

Supplementary Files

Table S1. Bond interactions and corresponding lengths from molecular docking studies.
(A) Vitexin interactions with *A. baumannii* regulators 5HM6 and 7ZL4, including the key amino acid residues involved. **(B)** Orientin interactions with *A. baumannii* regulators 5HM6 and 7ZL4, highlighting the participating amino acid residues.

(A)

Bond Interactions between Vitexin and 5HM6 of <i>A. baumannii</i>	No. of bonds	Bond length (Å)	Amino acid residue
Conventional Hydrogen bond	1	2.83	VAL A:109
Pi-Donar Hydrogen bond	1	3.52	THR A:23
Pi-Sigma	1	3.57	LEU A:22
Pi-Alkyl	3	5.01 4.54 4.47	PRO A:111

Bond Interactions between Vitexin and 7ZL4 of <i>A. baumannii</i>	No. of bonds	Bond length (Å)	Amino acid residue
Conventional Hydrogen bond	3	2.48 2.06 2.88	PHE B:35 GLY B:36
Carbon Hydrogen bond	1	2.50	ASN B:34
Alkyl and Pi-Alkyl	9	3.84 5.11 5.34 4.10 5.21 4.80 5.38 4.54 5.30	TRP B:42 LEU B:85 VAL B:94 ILE B:132 TYR B:145 LYS B:140

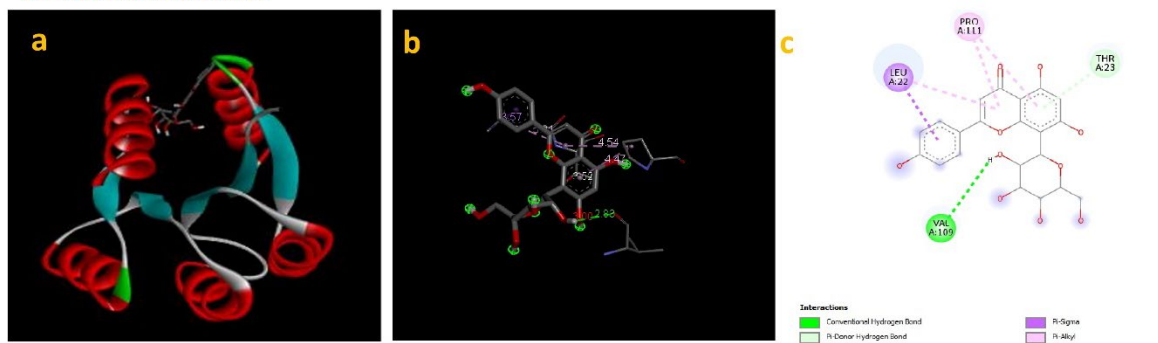
(B) Orientin interactions with *A. baumannii* regulators 5HM6 and 7ZL4, highlighting the participating amino acid residues.

Bond Interactions between Orientin and 5HM6 of <i>A. baumannii</i>	No. of bonds	Bond length (Å)	Amino acid residue
Conventional Hydrogen bond	5	1.88 3.16 2.97 3.26 2.64	LEU A:19 ASP A:16 THR A:23 VAL A:109
Pi-Alkyl	3	4.54 4.62 5.18	PRO A:108

Bond Interactions between Orientin and 7ZL4 of <i>A. baumannii</i>	No. of bonds	Bond length (Å)	Amino acid residue
Conventional Hydrogen bond	2	2.19 2.31 2.62	LYS B:140 GLY B:36
Carbon Hydrogen bond	1	3.44	ASP B:144
Pi-Anion	1	4.54	ASP B:144
Pi-Pi Stacked	1	4.67	TYR B:145
Pi-Alkyl	1	4.02	LYS B:37

Figures

A - Vitexin with 5HM6



B - Vitexin with 7ZL4

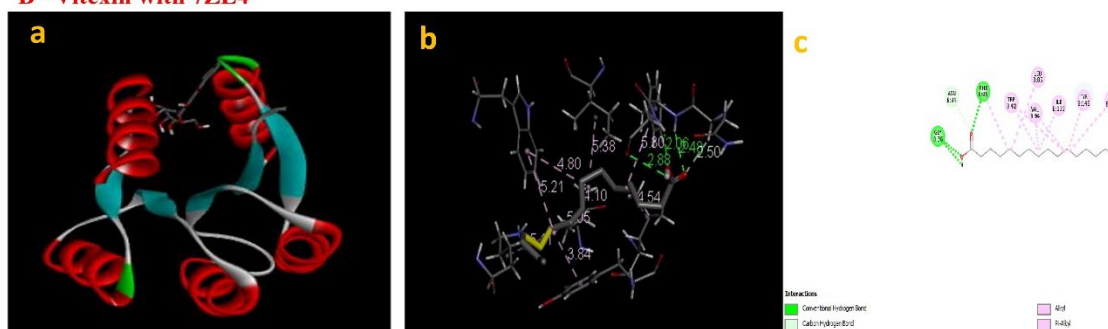
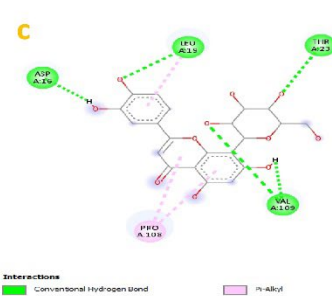
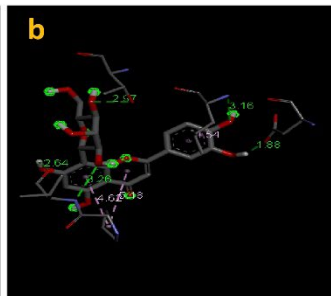


Figure S1. Docking analysis of Vitexin with *A. baumannii* regulators 5HM6 (A) and 7ZL4 (B). The figure illustrates (a) docked 3D conformations, (b) BIOVIA-generated 3D interaction profiles, and (c) corresponding 2D interaction visualizations.

a

A 3D ribbon diagram of the 19S proteasome structure. The structure is composed of two main parts: a large, complex core made of red and cyan subunits, and a smaller, yellow regulatory subunit attached to the side. The red subunits form a large, multi-layered structure, while the cyan subunits are interspersed within it. The yellow subunit is a smaller, more compact structure. The entire structure is set against a black background.

a

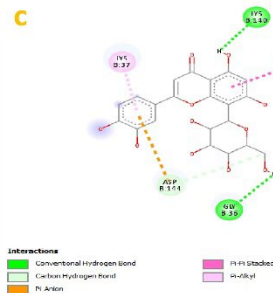
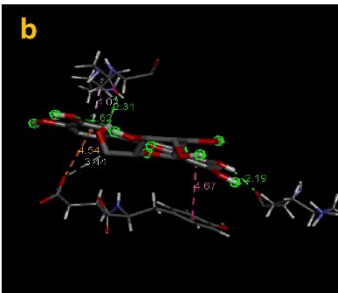


Figure S2. Docking analysis of Orientin with *A. baumannii* regulators 5HM6 (A) and 7ZL4 (B). The figure presents (a) docked 3D conformations, (b) BIOVIA-generated 3D interaction profiles, and (c) corresponding 2D interaction visualizations.