



## 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<sup>-1</sup>) of ligands and Cd(II) carboxylates.

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

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**Table S2.** <sup>1</sup>H-NMR data in ppm of o-methoxyphenylacetic acid and synthesized complexes.

| Proton            | MeOPhA | MeOPhA1     | MeOPhA2     |                              | MeOPhA3     |                                           |
|-------------------|--------|-------------|-------------|------------------------------|-------------|-------------------------------------------|
| -OH               | 11.0   | -           | -           |                              | -           |                                           |
| -CH <sub>2</sub>  | 3.49   | 3.20 s      | 3.22 s      |                              | 3.69 br     |                                           |
| -OCH <sub>3</sub> | 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 <sub>α</sub>    | -      | -           | 8.59        | 8.68-8.69 d J=4.8            | 8.81        | 9.08-9.10 dd<br><i>J</i> = 1.5 Hz, 4.2 Hz |
| H <sub>β</sub>    | -      | -           | 7.12        | 7.44-7.47 m                  | 7.26        | 7.79-7.83 m                               |
| H <sub>γ</sub>    | -      | -           | 7.66        | 7.92-7.98 m                  | 8.00        | 8.52-8.55 dd<br><i>J</i> = 1.5 Hz, 8.1 Hz |
| H <sub>δ</sub>    | -      | -           | 8.50        | 8.37-8.39<br><i>J</i> =8.1Hz | -           | -                                         |
| H <sub>ε</sub>    | -      | -           | -           | -                            | 7.55        | 8.02 s                                    |

**Table S3.** <sup>1</sup>H-NMR data in ppm of 2,4-chlorophenoxyacetic acid and synthesized complexes.

| Proton            | ClPhA | ClPhA1        | ClPhA2                 |                           | ClPhA3                  |                            |
|-------------------|-------|---------------|------------------------|---------------------------|-------------------------|----------------------------|
| -OH               | 11.0  | -             | -                      |                           | -                       |                            |
| -OCH <sub>2</sub> | 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> =9Hz | <i>J</i> = 2.7 Hz, 9Hz |                           | <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> =9Hz | <i>J</i> = 9 Hz        |                           | <i>J</i> = 9 Hz         |                            |
|                   |       |               | Bipy (free)            | Bipy (bound)              | Phen (free)             | Phen (bound)               |
| H <sub>α</sub>    | -     | -             | 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 <sub>β</sub>    | -     | -             | 7.26                   | 7.43-7.48 m               | 7.12                    | 7.80-7.84 dd               |
|                   |       |               |                        |                           |                         | <i>J</i> = 4.2 Hz, 8.1 Hz  |
| H <sub>γ</sub>    | -     | -             | 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 <sub>δ</sub>    | -     | -             | 7.55                   | 8.37-8.40 d               | -                       | -                          |
|                   |       |               |                        | <i>J</i> = 7.8 Hz         |                         |                            |
| H <sub>ε</sub>    | -     | -             | -                      | -                         | 8.50                    | 8.03 s                     |

**Table S4.**  $^{13}\text{C}$ -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 <sub>2</sub>  | 38.3   | 39.0    | 39.1               | 39.0                |                    |                     |
| -OCH <sub>3</sub> | 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               |                    |                     |
|                   |        |         | <b>Bipy (free)</b> | <b>Bipy (bound)</b> | <b>Phen (free)</b> | <b>Phen (bound)</b> |
| C $\alpha$        | -      | -       | 149.3              | 157.5               | 150.0              | 157.5               |
| C $\beta$         | -      | -       | 121.0              | 120.9               | 121.5              | 124                 |
| C $\gamma$        | -      | -       | 137.2              | 131.1               | 136.4              | 131.1               |
| C $\delta$        | -      | -       | 123                | 137.8               | 129.1              | 137                 |
| C $\epsilon$      | -      | -       | 155.4              | 157.5               | 127.5              | 128.9               |
| C $\zeta$         | -      | -       |                    |                     | 144.5              | 157.5               |

**Table S5.**  $^{13}\text{C}$ -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 <sub>2</sub> | 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) |
| C $\alpha$        | -     | -      | 149.3       | 149.7        | 150.0       | 150.7        |
| C $\beta$         | -     | -      | 121.0       | 120.8        | 121.5       | 122.5        |
| C $\gamma$        | -     | -      | 137.2       | 122.1        | 136.4       | 129.2        |
| C $\delta$        | -     | -      | 123.0       | 127.9        | 129.1       | 128.9        |
| C $\epsilon$      | -     | -      | 155.4       | 149.7        | 127.5       | 124.1        |
| C $\zeta$         | -     | -      |             |              | 144.5       | 145.6        |