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COMPUTATIONAL ASSESSMENT OF THE HUMAN HEALTH AND ECOTOXICOLOGICAL
EFFECT OF THE MAIN COMPOUNDS IDENTIFIED IN TARRAGON EXTRACTS

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• Introduction

Artemisia dracunculus L. — commonly known as tarragon (family Asteraceae) — is used in the food industry and in traditional medicine due to its well-known properties: antibacterial, antifungal, antihelmintic, antiseptic, anti-inflammatory, antipyretic, carminative, digestive, and stimulant. The plant contains essential oils with highly variable compositions, along with flavonoids, phenolic acids, coumarins, and alkamides.

In vivo studies have confirmed its traditional anti-inflammatory and analgesic uses and have also revealed additional biological activities, including antioxidant, immunomodulatory, antitumor, hepatoprotective, and hypoglycemic effects. However, research has also shown that, in addition to its beneficial effects, tarragon may exert certain negative impacts on human health and may pose ecotoxicological risks.

In summary, tarragon is valued for its wide range of health-promoting properties, but its potential adverse effects highlight the need for careful use and further investigation into its safety and environmental impact.

• Material and method

- admetSAR3.0
- ADMETLab3.0
- CLC-Pred2.0
- AntiBac-Pred
- A growth inhibition test using *Lemna minor* to evaluate the potential ecotoxicity of tarragon

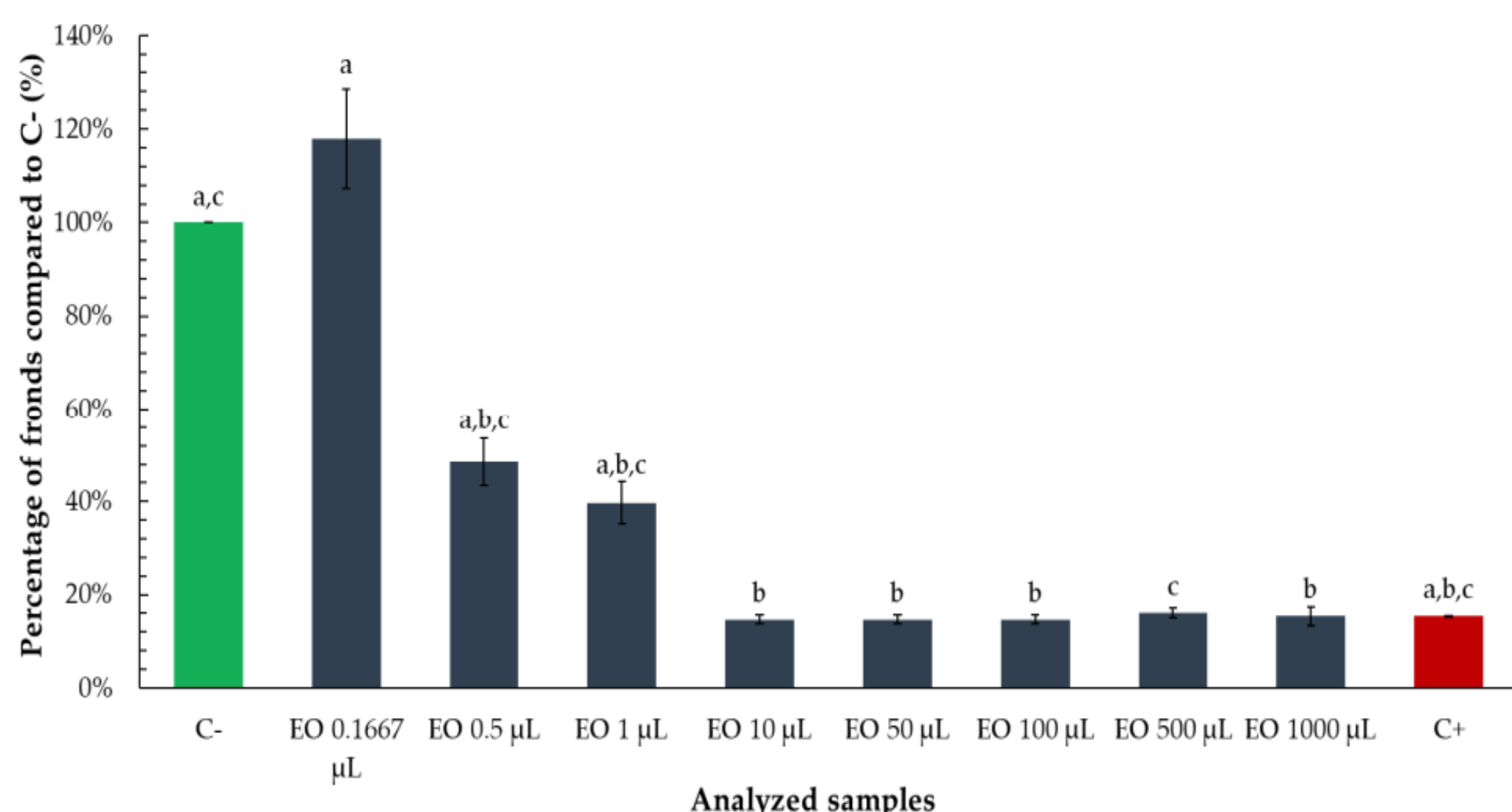


Figure 1. Percentage of *Lemna minor* fronds relative to the negative control (C-) following exposure to tarragon essential oil at various volumes. Bars labeled with different letters represent treatments that are significantly different from each other ($p < 0.05$; one-way ANOVA followed by post hoc test). Treatments sharing the same letter are not significantly different. If a bar has multiple letters (e.g., "ab"), it is not significantly different from any treatment sharing at least one of those letters.

• Conclusion

This study indicates that the compounds found in tarragon essential oils sold on the Romanian market exhibit generally acceptable ADMET profiles. However, some compounds may pose risks for skin sensitization and respiratory toxicity, and all of them have the potential to inhibit organic anion transporters OATP1 and OATP2. These toxicity concerns should be carefully considered, especially when individuals are exposed to high concentrations or use tarragon essential oils over extended periods. Additionally, several of the compounds studied were predicted to have antibacterial activity against certain *Staphylococcus*, *Streptococcus*, and *Prevotella* species and may also show toxic effects against various cancer cell types. The compounds present in higher concentrations in the tarragon essential oils are believed to have cytotoxic effects on a variety of cancer cell types. Additionally, predictions suggest that all of these compounds exhibit toxicity against cisplatin-resistant ovarian carcinoma cells. Among the identified compounds, caryophyllene oxide seems to be particularly effective against the majority of cancer cell types. Furthermore, the study predicts that all the compounds found in tarragon essential oils are capable of inhibiting the regulator of G-protein signaling 17 (RGS17). Essential oil demonstrated dose-dependent phytotoxicity, inhibiting growth at volumes of 0.5 μL and higher, with an ED50 value confirming its inhibitory potential.

• Results and discussions

Table 1. Toxicity profiles obtained using the admetSAR3.0 tool for the compounds identified in higher amounts in obtained tarragon essential oils: NT—neurotoxicity, hERG—cardiotoxicity, RT—respiratory toxicity, NphT—nephrotoxicity, SSens—skin sensitization, Ames—Ames mutagenesis, RepT—reproductive toxicity, and HemT—hemolytic toxicity. Red cells emphasize higher probabilities, orange cells emphasize reasonable probabilities, and yellow cells emphasize low probabilities of these compounds to produce the predicted toxicity

Compound/Toxicity	NT	hERG 10–30 μM	RT	NphT	SSens	Ames	RepT	HemT
Estragole	–2.295	0.256	0.143	0.893	0.839	0.240	0.223	0.166
α -Pinene	–2.633	0.465	0.477	0.704	0.923	0.074	0.172	0.361
cis- β -Ocimene	–2.537	0.569	0.269	0.629	0.971	0.098	0.063	0.407
trans- β -Ocimene	–2.536	0.556	0.272	0.626	0.971	0.098	0.062	0.408
Limonene	–2.618	0.565	0.275	0.592	0.916	0.069	0.095	0.424
Eugenol methyl ether	–2.203	0.379	0.121	0.846	0.684	0.308	0.195	0.101
Eugenol acetate	–2.542	0.470	0.079	0.711	0.476	0.452	0.235	0.054
Eugenol	–2.175	0.132	0.189	0.496	0.809	0.123	0.213	0.125
Caryophyllene oxide	–2.608	0.836	0.500	0.690	0.913	0.137	0.167	0.342

Table 2. Toxicity profiles obtained using the ADMETLab3.0 tool for the compounds identified in higher amounts in obtained tarragon essential oils: hERG—cardiotoxicity, H-HT—hepatotoxicity, Ames—Ames mutagenicity, SSens—skin sensitization, RT—respiratory toxicity, NT—neurotoxicity, NphT—nephrotoxicity, and HemT—hemolytic toxicity. Red cells emphasize higher probabilities, orange cells emphasize reasonable probabilities, and yellow cells empha-size low probabilities of these compounds to produce the predicted toxicity.

Compound /Toxicity	hERG 10 μM	H-HT	Ames	SSens	Carcinogenicity	RT	NT	NphT	HemT
Estragole	0.695	0.315	0.502	0.881	0.644	0.814	0.180	0.673	0.174
α -Pinene	0.796	0.331	0.016	0.938	0.629	0.844	0.008	0.655	0.124
cis- β -Ocimene	0.632	0.437	0.337	0.963	0.567	0.796	0.142	0.674	0.275
trans- β -Ocimene	0.470	0.624	0.510	0.928	0.499	0.827	0.307	0.544	0.372
Limonene	0.344	0.401	0.192	0.920	0.691	0.637	0.436	0.136	0.384
Eugenol methyl ether	0.625	0.345	0.468	0.880	0.649	0.815	0.172	0.702	0.214
Eugenol acetate	0.479	0.314	0.461	0.940	0.470	0.690	0.083	0.600	0.272
Eugenol	0.658	0.310	0.468	0.930	0.582	0.822	0.138	0.563	0.136
Caryophyllene oxide	0.540	0.476	0.556	0.815	0.715	0.621	0.208	0.618	0.416

Table 3. Predictions regarding the antibacterial properties of the main compounds of tarragon essential oils. The confidence of each prediction is given in the parentheses.

Compound	Antibacterial Property
cis- β -Ocimene and trans- β -Ocimene	<i>Staphylococcus simulans</i> (0.713), <i>Streptococcus mutans</i> (0.509)
α -Pinene	Resistant <i>Staphylococcus simulans</i> (0.714), <i>Staphylococcus sciuri</i> (0.593), <i>Staphylococcus simulans</i> (0.539)
Caryophyllene oxide	<i>Prevotella melaninogenica</i> (0.556), <i>Prevotella intermedia</i> (0.509)