Computationally guided identification of Akt-3, a serine/theronine kinase inhibitors: Insights from homology modelling, structure-based screening, molecular dynamics and quantum mechanical calculations

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Supplementary Information

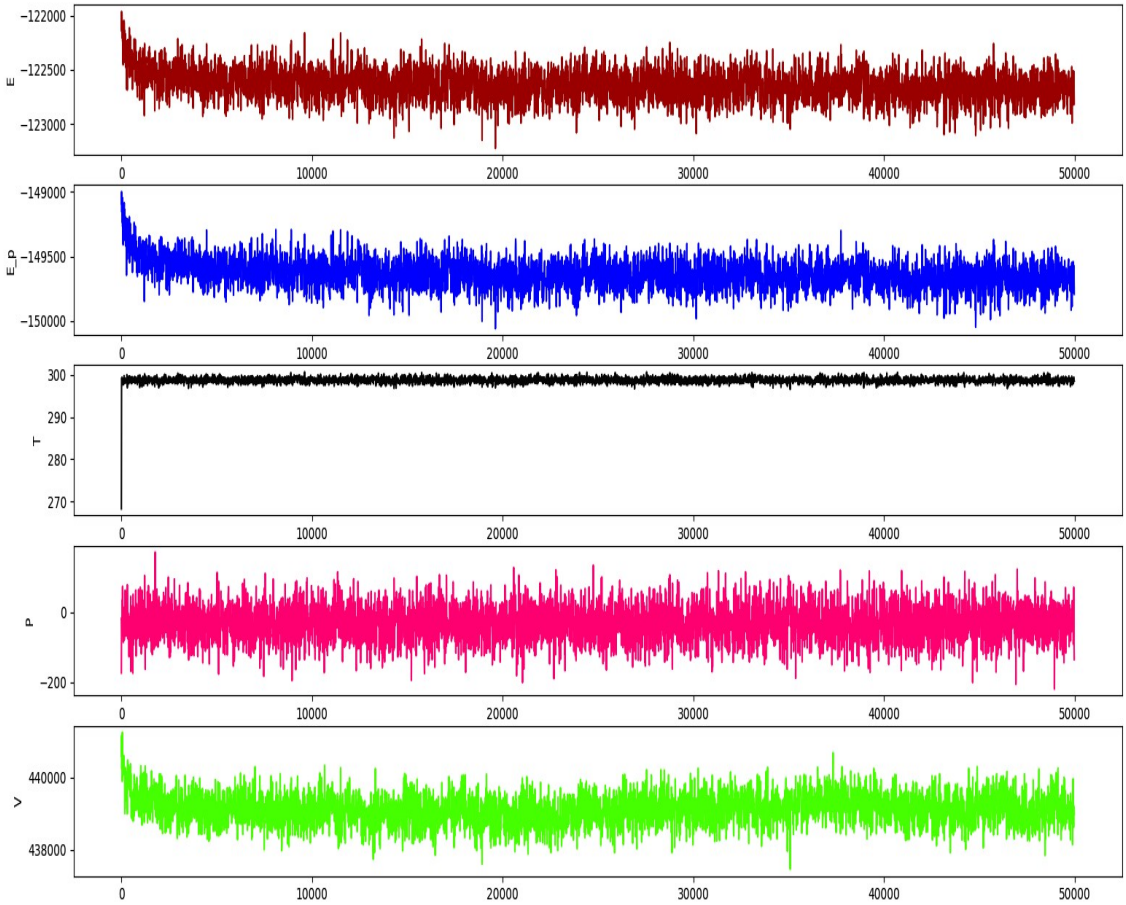

Figure S1: Simulation quality plot for apo protein

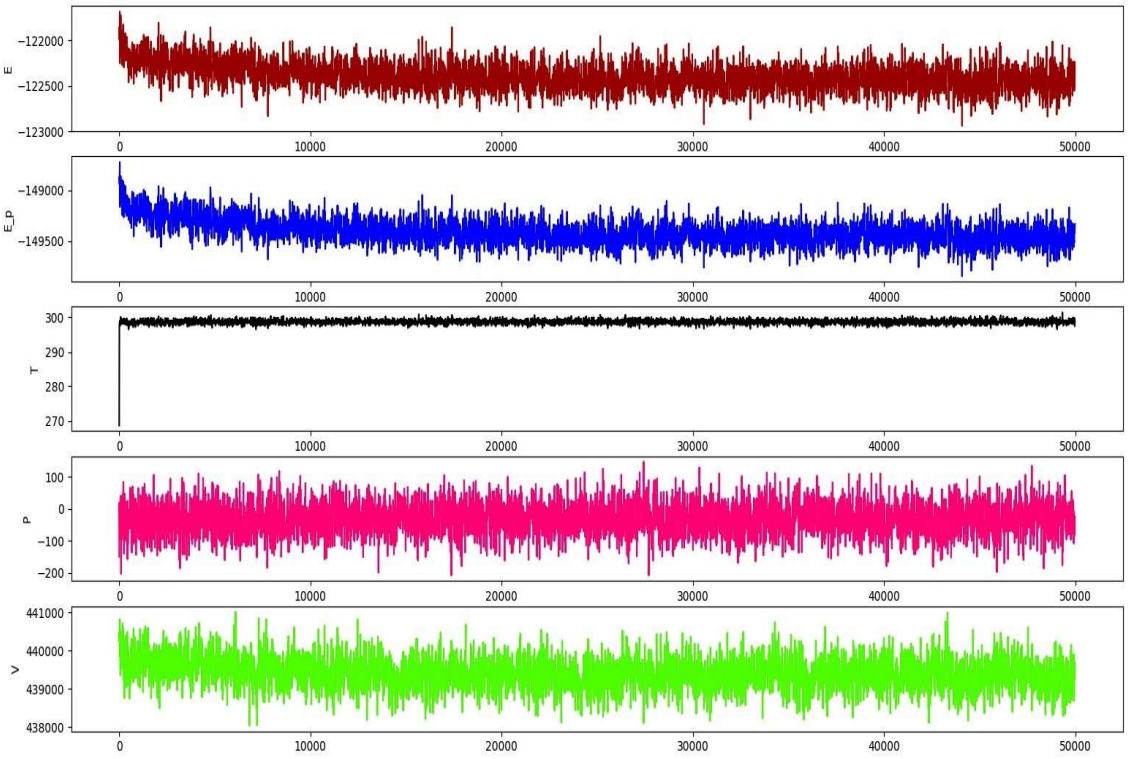

Figure S2: Simulation quality plot for ZINC04196061

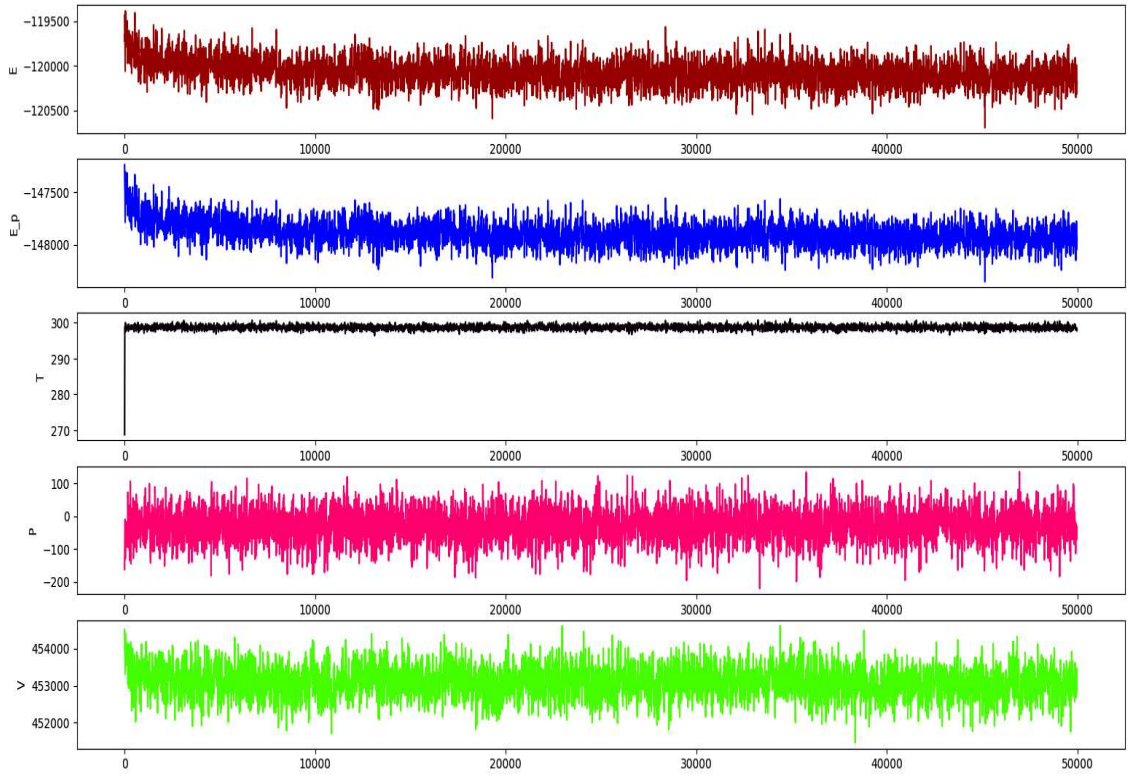

Figure S3: Simulation quality plot for ZINC08396840

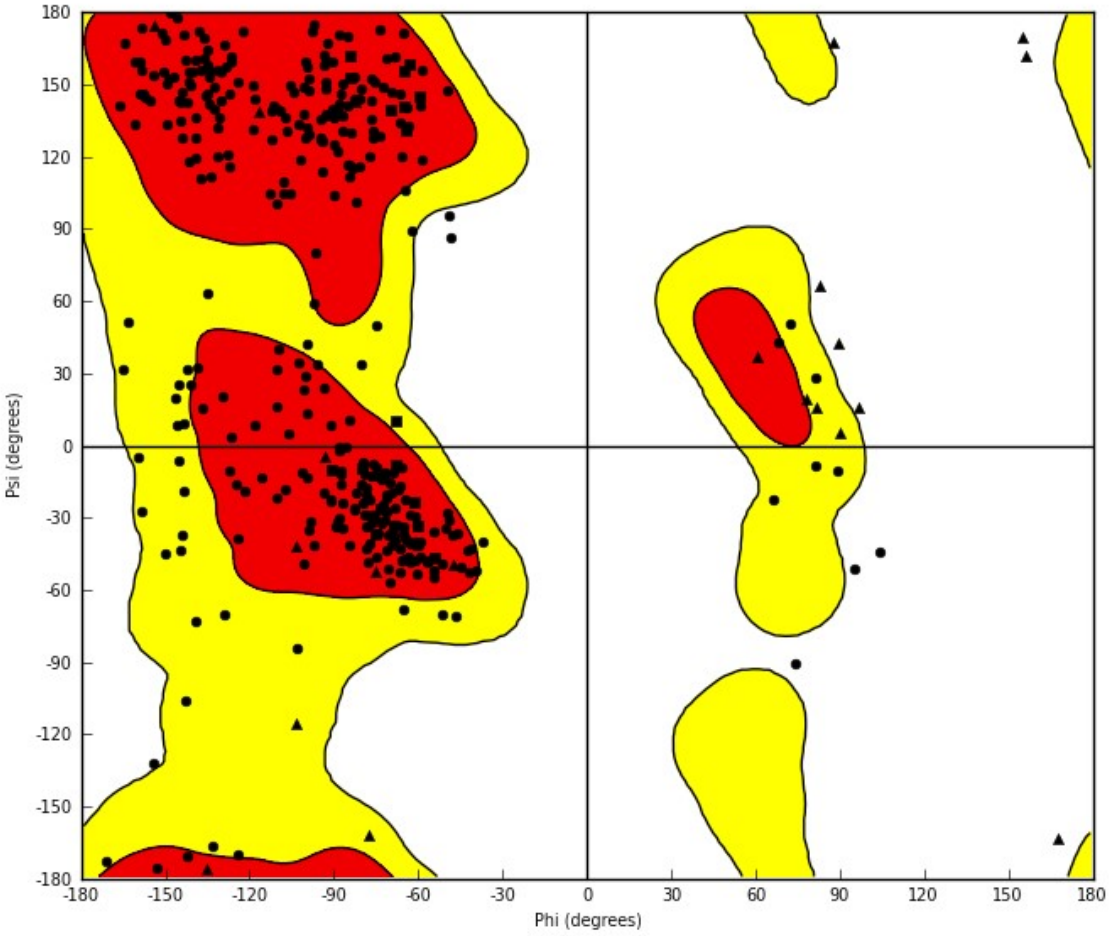

Figure S4: Ramachandran Plot of Akt-3 modelled protein post MD simulations