

Supplementary file

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

Hanan Y. Aati ^{1,*},[†], Mariyam Anwar², Jawaher Al-Qahtani ¹, Areej Al-Taweel ¹, Kashif-ur-Rehman Khan^{2,*},[†], Sultan Aati³, Faisal Usman⁴, Bilal Ahmad Ghalloo², Hafiz Muhammad Asif⁵, Jafir Hussain Shirazi⁶, Aliza Abbasi²

¹ Department of Pharmacognosy, College of Pharmacy, King Saud University, Riyadh 11495, Saudi Arabia

² Department of Pharmaceutical Chemistry, Faculty of Pharmacy, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan

³ UWA, University of Western Australia, Nedland, WA 6009, Australia

⁴ Department of Pharmaceutics, Faculty of Pharmacy, Bahauddin Zakariya University, Multan 60000, Pakistan

⁵ Faculty of Medicine and Allied Health Sciences, University College of Conventional Medicine, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan

⁶ Department of Pharmaceutics, Faculty of Pharmacy, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan

* Correspondence: hati@ksu.edu.pk (H.Y.A.); kashifur.rahman@iub.edu.pk (K.-u.-R.K.)

[†] These authors contributed equally to this work.

Citation: Aati, H.Y.; Anwar, M.; Al-Qahtani, J.; Al-Taweel, A.; Khan, K.-u.-R.; Aati, S.; Usman, F.; Ghalloo, B.A.; Asif, H.M.; Shirazi, J.H.; et al. Phytochemical profiling, *In vitro* Biological activities, and *In-Silico* Studies of *Ficus vasta* Forssk.: An unexplored plant. *Antibiotics* **2022**, *11*, 1155. <https://doi.org/10.3390/antibiotics11091155>

Academic Editor: Muhammad Jawad Nasim

Received: 5 July 2022

Accepted: 23 August 2022

Published: 26 August 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).

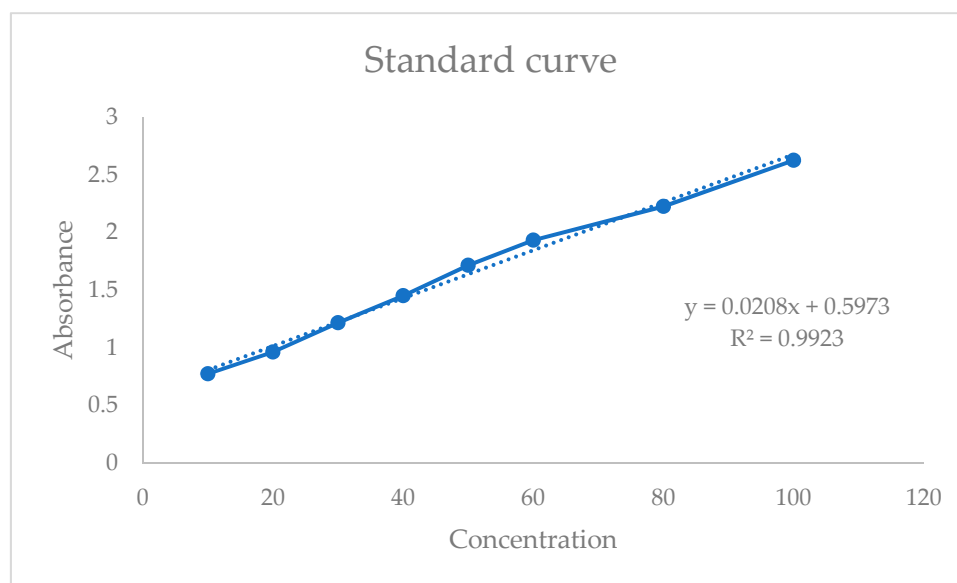


Figure S1. Standard curve, regression equation and R^2 for quantification of phenolics

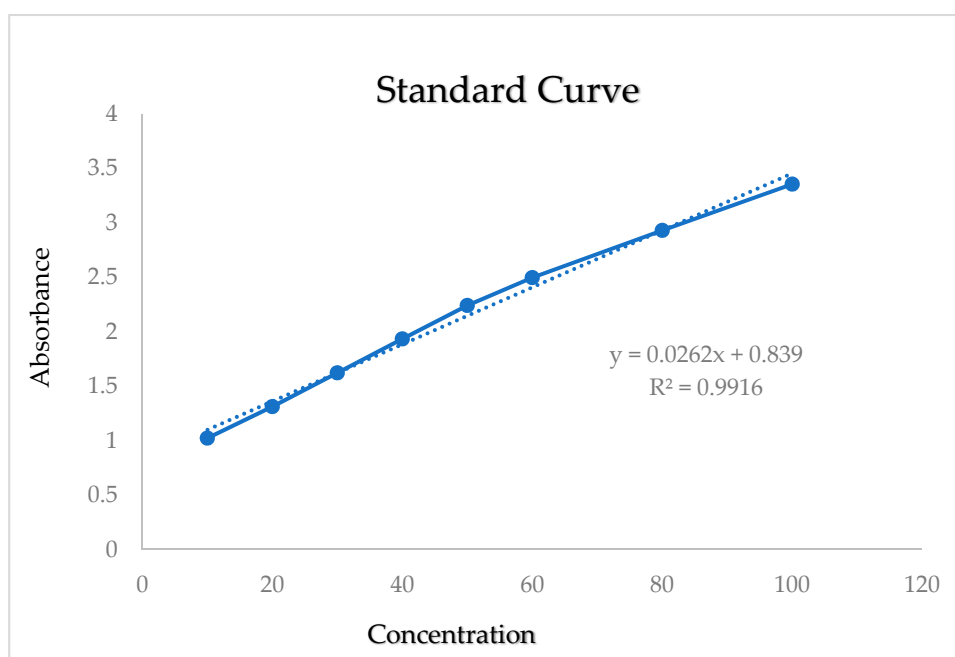


Figure S2. Standard curve, regression equation and R^2 for quantification of flavonoids

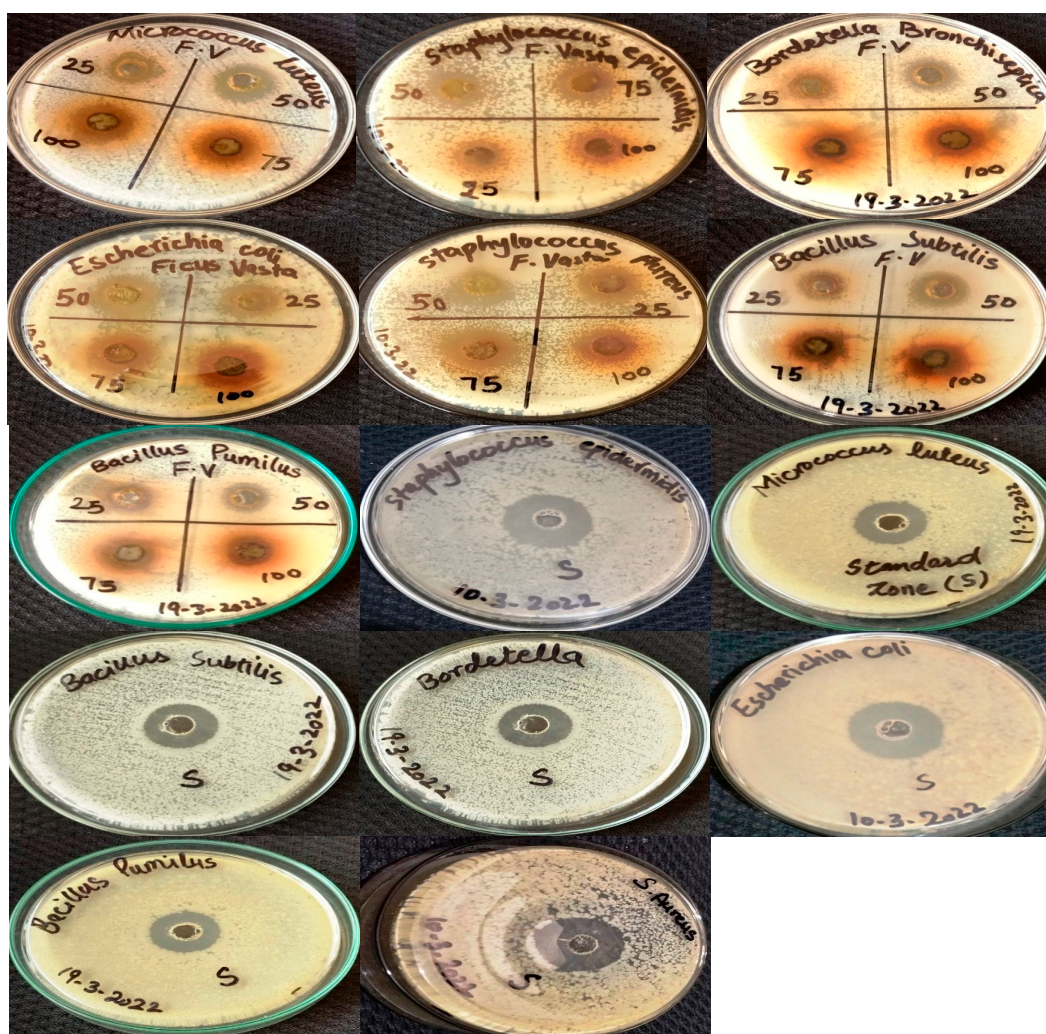
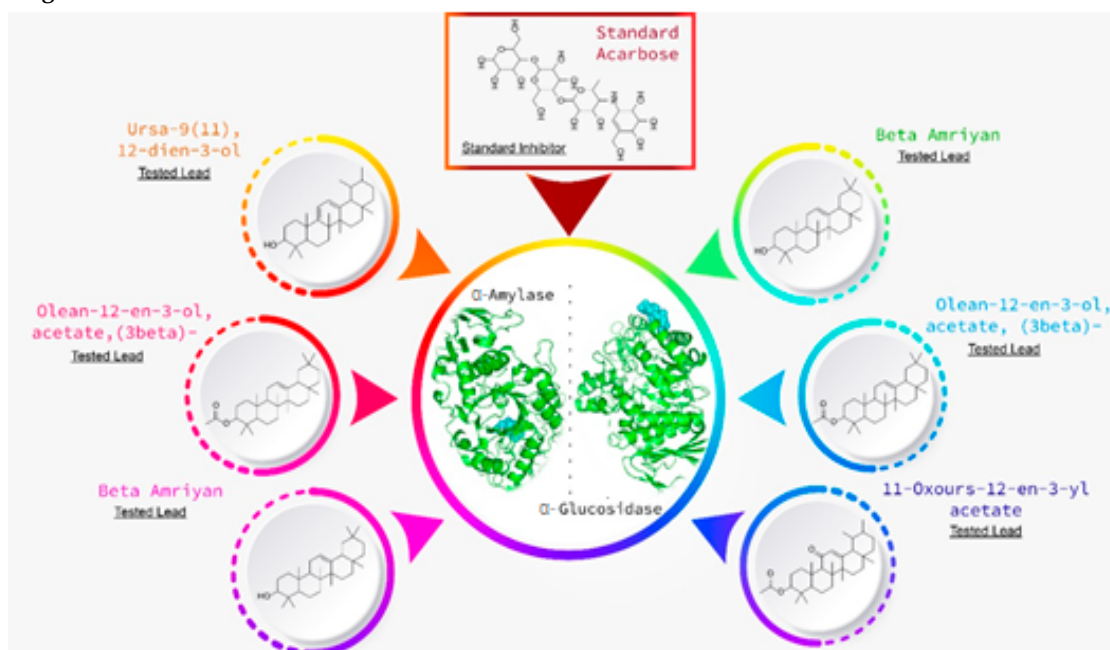


Figure S3. Antibacterial results of *F. vasta* ethanolic extract.**Figure S4.** Graphical representation of best three docked compounds and Acarbose against α -glucosidase and α -amylase.**Table S1.** Pharmacokinetic properties of best-docked compounds.

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: $LD_{50} > 5000$.

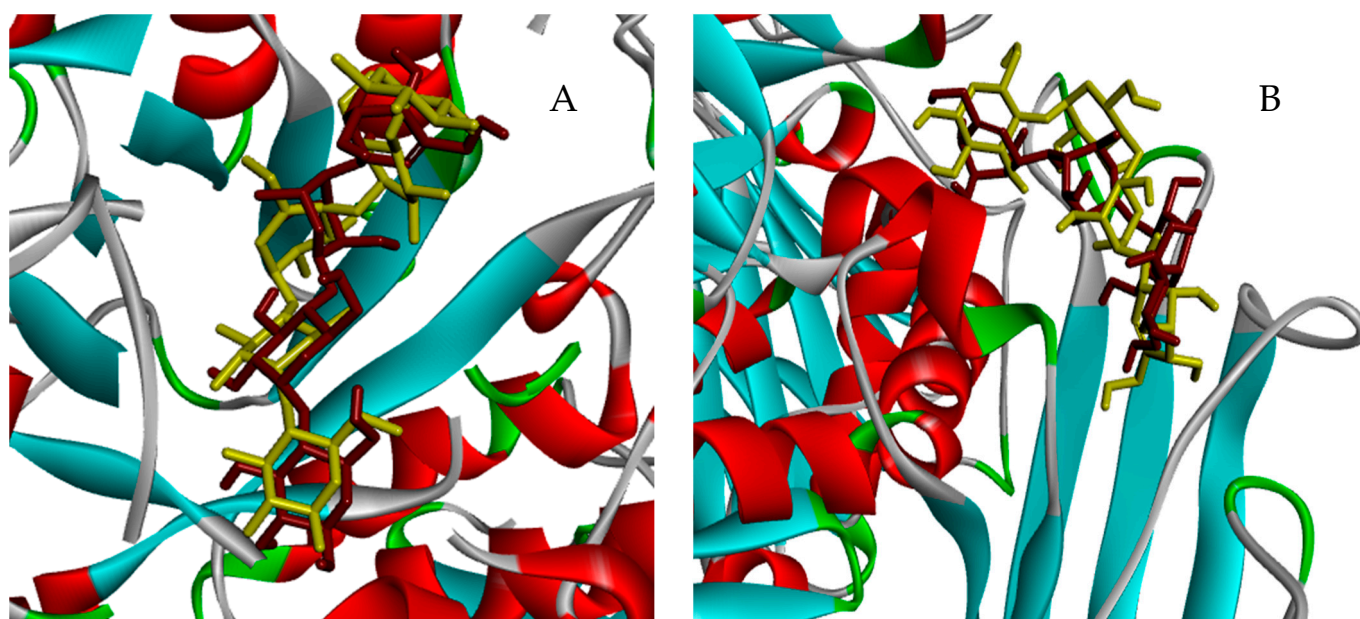


Figure S5. Superimposition of re-docked (Red) onto co-crystallized Acarbose (Yellow) in the active site. “A” α -amylase (RMSD value=1.525 Å) and “B” α -glucosidase (RMSD value=1.234 Å).