Supporting information

S1 Table. All PACMANS predicted fibrinogen α chain cleavage sites by cathepsin K from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 3B.

S2 Table. All PACMANS predicted fibrinogen β chain cleavage sites by cathepsin K from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 3B.

S3 Table. All PACMANS predicted fibrinogen γ chain cleavage sites by cathepsin K from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 3B.

S4 Table. All PACMANS predicted fibrinogen α chain cleavage sites by cathepsin L from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 4B.

S5 Table. All PACMANS predicted fibrinogen β chain cleavage sites by cathepsin L from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 4B.

S6 Table. All PACMANS predicted fibrinogen γ chain cleavage sites by cathepsin L from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 4B.

S7 Table. All PACMANS predicted fibrinogen α chain cleavage sites by cathepsin S from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 5B.

S8 Table. All PACMANS predicted fibrinogen β chain cleavage sites by cathepsin S from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 5B.

S9 Table. All PACMANS predicted fibrinogen γ chain cleavage sites by cathepsin S from PACMANS and how sequences relate to molecular docking models. Blue sequences with molecule docking model with the cathepsin active site facing the fibrinogen chain were included in Fig 5B.

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
182	1.06	26	DFLAEGGG	33	not in crystal structure
170	1.00	821	YYPGGSYD	828	not in crystal structure
168	0.96	167	KRLEVDID	174	allosteric/hairpin
165	0.96	667	TSLGGWLL	674	not in crystal structure
156	0.90	186	RALAREVD	193	allosteric/hairpin
155	0.91	111	EILRGDFS	118	active site facing
153	0.90	239	SQLQKVPP	246	not in crystal structure
152	0.87	202	KQLEQVIA	209	active site facing
150	0.88	490	DCPEAMDL	497	not in crystal structure
150	0.88	769	GSVEEGAE	776	not in crystal structure
145	0.83	259	MELERPGG	266	not in crystal structure
145	0.84	726	VELEDWAG	733	not in crystal structure
144	0.84	262	ERPGGNEI	269	not in crystal structure
144	0.86	759	EGTAGDAL	766	not in crystal structure
143	0.82	535	PMLGEFVS	542	not in crystal structure
142	0.83	498	GTLSGIGT	505	not in crystal structure
141	0.84	396	DSPGSGNA	403	not in crystal structure
141	0.83	764	DALIEGSV	771	not in crystal structure
139	0.81	132	EDLRSRIE	139	active site facing
138	0.82	244	VPPEWKAL	251	not in crystal structure
138	0.82	563	HHPGIAEF	570	not in crystal structure
136	0.79	27	FLAEGGGV	34	not in crystal structure
136	0.80	694	RGFGSLND	701	not in crystal structure
135	0.83	73	LIDEVNQD	80	active site facing
135	0.80	192	VDLKDYED	199	allosteric/hairpin
135	0.78	650	IKLPGSSK	657	not in crystal structure
135	0.79	765	ALIEGSVE	772	not in crystal structure
134	0.80	715	HLLTQRGS	722	not in crystal structure
133	0.79	21	DSGEGDFL	28	not in crystal structure
133	0.79	211	DLLPSRDR	218	no docking models near
133	0.81	699	LNDEGEGE	706	not in crystal structure
132	0.80	844	VSFRGADY	851	not in crystal structure
131	0.79	9	LVLSVVGT	16	not in crystal structure
131	0.77	565	PGIAEFPS	572	not in crystal structure
130	0.78	103	HSLTTNIM	110	no docking models near
130	0.75	495	MDLGTLSG	502	not in crystal structure
129	0.77	32	GGVRGPRV	39	not in crystal structure
128	0.75	90	NSLFEYQK	97	active site facing
128	0.76	377	SSVSGSTG	384	not in crystal structure
128	0.75	627	RPVRDCDD	634	not in crystal structure
127	0.75	300	SGPGSTGN	307	not in crystal structure
127	0.75	326	SGPGSTGS	333	not in crystal structure
127	0.77	724	LRVELEDW	731	not in crystal structure

Supp Table 1

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
169	0.98	110	CQLQEALL	117	no docking models near
158	0.92	210	QKLESDVS	217	no docking models near
156	0.92	94	GCLHADPD	101	no docking models near
155	0.91	339	ELLIEMED	346	globular
148	0.85	174	SELEKHQL	181	no docking models near
146	0.86	388	SQLMGENR	395	globular
144	0.84	57	PSLRPAPP	64	not in crystal structure
144	0.83	200	SILENLRS	207	active site facing
141	0.85	179	HQLYIDET	186	active site facing
139	0.82	376	RGTAGNAL	383	globular
137	0.82	28	VKSQGVND	35	not in crystal structure
137	0.84	105	LCPTGCQL	112	active site facing
136	0.82	59	LRPAPPPI	66	not in crystal structure
133	0.78	203	ENLRSKIQ	210	active site facing
132	0.78	304	GNVATNTD	311	globular
132	0.78	335	MGPTELLI	342	globular
129	0.75	316	CGLPGEYW	323	globular
127	0.76	89	APDAGGCL	96	no docking models near
127	0.75	317	GLPGEYWL	324	globular
127	0.73	322	YWLGNDKI	329	globular
126	0.73	115	ALLQQERP	122	no docking models near
125	0.73	254	MYLIQPDS	261	globular
125	0.73	414	GWLTSDPR	421	globular
124	0.76	20	LLLLCVFL	27	not in crystal structure
124	0.77	116	LLQQERPI	123	no docking models near
123	0.71	100	PDLGVLCP	107	no docking models near

Supp Table 2

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
166	0.98	426	HHLGGAKQ	433	not in crystal structure
160	0.92	222	KRLDGSVD	229	globular
156	0.89	64	KDLQSLED	71	allosteric
156	0.91	274	VELEDWNG	281	globular
154	0.90	90	IQLTYNPD	97	active site facing
153	0.91	445	DSLYPEDD	452	not in crystal structure
150	0.89	305	AYFAGGDA	312	globular
148	0.84	114	KMLEEIMK	121	active site facing
147	0.86	67	QSLEDILH	74	allosteric
147	0.85	155	AQLEAQCQ	162	active site facing
143	0.83	416	NRLTIGEG	423	globular
141	0.82	134	RYLQEIYN	141	active site facing
139	0.80	35	CILDERFG	42	not in crystal structure
137	0.83	438	HPAETEYD	445	not in crystal structure
136	0.83	244	LSPTGTTE	251	globular
135	0.80	148	VNLKEKVA	155	no docking models near
135	0.80	293	VGPEADKY	300	globular
134	0.82	317	DGFDFGDD	324	globular
132	0.78	26	AYVATRDN	33	not in crystal structure
130	0.78	18	LFLSSTCV	25	not in crystal structure
128	0.75	3	WSLHPRNL	10	not in crystal structure
127	0.77	272	LRVELEDW	279	globular
125	0.73	368	GHLNGVYY	375	globular

Supp Table 3

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
1006	0.95	498	GTLSGIGT	505	not in crystal structure
962	0.90	667	TSLGGWLL	674	not in crystal structure
944	0.89	377	SSVSGSTG	384	not in crystal structure
941	0.88	432	KLVTSKGD	439	not in crystal structure
921	0.88	765	ALIEGSVE	772	not in crystal structure
914	0.86	742	FRVGSEAE	749	not in crystal structure
909	0.86	239	SQLQKVPP	246	not in crystal structure
897	0.84	694	RGFGSLND	701	not in crystal structure
888	0.83	26	DFLAEGGG	33	not in crystal structure
887	0.83	495	MDLGTLSG	502	not in crystal structure
878	0.83	481	EVVTSEDG	488	not in crystal structure
878	0.82	634	DVLQTHPS	641	not in crystal structure
877	0.83	447	EKVTSGST	454	not in crystal structure
863	0.82	111	EILRGDFS	118	active site facing
852	0.80	8	CLVLSVVG	15	not in crystal structure
852	0.81	32	GGVRGPRV	39	not in crystal structure
846	0.80	326	SGPGSTGS	333	not in crystal structure
844	0.80	313	SGTGGTAT	320	not in crystal structure
837	0.80	769	GSVEEGAE	776	not in crystal structure
834	0.78	715	HLLTQRGS	722	not in crystal structure
832	0.79	756	SSYEGTAG	763	not in crystal structure
830	0.78	467	KTVIGPDG	474	not in crystal structure
829	0.78	259	MELERPGG	266	not in crystal structure
829	0.79	297	SGSSGPGS	304	not in crystal structure
828	0.79	414	EEVSGNVS	421	not in crystal structure
828	0.78	535	PMLGEFVS	542	not in crystal structure
823	0.78	697	GSLNDEGE	704	not in crystal structure
820	0.77	347	QNPGSPRP	354	not in crystal structure
816	0.77	501	SGIGTLDG	508	not in crystal structure
816	0.78	545	ESRGSESG	552	not in crystal structure
815	0.76	295	WNSGSSGP	302	not in crystal structure
806	0.76	323	PGSSGPGS	330	not in crystal structure
805	0.76	12	SVVGTAWT	19	not in crystal structure
805	0.75	186	RALAREVD	193	no docking models near
805	0.76	300	SGPGSTGN	307	not in crystal structure
804	0.76	9	LVLSVVGT	16	not in crystal structure
803	0.76	650	IKLPGSSK	657	not in crystal structure
803	0.76	815	ANLNGIYY	822	not in crystal structure
800	0.76	753	LQVSSYEG	760	not in crystal structure
794	0.75	504	GTLDGFRH	511	not in crystal structure
791	0.75	339	SGTGSTGN	346	not in crystal structure
789	0.75	132	EDLRSRIE	139	active site facing
789	0.74	321	WKPGSSGP	328	not in crystal structure

Supp Table 4

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
936	0.89	115	ALLQQERP	122	no docking models near
894	0.85	94	GCLHADPD	101	no docking models near
894	0.85	414	GWLTSDPR	421	globular
885	0.83	57	PSLRPAPP	64	not in crystal structure
862	0.81	26	FLVKSQGV	33	not in crystal structure
842	0.79	210	QKLESDVS	217	no docking models near
840	0.79	100	PDLGVLCP	107	no docking models near
839	0.80	185	ETVNSNIP	192	active site facing
823	0.78	330	SQLTRMGP	337	globular
822	0.78	339	ELLIEMED	346	globular
815	0.78	38	EGFFSARG	45	not in crystal structure
813	0.76	196	RVLRSILE	203	active site facing
802	0.77	58	SLRPAPPP	65	not in crystal structure
795	0.76	203	ENLRSKIQ	210	no docking models near
789	0.74	64	PPISGGGY	71	not in crystal structure
782	0.74	233	IPVVSGKE	240	globular
782	0.74	301	QGFGNVAT	308	globular
782	0.74	388	SQLMGENR	395	globular
776	0.74	135	EAVSQTSS	142	active site facing
776	0.73	381	NALMDGAS	388	globular
764	0.71	110	CQLQEALL	117	no docking models near
750	0.71	200	SILENLRS	207	active site facing
745	0.71	214	SDVSAQME	221	no docking models near
744	0.70	316	CGLPGEYW	323	globular
742	0.70	234	PVVSGKEC	241	globular
739	0.70	102	LGVLCPTG	109	no docking models near

Supp Table 5

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
989	0.92	426	HHLGGAKQ	433	not in crystal structure
915	0.87	239	EGFGHLSP	246	globular
894	0.83	64	KDLQSLED	71	no docking models near
877	0.83	16	ALLFLSST	23	not in crystal structure
861	0.81	18	LFLSSTCV	25	not in crystal structure
861	0.80	222	KRLDGSVD	229	globular
840	0.80	125	SILTHDSS	132	active site facing
828	0.78	259	IHLISTQS	266	globular
827	0.78	39	ERFGSYCP	46	not in crystal structure
804	0.76	305	AYFAGGDA	312	globular
803	0.76	155	AQLEAQCQ	162	allosteric facing
801	0.75	90	IQLTYNPD	97	active site facing
792	0.75	209	EIDGSGNG	216	globular
786	0.75	190	SGLYFIKP	197	globular
785	0.75	242	GHLSPTGT	249	globular
785	0.75	368	GHLNGVYY	375	globular
770	0.72	306	YFAGGDAG	313	globular
769	0.73	17	LLFLSSTC	24	not in crystal structure
766	0.72	262	ISTQSAIP	269	globular
759	0.71	416	NRLTIGEG	423	globular
758	0.71	291	FKVGPEAD	298	globular
748	0.70	53	DFLSTYQT	60	allosteric facing
748	0.71	108	ATLKSRKM	115	active site facing

Supp Table 6

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
735	0.99	26	DFLAEGGG	33	not in crystal structure
696	0.94	498	GTLSGIGT	505	not in crystal structure
685	0.93	377	SSVSGSTG	384	not in crystal structure
682	0.93	481	EVVTSEDG	488	not in crystal structure
674	0.91	769	GSVEEGAE	776	not in crystal structure
665	0.89	742	FRVGSEAE	749	not in crystal structure
642	0.87	239	SQLQKVPP	246	not in crystal structure
638	0.86	259	MELERPGG	266	not in crystal structure
637	0.85	432	KLVTSKGD	439	not in crystal structure
636	0.86	634	DVLQTHPS	641	not in crystal structure
636	0.86	726	VELEDWAG	733	not in crystal structure
627	0.85	447	EKVTSGST	454	not in crystal structure
624	0.84	495	MDLGTLSG	502	not in crystal structure
621	0.84	697	GSLNDEGE	704	not in crystal structure
621	0.83	715	HLLTQRGS	722	not in crystal structure
618	0.83	667	TSLGGWLL	674	not in crystal structure
607	0.82	9	LVLSVVGT	16	not in crystal structure
597	0.81	753	LQVSSYEG	760	not in crystal structure
596	0.80	535	PMLGEFVS	542	not in crystal structure
595	0.81	414	EEVSGNVS	421	not in crystal structure
595	0.80	764	DALIEGSV	771	not in crystal structure
592	0.81	111	EILRGDFS	118	active site facing
591	0.79	249	KALTDMPQ	256	not in crystal structure
590	0.80	12	SVVGTAWT	19	not in crystal structure
588	0.79	296	NSGSSGPG	303	not in crystal structure
588	0.80	765	ALIEGSVE	772	not in crystal structure
583	0.78	8	CLVLSVVG	15	not in crystal structure
581	0.79	800	AEVYGGGW	807	not in crystal structure
579	0.79	365	SERGSAGH	372	not in crystal structure
578	0.79	539	EFVSETES	546	not in crystal structure
576	0.78	132	EDLRSRIE	139	active site facing
572	0.77	211	DLLPSRDR	218	no docking models near
572	0.76	467	KTVIGPDG	474	not in crystal structure
567	0.76	751	YALQVSSY	758	not in crystal structure
567	0.77	756	SSYEGTAG	763	not in crystal structure
565	0.77	326	SGPGSTGS	333	not in crystal structure
565	0.76	605	DEAGSEAD	612	not in crystal structure
564	0.77	313	SGTGGTAT	320	not in crystal structure
560	0.76	815	ANLNGIYY	822	not in crystal structure
559	0.75	322	KPGSSGPG	329	not in crystal structure
556	0.76	339	SGTGSTGN	346	not in crystal structure
555	0.74	186	RALAREVD	193	no docking models near
553	0.75	545	ESRGSESG	552	not in crystal structure

Supp Table 7

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
652	0.89	115	ALLQQERP	122	no docking models near
646	0.87	94	GCLHADPD	101	no docking models near
644	0.87	414	GWLTSDPR	421	globular
639	0.86	57	PSLRPAPP	64	not in crystal structure
614	0.84	135	EAVSQTSS	142	active site facing
611	0.82	381	NALMDGAS	388	globular
605	0.82	210	QKLESDVS	217	no docking models near
585	0.80	114	EALLQQER	121	no docking models near
579	0.77	110	CQLQEALL	117	no docking models near
578	0.79	339	ELLIEMED	346	globular
577	0.78	330	SQLTRMGP	337	globular
575	0.77	196	RVLRSILE	203	active site facing
573	0.77	100	PDLGVLCP	107	no docking models near
572	0.78	203	ENLRSKIQ	210	active site facing
571	0.78	185	ETVNSNIP	192	active site facing
570	0.77	26	FLVKSQGV	33	not in crystal structure
567	0.77	214	SDVSAQME	221	no docking models near
563	0.76	132	NNVEAVSQ	139	active site facing
563	0.76	233	IPVVSGKE	240	globular
552	0.75	200	SILENLRS	207	active site facing
548	0.74	64	PPISGGGY	71	not in crystal structure
546	0.74	25	VFLVKSQG	32	not in crystal structure
546	0.74	234	PVVSGKEC	241	globular
546	0.74	388	SQLMGENR	395	globular
540	0.73	128	DELNNNVE	135	active site facing
539	0.72	254	MYLIQPDS	261	globular

Supp Table 8

Cumulative Score	Normalized Score	Fibriongen Sequence			Inclusion/Exclusion Rationale
687	0.92	426	HHLGGAKQ	433	not in crystal structure
634	0.86	18	LFLSSTCV	25	not in crystal structure
632	0.86	155	AQLEAQCQ	162	active site facing
630	0.84	64	KDLQSLED	71	no binding
604	0.81	90	IQLTYNPD	97	no docking models near
595	0.80	416	NRLTIGEG	423	globular
593	0.80	274	VELEDWNG	281	globular
589	0.80	209	EIDGSGNG	216	globular
584	0.79	125	SILTHDSS	132	active site facing
581	0.79	16	ALLFLSST	23	not in crystal structure
580	0.77	222	KRLDGSVD	229	globular
579	0.78	242	GHLSPTGT	249	globular
570	0.77	259	IHLISTQS	266	globular
561	0.76	305	AYFAGGDA	312	globular
550	0.74	67	QSLEDILH	74	no docking models near
537	0.73	53	DFLSTYQT	60	active site facing
536	0.72	71	DILHQVEN	78	no docking models near
536	0.72	291	FKVGPEAD	298	globular
535	0.73	368	GHLNGVYY	375	globular
532	0.71	35	CILDERFG	42	not in crystal structure
531	0.71	196	KPLKANQQ	203	globular
529	0.72	445	DSLYPEDD	452	not in crystal structure
524	0.70	306	YFAGGDAG	313	globular

Supp Table 9