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Spectroscopic Characterization, Molecular Docking and Machine Learning Studies of Sulphur containing Hydrazide Derivatives

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Figure S1. Optimized geometries of TSCZ(A-C) and TCHZ(D-F) at Basis set 6-31G(d, p), 6-31+G(d', p') and 6-311+G(d, p) respectively.

Figure S2. Experimental UV spectra of TSCZ and TCHZ.

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Figure S4. Ramchandran diagram of PDB IDs. 6CLU and 2WJE respectively.

Figure S5. 3D representation of hydrogen bonding interactions (A-D) and 2D representation of hydrogen bonding and hydrophobic interactions (E) of compound TSCZ with different amino acid residues at active site of protein (PDB ID. 6CLU).

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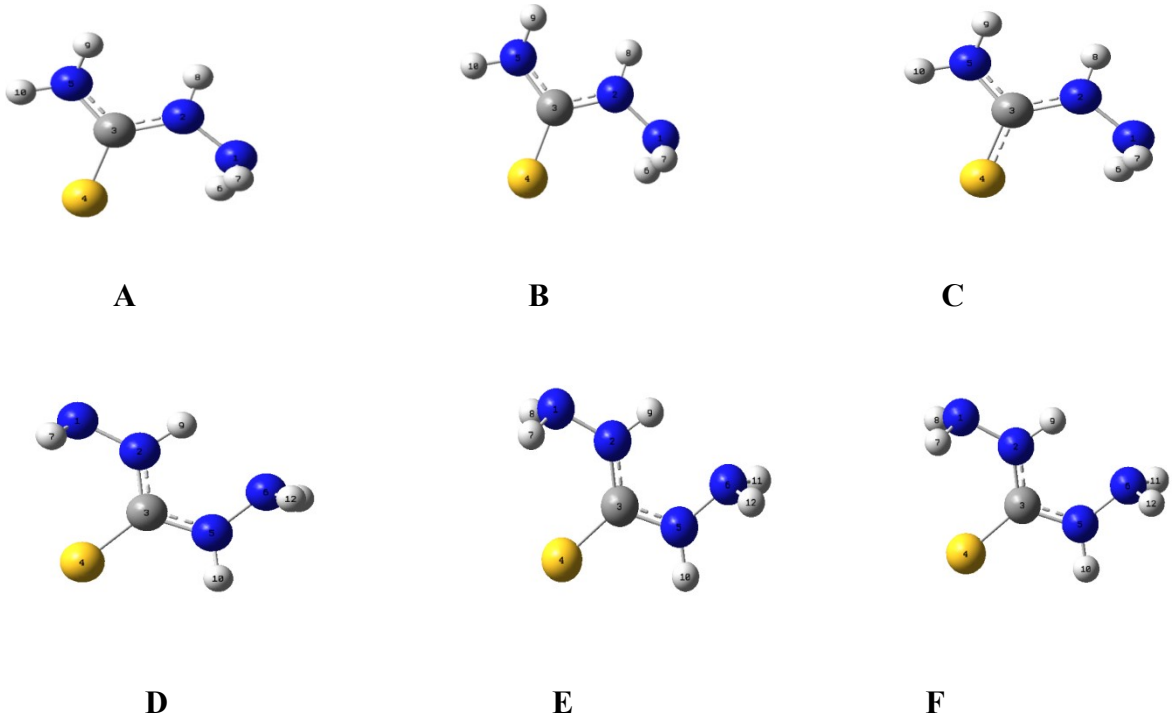
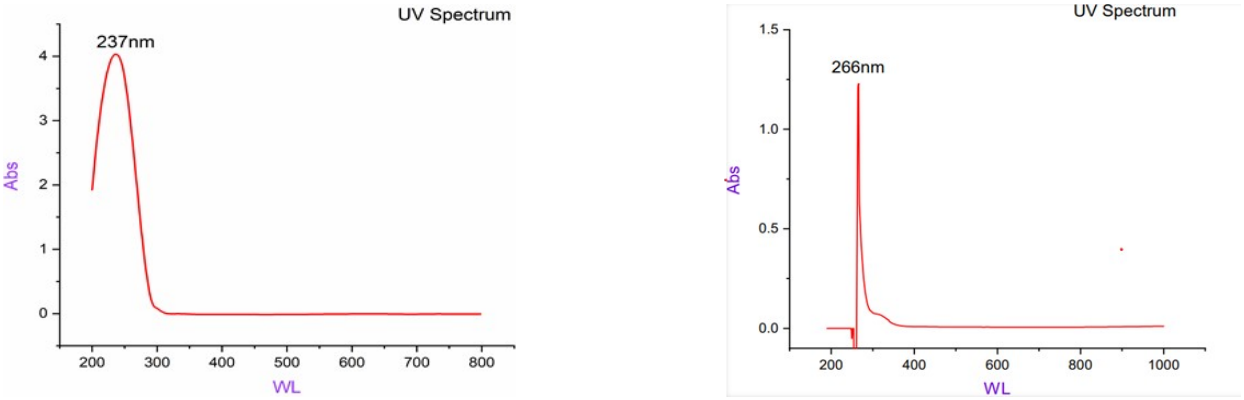
Figure S7. 3D representation of hydrogen bonding interactions (A-D) and 2D representation of hydrogen bonding and hydrophobic interactions (E) of compound TSCZ with different amino acid residues at active site of protein (PDB ID. 2WJE).

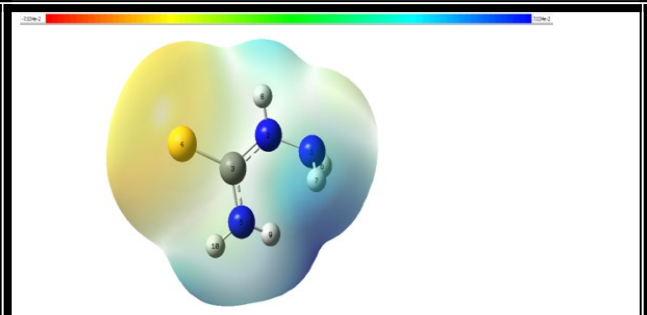
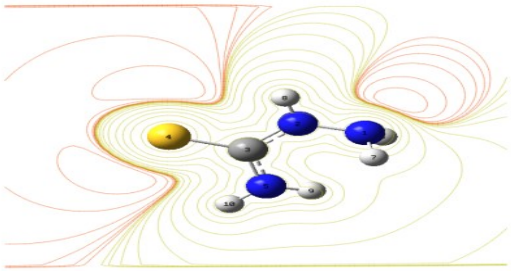
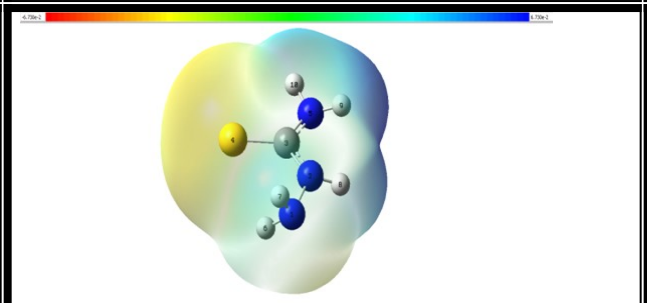
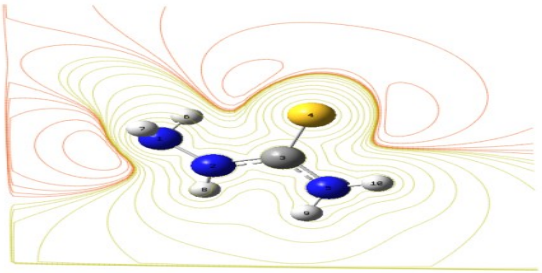
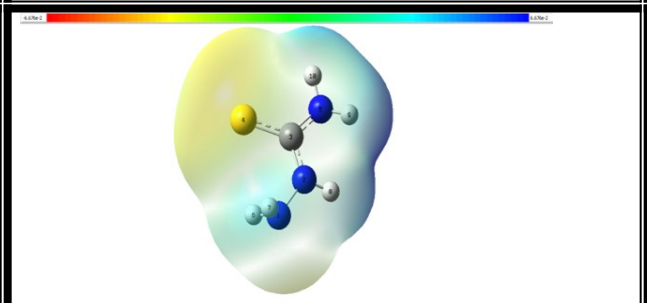
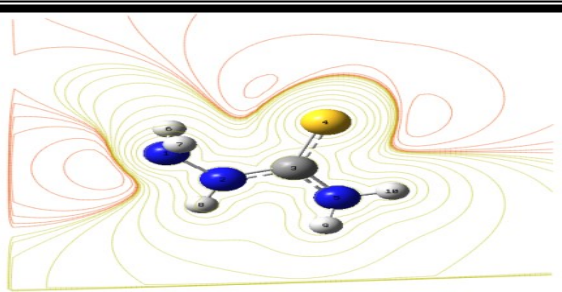
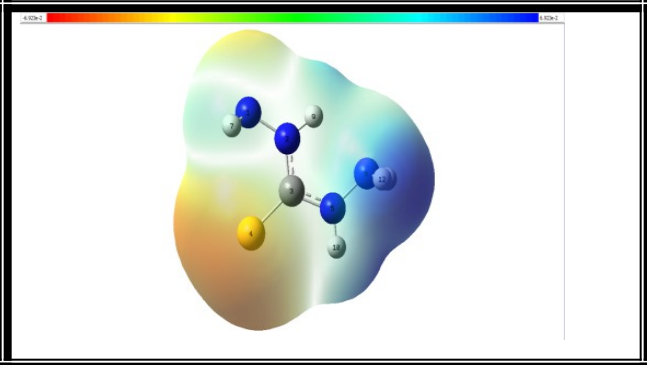
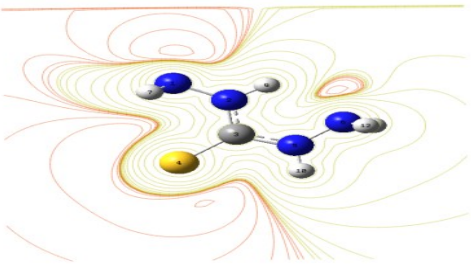
Figure S8. 3D representation of hydrogen bonding interactions (A-D) and 2D representation of hydrogen bonding and hydrophobic interactions (E) of compound TCHZ with different amino acid residues at active site of protein (PDB ID. 2WJE).

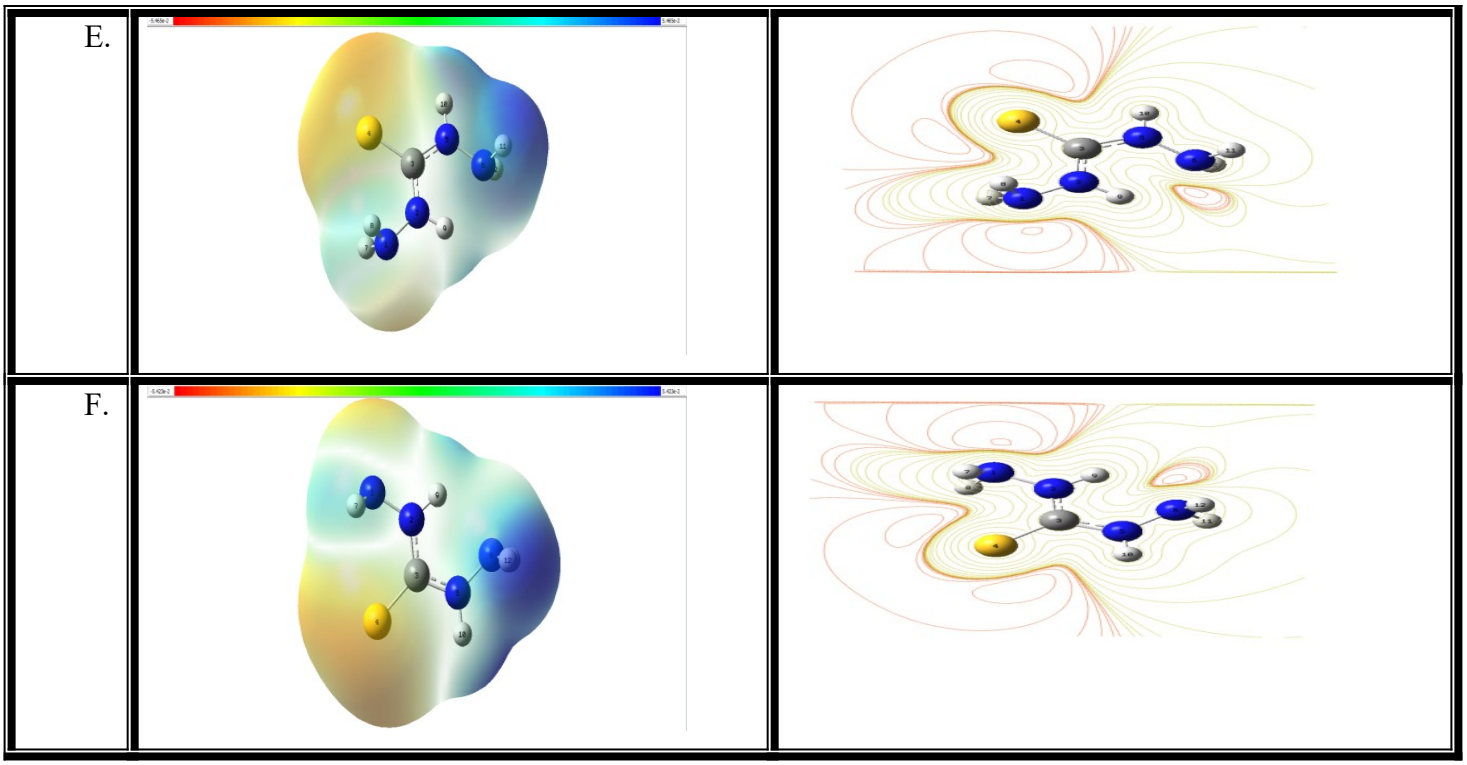


Supplementary Figure S1. Optimized geometries of TSCZ (A-C) and TCHZ (D-F) at Basis set 6-31G(d, p), 6-31+G(d', p') and 6-311+G(d, p) respectively.

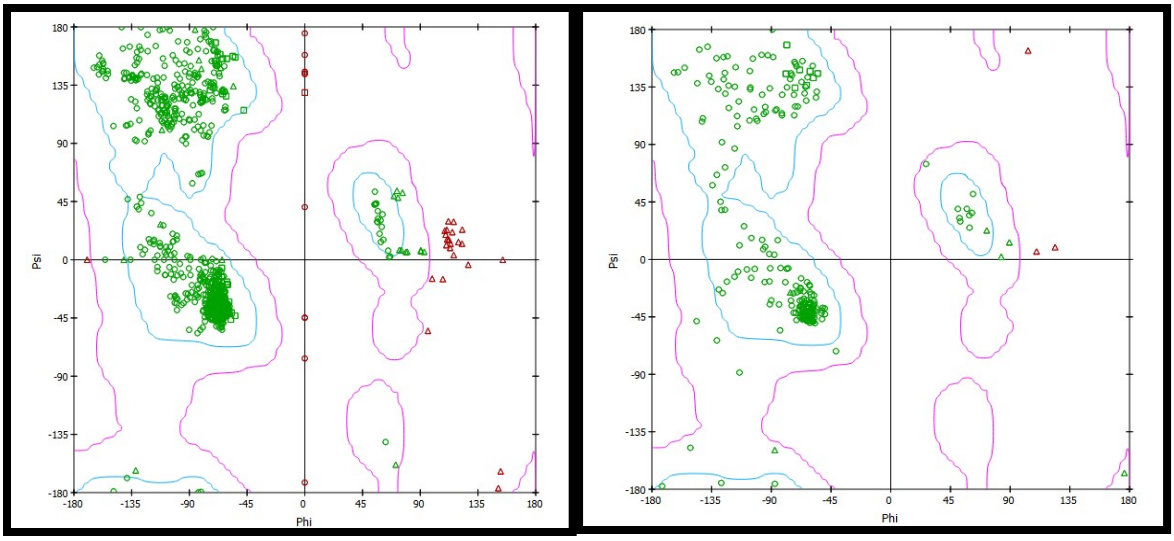


Supplementary Figure S2. Experimental UV spectra of TSCZ and TCHZ.

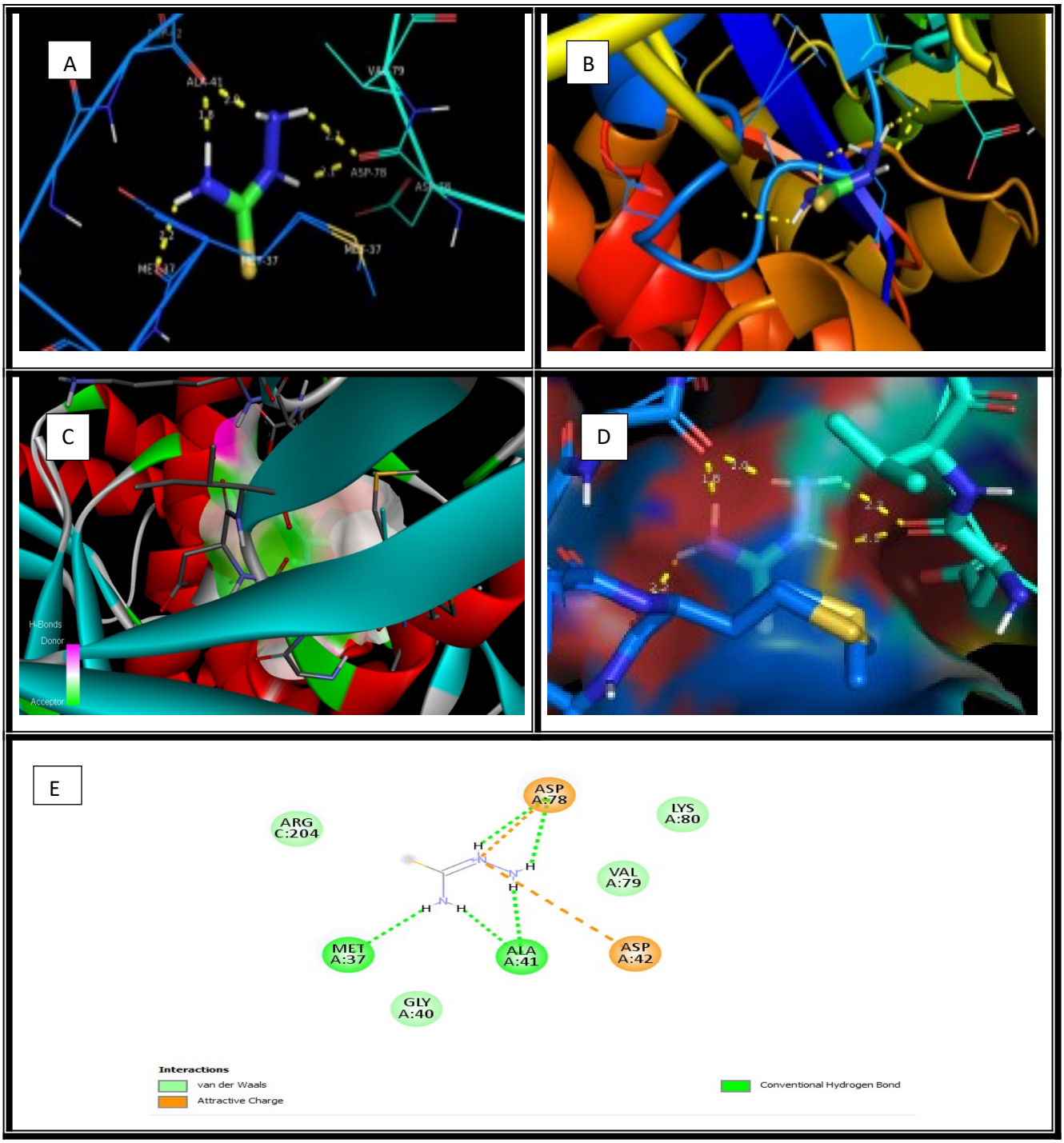
A.		
B.		
C.		
D.		



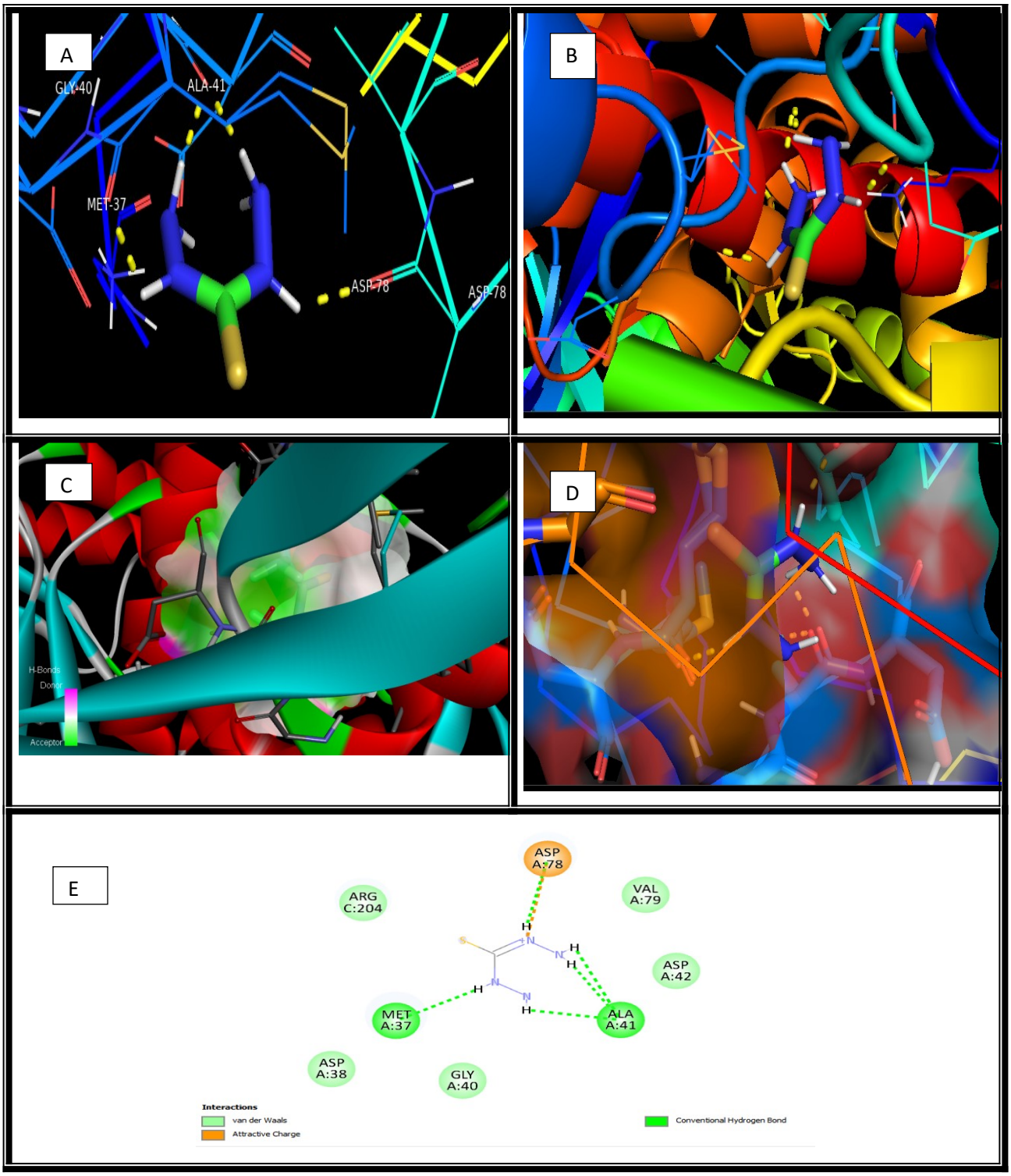
Supplementary Figure S3. MESP and ESP diagrams of TSCZ (A – C) and TCHZ (D – F).



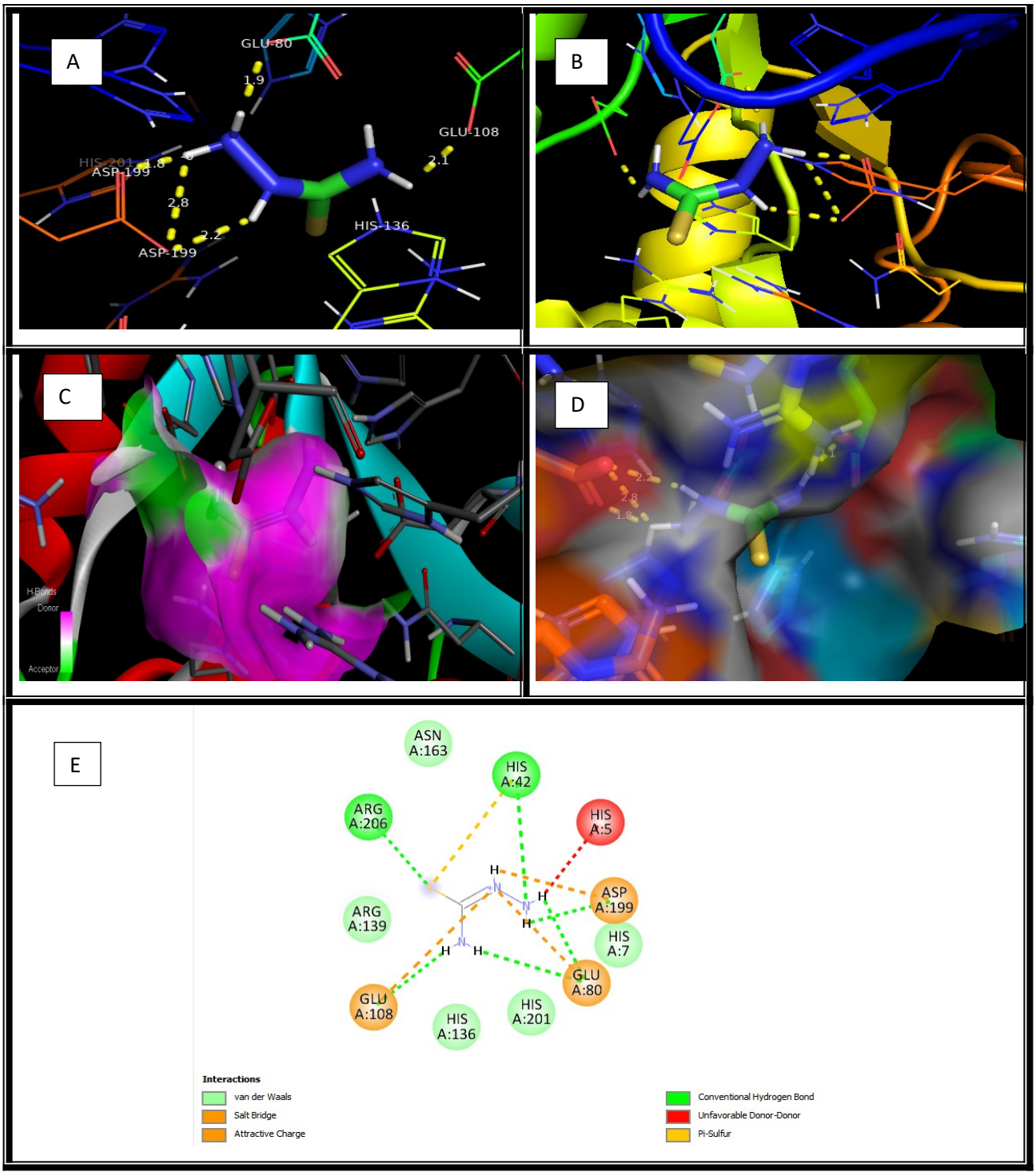
Supplementary Figure S4. Ramchandran diagram of PDB IDs. 6CLU and 2WJE respectively.



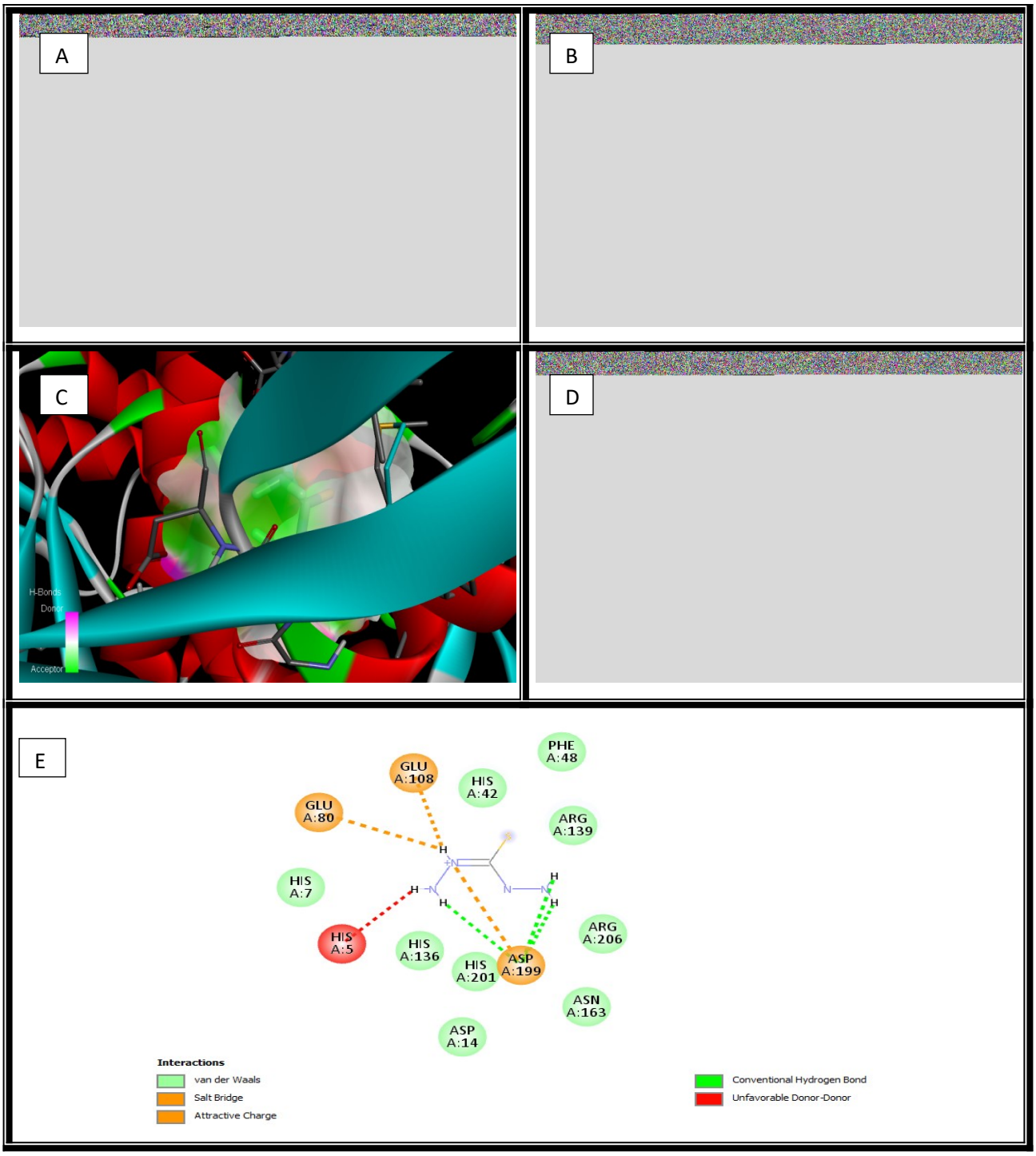
Supplementary Figure S5. 3D representation of hydrogen bonding interactions (A-D) and 2D representation of hydrogen bonding and hydrophobic interactions (E) of compound TSCZ with different amino acid residues at active site of protein (PDB ID. 6CLU).



Supplementary Figure S6. 3D representation of hydrogen bonding interactions (A-D) and 2D representation of hydrogen bonding and hydrophobic interactions (E) of compound TCHZ with different amino acid residues at active site of protein (PDB ID. 6CLU).



Supplementary Figure S7. 3D representation of hydrogen bonding interactions (A-D) and 2D representation of hydrogen bonding and hydrophobic interactions (E) of compound TSCZ with different amino acid residues at active site of protein (PDB ID. 2WJE).



Supplementary Figure S8. 3D representation of hydrogen bonding interactions (A-D) and 2D representation of hydrogen bonding and hydrophobic interactions (E) of compound TCHZ with different amino acid residues at active site of protein (PDB ID. 2WJE).