Supplementary Materials

Supplementary Table 1: Molecular docking results.

Supplementary Table 2: The top five components with binding energy less than −7.0 kcal/mol

Supplementary Figure 3:Interactions between the top five components of LHQW with the amino acids of targets related to IVP and NCP with binding energy less than -7.0 kcal/mol.

Supplementary Table 1: Molecular docking results

Serial number	Molecular	3CL	ACE2	COX2	HA	NA	IL6
		Affinity (kcal/mol)					
1	Isoforsythiaside	-8.8	-9.2	-9.5	-7	-7.2	-6.8
2	Luteolin	-7.4	-7.8	-7.9	-7.2	-7.4	-6.7
3	Guaiene	-5.3	-6.1	-6.3	-6.3	-6.4	-5.6
4	Rutin	-9	-8.3	-9	-7.1	-6.8	-5.6
5	Aloe emodin	-6.9	-7.5	-7.3	-6.4	-6.9	-6
6	Emodin	-7	-7.3	-6.9	-6.8	-7.1	-5.9
7	Patchouli alcohol	-5.1	-5.9	-5.2	-6	-6.1	-4.8
8	Quercitrin	-8.5	-7.9	-8.4	-7.1	-7.3	-6.4
9	α-gurjunene	-5	-5.6	-5.5	-5.8	-6.2	-4.7
10	Amygdalin	-8.1	-8.2	-8.5	-7.2	-7.6	-6.1
11	Chrysophanol	-6.9	-7.3	-7.6	-6.6	-7.3	-5.7
12	Liquiritin	-7.6	-7.1	-8.1	-7.1	-6.7	-6.1
13	Isochlorogenic acid B	-7.2	-8	-8.7	-7.7	-7.9	-7
14	Isochlorogenic acid C	-8.1	-7.6	-7.4	-6.8	-7.2	-5.7
15	Rhein	-7.2	-7.6	-7.7	-6.6	-7.2	-6.2
16	α-patchoulene	-5.2	-6	-5.7	-6.2	-6.3	-5.1
17	Salidroside	-7	-6.6	-7.5	-6.5	-6.3	-6.2
18	4-caffeoylquinic acid	-6.4	-6.6	-7.3	-7.3	-7.1	-6.2
19	Neochlorogenic acid	-6.7	-7.2	-6.8	-6.7	-7.2	-5.8
20	Phillyrin	-7.8	-8.6	-7.6	-6.9	-5.9	-5.7
21	(-)-Phillygenin	-6.9	-7.6	-6.9	-7.1	-6.1	-5.5
22	Forsythoside E	-8.4	-7.8	-8.7	-7.3	-7.4	-6.3
23	chlorogenic acid	-7.1	-7.6	-8.2	-6.6	-7.4	-6.2
24	Hyperin	-8.4	-8.2	-7.8	-7	-6.9	-5.5

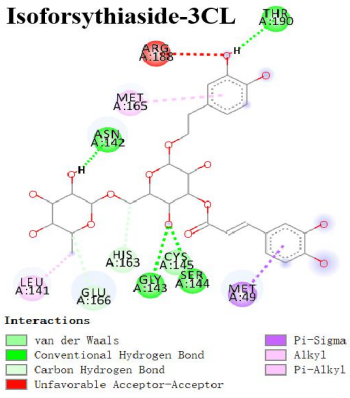
25	Glycyrrhizic acid	-7.9	-7.1	-6.1	-7.6	-2.9	-5
26	Mollugin	-7.1	-7.2	-6.7	-6.7	-7.2	-6
27	α-bulnesene	-5	-5.8	-6	-6.4	-6.4	-4.9
28	L-menthol	-4.7	-5.5	-5.9	-4.8	-5.2	-4.6
29	Hesperidin	-8.8	-9.1	-8.5	-8	-7.1	-6.8
30	Caffeic acid	-5.6	-5.8	-6.8	-5.2	-5.8	-5.4
31	β-patchoulene	-5.2	-6	-5.7	-6.2	-6.3	-5.1

Supplementary Table 2: The top five components with binding energy less than −7.0 kcal/mol.

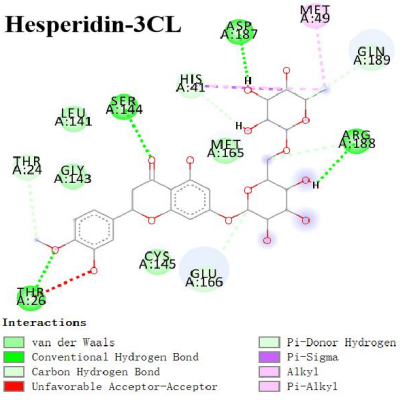
Composition	3CL	ACE2	COX2	HA	NA	IL6
−7.0 kcal/mol	Rutin	Isoforsythiaside A	Isoforsythiaside A	Hesperidin	Isochlorogenic acid B	Isochlorogenic acid B
	Isoforsythiaside A	Hesperidin	Rutin	Isochlorogenic acid B	Amygdalin	
	Hesperidin	Phillyrin	Isochlorogenic acid B	Glycyrrhizic acid	Forsythoside E	
	Quercetin	Rutin	Forsythoside E	Forsythoside E	Luteolin	
	Forsythoside E	Hypericin	Hesperidin	4-caffeoylquinic acid	Chlorogenic acid	

Supplementary Figure 3:Interactions between the top five components of LHQW with the amino acids of targets related to IVP and NCP with binding energy less than -7.0 kcal/mol.

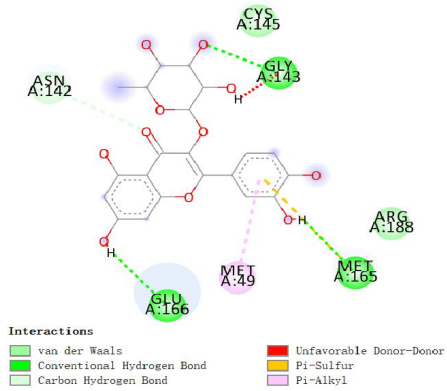
Isoforsythiaside-3CL



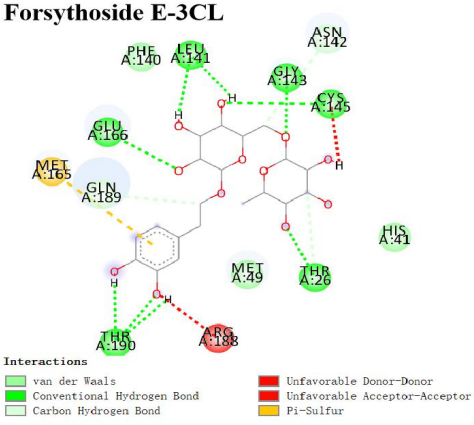
Hesperidin-3CL



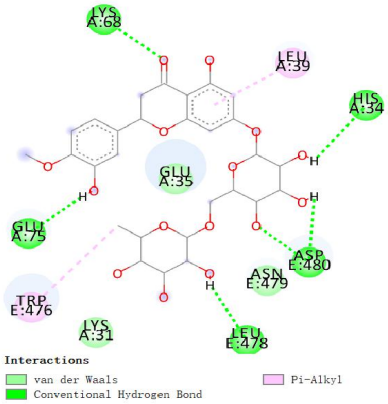
Quercetin-3CL



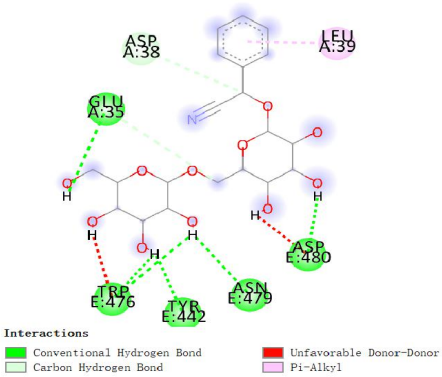
Forsythoside E-3CL



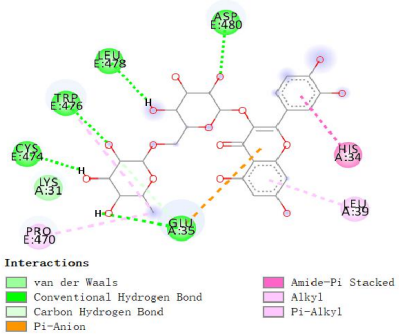
Hesperidin-ACE2



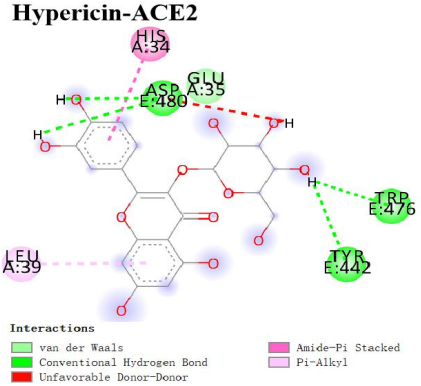
Phillyrin-ACE2



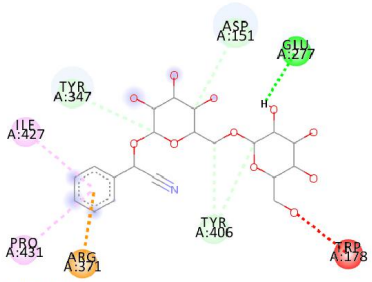
Rutin-ACE2



Hypericin-ACE2



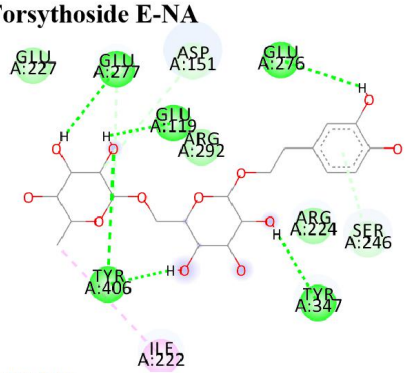
Amygdalin-NA



Interactions

Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Cation
Pi-Alkyl

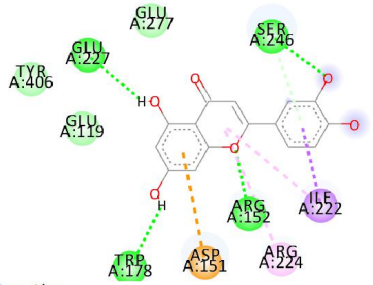
Forsythoside E-NA



Interactions

van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Pi-Donor Hydrogen Bond
Alkyl

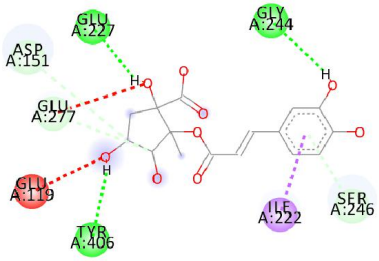
Luteolin-NA



Interactions

van der Waals
Conventional Hydrogen Bond
Pi-Anion
Pi-Donor Hydrogen Bond
Pi-Sigma
Pi-Alkyl

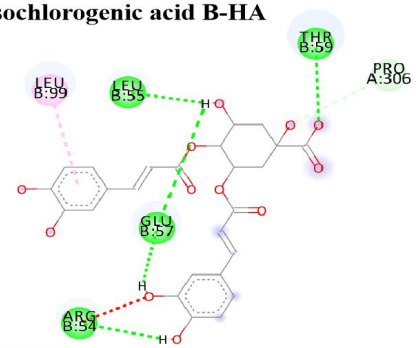
Chlorogenic acid-NA



Interactions

Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Donor Hydrogen Bond
Pi-Sigma

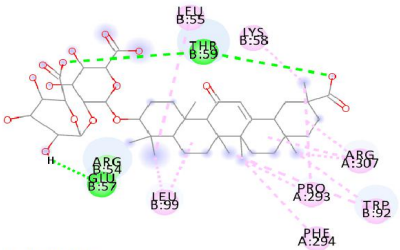
Isochlorogenic acid B-HA



Interactions

Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor
Pi-Alkyl

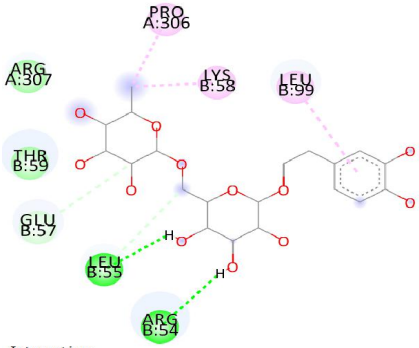
Glycyrrhizic acid-HA



Interactions

van der Waals
Conventional Hydrogen Bond
Alkyl
Pi-Alkyl

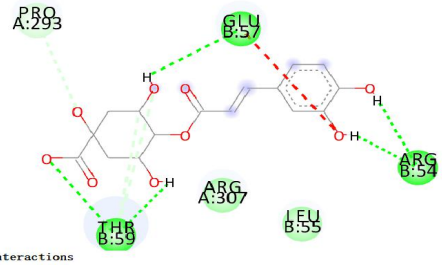
Forsythoside E-HA



Interactions

van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Alkyl
Pi-Alkyl

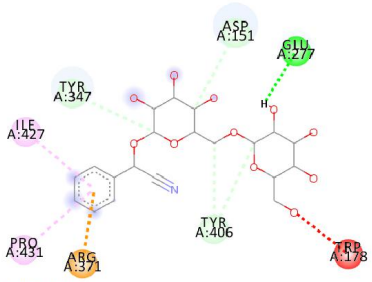
Caffeoylquinic acid 4-HA



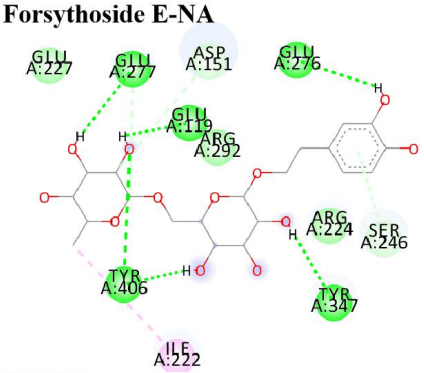
Interactions

van der Waals
Conventional Hydrogen Bond
Carbon Hydrogen Bond
Unfavorable Acceptor-Acceptor

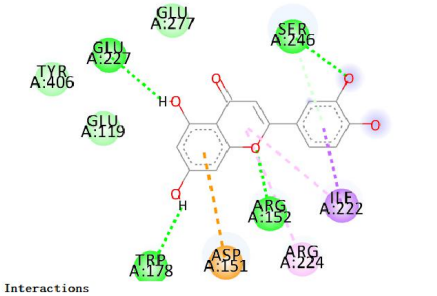
Amygdalin-NA



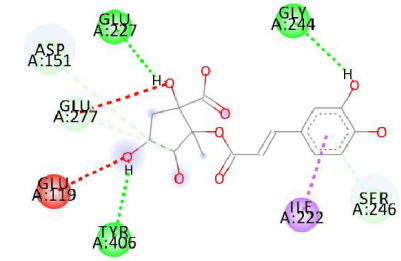
Forsythoside E-NA



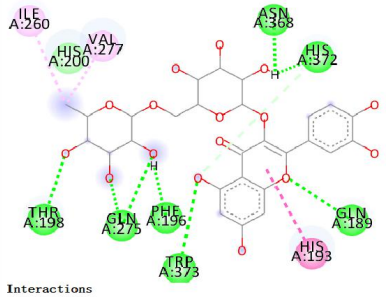
Luteolin-NA



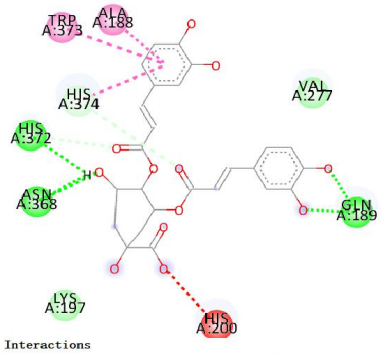
Chlorogenic acid-NA



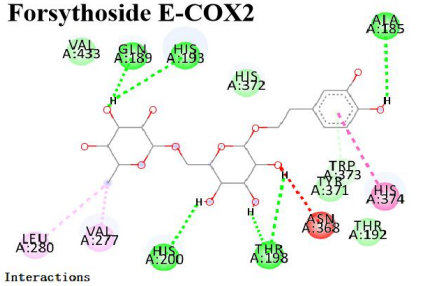
Rutin-COX2



Isochlorogenic acid B-COX2



Forsythoside E-COX2



Hesperidin-COX2