

*Supplementary Information for*

## **A Highly efficient Method for Suzuki Reactions in Aqueous Media**

Xinglong Zhou<sup>a</sup>, Xuming Guo<sup>a</sup>, Fangfang Jian<sup>a,\*</sup>, Gang Wei<sup>b</sup>

<sup>a</sup>School of Chemical Engineering and Pharmaceutics, Henan University of Science and Technology, Luoyang, Henan, P. R. China

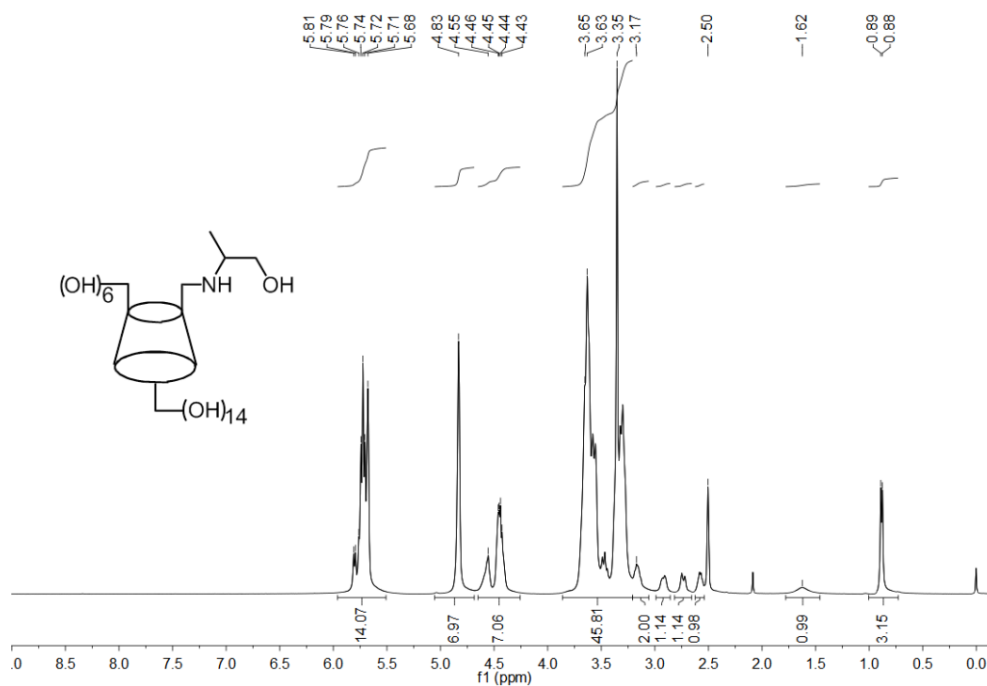
<sup>b</sup>CSIRO Manufacturing, 36 Bradfield Road, West Lindfield, PO Box 218, Lindfield, NSW 2070, Australia

Corresponding Author

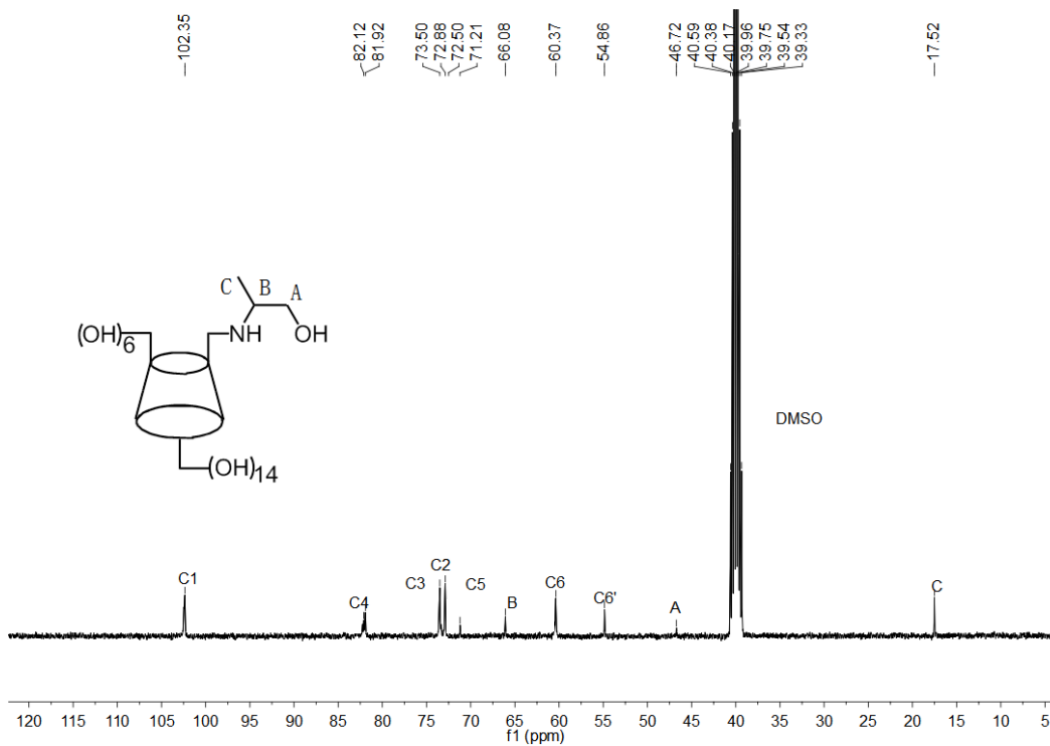
E-mail: [ffj2017@haust.edu.cn](mailto:ffj2017@haust.edu.cn); [ffj2013@163.com](mailto:ffj2013@163.com)

| <b>Table of contents</b>  | <b>Page</b>   |
|---|---------------|
| <b>1. Spectra data</b>  | <b>S2-S3</b>  |
| <b>2. Crystallographic data for (L<sub>n</sub>@β-CD)·H<sub>2</sub>O</b> | <b>S4</b>     |
| <b>3. <sup>1</sup>HNMR of biphenyl derivatives</b>                      | <b>S5-S10</b> |

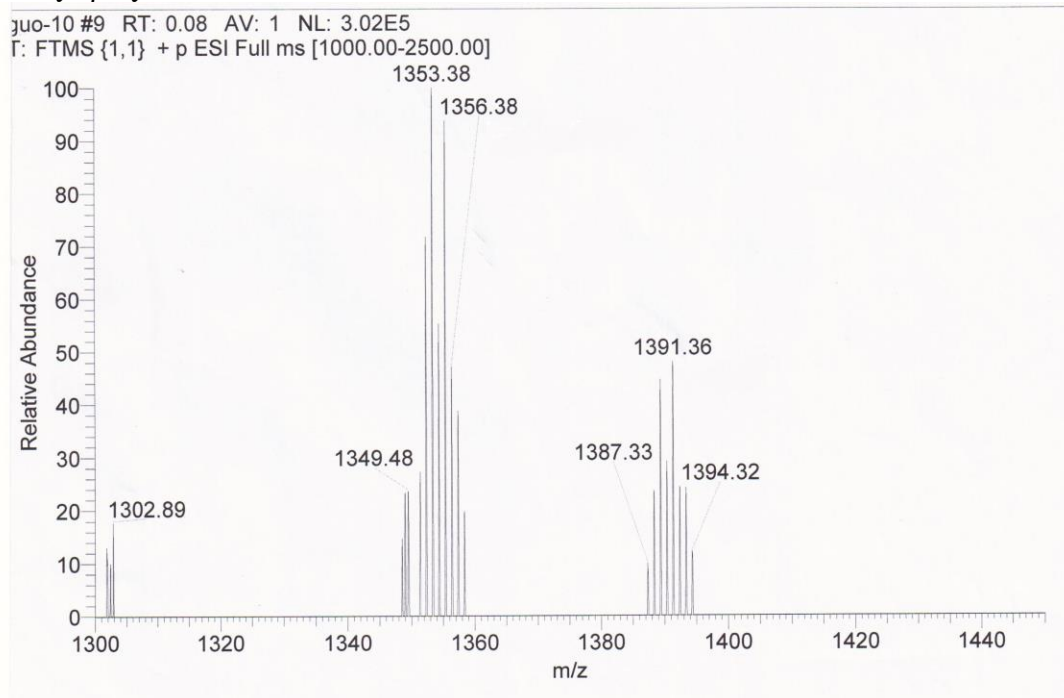
**Figure S1.**  $^1\text{H}$  NMR of 6-(L-amino propanol)-deoxy- $\beta$ -cyclodextrin ( $L_n@ \beta$ -CD)



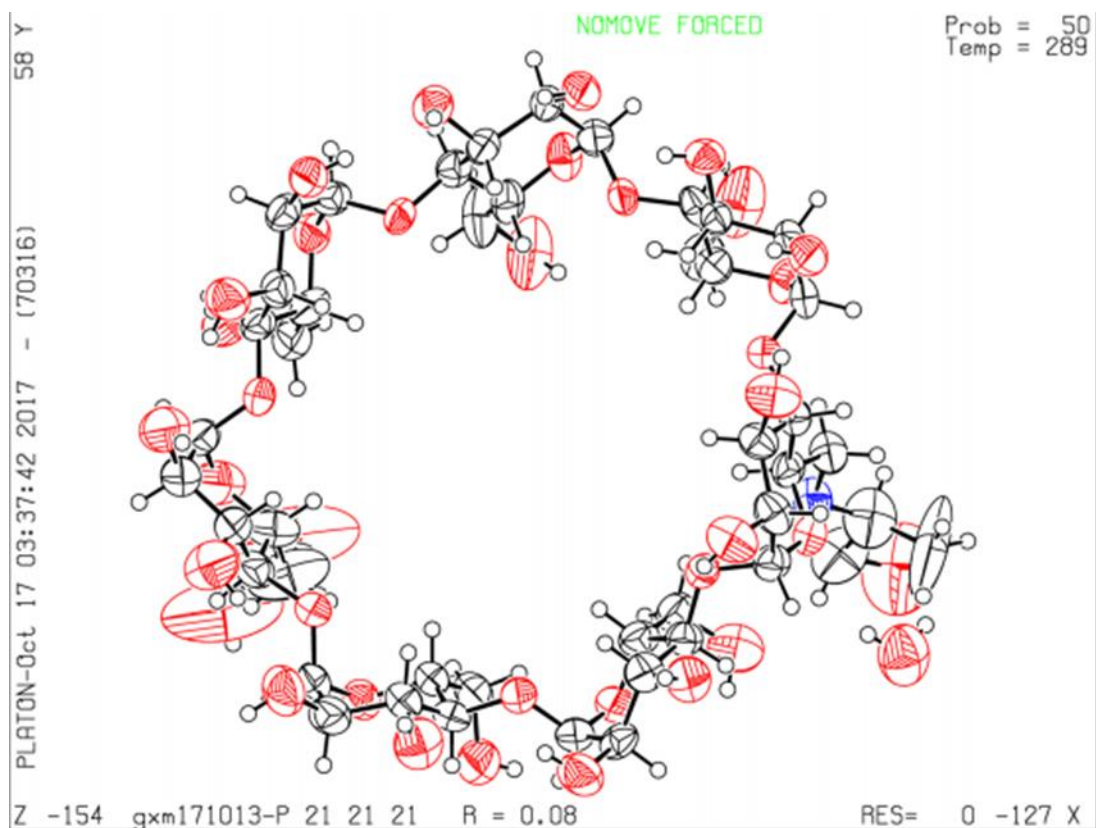
**Figure S2.**  $^{13}\text{C}$  NMR of 6-(L-amino propanol)-deoxy- $\beta$ -cyclodextrin ( $L_n@ \beta$ -CD)



**Figure S3.** Positive ion ESI full ms of the mixture of PdCl<sub>2</sub> with 6-(L-amino propanol)-deoxy- β-cyclodextrin in water

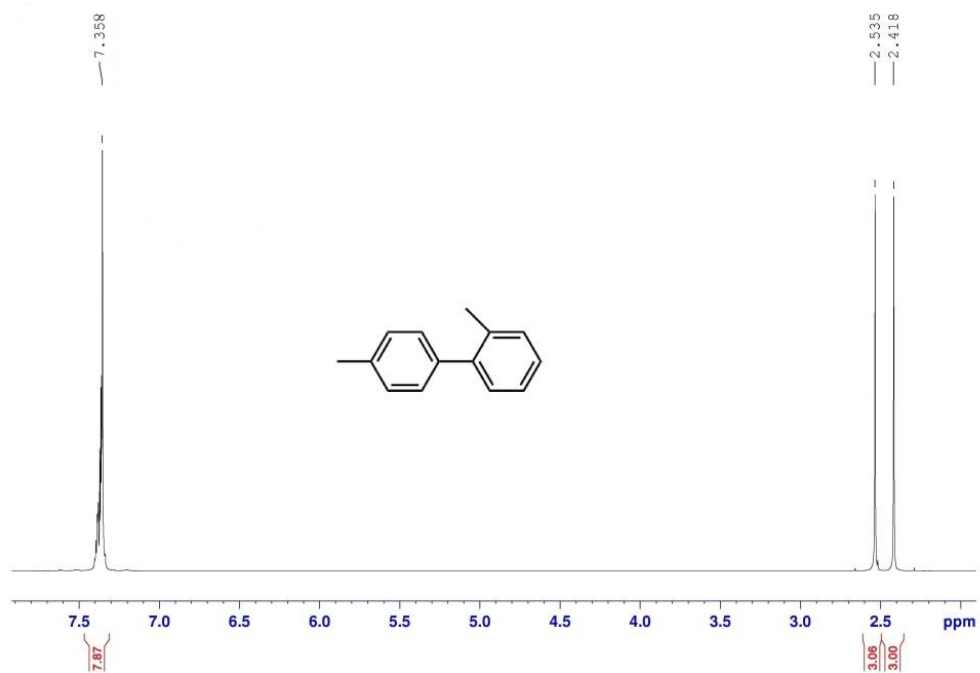
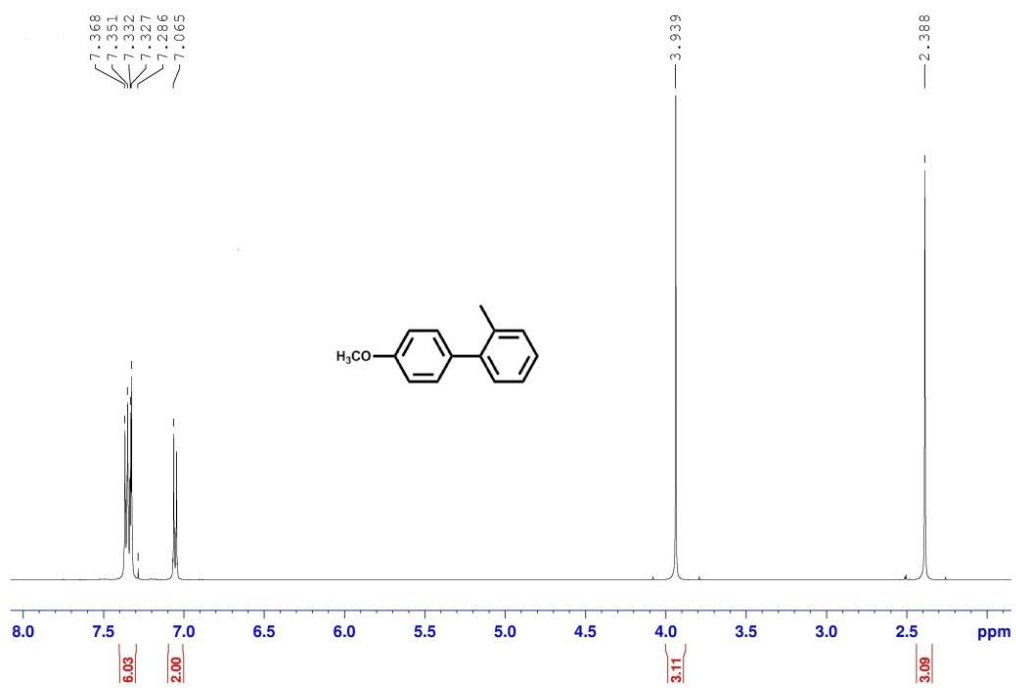


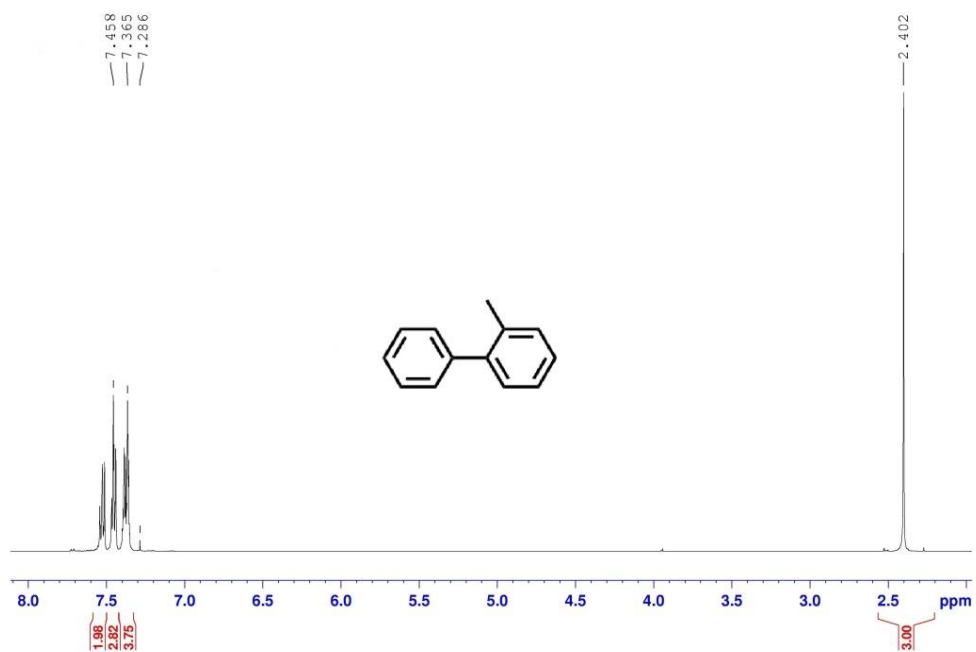
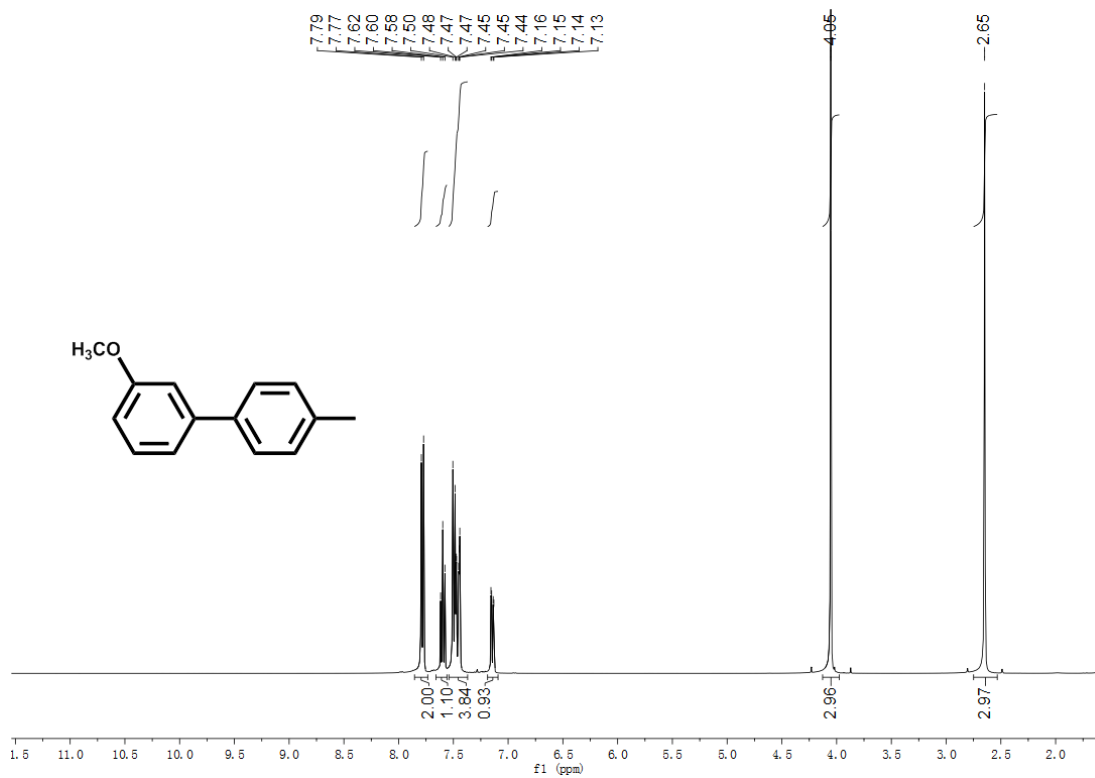
**Figure S4.** Crystal data and structure refinement for (L<sub>n</sub>@β-CD)·H<sub>2</sub>O

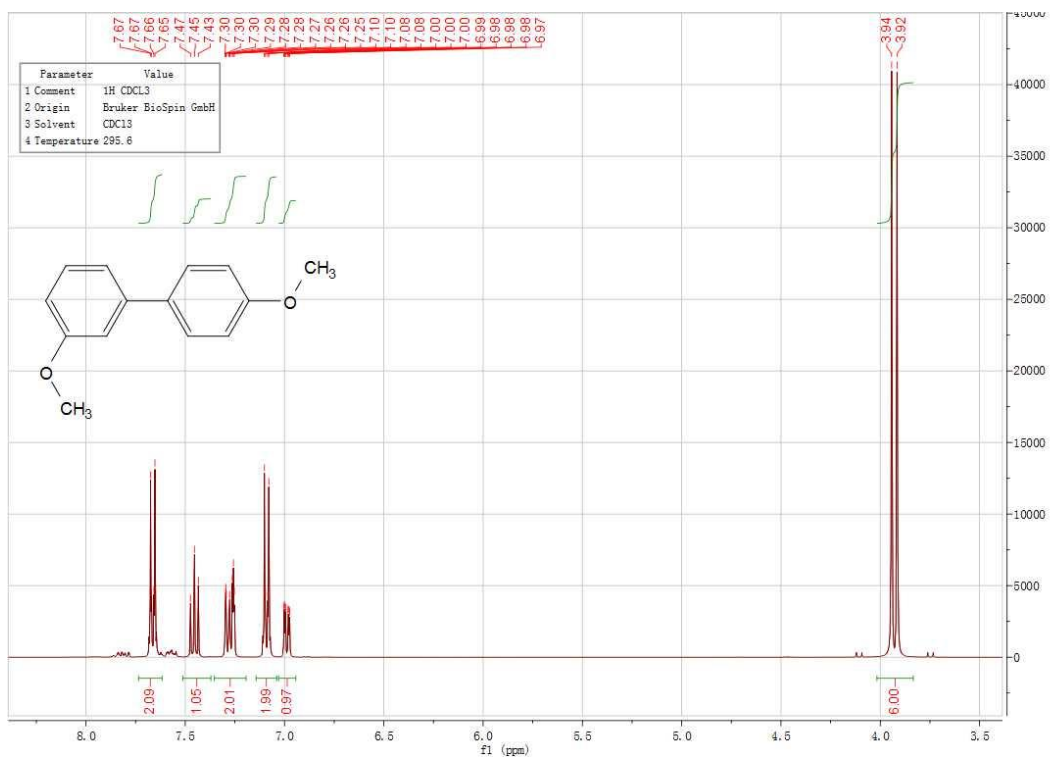
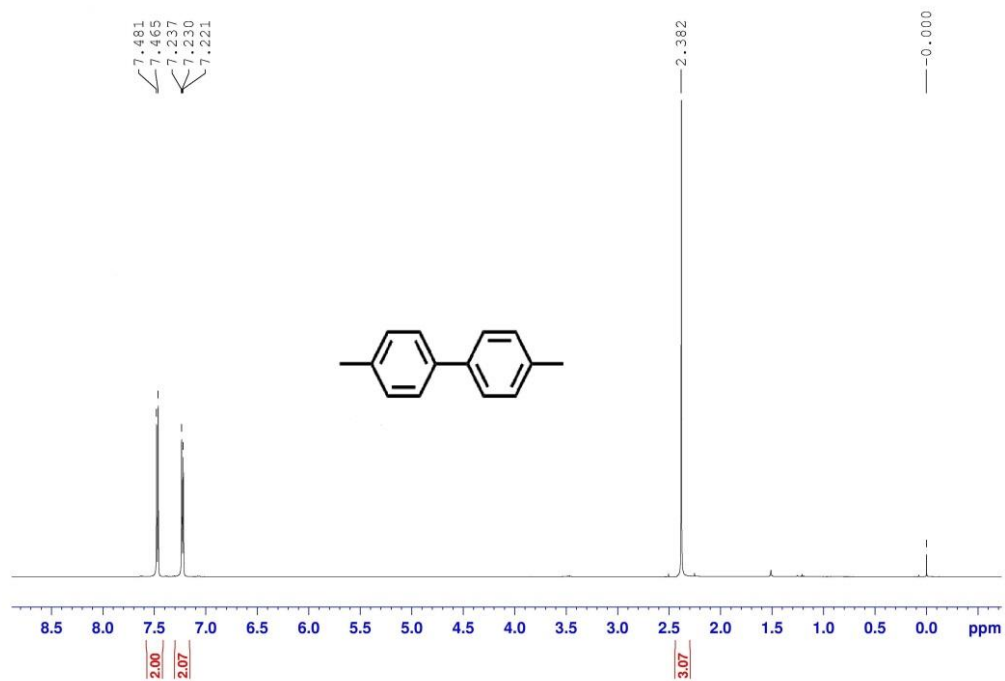


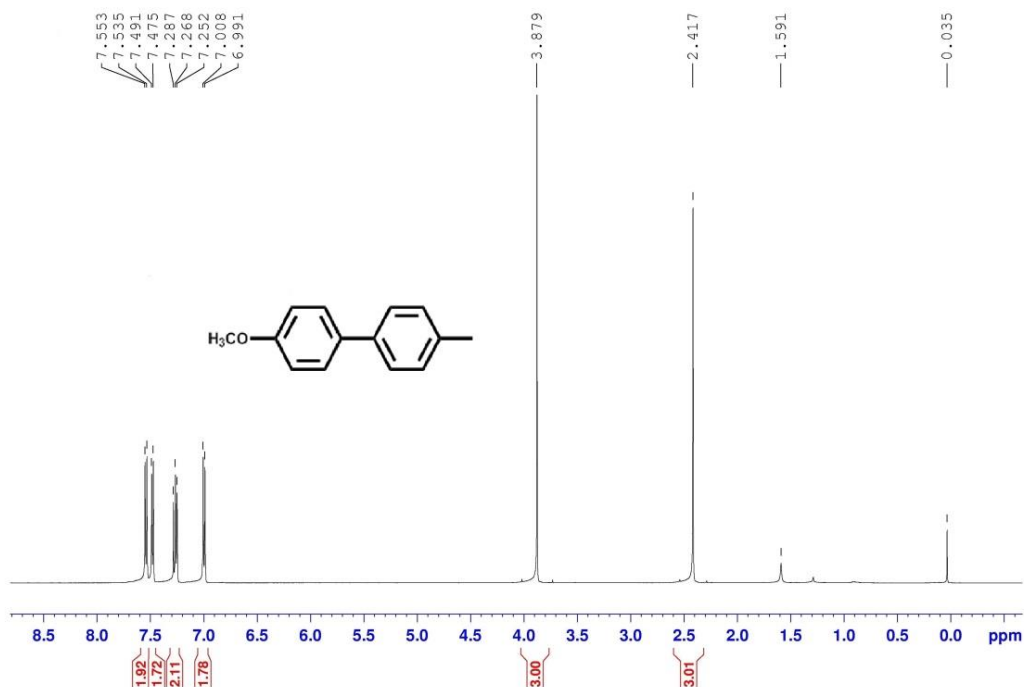
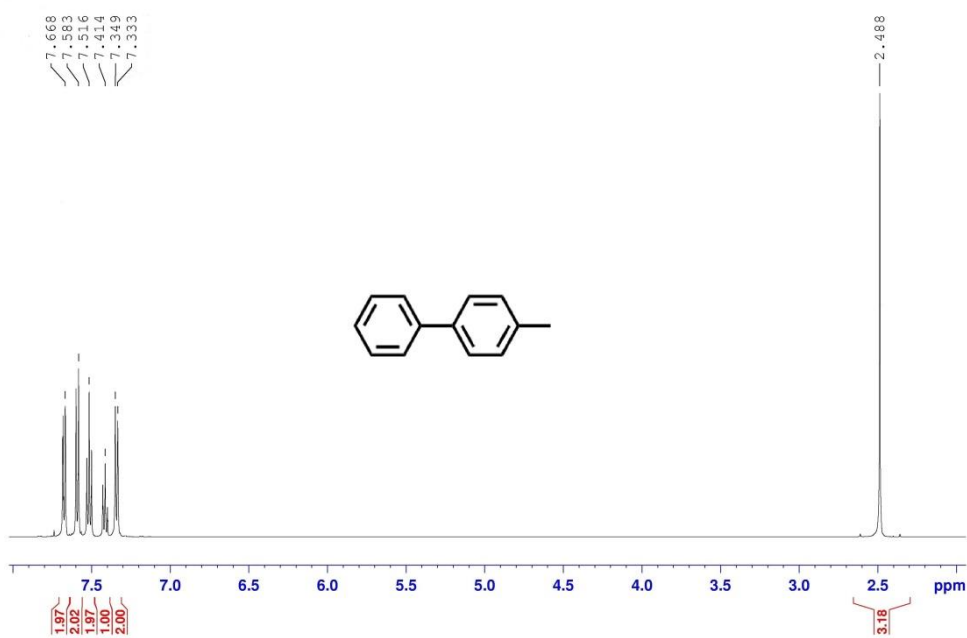
**Table S1.** Crystallographic data for ligand 6-(L-aminopropanol)-deoxy- $\beta$ - cyclodextrin ( $L_n@ \beta$ -CD $\cdot$ H<sub>2</sub>O)

|   |   |
|---|---|
| Identification code                         | gxm171013-1_sq  |
| Empirical formula                           | C <sub>45</sub> H <sub>79</sub> N <sub>3</sub> O <sub>36</sub>  |
| Formula weight                              | 1210.09   |
| Temperature/K                               | 289.03(14)  |
| Crystal system                              | orthorhombic  |
| Space group                                 | P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>                   |
| a/Å   | 13.1062(5)  |
| b/Å   | 19.3742(9)  |
| c/Å   | 27.0246(11)   |
| $\alpha$ /°                                 | 90  |
| $\beta$ /°                                  | 90  |
| $\gamma$ /°                                 | 90  |
| Volume/Å <sup>3</sup>                       | 6862.1(5)   |
| Z   | 4   |
| $\rho_{\text{calc}}$ /g/cm <sup>3</sup>     | 1.079   |
| $\mu$ /mm <sup>-1</sup>                     | 0.098   |
| F(000)                                      | 2229  |
| Crystal size/mm <sup>3</sup>                | 0.28 × 0.27 × 0.24  |
| Radiation                                   | MoK $\alpha$ ( $\lambda$ = 0.71073)                             |
| 2 $\theta$ range for data collection/°      | 6.564 to 49.994   |
| Index ranges                                | -15 ≤ h ≤ 15, -22 ≤ k ≤ 22, -30 ≤ l ≤ 30                        |
| Reflections collected                       | 64180   |
| Independent reflections                     | 11787 [ $R_{\text{int}}$ = 0.0594, $R_{\text{sigma}}$ = 0.0577] |
| Data/restraints/parameters                  | 11787/47/769  |
| Goodness-of-fit on F <sup>2</sup>           | 1.041   |
| Final R indexes [ $I > 2\sigma(I)$ ]        | $R_1$ = 0.0798, $wR_2$ = 0.2198                                 |
| Final R indexes [all data]                  | $R_1$ = 0.1114, $wR_2$ = 0.2391                                 |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.78/-0.37  |
| Flack parameter                             | 0.3(4)  |

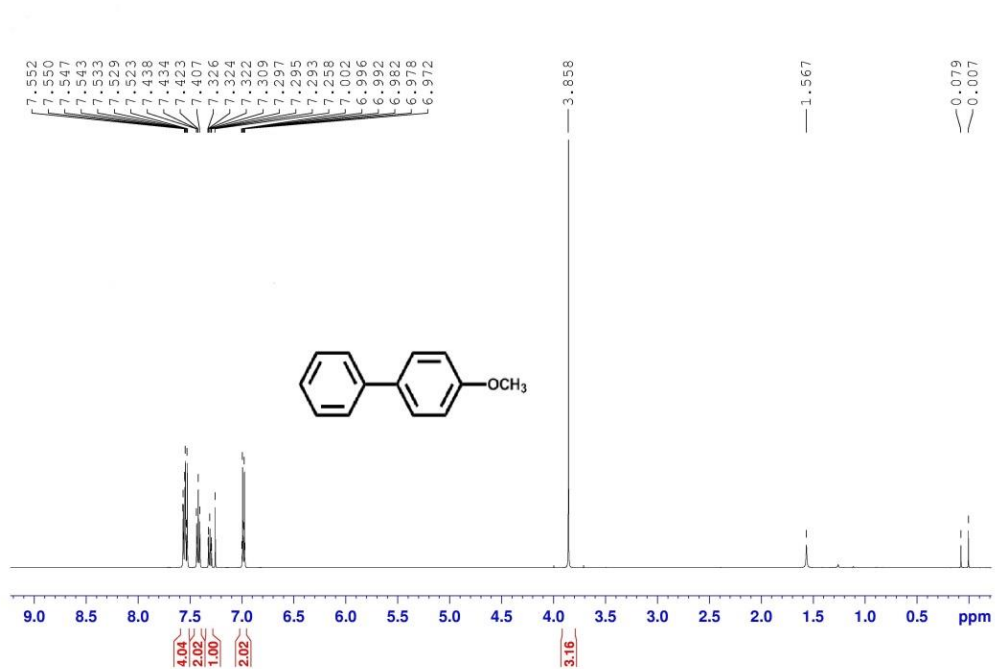
**Figure S5.**  $^1\text{H}$ NMR of 1-methyl-2-(4-methylphenyl)benzene.**Figure S6.**  $^1\text{H}$ NMR of 1-methoxy-4-(2-methylphenyl)benzene.

**Figure S7.**  $^1\text{H}$ NMR of 2-methylbiphenyl.**Figure S8.**  $^1\text{H}$ NMR of 3-methoxy-4'-methyl-1,1'-biphenyl.

**Figure S9.**  $^1\text{H}$ NMR of 3,4'-dimethoxy-1,1'-biphenyl.**Figure S10.**  $^1\text{H}$ NMR of 4,4'-dimethyl-1,1'-biphenyl.

**Figure S11.**  $^1\text{H}$ NMR of 4-methoxy-4'-methyl-1,1'-biphenyl.**Figure S12.**  $^1\text{H}$ NMR of 4-methyl-1,1'-biphenyl.



**Figure S13.**  $^1\text{H}$ NMR of 4-methoxy-1,1'-biphenyl**Figure S14.**  $^1\text{H}$ NMR of 4-nitro-1,1'-biphenyl.