Cyclam-based molybdenum carbonyl complexes as a novel class of cytotoxic agents

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SUPPORTING INFORMATION

Table SI1 – Thermoanalytical data of complexes **5-8**.

	TG range (°C)	DTG_{max} (°C)	Found (calcd %)		Assignment
			Weight loss	Total weight loss	
5	25-200	120	14.9 (14.7)	77.5 (74.7)	Loss of two CO molecules
	200-550	300, 480	62.6 (60.0)		Loss of $C_{10}H_{24}N_4$ + CO
6	140-180	160	8.8 (8.3)	83.6 (85.7)	Loss of two CO molecules
	180-600	280, 420, 500	74.8 (77.4)		Loss of $C_{32}H_{52}N_4$ + CO
7	150-200	180	7.0 (8.0)	82.0 (86.2)	Loss of two CO molecules
	200-650	300, 320, 440, 500, 580	75.0 (78.2)		Loss of $C_{26}H_{34}F_6N_4$ + CO
8	150-200	180	10.0 (9.1)	85.0 (84.5)	Loss of two CO molecules
	200-550	320, 510	75.0 (75.4)		Loss of $C_{28}H_{44}N_4$ + CO

Table SI2 - Crystal data and structure refinement for compound **5.CH_2Cl_2**.

Formula	$C_{14}H_{26}Cl_2MoN_4O_3$
Fw	465.23
Crystal form, colour	Block, yellow
Crystal size (mm)	0.20x0.20x0.24
Crystal system	Monoclinic
Space group	$P2_1/n$
***a*, Å**	8.933(1)
***b*, Å**	17.321(2)
***c*, Å**	13.139(2)
***α*, °**	90
***β*, °**	104.667(5)
***γ*, °**	90
Z	4
***V*, Å^3**	1966.7(4)
***T*, K**	150(2)
D_c, g cm^{-3}	1.527
***μ*(Mo Kα), mm^{-1}**	0.958
θ range (º)	1.987 – 29.567
refl. collected	61475
independent refl.	5506
R_{int}	0.0585
R_1[a], wR_2[b] [$I \geq 2\sigma(I)$]	0.0511, 0.0821
GOF on F^2	1.086

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$

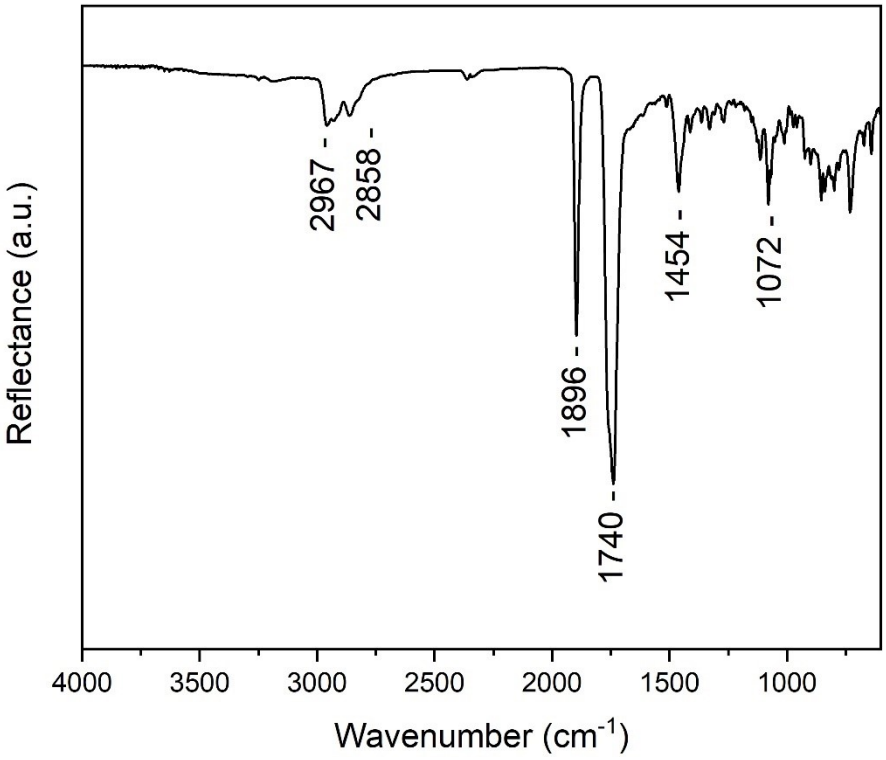

Figure S1: IR spectrum of **5**.

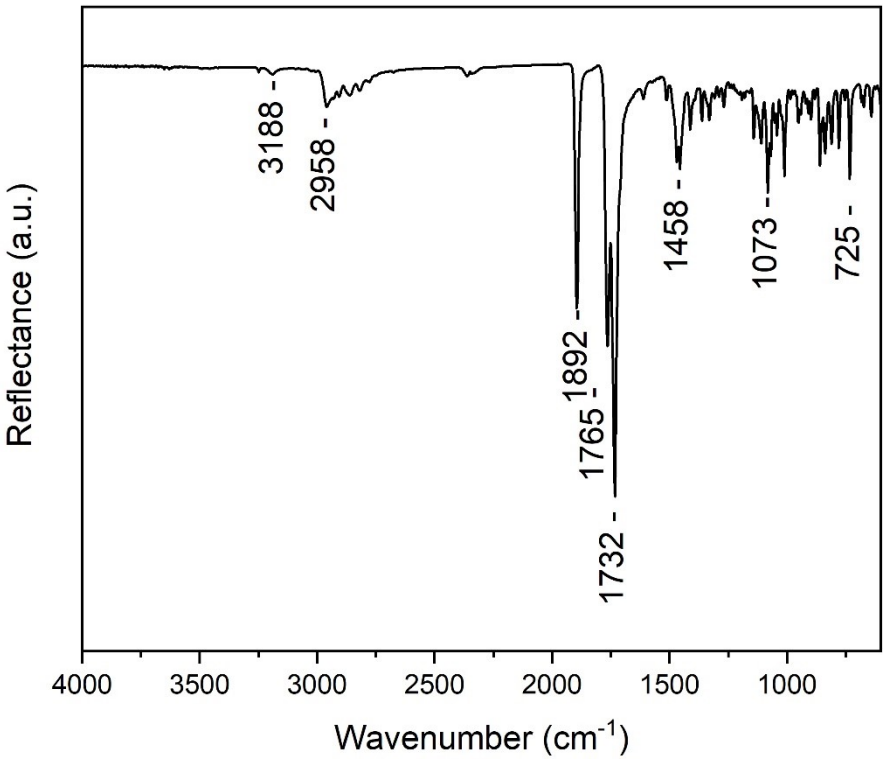

Figure S2: IR spectrum of **6**.

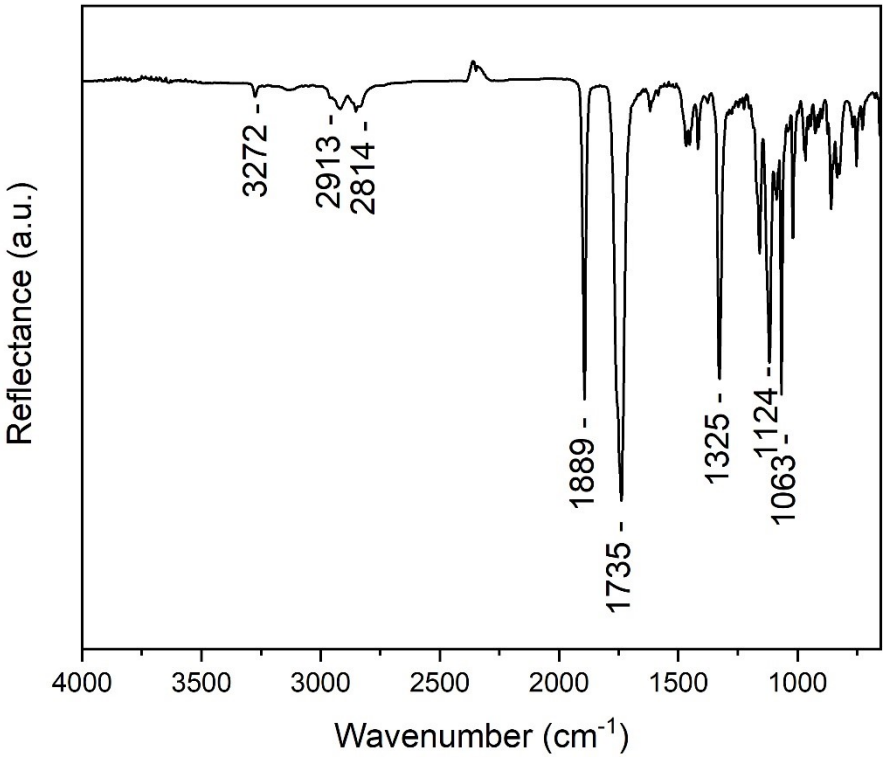

Figure S3: IR spectrum of **7**.

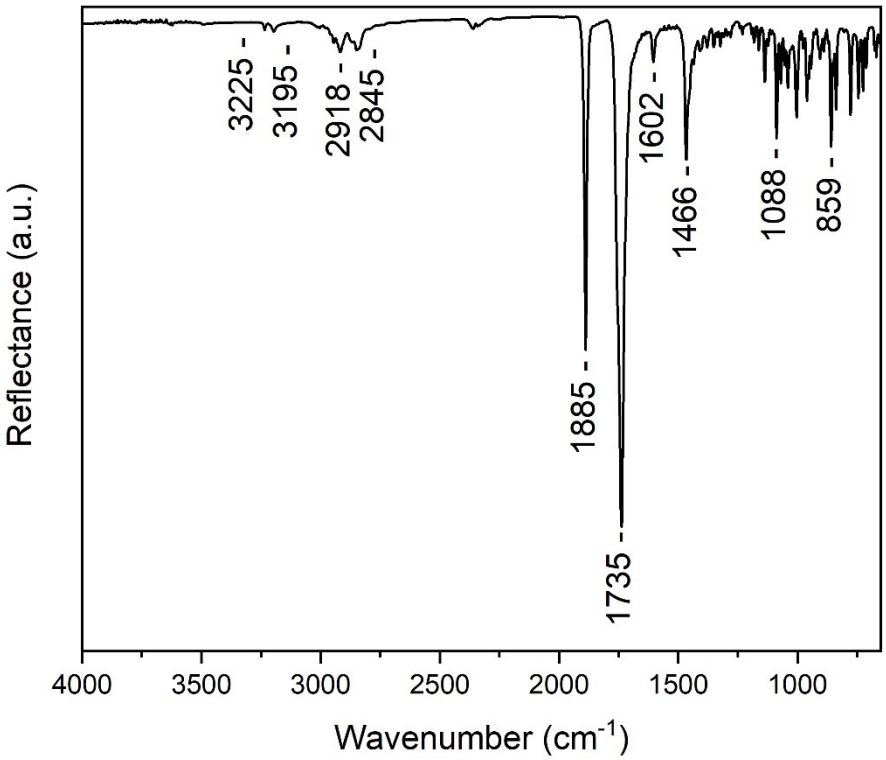

Figure S4: IR spectrum of **8**.

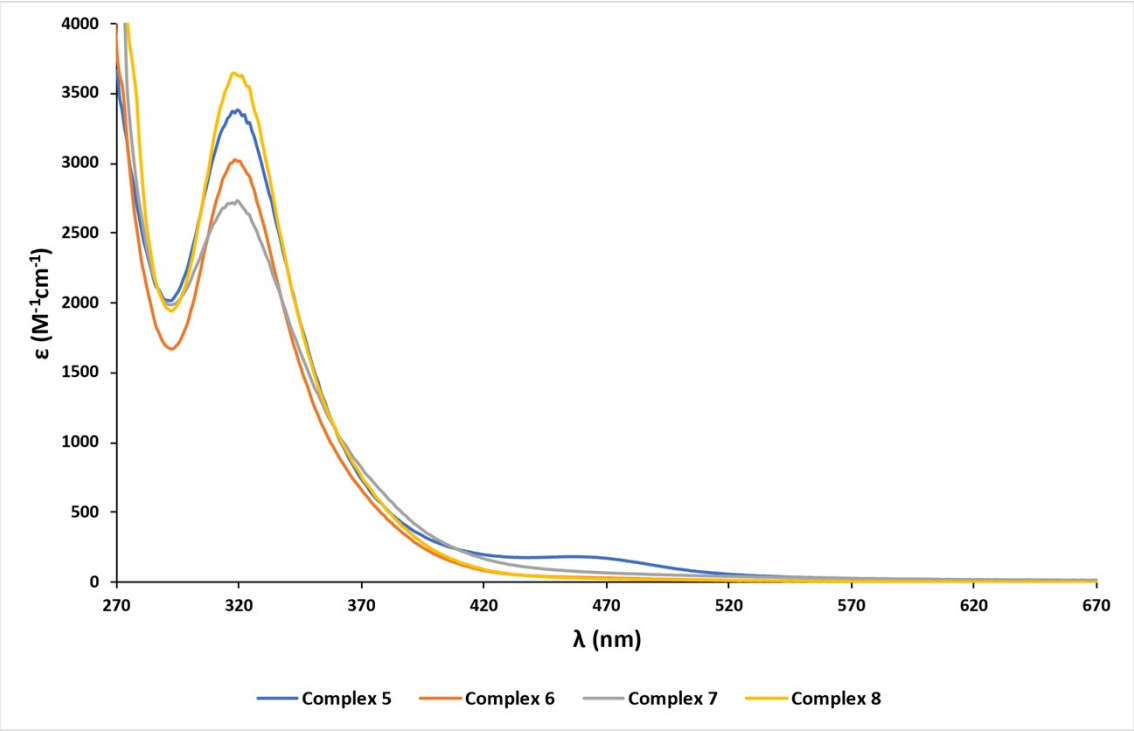

Figure S5: UV-Vis spectra of complexes **5-8** in DMSO.

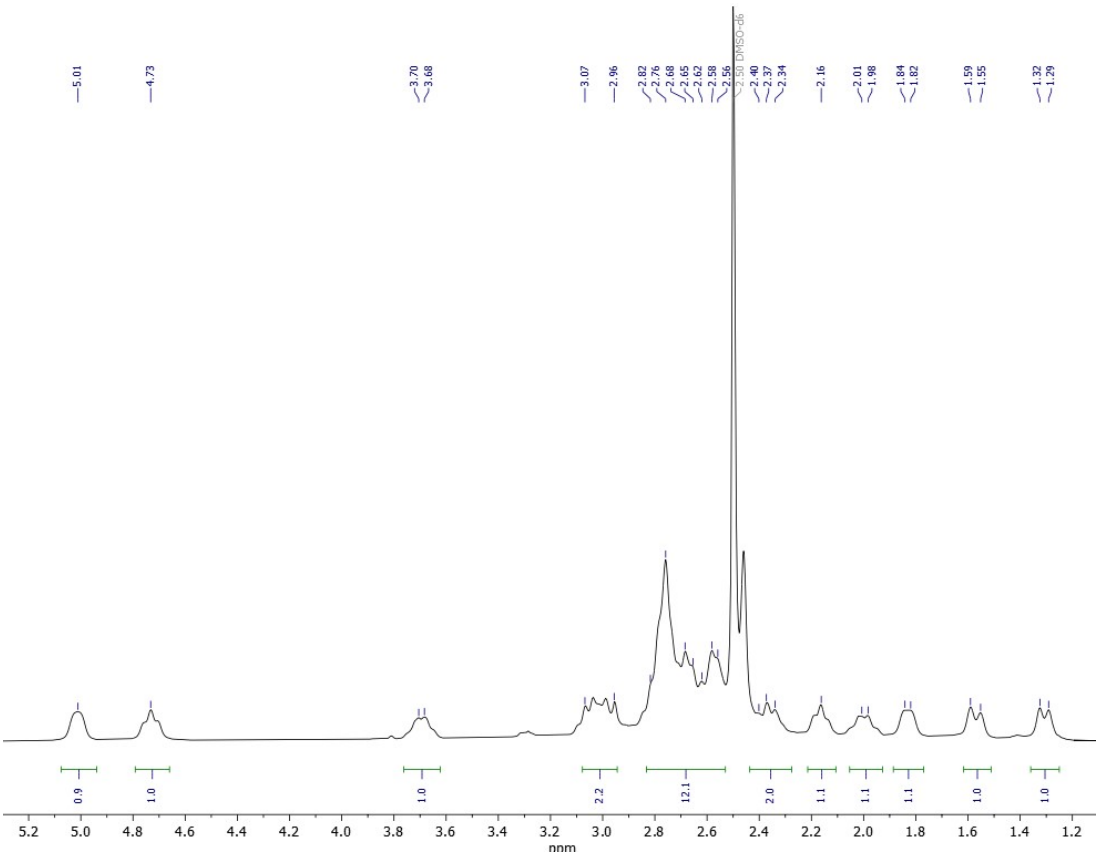

Figure S6A: ^{1}H NMR spectrum of **5** in DMSO-d_6.

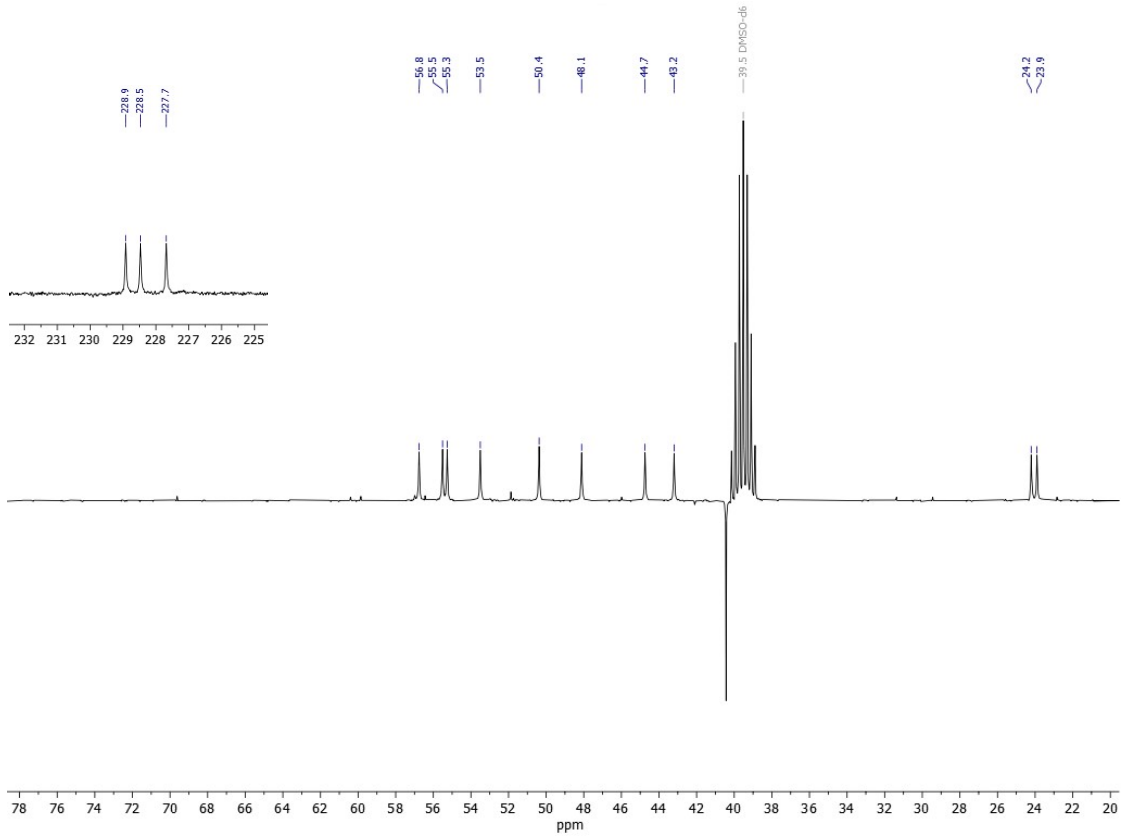

Figure S6B: $^{13}C\{^{1}H\}$ NMR spectrum of **5** in DMSO-d_6.

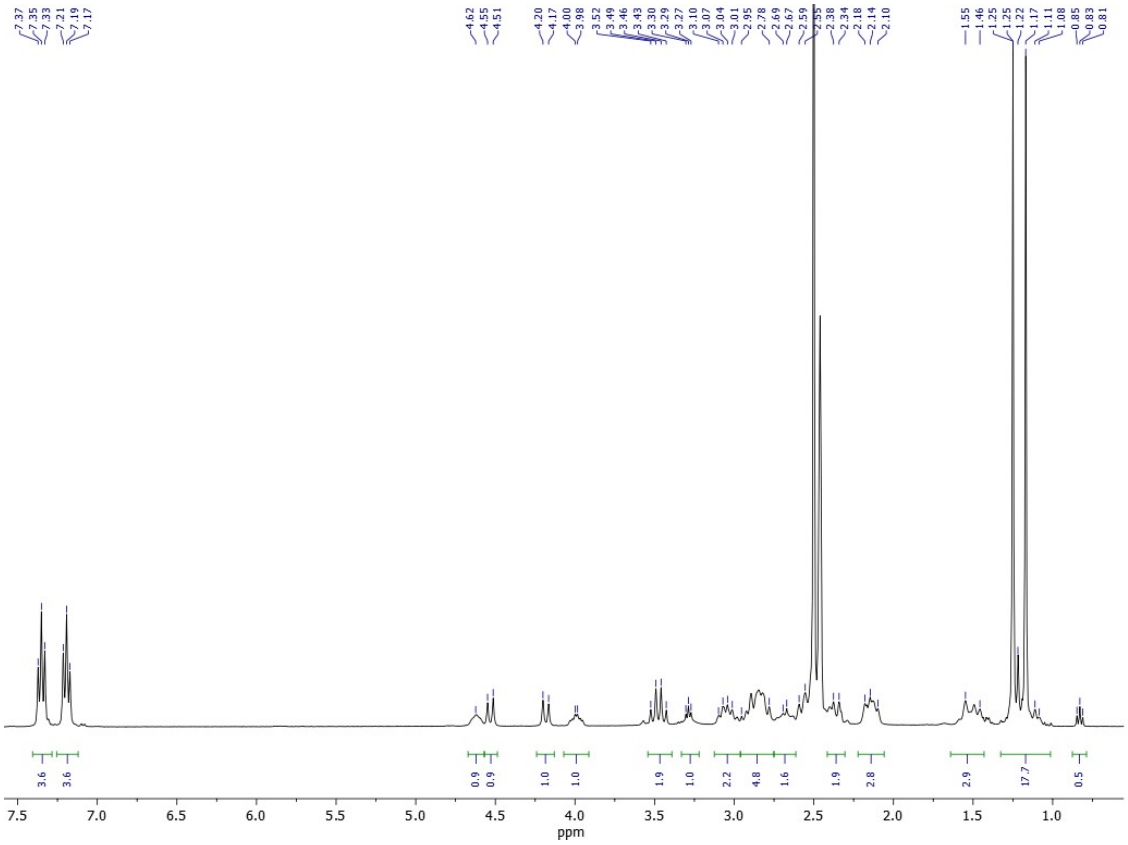

Figure S7A: ^{1}H NMR spectrum of **6** in DMSO-d_6.

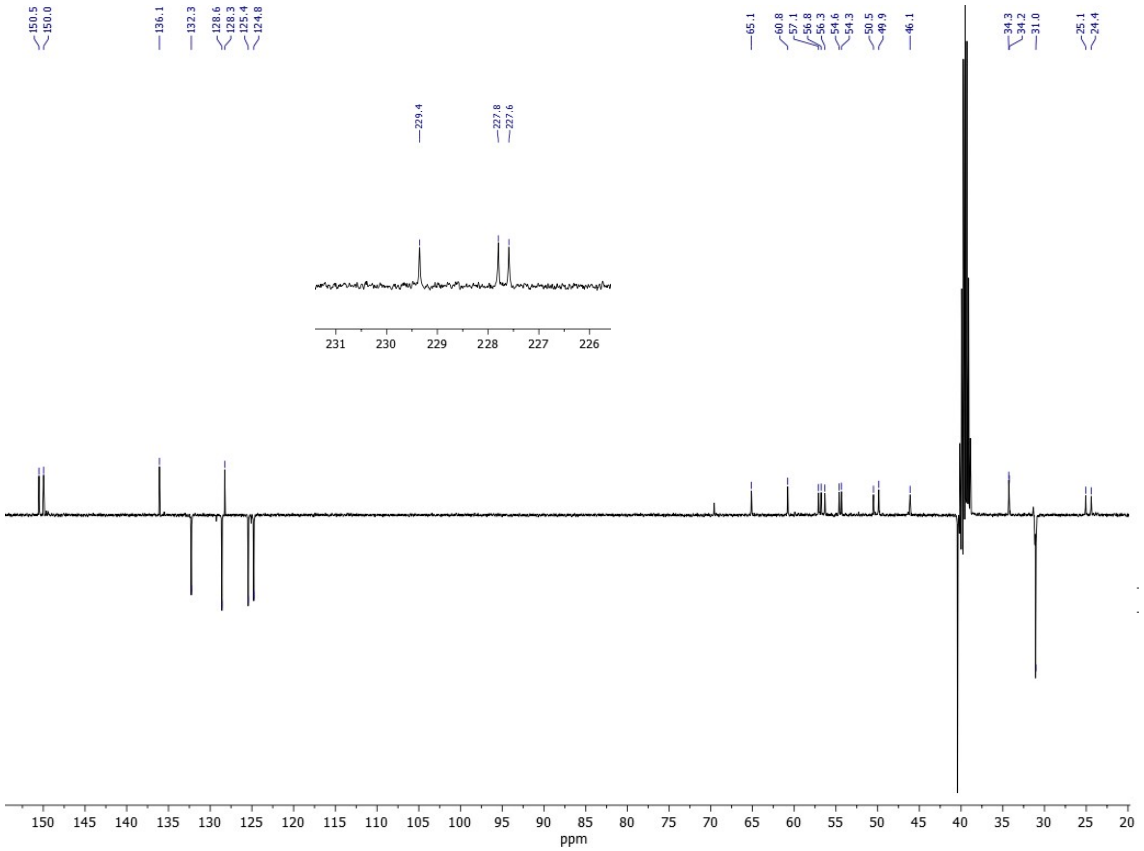

Figure S7B: $^{13}C\{^{1}H\}$ NMR spectrum of **6** in DMSO-d_6.

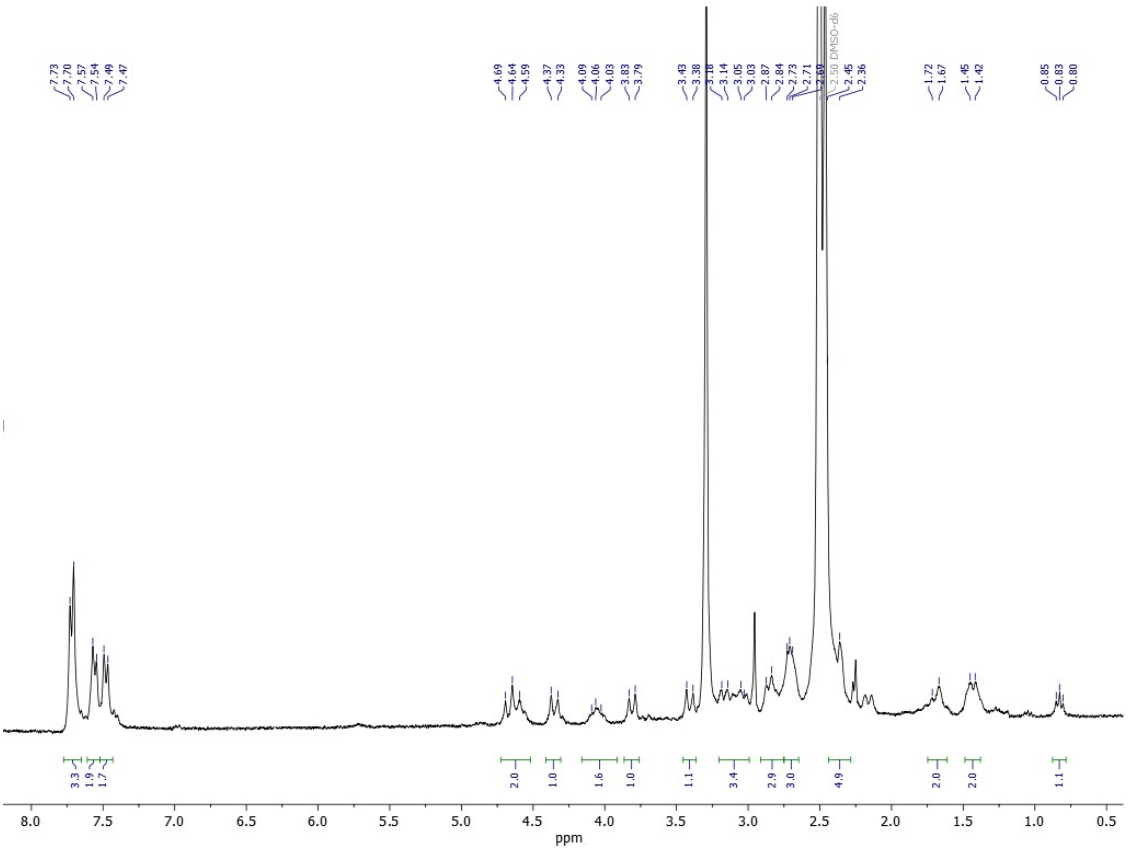

Figure S8A: ^{1}H NMR spectrum of **7** in DMSO-d_6.

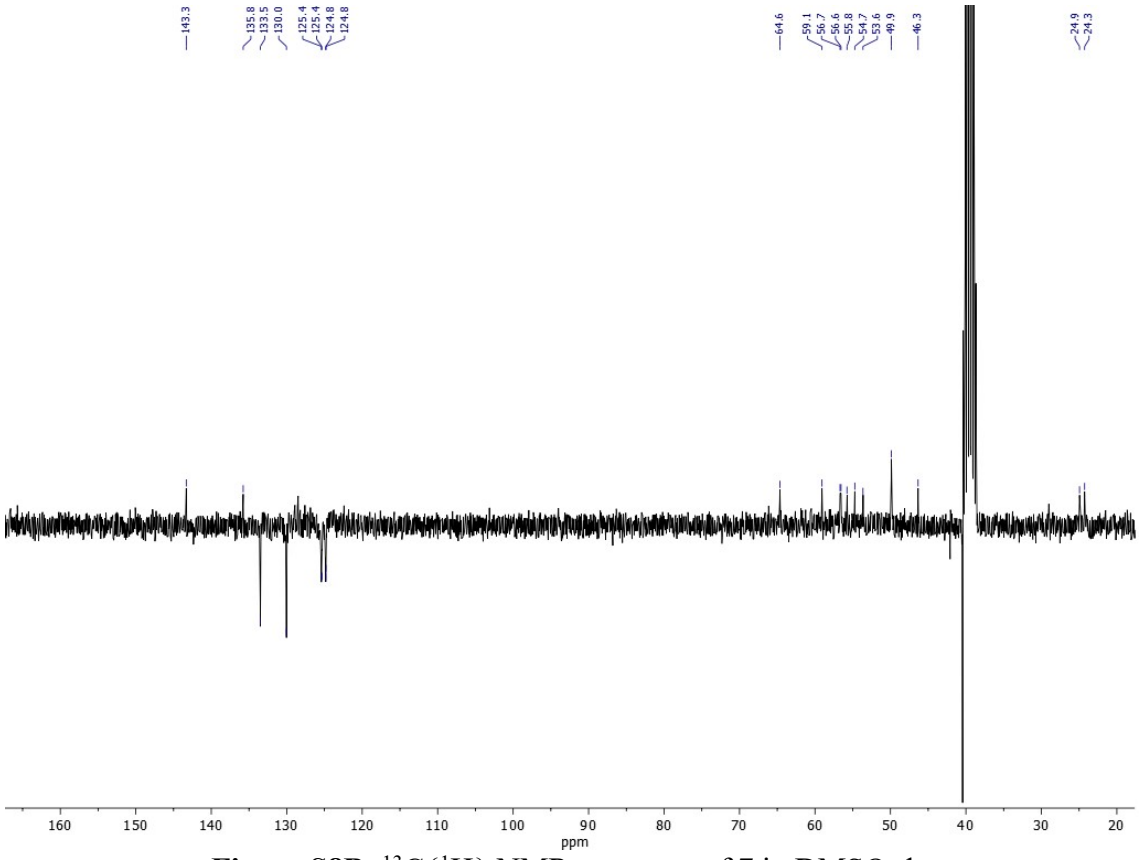

Figure S8B: $^{13}C\{^{1}H\}$ NMR spectrum of **7** in DMSO-d_6.

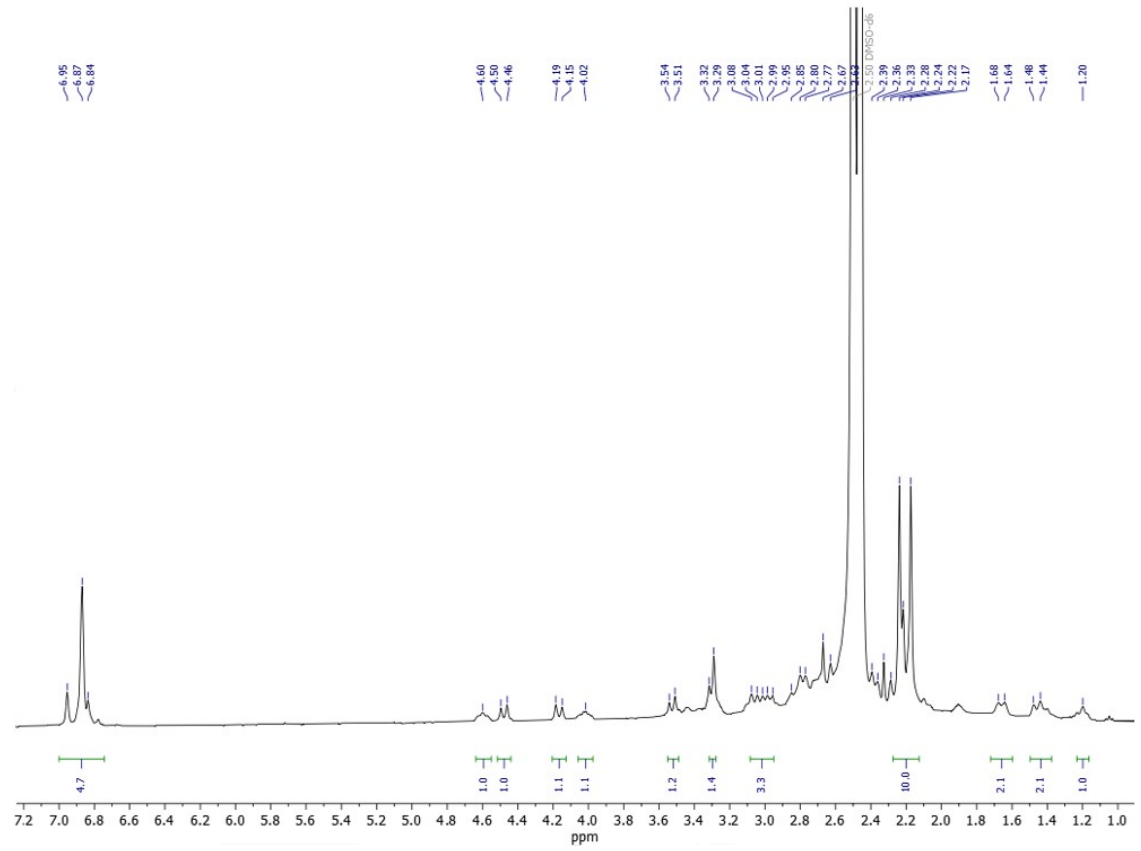

Figure S9A: ^{1}H NMR spectrum of **8** in DMSO-d_6.

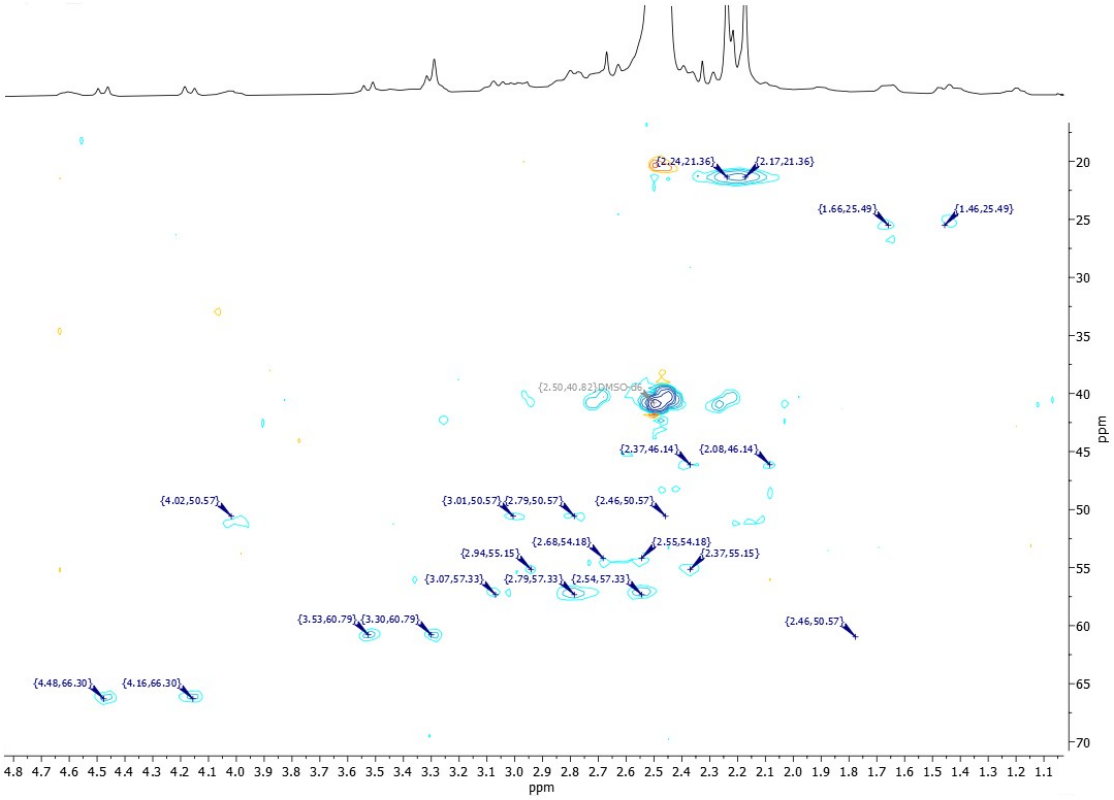

Figure S9B: ^{1}H-^{13}C HSQC spectrum of **8** in DMSO-d_6.

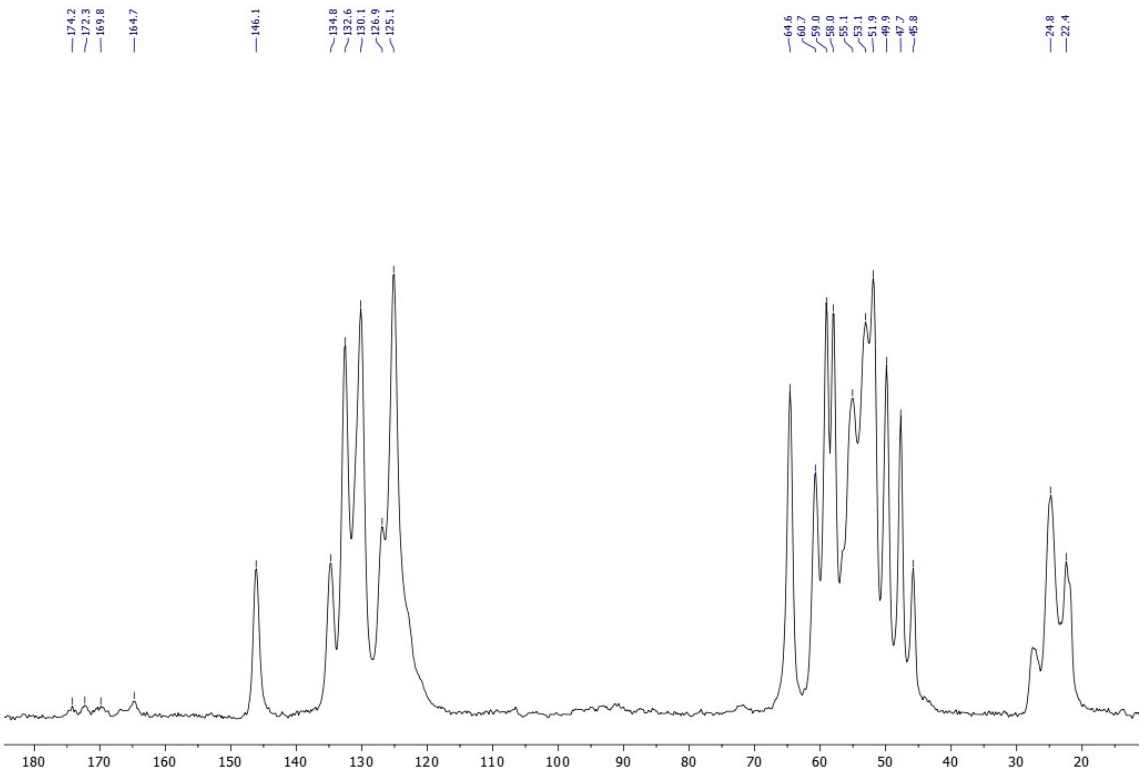

Figure S10: ^{13}C CP MAS TOSS spectrum of **7**.

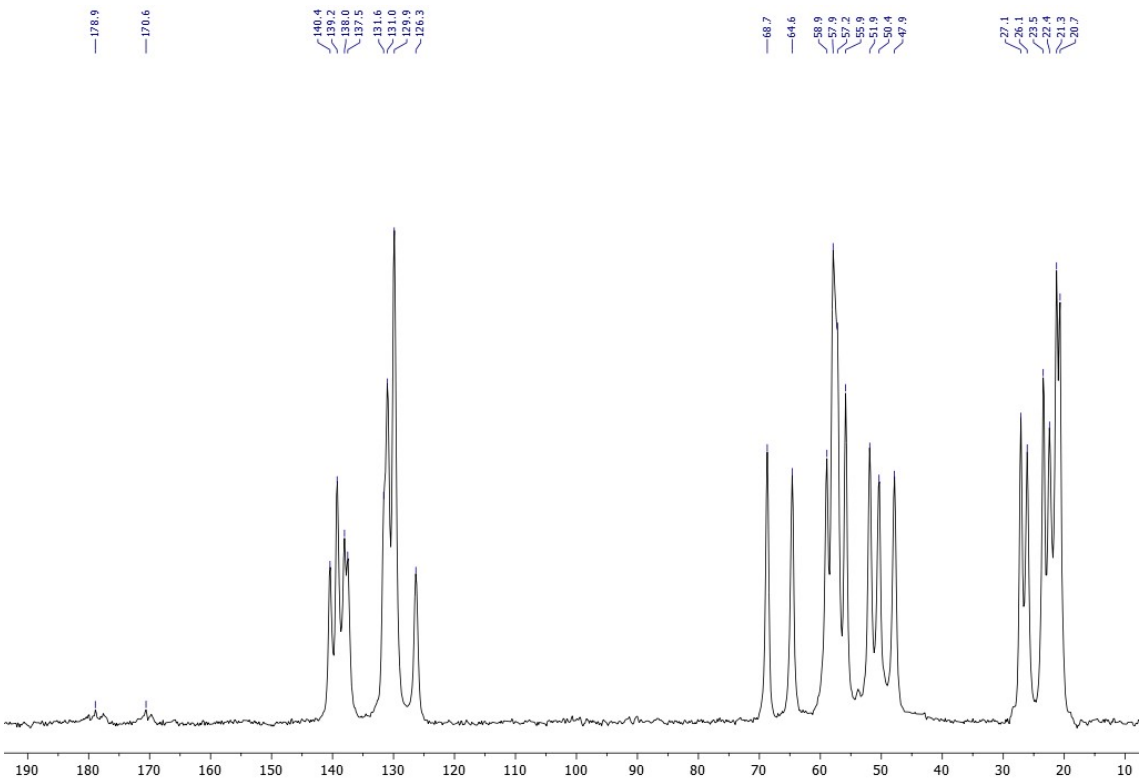

Figure S11: ^{13}C CP MAS TOSS spectrum of **8**.

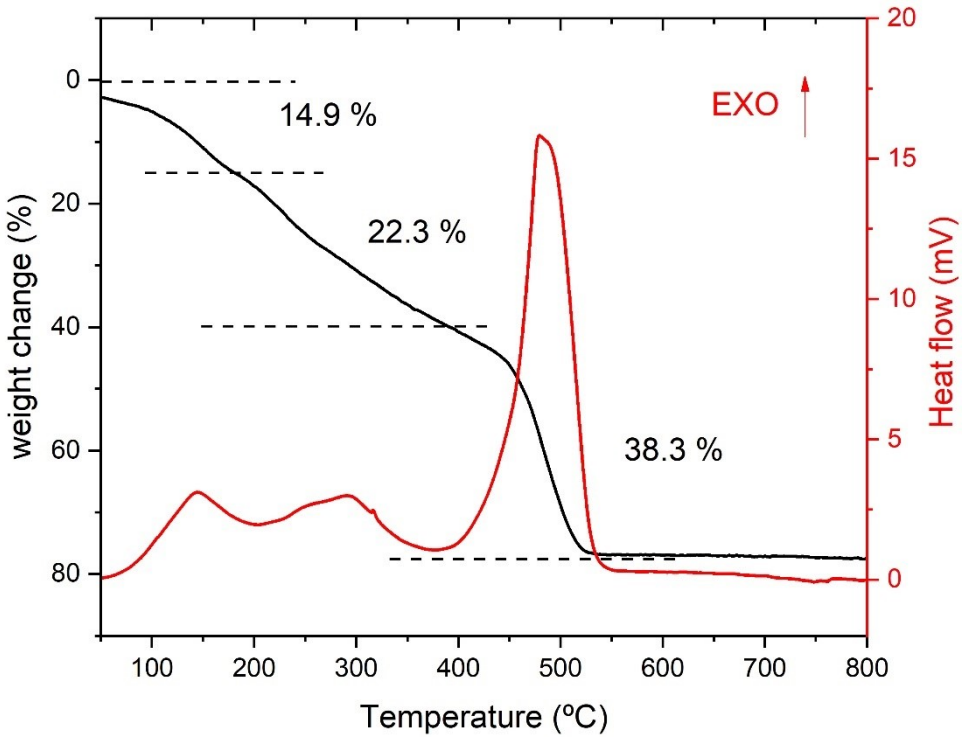

Figure S12: TG-DSC curves of **5**.

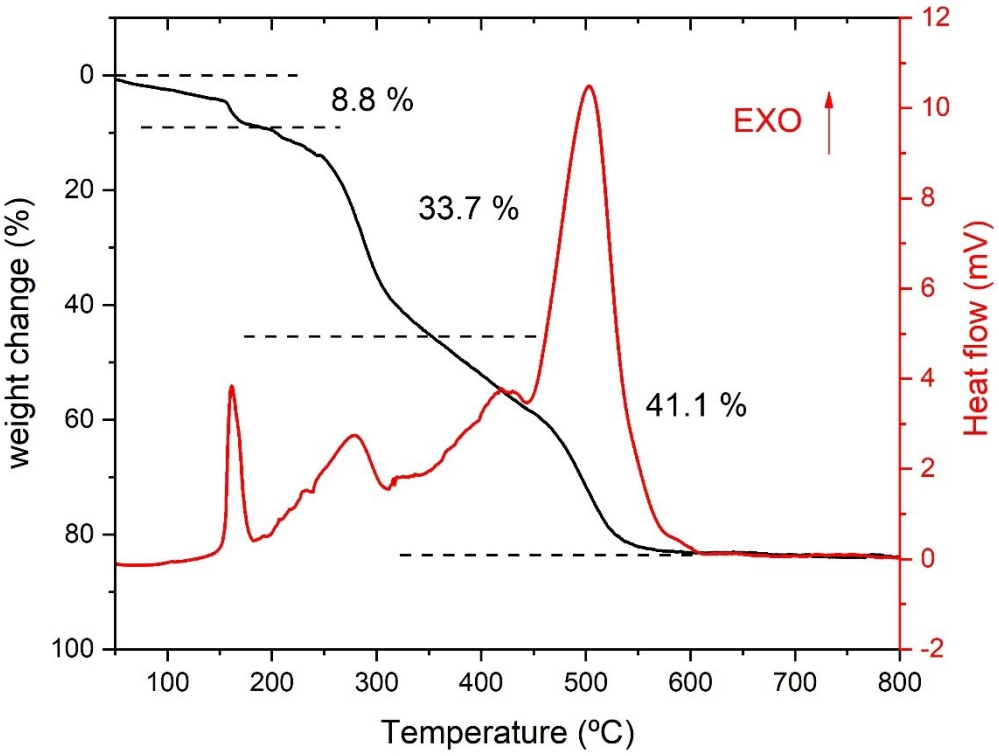

Figure S13: TG-DSC curves of **6**.

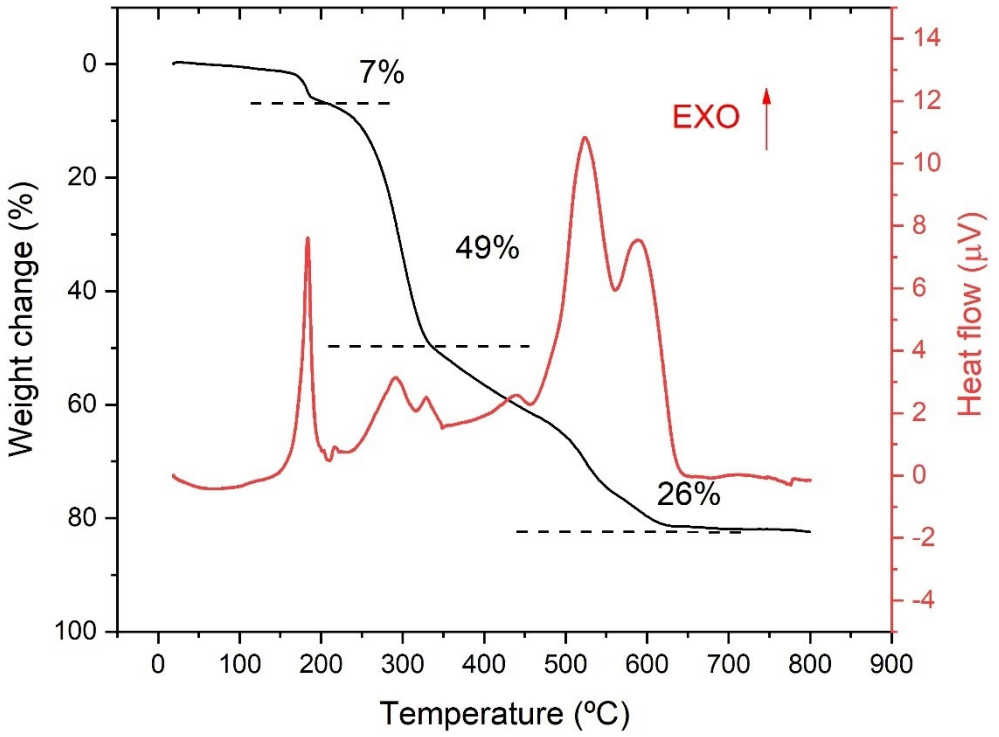

Figure S14: TG-DSC curves of **7**.

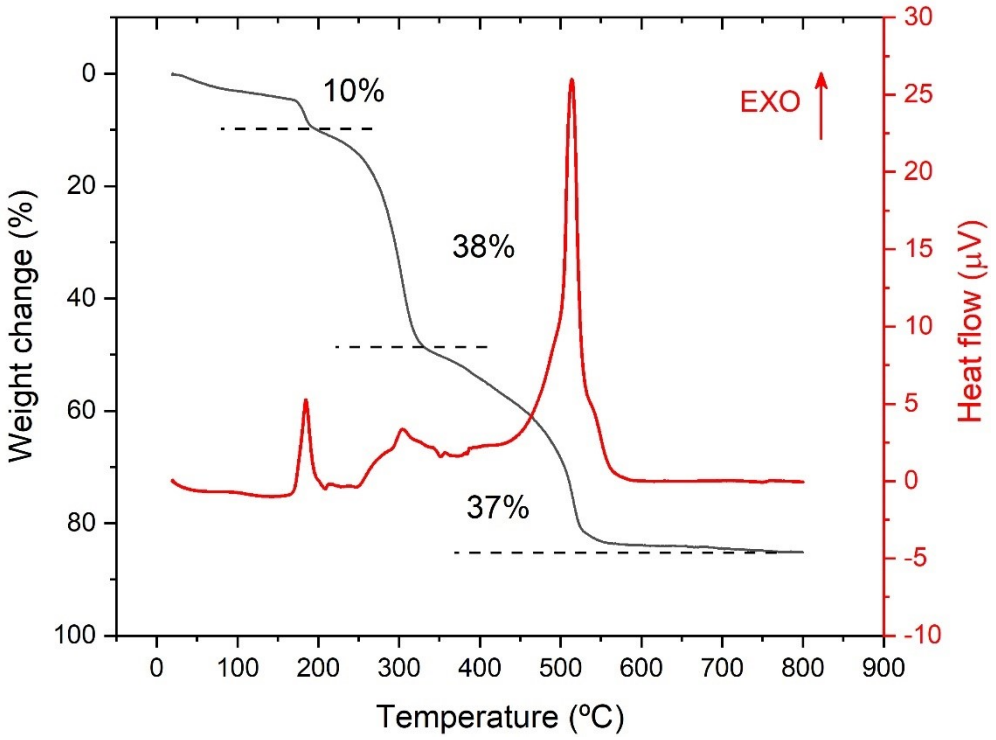

Figure S15: TG-DSC curves of **8**.

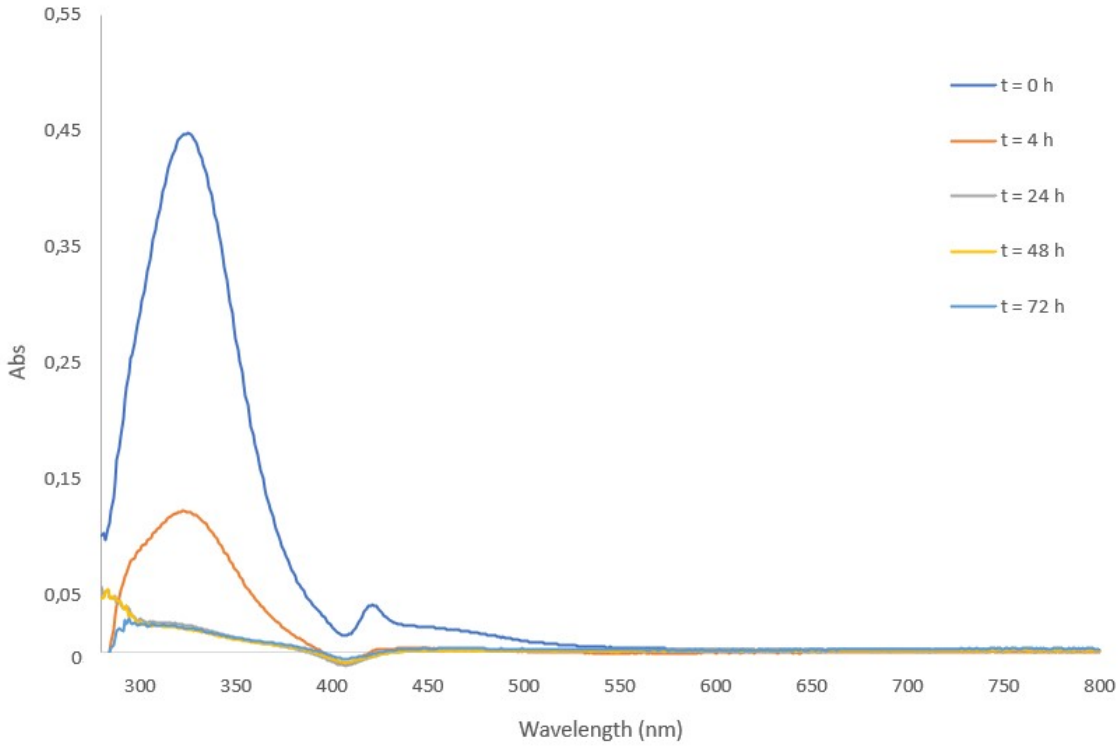

Figure S16: UV-Vis spectrum of **5** in DMEM supplemented with 10% FBS at t = 0, 4, 24, 48 and 72h.

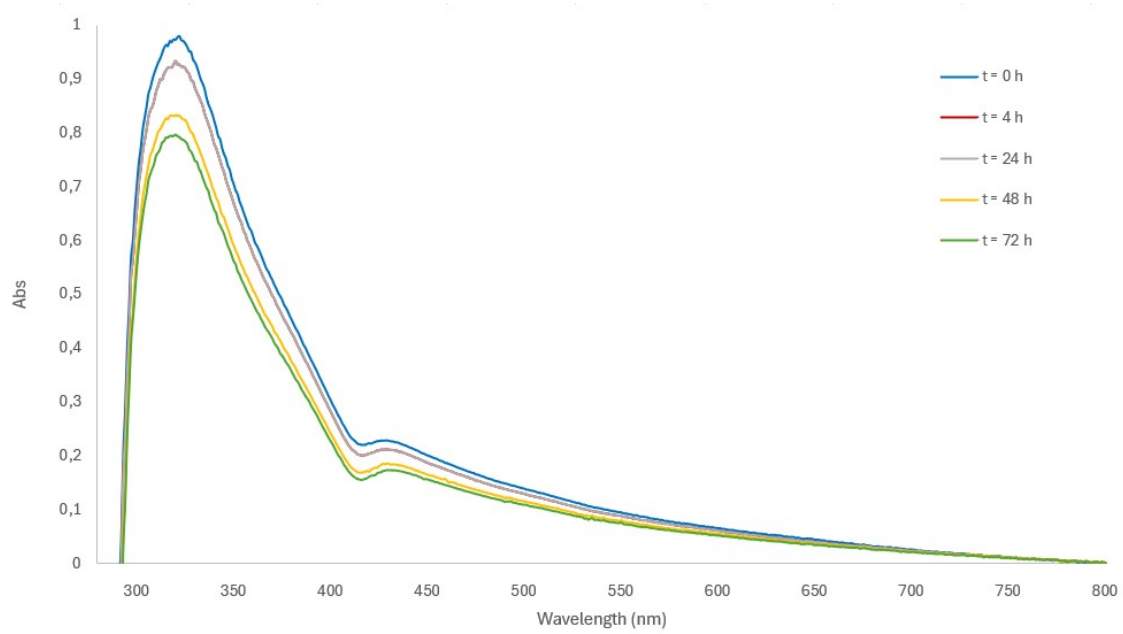

Figure S17: UV-Vis spectrum of **6** in DMEM supplemented with 10% FBS at t = 0, 4, 24, 48 and 72h..

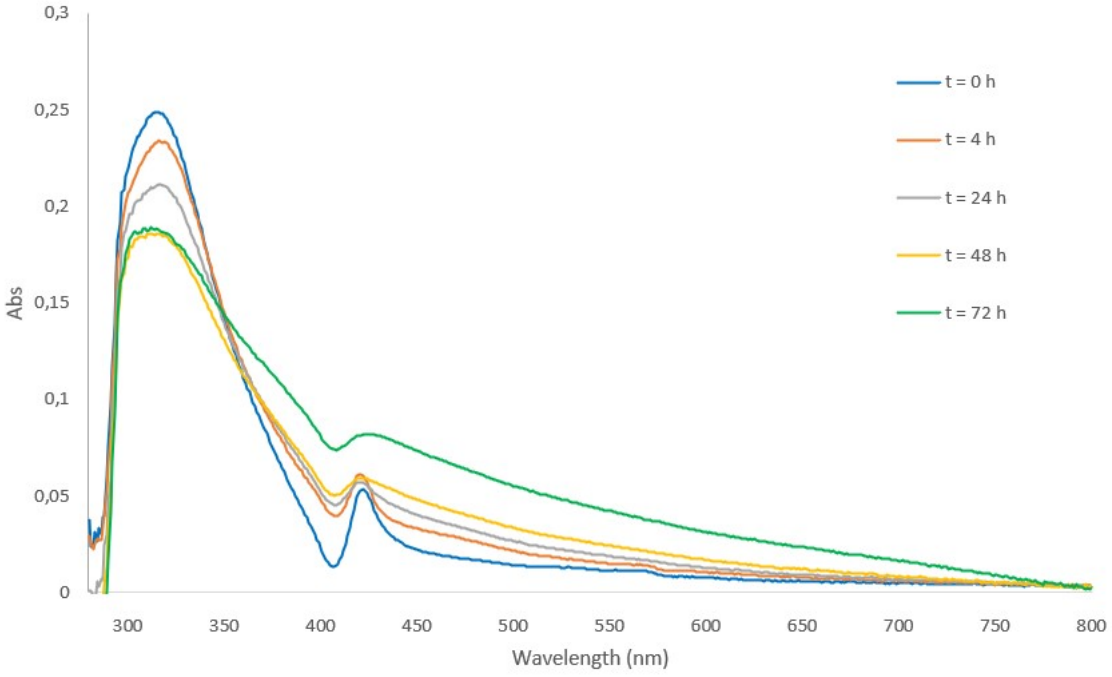

Figure S18: UV-Vis spectrum of **7** in DMEM supplemented with 10% FBS at t = 0, 4, 24, 48 and 72h.

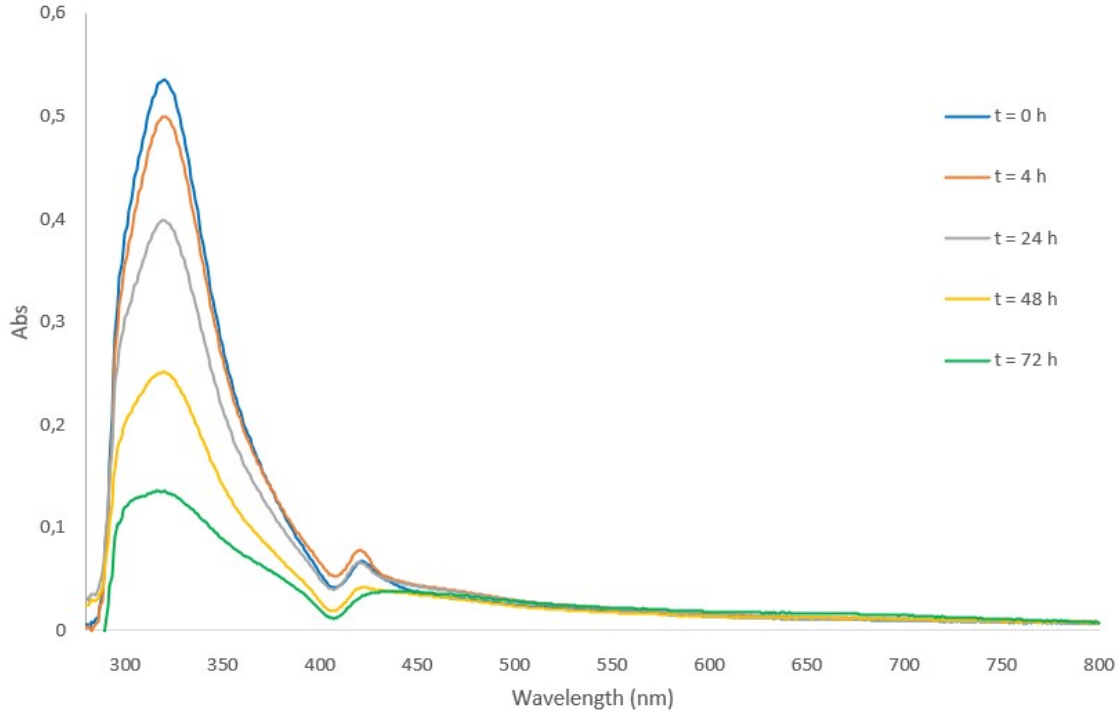

Figure S19: UV-Vis spectrum of **8** in DMEM supplemented with 10% FBS at t = 0, 4, 24, 48 and 72h.

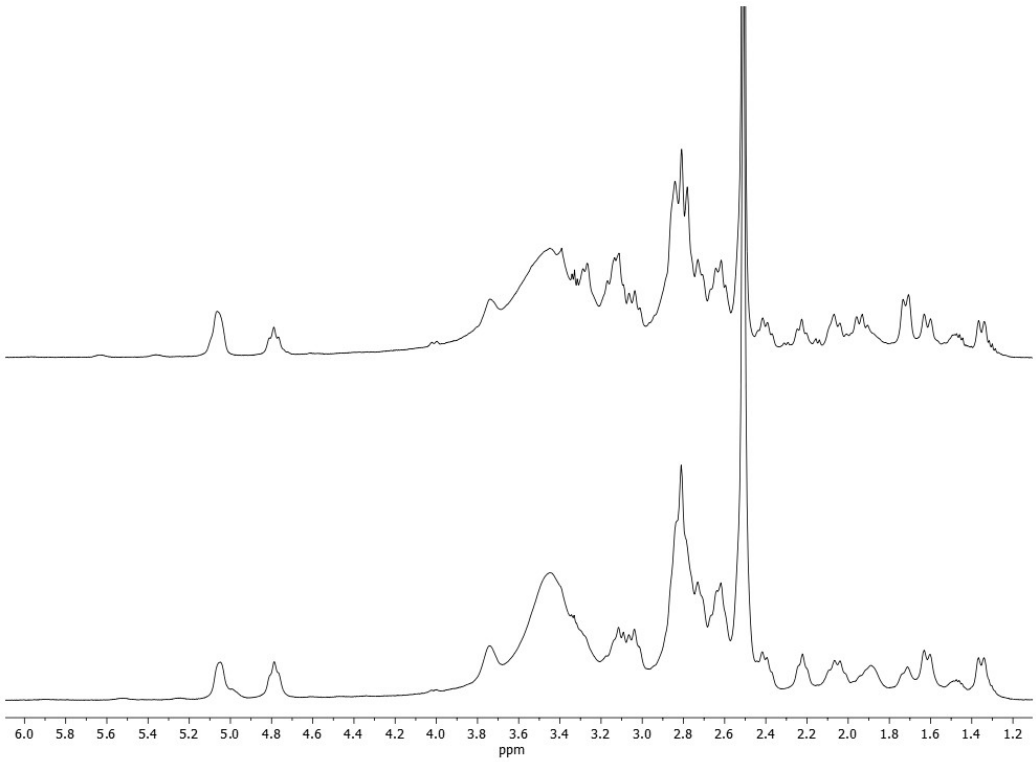

Figure S20: ^{1}H NMR spectrum of **5** initially (bottom) and after 6 days (top) in DMSO-d_6.

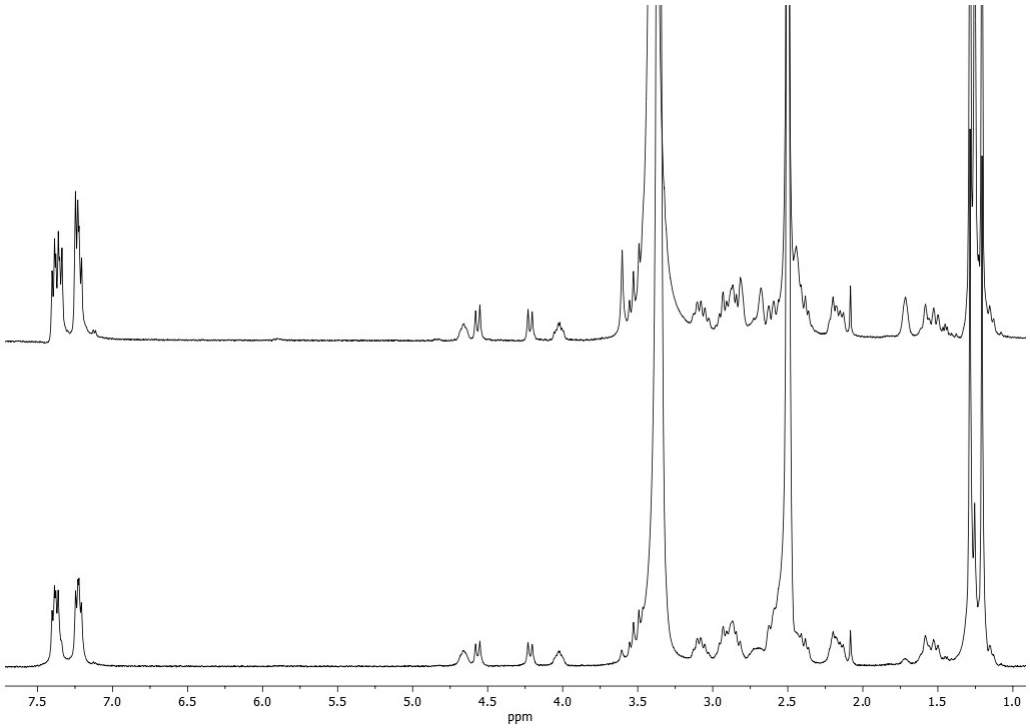

Figure S21: ^{1}H NMR spectrum of **6** initially (bottom) and after 6 days (top) in DMSO-d_6.

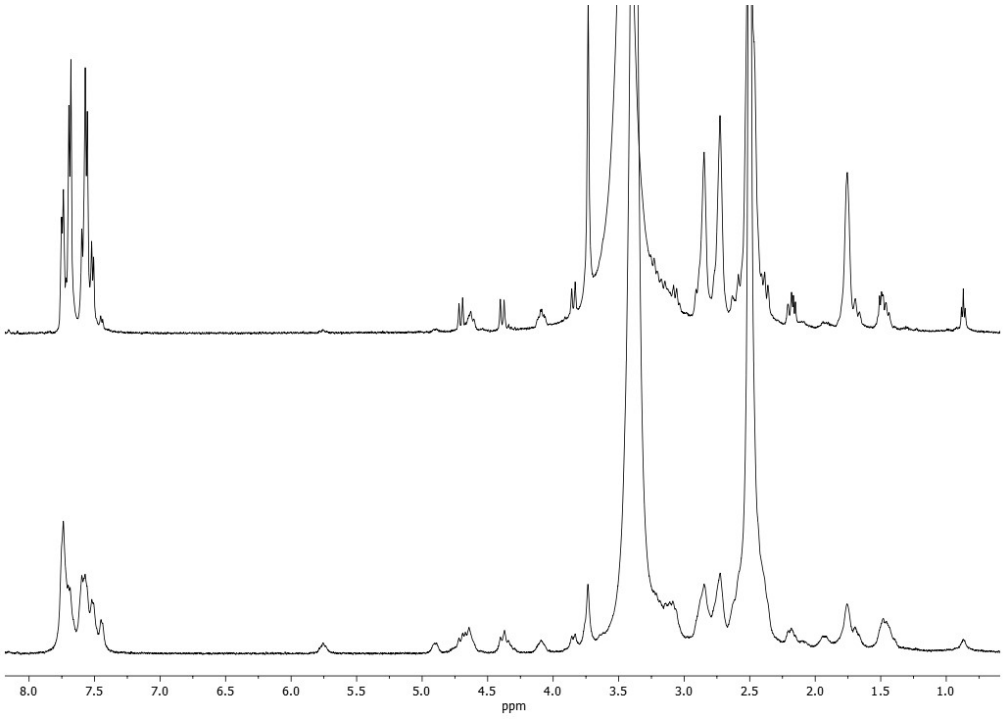

Figure S22: ^{1}H NMR spectrum of **7** initially (bottom) and after 6 days (top) in DMSO-d_6.

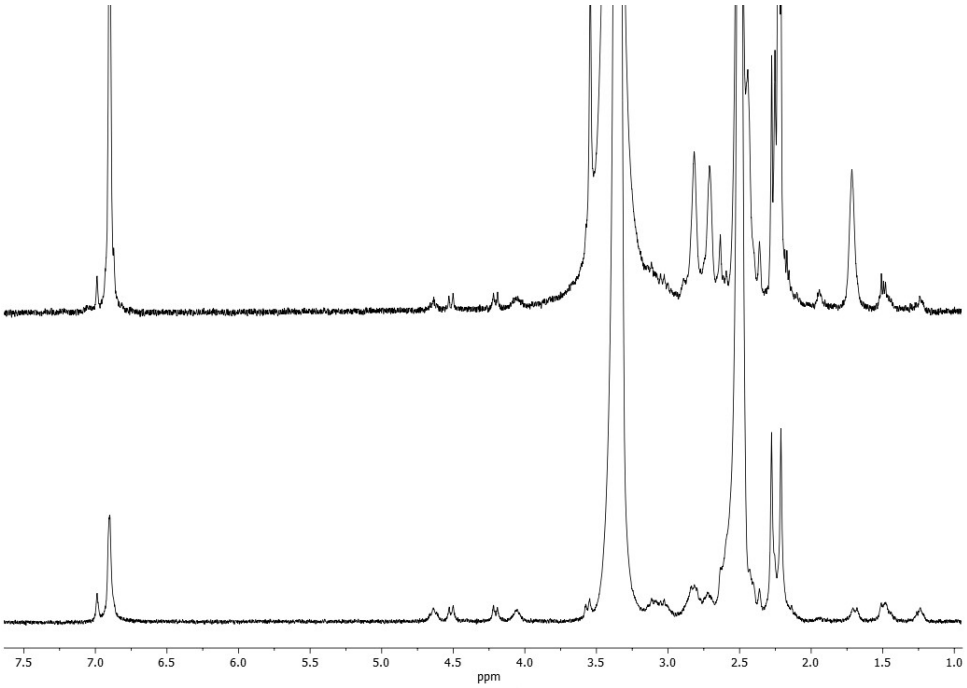

Figure S23: ^{1}H NMR spectrum of **8** initially (bottom) and after 6 days (top) in DMSO-d_6.