SUPPORTING INFORMATION:

Microwave-assisted click polymerization for the synthesis of Aβ(16-22) cyclic oligomers and their self-assembly into polymorphous aggregates

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$^{13}$C-NMR (75.5 MHz, CDCl$_3$/CD$_3$OD (9:1 v/v)) of Fmoc-Glu(OH)-propargyl amide 3.
$^1$H-NMR (300 MHz, DMSO-d$_6$) of peptide 1.
$^{13}$C-NMR (75.5 MHz, DMSO-d$_6$) of peptide 1.
$^1$H-COSY-NMR (300 MHz, DMSO-d$_6$) of peptide 1.
Analytical HPLC analysis of crude peptide 1 (top: UV; bottom: ELSD trace).
EI-MS spectrum of peptide 1; C_{46}H_{65}N_{11}O_{9} requires m/z [M + H]^+ monoisotopic 916.67, [M + H]^+ ave 918.19, [M + Na]^+ ave 940.21, [M + CH_3CN]^+ ave 940.21.
Preparative HPLC run of click polymerization product of peptide 1. (fractions # 3 – 5 represent peptide 9 and fractions # 7 – 8 represent peptide 8)
Analytical HPLC analysis of cyclic peptide 8.

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MALDI-TOF spectrum of peptide 8; C_{46}H_{65}N_{11}O_{9} requires m/z [M + H]^+ monoisotopic 916.672, [M + Na]^+ monoisotopic 938.627.
Analytical HPLC analysis of peptide 9.

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| Totals | | | 5393805 | 100.00 |

cinde
MALDI-TOF spectrum of peptide 9, C_{92}H_{130}N_{22}O_{18} requires 1830.994, found m/z (M + H)^+ monoisotopic 1831.542.
FTIR spectrum of peptide 1 (ν\(_{\text{max}}/\text{cm}^{-1} 2108 (N_3))$).

FTIR spectrum of the crude polymerization mixture (oligomers of peptide 1).
FTIR spectrum of peptide 8 (cyclic monomer of peptide 1).

FTIR spectrum of peptide 9 (cyclic dimer of peptide 1).
Computational modeling. A lowest energy conformation of peptides 1 and 8 were performed on a SiliconGraphics O2 workstation with MacroModel 7.0 using the organic builder and the peptide builder in the grow mode.\textsuperscript{1} MMFF94 was used as a force field.\textsuperscript{2} After construction, the structures were minimized on an Origin200 Server using Molecular Mechanics calculations with the following settings: MMFF94 (GB/SA water solvent model, planar N's),\textsuperscript{1} MCMM (Monte Carlo Multiple Minimum, conformational search), PCRG, CCrit 0.01 kJ(molÅ)\textsuperscript{-1}, iterations > max. Finally, a conformational search was carried out starting with the minimized structure using a Monte Carlo run which generated 1000 structures (all appropriate single bonds will become variable, all double bonds, amide bonds and ester bonds will become constrained, potential chiral centers will be set and flexible rings will be opened). The goal of the conformational searching was to locate the lowest-energy conformations of the structure of interest. The settings of a standard conformational search: Monte Carlo Multiple Minimum (MCMM), number of steps: 1000, solvent: H\textsubscript{2}O. After each MCMM step, the structure was again minimized (with the same settings as above).

2. MMFF94, or MMFF for short by T. A. Halgren, in: \textit{J. Comput. Chem.}, 1996, 17, issues 5 and 6, 490-641. This two-volume series contain five articles introducing MMFF94 as a good force field for biopolymers (peptides and proteins) and many organic molecules.

RCG: conjugate gradient minimization using the Polak-Ribiere first derivative method with restarts every 3N iterations; should not find saddle points; best general minimization method for energy minimization; BatchMin code for carrying out this method is highly vectorized for efficient operation on vector hardware, see: E. Polak, G. Ribiere, \textit{Revue Francaise Informat. Recherche Operationelle}, 1969, 16, 35.

Convergence criterion – energy, movement or gradient. Default is gradient (first derivative RMS) convergence (criterion = 0.01 kJ(molÅ)\textsuperscript{-1})

Iterations/stop: sets the maximum number of iterations Batchmin will use to energy minimize a structure; W. C. Still, A. Tempczyk, R. C. Hawley, T. Hendrickson, \textit{J. Am. Chem. Soc.}, 1990, 112, 6127-6129 (This solvent model provides a volume-based continuum model (the GB/SA model) for the electrostatic (polarization) component).
Image of the lowest energy conformation of peptide 1 (energy $-56.046 \text{ kJmol}^{-1}$).

Image of the lowest energy conformation of peptide 8 (energy $+6.372 \text{ kJmol}^{-1}$).