

Article

Phytochemical Profiling of the Ethanolic Extract of *Zaleya pentandra* L. Jaffery and Its Biological Activities by In-Vitro Assays and In-Silico Molecular Docking

Afia Shahid ¹, Kashif ur Rehman Khan ^{1,*}, Huma Rao ¹, Hanan Y. Aati ², Asmaa E. Sherif ^{3,4}, Duraiz Ahmed Khan ¹, Abdul Basit ^{1,5}, Muhammad Umair ⁶, Abdul Mueed ⁷, Tuba Esatbeyoglu ^{8,*} and Sameh A. Korma ^{9,10}

¹ Department of Pharmaceutical Chemistry, Faculty of Pharmacy, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan

² Department of Pharmacognosy, College of Pharmacy, King Saud University, Riyadh 11495, Saudi Arabia

³ Department of Pharmacognosy, College of Pharmacy, Prince Sattam bin Abdul Aziz University, Alkharj 11942, Saudi Arabia

⁴ Department of Pharmacognosy, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt

⁵ Department of Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, Prince of Songkla University, Hat Yai 90112, Songkla, Thailand

⁶ College of Pharmacy, Shenzhen Technology University, Shenzhen 518060, China

⁷ State Key Laboratory of Food Science and Technology, Nanchang University, Nanchang 330047, China

⁸ Department of Food Development and Food Quality, Institute of Food Science and Human Nutrition, Gottfried Wilhelm Leibniz University Hannover, Am Kleinen Felde 30, 30167 Hannover, Germany

⁹ Department of Food Science, Faculty of Agriculture, Zagazig University, Zagazig 44519, Egypt

¹⁰ School of Food Science and Engineering, South China University of Technology, Guangzhou 510641, China

* Correspondence: kashifur.rahman@iub.edu.pk (K.u.R.K.); esatbeyoglu@lw.uni-hannover.de (T.E.); Tel.: +92-33-6670-8638 (K.u.-R.K.); +49-51-1762-5589 (T.E.)

Table S2. Toxicity studies (PROTOX II) results of the best docked compounds.

Sr No.	Best Docked Compounds	LD ₅₀ mg/kg	Predicted Class	Hepatotoxic	Carcinogenic	Immunotoxic	Mutagenic	Cytotoxic
1	2-Hydroxy-n-(2-phenylethyl)benzamide	2530	5	-	-	-	-	-
2	1,2-Benzenedicarboxylic acid	1000	4	Inactive	Inactive	Inactive	Inactive	Inactive
3	[1,3] Diazepan-2,4-dione	1600	4	Inactive	Inactive	Inactive	Inactive	Inactive
4	Lactose	10000	6	Inactive	Inactive	Inactive	Inactive	Inactive
5	Tricyclo[4.3.1.1(3,8)]undecane-1-carboxylic acid	1000	4	Inactive	Inactive	Inactive	Inactive	Inactive
6	Cis-(-)-carvone-5,6-oxide	5000	5	Inactive	Inactive	Inactive	Inactive	Inactive
7	Phthalic acid, bis-7-methyloctyl ester	1340	4	Inactive	Active	Inactive	Inactive	Inactive
8	γ -Sitosterol	890	4	Inactive	Inactive	Active	Inactive	Inactive
9	Diethyl phthalate	1340	4	Inactive	Active	Inactive	Inactive	Inactive

Class I: (LD₅₀ less than equals to 5), **Class II:** (LD₅₀ greater than 5 but less than equals to 50), **Class III:** (LD₅₀ greater than 50 but less than equals to 300), **Class IV:** (LD₅₀ greater than 300 but less than equals to 2000), **Class V:** (LD₅₀ Greater than 2000 but less than equals to 5000), **Class VI:** LD₅₀ (greater than 5000).