

Supplementary Table 1: IUPAC name of Non-Peptidic, Non-Prenylic Inhibitors (bisubstrate analogue inhibitors).

S. No	Compound name	IUPAC Name
1	Compound1	methyl (2S)-2- {[4-(3-hexadecanamidopropanamido)phenyl]formamido}-4-(methylsulfanyl)butanoate
2	Compound2	methyl (2S)-2- {[4-(3-hexadecanamidopropanamido)benzene]sulfonamido}-4-(methylsulfanyl)butanoate
3	Compound3	methyl (2S)-2- ({4-[(3-hexadecanamido-2-oxopropyl)amino]phenyl} formamido)-4-(methylsulfanyl)butanoate
4	Compound4	N-(2,3-dimethylphenyl)-3-(3-hexadecanamidopropanamido)benzamide
5	Compound5	N-[2-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)ethyl]hexadecanamide
6	Compound6	N-[2-({3-[(2,3-dimethylnaphthalen-1-yl)sulfamoyl]phenyl} carbamoyl)ethyl]hexadecanamide
7	Compound7	N-[2-({3-[(naphthalen-1-ylmethyl)sulfamoyl]phenyl} carbamoyl)ethyl]hexadecanamide
8	Compound8	N- {2-[(3- {2-(1H-indol-3-yl)ethyl}sulfamoyl} phenyl) carbamoyl]ethyl} hexadecanamide
9	Compound9	N-[2-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)ethyl]tetradecanamide
10	Compound10	N-[2-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)ethyl]octadecanamide
11	Compound11	(9Z)-N-[2-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)ethyl]octadec-9-enamide
12	Compound12	(9Z,12Z)-N-[2-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)ethyl]octadeca-9,12-dienamide
13	Compound13	N-[2-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)ethyl]-N-methylhexadecanamide
14	Compound14	N-[({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)methyl]heptadecanamide
15	Compound15	N-[3-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)propyl]pentadecanamide
16	Compound16	(2E)-N-[2-({3-[(2,3-dimethylphenyl)sulfamoyl]phenyl} carbamoyl)ethyl]-3-(4-phenylphenyl)prop-2-enamide

Supplementary Table 2: IUPAC name of Peptidyl (acyloxy) methyl ketones.

S. No	Compound Name	IUPACName
1	(FABK(CH3)3)	(3S)-3-[(2S)-2-{{(benzyloxy)carbonyl}amino}-3-phenylpropanamido]-2-oxobutyl 2,4,6-trimethylbenzoate
2	Y(FGBK(CH3)2)	(3S)-3-[(2S)-2-[(2S)-2-acetamido-3-(4-hydroxyphenyl)propanamido]-3-phenylpropanamido]-2-oxobutyl 2,6-dimethylbenzoate
3	(FKBK(CH3)3)	(3S)-7-amino-3-[(2S)-2-{{(benzyloxy)carbonyl}amino}-3-phenylpropanamido]-2-oxoheptyl 2,4,6-trimethylbenzoate

Supplementary Table 3: Extra precision docking of Non-Peptidic, Non-preylic Inhibitors of the Prenyl Protein-specific Protease Rce1 and Peptidyl(acyloxy)methyl ketones with Human CAAX prenyl protease I.

S. No	Compound NAME	Docking Score	Glide Energy	Glide Evdw	Glide Ecol	Glide Emodel	Residues involved	ΔG_{bind}
Non-Peptidic, Non-preylic Inhibitors								
1	Compound6	-8.678	-55.192	-53.695	-1.497	-75.941	----	-86.550
2	Compound7	-8.356	-59.344	-54.432	-4.911	-83.122	Gln393	-97.332
3	Compound8	-8.294	-58.827	-54.648	-4.179	-84.461	Phe133, Ser134	-104.926
4	Compound10	-7.542	-52.975	-52.191	-0.784	-76.209	Ser134, Gln393, Phe394	-93.247
5	Compound4	-7.524	-52.179	-48.648	-3.532	-76.804	Gln393	-107.792
6	Compound12	-7.174	-48.859	-42.751	-6.108	-67.161	Gln393	-77.928
7	Compound1	-7.148	-55.166	-52.529	-2.637	-80.845	Glu88	-110.722
8	Compound2	-7.000	-53.253	-45.648	-7.605	-69.918	Ser27, Ser134, Gln393, Phe394, Ser397	-95.605
9	Compound3	-6.925	-56.861	-53.313	-3.548	-75.998	Ser134	-102.784
10	Compound5	-6.731	-46.607	-43.085	-3.522	-71.185	Phe133, Gln393	-86.552
11	Compound16	-6.672	-52.802	-52.950	0.148	-81.432	Ser134, Phe394,	-68.547
12	Compound14	-6.664	-48.793	-46.097	-2.696	-74.080	Ala130	-105.226
13	Compound13	-6.657	-52.534	-49.824	-2.710	-78.825	Glu88	-89.779
14	Compound9	-6.435	-53.026	-51.454	-1.572	-67.736	Glu88	-94.151
15	Compound11	-6.279	-52.516	-48.827	-3.689	-74.905	Ala130, Phe394, Gln393	-71.412
16	Compound15	-5.962	-52.043	-49.924	-2.119	-78.601	Glu88, Ser134	-81.641
Peptidyl(acyloxy)methyl ketones								
1	(FKBK(CH ₃) ₃)	-8.625	-60.572	-52.338	-8.234	-87.302	Glu88, Ser134	-97.443
2	(FABK(CH ₃) ₃)	-7.090	-52.620	-51.692	-0.928	-70.127	---	-80.749
3	Y(FGBK(CH ₃) ₂)	-7.005	-54.632	-47.665	-6.967	-79.855	Glu34	-76.961

Supplementary Table 4: Result of Drug Likeness properties prediction of compounds obtained from virtual screening against CAAX prenyl protease 1 using DruLiTo

S.No	Compound Code	MW	logP	Alogp	HB A	HB D	TPSA	AMR	nRB	nAtom	nAcidic	RC	nRingd b	nArom atic	nHB	SAlert s
1	SYN20008993 ^A	398.2	-0.19	-0.825	8	3	99.77	112.88	8	55	0	3	23	1	11	1
2	F0451-4356 ^L	322.06	0.97	-0.522	9	4	124.05	77.59	6	33	0	2	17	1	13	3
3	F02432-0154 ^L	405.13	1.337	-0.522	7	4	119.92	120.42	9	48	0	4	23	4	11	0
4	F0849-2472 ^L	362.13	1.46	-1.64	11	4	142.51	120.42	9	44	0	2	18	1	15	3
5	SYN15784346 ^A	361.15	1.416	0.164	7	3	85.83	107.83	4	46	0	4	26	2	10	0
6	LEG17766749 ^A	400.16	1.411	-0.638	7	2	116.17	109.4	9	52	0	3	21	2	9	1
7	SYN17739355 ^A	397.11	-0.797	-0.754	7	2	103.96	112.33	4	47	0	4	27	2	9	0
8	F0452-3342 ^L	370.1	1.86	0.26	9	4	124.05	82.79	8	39	0	2	19	1	13	4
9	KM09023 ^M	408.05	1.682	1.471	6	4	139.65	115.02	11	43	0	2	16	2	10	2
10	KM03725 ^M	355.09	-0.097	0.037	7	4	124.63	100.39	7	41	0	3	20	2	11	1
11	F04375-4375 ^L	278.05	0.381	-2.285	10	4	133.28	63.96	6	30	0	2	15	1	14	3
12	SYN19993980 ^A	419.16	0.191	-0.134	9	2	103.34	119.84	7	52	0	4	27	3	11	0
13	KM03692 ^M	477.06	1.556	2.086	6	3	112.6	107.77	8	45	0	3	26	2	9	2
14	JFD00284 ^M	330.11	0.588	1.022	6	2	93.06	93.25	9	42	0	2	16	2	8	2
15	JFD00284 ^M	330.11	0.588	1.022	6	2	93.06	93.25	9	42	0	2	16	2	8	2

^A-Asinex, ^L-Life chemicals, ^M-Maybridge

Supplementary Table 5: Result of Drug Likeness properties prediction of compounds obtained from virtual screening against CAAX prenyl protease 2 using DruLiTo

S.no	Compound_Code	MW	logP	Alogp	H B A	HB D	TPSA	AMR	nRB	nAtom	nAcidic	RC	nRingdb	nAromatic	nHB	SAlerts
1	F2721-0700 ^L	348.09	0.972	-1.137	5	3	106.07	91.31	8	41	0	2	17	2	8	1
2	F72721-0150 ^L	359.16	0.251	-1.246	5	3	97.87	97.96	10	48	0	2	17	2	8	2
3	DP01608 ^M	309.03	2.374	-0.412	2	1	46.26	84.25	4	33	0	2	17	2	3	1
4	RH00579 ^M	245.22	1.094	-1.267	3	2	76.97	68.41	4	33	0	2	15	2	5	0
5	SYN 15030991 ^A	329.19	0.476	-1.762	4	2	55.49	96.81	8	49	0	3	18	2	6	0
6	F2721-0715 ^L	342.16	1.367	-0.804	5	3	106.07	95.33	9	47	0	2	17	2	8	1
7	F1386-0017 ^L	274.05	2.405	0.29	3	1	55.6	54.96	3	27	0	2	16	2	4	2
8	SYN 19817855 ^A	324.14	0.272	-1.37	4	1	58.4	93.32	5	41	0	3	21	2	5	1
9	S15270 ^M	240.12	-1.532	-3875	6	2	83.64	55.67	2	33	0	2	16	0	8	1
10	SYN 10322709 ^A	319.16	0.714	-4.142	5	3	69.78	81.0	4	43	0	3	21	2	8	1
11	SYN 19819113 ^A	340.23	2.586	-2.625	4	1	58.4	92.27	6	53	0	3	21	1	5	0
12	SYN 17737972 ^A	330.12	0.898	-0.359	5	1	72.09	91.68	3	41	0	3	22	1	6	0
13	F1278-0573 ^L	390.13	0.57	-0.371	5	2	95.07	105.08	10	50	0	2	18	2	7	0
14	HTS02812 ^M	370.21	-0.052	-0.608	5	4	77.24	109.61	9	55	0	3	20	2	9	0
15	HTS02812 ^M	370.21	-0.052	-0.608	5	4	77.24	109.61	9	55	0	3	20	2	9	0

^A-Asinex, ^L-Life chemicals, ^M-Maybridge