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Supplementary Data

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. [1]H-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)**
Hα	-	-	8.59	8.68-8.69 d J=4.8	8.81	9.08-9.10 dd
						J = 1.5 Hz, 4.2 Hz
Hβ	-	-	7.12	7.44-7.47 m	7.26	7.79-7.83 m
Hγ	-	-	7.66	7.92-7.98 m	8.00	8.52-8.55 dd
						J = 1.5 Hz, 8.1 Hz
Hδ	-	-	8.50	8.37-8.39	-	-
				J =8.1Hz		
Hε			-		7.55	8.02 s

Table S3. [1]H-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	
						J = 2.4 Hz
H5	7.04	7.24-7.27 d	7.23-7.27 dd		7.21-7.25 dd	
		J=9Hz	*J* = 2.7 Hz, 9Hz		*J* = 2.4 Hz, 9 Hz	
H6	6.65	6.84-6.87 d	6.83-6.86 d		6.85 -6.88	
		J=9Hz	*J* = 9 Hz		*J* = 9 Hz	
			Bipy (free)	**Bipy (bound)**	**Phen (free)**	**Phen (bound)**
Hα	-	-	8.81	8.68-8.69 d	8.59	9.08-9.10 dd
				J=3.9 Hz		J = 1.5 Hz, 2.7 Hz
Hβ	-	-	7.26	7.43-7.48 m	7.12	7.80-7.84 dd
						J= 4.2 Hz, 8.1 Hz
Hγ	-	-	8.00	7.92-7.98 td	7.66	8.55-8.58 dd
				J = 1.8 Hz, 7.8 Hz		J = 1.5 Hz, 8.1 Hz)
Hδ	-	-	7.55	8.37-8.40 d	-	-
				J = 7.8 Hz		
Hε					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)**
Cα	-	-	149.3	157.5	150.0	157.5
Cβ	-	-	121.0	120.9	121.5	124
Cγ	-	-	137.2	131.1	136.4	131.1
Cδ	-	-	123	137.8	129.1	137
Cε	-	-	155.4	157.5	127.5	128.9
Cζ	-	-			144.5	157.5

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

Carbon	ClPhA	ClPhA1	ClPhA2		ClPhA3	
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