

Supporting information

SYNTHESIS.....	S2
Synthesis of homooligourea 5	S2
Synthesis of α -heptapeptide 6 on solid support	S2
Scheme S1 : Synthesis of peptide 6 on solid support using microwave irradiation.	S2
ADDITIONAL ^1H -NMR DATA.....	S3
Figure S1 . Amide NH resonances in the ^1H NMR spectrum of chimera 14-mer 1 recorded at 700 MHz in CD_3OH . Reported $^3J(\text{NH}, \alpha\text{CH})$ values for α -amino acid residues are in Hz.	S3
Figure S2 . $^1\text{H}, ^{15}\text{N}$ -HSQC spectrum of 1 recorded at 700 MHz in CD_3OH	S4
Figure S3 . Amide NH resonances in the ^1H NMR spectrum of chimera 13-mer 2 recorded at 700 MHz in CD_3OH . Reported $^3J(\text{NH}, \alpha\text{CH})$ values for α -amino acid residues are in Hz.	S5
Figure S4 . $^1\text{H}, ^{15}\text{N}$ -HSQC spectrum of 2 recorded at 700 MHz in CD_3OH	S6
Table S1 : $^3J(\text{NH}, ^\beta\text{CH})$ coupling constants (in Hertz) for ethylene diamine residues in the oligourea domains of chimera 1 in CD_3OH (700 MHz) at 4 mM	S6
Table S2 : $^3J(\text{NH}, ^\beta\text{CH})$ coupling constants (in Hertz) for ethylene diamine residues in the oligourea domains of chimera 2 in CD_3OH (700 MHz) at 4 mM	S6
CIRCULAR DICHROISM.....	S7
Figure S5 : CD spectra of chimera 2 in MeOH, oligourea 5 in MeOH and peptide 6 in MeOH and TFE, all recorded at 20°C at 0.05mM.	S7
Table S3 : Molar ellipticity values at 222 nm for chimera 2 , oligourea 5 and peptide 6 (0.05mM).	S7
Figure S6 : CD spectra of chimera 1 and oligourea 5 recorded at 20°C in MeOH at 0.05mM.	S8

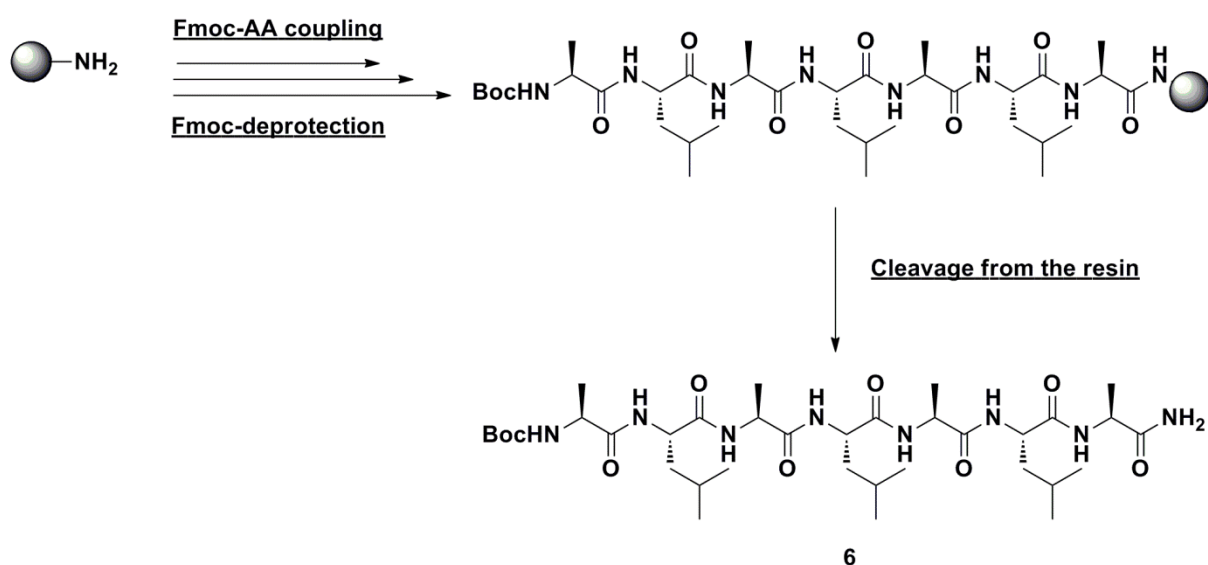
SYNTHESIS

Synthesis of homooligourea 5

Boc-Val^u-Ala^u-Leu^u-Val^u-Ala^u-Leu^u-NH₂ (5)

The synthesis of model homooligourea **5** was previously described¹.

Synthesis of α -heptapeptide 6 on solid support



Scheme S1 : Synthesis of peptide **6** on solid support using microwave irradiation.

Boc-Ala-Leu-Ala-Leu-Ala-Leu-Ala-NH₂ (6)

6 was synthesized according to GP1, GP2 and GP5, starting from Sieber resin (162mg, 0.10 mmol, loading: 0.62mmol/g) and Fmoc- α -AA (0.40 mmol, 4eq relative to the resin loading). The final product **6** was purified by semi preparative HPLC. 2 mg were obtained with total yield of 4%. **ESI-MS** (M_w 740.93) m/z 741.20 $[\text{M} + \text{H}]^+$, 763.53 $[\text{M} + \text{Na}]^+$; **HPLC** (H_2O (0.1% TFA), MeOH (0.1% TFA); gradient 50-100%, 5 min; 100%, 5min) $t_R = 5.74$ min.

¹ Y. R. Nelli, S. Antunes, A. Salaün, E. Thinon, S. Massip, B. Kauffmann, C. Douat, G. Guichard, *Chem. Eur. J.* **2015**, *21*, 2870-2880.

ADDITIONAL ^1H -NMR DATA

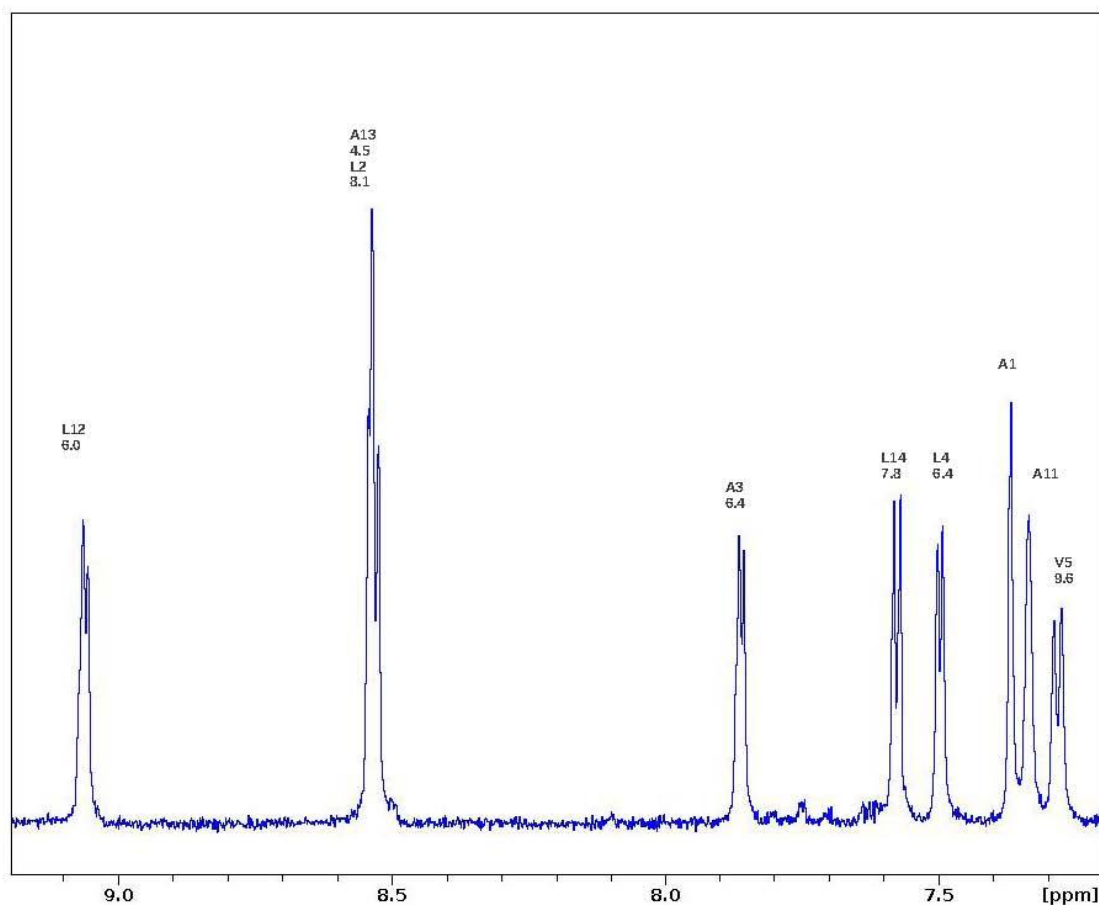


Figure S1. Amide NH resonances in the ^1H NMR spectrum of chimera 14-mer **1** recorded at 700 MHz in CD_3OH . Reported $^3\text{J}(\text{NH}, \alpha\text{CH})$ values for α -amino acid residues are in Hz.

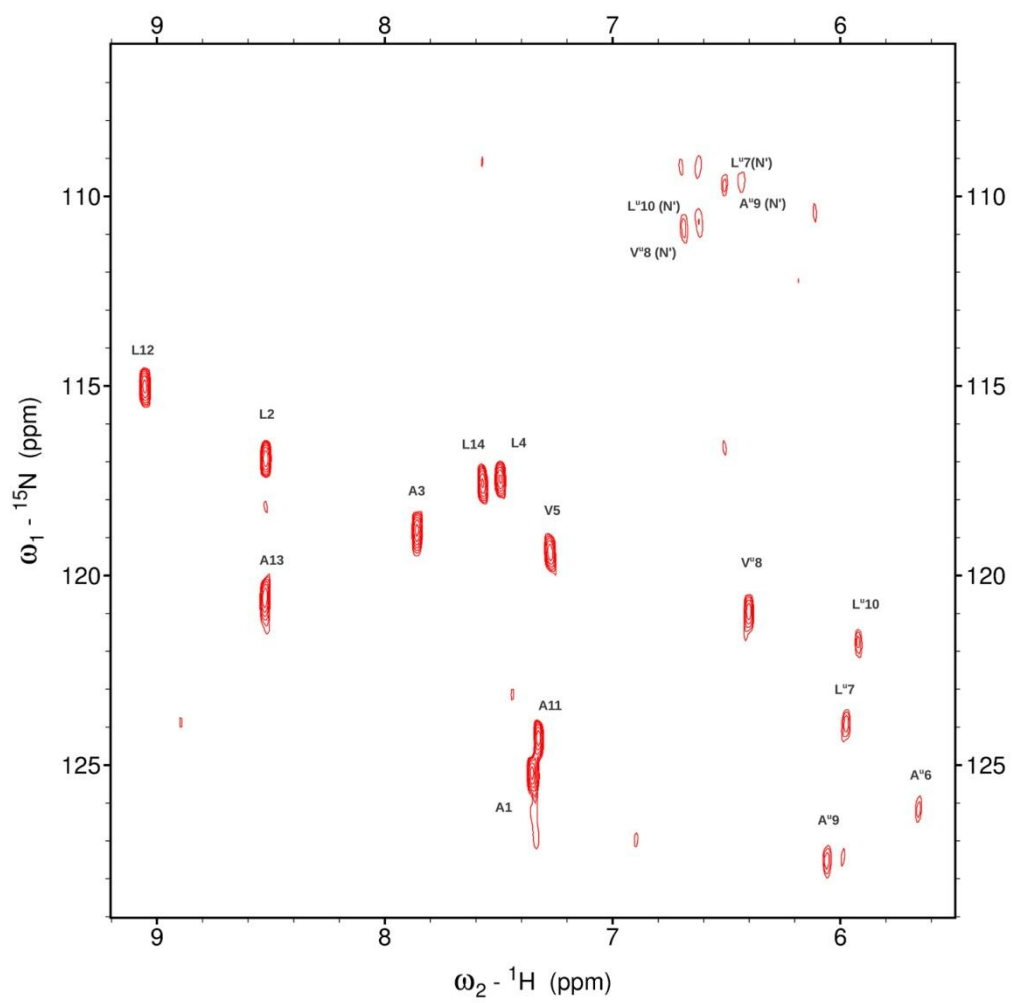


Figure S2. ^1H , ^{15}N -HSQC spectrum of **1** recorded at 700 MHz in CD_3OH .

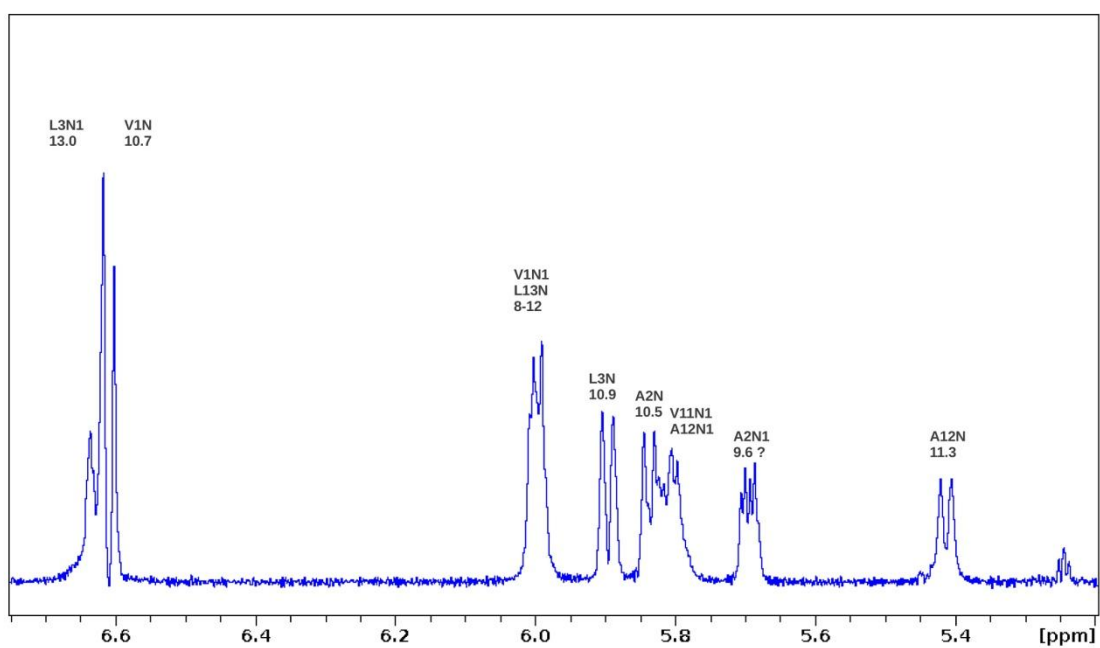
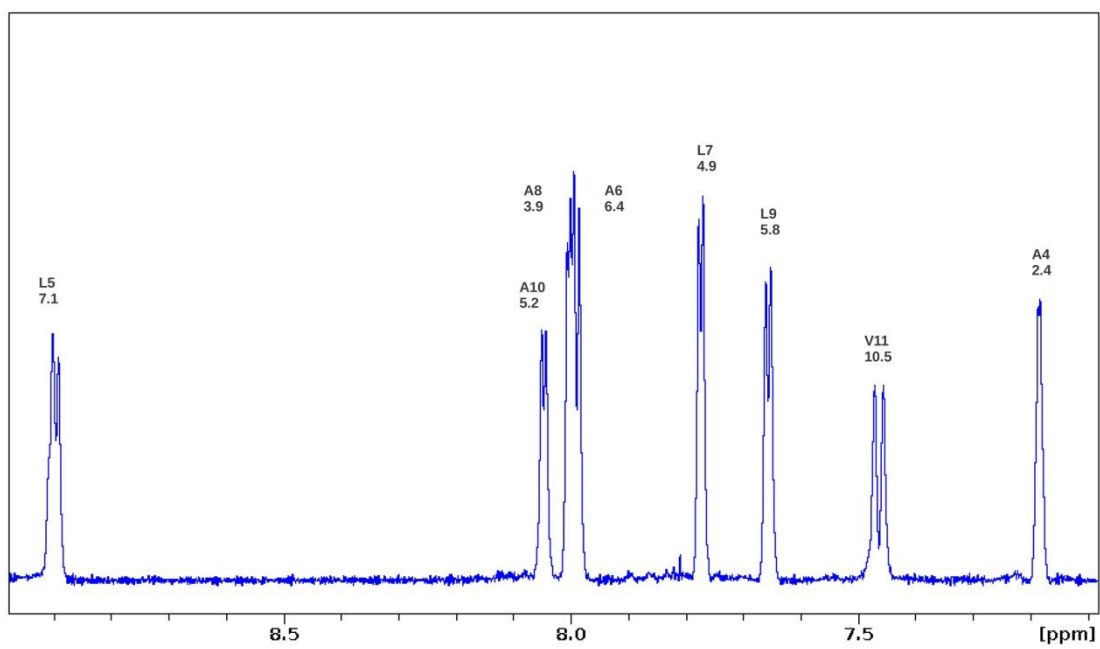


Figure S3. Amide NH resonances in the ^1H NMR spectrum of chimera 13-mer **2** recorded at 700 MHz in CD_3OH . Reported $^3\text{J}(\text{NH}, \alpha\text{CH})$ values for α -amino acid residues are in Hz.

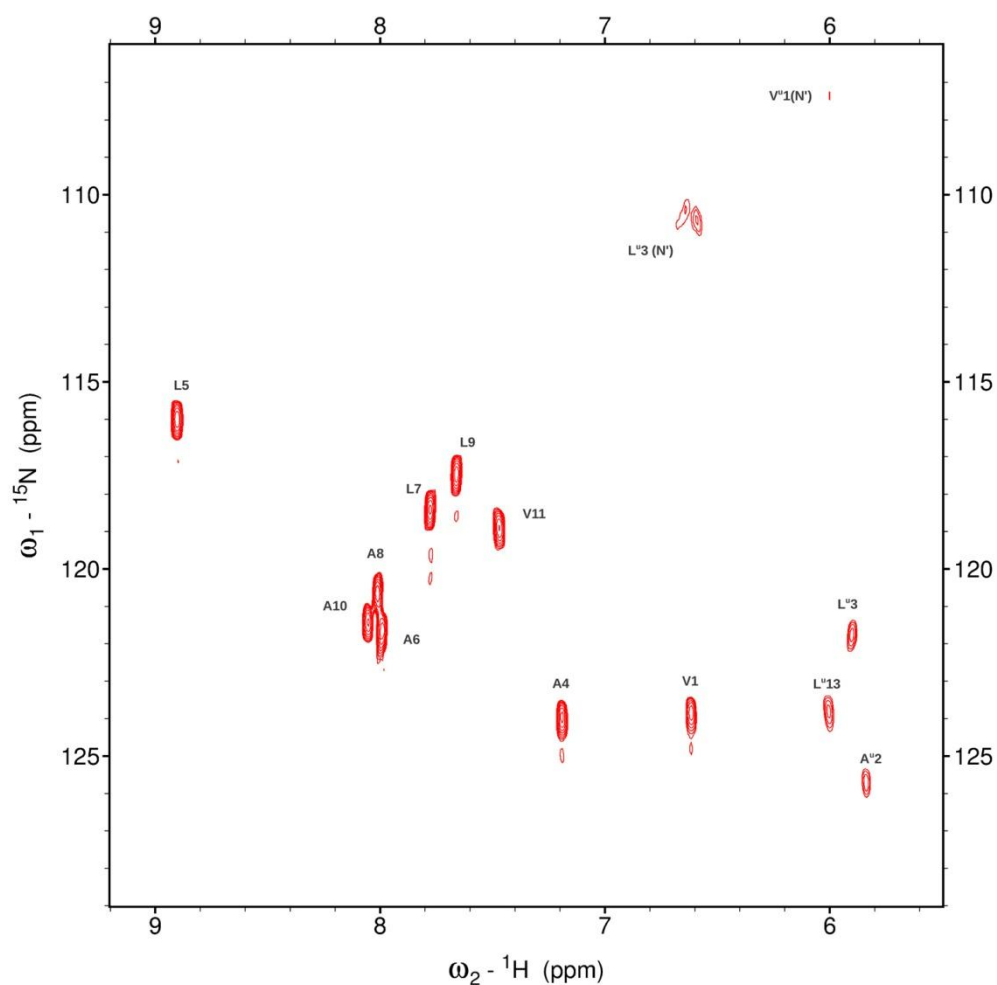


Figure S4. ^1H , ^{15}N -HSQC spectrum of **2** recorded at 700 MHz in CD_3OH .

Table S1 : $^3J(\text{NH}, ^\beta\text{CH})$ coupling constants (in Hertz) for ethylene diamine residues in the oligoureia domains of chimera **1** in CD_3OH (700 MHz) at 4 mM

Compd	Solvent	peptide	Val ^u	Ala ^u	Leu ^u	Val ^u	Ala ^u	Leu ^u	peptide
1	CD_3OH	Boc-A-L-A-L	9.6	11.5	12.5	12.3	10.7	12.1	A-L-A-L-NH ₂

Table S2 : $^3J(\text{NH}, ^\beta\text{CH})$ coupling constants (in Hertz) for ethylene diamine residues in the oligoureia domains of chimera **2** in CD_3OH (700 MHz) at 4 mM

Compd	Solvent	Boc-Val ^u	Ala ^u	Leu ^u	peptide	Val ^u	Ala ^u	Leu ^u -NH ₂
2	CD_3OH	10.7	9.6	10.9	A-L-A-L-A-L-A	10.5	11.3	ND

Circular dichroism

All CD spectra were recorded on a J-815 Jasco dichrographe (Jasco France, Nantes, France). Electronic Circular dichroism (ECD) spectra of chimeras **1** and **2**, oligourea **5** and heptapeptide **6** and were acquired between 300 and 180 nm at a concentration of 0.05 mM in MeOH or TFE using a quartz cell with a path length of 5 mm. Sample temperature was regulated at 20°C. Data were collected in continuous scan mode with a data pitch of 0.1 nm, a scanning speed of 50 nm.min⁻¹, 2 nm bandwidth and 2 accumulations per sample. Sample Data were collected as raw ellipticity (ψ in mdeg) and converted to molar ellipticity $[\theta]$ in deg.cm².dmol⁻¹ using the following equation:

$$[\theta] = \frac{\psi \times 10^{-3}}{l \times c}$$

Where l is the pathlength in cm, and c is the peptide concentration in dmol.cm⁻³

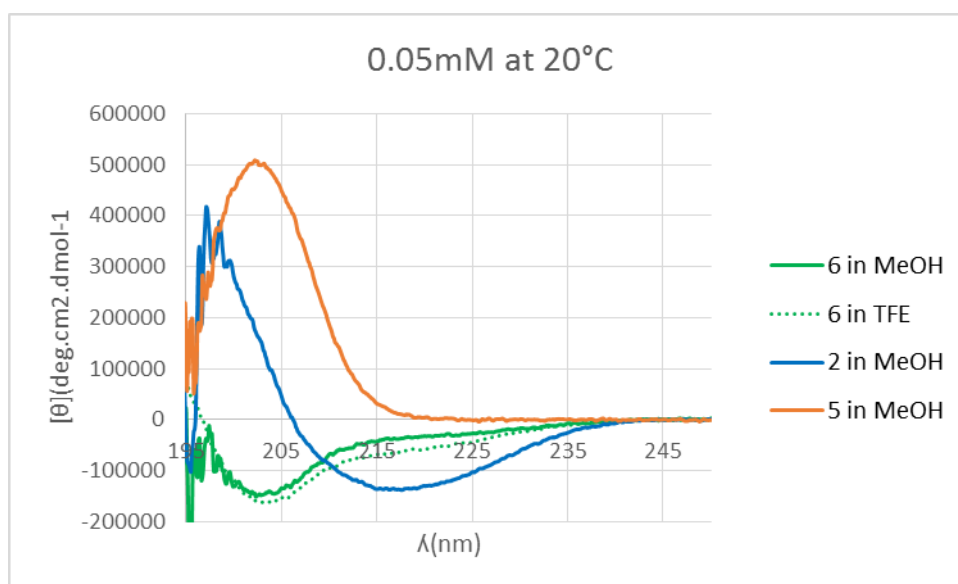


Figure S5: CD spectra of chimera **2** in MeOH, oligourea **5** in MeOH and peptide **6** in MeOH and TFE, all recorded at 20°C at 0.05mM.

Table S3: Molar ellipticity values at 222 nm for chimera **2**, oligourea **5** and peptide **6** (0.05mM).

		5	2	6
Solvent	Temperature	$[\theta]$ (deg.cm ² .dmol ⁻¹)	$[\theta]$ (deg.cm ² .dmol ⁻¹)	$[\theta]$ (deg.cm ² .dmol ⁻¹)
MeOH	20°C	2 181	-123 526	-31 267
TFE	20°C			-50 996

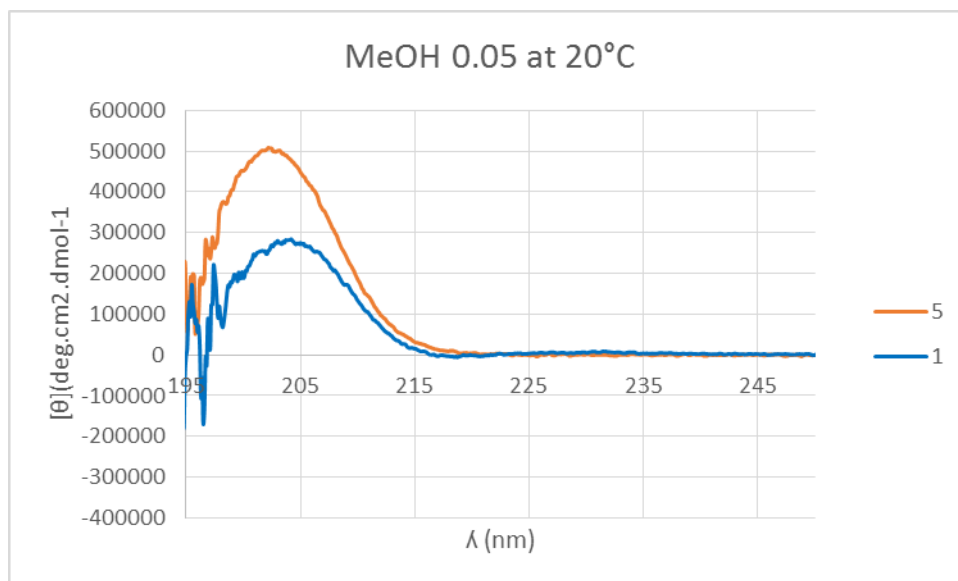


Figure S6: CD spectra of chimera **1** and oligourea **5** recorded at 20°C in MeOH at 0.05mM.