Breast Cancer is a leading death causing disease, also known as the supreme common cancer prevalent in women worldwide. Female breast cancer is noted as 15.3% among all new cancer cases in US alone, and recurrence is spotted amongst women aged 55 to 69 years. Recently it has been testified that over 2 million newfangled cases all over the globe suffering with the same disease. This disease is a common malignancy and a lifespan threat amongst women all-inclusive. In the contemporary era, computer aided drug design (CADD) approaches efficaciously have been pragmatic in drug development processes. In this strategy, chemical structures are designed after ascertaining them in clinical tests for suitability. The process is based on designing 3D structures and works in yielding therapeutic activity of those structures/compounds or molecules with their biological activity. In depth knowledge over human genome along with the sequential, proteomic, genomic and structural information is quintessential in the progress of satisfying targets and drug discovery. Structure based designing finds supplementing the 3D structure (binding and/or active site) of the target which has shown very promising results in the recent times. Effective new drugs particularly promising in fighting with cancer can be designed by having the deeper insight with molecular working of cancer progression. Cancer happens due to disturbances different cell signaling pathways such as PI3K/AKT Signaling Pathway, JAK/STAT Pathway, p53-Mediated Apoptosis Pathway etc. But being one of the most frequently activated pathway in cancer, much effort has been directed towards reticence of PI3K/AKT/mTOR pathway as a unique oncological therapeutic initiative. mTOR as a momentous target for the provocative ailments can act as a best suited therapeutic molecule, a gene accountable to cause cancer, and functions in controlling cell division at finest levels. Any aberration in the gene on that account, the division of breast cells will be modified and as a consequence the cancerous growth of cells will transpire in breast. In our study mTOR/FRB Domain’s recruitment cleft as well as substrate recruitment mechanism was targeted using structural based approach. A series of selective inhibitory small molecules have been designed and screened for the best inhibiting target binding triad of FRB Domain with better ADME and no detectable toxic effects. In the same study we have used computer-aided methodology for drug design, using modeller three
dimensional structure has been predicted which is followed by verification of designed structures using programs ProCheck & PROSA. Active site for the target protein has been predicted also after predicting active site performing literature search lead compound has been selected further the same lead molecule has been populated and strict hierarchical screening over bioavailability and chemical parameters yielded final molecules for binding analysis studies, and the most suitable candidate with enough binding energy and biosafety selected as a most promising candidate.