



Cd(II) Derivatives of Substituted Phenylacetic Acids, Synthesis, Spectroscopic Characterization and Binding Studies with DNA

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Table S1. The FT-IR data (cm⁻¹) of ligands and Cd(II) carboxylates.

Code	Compound	-OH	C=O/C-O		Δν	Cd-O	Cd-N	C-H
MeOPhA	2-methoxy phenylacetic acid	3400-2600	1682/1297					
			COO _{asymm}	COO _{symm}				
MeOPhA1	Cd(MeOPhA) ₂	-	1582	1410	172	526		
MeOPhA2	Cd(MeOPhA) ₂ (bipy)	-	1560	1386	174	490	590	734
MeOPhA3	Cd(MeOPhA) ₂ (phen)	-	1570	1390	180	507	607	856
ClPhA	2,4-dichlorophenyl acetic acid	3300-2400	1733/1290		-	-	-	-
ClPhA1	Cd(ClPhA) ₂	-	1611	1422	189	460		
ClPhA2	Cd(ClPhA) ₂ (bipy)	-	1613	1419	194	475	556	752
ClPhA3	Cd(ClPhA) ₂ (phen)	-	1611	1422	189	461	584	872

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Table S2. ¹H-NMR data in ppm of o-methoxyphenylacetic acid and synthesized complexes.

Proton	MeOPhA	MeOPhA1	MeOPhA2		MeOPhA3	
-OH	11.0	-	-		-	
-CH ₂	3.49	3.20 s	3.22 s		3.69 br	
-OCH ₃	3.73	3.70 br	3.70 s		3.69 br	
H3	6.65	6.77-6.86 m	6.77-6.86 m		6.76-6.86 m	
H4	6.96	7.06-7.66 m	7.06-7.15 m		7.06-7.14 m	
H5	6.70	6.77-6.86 m	6.77-6.86 m		6.76-6.86 m	
H6	6.95	7.09-7.15 m	7.06-7.15 m		7.06-7.14 m	
			Bipy (free)	Bipy (bound)	Phen (free)	Phen (bound)
H α	-	-	8.59	8.68-8.69 d J=4.8	8.81	9.08-9.10 dd <i>J</i> = 1.5 Hz, 4.2 Hz
H β	-	-	7.12	7.44-7.47 m	7.26	7.79-7.83 m
H γ	-	-	7.66	7.92-7.98 m	8.00	8.52-8.55 dd <i>J</i> = 1.5 Hz, 8.1 Hz
H δ	-	-	8.50	8.37-8.39 <i>J</i> = 8.1 Hz	-	-
H ϵ			-		7.55	8.02 s

Table S3. ¹H-NMR data in ppm of 2,4-chlorophenoxyacetic acid and synthesized complexes.

Proton	ClPhA	ClPhA1	ClPhA2		ClPhA3	
-OH	11.0	-	-		-	
-OCH ₂	4.88	4.28 s	4.25 s		4.29 s	
H3	7.17	7.47 s	7.43-7.48 m		7.45-7.46 d	
					<i>J</i> = 2.4 Hz	
H5	7.04	7.24-7.27 d	7.23-7.27 dd		7.21-7.25 dd	
		<i>J</i> = 9 Hz	<i>J</i> = 2.7 Hz, 9 Hz		<i>J</i> = 2.4 Hz, 9 Hz	
H6	6.65	6.84-6.87 d	6.83-6.86 d		6.85 -6.88	
		<i>J</i> = 9 Hz	<i>J</i> = 9 Hz		<i>J</i> = 9 Hz	
			Bipy (free)	Bipy (bound)	Phen (free)	Phen (bound)
H α	-	-	8.81	8.68-8.69 d	8.59	9.08-9.10 dd
				<i>J</i> = 3.9 Hz		<i>J</i> = 1.5 Hz, 2.7 Hz
H β	-	-	7.26	7.43-7.48 m	7.12	7.80-7.84 dd
						<i>J</i> = 4.2 Hz, 8.1 Hz
H γ	-	-	8.00	7.92-7.98 td	7.66	8.55-8.58 dd
				<i>J</i> = 1.8 Hz, 7.8 Hz		<i>J</i> = 1.5 Hz, 8.1 Hz)
H δ	-	-	7.55	8.37-8.40 d	-	-
				<i>J</i> = 7.8 Hz		
H ϵ					8.50	8.03 s

Table S4. ^{13}C -NMR data in ppm of o-methoxyphenylacetic acid (MeOPhA) and synthesized complexes.

Carbon	MeOPhA	MeOPhA1	MeOPhA2		MeOPhA3	
C=O	172.3	175.4	175.7		175.4	
-CH ₂	38.3	39.0	39.1		39.0	
-OCH ₃	55.1	55.6	55.6		55.5	
C1	124.1	126.7	124.7		126.7	
C2	159.1	157.5	149.7		150.5	
C3	114.7	110.6	110.6		110.6	
C4	128.6	128.6	126.8		127.1	
C5	121.5	120.1	120.1		120.1	
C6	130.8	131.2	128.4		128.5	
			Bipy (free)	Bipy (bound)	Phen (free)	Phen (bound)
C α	-	-	149.3	157.5	150.0	157.5
C β	-	-	121.0	120.9	121.5	124
C γ	-	-	137.2	131.1	136.4	131.1
C δ	-	-	123	137.8	129.1	137
C ϵ	-	-	155.4	157.5	127.5	128.9
C ζ	-	-			144.5	157.5

Table S5. ^{13}C -NMR data in ppm of 2,4-chlorophenoxyacetic acid (CIPhA) and synthesized complexes.

Carbon	CIPhA	CIPhA1	CIPhA2		CIPhA3	
C=O	167.0	170.7	170.3		171.1	
-OCH ₂	67.1	68.7	68.9		68.8	
C1	152.8	154.0	154.0		154.0	
C2	124.0	129.2	137.8		137.3	
C3	131.4	123.6	124.6		127.9	
C4	128.0	127.9	129.1		128.9	
C5	128.0	122.2	123.4		123.6	
C6	117.1	115.4	115.5		115.5	
			Bipy (free)	Bipy (bound)	Phen (free)	Phen (bound)
Cα	-	-	149.3	149.7	150.0	150.7
Cβ	-	-	121.0	120.8	121.5	122.5
Cγ	-	-	137.2	122.1	136.4	129.2
Cδ	-	-	123.0	127.9	129.1	128.9
Cε	-	-	155.4	149.7	127.5	124.1
Cζ	-	-			144.5	145.6