Chemistry of Natural Compounds, Vol. 45, No. 4, 2009

GC/MS STUDY OF ESSENTIAL OIL COMPONENTS FROM FLOWERS OF *Crataegus jackii*, *C. robesoniana*, AND *C. flabellata*

A. M. Kovaleva,[1*] N. F. Goncharov,[2] A. N. Komissarenko,[1] N. V. Sidora,[1] and S. V. Kovalev[1]

UDC 615.322; 582.711

Many species of the genus *Crataegus* are official and have been included in various pharmacopoeias.

North American species of *Crataegus* have been cultivated since the 18th century. The work of I. A. Samylina was dedicated to the study of Baltic and Tadzhik species of *Crataegus*. She also investigated certain North American species [1, 2]. Both wild and cultivated species in Russia and Ukraine are presently little studied. We have previously reported results from a study of phenolic, flavonoid, and polyphenol compounds and the elemental composition of several North American *Crataegus* species [3, 4].

During the research we established the component composition of essential oils from flowers of three *Crataegus* species, *C. jackii* Sarg., *C. robesoniana* Sarg., and *C. flabellata* (Bosc ex Spach; C. Koch) Rydb.

The species *C. jackii* (syn. *C. chrysocarpa* Sarg.) belongs to the section Rotundifoliae; *C. flabellata*, Tenuifoliae; *C. robesoniana* (*C. pedicellata* var. *robesoniana* Sarg.), Coccineae. Certain systematics suggest that *C. flabellata* is intermediate between *C. macrosperma* (Tenuifoliae) and *C. chrysocarpa* (Rotundifoliae). These three species have flowers with white petals but form different fruits. Those of *C. flabellata* are pink with yellow juicy pulp; *C. jackii*, from golden yellow to fiery red with juicy pulp; *C. robesoniana*, red with mealy dry sweet pulp [5, 6].

We studied flowers of *Crataegus* species that were collected near Kursk in May-June 2008 in order to compare the component composition of essential oils and to find distinct species using chemical taxonomy.

A method enabling essential oil to be isolated from a small quantity of plant material was used to obtain essential oil [7]. We used Agilent vials (22 mL, part number 5183–4536) with open tops and a silicone stopper in which an opening was drilled and an air condenser (an ordinary glass tube 50 cm long and 5–7 mm in diameter) was placed for the distillation. Essential oil was distilled by placing ground plant raw material (2.0–3.0 g) (a mixture of peduncles, calyxes, sepals, petals, stamens, and styles with stigmas) into a vial, filling half the vial with water, twisting the stopper with the condenser into the top, and placing the vial into a small sand bath with regulated heating.

The essential oil composition was studied on an Agilent Technology 6890N chromatograph with a 5973N mass-spectrometric detector. The analytical conditions were a quartz chromatographic column, HP-5MS capillary, column length 30 m, inner diameter 0.25 mm, He carrier gas, gas flow rate 1 mL/min, sample volume 0.1–0.5 μL (for essential oil solutions). Samples were introduced with a 1/50 flow division. The thermostat was set at 50°C with programming at 4°C/min to 220°C. The detector and vaporizer temperatures were 250°C.

Essential oil components were identified by comparing mass spectra of chemical compounds in essential oils that were obtained from the chromatography with library mass spectra from NIST02 (>174,000 compounds). Retention indices (RI) of components were calculated from analytical results for essential oils with added normal alkanes (C_{10}-C_{18}).

Calibration that showed that 0.5 mg of compound corresponded to 2.5×10^9 area units was made in order to estimate the content of each component in the oil sample. The contents of essential oils in *C. robesoniana* (0.03%), *C. flabellata* (0.04%), and *C. jackii* (0.08%) were found.

Table 1 lists the results.

1) National Pharmaceutical University, Ukraine, Kharkov, ul. Pushkinskaya, 53, fax: 8057 714 25 40, e-mail: allapharm@yahoo.com; 2) Kursk State Medical University, Russia, Kursk, ul. Karla Marksa, 3. Translated from Khimiya Prirodnykh Soedinenii, No. 4, pp. 490–491, July–August, 2009. Original article submitted February 16, 2009.

 0009-3130/09/4504-0582

TABLE 1. Essential Oil Composition in *C. robesoniana*, *C. flabellata*, and *C. jackii*

Compound	Retention time, min	*C. robesoniana*	*C. flabellata*	*C. jackii*
Decane	7.75	0.16	0.18	0.03
cis-Linalooloxide	10.11	0.15		0.28
trans-Linalooloxide	10.63	0.16		0.18
Linalool	11.06	0.41		0.56
Nonanal	11.18	0.22		
Syringaldehyde B	12.40			0.04
Syringaldehyde C	12.69			0.09
Syringaldehyde D	13.19			0.04
Borneol	13.29	1.23	0.09	
Terpinen-4-ol	13.64	0.34	0.07	
α-Terpineol	14.15	0.55	0.15	0.61
Undecane	14.28		0.11	0.04
Nerol	15.41			0.14
Geraniol	16.29			0.38
Anisaldehyde	16.43			0.54
Tridecane	17.62		0.14	0.10
β-Damascenone	20.41	0.15	0.08	0.08
Tetradecane	20.84	0.29	0.29	0.07
Caryophyllene	21.48	0.90		0.22
Humulene	22.55	0.80	0.31	0.57
γ-Curcumene	23.34	0.51		0.48
β-Ionone	23.58	0.26	0.20	0.31
Pentadecane	23.92	0.33		0.33
α-Farnesene	24.20			0.11
Caryophylleneoxide	26.29	0.80		0.18
Viridiflorol	26.54	5.94	0.76	0.36
Hexadecane	26.59			1.01
Heptadecane	28.46	0.69	0.58	0.71
β-Farnesene	28.55		0.43	
Octadecane	29.94	0.69	0.54	0.88
Hexahydrofarnesylacetone	30.56		0.48	0.67
Phthalate	30.91	5.20	7.60	6.28
Nonadecane	31.21	2.01	0.74	6.14
Phthalate	32.02	15.62	9.20	13.38
Eicosane	32.35	1.34	0.82	1.92
Heneicosene-1	33.08		1.22	12.53
Heneicosane	33.35	7.66	12.59	
Naphthylbenzyl ether	34.15			2.66
Docosane	34.30	2.28	1.97	3.06
Tricosane	35.20	11.11	19.21	17.88
Squalene	35.86	13.08	4.07	0.95
Tetracosane	36.05	7.26	2.46	2.59
Pentacosane	36.86	5.03	6.00	7.34
Nonacosane	37.12	6.99	11.22	2.00
Phthalate	37.31	4.56	4.89	
Heptacosane	37.32			3.58

The study of essential oils from flowers of three *Crataegus* species identified 46 compounds, among which were acyclic, monocyclic, and bicyclic mono- and sesquiterpenoids, norterpenoids, and triterpenoids, which are of scientific interest as chemotaxonomic markers for the genus *Crataegus*.

The component composition of essential oils from flowers of *C. robesoniana*, *C. flabellata*, and *C. jackii* was studied for the first time.

REFERENCES

1. I. A. Samylina and T. L. Kiseleva, *Farmatsiya*, **5**, 30 (1987).
2. I. A. Samylina, *Rastit. Resur.*, **25**, No. 2, 145 (1989).
3. A. M. Koval′ova, N. V. Sidora, O. M. Aleksandrov, and A. L. Vil′ker, *Farmakom*, **2**, 54 (2007).
4. A. M. Koval′ova, N. V. Sidora, S. V. Koval′ov, A. M. Komisarenko, and A. L. Vil′ker, *Visn. Farm.*, **2**, 16 (2005).
5. T. A. Dickinson and J. B. Phipps, *Am. J. Bot.*, **73**, 4, 116 (2000).
6. J. B. Phipps and J. O'Kennon, *Sida*, **20**, 115 (2002).
7. L. B. Chernogorod and B. A. Vinogradov, *Rastit. Resur.*, **42**, No. 2, 61 (2006).