

SUPPLEMENTARY DATA

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

Carlton Ranjith Wilson Alphonse¹, Rajaretinam Rajesh Kannan^{1*}, Nagasundaram Nagarajan^{1,2}

¹ *Neuroscience lab, Centre for Molecular and Nanomedical Sciences, Centre for Nanoscience and Nanotechnology, School of Bio and Chemical Engineering, Sathyabama Institute of Science and Technology, Chennai – 600119, Tamil Nadu, India.*

² *School of Biosciences and Technology, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India*

1. Carlton Ranjith Wilson Alphonse – carltonranjith@sathyabama.ac.in (ORCID Id: [0000-0002-0402-6385](https://orcid.org/0000-0002-0402-6385))
2. **Rajaretinam Rajesh Kannan*** - rajeshkannan.mnru@sathyabama.ac.in (ORCID Id: [0000-0001-6846-5777](https://orcid.org/0000-0001-6846-5777))
3. Nagasundaram Nagarajan- nagasundaram.n@vit.ac.in (ORCID Id: 0000-0002-9581-4781)

***Corresponding Author:** Dr Rajaretinam Rajesh Kannan, Centre for Nanoscience and Nanotechnology, School of Bio and Chemical Engineering, Sathyabama Institute of Science and Technology, Chennai – 600119, Tamil Nadu, India.

E-mail: rajeshkannan.mnru@sathyabama.ac.in (ORCID Id: [0000-0001-6846-5777](https://orcid.org/0000-0001-6846-5777))

Telephone no: +91 99405 10096

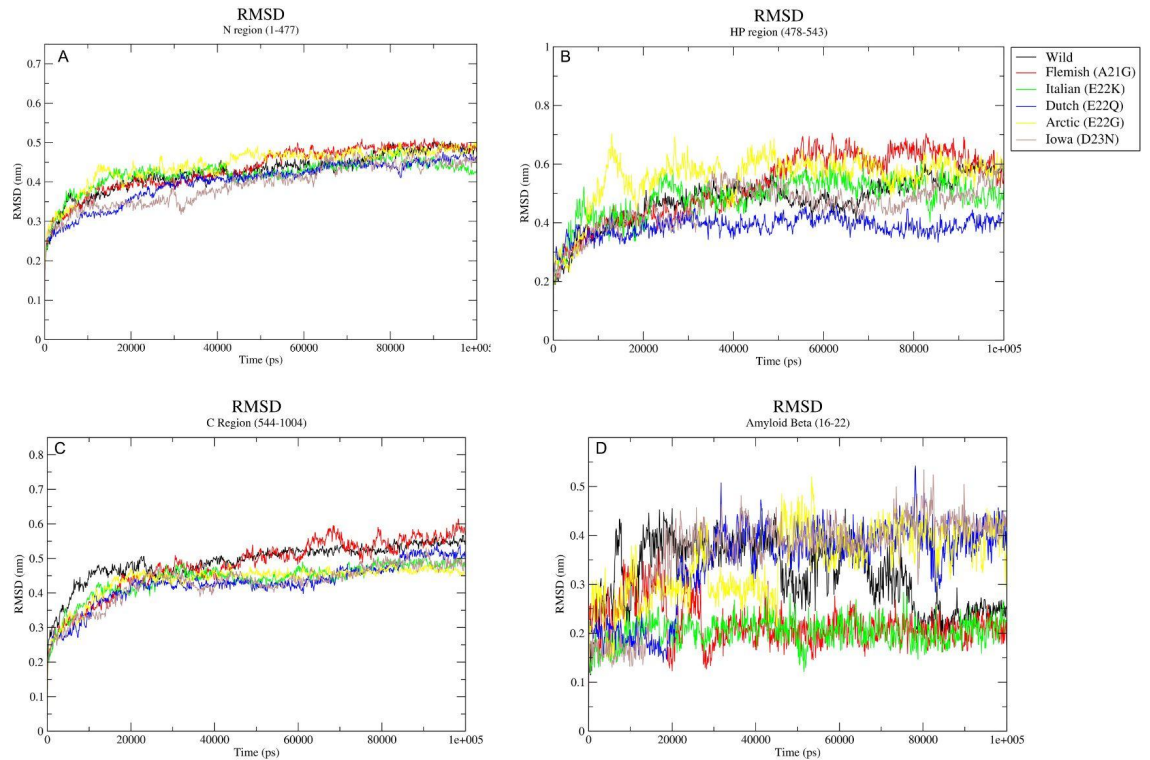


Figure S1: RMSD of 6 complex for a period of 100 ns. Black for native amyloid beta-PITRM complex, Green for Italian amyloid beta-PITRM complex, Blue for Dutch amyloid beta-PITRM complex, Yellow for Arctic amyloid beta-PITRM complex, Red for Flemish amyloid beta-PITRM complex and Brown for Iowa amyloid 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. (D) RMSD of Nonapeptide alone..

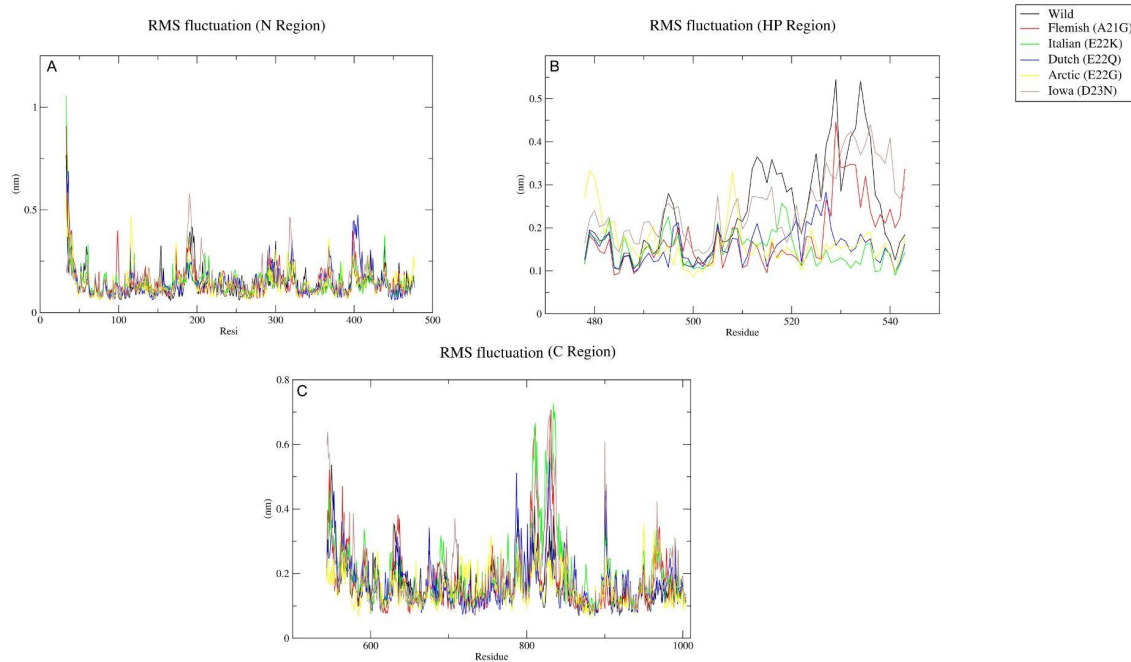


Figure S2: RMS fluctuations observed in PITRM1 during interaction with native and familial mutant amyloid beta (6 complex) for a period of 50 ns (last 50 ns of total 100ns). Black for native amyloid beta-PITRM complex, Green for Italian amyloid beta-PITRM complex, Blue for Dutch amyloid beta-PITRM complex,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

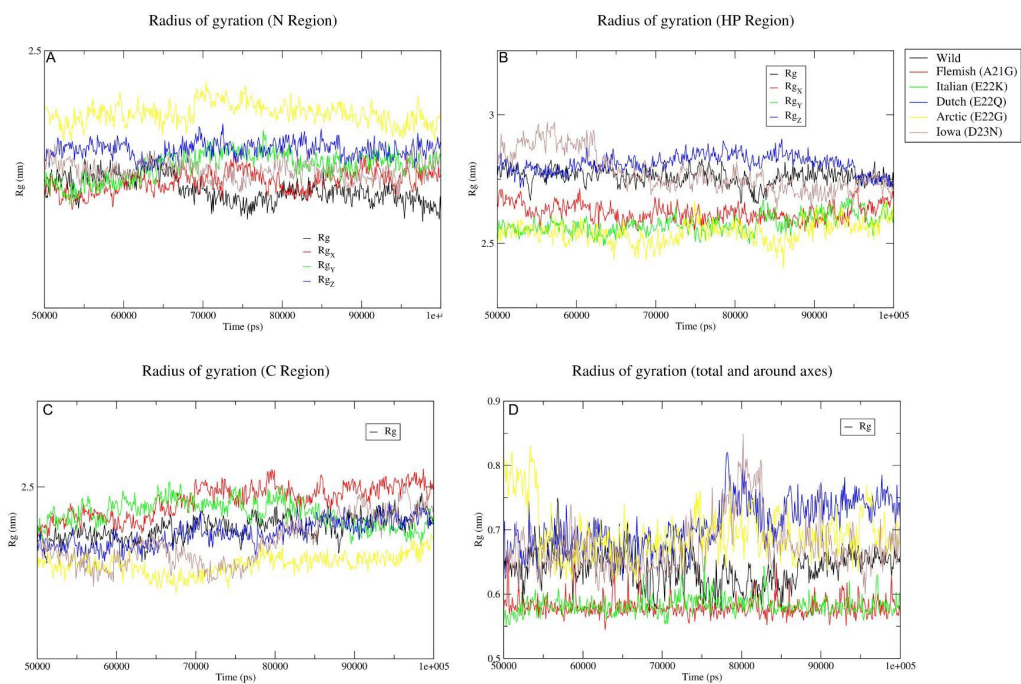


Figure S3: Radius of gyration observed in PITRM1 during interaction with native and familial mutant amyloid beta (6 complex) for a period of 50 ns (last 50 ns of total 100ns). Black for native amyloid beta-PITRM complex, Green for Italian amyloid beta-PITRM complex, Blue for Dutch amyloid beta-PITRM 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. (C) Radius of gyration of PITRM1-C region while interaction with amyloid beta. (D) Radius of gyration of amyloid beta (native and familial mutants) while interaction with PITRM1.

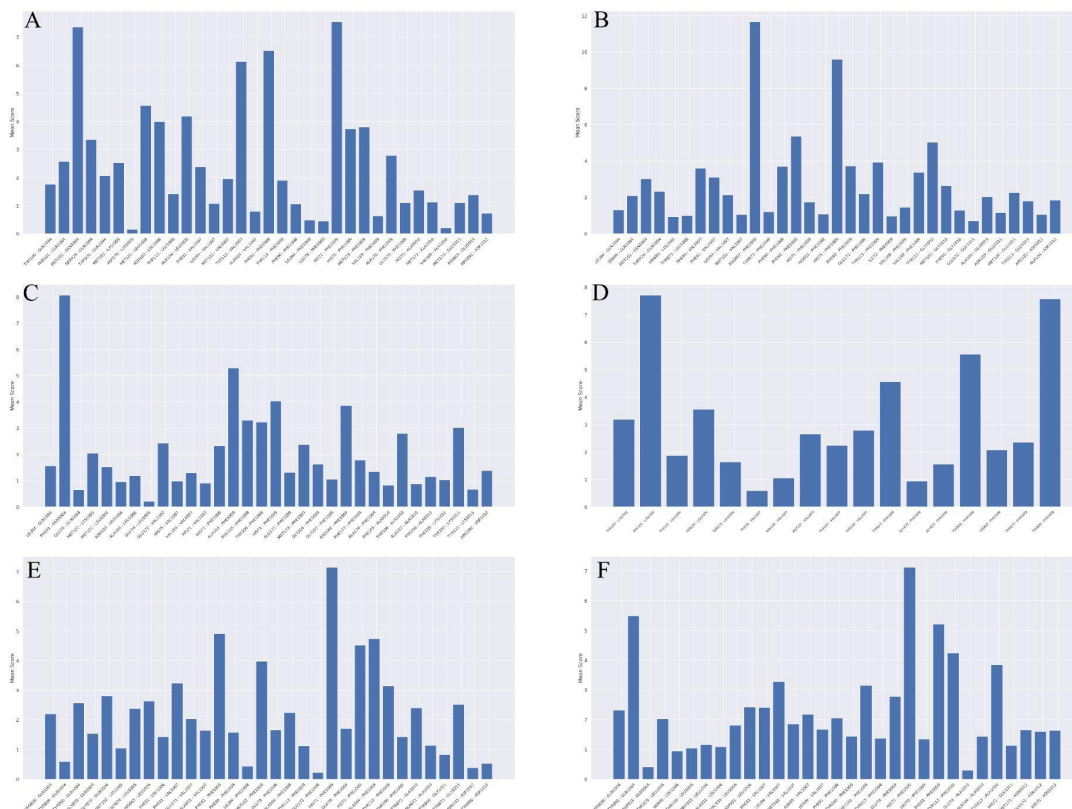


Figure S4:

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).

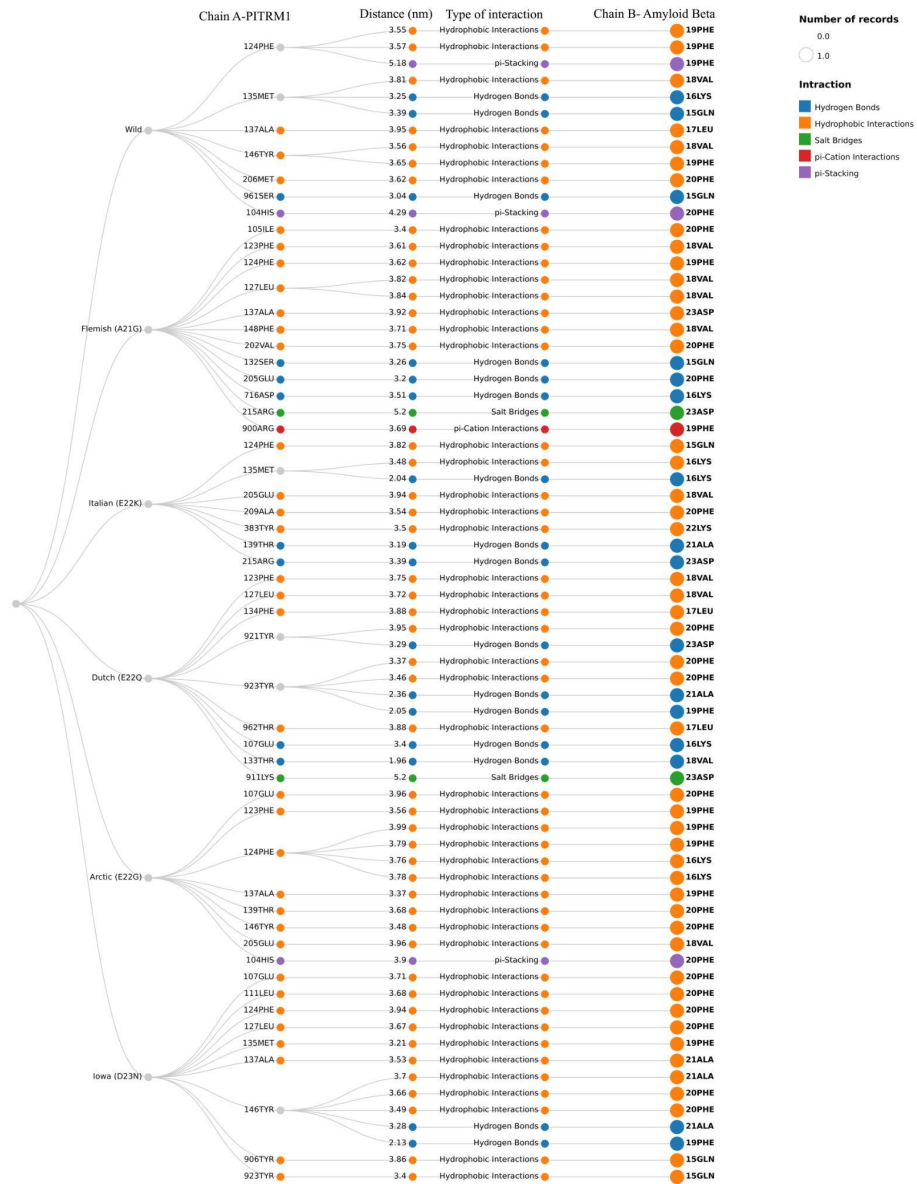


Figure S5: Distance and interaction between PITRM1 and amyloid beta of 6 MD simulated average complex.