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SUPPLEMENTARY

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

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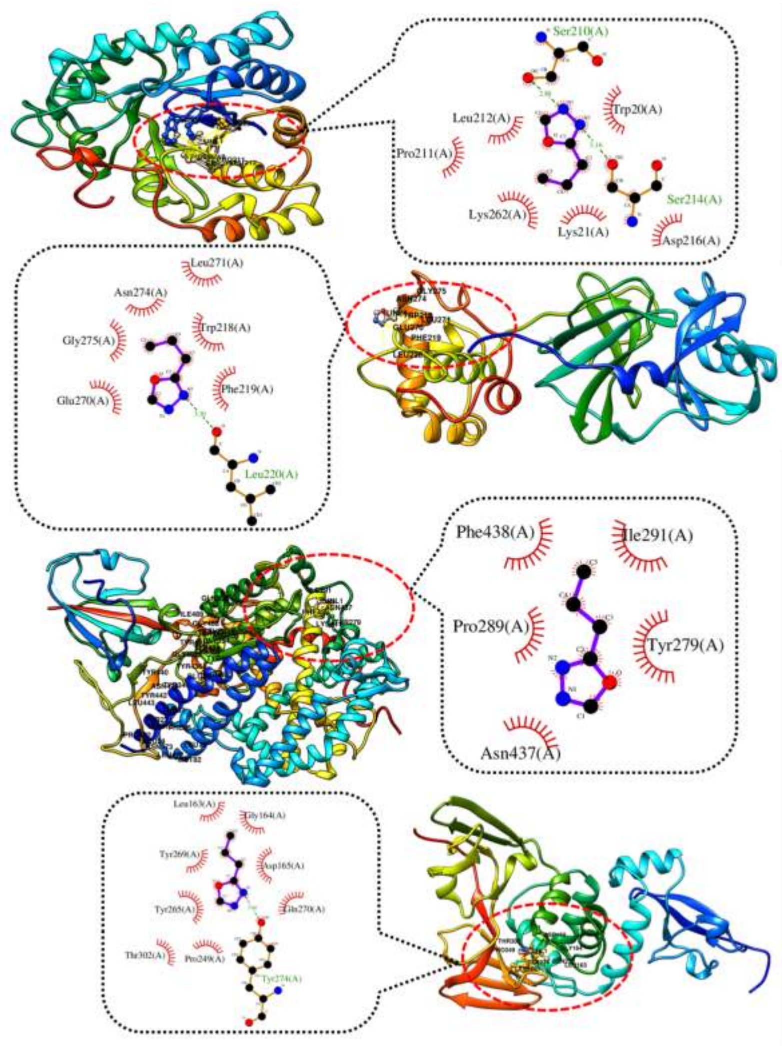

Fig. S1. Lowest binding energy docking pose of Oxa2 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

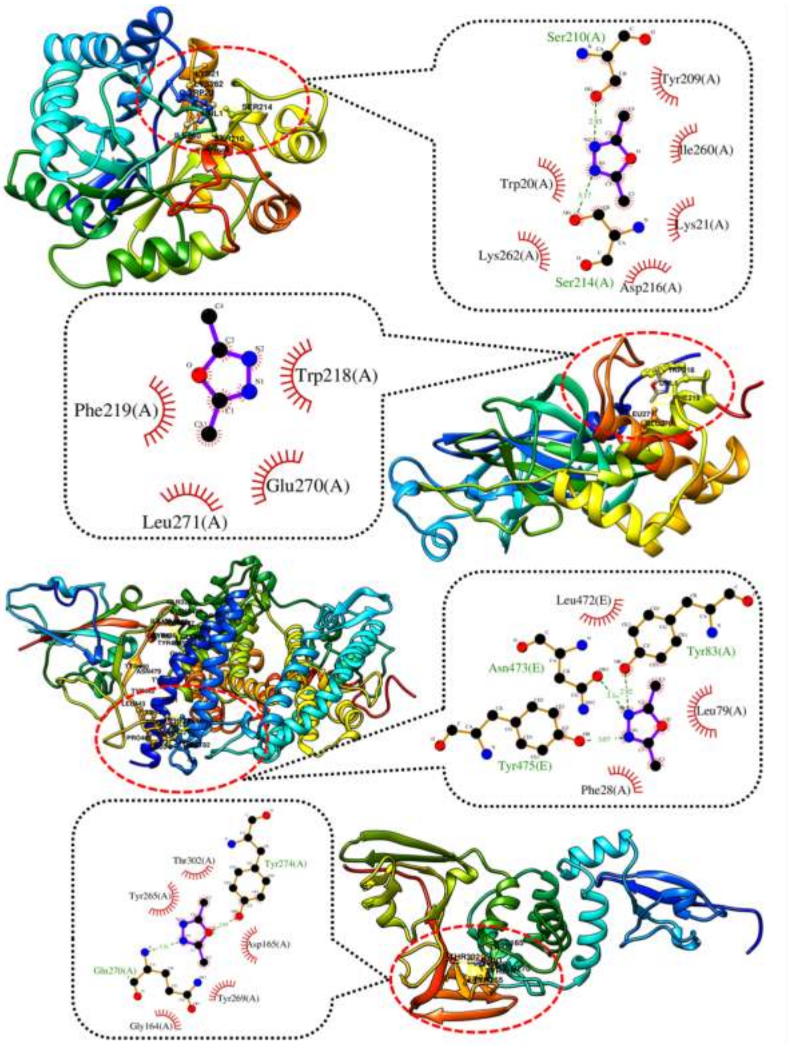

Fig. S2. Lowest binding energy docking pose of Oxa3 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

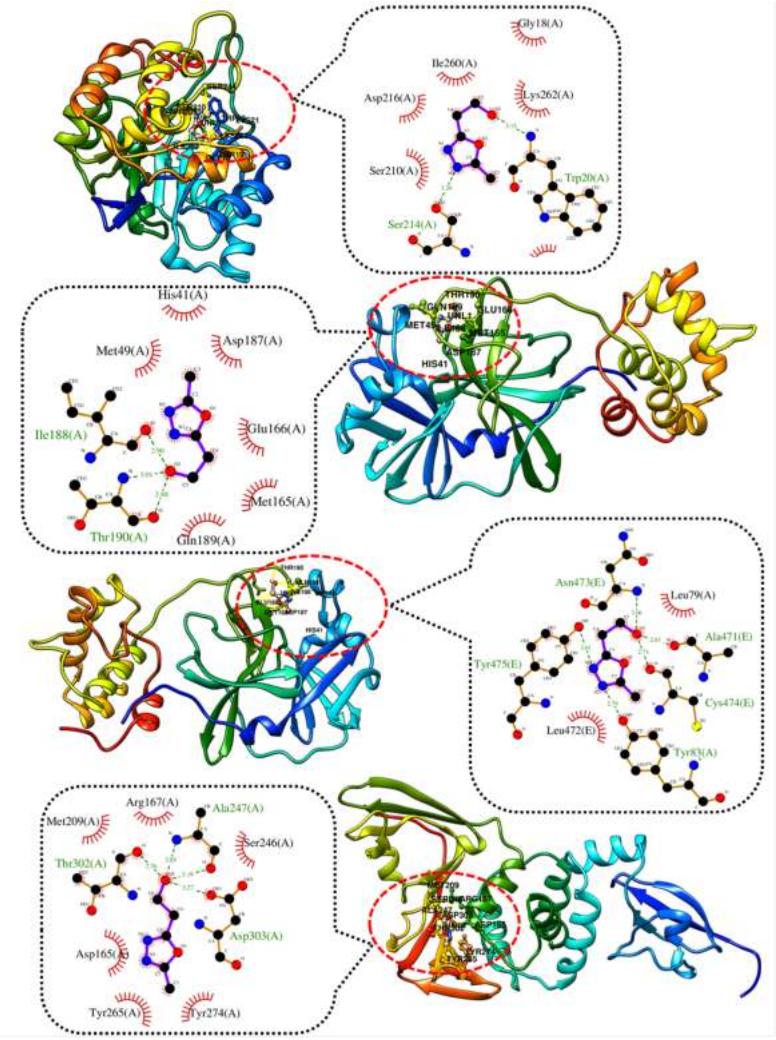

Fig. S3. Lowest binding energy docking pose of Oxa4 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

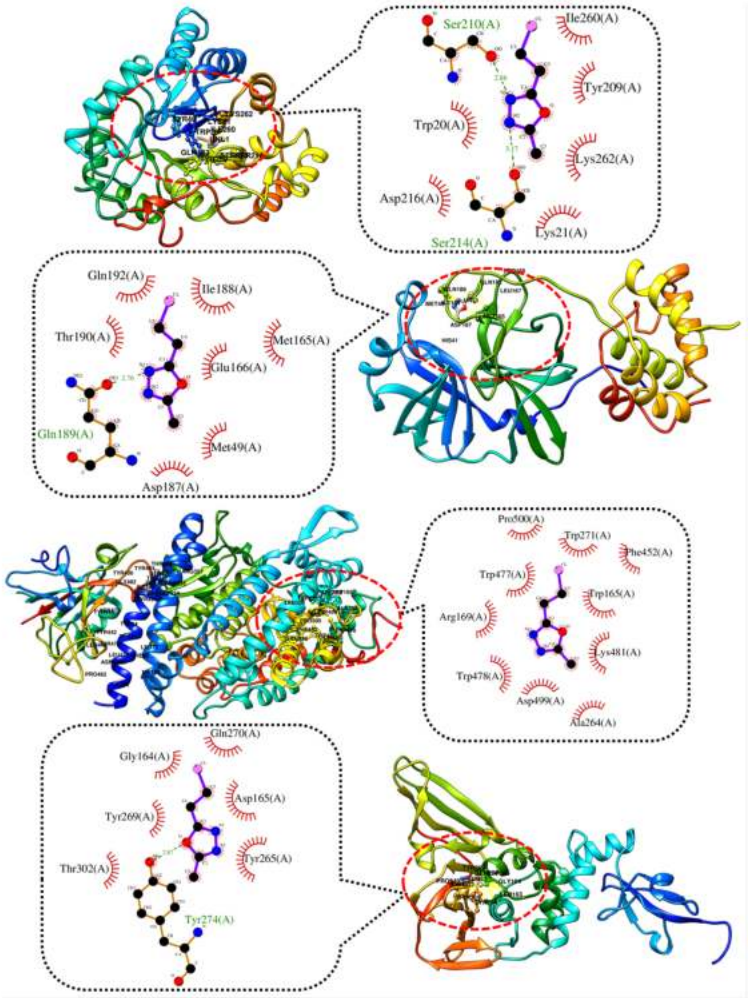

Fig. S4. Lowest binding energy docking pose of Oxa5 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

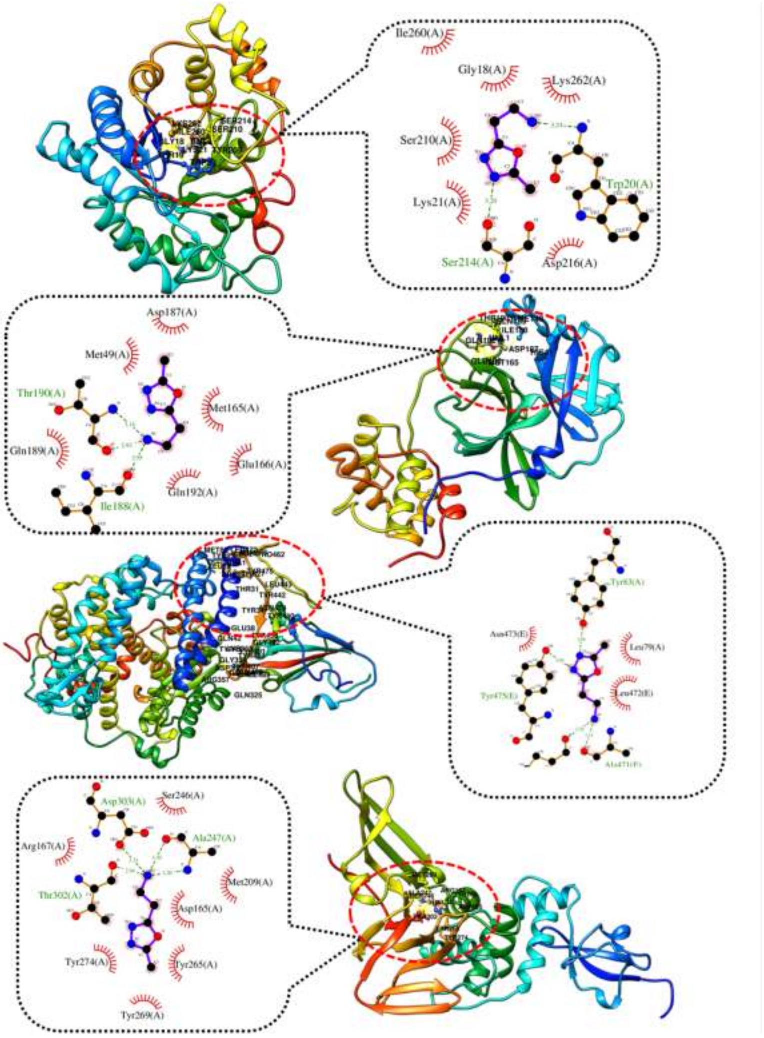

Fig. S5. Lowest binding energy docking pose of Oxa6 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S(3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

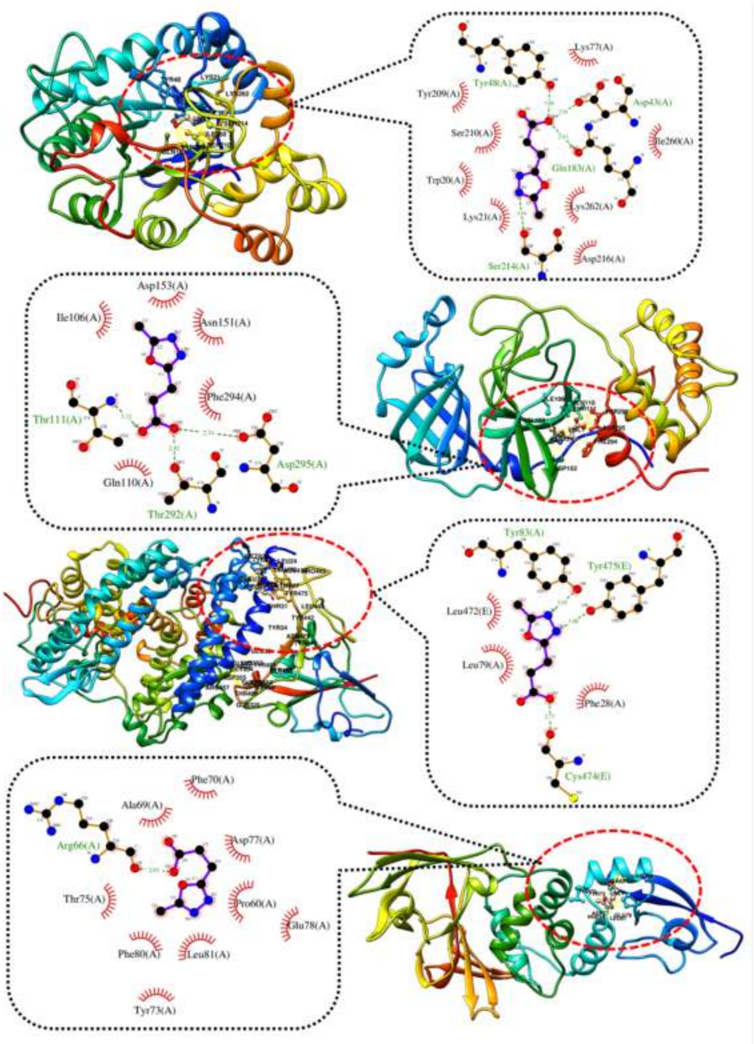

Fig. S6. Lowest binding energy docking pose of Oxa7 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S

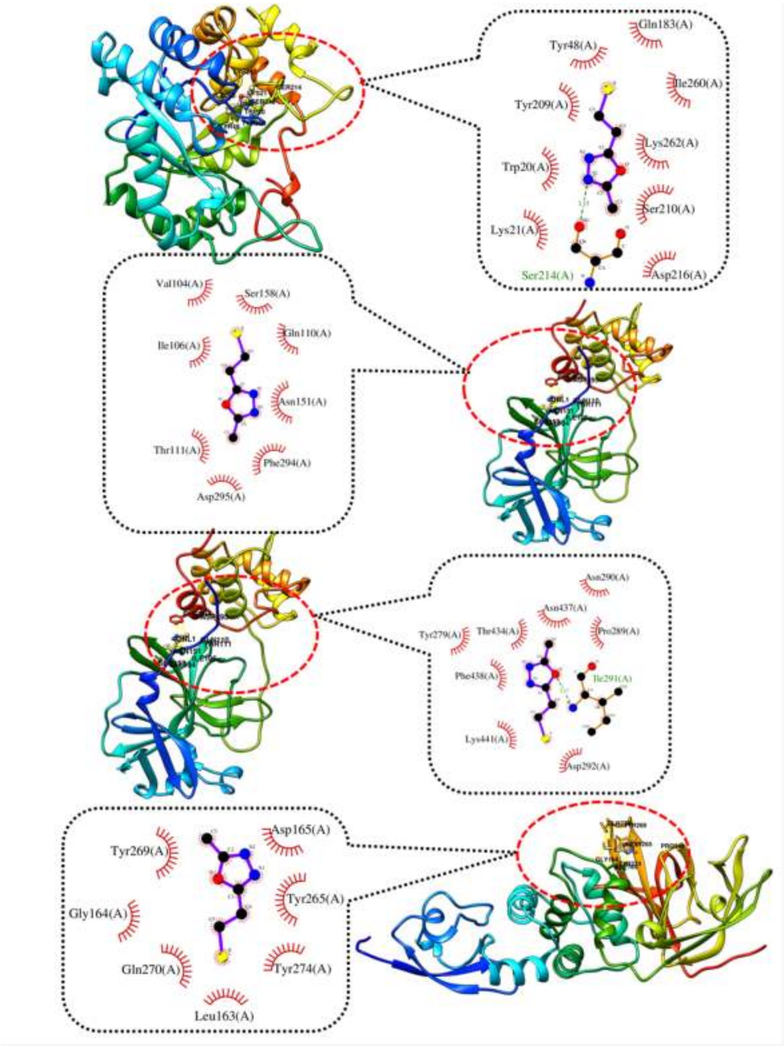

Fig. S7. Lowest binding energy docking pose of Oxa9 in the (a) transmembrane serine protease 2(TMPRSS2) PDB ID: 1Z8A; (b) angiotensin-converting enzyme 2 (ACE 2) PDB ID: 3D0G; (c) 3-chymotrypsin-like protease (3CLpro) PDB ID: 3AW0 and papain-like protease (PLpro) PDB ID: 3E9S