Supporting Information

Pathogenic Properties of Alzheimer's β-Amyloid Identified from Structure-Property Patient-Phenotype Correlations

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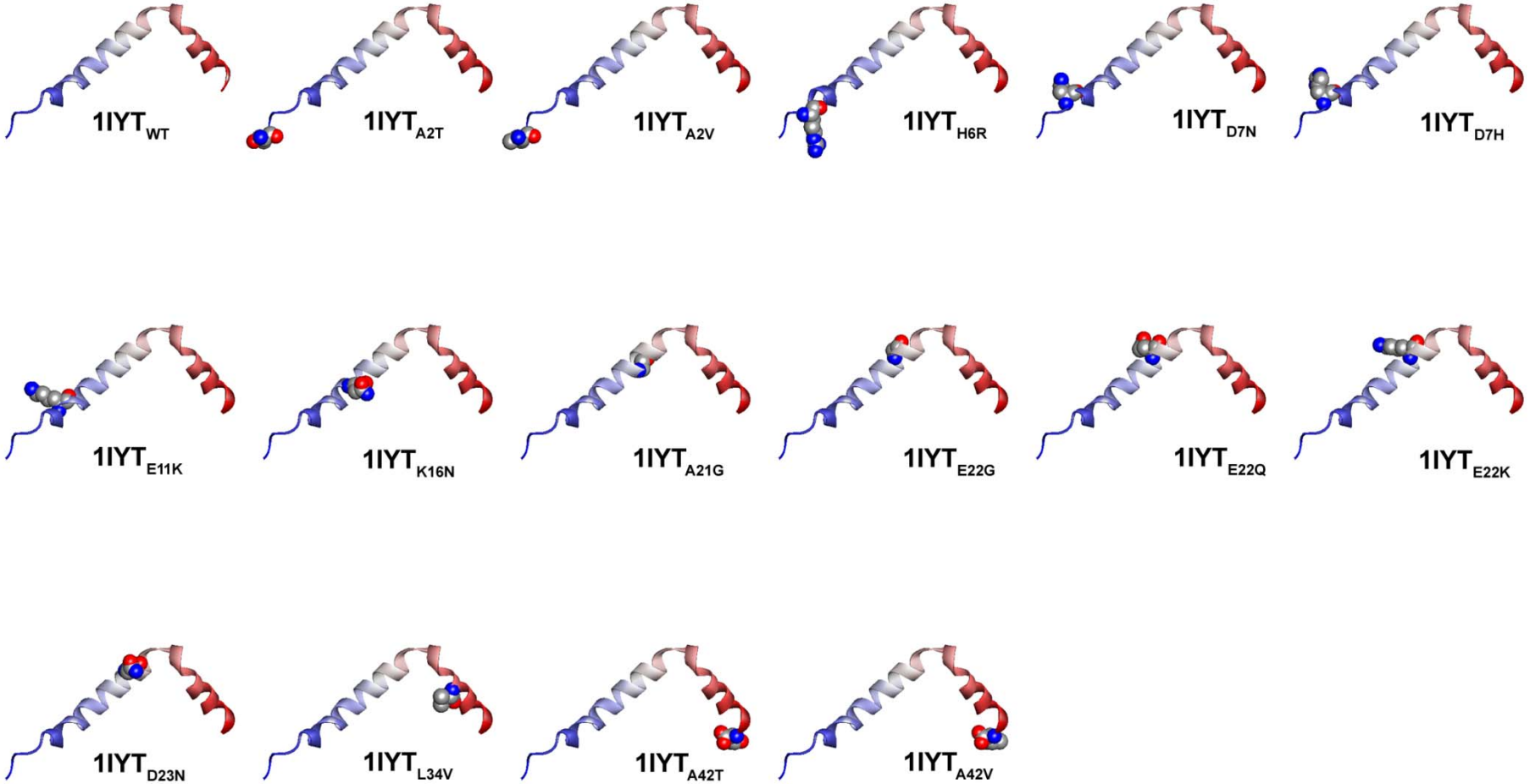

Figure S1. Orthographic view of Aβ$_{42}$ (1IYT) WT and mutant structures. The mutant residues are shown in CPK model and numbering is according to their respective PDB structure. The WT and mutant structures are represented with ribbon structure and are blue at the N-terminus to red at the C-terminus.

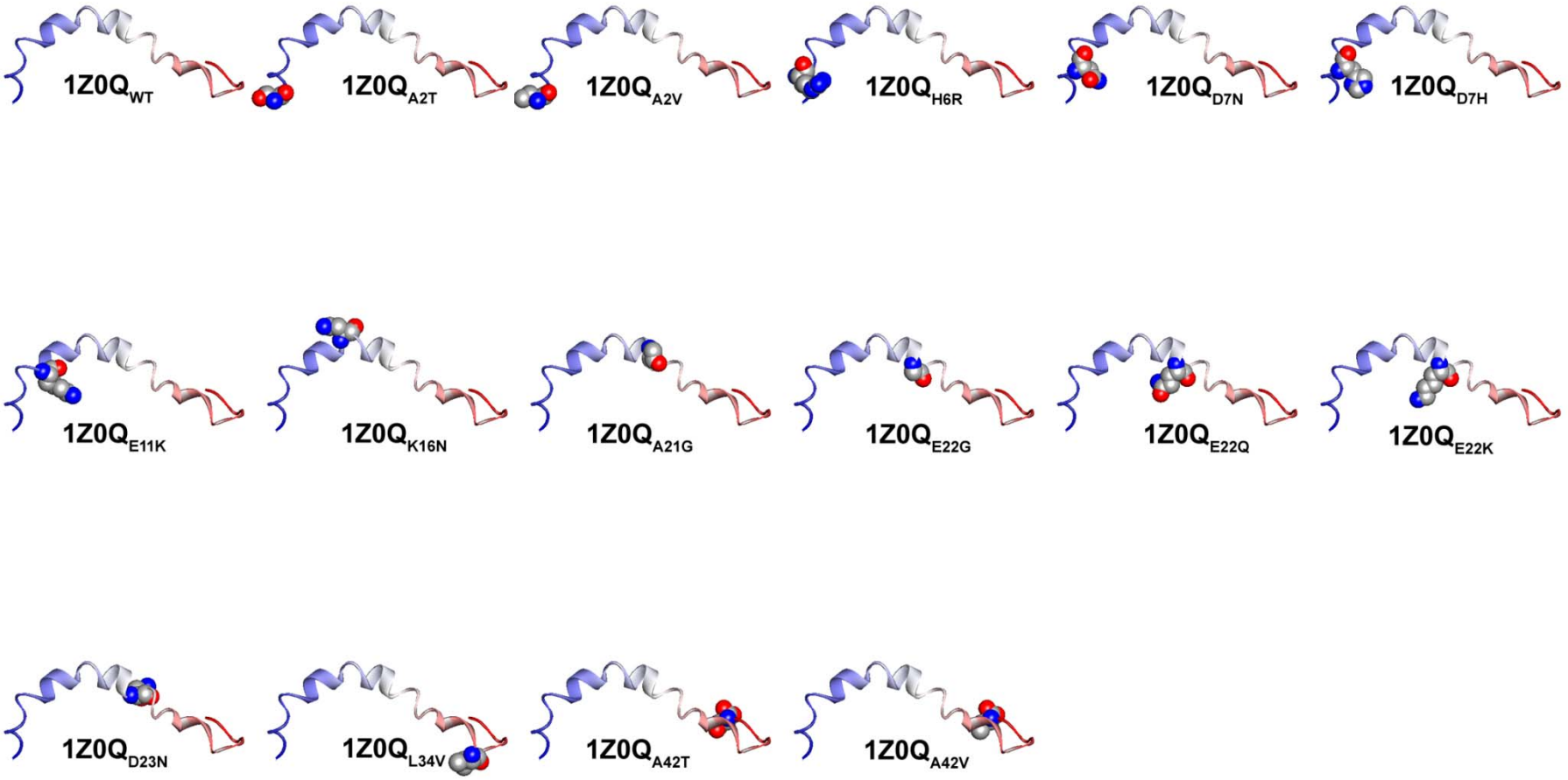

Figure S2. Orthographic view of Aβ$_{42}$ (1Z0Q) WT and mutant structures. The mutant residues are shown in CPK model and numbering is according to their respective PDB structure. The WT and mutant structures are represented with ribbon structure and are blue at the N-terminus to red at the C-terminus.

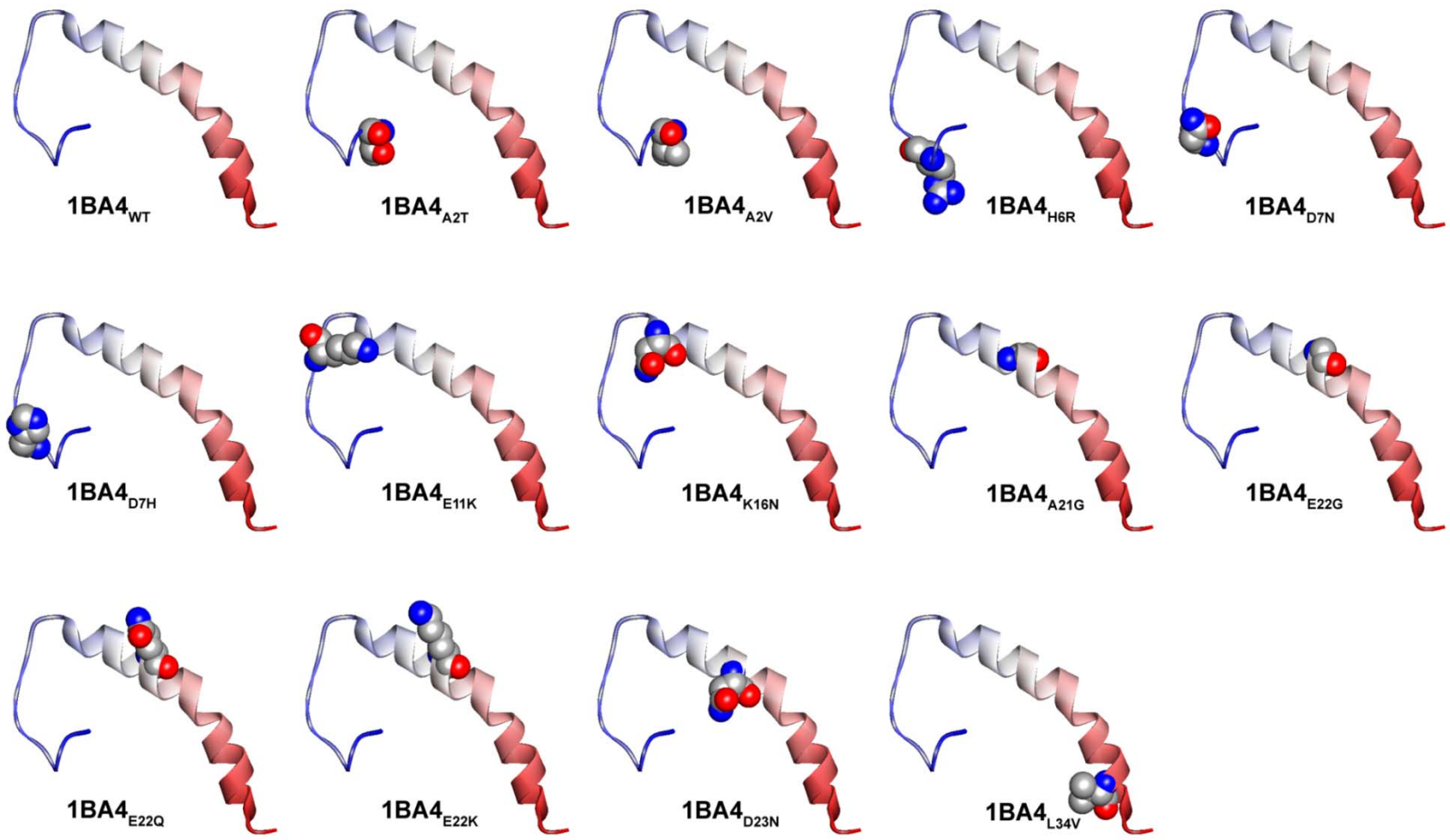

Figure S3. Orthographic view of Aβ$_{40}$ (1BA4) WT and mutant structures. The mutant residues are shown in CPK model and numbering is according to their respective PDB structure. The WT and mutant structures are represented with ribbon structure and are blue at the N-terminus to red at the C-terminus.

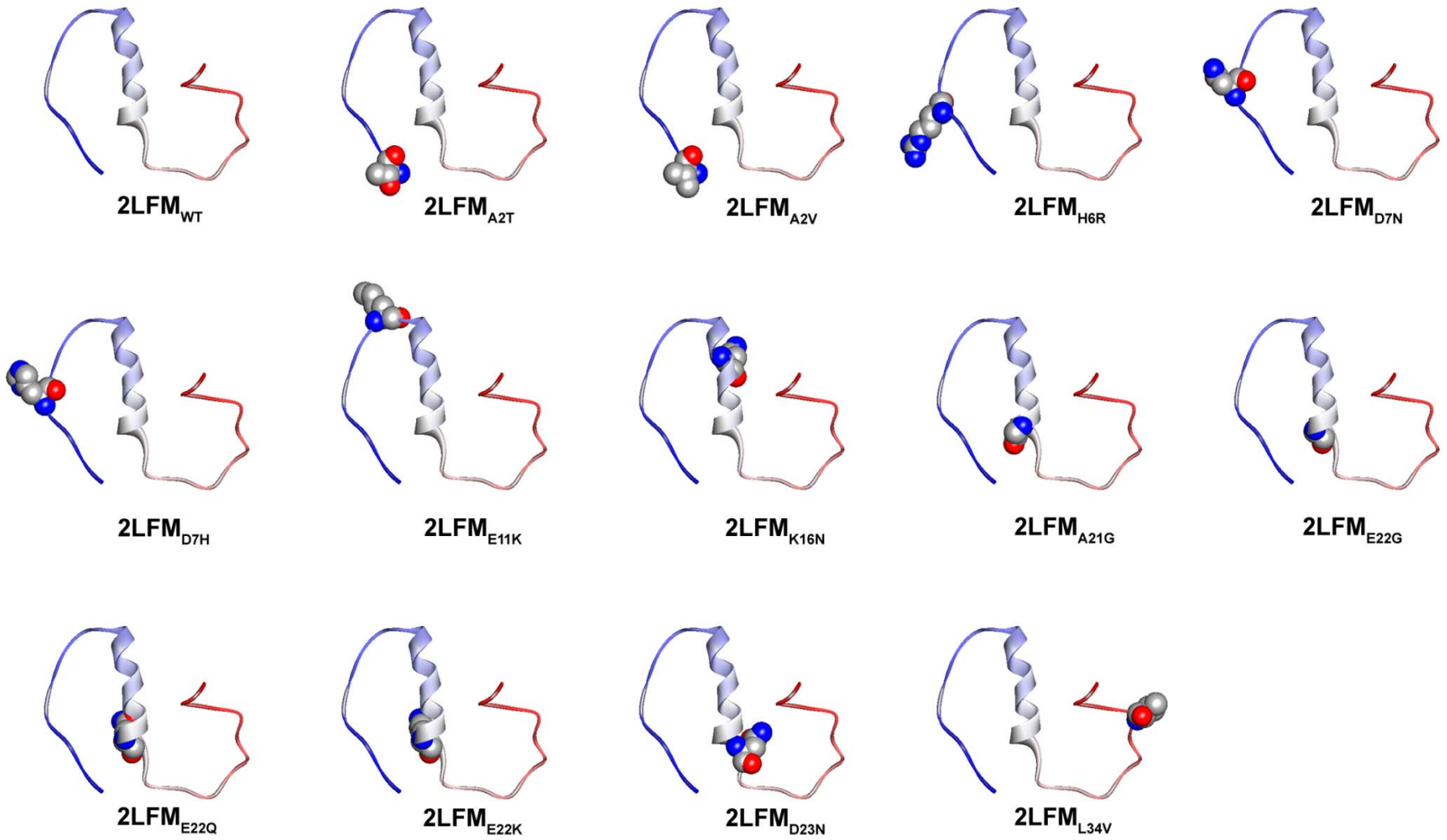

Figure S4. Orthographic view of Aβ$_{40}$ (2LFM) WT and mutant structures. The mutant site residues are shown in CPK model and numbering is according to their respective PDB structure. The WT and mutant structures are represented with ribbon structure and are blue at the N-terminus to red at the C-terminus.

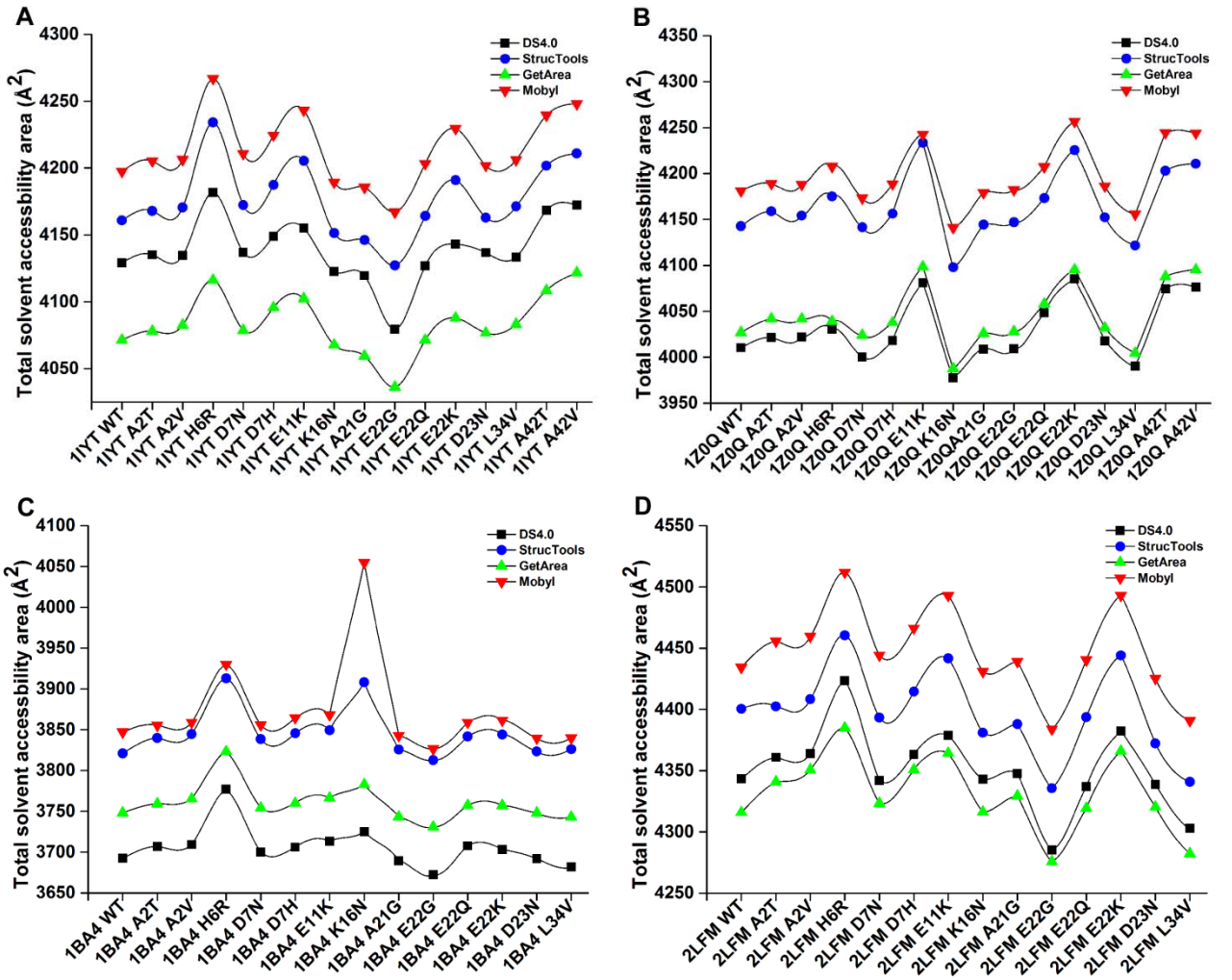

Figure S5. Calculated total solvent accessibility surface of WT and mutant Aβ$_{40}$ and Aβ$_{42}$ structures (method sensitivity) using various methods. (**A**) Total solvent accessibility surface for 1IYT WT and mutants Aβ$_{42}$. (**B**) Total solvent accessibility surface for 1Z0Q WT and mutants Aβ$_{42}$. (**C**) Total solvent accessibility surface for 1BA4 WT and mutants Aβ$_{40}$. (**D**) Total solvent accessibility surface for 2LFM WT and mutants Aβ$_{40}$. Total solvent accessibility surface for all the 60 structures were calculated using DS 4.0 (black square), Get area (green triangle), Struc tools (blue sphere) and Mobyl (red triangle).

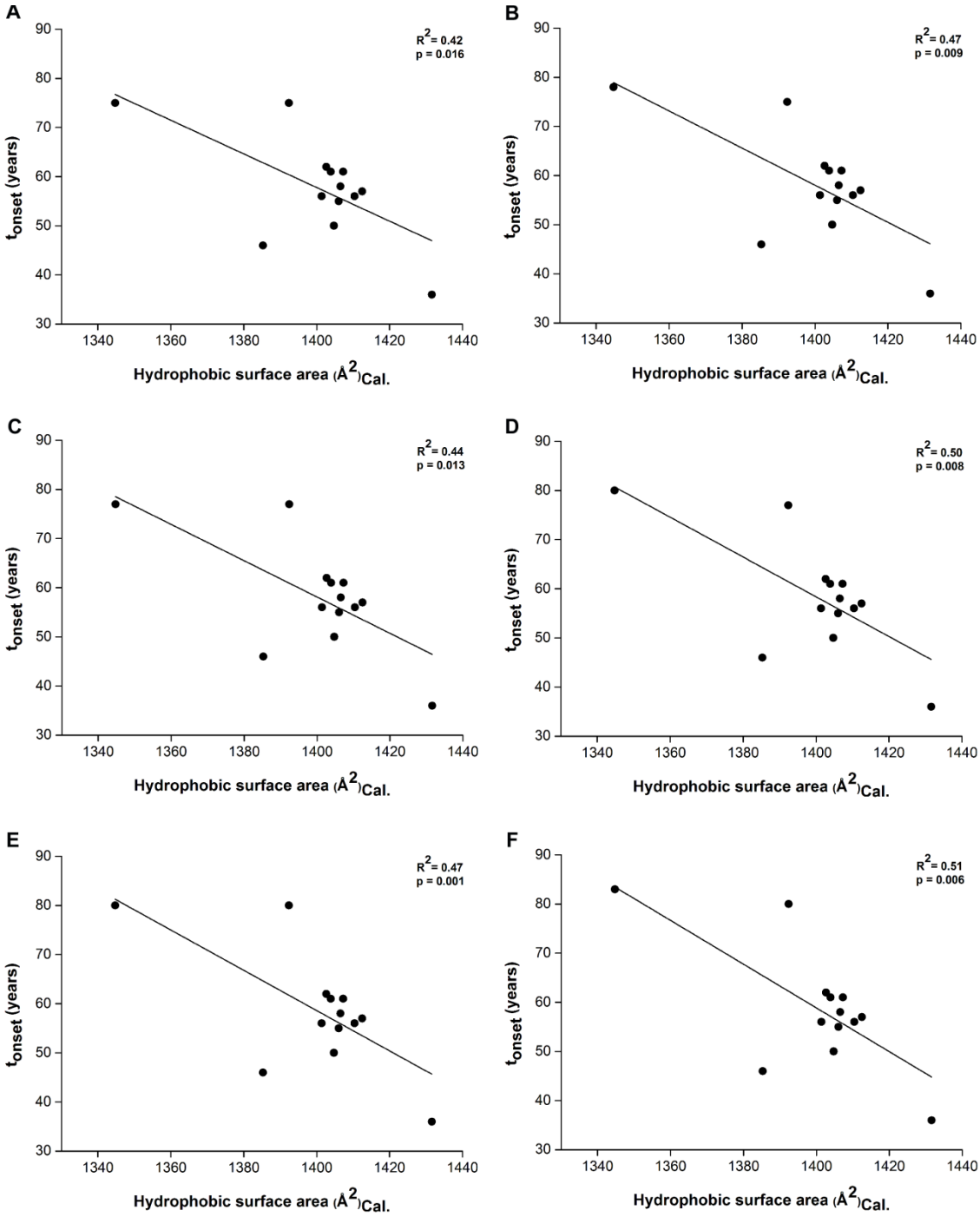

Figure S6 Correlation sensitivity to choice of t_{onset} for Aβ WT and protective A2T variant. The figures show the correlations between t_{onset} and hydrophobic surfaces of 2LFM wild type and mutants. (**A**) t_{onset} = 75 for WT and t_{onset} = 75 for A2T. (**B**) t_{onset} = 75 for WT and t_{onset} = 78 for A2T. (**C**) t_{onset} = 77 for WT and t_{onset} = 77 for A2T. (**D**) t_{onset} = 77 for WT and t_{onset} = 80 for A2T. (**E**) t_{onset} = 80 for WT and t_{onset} = 80 for A2T. (**E**) t_{onset} = 80 for WT and t_{onset} = 83 for A2T.

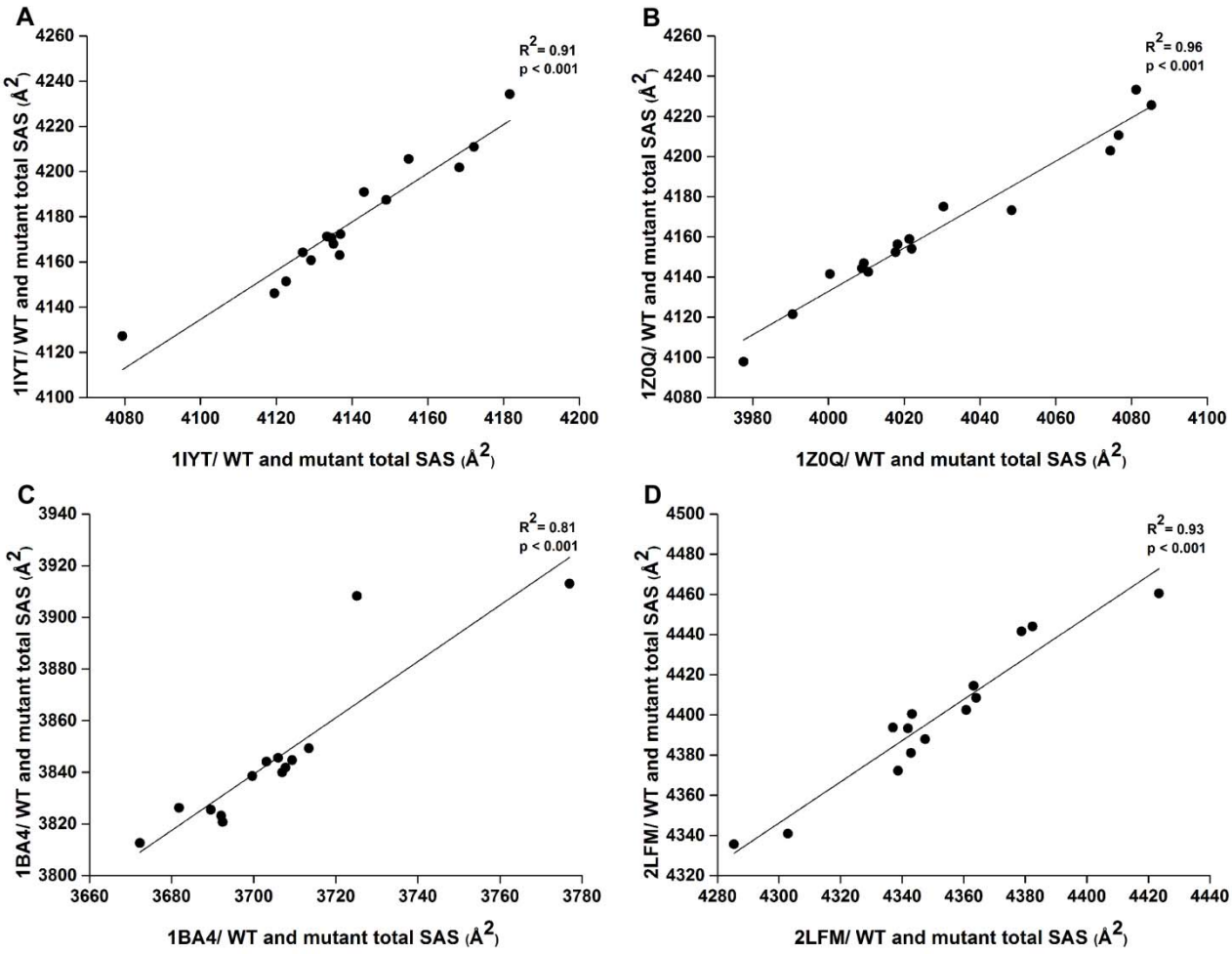

Figure S7. Correlation between calculated total solvent accessibility surface of WT and mutant $A\beta_{40}$ and $A\beta_{42}$ structures (structure and method sensitivity) using DS 4.0 (x-axis) and struc tools (y-axis). (**A**) Total solvent accessibility surface for 1IYT WT and mutants $A\beta_{42}$. (**B**) Total solvent accessibility surface for 1Z0Q WT and mutants $A\beta_{42}$. (**C**) Total solvent accessibility surface for 1BA4 WT and mutants $A\beta_{40}$. (**D**) Total solvent accessibility surface for 2LFM WT and mutants $A\beta_{40}$.

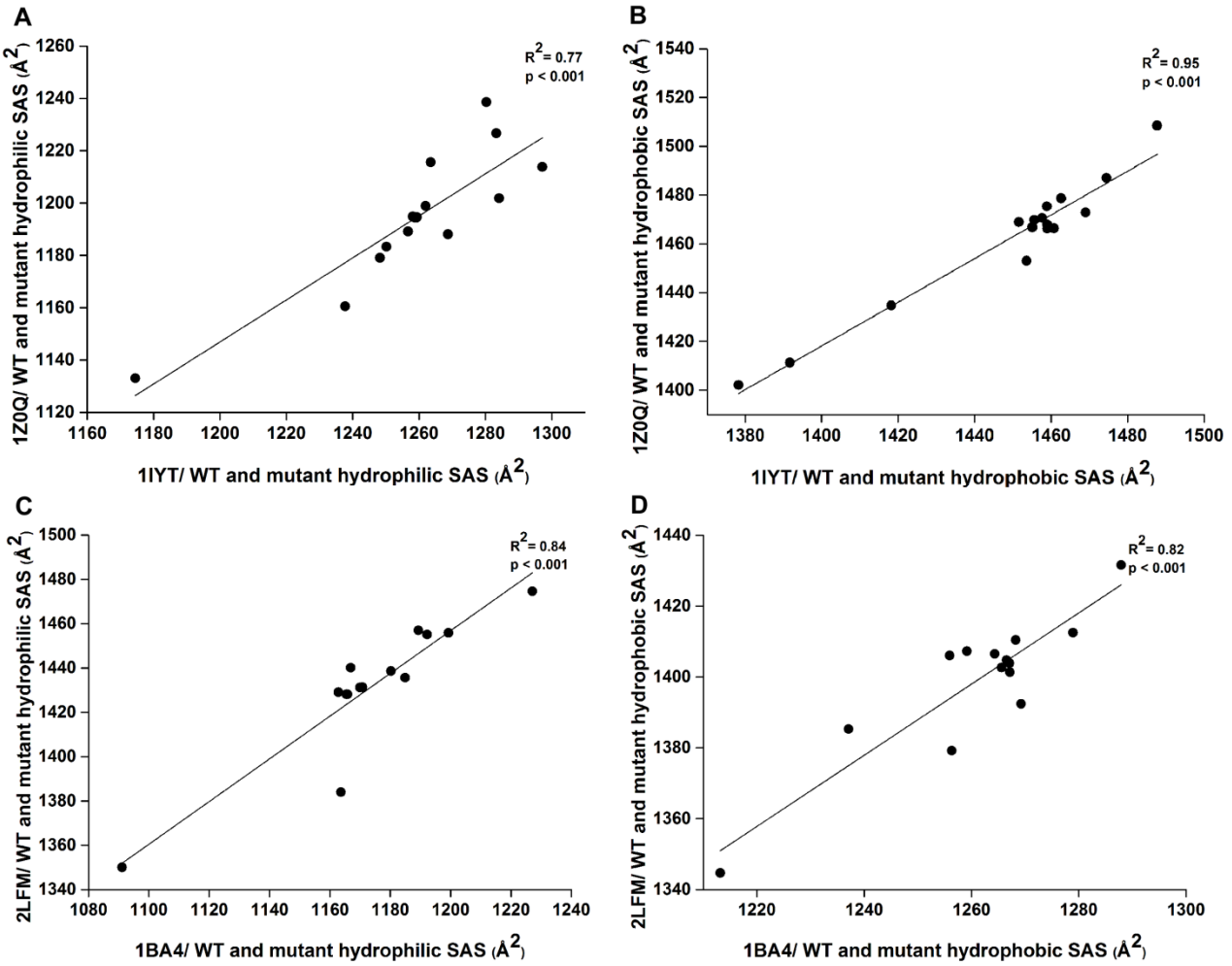

Figure S8. Correlation between calculated hydrophilic, hydrophobic surface of WT and mutant $A\beta_{40}$ and $A\beta_{42}$ structures using DS 4.0. (**A**) Hydrophilic surface for WT and mutants $A\beta_{42}$ (1IYT vs. 1Z0Q). (**B**) Hydrophobic surface for WT and mutants $A\beta_{42}$ (1IYT vs. 1Z0Q). (**C**) Hydrophilic surface for WT and mutants $A\beta_{40}$ (1BA4 vs. 2LFM). (**D**) Hydrophobic surface for WT and mutants $A\beta_{40}$ (1BA4 vs. 2LFM).

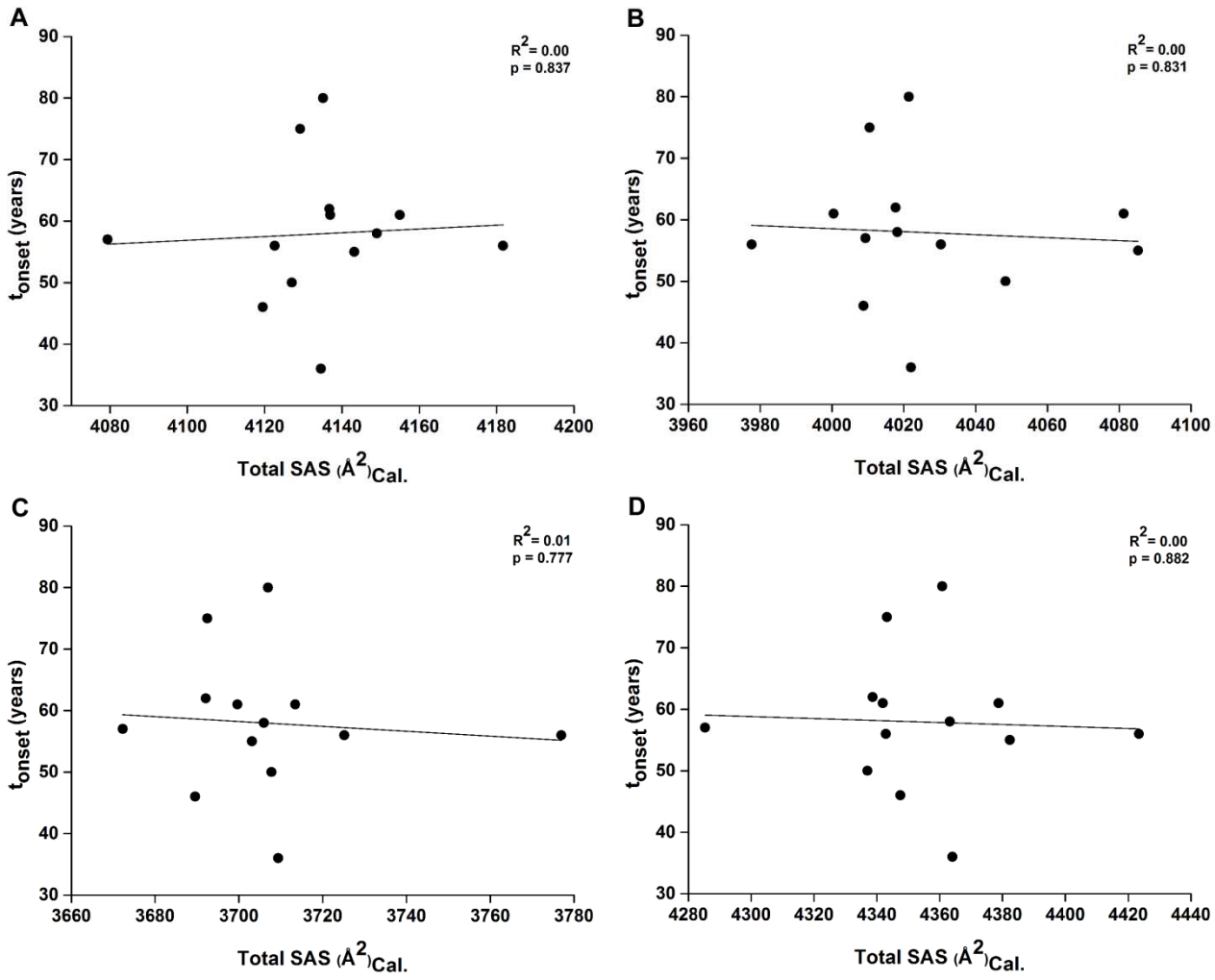

Figure S9. Correlation between t_{onset} and calculated total solvent accessibility surface (SAS) for WT and mutant $A\beta_{40}$ and $A\beta_{42}$. (**A**) vs. total solvent accessibility surface for 1IYT WT and mutants $A\beta_{42}$. (**B**) vs. total solvent accessibility surface for 1Z0Q WT and mutants $A\beta_{42}$. (**C**) vs. total solvent accessibility surface for 1BA4 WT and mutants $A\beta_{40}$. (**D**) vs. total solvent accessibility surface for 2LFM WT and mutants $A\beta_{40}$. Total solvent accessibility surface was calculated using DS 4.0**.**

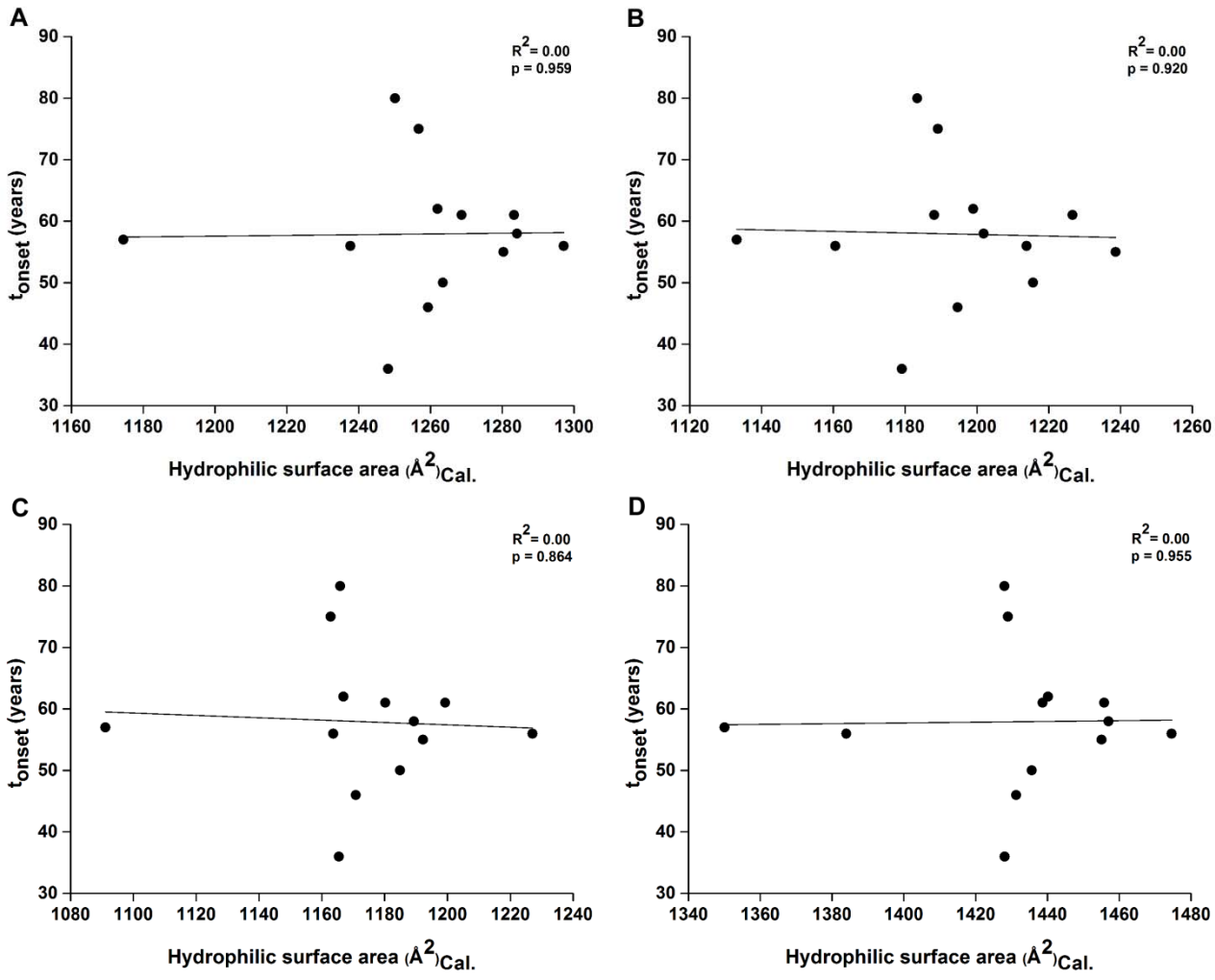

Figure S10. Correlation between t_{onset} and calculated hydrophilic surface for WT and mutant $A\beta_{40}$ and $A\beta_{42}$. (**A**) vs. hydrophilic surface for 1IYT WT and mutants $A\beta_{42}$. (**B**) vs. hydrophilic surface for 1Z0Q WT and mutants $A\beta_{42}$. (**C**) vs. hydrophilic surface for 1BA4 WT and mutants $A\beta_{40}$. (**D**) vs. hydrophilic surface for 2LFM WT and mutants $A\beta_{40}$. Hydrophilic surface was calculated using DS 4.0**.**

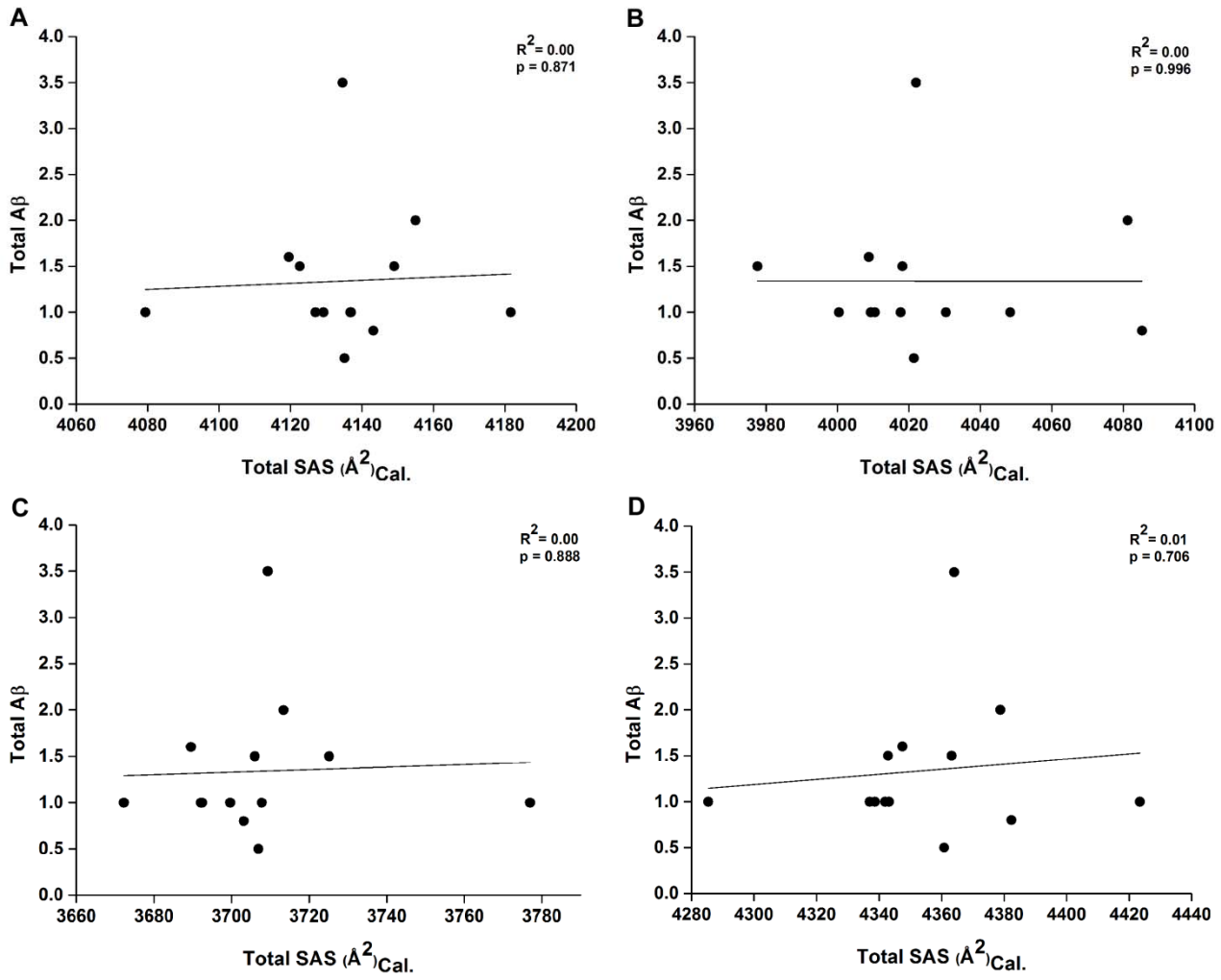

Figure S11. Correlation between total Aβ and calculated total solvent accessibility surface (SAS) for WT and mutant $A\beta_{40}$ and $A\beta_{42}$. (**A**) vs. total solvent accessibility surface for 1IYT WT and mutants $A\beta_{42}$. (**B**) vs. total solvent accessibility surface for 1Z0Q WT and mutants $A\beta_{42}$. (**C**) vs. total solvent accessibility surface for 1BA4 WT and mutants $A\beta_{40}$. (**D**) vs. total solvent accessibility surface for 2LFM WT and mutants $A\beta_{40}$. Total solvent accessibility surface was calculated using DS 4.0**.**

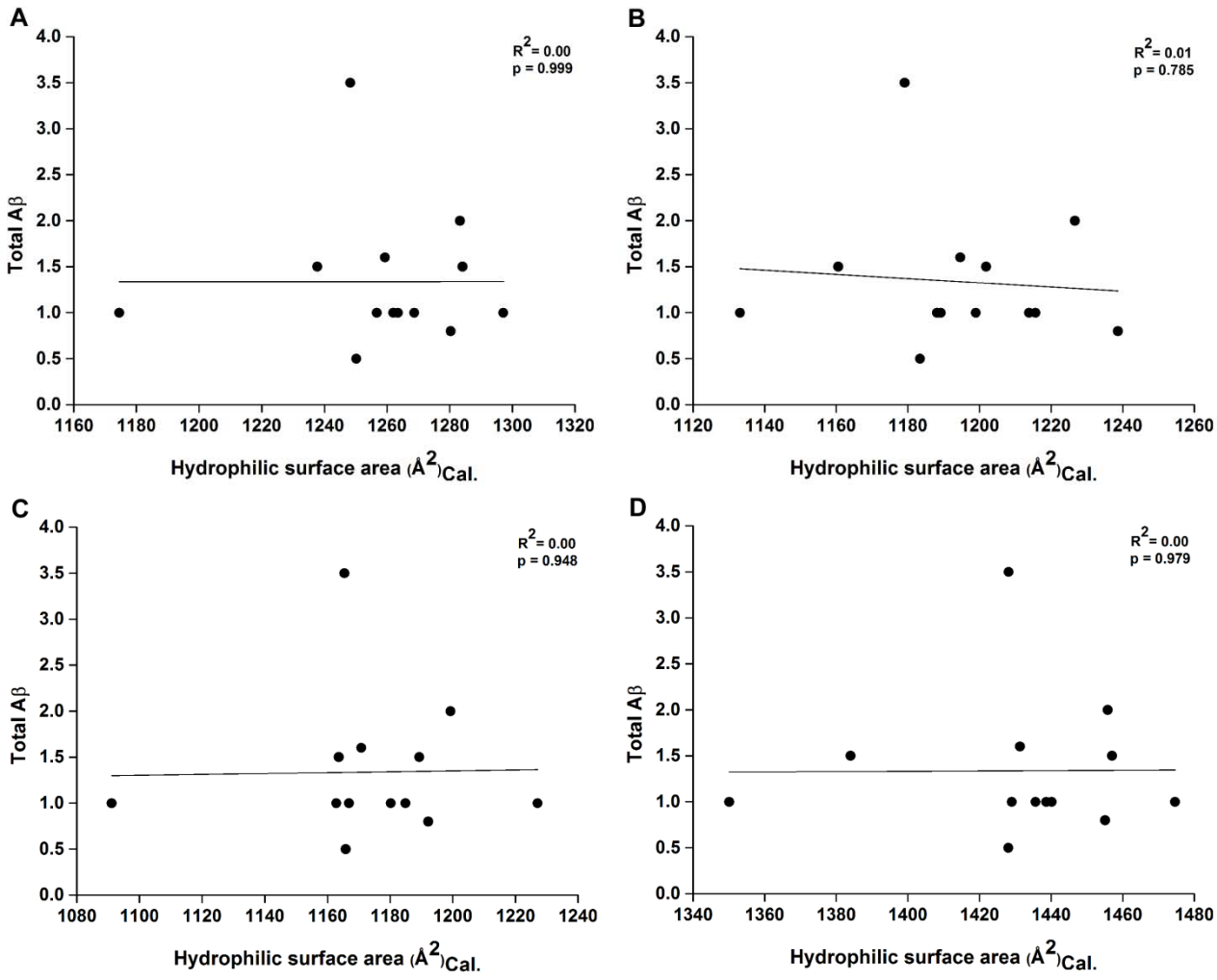

Figure S12. Correlation between total Aβ and calculated hydrophilic surface for WT and mutant $A\beta_{40}$ and $A\beta_{42}$. (**A**) vs. hydrophilic surface for 1IYT WT and mutants $A\beta_{42}$. (**B**) vs. hydrophilic surface for 1Z0Q WT and mutants $A\beta_{42}$. (**C**) vs. hydrophilic surface for 1BA4 WT and mutants $A\beta_{40}$. (**D**) vs. hydrophilic surface for 2LFM WT and mutants $A\beta_{40}$. Hydrophilic surface was calculated using DS 4.0**.**

Supporting Tables

Table S1. Effects of mutations on the total solvent accessibility surface area (Å^2) of Aβ$_{42}$ (1IYT). Total solvent accessibility surface area was calculated using DS 4.0, StrucTools, Get area and Mobyle.

Molecule	Total solvent accessibility (Å^2)			
	DS	StrucTools	Get Area	Mobyle
1IYT$_{wt}$	4129.19	4160.79	4071.28	4197.42
1IYT$_{A2T}$	4135.09	4167.95	4078.08	4205.32
1IYT $_{A2V}$	4134.58	4170.58	4082.61	4206.42
1IYT $_{H6R}$	4181.65	4234.21	4116.23	4266.86
1IYT $_{D7N}$	4136.93	4172.31	4078.75	4210.87
1IYT $_{D7H}$	4149.04	4187.49	4095.7	4224.50
1IYT $_{E11K}$	4154.98	4205.52	4102.44	4243.28
1IYT $_{K16N}$	4122.59	4151.42	4067.67	4189.41
1IYT $_{A21G}$	4119.54	4146.13	4059.51	4185.59
1IYT $_{E22G}$	4079.36	4127.24	4036.23	4167.09
1IYT $_{E22Q}$	4126.99	4164.27	4071.43	4203.34
1IYT $_{E22K}$	4143.16	4190.90	4087.8	4229.56
1IYT $_{D23N}$	4136.75	4162.99	4076.81	4201.8
1IYT $_{L34V}$	4133.40	4171.24	4083.22	4206.25
1IYT $_{A42T}$	4168.32	4201.83	4108.45	4239.44
1IYT $_{A42V}$	4172.19	4210.92	4121.76	4248.04

Table S2. Effects of mutations on total solvent accessibility surface area (Å^2) of Aβ$_{42}$ (1Z0Q). Total solvent accessibility surface area was calculated using DS 4.0, StrucTools, Get area and Mobyle.

Molecule	Total solvent accessibility (Å^2)			
	DS	StrucTools	Get Area	Mobyle
1Z0Q$_{wt}$	4010.51	4142.57	4026.95	4180.90
1Z0Q$_{A2T}$	4021.38	4158.91	4041.94	4189.04
1Z0Q$_{A2V}$	4022.00	4154.07	4041.72	4188.06
1Z0Q$_{H6R}$	4030.34	4175.02	4039.19	4207.52
1Z0Q$_{D7N}$	4000.42	4141.46	4023.99	4173.27
1Z0Q$_{D7H}$	4018.21	4156.24	4037.91	4188.54
1Z0Q$_{E11K}$	4081.21	4233.25	4098.52	4242.52
1Z0Q$_{K16N}$	3977.61	4097.87	3987.69	4141.06
1Z0Q$_{A21G}$	4008.83	4144.39	4026.03	4179.07
1Z0Q$_{E22G}$	4009.33	4146.88	4027.90	4182.22
1Z0Q$_{E22Q}$	4048.38	4173.22	4058.06	4207.14
1Z0Q$_{E22K}$	4085.24	4225.51	4095.27	4256.63
1Z0Q$_{D23N}$	4017.70	4152.34	4032.11	4186.08
1Z0Q$_{L34V}$	3990.54	4121.5	4004.63	4155.71
1Z0Q$_{A42T}$	4074.40	4202.89	4087.72	4244.48
1Z0Q$_{A42V}$	4076.57	4210.61	4095.24	4243.96

Table S3. Effects of mutations on the total solvent accessibility surface area (Å^2) of Aβ$_{40}$ (1BA4). Total solvent accessibility surface area was calculated using DS 4.0, StrucTools, Get area and Mobyle.

Molecule	Total solvent accessibility (Å^2)			
	DS	StrucTools	Get Area	Mobyle
1BA4$_{wt}$	3692.47	3820.8	3748.25	3847.18
1BA4$_{A2T}$	3706.95	3839.97	3759.28	3855.41
1BA4$_{A2V}$	3709.36	3844.71	3765.46	3858.9
1BA4$_{H6R}$	3776.95	3913.00	3823.24	3930.06
1BA4$_{D7N}$	3699.69	3838.54	3754.19	3855.7
1BA4$_{D7H}$	3705.98	3845.59	3759.98	3864.45
1BA4$_{E11K}$	3713.44	3849.29	3766.45	3868.22
1BA4$_{K16N}$	3725.15	3908.25	3782.90	4054.83
1BA4$_{A21G}$	3689.56	3825.55	3743.36	3842.86
1BA4$_{E22G}$	3672.25	3812.63	3730.97	3826.34
1BA4$_{E22Q}$	3707.77	3841.81	3757.27	3858.95
1BA4$_{E22K}$	3703.12	3844.15	3757.18	3861.57
1BA4$_{D23N}$	3692.06	3823.22	3748.23	3839.62
1BA4$_{L34V}$	3681.79	3826.25	3743.01	3839.93

Table S4. Effects of mutations on the total solvent accessibility surface area (Å^2) of Aβ$_{40}$ (2LFM). Total solvent accessibility surface area was calculated using DS 4.0, StrucTools, Get area and Mobyle.

Molecule	Total solvent accessibility (Å^2)			
	DS	**StrucTools**	**GETAREA**	**Mobyle**
2LFM$_{wt}$	4343.2	4400.49	4315.89	4434.33
2LFM$_{A2T}$	4360.81	4402.47	4340.91	4455.75
2LFM$_{A2V}$	4364.04	4408.47	4350.75	4459.57
2LFM$_{H6R}$	4423.44	4460.44	4384.94	4511.92
2LFM$_{D7N}$	4341.88	4393.33	4323.38	4444.16
2LFM$_{D7H}$	4363.23	4414.55	4350.87	4466.27
2LFM$_{E11K}$	4378.78	4441.61	4364.27	4492.97
2LFM$_{K16N}$	4342.89	4381.05	4316.36	4430.97
2LFM$_{A21G}$	4347.45	4387.95	4329.37	4439.02
2LFM$_{E22G}$	4285.35	4335.59	4275.77	4383.96
2LFM$_{E22Q}$	4337.00	4393.69	4319.45	4440.36
2LFM$_{E22K}$	4382.35	4444.08	4365.95	4493.06
2LFM$_{D23N}$	4338.65	4372.26	4320.47	4425.23
2LFM$_{L34V}$	4302.88	4340.88	4282.23	4390.84

Table S5. Effects of mutations on hydrophobic and hydrophilic surface area (Å^2) of Aβ$_{42}$ (1IYT). Hydrophobic and hydrophilic solvent accessibility surface area was calculated using DS 4.0.

Molecules	Solvent accessibility surface area (Å^2)	
	Hydrophobic	Hydrophilic
$1IYT_{wt}$	1458.98	1256.70
$1IYT_{A2T}$	1391.67	1250.16
$1IYT_{A2V}$	1474.48	1248.23
$1IYT_{H6R}$	1460.74	1297.13
$1IYT_{D7N}$	1457.62	1268.70
$1IYT_{D7H}$	1458.92	1284.11
$1IYT_{E11K}$	1458.88	1283.27
$1IYT_{K16N}$	1468.98	1237.72
$1IYT_{A21G}$	1418.15	1259.34
$1IYT_{E22G}$	1462.61	1174.49
$1IYT_{E22Q}$	1455.05	1263.49
$1IYT_{E22K}$	1451.56	1280.30
$1IYT_{D23N}$	1455.59	1261.99
$1IYT_{L34V}$	1453.56	1259.06
$1IYT_{A42T}$	1378.25	1258.09
$1IYT_{A42V}$	1487.74	1258.67

Table S6. Effects of mutations on hydrophobic and hydrophilic surface area (Å^2) of Aβ$_{42}$ (1Z0Q). Hydrophobic and hydrophilic solvent accessibility surface area was calculated using DS 4.0.

	Solvent accessibility surface area (Å^2)	
Molecules	**Hydrophobic**	**Hydrophilic**
1Z0Q$_{wt}$	1466.29	1189.16
1Z0Q$_{A2T}$	1411.31	1183.35
1Z0Q$_{A2V}$	1487.00	1179.10
1Z0Q$_{H6R}$	1466.36	1213.81
1Z0Q$_{D7N}$	1470.72	1188.13
1Z0Q$_{D7H}$	1467.95	1201.88
1Z0Q$_{E11K}$	1475.35	1226.69
1Z0Q$_{K16N}$	1472.88	1160.54
1Z0Q$_{A21G}$	1434.79	1194.65
1Z0Q$_{E22G}$	1478.67	1133.10
1Z0Q$_{E22Q}$	1466.86	1215.65
1Z0Q$_{E22K}$	1468.97	1238.64
1Z0Q$_{D23N}$	1469.85	1198.96
1Z0Q$_{L34V}$	1452.99	1194.44
1Z0Q$_{A42T}$	1402.15	1194.89
1Z0Q$_{A42V}$	1508.44	1194.47

Table S7. Effects of mutations on hydrophobic and hydrophilic surface area (Å^2) of Aβ$_{40}$ (1BA4). Hydrophobic and hydrophilic solvent accessibility surface area was calculated using DS 4.0.

	Solvent accessibility surface area	
Molecule	**Hydrophobic**	**Hydrophilic**
1BA4$_{wt}$	1269.24	1162.85
1BA4$_{A2T}$	1213.17	1165.88
1BA4$_{A2V}$	1287.88	1165.43
1BA4$_{H6R}$	1267.14	1227.05
1BA4$_{D7N}$	1267.09	1180.23
1BA4$_{D7H}$	1264.33	1189.33
1BA4$_{E11K}$	1259.16	1199.30
1BA4$_{K16N}$	1268.23	1163.68
1BA4$_{A21G}$	1237.07	1170.78
1BA4$_{E22G}$	1278.91	1091.13
1BA4$_{E22Q}$	1266.53	1184.88
1BA4$_{E22K}$	1255.94	1192.20
1BA4$_{D23N}$	1265.59	1166.86
1BA4$_{L34V}$	1256.31	1169.99

Table S8. Effects of mutations on hydrophobic and hydrophilic surface area (Å^2) of Aβ$_{40}$ (2LFM). Hydrophobic and hydrophilic solvent accessibility surface area was calculated using DS 4.0.

Molecule	Solvent accessibility surface area	
	Hydrophobic	Hydrophilic
2LFM$_{wt}$	1392.36	1429.05
2LFM$_{A2T}$	1344.73	1428.09
2LFM$_{A2V}$	1431.59	1428.10
2LFM$_{H6R}$	1401.36	1474.62
2LFM$_{D7N}$	1403.86	1438.64
2LFM$_{D7H}$	1406.52	1457.03
2LFM$_{E11K}$	1407.27	1455.84
2LFM$_{K16N}$	1410.42	1384.00
2LFM$_{A21G}$	1385.28	1431.29
2LFM$_{E22G}$	1412.48	1350.08
2LFM$_{E22Q}$	1404.72	1435.64
2LFM$_{E22K}$	1406.04	1455.09
2LFM$_{D23N}$	1402.64	1440.15
2LFM$_{L34V}$	1379.22	1431.18

Table S9. Normalized data for time of onset (t_{onset}) and total Aβ. (Aβ levels from Jonsson et al.[1])

Molecule	t_{onset} (years)	Total Aβ
WT	75	1
A673T (A2T)	80	0.5
A673V (A2V)	36	3.5
H677R (H6R)	56	1
D678N (D7N)	61	1
D678H (D7H)	58	1.5
E682K (E11K)	61	2
K687N (K16N)	56	1.5
A692G (A21G)	46	1.6
E693G (E22G)	57	1
E693K (E22K)	55	0.8
E693Q (E22Q)	50	1
D694N (D23N)	62	1

Table S10. Normalized data set on t_{onset} and total Aβ. (Aβ levels from Di Fede et al.[2])

Molecule	t_{onset} (years)	Total Aβ
WT	75	1
A673T (A2T)	80	0.5
A673V (A2V)	36	2.1
H677R (H6R)	56	1
D678N (D7N)	61	1
D678H (D7H)	58	1.5
E682K (E11K)	61	2
K687N (K16N)	56	1.5
A692G (A21G)	46	1.6
E693G (E22G)	57	1
E693K (E22K)	55	0.8
E693Q (E22Q)	50	1
D694N (D23N)	62	1

Table S11. Data for correlating t_{onset} with properties of 1IYT WT and mutant Aβ.

Molecule	t_{onset} (years)	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	75	4129.19	1458.98	1256.7
A673T (A2T)	80	4135.09	1391.67	1250.16
A673V (A2V)	36	4134.58	1474.48	1248.23
H677R (H6R)	56	4181.65	1460.74	1297.13
D678N (D7N)	61	4136.93	1457.62	1268.7
D678H (D7H)	58	4149.04	1458.92	1284.11
E682K (E11K)	61	4154.98	1458.88	1283.27
K687N (K16N)	56	4122.59	1468.98	1237.72
A692G (A21G)	46	4119.54	1418.15	1259.34
E693G (E22G)	57	4079.36	1462.61	1174.49
E693K (E22K)	55	4143.16	1451.56	1280.3
E693Q (E22Q)	50	4126.99	1455.05	1263.49
D694N (D23N)	62	4136.75	1455.59	1261.99

Table S12. **Data for correlating t_{onset} with properties of 1Z0Q WT and mutant Aβ.**

Molecule	t_{onset} (years)	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	75	4010.51	1466.29	1189.16
A673T (A2T)	80	4021.38	1411.31	1183.35
A673V (A2V)	36	4022.00	1487.00	1179.10
H677R (H6R)	56	4030.34	1466.36	1213.81
D678N (D7N)	61	4000.42	1470.72	1188.13
D678H (D7H)	58	4018.21	1467.95	1201.88
E682K (E11K)	61	4081.21	1475.35	1226.69
K687N (K16N)	56	3977.61	1472.88	1160.54
A692G (A21G)	46	4008.83	1434.79	1194.65
E693G (E22G)	57	4009.33	1478.67	1133.10
E693K (E22K)	55	4048.38	1466.86	1215.65
E693Q (E22Q)	50	4085.24	1468.97	1238.64
D694N (D23N)	62	4017.70	1469.85	1198.96

Table S13. Data for correlating t_{onset} with properties of 1BA4 WT and mutant Aβ.

Molecule	t_{onset} (years)	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	75	3692.47	1269.24	1162.85
A673T (A2T)	80	3706.95	1213.17	1165.88
A673V (A2V)	36	3709.36	1287.88	1165.43
H677R (H6R)	56	3776.95	1267.14	1227.05
D678N (D7N)	61	3699.69	1267.09	1180.23
D678H (D7H)	58	3705.98	1264.33	1189.33
E682K (E11K)	61	3713.44	1259.16	1199.30
K687N (K16N)	56	3725.15	1268.23	1163.68
A692G (A21G)	46	3689.56	1237.07	1170.78
E693G (E22G)	57	3672.25	1278.91	1091.13
E693K (E22K)	55	3707.77	1266.53	1184.88
E693Q (E22Q)	50	3703.12	1255.94	1192.20
D694N (D23N)	62	3692.06	1265.59	1166.86

Table S14. Data for correlating t_{onset} with properties of 2LFM WT and mutant Aβ.

Molecule	t_{onset} (years)	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	75	4343.2	1392.36	1429.05
A673T (A2T)	80	4360.81	1344.73	1428.09
A673V (A2V)	36	4364.04	1431.59	1428.1
H677R (H6R)	56	4423.44	1401.36	1474.62
D678N (D7N)	61	4341.88	1403.86	1438.64
D678H (D7H)	58	4363.23	1406.52	1457.03
E682K (E11K)	61	4378.78	1407.27	1455.84
K687N (K16N)	56	4342.89	1410.42	1384.00
A692G (A21G)	46	4347.45	1385.28	1431.29
E693G (E22G)	57	4285.35	1412.48	1350.08
E693K (E22K)	55	4337.00	1404.72	1435.64
E693Q (E22Q)	50	4382.35	1406.04	1455.09
D694N (D23N)	62	4338.65	1402.64	1440.15

Table S15. Total helix percentage calculated for WT and mutant $A\beta_{40}$ and $A\beta_{42}$.

Molecules	Total helix percentage			
	$A\beta_{40}$		$A\beta_{42}$	
	1BA4	2LFM	1IYT	1Z0Q
WT	55	22.5	71.4	33.3
A673T (A2T)	55	22.5	71.4	33.3
A673V (A2V)	55	22.5	71.4	33.3
H677R (H6R)	55	22.5	73.8	33.3
D678N (D7N)	55	22.5	71.4	33.3
D678H (D7H)	55	22.5	71.4	33.3
E682K (E11K)	55	22.5	71.4	33.3
K687N (K16N)	55	22.5	71.4	33.3
A692G (A21G)	55	22.5	71.4	33.3
E693G (E22G)	55	22.5	71.4	33.3
E693K (E22K)	55	22.5	71.4	33.3
E693Q (E22Q)	55	22.5	71.4	33.3
D694N (D23N)	55	22.5	71.4	33.3
L705V (L34V)	55	22.5	71.4	33.3
A713T (A42T)	NA	NA	71.4	33.3
A713V (A42V)	NA	NA	71.4	33.3

NA - Not Applicable

Table S16. Data for correlating total Aβ with properties of 1IYT WT and mutant Aβ.

Molecule	Total Aβ	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	1	4129.19	1458.98	1256.7
A673T (A2T)	0.5	4135.09	1391.67	1250.16
A673V (A2V)	3.5	4134.58	1474.48	1248.23
H677R (H6R)	1	4181.65	1460.74	1297.13
D678N (D7N)	1	4136.93	1457.62	1268.7
D678H (D7H)	1.5	4149.04	1458.92	1284.11
E682K (E11K)	2	4154.98	1458.88	1283.27
K687N (K16N)	1.5	4122.59	1468.98	1237.72
A692G (A21G)	1.6	4119.54	1418.15	1259.34
E693G (E22G)	1	4079.36	1462.61	1174.49
E693K (E22K)	0.8	4143.16	1451.56	1280.3
E693Q (E22Q)	1	4126.99	1455.05	1263.49
D694N (D23N)	1	4136.75	1455.59	1261.99

Table S17. Data for correlating total Aβ with properties of 1Z0Q WT and mutant Aβ.

Molecule	Total Aβ	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	1	4010.51	1466.29	1189.16
A673T (A2T)	0.5	4021.38	1411.31	1183.35
A673V (A2V)	3.5	4022.00	1487.00	1179.10
H677R (H6R)	1	4030.34	1466.36	1213.81
D678N (D7N)	1	4000.42	1470.72	1188.13
D678H (D7H)	1.5	4018.21	1467.95	1201.88
E682K (E11K)	2	4081.21	1475.35	1226.69
K687N (K16N)	1.5	3977.61	1472.88	1160.54
A692G (A21G)	1.6	4008.83	1434.79	1194.65
E693G (E22G)	1	4009.33	1478.67	1133.10
E693K (E22K)	0.8	4048.38	1466.86	1215.65
E693Q (E22Q)	1	4085.24	1468.97	1238.64
D694N (D23N)	1	4017.70	1469.85	1198.96

Table S18. Data for correlating total Aβ with properties of 1BA4 WT and mutant Aβ.

Molecule	Total Aβ	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	1	3692.47	1269.24	1162.85
A673T (A2T)	0.5	3706.95	1213.17	1165.88
A673V (A2V)	3.5	3709.36	1287.88	1165.43
H677R (H6R)	1	3776.95	1267.14	1227.05
D678N (D7N)	1	3699.69	1267.09	1180.23
D678H (D7H)	1.5	3705.98	1264.33	1189.33
E682K (E11K)	2	3713.44	1259.16	1199.30
K687N (K16N)	1.5	3725.15	1268.23	1163.68
A692G (A21G)	1.6	3689.56	1237.07	1170.78
E693G (E22G)	1	3672.25	1278.91	1091.13
E693K (E22K)	0.8	3707.77	1266.53	1184.88
E693Q (E22Q)	1	3703.12	1255.94	1192.20
D694N (D23N)	1	3692.06	1265.59	1166.86

Table S19. Data for correlating total Aβ with properties of 2LFM WT and mutant Aβ.

Molecule	Total Aβ	Solvent accessibility surface (Å^2)		
		Total	Hydrophobic	Hydrophilic
WT	1	4343.2	1392.36	1429.05
A673T (A2T)	0.5	4360.81	1344.73	1428.09
A673V (A2V)	3.5	4364.04	1431.59	1428.1
H677R (H6R)	1	4423.44	1401.36	1474.62
D678N (D7N)	1	4341.88	1403.86	1438.64
D678H (D7H)	1.5	4363.23	1406.52	1457.03
E682K (E11K)	2	4378.78	1407.27	1455.84
K687N (K16N)	1.5	4342.89	1410.42	1384.00
A692G (A21G)	1.6	4347.45	1385.28	1431.29
E693G (E22G)	1	4285.35	1412.48	1350.08
E693K (E22K)	0.8	4337.00	1404.72	1435.64
E693Q (E22Q)	1	4382.35	1406.04	1455.09
D694N (D23N)	1	4338.65	1402.64	1440.15

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