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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*

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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; Aviculoroside)	$C_{20}H_{18}O_{11}$	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-*p*-hydroxybenzoyl) galactoside	$C_{28}H_{24}O_{14}$	584.4818	583		463; 343; 301	301; 151	271; 179
24	Flavonol	Rutin (Quercetin 3-*O*-rutinoside)	$C_{27}H_{30}O_{16}$	610.5175	609		463; 343; 301; 255; 179	301	255; 179
25	Flavonol	Quercetin-3-(7-*O*-glucosyl)glucuronide *	$C_{27}H_{28}O_{18}$	640.5004		641	303; 256	256; 228	
26	Flavonol	Isorhamnetin-*O*-dihexoside*	$C_{28}H_{32}O_{17}$	640.5435		641	303; 176	229; 165	201
27	Flavone	Apigenin [5,7-Dixydroxy-2-(40Hydroxyphenyl)-4H-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'-Methoxytectochrysin*	$C_{17}H_{14}O_5$	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'-dimetoxyflavone]*	$C_{17}H_{14}O_7$	330.2889		331	318	301; 215	226
38	Flavone	Tricin [5,7,4'-trihydroxy-3',5'-dimetoxyflavone]*	$C_{17}H_{14}O_7$	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-*C*-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-*C*-[6"-acetyl-2"-*O*-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	Epiafzelechin [(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	Anthocianin	Cyanidin-3-*O*-glucoside [Cyanidin 3-*O*-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-*O*-glucoside*	$C_{21}H_{21}O_{12+}$	465.3905		465	303	257; 201; 165	229; 201
54	Anthocyanin	Petunidin-3-*O*-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-*O*-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	*p*-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] *	$C_{14}H_6O_8$	302.19		303	284; 181	256	240; 185
61	Phenolic acid	Chlorogenic acid [3-O-Caffeoylquinic acid]	$C_{16}H_{18}O_9$	354.31	353		191; 135	173; 127	
62	Phenolic acid	Neochlorogenic acid [5-O-Caffeoylquinic acid]	$C_{16}H_{18}O_9$	354.31	353		191	173	
63	Phenolic acid	3-*O*-Caffeoylquininc 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-*O*-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]	$C_9H_6O_3$	162.1421		163	145	117	
67	Coumarin	Scopoletin [Scopoletine; Gelseminic acid]	$C_{10}H_8O_4$	192.1681		193	133; 165	119	
68	Coumarin	Fraxetin	$C_{10}H_8O_5$	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-O-glucoside)	$C_{16}H_{18}O_{10}$	370.3081	369		207; 354	192	164; 120
72	Coumarin glucoside	Fraxetin-7-O-beta-glucuronide	$C_{16}H_{16}O_{11}$	384.2916	383		365; 285; 191	215; 149	171
73	Coumarin glucoside	Isofraxidin-7-glucoside [Calycanthoside; Eleuteroside 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-O-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] *	$C_4H_6O_4$	118.088		119	116		

Продолжение таблицы

1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*
81	Gamma-lactone	1-Isobenzofuranone*	$C_8H_6O_2$	134.1320		135	117		
82	2-hydroxycarboxylic acid (succinic acid)	Malic acid [DL-Malic acid] *	$C_4H_6O_5$	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-Hydroxyphnyl)Propanoic acid]*	$C_9H_{11}NO_3$	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 *	$C_{11}H_{12}N_2O_2$	204.2252		205	187	186; 139	183; 154
87	Organic sodium salt	Sodium ferulate*	$C_{10}H_9NaO_4$	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*	$C_{10}H_{13}N_5O_4$	267.2413		268	136	116	
92	Ribonucleoside composite of adenine (purine)	Inosine*	$C_{10}H_{12}N_4O_5$	268.2261		269	136	117	
93	Cannabioid	Cannabigerovarin (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	Cannabioid	Cannabigerol (CBG)*	$C_{21}H_{32}O_2$	316.4776		317	179; 121	145	
97	Cannabioid	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	Cannabioid	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	Cannabioid	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	Cannabioid	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	Vebonol*	$C_{30}H_{44}O_3$	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	Pterocarpans	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	*p*-Coumaroyl monotropein hexoside*	$C_{37}H_{62}O_{12}$	698.8810		699	537; 434; 343; 258	519; 375; 260	