



16-17 November, 2023

Identification and characterization of the chemical compounds responsible of the biological actions of *Artemisia vulgaris* and *Artemisia dracunculus*

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Abstract: The genus *Artemisia* L. is part of the Asteraceae family and includes approximately 500 species worldwide. In Europe, the genus *Artemisia* includes 57 species, and in Romania the presence of 16 species was observed. There is a long history of the use of *Artemisia* species in traditional medicine worldwide for treating numerous diseases such as: gastrointestinal problems, wounds, inflammatory diseases, menstrual pains, headache, malaria and intestinal parasites. In cooking, *Artemisia* species are used to give a particular flavor to food. Several studies also mention several toxicological effects of these plants when used in high quantities: neurotoxicity and liver injuries. Among these species, we focused our attention on *Artemisia vulgaris* and *Artemisia dracunculus* and identified the organic compounds that are found in higher quantities in these plants and are responsible for their use in medicine and food, but also for their toxicity. The identified compounds are: ascorbic acid, 17alpha-ethynylestradiol, caffeic acid, 1-methoxy-4-(2-propenyl)benzene, nerol, maltose, thujene, and methyleugenol. These compounds usually have low molecular weight, small number of hydrogen bond donors and acceptor and some of them are highly hydrophobic. These properties can be correlated with the biological activity and toxicity of investigated *Artemisia* species.

• Introduction

The *Artemisia* L. genus, belonging to the Asteraceae family, is one of the largest and widely spread groups, encompassing nearly 100 genera. Research on the *Artemisia* genus in its natural habitat in Romania is limited, with a particular gap in understanding the bioactive components of *Artemisia vulgaris* and *Artemisia dracunculus*. Despite this, various herbal supplements derived from these plants are readily available globally. These supplements are utilized for a range of purposes, including digestive aid, menstrual support, antibacterial and antifungal properties, anti-inflammatory effects, antioxidant benefits, etc.

TABLE 1. Plant species of the genus *Artemisia* (*Artemisia vulgaris* and *Artemisia dracunculus*), scientific name, picture, chemical composition, biological properties/usage

Species name	Picture	Chemical composition	Biological activities/ Usage
<i>Artemisia vulgaris</i> (Common Mugwort)		α -pinene; Camphene; Sabinene; Beta-pinene; Cymene; Limonene; α -thujone; β -thujone; Camphor; Pinocarvone; Borneol; Myrtenal; Carveol; Bicyclogermacrene; Caryophyllene	Digestive aid; Menstrual support; Antibacterial and antifungal; Anti-inflammatory; Antioxidant
<i>Artemisia dracunculus</i> (Tarragon)		Estragole; limonene; (E)- β -ocimene; β -pinene; (Z)- β -ocimene; Pinocembrin; Luteolin; quercetin; rutin; kaempferol; Annanenin; caffeic acid; Dracumerin; Scopoletin; Artemidiol; artemidin; Artemidinal	Antibacterial; antifungal; anti- inflammatory; Antidiabetic; Hepatoprotective; Gastroprotective; anticonvulsant

• Material and method

- FoodDB database
- PubChem database

• Results and discussions

TABLE 2. Physico-chemical properties of the organic compounds found in *Artemisia dracunculus* and *Artemisia vulgaris*: MW – molecular mass; logP – partition coefficient; HBD – the number of hydrogen bond donors; HBA – the number of hydrogen bond acceptors; RB – the number of rotatable bonds; TPSA – polar topological area, extras from PubChem

Organic compound	MW (g/mol)	logP	HBD	HBA	RB	TPSA (Å ²)
Caffeic acid	180.16 g/mol	1.15	3	4	2	77.8 Å ²
17alpha-ethynylestradiol	296.4 g/mol	3.67	2	2	1	40.5 Å ²
Anethole	148.20 g/mol	3.3	0	1	2	9.2 Å ²
1-Methoxy-4-(2-propenyl)benzene	148.20 g/mol	3.4	0	1	3	9.2 Å ²
Nerol	154.25 g/mol	3.47	1	1	4	20.2 Å ²
Maltose	342.30 g/mol	-4.7	8	11	4	190 Å ²
4(10)-Thujene	136.23 g/mol	3.1	0	0	1	0 Å ²
Methyleugenol	178.23 g/mol	2.5	0	2	4	18.5 Å ²
L-Ascorbic acid	176.12 g/mol	-1.85	4	6	2	107 Å ²

• Conclusions

The main identified compounds in plants from *Artemisia* sp. are: ascorbic acid, 17alpha-ethynylestradiol, caffeic acid, 1-methoxy-4-(2-propenyl)benzene, nerol, maltose, thujene, and methyleugenol. As revealed in Table 2, these compounds usually have low molecular weight, small number of hydrogen bond donors and acceptor and some of them are highly hydrophobic. Further studies will be done in order to correlate the properties of these compounds with the biological activity and possible toxicity to humans of plants from *Artemisia* species.