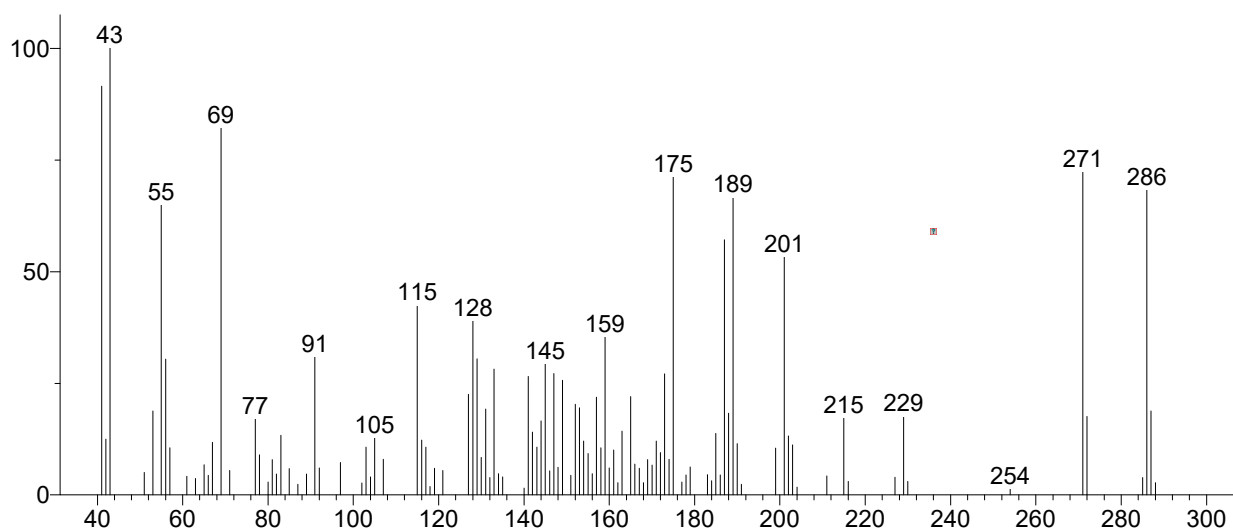


Unknown; InLib=-133



(Text File) Component at scan 2411 (14.278 min) [Model = +43u] in X:\ABBY GCMS\20211015\A_211015_024.D\DATA.MS

Name: Component at scan 2411 (14.278 min) [Model = +43u] in X:\ABBY GCMS\20211015\A_211015_024.D\DATA.MS

MW: N/A ID#: 1017 DB: Text File

10 largest peaks:

43 999	41 913	69 820	271 721	175 711	286 681	189 664	55 648	187 570	201 532
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111 m/z Values and Intensities:

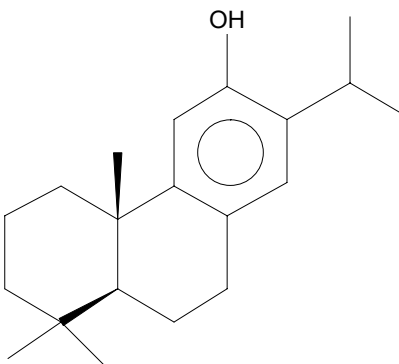
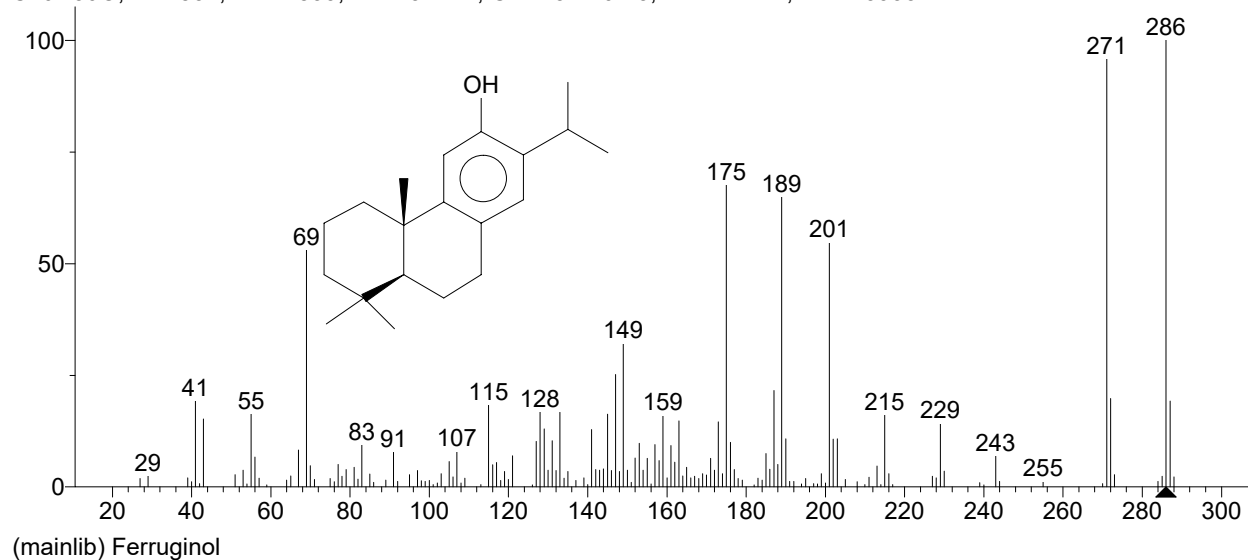
41 913	42 124	43 999	51 50	53 187	55 648	56 303	57 105	61 41	63 36
65 67	66 43	67 117	69 820	71 54	77 169	78 89	80 28	81 78	82 46
83 133	85 58	87 23	89 46	91 308	92 60	97 72	102 26	103 106	104 40
105 127	107 79	115 423	116 122	117 106	118 18	119 59	121 54	127 224	128 388
129 304	130 83	131 191	132 38	133 281	134 47	135 40	140 15	141 264	142 140
143 106	144 165	145 293	146 53	147 271	148 61	149 256	151 43	152 202	153 194
154 120	155 92	156 47	157 218	158 105	159 352	160 60	161 100	162 27	163 142
165 219	166 68	167 59	168 27	169 78	170 66	171 120	172 94	173 270	174 79
175 711	177 28	178 44	179 62	183 45	184 31	185 137	186 44	187 570	188 182
189 664	190 114	191 23	199 104	201 532	202 131	203 111	204 17	211 42	215 171
216 30	227 39	229 175	230 30	254 13	271 721	272 175	285 38	286 681	287 187
288 27									

Synonyms:

no synonyms.

Hit 1 : Ferruginol

C₂₀H₃₀O; MF: 834; RMF: 839; Prob 57.7%; CAS: 514-62-5; Lib: mainlib; ID: 243935.



Name: Ferruginol

Formula: C₂₀H₃₀O

MW: 286 Exact Mass: 286.229666 CAS#: 514-62-5 NIST#: 413241 ID#: 243935 DB: mainlib

Other DBs: None

Contributor: NIST Mass Spectrometry Data Center

InChIKey: QXNWVJOHUAQHLM-AZUAARDMSA-N Non-stereo

10 largest peaks:

286 999 | 271 956 | 175 675 | 189 648 | 201 546 | 69 530 | 149 320 | 147 251 | 187 215 | 272 197 |

153 m/z Values and Intensities:

27	18	29	24	39	20	40	11	41	192	42	7	43	151	51	27	53	37	54	6
55	163	56	66	57	19	59	4	64	15	65	24	67	82	69	530	70	47	71	16
75	18	76	11	77	50	78	23	79	38	81	43	82	17	83	93	85	28	86	10
89	15	91	77	92	12	95	27	97	36	98	13	99	12	100	14	101	5	102	8
103	29	105	56	106	22	107	79	108	8	109	19	113	5	115	182	116	49	117	54
118	14	119	34	120	16	121	69	126	4	127	101	128	167	129	129	130	37	131	103
132	36	133	166	134	19	135	34	137	14	139	20	140	5	141	128	142	38	143	37

144	40	145	162	146	36	147	251	148	34	149	320	150	37	151	10	152	64	153	97
154	37	155	63	156	6	157	94	158	58	159	159	160	20	161	92	162	55	163	147
164	24	165	43	166	20	167	23	168	18	169	29	170	26	171	63	172	37	173	145
174	29	175	675	176	99	177	38	178	18	179	15	182	4	183	19	184	15	185	74
186	39	187	215	188	50	189	648	190	107	191	12	192	12	194	6	195	18	197	7
198	6	199	29	200	8	201	546	202	106	203	107	205	16	208	11	210	5	211	21
213	46	214	5	215	160	216	29	217	5	227	23	228	20	229	141	230	35	239	9
240	4	243	68	244	12	255	12	270	7	271	956	272	197	273	27	284	12	285	23
286	999	287	191	288	22														

Synonyms:

1. Abieta-9(11),8(14),12-trien-12-ol #
2. trans-Ferruginol
3. Podocarpa-8,11,13-trien-12-ol, 13-isopropyl-

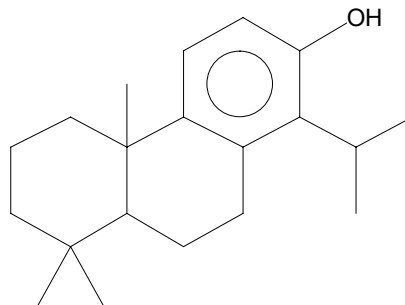
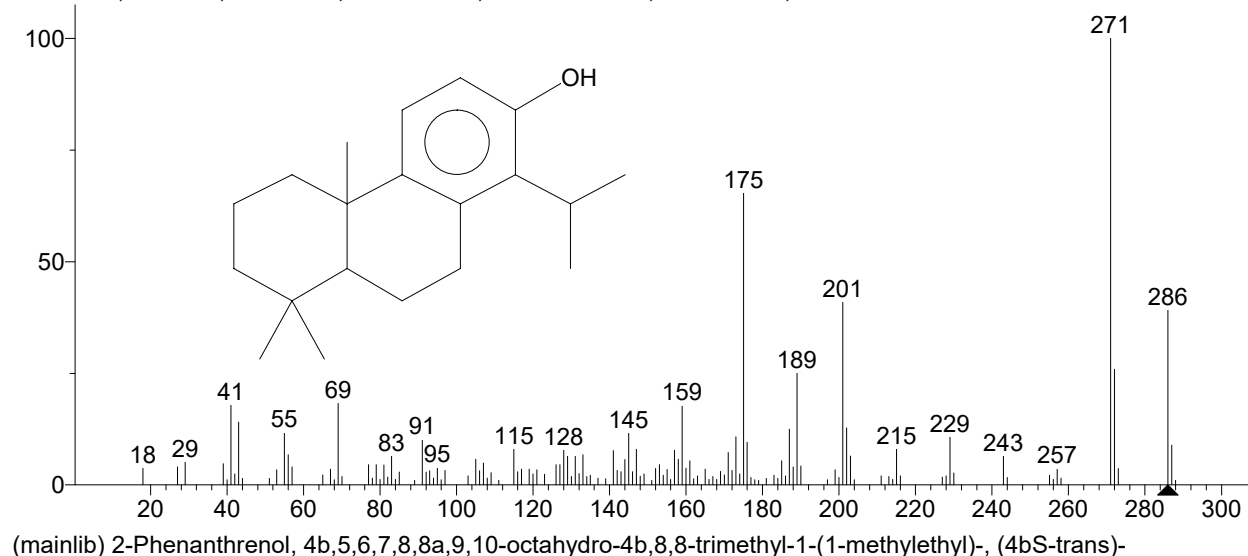
Experimental RI median±deviation (#data)

Semi-standard non-polar: 2325±0 (16)

Standard non-polar: 2283±N/A (1)

Polar: 2295±N/A (1)

Hit 2 : 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS-trans)-
C₂₀H₃₀O; MF: 820; RMF: 828; Prob 36.1%; CAS: 511-15-9; Lib: mainlib; ID: 238936.



Name: 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS-trans)-

Formula: C₂₀H₃₀O

MW: 286 Exact Mass: 286.229666 CAS#: 511-15-9 NIST#: 42592 ID#: 238936 DB: mainlib

Other DBs: NIH

Contributor: R RYHAGE MS-LAB KAROLINSKA INSTITUTET STOCKHOLM SWEDEN

InChIKey: ZRVDANDJSTYELM-UHFFFAOYSA-N Non-stereo

10 largest peaks:

271 999 | 175 653 | 201 409 | 286 391 | 272 258 | 189 249 | 69 182 | 41 178 | 159 177 | 43 140 |

136 m/z Values and Intensities:

18 37	27 40	29 51	39 47	40 11	41 178	42 24	43 140	44 14	51 14
53 33	55 117	56 67	57 40	65 22	67 35	68 11	69 182	70 18	77 45
78 15	79 45	80 12	81 44	82 17	83 65	84 12	85 28	89 10	91 101
92 28	93 31	94 15	95 38	96 11	97 32	103 20	105 57	106 31	107 48
108 15	109 27	111 10	115 80	116 29	117 35	119 35	120 24	121 33	123 23
126 45	127 45	128 77	129 63	130 18	131 63	132 25	133 67	134 18	135 21
137 15	139 13	141 76	142 32	143 29	144 56	145 116	146 29	147 79	148 19

149	24	151	10	152	36	153	45	154	21	155	34	156	12	157	77	158	57	159	177
160	37	161	53	162	13	163	20	165	35	166	12	167	18	168	12	169	30	170	22
171	72	172	32	173	107	174	24	175	653	176	95	177	16	178	11	179	10	181	14
183	21	184	14	185	53	186	20	187	124	188	40	189	249	190	42	197	11	199	33
200	16	201	409	202	127	203	64	204	11	211	20	213	18	214	12	215	80	216	20
227	17	228	20	229	107	230	26	243	64	244	16	255	21	256	12	257	36	258	15
271	999	272	258	273	36	286	391	287	88	288	10								

Synonyms:

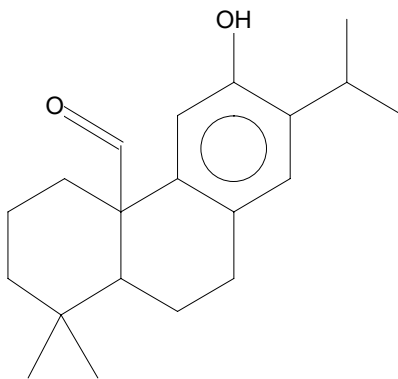
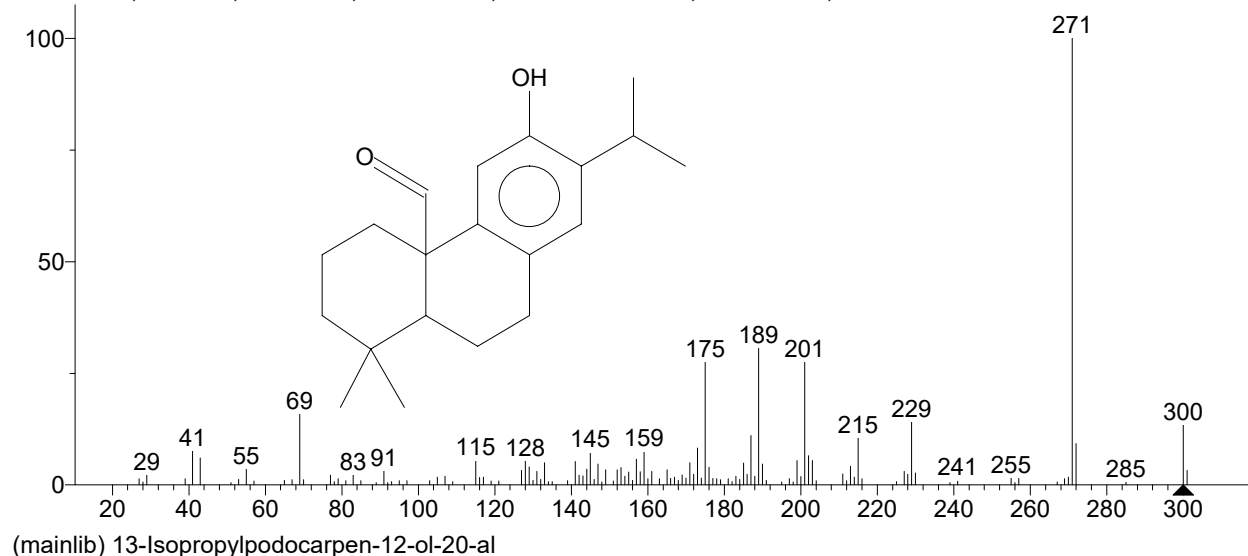
- 1.Podocarpa-8,11,13-trien-13-ol, 14-isopropyl-
- 2.Totarol
- 3.TOTAROL (B637832K176)
- 4.(+)-Totarol
- 5.14-Isopropylpodocarpa-8,11,13-trien-13-ol #
- 6.trans-Totarol

Experimental RI median±deviation (#data)

Semi-standard non-polar:2302±0 (14)

Standard non-polar: 2268±15 (7)

Hit 3 : 13-Isopropylpodocarpin-12-ol-20-al
 C₂₀H₂₈O₂; MF: 737; RMF: 788; Prob 3.53%; CAS: 24035-37-8; Lib: mainlib; ID: 238951.



Name: 13-Isopropylpodocarpin-12-ol-20-al
 Formula: C₂₀H₂₈O₂
 MW: 300 Exact Mass: 300.208931 CAS#: 24035-37-8 NIST#: 42992 ID#: 238951 DB: mainlib
 Other DBs: None
 Contributor: R RYHAGE MS-LAB KAROLINSKA INSTITUTET STOCKHOLM SWEDEN
 InChIKey: YPWYNONCSGZEQQ-UHFFFAOYSA-N Non-stereo
 10 largest peaks:

271 999 | 189 305 | 175 274 | 201 274 | 69 158 | 229 140 | 300 134 | 187 110 | 215 104 | 272 92 |
 125 m/z Values and Intensities:

27	13	28	6	29	21	39	13	41	75	43	60	51	5	53	12	55	35	57	8
65	10	67	11	69	158	70	11	77	21	78	7	79	13	81	9	83	22	85	9
89	5	91	31	92	5	93	7	95	9	97	9	103	9	105	17	107	19	109	7
115	54	116	16	117	17	119	8	121	8	127	32	128	53	129	40	130	10	131	30
132	12	133	49	134	7	135	7	139	9	141	52	142	21	143	20	144	35	145	72
146	12	147	46	148	6	149	33	151	8	152	33	153	38	154	19	155	28	156	10
157	57	158	29	159	74	160	13	161	30	163	13	165	33	166	14	167	17	168	10

169	22	170	15	171	49	172	23	173	82	174	15	175	274	176	39	177	14	178	13
179	11	181	13	182	7	183	19	184	12	185	48	186	23	187	110	188	19	189	305
190	46	191	10	195	6	197	13	198	6	199	54	200	18	201	274	202	65	203	54
204	9	211	24	212	9	213	41	214	17	215	104	216	13	225	7	227	30	228	23
229	140	230	26	239	5	241	10	255	15	256	5	257	14	267	6	269	13	270	17
271	999	272	92	285	7	300	134	301	32										

Synonyms:

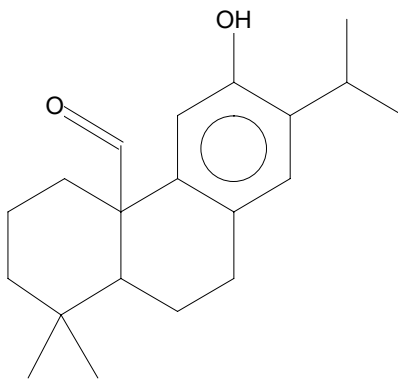
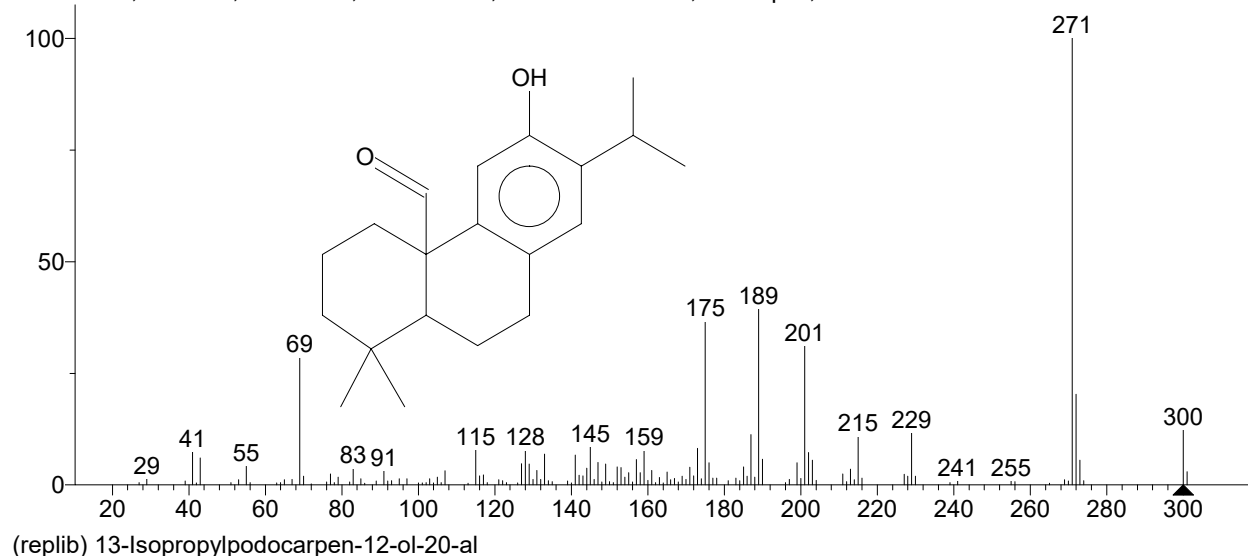
1.12-Hydroxyabieta-9(11),8(14),12-trien-20-al #

Experimental RI median±deviation (#data)

Semi-standard non-polar:2569±N/A (1)

Standard non-polar: 2502±0 (2)

Hit 4 : 13-Isopropylpodocarpin-12-ol-20-al
 C₂₀H₂₈O₂; MF: 737; RMF: 788; Prob 3.53%; CAS: 24035-37-8; Lib: replib; ID: 37061.



Name: 13-Isopropylpodocarpin-12-ol-20-al
 Formula: C₂₀H₂₈O₂
 MW: 300 Exact Mass: 300.208931 CAS#: 24035-37-8 NIST#: 414191 ID#: 37061 DB: replib
 Other DBs: None
 Contributor: NIST Mass Spectrometry Data Center
 InChIKey: YPWYNONCSGZEQQ-UHFFFAOYSA-N Non-stereo
 10 largest peaks:

271 999 | 189 392 | 175 365 | 201 310 | 69 284 | 272 202 | 300 122 | 229 116 | 187 112 | 215 108 |
 137 m/z Values and Intensities:

27	5	29	13	39	8	41	73	42	4	43	60	51	5	53	11	55	41	56	5
63	4	64	5	65	11	67	12	69	284	70	19	72	2	76	6	77	24	78	5
79	17	82	6	83	36	85	13	86	3	89	8	91	31	92	8	93	9	95	13
97	13	100	4	101	4	102	5	103	13	104	4	105	17	106	5	107	31	113	3
115	78	116	20	117	22	118	5	121	11	122	9	123	5	126	4	127	47	128	76
129	46	130	12	131	32	132	12	133	68	134	9	135	7	139	8	140	4	141	66
142	21	143	20	144	37	145	84	146	12	147	50	148	6	149	46	150	7	151	5

152	40		153	38		154	17		155	27		156	6		157	56		158	27		159	76		160	10		161	32	
162	5		163	16		164	4		165	28		166	11		167	14		168	6		169	19		170	12		171	39	
172	20		173	81		174	13		175	365		176	49		177	15		178	15		181	9		183	15		184	9	
185	40		186	19		187	112		188	17		189	392		190	57		196	5		197	12		199	49		200	14	
201	310		202	72		203	55		204	10		211	24		212	7		213	35		214	11		215	108		216	15	
227	23		228	19		229	116		230	19		239	5		241	9		255	9		256	7		265	3		269	11	
270	8		271	999		272	202		273	55		274	9		300	122		301	29										

Synonyms:

1.12-Hydroxyabieta-9(11),8(14),12-trien-20-al #

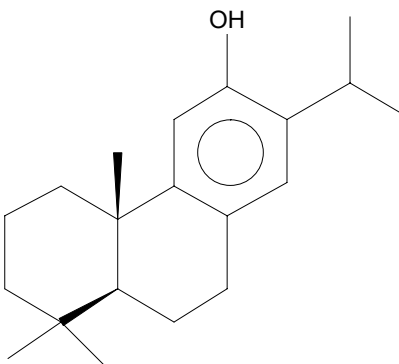
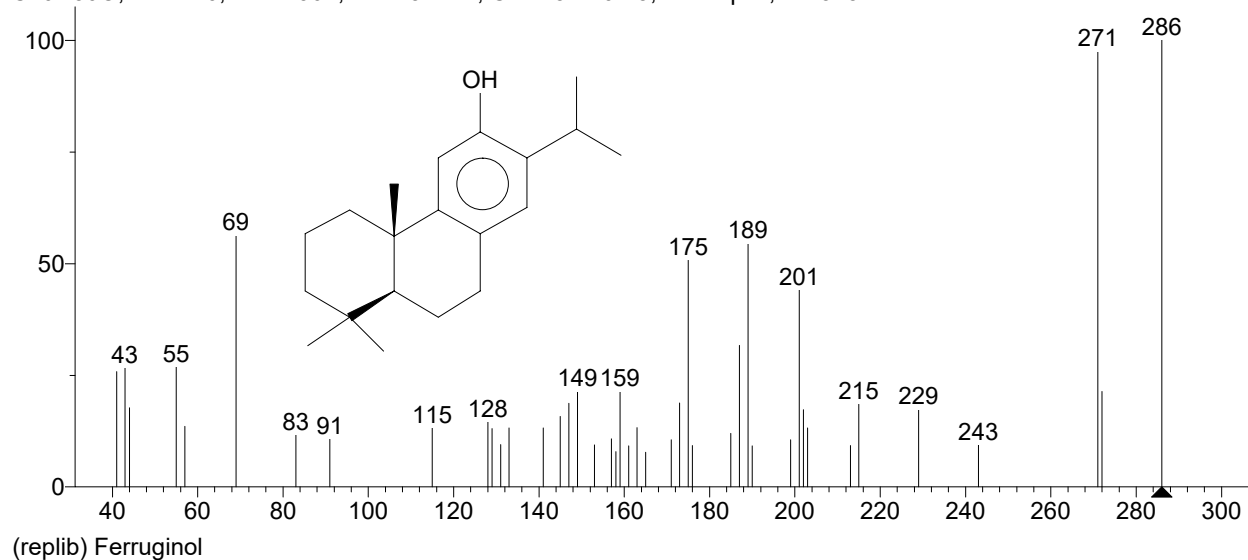
Experimental RI median±deviation (#data)

Semi-standard non-polar:2569±N/A (1)

Standard non-polar: 2502±0 (2)

Hit 5 : Ferruginol

C₂₀H₃₀O; MF: 710; RMF: 904; Prob 57.7%; CAS: 514-62-5; Lib: replib; ID: 37524.



Name: Ferruginol

Formula: C₂₀H₃₀O

MW: 286 Exact Mass: 286.229666 CAS#: 514-62-5 NIST#: 148606 ID#: 37524 DB: replib

Other DBs: None

Contributor: ASES Database, Dalian Institute, P.R. China

InChIKey: QXNWVJOHUAQHLM-AZUAARDMSA-N Non-stereo

10 largest peaks:

286 999 | 271 973 | 69 562 | 189 544 | 175 506 | 201 440 | 187 316 | 55 268 | 43 265 | 41 257 |

43 m/z Values and Intensities:

41 257 | 43 265 | 44 176 | 55 268 | 57 135 | 69 562 | 83 116 | 91 106 | 115 132 | 128 145 |
129 130 | 131 94 | 133 131 | 141 131 | 145 157 | 147 186 | 149 213 | 153 93 | 157 107 | 158 78 |
159 213 | 161 91 | 163 132 | 165 77 | 171 105 | 173 187 | 175 506 | 176 92 | 185 119 | 187 316 |
189 544 | 190 91 | 199 105 | 201 440 | 202 172 | 203 131 | 213 92 | 215 184 | 229 173 | 243 93 |
271 973 | 272 213 | 286 999 |

Synonyms:

1.Abieta-9(11),8(14),12-trien-12-ol #

2.trans-Ferruginol

3.Podocarpa-8,11,13-trien-12-ol, 13-isopropyl-

Experimental RI median \pm deviation (#data)

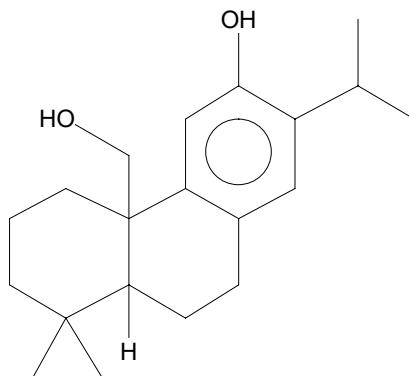
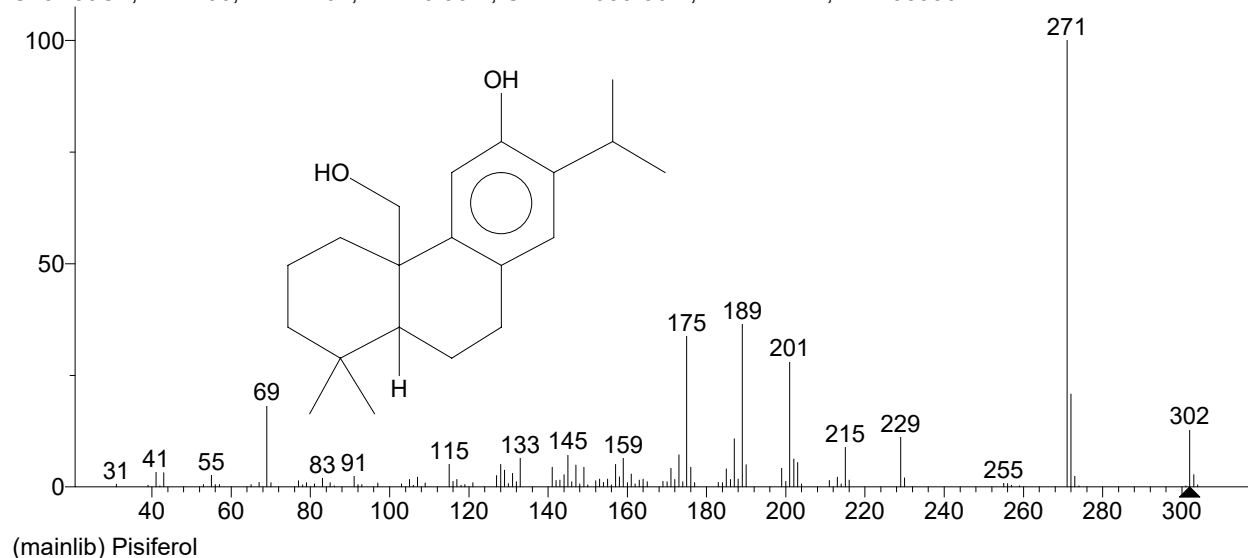
Semi-standard non-polar:2325 \pm 0 (16)

Standard non-polar: 2283 \pm N/A (1)

Polar: 2295 \pm N/A (1)

Hit 6 : Pisiferol

C₂₀H₃₀O₂; MF: 706; RMF: 767; Prob 0.96%; CAS: 24035-36-7; Lib: mainlib; ID: 238950.



Name: Pisiferol

Formula: C₂₀H₃₀O₂

MW: 302 Exact Mass: 302.22458 CAS#: 24035-36-7 NIST#: 414875 ID#: 238950 DB: mainlib

Other DBs: None

Contributor: NIST Mass Spectrometry Data Center

InChIKey: NKGGFTFDYGTUSL-UHFFFAOYSA-N Non-stereo

10 largest peaks:

271	999	189	364	175	337	201	280	272	207	69	181	302	128	229	111	187	107	215	88
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108 m/z Values and Intensities:

31	7	39	3	41	33	42	2	43	31	53	5	55	27	56	5	57	5	65	5
67	10	69	181	70	9	77	13	78	4	79	9	81	6	83	20	85	9	86	2
91	25	92	5	93	5	97	8	103	6	105	16	106	3	107	21	109	8	115	51
116	12	117	16	118	3	119	5	121	9	127	25	128	50	129	37	130	7	131	30
132	11	133	64	141	43	142	14	143	15	144	27	145	72	146	11	147	48	148	6
149	43	150	4	152	13	153	17	154	10	155	17	156	4	157	50	158	22	159	65
160	9	161	28	162	6	163	15	164	17	165	11	169	12	170	11	171	41	172	16

173	71	174	11	175	337	176	43	177	9	183	10	184	9	185	40	186	16	187	107
188	17	189	364	190	49	199	41	200	12	201	280	202	62	203	54	204	6	211	14
213	21	214	6	215	88	216	15	229	111	230	20	255	9	256	7	257	3	259	2
271	999	272	207	273	23	274	2	301	2	302	128	303	27	304	4				

Synonyms:

1.4a(2H)-Phenanthrenemethanol, 1,3,4,9,10,10a-hexahydro-6-hydroxy-1,1-dimethyl-7-(1-methylethyl)-, (4aR,10aS)-

2.4a(2H)-Phenanthrenemethanol, 1,3,4,9,10,10a-hexahydro-6-hydroxy-1,1-dimethyl-7-(1-methylethyl)-, (4aR-trans)-

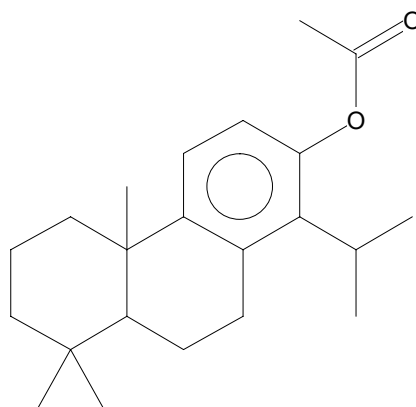
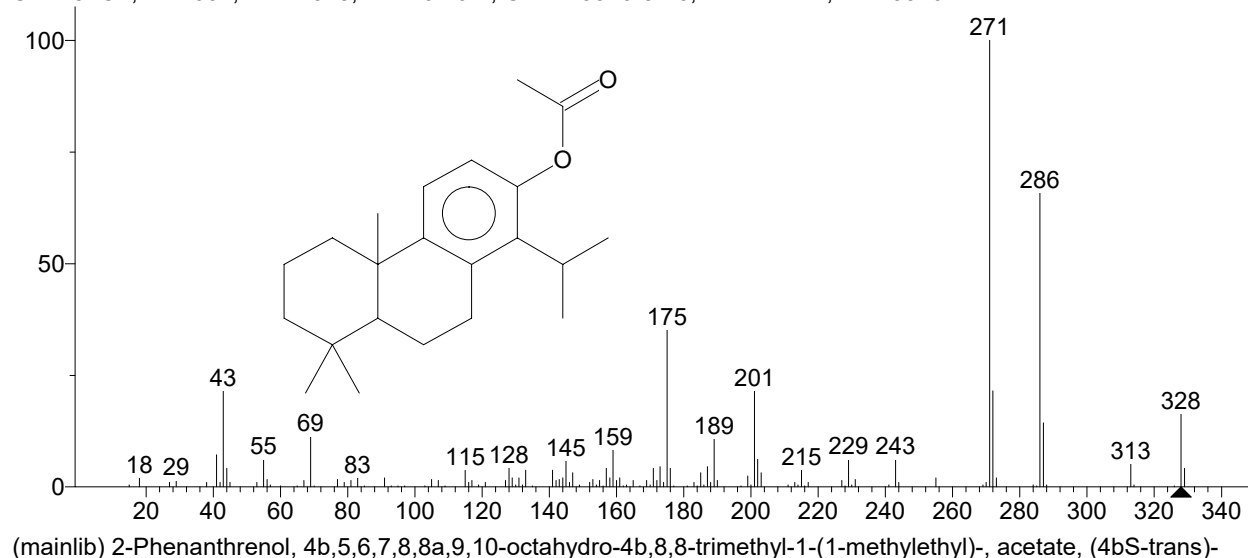
3.Podocarpa-8,11,13-triene-12,17-diol, 13-isopropyl-

4.(+)-Pisiferol

Experimental RI median±deviation (#data)

Semi-standard non-polar:2615±N/A (1)

Hit 7 : 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, acetate, (4bS-trans)-C₂₂H₃₂O₂; MF: 661; RMF: 678; Prob 0.20%; CAS: 15340-82-6; Lib: mainlib; ID: 239104.



Name: 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, acetate, (4bS-trans)-

Formula: C₂₂H₃₂O₂

MW: 328 Exact Mass: 328.24023 CAS#: 15340-82-6 NIST#: 15316 ID#: 239104 DB: mainlib

Other DBs: None

InChIKey: ORVBSFQTFRBNRP-UHFFFAOYSA-N Non-stereo

10 largest peaks:

271 999 | 286 657 | 175 351 | 43 214 | 201 214 | 272 214 | 328 163 | 287 143 | 69 112 | 189 106 |

121 m/z Values and Intensities:

15	4	18	20	27	10	29	14	38	10	41	71	42	10	43	214	44	41	45	10
53	10	55	61	56	16	57	4	60	2	65	2	67	14	69	112	70	2	77	16
79	10	81	14	83	20	85	2	91	20	93	2	95	2	97	2	103	2	105	16
107	14	109	2	115	37	116	10	117	14	119	4	121	10	127	14	128	41	129	20
130	4	131	20	132	4	133	37	135	2	141	37	142	14	143	16	144	20	145	57
146	10	147	31	149	4	152	10	153	16	154	4	155	14	156	2	157	41	158	20
159	82	160	14	161	20	162	2	163	4	165	14	167	2	169	14	170	4	171	41
172	14	173	45	174	10	175	351	176	41	177	2	181	2	183	10	184	2	185	31

186	4	187	45	188	10	189	106	190	14	197	2	199	24	200	4	201	214	202	61
203	31	211	4	213	10	214	4	215	37	216	2	217	10	227	14	228	2	229	61
230	4	231	16	241	4	243	61	244	10	255	20	269	4	270	10	271	999	272	214
273	20	284	4	285	2	286	657	287	143	288	4	313	51	314	4	326	2	328	163
329	41																		

Synonyms:

1.Podocarpa-8,11,13-trien-13-ol, 14-isopropyl-, acetate

2.Totaryl acetate

3.14-Isopropylpodocarpa-8,11,13-trien-13-yl acetate #

4.Totarol acetate

5.2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, 2-acetate, (4bS,8aS)-

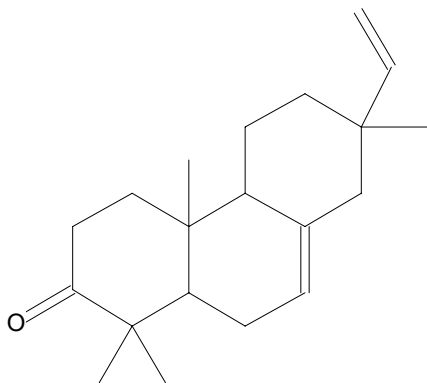
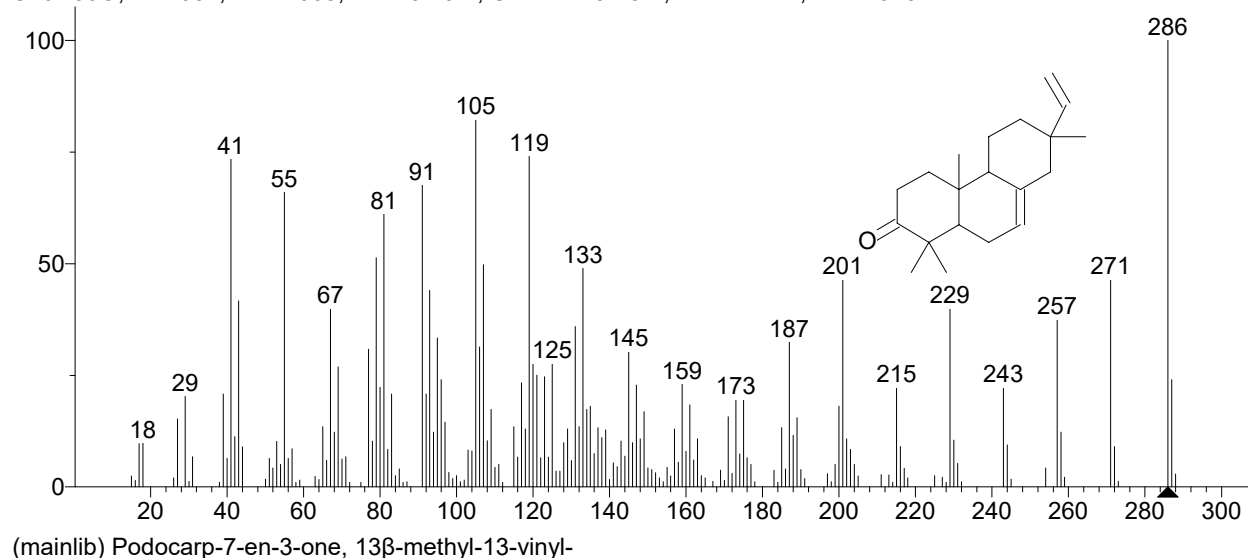
6.2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, acetate, (4bS,8aS)-

Experimental RI median±deviation (#data)

Semi-standard non-polar:2417±0 (2)

Standard non-polar: 2437±0 (2)

Hit 8 : Podocarp-7-en-3-one, 13 β -methyl-13-vinyl-
C₂₀H₃₀O; MF: 661; RMF: 668; Prob 0.20%; CAS: 7715-48-2; Lib: mainlib; ID: 243782.



Name: Podocarp-7-en-3-one, 13 β -methyl-13-vinyl-

Formula: C₂₀H₃₀O

MW: 286 Exact Mass: 286.229666 CAS#: 7715-48-2 NIST#: 42588 ID#: 243782 DB: mainlib

Other DBs: None

Contributor: R RYHAGE MS-LAB KAROLINSKA INSTITUTET STOCKHOLM SWEDEN

InChIKey: YAXFLCDQLAZOPS-UHFFFAOYSA-N Non-stereo

10 largest peaks:

286 999	105 821	119 740	41 732	91 675	55 659	81 610	79 512	107 496	133 488
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177 m/z Values and Intensities:

15 24	16 14	17 96	18 98	26 20	27 151	29 202	30 12	31 67	38 10
39 207	40 63	41 732	42 112	43 415	44 89	50 17	51 63	52 42	53 101
54 50	55 659	56 63	57 85	58 10	59 15	63 23	64 16	65 134	66 59
67 398	68 122	69 268	70 62	71 67	72 10	75 10	77 307	78 102	79 512
80 222	81 610	82 83	83 207	84 25	85 40	86 10	87 11	91 675	92 207
93 439	94 122	95 332	96 239	97 144	98 32	99 18	100 25	101 11	102 15
103 82	104 80	105 821	106 312	107 496	108 103	109 173	110 43	111 50	112 10

115 134	116 66	117 232	118 129	119 740	120 276	121 249	122 65	123 246	124 66
125 276	126 35	127 35	128 98	129 129	130 58	131 358	132 134	133 488	134 173
135 180	136 74	137 132	138 110	139 127	140 16	141 53	142 45	143 102	144 68
145 302	146 98	147 227	148 107	149 168	150 42	151 38	152 31	153 20	154 11
155 43	156 24	157 129	158 55	159 229	160 79	161 183	162 60	163 107	164 25
165 20	167 12	169 37	170 14	171 156	172 30	173 195	174 73	175 195	176 65
177 50	178 11	183 37	184 10	185 132	186 40	187 324	188 115	189 154	190 38
191 18	197 29	198 11	199 50	200 180	201 463	202 107	203 83	204 50	205 24
211 27	213 26	214 10	215 222	216 90	217 41	218 20	225 25	227 21	228 10
229 398	230 104	231 52	232 11	243 222	244 93	245 17	254 42	257 374	258 122
259 21	271 463	272 90	273 12	286 999	287 239	288 28			

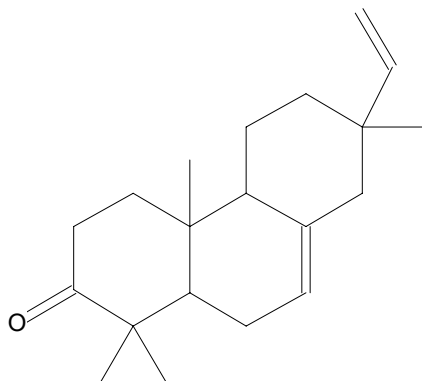
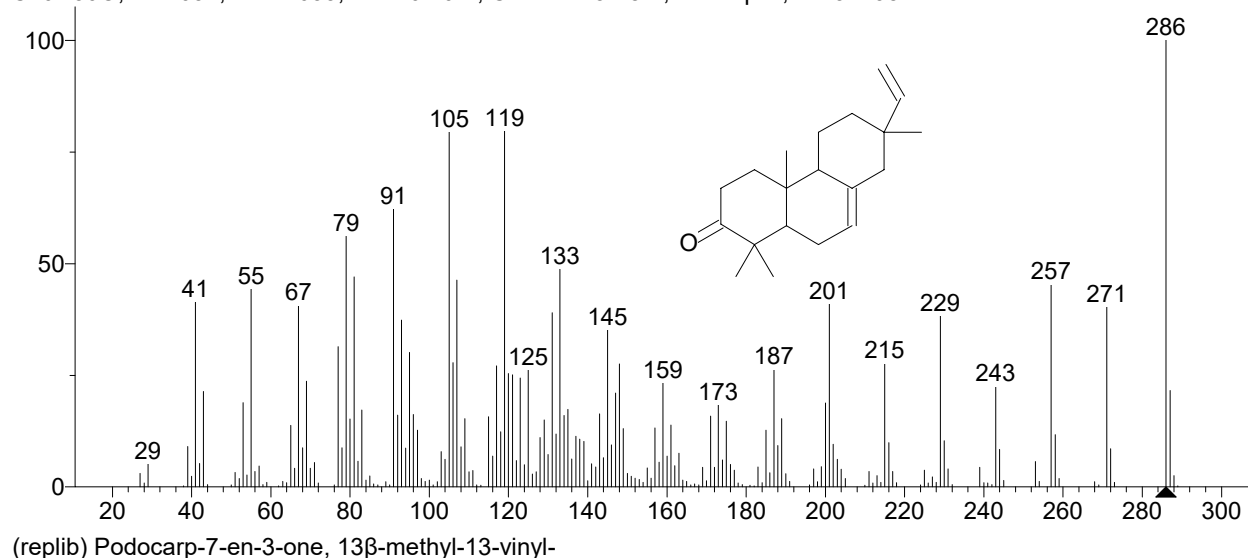
Synonyms:

1.Pimara-7,15-dien-3-one #

Experimental RI median±deviation (#data)

Semi-standard non-polar:2257±22 (3)

Hit 9 : Podocarp-7-en-3-one, 13 β -methyl-13-vinyl-
C₂₀H₃₀O; MF: 651; RMF: 653; Prob 0.20%; CAS: 7715-48-2; Lib: replib; ID: 37498.



Name: Podocarp-7-en-3-one, 13 β -methyl-13-vinyl-

Formula: C₂₀H₃₀O

MW: 286 Exact Mass: 286.229666 CAS#: 7715-48-2 NIST#: 466212 ID#: 37498 DB: replib

Other DBs: None

Contributor: NIST Mass Spectrometry Data Center

InChIKey: YAXFLCDQLAZOPS-UHFFFAOYSA-N Non-stereo

10 largest peaks:

286 999	119 796	105 793	91 621	79 560	133 486	81 469	107 462	257 452	55 442
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193 m/z Values and Intensities:

27 30	28 8	29 51	38 2	39 90	40 23	41 413	42 52	43 213	44 5
50 4	51 32	52 18	53 188	54 26	55 442	56 34	57 46	58 5	59 10
62 2	63 12	64 9	65 137	66 41	67 405	68 87	69 236	70 41	71 54
72 8	76 4	77 313	78 87	79 560	80 151	81 469	82 57	83 171	84 15
85 24	86 6	87 4	89 11	90 4	91 621	92 160	93 372	94 86	95 300
96 161	97 126	98 18	99 12	100 15	101 4	102 11	103 78	104 61	105 793
106 277	107 462	108 89	109 152	110 33	111 36	112 4	113 3	115 156	116 68

117 270	118 123	119 796	120 253	121 250	122 58	123 243	124 49	125 261	126 28
127 33	128 110	129 149	130 72	131 389	132 118	133 486	134 159	135 173	136 62
137 113	138 106	139 101	140 13	141 51	142 44	143 163	144 65	145 351	146 93
147 209	148 274	149 130	150 30	151 23	152 19	153 16	154 10	155 42	156 19
157 131	158 55	159 232	160 68	161 138	162 47	163 75	164 15	165 12	166 4
167 6	168 4	169 43	170 13	171 158	172 43	173 183	174 60	175 146	176 50
177 37	178 8	179 5	181 3	182 2	183 44	184 9	185 126	186 31	187 262
188 92	189 152	190 29	191 12	196 4	197 40	198 11	199 45	200 187	201 409
202 95	203 61	204 39	205 18	210 3	211 34	212 8	213 25	214 10	215 276
216 98	217 34	218 9	224 4	225 37	226 8	227 22	228 10	229 382	230 103
231 40	232 5	239 43	240 9	241 8	242 5	243 224	244 83	245 14	253 56
254 12	257 452	258 116	259 18	268 11	269 4	271 402	272 85	273 10	286 999
287 215	288 25	289 2							

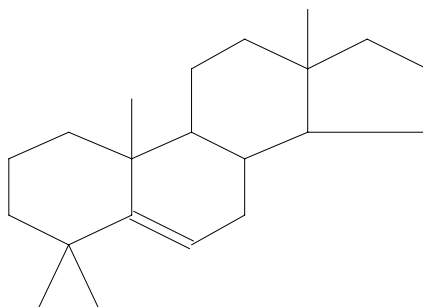
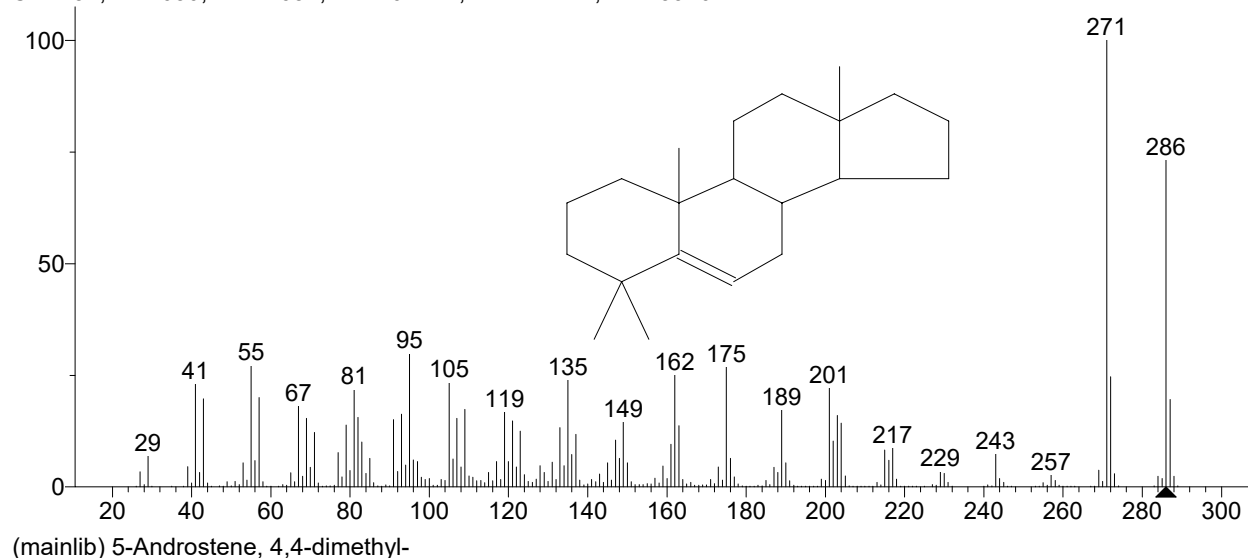
Synonyms:

1.Pimara-7,15-dien-3-one #

Experimental RI median±deviation (#data)

Semi-standard non-polar:2257±22 (3)

Hit 10 : 5-Androstene, 4,4-dimethyl-
 C₂₁H₃₄; MF: 650; RMF: 651; Prob 0.14%; Lib: mainlib; ID: 239102.



Name: 5-Androstene, 4,4-dimethyl-

Formula: C₂₁H₃₄

MW: 286 Exact Mass: 286.26605 NIST#: 194154 ID#: 239102 DB: mainlib

Contributor: Chemical Concepts

InChIKey: RAYCKELWUDCADQ-UHFFFAOYSA-N Non-stereo

10 largest peaks:

271 999 | 286 730 | 95 298 | 55 271 | 175 268 | 162 250 | 272 246 | 135 239 | 105 233 | 41 229 |

231 m/z Values and Intensities:

26	1	27	33	28	5	29	68	30	1	35	1	38	1	39	45	40	8	41	229
42	32	43	196	44	8	45	1	47	2	48	1	49	11	50	2	51	12	52	5
53	53	54	15	55	271	56	58	57	199	58	11	59	1	60	Tr	62	Tr	63	5
64	3	65	31	66	11	67	180	68	23	69	153	70	43	71	121	72	8	73	1
74	2	75	2	76	3	77	76	78	22	79	138	80	36	81	217	82	155	83	100
84	30	85	63	86	9	87	2	88	1	89	4	90	2	91	150	92	34	93	162
94	48	95	298	96	60	97	56	98	21	99	16	100	18	101	3	102	3	103	16
104	14	105	233	106	62	107	153	108	44	109	173	110	24	111	21	112	13	113	14

114	9	115	32	116	13	117	56	118	16	119	167	120	56	121	147	122	44	123	124
124	27	125	12	126	10	127	17	128	47	129	32	130	12	131	55	132	16	133	132
134	47	135	239	136	72	137	117	138	15	139	4	140	6	141	16	142	11	143	28
144	10	145	53	146	15	147	104	148	63	149	144	150	53	151	11	152	5	153	5
154	5	155	7	156	6	157	19	158	8	159	46	160	18	161	95	162	250	163	136
164	16	165	6	166	10	167	3	168	3	169	4	170	4	171	16	172	7	173	44
174	15	175	268	176	63	177	22	178	6	179	2	180	1	181	1	182	1	183	3
184	2	185	14	186	5	187	43	188	32	189	171	190	53	191	13	192	3	193	Tr
194	Tr	195	1	196	Tr	197	1	198	1	199	17	200	14	201	221	202	102	203	159
204	142	205	24	206	2	207	Tr	208	Tr	209	Tr	210	Tr	211	Tr	212	Tr	213	10
214	4	215	82	216	59	217	86	218	17	219	1	220	Tr	221	Tr	222	Tr	223	Tr
225	Tr	227	5	228	3	229	34	230	30	231	10	232	1	240	Tr	241	4	242	2
243	73	244	18	245	10	246	1	247	Tr	253	Tr	254	Tr	255	9	256	3	257	27
258	14	259	3	260	Tr	261	Tr	262	Tr	263	Tr	267	1	268	1	269	37	270	12
271	999	272	246	273	29	274	2	283	2	284	23	285	18	286	730	287	195	288	23
289	2																		

Synonyms:

1,4,4,10,13-Tetramethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene

2,4,4-Dimethylandrosta-5-ene #

Experimental RI median±deviation (#data)

Semi-standard non-polar:2219±N/A (1)