

# **Molecular Assembly of Highly Symmetric Molecules under Hydrogen Bond Framework Controlled by Alkyl Building Blocks: A Simple Approach to Fine-tune Nano-scale Structures**

*Pimsai Tanphibal<sup>a</sup>, Kohji Tashiro<sup>\*\*b</sup> and Suwabun Chirachanchai<sup>\*,a,c</sup>*

*<sup>a</sup>The Petroleum and Petrochemical College, Chulalongkorn University, Bangkok 10330, Thailand*

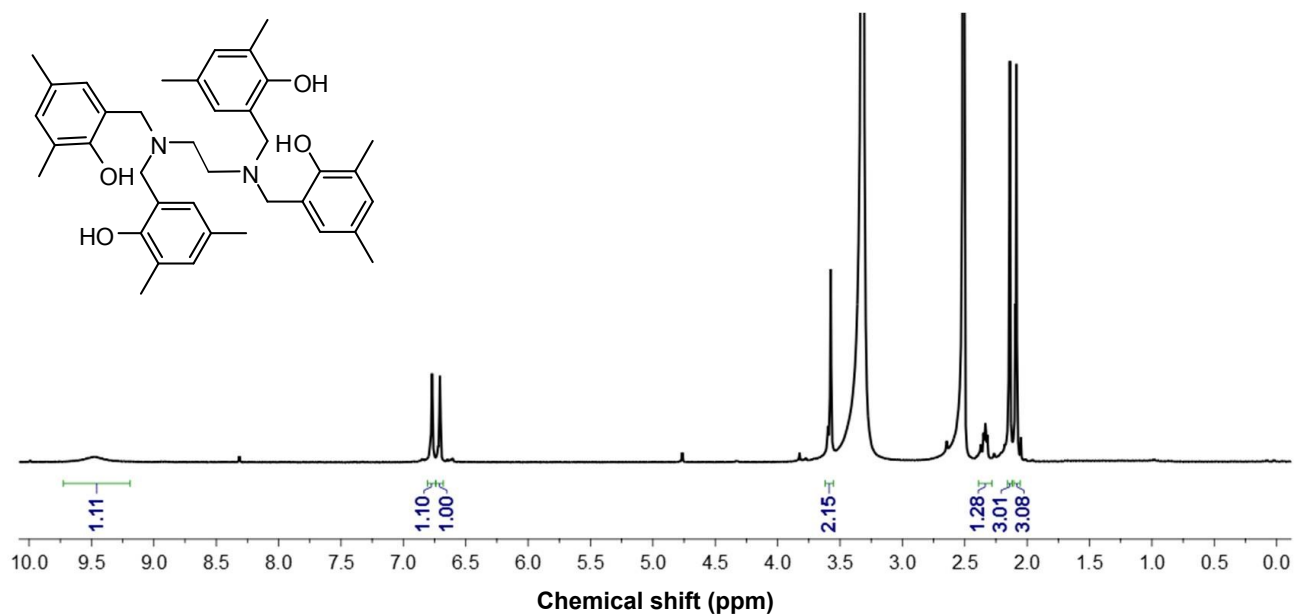
*<sup>b</sup>Department of Future Industry-oriented Basic Science and Materials, Toyota Technological Institute,*

*Tempaku, Nagoya 468-8511, Japan*

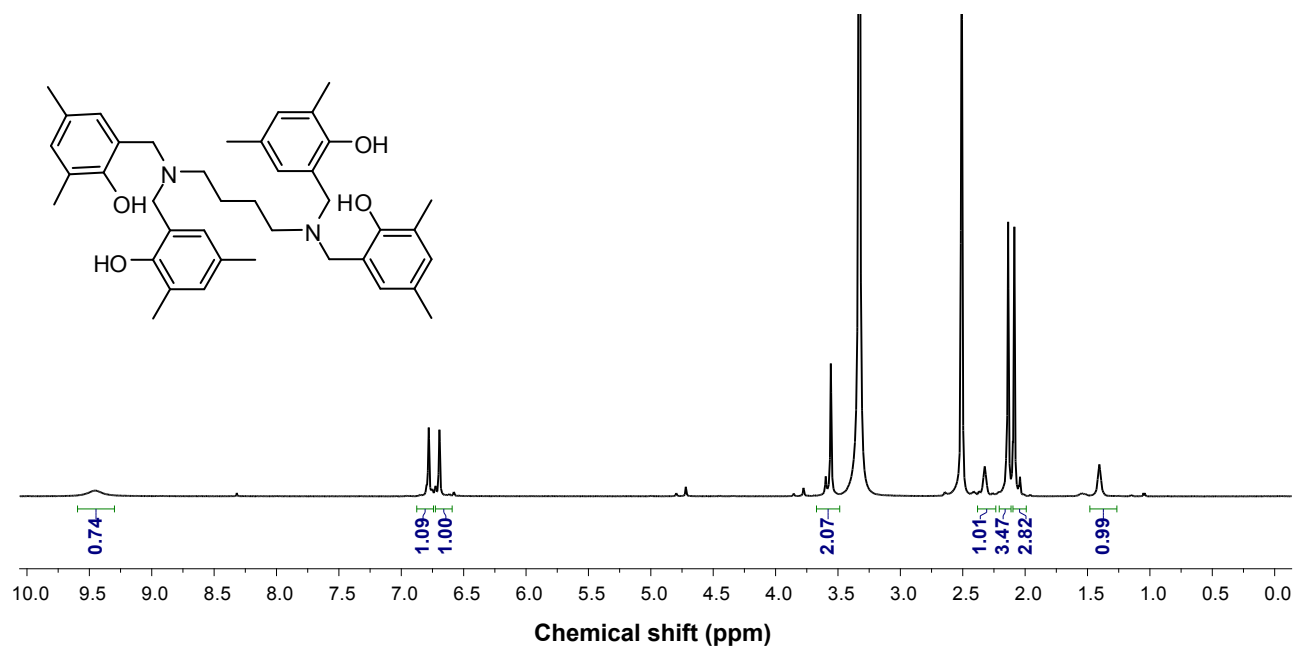
*<sup>c</sup>Center for Petroleum, Petrochemical, and Advance Materials, Chulalongkorn University, Bangkok*

*10330, Thailand*

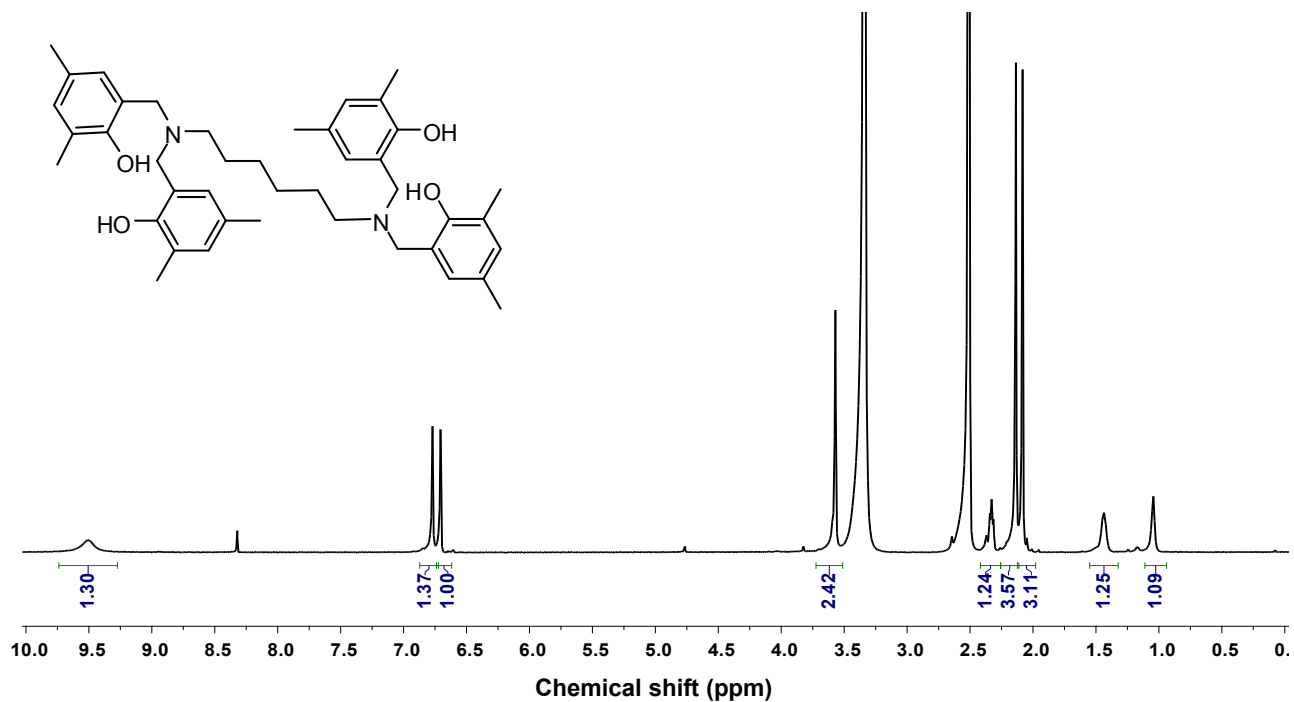
Corresponding author E-mail address: \*[csuwabun@chula.ac.th](mailto:csuwabun@chula.ac.th), \*\*[ktashiro@toyota-ti.ac.jp](mailto:ktashiro@toyota-ti.ac.jp)



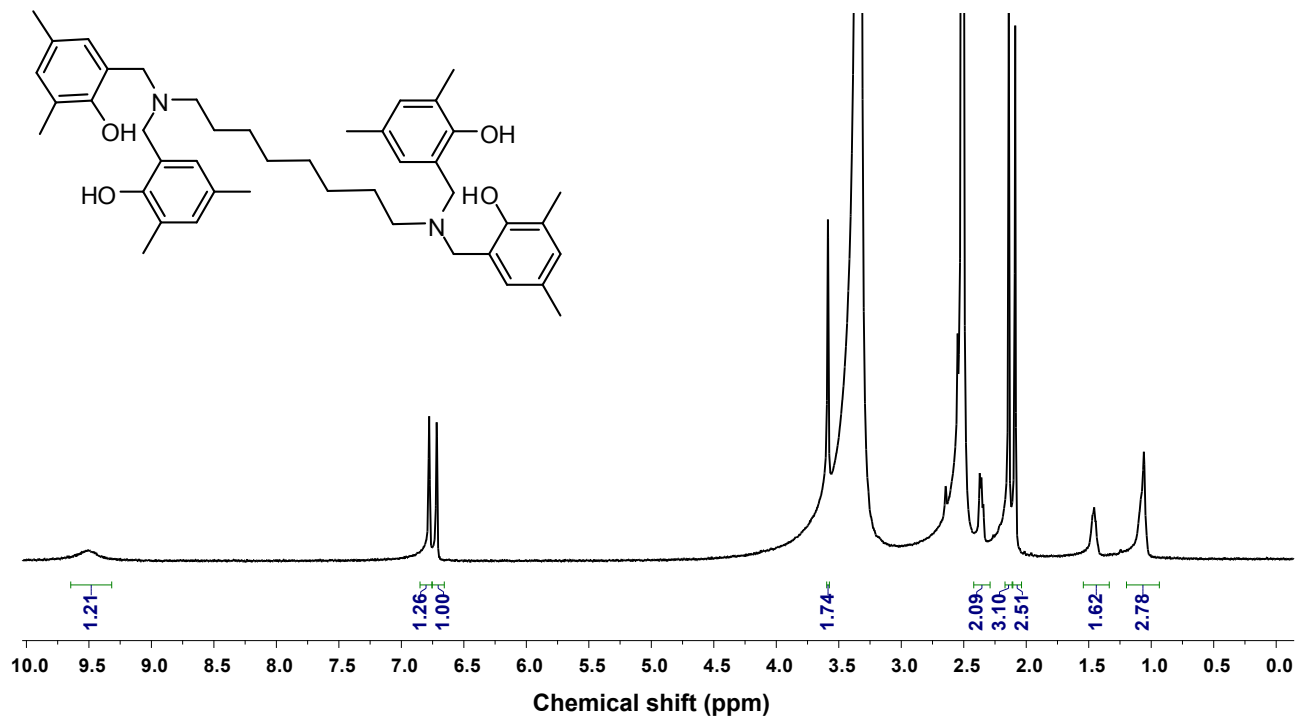
**Figure S1.**  $^1\text{H-NMR}$  spectrum of **C2** in  $\text{DMSO-}d_6$  (500 MHz) at 25 °C.



**Figure S2.**  $^1\text{H-NMR}$  spectrum of **C4** in  $\text{DMSO-}d_6$  (500 MHz) at 25 °C.



**Figure S3.** <sup>1</sup>H-NMR spectrum of C6 in DMSO-*d*<sub>6</sub> (500 MHz) at 25 °C.

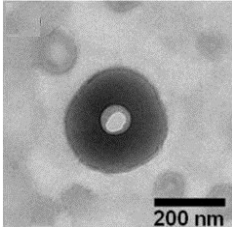
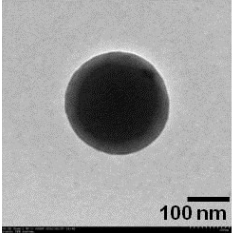
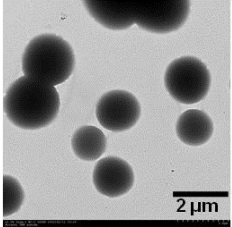
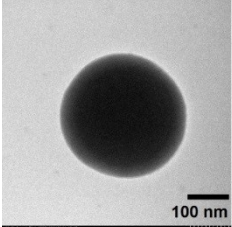
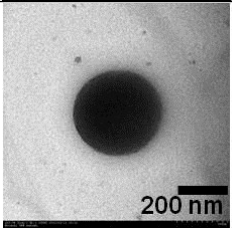
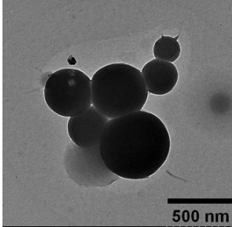


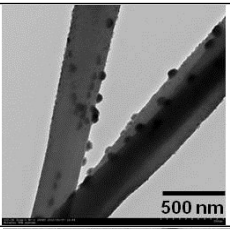
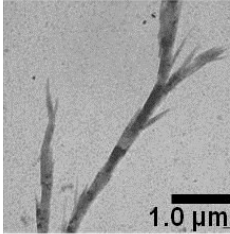
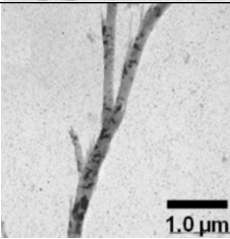
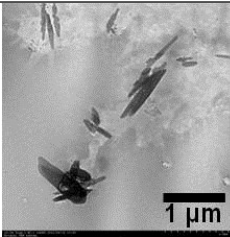
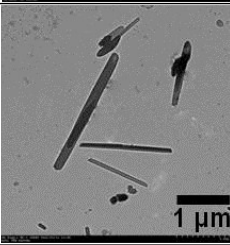
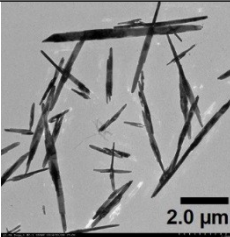
**Figure S4.** <sup>1</sup>H-NMR spectrum of C8 in DMSO-*d*<sub>6</sub> (500 MHz) at 25 °C.

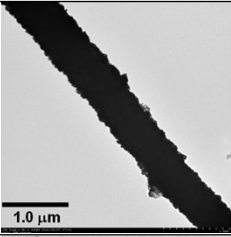
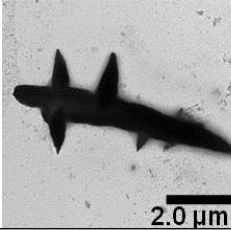
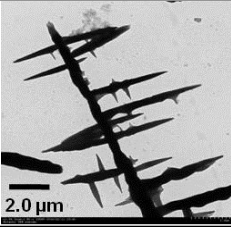
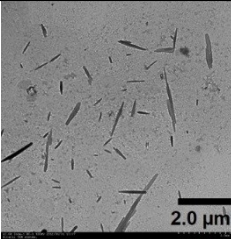
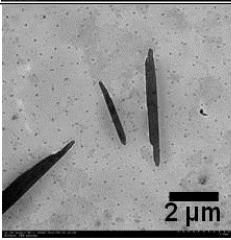
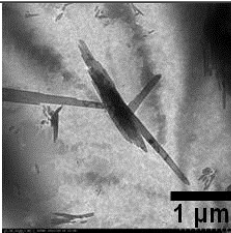
**Table S1.** Crystal data and structure refinement parameters for **C2**, **C4**, **C6**, and **C8**.

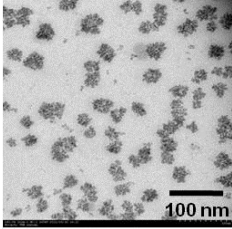
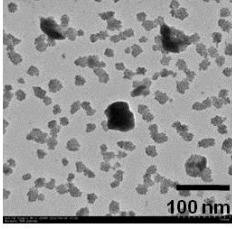
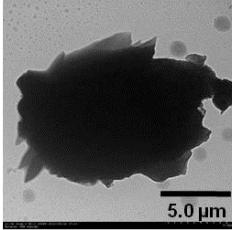
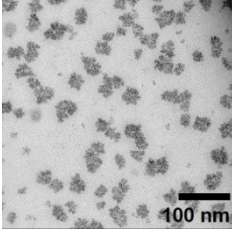
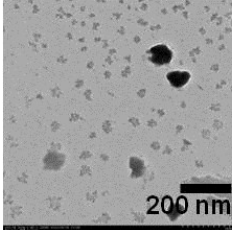
<b>Compound</b>	<b>C2</b>	<b>C4</b>	<b>C6</b>	<b>C8</b>
Empirical Formula	C <sub>38</sub> H <sub>48</sub> N <sub>2</sub> O <sub>4</sub>	C <sub>42</sub> H <sub>58</sub> N <sub>2</sub> O <sub>5</sub> S	C <sub>42</sub> H <sub>56</sub> N <sub>2</sub> O <sub>6</sub>	C <sub>44</sub> H <sub>60</sub> N <sub>2</sub> O <sub>4</sub>
Formula weight	596.81	702.99	652.92	680.97
Crystal system	Triclinic	Monoclinic	Monoclinic	Tetragonal
Space group	$P\bar{1}$	$P2_1/c$	$C2/c$	$P4_212$
<i>Unit cell dimension</i>				
<i>a</i> / Å	8.324(2)	9.8772(6)	10.426(4)	10.369(6)
<i>b</i> / Å	9.203(2)	18.7760(11)	26.794(9)	10.369(6)
<i>c</i> / Å	11.889(3)	12.3743(7)	14.099(5)	37.645(2)
$\alpha$ / °	84.965(3)	90.000	90.000	90.000
$\beta$ / °	88.978(3)	98.3301(17)	107.728(3)	90.000
$\gamma$ / °	69.436(3)	90.000	90.000	90.000
Unit cell volume/ Å <sup>3</sup>	849.3(3)	2270.6(2)	3752	4047.3(4)
Temperature/ K	296(1)	296(1)	296(1)	296(1)
Z	1	2	4	4
Radiation type	MoK $\alpha$	MoK $\alpha$	MoK $\alpha$	MoK $\alpha$
Absorption coefficient, $\mu$ / cm <sup>-1</sup>	0.748	1.103	0.732	0.703
No. of reflection measured	8361	22337	18478	5836
No. of independent reflections	3855	5187	4314	4627
R <sub>int</sub>	0.0408	0.0652	0.0272	0.0347
Final R <sub>1</sub> values	0.0665 [ $I > 2.5\sigma(I)$ ]	0.1066 [ $I > 3\sigma(I)$ ]	0.0791 [ $I > 2\sigma(I)$ ]	0.0505 [ $I > 2\sigma(I)$ ]
Final wR(F <sup>2</sup> ) values	0.1295 [ $I > 2.5\sigma(I)$ ]	0.1716 [ $I > 3\sigma(I)$ ]	0.1453 [ $I > 2\sigma(I)$ ]	0.0923 [ $I > 2\sigma(I)$ ]
Goodness of fit on $F^2$	2.766	9.108	2.541	1.513

**Table S2.** Morphologies of **C2**, **C4**, **C6**, and **C8** obtained from DMSO and chloroform at different concentrations.

Compound	Solvent	Concentration (mM)	Morphology
<b>C2</b>	DMSO	0.001	
		1.0	
		100	
	CHCl <sub>3</sub>	0.001	
		1.0	
		100	

Compound	Solvent	Concentration (mM)	Morphology
C4	DMSO	0.001	
		1.0	
		100	
	CHCl <sub>3</sub>	0.001	
		1.0	
		100	

Compound	Solvent	Concentration (mM)	Morphology
C6	DMSO	0.001	
		1.0	
		100	
	CHCl <sub>3</sub>	0.001	
		1.0	
		100	

Compound	Solvent	Concentration (mM)	Morphology
C8	DMSO	0.001	
		1.0	
		100	
	CHCl <sub>3</sub>	0.001	
		1.0	
		100	