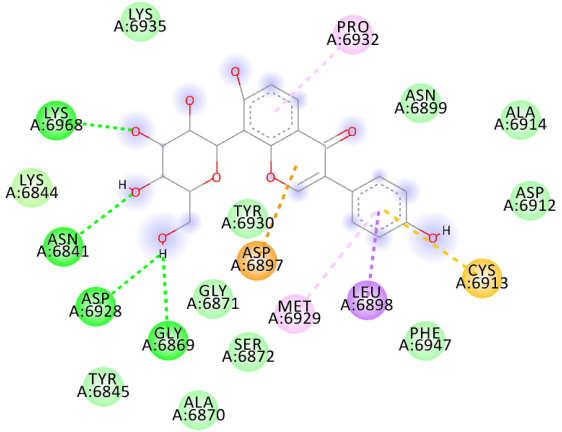
Table (S) The docking binding free energies of polyphenols (flavonoids and coumarins) and the co-crystallized ligands against SARS-COV-2 target proteins.

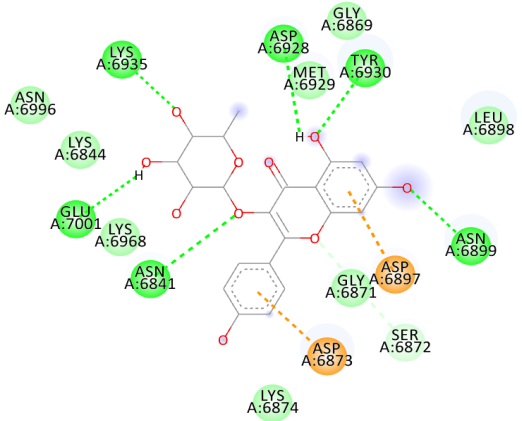
Ligands	COVID-19 3CL^{pro}	Docking energy	2' *O*-RNA mtase	Docking energy
	Bond type /Involved amino acids/ Distance in (Å)	Scores in kcal/mol	Bond type /Involved amino acids/ Distance in (Å)	Scores in kcal/mol
(N3)	H-Bond/ CYS145/3.65; H-Bond/; CYS145/3.66; H-Bond/ GLN189/3.63; H-Bond/ GLN189/2.35; H-Bond/ THR26/2.79; H-Bond/ HIS163/2.12; H-Bond/ GLU166/3.47; C-H Bond/ HIS41/4.09; Pi-Anion/ MET49/3.99; Pi-Sigma/ MET165/4.33; Alkyl MET49/4.33; Alkyl/MET165/5.44	-7.6	-----	-----
(Sinefungin)	-----	---	H-Bond/ASN6841/2.26; H-Bond/LYS6844/2.32; H-Bond/LYS6968/2.25; H-Bond/GLU7001/2.47; H-Bond/ASP6897/2.61; H-Bond/LEU6898/2.26; H-Bond/ASP6897/2.78; H-Bond/ASP6897/2.78; C-H Bond/ASN6841/3.43; Pi-Anion/ASP6928/4.57	-7.8
Comp. 14 (Scopoletin)	H-Bond/SER144/3.17; C-H Bond/PHE140/3.45; C-H Bond/GLU166/3.71; Pi-Donor H-Bond/CYS145/3.74	-5.4	H-Bond/MET6929/2.92; C-H Bond/ASP6897/3.45; Pi-Sigma/LEU6898/3.37; Pi-Pi T-shaped/PHE6947/5.15; Pi-Alkyl/LEU6898/4.94; Pi-Alkyl/CYS6913/5.05; Pi-Alkyl/MET6929/4.48	-6.1
Comp. 19 (Daphnetin)	H-Bond/SER144/3.21; H-Bond/CYS145/3.35; H-Bond/LEU141/1.90; H-Bond/SER144/2.21; Pi-Donor H-Bond/CYS145/4.03;	-5.9	H-Bond/CYS6913/2.30; Pi-Sigma/LEU6898/3.34; Pi-Pi T-shaped/PHE6947/4.81; Pi-Alkyl/LEU6898/5.17; Pi-Alkyl/MET6929/4.68	-6.7
Comp. 23 Esculin	H-Bond/CYS145/3.21; H-Bond/LEU141/1.91; H-Bond/SER144/2.40; H-Bond/ LEU141/2.27; Pi-Alkyl/MET165/4.91	-7.2	H-Bond/LYS6844/2.69; H-Bond/LYS6844/1.81; H-Bond/LEU6898/2.56; H-Bond/ASP6928/2.24; H-Bond/ASP6928/2.13	-7.4
Comp. 10 (Kaempferol-3-*O*-Alpha-L-Rhamnoside)	H-Bond/GLY143/3.13; H-Bond/CYS145/3.25; H-Bond/TYR54/2.79; H-Bond/LEU141/3.00; Pi-Sulfur/MET49/4.80; Pi-Sulfur/MET165/5.68; Pi-Pi Stacked/HIS41/4.20	-8.3	H-Bond/ASN6841/2.24; H-Bond/ASN6899/2.49; H-Bond/TYR6930/2.68; H-Bond/LYS6935/1.96; H-Bond/ASP6928/2.72; H-Bond/GLU7001/2.12; C-H Bond/SER6872/3.48; Pi-Anion/ASP6873/3.52; Pi-Anion/ASP6897/4.01	-7.7
Comp. 17 Kaempferol-3-*O*-(6‴ -p-coumaroyl)-glucoside	H-Bond/TYR54/3.19; H-Bond/CYS145/3.73; H-Bond/GLN192/3.08; H-Bond/PHE140/2.72 H-Bond/LEU141/2.55; H-Bond/THR26/2.52; H-Bond/GLN192/3.00; C-H Bond/ARG188/3.55; C-H Bond/ASN142/3.40; Pi-Sulfur/MET165/4.88; Pi-Alkyl/MET49/4.99; Pi-Alkyl/CYS145/5.31; Pi-Alkyl/MET49/4.34; Pi-Alkyl/CYS145/4.89; Pi-AlkylPRO168/5.18.	-9.2	H-Bond/ASN6841/2.21; H-Bond/ASN6899/2.59; H-Bond/CYS6913/2.25; H-Bond/LYS6968/2.31; H-Bond/GLY6869/1.91; H-BondGLY68769/1.86; H-Bond/GLY6871/3.02; H-Bond/ASP6928/2.47; H-Bond/ASN6996/2.29; C-H Bond/TYR6930/2.97; Pi-Cation/LYS6844/4.38; Pi; Cation/LYS6844/3.91; Pi-Cation/LYS6935/4.88; Pi-Donor H Bond/ASN6996/3.22; Pi-Sigma/LEU6898/3.44; Pi-Sulfur/MET6929/3.69; Pi-Alkyl/LEU6898/4.89; Pi-Alkyl/CYS6913/5.42	-10.2
Comp. 12	H-Bond/PHE140/2.36; H-Bond/GLU166/2.50;	-8.7	H-Bond/LYS6935/2.61; H-Bond/SER6998/2.18;	-8.8

Datiscin	H-Bond/LEU141/1.77; H-Bond/SER144/2.29; H-Bond/CYS145/2.69; H-BondTYR54/2.47; Pi-Sulfur/CYS145/5.17; Pi-Alkyl/MET49/5.00; Pi-Alkyl/MET49/4.49		Pi-Cation/LYS6822/3.35; Pi-Anion/GLU6971/4.55; Pi-Pi Stacked/TYR6828/4.52; Pi-Pi Stacked/TYR6828/3.68	
Comp. 29 Isorhamnetin-3-*O*-Rutinoside	H-Bond/LEU141/.198; H-Bond/TYR54/2.62; H-Bond/ASP187/2.15; H-Bond/GLU166/1.94; Pi-SulfurCYS145/5.14; Pi-Alkyl/MET49/4.94; Pi-Alkyl/MET49/4.54	-8.9	H-Bond/LEU6825/1.74; H-Bond/GLY6829/2.70; H-Bond/HIS6972/2.88; H-Bond/ASP6830/2.90; H-Bond/SER6998/1.83; H-Bond/ASN6996/2.82; H-Bond/SER6998/2.43; C-H Bond/HIS6972/3.77; Pi-Cation/LYS6822/4.09; Pi-Cation;Pi-Donor H- bond/LYS6822/2.41; Pi-Pi Stacked/TYR6828/4.66; Pi-Pi Stacked/TYR6828/3.67	-8.9
Comp. 15 Apigenin-7-*O*-Glucoside	H-Bond/SER144/3.01; H-Bond/SER144/3.23; H-Bond/cys145/3.36; H-Bond/HIS163/2.21; C-H Bond/GLN189/3.42; Pi-Sigma/PRO168/3.50	-8.1	H-Bond/LYS6844/2.70; H-Bond/ASN6899/2.76; H-Bond/CYS6913/1.95; H-Bond/CYS6913/1.98; H-Bond/TYR6930/2.13; H-Bond/LYS6968/2.37; H-Bond/GLU7001/1.91; H-Bond/ASP6912/2.29; C-H Bond/MET6929/3.25; Pi-Sigma/LEU6898/3.46; Pi-Sulfur/MET6929/3.66; Pi-Alkyl/LEU6898/4.84; Pi-Alkyl/CYS6913/5.36	-9.5
Comp. 22 Acacetin	H-Bond/LEU141/1.79; H-Bond/SER144/2.50; C-H Bond/MET49/3.28; Pi-Donor H-Bond/GLU166/4.04; Pi-Sulfur/CYS145/5.44; Pi-Sulfur/CYS145/5.41; Pi-Alkyl/MET49/4.75	-7.2	H-Bond/LYS6814/2.71; H-Bond/TRP6988/2.11; H-Bond/ARG7014/1.78; Pi-Cation/LYS6814/4.19; Pi-Cation/ARG7014/4.53; Pi-Cation/ARG7014/4.34; Pi-Anion/GLU7015/3.29; Pi-Sulfur/MET6815/5.79; Pi-Sulfur/MET6815/5.49; Pi-Alkyl/LYS6814/4.08; Pi-Alkyl/LYS6814/4.24	-7.6
Comp. 11 Baicalein-7-*O*-glucouronoide	H-Bond/SER144/3.04; H-Bond/CYS145/3.69; H-Bond/GLU166/2.66; H-Bond/PHE140/2.88 H-Bond/CYS145/2.25; Pi-Donor H-Bond/HIS41/2.78; Pi-Sulfur/MET165/4.72; Pi-Pi T-shaped/HIS41/5.68;Pi-Alkyl/PRO168/5.18	-8.2	H-Bond/LYS6844/2.16; H-Bond/ASN6899/2.23; H-Bond/LYS6968/1.96; Pi-Sigma/LEU6898/3.42; Pi-Alkyl/LEU6898/4.91; Pi-Alkyl/MET6929/4.38;	-8.7
Comp. 18 Apigenin	H-Bond/SER144/2.49; H-Bond/TYR54/2.49; Pi-Donor H Bond/GLU166/4.07; Pi-Sulfur/CYS145/5.45; Pi-Sulfur/CYS145/5.17; Pi-Alkyl/MET49/4.66	-7.8	H-Bond/ASN6899/2.58; H-Bond/CYS6913/2.67; H-Bond/CYS6913/2.04; H-Bond/TYR6930/2.32; H-Bond/ASP6928/2.18; C-H Bond/MET6929/3.33; Pi-Anion/ASP6897/3.45; Pi-Anion/ASP6897/4.05; Pi-Sigma/LEU6898/3.37; Pi-Sulfur/MET6929/3.76; Pi-Alkyl/LEU6898/4.87; Pi-Alkyl/CYS6913/5.42;	-8.8
Comp. 20 3,5,7-trihydroxy-4'-methoxyflavanone	H-Bond/ GLU166/2.46; H-Bond/ SER144/2.16; C-H Bond/ MET49/3.26; Pi-Sulfur/ CYS145/5.45; Pi-Alkyl/ MET49/4.92; Pi-Alkyl/ MET165/5.43	-7.1	H-Bond/ ASN6899/2.80; C-H Bond/ ASP6912/3.46; C-H Bond/ ASP6897/3.27; Pi-Sigma/ LEU6898/3.56; Pi-Alkyl/ LEU6898/5.04; Pi-Alkyl/ MET6929/4.39;	-8.4
Comp. 24 4'-hydroxyisoflavone-7-O-glucoside	H-Bond/GLU166/3.07; H-Bond/SER144/2.81; C-H Bond/THR190/3.51; Pi-Sulfur/MET165/5.73; Pi-Sulfur/MET165/5.51; Amide-Pi Stacked/THR190/3.62; Pi-Alkyl/PRO168/5.3; Pi-Alkyl/ALA191/4.98	-7.9	H-Bond/CYS6913/2.08; H-Bond/ASP6873/2.06; H-Bond/ASP6912/2.51; C-H Bond/SER6872/3.40; Pi-Anion/ASP6897/4.11; Pi-Anion/ASP6897/3.38; Pi-Sigma/LEU6898/3.51; Pi-Sulfur/MET6929/3.67;	-8.8

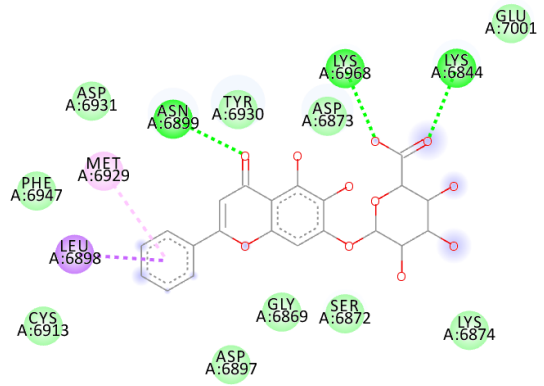
			Pi-Alkyl/LEU6898/4.86; Pi-Alkyl/CYS6913/5.47;	
Comp. 13 **Formononetin**	H-Bond/CYS145/3.39; C-H Bond/MET165/3.51; C-H Bond/ASP187/3.56;C-H Bond/GLN189/3.64; Pi-Alkyl/MET49/4.82	-6.9	Pi-Pi Stacked/TYR7020/4.05; Pi-Pi Stacked/TYR7020/3.69; Pi-Alkyl/VAL7021/4.93	-7.2
Comp. 6 **Daidzein-8-c-glucoside**	H-Bond/GLY143/2.81; H-Bond/SER144/3.05; H-Bond/HIS163/2.26; H-Bond/LEU141/1.69; H-Bond/SER144/2.88; H-Bond/HIS164/1.93; Pi-Alkyl/PRO168/4.93; Pi-Alkyl/MET165/5.03	-7.8	H-Bond/ASN6841/2.41; H-Bond/LYS6968/2.18; H-Bond/GLY6869/2.55; H-Bond/ASP6928/2.46; Pi-Anion/ASP6897/4.43; Pi-Sigma/LEU6898/3.40; Pi-Sulfur/CYS6913/5.76; Pi-Alkyl/LEU6898/4.84; Pi-Alkyl/MET6929/4.18; Pi-Alkyl/PRO6932/4.82	-9.3
Comp. 29 **Myricetin**	H-Bond/SER144/3.09; H-Bond/HIS163/1.95 H-Bond/MET165/2.94; C-H Bond/GLN189/3.42 Pi-Donor H Bond/CYS145/4.16; Pi-Sulfur/MET165/5.24	-7.5	H-Bond/LEU6898/2.27' H-Bond/CYS6913/2.90; H-Bond/ASP6928/1.94; H-Bond/ASP6897/2.61; C- H Bond/ASP6897/3.21; Pi-Anion ASP/6897/3.29; Pi-Sigma/LEU6898/3.40; Pi-Sigma/LEU6898/3.46; Pi-Pi T-shaped/PHE6947/4.73; Pi-Alkyl/LEU6898/4.97; Pi-Alkyl/MET6929/4.38; Pi-Alkyl/LEU6898/5.31; Pi-Alkyl/MET6929/5.09	-9.3



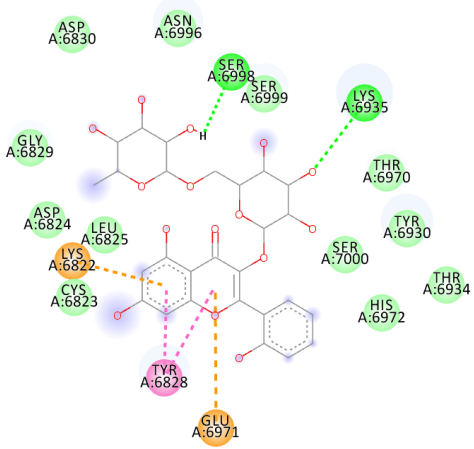
Daidzein-8-C-glucoside (6)



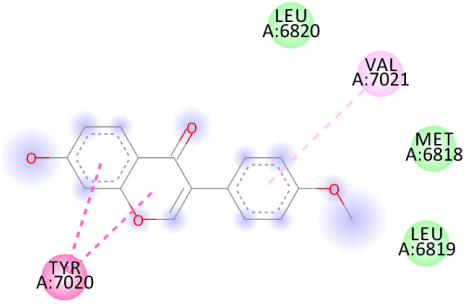
Kaempferol-3-O-alpha-L-rhamnoside (10)



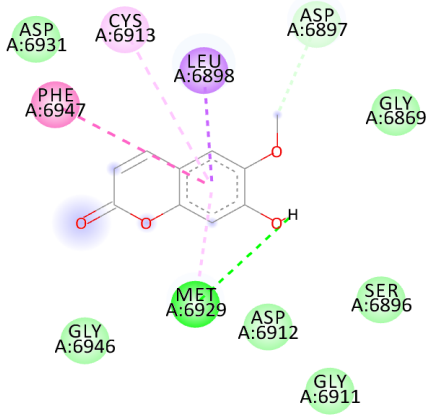
Baicalein-7-*O*-glucouronoide (11)



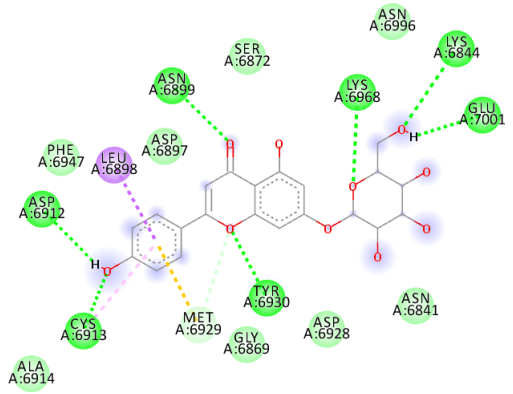
Datiscin (12)



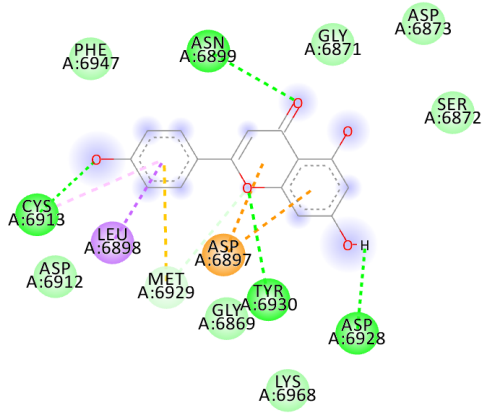
Formononetin (13)



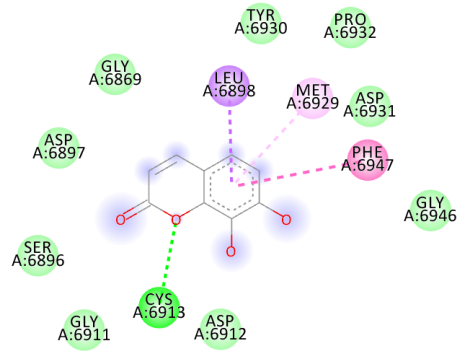
Scopoletin (14)



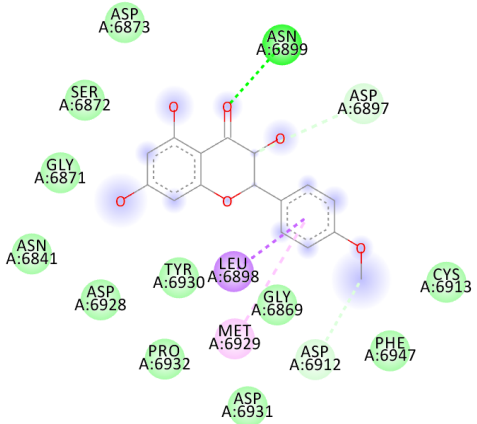
Apigenin-7-O-glucoside (15)



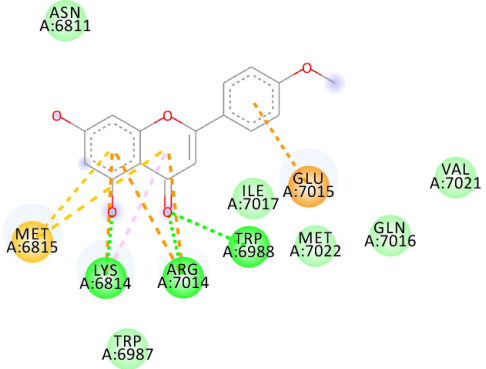
Apigenin (18)



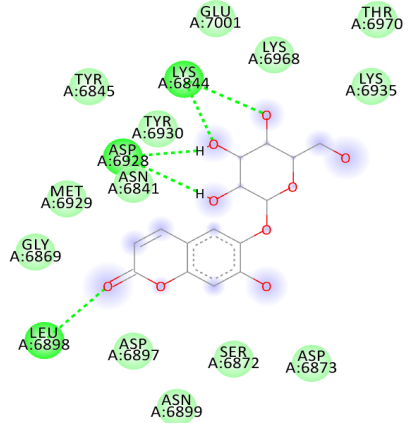
Daphnetin (19)



3, 5, 7-trihydroxy-4'-methoxyflavanone (20)



Acacetin (22)



Esculin (23)

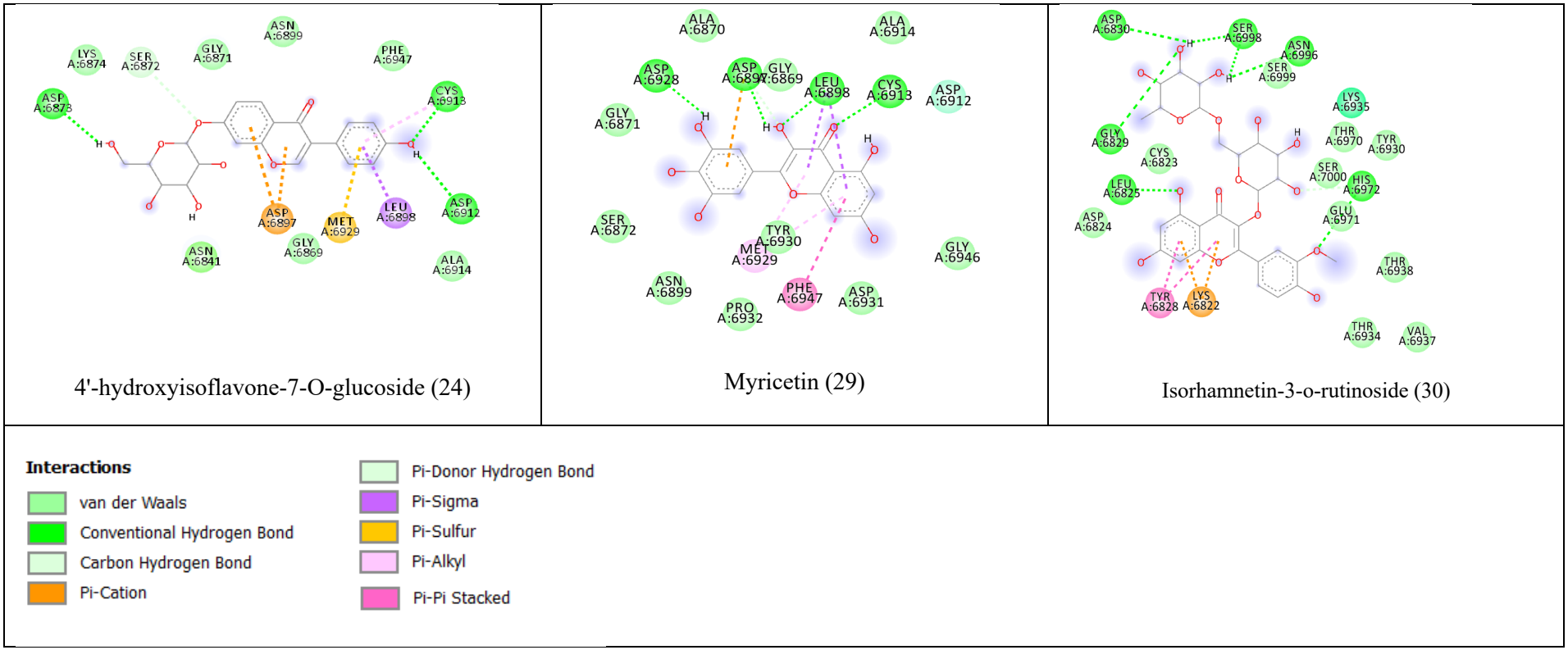
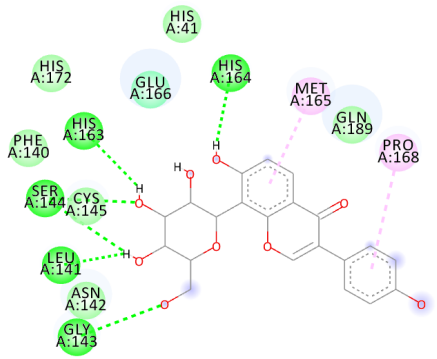
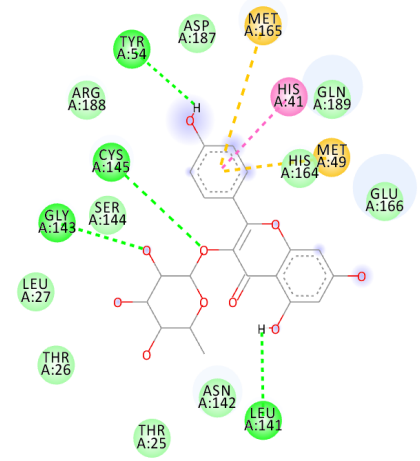


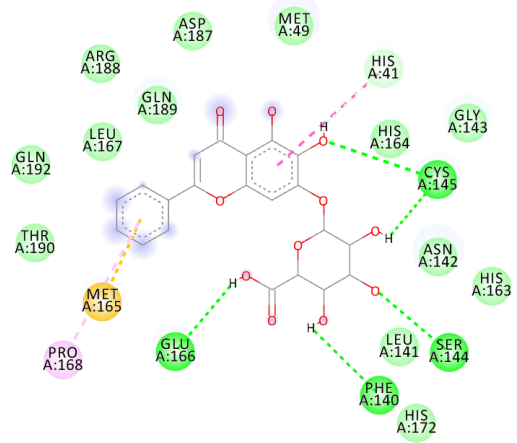
Figure S1: **2D visualization of molecular interaction of 2′-O-RNA methyltransferase (PDB code 6WKQ) binding with Daidzein-8-C-glucoside (6), Kaempferol-3-*O*-alpha-L-rhamnoside (10), Baicalein-7-*O*-glucouronoide (11), Datiscin (12), Formononetin (13), Scopoletin (14), Apigenin-7-*O*-glucoside (15), Apigenin (18), Daphnetin (19), 3, 5, 7-trihydroxy-4'-methoxyflavanone (20), Acacetin (22), Esculin (23), 4'-hydroxyisoflavone-7-*O*-glucoside (24), Myricetin (29) and Isorhamnetin-3-*O*-rutinoside (30).**



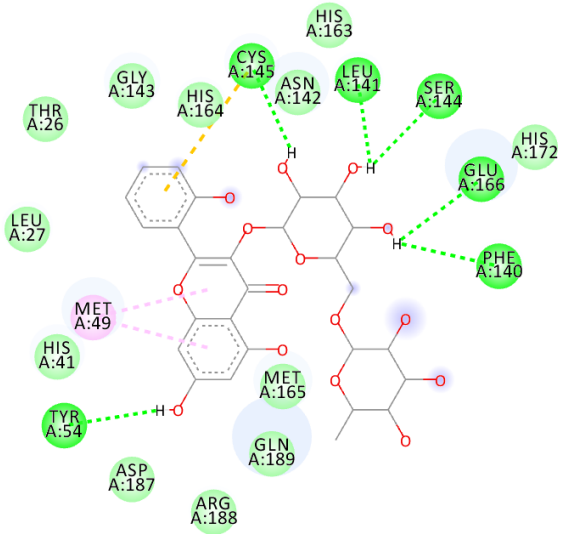
Daidzein-8-C-glucoside (6)

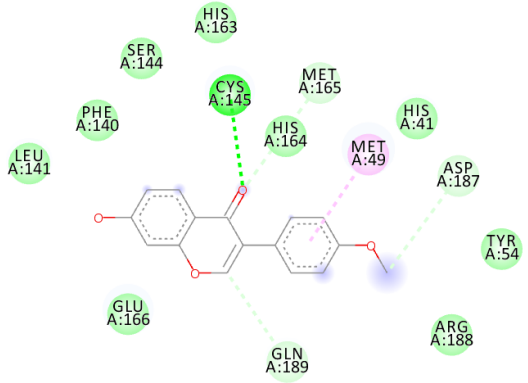


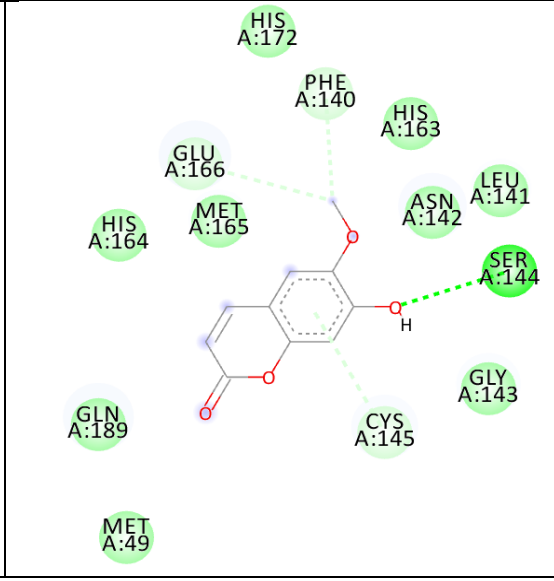
Kaempferol-3-O-alpha-L-rhamnoside (10)

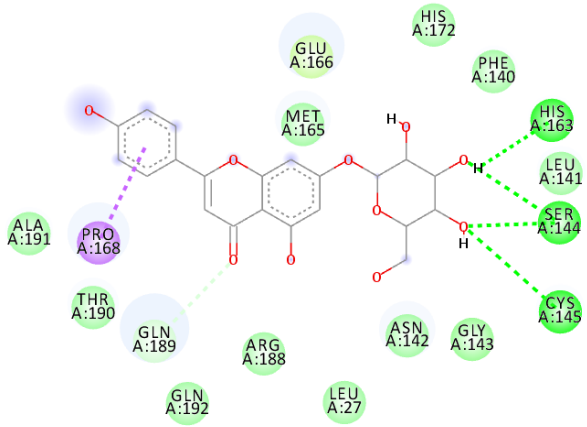
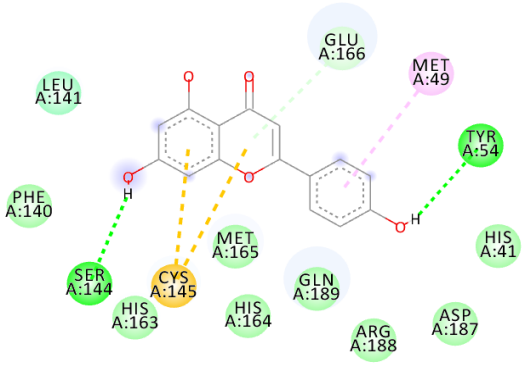
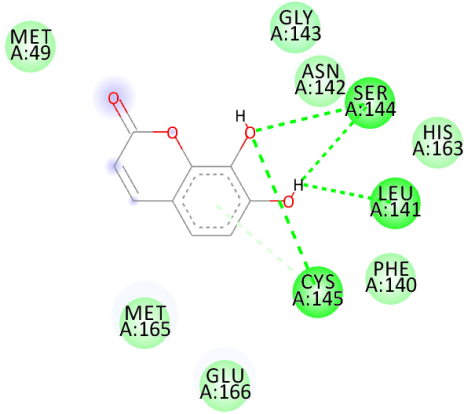
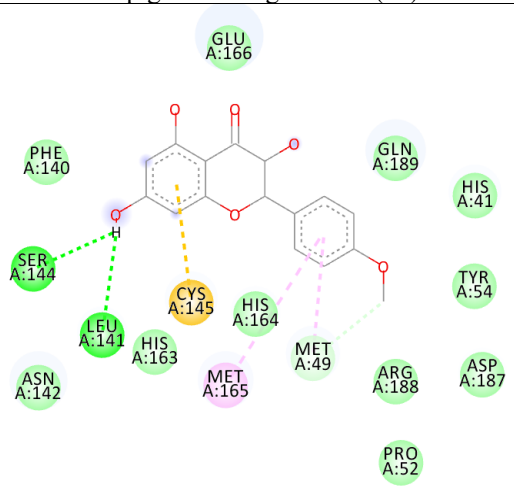
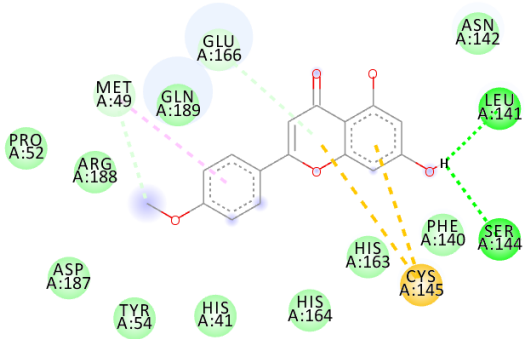
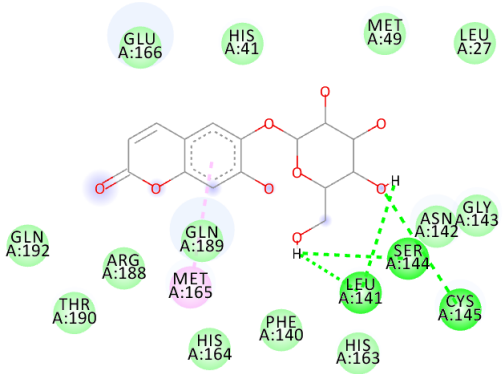


Baicalein-7-*O*-glucouronoide (11)







Datiscin (12)	Formononetin (13)	Scopoletin (14)
		
Apigenin-7-O-glucoside (15)	Apigenin (18)	Daphnetin (19)
		
3,5, 7-Trihydroxy-4'-methoxyflavanone (20)	Acacetin (22)	Esculin (23)

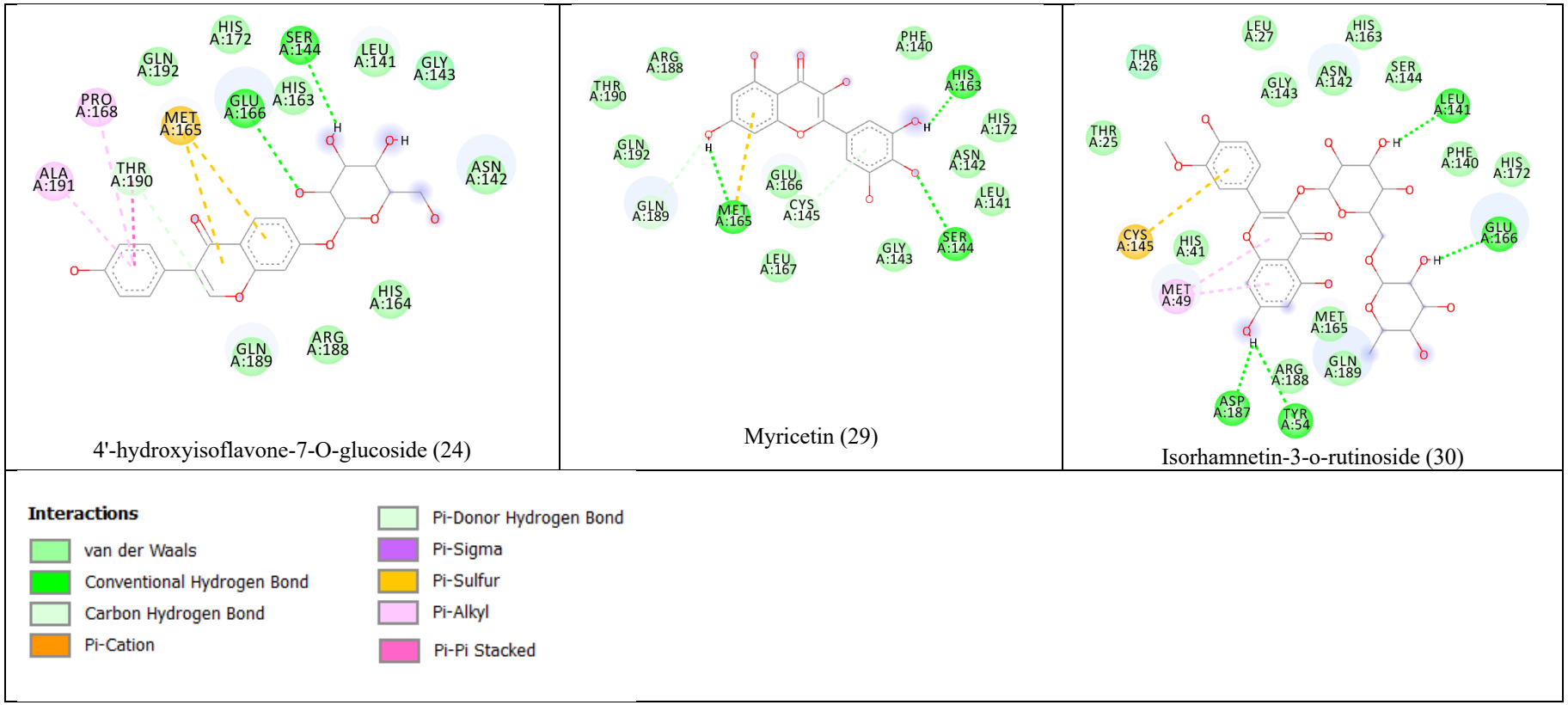


Figure S2: 2D visualization of docking analysis of 6LU7 protease binding with Daidzein-8-C-glucoside (6), Kaempferol-3-O-alpha-L-rhamnoside (10), Baicalein-7-*O*-glucouronoide (11), Datiscin (12), Formononetin (13), Scopoletin (14), Apigenin-7-*O*-glucoside (15), Apigenin (18), Daphnetin (19), 3, 5, 7-trihydroxy-4'-methoxyflavanone (20), Acacetin (22), Esculin (23), 4'-hydroxyisoflavone-7-*O*-glucoside (24), Myricetin (29) and Isorhamnetin-3-*O*-rutinoside (30).