Molecular Docking methods
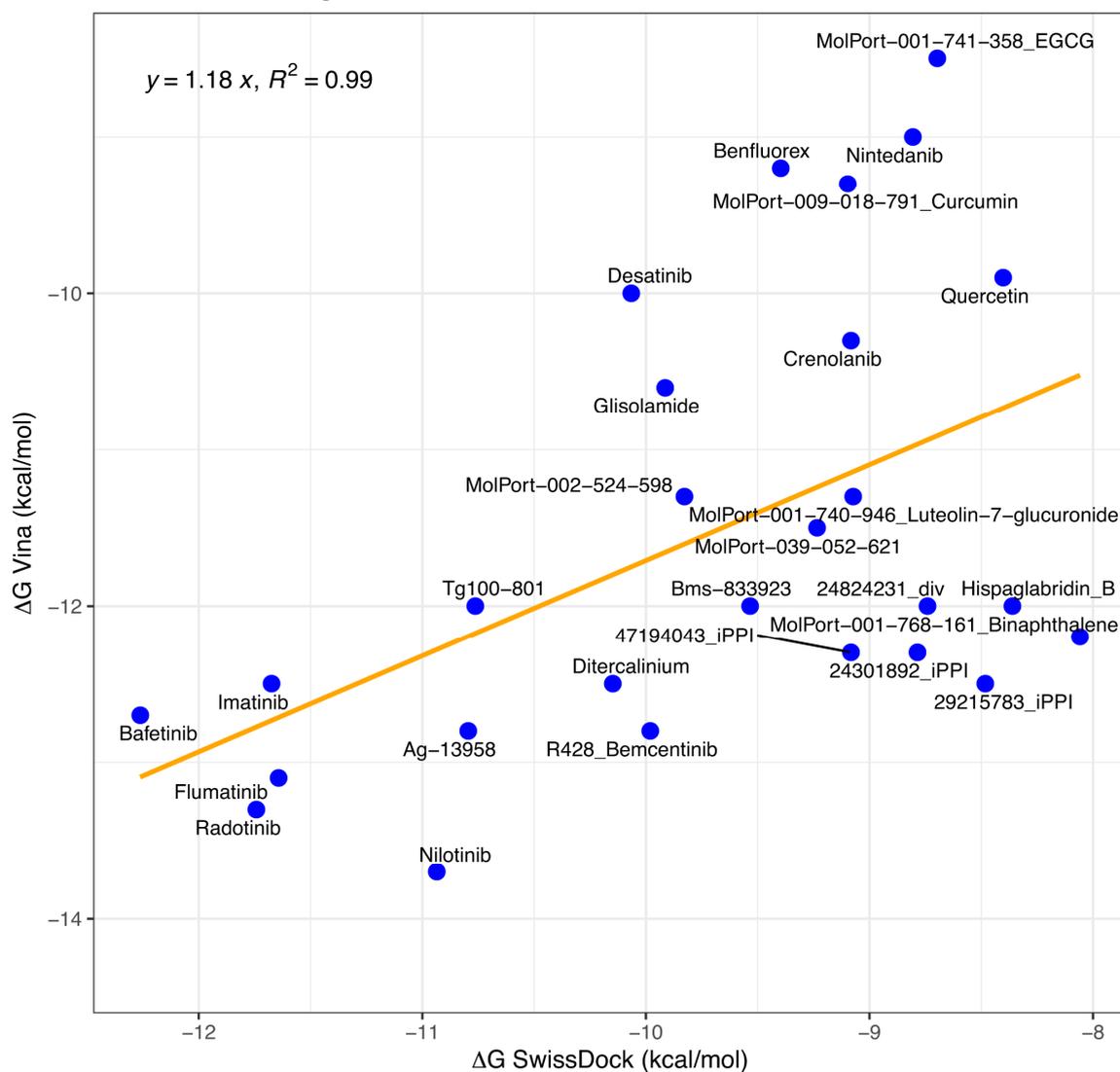

$y = 1.18\ x,\ R^2 = 0.99$

(Plot axes: x-axis "ΔG SwissDock (kcal/mol)", y-axis "ΔG Vina (kcal/mol)")

Data point labels: MolPort–001–741–358_EGCG, Benfluorex, Nintedanib, MolPort–009–018–791_Curcumin, Desatinib, Quercetin, Crenolanib, Glisolamide, MolPort–002–524–598, MolPort–001–740–946_Luteolin–7–glucuronide, MolPort–039–052–621, Tg100–801, Bms–833923, 24824231_div, Hispaglabridin_B, 47194043_iPPI, MolPort–001–768–161_Binaphthalene, Ditercalinium, 24301892_iPPI, 29215783_iPPI, Imatinib, Bafetinib, Ag–13958, R428_Bemcentinib, Flumatinib, Radotinib, Nilotinib

Figure S1: Correlation between the two molecular docking algorithms used (Autodock Vina-based docking genetic algorithm and EADock DSS algorithm).

Tables S1–S5. List of compounds included in the libraries used for structure-based virtual screening against the human intracellular PDGFRα.