Supplemental material for:

Hydrodistillation extraction kinetics regression models for essential oil yield and composition in *Juniperus virginiana*, *J. excelsa*, and *J. sabina*

Ivanka B. Semerdjieva [1], Santosh Shiwakoti [2], Charles L. Cantrell [3], Valtcho D. Zheljazkov [2,*], Tess Astatkie [4], Vicki Schlegel [5], Tzenka Radoukova [6]

[1] Department of Botany and Agrometeorology, Agricultural University, Mendeleev 12, 4000 Plovdiv, Bulgaria; v_semerdjieva@abv.bg

[2] Crop and Soil Science Department, Oregon State University, 3050 SW Campus Way, 109 Crop Science Building, Corvallis, OR 97331, USA; santoshcwakoti@gmail.com (S.H.); Valtcho.jeliazkov@oregonstate.edu (V.D.Z.)

[3] National Center for Natural Products Research, Agricultural Research Service, United States Department of Agriculture, University, MS 38677, USA; clcantr1@olemiss.edu

[4] Faculty of Agriculture, Dalhousie University, PO Box 550, Truro, NS B2N 5E3, Canada; astatkie@dal.ca

[5] Department of Food Science and Technology, University of Nebraska – Lincoln, 327 Food Technology Complex, Lincoln, NE 68583, USA; vschlegel3@unl.edu
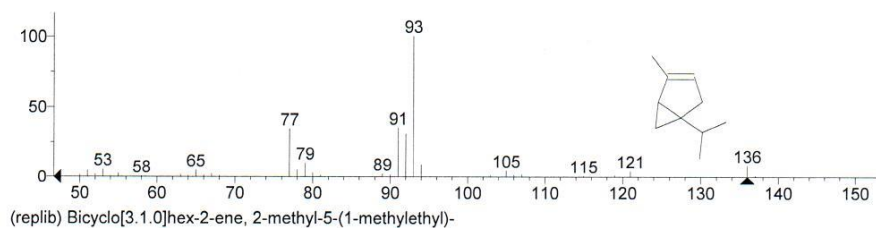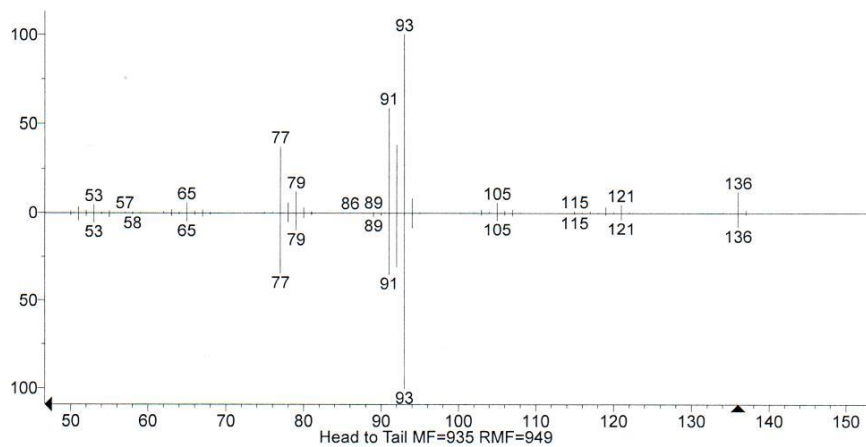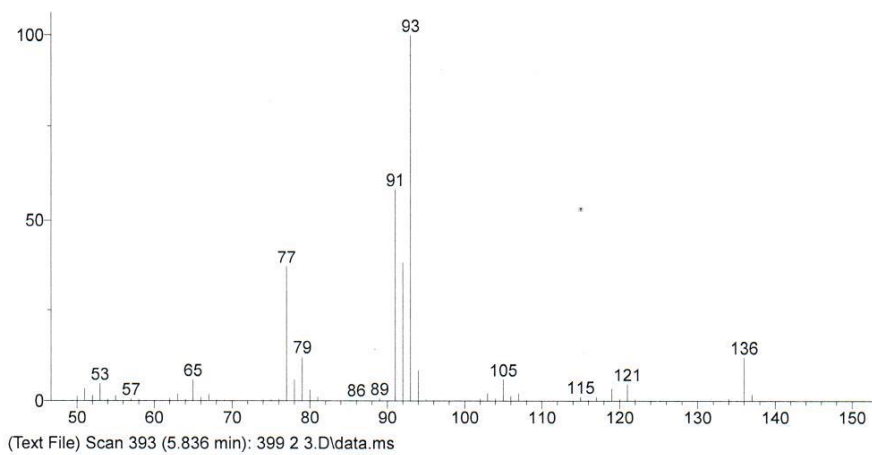
[6] Department of Botany and Methods of Biology Teaching, Faculty of Biology, University of Plovdiv "Paisii Hilendarski", 24 Tzar Assen, 4000 Plovdiv, Bulgaria; kiprei@abv.bg

* Correspondence: Valtcho.jeliazkov@oregonstate.edu

Supplemental Table 1. Observed and reported retention index values for compounds identified by Kovat analysis only.
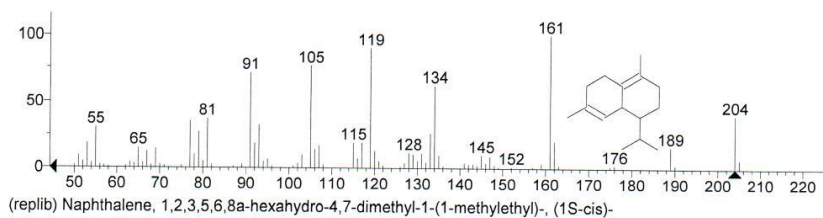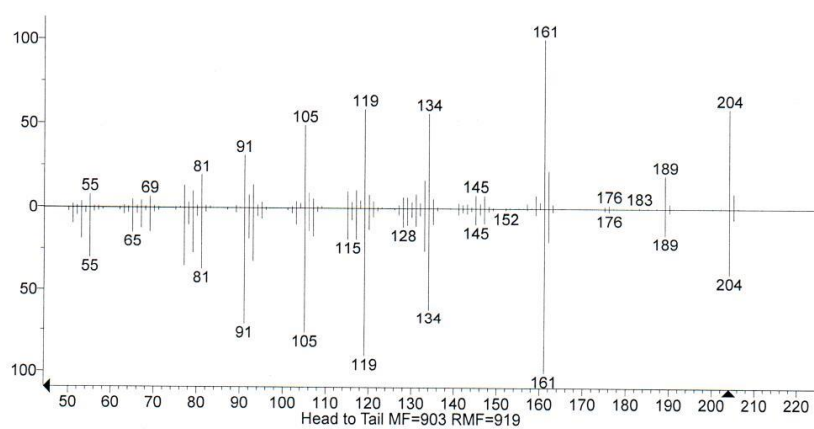
Compound	Observed RI	Calculated RI	Identification Methods
pregeijerene B	KI = 1276	RI = 1277.56	RI, Kovat
α-thujene	KI = 930	RI = 928.52	RI, Kovat, NIST
δ-cadinene	KI = 1523	RI = 1523.61	RI, Kovat, NIST
elemol	KI = 1550	RI = 1554.91	RI, Kovat, NIST
elemicin	KI = 1557	RI = 1553.35	RI, Kovat, NIST

α-Thujene

(Text File) Scan 393 (5.836 min): 399 2 3.D\data.ms

Head to Tail MF=935 RMF=949
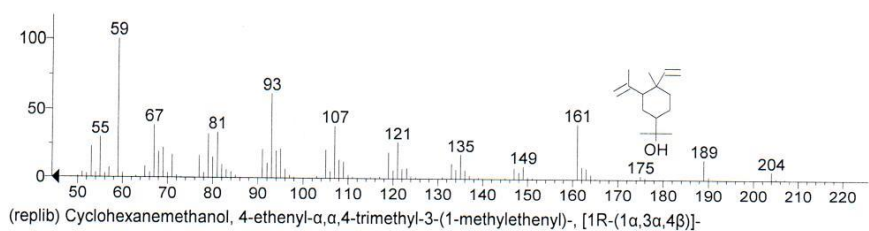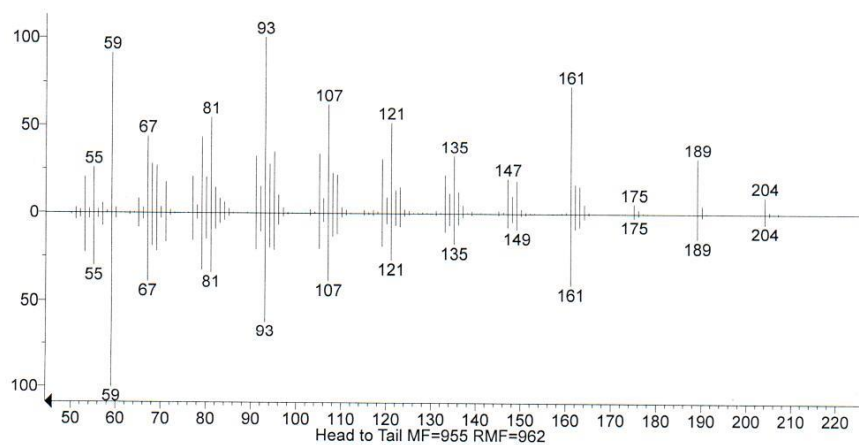
(replib) Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-

Supplemental Figure 1. Comparison of actual mass spectrum for α-thujene and NIST database mass spectrum.

Cadinene <delta>

(Text File) Scan 4463 (29.124 min): 397_Cb.D\data.ms

Head to Tail MF=903 RMF=919

(replib) Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-
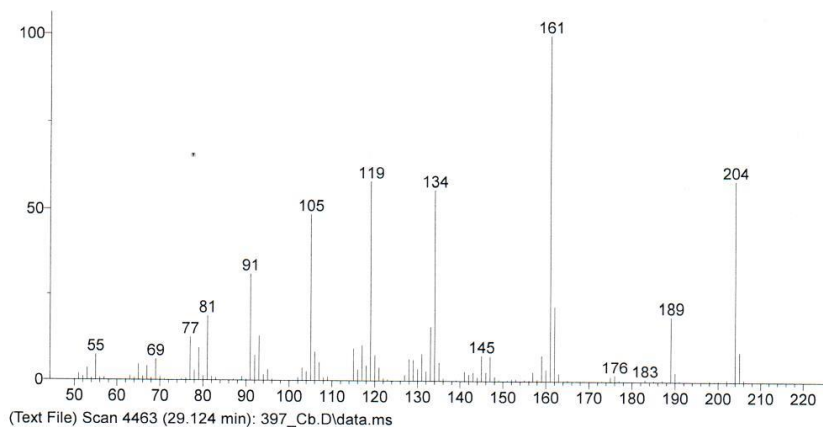
Supplemental Figure 2. Comparison of actual mass spectrum for δ-cadinene and NIST database mass spectrum.

Elemol

(Text File) Scan 4649 (30.188 min): 397_Cb.D\data.ms

Head to Tail MF=955 RMF=962

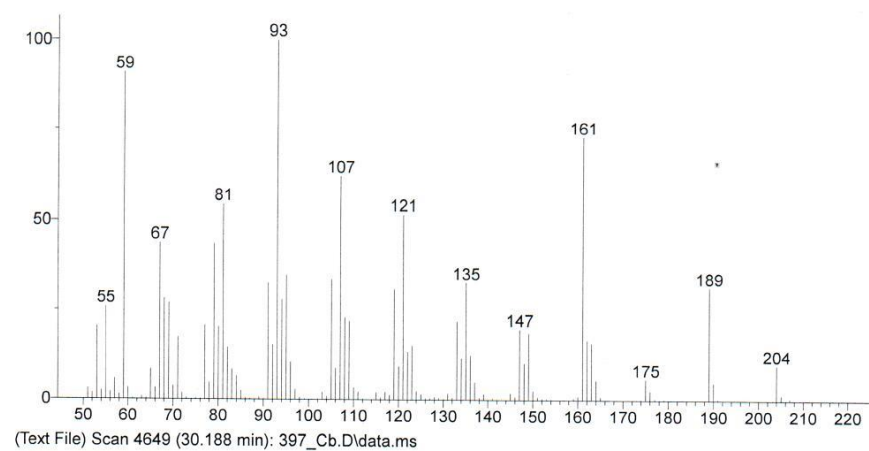(replib) Cyclohexanemethanol, 4-ethenyl-α,α,4-trimethyl-3-(1-methylethenyl)-, [1R-(1α,3α,4β)]-

Supplemental Figure 3. Comparison of actual mass spectrum for elemol and NIST database mass spectrum.

Elemicin

(Text File) Scan 4679 (30.360 min): 397_Cb.D\data.ms

Head to Tail MF=929 RMF=933
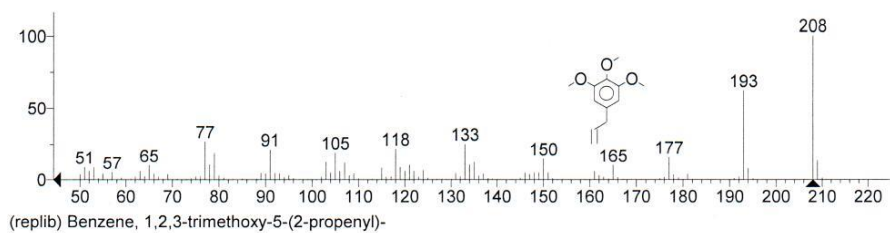
(replib) Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
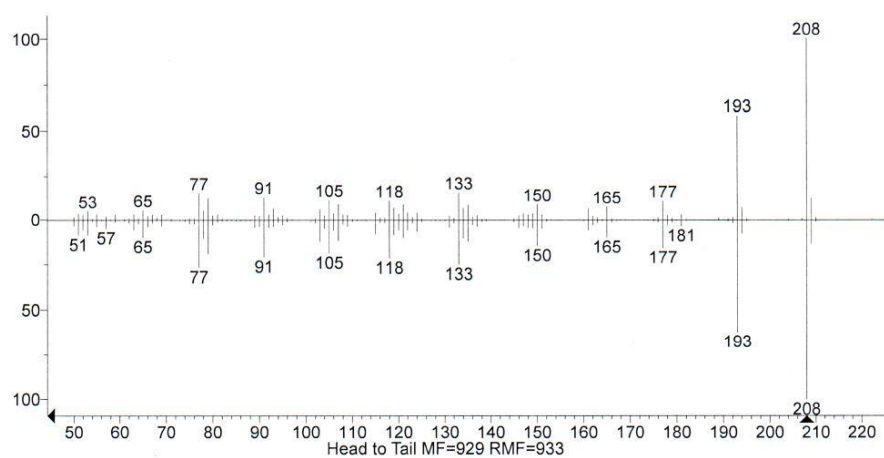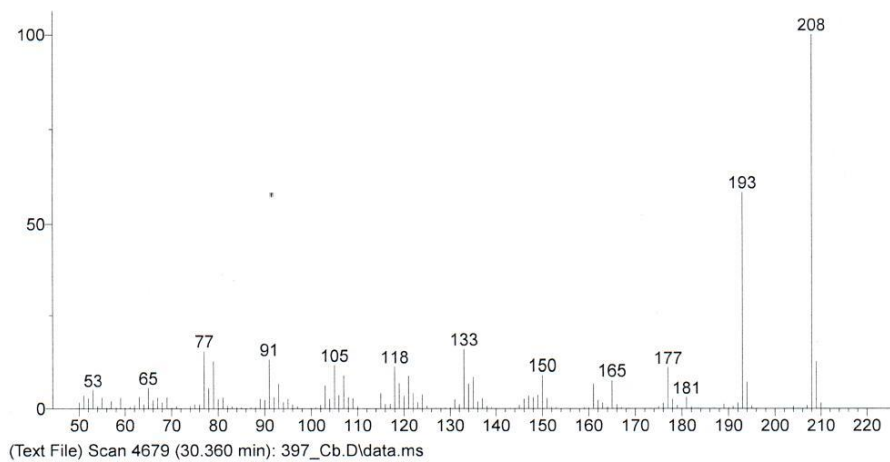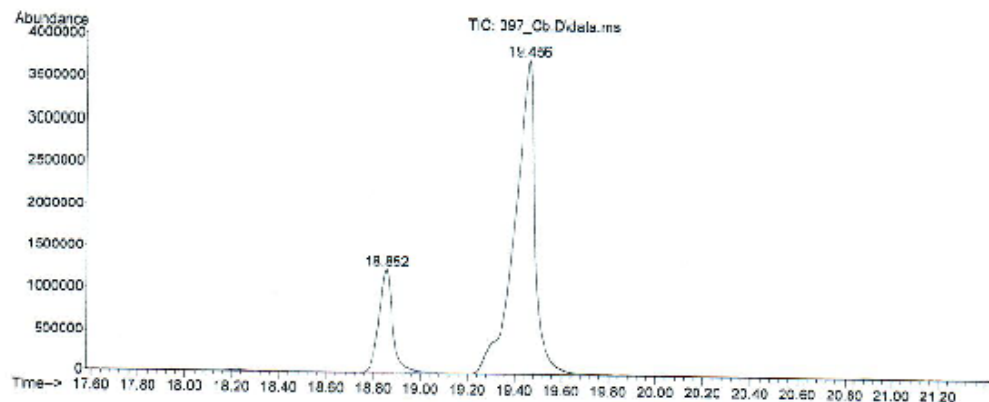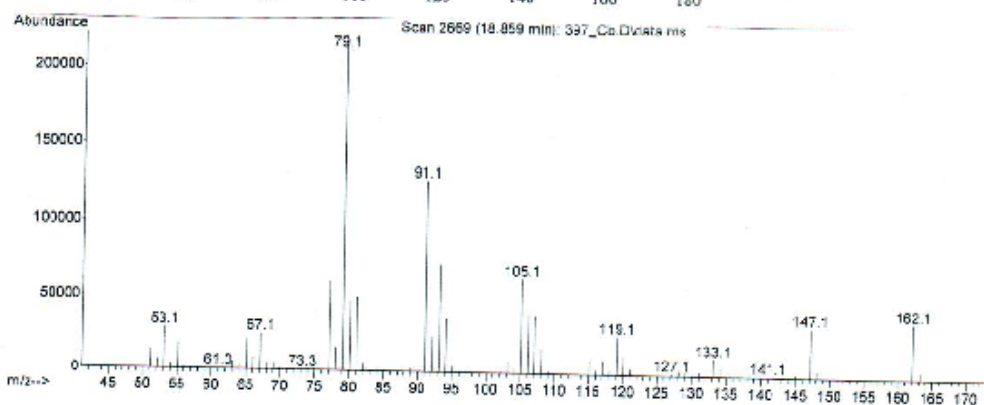
Supplemental Figure 4. Comparison of actual mass spectrum for elemicin and NIST database mass spectrum.

File   :C:\msdchem\1\data\Valtcho 2015\JuniperusVirginianus_180308\3
...   97_Cb.D
Operator : SG3
Instrument :   USDA 5975
Acquired : 8 Mar 2018 16:43   using AcqMethod USDA KOVAT.M
Sample Name: 397_Cb
Misc Info :

RT: 19.05   AI: 1274   KI: 1276   Pregeijerene B
CAS#: 556799-96-3   MF: C12 H18   FW: 162   MSD LIB#: 1758
CN: 1,4,7-cyclodecatriene, 1,7-dimethyl-,(1E,4E,7E)-
Synonyms: erectopatene
Source: *Juniperus erectopatens* leaf oil, Cool & RP Adams, Phytochem. 63:105(2003)
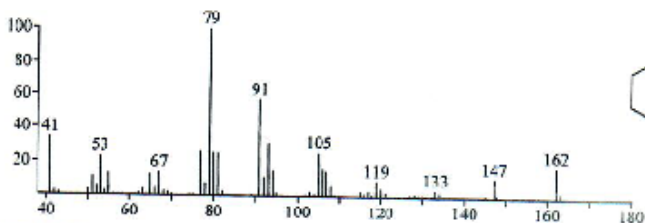
Supplemental Figure 5. Comparison of actual mass spectrum for pregeijerene B and Kovat reported mass spectrum.

Distillation study with Juniperus virginiana from Bulgaria conducted on Jan 4, 2018

Sample # Timeframe, repliate	Species	g oil
0-5 min rep 1	Juniperus virginiana	0.1195
0-5min rep 2	Juniperus virginiana	0.1056
0-5min rep 3	Juniperus virginiana	0.1330
5-10min rep1	Juniperus virginiana	0.0156
5-10min rep2	Juniperus virginiana	0.0490
5-10 min rep 3	Juniperus virginiana	0.1528
10-20 min rep1	Juniperus virginiana	0.0943
10-20 min rep2	Juniperus virginiana	0.0771
10-20 min rep 3	Juniperus virginiana	0.0280
20-40 min rep 1	Juniperus virginiana	0.1340
20-40 min rep 2	Juniperus virginiana	0.1523
20-40 min rep 3	Juniperus virginiana	0.1809
40-80 min rep 1	Juniperus virginiana	0.1714
40-80 min rep 2	Juniperus virginiana	0.2277
40-80 min rep 3	Juniperus virginiana	0.2130
80-160 min rep 1	Juniperus virginiana	0.1462
80-160 min rep 2	Juniperus virginiana	0.2412
80-160 min rep 3	Juniperus virginiana	0.0675
160-240 min rep 1	Juniperus virginiana	0.1006
160-240 min rep 2	Juniperus virginiana	0.0798
160-240 min rep 3	Juniperus virginiana	0.0586
Controll 0-240 min	Juniperus virginiana	1.1982
Control 0-240 min	Juniperus virginiana	1.0444

Distillation study with Juniperus excelsa from Bulgaria, conducted on Jan 5 2018

Timeframe, replicate	Species	g oil
0-5 min rep 1	Juniperus excelsa	0.3552
0-5min rep 2	Juniperus excelsa	0.2522
0-5min rep 3	Juniperus excelsa	0.2717
5-10min rep1	Juniperus excelsa	0.0683
5-10min rep2	Juniperus excelsa	0.0665
5-10 min rep 3	Juniperus excelsa	0.0747
10-20 min rep1	Juniperus excelsa	0.0996
10-20 min rep2	Juniperus excelsa	0.0709
10-20 min rep 3	Juniperus excelsa	0.0728
20-40 min rep 1	Juniperus excelsa	0.0149
20-40 min rep 2	Juniperus excelsa	0.0992
20-40 min rep 3	Juniperus excelsa	0.1249
40-80 min rep 1	Juniperus excelsa	0.0000
40-80 min rep 2	Juniperus excelsa	0.0000
40-80 min rep 3	Juniperus excelsa	0.0000
80-160 min rep 1	Juniperus excelsa	0.0000
80-160 min rep 2	Juniperus excelsa	0.0000
80-160 min rep 3	Juniperus excelsa	0.0318
160-240 min rep 1	Juniperus excelsa	0.0163

160-240 min rep 2	*Juniperus excelsa*	0.0000
160-240 min rep 3	*Juniperus excelsa*	0.0000
Controll 0-240 min	*Juniperus excelsa*	0.7180
Control 0-240 min	*Juniperus excelsa*	1.1434

Distillation study with Juniperus sabina collected in Bulgaria

Replicate, timeframe in mi	Species	g of oil
rep1-time1; 0-3min	*Junipers sabina*	0.4625
rep2-time1; 0-3min	*Junipers sabina*	0.7038
rep3-time1; 0-3min	*Junipers sabina*	0.5532
rep1-time2; 3-5min	*Junipers sabina*	0.3036
rep2-time2; 3-5min	*Junipers sabina*	0.1110
rep3-time2; 3-5min	*Junipers sabina*	0.1753
rep1-time3; 5-10min	*Junipers sabina*	0.1710
rep2-time3; 5-10min	*Junipers sabina*	0.2388
rep3-time3; 5-10min	*Junipers sabina*	0.1878
rep1-time4; 10-20min	*Junipers sabina*	0.1089
rep2-time4; 10-20min	*Junipers sabina*	0.1188
rep3-time4; 10-20min	*Junipers sabina*	0.1125
rep1-time5; 20-40min	*Junipers sabina*	0.1430
rep2-time5; 20-40min	*Junipers sabina*	0.1887
rep3-time5; 20-40min	*Junipers sabina*	0.1033
rep1-time6; 40-80min	*Junipers sabina*	0.2273
rep2-time6; 40-80min	*Junipers sabina*	0.2248
rep3-time6; 40-80min	*Junipers sabina*	0.2236
Control; 0-80min	*Junipers sabina*	1.5801
Control; 0-80min	*Junipers sabina*	1.7085