



Homo- and Heteroleptic Cd(II) 4-Phenylbutyrates, Synthesis, Exploration of Chemistry, DNA Binding Study and Antileishmanial Activity

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Table S1: Physical data of ligand and its synthesized complexes.

Code	Compound	Mol. Formula	Mol. Wt (g/mol)	M.P (°C)	Yield (%)
4-PBA	4-Phenylbutyric acid	C ₁₀ H ₁₂ O ₂	164.08	49-51	-
4-PB1	[Cd(4-PBA) ₂]	C ₂₀ H ₂₂ CdO ₄	438.80	250-253	67
4-PBB	[Cd(4-PBA) ₂ BPY]	C ₃₀ H ₃₀ CdN ₂ O ₄	596.12	123-125	73
4-PBP	[Cd(4-PBA) ₂ PHEN]	C ₃₂ H ₃₀ CdN ₂ O ₄	620.12	179-180	85
4-PBD	[Cd(4-PBA) ₂ (Me ₂ PHEN)]	C ₃₄ H ₃₄ CdN ₂ O ₄	647.07	156-158	83

Table S2: FT-IR data of ligand and its synthesized complexes.

Code	Compound	-OH	C=O/C-O		Δν	Cd-O	Cd-N	C-H
4-PBA	4-Phenylbutyric acid	3340-2500	1685/1292		-	-	-	-
			COO ⁻ _{asymm}	COO ⁻ _{symm}				
4-PB1	[Cd(4-PBA) ₂]	-	1546	1398	148	462	524	-
4-PBB	[Cd(4-PBA) ₂ BPY]	-	1550	1407	143	420	533	763, 722
4-PBP	[Cd(4-PBA) ₂ PHEN]	-	1554	1409	145	427	566	849, 728
4-PBD	[Cd(4-PBA) ₂ (Me ₂ PHEN)]	-	1548	1410	138	418	550	859, 731

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Table S3: CV Data indicating binding parameters with DNA.

Code	Before DNA			After DNA			Change in E		Remarks
	E _a	E _c	E _a '	E _c '	E _a	E _c	ΔE _a	ΔE _c	
4-PB1	-0.3803	-0.6696	-0.2219	-0.6041	0.1584	0.0655			Positive shift
	-0.9700	-1.4197	-1.0405	-1.3277	-0.0705	0.092			Positive shift
	-	-2.057	-	-1.9562	-	0.1008			Positive shift
4-PBB	0.4271	-	Disappear	-	Disappear	-			-
	-0.4812	-0.6473	Disappear	-0.5992	-	0.0481			Positive shift
	-	-1.661	-	-1.614	-	0.047			Positive shift
4-PBP	-1.778	-2.204	-1.693	-2.176	0.085	0.028			Positive and Negative shift
	-1.6036	-	Disappear	-	Disappear	-			New peak
	0.3985		Disappear						-
4-PBD	-0.5605	-0.6742	-	-0.6600	-	0.0142			Positive shift
	-1.095	-	disappear	-	Disappear	-			-
	-1.286	-1.488	-1.13040	-1.6031	0.1556	-0.1151			Positive and negative shift
4-PBD	-1.855	-1.8905	-1.7984	-1.9592	0.0566	-0.0687			Positive and negative shift
	-	-0.640	-	-0.614	-	0.026			Positive shift
	-1.859	-	-1.768	-	0.091	-			Positive shift
	-1.255	-1.732	-1.244	-1.671	0.011	0.061			Positive and Negative shift