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Table 1. Relative ion intensities for the dissociated ions of ligands in the L-289 library. The ion intensity of each ligand was normalized to that of Gly-Gly compound. The uncertainty is 10-20% (precision of the three measurements, not accuracy).

L-AA	Phe	Tyr	Leu	Ile	Val	Ala	His	Thr	Gly	Gln	Asn	Ser	Pro	Lys	Arg	Glu	Asp
Phe	3.13	3.09	4.07	4.07	2.52	1.53	1.24	1.41	1.80	1.54	1.04	1.15	2.48	1.74	1.46	1.09	1.11
Tyr		3.37	4.35	4.35	2.98	1.15	1.17	1.52	1.54	1.26	0.87	1.00	1.70	1.33	1.15	0.87	1.00
Leu			3.80	3.80	2.39	2.48	2.07	2.13	2.37	2.22	1.70	1.93	2.50	2.28	1.96	1.04	0.75
Ile				3.80	2.39	2.48	2.07	2.13	2.37	2.22	1.70	1.93	2.50	2.28	1.96	1.04	0.75
Val					1.76	2.37	1.35	1.93	1.74	1.70	1.13	1.50	1.43	1.33	1.20	0.85	0.72
Ala						0.63	0.52	0.70	0.65	0.85	0.50	0.50	0.65	0.72	1.13	0.67	0.30
His							0.46	0.72	0.57	0.54	0.46	0.50	0.76	0.72	0.63	0.39	0.43
Thr								1.02	0.50	0.63	0.54	0.59	0.63	0.98	0.48	0.67	0.28
Gly									1.00	0.50	0.26	0.46	0.85	0.48	0.74	0.30	0.37
Gln										0.70	0.65	0.54	0.93	0.48	0.52	0.43	0.30
Asn											0.70	0.30	0.83	0.63	0.46	0.30	0.39
Ser												0.54	0.59	0.35	0.33	0.28	0.35
Pro													0.26	0.63	0.65	0.48	0.67
Lys														0.70	0.46	0.48	0.33
Arg															0.43	0.41	0.37
Glu																0.52	0.74
Asp																	0.46

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Table 2. Relative ion intensities for the dissociated ions of ligands in the D-256 library. The ion intensity of each ligand was normalized to that of Gly-Gly compound. The uncertainty is 10-20% (precision of the three measurements, not accuracy).

D-AA	Phe	Tyr	Leu	Val	Ala	His	Thr	Gly	Gln	Asn	Ser	Pro	Lys	Arg	Glu	Asp
Phe	1.49	1.43	2.13	1.57	0.97	0.93	1.16	1.15	0.92	0.76	0.86	0.71	0.66	0.54	0.47	0.47
Tyr		1.42	2.09	1.77	0.86	0.75	1.01	0.93	0.68	0.62	0.98	0.66	0.59	0.47	0.54	0.33
Leu			2.47	2.01	1.25	1.33	1.71	1.53	1.47	1.22	1.53	0.61	0.85	0.89	0.67	0.88
Val				1.72	1.53	1.25	1.53	1.42	1.22	0.87	1.38	0.49	1.08	0.84	0.88	0.85
Ala					0.84	0.51	0.63	0.76	0.62	0.55	0.76	0.61	0.45	0.82	0.38	0.42
His						0.48	0.55	0.58	0.39	0.37	0.61	0.58	0.39	0.28	0.24	0.15
Thr							0.54	0.76	0.41	0.52	0.99	0.58	0.36	0.29	0.59	0.34
Gly								1.00	0.55	0.52	0.78	0.92	0.50	0.58	0.42	0.30
Gln									0.51	0.38	0.52	0.53	0.17	0.34	0.45	0.25
Asn										0.59	0.53	0.60	0.40	0.21	0.25	0.30
Ser											1.10	0.77	0.48	0.29	0.34	0.34
Pro												0.29	0.38	0.40	0.70	0.64
Lys													0.29	0.28	0.29	0.29
Arg														0.24	0.26	0.20
Glu															0.36	0.23
Asp																0.26

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Table 3. The amino acid analysis shows that each amino acid in the two libraries has a similar molar ratio.^a
The analyses were provided by the Harvard Microchemistry Facility.

Amino acids	Asx ^b	Glx ^b	Ser	Gly	His	Arg	Thr+ β -Ala ^c	Ala	Pro	Tyr	Val	Ile	Leu	Phe	Lys
D-form	1.86	1.97	0.80	1.00	1.10	1.04	8.93	1.07	0.98	0.87	0.82	0.63	1.03	1.10	1.07
L-form	2.00	1.93	0.82	1.00	0.96	1.02	8.37	0.92	0.97	0.69	0.88	d	0.91	1.01	0.77

^aThe molar ratio of each amino acid was normalized based on Gly. ^bAmino acid analysis can not distinguish between Asp and Asn (Asx), and between Glu and Gln (Glx). ^cThr and β -Ala coelute in the HPLC analysis and can not be distinguished. ^d D-Ile is excluded in the D-library.

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Table 4. Correlation of binding constants in solution with relative ion intensities for the seven individual peptide inhibitors.

AA ₁ , AA ₂	Ion Intensity ^a	K _b (x10 ⁶ , M ⁻¹) ^b	ΔG _b (kcal/mol) ^b
L-Leu	3.8	140	-11.2
D-Leu	2.4	41	-10.5
L-Thr	1.0	8.8	-9.5
D-Thr	0.5	5.8	-9.3
L-Ser	0.5	7.5	-9.4
D-Ser	1.1	16	-9.9
Gly	1.0	4.9	-9.2

^aThe ion intensity of each ligand in both libraries is normalized to that of Gly-Gly. The uncertainty determined from three experiments is 20%. ^bThe binding affinity of these ligands were measured in 20 mM phosphate buffer (pH = 7.5) at 37 °C. The uncertainty of K_b is 10%.