Supporting Information

Positional Scanning Identifies the Molecular Determinants of a High Affinity Multi-Leucine Inhibitor for Furin and PACE4

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Table S1. Analytical data of the peptides used in the present study.

Analog	Peptide Sequence	Retention time[a] t_R [min]	Molecular mass		
			calculated	found[b]	$(M+3H)^{3+}$ calculated/**observed**[c]
2	Ac-LLLLRVK-Amba	22.86	1027.35	1026.95	343.24/**343.24**
3	Ac-LLL**A**RVK-Amba	21.55	985.08	984.81	-
4	Ac-LLL**D**RVK-Amba	20.06	1029.09	1028.80	-
5	Ac-LLL**E**RVK-Amba	20.45	1043.12	1041.44	-
6	Ac-LLL**F**RVK-Amba	23.84	1061.18	1060.93	-
7	Ac-LLL**G**RVK-Amba	20.82	971.06	970.81	-
8	Ac-LLL**H**RVK-Amba	19.56	1051.15	1050.86	-
9	Ac-LLL**I**RVK-Amba	23.11	1027.35	1027.33	-
10	Ac-LLL**K**RVK-Amba	18.66	1042.18	1041.66	-
11	Ac-LLL**M**RVK-Amba	21.72	1045.20	1044.25	-
12	Ac-LLL**N**RVK-Amba	19.80	1028.11	1027.58	-
13	Ac-LLL**P**RVK-Amba	20.95	1011.12	1010.94	-
14	Ac-LLL**Q**RVK-Amba	20.24	1042.14	1041.85	-
15	Ac-LLL**R**RVK-Amba	19.98	1070.19	1069.51	-
16	Ac-LLL**S**RVK-Amba	20.87	1001.09	1000.84	-
17	Ac-LLL**T**RVK-Amba	20.83	1015.11	1014.61	-
18	Ac-LLL**V**RVK-Amba	22.28	1013.14	1012.88	-
19	Ac-LLL**W**RVK-Amba	23.51	1100.22	1099.88	-
20	Ac-LLL**Y**RVK-Amba	21.92	1077.18	1076.93	-
21	Ac-LL**A**LRKV-Amba	15.54[d]	985.08	-	329.22/ **329.23**
22	Ac-LL**D**LRKV-Amba	25.81[e]	1029.09	-	343.89/**343.89**
23	Ac-LL**E**LRKV-Amba	16.03[f]	1043.12	-	348.56/**348.56**
24	Ac-LL**F**LRKV-Amba	31.82[e]	1061.18	-	354.57/**354.57**
25	Ac-LL**G**LRKV-Amba	15.26[d]	971.06	-	324.55/**324.55**
26	Ac-LL**H**LRKV-Amba	14.14[d]	1051.15	-	351.23/**351.23**
27	Ac-LL**I**LRKV-Amba	18.63[d]	1027.35	-	343.24/**343.24**
28	Ac-LL**K**LRKV-Amba	13.95[d]	1042.18	-	348.24/**348.25**
29	Ac-LL**M**LRKV-Amba	18.08[d]	1045.20	-	349.22/**349.23**
30	Ac-LL**N**LRKV-Amba	15.01[d]	1028.11	-	343.56/**343.56**

31	Ac-LL**P**LRKV-Amba	15.35[d]	1011.12	-	337.89/**337.90**
32	Ac-LL**Q**LRKV-Amba	15.00[d]	1042.14	-	348.23/**348.23**
33	Ac-LL**R**LRKV-Amba	14.17[d]	1070.19	-	357.58/**357.58**
34	Ac-LL**S**LRKV-Amba	15.39[f]	1001.09	-	334.55/**334.56**
35	Ac-LL**T**LRKV-Amba	15.54[d]	1015.11	-	339.23/**339.23**
36	Ac-LL**V**LRKV-Amba	17.30[d]	1013.14	-	338.57/**338.57**
37	Ac-LL**W**LRKV-Amba	19.58[d]	1100.22	-	367.57/**367.57**
38	Ac-LL**Y**LRKV-Amba	17.49[d]	1077.18	-	359.90/**359.90**
39	Ac-L**A**LLRVK-Amba	20.67	985.08	985.24	-
40	Ac-L**D**LLRVK-Amba	20.12	1029.09	1028.70	-
41	Ac-L**E**LLRVK-Amba	20.43	1043.12	1043.12	-
42	Ac-L**F**LLRVK-Amba	22.91	1061.18	1061.13	-
43	Ac-L**G**LLRVK-Amba	20.14	971.06	970.67	-
44	Ac-L**H**LLRVK-Amba	18.23	1051.15	1051.30	-
45	Ac-L**I**LLRVK-Amba	22.28	1027.35	1027.33	-
46	Ac-L**K**LLRVK-Amba	18.52	1042.18	1042.36	-
47	Ac-L**M**LLRVK-Amba	22.01	1045.20	1046.66	-
48	Ac-L**N**LLRVK-Amba	19.82	1028.11	1028.10	-
49	Ac-L**P**LLRVK-Amba	20.71	1011.12	1011.29	-
50	Ac-L**Q**LLRVK-Amba	20.04	1042.14	1042.12	-
51	Ac-L**R**LLRVK-Amba	18.75	1070.19	1070.12	-
52	Ac-L**S**LLRVK-Amba	20.04	1001.09	1000.72	-
53	Ac-L**T**LLRVK-Amba	20.20	1015.11	1014.26	-
54	Ac-L**V**LLRVK-Amba	21.32	1013.14	1013.30	-
55	Ac-L**W**LLRVK-Amba	23.16	1100.22	1100.38	-
56	Ac-L**Y**LLRVK-Amba	21.21	1077.18	1077.33	-
57	Ac-**A**LLLRVK-Amba	20.54	985.08	984.72	-
58	Ac-**D**LLLRVK-Amba	20.32	1029.09	1028.92	-
59	Ac-**E**LLLRVK-Amba	20.64	1043.12	1042.98	-
60	Ac-**F**LLLRVK-Amba	22.96	1061.18	1060.97	-
61	Ac-**G**LLLRVK-Amba	19.84	971.06	970.66	-
62	Ac-**H**LLLRVK-Amba	18.02	1051.15	1050.98	-
63	Ac-**I**LLLRVK-Amba	22.64	1027.35	1027.12	-
64	Ac-**K**LLLRVK-Amba	18.10	1042.18	1042.03	-
65	Ac-**M**LLLRVK-Amba	21.42	1045.20	1044.95	-
66	Ac-**N**LLLRVK-Amba	19.67	1028.11	1028.08	-
67	Ac-**P**LLLRVK-Amba	21.62	1011.12	1011.04	-

68	Ac-**Q**LLLRVK-Amba	20.01	1042.14	1041.98	-
69	Ac-**R**LLLRVK-Amba	18.62	1070.19	1069.27	-
70	Ac-**S**LLLRVK-Amba	19.70	1001.09	1000.94	-
71	Ac-**T**LLLRVK-Amba	19.91	1015.11	1014.56	-
72	Ac-**V**LLLRVK-Amba	21.64	1013.14	1012.99	-
73	Ac-**W**LLLRVK-Amba	23.76	1100.22	1100.02	-
74	Ac-**Y**LLLRVK-Amba	21.37	1077.18	1076.98	-
76	FITC-βAla-LLLRRVKAmba	31.07[e]	1488.80	-	496.93/**496.93**
77	FITC-βAla-LLLIRVKAmba	34.46[e]	1445.77	-	482.59/**482.59**
78	Ac-LL**II**RVK-Amba	28.65[e]	1027.35	-	343.24/**343.24**
79	Ac-[DLeu]L**II**RVK-Amba	29.51[e]	1027.35	-	343.24/**343.24**

[a]linear gradient from 1 to 80% of B in A for 30 min, flow rate 1 mL/min, RP-HPLC system Shimadzu, Jupiter 4µ Proteo 90 Å (Phenomenex), 250 × 4,60 mm column; [b] molecular masses were determined by the deconvolution of data obtained from the analysis of peptides using LCMS ESI IT-TOF mass spectrometer; [c] molecular masses were obtained by high-resolution mass spectrometry; [d] linear gradient from 10 to 70% of B in A for 40 min, RP-HPLC system Agilent, Elipse XDB C18 column (Agilent); [e] linear gradient from 10 to 70% of B in A for 50 min, RP-HPLC system Agilent, Jupiter C18 column (Phenomenex); ; [f] linear gradient from 10 to 70% of B in A for 30 min, RP-HPLC system Agilent, Elipse XDB C18 column (Agilent); A: 0.1% aqueous TFA, B: 80% acetonitrile in water containing 0.1% of TFA