Human Fibrinogen inhibits amyloid assembly of most Phenol Soluble Modulins (PSM) from *Staphylococcus aureus*

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Supplementary Information

TABLES

Table S1. Deconvolution results from FTIR of PSMs incubated with Fg

Peptide	[Fg] (mg/ml)	Peak position (cm^{-1})	% β-sheet content	% α-helix content
PSMα1	0	1628, 1655	73.6	26.4
PSMα1	0.25	1625, 1651	43.36	56.6
PSMα1	1	1621, 1650	11	89.0
PSMα3 (+Fg)	0-1	1685, 1653	4.4	95.6
PSMβ1	0	1630, 1660	71.1	28.9*
PSMβ1	0.25	1630, 1659	63.6	36.4*
PSMβ1	0.5	1629, 1657	68	32*
PSMβ2	0	1626, 1660	71.2	28.8*
PSMβ2	0.25	1621, 1650	8	92
PSMβ2	1	1619, 1650	2	98

Notes:

* Peak position at 1660 cm^{-1} mainly matches to β-turn

Table S2: *p*-values of multiple regression analysis of the correlation between signal intensity of alanine scans from peptide arrays and the two parameters charge and hydrophobicity

Peptide	Charge	Hydrophobicity
PSMα1	8.4×10^{-5}	0.008
PSMα3	2.9×10^{-5}	5.7×10^{-5}
PSMβ1	1.6×10^{-7}	0.1
PSMβ2	1.6×10^{-7}	0.1

FIGURES

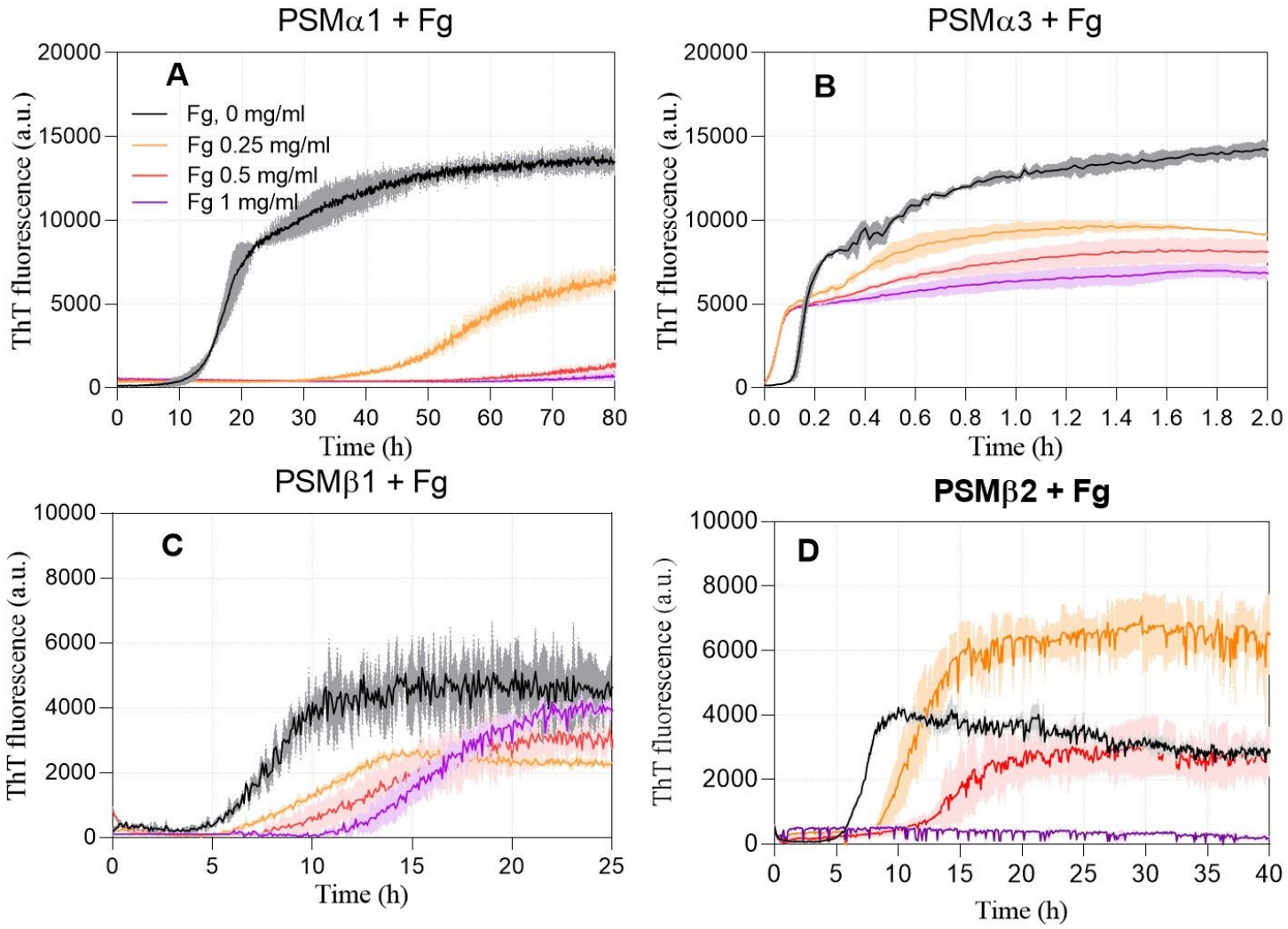

Figure S1. Kinetics of PSM amyloid formation in presence and absence of fibrinogen monitored by ThT fluorescence. A) PSMα1, B) PSMα3, C) PSMβ1 and D) PSMβ2. Colour codes from panel A also apply to panels B-D.

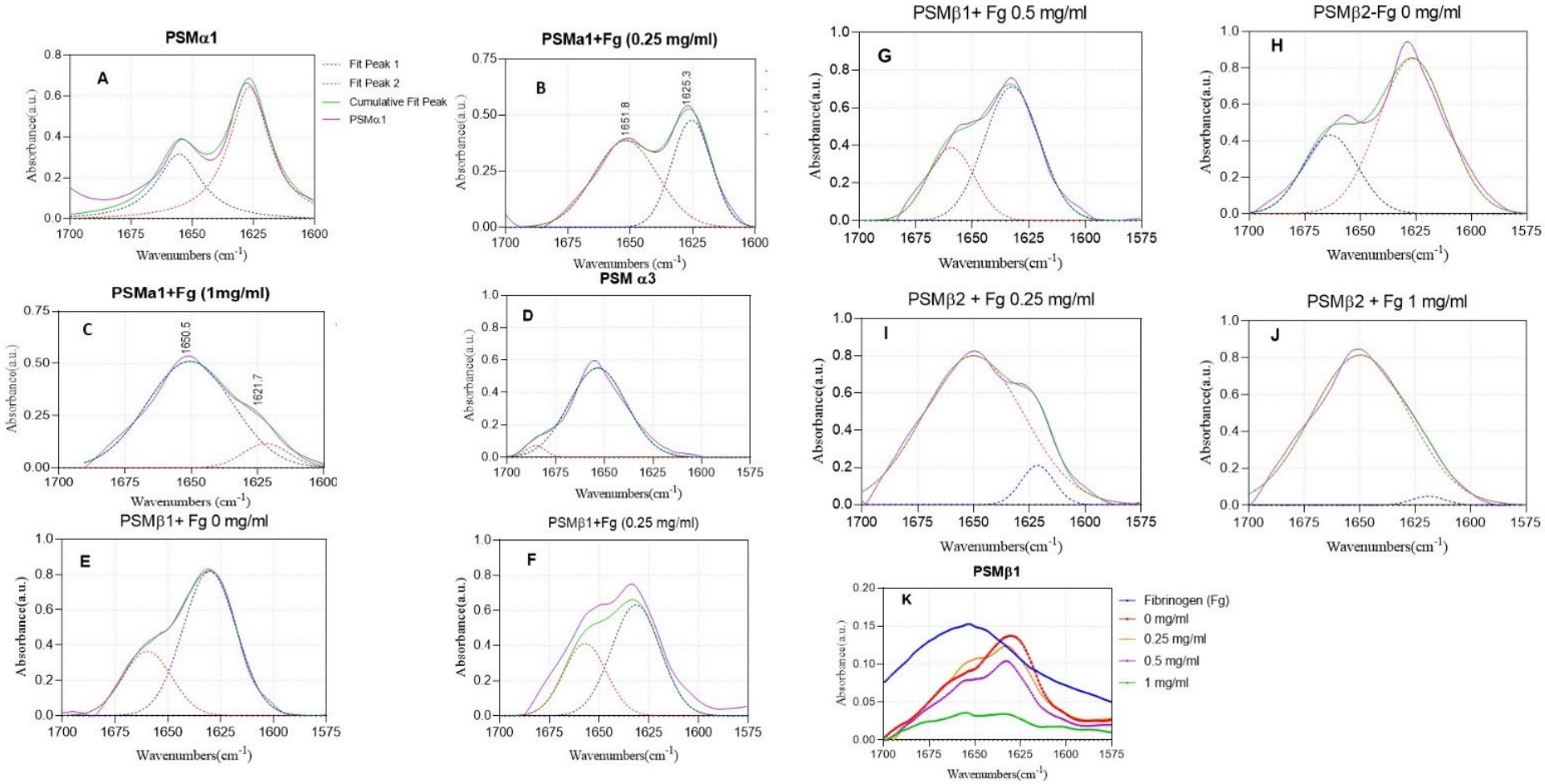

Figure S2. FTIR analysis of the secondary structure of PSMs peptides in presence of different concentrations of fibrinogen. Deconvolution of peaks carried out in Origin. A) PSMα1 (0 mg/ml Fg), B) PSMα1 (0.25 mg/ml Fg), C) PSMα1 (1 mg/ml Fg) (D) PSMα3 (0-1 mg/ml Fg), E) PSMβ1 (0 mg/ml Fg), F) PSMβ1 (0.25 mg/ml Fg), G) PSMβ1 (0.5 mg/ml Fg) H) PSMβ2 (0 mg/ml Fg), I) PSMβ2 (0.25 mg/ml Fg), J) PSMβ2 (1 mg/ml Fg). Colour code from panel A applies to panels B-J. K) FTIR curves of PSMβ1(0.2 mg/ml) in presence of 0-1 mg/ml Fg.

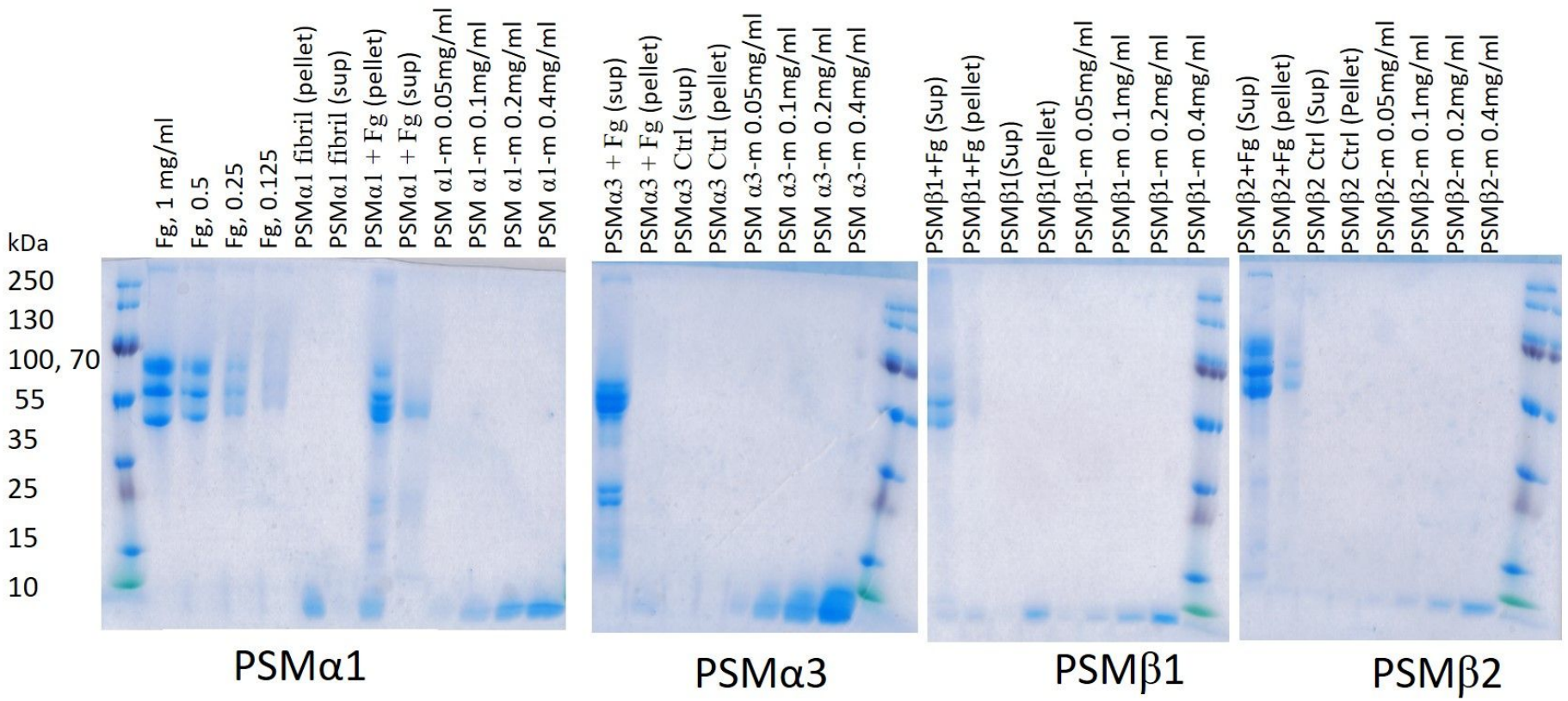

Figure S3. SDS-PAGE of pellet and supernatants of aggregates formed in presence of 1 mg/ml Fg densitometrically quantified using ImageJ.

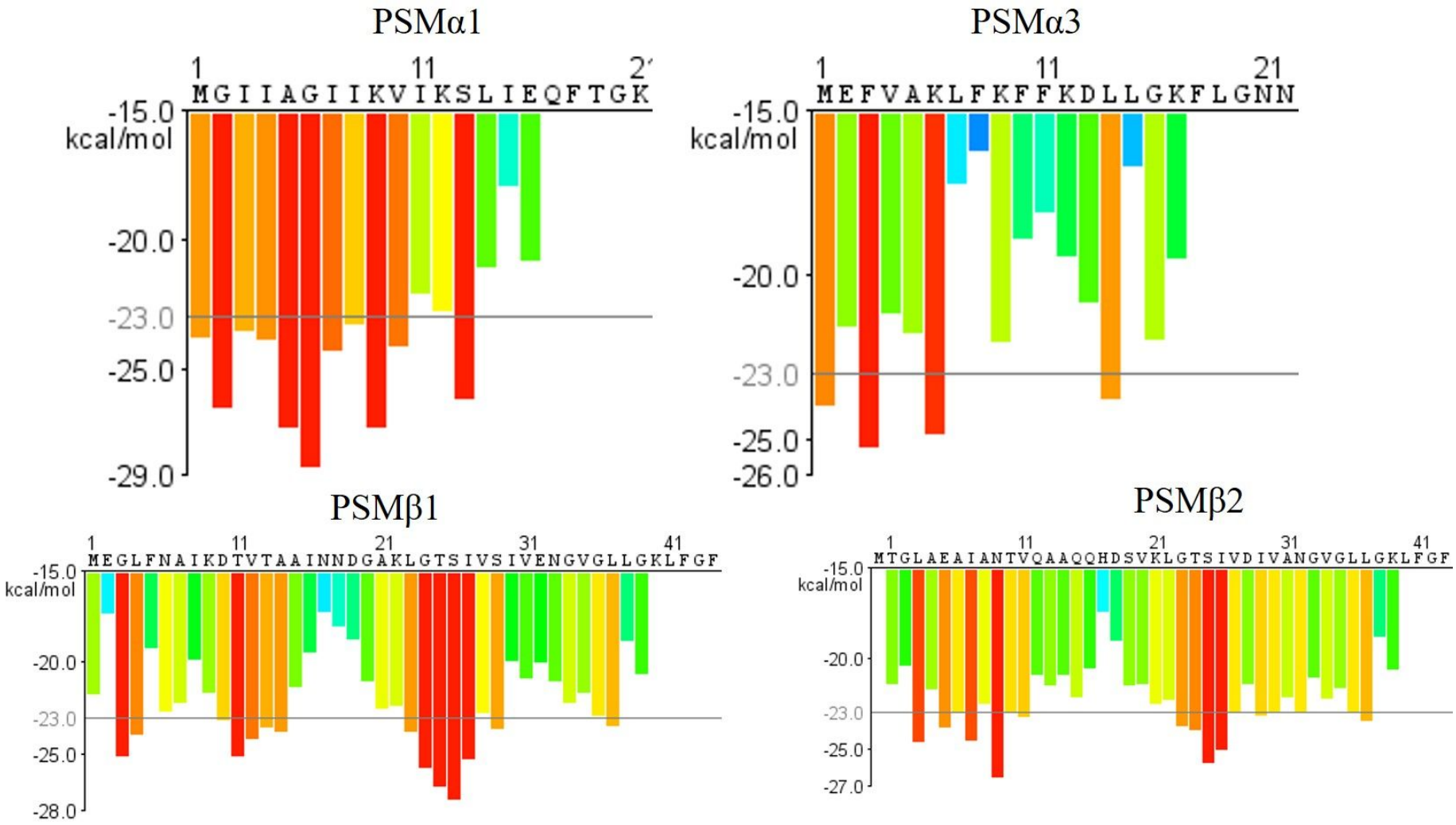

Figure S4. Computational prediction of aggregation propensity of different PSMs based on Rosetta energies that predict amyloid propensity in hexapeptides. Orange – red segments (energies < -23 kcal/mol) predicted to take part in fibril formation through higher aggregation propensity. Letters on x-axis denote the first residue of each hexapeptide.