Supporting Information

Multi-Target Chemometric Modelling, Fragment Analysis and Virtual Screening with ERK Inhibitors as Potential Anticancer Agents

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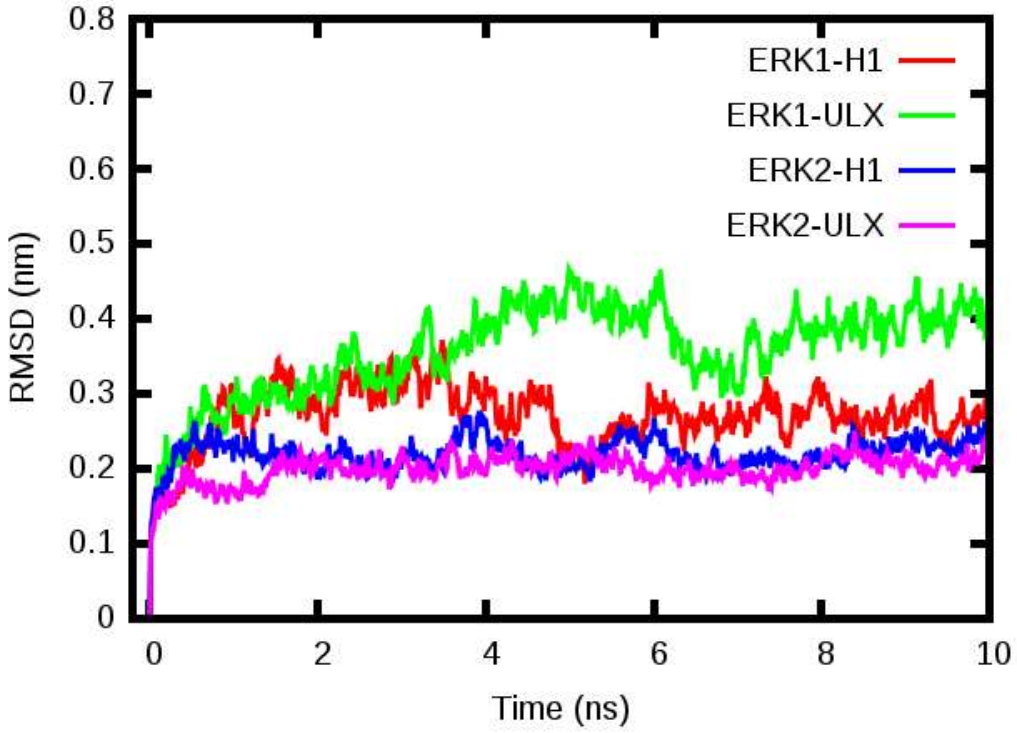

Figure S1. The root mean square deviation (RMSD) plots of backbone atoms of the receptor-ligand complexes.

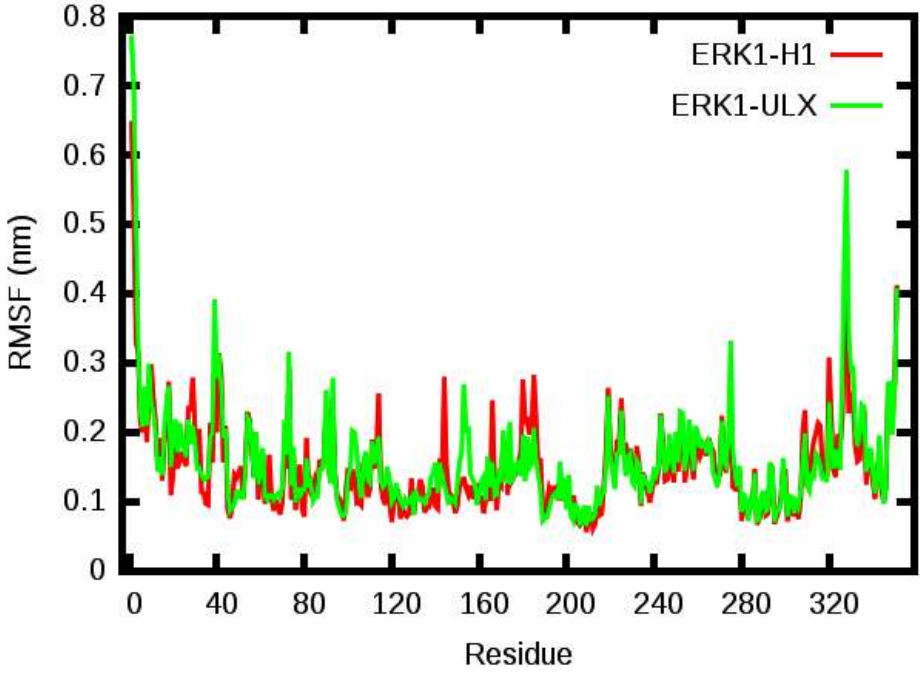

Figure S2. The root mean square fluctuation (RMSF) plots of ERK-1 complexes.

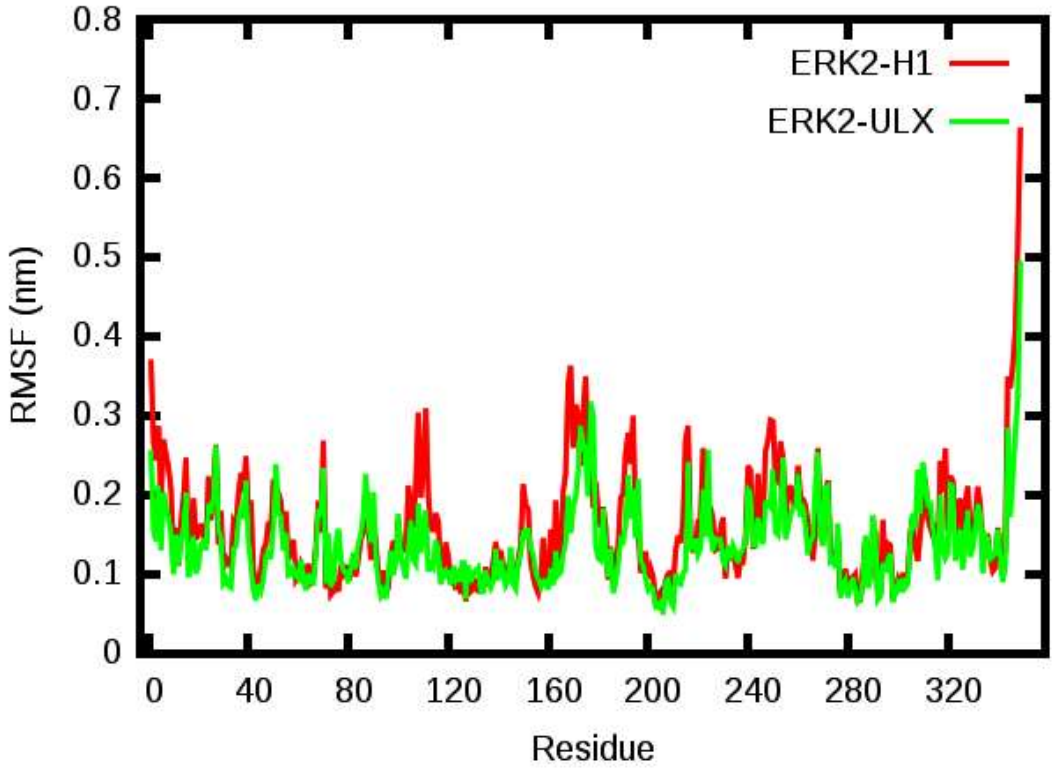

Figure S3. The root mean square fluctuation (RMSF) plots of ERK-2 complexes.

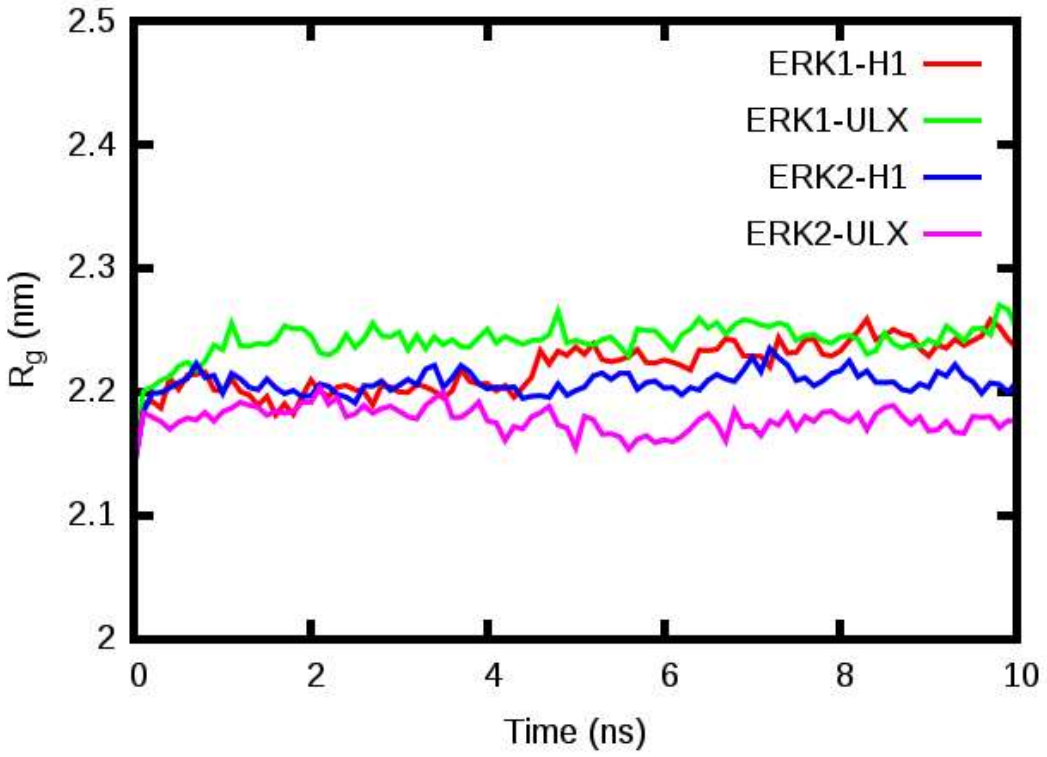

Figure S4. The radius of gyration (Rg) plots of ERK-1 and ERK-2 complexes

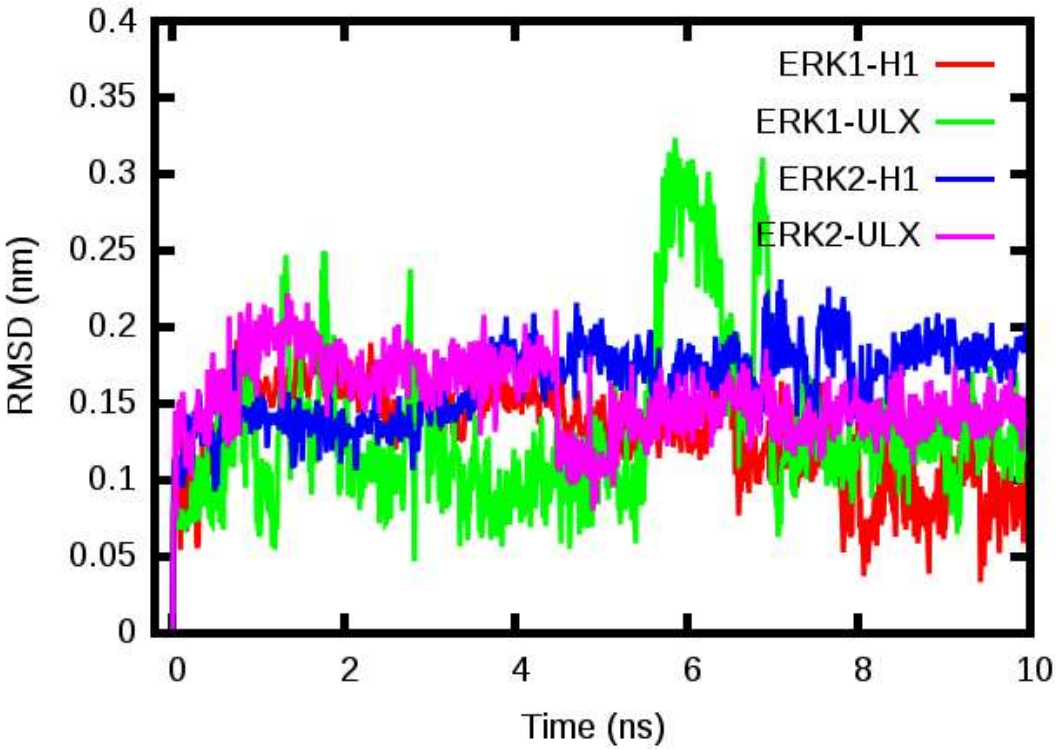

Figure S5. The root mean square deviation (RMSD) plots of bound ligands of the receptor-ligand complexes.

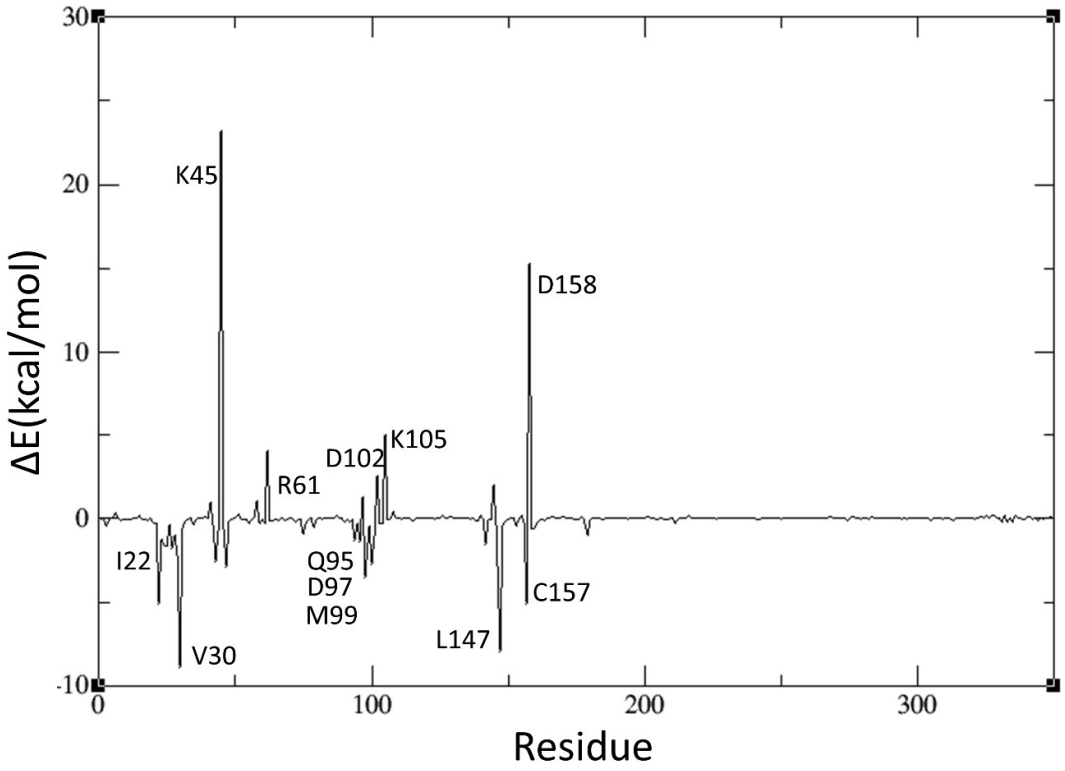

Figure S6. Per-residue decomposition profile of ERK2-ULX complex