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ORIGINAL RESEARCH ARTICLE

Effect of Darjeeling black tea aromatics on central nervous system function: An *in silico* study of glutamate receptor–ligand interactions

Supplementary Files

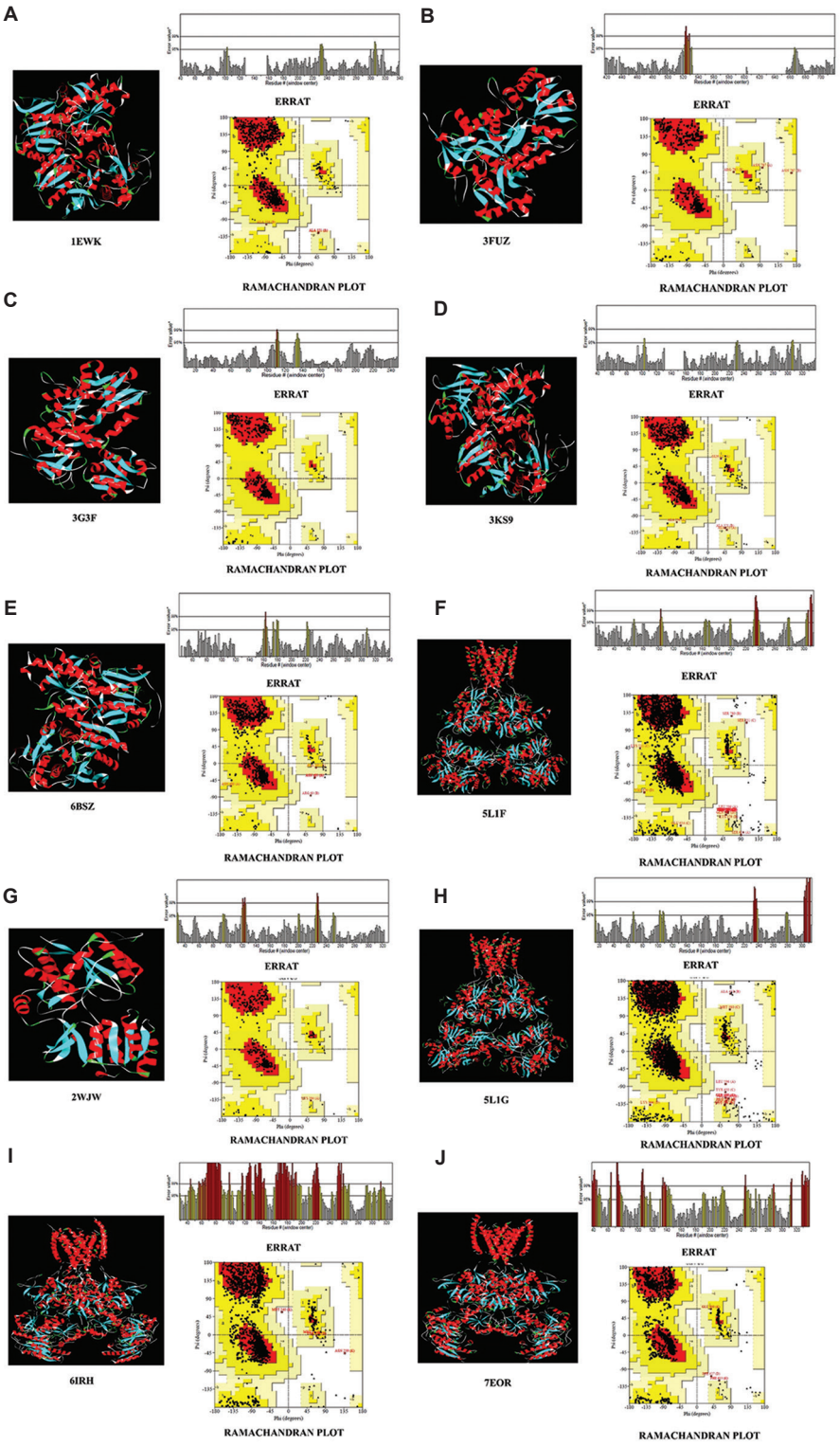

Figure S1. Structure quality assessment parameters for the selected receptor proteins. (A) GluR subtype 1. (B) GluR5. (C) GluR6. (D) mGluR1. (E) mGlu8. (F) AMPA-type glutamate receptor GluA2 complexed with perampanel. (G) AMPA-type glutamate receptor GluA2. (H) AMPA-type glutamate receptor GluA2 complexed with GYKI-Br. (I) NMDA-type glutamate receptor GluN1/GluN2A. (J) NMDA-type glutamate receptor GluN1/GluN2A.
Abbreviations: AMPA: α-amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid receptor; GluR: Glutamate receptors; mGlu: Metabotropic glutamate receptor; NMDA: N-methyl-D-aspartate receptor.

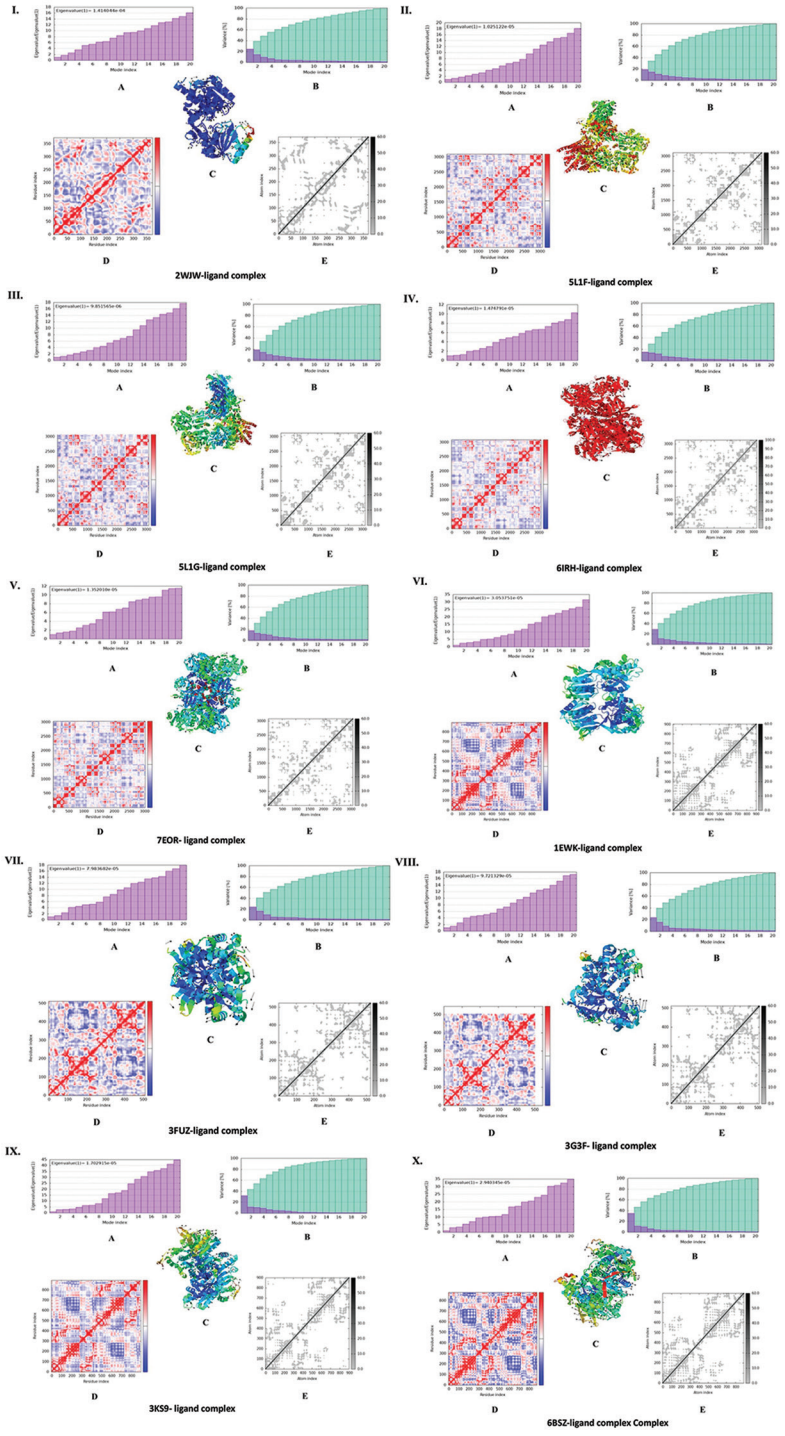

Figure S2. iMod server predictions for the selected receptor proteins and their respective ligand complexes. (A) Eigenvalue plot. (B) Variance plot. (C) iMODVIEW visualization of receptor–ligand 3D models showing vibrational modes and conformational transitions. (D) Covariance map. (E) Elastic network model. Panels I-X correspond to the following receptor–ligand systems: (I) GluR AMPA ionotropic receptor subtype–safranal complex. (II) AMPA-type glutamate receptor GluA2–α-ionone complex. (III) AMPA-type ionotropic glutamate receptor GluA2–GYKI-Br complex and GluA2–α-ionone complex. (IV) NMDA-type ionotropic receptor GluN1/GluN2A–α-ionone complex. (V) NMDA-type ionotropic receptor GluN1/GluN2A (different pH condition)–α-ionone complex. (VI) GluR1 receptor–(E,E)-2,4-decadienal complex. (VII) GluR5 receptor–safranal complex. (VIII) GluR6 receptor–α-ionone complex. (IX) GluR1 receptor–α-ionone complex. (X) Metabotropic glutamate receptor mGlu8–2-acetyl-3,5-dimethyl pyrazine complex.

Abbreviations: AMPA: α-amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid receptor; GluR: Glutamate receptors; NMDA: N-methyl-D-aspartate receptor.