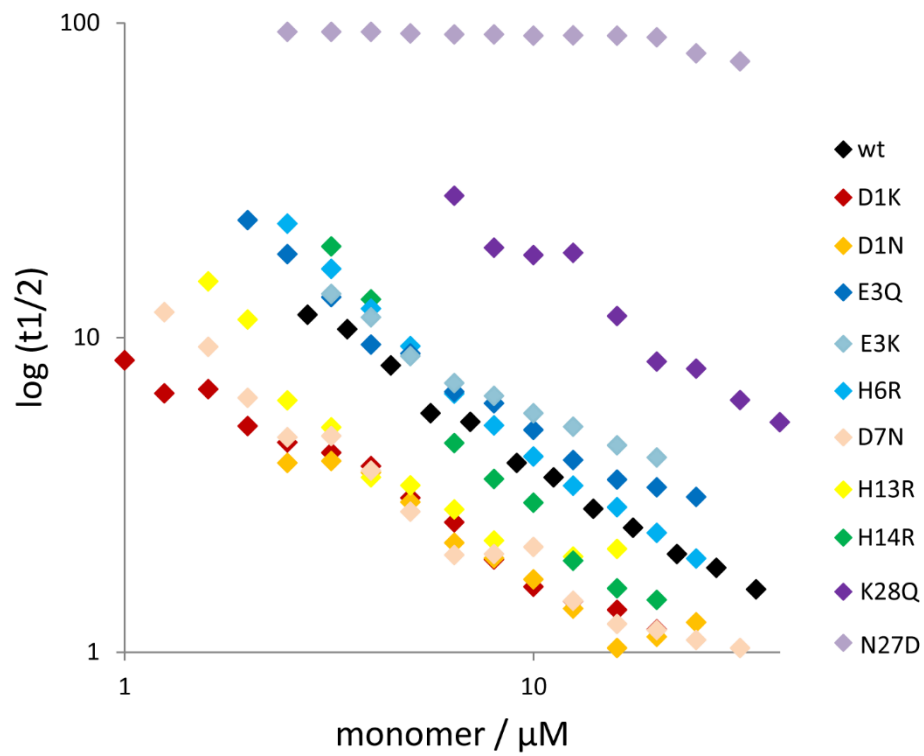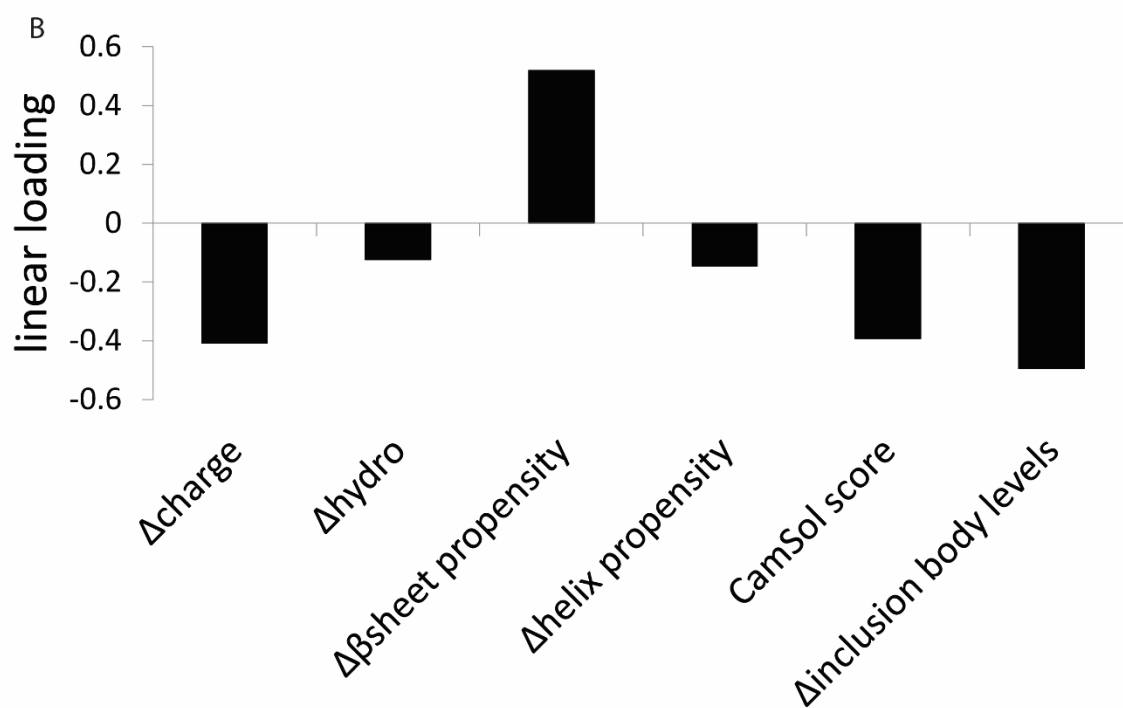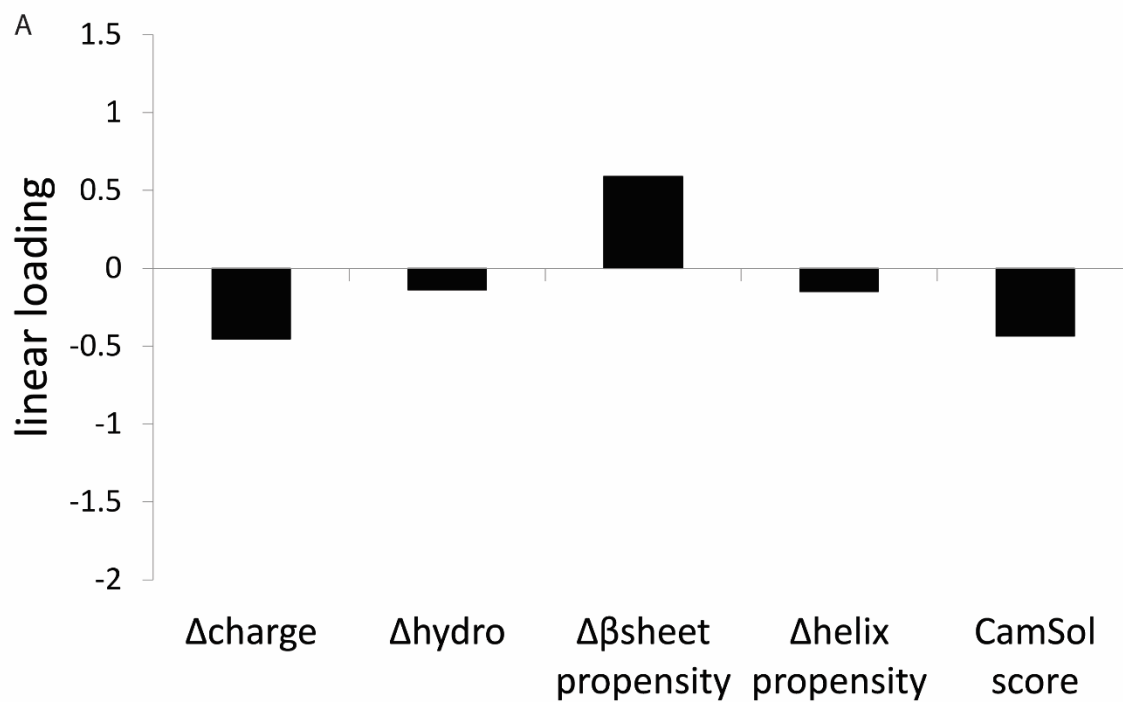# A method of predicting the *in vitro* fibril formation propensity of Aβ40 mutants based on their inclusion body levels in *E. coli*

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Supplementary Figure S1. Plot showing half-time of aggregation versus peptide concentration for Aβ40 wild-type (wt) and different charge variants (D1K, D1N, E3Q, E3K, H6R, D7N, H13R, H14R, K28Q and N27D).
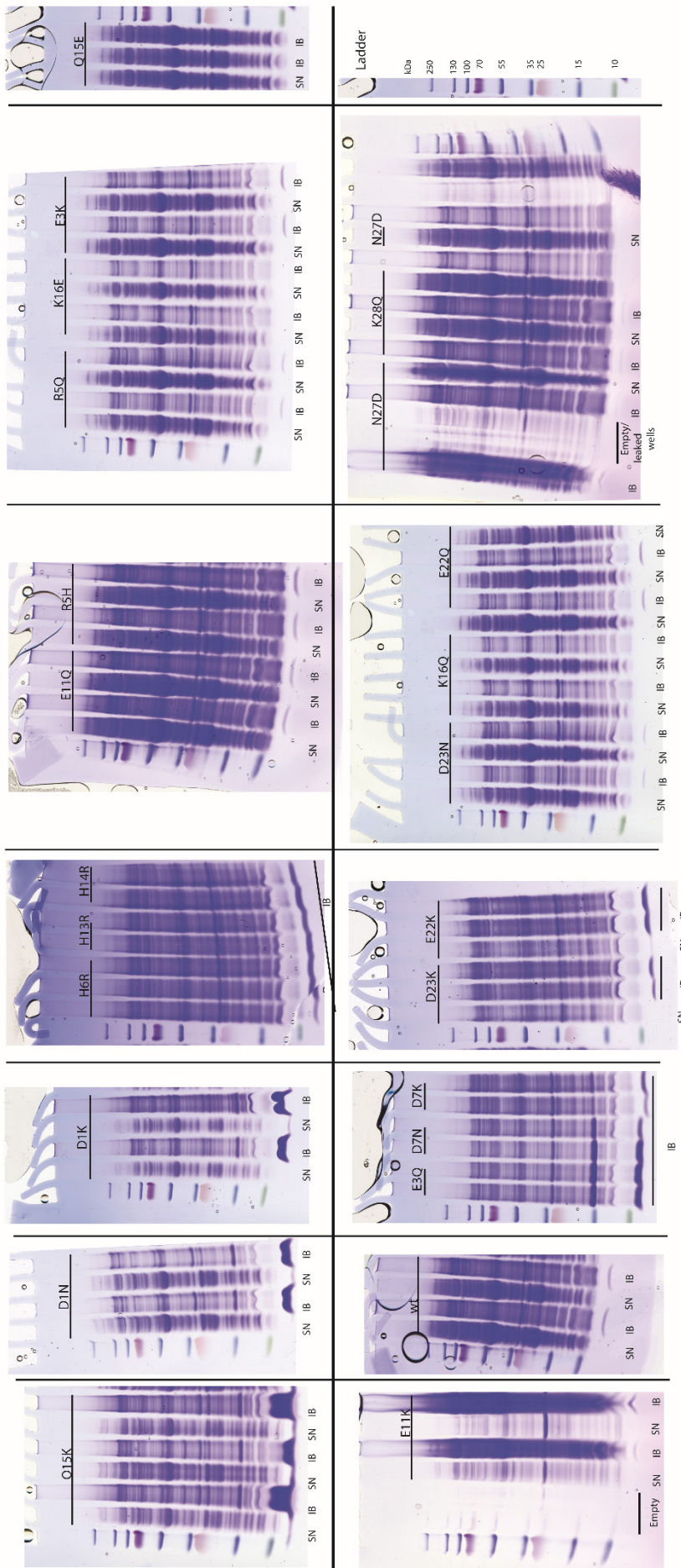
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30 **Supplementary Figure S2.** Parameter loadings for linear components used in A. Figure 8C (without

31 inclusion body levels) and B. 8D (with inclusion body levels).

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Supplementary Figure S3. SDS-PAGE analysis of inclusion body formation of Aβ40 charge mutants. Mutants were expressed on different days and were run on different SDS-PAGE gels. Duplicates of each sample were shown. Wells labelled with the mutation, lines indicate the wells included for each sample. Both supernatant (SN) and inclusion bodies (IB) were analyzed on SDS-PAGE gel. Gel bands shown in Figure 2 were cut from these gels.
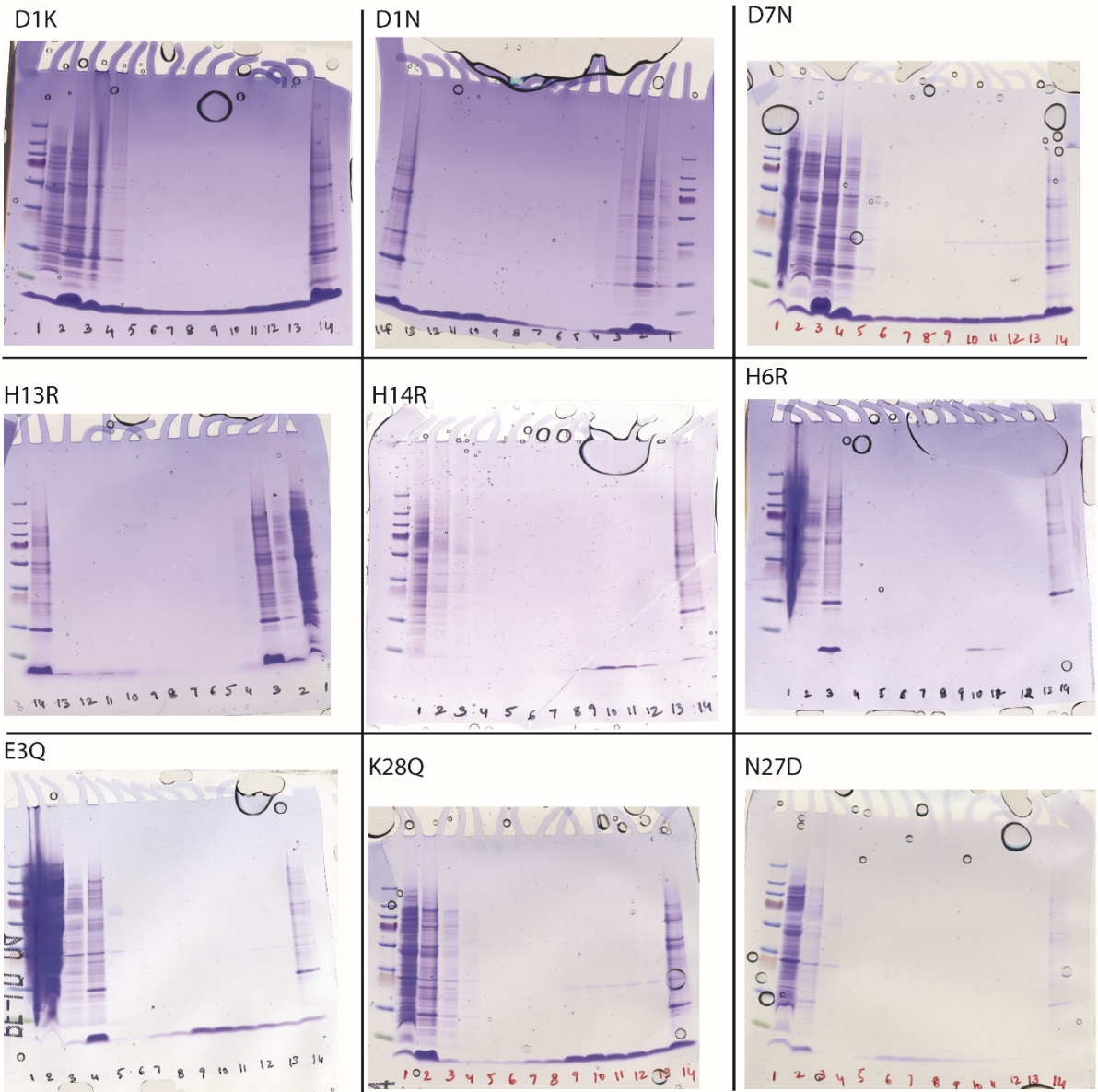
Supplementary Figure S4. Ion exchange chromatography of Aβ40 charge mutants. Uncropped SDS-PAGE gels for Figure 9. The details of samples in different wells is explained in Figure 9.

	Mutant	before	after	Δcharge	before	after	Δhydro	before	after	Δβsheet prop	CamSol score	pI
1	D1N	-3	-2	1	3.81	1.91	-1.9	0.72	0.40	-0.32	0.62	5.5
2	D1K	-3	-1	2	3.81	2.77	-1.04	0.72	0.34	-0.38	0.64	6
3	E3Q	-3	-2	1	2.91	1.30	-1.61	0.35	0.34	-0.01	0.57	5.48
4	E3K	-3	-1	2	2.91	2.77	-0.14	0.35	0.34	-0.01	0.62	5.99
5	R5H	-3	-4	-1	3.95	0.64	-3.31	0.35	0.37	0.02	0.59	5.03
6	R5Q	-3	-4	-1	3.95	1.30	-2.65	0.35	0.34	-0.01	0.60	4.74
7	H6R	-3	-2	1	0.64	3.95	3.31	0.37	0.35	-0.02	0.75	5.21
8	D7N	-3	-2	1	3.81	1.91	-1.9	0.72	0.40	-0.32	0.60	5.5
9	D7K	-3	-1	2	3.81	2.77	-1.04	0.72	0.34	-0.38	0.64	6
10	E11Q	-3	-2	1	2.91	1.30	-1.61	0.35	0.34	-0.01	0.60	5.48
11	E11K	-3	-2	2	2.91	1.30	-1.61	0.35	0.34	-0.01	0.66	5.99
12	H13R	-3	-2	1	0.64	3.95	3.31	0.37	0.35	-0.02	0.74	5.21
13	H14R	-3	-2	1	0.64	3.95	3.31	0.37	0.35	-0.02	0.79	5.21
14	Q15E	-3	-4	-1	1.30	2.91	1.61	0.34	0.35	0.01	0.82	4.83
15	Q15K	-3	-2	1	1.30	2.77	1.47	0.34	0.34	0	0.82	5.51
16	K16Q	-3	-4	-1	2.77	1.30	-1.47	0.34	0.34	0	0.46	4.74
17	K16E	-3	-5	-2	2.77	2.91	0.14	0.34	0.35	0.01	0.75	4.55
18	E22Q	-3	-2	1	2.91	1.30	-1.61	0.35	0.34	-0.01	0.43	5.48
19	E22K	-3	-1	2	2.91	2.77	-0.14	0.35	0.34	-0.01	0.60	5.99

20	D23K	-3	-1	2	3.81	2.77	-1.04	0.72	0.34	-0.38	0.61	6
21	D23N	-3	-2	1	3.81	1.91	-1.9	0.72	0.40	-0.32	0.53	5.5
22	N27D	-3	-4	-1	1.91	3.81	1.9	0.40	0.72	0.32	0.70	4.78
23	K28Q	-3	-4	-1	2.77	1.30	-1.47	0.34	0.34	0	0.59	4.74
24	K28E	-3	-5	-2	2.77	2.91	0.14	0.34	0.35	0.01	0.68	4.55

Supplementary Table S1. Aβ40 charge mutant peptides. Details of variation in charge,

hydrophobicity and β sheet propensity before and after mutation while CamSol score and isoelectric

point (pI) of each mutant calculated based on the sequence using protein pI calculator by Kozlowski

LP, 2016 are included.