Electronic Supplementary Material (ESI) for MedChemComm.

SUPPLEMENTARY INFORMATION

LIPOPHILICITY PREDICTION OF PEPTIDES AND PEPTIDE DERIVATIVES BY CONSENSUS MACHINE LEARNING

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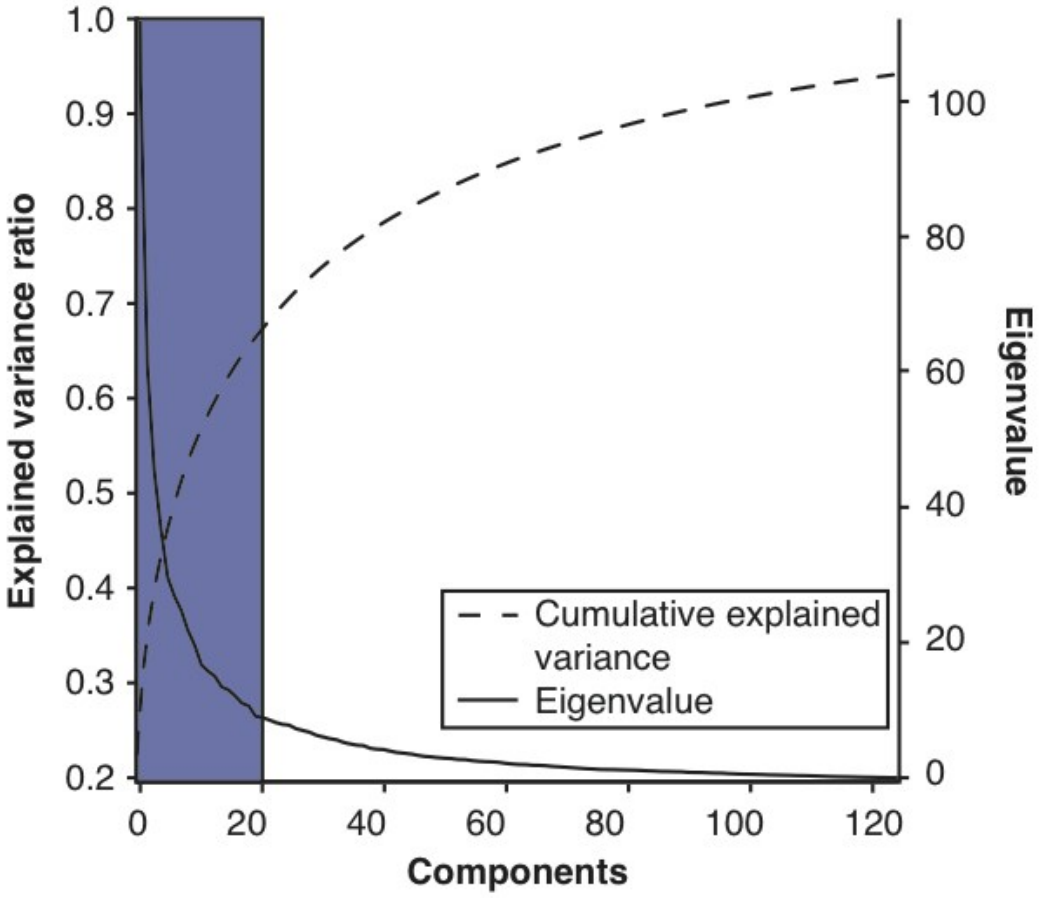


Figure S1. PCA Scree plot. Cumulative sum of explained variance (dashed line) and Eigenvalues of the respective principal components (straight line). 20 components were selected (blue area) and the calculated scores serve as a reduced feature set.

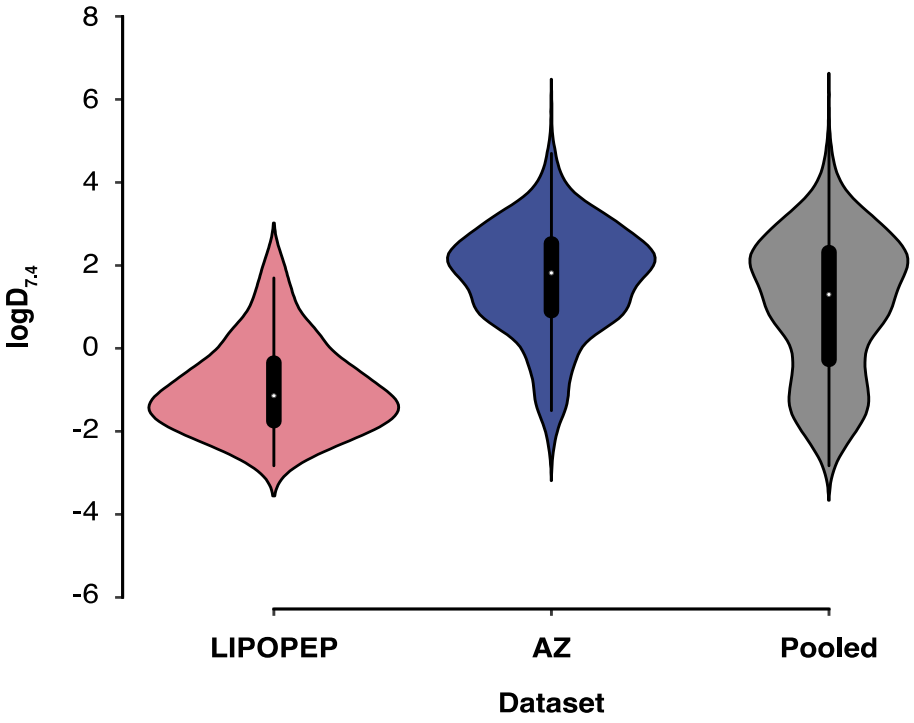


Figure S2. Violin plots showing $logD_{7.4}$ distributions of LIPOPEP, AZ and the pooled data set.

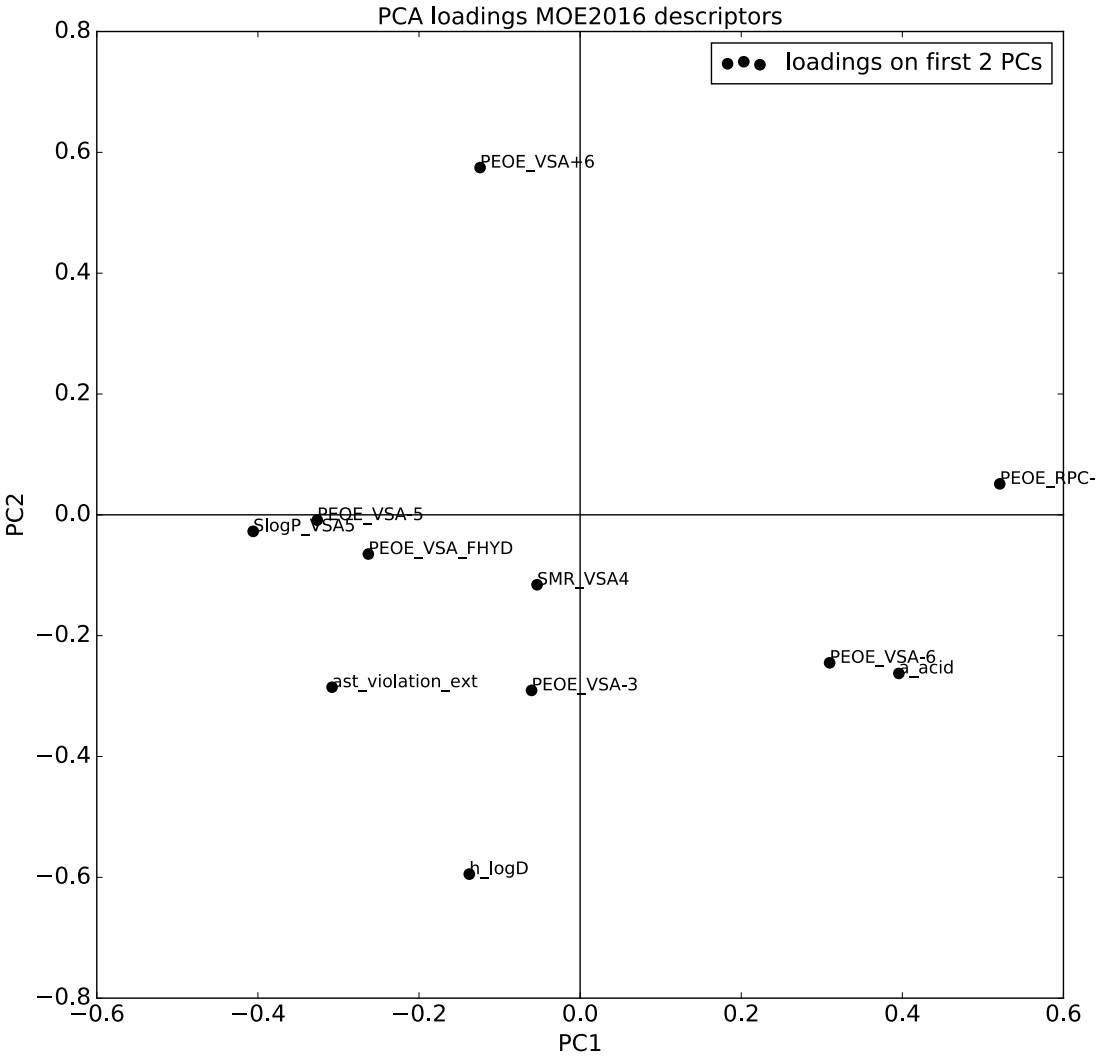


Figure S3. PCA Loadings of the LASSO selected features on the first two principal components.

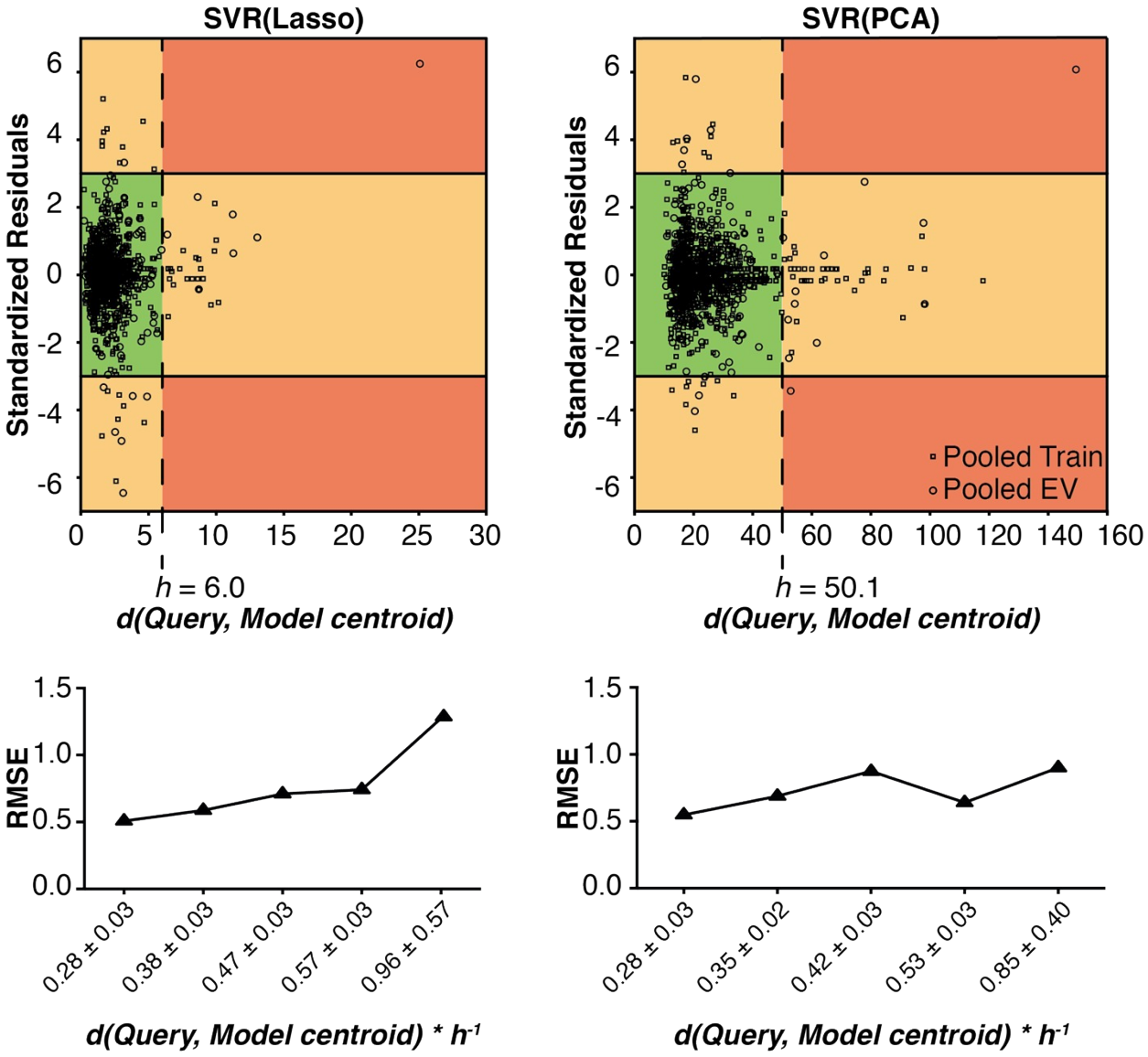


Figure S4. Top: Williams plots of standardized residuals vs. leverages for compound in pooled training Set (squares) and external validation (circles) for SVR(Lasso) and SVR(PCA). The vertical line depicts the warning leverage *h*. Horizontal lines indicate standardized residuals at -3 and 3. Observations in the green rectangle are within AD and cover 99.7% of normally distributed error (approximately 95% of the data for SVR(Lasso) and SVR(PCA). Observations in light orange exceed one of the thresholds, observations in dark orange exceed both. Bottom: RMSE in relation to "Novelty" of a query. Novelty is quantified as the ratio of distance to model centroid divided by *h*. Objects in external validation partitions were sorted according to their novelty and binned into five equally sized groups. Lines connecting the markers are introduced for visualisation and do not display a function.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}\left(\hat{y}_i - y_i\right)^2}{n}} \qquad \%accurate = \frac{\sum\left(\hat{y}_i - y_i\right) < 0.5}{n}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n_{TR}}\left(y_i - \hat{y}_i\right)^2}{\sum_{i=1}^{n_{TR}}\left(y_i - \bar{y}_{TR}\right)^2} \qquad Q^2_{F1} = 1 - \frac{\sum_{i=1}^{n_{CV}}\left(y_i - \hat{y}_{i/i}\right)^2}{\sum_{i=1}^{n_{CV}}\left(y_i - \bar{y}_{TR}\right)^2}$$

Figure S5. Regression metrics used to evaluate the performance of the models.

Table S1. List of descriptors after feature selection with LASSO.

Name	Description
h_logD	Octanol/water distribution coefficient at pH 7 calculated as a state average: log sum $\{10^{h\_logP_i - pC_i}\}$. Here, h_logP is the pH-independent octanol/water partition coefficient using an eight parameter model based on Hueckel Theory [unpublished] with R^2 = 0.84, RMSE=0.59 on 1,836 small molecules. Peptides or peptidic structures were not subject of the training set.
PEOE_VSA-6	Partial Equalization of Orbital Electronegativities (PEOE) (Gasteiger 1980) that calculates atomic partial charges only from elements, formal charges and connectivity information of the molecule. Here: sum of vdW surface of atom i (vi) where the partial charge of atom i (qi) is < -0.30. Most negative partial charge category. vi is calculated by a connection table approximation.
SMR_VSA4	Subdivided surface area: Sum of vi such that the atomic contribution to molar refractivity (model CrippenÊ1999) is in range [0.39, 0.44]. Representation of polarizability of a molecule.
SlogP_VSA5	Subdivided surface area: Sum of vi such that the atomic contribution to logP (model CrippenÊ1999) is in range [0.15, 0.20]. Intermediate hydrophobic contribution.
a_acid	Number of acidic atoms
PEOE_RPC-	Relative negative partial charge: the smallest negative qi divided by the sum of the negative qi.
PEOE_VSA-5	Sum of vi where qi is in range [-0.25, -0.3]. Second highest negative partial charge category.
PEOE_VSA_FHYD	Fractional hydrophobic vdW surface area, also calculated by vi and qi
PEOE_VSA+6	Sum of vi where qi is > 0.3. Most positive partial charge category.
ast_violation_ext	Astex fragment like violation count (rule of three: hbd < 3, hba < 3, clogP < 3)
PEOE_VSA-3	Sum of vi where qi is in range [-0.15, -0.2]. Intermediate negative partial charge category.

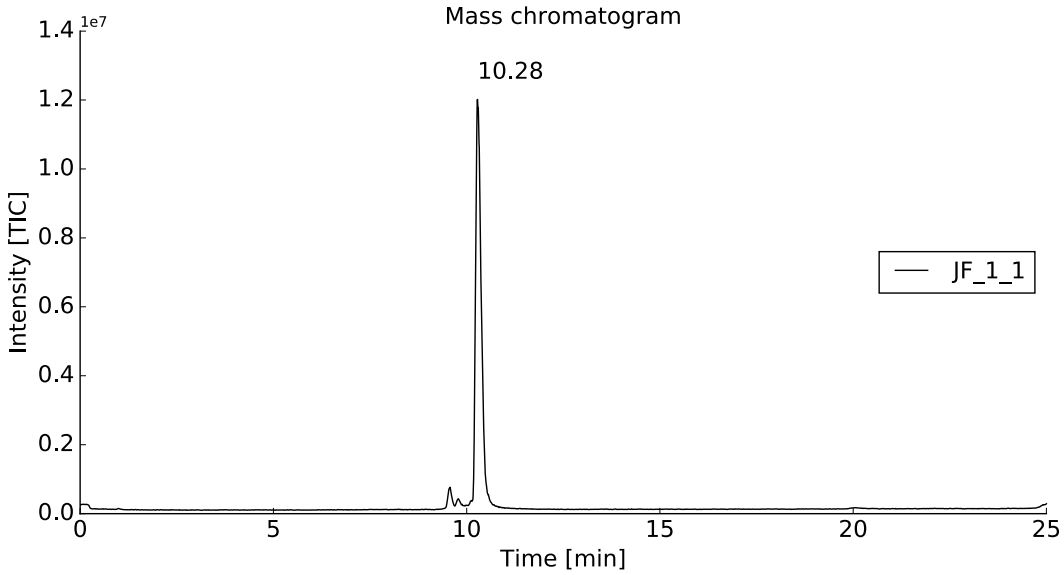
Table S2. Model performance before and after y–randomization.

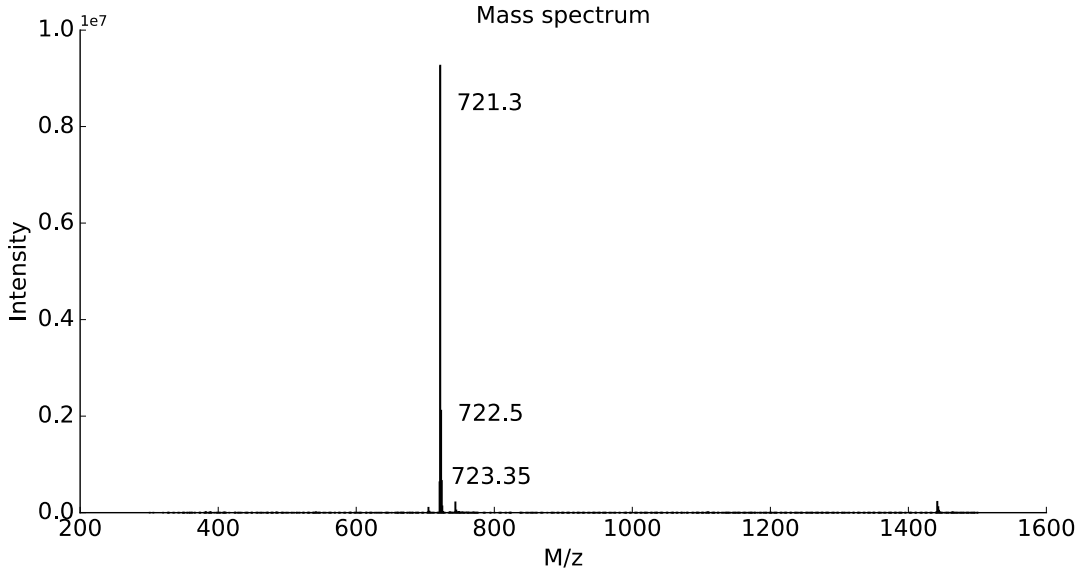
		Original Training			Original Cross Validation		
Dataset	**Model**	**RMSE***	**% accurate***	**R2**	**RMSE***	**% accurate***	**Q2F1**
LIPOPEP	Lasso (MOE)	0.52 ± 0.02	78.6 ± 1.6	0.79	0.60 ± 0.09	75.5 ± 7.4	0.68
	SVR (MOE)	0.37 ± 0.02	91.2 ± 1.0	0.88	0.47 ± 0.13	86.0 ± 3.1	0.80
	SVR (PCA)	0.4 ± 0.01	83.9 ± 1.1	0.87	0.59 ± 0.11	73.8 ± 4.1	0.69
Pooled	SVR (MOE)	0.69 ± 0.01	68.8 ± 1.5	0.83	0.77 ± 0.05	65.2 ± 3.1	0.79
	SVR (PCA)	0.59 ± 0.01	72.9 ± 1.5	0.78	0.78 ± 0.04	58.9 ± 3.3	0.78
		y - Randomized Training			**y - Randomized Cross Validation**		
Dataset	**Model**	**RMSE***	**% accurate***	**R2**	**RMSE***	**% accurate***	**Q2F1**
LIPOPEP	Lasso (MOE)	1.06 ± 0.03	36.3 ± 2.2	0.03	1.08 ± 0.11	35.3 ± 7.0	0.85
	SVR (MOE)	1.03 ± 0.03	45.6 ± 2.2	0.10	1.13 ± 0.12	35.9 ± 6.8	0.84
	SVR (PCA)	0.98 ± 0.03	50.9 ± 2.3	0.21	1.14 ± 0.12	35.8 ± 6.4	0.84
Pooled	SVR (MOE)	1.65 ± 0.02	26.5 ± 1.0	0.06	1.75 ± 0.07	21.1 ± 2.6	0.04
	SVR (PCA)	1.54 ± 0.02	34.1 ± 1.1	0.18	1.78 ± 0.07	20.6 ± 2.6	-0.01

*Average values and standard deviation are given

Analytics of in-house peptide JF_1_1

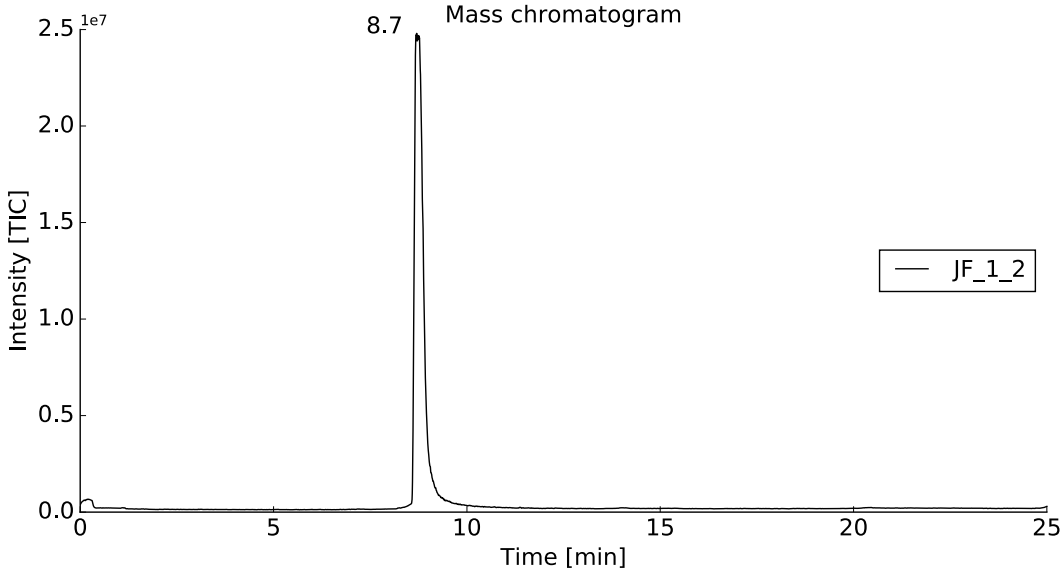
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
ALIWGY-NH_2	720.86	0.92±0.02	1

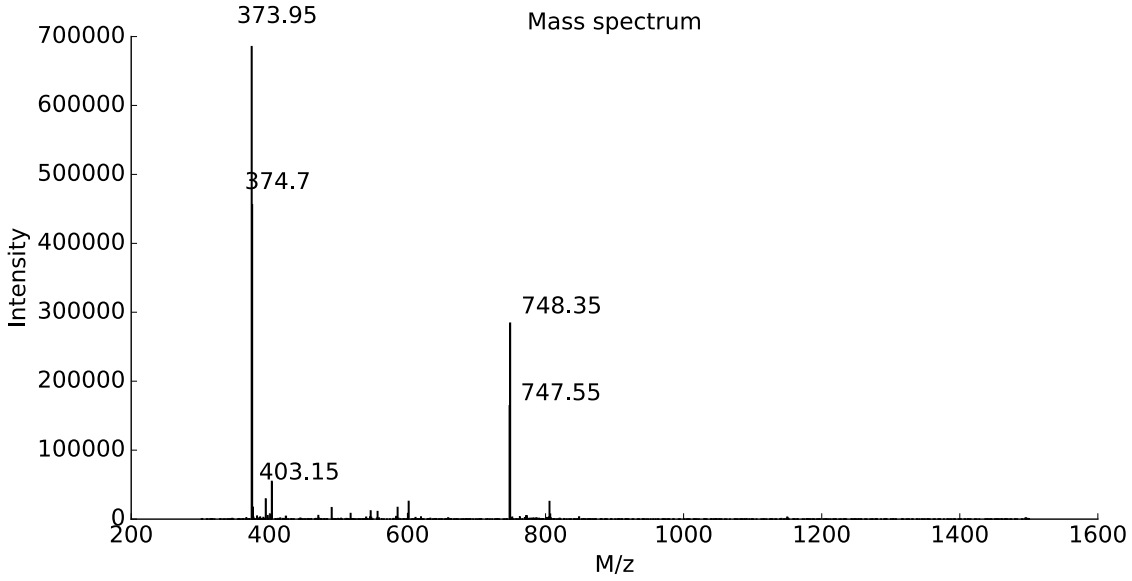




Analytics of in-house peptide JF_1_2

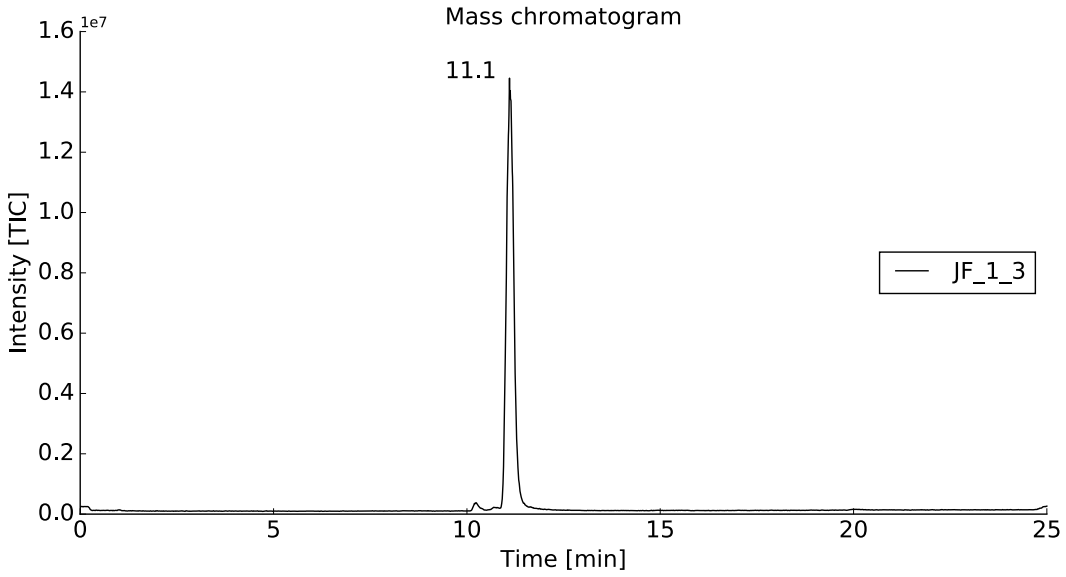
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
FLGKVW-NH_2	747.93	-0.99±0.02	2

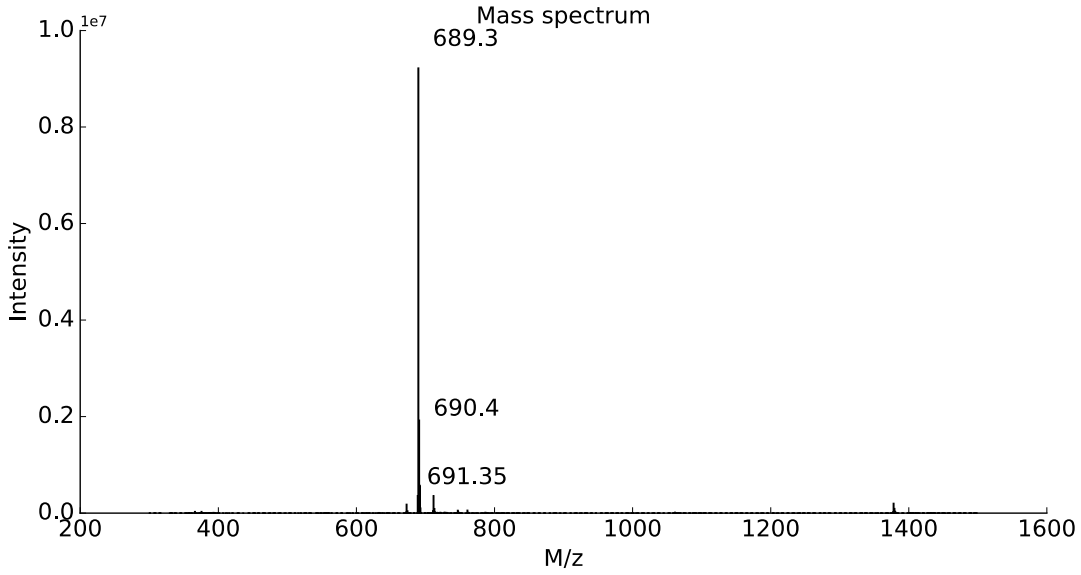




Analytics of in-house peptide JF_1_3

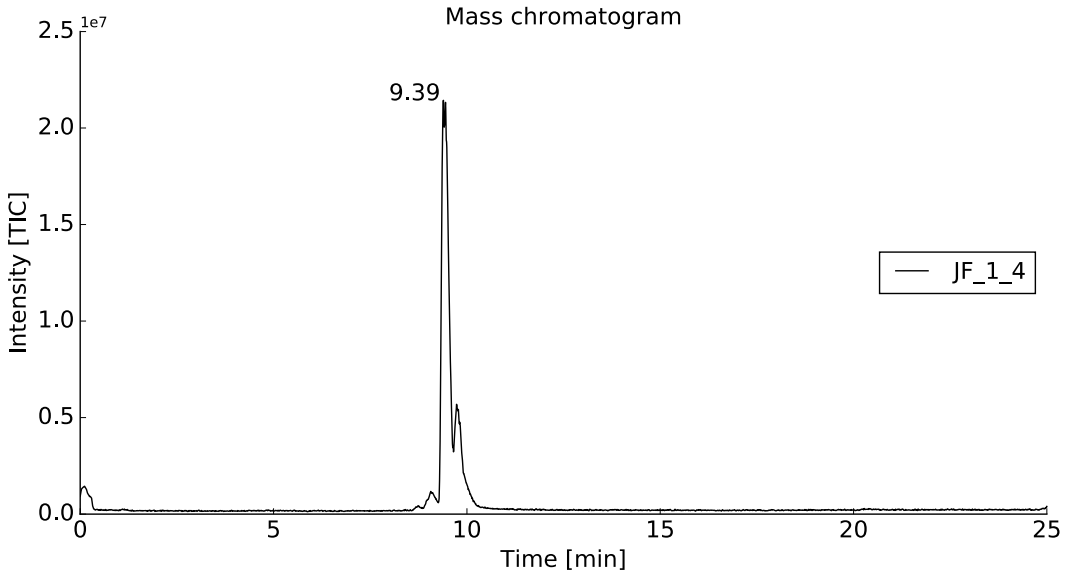
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
GAWPFL-NH_2	688.81	0.80±0.01	1

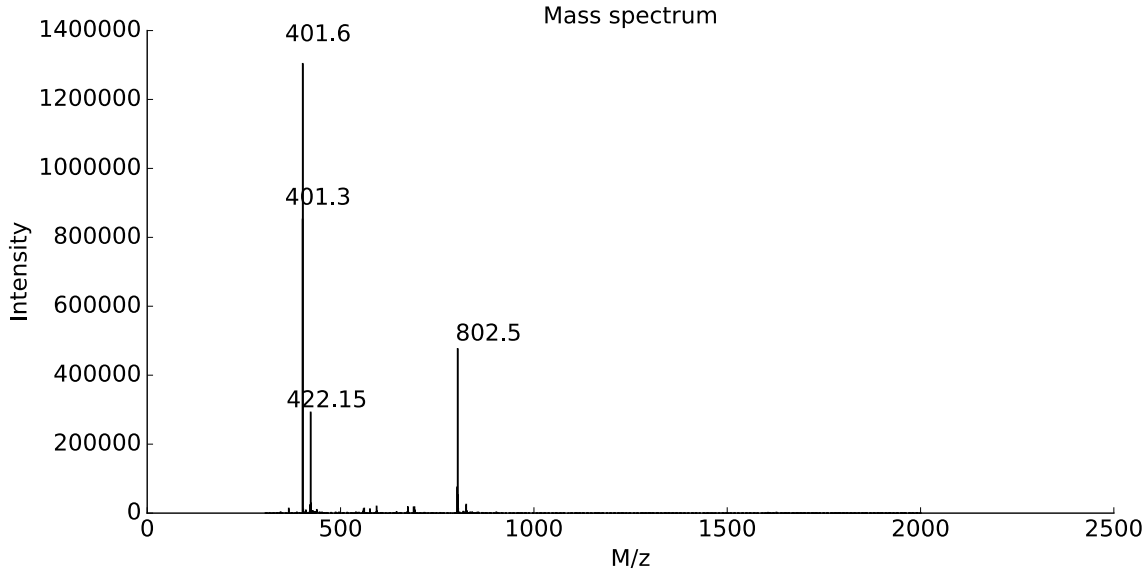




Analytics of in-house peptide JF_1_4

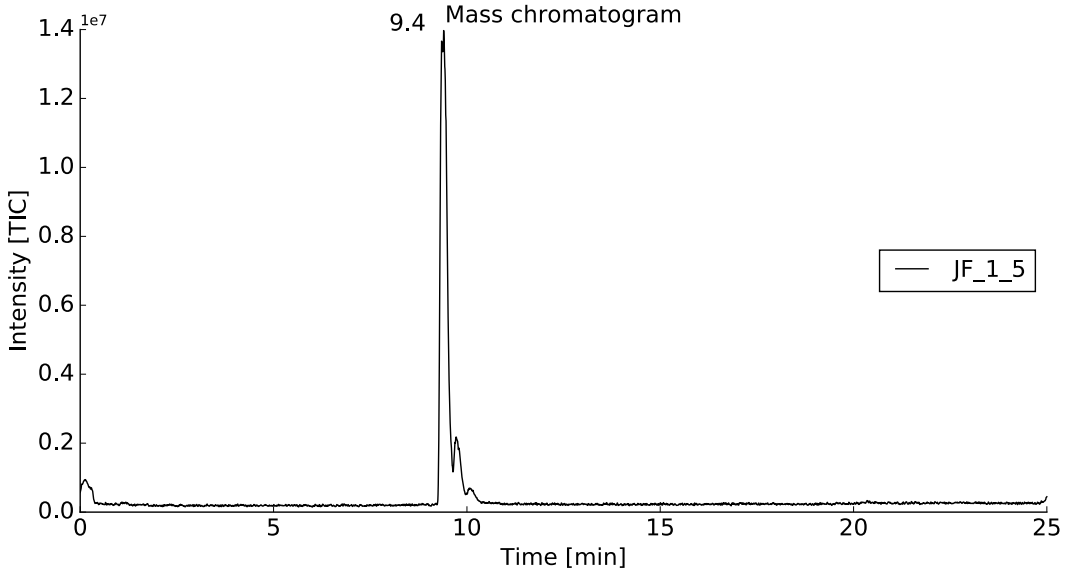
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
IPFWKL-NH_2	802.02	-0.85±0.03	2

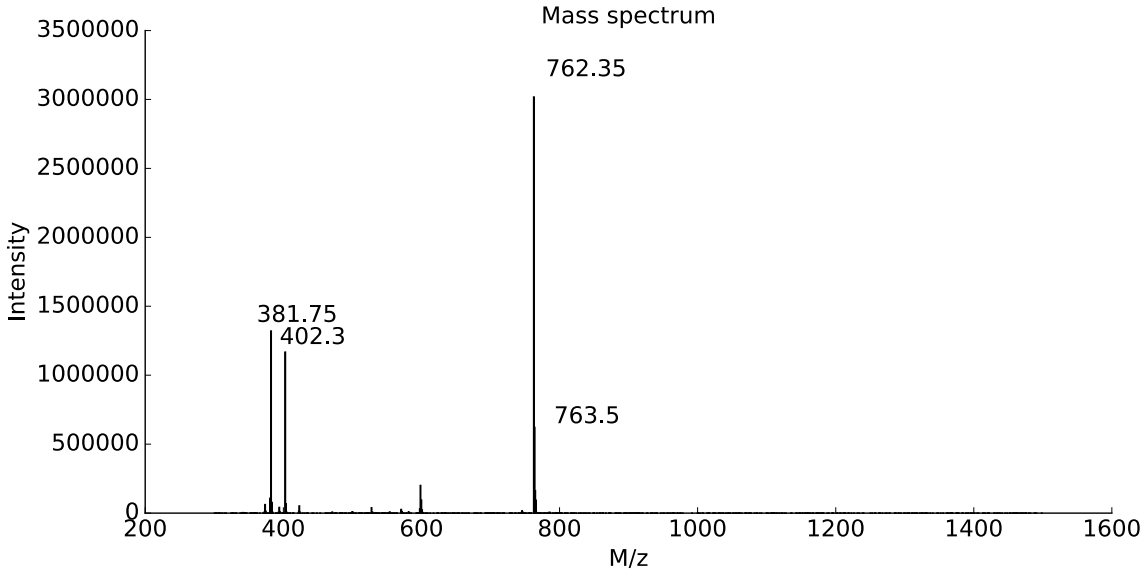




Analytics of in-house peptide JF_1_5

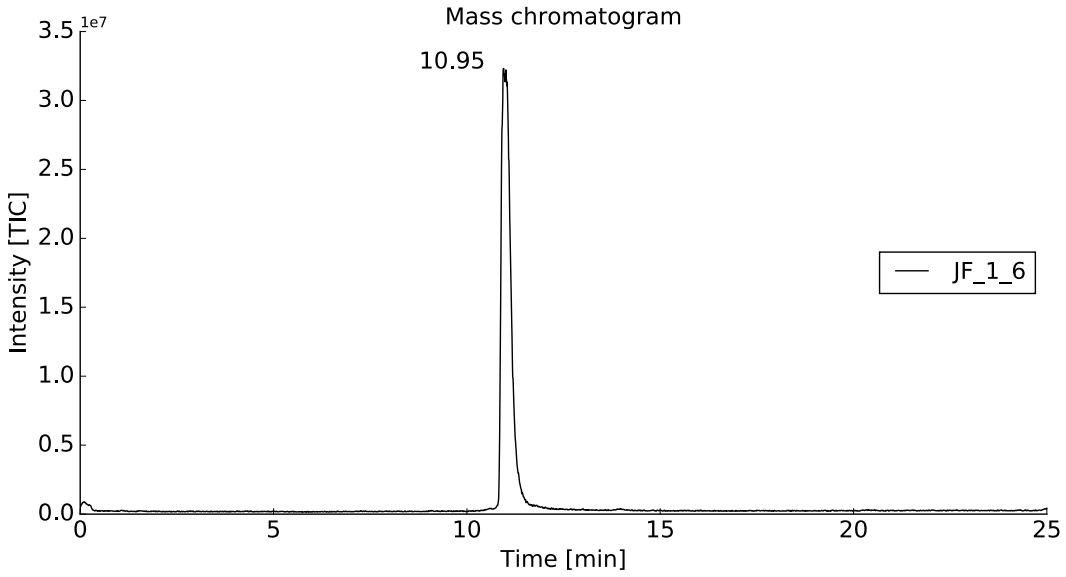
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
KLVWAF-NH_2	761,95	-1.13±0.02	2

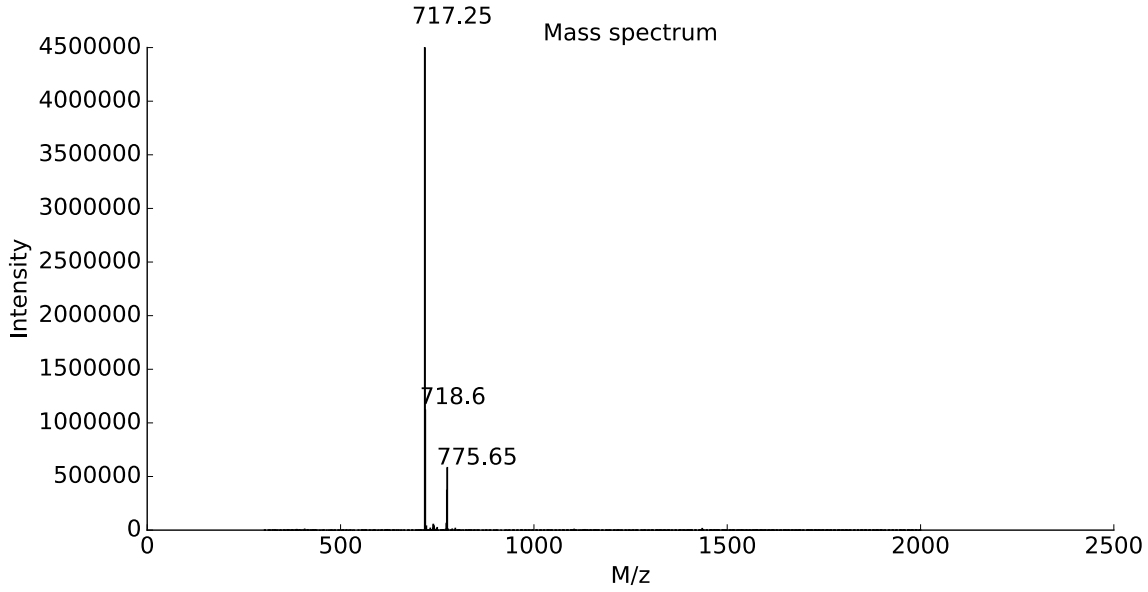




Analytics of in-house peptide JF_1_6

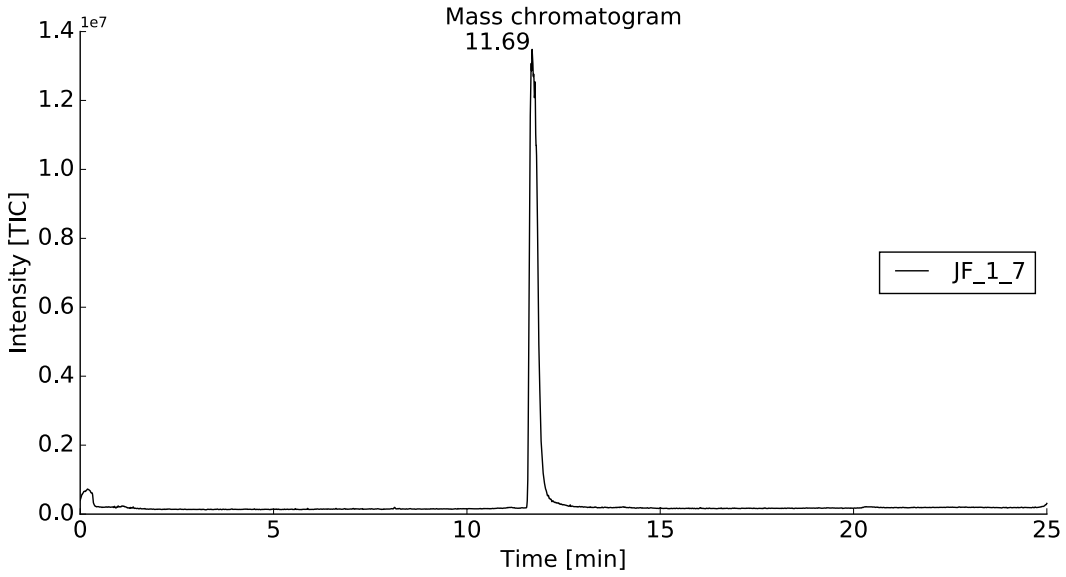
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
LPVGWF-NH_2	716.87	1.12±0.02	1

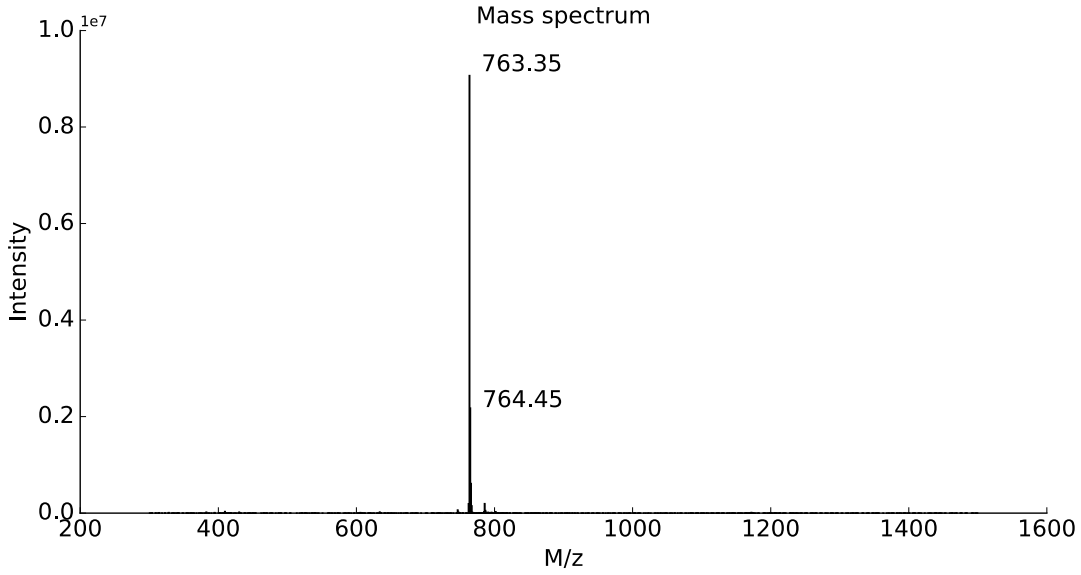




Analytics of in-house peptide JF_1_7

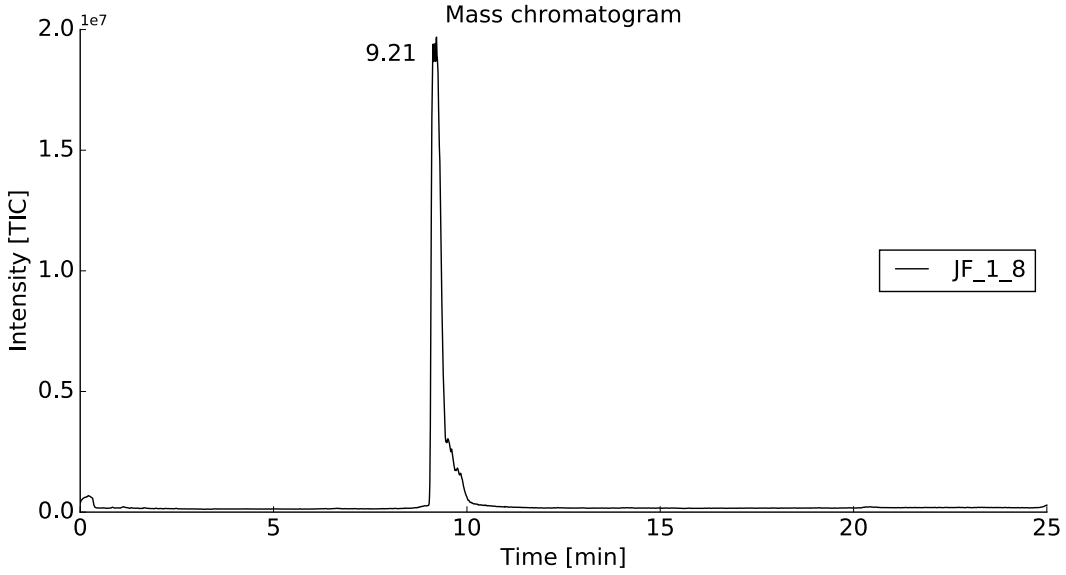
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
LYLGWI-NH_2	762.94	2.16±0.27	1

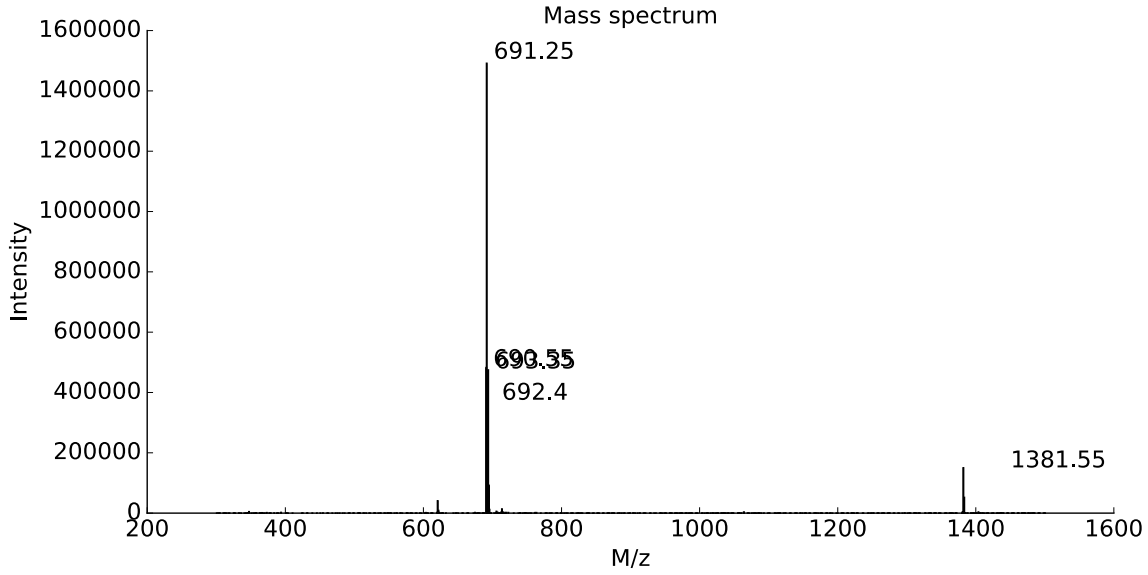




Analytics of in-house peptide JF_1_8

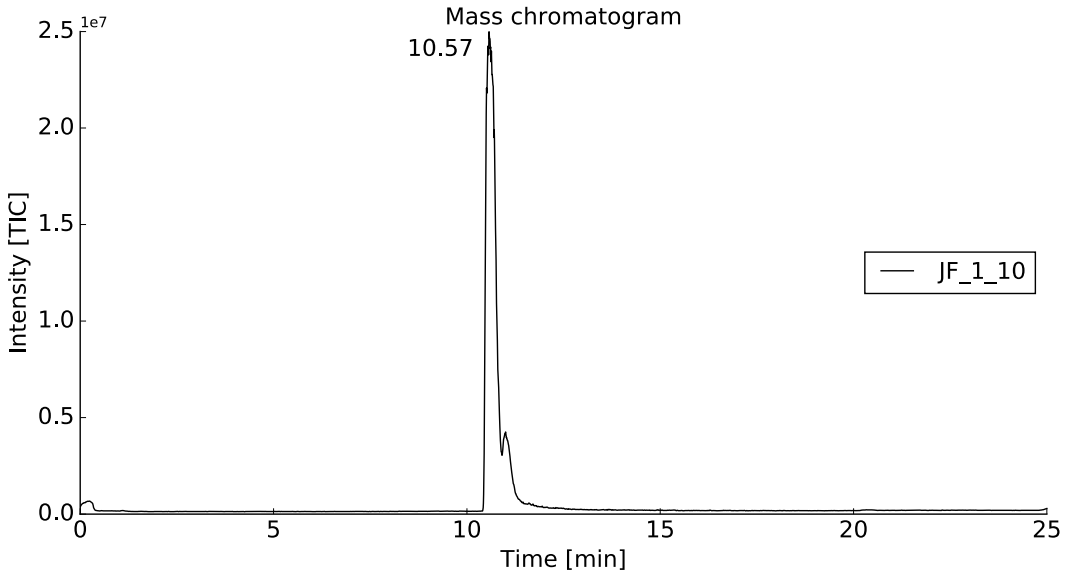
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
PWGYVA-NH_2	690.79	-0.38±0.01	1

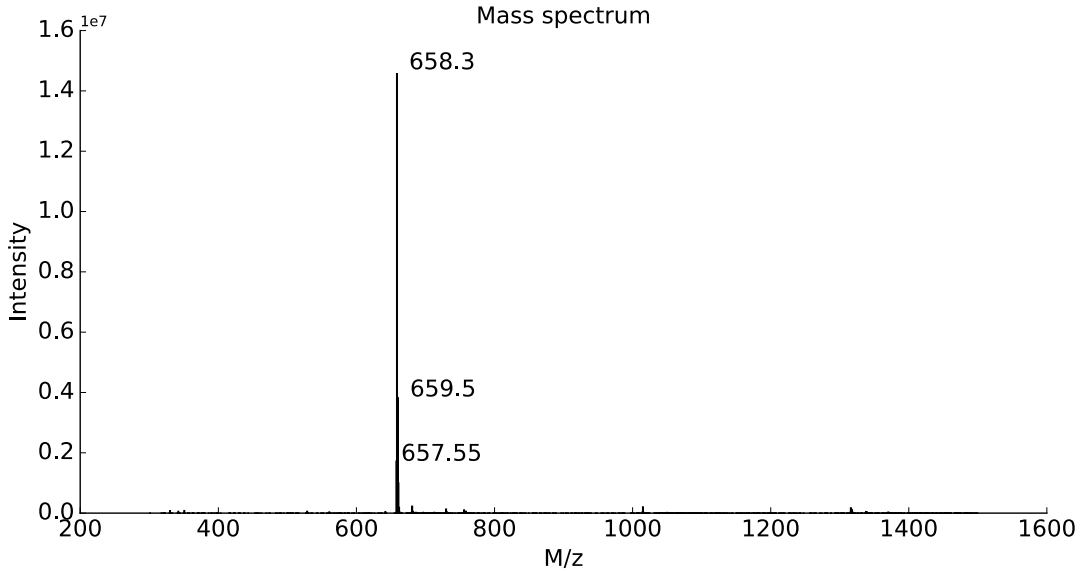




Analytics of in-house peptide JF_1_10

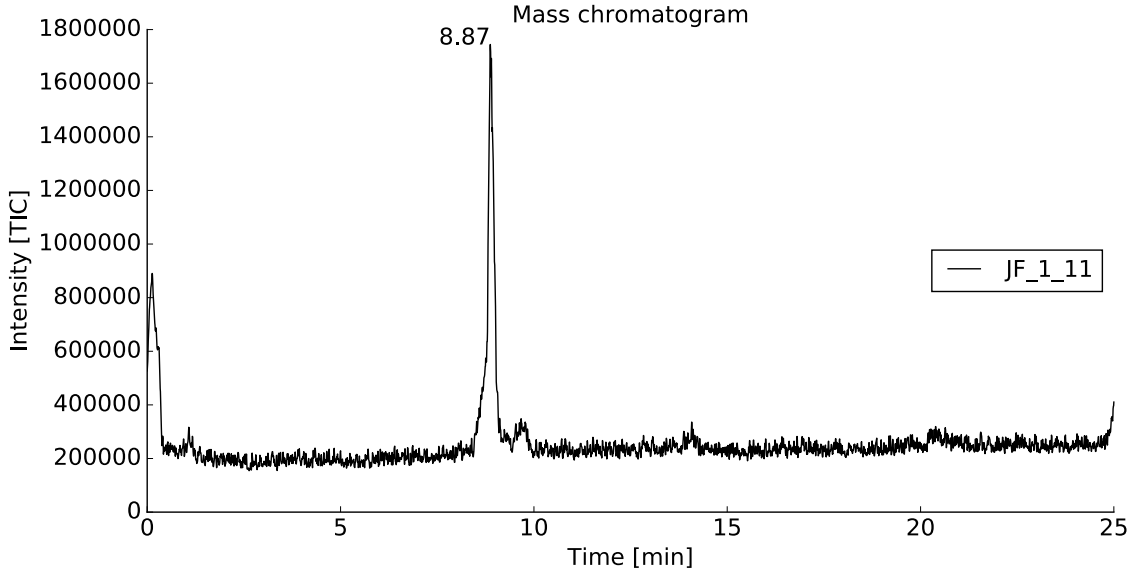
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
VPAFII-NH_2	657.84	0.66±0.02	1

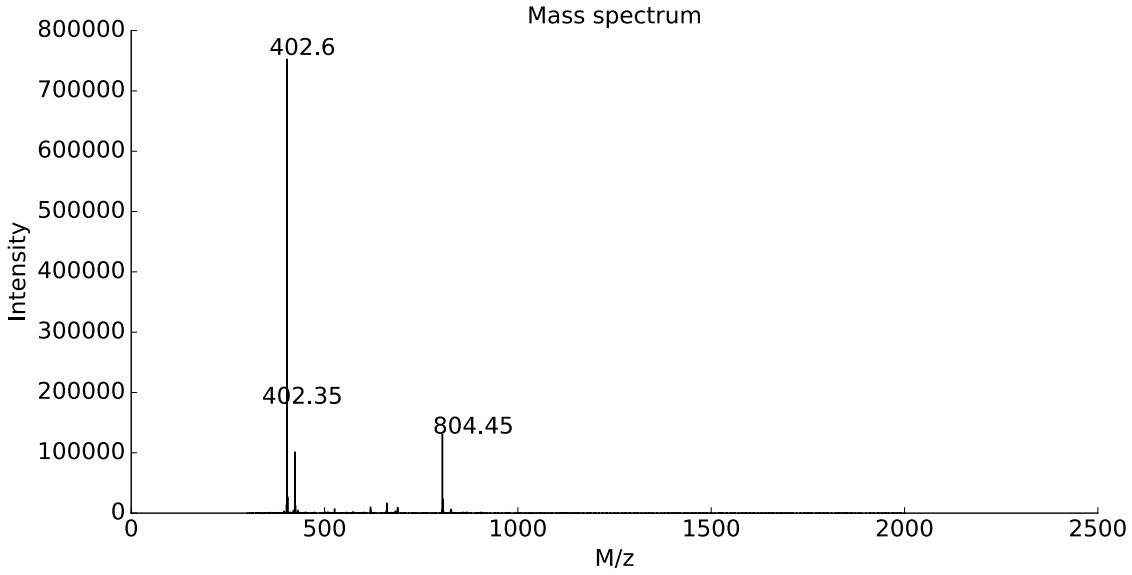




Analytics of in-house peptide JF_1_11

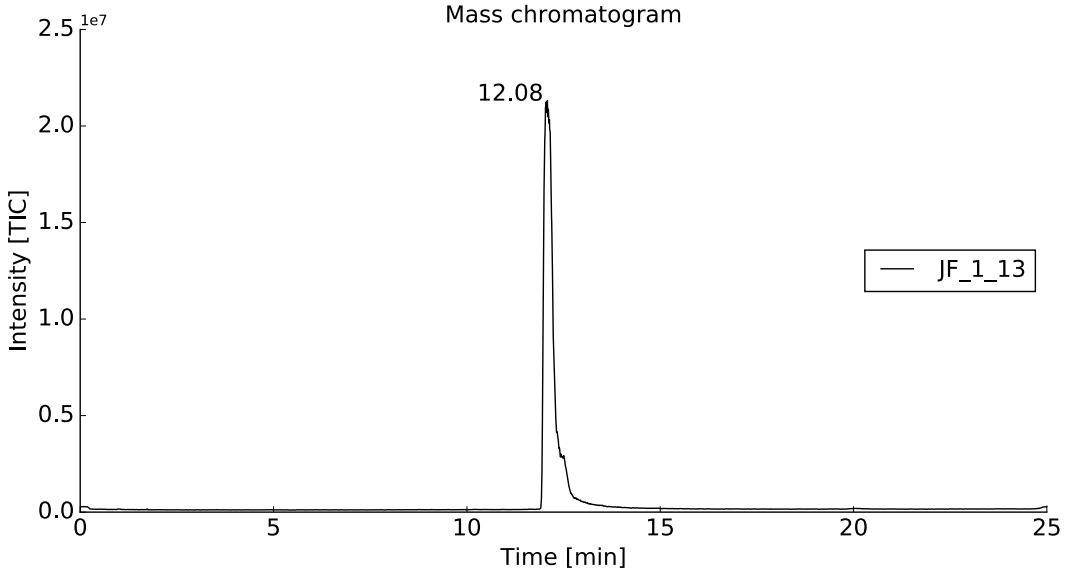
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
WPKIYV-NH_2	803.99	-1.82±0.19	2

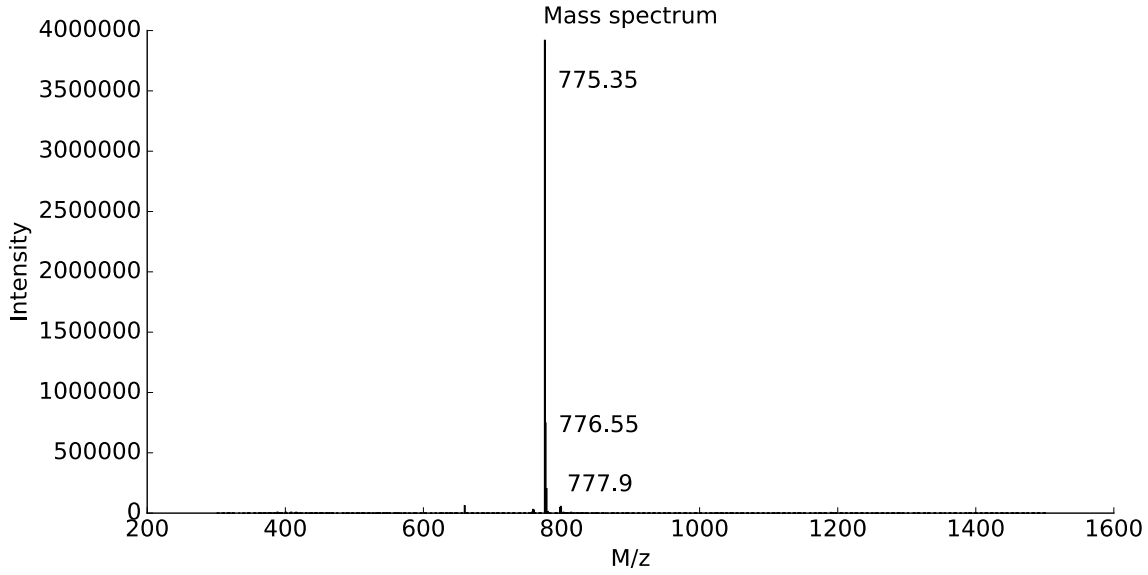




Analytics of in-house peptide JF_1_13

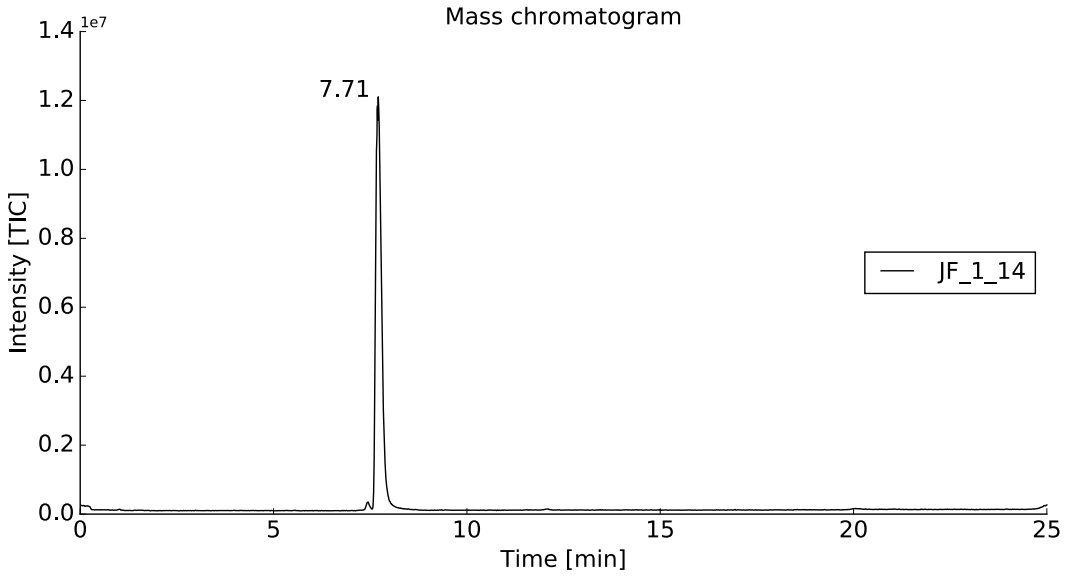
Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
VLIWFV-NH_2	774.99	2.35±0.31	1





Analytics of in-house peptide JF_1_14

Sequence	Mw	Exp. $logD_{7.4}$	Basic functions
SVYLQP-NH_2	704.81	-1.59±0.08	1



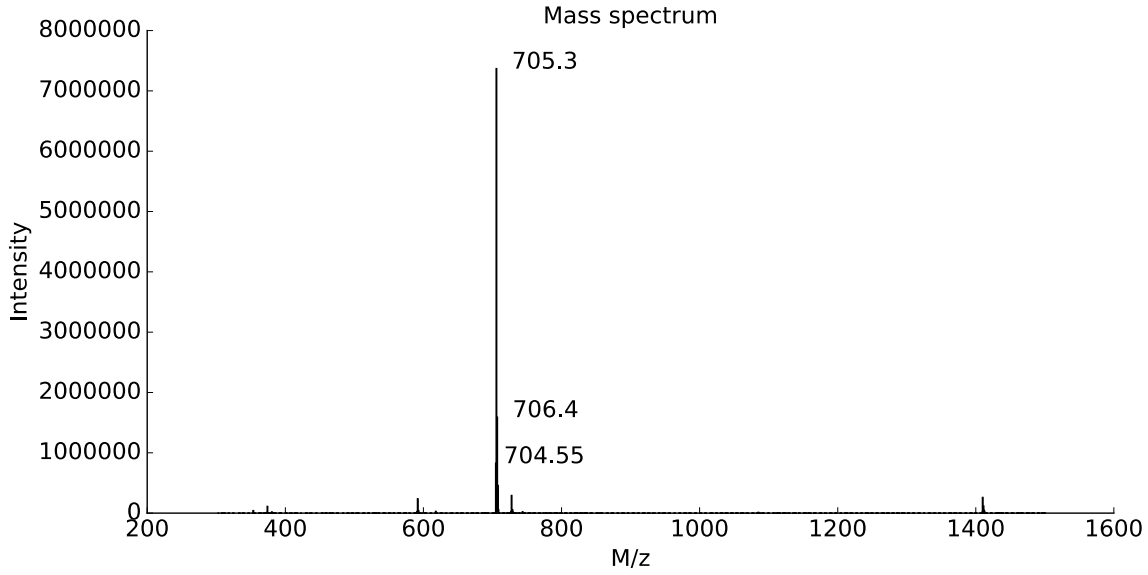


Table S3. LogD data of LIPOPEP and the In-House measured peptides. pH (aq) = pH of the aqueous of both phases at which SFM was conducted.

ID	Sequence	SMILES	C-Terminus	N-Terminus	Ionisable	logD (exp)	pH (aq)	Ref
LIPOPEP								
1	AGA	[H]N(C(C)=O)[C@H](C(NCC(N[C@H](C(NC(C)(C)C)=O)C)=O)=O)C	CONHt-Butyl	NHCOCH3	No	-0.6	7.2	1
2	AAA	[H]N(C(C)=O)[C@H](C(NC(C)C(N[C@H](C(NC(C)(C)C)=O)C)=O)=O)C	CONHt-Butyl	NHCOCH3	No	-0.51	7.2	1
3	AFA	[H]N(C(C)=O)[C@H](C(NC(CC1=CC=CC=C1)C(N[C@H](C(NC(C)(C)C)=O)C)=O)=O)C	CONHt-Butyl	NHCOCH3	No	1.01	7.2	1
4	AWA	[H]N(C(C)=O)[C@H](C(N[C@H](C(N[C@H](C(NC(C)(C)C)=O)C)=O)CC1=CNC2=C1C=CC=C2)=O)C	CONHt-Butyl	NHCOCH3	No	1.25	7.2	1
5	APA	[H]N(C(C)=O)[C@H](C(N1CCC[C@H]1C(N[C@H](C(NC(C)(C)C)=O)C)=O)=O)C	CONHt-Butyl	NHCOCH3	No	-0.39	7.2	1
6	AHA	O=C(N[C@H](C(=O)N[C@@H](Cc1[nH]cnc1)C(=O)N[C@H](C(=O)NC(C)(C)C)C)C)C	CONHt-Butyl	NHCOCH3	Yes	-0.48	7.2	1
7	ADA	[H]N(C(C)=O)[C@H](C(N[C@H](C(N[C@H](C(NC(C)(C)C)=O)C)=O)CC(O)=O)=O)C	CONHt-Butyl	NHCOCH3	No	-0.74	7.2	1
8	AEA	[H]N(C(C)=O)[C@H](C(N[C@@H](CCC(O)=O)C(N[C@H](C(NC(C)(C)C)=O)C)=O)=O)C	CONHt-Butyl	NHCOCH3	No	-0.67	7.2	1
9	(D-)FG	O=C([O-])CNC(=O)[C@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-2.16	7.2	2
10	(D-)F(D-)FG	O=C(N[C@H](Cc1ccccc1)C(=O)N[C@H](Cc1ccccc1)C(=O)[O-])C[NH3+]	COOH	NH2	Yes	-1.46	7.2	2
11	(D-)F(D-)F(D-)FG	O=C([O-])CNC(=O)[C@H](NC(=O)[C@H](NC(=O)[C@H]([NH3+])Cc1ccccc1)Cc1ccccc1)Cc1ccccc1	COOH	NH2	Yes	-0.66	7.2	2
12	(D-)F(D-)F	[H]N(C(C)=O)[C@@H](C(N[C@@H](C(N)=O)CC1=CC=CC=C1)=O)CC2=CC=CC=C2	CONH2	NHCOCH3	No	1.19	7.2	2
13	(D-)F(D-)F(D-)F	[H]N(C(C)=O)[C@@H](C(N[C@@H](C(N[C@@H](C(N)=O)CC1=CC=CC=C1)=O)CC2=CC=CC=C2)=O)CC3=CC=CC=C3	CONH2	NHCOCH3	No	2.3	7.2	2
14	FL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-1.17	7.0	3
15	LF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-1.15	7.0	3
16	FF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-0.85	7.0	3
17	LL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-1.46	7.0	3
18	LV	O=C(N[C@@H](C(C)C)C(=O)[O-])[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-2.05	7.0	3
19	VL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H]([NH3+])C(C)C	COOH	NH2	Yes	-2.07	7.0	3
20	AI	O=C(N[C@@H]([C@H](CC)C)C(=O)[O-])[C@@H]([NH3+])C	COOH	NH2	Yes	-2.60	7.0	3
21	II	O=C(N[C@@H]([C@H](CC)C)C(=O)[O-])[C@@H]([NH3+])[C@H](CC)C	COOH	NH2	Yes	-1.82	7.0	3
22	LI	O=C(N[C@@H]([C@H](CC)C)C(=O)[O-])[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-1.64	7.0	3
23	VV	O=C(N[C@@H](C(C)C)C(=O)[O-])[C@@H]([NH3+])C(C)C	COOH	NH2	Yes	-2.82	7.0	3
24	WW	O=C(N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)[O-])[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	-0.27	7.0	3
25	WF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	-0.47	7.0	3
26	WA	O=C(N[C@H](C(=O)[O-])C)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	-1.98	7.0	3
27	WL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	-0.73	7.0	3
28	WY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)C(=O)[O-]	COOH	NH2	Yes	-1.13	7.0	3

29	LY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.94	7.0	3
30	YL	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.75	7.0	3
31	VY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])C(C)C)C(=O)[O-]	COOH	NH2	Yes	-2.52	7.0	3
32	FY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)C(=O)[O-]	COOH	NH2	Yes	-1.68	7.0	3
33	YY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])Cc1ccc(O)cc1)C(=O)[O-]	COOH	NH2	Yes	-1.87	7.0	3
34	LM	S(CC[C@H](NC(=O)[C@@H]([NH3+])CC(C)C)C(=O)[O-])C	COOH	NH2	Yes	-1.87	7.0	3
35	ML	S(CC[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)[O-])C	COOH	NH2	Yes	-1.84	7.0	3
36	MV	S(CC[C@H]([NH3+])C(=O)N[C@@H](C(C)C)C(=O)[O-])C	COOH	NH2	Yes	-2.53	7.0	3
37	FM	S(CC[C@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)C(=O)[O-])C	COOH	NH2	Yes	-1.59	7.0	3
38	SL	OC[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-2.49	7.0	3
39	PF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@H]1[NH2+]CCC1	COOH	NH2	Yes	-2.07	7.0	3
40	PL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@H]1[NH2+]CCC1	COOH	NH2	Yes	-2.41	7.0	3
41	PI	O=C(N[C@@H]([C@H](CC)C)C(=O)[O-])[C@H]1[NH2+]CCC1	COOH	NH2	Yes	-2.56	7.0	3
42	FP	O=C([O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-1.36	7.0	3
43	LP	O=C([O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-1.76	7.0	3
44	IP	O=C([O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])[C@H](CC)C	COOH	NH2	Yes	-1.79	7.0	3
45	FFF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)Cc1ccccc1	COOH	NH2	Yes	-0.02	7.0	3
46	GFF	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])C[NH3+]	COOH	NH2	Yes	-1.33	7.0	3
47	FVG	O=C([O-])CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)C(C)C	COOH	NH2	Yes	-2.33	7.0	3
48	FVF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)C(C)C	COOH	NH2	Yes	-0.76	7.0	3
49	FVA	O=C(N[C@H](C(=O)[O-])C)[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)C(C)C	COOH	NH2	Yes	-2.19	7.0	3
50	LVV	O=C(N[C@@H](C(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)C(C)C	COOH	NH2	Yes	-2.10	7.0	3
51	LII	O=C(N[C@@H]([C@H](CC)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-1.11	7.0	3
52	LVL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)C(C)C	COOH	NH2	Yes	-1.57	7.0	3
53	LAL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)C	COOH	NH2	Yes	-2.03	7.0	3
54	LLL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	-0.94	7.0	3
55	WGG	O=C(NCC(=O)[O-])CNC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	-2.72	7.0	3
56	WFA	O=C(N[C@H](C(=O)[O-])C)[C@@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)Cc1ccccc1	COOH	NH2	Yes	-1.00	7.0	3

57	WWL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	0.36	7.0	3
58	LLY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.34	7.0	3
59	VFY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])C(C)C)Cc1ccccc1)C(=O)[O-]	COOH	NH2	Yes	-1.50	7.0	3
60	GFY	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H](NC(=O)C[NH3+])Cc1ccccc1)C(=O)[O-]	COOH	NH2	Yes	-1.96	7.0	3
61	YLV	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.45	7.0	3
62	YVF	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-]	COOH	NH2	Yes	-1.37	7.0	3
63	YGF	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)NCC(=O)N[C@@H](C(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.86	7.0	3
64	YYL	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])Cc1ccc(O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.38	7.0	3
65	AYI	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])C)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-]	COOH	NH2	Yes	-2.04	7.0	3
66	IYV	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C(=O)N[C@@H](C(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.77	7.0	3
67	MLF	S(CC[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])C	COOH	NH2	Yes	-1.03	7.0	3
68	LSL	OC[C@H](NC(=O)[C@@H]([NH3+])CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-2.35	7.0	3
69	ISL	OC[C@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-2.28	7.0	3
70	ISI	OC[C@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-]	COOH	NH2	Yes	-2.64	7.0	3
71	SLI	OC[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-]	COOH	NH2	Yes	-1.99	7.0	3
72	SLL	OC[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-2.03	7.0	3
73	FIT	O=C(N[C@@H]([C@H](CC)C)C(=O)N[C@@H]([C@H](O)C)C(=O)[O-])[C@@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-1.95	7.0	3
74	LIT	O=C(N[C@@H]([C@H](CC)C)C(=O)N[C@@H]([C@H](O)C)C(=O)[O-])[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-2.14	7.0	3
75	IIT	O=C(N[C@@H]([C@H](O)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)[C@H](CC)C	COOH	NH2	Yes	-2.23	7.0	3
76	LTI	O=C(N[C@@H]([C@H](O)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-2.30	7.0	3
77	TLI	O=C(N[C@@H]([C@H](CC)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])[C@H](O)C)CC(C)C	COOH	NH2	Yes	-1.66	7.0	3
78	TVL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])[C@H](O)C)C(C)C	COOH	NH2	Yes	-1.97	7.0	3
79	PLL	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-])[C@H]1[NH2+]CCC1	COOH	NH2	Yes	-1.64	7.0	3
80	LPL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-1.56	7.0	3
81	LLP	O=C([O-])[C@H]1N(CCC1)C(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	-1.58	7.0	3
82	IPI	O=C(N[C@@H]([C@H](CC)C)C(=O)[O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])[C@H](CC)C	COOH	NH2	Yes	-1.65	7.0	3
83	FGGF	O=C(NCC(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-1.51	7.0	3
84	VAAF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])C(C)C)C)C	COOH	NH2	Yes	-1.91	7.0	3
85	LLVF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C)C(C)C	COOH	NH2	Yes	-0.25	7.0	3

86	LLLV	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	-0.51	7.0	3
87	VGFF	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H]([NH3+])C(C)C	COOH	NH2	Yes	-0.51	7.0	3
88	AVLL	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])C)C(C)C	COOH	NH2	Yes	-1.74	7.0	3
89	IAGF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C	COOH	NH2	Yes	-1.78	7.0	3
90	FFFF	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)Cc1ccccc1	COOH	NH2	Yes	1.63	7.0	3
91	LLGF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	-0.42	7.0	3
92	LLAF	O=C(N[C@H](C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])C)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	-1.00	7.0	3
93	LLLF	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	0.24	7.0	3
94	IIVV	O=C(N[C@@H](C(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)[C@H](CC)C)C(C)C	COOH	NH2	Yes	-1.41	7.0	3
95	IIGF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)[C@H](CC)C	COOH	NH2	Yes	-0.99	7.0	3
96	IAAI	O=C(N[C@H](C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])C)[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C	COOH	NH2	Yes	-2.82	7.0	3
97	FFGF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)Cc1ccccc1	COOH	NH2	Yes	0.17	7.0	3
98	VLVL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])C(C)C)CC(C)C)C(C)C	COOH	NH2	Yes	-1.23	7.0	3
99	WLLV	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)CC(C)C	COOH	NH2	Yes	0.23	7.0	3
100	WGLL	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-])CNC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	0.06	7.0	3
101	YILG	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](CC(C)C)C(=O)NCC(=O)[O-]	COOH	NH2	Yes	-1.49	7.0	3
102	FVYF	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-]	COOH	NH2	Yes	-0.32	7.0	3
103	IYIV	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](C(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.09	7.0	3
104	VFLT	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H]([C@H](O)C)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])C(C)C)Cc1ccccc1	COOH	NH2	Yes	-1.32	7.0	3
105	MILI	S(CC[C@H]([NH3+])C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H]([C@	COOH	NH2	Yes	-0.49	7.0	3

		H](CC)C)C(=O)[O-])C						
106	VMFI	S(CC[C@H](NC(=O)[C@@H]([NH3+])C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])C	COOH	NH2	Yes	-0.63	7.0	3
107	PLLL	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-])[C@H]1[NH2+]CCC1	COOH	NH2	Yes	-1.06	7.0	3
108	LPLL	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])CC(C)C	COOH	NH2	Yes	-0.92	7.0	3
109	LLPL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@H]1N(CCC1)C(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	-1.00	7.0	3
110	LLLP	O=C([O-])[C@H]1N(CCC1)C(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)CC(C)C)CC(C)C	COOH	NH2	Yes	-1.18	7.0	3
111	IPGI	O=C(NCC(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])[C@H](CC)C	COOH	NH2	Yes	-1.69	7.0	3
112	VPVL	O=C(N[C@@H](C(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])C(C)C	COOH	NH2	Yes	-1.91	7.0	3
113	VPGV	O=C(NCC(=O)N[C@@H](C(C)C)C(=O)[O-])[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])C(C)C	COOH	NH2	Yes	-2.83	7.0	3
114	YPGW	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N1CCC[C@H]1C(=O)NCC(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)[O-]	COOH	NH2	Yes	-1.25	7.0	3
115	YPGI	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N1CCC[C@H]1C(=O)NCC(=O)N[C@@H]([C@H](CC)C)C(=O)[O-]	COOH	NH2	Yes	-1.65	7.0	3
116	GGFVF	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)C[NH3+]	COOH	NH2	Yes	-1.40	7.0	3
117	VFVGL	O=C(N[C@@H](CC(C)C)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])C(C)C)Cc1ccccc1)C(C)C	COOH	NH2	Yes	-0.97	7.0	3
118	VGFVF	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H]([NH3+])C(C)C	COOH	NH2	Yes	-0.50	7.0	3
119	GAALL	O=C(N[C@H](C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-])C)C)C[NH3+]	COOH	NH2	Yes	-2.55	7.0	3
120	AFGVF	O=C(N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])C)Cc1ccccc1	COOH	NH2	Yes	-0.59	7.0	3
121	AGFVF	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H]([NH3+])C	COOH	NH2	Yes	-1.10	7.0	3
122	LIIGA	O=C(N[C@H](C(=O)[O-])C)CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)[C@H](CC)C)[C@H](CC)C	COOH	NH2	Yes	-1.65	7.0	3
123	GLLGF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C[NH3+])CC(C)C)CC(C)C	COOH	NH2	Yes	-0.18	7.0	3
124	ALLGF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])C)CC(C)C)CC(C)C	COOH	NH2	Yes	-0.63	7.0	3
125	IIIIG	O=C([O-])CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)[C@H](CC)C)[C@H](CC)C)[C@H](CC)C	COOH	NH2	Yes	-0.97	7.0	3
126	IVVVI	O=C(N[C@@H](C(C)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C(C)C)C(C)C	COOH	NH2	Yes	-0.89	7.0	3

127	FGAGI	O=C(N[C@H](C(=O)NCC(=O)N[C@@H]([C@H](CC)C)C(=O)[O-])C)CNC(=O)[C@@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-1.87	7.0	3
128	FAAAL	O=C(N[C@@H](CC(C)C)C(=O)[O-])[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)C)C)C	COOH	NH2	Yes	-2.23	7.0	3
129	WGGFV	O=C(NCC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)[O-])CNC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	-0.44	7.0	3
130	WLFAA	O=C(N[C@H](C(=O)N[C@H](C(=O)[O-])C)C)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)CC(C)C)Cc1ccccc1	COOH	NH2	Yes	-0.32	7.0	3
131	IAYWG	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])[C@H](CC)C)C)C(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)NCC(=O)[O-]	COOH	NH2	Yes	-1.47	7.0	3
132	GLSVL	OC[C@H](NC(=O)[C@@H](NC(=O)C[NH3+])CC(C)C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.64	7.0	3
133	SLAIV	OC[C@H]([NH3+])C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](C(C)C)C(=O)[O-])C	COOH	NH2	Yes	-1.94	7.0	3
134	YTGFL	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N[C@@H]([C@H](O)C)C(=O)NCC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-1.18	7.0	3
135	LVGTF	O=C(N[C@@H]([C@H](O)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CC(C)C)C(C)C	COOH	NH2	Yes	-1.18	7.0	3
136	YGGFL	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)NCC(=O)NCC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)[O-]	COOH	NH2	Yes	-0.80	7.0	3
137	YGGFM	S(CC[C@H](NC(=O)[C@@H](NC(=O)CNC(=O)CNC(=O)[C@@H]([NH3+])Cc1ccc(O)cc1)Cc1ccccc1)C(=O)[O-])C	COOH	NH2	Yes	-1.39	7.0	3
138	FF	O=C(N[C@@H](Cc1ccccc1)C(=O)[O-])[C@@H]([NH3+])Cc1ccccc1	COOH	NH2	Yes	-0.94	7.4	4
139	WW	O=C(N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)[O-])[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	-0.35	7.4	4
140	WWW	O=C(N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)[O-])[C@@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)Cc1c2c([nH]c1)cccc2	COOH	NH2	Yes	0.51	7.4	4
141	WMDF	S(CC[C@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](CC(=O)[O-])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	COOH	NH3	Yes	1.60	7.4	5
142	WMRF	S(CC[C@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](CCCNC(=[NH2+])N)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	COOH	NH4	Yes	1.90	7.4	5
143	WDMF	S(CC[C@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)CC(=O)[O-])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	COOH	NH5	Yes	1.70	7.4	5
144	SQDG	OC[C@H]([NH3+])C(=O)N[C@@H](CCC(=O)N)C(=O)N[C@@H](CC(=O)[O-])C(=O)NCC(=O)N	COOH	NH6	Yes	-2.40	7.4	5
145	SQRG	OC[C@H]([NH3+])C(=O)N[C@@H](CCC(=O)N)C(=O)N[C@@H](CCCNC(=[NH2+])N)C(=O)NCC(=O)N	COOH	NH7	Yes	-2.40	7.4	5
146	GV	[H]N(C(C)=O)CC(N[C@@H](C(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	-1.33	7.0	
147	AV	[H]N(C(C)=O)[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)C	CONH2	NHCOCH3	No	-1.13	7.0	6
148	LV	[H]N(C(C)=O)[C@@H](CC(C)C)C(N[C@@H](C(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	0.26	7.0	6
149	GF	[H]N(C(C)=O)CC(N[C@H](C(N)=O)CC1=CC=CC=C1)=O	CONH2	NHCOCH3	No	-0.56	7.0	6
150	IV	[H]N(C(C)=O)[C@]([H])(C(N[C@H](C(N)=O)C(C)C)=O)[C@@H](C)CC	CONH2	NHCOCH3	No	0.16	7.0	6
151	VV	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@@H](C(C)C	CONH2	NHCOCH3	No	-0.32	7.0	6

		)C(N)=O)=O						
152	FV	[H]N(C(C)=O)[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)CC1=CC=CC=C1	CONH2	NHCOCH3	No	0.43	7.0	6
153	AL	[H]N(C(C)=O)[C@H](C(N[C@@H](CC(C)C)C(N)=O)=O)C	CONH2	NHCOCH3	No	-0.54	7.0	6
154	AA	[H]N(C(C)=O)[C@H](C(N[C@H](C(N)=O)C)=O)C	CONH2	NHCOCH3	No	-2.01	7.0	6
155	GL	[H]N(C(C)=O)CC(N[C@@H](CC(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	-0.78	7.0	6
156	LI	[H]N(C(C)=O)[C@@H](CC(C)C)C(N[C@]([C@@H](C)CC)([H])C(N)=O)=O	CONH2	NHCOCH3	No	0.68	7.0	6
157	FG	[H]N(C(C)=O)[C@H](C(NCC(N)=O)=O)CC1=CC=CC=C1	CONH2	NHCOCH3	No	-0.5	7.0	6
158	VA	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@H](C(N)=O)C)=O	CONH2	NHCOCH3	No	-1.14	7.0	6
159	YV	[H]N(C(C)=O)[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)CC1=CC=C(O)C=C1	CONH2	NHCOCH3	No	-0.2	7.0	6
160	YL	[H]N(C(C)=O)[C@H](C(N[C@@H](CC(C)C)C(N)=O)=O)CC1=CC=C(O)C=C1	CONH2	NHCOCH3	No	0.32	7.0	6
161	YF	[H]N(C(C)=O)[C@H](C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O)CC2=CC=C(O)C=C2	CONH2	NHCOCH3	No	0.54	7.0	6
162	WV	[H]N(C(C)=O)[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)CC1=CNC2=C1C=CC=C2	CONH2	NHCOCH3	No	0.73	7.0	6
163	MV	[H]N(C(C)=O)[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)CCSC	CONH2	NHCOCH3	No	-0.28	7.0	6
164	MF	[H]N(C(C)=O)[C@H](C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O)CCSC	CONH2	NHCOCH3	No	0.42	7.0	6
165	SV	[H]N(C(C)=O)[C@@H](CO)C(N[C@@H](C(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	-1.53	7.0	6
166	SF	[H]N(C(C)=O)[C@@H](CO)C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O	CONH2	NHCOCH3	No	-0.79	7.0	6
167	TV	[H]N(C(C)=O)[C@]([C@@H](C)O)([H])C(N[C@@H](C(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	-1.25	7.0	6
168	TI	[H]N(C(C)=O)[C@]([C@@H](C)O)([H])C(N[C@]([C@@H](C)CC)([H])C(N)=O)=O	CONH2	NHCOCH3	No	-0.86	7.0	6
169	NV	[H]N(C(C)=O)[C@@H](CC(N)=O)C(N[C@@H](C(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	-1.85	7.0	6
170	NI	[H]N(C(C)=O)[C@@H](CC(N)=O)C(N[C@]([C@@H](C)CC)([H])C(N)=O)=O	CONH2	NHCOCH3	No	-1.43	7.0	6
171	NF	[H]N(C(C)=O)[C@@H](CC(N)=O)C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O	CONH2	NHCOCH3	No	-1.14	7.0	6
172	LN	[H]N(C(C)=O)[C@@H](CC(C)C)C(N[C@@H](CC(N)=O)C(N)=O)=O	CONH2	NHCOCH3	No	-1.3	7.0	6
173	IN	[H]N(C(C)=O)[C@]([C@H](CC)C)([H])C(N[C@@H](CC(N)=O)C(N)=O)=O	CONH2	NHCOCH3	No	-1.41	7.0	6
174	QV	[H]N(C(C)=O)[C@@H](CCC(N)=O)C(N[C@@H](C(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	-1.85	7.0	6
175	QL	[H]N(C(C)=O)[C@@H](CCC(N)=O)C(N[C@@H](CC(C)C)C(N)=O)=O	CONH2	NHCOCH3	No	-1.32	7.0	6
176	QF	[H]N(C(C)=O)[C@@H](CCC(N)=O)C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O	CONH2	NHCOCH3	No	-1.14	7.0	6
177	FQ	[H]N(C(C)=O)[C@H](C(N[C@@H](CCC(N)=O)C(N)=O)=O)CC1=CC=CC=C1	CONH2	NHCOCH3	No	-1.03	7.0	6
178	VQ	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@@H](CCC(N)=O)C(N)=O)=O	CONH2	NHCOCH3	No	-1.82	7.0	6
179	KF	O=C(N[C@@H](CCCC[NH3+])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-2.43	7.0	6
180	FK	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CCCC[NH3+])C(=O)N)C	CONH2	NHCOCH3	Yes	-2.23	7.0	6
181	OrnF	O=C(N[C@@H](CCC[NH3+])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-2.23	7.0	6
182	VAA	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@H](C(N[C@H](C(N)=O)C)=O)C)=O	CONH2	NHCOCH3	No	-1.4	7.0	6
183	VAV	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)C)=O	CONH2	NHCOCH3	No	-0.67	7.0	6
184	VIG	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@]([C@@H](C)CC)([H])C(NCC(N)=O)=O)=O	CONH2	NHCOCH3	No	-0.45	7.0	6

185	ALV	[H]N(C(C)=O)[C@H](C(N[C@@H](CC(C)C)C(N[C@@H](C(C)C)C(N)=O)=O)=O)C	CONH2	NHCOCH3	No	-0.14	7.0	6
186	VFA	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@H](C(N[C@H](C(N)=O)C)=O)CC1=CC=CC=C1)=O	CONH2	NHCOCH3	No	0.06	7.0	6
187	AVI	[H]N(C(C)=O)[C@H](C(N[C@@H](C(C)C)C(N[C@]([C@@H](C)CC)([H])C(N)=O)=O)=O)C	CONH2	NHCOCH3	No	-0.2	7.0	6
188	IFA	[H]N(C(C)=O)[C@]([C@H](CC)C)([H])C(N[C@H](C(N[C@H](C(N)=O)C)=O)CC1=CC=CC=C1)=O	CONH2	NHCOCH3	No	0.52	7.0	6
189	GAV	[H]N(C(C)=O)CC(N[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)C)=O	CONH2	NHCOCH3	No	-1.56	7.0	6
190	AGF	[H]N(C(C)=O)[C@H](C(NCC(N[C@H](C(N)=O)CC1=CC=CC=C1)=O)=O)C	CONH2	NHCOCH3	No	-0.71	7.0	6
191	IAV	[H]N(C(C)=O)[C@]([C@H](CC)C)([H])C(N[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)C)=O	CONH2	NHCOCH3	No	-0.21	7.0	6
192	FGL	[H]N(C(C)=O)[C@H](C(NCC(N[C@@H](CC(C)C)C(N)=O)=O)=O)CC1=CC=CC=C1	CONH2	NHCOCH3	No	0.6	7.0	6
193	FIG	[H]N(C(C)=O)[C@H](C(N[C@]([C@@H](C)CC)([H])C(NCC(N)=O)=O)=O)CC1=CC=CC=C1	CONH2	NHCOCH3	No	0.34	7.0	6
194	VVI	[H]N(C(C)=O)[C@@H](C(C)C)C(N[C@@H](C(C)C)C(N[C@]([C@@H](C)CC)([H])C(N)=O)=O)=O	CONH2	NHCOCH3	No	0.49	7.0	6
195	GLG	[H]N(C(C)=O)CC(N[C@@H](CC(C)C)C(NCC(N)=O)=O)=O	CONH2	NHCOCH3	No	-1.23	7.0	6
196	AYL	[H]N(C(C)=O)[C@H](C(N[C@H](C(N[C@@H](CC(C)C)C(N)=O)=O)CC(C=C1)=CC=C1O)=O)C	CONH2	NHCOCH3	No	-0.04	7.0	6
197	AYF	[H]N(C(C)=O)[C@H](C(N[C@H](C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O)CC(C=C2)=CC=C2O)=O)C	CONH2	NHCOCH3	No	0.26	7.0	6
198	WAA	[H]N(C(C)=O)[C@H](C(N[C@H](C(N[C@H](C(N)=O)C)=O)C)=O)CC1=CNC2=C1C=CC=C2	CONH2	NHCOCH3	No	-0.38	7.0	6
199	WIG	[H]N(C(C)=O)[C@H](C(N[C@]([C@@H](C)CC)([H])C(NCC(N)=O)=O)=O)CC1=CNC2=C1C=CC=C2	CONH2	NHCOCH3	No	0.62	7.0	6
200	WGF	[H]N(C(C)=O)[C@H](C(NCC(N[C@H](C(N)=O)CC1=CC=CC=C1)=O)=O)CC2=CNC3=C2C=CC=C3	CONH2	NHCOCH3	No	0.99	7.0	6
201	WAV	[H]N(C(C)=O)[C@H](C(N[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)C)=O)CC1=CNC2=C1C=CC=C2	CONH2	NHCOCH3	No	0.36	7.0	6
202	AMV	[H]N(C(C)=O)[C@H](C(N[C@H](C(N[C@@H](C(C)C)C(N)=O)=O)CCSC)=O)C	CONH2	NHCOCH3	No	-0.63	7.0	6
203	IMF	[H]N(C(C)=O)[C@]([C@H](CC)C)([H])C(N[C@H](C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O)CCSC)=O	CONH2	NHCOCH3	No	1.28	7.0	6
204	LSF	[H]N(C(C)=O)[C@@H](CC(C)C)C(N[C@@H](CO)C(N[C@H](C(N)=O)CC1=CC=CC=C1)=O)=O	CONH2	NHCOCH3	No	0.23	7.0	6
205	LTL	[H]N(C(C)=O)[C@@H](CC(C)C)C(N[C@]([C@H](O)C)([H])C(N[C@@H](CC(C)C)C(N)=O)=O)=O	CONH2	NHCOCH3	No	0.24	7.0	6
206	KFV	O=C(N[C@@H](CCCC[NH3+])C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-2.13	7.0	6
207	KIF	O=C(N[C@@H](CCCC[NH3+])C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.46	7.0	6
208	KFL	O=C(N[C@@H](CCCC[NH3+])C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.51	7.0	6
209	LKF	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CCCC[NH3+])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.41	7.0	6
210	OrnFL	O=C(N[C@@H](CCC[NH3+])C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.37	7.0	6
211	LOrnF	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CCC[NH3+])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.38	7.0	6
212	RIF	O=C(N[C@@H](CCCNC(=[NH2+])N)C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-0.90	7.0	6
213	RFL	O=C(N[C@@H](CCCNC(=[NH2+])N)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.04	7.0	6
214	LRF	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CCCNC(=[NH2+])N)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-0.76	7.0	6
215	LFR	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CCCNC(=[NH2+])N)C(=O)N)C	CONH2	NHCOCH3	Yes	-0.93	7.0	6

216	IFR	O=C(N[C@@H]([C@H](CC)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CCCNC(=[NH2+])N)C(=O)N)C	CONH2	NHCOCH3	Yes	-0.93	7.0	6
217	HIF	O=C(N[C@@H](Cc1[nH]cnc1)C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	0.36	7.0	6
218	FHL	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1[nH]cnc1)C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	0.46	7.0	6
219	IHV	O=C(N[C@@H]([C@H](CC)C)C(=O)N[C@@H](Cc1[nH]cnc1)C(=O)N[C@@H](C(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-0.33	7.0	6
220	GFH	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1[nH]cnc1)C(=O)N)CNC(=O)C	CONH2	NHCOCH3	Yes	-1.09	7.0	6
221	WHV	O=C(N[C@@H](Cc1[nH]cnc1)C(=O)N[C@@H](C(C)C)C(=O)N)[C@@H](NC(C)=C)Cc1c2c([nH]c1)cccc2	CONH2	NHCOCH3	Yes	0.16	7.0	6
222	FWH	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](Cc1[nH]cnc1)C(=O)N)C	CONH2	NHCOCH3	Yes	0.89	7.0	6
223	DFL	O=C(N[C@@H](CC(=O)[O-])C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.39	7.0	6
224	FDL	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(=O)[O-])C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.19	7.0	6
225	LDL	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CC(=O)[O-])C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.55	7.0	6
226	ILD	O=C(N[C@@H]([C@H](CC)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(=O)[O-])C(=O)N)C	CONH2	NHCOCH3	Yes	-1.90	7.0	6
227	EFL	O=C(N[C@@H](CCC(=O)[O-])C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.52	7.0	6
228	EIF	O=C(N[C@@H](CCC(=O)[O-])C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.57	7.0	6
229	FEF	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CCC(=O)[O-])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.08	7.0	6
230	LEF	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(=O)[O-])C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C	CONH2	NHCOCH3	Yes	-1.25	7.0	6
231	LIE	O=C(N[C@@H](CC(C)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](CCC(=O)[O-])C(=O)N)C	CONH2	NHCOCH3	Yes	-1.87	7.0	6
232	(D-)F(D-)F(D-)F	[H]N(C(C)=O)[C@@H](C(N[C@@H](C(N[C@@H](C(N)=O)CC1=CC=CC=C1)=O)CC2=CC=CC=C2)=O)CC3=CC=CC=C3	CONH2	NHCOCH3	No	2.3	7.2	7
233	YPWF	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](Cc1ccccc1)C(=O)N	CONH2	NH2	Yes	1.10	7.4	8
234	Y(D-)AWF	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N[C@@H](C(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](Cc1ccccc1)C(=O)[O-])C	CONH2	NH2	Yes	1.29	7.4	8
235	YPIDV	Oc1ccc(cc1)C[C@H](NC(=O)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H](CC(=O)[O-])C(=O)N[C@@H](C(C)C)C(=O)N	CONH2	NHCOCH3	Yes	-1.85	7.2	9
236	YPINV	NC([C@H](C(C)C)NC([C@H](CC(N)=O)NC([C@@]([C@@H](C)CC)([H])NC([C@@H]1CCCN1C([C@@H](NC(C)=O)CC2=CC=C(O)C=C2)=O)=O)=O)=O)=O	CONH2	NHCOCH3	No	-0.42	7.2	9
237	YPGNV	NC([C@H](C(C)C)NC([C@H](CC(N)=O)NC(CNC([C@@H]1CCCN1C([C@@H](NC(C)=O)CC2=CC=C(O)C=C2)=O)=O)=O)=O)=O	CONH2	NHCOCH3	No	-2.06	7.2	9
238	YPIIV	NC([C@H](C(C)C)NC([C@@]([C@@H](C)CC)([H])NC([C@@]([C@@H](C)CC)([H])NC([C@@H]1CCCN1C([C@@H](NC(C)=O)CC2=CC=C(O)C=C2)=O)=O)=O)=O)=O	CONH2	NHCOCH3	No	1.13	7.2	9
239	YPGIV	NC([C@H](C(C)C)NC([C@@]([C@@H](C)CC)([H])NC(CNC([C@@H]1CCCN1C([C@@H](NC(C)=O)CC2=CC=C(O)C=C2)=O)=O)=O)=O)=O	CONH2	NHCOCH3	No	-0.2	7.2	9
240	FPIIV	[H]N(C(C)=O)[C@H](C(N1CCC[C@H]1C(N[C@]([C@@H](C)CC)([H])C(N[C@]([C@@H](C)CC)([H])C(N[C@@H](C(C)C)C(N)=O)=O)=O)=O)=O)CC2=	CONH2	NHCOCH3	No	1.61	7.2	9

		CC=CC=C2						
241	FPGIV	[H]N(C(C)=O)[C@H](C(N1CCC[C@H]1C(NCC(N[C@]([C@@H](C)CC)([H])C(N[C@@H](C(C)C)C(N)=O)=O)=O)=O)=O)CC2=CC=CC=C2	CONH2	NHCOCH3	No	1.96	7.2	9
242	FPII	[H]N(C(C)=O)[C@H](C(N1CCC[C@H]1C(N[C@]([C@@H](C)CC)([H])C(N[C@]([C@@H](C)CC)([H])C(N)=O)=O)=O)=O)CC2=CC=CC=C2	CONH2	NHCOCH3	No	1.17	7.2	9
243	FPGI	[H]N(C(C)=O)[C@H](C(N1CCC[C@H]1C(NCC(N[C@]([C@@H](C)CC)([H])C(N)=O)=O)=O)=O)CC2=CC=CC=C2	CONH2	NHCOCH3	No	2	7.2	9
In-House Set								
1	GPG	O=C(NCC(=O)N)[C@H]1N(CCC1)C(=O)C[NH3+]	CONH2	NH2	Yes	-3.05	7.4	10
2	YPWF	Oc1ccc(cc1)C[C@H]([NH3+])C(=O)N1CCC[C@H]1C(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](Cc1ccccc1)C(=O)N	CONH2	NH2	Yes	1.29	7.4	10
3	QWL	NC([C@H](CC(C)C)NC([C@@H](NC([C@H](CCC(N)=O)N(C(C)=O)[H])=O)CC1=CNC2=C1C=CC=C2)=O)=O	CONH2	NHCOCH3	No	0.07	7.4	10
4	FLGKVW	O=C(N[C@@H](CCCC[NH3+])C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N)CNC(=O)[C@@H](NC(=O)[C@@H]([NH3+])Cc1ccccc1)CC(C)C	CONH2	NH2	Yes	-0.99	7.4	10
5	KLVWAF	O=C(N[C@H](C(=O)N[C@@H](Cc1ccccc1)C(=O)N)C)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CCCC[NH3+])CC(C)C)C(C)C)Cc1c2c([nH]c1)cccc2	CONH2	NH2	Yes	-1.13	7.4	10
6	LPVGWF	O=C(N[C@@H](C(C)C)C(=O)NCC(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](Cc1ccccc1)C(=O)N)[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])CC(C)C	CONH2	NH2	Yes	1.12	7.4	10
7	LYLGWI	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H]([NH3+])CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)NCC(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H]([C@H](CC)C)C(=O)N	CONH2	NH2	Yes	2.16	7.4	10
8	PWGYVA	Oc1ccc(cc1)C[C@H](NC(=O)CNC(=O)[C@@H](NC(=O)[C@H]1[NH2+]CCC1)Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](C(C)C)C(=O)N[C@H](C(=O)N)C	CONH2	NH2	Yes	-0.38	7.4	10
9	VPAFII	O=C(N[C@H](C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H]([C@H](CC)C)C(=O)N[C@@H]([C@H](CC)C)C(=O)N)C)[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])C(C)C	CONH2	NH2	Yes	0.66	7.4	10
10	ALIWGY	Oc1ccc(C[C@@H](C(N)=O)NC(CNC([C@H](Cc2c[nH]c3ccccc23)NC([C@H]([C@@H](C)CC)NC([C@H](CC(C)C)NC([C@H](C)[NH3+])=O)=O)=O)=O)=O)cc1	CONH2	NH2	Yes	0.92	7.4	10
11	GAWPFL	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)N)[C@H]1N(CCC1)C(=O)[C@@H](NC(=O)[C@@H](NC(=O)C[NH3+])C)Cc1c2c([nH]c1)cccc2	CONH2	NH2	Yes	0.80	7.4	10
12	VLIWFV	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)N)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])C(C)C)CC(C)C)[C@H](CC)C)Cc1c2c([nH]c1)cccc2	CONH2	NH2	Yes	2.35	7.4	10
13	SVYLQP	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H]([NH3+])CO)C(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(=O)N)C(=O)N1CCC[C@H]1C(=O)N	CONH2	NH2	Yes	-1.59	7.4	10
14	IPFWKL	O=C(N[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1c2c([nH]c1)cccc2)C(=O)N[C@@H](CCCC[NH3+])C(=O)N[C@@H](CC(C)C)C(=O)N)[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])[C@H](CC)C	CONH2	NH2	Yes	-0.85	7.4	10
15	WPKIYV	Oc1ccc(cc1)C[C@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]1N(CCC1)C(=O)[C@@H]([NH3+])Cc1c2c([nH]c1)cccc2)CCCC[NH3+])[C@H](	CONH2	NH2	Yes	-1.82	7.4	10

		CC)C)C(=O)N[C@@H](C(C)C)C(=O)N						

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