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Research article

Wound-healing, antibacterial, and immunomodulatory effects of laevicaulis alte slug extract: An Integrated *in vitro*, *in vivo*, and *in silico* study

Mostafa Yahia Morad[1,*], Heba El-Sayed[2,*], Ahmed A. Elhenawy[3,4], Hana Sonbol[5], Olfat Hammam[6], Asmaa F. Abdelmonem[2], Amina Ibrahim[7] and Marwa A. Hamada[2,*]

[1] Zoology and Entomology Department, Faculty of Science, Capital University (Formerly Helwan University), Helwan 11795, Egypt
[2] Botany and Microbiology Department, Faculty of Science, Capital University (Formerly Helwan University), Helwan 11795, Egypt
[3] Chemistry Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo 11884, Egypt
[4] Chemistry Department, Faculty of Science and Art, Al Baha University, P.O. Box 1988, Mukhwah, Al Baha 6531, Saudi Arabia
[5] Department of Biology, College of Science, Princess Nourah bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia
[6] Pathology Departments, Theodor Bilharz Research Institute, Giza 12411, Egypt
[7] Medical Malacology Department, Theodor Bilharz Research Institute, Giza 12411, Egypt

* **Correspondence:** Email: HebaElSayed@science.capu.edu.eg; mustafa_ali@science.capu.edu.eg; marwa.hamada@science.capu.edu.eg.

Supplementary

Table S1. Complete molecular docking scores for the 12 GC-MS-identified compounds from *Laeviculus alte* extract against four molecular targets: *S. aureus* DNA gyrase (PDB: 2XCT), TNF-α (PDB: 2AZ5), IL-6 (PDB: 1ALU), and IL-10 (PDB: 1Y6K).

Compound	Target (PDB)	B.E. (kcal/mol)	RMSD (Å)	E_Int (kcal/mol)
Heptadecane, 2,6,10,15-tetramethyl	2XCT	−5.203	1.85	−15.2
	2AZ5	−4.85	1.1	−12.5
	1ALU	−4.5	1.95	−11.8
	1Y6K	−4.92	1.75	−13.1
7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	2XCT	−6.12	1.42	−18.5
	2AZ5	−5.45	1.65	−16.2
	1ALU	−5.2	1.5	−15.8
	1Y6K	−5.6	1.38	−17
Stearic acid	2XCT	−5.85	1.55	−17.2
	2AZ5	−5.1	1.8	−14.5
	1ALU	−4.95	1.7	−14
	1Y6K	−5.35	1.6	−15.5
1-Octadecyne	2XCT	−5.4	1.9	−16
	2AZ5	−4.75	2.05	−13.2
	1ALU	−4.6	1.85	−12.8
	1Y6K	−5.05	1.75	−14.1
2-Pentadecyn-1-ol	2XCT	−5.65	1.65	−16.8
	2AZ5	−5	1.9	−14.8
	1ALU	−4.85	1.8	−14.2
	1Y6K	−5.25	1.7	−15.6
Octadecanoic acid, ethyl ester	2XCT	−6.852	1.009	−19.5
	2AZ5	−5.3	1.55	−15.5
	1ALU	−5.1	1.6	−15
	1Y6K	−5.5	1.45	−16.2
1,11-Dodecadiyne	2XCT	−5.3	1.95	−15.5
	2AZ5	−4.65	2.15	−12.8
	1ALU	−4.45	2	−12.2
	1Y6K	−4.8	1.85	−13.5
Oxirane, tetradecyl-	2XCT	−5.55	1.75	−16.5
	2AZ5	−4.9	1.95	−14
	1ALU	−4.75	1.85	−13.5
	1Y6K	−5.15	1.7	−14.8
1,5,9-Undecatriene,2,6,10-trimethyl-, (Z)-	2XCT	−5.45	1.8	−16.2
	2AZ5	−4.8	2	−13.8
	1ALU	−4.65	1.9	−13.2
	1Y6K	−5	1.75	−14.5

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Compound	Target (PDB)	Target (PDB)	RMSD (Å)	RMSD (Å)
Cholesterol	2XCT	−6.924	1.25	−20.1
	2AZ5	−5.693	1.4	−16.8
	1ALU	−5.4	1.5	−16
	1Y6K	−5.997	1.3	−17.5
Phenol,2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)	2XCT	−7.523	1.15	−32.540
	2AZ5	−6.663	1.35	−22.5
	1ALU	−5.85	1.45	−18.2
	1Y6K	−7.188	1.2	−24.5
Tris(2,4-di-tert-butylphenyl) phosphate	2XCT	−7.509	1.1	−21.436
	2AZ5	−6.373	1.3	−20.5
	1ALU	−5.163	1.55	−17.8
	1Y6K	−7.433	1.05	−25.2

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