Article

Curcumin-based β-diketo ligands for Ga^{3+}: on the way to develop new antineoplastic agents

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Figure S1.

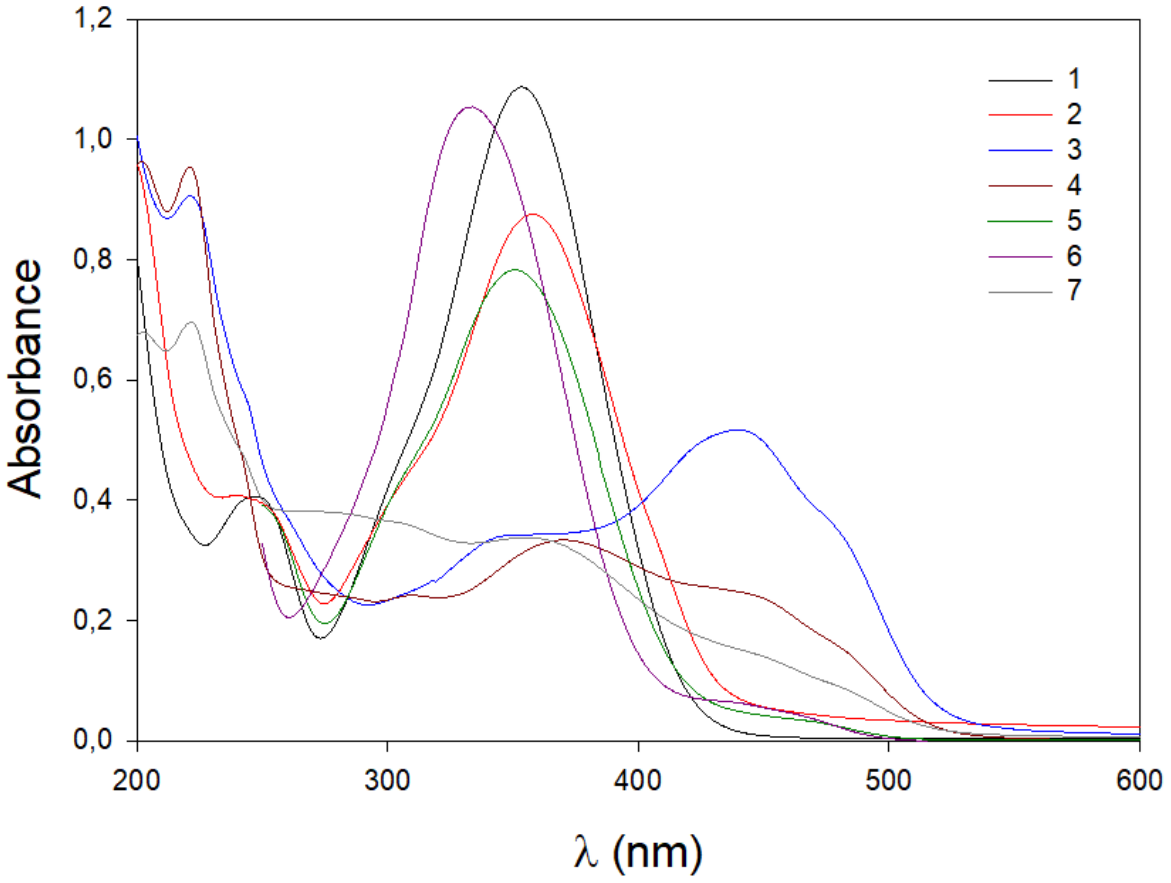

Figure S1. UV-Vis spectra of the investigated compounds at 25°C in aqueous solution ([L] = 50 μM, [$NaNO_3$] = 0.1 M, 298 K).

Figure S2.

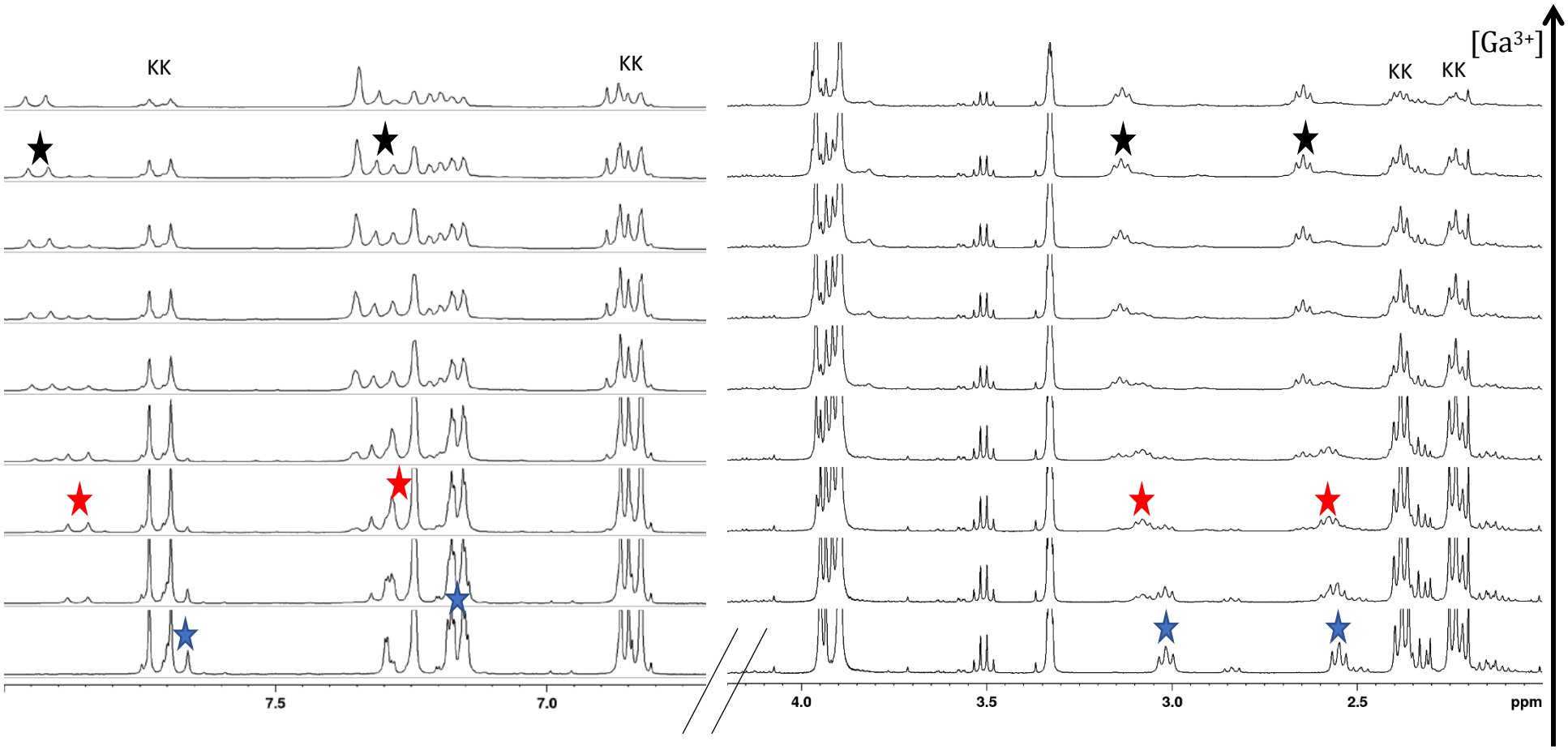

Figure S2. ^{1}H NMR spectra of compound **7** in MeOD-*d*$_4$ at 298K (@600 MHz) at increasing addition of Ga^{3+} MeOD-*d*$_4$ solution up to the metal-to-ligand 1:1.5 molar ratio. Stars highlights resonances of protons H-3, H-4, H-11 and H-12 in the free ligand (blue), M:L 1:2 complex (red) and M:L 1:1 complex (black). Analogous resonances for the di-keto form are labelled with KK and are unaffected by metal addition.

Figure S3.

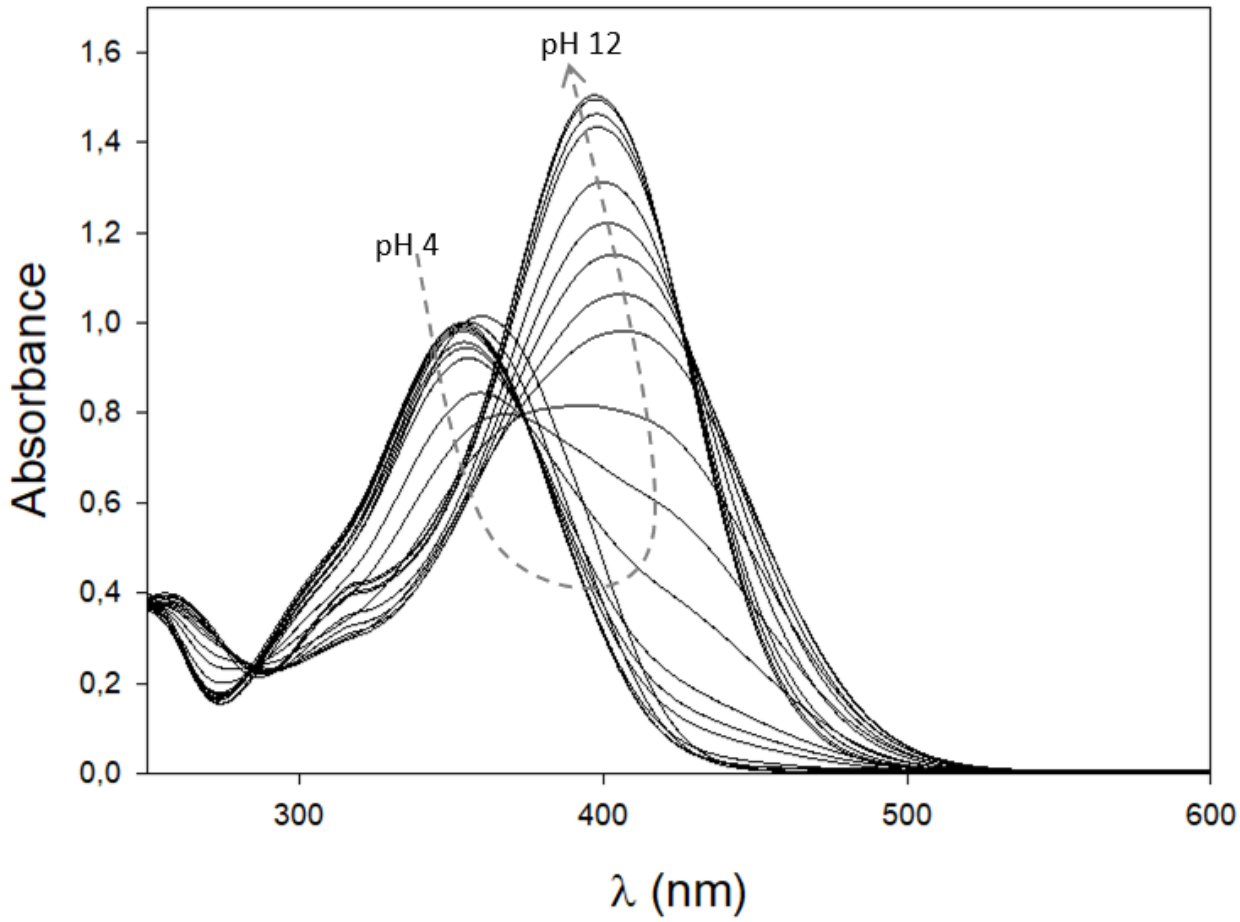

Figure S3. pH-metric spectrophotometric titration of Ga^{3+}:1 1:1 system in aqueous solution ([L] = 50μM; [$NaNO_3$] = 0.1 M, 298 K).

Figure S4.

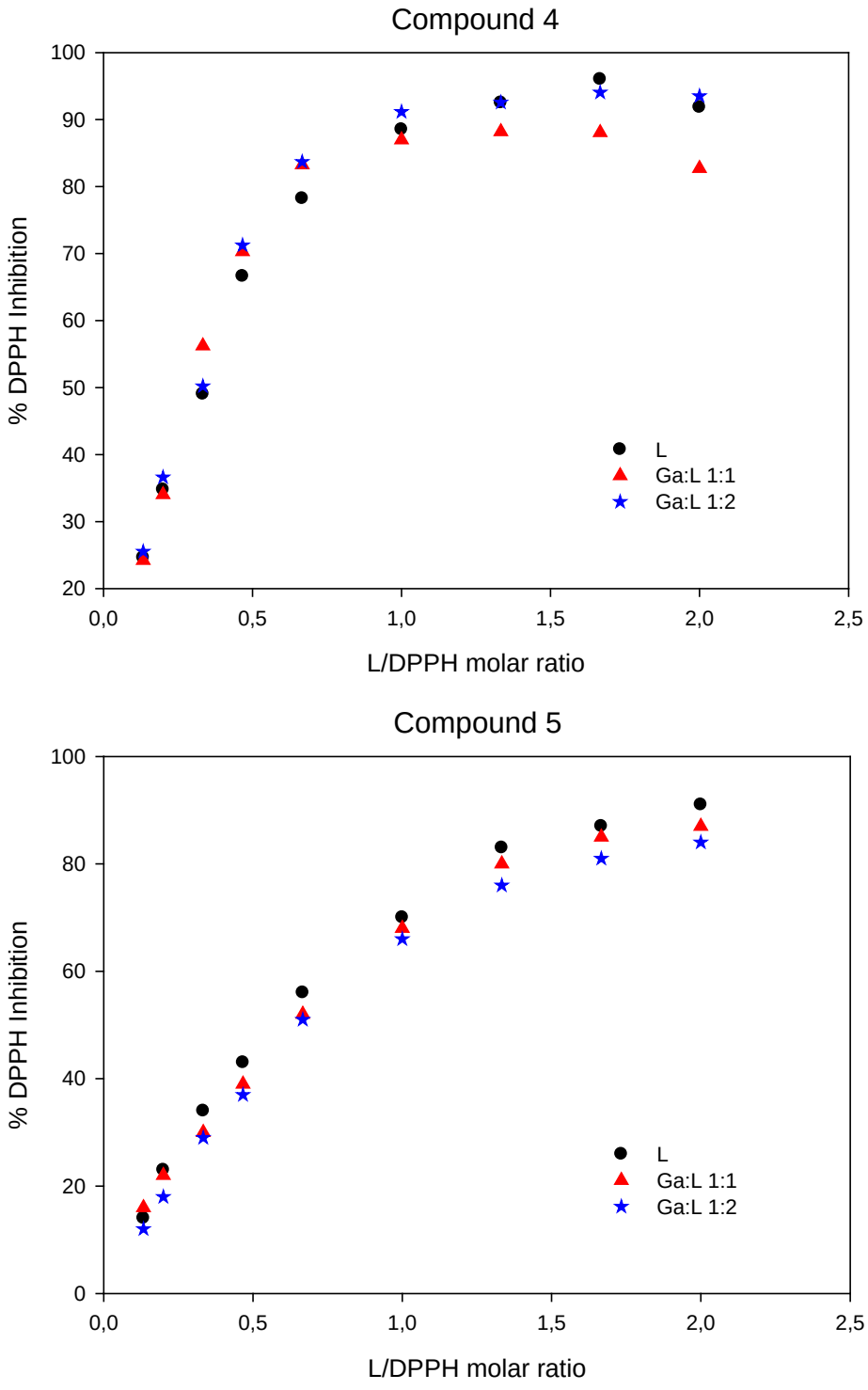

Figure S4. Radical scavenging ability of derivatives **4** and **5** together with their Ga^{3+} metal complexes. Percentage of inhibition of free DPPH radical ([$DPPH^{\cdot}$] = 60 μM) in the presence of the compound (free ligand (L) and gallium complexes) at increasing concentration. Compound concentration is expressed as molar ratio (L/DPPH).

Table S1. Liquid chromatography/mass spectrometry (LC/MS) results (*m*/*z*) for Gallium(III) complexes.

Compound	Formula	$[M+H]^+$
1	$[Ga(C_{13}H_{13}O_4)_2]^+$	536.11
2	$[Ga(C_{16}H_{18}BrO_4)_2]^+$	776.02
3	$[Ga(C_{29}H_{22}NO_6)_2]^+$	1046.30
4	$[Ga(C_{32}H_{28}NO_8)_2]^+$	1178.35
5	$[Ga(C_{30}H_{24}NO_6)_2]^+$	1058.29
6	$[GaC_{23}H_{22}O_6]^+$	448.09
7	$[GaC_{25}H_{26}O_8]^+$	524.12