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Evaluation of predictive machine learning models for drug repurposing against delta variant of SARS-CoV-2 spike protein

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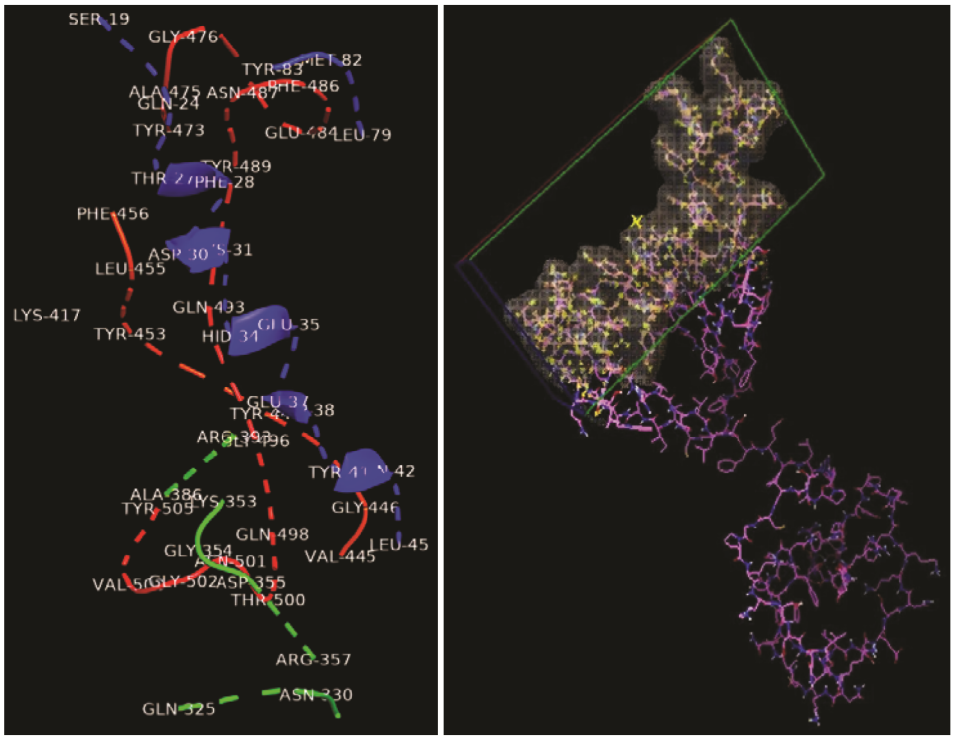
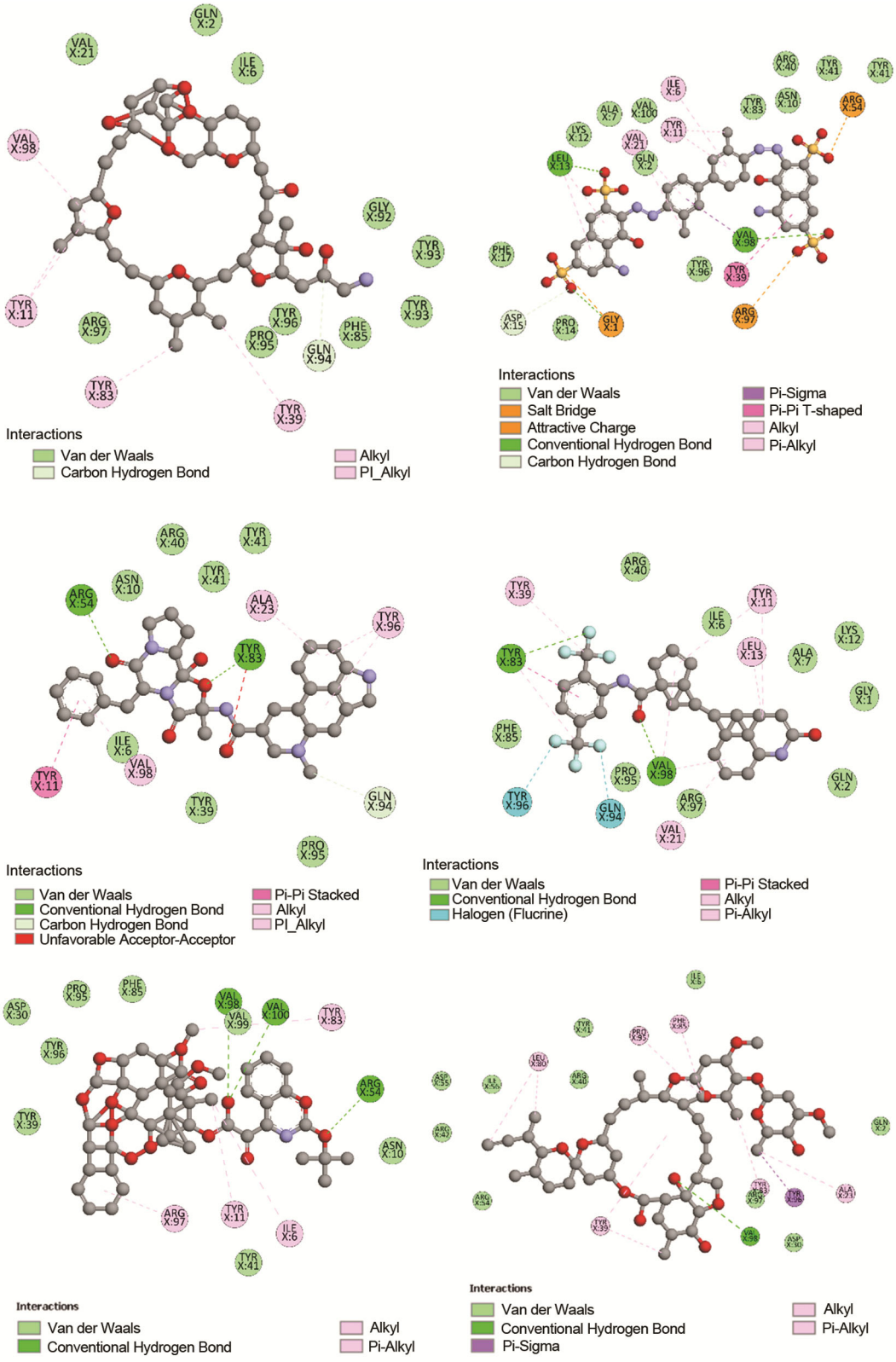
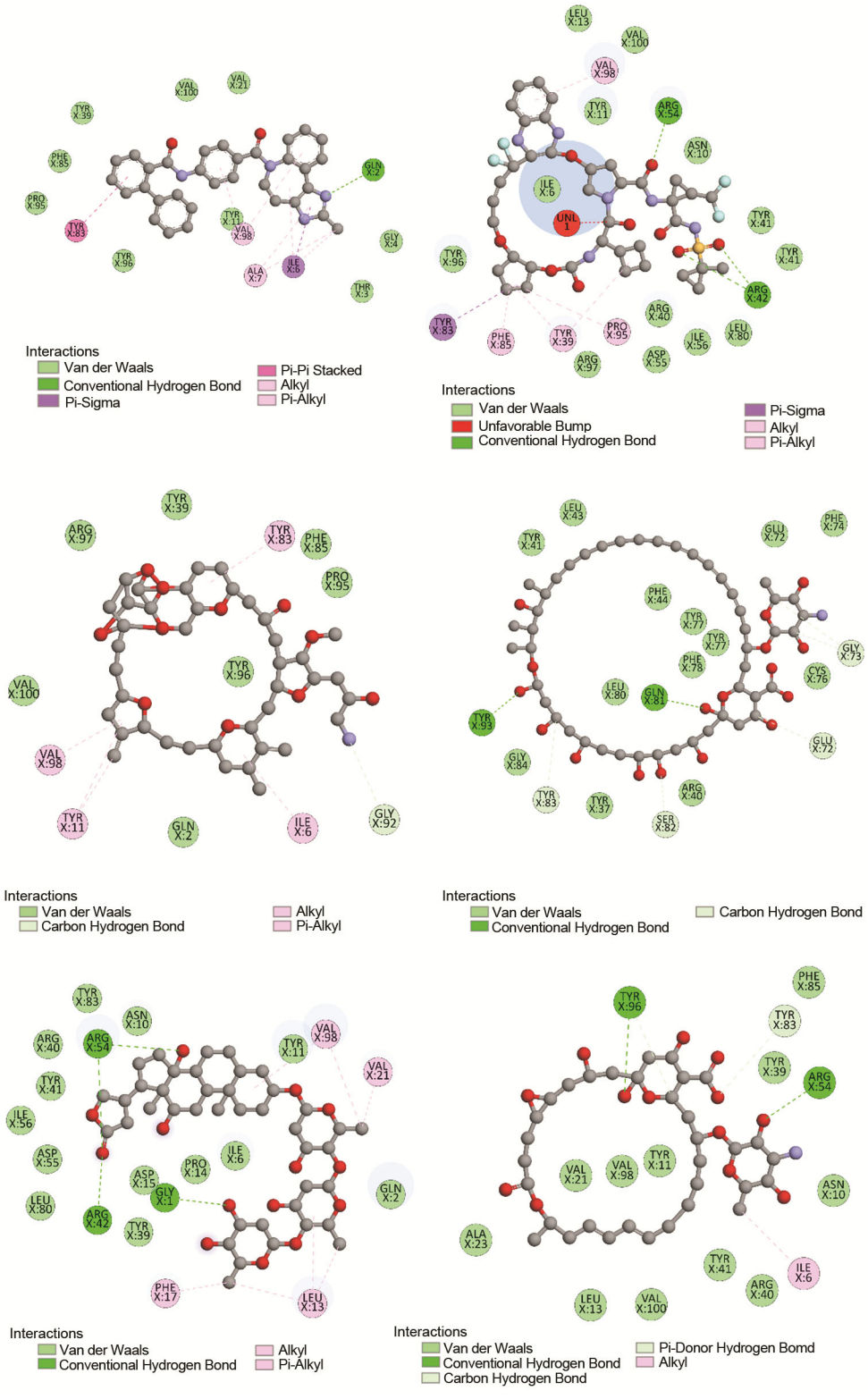
Supplementary Data



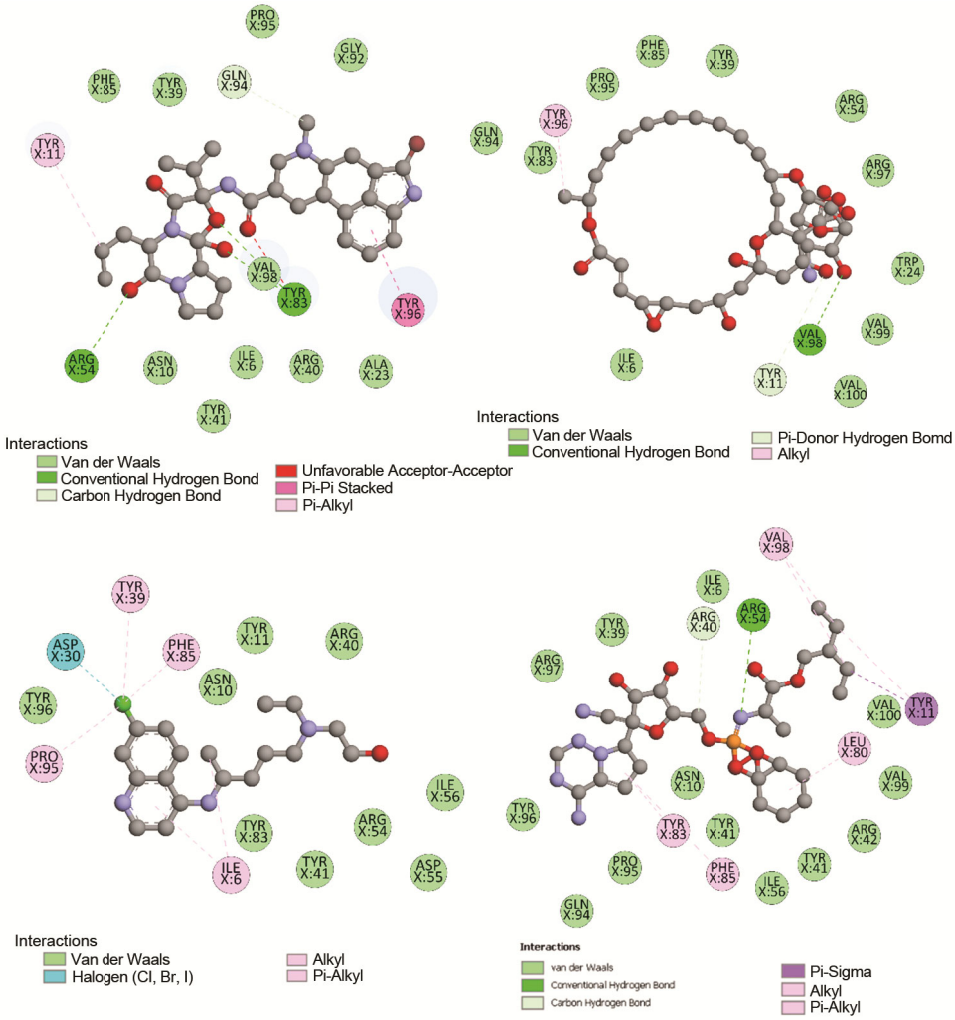
Suppl. Fig. 1 — (A) Predicted active site residues; and (B) Docking grid generation by Autodock Vina on the modelled spike protein. Docking Grid Dimensions: Grid box = 56 × 60 × 112 with a spacing of 0.375. The binding pocket was set at x = 78.999, y = -17.378, and z = -13.748


Interactions
Van der Waals
Carbon Hydrogen Bond
Alkyl
PI_Alkyl
Interactions
Van der Waals
Salt Bridge
Attractive Charge
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Sigma
Pi-Pi T-shaped
Alkyl
Pi-Alkyl
Interactions
Van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Pi Stacked
Alkyl
PI_Alkyl
Interactions
Van der Waals
Conventional Hydrogen Bond
Halogen (Flucrine)
Pi-Pi Stacked
Alkyl
Pi-Alkyl
Interactions
Van der Waals
Conventional Hydrogen Bond
Alkyl
Pi-Alkyl
Interactions
Van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Alkyl
Pi-Alkyl

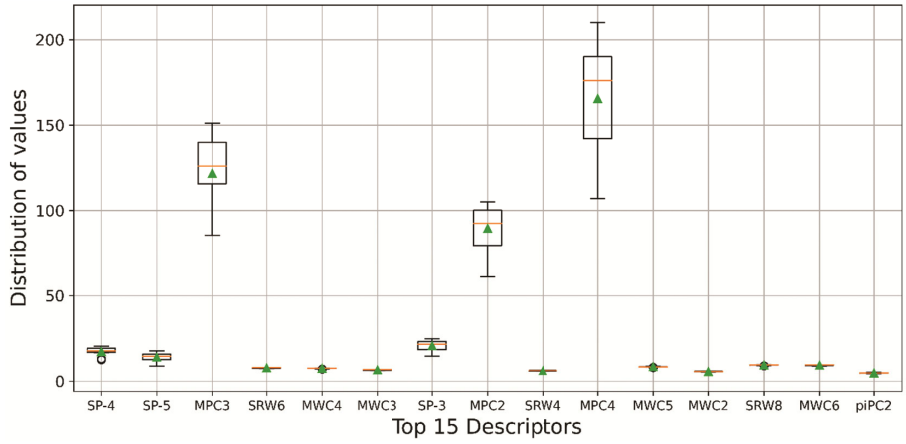
(*Contd*).


Interactions
Van der Waals
Conventional Hydrogen Bond
Pi-Sigma
Pi-Pi Stacked
Alkyl
Pi-Alkyl
Interactions
Van der Waals
Unfavorable Bump
Conventional Hydrogen Bond
Pi-Sigma
Alkyl
Pi-Alkyl
Interactions
Van der Waals
Carbon Hydrogen Bond
Alkyl
Pi-Alkyl
Interactions
Van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Interactions
Van der Waals
Conventional Hydrogen Bond
Alkyl
Pi-Alkyl
Interactions
Van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Donor Hydrogen Bomd
Alkyl

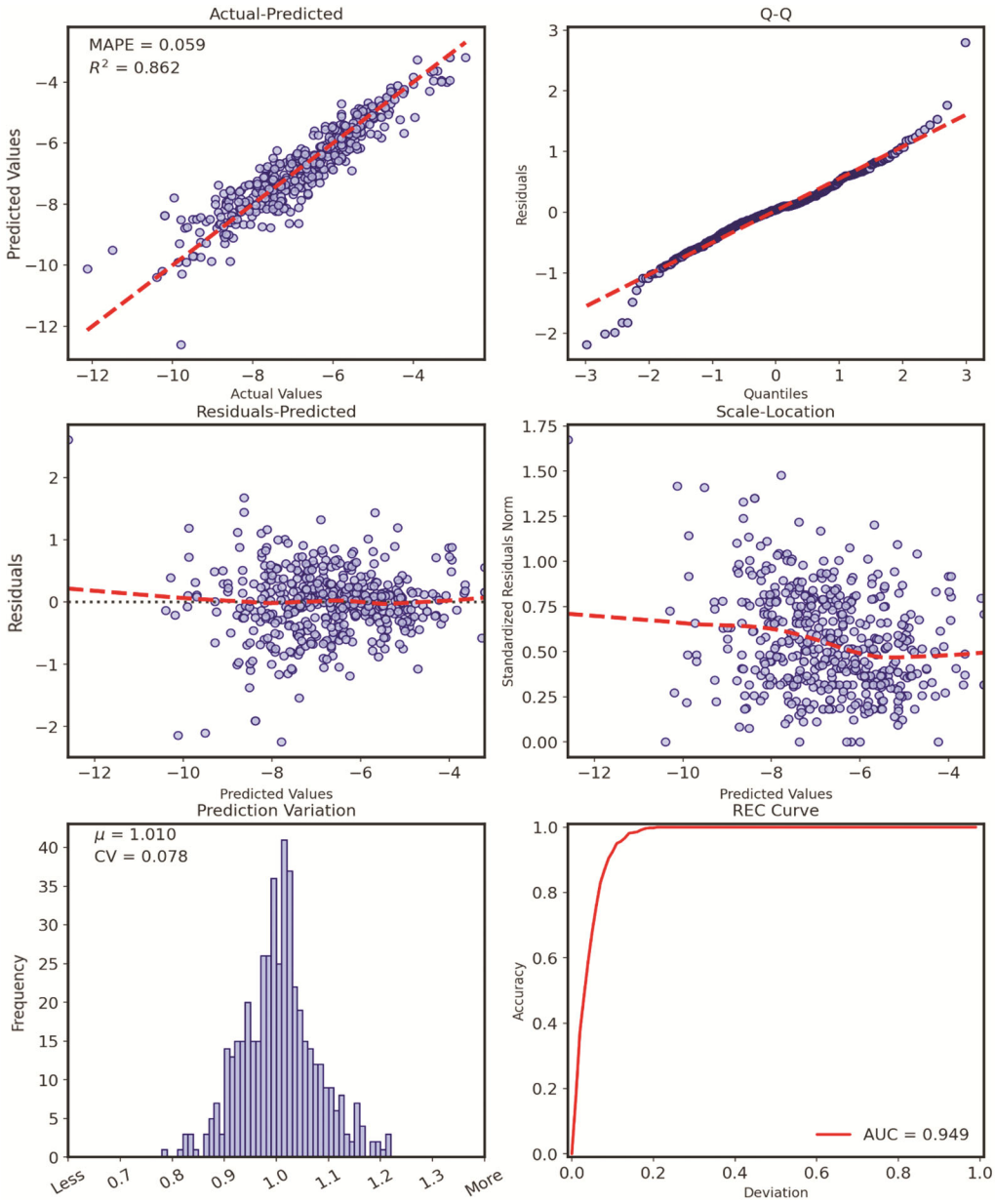
(*Contd*).



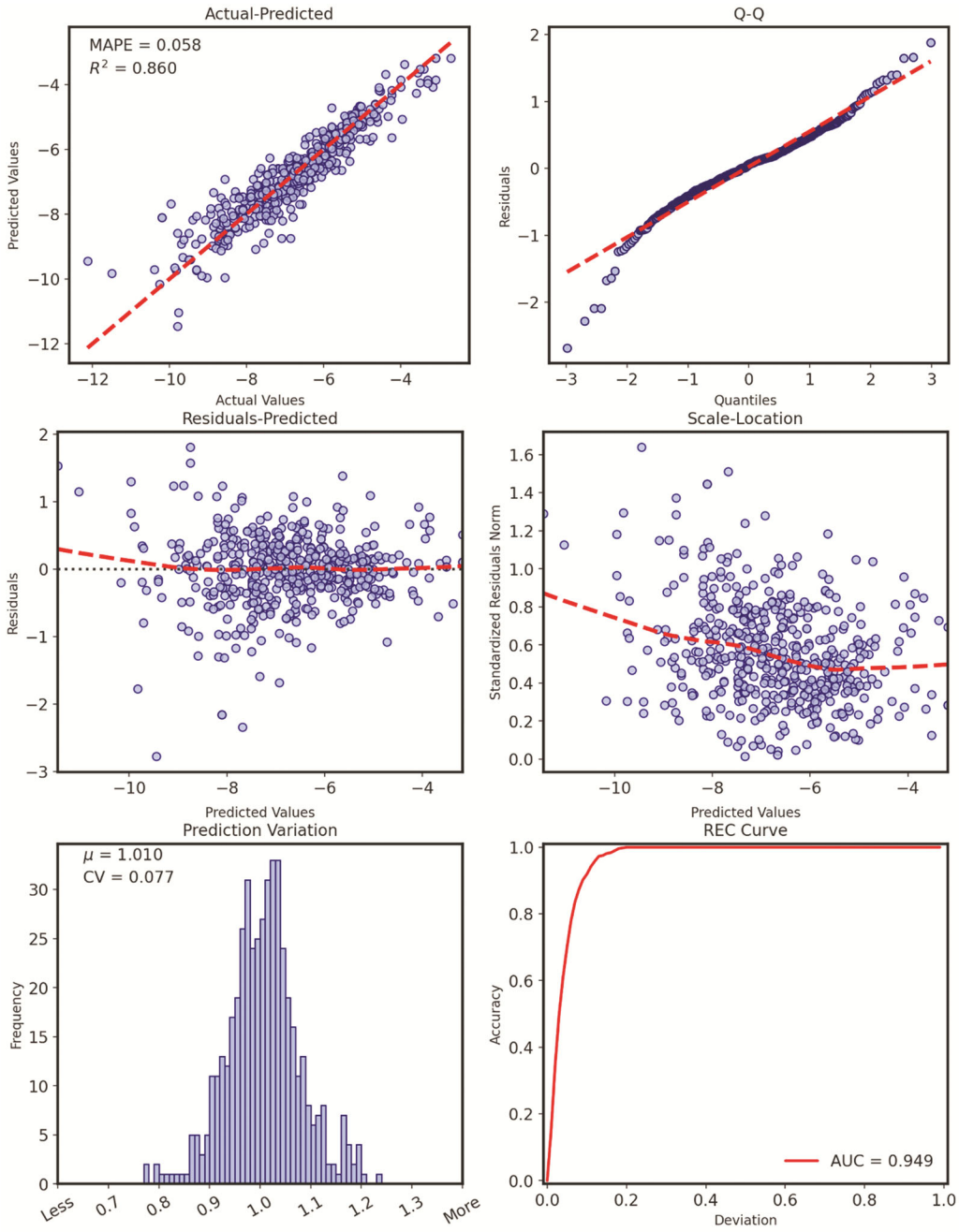
Suppl. Fig. 2 (A-P) — 2D interaction diagram of top 7-20 potential drugs that can inhibit the binding of spike protein and hACE2 protein (A) ZINC000169621219, (B) ZINC000169289767, (C) ZINC000003978005, (D) ZINC000003932831, (E) ZINC000085536932, (F) ZINC000253630390, (G) ZINC000012503187, (H) ZINC000164528615, (I) ZINC000169344691, (J) ZINC000253387843, (K) ZINC000242548690, (L) ZINC000169621220, (M) ZINC000053683151, (N) ZINC000008220909 (O) Hydroxychloroquine (P) Remdesivir



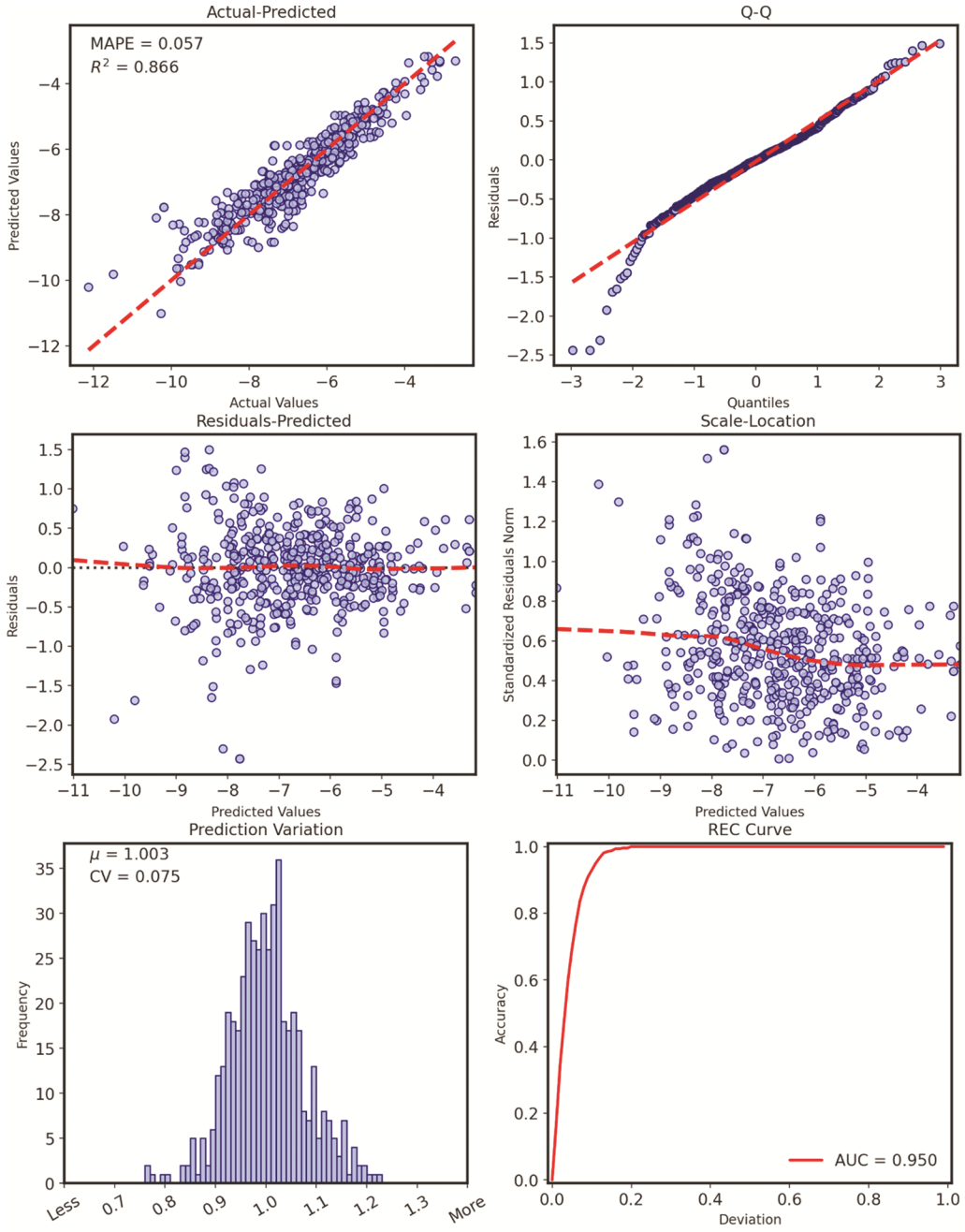
Suppl. Fig. 3 — Graph of the top 15 molecular descriptors and their range of values for the top 20 potential drugs/inhibitors



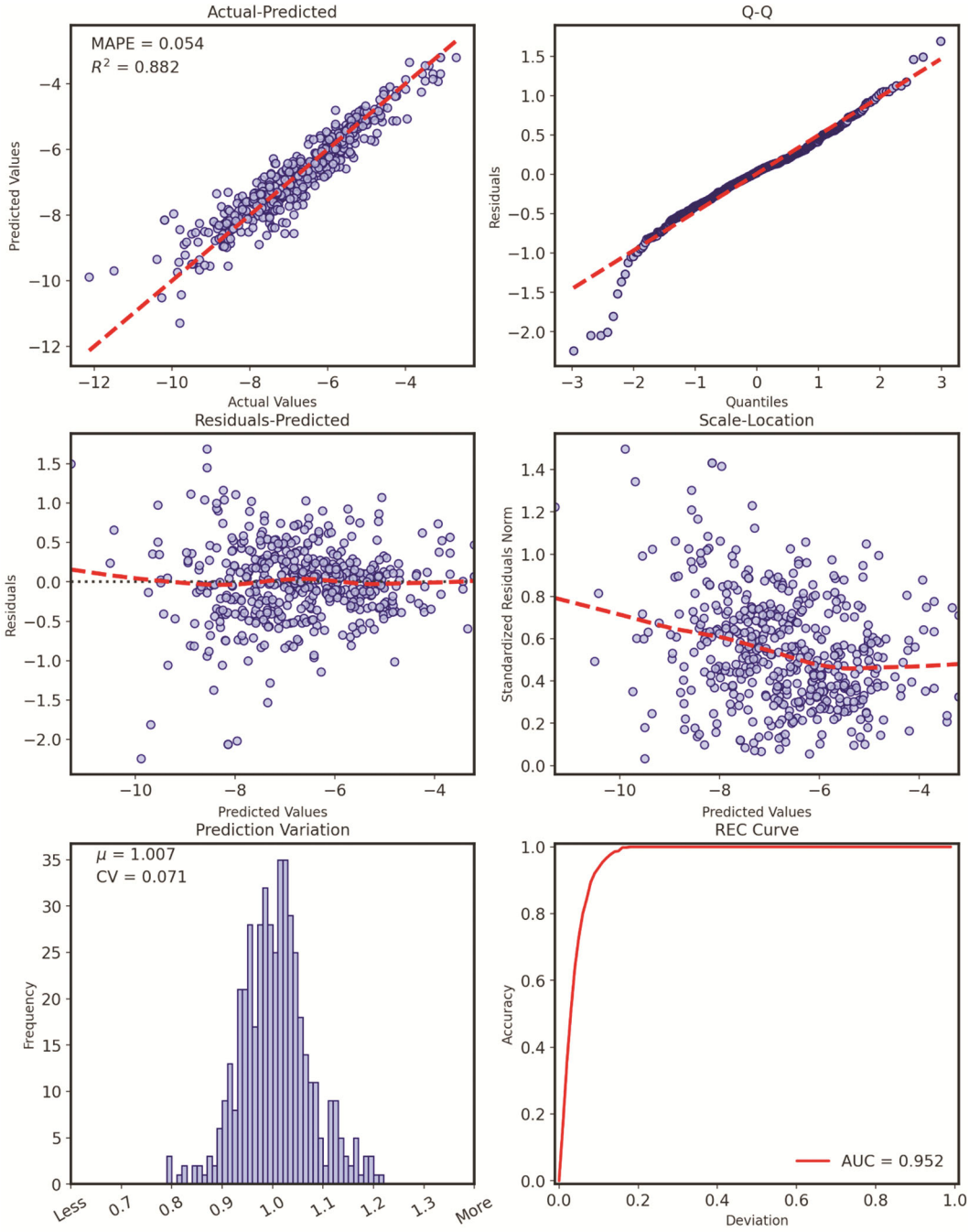
Suppl. Fig. 4 — SlickML evaluation results for K-Nearest Neighbor algorithm



Suppl. Fig. 5 — SlickML evaluation results for Random Forest algorithm



Suppl. Fig. 6 — SlickML evaluation results for Support Vector Machine algorithm



Suppl. Fig. 7 — SlickML evaluation results for Ensemble Stacking method