

# Supplementary data

## Peptide foldamers composed of six-membered ring $\alpha,\alpha$ - disubstituted $\alpha$ -amino acid with two changeable chiral acetal moieties

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**Table S1.** Crystal and diffraction parameters of peptides **7** and **8'**. ----- S2

**Figure S1.** Plots of N-H chemical shifts and the bandwidth of the N-H protons

of Cbz- $\{(R,R)\text{-Ac}_6\text{C}^{35\text{dBu}}\}_4\text{-OMe}$  (**9**). ----- S3

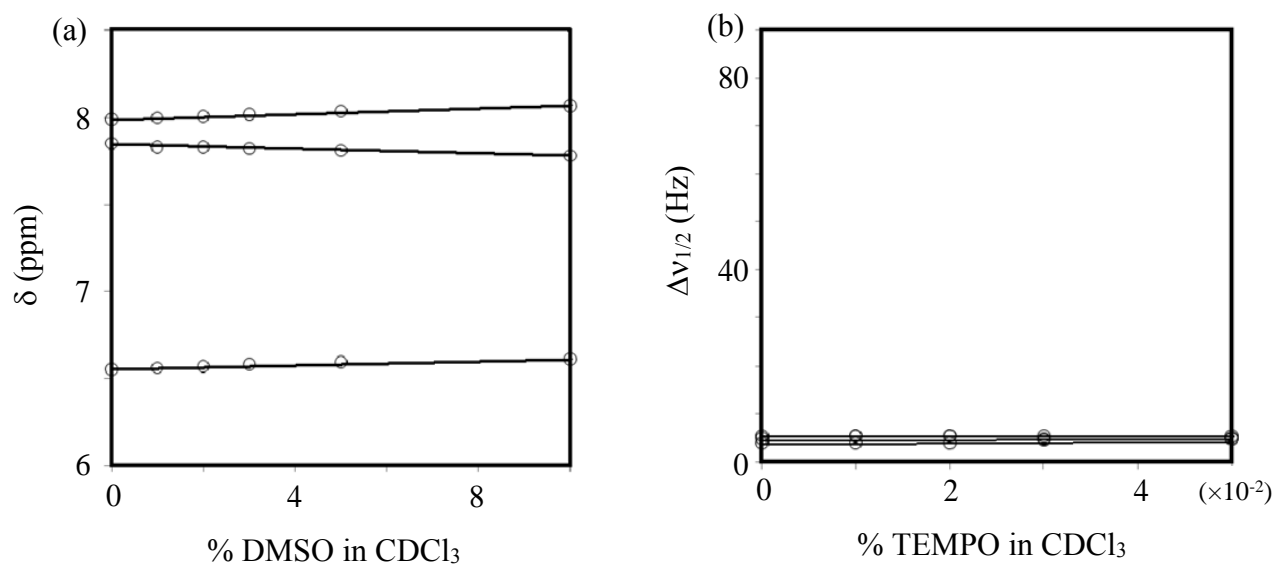
**Figure S2.** CD spectrum of Cbz- $\{(R,R)\text{-Ac}_6\text{C}^{35\text{dBu}}\}_4\text{-OMe}$  (**9**) in TFE solution. ----- S4

**Figure S3.** ORTEP drawing of **7** and **8'** ----- S5-6

Table S1. Crystal and diffraction parameters of peptides 7 and 8'.

	Dipeptide 7	Tripeptide acid 8'
empirical formula	C <sub>39</sub> H <sub>56</sub> N <sub>2</sub> O <sub>13</sub> , C <sub>2</sub> H <sub>6</sub> O	C <sub>53</sub> H <sub>77</sub> N <sub>3</sub> O <sub>18</sub>
<i>Mr</i>	806.93	1044.18
crystal dimensions [mm]	0.50×0.40×0.30	0.40×0.40×0.15
crystal system	monoclinic	monoclinic
lattice parameters:		
<i>a</i> , <i>b</i> , <i>c</i> [Å]	36.527, 15.063, 17.016	10.0377, 19.7698, 28.323
$\alpha$ , $\beta$ , $\gamma$ [°]	90, 112.83, 90	90, 90.707, 90
<i>V</i> [Å <sup>3</sup> ]	8629	5620.1
space group	<i>C</i> 2	<i>P</i> 2 <sub>1</sub>
<i>Z</i> value	8	4
<i>D</i> <sub>calc</sub> [g/cm <sup>3</sup> ]	1.242	1.234
$\mu$ (MoK $\alpha$ ) [cm <sup>-1</sup> ]	0.93	0.93
no. of observations ( <i>I</i> > - 10.0 $\sigma$ <i>I</i> )	9175	10975
no. of variables	1026	1333
<i>R</i> <sub><i>I</i></sub> , <i>R</i> <sub><i>W</i></sub>	0.0626, 0.1386	0.0583, 0.1473
solvent	EtOH	petroleum ether/CHCl <sub>3</sub>

**Figure S1.** (a) Plots of N-H chemical shifts in the  $^1\text{H}$  NMR spectra of Cbz- $\{(R,R)\text{-Ac}_6\text{C}^{35\text{dBu}}\}_4\text{-OMe}$  (**9**) as a function of increasing percentage of DMSO (v/v) added to the  $\text{CDCl}_3$  solution and (b) plots of the bandwidth of the N-H protons of **9** as a function of increasing percentage of TEMPO (w/v) added to the  $\text{CDCl}_3$  solution. One N-H proton overlapped with Cbz-protecting group. Peptide concentration 1.0 mM.



**Figure S2.** CD spectrum of Cbz- $\{(R,R)\text{-Ac}_6\text{C}^{35\text{dBu}}\}_4\text{-OMe}$  in TFE solution. Peptide concentration 0.1 mM.

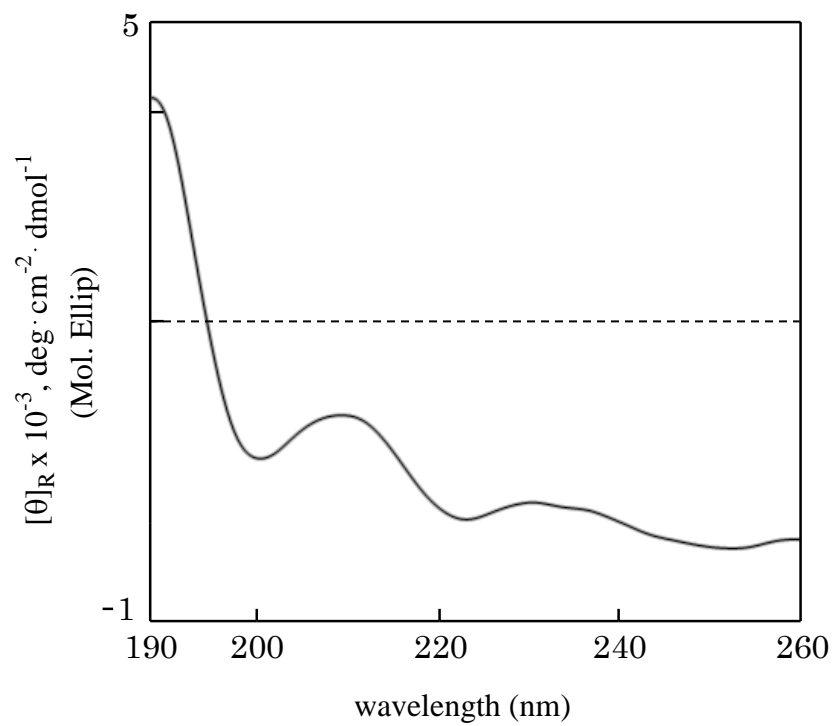
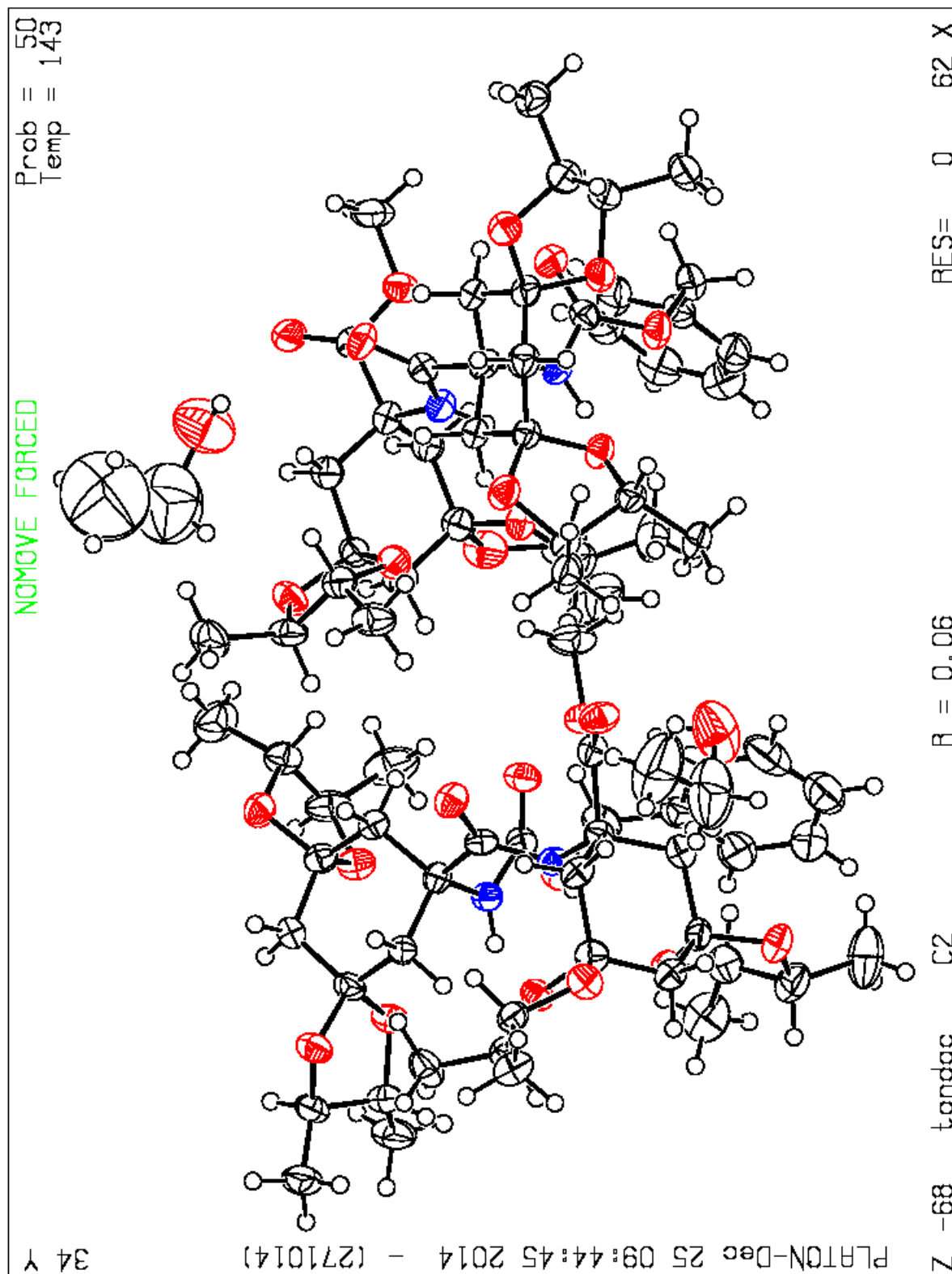


Figure S3. ORTEP drawings

a) Dipeptide (7)



b) Tripeptide acid (8')

