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# Solvent Effects on Chelate Cooperativity

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## Data analysis for complexes that show additional equilibria

**Table S1** Binding constant for selected complexes fitted to 1:1 and 1:1 plus 2:5 binding isotherms in TCE at 298K.

| | | 1:1 fit | | 1:1 plus 5:2 fit | | |
|---|---|---|---|---|---|---|
| | | $K_{1:1}/M^{-1}$ | R factor | $K_{1:1}/M^{-1}$ | $K_{2:5}/M^{-6}$ | R factor |
| **P1a** | **L1a** | $2.1x10^{3}$ | 4.4 | $4.6x10^{3}$ | $2.4x10^{17}$ | 7.7 |
| **P3a** | **L1a** | $2.4x10^{3}$ | 2.4 | $2.4x10^{3}$ | $2.6x10^{15}$ | 2.5 |
| **P4a** | **L1a** | $1.5x10^{3}$ | 5.3 | $1.6x10^{3}$ | $6.1x10^{15}$ | 5.5 |
| **P4a** | **L2a** | $2.2x10^{3}$ | 6.4 | $2.8x10^{3}$ | $4.0x10^{16}$ | 10 |
| **P2a** | **L5a** | $1.2x10^{4}$ | 6.1 | $1.2x10^{4}$ | $1.1x10^{20}$ | 6.0 |
| **P3a** | **L5a** | $1.8x10^{4}$ | 4.8 | $2.1x10^{4}$ | $1.1x10^{22}$ | 4.6 |
| **P4a** | **L5a** | $1.8x10^{4}$ | 6.2 | $1.9x10^{4}$ | $9.9x10^{18}$ | 6.4 |

## Partially Bound States Analysis

**One H-bond.** For complexes that can make a single intramolecular H-bond, the observed association constant is given by the sum of the equilibrium constants for the fully bound and partially bound states (Equation S1).

$$K_{obs} = K_0(1 + \sigma_1 K_1 EM_1) \quad \text{(S1)}$$

where $K_0$ is intermolecular association constant for formation of the zinc-nitrogen interaction, $K_1$ is the intermolecular association constant for formation of the H-bonding interaction, $EM_1$ is the effective molarity for the intramolecular interaction, and $\sigma_1$ is a statistical factor that describes the degeneracy of the fully bound state. In the complexes discussed here, the porphyrins all have four identical H-bond donor sites, so $\sigma_1 = 4$.

So, the parameter *f* required for the determination of *EM* using the double mutant cycle analysis is given by Equation S2.

$$f = 1 + \sigma_1 K_1 EM_1 \quad \text{(S2)}$$

The population of the fully bound state, $P_b$, is given by

$$P_b = \frac{\sigma_1 K_1 EM_1}{1 + \sigma_1 K_1 EM_1} \quad \text{(S3)}$$

and the population of the partially bound state, $P_f$, where the intramolecular H-bond is not made is given by

$$P_f = \frac{1}{1 + \sigma_1 K_1 EM_1} \quad \text{(S4)}$$

**Two H-bonds.** For complexes that can make two different intramolecular H-bonds, ie an ester-phenol and a phosphonate diester-phenol H-bond, the observed association constant is given by the sum of the equilibrium constants for the fully bound and three partially bound states, so the parameter *f* required for the determination of *EM* using the double mutant cycle analysis is given by Equation S5.

$$f = 1 + \sigma_1 K_1 EM_1 + \sigma_2 K_2 EM_2 + \sigma_{12} K_1 EM_1 K_2 EM_2 \quad \text{(S5)}$$

where $K_i$ is the intermolecular association constant for formation of the ith H-bonding interaction, $EM_i$ is the effective molarity for the ith intramolecular interaction, $\sigma_i$ is the statistical factor that describes the degeneracy of singly H-bonded complexes, and $\sigma_{12}$ is the statistical factor that describes the degeneracy of doubly H-bonded complex.

We used the DMC in Figure 9 of the main text to determine the free energy contribution from phosphonate diester-phenol H-bonding in these complexes. If we consider the partially bound states that are possible in complexes A and B in Figure 9, the value of $\Delta\Delta G°$ measured by this double mutant cycle is given by Equation S6.

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$$e^{-\Delta\Delta G^\circ/RT} = \frac{1+\sigma_1 K_1 EM_1 + \sigma_2 K_2 EM_2 + \sigma_{12} K_1 EM_1 K_2 EM_2}{1+\sigma_1 K_1 EM_1} \quad \text{(S6)}$$

The value of $K_iEM_i$ for the formation of the intramolecular ester-phenol H-bond can be determined from the double mutant cycle for the relevant singly H-bonded complex. Thus Equation S6 can be rearranged to determine $K_2EM_2$ for the phosphonate diester-phenol H-bond (Equation S7).

$$K_2 EM_2 = \frac{(1+\sigma_1 K_1 EM_1)(e^{-\Delta\Delta G^\circ/RT} - 1)}{\sigma_2 + \sigma_{12} K_1 EM_1} \quad \text{(S7)}$$

We assume that the effective molarity for the formation of the first ester-phenol H-bond is not affected by the formation of the second phosphonate-diester H-bond: in other words, $K_1EM_1$ is a constant. Cases where this assumption may not be valid are discussed below. We must also make some assumptions about the values of the statistical factors, $\sigma_1$, $\sigma_2$ and $\sigma_{12}$. For the partially bound, singly H-bonded complexes, there is no ambiguity: $\sigma_1 = \sigma_2 = 4$. For the fully bound, doubly H-bonded complex, there are four degenerate states in which two H-bonds are made with phenol groups on trans-related meso positions on the porphyrin, and eight degenerate states in which two H-bonds are made with phenol groups on cis-related meso positions. Models suggest that the geometry of the ester-phosphatodiester ligands precludes the trans arrangement, and so we assume that $\sigma_{12} = 8$. This assumption affects the precise values of *EM* quoted here, but does not qualitatively alter the results.

For complexes that can make two identical intramolecular H-bonds, the observed association constant is given by the sum of the equilibrium constants for the fully bound and two partially bound states (Equation S8).

$$f = 1 + \sigma_1 K_1 EM_1 + \sigma_{11} (K_1 EM_1)^2 \quad \text{(S8)}$$

Again, we assume that the effective molarity for the formation of the first H-bond is not affected by the formation of the second H-bond, so that $K_1EM_1$ is a constant (Equation S9).

$$K_1 EM_1 = \frac{-\sigma_1 + \sqrt{\sigma_1^{\,2} - 4\sigma_{11}(1 - e^{-\Delta\Delta G^\circ/RT})}}{2\sigma_{11}} \quad \text{(S9)}$$

Again assumptions about the statistical factors are required in order to deduce values of $K_1EM_1$. For the partially bound, singly H-bonded complex, $\sigma_1 = 8$. For the fully bound, doubly H-bonded complex, there are two degenerate states in which two H-bonds are made with phenol groups on trans-related meso positions on the porphyrin, and four degenerate states in which two H-bonds are made with phenol groups on cis-related meso positions. Models suggest that all states are equally accessible, so $\sigma_{11} = 6$, but this value may be as low as 2, if the cis states are inaccessible.

**Four H-bonds.** For complexes that can make four intramolecular H-bonds, the observed association constant is given by the sum of the equilibrium constants for all possible states (Equation S10).

$$\begin{aligned} f = {} & 1 + \sigma_1 K_1 EM_1 + \sigma_2 K_2 EM_2 + \sigma_3 K_3 EM_3 + \sigma_4 K_4 EM_4 \\ & + \sigma_{12} K_1 EM_1 K_2 EM_2 + \sigma_{13} K_1 EM_1 K_3 EM_3 + \sigma_{14} K_1 EM_1 K_4 EM_4 \\ & + \sigma_{23} K_2 EM_2 K_3 EM_3 + \sigma_{24} K_2 EM_2 K_4 EM_4 + \sigma_{34} K_3 EM_3 K_4 EM_4 \\ & + \sigma_{123} K_1 EM_1 K_2 EM_2 K_3 EM_3 + \sigma_{124} K_1 EM_1 K_2 EM_2 K_4 EM_4 + \sigma_{134} K_1 EM_1 K_3 EM_3 K_4 EM_4 \\ & + \sigma_{234} K_2 EM_2 K_3 EM_3 K_4 EM_4 + \sigma_{1234} K_1 EM_1 K_2 EM_2 K_3 EM_3 K_4 EM_4 \end{aligned} \quad \text{(S10)}$$

If we assume that the values of $K_iEM_i$ for the ester and phosphonate diester H-bonds are constants for the symmetric ligands studied here, this equation simplifies to Equation S11.

$$\begin{aligned} f = {} & 1 + \sigma_1 K_1 EM_1 + \sigma_2 K_2 EM_2 + \sigma_{11} (K_1 EM_1)^2 + \sigma_{22} (K_2 EM_2)^2 + \sigma_{12} K_1 EM_1 K_2 EM_2 \\ & + \sigma_{112} (K_1 EM_1)^2 K_2 EM_2 + \sigma_{122} K_1 EM_1 (K_2 EM_2)^2 + \sigma_{1122} (K_1 EM_1)^2 (K_2 EM_2)^2 \end{aligned} \quad \text{(S11)}$$

where the σ subscripts reflect the symmetries of the complexes.

We used the DMC in Figure 9 of the main text to determine the free energy contribution from phosphonate diester-phenol H-

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bonding in these complexes. If we consider the partially bound states that are possible in complexes A and B in Figure 9, the value of $\Delta\Delta G°$ measured by the DMC is given by Equation S12.

$$e^{-\Delta\Delta G/RT} = \frac{\left\{\begin{array}{l} 1+\sigma_1 K_1 EM_1 + \sigma_2 K_2 EM_2 + \sigma_{11}(K_1 EM_1)^2 + \sigma_{22}(K_2 EM_2)^2 + \sigma_{12} K_1 EM_1 K_2 EM_2 \\ +\sigma_{112}(K_1 EM_1)^2 K_2 EM_2 + \sigma_{122} K_1 EM_1 (K_2 EM_2)^2 + \sigma_{1122}(K_1 EM_1)^2 (K_2 EM_2)^2 \end{array}\right\}}{1+\sigma_1 K_1 EM_1 + \sigma_{11}(K_1 EM_1)^2} \quad \text{(S12)}$$

The value of $K_1EM_1$ for the formation of intramolecular ester-phenol H-bonds can be determined from the DMC for the relevant doubly H-bonded complex, so Equation S12 can be rearranged to determine $K_2EM_2$ for the phosphatodiester H-bonds (Equation S13).

$$K_2 EM_2 = \frac{\left\{\begin{array}{l} -\left(\sigma_2 + \sigma_{12} K_1 EM_1 + \sigma_{112}(K_1 EM_1)^2\right) \\ +\sqrt{\left(\sigma_2 + \sigma_{12} K_1 EM_1 + \sigma_{112}(K_1 EM_1)^2\right)^2 - 4\left(\sigma_{22} + \sigma_{122} K_1 EM_1 + \sigma_{1122}(K_1 EM_1)^2\right)\left(1+\sigma_1 K_1 EM_1 + \sigma_{11}(K_1 EM_1)^2\right)\left(1-e^{-\Delta\Delta G/RT}\right)} \end{array}\right\}}{2\left(\sigma_{22} + \sigma_{122} K_1 EM_1 + \sigma_{1122}(K_1 EM_1)^2\right)} \quad \text{(S13)}$$

For the singly H-bonded complexes, $\sigma_1 = \sigma_2 = 8$. For the complexes that form two ester H-bonds or two phosphatodiester H-bonds, we assume that *trans* and *cis* arrangements are equally likely, so $\sigma_{11} = \sigma_{22} = 6$. However, formation of H-bonds to both the ester and phosphonate diester groups on the same side chain can only be made in the cis arrangement, so $\sigma_{12} = 40$. Using the same assumptions for the triply H-bonded complexes, $\sigma_{112} = \sigma_{122} = 16$, and for the complex where all four H-bonds are made, $\sigma_{1122} = 8$ (see Figure S1 for details of the statistical analysis).

**Table S2** Statistical factors for complexes formed with ligands **L1a-L6a**.

| | Ligand | | | | | |
|---|---|---|---|---|---|---|
| | **L1a** | **L2a** | **L3a** | **L4a** | **L5a** | **L6a** |
| $\sigma_1 = \sigma_2$ | 4 | 4 | 8 | 4 | 4 | 8 |
| $\sigma_{11} = \sigma_{22}$ | | | 12 | | | 12 |
| $\sigma_{12}$ | | | | | 8 | 40 |
| $\sigma_{112} = \sigma_{122}$ | | | | | | 32 |
| $\sigma_{1122}$ | | | | | | 16 |

**Table S3** Statistical factors for complexes formed with ligands **L1b-L6b**.

| | Ligand | | | | | |
|---|---|---|---|---|---|---|
| | **L1b** | **L2b** | **L3b** | **L4b** | **L5b** | **L6b** |
| $\sigma_1 = \sigma_2$ | | | | | 4 | 8 |
| $\sigma_{11} = \sigma_{22}$ | | | | | | 12 |

## Statistically-corrected equilibrium constants for formation of intramolecular H-bonds

**Table S4** *K EM* values for formation of an intramolecular phosphonate diester-phenol H-bond.[a]

| | | Ligand | | | | | |
|---|---|---|---|---|---|---|---|
| | | **L1a** | **L2a** | **L3a** | **L4a** | **L5a** | **L6a** |
| **Porphyrin** | **P1a** | | 9.1 | 6.6 | 2.4 | 2.6 | 3.1 |
| | **P2a** | 0.3 | 0.6 | 0.2 | 0.6 | 0.6 | 0.6 |
| | **P3a** | 0.3 | 2.2 | 0.9 | 2.5 | 1.0 | 1.2 |
| | **P4a** | | 1.5 | 0.2 | 1.9 | 3.3 | 1.2 |

[a] Errors are ±40%.

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**Table S5** *K EM* values for formation of an intramolecular ester-phenol H-bond.[a]

| | | Ligand | | | | | |
|---|---|---|---|---|---|---|---|
| | | **L1b** | **L2b** | **L3b** | **L4b** | **L5b** | **L6b** |
| **Porphyrin** | **P1a** | | | | | 0.4 | 0.5 |
| | **P2a** | | | | | 0.2 | 0.3 |
| | **P3a** | | | | | 0.6 | 0.6 |
| | **P4a** | | | | | | |

[a] Errors are ±40%.

## H-bond occupancy

**Table S6** Occupancy of the H-bonded state for phosphonate diester-phenol H-bonds (%).

| | | Ligand | | | | | |
|---|---|---|---|---|---|---|---|
| | | **L1a** | **L2a** | **L3a** | **L4a** | **L5a** | **L6a** |
| **Porphyrin** | **P1a** | | 97 | 95 | 90 | 88 | 86 |
| | **P2a** | 53 | | 43 | 70 | 63 | 58 |
| | **P3a** | 50 | 90 | 74 | 91 | 71 | 70 |
| | **P4a** | 38 | 85 | 39 | 88 | 93 | 79 |

**Table S7** Occupancy of the H-bonded state for ester-phenol H-bonds in the control ligand complexes (%).

| | | Ligand | | | | | |
|---|---|---|---|---|---|---|---|
| | | **L1b** | **L2b** | **L3b** | **L4b** | **L5b** | **L6b** |
| **Porphyrin** | **P1a** | | | | | 58 | 61 |
| | **P2a** | | | | | 48 | 49 |
| | **P3a** | | | | | 70 | 67 |
| | **P4a** | | | | | | |

**Table S8** Occupancy of the H-bonded state for ester-phenol H-bonds in the phosphonate diester ligand complexes (%).

| | | Ligand | | | | | |
|---|---|---|---|---|---|---|---|
| | | **L1a** | **L2a** | **L3a** | **L4a** | **L5a** | **L6a** |
| **Porphyrin** | **P1a** | | | | | 59 | 45 |
| | **P2a** | | | | | 54 | 37 |
| | **P3a** | | | | | 64 | 54 |
| | **P4a** | | | | | | |

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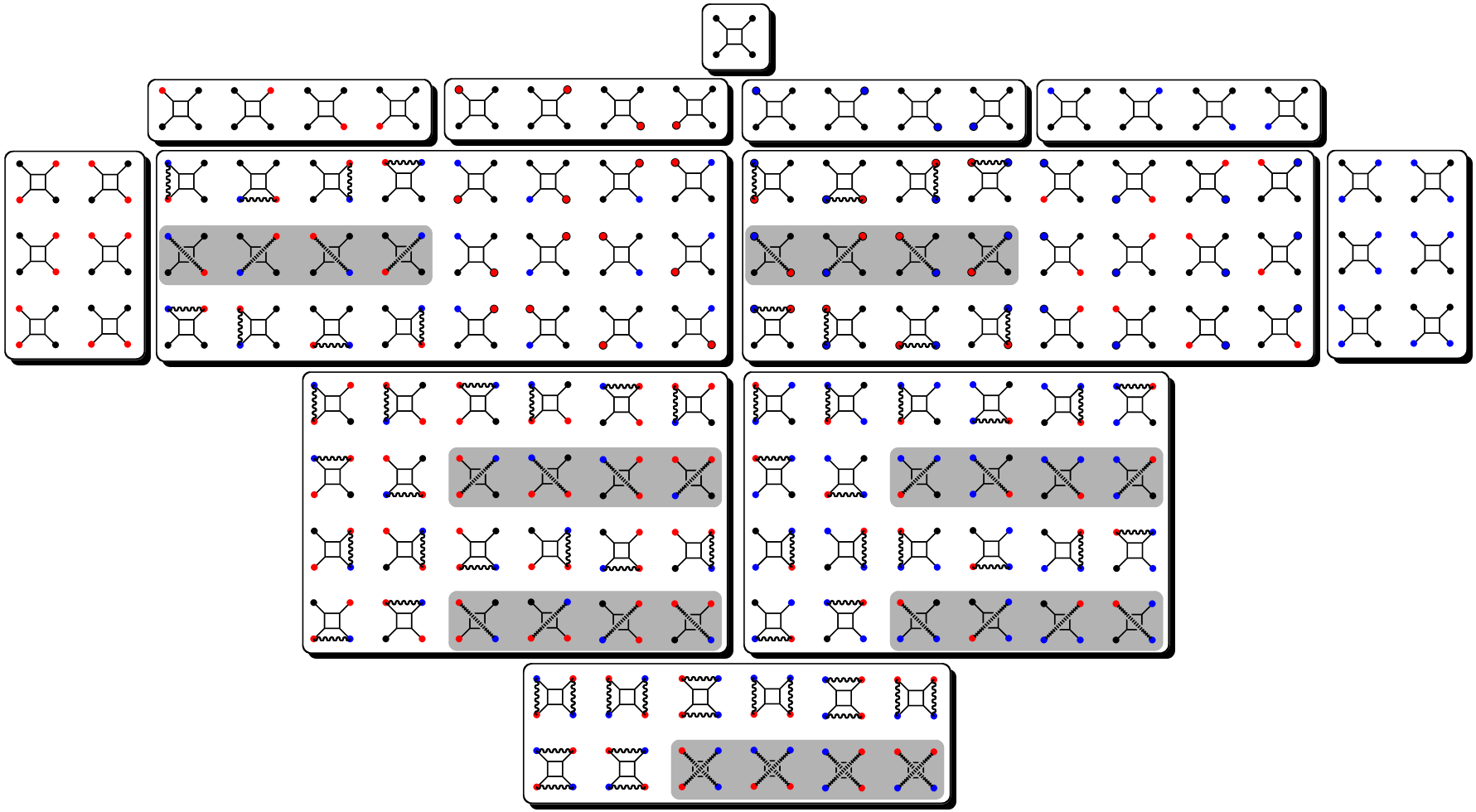

**Fig. S1** Degenerate states for the complex where four intramolecular H-bonds are possible. Unbound phenol OH groups on the porphyrin are represented by black dots, phenol groups H-bonded to phosphonate diesters are represented by red dots and phenol groups H-bonded to esters are represented by blue dots. The connectivity between phosphonate diester and ester groups on the same side chain are represented by wiggly lines. In complexes where the two side chains are non-equivalent, i.e. one is bound and one is free, the side chains are distinguished by large and small dots. The shaded complexes are structures that models suggest are geometrically impossible. The panels are orders zero, one, two, three and four H-bonds from top to bottom and grouped by symmetry.

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## NMR structures

**P1a•L2a** NMR stucture Cartesian coordinates

| | | | |
|---|---|---|---|
| N | -1.051600 | -1.043900 | -1.955600 |
| N | -3.450700 | -1.143700 | -3.585900 |
| N | 0.443800 | 0.135100 | -4.158400 |
| N | -1.956000 | -0.004200 | -5.833700 |
| C | 0.220400 | -0.983100 | -1.369300 |
| C | -1.902700 | -1.675600 | -1.059100 |
| C | -3.241800 | -1.996500 | -1.251400 |
| C | 0.142500 | -1.578100 | 0.000800 |
| C | -5.333800 | -2.208000 | -2.715900 |
| C | -5.650200 | -1.856900 | -3.997800 |
| C | -4.459200 | -1.188200 | -4.581600 |
| C | -1.138500 | -1.996000 | 0.190200 |
| C | 1.466400 | 0.012200 | -3.271800 |
| C | 2.735100 | 0.453600 | -3.895600 |
| C | 1.381200 | -0.492900 | -1.932300 |
| C | 0.985900 | 0.620600 | -5.376000 |
| C | -3.938000 | -1.758400 | -2.471400 |
| C | 0.305200 | 0.811400 | -6.562800 |
| C | -4.355800 | -0.746300 | -5.881800 |
| C | -3.176500 | -0.182300 | -6.465400 |
| C | -3.075500 | 0.262700 | -7.847000 |
| C | -1.770700 | 0.696000 | -8.038100 |
| C | -1.075200 | 0.517900 | -6.774100 |
| C | 2.436700 | 0.828900 | -5.179100 |
| C | -7.777400 | -1.147800 | -8.425400 |
| C | -7.211500 | -2.267800 | -7.820700 |
| C | -6.095400 | -2.141500 | -6.997200 |
| C | -5.531100 | -0.878300 | -6.761100 |
| C | -6.088700 | 0.256100 | -7.356600 |
| C | -7.206900 | 0.110300 | -8.191300 |
| C | -5.411000 | -3.879400 | 1.926500 |
| C | -5.081200 | -4.590100 | 0.778400 |
| C | -4.374100 | -3.983700 | -0.258800 |
| C | -3.985100 | -2.641200 | -0.162300 |
| C | -4.311700 | -1.910800 | 0.988300 |
| C | -5.018200 | -2.535500 | 2.022900 |
| C | 4.988900 | -0.487000 | 0.376000 |
| C | 4.053200 | 0.552300 | 0.502600 |
| C | 2.870300 | 0.557200 | -0.251100 |
| C | 2.618700 | -0.490800 | -1.139200 |
| C | 3.548200 | -1.533500 | -1.268100 |
| C | 4.720500 | -1.524100 | -0.514200 |
| C | 2.477700 | 2.345400 | -9.918900 |
| C | 2.365700 | 0.963700 | -9.715300 |
| C | 1.652800 | 0.447500 | -8.620800 |
| C | 1.057300 | 1.332400 | -7.718000 |
| C | 1.171200 | 2.718300 | -7.915800 |
| C | 1.872200 | 3.214100 | -9.012400 |
| O | 2.933100 | 0.039800 | -10.563700 |
| O | -7.703800 | 1.267800 | -8.750500 |
| O | 4.352100 | 1.557700 | 1.390300 |
| O | -5.367500 | -1.874300 | 3.181000 |
| Zn | -1.573400 | -0.252100 | -3.790600 |
| H | -7.241300 | 2.015900 | -8.345400 |
| H | -5.932800 | -2.725100 | -1.970700 |
| H | -6.573700 | -2.020000 | -4.550300 |
| H | 3.689600 | 0.449900 | -3.375800 |
| H | 3.100000 | 1.204400 | -5.956100 |
| H | -3.889900 | 0.241900 | -8.565900 |
| H | -1.322400 | 1.097800 | -8.942000 |
| H | -8.655800 | -1.247800 | -9.077500 |
| H | -7.652300 | -3.260700 | -7.994600 |
| H | -5.649300 | -3.029800 | -6.526100 |
| H | -5.666500 | 1.256300 | -7.182300 |
| H | -5.967400 | -4.345300 | 2.751900 |
| H | -5.385500 | -5.643400 | 0.686200 |
| H | -4.121700 | -4.556300 | -1.163800 |
| H | -4.012500 | -0.856200 | 1.074400 |
| H | 5.908500 | -0.469500 | 0.975100 |
| H | 2.153800 | 1.388600 | -0.129200 |
| H | 3.349700 | -2.358400 | -1.969200 |
| H | 5.444500 | -2.345400 | -0.624000 |
| H | 1.574800 | -0.640600 | -8.484300 |
| H | 0.700700 | 3.408300 | -7.199100 |
| H | 1.950800 | 4.301200 | -9.163000 |
| H | 3.033900 | 2.737400 | -10.781700 |
| H | -5.117100 | -0.944200 | 3.079600 |
| H | 3.667700 | 2.244000 | 1.298100 |
| H | 3.701700 | 0.453200 | -10.982100 |
| H | 1.003400 | -1.634400 | 0.665200 |
| H | -1.593900 | -2.480300 | 1.050000 |
| N | -1.370200 | 2.386100 | -3.689500 |
| C | 4.559700 | 6.619900 | -2.337600 |
| C | 5.007000 | 6.057900 | 2.917300 |
| C | -1.645300 | 5.193000 | -3.640600 |
| C | -2.075000 | 4.457600 | -4.742300 |
| C | -0.937600 | 3.101300 | -2.629500 |
| C | -0.645400 | 5.275300 | -1.388400 |
| C | -1.925400 | 3.058800 | -4.724600 |
| C | 3.909300 | 5.058400 | 2.658200 |
| C | 0.862300 | 5.454800 | 0.447200 |
| C | 3.520600 | 5.692700 | -1.748100 |
| C | -1.062600 | 4.505700 | -2.563500 |
| O | 2.983000 | 3.715800 | 0.447400 |
| O | -1.069800 | 6.366300 | -1.008300 |
| O | 0.363000 | 4.693300 | -0.648700 |
| O | 2.840900 | 5.709800 | 1.997300 |
| O | 3.217500 | 6.098700 | -0.428600 |
| P | 2.476600 | 5.081400 | 0.564300 |
| H | -2.529800 | 4.950900 | -5.614000 |
| H | 0.680600 | 6.551200 | 0.267100 |
| H | 3.938900 | 4.647300 | -1.678300 |
| H | 4.663000 | 6.829900 | 3.647300 |
| H | 0.266900 | 5.202500 | 1.364300 |
| H | 5.066700 | 7.196600 | -1.526600 |
| H | 3.510600 | 4.619800 | 3.615500 |
| H | 5.322200 | 6.016900 | -2.887300 |
| H | 4.095500 | 7.344500 | -3.047100 |
| H | 5.295100 | 6.573600 | 1.970100 |
| H | 4.260400 | 4.223700 | 1.987700 |
| H | 2.580300 | 5.685200 | -2.366900 |
| H | -1.760400 | 6.287500 | -3.598900 |

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| | | | |
|---|---|---|---|
| H | 5.897500 | 5.529900 | 3.334300 |
| H | -2.270500 | 2.441900 | -5.583700 |
| H | -0.471700 | 2.535100 | -1.794600 |

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**P4a•L6a** NMR structure Cartesian coordinates

| | | | |
|---|---|---|---|
| N | 1.693200 | -3.091200 | -1.523400 |
| N | 0.744400 | -3.586200 | 1.206600 |
| N | 2.736300 | -1.696300 | 2.228700 |
| N | 3.681800 | -1.246800 | -0.479500 |
| C | 5.254000 | -0.372900 | -1.995100 |
| C | 3.739800 | -0.598500 | -4.943900 |
| C | 4.047600 | -1.242100 | -1.828600 |
| C | 3.449200 | -1.933000 | -2.866500 |
| C | 3.364600 | 3.192200 | -8.292800 |
| C | 1.748700 | -3.619500 | -3.790100 |
| C | 0.747300 | -4.376400 | -3.242000 |
| C | 1.509400 | -4.249800 | 5.787200 |
| C | 0.705000 | -4.070500 | -1.795700 |
| C | 2.341600 | -2.824200 | -2.689200 |
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| C | 4.608200 | -0.472300 | 0.213800 |
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| C | 2.931500 | -1.483600 | 4.558800 |
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| C | 10.849300 | -1.405700 | 3.466300 |
| C | 6.484000 | 2.846600 | 2.722300 |
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| C | 7.693200 | 2.312100 | 3.160500 |
| C | -2.125900 | -1.180000 | 7.656800 |
| C | 7.922300 | 0.931000 | 3.081400 |
| C | 6.923200 | 0.099400 | 2.558600 |
| C | -4.398700 | -2.768900 | 8.015400 |
| C | 3.978300 | -1.777400 | -4.227500 |
| C | -2.930900 | -7.564000 | -2.323300 |
| C | 4.662600 | -0.248400 | 1.581800 |
| C | -3.344000 | -6.245900 | -2.082300 |
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| C | 4.960200 | 1.701300 | -7.264500 |
| C | 3.937400 | 0.782700 | -6.991000 |
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| C | 9.962400 | 1.037700 | 4.499300 |
| C | 5.491600 | 2.016500 | 2.205300 |
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