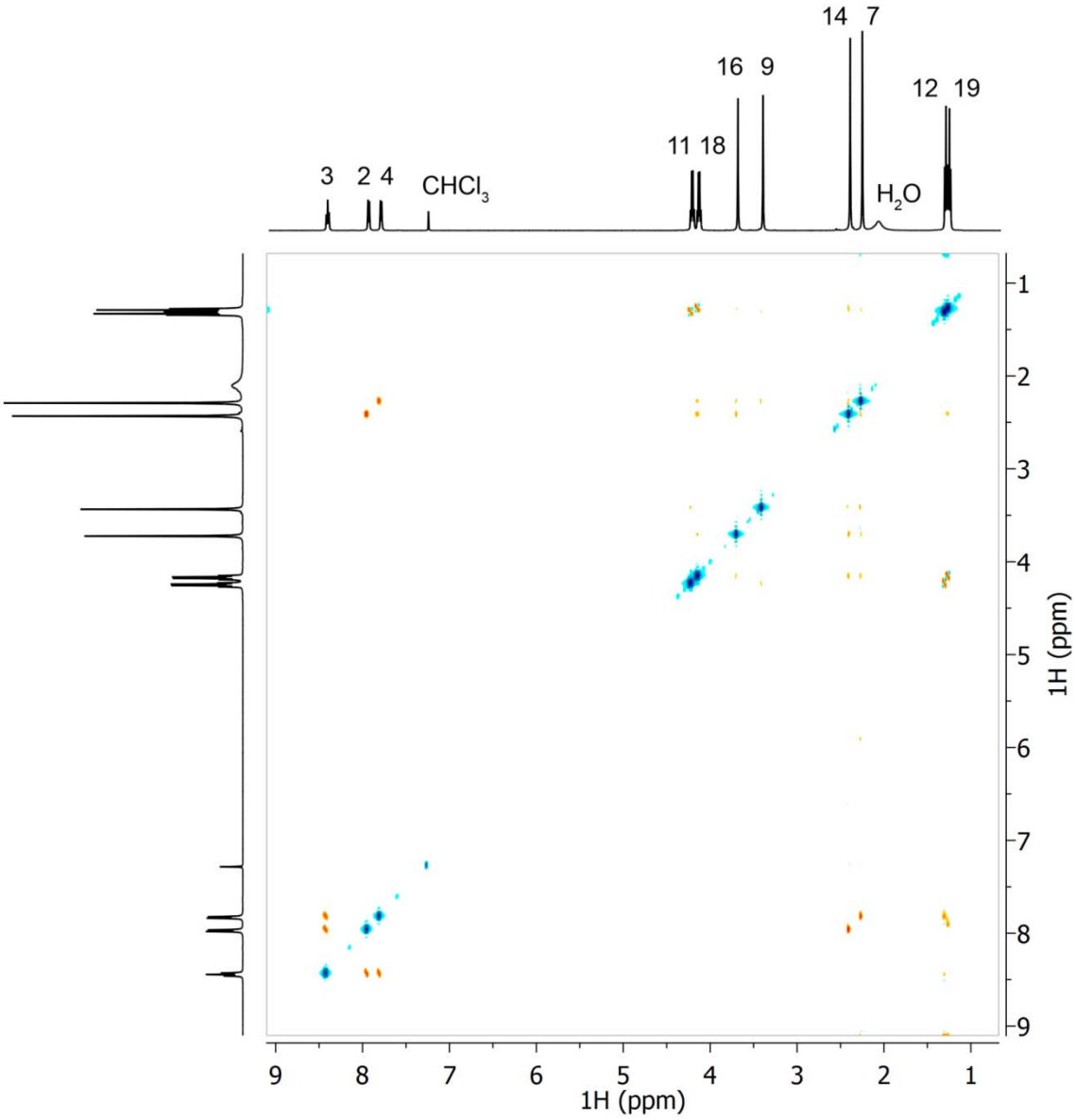

Figure S6. ROESY spectrum of **1** in $CDCl_3$.

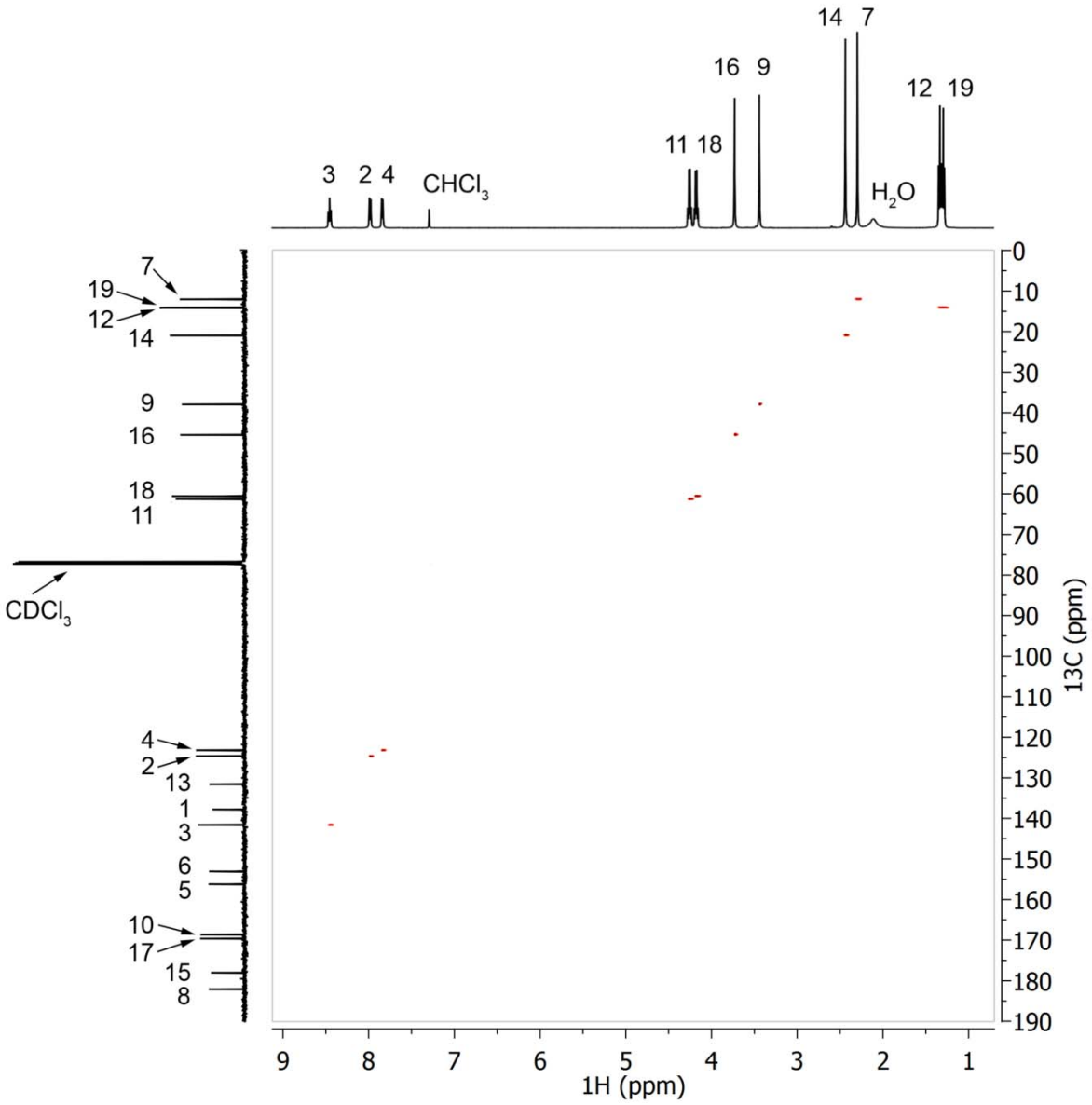

Figure S7. $^{1}H-^{13}C$ HSQC NMR spectrum of **1** in $CDCl_3$.

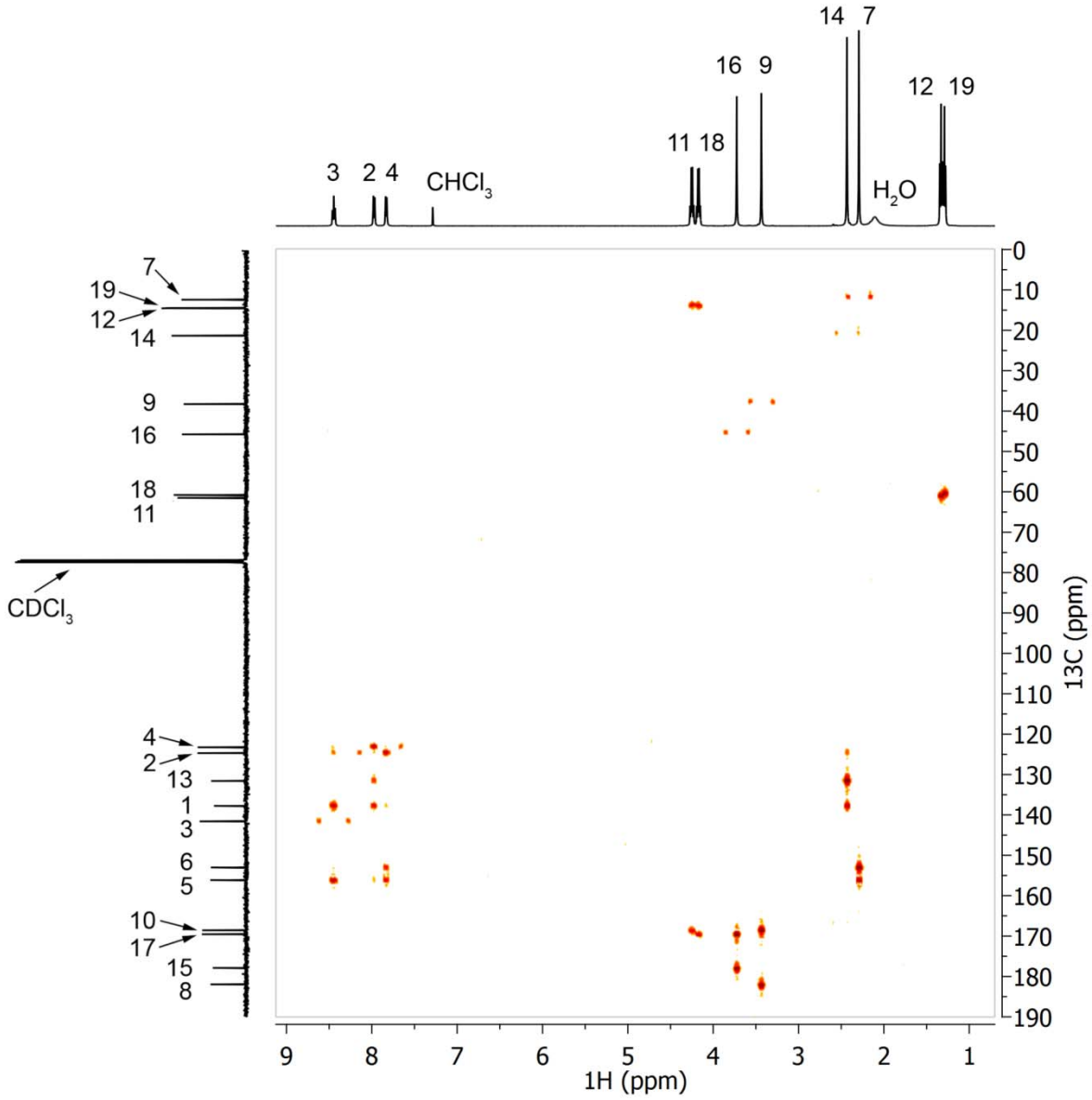

Figure S8. $^{1}H-^{13}C$ HMBC NMR spectrum of **1** in $CDCl_3$.

Table S1. Experimental and calculated ^{1}H NMR chemical shifts of **1.**

Assignation	Experimental chemical shift δ (ppm)	Calculated chemical shift δ (ppm)
H−C3	8.44	8.22577
H−C4	7.83	7.86877
H−C2	7.97	7.68497
H−C7	2.29	2.38157
H−C14	2.43	2.57017
H−C9	3.44	3.13757
H−C16	3.72	4.10837
H−C11	4.25	4.00027
H−C18	4.17	4.14927
H−C12	1.33	1.31587
H−C19	1.29	1.32397
H_2O	2.11	2.31637
		9.68517

Table S2. Experimental and calculated ^{13}C NMR chemical shifts of **1**

Assignation	Experimental chemical shift δ (ppm)	Calculated chemical shift δ (ppm)
C3	141.60	136.0176
C4	123.19	118.5201
C2	124.64	119.9311
C5	156.28	150.5638
C1	137.80	139.1615
C6	153.08	158.8117
C13	131.57	138.3357
C7	12.06	16.3772
C14	20.98	22.2051
C8	182.10	166.0884
C15	178.04	175.0396
C9	37.96	45.1723
C16	45.48	50.8007
C10	168.66	170.9611
C17	169.76	165.6791
C11	61.29	64.2114
C18	60.58	63.5428
C12	14.18	14.3748
C19	14.11	14.4742

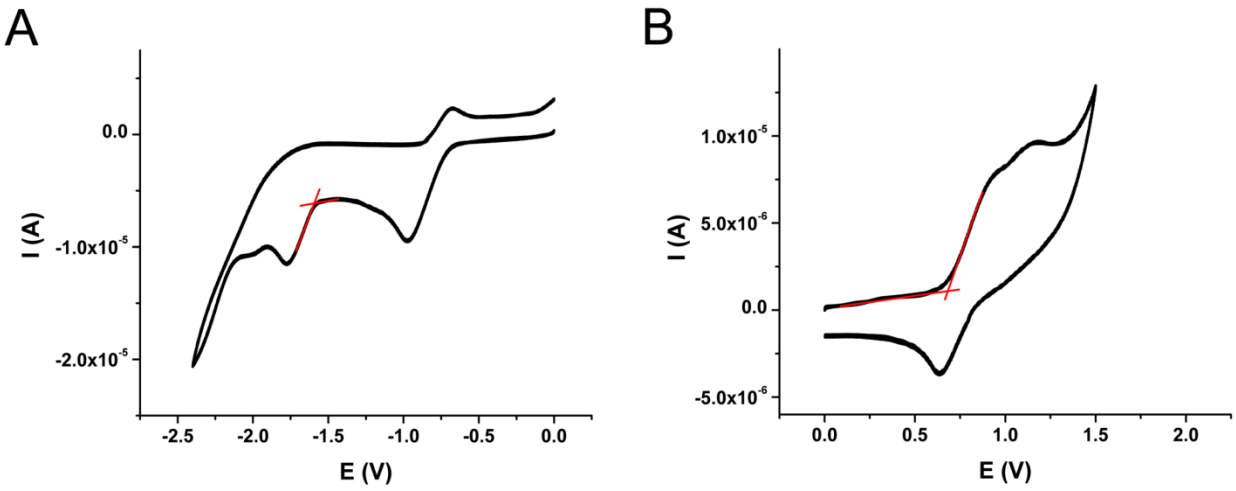

Figure S9. Cyclic voltammograms of **1** in anhydrous DMSO containing 0.10 M [*n*-Bu_4N][PF_6] at a scan rate of 100 mVs^{-1} using a glassy carbon working electrode in the potential range from –2.5 to 0.0 V (A) and from 0.0 to +1.5 V (B).

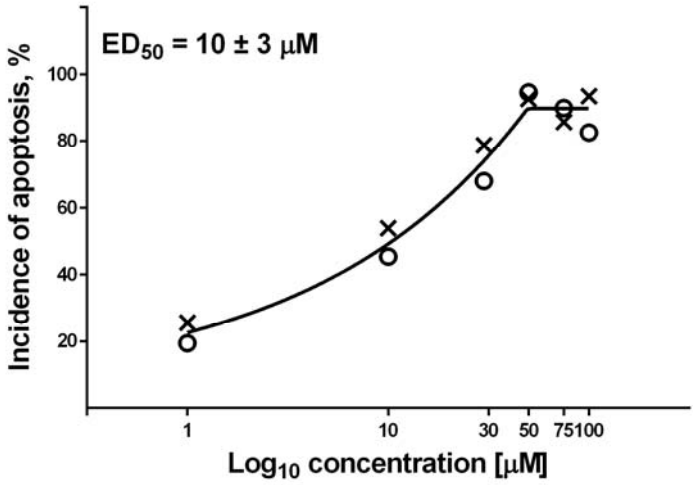

Figure S10. Concentration-response curve and ED_{50} value for **1** on THP-1 cells treated during 24 h incubation. Results are presented as percentage of apoptotic events determined by means of Annexin V/PI double staining in two independent experiments (circles and crosses) with asymmetric five-parameter sigmoidal curve computed for both replicated in GraphPad Prism software.

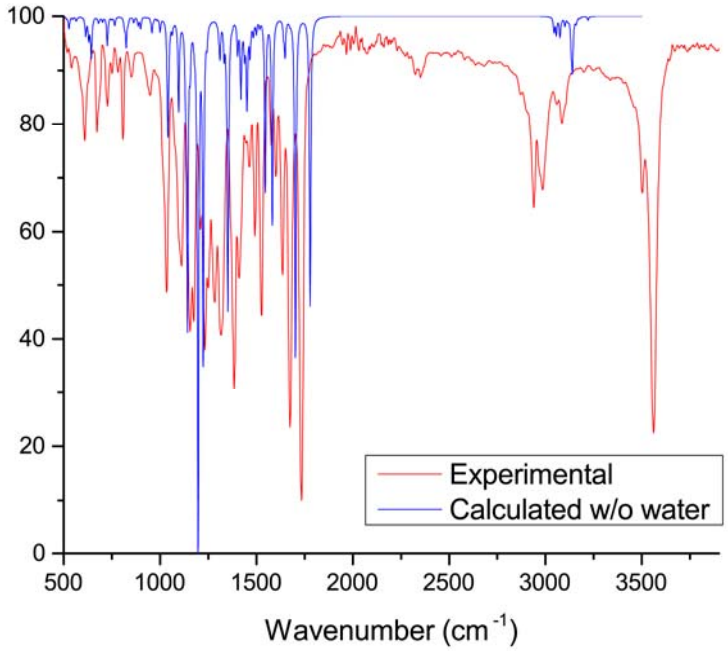

Figure S11. Comparison of experimental IR spectrum and calculated IR spectrum for the structure with coordination of the carbonylic oxygen of the hydrazonic arm.

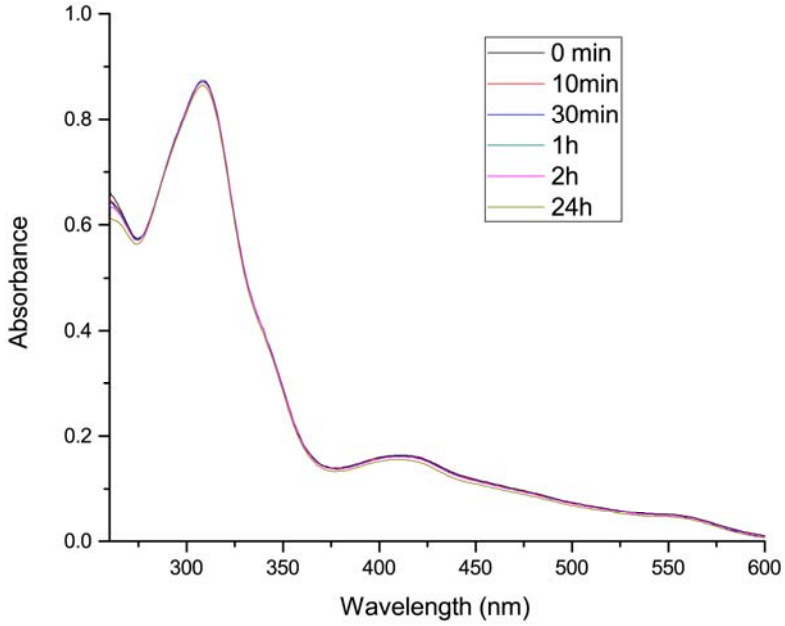

Figure S12. UV-VIS spectra of **1** in DMSO over 24 hour period.

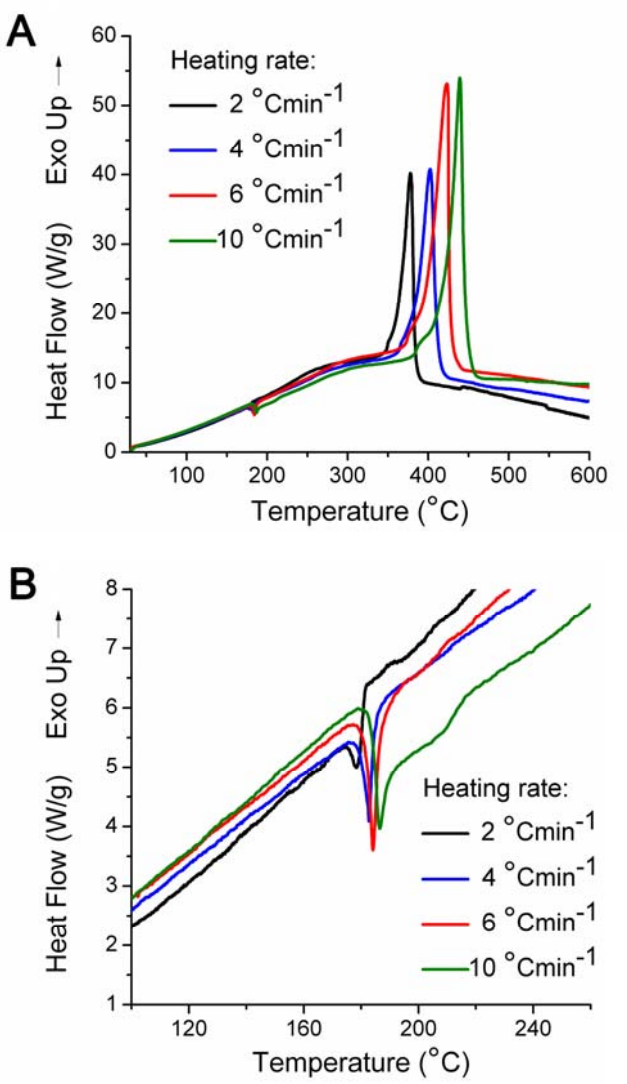

Figure 13. DSC curves in air with subtracted baselines at different heating rates (A), with enhanced region of the first degradation peak (B).

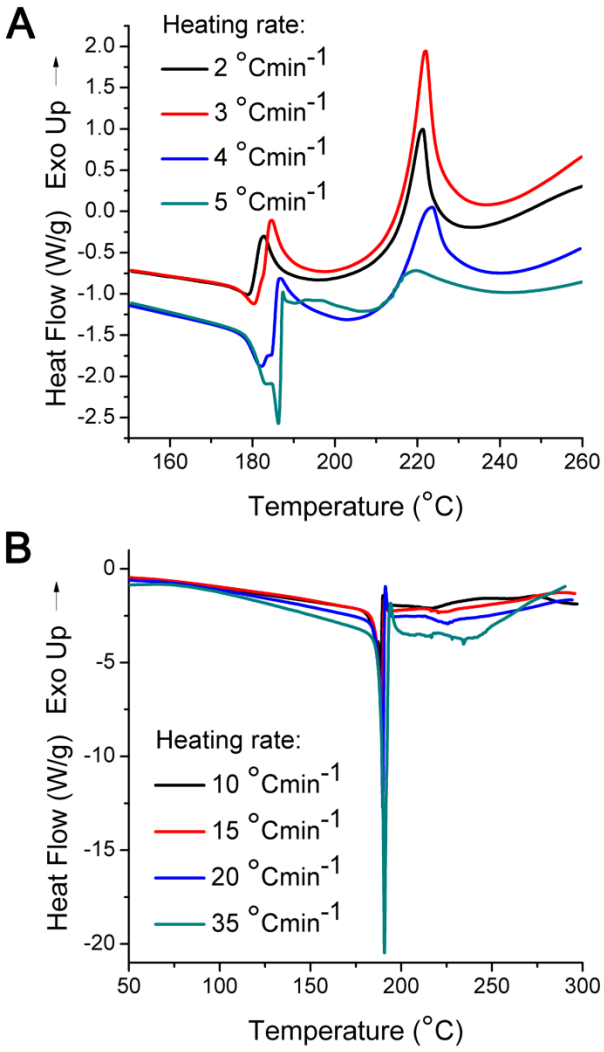

Figure S14. DSC recorded in nitrogen at lower (A) and higher (B) heating rates.