ChemBioChem

Supporting Information

Synthesis and Biological Studies of Dodecameric Cationic Antimicrobial Peptides Containing Tetrahydrofuran Amino Acids

Uttam Ghosh, Isha Soni, Grace Kaul, Priyanka Trivedi, Vinita Chaturvedi, Sidharth Chopra, and Tushar Kanti Chakraborty*

Supporting Information

^1H NMR spectrum (400 MHz, CDCl_3) of compound **2a**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **2a**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **3**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **3**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **4a**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4a**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **4b**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4b**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **5a**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **5a**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **1a**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **1a**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **1c**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **1c**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **6**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **6**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **2b**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **2b**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **1b**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **1b**

^1H NMR spectrum (400 MHz, CDCl_3) of compound **1d**

^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **1d**

^1H NMR spectrum of compound **9a** in $\text{DMSO}-d_6$ (400 MHz, 300K)

^1H NMR spectrum of compound **9b** in $\text{DMSO}-d_6$ (400 MHz, 300K)

Variable temperature study of peptide **9b** in DMSO-*d*₆ (400 MHz)

NH	303K	313K	323K	333K	$\Delta\delta/\Delta T$ (ppb/°K)
SAA ¹	6.66	6.60	6.52	6.44	7.33
Val ²	7.49	7.45	7.41	7.38	3.66
Orn ³	8.10	7.99	7.94	7.89	7.00
Orn ³ (sc)	6.54	6.48	6.41	6.32	7.33
Leu ⁴	7.52	7.47	7.43	7.41	4.33
SAA ⁵	7.76	7.71	7.65	7.60	5.33
Val ⁶	7.42	7.39	7.36	7.32	3.33
Orn ⁷	8.13	8.06	8.01	7.96	5.66
Orn ⁷ (sc)	7.89	7.84	7.77	7.71	6.00
Leu ⁸	7.67	7.62	7.56	7.51	5.33
SAA ⁹	7.86	7.81	7.75	7.68	6.00
Val ¹⁰	7.36	7.34	Mixed with phenyl region	Mixed with phenyl region	
Orn ¹¹	8.18	8.11	8.05	7.99	6.33
Orn ¹¹ (sc)	8.03	7.97	7.92	7.86	5.66
Leu ¹²	7.69	7.64	7.59	7.54	5.00

¹H NMR spectra of peptide **9b** at temperatures from 303-333 K (400 MHz, DMSO-*d*₆)

2D ^1H - ^1H TOCSY Spectrum of peptide **9b** (500 MHz, $\text{DMSO}-d_6$, 300 K)

CD Data Analysis: CD spectra were recorded at 298 K on Jasco J-815 spectrometer using 0.1 cm path length quartz cells. The peptides were prepared at concentrations of 0.1 mM in MeOH.

CD for tetrapeptide

CD for octapeptide

CD for dodecapeptide

^1H NMR spectrum of compound **9c** in $\text{DMSO}-d_6$ (400 MHz, 300 K)

^1H NMR spectrum of compound **9d** in $\text{DMSO}-d_6$ (400 MHz, 300 K)

^1H NMR spectrum of compound **10a** in $\text{DMSO-}d_6$ (400 MHz, 300 K)

^1H NMR spectrum of compound **10b** in $\text{DMSO-}d_6$ (400 MHz, 300 K)

^1H NMR spectrum of compound **10c** in $\text{DMSO-}d_6$ (400 MHz, 300 K)

^1H NMR spectrum of compound **10d** in $\text{DMSO-}d_6$ (400 MHz, 300 K)