

**Characterization of Possible α -Glucosidase Inhibitors from *Trigonella stellata*
Extract Using LC-MS and In-Silico Molecular Docking**

(SUPPLEMENTARY MATERIAL)

Ahlam Elwekeel^{1†}, Dalia El Amir^{1†}, Enas I. A. Mohamed¹, Elham Amin^{1,2}, Marwa H.
A. Hassan^{1*} and Mohamed A. Zaki^{1*}

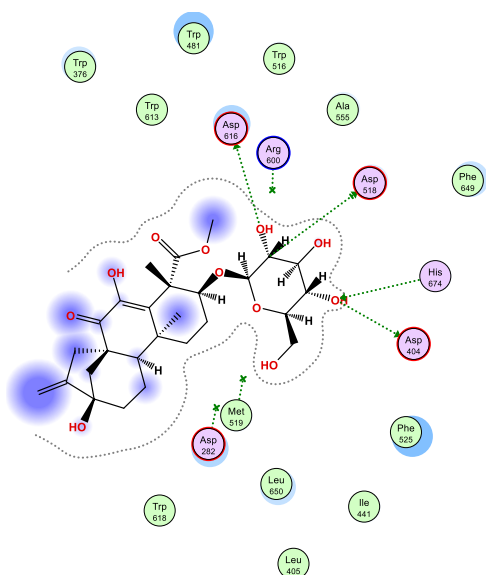
¹Department of Pharmacognosy, Faculty of Pharmacy, Beni-Suef University, Beni-Suef 62514, Egypt.

²Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, Qassim University, Buraidah 52571, Saudi Arabia

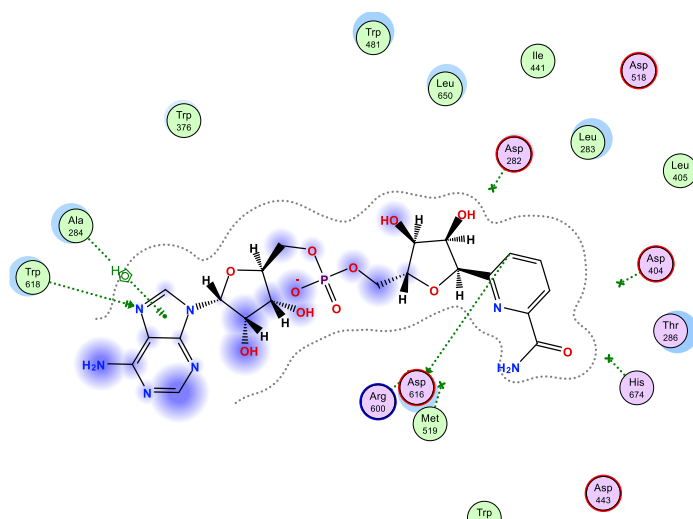
*Corresponding authors

[†]Authors with equal contributions

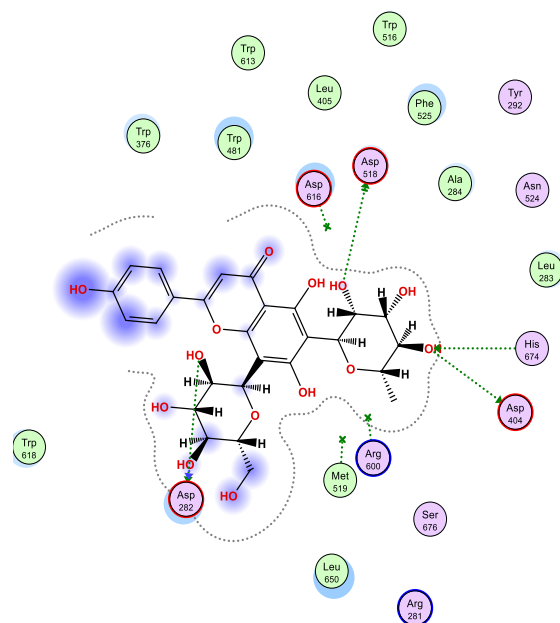
Figure S1: 2D diagram of the binding interactions of compounds detected in *Trigonella stellata* to α -glucosidase enzyme (PDB: 5NN8) binding site.



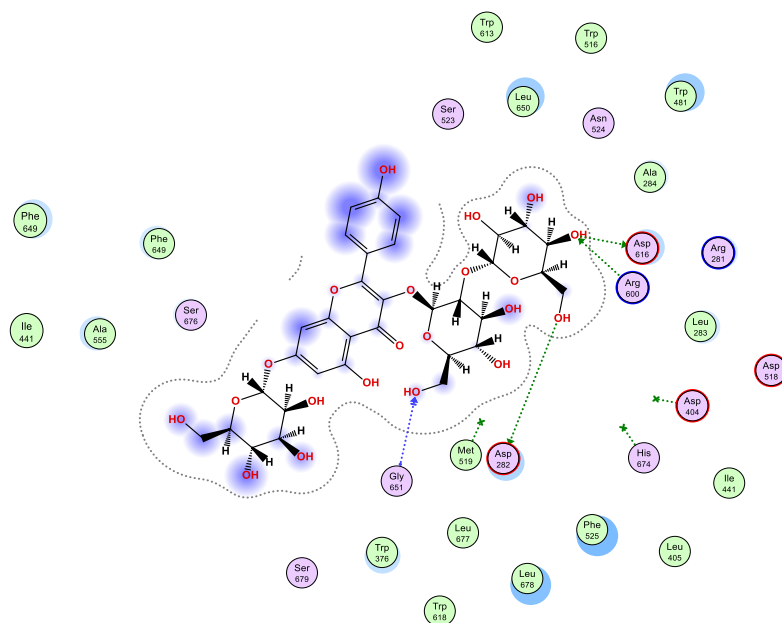
Graecumoside A



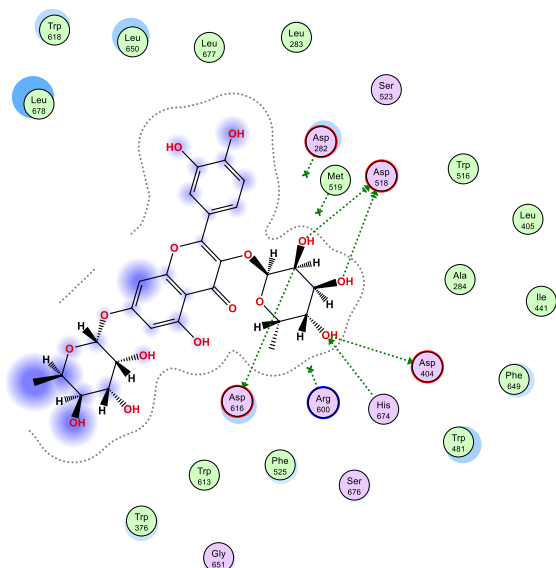
Fenugreekine



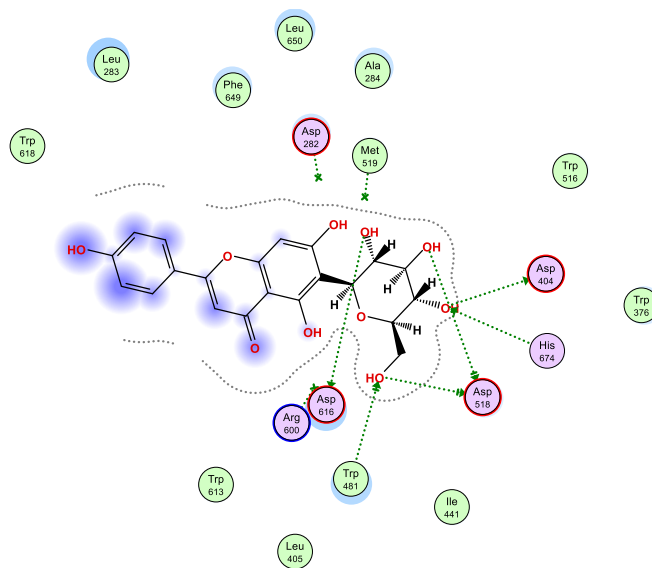
Apigenin-6,8-di-C-rhamnosyl-glucosyl



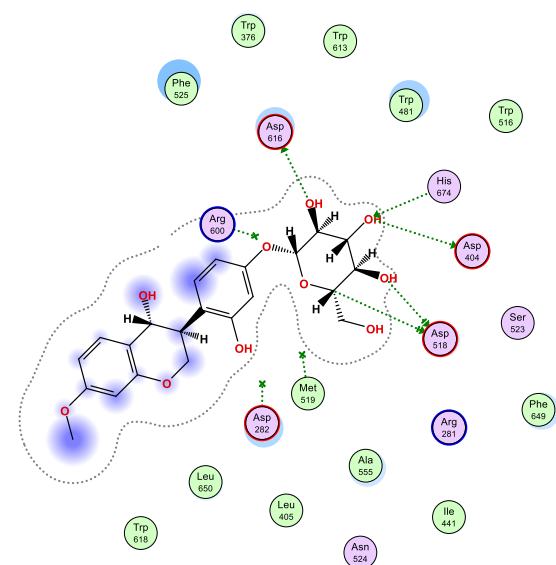
Kaempferol 3-O- β -D-glucosyl (1 \rightarrow 2) β -D-galactoside 7-O- β -D-glucoside



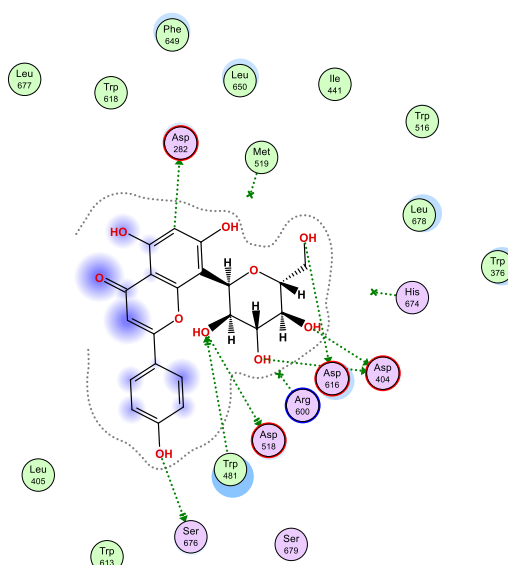
Quercetin-3,7-*O*- α -L dirhamnoside



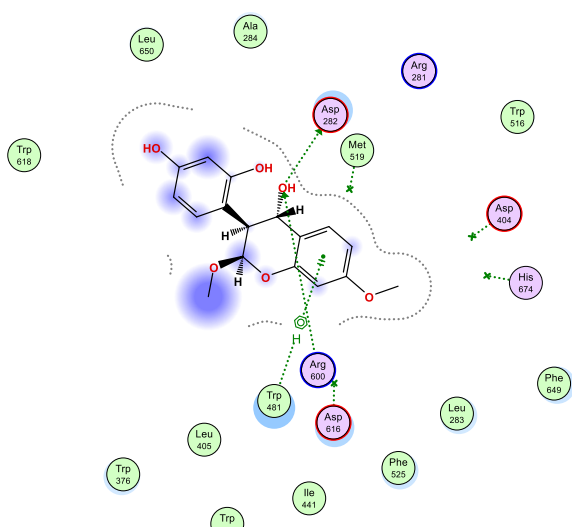
Isovitexin



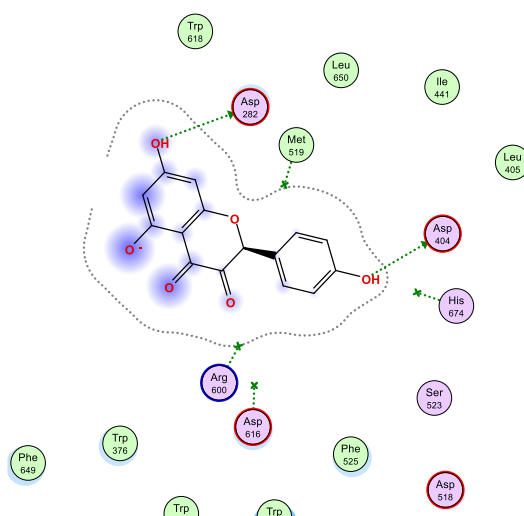
4,2',4'-trihydroxy-7-methoxyisoflavan-4'-*O*- β -D-glucopyranoside



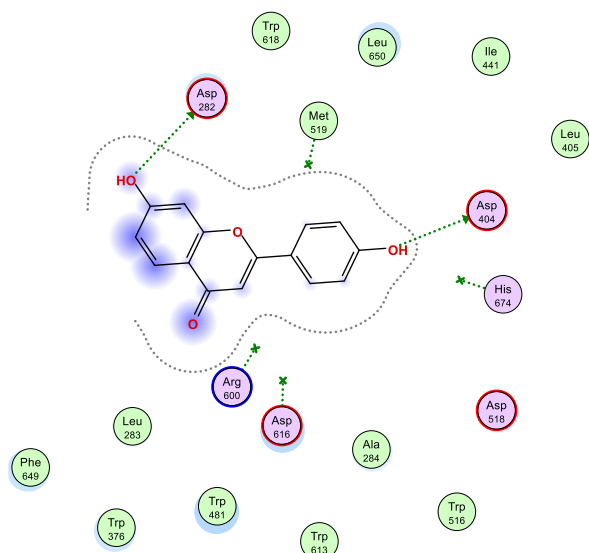
Vitexin



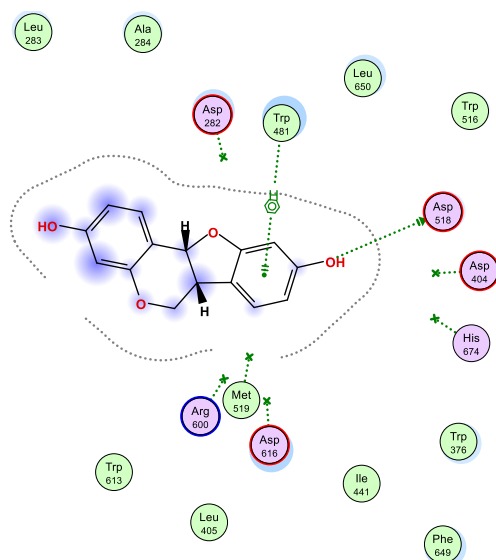
4,2',4'-trihydroxy-2,7dimethoxy isoflavan



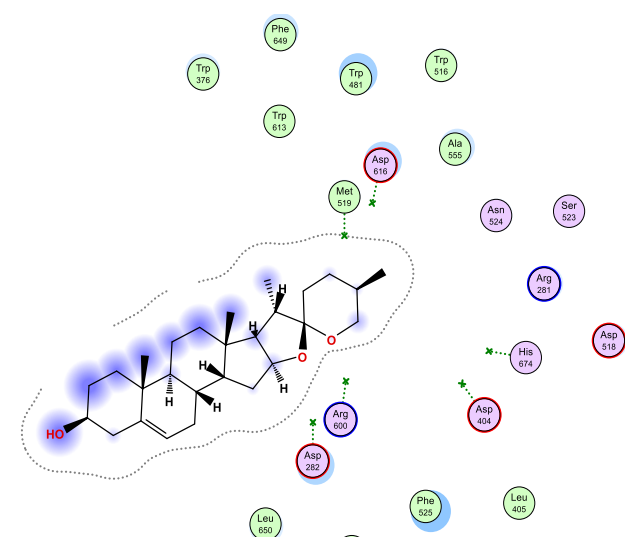
Kaempferol



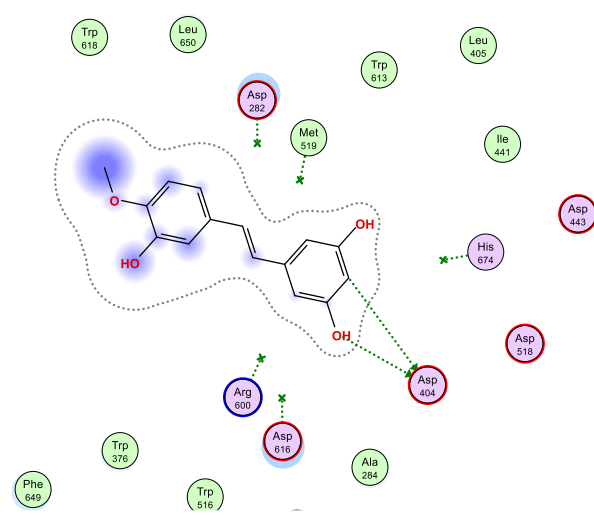
7,4'-dihydroxyflavone



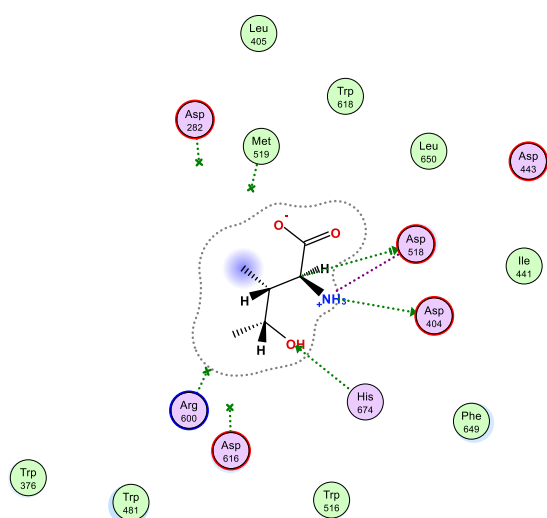
Demethylmedicarpin



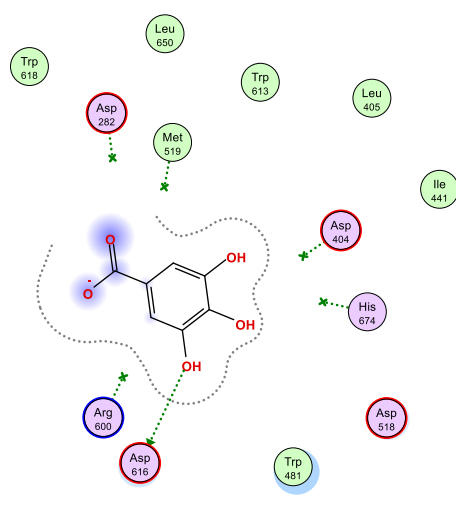
Diosgenin



Rhapontigenin



4-Hydroxyisoleucine



Gallic acid

Table S1: Molecular docking data of compounds detected in *Trigonella stellata* against α -glucosidase enzyme (PDB: 5NN8).

Compound	S	E_place	E_refine
Quercetin3,7-O- α -L dirhamnoside	-8.4145	-122.8735	-56.2776
Kaempferol 3-O- β -D-glucosyl (1 \rightarrow 2) β -D-galactoside 7-O- β -D glucoside	-8.2965	-124.818	-50.5163
Apigenin-6,8-di-C-rhamnosyl-glucosyl	-7.9316	-70.4017	-48.7354
4,2',4'-trihydroxy-7-methoxyisoflavan-4'-O- β -D-glucopyranoside	-7.5373	-79.0674	-43.2596
Graecumoxide A	-7.5332	-79.6454	-44.9570
Fenugreekine	-7.4232	-67.1776	-43.5502
Isovitexin	-7.6797	-81.5558	-53.8580
Vitexin	-7.3030	-76.0586	-37.0603
Diosgenin	-5.7770	-50.8094	-25.5028
4,2',4'-trihydroxy-2,7dimethoxy isoflavan	-5.3993	-56.7509	-26.3511
Kaempferol	-5.1935	-49.4873	-20.8675
4-Hydroxyisoleucine	-5.1152	-50.5002	-22.1747
Rhapontigenin	-5.0388	-66.4366	-21.5091
7,4'-dihydroxyflavone	-4.8529	-87.7661	-20.3868
Demethylmedicarpin	-4.8493	-62.5706	-22.8222
Gallic acid	-4.2908	-57.5793	-14.8477