

Electronic supplementary material

UDC 581.19

**THE FIRST DETECTION OF CANNABINOIDS IN SMOKE FROM THE INCENSE
OF *RHODODENDRON TOMENTOSUM* (*LEDUM PALUSTRE* L.), USED IN THE
FOLK SHAMANIC PRACTICE OF THE UDEGE PEOPLE BY HPLC-ESI-MS/MS
SPECTROMETRY***

© *V.I. Dunkay¹, M.P. Razgonova^{2,3}, A.M. Zakharenko^{1,3,4}, A.V. Razgonov², A.M. Panichev⁴,
K.S. Golokhvast^{1,3,4**}*

¹ *Siberian Federal Scientific Centre of Agrobiotechnology RAS, st. Centralnaya,
Presidium, Krasnoobsk, 633501, Russia, droopy@mail.ru*

² *N.I. Vavilov All-Russian Institute of Plant Genetic Resources, st. B. Morskaya, 42-44,
Saint-Petersburg, 190000, Russia*

³ *Far Eastern Federal University, 10 Ajax Bay settlement, Russkiy Island, Vladivostok,
690950, Russia*

⁴ *National Research Tomsk State University, ave. Lenina, 36, Tomsk, 634050, Russia*

⁵ *Pacific Institute of Geography of the Far Eastern Branch of the Russian Academy of
Sciences, st. Radio, 7, Vladivostok, 690041, Russia*

* This article has electronic supplementary material (appendix), which is available to readers on the journal's website.
<https://doi.org/10.14258/jcprm.20260316678s>.

** Corresponding author.

Compounds identified from the extracts of *L. palustre* in positive and negative ionization modes by HPLC-ion trap-MS/MS

№	Class of compounds	Identified compounds	Formula	Mass	Molecular ion [M-H] ⁻	Molecular ion [M+H] ⁺	2 fragmentation MS/MS	3 fragmentation MS/MS	4 fragmentation MS/MS
1	2	3	4	5	6	7	8	9	10
Polyphenols									
1	Flavonol	Kaempferol [3,5,7-Trihydroxy-2-(4-hydro-xyphenyl)-4H-chromen-4-one]	C ₁₅ H ₁₀ O ₆	286.2363		287	286; 205; 163	181	163
2	Flavonol	Dihydrokaempferol [Aromadendrin; Katuranin] *	C ₁₅ H ₁₂ O ₆	288.2522	287		269; 241; 185; 141	267; 185	
3	Flavonol	Kaempferol 5-methyl ether	C ₁₆ H ₁₂ O ₆	300.2629	299		271; 243; 225; 199; 177	268; 243; 227; 187; 177	241; 201
4	Flavonol	Quercetin	C ₁₅ H ₁₂ O ₇	302.2357	301	303	285; 163	181; 145	163
5	Flavonol	Herbacetin [3,5,7,8-Tetrahydroxy-2-(4-hydro-xyphenyl)-4H-chromen-4-one] *	C ₁₅ H ₁₀ O ₇	302.2357		303	275; 202	175	
6	Flavonol	Dihydroquercetin [Taxifolin; Taxifoliol]	C ₁₅ H ₁₂ O ₇	304.2516	303		285	267; 241; 215; 135	171
7	Flavonol	Rhamnetin I [beta-Rhamnocitrin; Quercetin 7-Methyl ether]	C ₁₆ H ₁₂ O ₇	316.2623		317	257; 269; 216	230	
8	Flavonol	Rhamnetin II*	C ₁₆ H ₁₂ O ₇	316.2623	315		300; 165	299; 271; 151; 124	243
9	Flavonol	Isorhamnetin [Isorhamnetol; Quercetin 3'-Methyl ether; 3-Methylquercetin]	C ₁₆ H ₁₂ O ₇	316.2623	315		300; 165; 121	271; 226; 151	271; 243
10	Flavonol	Myricetin [3,5,7-Trihydroxy-2-(3,4,5-Trihydroxyphenyl)-4H-Chromen-4-One]	C ₁₅ H ₁₀ O ₈	318.2351		319	273; 245; 219	245; 217	
11	Flavonol	Ampelopsin [Dihydromyricetin; Ampeloptin]	C ₁₅ H ₁₂ O ₈	320.251	319		317; 275	257; 217	
12	Flavonol	Myricetin 5-Methyl ether [5-O-Methylmyricetin]	C ₁₆ H ₁₂ O ₈	332.2617		333	318	301; 244; 153	193
13	Flavonol	Syringetin*	C ₁₇ H ₁₄ O ₈	346.2883		347	331; 280	317; 257	261; 233; 191
14	Flavonol	Avicularin (Quercetin 3-Alpha-L-Arabinofuranoside; Avicularoside)	C ₂₀ H ₁₈ O ₁₁	434.3503		435	303	257; 201; 165	229; 201; 145
15	Flavonol	Quercetin-3-O-arabinoside*	C ₂₀ H ₁₈ O ₁₁	434.3503	433		301	179; 121	151
16	Flavonol	Methylquercetin-pentoside*	C ₂₁ H ₂₀ O ₁₁	448.3769		449	317	301	228; 153
17	Flavonol	Quercitrin [Quercetin 3-L- rhamnoside; Quercetrin]	C ₂₁ H ₂₀ O ₁₁	448.3769	447		301	271; 151	
18	Flavonol	Myricetin-3-O-alpha-arabinofuranoside*	C ₂₀ H ₁₈ O ₁₂	450.3497	449		317; 284	299; 227; 178	151
19	Flavonol	Hyperoside (Quercetin 3-O- galactoside; Hyperin)	C ₂₁ H ₂₀ O ₁₂	464.3763		465	303	257; 191	229; 173
20	Flavonol	Quercetin 3-O- glucoside	C ₂₁ H ₂₀ O ₁₂	464.3763	463		301; 179	271; 179; 151	151
21	Flavonol	Isorhamnetin 3-O-glucoside*	C ₂₂ H ₂₂ O ₁₂	478.4029		479	317; 290	301; 253	274
22	Flavonol	Quercetin acetyl hexoside*	C ₂₃ H ₂₂ O ₁₃	506.413		507	303; 485; 431; 407; 353; 291	257; 187	

Продолжение таблицы

1	2	3	4	5	6	7	8	9	10
23	Flavonol	Quercetin 3-beta-D (6- <i>p</i> -hydroxybenzoyl) galactoside	C ₂₈ H ₂₄ O ₁₄	584.4818	583		463; 343; 301	301; 151	271; 179
24	Flavonol	Rutin (Quercetin 3- <i>O</i> -rutinoside)	C ₂₇ H ₃₀ O ₁₆	610.5175	609		463; 343; 301; 255; 179	301	255; 179
25	Flavonol	Quercetin-3-(7- <i>O</i> -glucosyl)glucuronide *	C ₂₇ H ₂₈ O ₁₈	640.5004		641	303; 256	256; 228	
26	Flavonol	Isorhamnetin- <i>O</i> -dihexoside*	C ₂₈ H ₃₂ O ₁₇	640.5435		641	303; 176	229; 165	201
27	Flavone	Apigenin [5,7-Dihydroxy-2-(4 <i>H</i> -hydroxyphenyl)-4 <i>H</i> -chromen-4-one]	C ₁₅ H ₁₀ O ₅	270.2369		271	253; 199	224; 193	
28	Flavone	Acacetin [Linarigenin; Buddleoflavonol] *	C ₁₆ H ₁₂ O ₅	284.2635		285	270; 241; 225; 184; 166	242; 214	213; 197; 187; 167
29	Flavone	Genkwanin [Gengkwanin; Puddumetin; Apigenin 7-Methyl Ether] *	C ₁₆ H ₁₂ O ₅	284.2635		285	269; 167	242	197; 120
30	Flavone	4'-Methoxytecto-chrysin*	C ₁₇ H ₁₄ O ₅	298.2901	297		282; 178	253	238
31	Flavone	Apigenin-7, 4'-dimethyl ether*	C ₁₇ H ₁₄ O ₅	298.2901		299	284	256; 165	255; 211
32	Flavone	Diosmetin*	C ₁₆ H ₁₂ O ₆	300.2629	299		283; 256		
33	Flavone	Chrysoeriol [Chryseriol]*	C ₁₆ H ₁₂ O ₆	300.2629		301	298	283; 167	256
34	Flavone	Cirsimaritin*	C ₁₇ H ₁₄ O ₆	314.2895	313		298; 269	271	269
35	Flavone	Dihydroxy-trimethoxy dihydroxyisoflavone*	C ₁₇ H ₁₆ O ₆	316.3053		317	288; 221; 155	214; 164	187
36	Flavone	Salvigenin*	C ₁₈ H ₁₆ O ₆	328.3160		329	314	296	268
37	Flavone	Jaceosidin [5,7,4'-trihydroxy-6',5'-dimethoxyflavone]*	C ₁₇ H ₁₄ O ₇	330.2889		331	318	301; 215	226
38	Flavone	Tricin [5,7,4'-trihydroxy-3',5'-dimethoxyflavone]*	C ₁₇ H ₁₄ O ₇	330.2889	329		314	299	271; 243
39	Flavone	Dihydroxy-trimethoxy(iso)flavone*	C ₁₈ H ₁₆ O ₇	344.3154		345	329	315; 179	287; 167
40	Flavone	Gardenin B [Demethyltangeretin]*	C ₁₉ H ₁₈ O ₇	358.342		359	344	329; 191	301
41	Flavone	Thymonin [5,6,4'-trihydroxy-7,8,3'-tri-methoxyflavone]*	C ₁₈ H ₁₆ O ₈	360.3148		361	346; 331	331	303; 275; 247; 219; 205
42	Flavone	Dihydroxy-tetramethoxy(iso)flavone*	C ₁₉ H ₁₈ O ₈	374.3414		375	360; 328	345; 314	314
43	Flavone	Luteolin 6- <i>C</i> -glucoside [Isoorientin; Homoorientin] *	C ₂₁ H ₂₀ O ₁₁	448.3769		449	431; 337	387; 225	369; 233; 180
44	Flavone	Nevadensin*	C ₁₈ H ₁₆ O ₇	344.3154		345	330	315; 179	287; 259; 167
45	Flavone	Apigenin derivative	C ₂₄ H ₂₆ O ₁₃	522.4554		523	273	175; 245; 121	
46	Flavone	Apigenin 6- <i>C</i> -[6"-acetyl-2"- <i>O</i> -deoxyhexoside]-glucoside*	C ₂₉ H ₃₂ O ₁₅	620.5554		621	561	461	433
47	Flavanone	Naringenin [Naringetol; Naringenine]	C ₁₅ H ₁₂ O ₅	272.5228		273	256; 188	212; 188; 171	
48	Flavan-3-ol	Epi-afzelechin [(epi)Afzelechin] *	C ₁₅ H ₁₄ O ₅	274.2687		275	244; 175	215; 175; 143	175
49	Flavan-3-ol	Catechin [D-Catechol]	C ₁₅ H ₁₄ O ₆	290.2681		291	271; 233; 216; 193	255; 245; 215	
50	Flavan-3-ol	(epi)Catechin	C ₁₅ H ₁₄ O ₆	290.2681		291	273	245; 148	
51	Flavan-3-ol	Gallocatechin [+(-) Gallocatechin]	C ₁₅ H ₁₄ O ₇	306.2675		307	275; 207	206; 111	
52	Anthocyanin	Cyanidin-3- <i>O</i> -glucoside [Cyanidin 3- <i>O</i> -beta-D-Glucoside; Kuromarin]	C ₂₁ H ₂₁ O ₁₁ +	449.3848		449	287; 213; 137	185; 115	

Продолжение таблицы

1	2	3	4	5	6	7	8	9	10
53	Anthocyanidin	Delphinidin 3- <i>O</i> -glucoside*	C ₂₁ H ₂₁ O ₁₂ +	465.3905		465	303	257; 201; 165	229; 201
54	Anthocyanin	Petunidin-3- <i>O</i> -glucoside*	C ₂₂ H ₂₃ O ₁₂ +	479.4108		479	317; 275	302	273; 227; 153
55	Anthocyanin	Delphinidin 3-acetylglucoside [Delphinidin-3-(6"-Acetyl-Glucoside)] *	C ₂₃ H ₂₃ O ₁₃ +	507.4209		507	303	257; 229; 165	229; 201
56	Anthocyanin	Peonidin 3-(6- <i>O</i> -coumaroyl)glucoside *	C ₃₁ H ₂₉ O ₁₃	609.554		609	302	285; 257; 229	229
57	Condensed tannin	Procyanidin A-type dimer*	C ₃₀ H ₂₄ O ₁₂	576.5044		577	425; 559; 287	287	227; 137
58	Condensed tannin	Proanthocyanidin B3 [Proanthocyanidin; Catechin-(4 alpha->8)-catechin]	C ₃₀ H ₂₆ O ₁₂	578.5202		579	409	297; 259	245; 203
59	Phenolic acid	<i>p</i> -Hydroxybenzoic acid hexoside*	C ₁₃ H ₁₆ O ₈	300.2613	299		281; 169	253; 211; 127	183
60	Phenolic acid	Ellagic acid [Benzoaric acid; Elagostasine; Lagistase; Eleagic acid] *	C ₁₄ H ₆ O ₈	302.19		303	284; 181	256	240; 185
61	Phenolic acid	Chlorogenic acid [3- <i>O</i> -Caffeoylquinic acid]	C ₁₆ H ₁₈ O ₉	354.31	353		191; 135	173; 127	
62	Phenolic acid	Neochlorogenic acid [5- <i>O</i> -Caffeoylquinic acid]	C ₁₆ H ₁₈ O ₉	354.31	353		191	173	
63	Phenolic acid	3- <i>O</i> -Caffeoylquinic acid methyl ether*	C ₁₇ H ₂₀ O ₉	368.3353		369	207; 271; 339	207	153
64	Phenolic acid	Ellagic acid pentoside [Ellagic acid 4- <i>O</i> -xylopyranoside]*	C ₁₉ H ₁₄ O ₁₂	434.3073	433		301	271; 179	151
65	Phenolic acid	Ellagic acid - hexoside*	C ₂₀ H ₁₆ O ₁₃	464.3332		465	303	257; 201; 165	229
66	Hydroxycoumarin	Umbelliferone [Skimmetin; Hydragin]	C ₉ H ₆ O ₃	162.1421		163	145	117	
67	Coumarin	Scopoletin [Scopoletine; Gelseminic acid]	C ₁₀ H ₈ O ₄	192.1681		193	133; 165	119	
68	Coumarin	Fraxetin	C ₁₀ H ₈ O ₅	208.1675		209	148.96	120.96	
69	Coumarin	Esculin [Aesculin; Esculoside; Polichrome]	C ₁₅ H ₁₆ O ₉	340.2821		341	281; 217; 151	174.96	
70	Coumarin	Scopolin [Scopoloside; Scopoletin-7-glucoside; Murrayin]	C ₁₆ H ₁₈ O ₉	354.3087	353		191		
71	Coumarin glucoside	Fraxin (Fraxetin-8- <i>O</i> -glucoside)	C ₁₆ H ₁₈ O ₁₀	370.3081	369		207; 354	192	164; 120
72	Coumarin glucoside	Fraxetin-7- <i>O</i> -beta-glucuronide	C ₁₆ H ₁₆ O ₁₁	384.2916	383		365; 285; 191	215; 149	171
73	Coumarin glucoside	Isofraxidin-7-glucoside [Calycanthoside; Eleuterioside B1] *	C ₁₇ H ₂₀ O ₁₀	384.3347	383		191	127; 172	
74	Lignan	Secoisolariciresinol*	C ₂₀ H ₂₆ O ₆	362.4168		363	261; 163	233; 179	215; 151; 127
75	Lignan	Medioresinol*	C ₂₁ H ₂₄ O ₇	388.4111		389	209; 124	149	
76	Stilbenoids	Pterostilbene*	C ₁₆ H ₁₆ O ₃	256.2964		257	197	155	
77	Stilbenoids	Resveratrol [trans-Resveratrol; 3,4',5-Trihydroxystilbene; Stilbentriol] *	C ₁₄ H ₁₂ O ₃	228.2433		229	211; 135		
78	Gallate ester	Beta-Glucogallin [1- <i>O</i> -Galloyl-Beta-D-Glucose; Galloyl glucose] *	C ₁₃ H ₁₆ O ₁₀	332.2601		333	314; 273		
79	Dihydrochalcone	Phloretin [Dihydronaringenin; Phloretol] *	C ₁₅ H ₁₄ O ₅	274.2687		275	257; 175	239; 175	183
Others									
80	Alpha, omega-dicarboxylic acid	Succinic acid [Butanedioic acid; Amber acid; Asuccin; Wormwood acid] *	C ₄ H ₆ O ₄	118.088		119	116		

1	2	3	4	5	6	7	8	9	10
81	Gamma-lactone	1-Isobenzofuranone*	C ₈ H ₆ O ₂	134.1320		135	117		
82	2-hydroxycarboxylic acid (succinic acid)	Malic acid [DL-Malic acid] *	C ₄ H ₆ O ₅	134.0874		135	115; 119		
83	Cyclohexanecarboxylic acid	Perillic acid*	C ₁₀ H ₁₄ O ₂	166.217		167	121; 149	121	
84	Amino acid	Tyrosine [(2S)-2-Amino-3-(4-Hydroxyphenyl)Propanoic acid]*	C ₉ H ₁₁ NO ₃	181.1885		182	165; 136	147	119
85	Polysaturated fatty acid	Dodecapentaenoic acid*	C ₁₂ H ₁₄ O ₂	190.2384		191	179		
86	Amino acid	L-Tryptophan *	C ₁₁ H ₁₂ N ₂ O ₂	204.2252		205	187	186; 139	183; 154
87	Organic sodium salt	Sodium ferulate*	C ₁₀ H ₉ NaO ₄	216.1658		217	119; 199	117	
88	Sesquiterpenoid	Caryophyllene oxide [Caryophyllene-alpha-oxide]	C ₁₅ H ₂₄ O	220.3505		221	121; 291	119	
89	Omega-5 fatty acid	Myristoleic acid [Cis-9-Tetradecanoic acid] *	C ₁₄ H ₂₆ O ₂	226.3550		227	209	192; 139	122
90	Omega-3 unsaturated fatty acid	Hexadecatrienoic acid [Hexadeca-2,4,6-trienoic acid]*	C ₁₆ H ₂₆ O ₂	250.3764		251	195; 232; 135	167; 135	149; 121
91	Ribonucleoside composite of adenine (purine)	Adenosine*	C ₁₀ H ₁₃ N ₅ O ₄	267.2413		268	136	116	
92	Ribonucleoside composite of adenine (purine)	Inosine*	C ₁₀ H ₁₂ N ₄ O ₅	268.2261		269	136	117	
93	Cannabiod	Cannabigerovar (CBGV) [Cannabigerovarol] *	C ₁₉ H ₂₈ O ₂	288.4244		289	189; 228; 272	171	
94	Abietane diterpenoid	Tanshinone IIA [Tanshinone II; Dan Shen Ketone; Tanshinone B] *	C ₁₉ H ₁₈ O ₃	294.3444		293	275; 231; 171	231; 177	
95	Higher-molecular-weight carboxylic acid	Oxo-nonadecanoic acid*	C ₁₉ H ₃₆ O ₃	312.4873		313	298	270; 297	181
96	Cannabiod	Cannabigerol (CBG)*	C ₂₁ H ₃₂ O ₂	316.4776		317	179; 121	145	
97	Cannabiod	Delta9-Tetrahydrocannabinol (Delta9-THC)	C ₂₁ H ₃₀ O ₂	314.4617		315	299	272	257; 243; 201; 167
98	Terpenoid trilactone	Bilobalide [(-)-Bilobalide] *	C ₁₅ H ₁₈ O ₈	326.30	325		183	183; 119	119
99	Oxylipin	9,10-Dihydroxy-8-oxooctadec-12-enoic acid [oxo-DHODE; oxo-Dihydroxy-octadecenoic acid]*	C ₁₈ H ₃₂ O ₅	328.4437	327		229; 211; 171	209; 125	191; 165; 125
100	Oxylipin	13- Trihydroxy-Octadecenoic acid [THODE]*	C ₁₈ H ₃₄ O ₅	330.4596	329		211; 171	183; 155	
101	Cannabiod	11-Hydroxy-Δ9-Tetrahydrocannabinol (11-OH-THC) [11-Hydroxytetrahydrocannabinol]*	C ₂₁ H ₃₀ O ₃	330.4611		331	313	293; 257; 211; 152	134
102	Cannabiod	11-nor-9-carboxy-THC (THC-COOH) [THC-11-Oic acid; Delta-9-11-Carboxytetrahydrocannabinol] *	C ₂₁ H ₂₈ O ₄	344.4446		345	327; 165	239; 149; 119	
103	Cannabiod	Cannabidiolic acid (CBD-A) *	C ₂₂ H ₃₀ O ₄	358.4712		359	341; 289; 239; 197	279; 199	

Окончание таблицы

1	2	3	4	5	6	7	8	9	10
104	Sterol	Fucosterol [Fucostein; Trans-24-Ethylidenecholesterol] *	C ₂₉ H ₄₈ O	412.6908		413	395; 357; 203	333.10; 233	
105	Sterol	Beta-Sitostenone [Stigmast-4-En-3-One; Sitostenone]	C ₂₉ H ₄₈ O	412.6908		413	393; 301; 230	189	
106	Iridoid monoterpenoid	Dihydroisovaltrate*	C ₂₂ H ₃₂ O ₈	424.4847		425	365; 207	309; 235	235
107	Triterpenoid	Uvaol	C ₃₀ H ₅₀ O ₂	442.7168		443	425; 233	407; 325	389; 231
108	Anabolic steroid; Androgen; Androgen ester	Vebronol*	C ₃₀ H ₄₄ O ₃	452.6686		453	435; 389; 336; 276; 226	336; 258; 226; 182	
109	Triterpenoid	Oleanoic acid	C ₃₀ H ₄₈ O ₃	456.70		457	439; 411; 357; 326; 291; 239; 221; 175	421; 395; 311; 286; 250; 228; 201; 175	
110	Triterpenoid	Ursolic acid	C ₃₀ H ₄₈ O ₃	456.7003		457	439; 357; 203	421; 367; 211; 135	322
111	Phytohormone	GA8-hexose gibberellin*	C ₂₅ H ₃₄ O ₁₂	526.53		527	365	305; 275; 203	144
112	Pterocarpan	9,10-DiMP-3-O-malonyl-glucoside	C ₂₆ H ₂₈ O ₁₃	548.4927		549	531; 379; 303; 247	285; 165	
113	Iridoid monoterpenoid	<i>p</i> -Coumaroyl monotropein hexoside*	C ₃₇ H ₆₂ O ₁₂	698.8810		699	537; 434; 343; 258	519; 375; 260	