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3D modelling and MD simulation analysis of wild and mutated Serine/threonine-protein kinase B-raf (BRAF) ABSTRACT BRAF kinase protein is a serine-threonine kinase encoded on chromosome 7q34, an important signal transduction molecule. BRAF is a 766 amino acid long with 84,437 Da of mass. As per the KEGG database, the wild and mutated form of BRAF kinase is involved in 42 metabolic pathway including MAPK signalling pathway, Breast cancer, Glioma, etc. In the present work, we are focused on amino acid position 600 in BRAF kinase, where V600E is highly involved with Glioma. Understanding the molecular structural features of this protein will help us to develop new inhibitor and treatment methodology.

As V600E is a widely studied mutation in BRAF, from the literature sources, we have mined out numerous mutations. Implementing the homology and fold based protein structure modelling methods we have modelled the BRAF kinase using Phyre2 server and mutated with V600D, V600E and V600G, evaluated the protein quality with Ramachandran Plot analysis and studied the molecular dynamic behaviour of the proteins. All the mutated proteins exhibited a stable conformation and acceptable occurrence in the Ramachandran plot. After the MD simulation the total energy of Wild type BRAF kinase structure is reported as -2.81604 e+06, V600D (-2.81686 e+06), V600E (-2.81547 e+06) and V600G (-2.81587 e+06) structure. Keyword: BRAF, Kinase, V600E, Molecular modelling, Molecular dynamic simulation.

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