Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Table S1. Molecular descriptors, experimental and predicted pIC_{50}s of 19 flavonoids and compounds **1-3** during 2D QSAR analysis.

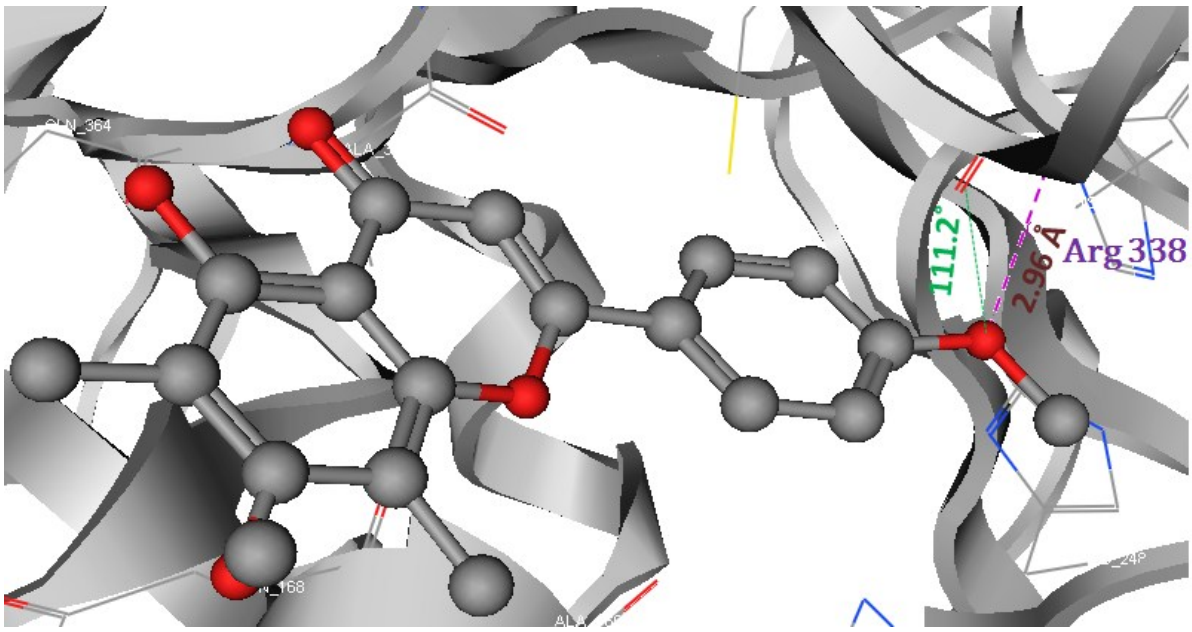
S.No	Compound	b_rotN	Weight	mr	HBA	HBD	TPSA	cLogp (o/w)	pIC50	$PRED	$RES	$Z-SCORE	$XPRED	$XRES	$XZ-SCORE	PCA1	PCA2	PCA3
1	Apigenin	1.00	270.24	7.00	4.00	3.00	86.99	2.53	3.86	3.74	-0.05	1.09	3.92	-0.06	0.15	-0.67	0.43	0.26
2	Baicalein	1.00	270.24	7.01	4.00	3.00	86.99	2.49	3.53	3.52	-0.36	0.75	3.93	-0.70	-0.51	-0.07	-0.51	-0.07
3	Chrysin	1.00	254.24	6.88	3.00	2.00	66.76	2.84	3.51	3.53	-0.16	0.61	3.69	-0.18	0.43	-1.00	0.30	-0.16
4	Diadzein	1.00	254.24	6.88	3.00	2.00	66.76	2.18	3.25	3.31	-0.12	0.02	3.43	-0.18	0.43	-0.59	1.26	-3.01
5	Dihydromyricetin	1.00	320.25	7.41	8.00	6.00	147.68	1.17	3.80	3.66	0.09	0.22	3.66	0.13	0.32	0.37	-1.72	1.31
6	Fistein	1.00	286.23	7.12	5.00	4.00	107.22	2.30	3.92	4.14	-0.28	0.77	4.23	-0.31	0.75	-0.39	-0.78	0.29
7	Formononetin	2.00	268.26	7.39	3.00	1.00	55.76	2.45	2.69	2.56	-0.51	0.93	3.29	-0.60	1.47	-0.67	0.43	0.26
8	Genistein	1.00	270.24	7.00	4.00	3.00	86.99	1.91	3.82	3.75	0.18	0.23	3.61	0.20	0.49	-0.74	-0.18	-0.16
9	Hesperetin	2.00	302.28	7.69	6.00	3.00	96.22	2.37	3.48	3.36	0.28	0.37	3.09	0.38	0.92	-0.54	0.25	-0.75
10	Kaempferol	1.00	286.23	7.12	5.00	4.00	107.22	2.30	3.90	4.14	-0.30	0.72	4.23	-0.33	0.80	-0.38	-0.80	0.32
11	Liquiritigenin	1.00	256.25	6.94	4.00	2.00	66.76	2.65	3.06	3.31	0.22	0.55	2.75	0.30	0.88	-0.93	-0.38	-0.24
12	Luteolin	1.00	286.23	7.12	5.00	4.00	107.22	2.26	4.45	4.26	0.26	1.67	4.14	0.30	0.71	-0.28	0.41	0.95
13	Myricetin	1.00	318.23	7.35	7.00	6.00	147.68	1.75	4.11	4.06	-0.62	1.38	4.95	-0.84	2.13	0.20	0.51	1.59
14	Myricitrin	3.00	464.37	10.51	11.00	8.00	206.60	0.53	4.00	4.95	-0.24	3.16	4.30	-0.30	0.72	1.69	-1.60	0.64
15	Naringenin	1.00	272.25	7.06	5.00	3.00	86.90	2.38	2.33	2.32	-0.76	0.02	3.25	-0.92	2.34	-0.59	1.26	-3.01
16	Puerarin	3.00	416.38	10.16	8.00	6.00	156.91	-0.28	3.03	3.03	-0.37	1.28	3.66	-0.63	1.53	0.76	-0.76	-0.79
17	Quercetin	1.00	302.23	7.24	6.00	5.00	127.45	2.03	4.95	4.85	0.48	2.03	4.35	0.59	1.56	0.08	0.46	1.65
18	Rutin	6.00	610.52	13.68	15.00	10.00	265.52	-1.11	4.17	4.06	-0.05	0.36	4.27	-0.10	0.24	2.58	0.04	-2.11
19	Tangeretin	6.00	372.37	9.81	6.00	0.00	72.45	2.41	2.33	2.32	-0.87	0.02	4.59	-2.26	6.48	-0.59	1.26	-3.01
20	Compound **1**	3.00	326.34	8.94	4.00	1.00	64.99	3.57	4.22	4.10	0.87	2.09	2.89	1.32	3.75	-0.57	1.20	-0.07
21	Compound **2**	4.00	448.38	10.43	10.00	7.00	186.37	0.04	4.54	3.94	0.25	0.61	4.20	0.33	0.79	1.54	2.76	1.08
22	Compound **3**	3.00	432.38	10.28	9.00	6.00	166.14	1.07	4.33	4.50	0.61	1.47	3.62	0.70	1.77	0.96	-0.93	-0.30

b_rotN: Number of rotatable, **Weight:** Molecular weight, **mr:** Molecular refractivity, **HBA**: H-bond acceptor atoms, **HBD:** H-bond donor atoms, **TPSA:** Topological polar surface area, **clogP:** Log octanal/water partition coefficient, **pIC50:** experimentally calculated log IC_{50}, **$PRED, $RES and $Z-SCORE** predicted pIC_{50}, residual and Z-score values, **$XPRED, $XRES and $XZ-SCORE:** The corresponding cross-validation properties, **PCA1, PCA2 and PCA3:** Selected three Principal Components.

Table S2. Prediction of Adsorption, distribution, metabolism and excretion properties for 19 flavonoids and compound 1-3 using pre ADMET server.

Compounds	**Human intestinal absorption (%)**	**In vitro Caco2 cell permeability (nm/sec)**	**In vitro MDCK cell permeability (nm/sec)**	**In vitro Plasma protein binding (%)**	**In vivo blood brain barrier penetration (C. brain/C. blood)**
Kaemferol	79.431	9.572	29.62	89.60	0.286
Quercetin	63.481	3.412	13.523	93.236	0.172
Apigenin	88.122	10.546	44.322	97.253	0.565
Genistein	88.121	5.747	39.433	89.738	0.178
Diadzein	92.646	7.720	31.422	88.706	0.193
Formononetin	95.552	7.601	19.256	85.062	0.063
Chrysin	92.643	2.478	42.133	95.095	0.935
Hesperetin	85.960	6.962	3.680	68.721	0.0868
Liquiritigenin	92.472	21.049	128.8	100.000	1.786
Baicalein	88.105	1.280	101.909	98.983	0.770
Naringenin	87.318	10.521	44.638	100.000	0.596
Luteolin	81.852	16.048	182.904	100.000	0.873
Myricitrin	24.943	8.115	0.401	65.414	0.035
Myricetin	40.964	0.991	4.882	96.984	0.110
Dihydromyricetin	37.042	0.997	3.582	99.901	0.105
Fisetin	79.431	9.575	69.192	88.728	0.316
Tangeretin	98.886	53.605	0.629	87.173	0.027
Luteolin glycoside	34.093	6.943	1.222	82.898	0.035
Rutin	2.861	7.912	0.326	43.897	0.028
Puerarin	62.134	16.326	8.458	70.062	0.045
Compound **1**	95.97	42.682	0.394	89.515	0.190
Compound **2**	25.171	11.455	1.147	57.175	0.035
Compound **3**	46.49	8.19	1.928	65.99	0.042

A



B

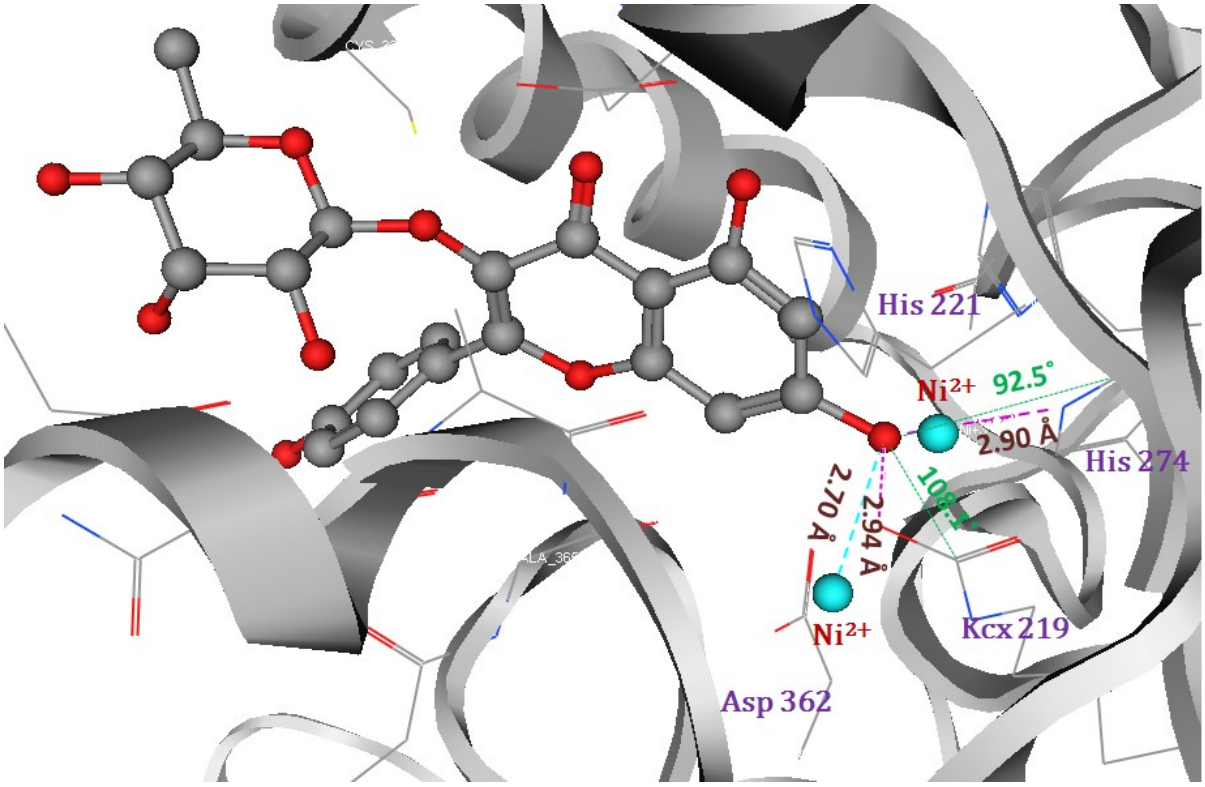


Fig. S1. Molecular interactions of Compound **1** (**A**) and **3** (**B**) with active site amino acid residues of *H. pylori* urease.

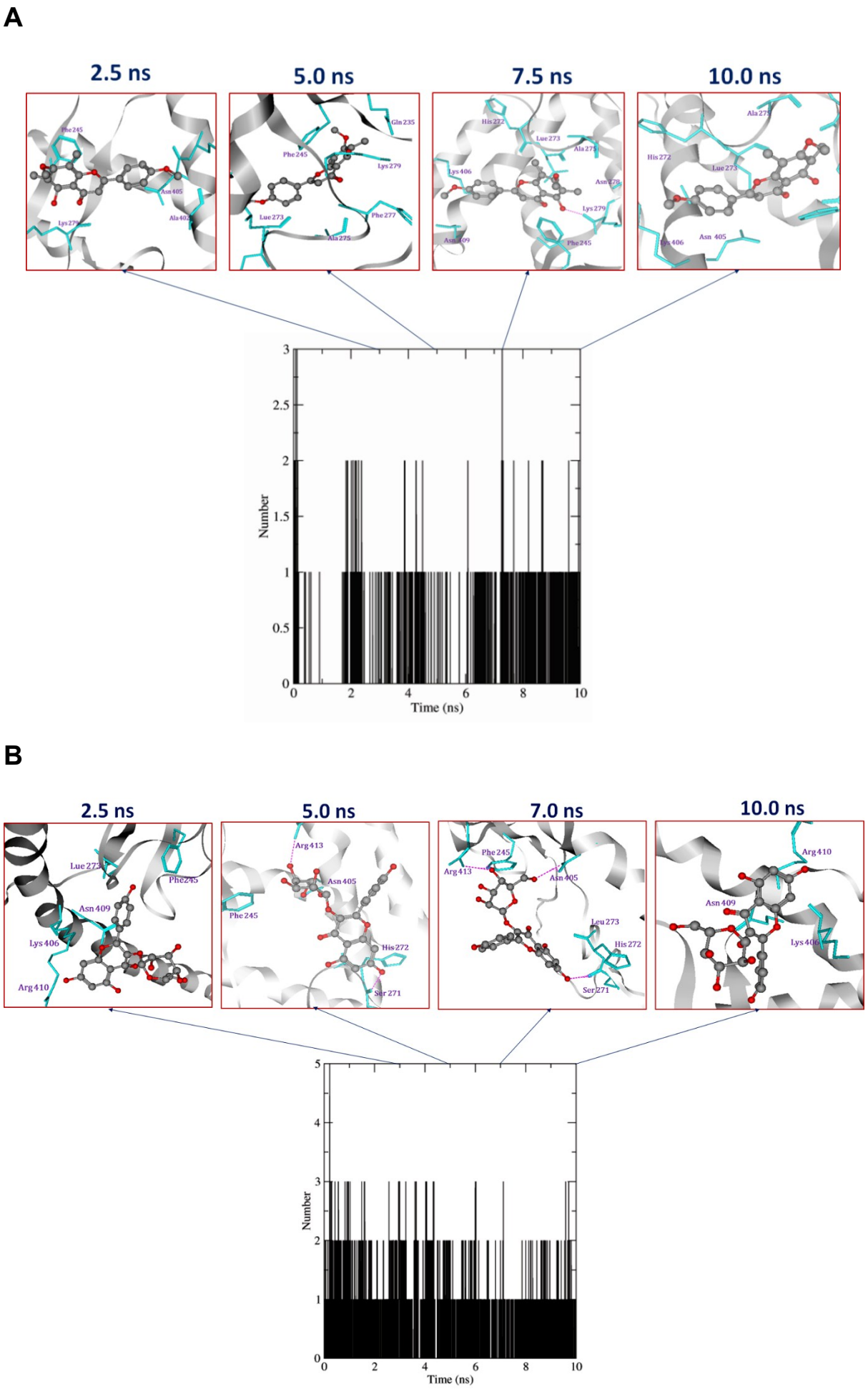


Fig S2. The snapshots of docking pose of compound **1 (A), 2 (B)** and total H-bond intensity at various time scale intervals in 10 ns complex MD simulations with Cag A.