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COMPUTATIONAL EVALUATION OF THE COMPOUNDS IDENTIFIED IN THE HIGHEST CONCENTRATION IN THE ESSENTIAL OIL OF *ARTEMISIA DRACUNCULUS*

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Abstract: *Artemisia dracunculus* (tarragon) is a perennial plant, used in traditional medicine and the food industry. The plant is known to have beneficial effects on health, such as: antibacterial, antifungal, antiseptic, carminative, anti-inflammatory, antipyretic, anthelmintic, etc. The aim of this study was to identify the compounds in the highest concentration in the essential oil of *Artemisia dracunculus* and evaluate their biological activity using ADMETlab3.0 and admetSAR3.0 programs. Compounds were identified by gas chromatography-mass spectrometry method using a Shimadzu QP 2010 Plus instrument (Columbia, SC, USA). The compounds identified in the largest quantity are: estragole, cis-beta-ocimene, trans-beta-ocimene, D-limonene, eugenol methyl ether, eugenol acetate, eugenol, caryophyllene oxide. With the help of the PubChem database, the SMILES formulas of the chemical compounds were identified, which were later used to evaluate the biological activity of each individual compound. The results obtained showed us that trans-beta-ocimene can be carcinogenic and hepatotoxic. Eugenol can inhibit glycoprotein P and that it is carcinogenic. Eugenol methyl ether, eugenol acetate, D-limonene, Cis-beta-ocimene, caryophyllene oxide and estragole can produce respiratory toxicity and can be carcinogenic. Most chemical compounds are considered inhibitors of organic anion and cation transporters.

• Introduction

Artemisia dracunculus L. – tarragon has a long history of use as a spice and remedy, because its known antibacterial, antifungal, antihemintic, antiseptic, anti-inflammatory, antipyretic, carminative, digestive and stimulant activities. The plant contain essential oils with highly variable compositions, along with flavonoids, phenolic acids, coumarins, and alkamides. In vivo studies mainly in rodents, highlight potential anti-inflammatory, hepatoprotective, and antihyperglycemic effects.



Fig 1. *Artemisia dracunculus*-Tarragon

• Material and method

- Shimadzu QP 2010 Plus instrument
- Database PubChem
- Program ADMETlab3.0
- Program admetSAR3.0



Fig. 2. Shimadzu QP 2010 Plus instrument

• Results and discussions

Table 1. The compounds identified in the highest concentration in the essential oil of *Artemisia dracunculus* and their SMILES formulas

Compound	SMILES formule
Estragole	<chem>COC1=CC=C(C=C1)CC=C</chem>
Cis-beta-ocimene	<chem>CC(=CC/C=C/C/C)C=C</chem>
Trans-beta-ocimene	<chem>CC(=CC/C=C/C/C)C=C</chem>
D-limonene	<chem>CC1=CC(C@H)C(C1)C=C</chem>
Eugenol methyl ether	<chem>COC1=CC(C=C(C=C1)CC=C)OC</chem>
Eugenol acetate	<chem>CC(=O)OC1=CC(C=C(C=C1)CC=C)OC</chem>
Eugenol	<chem>COC1=CC(C=C(C=C1)CC=C)O</chem>
Caryophyllene oxide	<chem>C[C@]12CC[C@H]3[C@H](C3)C(C)C(=C)CC[C@H]1O2</chem>

Table 2. Chemical compounds and their potential for inhibition of organic anion and cation transporters

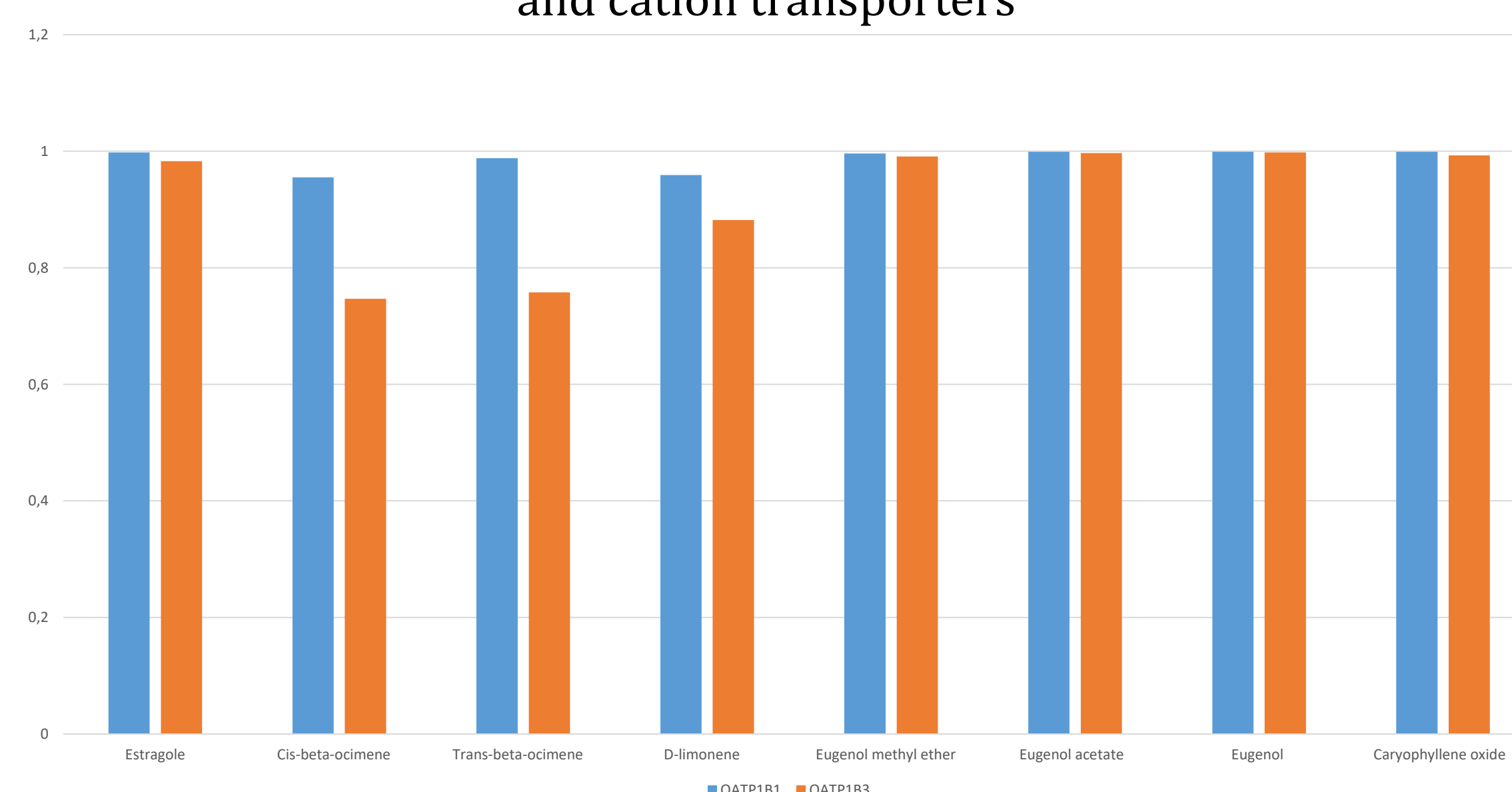


Table 3. Chemical compounds and their potential for toxicity

Compound	Skin sensitization	Carcinogenity	Eye corrosion	Respiratory	Human hepatotoxicity
Estragole	Yes	Yes	Yes	Yes	Yes
Cis-beta-ocimene	Yes	Yes	Yes	Yes	Yes
Trans-beta-ocimene	Yes	Yes	Yes	Yes	Yes
D-limonene	Yes	Yes	Yes	Yes	Yes
Eugenol methyl ether	Yes	Yes	Yes	Yes	Yes
Eugenol acetate	Yes	Yes	Yes	Yes	Yes
Eugenol	Yes	Yes	Yes	Yes	Yes
Caryophyllene oxide	Yes	Yes	Yes	Yes	Yes

• Conclusions

The results obtained showed us that trans-beta-ocimene can be carcinogenic and hepatotoxic. Eugenol can inhibit glycoprotein P which it is carcinogenic. Eugenol methyl ether, eugenol acetic acid derivation, D-limonene, Cis-beta-ocimene, caryophyllene oxide and estragole can create respiratory toxicity and can be carcinogenic. Most chemical compounds are considered inhibitors of organic anion and cation transporters.