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Supporting information

Formation of toroid by self-assembly of α-α corner mimetic: supramolecular cyclization

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ESI Figure 1. Concentration dependent absorption spectra of peptidomimetic **1** in MeOH. With increasing concentration not only the intensity increasing but also the band at 212 nm shifted to 218 nm.



ESI Figure 2. Concentration dependent emission spectra of peptidomimetic 1 in MeOH.



ESI Figure 3: Time dependent SEM images showing the toroids formation.(a) 0h (b) 3h (c) 6h (d) 12h



ESI Figure 4. The ORTEP diagram of peptidomimetic **1** with atomic numbering scheme. 50% probability.



ESI Figure 5. Rod like supramolecular helical assembly of peptidomimetic 1 through water mediated inter molecular hydrogen bonding.



ESI Figure 6. Ball and stick model of cyclic supramolecular polymer of peptidomimetic **1** through water mediated inter molecular hydrogen bonding.



ESI Figure 7. (a) UV-vis spectra and (b) Fluorescence spectra of peptidomimetic 1 with increasing concentration of sulfamethoxazole

ESI Table 1.	SI Table 1. Selected backbone torsion angles (deg) for compound 1							
		Leucine	Tyrosine	Aib				
	ф/°	-72.31	-78.94	-49.25				
	$\psi/^{\circ}$	-4.93	-6.91	-34.90				

ESI Table 2. Hydrogen bonding parameters of Compound 1

D-HA	DH(Å)	HA(Å)	DA(Å)	D-HA (°)	
N2-H2O5	0.86	2.39	3.242(4)	172	
N1-H1O4	0.86	2.08	2.905(4)	162	
07.117.4 018	0.85	2.02	2 844(5)	164	
0/-н/А01"	0.85	2.02	2.844(5)	104	
O7-H7BO2 ^b	0.85	2.02	2.840(4)	164	

Symmetry equivalent

a = y, 1+x,-1-zb = 1/2+y,-3/2-x, 1/4+z

0 = 1/2 + y, -3/2 - x, 1/4 + 2



Scheme 1: Reactions and conditions: (a)H-Aib-OMe, DCC, HOBt, dry DCM, 0^oC, ,48h, 78% (b) 2(N) NaOH, MeOH, 12h, 87%(C)DCM,H-Tyr-OMe, DCC, HOBt, 0^oC,48h,70% (d)2(N) NaOH, MeOH, 12h, 83% (e)m-xylylenediamine,EDC,HOBt,0^oC,48h,Dry DCM,59%



Figure S1: ¹H NMR (500 MHz, DMSO-*d*₆) spectra of Boc-Leu-OH.



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Figure S3: ¹H NMR (500 MHz, CDCl₃) spectra of Boc-Leu-Aib-OMe.



Figure S4: ¹³C NMR (125 MHz, CDCl₃) spectra of Boc-Leu-Aib-OMe.



Figure S5:¹H NMR (500 MHz, DMSO- d_6) spectra of Boc-Leu-Aib-OH.



Figure S6: ¹³C NMR (125 MHz, DMSO-*d*₆) spectra of Boc-Leu-Aib-OH.



Figure S7: ¹H NMR (500 MHz, CDCl₃) spectra of Boc-Leu-Aib-Tyr-OMe.



Figure S8: ¹³C NMR (125 MHz, CDCl₃) spectra of Boc-Leu-Aib-Tyr-OMe.



Figure S9: Mass spectra of Boc-Leu-Aib-Tyr-OMe.



Figure S10 :¹H NMR (400 MHz, DMSO-*d*₆) spectra of Boc-Leu-Aib-Tyr-COOH.



Figure S11: ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of Boc-Leu-Aib-Tyr-COOH.



Figure S12: Mass spectra of Boc-Leu-Aib-Tyr-COOH.



Figure S14:¹³C NMR (100 MHz, DMSO- d_6) spectra of Compound 1.



Figure S15: Mass spectra of compound 1.