Supplementary file

Phytochemical profiling, *In vitro* Biological activities, and *In-Silico* Studies of *Ficus vasta Forssk.*: An unexplored plant

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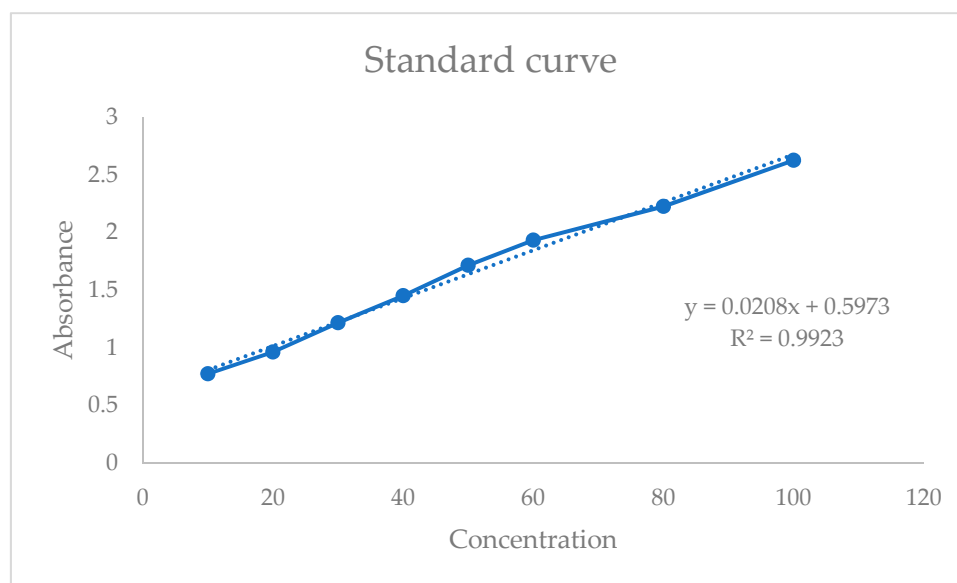† These authors contributed equally to this work.

Figure S1. Standard curve, regression equation and R^2 for quantification of phenolics
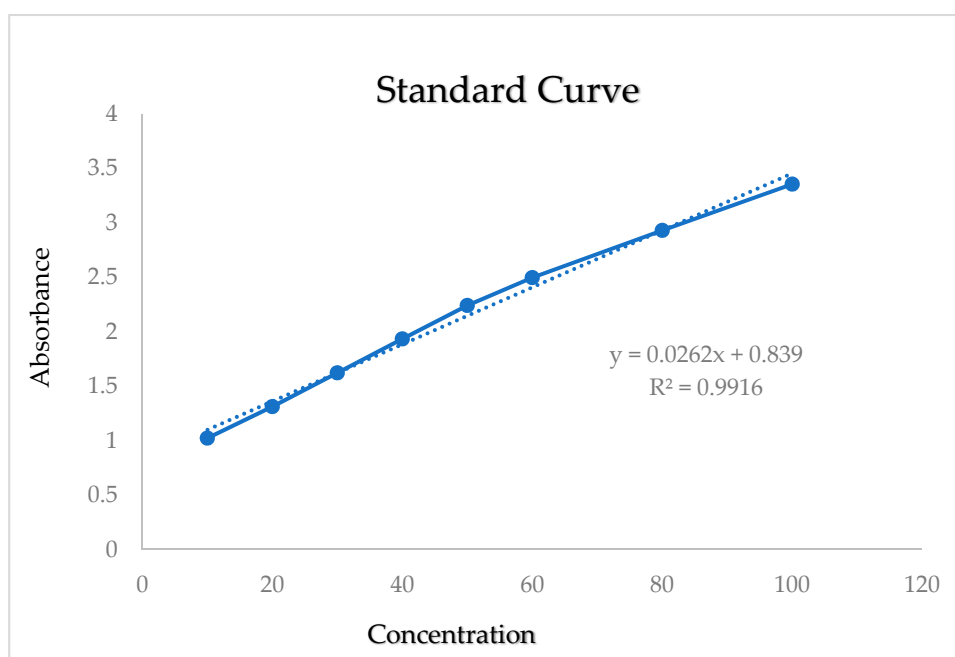
Figure S2. Standard curve, regression equation and R² for quantification of flavonoids
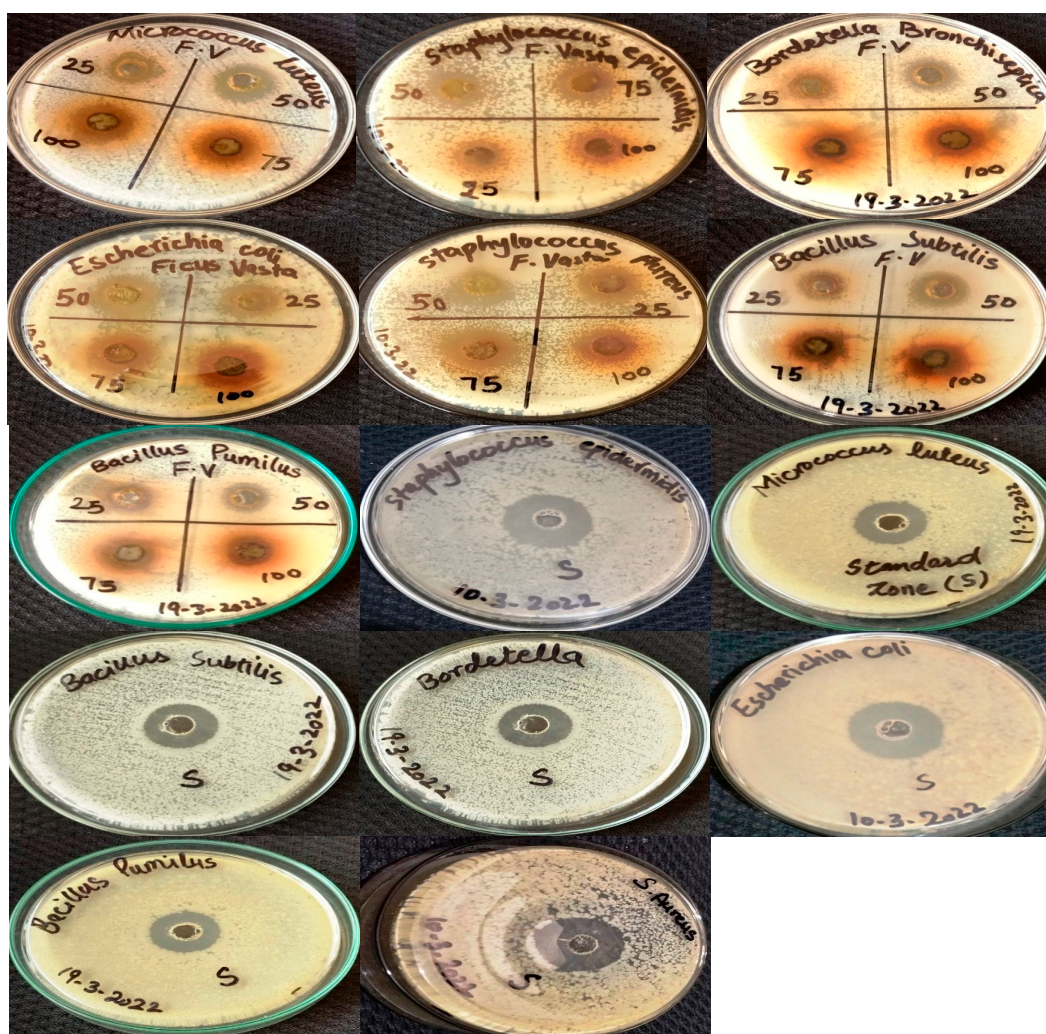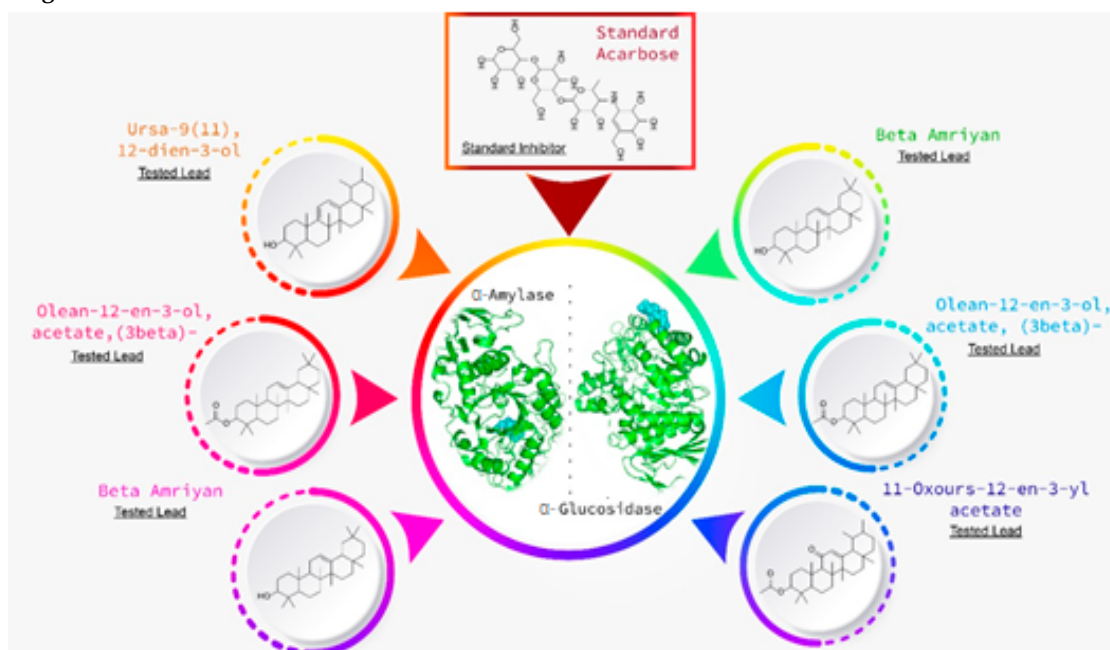
Figure S3. Antibacterial results of *F. vasta* ethanolic extract.

Figure S4. Graphical representation of best three docked compounds and Acarbose against α-glucosidase and α-amylase.

Table S1. Pharmacokinetic properties of best-docked compounds.

Sr no.	Best docked compounds	Gastrointestinal absorption	Blood-brain barrier	P-glycoprotein substrate	CYP inhibitors					log Kp skin permeation (cm/s)
					CYP 1A2	CYP 2C19	CYP 2C9	CYP 2D6	CYP 3A4	
1	Ursa-9(11),12-dien-3-ol	Low	✗	✗	✗	✗	✗	✗	✗	-2.69
2	Olean-12-en-3-ol, acetate, (3beta)-	Low	✗	✗	✗	✗	✗	✗	✗	-2.25
3	Beta-Amyrin	Low	✗	✗	✗	✗	✗	✗	✗	-2.41
4	11-Oxours-12-en-3-yl acetate	Low	✗	✗	✗	✗	✗	✗	✗	-3.2
5	Campesterol	Low	✗	✗	✗	✗	✗	✗	✗	-2.5
6	Beta-Sitosterol	Low	✗	✗	✗	✗	✗	✗	✗	-2.2
7	Stigmasterol	Low	✗	✗	✗	✗	✓	✗	✗	-2.74

✗; NO, and ✓; yes.

Table S2. Toxicity profiles of best-docked compounds.

Sr no.	Best docked compounds	LD50 mg/kg	Predicted class	Hepatotoxic	Carcinogenic	Immunotoxic	Mutagenic	Cytotoxic
1	Ursa-9(11),12-dien-3-ol	288	3	✗	✗	✓	✗	✗
2	Olean-12-en-3-ol, acetate, (3beta)-	3460	5	✗	✓	✓	✗	✗
3	Beta-Amyrin	70000	6	✗	✗	✓	✗	✗
4	11-Oxours-12-en-3-yl acetate	3300	5	✗	✓	✓	✗	✗
5	Campesterol	890	4	✗	✗	✓	✗	✗
6	Beta-Sitosterol	890	4	✗	✗	✓	✗	✗
7	Stigmasterol	890	4	✗	✗	✓	✗	✗

✓: Active, ✗: Inactive, Class I: $LD_{50} \leq 5$, class ii: $5 < LD_{50} \leq 50$, class iii: $50 < LD_{50} \leq 300$, class iv: $300 < LD_{50} \leq 2000$, class v: $2000 < LD_{50} \leq 5000$, and class vi: $LD_{50} > 5000$.
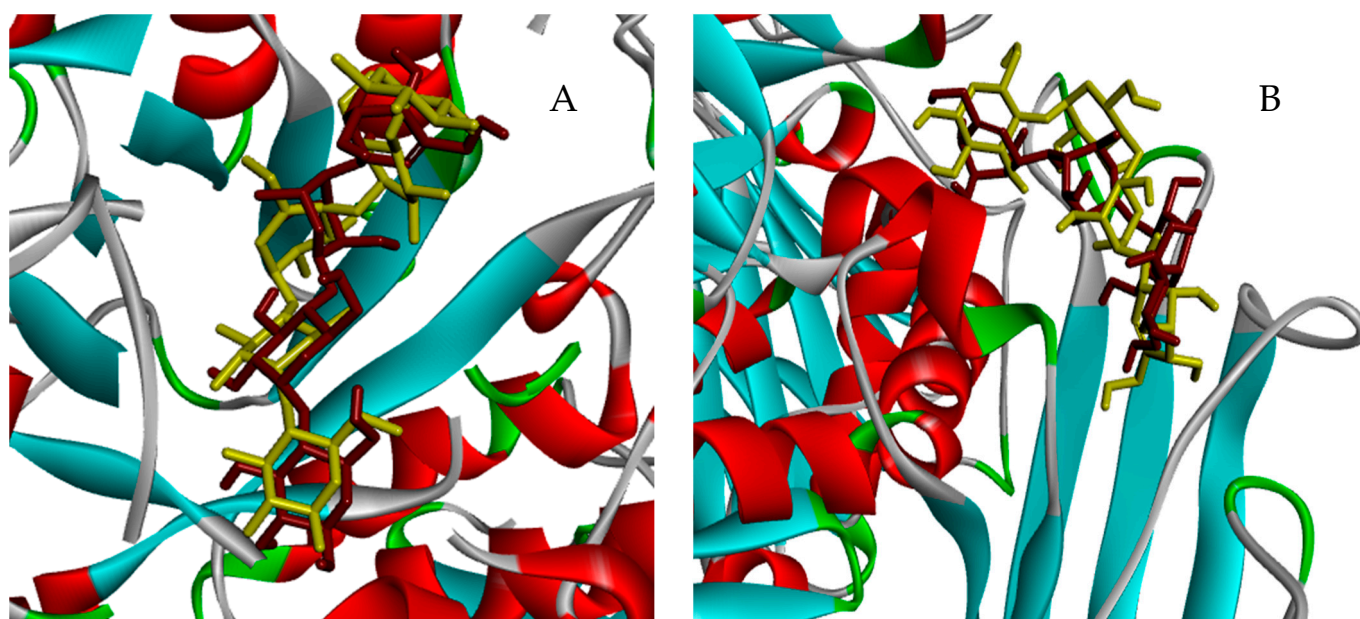
Figure S5. Superimposition of re-docked (Red) onto co-crystallized Acarbose (Yellow) in the active site. "A" α-amylase (RMSD value=1.525 Å) and "B" α-glucosidase (RMSD value=1.234 Å).