

## **Supplementary Materials**

### ***Foeniculum vulgare* Miller, a new chemotype from Montenegro**

**Mijat Božović<sup>1,✉</sup>, Stefania Garzoli<sup>2,✉</sup>, Svetlana Vujović<sup>3</sup>, Filippo Sapienza<sup>2</sup>, Rino Ragno<sup>2</sup>**

#### **Affiliation**

<sup>1</sup> Faculty of Natural Sciences and Mathematics, University of Montenegro, Podgorica, Montenegro

<sup>2</sup> Department of Drug Chemistry and Technology, Sapienza University, Rome, Italy

<sup>3</sup> Institute for Medicines and Medical Devices in Montenegro, Podgorica, Montenegro

#### **Correspondence**

##### ***Dr. Mijat Božović***

Faculty of Natural Sciences and Mathematics

University of Montenegro

Podgorica, Montenegro

Tel.: +382-20-243-816

Fax: +382-20-244-608

mijatboz@ucg.ac.me

##### ***Dr. Rino Ragno***

Department of Drug Chemistry and Technology

Sapienza University

Rome, Italy

Tel.: +39-6-4991-3937

Fax: +39-6-4991-3627

rino.ragno@uniroma1.it

<sup>¶</sup> Contributed equally to the paper

**Contents:**

**Figure S1:** Trend of major compounds for F1-F4 samples.

**Figure S2:** Trend of major compounds for F5-F8 samples.

**Figure S3:** Trend of major compounds for F9-F12 samples.

**Figure S4:** Trend of the low-boiling compounds for F1-F4 samples.

**Figure S5:** Trend of the low-boiling compounds for F5-F8 samples.

**Figure S6:** Trend of the low-boiling compounds for F9-F12 samples.

**Figure S7:** Doclea, Podgorica; natural habitat of *Foeniculum vulgare* Miller (FV) (photo by Svetlana Vujović).

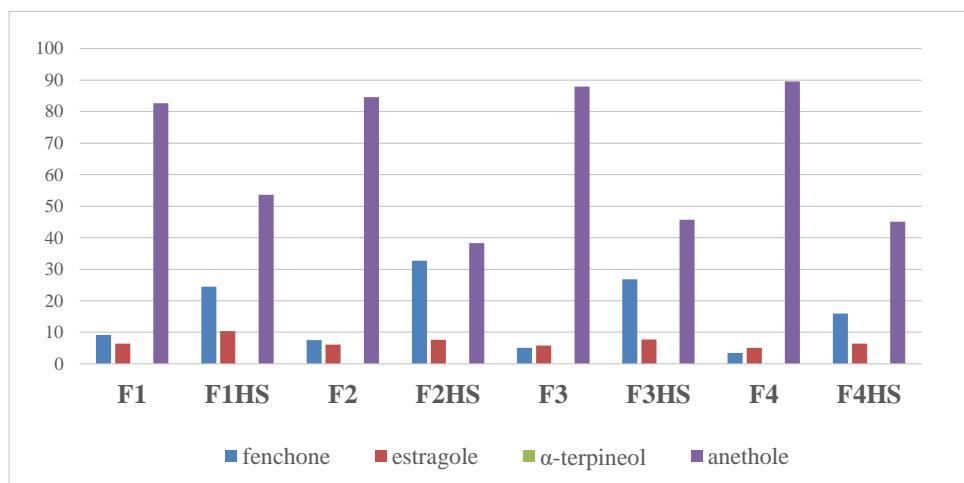
**Figure S8:** Uzdomir, Nikšić; natural habitat of FV (photo by Svetlana Vujović).

**Figure S9:** St. John's Fortress, Kotor; natural habitat of FV (photo by Svetlana Vujović).

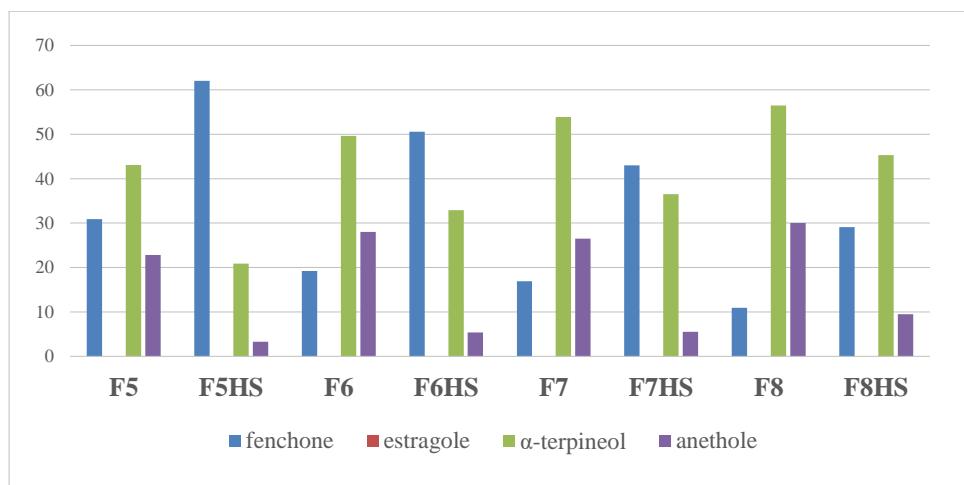
**Table S1:** Yield % of FV from Montenegro.

**Table S2:** Most characterizing components of FV essential oils (FVEOs) from Montenegro: chemical structures, MWs and CAS numbers.

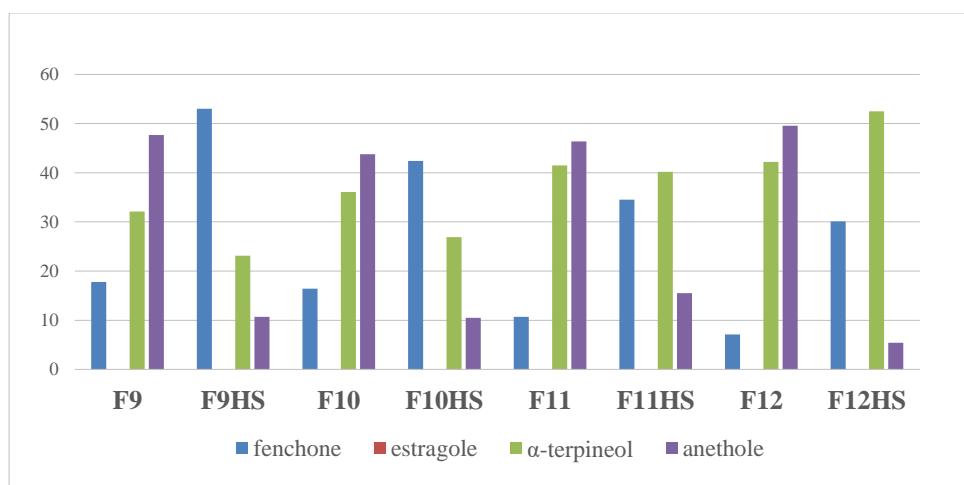
**Table S3:** Chemical composition (%) of various FVEOs as listed in the <http://eo.3d-qsar.com> site.



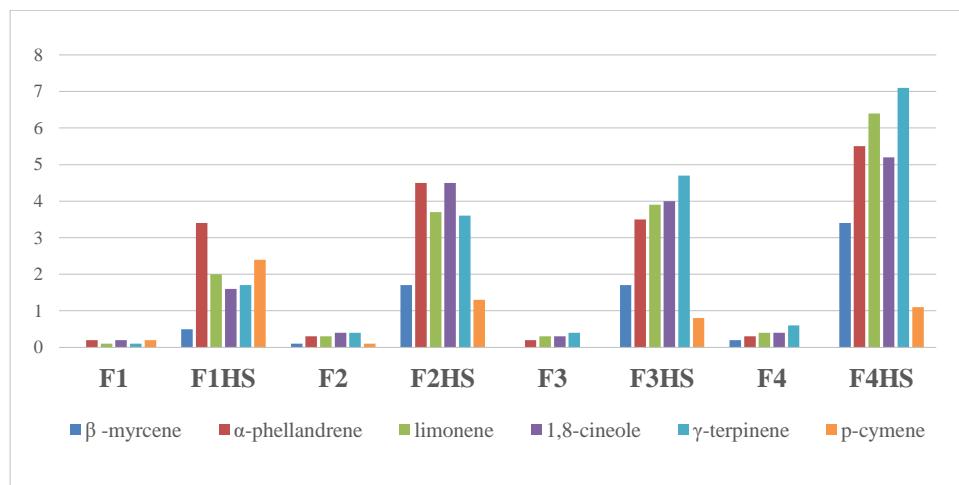
**Figure S1:** Trend of major compounds for F1-F4 samples.



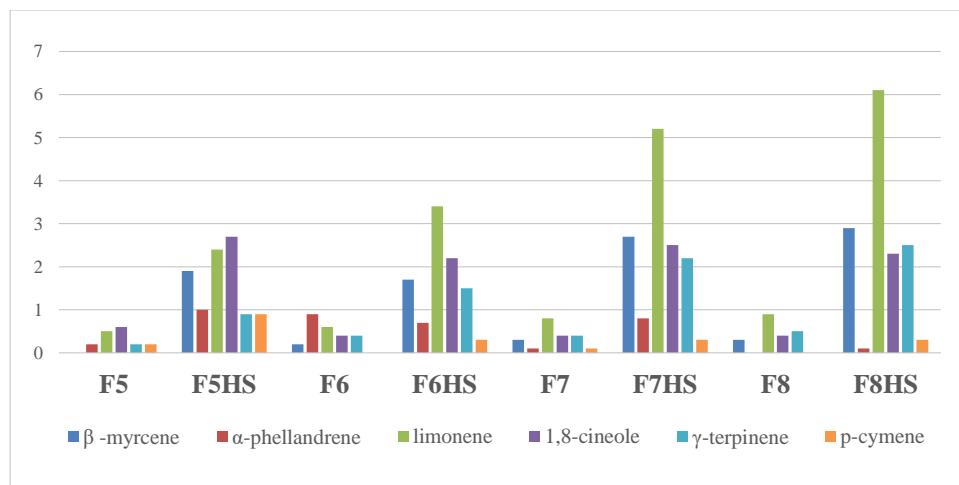
**Figure S2:** Trend of major compounds for F5-F8 samples.



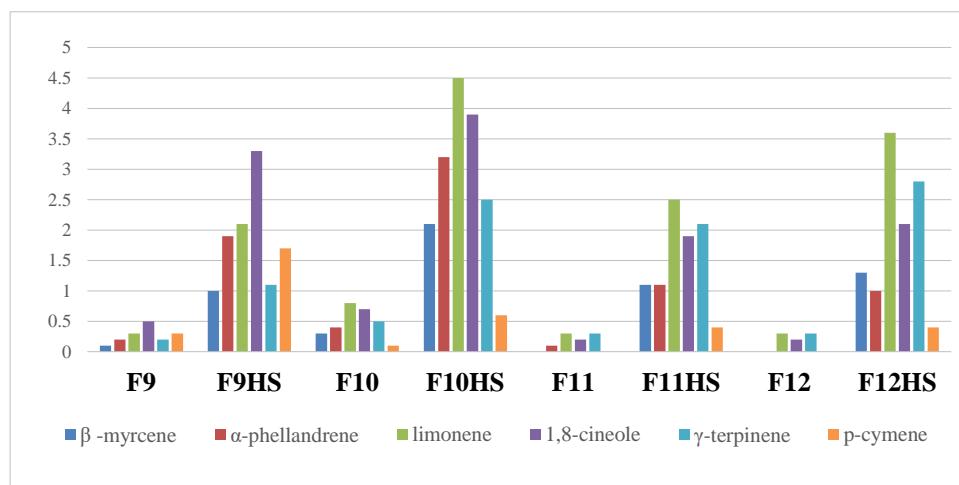
**Figure S3:** Trend of major compounds for F9-F12 samples.



**Figure S4:** Trend of the low-boiling compounds for F1-F4 samples.



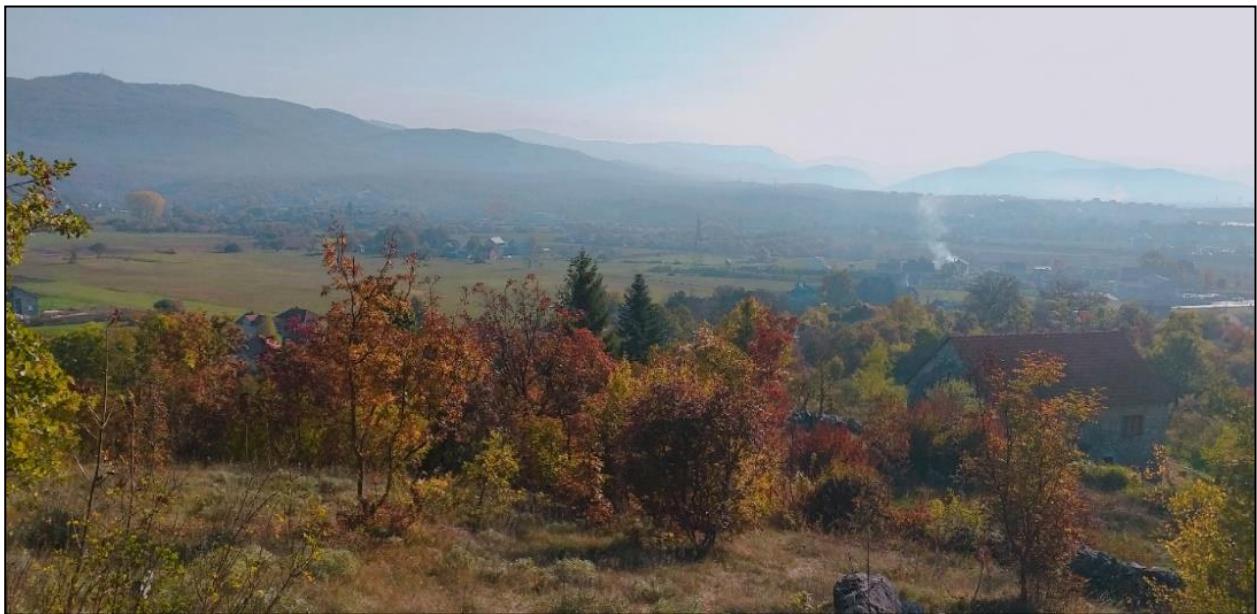
**Figure S5:** Trend of the low-boiling compounds for F5-F8 samples.



**Figure S6:** Trend of the low-boiling compounds for F9-F12 samples.



**Figure S7:** Doclea, Podgorica; natural habitat of *Foeniculum vulgare* Miller (FV) (photo by Svetlana Vujović).



**Figure S8:** Uzdomir, Nikšić; natural habitat of FV (photo by Svetlana Vujović).



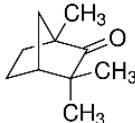
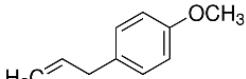
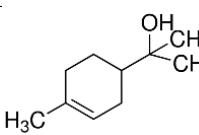
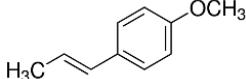
**Figure S9:** St. John's Fortress, Kotor; natural habitat of FV (photo by Svetlana Vujović).

**Table S1:** Yield % of FV from Montenegro.

locality	extraction time											
	1h			2h			3h			6h		
	y <sup>a</sup>	cy <sup>b</sup>	s <sup>c</sup>	y <sup>a</sup>	cy <sup>b</sup>	s <sup>c</sup>	y <sup>a</sup>	cy <sup>b</sup>	s <sup>c</sup>	y <sup>a</sup>	cy <sup>b</sup>	s <sup>c</sup>
Podgorica	0.92	0.92	31.72	0.82	1.74	28.27	0.5	2.24	17.24	0.66	2.9	22.76
Nikšić	1.88	1.88	64.38	0.44	2.32	15.06	0.32	2.64	10.95	0.28	2.92	9.44
Kotor	1.15	1.15	49.35	0.74	1.86	32.61	0.22	2.11	9.44	0.22	2.33	9.59

<sup>a</sup> Yield % calculated on the dried FV plant material. <sup>b</sup> Cumulative yield % of FVEOs over time. <sup>c</sup> Shared % of the total yield.

**Table S2:** Most characterizing components of FV essential oils (FVEOs) from Montenegro: chemical structures, MWs and CAS numbers.

# <sup>1</sup>	Chemical Structure	Name	MW	CAS
12		fenchone	152.23	7787-20-4
16		estragole	148.20	140-67-0
17		$\alpha$ -terpineol	154.25	98-55-5
18		anethole	148.20	4180-23-8

<sup>1</sup> # indicates the compound identification number.

**Table S3:** Chemical composition (%) of various FVEOs as listed in the <http://eo.3d-qsar.com> site. Components displaying an average composition lower than 2 were omitted.

DOI	Extraction Type	Extraction Yield	Extraction Time	Plant Part	Plant State	Country	alpha-pinene	pha-phellandren	camphor	limonene	Fenchone	Estragole	anethole
10.1080/03235408.2013.853456	Hydro Distillation	3.5	NA	Seeds	Dry	Iran	0.0	2.7	0.0	0.0	9.4	3.5	75.2
10.2478/pjct-2019-0018	Hydro Distillation	4.18	2.0 h	Fruits	Fresh	Poland	2.9	0.0	0.3	2.3	18.1	2.6	70.0
10.1016/j.bjp.2015.02.009	Hydro Distillation	NA	3.0 h	Leaves	Fresh	Brazil	1.5	0.0	0.0	21.3	1.2	1.8	70.2
Progetto_OE_Commerciali	Commercial	NA	NA	NA	NA	NA	1.0	0.0	0.0	3.4	3.4	2.2	78.1
10.1016/j.biopha.2016.10.013	NA	NA	NA	NA	NA	NA	5.6	3.7	0.3	6.3	5.2	8.1	56.3
10.1080/14786419.2017.1292266	Hydro Distillation	2.2	3.0 h	Areal Part	Fresh	Portugal	10.1	11.0	0.1	3.6	10.8	4.0	47.0
10.1080/10412905.2015.1025919	Steam Distillation	NA	NA	Seeds	NA	NA	4.7	1.0	0.0	4.0	14.3	2.1	71.3
10.1007/s10340-016-0759-2	Hydro Distillation	NA	4.0 h	Fruits	Fresh	Poland	2.8	0.0	0.6	2.1	33.4	0.0	39.2
10.1371/journal.pone.0165667	Hydro Distillation	NA	4.0 h	Seeds	Dry	NA	1.1	0.0	0.0	10.5	4.6	80.8	1.0
10.3390/molecules23071549	Commercial	NA	NA	NA	NA	NA	3.6	0.5	0.1	11.5	6.5	0.6	75.1
10.1007/s11274-011-0939-4	Hydro Distillation	NA	NA	NA	Dry	NA	0.0	0.0	0.4	1.6	0.0	0.0	88.9
10.1016/j.indcrop.2012.10.012	Hydro Distillation	1.95	6.0 h	Seeds	Dry	Egypt	1.6	0.0	0.0	4.2	8.3	10.4	56.4
10.1016/j.indcrop.2019.111854	Hydro Distillation	3.6	3.0 h	Fruits	Dry	Serbia	0.5	0.2	0.5	1.1	22.6	2.7	69.9
10.1016/j.indcrop.2019.111854	Hydro Distillation	4	3.0 h	Fruits	Dry	Serbia	2.0	0.4	0.5	2.3	23.1	2.6	64.9
10.24193/subbchem.2019.2.11	Hydro Distillation	1.7	4.0 h	Seeds	Dry	Romania	0.0	0.0	0.0	7.3	1.3	1.3	89.6
10.1080/10412905.2016.1146169	Hydro Distillation	NA	2.0 h	Seeds	Dry	Iran	3.6	0.1	0.0	20.6	7.2	57.9	5.0
10.1016/j.indcrop.2016.02.064	Hydro Distillation	NA	3.0 h	Fruits	Dry	Romania	0.0	0.0	21.3	0.0	0.5	0.6	58.1
10.3109/09637486.2014.953454	Commercial	NA	NA	Areal Part	Flowering	Scotland	1.7	1.1	0.0	2.8	7.1	8.1	58.7