

Table S2 - Docking scores (ds), mass and number of Non-H atoms of the 241 peptides with unknown bioactive properties.

Peptide ID	Peptide code	ds 4APH	ds 6EN5	Mass (Da)	Non-H Atoms	Peptide ID	Peptide code	ds 4APH	ds 6EN5	Mass (Da)	Non-H Atoms	Peptide ID	Peptide code	ds 4APH	ds 6EN5	Mass (Da)	Non-H Atoms
Ref1	BJ2	99.14	119.68	428.44	30	#80	QQTM	91.16	111.71	506.579	34	#161	EQSL	104.28	100.8	475.497	33
Ref2	ANG	104.65	111.66	1046.19	75	#81	QQQQL	97.04	122.3	643.696	45	#162	EPTF	97.71	103.79	492.527	35
#1	SCTEK	97.29	117.33	566.631	38	#82	QPVL	95.66	102.9	455.554	32	#163	EM	72.92	82.54	278.328	18
#2	VVVVTK	103.96	123.22	643.824	45	#83	QM	73.05	74.38	277.344	18	#164	EITVGK	104.97	129.72	645.752	45
#3	VVTY	97.44	110.28	480.56	34	#84	QGR	93.25	93.76	359.385	25	#165	EITSH	108.39	119.13	585.613	41
#4	VVQGAPL	96.51	113.89	682.817	48	#85	QGGGVSR	108.32	130.16	659.699	46	#166	EISH	94.42	113.15	484.508	34
#5	VVN	84.25	82.87	330.383	23	#86	QER	95.11	109.79	431.448	30	#167	EGVCCL	102.22	111.68	622.762	41
#6	VVAGSTL	114.54	119.67	645.752	45	#87	QEM	87.09	101.74	406.458	27	#168	EEK	90.7	107.67	404.418	28
#7	VTTK	94.39	103.2	447.531	31	#88	QCVQN	105.6	116.6	590.657	40	#169	EDITL	103.16	114.55	589.64	41
#8	VTL	80.55	89.28	331.411	23	#89	QATVVL	106.65	122.22	629.753	44	#170	EDIGK	112.52	111.17	560.603	39
#9	VTGN	84.06	93.87	389.407	27	#90	QATM	92.48	106.4	449.527	30	#171	EAVL	88.45	100.26	430.5	30
#10	VSEAM	92.19	111.04	535.617	36	#91	QAR	97.12	102.05	373.412	26	#172	EAVADR	116.98	117.15	659.695	46
#11	VSAY	86.83	108.38	438.479	31	#92	QAH	85.61	94.02	354.366	25	#173	EAEEGQF	116.28	138.65	808.796	57
#12	VQY	93.6	94.19	408.453	29	#93	QAF	90.51	100.16	364.401	26	#174	DVVEPDQY	119.22	123.63	963.992	68
#13	VQL	86.17	96.63	358.437	25	#94	PVR	82.39	93.86	370.452	26	#175	DVTN	95.56	101.64	447.443	31
#14	VQK	90.99	98.62	373.452	26	#95	PVPAW	95.04	113.11	568.673	41	#176	DTPDQF	102.19	115.36	721.718	51
#15	VQH	89.9	92.35	382.419	27	#96	PVDIH	89.51	112.29	579.653	41	#177	DTK	91.55	106.65	362.381	25
#16	VIGL	82.6	98.3	400.518	28	#97	PSQDQK	103.44	120.72	701.732	49	#178	DTF	91.54	105.23	381.384	27
#17	VIDIIN	90.24	129.46	685.817	48	#98	PQM	86.06	94.85	374.46	25	#179	DPY	88.11	93.08	393.395	28
#18	VGW	87.4	94.16	360.413	26	#99	PIVY	88.05	106.81	490.599	35	#180	DPGR	97.23	103.03	443.459	31
#19	VGPK	80.27	97.11	399.49	28	#100	PGIK	86.15	99.85	413.517	29	#181	DPDL	89.13	98.25	458.466	32
#20	VEAM	87.34	103.68	448.539	30	#101	PGGSATSR	131.15	125.17	731.762	51	#182	DL	81.47	81.22	246.262	17
#21	VCL	80.71	87.47	333.451	22	#102	PGAGGGGAGR	123.36	121.94	755.788	53	#183	DIAVF	93.32	108.12	563.65	40
#22	VAVATSR	116.91	122.87	702.808	49	#103	PEY	93.57	87.42	407.421	29	#184	DGIH	94.6	106.29	440.455	31
#23	VAPR	95.53	100.22	441.531	31	#104	PEW	92.11	97.89	430.459	31	#185	DEVF	97.14	118.63	508.526	36
#24	VAL	86.04	86.86	301.385	21	#105	PETSDTL	106.8	120.48	761.78	53	#186	DESVY	103.07	130.1	611.603	43
#25	TVVSGSTR	130.6	128.14	805.884	56	#106	PETETVL	112.9	120.29	787.862	55	#187	DDVVVTAGQCAH	132.52	116.24	1214.32	84
#26	TVVPF	90.94	107.4	561.677	40	#107	PEPDK	96.28	122.26	584.625	41	#188	DDK	88.59	100.08	376.365	26

#27	TVPCGTF	101.14	113.74	723.846	50	#108	PEM	80.77	87.02	375.445	25	#189	DAL	81.46	97.32	317.341	22
#28	TVIDAIVK	110.82	127.17	858.044	60	#109	PEDVK	97.46	121.45	586.64	41	#190	CY	72.51	77.17	284.335	19
#29	TVGF	88.29	107.66	422.48	30	#110	PCIAEIVSTVR	140.78	121.64	1187.42	82	#191	CVK	81.58	93.63	348.466	23
#30	TTVVAGR	120.97	115.54	702.808	49	#111	PATVS	90.29	101.31	473.525	33	#192	CSAAPAQSVQDDR	131.25	115.46	1347.42	93
#31	TTAGIAF	103.49	123.93	679.769	48	#112	PATL	84.79	89.73	400.474	28	#193	CR	71.59	75.89	277.348	18
#32	TSSPEEASDEM	127.45	118.92	1182.18	81	#113	PAQSGGCICR	120.65	121.23	1048.21	71	#194	CQPN	89.13	90.69	460.51	31
#33	TSEAN	91.67	112.55	520.494	36	#114	IVTDQSEK	124.15	128.14	918.996	64	#195	CQH	89.89	90.27	386.432	26
#34	TPW	83.56	88.17	402.449	29	#115	IVL	85.57	94.17	343.466	24	#196	CM	68.12	69.53	252.358	15
#35	TIGDSSSECSIF	130.69	144.4	1245.32	86	#116	IVGGK	101.48	103.82	472.585	33	#197	CL	65.94	69.73	234.319	15
#36	TGL	79.41	83.66	289.331	20	#117	ITM	88.74	93.52	363.477	24	#198	CK	71.75	78.58	249.334	16
#37	TEDW	95.77	109.12	549.535	39	#118	ISSCVGDIGSPL	115.93	137.23	1147.31	79	#199	CIQ	84.96	86.23	362.449	24
#38	TDDSTF	122.29	135.79	684.654	48	#119	ISDEVTVAVTATETM	105.41	110.36	1665.87	115	#200	CIEI	89.07	102.36	476.593	32
#39	TCPGTETCCTTPQGEEGCCPY	21.73	66.23	2180.42	147	#120	ISAIGVPH	105.24	114.21	792.932	56	#201	CGGAL	96.23	101.65	419.501	28
#40	TCDSL	94.89	127.47	537.589	36	#121	ISAEIEVL	113.25	118.46	873.011	61	#202	CGF	82.22	90.92	325.388	22
#41	TAVAL	89.99	113.77	473.569	33	#122	IPF	80.12	91.28	375.467	27	#203	CEN	84.77	89.83	364.378	24
#42	TAL	84.38	89.77	303.358	21	#123	IK	76.95	74.67	259.349	18	#204	CDAR	87.81	110.34	463.514	31
#43	TAIR	88.07	106.25	459.546	32	#124	IIGM	86.45	101.99	432.584	29	#205	CCSL	93.39	93.62	424.541	27
#44	SVW	88.01	104.45	390.438	28	#125	IIDEDIPL	113.34	121.44	927.059	65	#206	CCPSGTVCDEDH	126.66	118.11	1265.36	85
#45	SVSIQW	102.03	131.06	718.806	51	#126	IGVVSUW	110.04	128.58	659.782	47	#207	CAL	77.26	81.72	305.398	20
#46	SVF	84.74	90.41	351.402	25	#127	IGF	88.74	95.51	335.403	24	#208	AVVAL	86.22	105.61	471.597	33
#47	STVF	89.64	108.7	452.506	32	#128	IEIL	93.56	105.25	486.607	34	#209	AVR	88.02	89.11	344.414	24
#48	STQDSSCF	135.02	132.39	873.892	60	#129	IDIVSL	108.07	126.69	658.791	46	#210	AVASW	94.19	112.94	532.596	38
#49	SSY	94.98	97.24	355.346	25	#130	IDCSR	102.2	129.11	592.673	40	#211	ATVCACAL	101.83	110.78	750.937	50
#50	SSR	81.24	99.68	348.359	24	#131	ICSGPVTGK	119.88	127.01	861.028	59	#212	ATR	73.66	90.53	346.386	24
#51	SSN	72.37	89.35	306.274	21	#132	IAH	86.47	92.75	339.395	24	#213	ATPTY	85.26	107.13	551.595	39
#52	SSL	81.59	90.8	305.33	21	#133	GVPCAAVR	114.89	119.57	771.939	53	#214	ATL	75.43	81.78	303.358	21
#53	SR	80.53	80.2	261.281	18	#134	GVL	76.02	80.22	287.359	20	#215	ATIVL	89.35	109.02	515.649	36
#54	SPM	72.51	84.81	333.408	22	#135	GVCH	84.77	98.67	414.485	28	#216	ATAIL	93.07	105.33	487.596	34
#55	SN	66.8	71.01	219.196	15	#136	GTL	74.34	85.51	289.331	20	#217	ASEF	88.98	102.87	452.462	32
#56	SITAH	89.37	117.29	527.577	37	#137	GSTSN	96	108.95	464.43	32	#218	AQQQL	107.42	121.71	586.644	41

#57	SIL	82.48	92.86	331.411	23	#138	GSSF	86.56	104.47	396.399	28	#219	AQAATL	105.44	122.23	573.645	40
#58	SICVDAF	107.03	120.59	753.872	52	#139	GSL	73.62	83.79	275.304	19	#220	APR	77.67	82.9	342.398	24
#59	SGW	87.81	97.1	348.358	25	#140	GQSTL	95.12	110.18	504.539	35	#221	AN	63.09	64.09	203.197	14
#60	SGVSSH	113.49	114.93	572.574	40	#141	GPGL	85.71	86.52	342.394	24	#222	AK	68.13	78.92	217.268	15
#61	SGPL	79.97	95.4	372.42	26	#142	GN	63.44	63.53	189.17	13	#223	AIR	84.62	90.63	358.441	25
#62	SGEVW	99.4	113.95	576.605	41	#143	GGVPVR	105.3	121.47	583.688	41	#224	AIN	82.62	81.65	316.357	22
#63	SER	94.59	101.66	390.395	27	#144	GGSL	86.81	95.76	332.356	23	#225	AGY	87.28	83.51	309.321	22
#64	SEDGR	97.29	112.66	562.535	39	#145	GGQESDVL	113.31	133.44	803.821	56	#226	AGGR	86.46	96.06	359.385	25
#65	SDW	88.72	101.28	406.394	29	#146	GGM	76.44	78.41	263.317	17	#227	AGF	72.97	86.81	293.322	21
#66	SDK	84.12	94.71	348.355	24	#147	GGGSGGAAGR	120.01	122.93	802.801	56	#228	AGAL	85.44	93.16	330.383	23
#67	SAVPVVL	100.37	118.38	683.845	48	#148	GEGGDF	105.74	125.35	580.549	41	#229	AEVTIPTVN	132.44	127.7	1042.19	73
#68	SAVH	84.36	101.38	412.445	29	#149	GDFV	87.48	89.88	436.463	31	#230	ADIN	94.72	92.61	431.444	30
#69	SAPL	77.74	96.02	386.447	27	#150	GDAAPSAVH	112.14	113.55	823.859	58	#231	ACTCK	102.04	118.17	524.662	34
#70	SAL	67.93	83.8	289.331	20	#151	GCVK	92.29	103.57	405.518	27	#232	AAR	74.81	87.71	316.361	22
#71	SAK	75.27	89.52	304.346	21	#152	GCTAAGAF	111.53	112.44	696.78	48	#233	AAQAEVQK	122.69	124.46	843.933	59
#72	QVR	94.86	104.79	401.466	28	#153	GCCVAVASF	115.84	121.89	856.033	58	#234	AAPSAGH	104.75	103.37	609.639	43
#73	QVK	85.62	104.86	373.452	26	#154	GAY	76.7	88.69	309.321	22	#235	AAM	71.98	82.31	291.371	19
#74	QVF	84.76	107.59	392.454	28	#155	GAPAAGDCVSASPQAL	117.77	133.15	1414.56	98	#236	AAL	71.76	82.93	273.332	19
#75	QTW	88.06	108.51	433.463	31	#156	GAGSR	95.81	110.89	446.463	31	#237	AAISCGW	118.86	124.6	706.819	49
#76	QTSL	94.79	103.53	447.487	31	#157	GAAL	75.89	92.5	330.383	23	#238	AAGAGGSR	114.67	120.78	645.672	45
#77	QTIIR	98.24	135.05	629.757	44	#158	EVCL	88.64	103.68	462.566	31	#239	AADR	82.84	98.91	431.448	30
#78	QTAAPGPPTW	112.12	131.44	1025.13	73	#159	ETL	87.81	97.88	361.393	25	#240	AADL	82.96	90.97	388.419	27
#79	QR	80.87	86.94	302.334	21	#160	ESM	86.19	101	365.406	24	#241	AACVSAAVL	110.08	114.43	803.976	55

Table S3 – Intermolecular interactions between the ligands (peptides and reference structures) and the enzyme targets (N- and C-domain of sACE).

[illegible]

C-domain (PDB ID:4APH)	drophobic interactions	201	TRP	x	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		257	TRP	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		332	ALA	x	-	-	-	-	-	-	x	-	-	-	-	x	-	-	-	-
		335	TRP	-	-	-	-	x	-	x	x	-	x	-	-	-	-	-	x	-
		338	TYR	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		358	THR	x	-	-	-	x	x	-	-	-	-	x	-	-	-	-	x	-
		361	HIS	x	x	-	-	-	-	-	-	-	x	-	-	-	-	-	-	-
		369	TYR	-	-	-	-	-	-	-	-	-	x	-	-	-	-	-	-	-
		381	ARG	-	-	-	-	-	-	-	-	-	x	-	x	-	-	-	-	-
		385	PRO	-	-	-	-	-	-	-	-	-	x	-	x	-	-	-	-	-
		388	HIS	-	-	-	-	-	x	-	-	-	-	x	-	x	-	-	-	-
		435	PHE	-	x	x	x	-	x	-	x	x	-	-	-	-	x	-	-	-
		490	PHE	x	x	-	-	-	-	x	-	-	-	-	x	-	-	-	-	x
		496	THR	x	-	-	x	x	-	-	-	-	-	-	x	-	-	-	-	x
		497	PRO	x	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		501	TYR	x	-	-	x	x	-	x	x	x	x	x	x	x	x	x	x	x
		505	PHE	-	x	x	-	-	x	-	x	-	-	-	x	-	x	-	-	-
	Salt bridges	331	HIS	x	-	x	x	x	-	-	x	x	x	-	-	-	x	x	-	x
		350	ARG	-	-	-	-	-	-	-	-	-	-	-	-	x	-	-	-	-
		361	HIS	-	-	-	-	-	-	-	-	-	-	-	-	x	-	x	-	x
		365	HIS	x	-	-	-	-	-	-	x	x	-	-	-	-	x	x	-	x
		388	HIS	x	-	-	-	-	-	-	x	x	x	-	-	-	x	x	x	-
		393	ASP	-	-	-	-	x	-	x	-	-	x	-	-	-	-	-	-	-
		431	GLU	-	-	-	-	-	-	x	-	-	-	-	-	-	-	-	-	-
		489	LYS	x	-	x	x	x	x	x	x	x	x	x	x	-	x	x	-	x
		491	HYS	x	-	x	x	x	x	x	x	x	x	x	x	x	x	x	-	x
	π-Stacking	500	ARG	-	-	-	-	-	-	-	-	-	-	x	x	-	-	-	-	-
		490	PHE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	x	-
		505	PHE	-	-	-	x	-	-	-	-	-	-	-	-	-	-	-	x	-
		335	TRP	-	x	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C-domain (PDB ID:4APH)	Hydrogen bonds	66	ASN	-	x	-	-	-	-	-	-	x	-	x	-	x	x	-	-	x
		70	ASN	-	-	-	-	-	x	-	-	-	-	-	-	-	-	-	x	-
		123	GLU	x	-	-	-	-	-	-	-	-	-	x	-	-	-	-	-	-
		124	ARG	x	-	-	-	-	-	-	-	-	-	x	-	-	-	-	-	-
		143	GLU	-	-	-	-	-	-	-	x	-	-	-	-	-	-	-	-	-
		281	GLN	-	x	-	-	-	-	x	-	-	x	-	-	-	-	x	-	x
		282	THR	-	-	-	-	-	-	-	-	-	x	-	-	-	-	-	-	-

353	HIS	-	-	-	-	X	X	X	-	-	X	-	-	-	-	X	X	X
354	ALA	-	-	-	-	X	X	X	-	-	X	X	X	X	-	-	-	-
356	ALA	-	X	X	X	X	X	X	-	-	X	X	-	X	X	X	-	X
358	ASP	-	-	X	X	-	-	-	-	-	-	X	-	X	-	-	-	X
360	TYR	-	-	X	-	X	-	X	X	-	-	X	-	X	-	-	X	X
368	LYS	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	X	-
384	GLU	-	-	X	-	-	-	-	X	-	-	-	-	X	X	-	X	-
394	TYR	-	-	X	-	-	-	-	X	-	-	-	-	X	-	-	-	-
402	ARG	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-
403	GLU	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-
404	GLY	-	-	-	-	-	-	X	X	-	-	-	-	-	-	-	X	-
411	GLU	-	-	-	-	-	-	X	X	X	-	X	-	-	X	-	-	-
415	ASP	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
453	ASP	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
454	LYS	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
511	LYS	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X
513	HIS	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
516	SER	-	-	-	-	-	-	-	-	-	-	-	-	X	X	-	-	-
517	SER	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-
520	TYR	-	X	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-
522	ARG	X	-	-	-	-	X	X	-	X	-	X	X	-	X	-	X	-
523	TYR	X	-	X	X	-	X	-	-	-	-	X	-	X	X	-	X	-
59	TRP	-	X	-	X	-	-	-	-	-	-	X	-	-	-	-	-	-
62	TYR	-	X	-	-	-	-	-	-	-	-	X	X	X	X	-	-	-
63	ALA	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-
88	ILE	-	X	-	-	-	-	-	-	-	-	X	-	X	-	-	-	-
92	THR	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
118	LYS	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-
123	GLU	X	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-
124	ARG	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
220	TRP	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
282	THR	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
354	ALA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	X
357	TRP	-	X	-	-	X	-	X	-	-	X	-	X	-	X	-	-	-
358	ASP	-	-	-	X	-	-	-	-	X	-	-	-	-	-	-	-	-
360	TYR	-	X	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-
376	GLU	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Hydrophobic interactions

		387	HIS	-	x	-	-	-	-	-	x	-	-	-	-	-	-	-	-
		391	PHE	x	x	-	-	x	-	-	x	x	-	-	-	-	-	-	x
		403	GLU	-	-	-	-	-	-	x	-	-	-	-	-	-	-	x	-
		407	PRO	x	-	x	-	-	x	-	x	x	-	-	-	-	-	x	-
		410	HIS	x	-	-	-	-	-	-	-	x	-	-	-	-	-	x	-
		457	PHE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	x
		512	PHE	-	-	-	-	x	-	-	x	-	-	-	-	-	-	-	x
		518	VAL	-	-	-	-	-	x	-	x	-	-	-	x	-	x	-	x
		519	PRO	x	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		520	TYR	-	x	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		522	ARG	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
		523	TYR	-	x	-	-	-	-	-	-	-	-	-	x	-	-	-	-
		527	PHE	-	x	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	Salt bridges	123	GLU	-	-	-	-	x	-	-	-	-	-	-	-	-	-	-	-
		124	ARG	-	-	-	-	-	-	-	-	-	-	x	-	x	-	-	-
		353	HIS	-	-	-	-	-	-	-	-	x	-	-	-	-	x	-	-
		368	LYS	-	-	-	-	-	-	-	x	-	-	x	-	-	-	-	-
		383	HIS	x	-	-	-	-	-	-	x	x	-	-	x	-	x	x	-
		387	HIS	x	-	-	-	-	-	-	x	x	x	-	x	x	x	x	-
		403	GLU	-	-	-	-	x	-	-	-	-	-	-	-	-	-	-	-
		410	HIS	-	-	-	-	-	-	-	x	-	x	-	-	x	-	x	-
		453	ASP	-	-	-	-	-	-	-	-	-	x	-	-	-	-	-	-
		511	LYS	-	-	-	-	-	-	-	-	-	x	-	-	-	-	x	-
		513	HIS	-	-	-	-	-	-	-	-	-	x	-	-	-	-	x	-
		522	ARG	-	-	x	-	-	x	-	-	x	-	-	-	x	x	x	-
	π -Stacking	59	TRP	-	x	-	x	-	-	-	-	-	-	-	-	x	-	-	-
		457	PHE	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	x
	π -Cation Interactions																		
		457	PHE	-	-	-	-	-	-	-	-	-	x	-	-	-	-	-	-