Uncovering the potential of Fatty Acid Binding Proteins for predicting radiation-induced gastrointestinal injury

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Supplementary Information

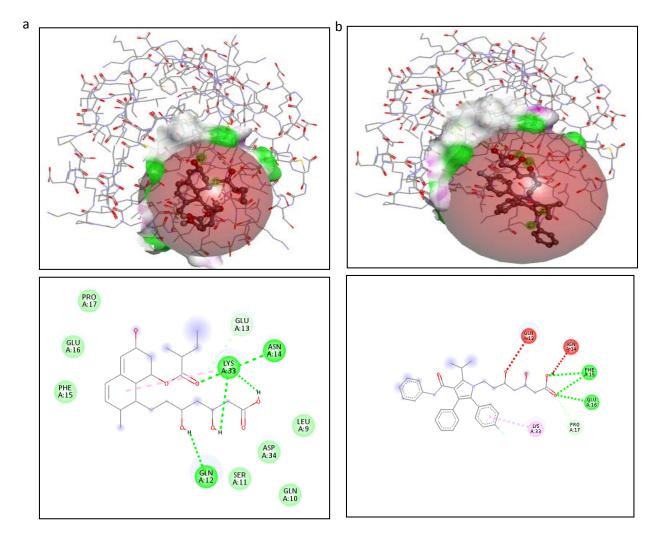


Figure S1 Molecular docking studies of mice FABP1 protein with pravastatin and atorvastatin: The 2D and 3D images of the ligand were retrieved from PubChem database (a) 3D and 2D image displaying mice FABP1 interaction with pravastatin through strong various amino acid residues with binding energy of -5.5 kcal/mol. (b) 3D and 2D images showing mice FABP1 interaction with atorvastatin through few amino residues and binding energy of -6.1 kcal/mol. The details of the interacting amino acid residues are given in the text.

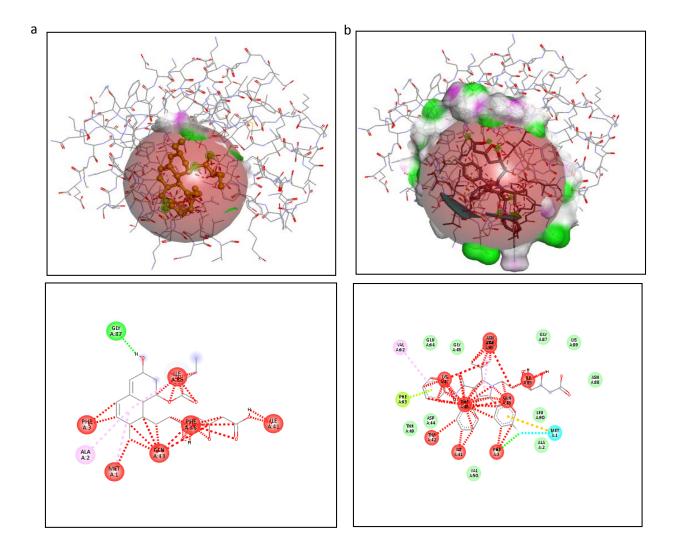


Figure S2 Molecular docking studies of mice FABP2 protein with pravastatin and atorvastatin: The 2D and 3D images of the ligand were retrieved from PubChem database (a) FABP2 - Pravastatin interaction binds through variety of amino acid residues and a binding energy of -5.4 Kcal/mol (b) FABP2 interacts with atorvastatin through different amino acids residues and displayed binding energy of -5.9 kcal/mol. The details of the interacting amino acid residues are given in the text.