

Supplementary Information

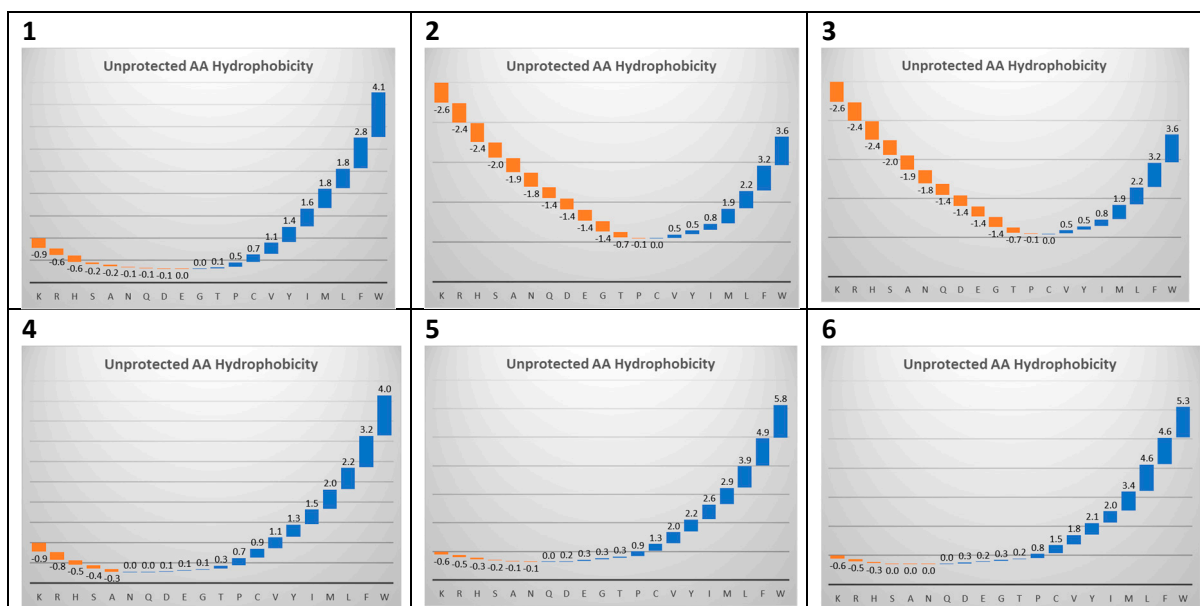
Supplementary Table S1. Hydrophobicity index of protected amino acids.

Amino acid	Hydrophobicity index (min) $\Delta t_{R(\text{peptide} - \text{Gly-peptide})}$					
	Sequence 1	Sequence 2	Sequence 3	Sequence 4	Sequence 5	Sequence 6
G	0.0	0.0	0.0	0.0	0.0	0.0
H(Trt)	8.1	7.8	9.9	8.46	10.0	9.9
Q(Trt)	11.0	10.9	12.7	11.38	12.9	12.7
N(Trt)	11.0	10.9	12.5	11.42	12.9	12.5
C(Trt)	11.9	13.0	14.5	12.36	14.8	14.3
K(Boc)	5.1	4.4	6.9	5.46	6.6	6.4
W(Boc)	9.5	10.1	12.0	9.92	12.0	11.7
E(tBu)	4.4	4.3	6.2	5.3	5.9	5.7
Y(tBu)	6.2	6.5	8.4	6.25	8.3	7.6
D(tBu)	3.6	3.9	5.2	4.2	5.7	4.8
S(tBu)	2.8	2.7	4.6	2.8	4.5	3.6
T(tBu)	3.4	3.6	5.4	3.9	5.1	5
R(Pbf)	8.9	8.1	10.1	9.47	10.4	10.2

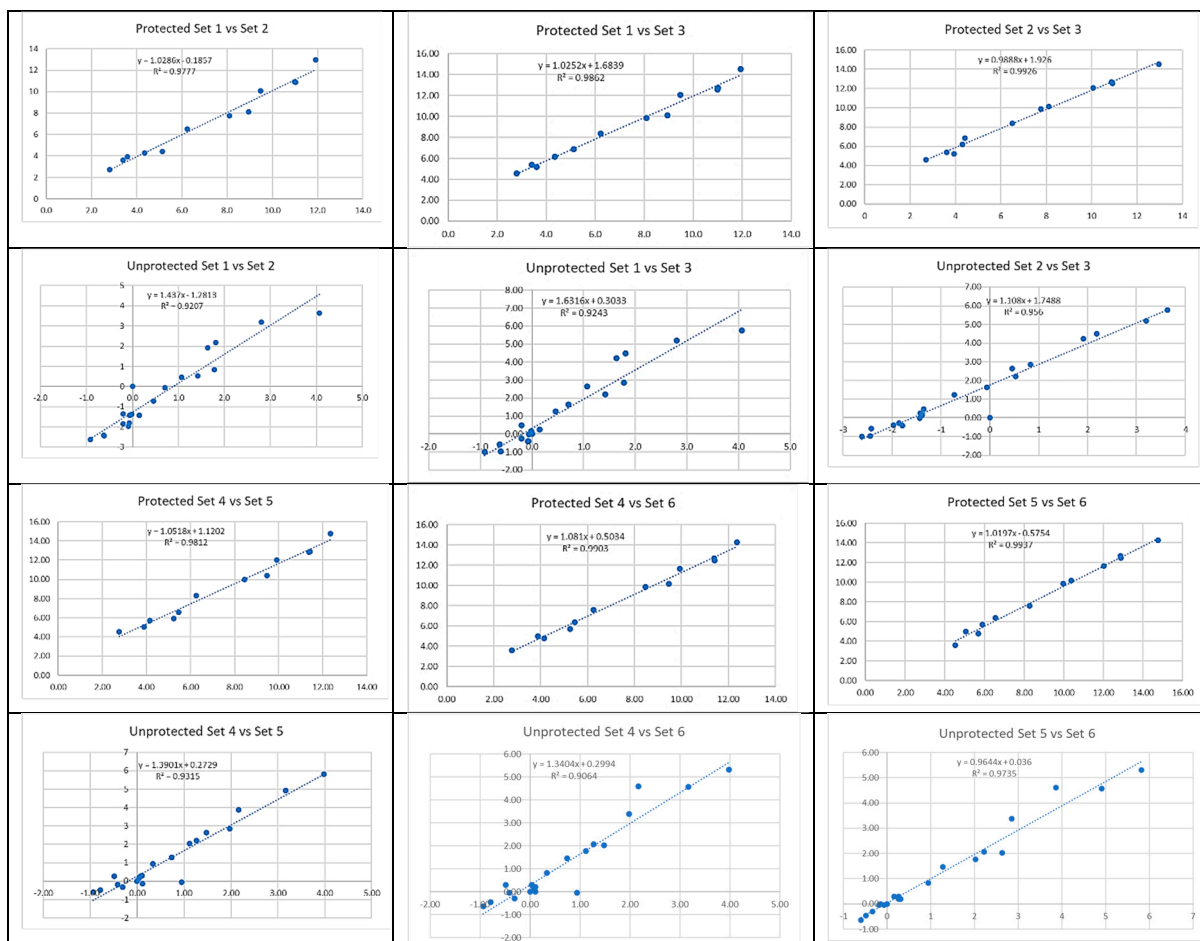
$\Delta t_{R(\text{pept-G})}$: retention time of AA-peptide minus the retention time of Gly-peptide.

Supplementary Table S2. Hydrophobicity index for unprotected amino acids

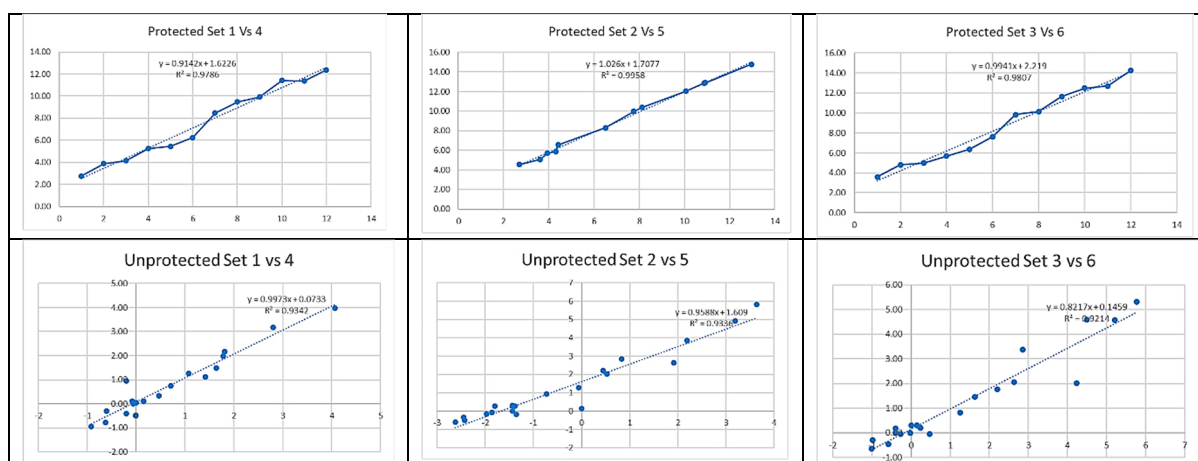
Amino acid	Hydrophobicity index (min)					
	Sequence 1	Sequence 2	Sequence 3	Sequence 4	Sequence 5	Sequence 6
G	0.0	0.0	0.0	0.0	0.0	0.0
H	-0.6	-2.4	-1.0	-0.3	-0.3	-0.3
Q	-0.1	-1.8	-0.4	0.1	0.3	0.2
N	-0.1	-2.0	-0.4	0.1	-0.1	0.0
C	0.7	-0.1	1.6	0.7	1.3	1.5
K	-0.9	-2.6	-1.0	-0.9	-0.6	-0.6
W	4.1	3.6	5.8	4.0	5.8	5.3
E	0.0	-1.4	0.2	-0.5	0.3	0.3
Y	1.4	0.5	2.2	1.1	2.0	1.8
D	-0.1	-1.4	0.0	0.0	0.0	0.0
S	-0.2	-1.9	-0.3	0.9	-0.1	0.0
T	0.1	-1.4	0.2	0.1	0.3	0.2
R	-0.6	-2.4	-0.6	-0.8	-0.5	-0.5
A	-0.2	-1.4	0.5	-0.4	-0.2	0.0
M	1.8	0.8	2.9	2.0	2.9	3.4
P	0.5	-0.7	1.2	0.3	0.9	0.8
V	1.1	0.5	2.6	1.3	2.2	2.1
F	2.8	3.2	5.2	3.2	4.9	4.6
I	1.6	1.9	4.2	1.5	2.6	2.0
L	1.8	2.2	4.5	2.2	3.9	4.6



Supplemental Figure S1. Hydrophobicity index for the unprotected amino acids in different positions of the peptide chains. The figure number represents the sequence of the peptide as per Figure 1.



Supplemental Figure S2. Correlation among hydrophobicity indices for the protected and unprotected amino acids in different positions of the peptide chains.



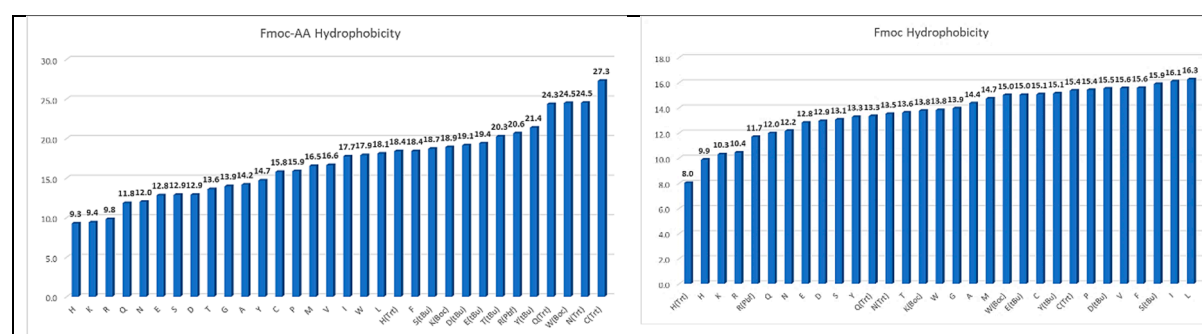
Supplemental Figure S3. Correlation among hydrophobicity indices for the protected and unprotected amino acids in acid and peptide amides.

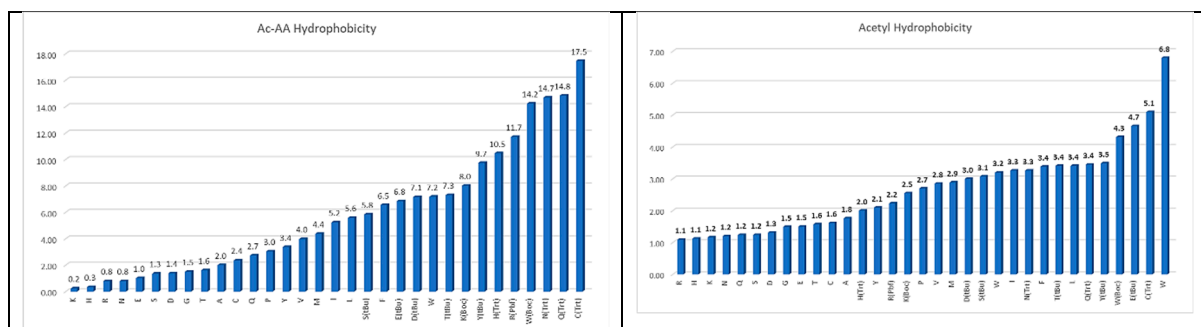
Supplementary Table S3. Hydrophobicity index for Fmoc, Fmoc-amino acid.

Amino acid	Fmoc group Hydrophobicity index (min) Δt_R (Fmoc-peptide – H-peptide)	Fmoc-amino acid Hydrophobicity index (min) Δt_R (Fmoc-peptide – H-Gly-peptide)
H(Trt)	8.0	18.4
Q(Trt)	13.3	24.3
N(Trt)	13.5	24.5
C(Trt)	15.4	27.3
K(Boc)	13.8	18.9
W(Boc)	15.0	24.5
E(tBu)	15.0	19.4
Y(tBu)	15.1	21.4
D(tBu)	15.5	19.1
S(tBu)	15.9	18.7
T(tBu)	16.8	20.3
R(Pbf)	11.7	20.6
H	9.9	9.3
Q	12.0	11.8
N	12.2	12.0
C	15.1	15.8
K	10.3	9.4
W	13.8	17.9
E	12.8	12.8
Y	13.3	14.7
D	12.9	12.9
S	13.1	12.9
T	13.6	13.6
R	10.4	9.8
G	13.9	13.9
A	14.4	14.2
M	14.7	16.5
P	15.4	15.9
V	15.6	16.6
F	15.6	18.4
I	16.1	17.7
L	16.3	18.1

Supplementary Table S4. Hydrophobicity index for Acetyl, Ac-amino acid.

Amino acid	Acetyl group Hydrophobicity index (min) Δt_R (Ac-peptide – H-peptide)	Ac-amino acid Hydrophobicity index (min) Δt_R (Ac-peptide – H-G-peptide)
H(Trt)	1.1	0.8
Q(Trt)	1.2	0.8
N(Trt)	1.6	2.4
C(Trt)	1.5	1.5
K(Boc)	1.2	0.2
W(Boc)	1.2	1.3
E(tBu)	1.3	1.4
Y(tBu)	1.2	2.7
D(tBu)	1.5	1.0
S(tBu)	1.6	1.6
T(tBu)	1.8	2.0
R(Pbf)	1.1	0.3
H	2.1	3.4
Q	2.7	3.0
N	2.5	8.0
C	3.3	5.2
K	2.2	11.7
W	3.5	9.7
E	3.1	5.8
Y	3.4	6.5
D	2.9	4.4
S	2.8	4.0
T	3.2	7.2
R	2.0	10.5
G	3.0	7.1
A	3.3	14.7
M	3.4	14.8
P	3.4	7.3
V	3.4	5.6
F	4.7	6.8
I	4.3	14.2
L	5.1	17.5





Supplemental Figure S4. Hydrophobicity indices for: Fmoc-amino acid (protected and unprotected), Fmoc protecting group, Ac-amino acid (protected and unprotected), and Acetyl group.