

Study of Oxadiazole derivatives as precursor for multi-functional inhibitor to SARS-CoV-2: A detailed virtual

Vikash Kumar, <https://orcid.org/0009-0001-2422-2965>

Sumit Kumar*, <https://orcid.org/0000-0002-5695-5944>

Department of Chemistry, Magadh University, Bodh Gaya 824234, Bihar, India

Accepted manuscript
Supplementary

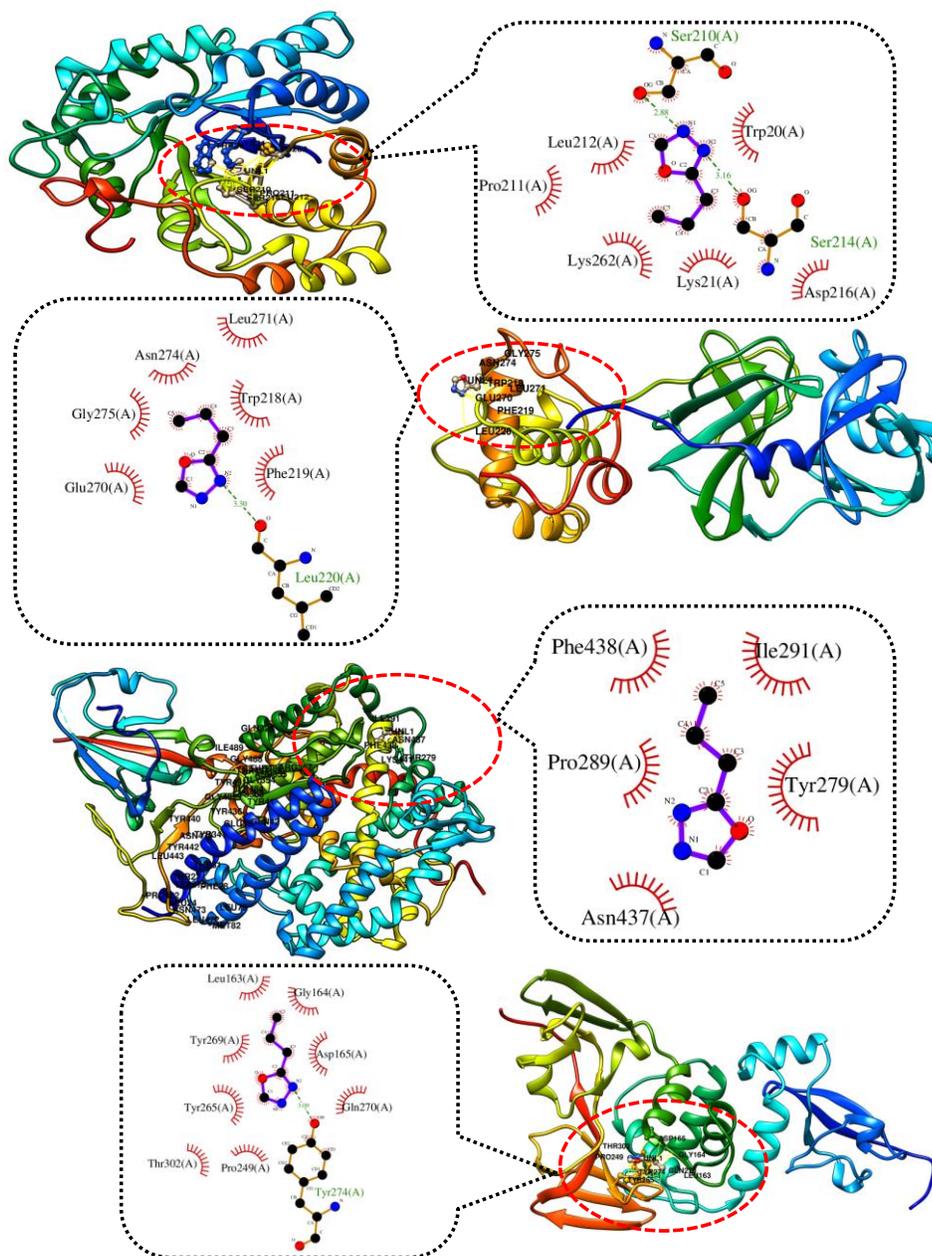


Fig. S1. Lowest binding energy docking pose of oxa2 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

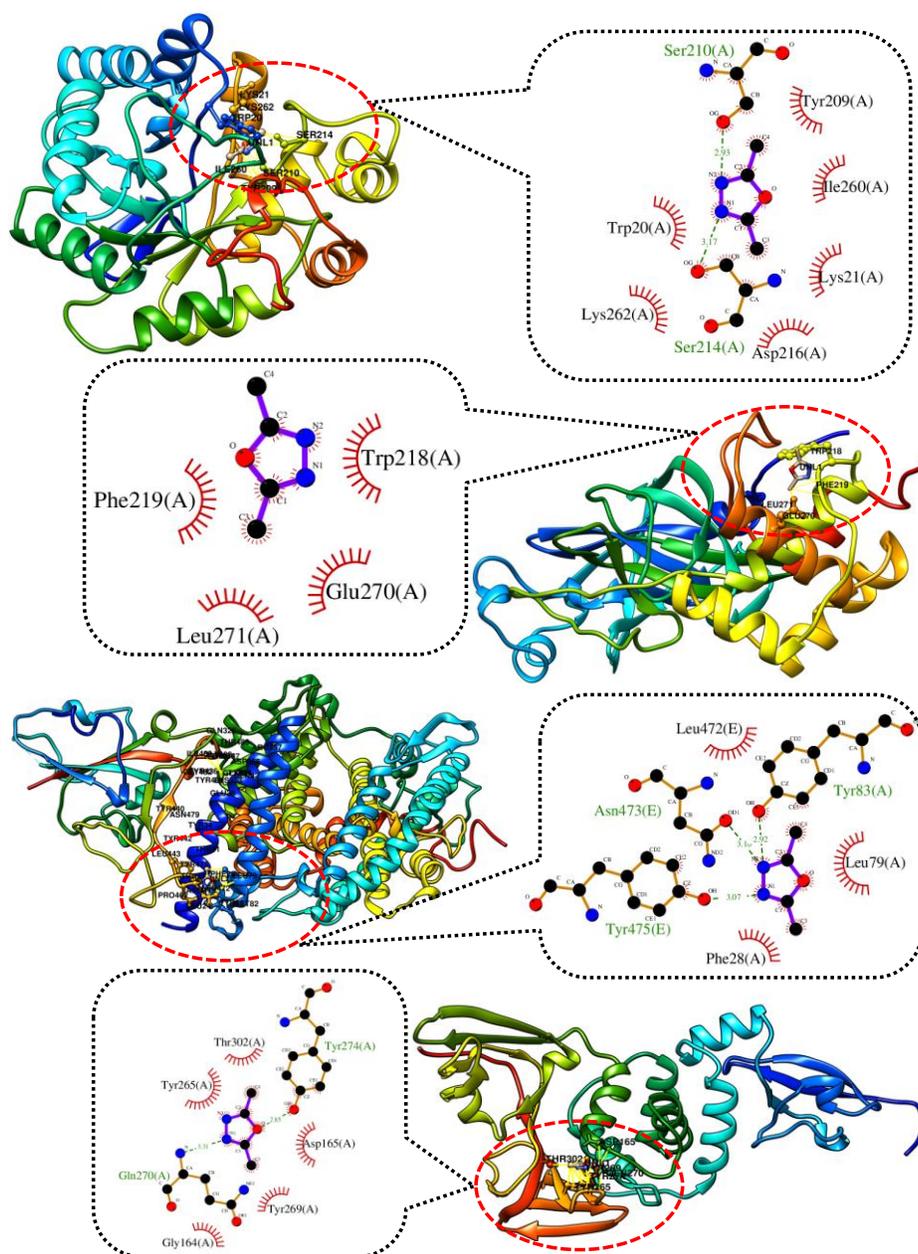


Fig. S2. Lowest binding energy docking pose of oxa3 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

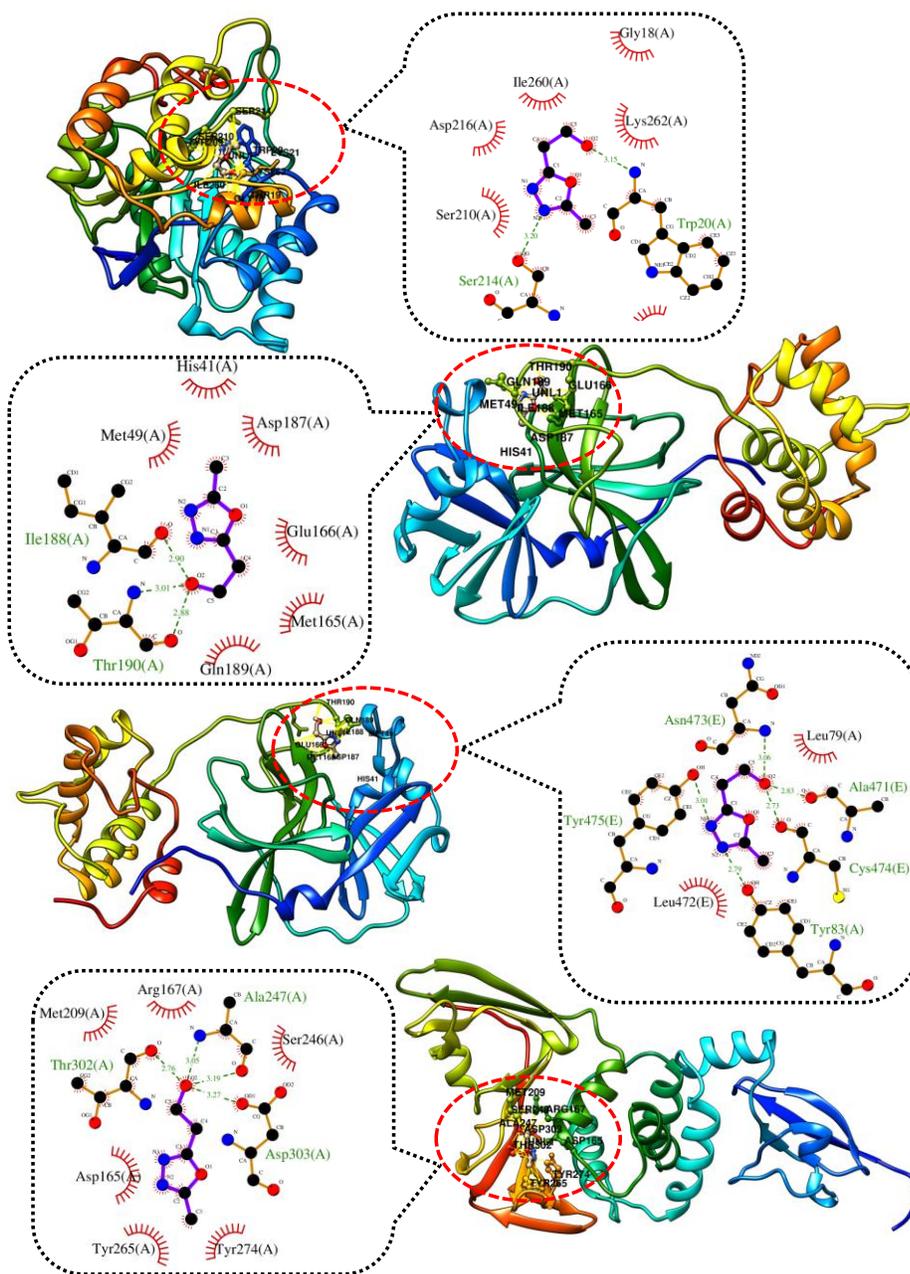


Fig. S3. Lowest binding energy docking pose of oxa4 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

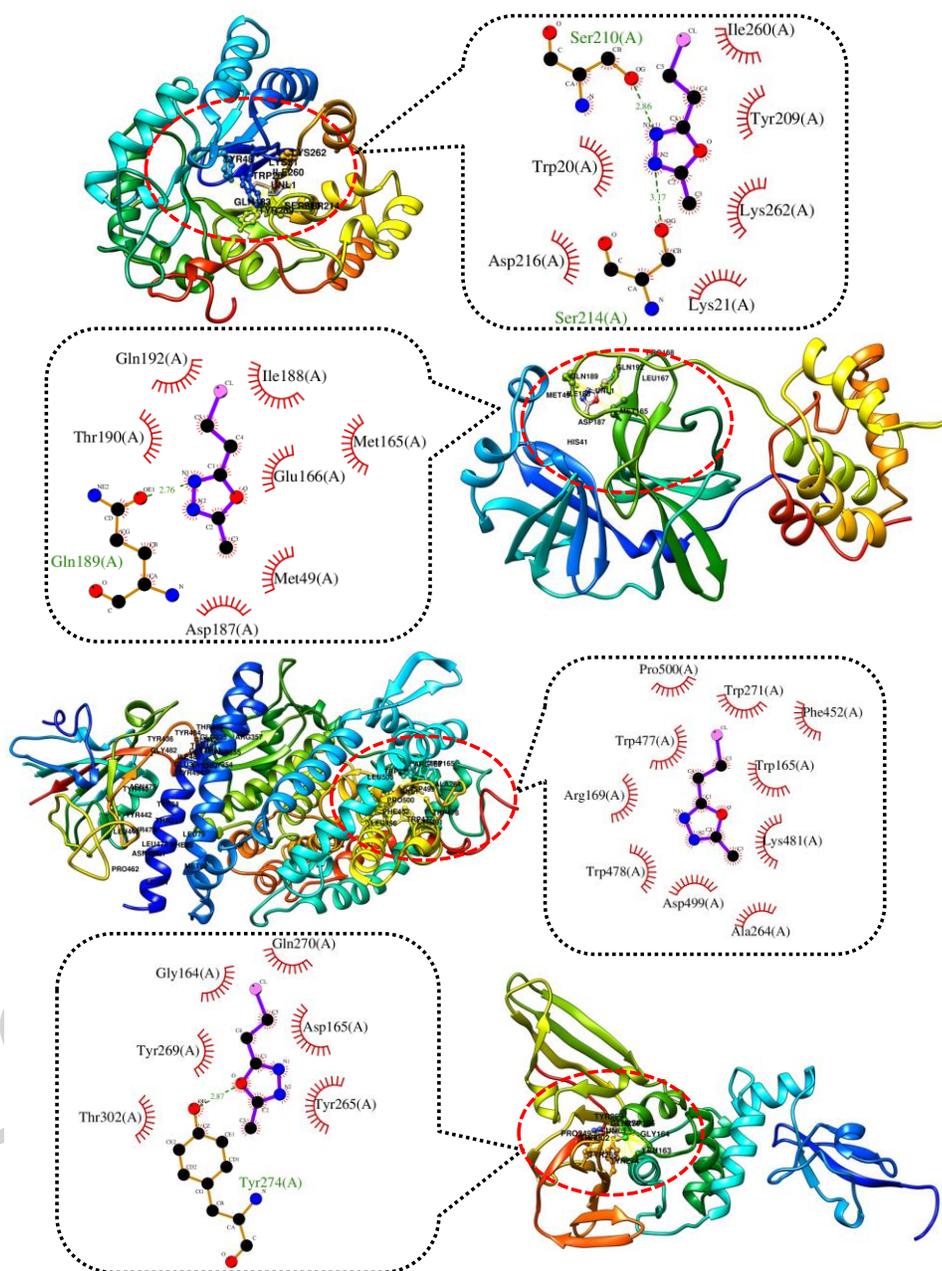


Fig. S4. Lowest binding energy docking pose of oxa5 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

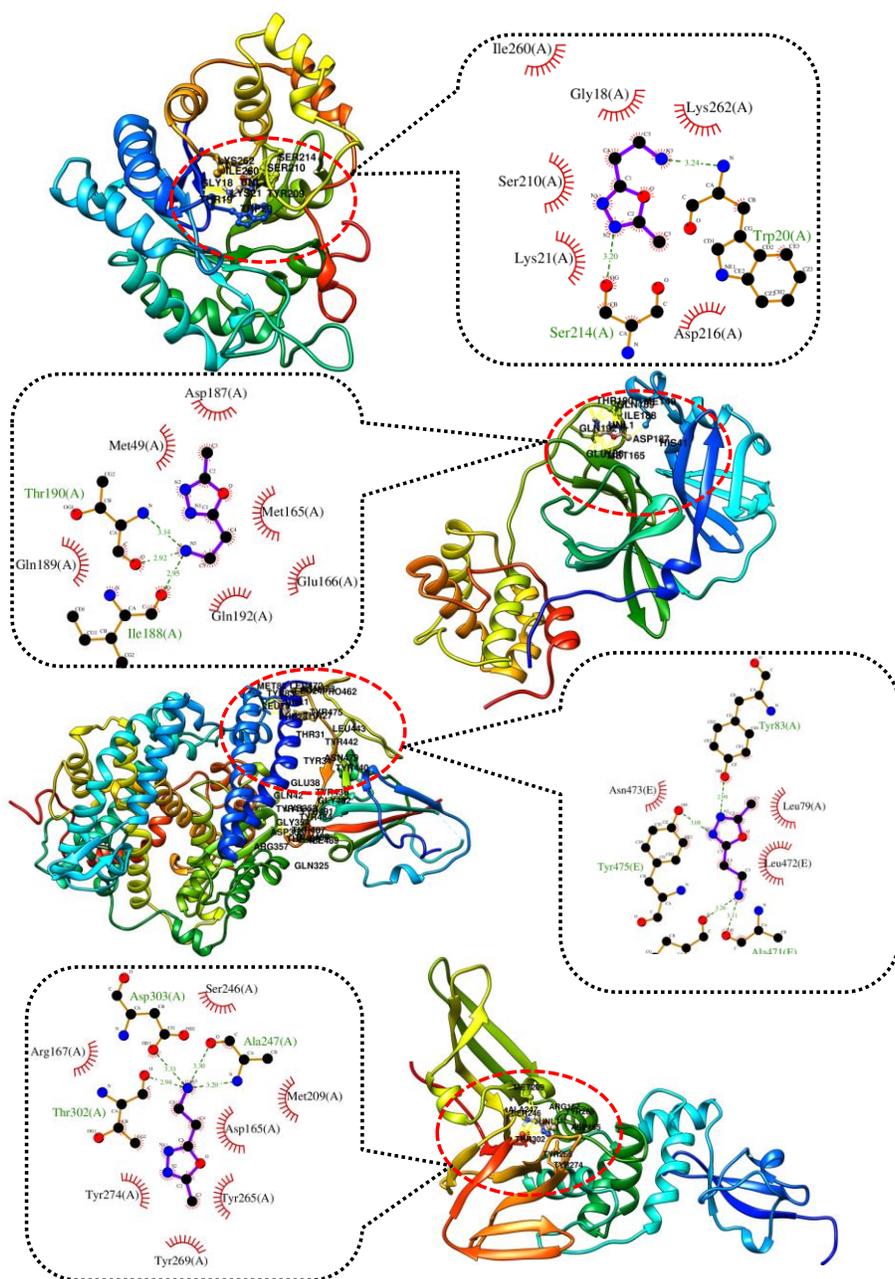


Fig. S5. Lowest binding energy docking pose of oxa6 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

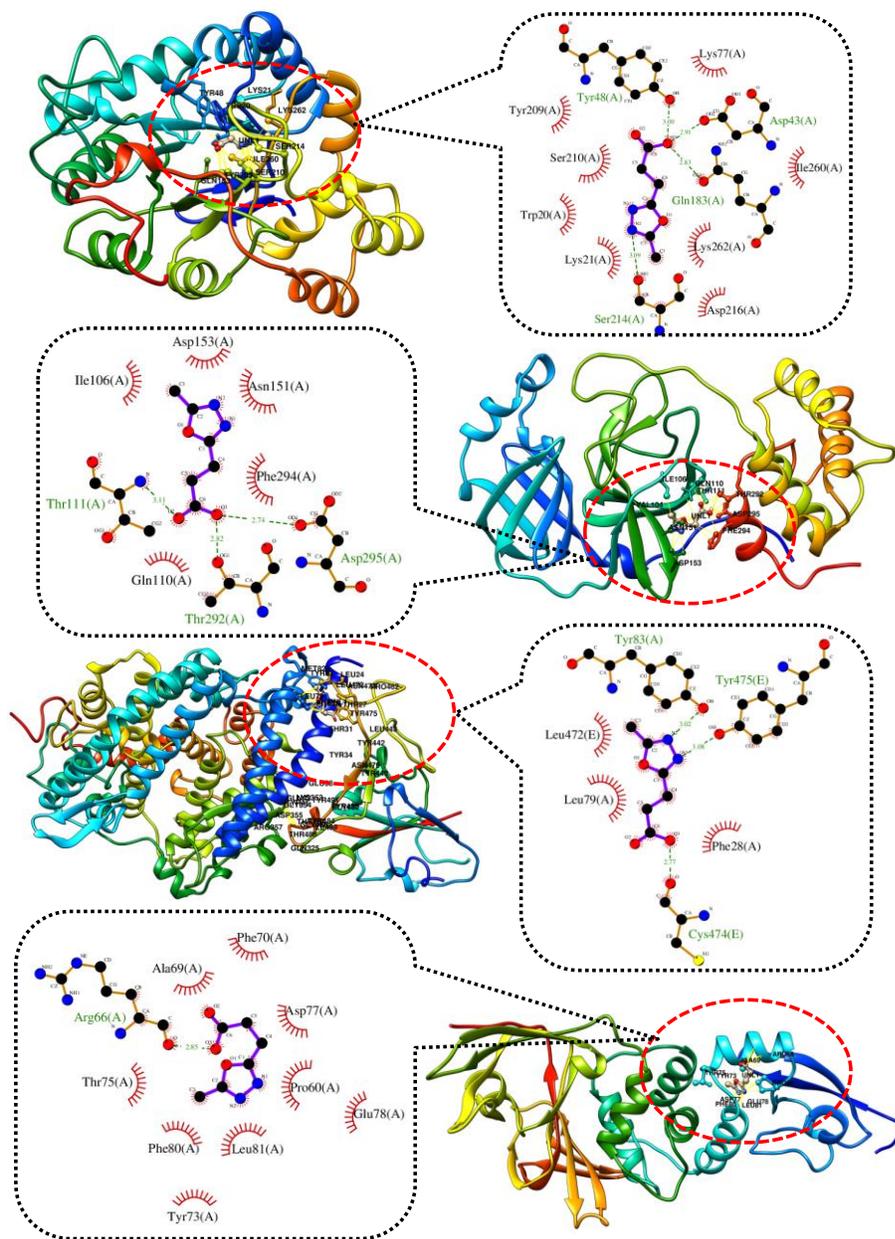


Fig. S6. Lowest binding energy docking pose of oxa7 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

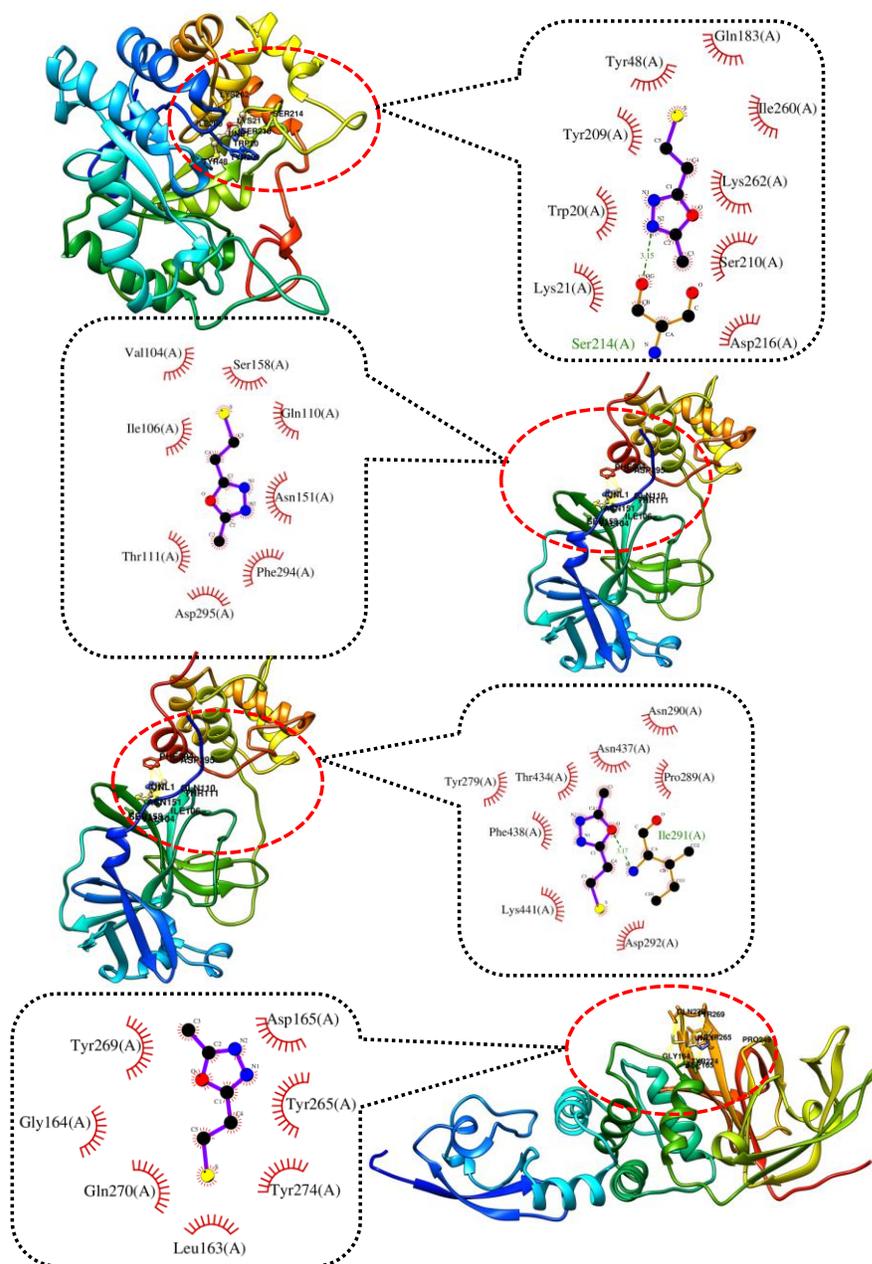


Fig. S7. Lowest binding energy docking pose of oxa9 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S