C^{α} -Methyl-L-Valine: A Preferential Choice over α -Aminoisobutyric Acid for Designing Right-Handed α -Helical Scaffolds

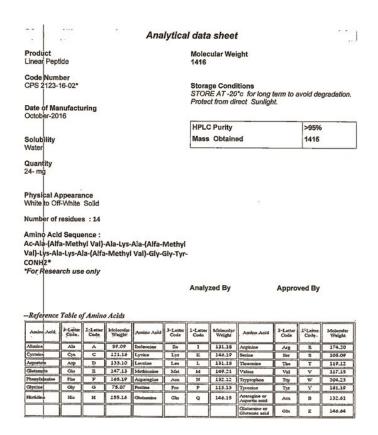
Raja Banerjee,*‡# Tridip Sheet,# Srijan Banerjee,# Barbara Biondi,† Fernando Formaggio,† Claudio Toniolo† and Cristina Peggion*†

[‡]Department of Biotechnology, and [#]Department of Bioinformatics, Maulana Abul Kalam Azad University of Technology, West Bengal (formerly known as West Bengal University of Technology), Salt Lake, Kolkata 700064, India [†] Department of Chemical Sciences, University of Padova, 35131 Padova, Italy, and Institute of Biomolecular Chemistry, Padova Unit, CNR, 35131 Padova, Italy

Supplementary Information

Figure S1	Mass spectrum of the 14-mer peptide
Figure S2	HPLC chromatogram of the 14-mer peptide
Figure S ₃	Singular Value Decomposition (SVD) analysis of the ECD spectral data.
Figure S ₄	Temperature dependence of the amide NH proton chemical shifts ($\Delta\delta/\Delta T$) in water
Figure S ₅	NMR NH-NH ROESY regions
Figure S6	NMR ROESY regions in 20%TFE
Table Sı	Distribution of sequential and non-sequential cross peaks

Figure S1: Mass spectrum of the 14-mer peptide



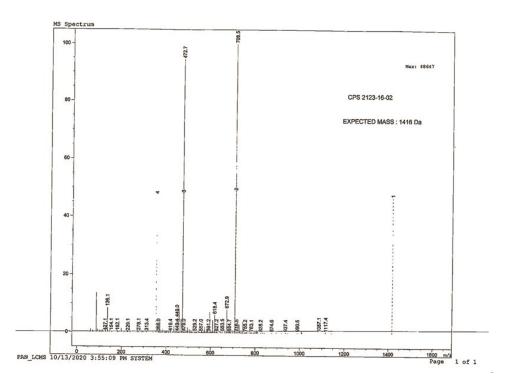


Figure S2: HPLC chromatogram of the 14-mer peptide

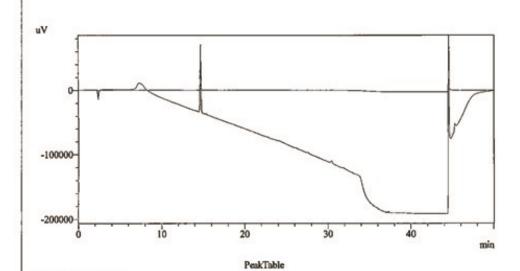
USV PVT. LIMITED GOVANDI

Acquired by Sample Name Sample ID Tray# Vail# : Admin : CPS 2123-16-02 : CPS 2123-16-02

:1:31

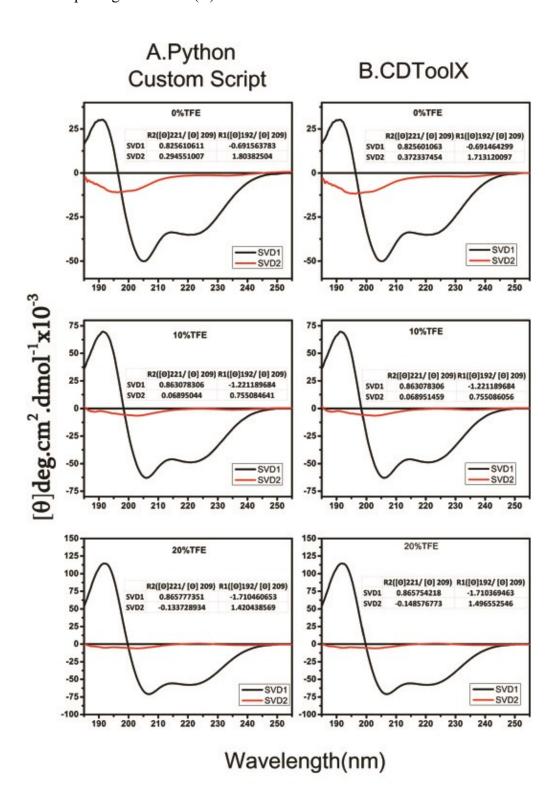
: 10 uL : CPS 2123-16-02 : Default.lcr : 10/27/2016 10:03:21 AM Injection Volume Data Filename Report Filename Date Acquired Data Processed

: 12/15/2016 4:26:13 PM



Peak#	Ret. Time	Area	Area %	
1	14.25	3784	0.52	
2	14.58	14027	1.93	
3	14.70	703003	96.74	
4	14.99	168	0.02	
5	15.36	5396	0.74	
6	15.48	316	0.04	
Total		726695	100.00	

Figure S₃: Singular Value Decomposition (SVD) analysis of the temperature-dependent ECD spectra of the L-AMV peptide analog under all solvent conditions based on the Scikit Learn library (A) and using the software package CDtoolX (B) to understand the conformational transition



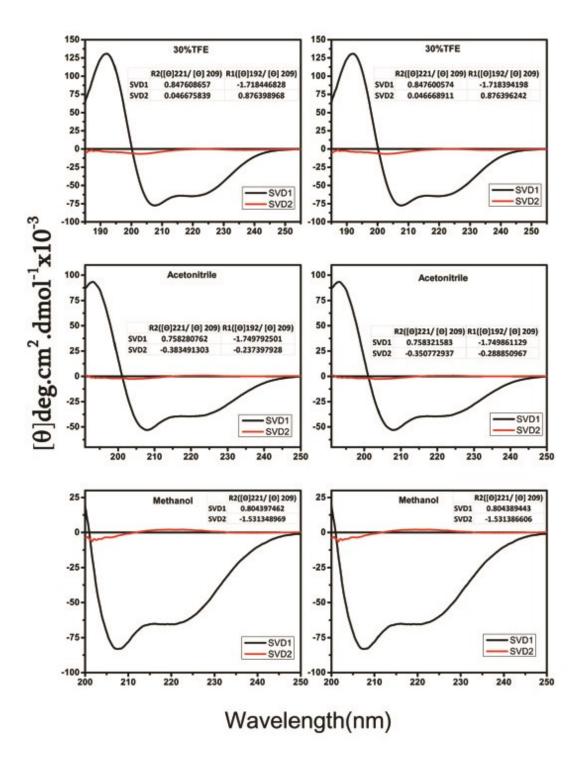


Figure S4: Temperature dependence of the amide NH proton chemical shifts ($\Delta\delta/\Delta T$) in aqueous conditions

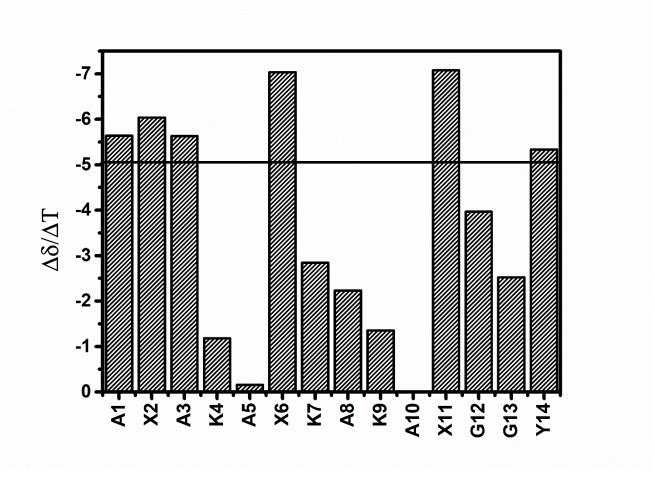
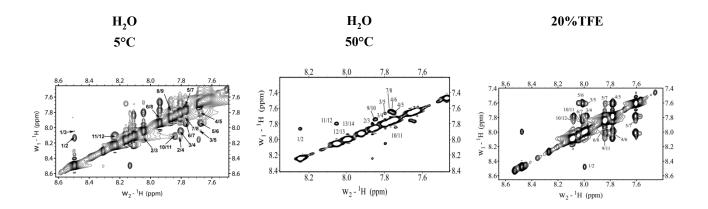


Figure S₅: Regions of the ROESY spectrum of the 14-mer peptide in the different solvents and temperatures examined. The NHi \rightarrow NHi+1 cross peaks are visible.



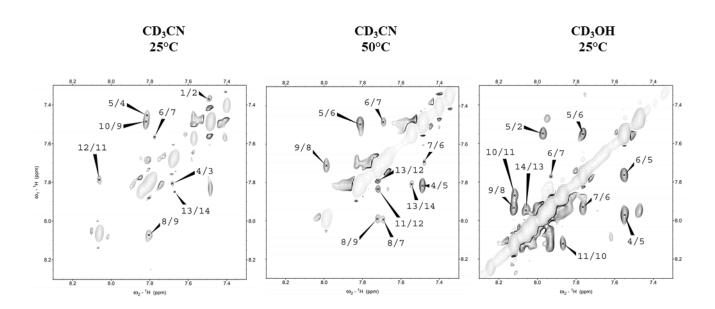


Figure S6: Regions of the ROESY spectrum of the 14-mer L-AMV peptide 1 showing the non-sequential NOEs in 20%TFE at 5° C. The long-range β CHi \rightarrow NHi+3, β CHi \rightarrow NHi+4 NOEs (top) and α CHi \rightarrow NHi+3, α CHi \rightarrow NHi+4 NOEs (bottom) are visible.

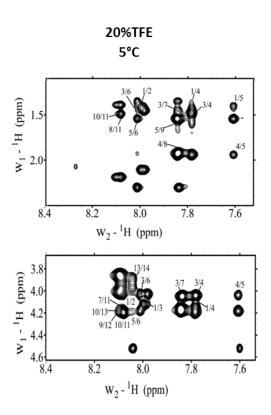


Table S1: Distribution of sequential and non-sequential cross peaks observed in all aqueous conditions

Cross- peaks	0% TFE		20% TFE		Cross-peaks	0% TFE		20% TFE	
pouno	5°C	50°C	5°C	25°C		5°C	50°C	5°C	25°C
αN (i, i+1)	1-2 4-5 5-6 7-8	1-2 4-5 5-6 7-8	1-2 3-4 4-5 5-6	1-2 4-5 5-6	βN (i, i+1)	1-2 2-3 3-4 4-5 5-6 6-7 7-8	1-2 2-3 3-4 4-5 5-6 6-7 7-8	1-2 2-3 4-5 5-6 6-7	1-2 2-3 3-4 4-5 5-6 6-7 7-8
	9-10 10-11	9-10 10-11	10-11	10-11 12-13		8-9 9-10 11-12	8-9 9-10 11-12	9-10 10-11 11-12	8-9 10-11 11-12
	13-14		13-14	13-14					
	1-3		1-3						
αN (i, i+2)	5-7	3-5 4-6		4-6	βN (i, i+2)	5-7	4-6 5-7		3-5 4-6
		8-10					8-10		8-10
	10-12			10-12			9-11		10-12
	1-4		1-4			1-4	1-4	1-4	1-4
αN (i, i+3)	3-6 4-7 5-8	3-6 4-7	3-6	3-6	βN (i, i+3)		3-6	3-6 4-7 5-8	3-6 4-7
	7-10 8-11 9-12	8-11	9-12 10-13	8-11 10-13		7-10	7-10 8-11	6-9 7-10 8-11	10-13
			10-13	10-13		1-5	1-5	1-5	1-5
αN (i, i+4)	3-7 4-8 5-9		3-7		βN (i, i+4)	3-7 4-8 5-9	5-9	3-7 4-8 5-9	3-7
	8-12		7-11	7-11 8-12					
NN (i, i+1)	1-2 2-3 3-4 4-5 5-6 6-7 7-8	1-2 2-3 3-4 4-5	1-2 3-4 4-5 5-6 6-7	3-4 4-5 5-6	NN (i, i+2)	1-3 2-4 3-5 4-6 5-7 6-8	3-5 4-6	4-6 5-7 6-8	4-6 6-8
	8-9 10-11 11-12	9-10 10-11 11-12 12-13 13-14	10-11	8-9 11-12				9-11 10-12	8-10