

Supplementary data

Downsizing the BAD BH3 peptide to small constrained α -helices with improved ligand efficiency

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Table 1. Compound characterisation data

#	Sequence	[M+H] ⁺ Calc.	[M+H] ⁺ Found	HPLC R _t
BAD-BH3	Ac-NLWAAQRYGRELRRMSDEFVDSFKK-NH ₂	3142.59	3142.97	14.67
Flu-BAD	Flu-AHA-NLWAAQRYGRELRRMSDEFVDSFKK-NH ₂	3571.05	3571.34	14.34
1	Ac-NLWAAQRYGRELRRMle-NH ₂	1943.25	1943.11	14.17
2	Ac-QRYGRELRRNleSDEF-NH ₂	1866.08	1866.67	14.68
3	Ac-LRRNleSDEFVDSFKK-NH ₂	1781.05	1780.59	14.53
4	Ac-QRYGRELRRNleSDEFVDSFKK-NH ₂	2570.90	2570.55	14.25
5	Ac-QRYGREL[RKleSDD]FVDSFKK-NH ₂	2510.85	2510.32	14.58
6	Ac-YARELR[KleADD]F-NH ₂	1518.79	1518.64	14.75
7	Ac-LR[KleADD]F-NH ₂	999.04	999.55	15.33
8	Ac-[KNLWD]AQ[KYARD]L-NH ₂	1625.86	1625.21	15.04
9	Ac-[KYARD]LR[KMADD]F-NH ₂	1632.89	1632.44	15.22
10	Ac-Y[KRELD][KMADD]F-NH ₂	1534.72	1535.26	15.81
11	Ac-LR[KleADD]FV[KSFKD]-NH ₂	1685.93	1686.03	15.38
12	Ac-[KYGRD]LR[KleSDD]FV[KSFKD]-NH ₂	2304.64	2305.28	15.29
13	Ac-INalR[KleADD]F-NH ₂	1083.55	1083.53	15.74
14	Ac-INalRRNleADEF-NH ₂	1143.58	1143.89	14.74
15	Ac-INal Aib[KleADD]F-NH ₂	955.48	955.66	16.31
16	Ac-INal Aib[KleADD]Phe(Cl ₂)-NH ₂	1042.88	1042.51	16.02
17	Ac-INal Aib[KleADD]2Nal-NH ₂	1062.52	1063.34	16.35
18	Ac-LR[KleADD]hPhe-NH ₂	1013.57	1012.97	15.24
19	Ac-LR[KFADD]hPhe-NH ₂	1047.55	1046.86	15.55
20	Ac-LR[KINalADD]hPhe-NH ₂	1047.55	1046.86	15.24

21	Ac-FR[KNleADD] <i>hPhe</i> -NH ₂	1047.55	1047.59	15.56
22	Ac-FR[KFADD] <i>hPhe</i> -NH ₂	1081.53	1081.49	15.55
23	Ac-FR[KINalADD] <i>hPhe</i> -NH ₂	1131.55	1131.40	16.11
24	Ac-INalR[KNleADD] <i>hPhe</i> -NH ₂	1097.51	1097.57	16.16
25	Ac-INalR[KFADD] <i>hPhe</i> -NH ₂	1131.45	1131.55	16.11
26	Ac-INalR[KINalADD] <i>hPhe</i> -NH ₂	1181.38	1181.56	16.74
27	Ac-LR[KFADD]F-NH ₂	1033.53	1032.91	15.18
28	Ac-LR[KINalADD]F-NH ₂	1083.55	1082.84	15.89
29	Ac-FR[KNleADD]F-NH ₂	1033.53	1033.65	15.23
30	Ac-FR[KFADD]F-NH ₂	1067.61	1067.52	15.24
31	Ac-FR[KINalADD]F-NH ₂	1117.53	1117.41	15.77
32	Ac-INalR[KFADD]F-NH ₂	1117.53	1117.51	15.65
33	Ac-INalR[KINalADD]F-NH ₂	1167.55	1167.33	16.19
34	Ac-LR[KNleADD] <i>Nle</i> -NH ₂	965.57	965.81	15.21
35	Ac-LR[KFADD] <i>Nle</i> -NH ₂	999.55	999.72	15.01
36	Ac-LR[KINalADD] <i>Nle</i> -NH ₂	1049.57	1049.65	15.80
37	Ac-FR[KNleADD] <i>Nle</i> -NH ₂	999.55	999.66	15.17
38	Ac-FR[KFADD] <i>Nle</i> -NH ₂	1033.53	1033.61	14.98
39	Ac-FR[KINalADD] <i>Nle</i> -NH ₂	1083.55	1083.51	15.56
40	Ac-INalR[KNleADD] <i>Nle</i> -NH ₂	1049.57	1049.38	16.67
41	Ac-INalR[KFADD] <i>Nle</i> -NH ₂	1083.55	1083.66	15.61
42	Ac-INalR[KINalADD] <i>Nle</i> -NH ₂	1133.22	1133.57	16.24
43	Ac-INapCH ₂ CH ₂ CO-Aib[KNleADD] <i>Nle</i> -NH ₂	955.66	955.48	16.72
44	Ac-INapCHCHCO-Aib[KFADD] <i>Nle</i> -NH ₂	953.46	953.85	16.95
45	Ac-INapOCH ₂ CO-Aib[KINalADD] <i>Nle</i> -NH ₂	1028.88	1028.51	16.61

HPLC conditions: Phenomenex C18 column, 5µm 100 Å 4.6×250 mm, 214 nm, Solvent A=0.1% TFA in H₂O, Solvent B=0.1% TFA, 10% H₂O in acetonitrile. Gradient: 0% B to 100% B over 30 min).