

TABLE S1a Houghten et. al.¹³

Mixture		IC ₅₀ uM	Mixture	
Ac-DVXXXX-NH2		250		Ac-DVPXXX-NH2
Constituent Mixtures		IC₅₀ uM	Constituent Mixtures	
Ac-DVPXXX-NH2		41		Ac-DVPDXX-NH2
Ac-DVEXXX-NH2		146		Ac-DVPAXX-NH2
Ac-DVQXXX-NH2		215		Ac-DVPEXX-NH2
Ac-DVMXXX-NH2		451		Ac-DVPFXX-NH2
Ac-DVRXXX-NH2		906		Ac-DVPGXX-NH2
Ac-DVAXXX-NH2		1,107		Ac-DVPHXX-NH2
Ac-DVDXXX-NH2		1,400		Ac-DVPIXX-NH2
Ac-DVFXXX-NH2		1,400		Ac-DVPKXX-NH2
Ac-DVGXXX-NH2		1,400		Ac-DVPLXX-NH2
Ac-DVHXXX-NH2		1,400		Ac-DVPMXX-NH2
Ac-DVIXXX-NH2		1,400		Ac-DVPNXX-NH2
Ac-DVKXXX-NH2		1,400		Ac-DVPPXX-NH2
Ac-DVLXXX-NH2		1,400		Ac-DVPQXX-NH2
Ac-DVNXXX-NH2		1,400		Ac-DVPRXX-NH2
Ac-DVSXXX-NH2		1,400		Ac-DVPSXX-NH2
Ac-DVTXXX-NH2		1,400		Ac-DVPTXX-NH2
Ac-DVVXXX-NH2		1,400		Ac-DVPVXX-NH2
Ac-DVYXXX-NH2		1,400		Ac-DVPYXX-NH2
		Predicted Value	Scaled Error	
Arithmetic Mean		1,093	3.37	Arithmetic Mean
Geometric Mean		827	2.31	Geometric Mean
Harmonic Mean		370	0.48	Harmonic Mean

TABLE S1b Dooley et. al.¹⁴

Mixture		IC ₅₀ nM	Mixture	
Ac-rfxxxx-NH ₂		14,000		Ac-rfwxxx-NH ₂
Constituent Mixtures		IC₅₀ nM	Constituent Mixtures	
Ac-rfwxxx-NH ₂		900		Ac-rfwvxx-NH ₂
Ac-rffxxx-NH ₂		2,000		Ac-rfwixx-NH ₂
Ac-rfhxxx-NH ₂		2,400		Ac-rfwlxx-NH ₂
Ac-rfyxxx-NH ₂		2,500		Ac-rfwmxx-NH ₂
Ac-rfixxx-NH ₂		5,500		Ac-rfwfxx-NH ₂
Ac-rfvxxx-NH ₂		6,900		Ac-rfwyxx-NH ₂
Ac-rfmxxx-NH ₂		12,000		Ac-rfwrxx-NH ₂
Ac-rfxxxx-NH ₂		12,000		Ac-rfwsxx-NH ₂
Ac-rflxxx-NH ₂		13,000		Ac-rfwgxx-NH ₂

Ac-rfsxxx-NH ₂	14,000		Ac-rfwhxx-NH ₂
Ac-rfrxxx-NH ₂	15,000		Ac-rfwpxx-NH ₂
Ac-rftxxx-NH ₂	21,000		Ac-rfwaxx-NH ₂
Ac-rfnxxx-NH ₂	21,000		Ac-rfwvxx-NH ₂
Ac-rfqxxx-NH ₂	23,000		Ac-rfwtxx-NH ₂
Ac-rfkxxx-NH ₂	23,000		Ac-rfwqxx-NH ₂
Ac-rfdxxx-NH ₂	50,000		Ac-rfwkxx-NH ₂
Ac-rfexxx-NH ₂	68,000		Ac-rfwnxx-NH ₂
Ac-rfpxxx-NH ₂	69,000		Ac-rfwexx-NH ₂
Ac-rfgxxx-NH ₂	69,000		Ac-rfwdx-NH ₂
Predicted Value		Scaled Error	
Arithmetic Mean	22,642	0.62	Arithmetic Mean
Geometric Mean	12,414	0.11	Geometric Mean
Harmonic Mean	5,618	0.60	Harmonic Mean

TABLE S1c Dooley et. al.¹⁵

Mixture	IC ₅₀ nM	Mixture
Ac-RFXXXX-NH ₂	2,701	Ac-RFMXXX-NH ₂
Constituent Mixtures		
Ac-RFMXXX-NH ₂	723	Ac-RFMWXX-NH ₂
Ac-RFLXXX-NH ₂	1,252	Ac-RFMSXX-NH ₂
Ac-RFIXXX-NH ₂	1,432	Ac-RFMAXX-NH ₂
Ac-RFWXXX-NH ₂	3,009	Ac-RFMGXX-NH ₂
Ac-RFFXXX-NH ₂	3,031	Ac-RFMIXX-NH ₂
Ac-RFGXXX-NH ₂	4,484	Ac-RFMVXX-NH ₂
Ac-RFYXXX-NH ₂	7,204	Ac-RFMMXX-NH ₂
Ac-RFHXXX-NH ₂	7,296	Ac-RFMRXX-NH ₂
Ac-RFNXXX-NH ₂	7,377	Ac-RFMHXX-NH ₂
Ac-RFRXXX-NH ₂	7,980	Ac-RFMTXX-NH ₂
Ac-RFQXXX-NH ₂	11,519	Ac-RFMNXX-NH ₂
Ac-RFTXXX-NH ₂	11,561	Ac-RFMKXX-NH ₂
Ac-RFAXXX-NH ₂	12,972	Ac-RFMQXX-NH ₂
Ac-RFKXXX-NH ₂	14,003	Ac-RFMYXX-NH ₂
Ac-RFSXXX-NH ₂	14,145	Ac-RFMDXX-NH ₂
Ac-RFPXXX-NH ₂	23,895	Ac-RFMFXX-NH ₂
Ac-RFVXXX-NH ₂	30,282	Ac-RFMLXX-NH ₂
Ac-RFDXXX-NH ₂	44,588	Ac-RFMPXX-NH ₂
Ac-RFEXXX-NH ₂	77,533	Ac-RFMEXX-NH ₂
Predicted Value		Scaled Error
Arithmetic Mean	14,962	4.54
Geometric Mean	7,989	1.96
Harmonic Mean	3,954	0.46

TABLE S1d Pinilla et. al.¹⁶

Mixture		IC ₅₀ nM	Mixture
YGGXXX-NH2		1,000	YGFXXX-NH2
Constituent Mixtures		IC ₅₀ nM	Constituent Mixtures
YGGFXX-NH2		48	YGFLXX-NH2
YGGLXX-NH2		1,160	YGFWXX-NH2
YGGWXX-NH2		6,840	YGFMXX-NH2
YGGIXX-NH2		18,220	YGFIXX-NH2
YGGMXX-NH2		26,680	YGFTXX-NH2
YGGYXX-NH2		98,220	YGFFXX-NH2
YGGRXX-NH2		179,780	YGFSXX-NH2
YGGGXX-NH2		253,500	YGFRXX-NH2
YGGTXX-NH2		399,620	YGFYXX-NH2
YGGVXX-NH2		517,060	YGFEXX-NH2
YGGQXX-NH2		732,040	YGFDXX-NH2
YGGAXX-NH2		800,000	YGFQXX-NH2
YGGPXX-NH2		1,081,160	YGFVXX-NH2
YGGHXX-NH2		1,232,200	YGFNXX-NH2
YGGSXX-NH2		1,690,580	YGFHXX-NH2
YGGNXX-NH2		1,750,000	YGFAXX-NH2
YGGEXX-NH2		1,750,000	YFGGXX-NH2
YGGKXX-NH2		1,750,000	YGFPXX-NH2
YGGDXX-NH2		1,750,000	YGFKXX-NH2
		Predicted Value	Scaled Error
Arithmetic Mean		738,795	737.80
Geometric Mean		168,921	167.92
Harmonic Mean		865	0.14

TABLE S1e Houghten et. al.¹⁷

Mixture		IC ₅₀ nM	Mixture
Ac-PYXXXX-NH2		20,000	Ac-PYPXXX-NH2
Constituent Mixtures		IC ₅₀ nM	Constituent Mixtures
Ac-PYPXXX-NH2		860	Ac-PYPNXX-NH2
Ac-PYGXXX-NH2		12,056	Ac-PYPHXX-NH2
Ac-PYQXXX-NH2		20,104	Ac-PYPGXX-NH2
Ac-PYAXXX-NH2		39,380	Ac-PYPTXX-NH2
Ac-PYKXXX-NH2		72,320	Ac-PYPQXX-NH2
Ac-PYHXXX-NH2		85,640	Ac-PYPAXX-NH2
Ac-PYLXXX-NH2		89,920	Ac-PYPDXX-NH2
Ac-PYRXXX-NH2		102,120	Ac-PYPEXX-NH2
Ac-PYSXXX-NH2		152,000	Ac-PYPFXX-NH2
Ac-PYMXXX-NH2		162,000	Ac-PYPIXX-NH2
Ac-PYNXXX-NH2		194,000	Ac-PYPKXX-NH2
Ac-PYYXXX-NH2		256,000	Ac-PYPLXX-NH2

Ac-PYTXXX-NH2	268,000		Ac-PYPMXX-NH2
Ac-PYEXXX-NH2	392,000		Ac-PYPPXX-NH2
Ac-PYIXXX-NH2	446,000		Ac-PYPRXX-NH2
Ac-PYVXXX-NH2	792,000		Ac-PYPSXX-NH2
Ac-PYFXXX-NH2	876,000		Ac-PYPVXX-NH2
Ac-PYWXXX-NH2	1,420,000		Ac-PYPWXX-NH2
Ac-PYDXXX-NH2	1,420,000		Ac-PYPYXX-NH2
Predicted Value		Scaled Error	
Arithmetic Mean	357,916	16.90	Arithmetic Mean
Geometric Mean	136,593	5.83	Geometric Mean
Harmonic Mean	13,557	0.32	Harmonic Mean

TABLE S1f Appel et. al.¹⁸

Mixture	IC ₅₀ nM		Mixture
Ac-YPXXXX-NH2	200,000		Ac-YPNXXX-NH2
Constituent Mixtures		IC ₅₀ nM	Constituent Mixtures
Ac-YPNXXX-NH2	7,329		Ac- YPNLXX-NH2
Ac- YPYXXX-NH2	12,780		Ac- YPNIXX-NH2
Ac-YPAXXX-NH2	1,400,000		Ac- YPNMXX-NH2
Ac- YPDXXX-NH2	1,400,000		Ac- YPNVXX-NH2
Ac- YPEXXX-NH2	1,400,000		Ac- YPNFXX-NH2
Ac- YPFXXX-NH2	1,400,000		Ac- YPNDXX-NH2
Ac- YPGXXX-NH2	1,400,000		Ac- YPNTXX-NH2
Ac- YPHXXX-NH2	1,400,000		Ac- YPNAXX-NH2
Ac- YPIXXX-NH2	1,400,000		Ac- YPN8XX-NH2
Ac- YPKXXX-NH2	1,400,000		Ac- YPNRXX-NH2
Ac- YPLXXX-NH2	1,400,000		Ac- YPNWXX-NH2
Ac- YPMXXX-NH2	1,400,000		Ac- YPNEXX-NH2
Ac- YPPXXX-NH2	1,400,000		Ac- YPNGXX-NH2
Ac- YPQXXX-NH2	1,400,000		Ac- YPNKXX-NH2
Ac- YPRXXX-NH2	1,400,000		Ac- YPNHXX-NH2
Ac- YPSXXX-NH2	1,400,000		Ac- YPNQXX-NH2
Ac- YPTXXX-NH2	1,400,000		Ac- YPNPXX-NH2
Ac- YPVXXX-NH2	1,400,000		Ac- YPNNXX-NH2
Ac- YPWXXX-NH2	1,400,000		Ac- YPNYXX-NH2
Predicted Value		Scaled Error	
Arithmetic Mean	1,253,690	5.27	Arithmetic Mean
Geometric Mean	829,323	3.15	Geometric Mean
Harmonic Mean	83,762	0.58	Harmonic Mean

TABLE S1g Davis et. al.¹⁹

Mixture	IC ₅₀ uM		Mixture
(noC)XXXT	30		(noC)(noC)XXT
Constituent Mixtures		IC ₅₀ uM	Constituent Mixtures

(noC)(dG)XXT	100		(noC)(noC)(dG)XT
(noC)(T)XXT	100		(noC)(noC)(T)XT
(noC)(mA)XXT	100		(noC)(noC)(mA)XT
(noC)(mU)XXT	100		(noC)(noC)(mU)XT
(noC)(BT1)XXT	35		(noC)(noC)(BT1)XT
(noC)(BT2)XXT	100		(noC)(noC)(BT2)XT
(noC)(egNH)XXT	100		(noC)(noC)(egNH)XT
(noC)(noC)XXT	20		(noC)(noC)(noC)XT
(noC)(mmU)XXT	100		(noC)(noC)(mmU)XT
(noC)(peG)XXT	35		(noC)(noC)(peG)XT
(noC)(egCB)XXT	100		(noC)(noC)(egCB)XT
(noC)(egIM)XXT	100		(noC)(noC)(egIM)XT
Predicted Value		Scaled Error	
Arithmetic Mean	83	1.75	Arithmetic Mean
Geometric Mean	73	1.45	Geometric Mean
Harmonic Mean	61	1.03	Harmonic Mean

TABLE S1h Ecker et. al.²⁰

Mixture	IC₅₀ uM		Mixture
XXXXCXCXX	4		XXCXCXCXX
Constituent Mixtures		IC₅₀ uM	Constituent Mixtures
XXAXCXCXX	10		XXCACXCXX
XXCXCXCXX	0.5		XXCCCXCXX
XXGXCXCXX	10		XXCGXCXCXX
XXUXCXCXX	10		XXCUCXCXX
Predicted Value		Scaled Error	
Arithmetic Mean	7.6	0.91	Arithmetic Mean
Geometric Mean	4.7	0.18	Geometric Mean
Harmonic Mean	1.7	0.57	Harmonic Mean

IC ₅₀ uM		Mixture	IC ₅₀ uM	
41		Ac-DVPDXX-NH2	4.4	
IC ₅₀ uM		Constituent Mixtures	IC ₅₀ uM	
4		Ac-DVPDYX-NH2	0.38	
1400		Ac-DVPDAX-NH2	1,400	
1,400		Ac-DVPDDX-NH2	1,400	
1,400		Ac-DVPDEX-NH2	1,400	
1,400		Ac-DVPDFX-NH2	1,400	
1,400		Ac-DVPDGX-NH2	1,400	
1,400		Ac-DVPDHX-NH2	1,400	
1,400		Ac-DVPDIX-NH2	1,400	
1,400		Ac-DVPDKX-NH2	1,400	
1,400		Ac-DVPDLX-NH2	1,400	
1,400		Ac-DVPDMX-NH2	1,400	
1,400		Ac-DVPDNX-NH2	1,400	
1,400		Ac-DVPDPX-NH2	1,400	
1,400		Ac-DVPDQX-NH2	1,400	
1,400		Ac-DVPDRX-NH2	1,400	
1,400		Ac-DVPDSX-NH2	1,400	
1,400		Ac-DVPDTX-NH2	1,400	
1,400		Ac-DVPDVX-NH2	1,400	
Predicted Value	Scaled Error		Predicted Value	Scaled Error
1,322	31.26	Arithmetic Mean	1,322	299.51
1,016	23.79	Geometric Mean	887	200.63
75	0.83	Harmonic Mean	7	0.55

IC ₅₀ nM		Mixture	IC ₅₀ nM	
1,500		Ac-rfwixx-NH ₂	480	
IC ₅₀ nM		Constituent Mixtures	IC ₅₀ nM	
400		Ac-rfwinx-NH ₂	200	
500		Ac-rfwiax-NH ₂	350	
1,000		Ac-rfwikx-NH ₂	370	
1,000		Ac-rfwirx-NH ₂	460	
1,000		Ac-rfwisx-NH ₂	490	
1,500		Ac-rfwimx-NH ₂	500	
2,000		Ac-rfwifx-NH ₂	690	
2,300		Ac-rfwilx-NH ₂	700	
2,400		Ac-rfwitx-NH ₂	780	

2,400		Ac-rfwigx-NH ₂	1,100	
2,700		Ac-rfwiwix-NH ₂	1,200	
2,800		Ac-rfwihx-NH ₂	1,300	
3,700		Ac-rfwivx-NH ₂	1,500	
3,800		Ac-rfwiyx-NH ₂	1,500	
4,200		Ac-rfwiqx-NH ₂	2,300	
4,400		Ac-rfwix-NH ₂	2,800	
4,500		Ac-rfwipx-NH ₂	3,700	
15,000		Ac-rfwidx-NH ₂	8,000	
33,000		Ac-rfwieix-NH ₂	11,000	
Predicted Value	Scaled Error		Predicted Value	Scaled Error
4,663	2.11	Arithmetic Mean	2,049	3.27
2,494	0.66	Geometric Mean	1,122	1.34
1,586	0.06	Harmonic Mean	729	0.52

IC ₅₀ nM		Mixture	IC ₅₀ nM	
907		Ac-RFMWXX-NH ₂	106	
IC ₅₀ nM		Constituent Mixtures	IC ₅₀ nM	
174		Ac-RFMWMX-NH ₂	30	
541		Ac-RFMWVX-NH ₂	54	
595		Ac-RFMWQX-NH ₂	83	
641		Ac-RFMWIX-NH ₂	108	
730		Ac-RFMWYX-NH ₂	125	
790		Ac-RFMWLX-NH ₂	180	
870		Ac-RFMWRX-NH ₂	187	
882		Ac-RFMWAX-NH ₂	204	
927		Ac-RFMWKX-NH ₂	210	
1,048		Ac-RFMWGX-NH ₂	313	
1,169		Ac-RFMWTX-NH ₂	321	
1,310		Ac-RFMWSX-NH ₂	327	
1,375		Ac-RFMWWX-NH ₂	327	
1,468		Ac-RFMWHX-NH ₂	348	
1,908		Ac-RFMWFX-NH ₂	378	
2,004		Ac-RFMWNX-NH ₂	454	
2,166		Ac-RFMWPX-NH ₂	616	
2,626		Ac-RFMWEX-NH ₂	795	
3,912		Ac-RFMWDX-NH ₂	952	
Predicted Value	Scaled Error		Predicted Value	Scaled Error
1,323	0.46	Arithmetic Mean	316	1.99
1,077	0.19	Geometric Mean	231	1.18
828	0.09	Harmonic Mean	151	0.42

IC ₅₀ nM		Mixture	IC ₅₀ nM	
400		YGGFXX-NH2	48	
IC ₅₀ nM		Constituent Mixtures	IC ₅₀ nM	
400		YGGFMX-NH2	6.6	
400		YGGFIX-NH2	7.2	
1,400		YGGFLX-NH2	8.8	
1,520		YGGFTX-NH2	22	
1,660		YGGFSX-NH2	28	
2,300		YGGFFX-NH2	28	
3,420		YGGFQX-NH2	28	
3,640		YGGFYX-NH2	34	
3,760		YGGFHX-NH2	34	
3,840		YGGFEX-NH2	36	
3,960		YGGFNX-NH2	38	
4,140		YGGFVX-NH2	50	
4,880		YGGFGX-NH2	56	
5,060		YGGFDX-NH2	56	
5,300		YGGFAX-NH2	62	
5,860		YGGFWX-NH2	64	
7,160		YGGFKX-NH2	146	
7,980		YGGFRX-NH2	246	
14,400		YGGFPX-NH2	352	
Predicted Value	Scaled Error		Predicted Value	Scaled Error
4,267	9.67	Arithmetic Mean	69	0.43
3,118	6.79	Geometric Mean	40	0.17
1,882	3.71	Harmonic Mean	25	0.49

IC ₅₀ nM		Mixture	IC ₅₀ nM	
860		Ac-PYPNXX-NH2	90	
IC ₅₀ nM		Constituent Mixtures	IC ₅₀ nM	
90		Ac-PYPNLX-NH2	6	
132,000		Ac-PYPNVX-NH2	69	
136,000		Ac-PYPNMX-NH2	85	
240,000		Ac-PYPNIX-NH2	88	
318,000		Ac-PYPNFX-NH2	461	
1,420,000		Ac-PYPNXX-NH2	615	
1,420,000		Ac-PYPNTX-NH2	3,662	
1,420,000		Ac-PYPNAX-NH2	4,719	
1,420,000		Ac-PYPNHX-NH2	8,138	
1,420,000		Ac-PYPNSX-NH2	8,447	
1,420,000		Ac-PYPNYX-NH2	9,307	
1,420,000		Ac-PYPNQX-NH2	10,663	

1,420,000		Ac-PYPNWX-NH2	12,625	
1,420,000		Ac-PYPNPX-NH2	36,759	
1,420,000		Ac-PYPNEX-NH2	67,596	
1,420,000		Ac-PYPNGX-NH2	89,080	
1,420,000		Ac-PYPNKX-NH2	91,700	
1,420,000		Ac-PYPNDX-NH2	113,446	
1,420,000		Ac-PYPNRX-NH2	183,400	
Predicted Value	Scaled Error		Predicted Value	Scaled Error
1,089,794	1266.20	Arithmetic Mean	33,730	373.78
560,506	650.75	Geometric Mean	4,149	45.10
1,705	0.98	Harmonic Mean	91	0.01

IC₅₀ nM		Mixture	IC₅₀ nM	
7,329		Ac- YPNLXX-NH2	376	
IC₅₀ nM		Constituent Mixtures	IC₅₀ nM	
376		Ac- YPNLPX-NH2	164	
4,710		Ac- YPNLSX-NH2	257	
5,500		Ac- YPNLQX-NH2	276	
7,700		Ac-YPNLRX-NH2	292	
30,000		Ac- YPNLEX-NH2	339	
31,000		Ac-YPNLTX-NH2	348	
112,000		Ac- YPNLGX-NH2	358	
374,000		Ac- YPNLDX-NH2	379	
1,400,000		Ac- YPNLMX-NH2	389	
1,400,000		Ac- YPNLKX-NH2	420	
1,400,000		Ac: YPNLNX-NH2	499	
1,400,000		Ac- YPNLAX-NH2	529	
1,400,000		Ac-YPNLVX-NH2	533	
1,400,000		Ac- YPNLHX-NH2	601	
1,400,000		Ac- YPNLIX-NH2	614	
1,400,000		Ac- YPNLFX-NH2	797	
1,400,000		Ac-YPNLYX-NH2	841	
1,400,000		Ac- YPNLLX-NH2	858	
1,400,000		Ac-YPNLWX-NH2	1,274	
Predicted Value	Scaled Error		Predicted Value	Scaled Error
840,278	113.65	Arithmetic Mean	514	0.37
208,754	27.48	Geometric Mean	456	0.21
5,813	0.21	Harmonic Mean	407	0.08

IC₅₀ uM	
20	
IC₅₀ uM	

10	
50	
50	
50	
50	
50	
50	
20	
45	
15	
50	
50	
Predicted Value	Scaled Error
41	1.04
36	0.82
30	0.50

IC₅₀ uM		Mixture	IC₅₀ uM	
0.5		XXCCCXCXX	0.15	
IC₅₀ uM		Constituent Mixtures	IC₅₀ uM	
10		XXCCCACXX	0.08	
0.15		XXXXXXXXXX	1	
10		XXXXCGCXX	0.4	
10		XXXXCUCXX	1	
Predicted Value	Scaled Error		Predicted Value	Scaled Error
7.54	14.08	Arithmetic Mean	0.62	3.13
3.50	6.00	Geometric Mean	0.42	1.82
0.57	0.15	Harmonic Mean	0.24	0.57

Mixture	IC ₅₀ uM	
Ac-DVPDYX-NH ₂	0.38	
Constituent Compounds		
Constituents	IC ₅₀ uM	
Ac-DVPDYA-NH ₂	0.03	
Ac-DVPDYS-NH ₂	0.27	
Ac-DVPDYV-NH ₂	1.1	
Ac-DVPDYT-NH ₂	1.5	
Ac-DVPDYG-NH ₂	1.6	
Ac-DVPDYE-NH ₂	4.06	
Ac-DVPDYI-NH ₂	5.29	
Ac-DVPDYM-NH ₂	7.7	
Ac-DVPDYQ-NH ₂	8.18	
Ac-DVPDYH-NH ₂	8.99	
Ac-DVPDYL-NH ₂	9.98	
Ac-DVPDYR-NH ₂	10.9	
Ac-DVPDYF-NH ₂	12.02	
Ac-DVPDYN-NH ₂	15.56	
Ac-DVPDYK-NH ₂	17.6	
Ac-DVPDYY-NH ₂	22.48	
Ac-DVPDYP-NH ₂	26.14	
Ac-DVPDYD-NH ₂	48	
	Predicted Value	Scaled Error
Arithmetic Mean	11	28.44
Geometric Mean	5	11.89
Harmonic Mean	0	0.17

Mixture	IC ₅₀ nM	
Ac-rfwinx-NH ₂	110	
Constituent Compounds		
Constituents	IC ₅₀ nM	
Ac-rfwink-NH ₂	18	
Ac-rfwir-NH ₂	27	
Ac-rfwina-NH ₂	37	
Ac-rfwins-NH ₂	130	
Ac-rfwinp-NH ₂	130	
Ac-rfwinn-NH ₂	130	
Ac-rfwinq-NH ₂	140	
Ac-rfwing-NH ₂	170	
Ac-rfwim-NH ₂	180	

Ac-rfwinh-NH ₂	200	
Ac-rfwint-NH ₂	230	
Ac-rfwihy-NH ₂	460	
Ac-rfwini-NH ₂	680	
Ac-rfwinf-NH ₂	770	
Ac-rfwinw-NH ₂	790	
Ac-rfwine-NH ₂	960	
Ac-rfwind-NH ₂	1,100	
Ac-rfwinv-NH ₂	1,300	
Ac-rfwini-NH ₂	5,600	
	Predicted Value	Scaled Error
Arithmetic Mean	687	5.24
Geometric Mean	265	1.41
Harmonic Mean	106	0.04

Mixture	IC ₅₀ nM	
Ac-RFMWMX-NH ₂	24	
Constituent Compounds	IC ₅₀ nM	
Ac-RFMWMK-NH ₂	5	
Ac-RFMWMT-NH ₂	5	
Ac-RFMWMR-NH ₂	6	
Ac-RFMWMS-NH ₂	7	
Ac-RFMWVG-NH ₂	10	
Ac-RFMWMN-NH ₂	11	
Ac-RFMWMQ-NH ₂	12	
Ac-RFMWMA-NH ₂	15	
Ac-RFMWMV-NH ₂	17	
Ac-RFMWMY-NH ₂	17	
Ac-RFMWMM-NH ₂	18	
Ac-RFMWML-NH ₂	20	
Ac-RFMWMH-NH ₂	20	
Ac-RFMWMP-NH ₂	24	
Ac-RFMWMW-NH ₂	46	
Ac-RFMWMI-NH ₂	67	
Ac-RFMWMF-NH ₂	68	
Ac-RFMWME-NH ₂	96	
Ac-RFMWMD-NH ₂	109	
	Predicted Value	Scaled Error
Arithmetic Mean	30	0.26
Geometric Mean	19	0.20
Harmonic Mean	13	0.45

Mixture	IC ₅₀ nM	
YGGFMX-NH2	6.6	
Constituent Compounds	IC ₅₀ nM	
YGGFMT-NH2	3.2	
YGGFMS-NH2	4.3	
YGGFME-NH2	4.4	
YGGFML-NH2	6	
YGGFMR-NH2	6	
YGGFMN-NH2	6.2	
YGGFMK-NH2	6.3	
YGGFMI-NH2	6.3	
YGGFMA-NH2	6.7	
YGGFMH-NH2	7.1	
YGGFMP-NH2	7.1	
YGGFMV-NH2	7.4	
YGGFMD-NH2	7.5	
YGGFMG-NH2	7.7	
YGGFMQ-NH2	8.3	
YGGFMM-NH2	11.3	
YGGFMY-NH2	16	
YGGFMF-NH2	25.8	
YGGFMW-NH2	25.8	
	Predicted Value	Scaled Error
Arithmetic Mean	9.1	0.38
Geometric Mean	7.7	0.17
Harmonic Mean	6.9	0.04

Mixture	IC ₅₀ nM	
Ac-PYPNLX-NH2	6	
Constituent Compounds	IC ₅₀ nM	
Ac-PYPNLP-NH2	4	
Ac-PYPNLT-NH2	5	
Ac-PYPNLS-NH2	6	
Ac-PYPNLQ-NH2	8	
Ac-PYPNLG-NH2	9	
Ac-PYPNLA-NH2	9	
Ac-PYPNLH-NH2	9	
Ac-PYPNLK-NH2	9	
Ac-PYPNLD-NH2	11	
Ac-PYPNLE-NH2	12	
Ac-PYPNLI-NH2	13	
Ac-PYPNLN-NH2	14	

Ac-PYPNLM-NH2	15	
Ac-PYPNLR-NH2	17	
Ac-PYPNLL-NH2	17	
Ac-PYPNLF-NH2	18	
Ac-PYPNLW-NH2	29	
Ac-PYPNLY-NH2	35	
Ac-PYPNLV-NH2	39	
Predicted Value		Scaled Error
Arithmetic Mean	15	1.45
Geometric Mean	12	1.04
Harmonic Mean	10	0.72

Mixture	IC ₅₀ nM	Mixture	IC ₅₀ nM
Ac- YPNLSX-NH2	257	Ac- YPYXXX-NH2	12,780
Constituent Mixtures		Constituent Mixtures	
Ac-YPNLSX-NH2	257	Ac-YPYXXX-NH2	12,780
Ac-YPNLSY-NH2	153	Ac-YPYGXX-NH2	34,000
Ac-YPNLSH-NH2	157	Ac-YPYAXX-NH2	50,000
Ac-YPNLSV-NH2	158	Ac-YPYKXX-NH2	108,000
Ac-YPNLST-NH2	161	Ac-YPYNXX-NH2	186,000
Ac-YPNLSD-NH2	177	Ac-YPYMXX-NH2	196,000
Ac-YPNLSF-NH2	180	Ac-YPYHXX-NH2	314,000
Ac-YPNLSQ-NH2	190	Ac-YPYRXX-NH2	378,000
Ac-YPNLSK-NH2	223	Ac-YPYYXX-NH2	452,000
Ac-YPNLSN-NH2	245	Ac-YPYDXX-NH2	546,000
Ac-YPNLSM-NH2	250	Ac-YPYEXX-NH2	558,000
Ac-YPNLSL-NH2	277	Ac-YPYSXX-NH2	618,000
Ac-YPNLSW-NH2	301	Ac-YPYVXX-NH2	640,000
Ac-YPNLSP-NH2	307	Ac-YPYTXX-NH2	740,000
Ac-YPNLSR-NH2	311	Ac-YPYFXX-NH2	1,400,000
Ac-YPNLSE-NH2	367	Ac-YPYWXX-NH2	1,400,000
Ac-YPNLSA-NH2	429	Ac-YPYIXX-NH2	1,400,000
Ac-YPNLSE-NH2	507	Ac-YPYLXX-NH2	1,400,000
Ac-YPNLSI-NH2	1,151	Ac-YPYQXX-NH2	1,400,000
Predicted Value		Predicted Value	
Arithmetic Mean	299	Arithmetic Mean	622,127
Geometric Mean	255	Geometric Mean	292,158
Harmonic Mean	230	Harmonic Mean	7,481

Mixture		IC ₅₀ uM	Mixture		IC ₅₀ uM
XXCCCACXX		0.08	XXCCCACAX		0.05
Constituent Mixtures		IC ₅₀ uM	Constituent Mixtures		IC ₅₀ uM
XXCCCACAX		0.05	XACCCACAX		0.1
XXCCCACCX		0.5	XCCCCACAX		0.1
XXCCCACGX		0.08	XGCCCACAX		0.03
XXCCCACUX		0.5	XUCCCACAX		0.1
		Predicted Value			Predicted Value
Arithmetic Mean		0.28	Scaled Error		2.53
Geometric Mean		0.18	Arithmetic Mean		0.08
Harmonic Mean		0.11	Geometric Mean		0.07
			Harmonic Mean		0.06

	Mixture	IC ₅₀ nM		Mixture
	Ac- YPYPXX-NH2	408		Ac-YPYPNX-NH2
	Constituent Mixtures	IC ₅₀ nM		Constituent Compounds
	Ac-YPYPNX-NH2	37		Ac-YPYPNL-NH2
	Ac- YPYPHX-NH2	56,993		Ac- YPYPNM-NH2
	Ac- YPYPGX-NH2	104,973		Ac- YPYPNI-NH2
	Ac- YPYPQX-NH2	162,400		Ac-YPYPNV-NH2
	Ac- YPYPIX-NH2	276,000		Ac-YPYPNF-NH2
	Ac-YPYPFX-NH2	318,000		Ac- YPYPNK-NH2
	Ac- YPYPEX-NH2	436,000		Ac- YPYPNT-NH2
	Ac- YPYPTX-NH2	523,200		Ac- YPYPNA-NH2
	Ac- YPYPDX-NH2	530,000		Ac-YPYPNS-NH2
	Ac- YPYPSX-NH2	980,000		Ac- YPYPNQ-NH2
	Ac- YPYPVX-NH2	1,400,000		Ac- YPYPNH-NH2
	Ac- YPYPLX-NH2	1,400,000		Ac-YPYPNP-NH2
	Ac- YPYPWX-NH2	1,400,000		Ac-YPYPNY-NH2
	Ac-YPYPAX-NH2	1,400,000		Ac-YPYPNW-NH2
	Ac- YPYPRX-NH2	1,400,000		Ac- YPYPNN-NH2
	Ac- YPYPPX-NH2	1,400,000		Ac-YPYPNG-NH2
	Ac- YPYPMX-NH2	1,400,000		Ac-YPYPNR-NH2
	Ac- YPYPKX-NH2	1,400,000		Ac- YPYPNE- NH2
	Ac- YPYPYX-NH2	1,400,000		Ac- YPYPND-NH2
Scaled Error		Predicted Value	Scaled Error	
47.68	Arithmetic Mean	841,453	2061.38	Arithmetic Mean
21.86	Geometric Mean	374,148	916.03	Geometric Mean
0.41	Harmonic Mean	702	0.72	Harmonic Mean

	Mixture	IC₅₀ uM		Mixture
	XGCCCACAX	0.03		XGCCCACAC
	Constituent Mixtures	IC₅₀ uM		Constituent Compounds
	XGCCCACAA	0.05		AGCCCACAC
	XGCCCACAC	0.02		CGCCCACAC
	XGCCCACAG	0.05		GGCCCACAC
	XGCCCACAU	0.042		UGCCCACAC
Scaled Error		Predicted Value	Scaled Error	
0.65	Arithmetic Mean	0.041	0.35	Arithmetic Mean
0.48	Geometric Mean	0.038	0.27	Geometric Mean
0.26	Harmonic Mean	0.035	0.17	Harmonic Mean

IC ₅₀ nM	
37	

IC ₅₀ nM	
2	
14	
14	
20	
176	
357	
358	
427	
1,733	
2,777	
2,809	
3,302	
4,741	
4,971	
5,679	
6,128	
6,746	
8,547	
67,480	

Predicted Value	Scaled Error
6,120	164.41
788	20.29
27	0.28

IC₅₀ uM	
0.02	
IC₅₀ uM	
0.03	
0.05	
0.02	
0.01	
Predicted Value	Scaled Error
0.028	0.38
0.023	0.17
0.020	0.02