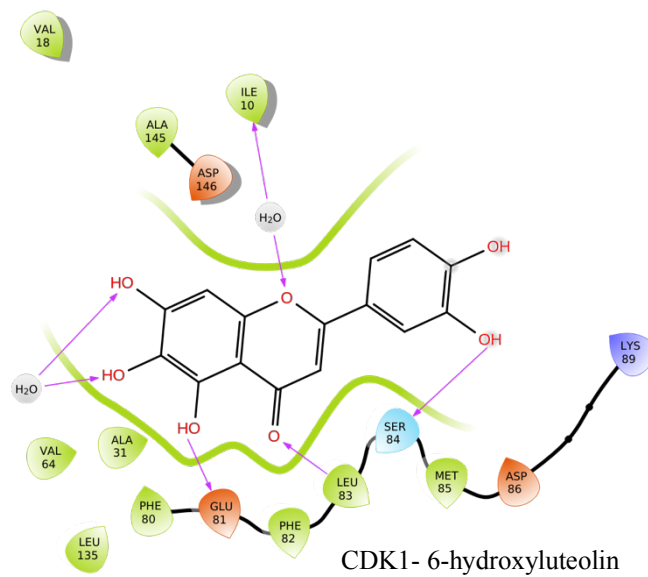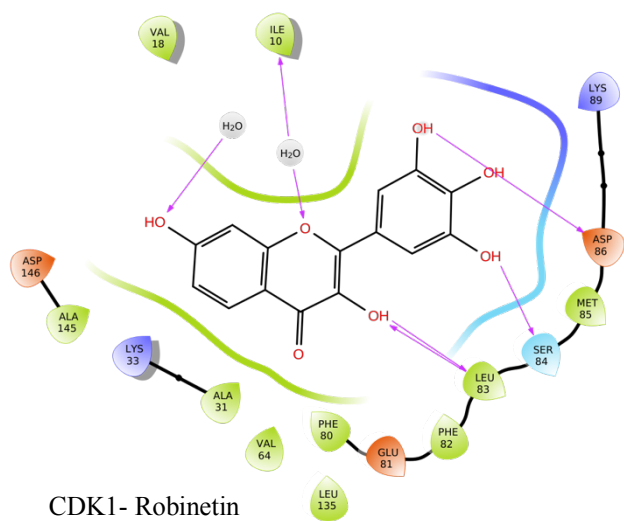Table 1. Molecular Docking results

Compound	Pubchem ID	Docking score	MMGBSA dG Bind
Co-lig (LZ9)	24864079	-13.993	-90.48
Quercetin 4-O-glucoside	5320844	-12.470944	-71.23
Robinetin	5281692	-12.216882	-59.84
6-hydroxyluteolin	5281642	-12.069299	-74.77
Quercetagetin	5281680	-12.065921	-60.97

Table 2: ADME properties of the compounds from QikProp

Compound	Mol_ MW	Donor HB	Accpt HB	SASA	QPlogPo/w	QPlogS	QPlogHERG	QPlogBB	QPPCaco	Rule Of Five
Co-lig (LZ9)	360.295	1	4.5	605.515	3.835	-5.51	-6.227	-0.704	577.385	0
Quercetin 4_O glucoside	464.382	7	13.75	693.403	-1.434	-2.8	-5.518	-3.996	2.275	2
Robinetin	302.24	5	6.25	509.856	-0.16	-2.524	-4.907	-2.348	18.577	0
6hydroxyluteolin	302.24	4	5.25	510.091	0.333	-2.772	-4.908	-2.344	18.748	0
Quercetagetin	318.239	5	6	516.226	-0.225	-2.471	-4.807	-2.673	9.915	1

[a]Molecular weight (acceptable range <500)

[b]Hydrogen bonds donor, HB donor = 0.0-6.0

[c]Hydrogen bonds acceptor' HB acceptor = 2.0-20.0

[d]Total solvent accessible surface area, SASA = 300.0-1000.0

[e]Predicted octanol/water partition coefficient, QP log Po/w = -2.0-6.5

[f]Predicted aqueous solubility, QPlogS = -6.5-0.5

[g]Predicted IC_{50} value for blockage of HERG K+ channels, QPlogHERG = Concern below -5

[h]Predicted blood/brain partition coefficient, QPlogBB = -3.0-1.2

CDK1-Co-Lig

CDK1- Quercetin 4-O-glucoside

CDK1- Robinetin

CDK1- 6-hydroxyluteolin

CDK1- Quercetagetin
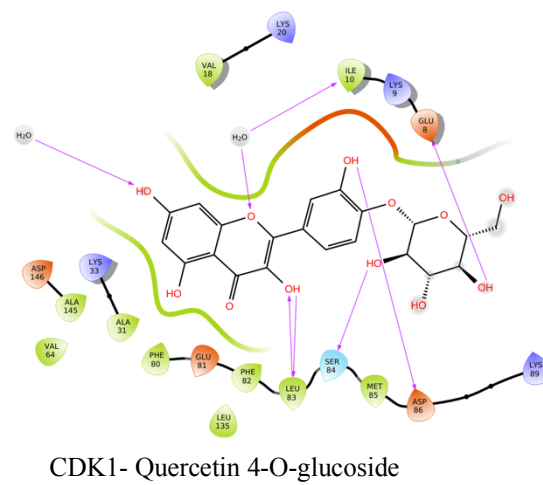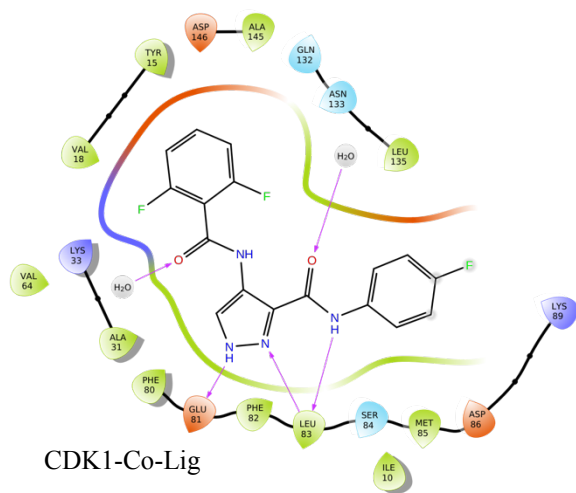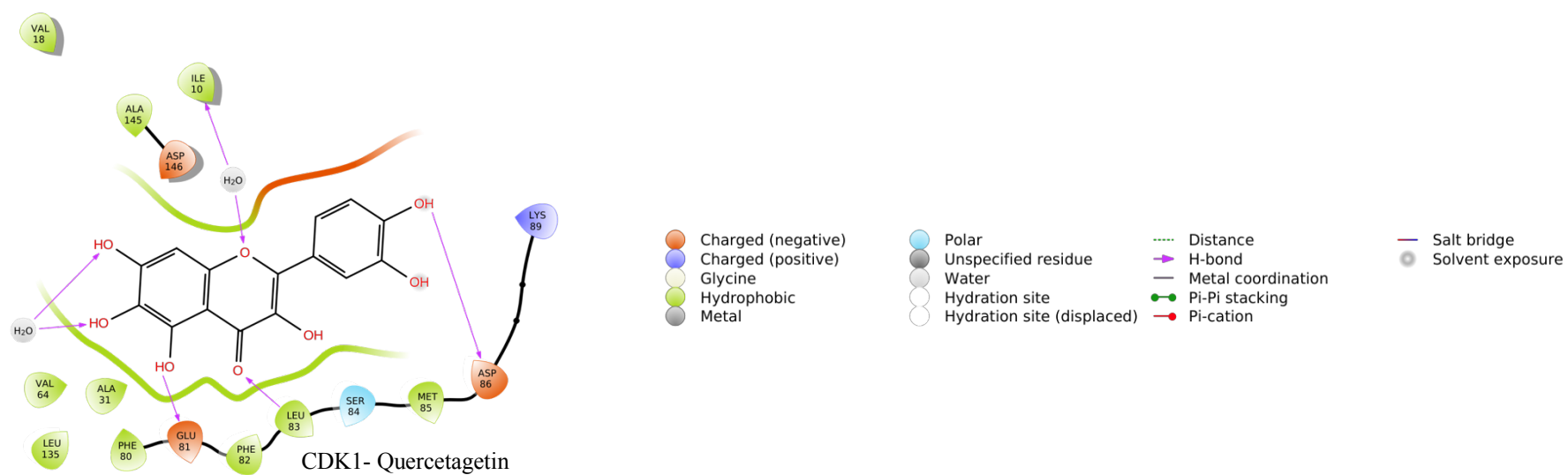
2D Protein-ligand interaction diagrams of CDK1 and the lead compounds