

## Supporting Information

**Table S1.** Summary of X-ray Crystallography Data of **2b**

|                                |  |
|--------------------------------|--|
| Emp. Formula                   | C <sub>76</sub> H <sub>118</sub> N <sub>2</sub> O <sub>6</sub> Zn <sub>2</sub> |
| Form. Weight                   | 1286.46  |
| Crystal system                 | Triclinic  |
| Space group                    | P-1  |
| a (Å)                          | 11.0687(8)   |
| b (Å)                          | 13.2741(10)  |
| c (Å)                          | 14.1357(11)  |
| • • •                          | 72.1170(10)  |
| • • •                          | 80.5380(10)  |
| • • •                          | 67.6900(010)   |
| Volume (Å <sup>3</sup> )       | 1825.9(2)  |
| Z                              | 1  |
| Density                        | 1.170  |
| F(000)                         | 696.0  |
| Crystal size(mm <sup>3</sup> ) | 0.52 x 0.48 x 0.45   |
| • • range                      | 1.97 to 25.99°   |
| Index ranges                   | -13<=h<=12<br>-16<=k<=8<br>-17<=l<=16  |
| Ref. collected                 | 10257  |
| Ind. Reflections               | 7039 [R(int) = 0.0144]   |
| Complete to • •                | 98.1   |
| Max. and min transmission      | 1.000000 and 0.3298  |
| Data / Restraints/ parameters  | 7039 / 0 / 398   |
| GOF                            | 1.035  |
| Final R indices                | R1=0.0374  |
| [I > 2 sigma (I)]              | wR2=0.1052   |
| R indices                      | R1 = 0.0420  |
| (all data)                     | wR2 = 0.1093   |
| Largest diff. Peak and hole    | 0.447 and -0.438 e.Å <sup>-3</sup>   |
| Temperature                    | 293(2)   |
| Wavelength                     | 0.71073  |
| Abs. correction                | SADABS   |
| Refine. Method                 | Full-matrix least-squares on F <sup>2</sup>                                    |

$$^a R1 = (|F_o| - |F_c|) / |F_o|$$

$${}^bR2 = \{[w(F_o^2 - F_c^2)^2] / [w](F_o^2)^2\}^{1/2}, w = 0.10.$$

$${}^cGoF = [w(F_o^2 - F_c^2)^2] / (N_{\text{rflns}} - N_{\text{params}})^{1/2}.$$

**Table S2** Selected bond lengths (Å) and angle (°) of 2b

|                | bond lengths (Å) |
|----------------|------------------|
| Zn-O(1)        | 1.9028(13)       |
| Zn-O(2)        | 1.9766(13)       |
| Zn-O(2)#1      | 1.9827(13)       |
| Zn-N           | 2.1015(15)       |
|                | bond angle (°)   |
| O(1)-Zn-O(2)   | 123.74(6)        |
| O(1)-Zn-O(2)#1 | 108.43(6)        |
| O(2)-Zn-O(2)#1 | 82.42(5)         |
| O(1)-Zn-N      | 100.07(6)        |
| O(2)-Zn-N      | 124.13(6)        |
| O(2)#1-Zn-N    | 117.25(6)        |