

Computational identification of potential tissue plasminogen activator (tPA) inhibitors from *Paris polyphylla* phytoconstituents through molecular docking and molecular dynamics simulations for anti-inflammatory therapy

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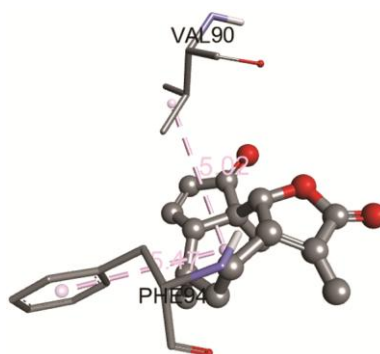
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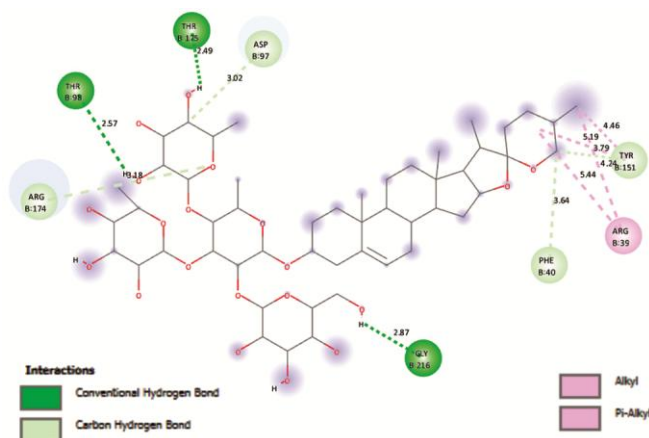
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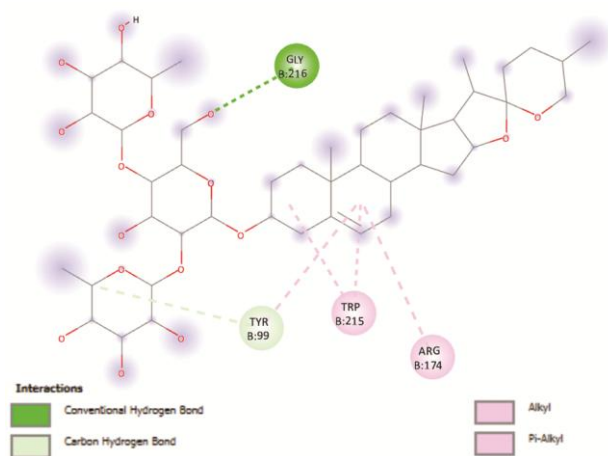
Supplementary data



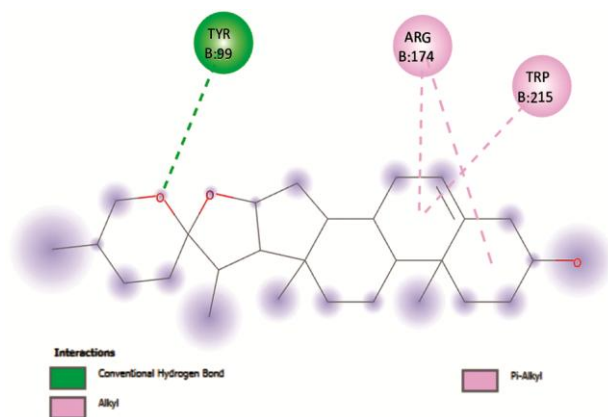
Suppl. Fig. S1 — 3D molecular interaction profiles of Ambrosin with tPA (PDB ID: 1A5H)



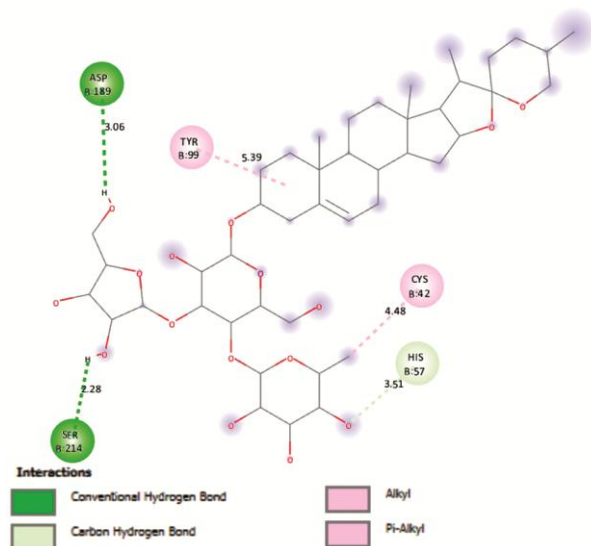
Suppl. Fig. S2 — 2D molecular interaction profiles of Polyphyllin F with tPA (PDB ID: 1A5H)



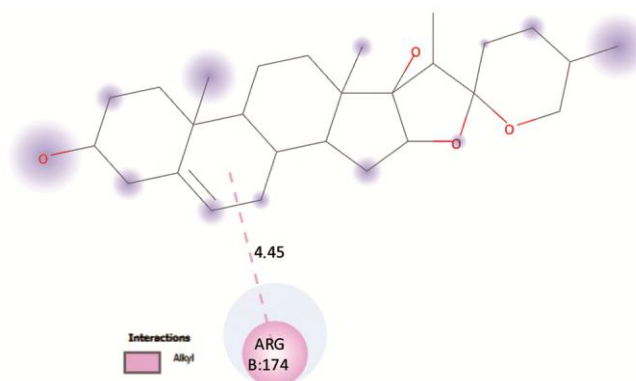
Suppl. Fig. S3 — 2D molecular interaction profiles of Dioscin with tPA (PDB ID: 1A5H)



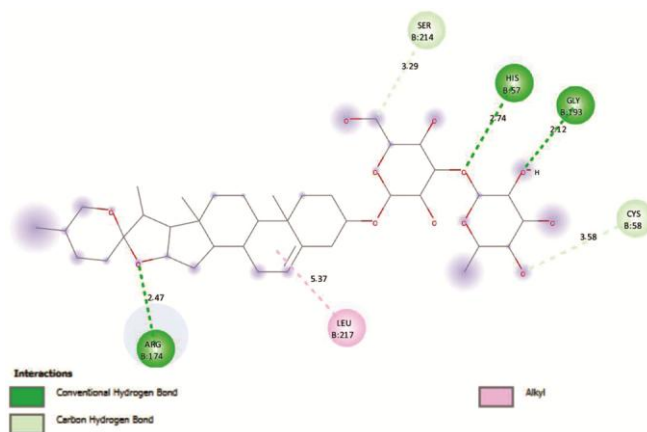
Suppl. Fig. S4 — 2D molecular interaction profiles of Diosgenin with tPA (PDB ID: 1A5H)



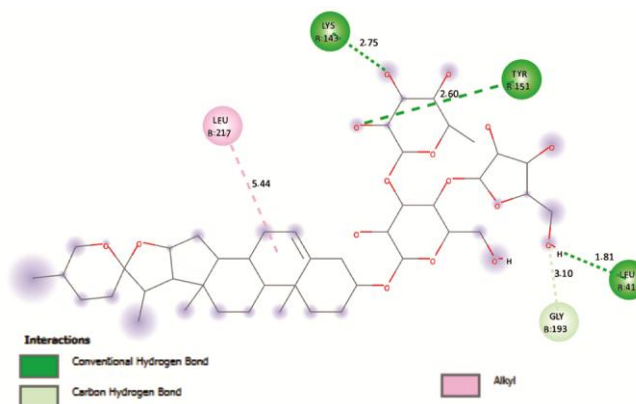
Suppl. Fig. S5 — 2D molecular interaction profiles of Pariphyllin with tPA (PDB ID: 1A5H)



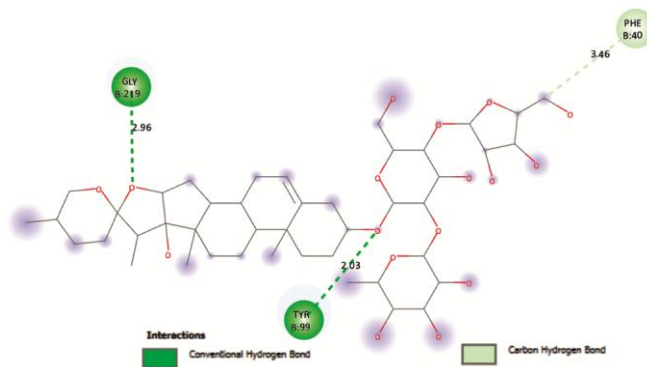
Suppl. Fig. S6 — 2D molecular interaction profiles of Pennogenin with tPA (PDB ID: 1A5H)



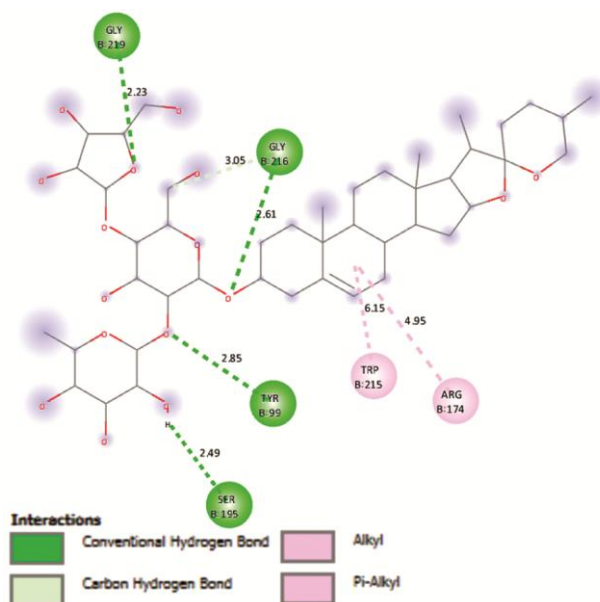
Suppl. Fig. S7 — 2D molecular interaction profiles of Polyphyllin C with tPA (PDB ID: 1A5H)



Suppl. Fig. S8 — 2D molecular interaction profiles of Polyphyllin d with tPA (PDB ID: 1A5H)



Suppl. Fig. S9 — 2D molecular interaction profiles of Polyphyllin H with tPA (PDB ID: 1A5H)



Suppl. Fig. S10 — 2D molecular interaction profiles of Polyphyllin I with tPA (PDB ID: 1A5H)