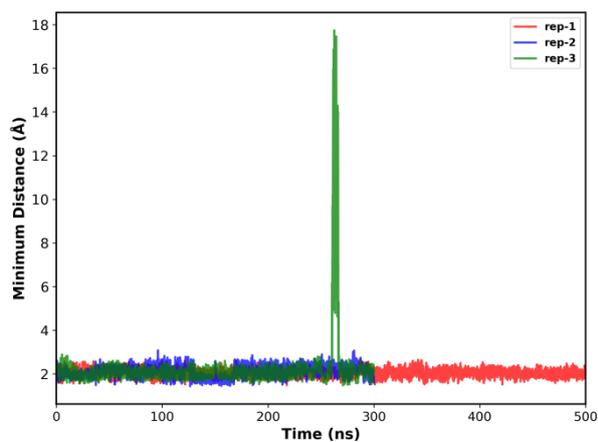# Supplementary Information

Computational analysis of dihydroxyflavone and benzylideneoxyindole derivative for glaucoma-associated myocilin: Insights into their molecular interactions and influence on hydration dynamics
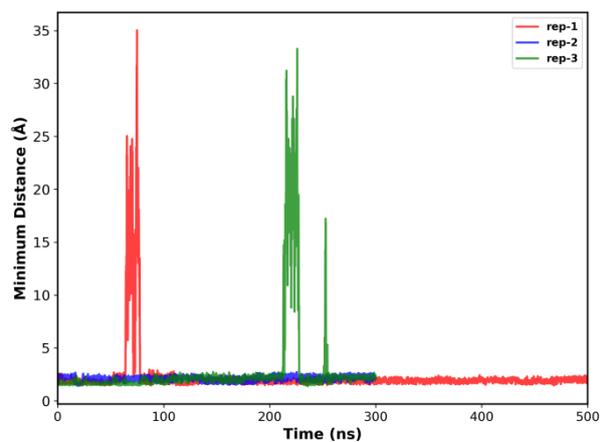
Aziza Rahman[a], Priya Dey*[b], and Anupual Baruah*[a]

[a]Department of Chemistry, Dibrugarh University, Dibrugarh, Assam, India, 786004
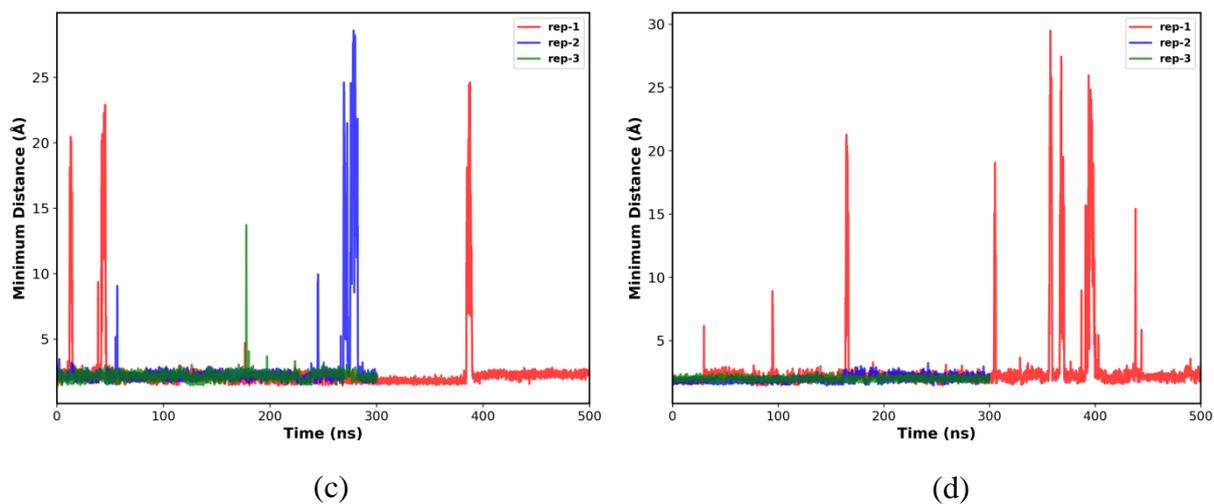[b]Institute of Integrated Cell-Material Science, Kyoto University, Kyoto, Japan

(a)

(b)

(c)

(d)

Figure S1: Minimum distance between the ligand and the protein estimated across three replicates in (a) MT-I477N-BOD System (b) MT-I477N-DHF System (c) WT-8FRR-BOD System (d) WT-8FRR-DHF System. In all cases where stable protein-ligand association is inferred from the COM distance analysis (Fig. 6), the minimum protein–ligand distance is also observed to remain low.