SUPPLEMENTARY DATA

PITRM1 interaction studies with amyloidogenic nonapeptide mutants of familial Alzheimer's disease

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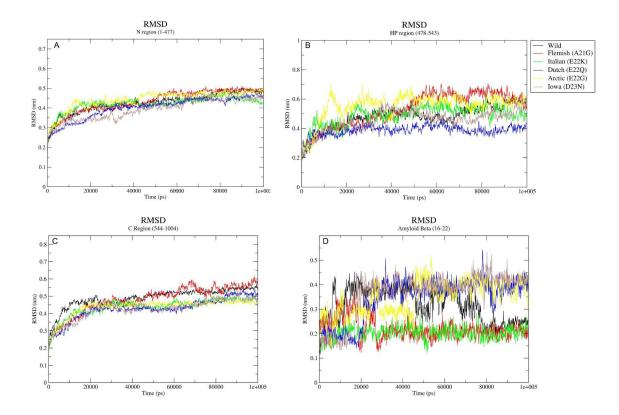


Figure S1: RMSD of 6 complex for a period of 100 ns. Black for native amyloid beta-PITRM complex, Green for Italian amyloid beta-PITRM complex, Blue for Dutch amyloid beta-PITRM complex, Yellow for Arctic amyloid beta-PITRM complex, Red for Flemish amyloid beta-PITRM complex and Brown for Iowa amyloid beta-PITRM complex. (A) RMSD of PITRM1-N region during interaction with Nonapeptide. (B) RMSD of PITRM1-HP region during interaction with Nonapeptide. (C) RMSD of PITRM1-C region during interaction with Nonapeptide alone..

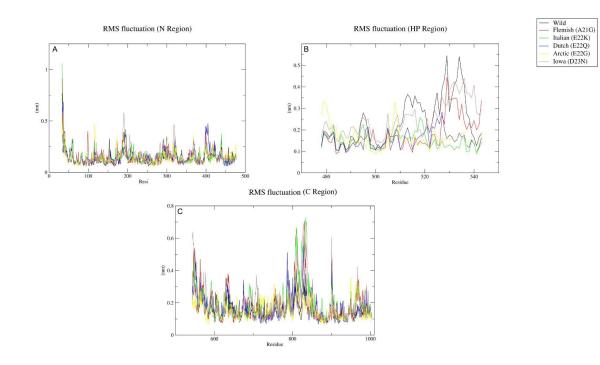


Figure S2: RMS fluctuations observed in PITRM1 during interaction with native and familial mutant amyloid beta (6 complex) for a period of 50 ns (last 50 ns of total 100ns). Black for native amyloid beta-PITRM complex, Green for Italian amyloid beta-PITRM complex, Blue for Dutch amyloid beta-PITRM complex, Yellow for Arctic amyloid beta-PITRM complex, Red for Flemish amyloid beta-PITRM complex and Brown for Iowa amyloid beta-PITRM complex. (A) RMS fluctuations of PITRM1-N region while interaction with amyloid beta. (C) RMS fluctuations of PITRM1-C region while interaction with amyloid beta.

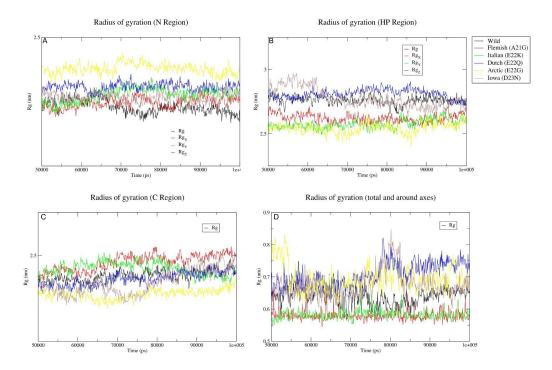


Figure S3: Radius of gyration observed in PITRM1 during interaction with native and familial mutant amyloid beta (6 complex) for a period of 50 ns (last 50 ns of total 100ns). Black for native amyloid beta-PITRM complex, Green for Italian amyloid beta-PITRM complex, Blue for Dutch amyloid beta-PITRM complex, Yellow for Arctic amyloid beta-PITRM complex, Red for Flemish amyloid beta-PITRM complex and Brown for Iowa amyloid beta-PITRM complex. (A) Radius of gyration of PITRM1-N region while interaction with amyloid beta. (B) Radius of gyration of PITRM1-HP region while interaction with amyloid beta. (D) Radius of gyration of amyloid beta (native and familial mutants) while interaction with PITRM1.

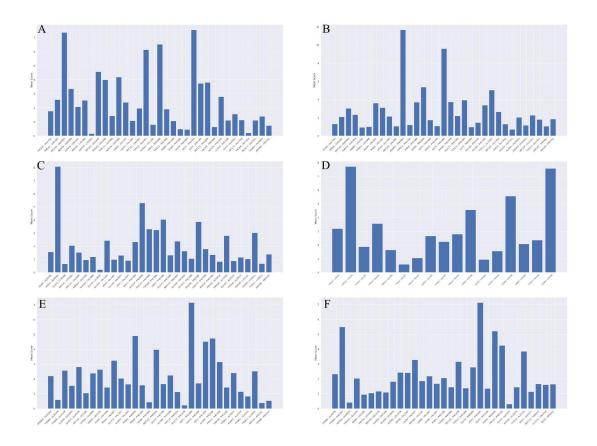


Figure S4:

Mean score of bond formation between PITRM1 and amyloid beta (wild and familial mutants) 6 complex for a period of 50 ns (last 50 ns of total 100ns).

	Chain A-PITRM1	Distance (nm)	Type of interaction Hydrophobic Interactions	Chain B- Amyloid Beta
	124PHE	3.57	Hydrophobic Interactions	19PHE
		5.18	pi-Stacking 🔵	19PHE
		3.81 🔴	Hydrophobic Interactions 🔴	18VAL
	135MET	3.25	Hydrogen Bonds	16LYS
	Vild 137ALA	3.39	Hydrogen Bonds	15GLN
		3.56	Hydrophobic Interactions	18VAL
	146TYR 😑	3.65	Hydrophobic Interactions	19PHE
	206MET	3.62	Hydrophobic Interactions	20PHE
	961SER •	3.04 🔵	Hydrogen Bonds 🔵	15GLN
	104HIS	4.29	pi-Stacking 🔵	20PHE
	105ILE	3.4 🔴	Hydrophobic Interactions	020PHE
	123PHE •	3.61	Hydrophobic Interactions	= 18VAL
		3.82	Hydrophobic Interactions	18VAL
	127LEU 🔴	3.84	Hydrophobic Interactions	18VAL
	137ALA 🔴	3.92	Hydrophobic Interactions	23ASP
Flemish (A2		3.71 😑	Hydrophobic Interactions 😑	- 18VAL
	202VAL 🔴	3.75 🔴	Hydrophobic Interactions 🔴	20PHE
	1325ER •	3.26	Hydrogen Bonds	15GLN
	205GLU • 716ASP •	3.2	Hydrogen Bonds 🔵 Hydrogen Bonds 🔵	20PHE 16LYS
	215ARG	5.2	Salt Bridges	23ASP
	900ARG	3.69	pi-Cation Interactions	19PHE
	124PHE	3.82	Hydrophobic Interactions	15GLN
	135MET	3.48 🔴	Hydrophobic Interactions	16LYS
		2.04	Hydrogen Bonds 🔵	16LYS
Italian (E2	205GLU O	3.94	Hydrophobic Interactions	_ 18VAL
	209ALA -	3.54	Hydrophobic Interactions	20PHE
	139THR	3.19	Hydrogen Bonds	21414
	215ARG	3.39	Hydrogen Bonds	23ASP
	123PHE 🔴	3.75 😑	Hydrophobic Interactions 😑	18VAL
	127LEU	3.72 😑	Hydrophobic Interactions 😑	18VAL
	134РНЕ 😑	3.88 😐	Hydrophobic Interactions 🔴	- 17LEU
	921TYR	3.95	Hydrophobic Interactions 🔴 Hydrogen Bonds 🔵	20PHE
		3.37	Hydrogen Bonds	23ASP
Dutch (E220	220	3.46	Hydrophobic Interactions	20PHE
	923TYR	2.36	Hydrogen Bonds	21ALA
		2.05	Hydrogen Bonds 🔵	19PHE
	962THR 🔴	3.88 😑	Hydrophobic Interactions 🔴	- 17LEU
	107GLU •	3.4 🔵	Hydrogen Bonds	16LYS
	133THR • 911LYS •	1.96 • 5.2 •	Hydrogen Bonds 🔵 Salt Bridges 🌰	18VAL
	107GLU	3.96	Salt Bridges	23ASP
	123PHE	3.56	Hydrophobic Interactions	19PHE
	1/	3.99	Hydrophobic Interactions	19PHE
	124PHE	3.79 😑	Hydrophobic Interactions	- 19PHE
		3.76	Hydrophobic Interactions 🔴	16LYS
Arctic (E2		3.78	Hydrophobic Interactions	e 16LYS
	137ALA 🔴 139THR 😑	3.37	Hydrophobic Interactions 🔴	9PHE
	1391HR •	3.68	Hydrophobic Interactions	20PHE
	205GLU	3.96	Hydrophobic Interactions	18VAL
	104HIS	3.9 🔵	pi-Stacking	20PHE
	107GLU 😑	3.71 😑	Hydrophobic Interactions	020PHE
	111LEU 🔴	3.68 😑	Hydrophobic Interactions	020PHE
	124PHE 🔴	3.94 🔴	Hydrophobic Interactions 😑	0 20PHE
	127LEU	3.67	Hydrophobic Interactions	20PHE
	135MET 0 137ALA 0	3.21	Hydrophobic Interactions	19PHE
Iowa (D2		3.53	Hydrophobic Interactions	21ALA
10410 (D2		3.66	Hydrophobic Interactions	20PHE
	146TYR	3.49	Hydrophobic Interactions	20PHE
		3.28	Hydrogen Bonds 🔵	21ALA
	906TYR 😑	3.28 • 2.13 • 3.86 •	Hydrogen Bonds Hydrogen Bonds Hydrogen Bonds	21ALA 19PHE 15GLN

Number of records 0.0 1.0 Intraction

Hydrogen Bonds Hydrophobic Interactions Salt Bridges pi-Cation Interactions pi-Stacking

Figure S5: Distance and interaction between PITRM1 and amyloid beta of 6 MD simulated average complex.