Simple N,N′-Dicyclohexylurea adduct of β-alanine can self-assemble to generate nano-morphological versatility in response to different environmental conditions

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Fourier-transform infrared spectra of as synthesized Boc-β-Ala-N,N'-Dicyclohexylurea.

Fourier-transform infrared spectra of methanol treated Boc-β-Ala-N,N'-Dicyclohexylurea.

**Fig. S1** Fourier-transform infrared spectra of as synthesized Boc-β-Ala-N,N'-Dicyclohexylurea and methanol treated Boc-β-Ala-N,N'-Dicyclohexylurea.
Table S1 Contact angle measurement study of de-ionized water on different SAM grown on glass surface.

<table>
<thead>
<tr>
<th>Type</th>
<th>Contact angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-NH2 SAM</td>
<td>50.11</td>
</tr>
<tr>
<td>-SH SAM</td>
<td>68.93</td>
</tr>
<tr>
<td>-CH₃ SAM</td>
<td>92.06</td>
</tr>
<tr>
<td>-C8 SAM</td>
<td>99.4</td>
</tr>
</tbody>
</table>

Fig. S2 TEM image showing rupture of Boc-β-Ala-N,N′-Dicyclohexylurea vesicles by addition of bio-compatible Potassium salt (10 mM KCL salt solution).
$^1$H NMR spectrum of Boc-β-Ala-N,N'-Dicyclohexylurea in CDCl₃ (300 MHz).


An ORTEP representation of the molecular structures of BocNH(CH₂)₂CON(C₆H₁₁)CONH(C₆H₁₁), in the solid state. The thermal ellipsoids are shown to the 50% probability level.
Crystal data: C21H37N3O4, Mr = 395.54, monoclinic, \( a = 16.015(10) \text{Å}, b = 9.068(3) \text{Å}, c = 17.893(21) \text{Å}, \beta = 114.432(2)°, V = 2365.7(2) \text{Å}^3, T = 294 \text{K}, \) space group P21/c, \( Z = 4, \mu = 0.077 \text{mm}^{-1}, \) 7459 reflections measured, 3973 unique reflections, \( R_{int} = 0.031. \)

The experimental data were collected at room temperature using a Nonius-Kappa CCD diffractometer with Mo–Kα radiation (\( \lambda = 0.7107 \text{ Å} \)) and the \( \phi-\omega \) scan technique [0 ≤ \( h \) ≤ 18, 0 ≤ \( 0 \) ≤ 10, −20 ≤ \( l \) ≤ 18]. The structure was solved by direct methods (SHELXS-97). The non-hydrogen atoms were refined anisotropically using full-matrix least squares on \( F^2 \) (SHELXL-97). The final R-value was 0.0624 for 3064 \( F_o > 4\sigma(F_o) \), \( wR^2 = 0.1813, S = 1.066 \) using 386 parameters and no restraints. The weighting scheme,

\[
  w = \frac{1}{[\sigma^2(Fo^2) + (0.0828*P)^2 + 0.87*P]} where \ P = (\text{Max}(Fo^2, 0) + 2*Fc^2)/3 gave satisfactory analysis of the variance.
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