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Research article

In-vitro biological activity and in-silico studies of some volatile phytochemicals from the ethanol extract of *Eugenia uniflora*

Abdulrahman Mahmoud Dogara[1,2], Ateeq Ahmed Al-Zahrani[3,*], Sarwan W. Bradosty[4], Saber W. Hamad[5,6], Aisha Abdullahi Mahmud[7], Hussain D. Almalki[3], Mustapha Abdullahi[8], Abubakar Abdullahi Lema[9] and Hasan Nudin Nur Fatihah[2]

[1] Biology Education Department, Tishk International University, Erbil, Iraq
[2] Faculty of Bioresources and Food Industry, Universiti Sultan Zainal Abidin, Besut Campus, 22200 Besut, Terengganu, Malaysia
[3] Chemistry Department, University College at Al-Qunfudhah, Umm Al-Qura University, Saudi Arabia
[4] Department of Medical Laboratory Science, College of Science, Cihan University-Erbil, Kurdistan Region, Iraq
[5] Department of Field Crops and Medicinal Plants, College of Agricultural Engineering Sciences, Salahaddin University-Erbil, Erbil, Kurdistan Region, Iraq
[6] Department of Medical Laboratory Science, College of Science, Knowledge University, Kirkuk Road, 44001 Erbil, Iraq
[7] Department of Plant Science and Biotechnology, Faculty of Life Science, Federal University Dutsin-Ma, Katsina State, Nigeria
[8] Department of Pure and Applied Chemistry, Kaduna State University, Kaduna, Nigeria
[9] Department of Biological Sciences, College of Natural and Applied Sciences, AL-Qalam University Katsina, Katsina State Nigeria

* **Correspondence:** Email: aaalzahrani@uqu.edu.sa; Tel: +966547393953.

Abstract: Throughout history, humans have heavily relied on plants for both nourishment and the treatment of diseases. Breast cancer chemotherapies are expensive, have side effects, and may develop resistant cells. This shows the need for natural therapies to reduce the side effects of pharmacological remedies. Our objective was to isolate phytochemicals from the ethanol extract of the *Eugenia uniflora* plant. Another objective was to assess the antioxidant activity of the crude ethanolic extract of *E. uniflora* leaves and predict the drug-likeness, pharmacokinetics, and binding potentials of the identified

phytochemicals as anti-breast cancer agents. From the results, fifteen phytochemicals were isolated and identified. The average total phenolic content (TPC), total flavonoid content (TFC), radical scavenging activity (DPPH), and ferric reducing antioxidant power (FRAP) values for the ethanol extract were 119.5 mg GAE/g, 141.16 mg GAE/g, 37.8 µg/mL, and 7.2 mmol/g, respectively. The chemical composition revealed 15 compounds: 3-Undecene, Acetic acid, Benzofuran, Hydroquinone, alpha-L-Galactopyranose, Methyl hexofuranoside, Nonadecanoic acid, 10-Octadecenoic acid, 2-Nonen-1-ol, Z-8-Methyl-9-tetradecenoic, 10-Undecenal, 2-Octylcyclopropene-1-heptanol, 1,5-Cyclododecadiene, Allantoic acid, and Stearic acid hydrazide. The drug-likeness and ADME properties of the fifteen identified compounds revealed non-violation of Lipinski's rules of five requirements. The docking screening of the fifteen identified phytochemicals with the human placental aromatase target revealed Stearic acid hydrazide, with the highest binding affinity of −7.86 kcal/mol, which can serve as a competitive aromatase inhibitor. The *in-silico* study gave a high probability that some of these compounds could be used as aromatase inhibitors and thus play a role in treating breast cancer. As far as we are aware, there has been no prior research conducted on the potential inhibitory effects of certain compounds found in *E. uniflora* on the aromatase enzyme.
Keywords: flavonoids; *Eugenia uniflora*; antioxidant activity; *in silico*; cancer

Supplementary

Supplementary Table 1. Solubility predictions of the identified compounds.

S/N.	PubChem CID	Solubility parameters		
		Log S (ESOL)	**Log S (Ali)**	**Log S (SILICOS-IT)**
1	5362751	−3.64 (soluble)	−4.99 (moderately soluble)	−3.56 (soluble)
2	176	−0.08 (very soluble)	−0.12 (very soluble)	0.53 (soluble)
3	9223	−2.99 (soluble)	−2.6 (soluble)	−3.23 (soluble)
4	785	−1.45 (very soluble)	−1.01 (very soluble)	−1.18 (soluble)
5	439554	−1.67 (very soluble)	−2.24 (soluble)	−0.15 (soluble)
6	134493	0.45 (highly soluble)	0.49 (highly soluble)	1.91 (soluble)
7	12591	−6.08 (poorly soluble)	−9.41 (poorly soluble)	−6.51 (poorly soluble)
8	5282760	−5.41 (moderately soluble)	−8.26 (poorly soluble)	−5.39 (moderately soluble)
9	61896	−2.23 (soluble)	−3.11 (soluble)	−2.19 (soluble)
10	5364410	−4.03 (moderately soluble)	−5.97 (moderately soluble)	−3.82 (soluble)
11	8187	−2.68 (soluble)	−3.85 (soluble)	−3.51 (soluble)
12	534620	−3.36 (soluble)	−4.97 (moderately soluble)	−2.85 (soluble)
13	5364368	−3.96 (soluble)	−4.67 (moderately soluble)	−2.27 (soluble)
14	203	1.01 (highly soluble)	0.01 (highly soluble)	1.42 (soluble)
15	20088	−4.61 (moderately soluble)	−7.37 (poorly soluble)	−6.38 (poorly soluble)

Supplementary Table 2. Pharmacokinetic predictions of the 16 identified phyto-chemicals.

	Absorption		Distribution		Metabolism		Excretion	Toxicity
S/N	Intestinal absorption (human) %	Skin Permeability (log Kp)	BBB permeability	CNS permeability	CYP3A4 substrate	CYP3A4 inhibitor	Total Clearance	AMES toxicity
1	93.27	−1.027	0.834	−1.637	No	No	1.716	No
2	95.463	−2.788	−0.321	−2.69	No	No	0.595	No
3	95.557	−1.506	0.276	−1.797	No	No	0.353	No
4	86.856	−2.618	−2.618	−2.076	No	No	0.52	No
5	21.51	−3.041	−0.943	−0.943	No	No	0.626	No
6	45.236	−3.276	−0.756	−4.001	No	No	0.696	No
7	90.973	−2.729	0.237	−1.652	Yes	No	1.866	No
8	91.823	−2.725	−0.168	−1.654	Yes	No	1.884	No
9	92.715	−1.403	0.656	−2.066	No	No	0.456	No
10	93.572	−1.034	0.006	−1.931	No	No	1.716	No
11	94.526	−1.436	0.735	−1.837	No	No	1.754	No
12	92.489	−2.817	0.806	−1.682	Yes	No	1.708	No
13	94.546	−1.953	0.652	−2.919	No	No	1.511	No
14	16.327	−2.737	−0.784	−0.784	No	No	0.884	No
15	88.892	−2.771	−0.556	−2.939	Yes	No	2.175	No