Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Boc-Val-Val-OMe ($A\beta_{39-40}$) and Boc-Ile-Ala-OMe ($A\beta_{41-42}$) crystallize in parallel β-sheet arrangement but generate different morphology

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Synthetic scheme and 2D NMR data:

Synthesis of peptide 1

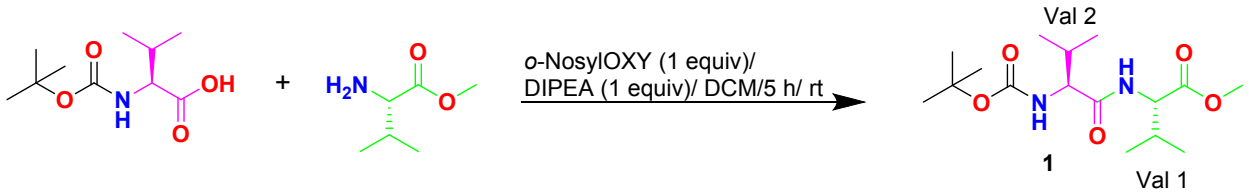

Table S1. Proton chemical shifts (ppm) for peptide **1**

Amino acid	HN	Hα	Hβ	Hγ	Hδ	Others
Val 1	6.69-6.67	3.87-3.84	1.92-1.88			Boc CH_3 1.37
Val 2	7.98-7.97	4.18-4.16	2.06-2.00	0.89-0.81		OCH_3 3.34

Synthesis of peptide 2

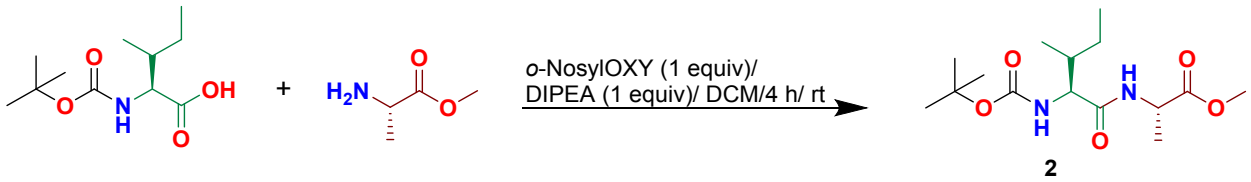

Table S2. Proton chemical shifts (ppm) for peptide **2**

Amino acid	HN	Hα	Hβ	Hγ	Hδ	Others
Ala	8.27-8.26	4.28-4.23	1.27-1.26			Boc CH_3 1.37
Ile	6.61-6.59	3.85-3.83	1.66-1.64	0.84-0.79 (γCH_3) & 1.10-1.03 (γCH_2)	0.84-0.79	OCH_3 3.33

Crystal images:

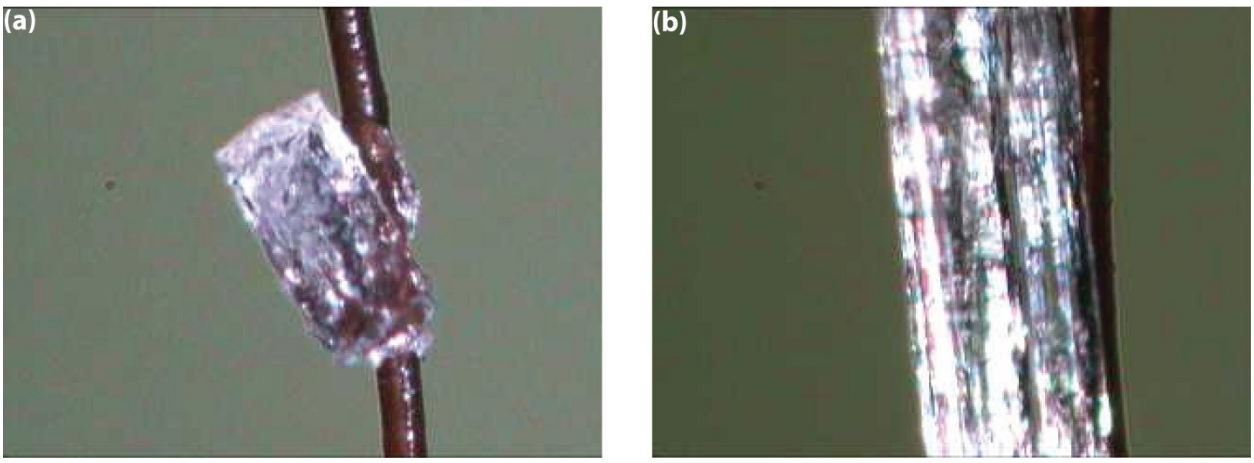

Figure S1. Block shape crystal structure of (a) Boc-Val-Val-OMe **1** and (b) Boc-Ile-Ala-OMe **2**

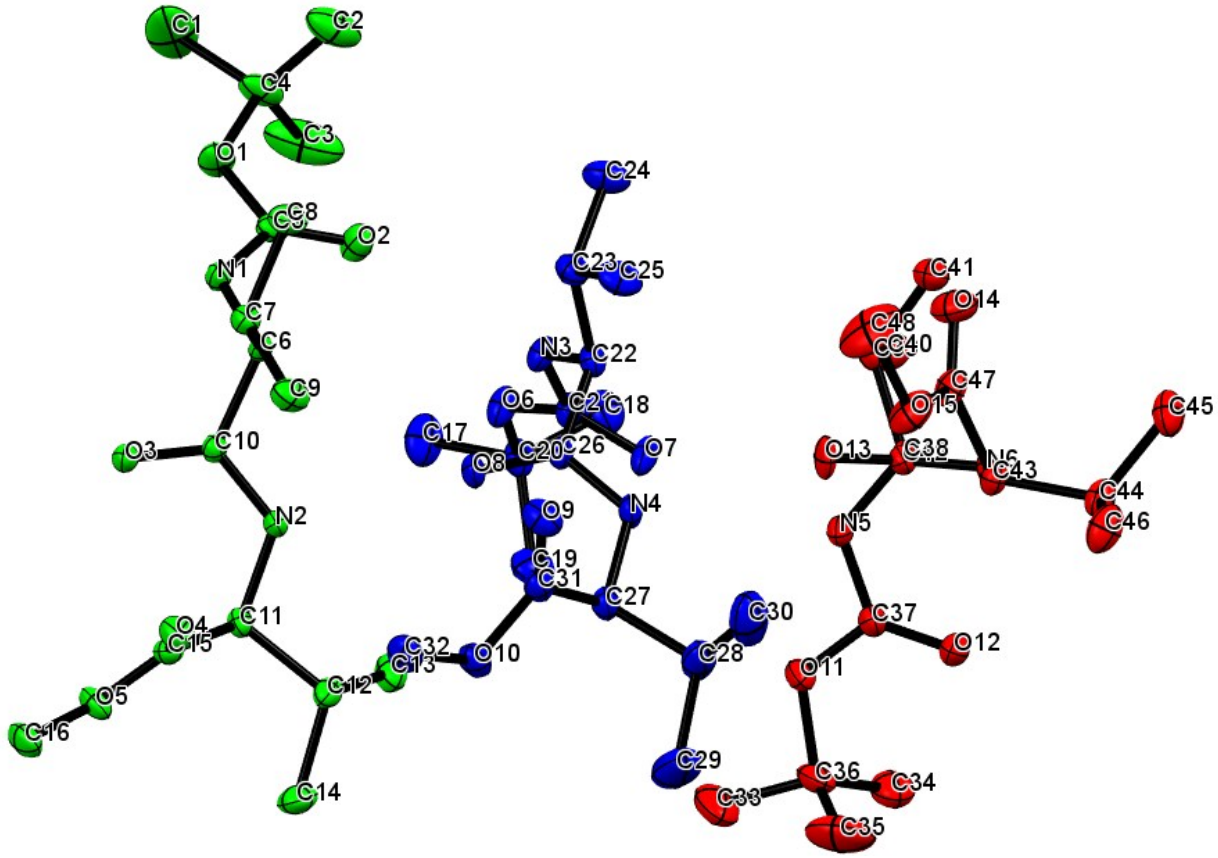

Figure S2. The ORTEP diagram with ellipsoid of 30% probability of three molecules in an asymmetric unit of Boc-Val-Val-OMe (**1**)

Table S3: Hydrogen bonding distances (Å) and Bond angles (º) of peptide **1** and **2**

molecule	D−H···A	*d*(D···H) /Å	*d*(H···A)/ Å	*d*(D···A)/ Å	<D−H··· A/°	Symmetry codes
Boc-VV-OMe (**1**)	N1-H1N···O12	0.86	2.23	2.956(5)	142	3/2-x, 1-y, 1/2+z
	N2-H2N···O8	0.86	1.96	2.810(5)	172	
	N3-H3N···O2	0.86	2.14	2.963(5)	160	
	N4-H4N···O13	0.86	1.92	2.782(5)	178	
	N5-H5N···O7	0.86	2.07	2.921(5)	169	

	N6-H6N···O3	0.86	2.05	2.882(5)	164	
Boc-IA-OMe (**2**)	N1-H1N···O2	0.86	2.11	2.957(6)	168	1+x, y, z
	N2-H2N···O3	0.86	2.14	2.996(6)	172	-1+x, y, z
	C12-H12···O4	0.98	2.37	3.293(10)	156	1-x, -1/2+y, 1/2-z
	C13-H13A···O4	0.96	2.44	3.240(17)	141	-x, -1/2+y, 1/2-z

Hirshfeld surfaces:

Table S4. Relative contributions of various interactions in percentages from Hirshfeld surface area analysis.

	Boc-VV-OMe (**1**)	Boc-IA-OMe (**2**)
O···O	0.7	0.2
N···O	0.0	0.0
C···O	0.0	0.0
H···O	18.6	21.0
C···N	0.0	0.0
N···H	0.0	1.2
C···H	0.5	2.0
C···C	0.0	0.0
H···H	80.0	75.6
Volume	504.32 $Å^3$	454.68 $Å^3$
Area	419.99 $Å^2$	398.19 $Å^2$
Globularity	0.730	0.718
Asphericity	0.113	0.176

Spectra:

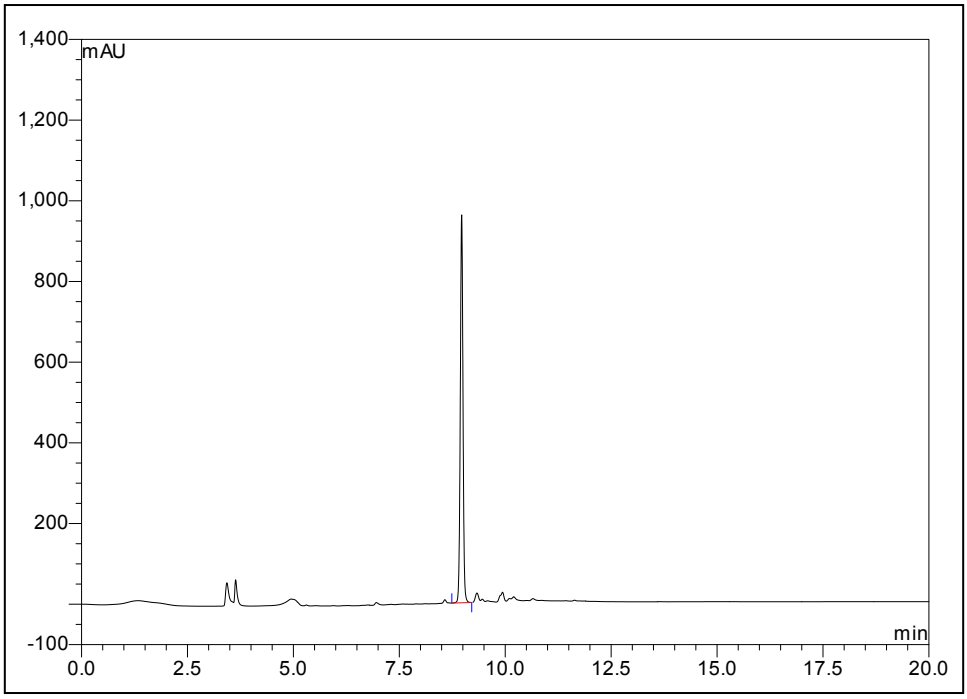

Figure S3: HPLC profile picture of purified peptide **1**

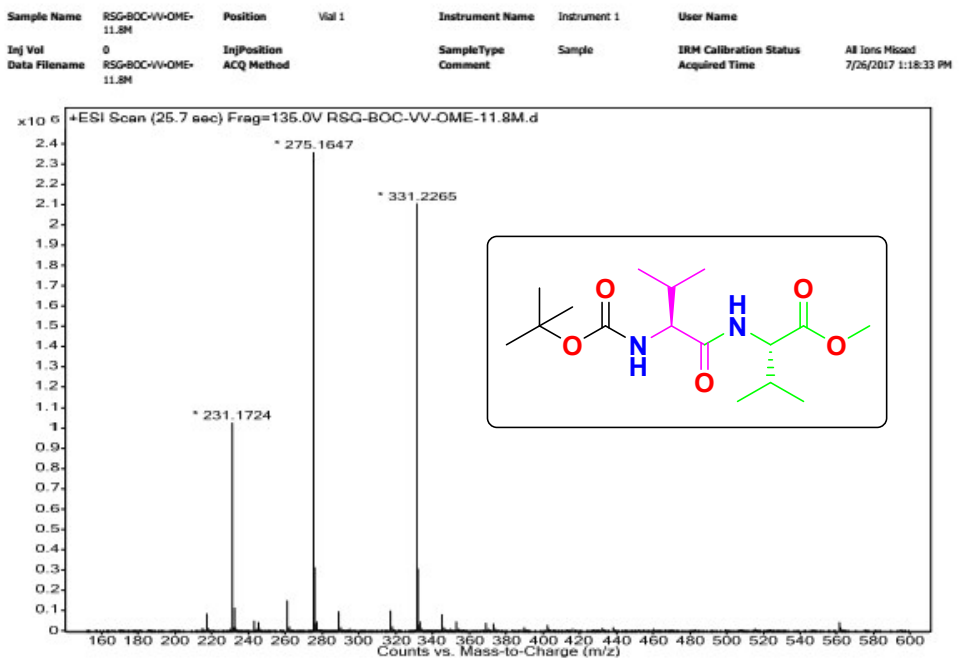

Figure S4: MS spectra of peptide**1**

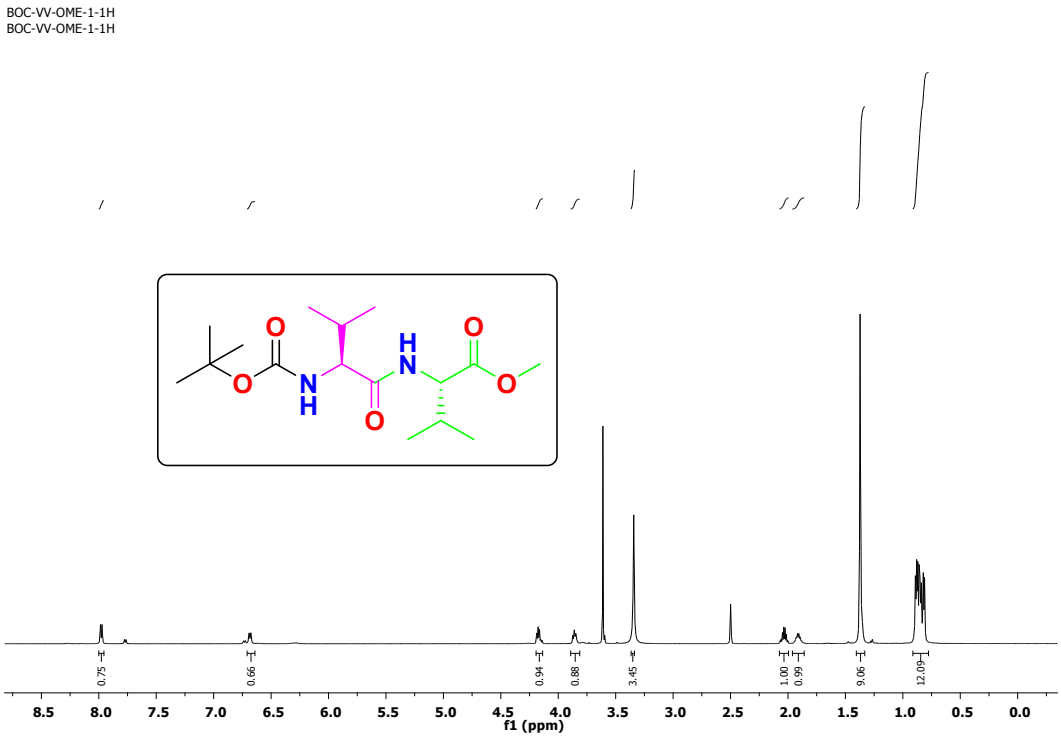

Figure S5: ^{1}H NMR spectra of peptide **1**

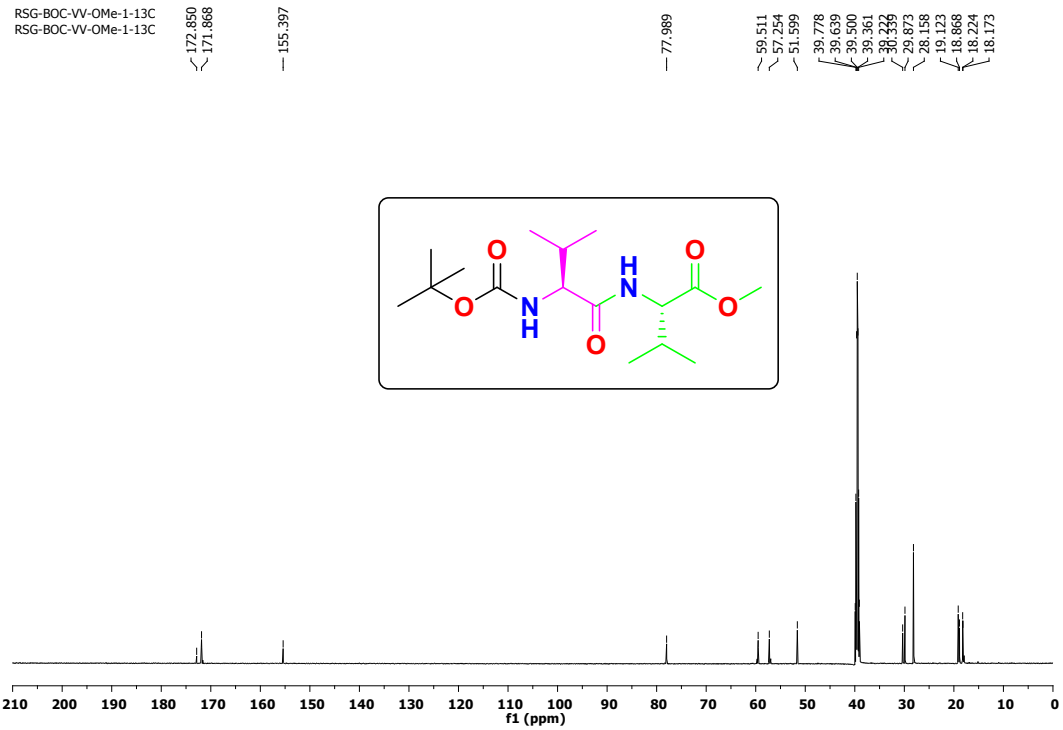

Figure S6: ^{13}C NMR spectra of peptide **1**

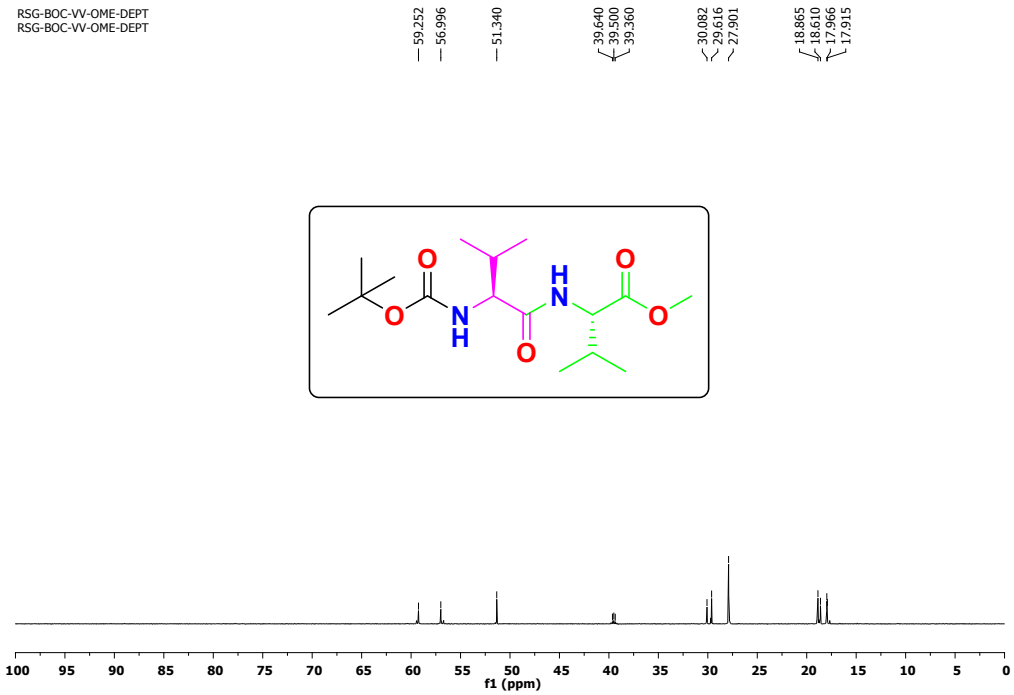

Figure S7: DEPT 135 spectra of peptide **1**

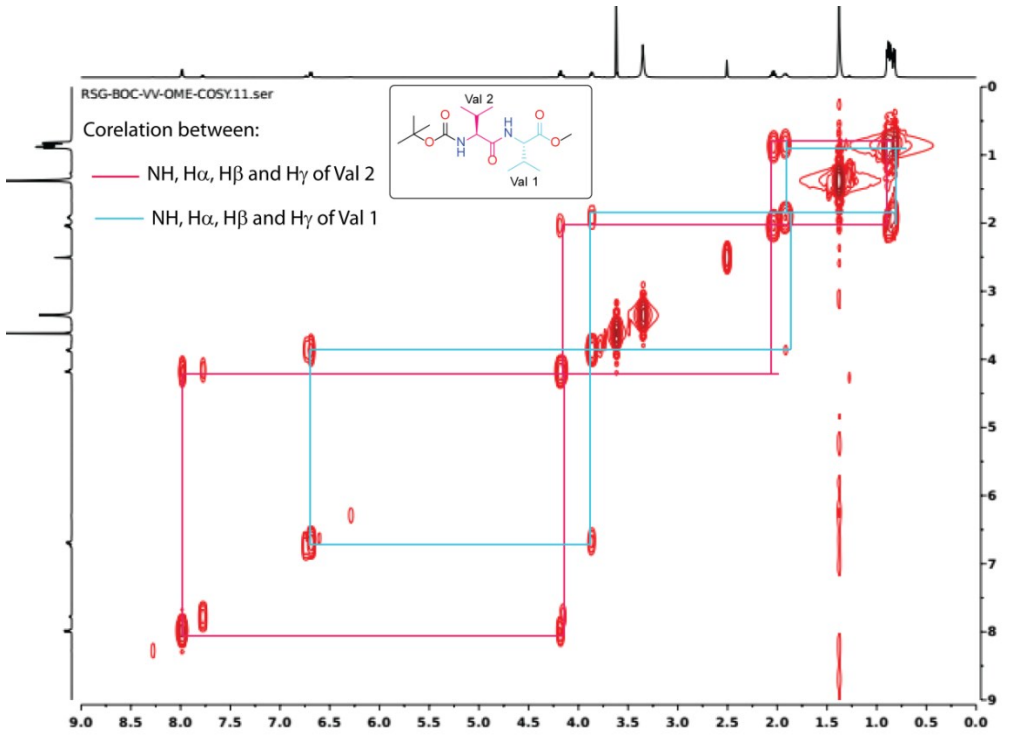

Figure S8: COSY spectra of peptide **1**

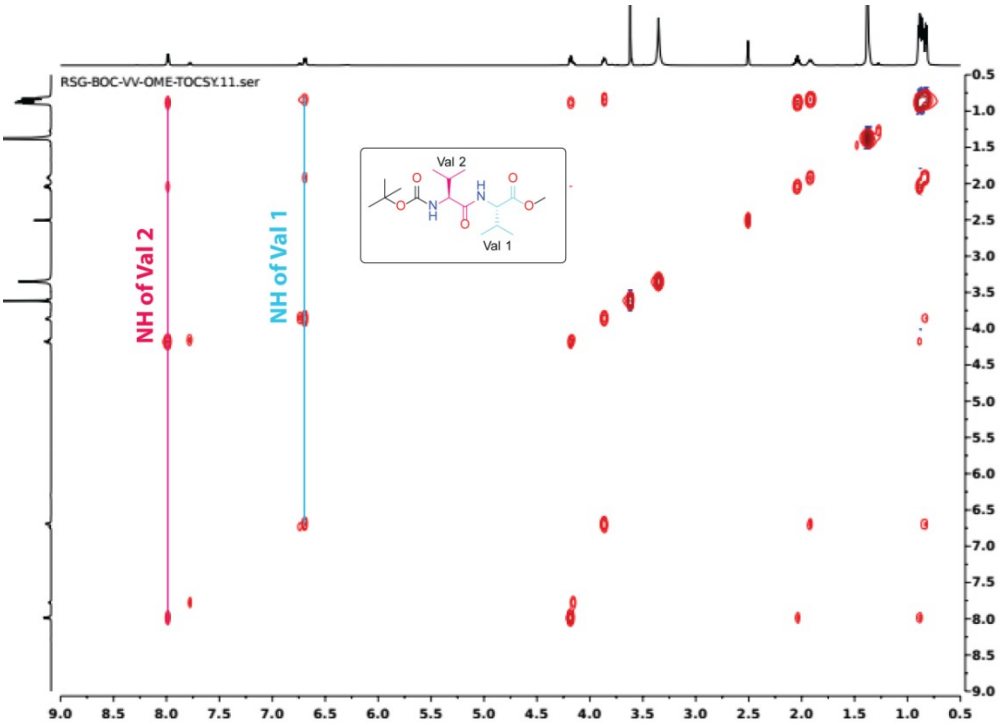

Figure S9: TOCSY spectra of peptide **1**

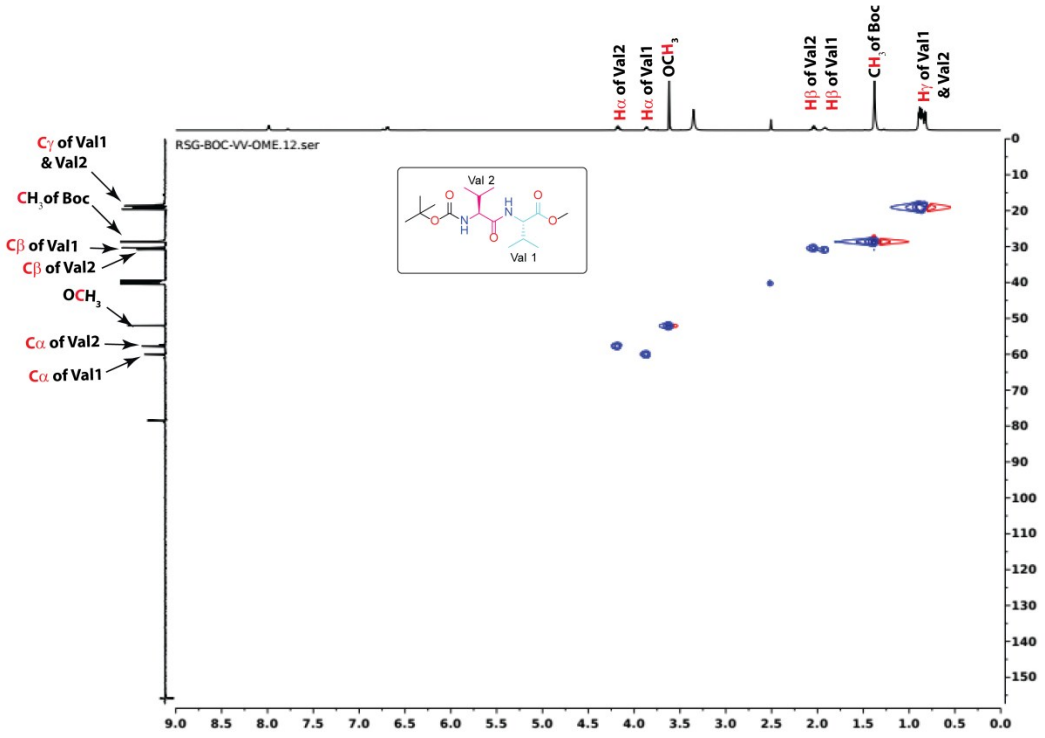

Figure S10: HSQC spectra of peptide **1**

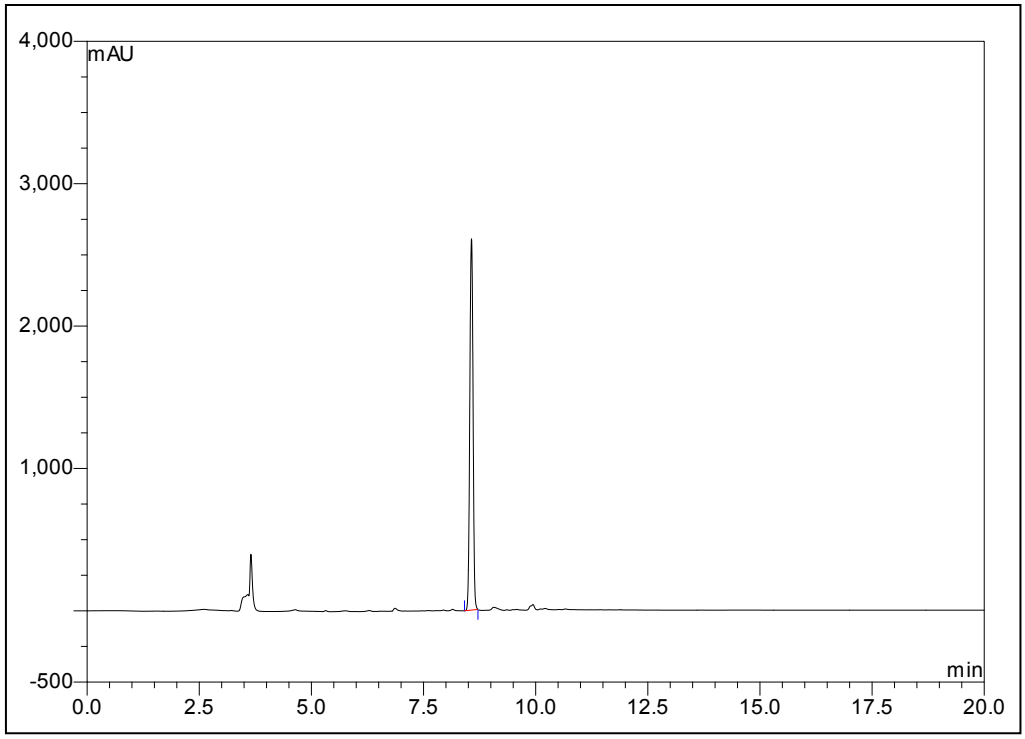

Figure S11: HPLC profile picture of purified peptide **2**

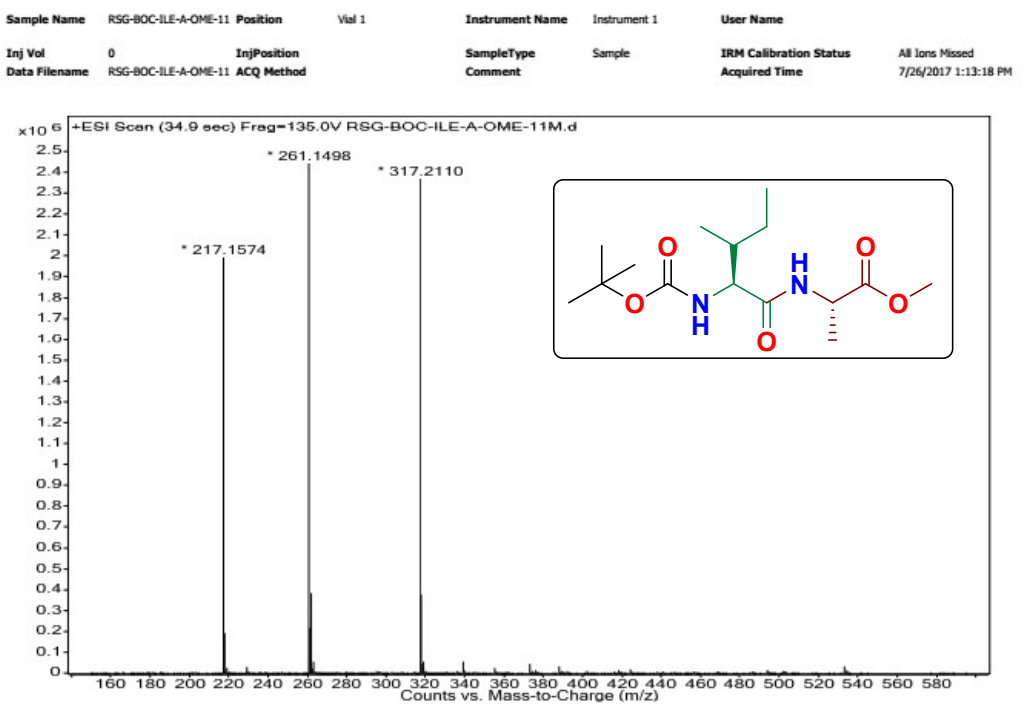

Figure S12: MS spectra of peptide **2**

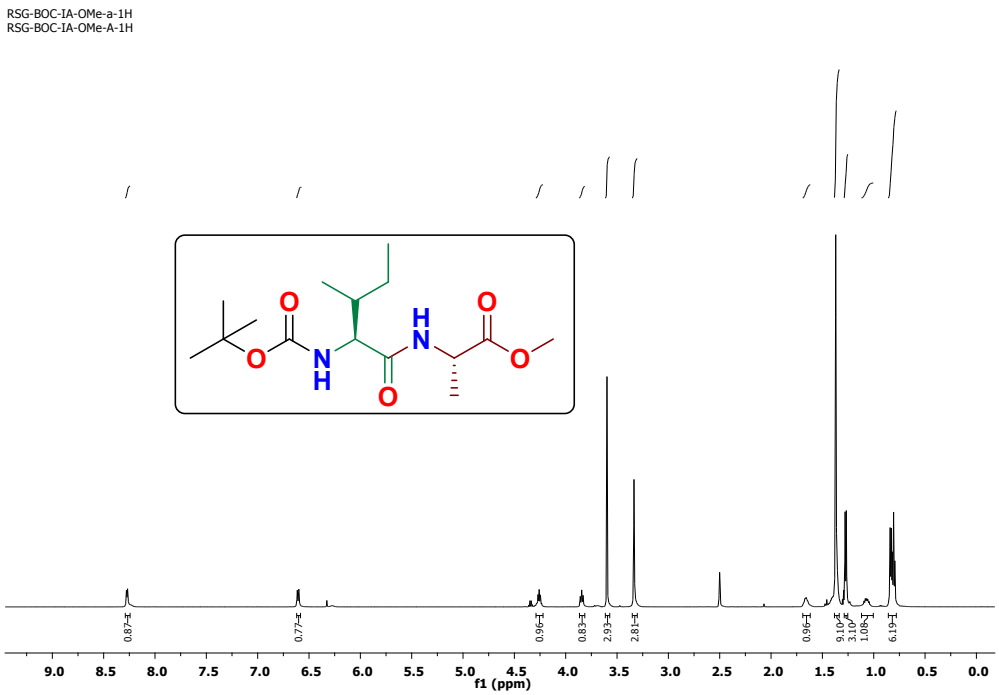

Figure S13: ^{1}H NMR spectra of peptide **2**

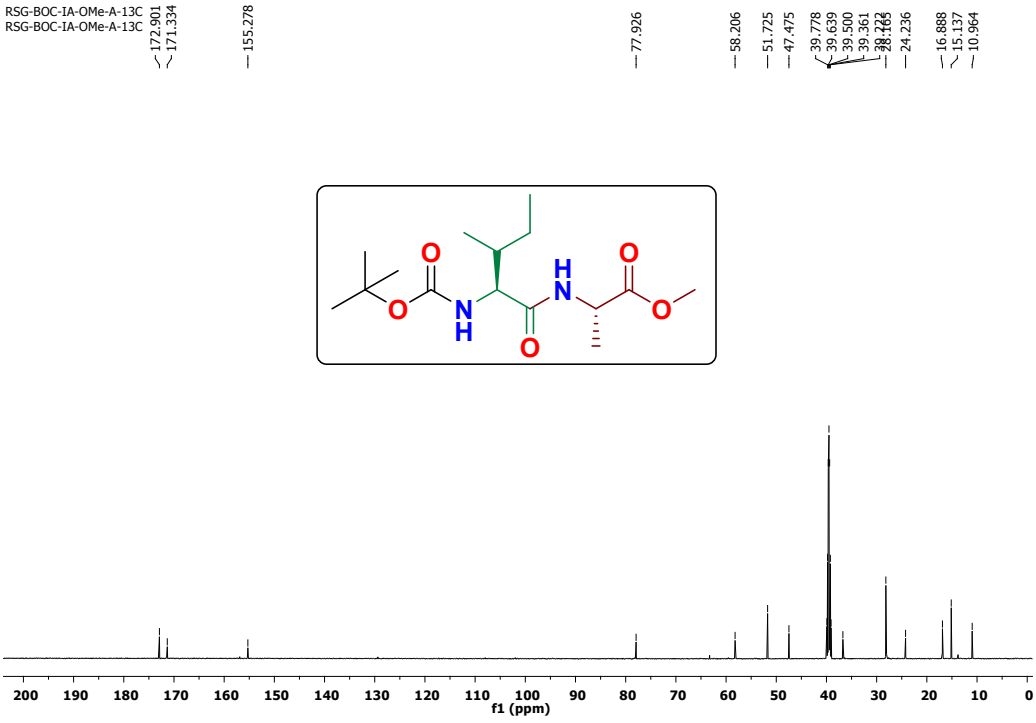

Figure S14: ^{13}C NMR spectra of peptide **2**

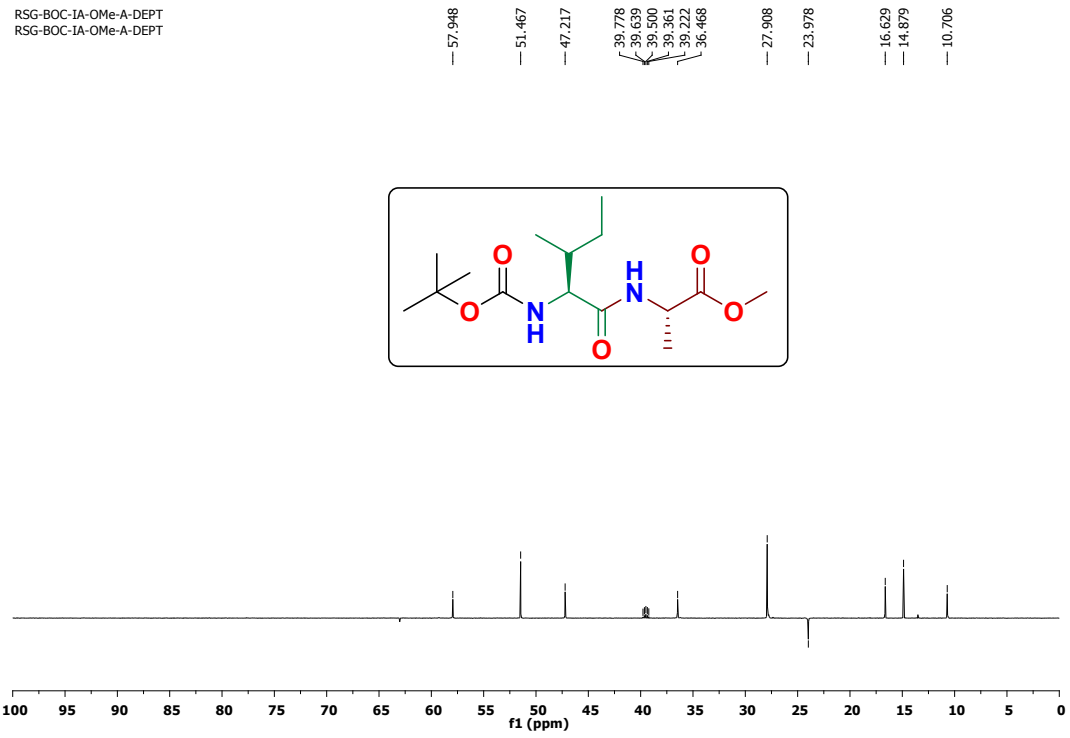

Figure S15: DEPT 135 spectra of peptide **2**

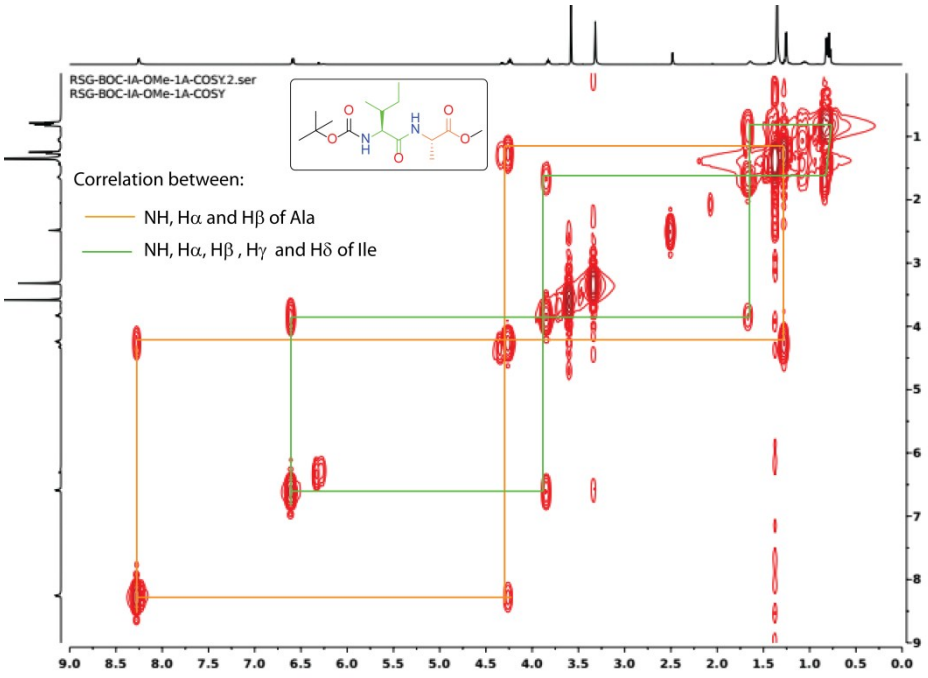

Figure S16: COSY spectra of peptide **2**

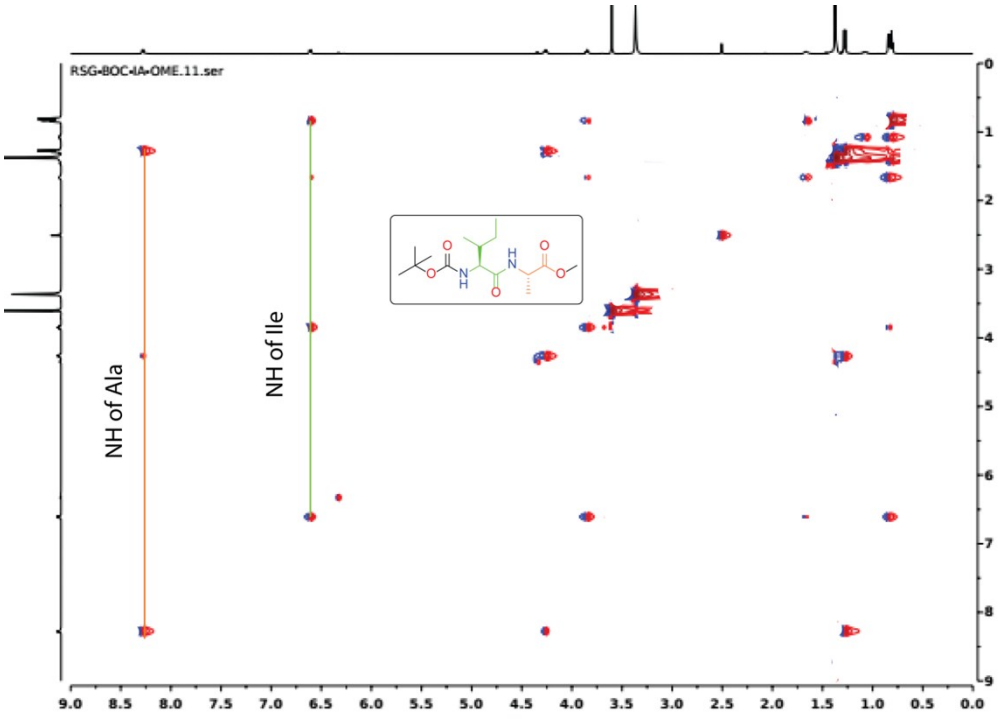

Figure S17: TOCSY spectra of peptide **2**

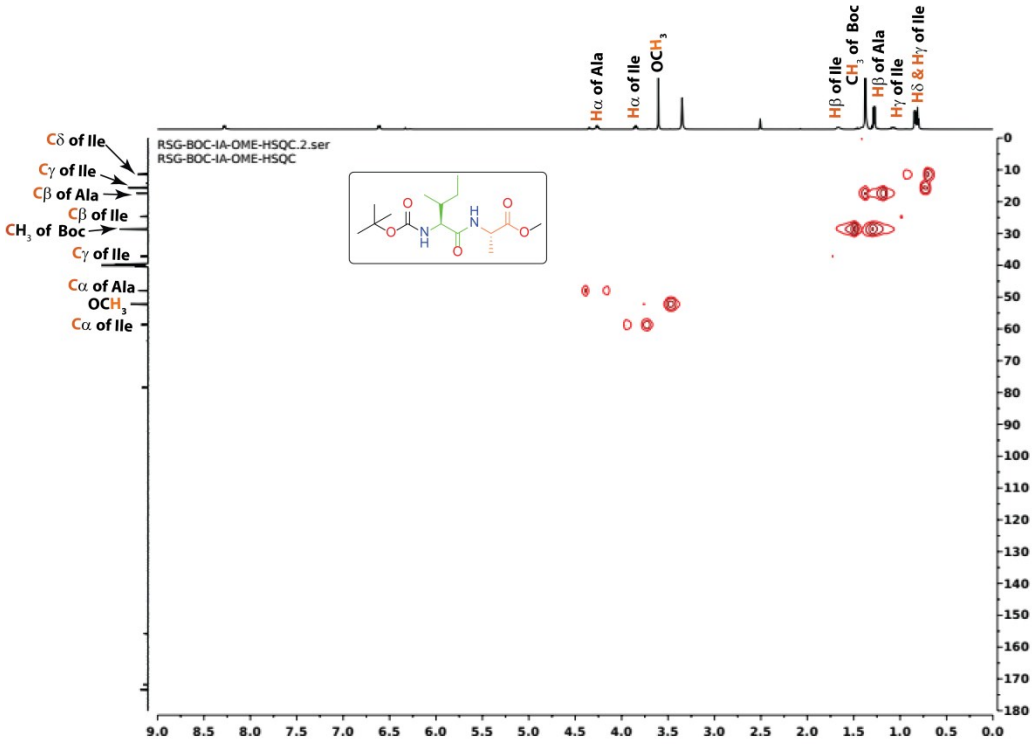

Figure S18: HSQC spectra of peptide **2**