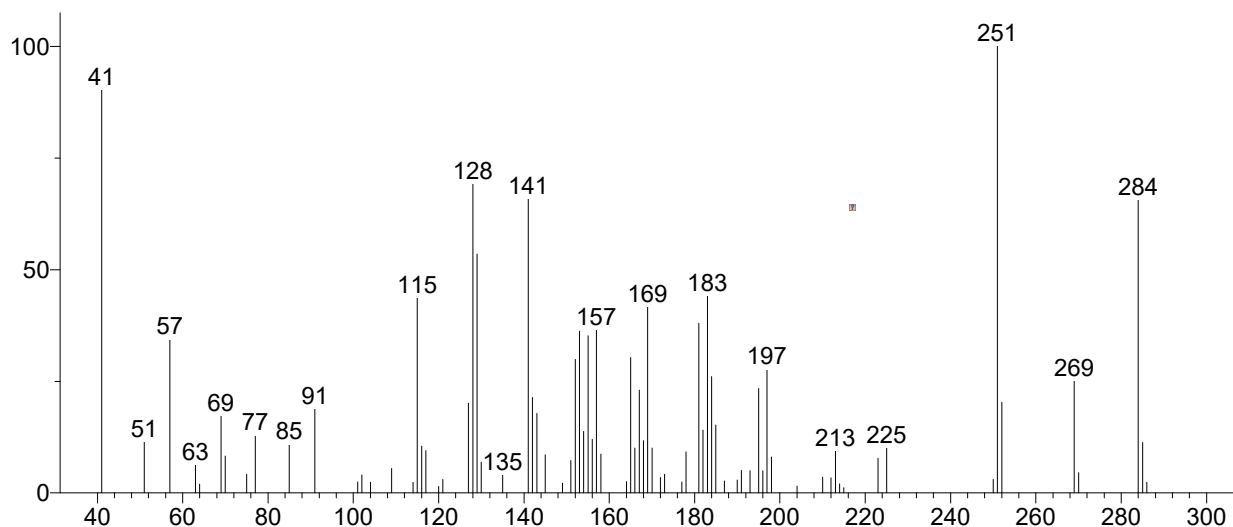


Unknown; InLib=-1302



(Text File) Component at scan 2581 (15.002 min) [Model = +284u] in X:\ABBY GCMS\20211015\A_211015_020.D\DATA.MS

Name: Component at scan 2581 (15.002 min) [Model = +284u] in X:\ABBY GCMS\20211015\A_211015_020.D\DATA.MS

MW: N/A ID#: 1016 DB: Text File

10 largest peaks:

251 999	41 901	128 690	141 657	284 654	129 533	183 440	115 435	169 415	181 379
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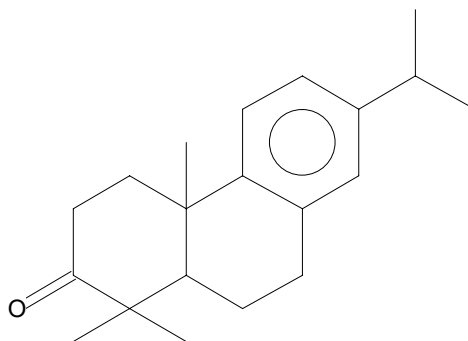
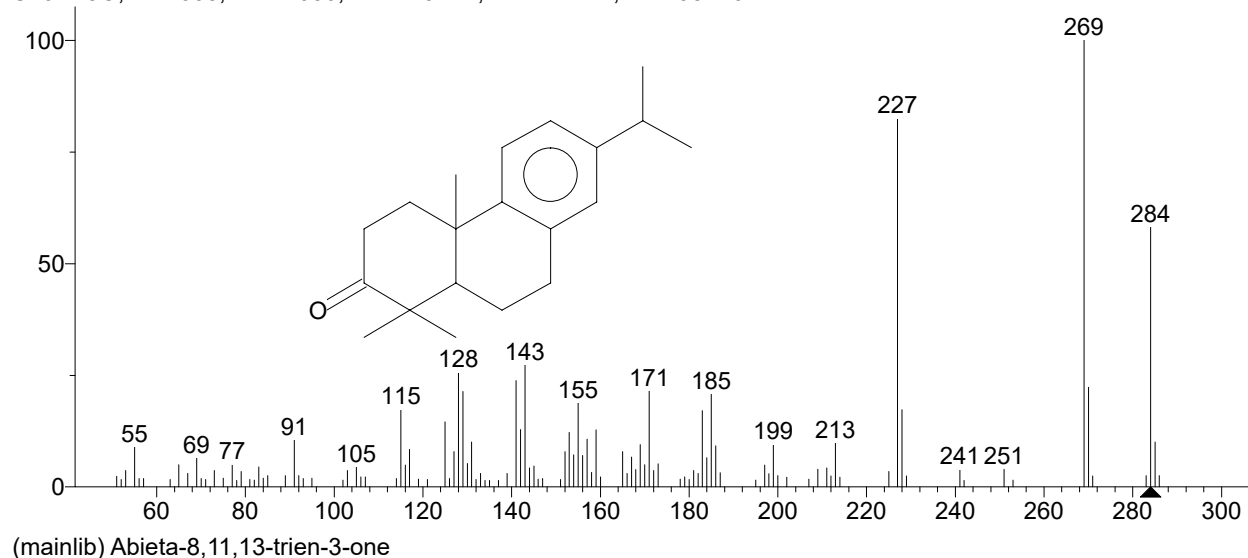
79 m/z Values and Intensities:

41 901	51 114	57 342	63 62	64 19	69 171	70 82	75 41	77 128	85 108
91 188	101 24	102 40	104 23	109 54	114 23	115 435	116 104	117 94	120 14
121 30	127 200	128 690	129 533	130 68	135 39	141 657	142 213	143 177	145 85
149 21	151 72	152 298	153 361	154 137	155 351	156 119	157 363	158 86	164 25
165 302	166 100	167 229	168 116	169 415	170 100	172 34	173 41	177 24	178 91
181 379	182 140	183 440	184 259	185 151	187 26	190 28	191 50	193 49	195 233
196 49	197 276	198 80	204 15	210 35	212 33	213 93	214 20	215 11	223 77
225 100	250 30	251 999	252 202	269 249	270 45	284 654	285 112	286 23	

Synonyms:

no synonyms.

Hit 1 : Abieta-8,11,13-trien-3-one
 C₂₀H₂₈O; MF: 608; RMF: 630; Prob 13.4%; Lib: mainlib; ID: 238140.



Name: Abieta-8,11,13-trien-3-one

Formula: C₂₀H₂₈O

MW: 284 Exact Mass: 284.214016 NIST#: 386463 ID#: 238140 DB: mainlib

Contributor: Robert E. Cox et al. Biochemical Systematics and Ecology 35 (2007) 342-362

InChIKey: ANVLVIISBTWDRN-UHFFFAOYSA-N Non-stereo

10 largest peaks:

269 999 | 227 823 | 284 581 | 143 272 | 128 255 | 141 237 | 270 222 | 171 214 | 129 213 | 185 208 |

114 m/z Values and Intensities:

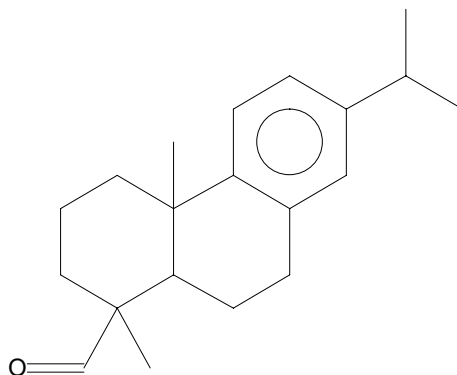
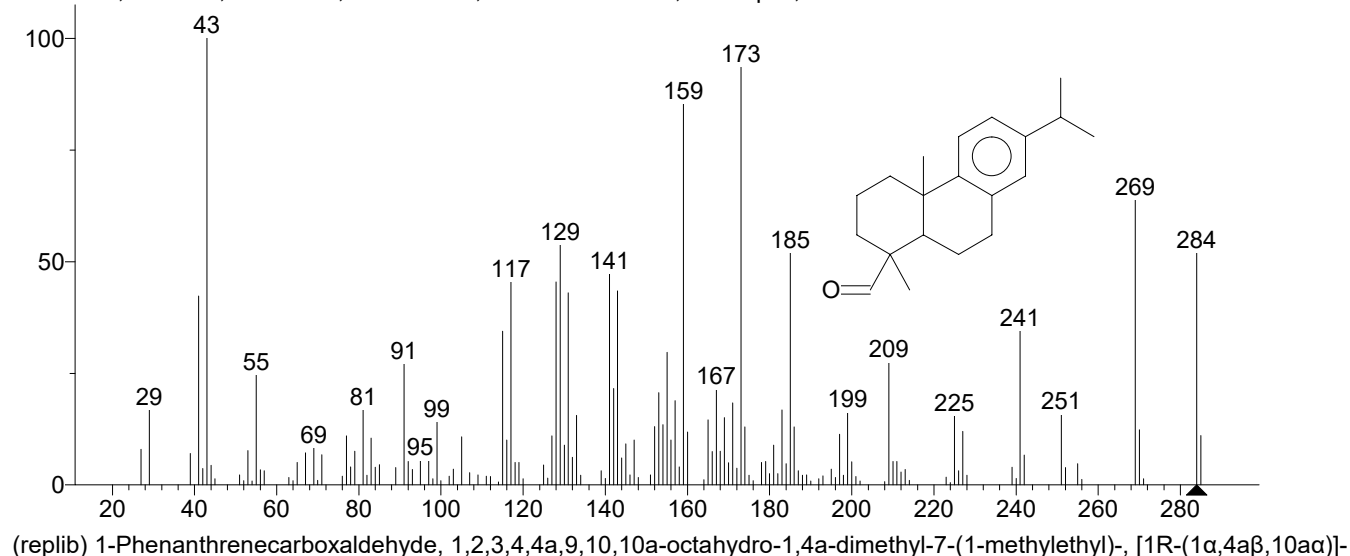
51	23	52	16	53	36	55	89	56	18	57	18	63	16	65	49	67	30	69	65
70	18	71	16	73	36	75	19	77	50	78	14	79	34	81	16	82	15	83	44
84	19	85	25	89	25	91	105	92	25	93	18	95	19	102	15	103	36	105	44
106	22	107	22	114	18	115	173	116	48	117	83	119	17	121	16	125	145	126	18
127	78	128	255	129	213	130	52	131	100	132	16	133	30	134	14	135	14	137	14
139	30	141	237	142	128	143	272	144	42	145	46	146	17	147	18	151	16	152	78
153	121	154	71	155	188	156	70	157	106	158	32	159	127	160	22	165	78	166	30
167	66	168	38	169	94	170	49	171	214	172	36	173	51	178	17	179	22	180	16

181	36		182	30		183	170		184	65		185	208		186	91		187	31		195	15		197	48		198	29	
199	94		200	25		202	21		207	17		209	39		211	42		212	24		213	98		214	21		225	34	
227	823		228	172		229	24		241	38		242	14		251	39		253	15		269	999		270	222		271	24	
283	25		284	581		285	100		286	25																			

Synonyms:

no synonyms.

Hit 2 : 1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1 α ,4 α ,10 α)]-



Name: 1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1 α ,4 α ,10 α)]-

Formula: C₂₀H₂₈O

MW: 284 Exact Mass: 284.214016 CAS#: 13601-88-2 NIST#: 384007 ID#: 3937 DB: replib

Other DBs: None

Contributor: NIST Mass Spectrometry Data Center, 2010

InChIKey: YCLCHPWGSDZKL-UHFFFAOYSA-N Non-stereo

10 largest peaks:

43 999 | 173 933 | 159 851 | 269 637 | 129 536 | 185 518 | 284 518 | 141 471 | 117 454 | 128 453 |

146 m/z Values and Intensities:

27	79	29	167	39	70	41	422	42	36	43	999	44	43	45	13	51	22	52	9
53	76	54	8	55	245	56	33	57	31	63	16	64	9	65	50	67	71	69	82
70	10	71	67	76	19	77	109	78	40	79	75	81	167	82	21	83	104	84	39
85	45	89	38	91	270	92	52	93	34	95	54	97	53	98	13	99	140	100	9
102	19	103	35	105	107	107	27	109	22	111	19	112	18	114	6	115	343	116	100
117	454	118	50	119	50	120	13	125	44	126	15	127	109	128	453	129	536	130	88

131	429	132	61	133	155	134	21	139	31	140	14	141	471	142	215	143	433	144	60
145	91	146	22	147	100	148	16	151	22	152	130	153	206	154	134	155	296	156	100
157	188	158	40	159	851	160	118	164	11	165	145	166	74	167	213	168	75	169	150
170	49	171	183	172	37	173	933	174	129	175	21	176	9	178	50	179	52	180	25
181	88	182	25	183	167	184	47	185	518	186	129	187	31	188	21	189	22	190	8
192	13	193	20	195	35	196	16	197	113	198	21	199	161	200	51	201	18	202	8
208	7	209	273	210	52	211	52	212	28	213	34	214	10	223	17	224	5	225	154
226	31	227	119	228	21	239	39	240	14	241	344	242	66	251	157	252	38	255	47
256	12	269	637	270	123	271	13	284	518	285	110								

Synonyms:

- 1.(1R,4aS,10aR)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-carbaldehyde
- 2.Podocarpa-8,11,13-trien-15-al, 13-isopropyl-
- 3.Dehydroabietal
- 4.Dehydroabietic aldehyde
- 5.Dehydroabietinal
- 6.Abietaldehyde, dehydro-
- 7.Abietal-8,11,13-trien-18-al #

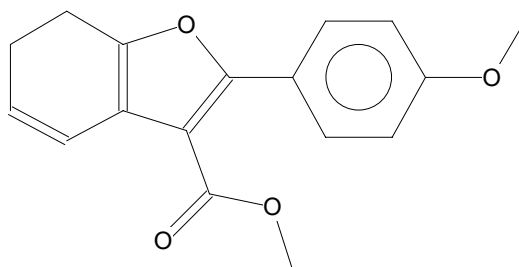
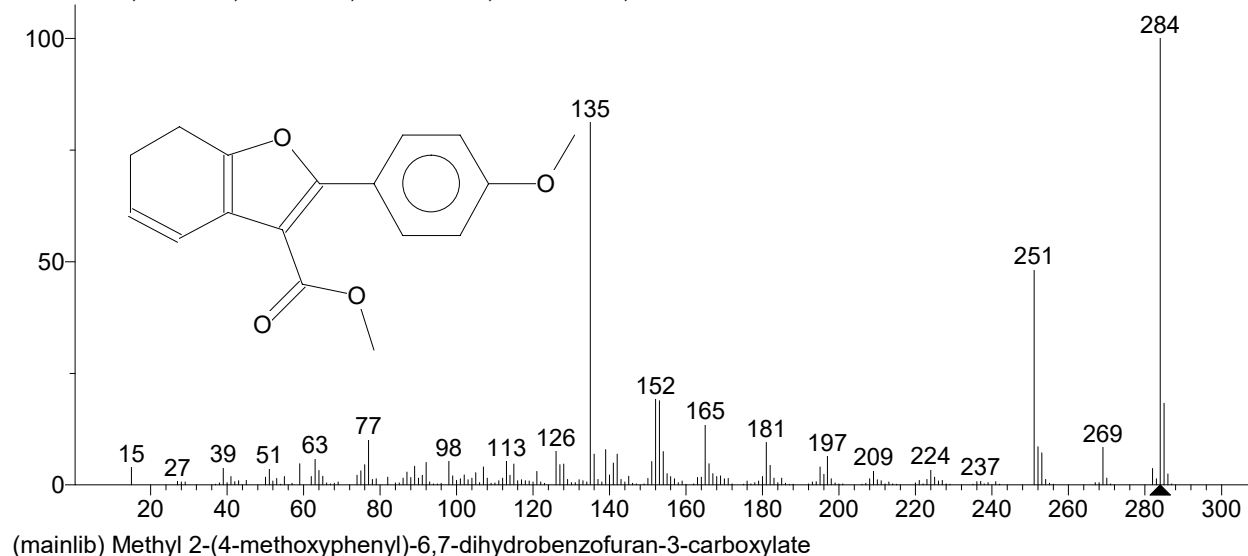
Experimental RI median±deviation (#data)

Semi-standard non-polar:2263±2 (8)

Standard non-polar: 2255±13 (7)

Polar: 2979±3 (2)

Hit 3 : Methyl 2-(4-methoxyphenyl)-6,7-dihydrobenzofuran-3-carboxylate
 C₁₇H₁₆O₄; MF: 605; RMF: 611; Prob 11.9%; Lib: mainlib; ID: 243098.



Name: Methyl 2-(4-methoxyphenyl)-6,7-dihydrobenzofuran-3-carboxylate

Formula: C₁₇H₁₆O₄

MW: 284 Exact Mass: 284.104858 NIST#: 458204 ID#: 243098 DB: mainlib

Contributor: NIH Small Molecule Repository/NIST Mass Spectrometry Data Center, 2012

InChIKey: DRZLMVKTTVZMGY-UHFFFAOYSA-N Non-stereo

10 largest peaks:

284 999 | 135 811 | 251 481 | 152 192 | 153 188 | 285 182 | 165 135 | 77 101 | 181 95 | 252 85 |

187 m/z Values and Intensities:

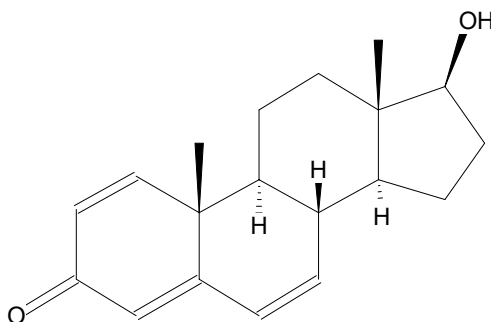
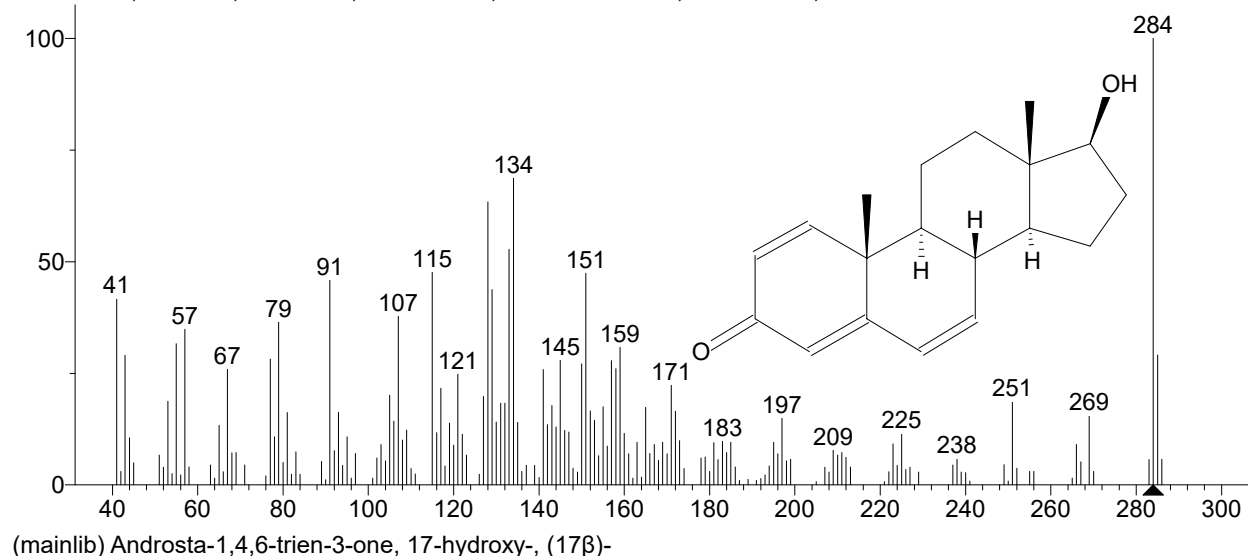
15	39	27	9	28	6	29	6	37	1	38	4	39	38	40	5	41	18	42	7
43	9	45	10	50	17	51	36	52	8	53	14	54	1	55	18	57	3	59	47
62	18	63	58	64	32	65	19	66	4	67	2	68	3	69	6	74	21	75	31
76	45	77	101	78	12	79	13	82	17	84	4	85	4	86	15	87	28	88	16
89	41	90	15	91	21	92	50	93	6	94	2	95	2	96	3	98	53	99	20
100	10	101	13	102	22	103	11	104	15	105	27	106	5	107	40	108	15	109	3
110	4	111	9	112	15	113	53	114	21	115	46	116	9	117	11	118	9	119	8
120	6	121	30	122	6	123	3	126	75	127	45	128	46	129	12	130	5	131	5

132	11		133	9		134	6		135	811		136	68		137	12		138	6		139	78		140	22		141	48	
142	68		143	12		144	6		145	19		146	3		147	2		149	2		150	14		151	52		152	192	
153	188		154	74		155	25		156	18		157	13		158	5		159	8		160	1		162	2		163	16	
164	17		165	135		166	47		167	25		168	18		169	20		170	13		171	14		172	2		175	1	
176	8		177	2		178	5		179	8		180	18		181	95		182	43		183	15		184	5		185	15	
186	3		187	1		188	1		192	2		193	6		194	7		195	40		196	23		197	64		198	13	
199	4		200	2		201	2		206	1		207	3		208	13		209	32		210	11		211	9		212	2	
213	6		214	2		215	1		220	4		221	10		222	2		223	12		224	34		225	17		226	8	
227	10		228	2		229	1		235	1		236	7		237	10		238	2		239	5		241	7		242	1	
251	481		252	85		253	71		254	12		255	3		256	1		267	5		268	5		269	84		270	15	
271	2		282	36		283	13		284	999		285	182		286	24		287	2										

Synonyms:

no synonyms.

Hit 4 : Androsta-1,4,6-trien-3-one, 17-hydroxy-, (17 β)-
C₁₉H₂₄O₂; MF: 603; RMF: 609; Prob 10.9%; CAS: 4075-12-1; Lib: mainlib; ID: 243096.



Name: Androsta-1,4,6-trien-3-one, 17-hydroxy-, (17 β)-

Formula: C₁₉H₂₄O₂

MW: 284 Exact Mass: 284.17763 CAS#: 4075-12-1 NIST#: 126884 ID#: 243096 DB: mainlib

Other DBs: None

Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892

InChIKey: WGFQJPRCLLMHRT-DYKIIIFRCSA-N Non-stereo

10 largest peaks:

284 999	134 686	128 632	133 526	115 476	151 474	91 458	129 436	41 416	107 377
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163 m/z Values and Intensities:

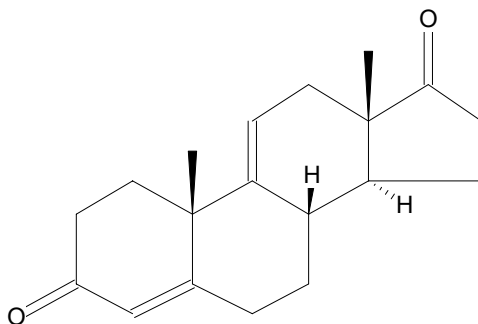
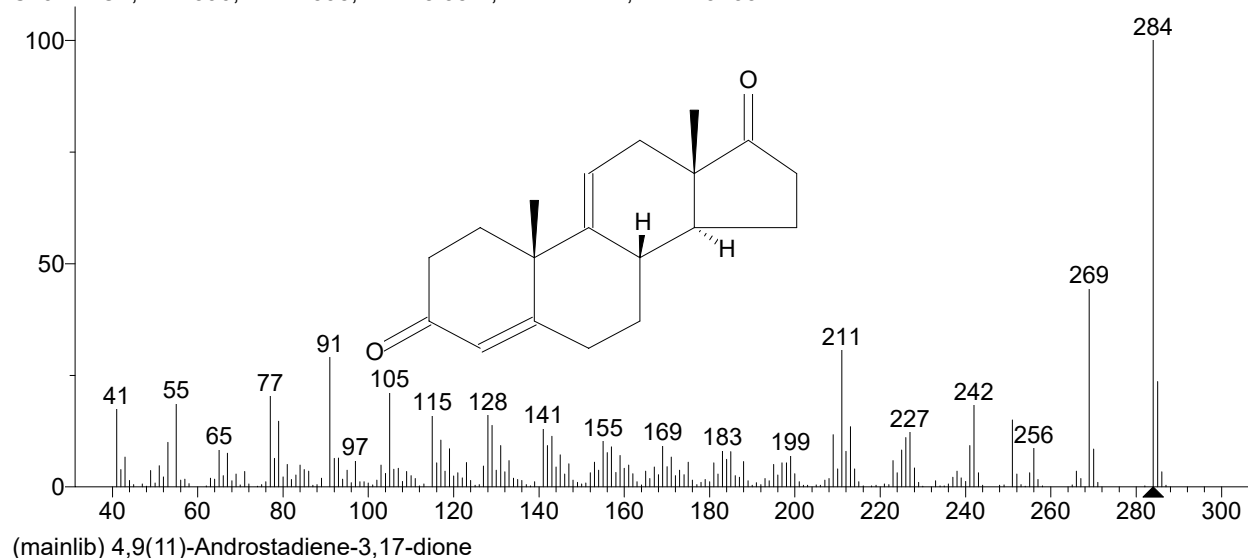
41 416	42 30	43 289	44 105	45 49	51 66	52 39	53 186	54 25	55 315
56 22	57 348	58 40	63 44	64 15	65 133	66 29	67 259	68 71	69 72
71 44	76 20	77 281	78 107	79 364	80 50	81 161	82 23	83 73	84 23
89 52	90 11	91 458	92 76	93 162	94 43	95 107	96 15	97 70	101 15
102 60	103 90	104 53	105 200	106 142	107 377	108 100	109 122	110 36	111 24
115 476	116 116	117 216	118 42	119 138	120 88	121 248	122 113	123 66	126 23
127 197	128 632	129 436	130 140	131 182	132 182	133 526	134 686	135 139	136 30

137	43	139	43	140	16	141	257	142	134	143	177	144	129	145	279	146	121	147	118
148	37	149	28	150	270	151	474	152	165	153	144	154	65	155	174	156	86	157	277
158	259	159	307	160	115	161	69	162	15	163	95	164	17	165	173	166	70	167	90
168	55	169	95	170	69	171	223	172	164	173	98	174	36	178	60	179	62	180	30
181	94	182	56	183	98	184	72	185	95	186	40	187	10	189	12	191	10	192	14
193	22	194	42	195	95	196	69	197	150	198	53	199	57	205	7	207	39	208	28
209	77	210	66	211	72	212	61	213	40	221	7	222	29	223	91	224	43	225	115
226	34	227	39	229	28	237	44	238	58	239	28	240	27	241	8	249	45	250	8
251	186	252	37	255	30	256	30	265	15	266	90	267	51	269	155	270	30	283	56
284	999	285	290	286	57														

Synonyms:

- 1.Androsta-1,4,6-trien-3-one, 17 β -hydroxy-
- 2.1,4,6-Androstatrien-17 β -ol-3-one
- 3.1,4,6-Androstatrien-3-one-17 β -ol
- 4.17-Hydroxyandrosta-1,4,6-trien-3-one-, (17 β)-
- 5.(17 β)-17-Hydroxyandrosta-1,4,6-trien-3-one

Hit 5 : 4,9(11)-Androstadiene-3,17-dione
C₁₉H₂₄O₂; MF: 596; RMF: 598; Prob 8.38%; Lib: mainlib; ID: 243233.



Name: 4,9(11)-Androstadiene-3,17-dione

Formula: C₁₉H₂₄O₂

MW: 284 Exact Mass: 284.17763 NIST#: 126893 ID#: 243233 DB: mainlib

Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892

InChIKey: HJTUINCBGMVXOB-LNMJFAINSA-N Non-stereo

10 largest peaks:

284 999	269 443	211 306	91 289	285 235	105 211	77 203	55 186	242 183	41 174
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211 m/z Values and Intensities:

41 174	42 38	43 66	44 14	45 5	47 6	48 1	49 36	50 8	51 47
52 22	53 99	55 186	56 15	57 17	58 7	62 2	63 19	64 17	65 83
66 25	67 75	68 13	69 28	70 4	71 34	72 6	74 1	75 5	76 11
77 203	78 63	79 146	80 22	81 50	82 16	83 26	84 48	85 38	86 35
87 3	88 5	89 19	91 289	92 63	93 64	94 17	95 37	96 9	97 58
98 11	99 11	100 8	101 4	102 15	103 48	104 30	105 211	106 39	107 41
108 12	109 34	110 25	111 18	112 2	113 6	115 159	116 53	117 104	118 35
119 85	120 24	121 31	122 20	123 54	124 14	125 3	126 5	127 46	128 160

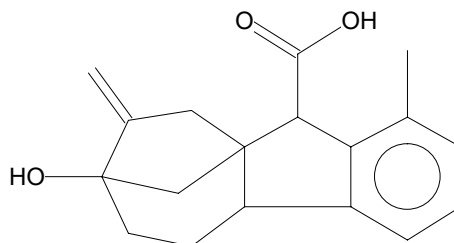
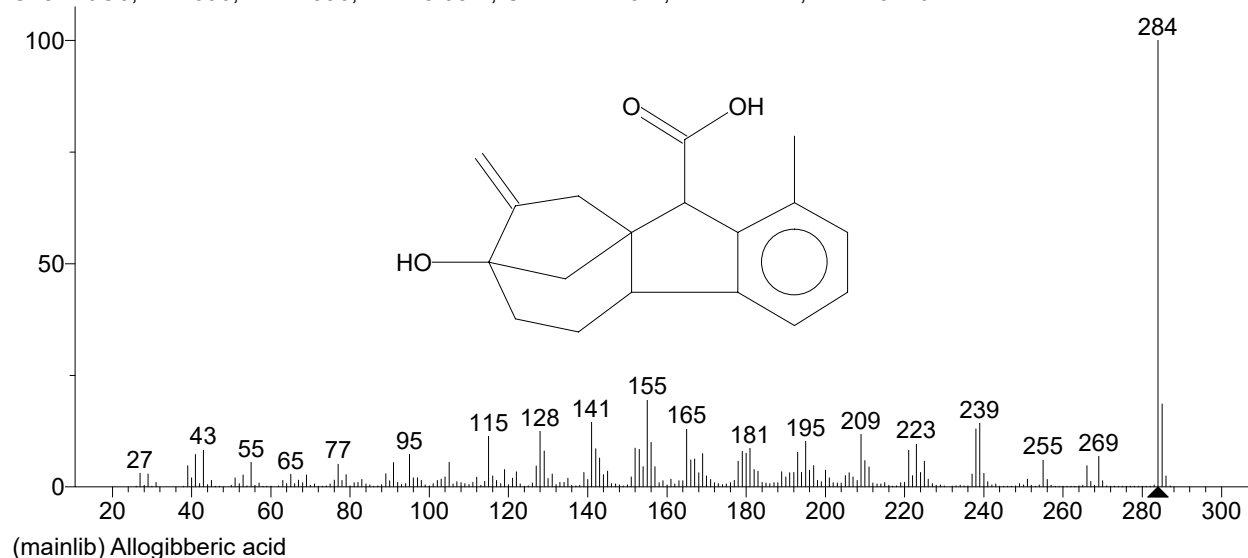
129	137	130	37	131	92	132	33	133	58	134	19	135	16	136	14	137	5	138	2
139	11	141	130	142	92	143	113	144	44	145	71	146	28	147	51	148	15	149	10
150	6	151	8	152	31	153	55	154	37	155	102	156	76	157	89	158	32	159	70
160	41	161	48	162	29	163	11	164	4	165	35	166	18	167	44	168	27	169	92
170	45	171	66	172	25	173	37	174	27	175	55	176	15	177	5	178	10	179	16
180	11	181	53	182	28	183	81	184	61	185	78	186	25	187	21	188	56	189	13
190	3	191	9	192	5	193	18	194	13	195	50	196	26	197	53	198	53	199	70
200	29	201	11	202	3	203	3	205	4	206	3	207	15	208	18	209	116	210	40
211	306	212	79	213	134	214	40	215	11	216	2	218	2	219	3	221	6	222	5
223	58	224	31	225	82	226	110	227	122	228	42	229	10	230	Tr	233	13	234	2
235	2	236	6	237	21	238	35	239	20	240	12	241	92	242	183	243	31	244	3
248	3	249	4	251	149	252	28	253	5	254	1	255	31	256	86	257	16	258	2
265	4	266	35	267	18	269	443	270	84	271	10	282	2	284	999	285	235	286	33
287	3																		

Synonyms:

1.Androst-4,9-dien-3,17-dione

Hit 6 : Allogibberic acid

C₁₈H₂₀O₃; MF: 596; RMF: 596; Prob 8.38%; CAS: 427-79-2; Lib: mainlib; ID: 243120.



Name: Allogibberic acid

Formula: C₁₈H₂₀O₃

MW: 284 Exact Mass: 284.141245 CAS#: 427-79-2 NIST#: 151230 ID#: 243120 DB: mainlib

Other DBs: None

Contributor: Chemical Concepts

InChIKey: IFYWTLQMNWNCFH-UHFFFAOYSA-N Non-stereo

10 largest peaks:

284 999 | 155 195 | 285 185 | 141 144 | 239 143 | 165 130 | 238 129 | 128 124 | 209 118 | 115 114 |

252 m/z Values and Intensities:

26	1	27	31	28	3	29	28	30	1	31	10	38	1	39	47	40	20	41	72
42	7	43	83	44	5	45	14	46	Tr	47	1	50	3	51	20	52	7	53	26
54	2	55	55	56	3	57	8	58	1	59	Tr	60	1	62	2	63	14	64	7
65	28	66	7	67	15	68	9	69	26	70	3	71	6	72	1	73	Tr	74	2
75	6	76	15	77	52	78	14	79	27	80	2	81	9	82	10	83	16	84	6
85	4	86	1	87	2	88	5	89	29	90	13	91	54	92	10	93	5	94	7
95	73	96	20	97	20	98	14	99	4	100	2	101	7	102	14	103	17	104	22

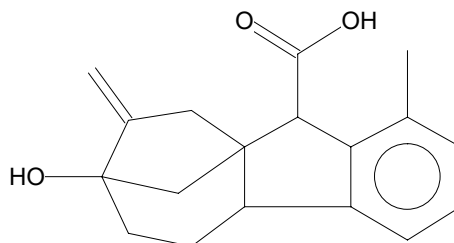
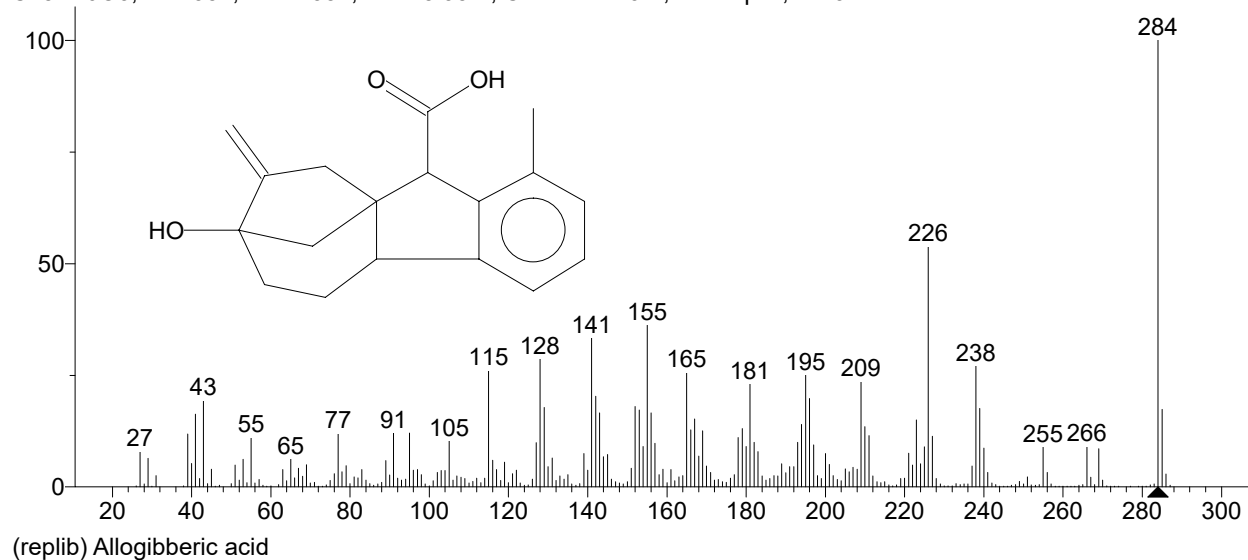
105	55	106	6	107	11	108	9	109	7	110	5	111	10	112	21	113	3	114	12
115	114	116	24	117	14	118	7	119	38	120	5	121	19	122	33	123	6	124	1
125	2	126	8	127	46	128	124	129	80	130	18	131	28	132	5	133	10	134	10
135	19	136	3	137	2	138	3	139	32	140	16	141	144	142	85	143	64	144	27
145	35	146	7	147	6	148	4	149	2	150	4	151	22	152	86	153	83	154	45
155	195	156	99	157	45	158	9	159	13	160	4	161	17	162	6	163	13	164	13
165	130	166	60	167	62	168	31	169	74	170	24	171	16	172	9	173	7	174	5
175	6	176	9	177	14	178	57	179	79	180	75	181	87	182	38	183	35	184	10
185	8	186	7	187	9	188	9	189	33	190	22	191	31	192	32	193	77	194	32
195	102	196	37	197	47	198	14	199	11	200	37	201	20	202	9	203	8	204	8
205	25	206	31	207	22	208	14	209	118	210	58	211	44	212	8	213	6	214	6
215	9	216	3	217	1	218	2	219	9	220	10	221	81	222	25	223	97	224	32
225	57	226	17	227	7	228	3	229	4	230	2	232	1	233	2	234	3	235	2
236	2	237	28	238	129	239	143	240	30	241	11	242	4	243	6	244	1	245	Tr
246	Tr	247	Tr	248	2	249	7	250	4	251	17	252	3	253	1	254	4	255	61
256	16	257	3	258	Tr	259	Tr	260	Tr	261	Tr	262	Tr	263	1	264	2	265	3
266	47	267	12	268	3	269	69	270	13	271	2	272	Tr	273	Tr	274	Tr	275	Tr
276	Tr	277	Tr	278	Tr	279	1	280	Tr	281	Tr	282	1	283	4	284	999	285	185
286	24	287	2																

Synonyms:

1.7-Hydroxy-1-methyl-8-methylenegibba-1,3,4a(10a)-triene-10-carboxylic acid #

Hit 7 : Allogibberic acid

C₁₈H₂₀O₃; MF: 587; RMF: 587; Prob 8.38%; CAS: 427-79-2; Lib: replib; ID: 37421.



Name: Allogibberic acid

Formula: C₁₈H₂₀O₃

MW: 284 Exact Mass: 284.141245 CAS#: 427-79-2 NIST#: 151229 ID#: 37421 DB: replib

Other DBs: None

Contributor: Chemical Concepts

InChIKey: IFYWTLMNWNCFH-UHFFFAOYSA-N Non-stereo

10 largest peaks:

284 999 | 226 537 | 155 361 | 141 333 | 128 286 | 238 270 | 115 260 | 165 255 | 195 249 | 209 235 |

250 m/z Values and Intensities:

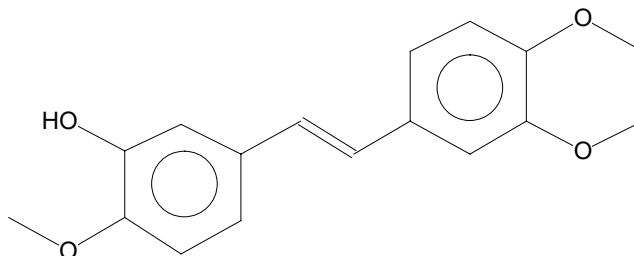
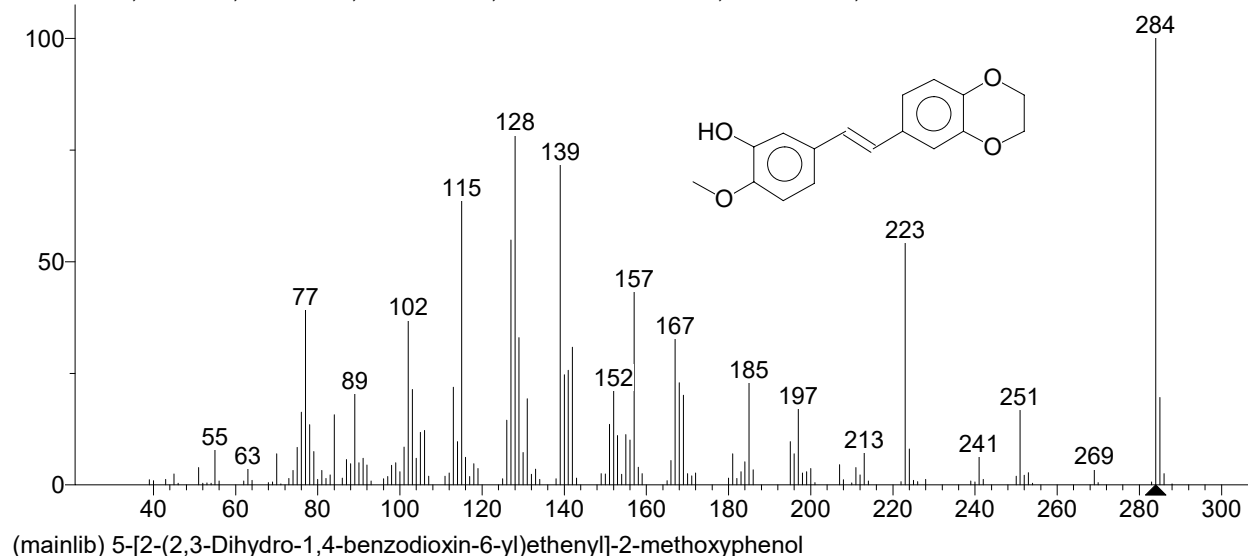
26	2	27	79	28	6	29	63	30	1	31	25	38	2	39	118	40	52	41	162
42	18	43	193	44	7	45	39	46	1	47	3	50	7	51	48	52	15	53	61
54	9	55	110	56	8	57	16	58	3	59	1	60	2	62	5	63	38	64	13
65	62	66	20	67	41	68	23	69	49	70	8	71	10	72	1	73	1	74	4
75	14	76	29	77	119	78	33	79	47	80	7	81	22	82	20	83	38	84	15
85	7	86	3	87	6	88	10	89	58	90	26	91	120	92	19	93	15	94	17
95	120	96	37	97	38	98	27	99	6	100	2	101	13	102	32	103	36	104	36

105	103	106	15	107	24	108	21	109	18	110	8	111	12	112	19	113	9	114	19
115	260	116	59	117	38	118	14	119	55	120	9	121	29	122	37	123	8	124	3
125	4	126	17	127	98	128	286	129	177	130	45	131	64	132	14	133	24	134	17
135	27	136	6	137	3	138	7	139	74	140	37	141	333	142	202	143	165	144	67
145	72	146	17	147	11	148	8	149	6	150	11	151	41	152	179	153	171	154	90
155	361	156	165	157	97	158	27	159	39	160	9	161	38	162	13	163	22	164	25
165	255	166	127	167	151	168	68	169	125	170	46	171	32	172	15	173	16	174	11
175	10	176	19	177	27	178	110	179	130	180	90	181	229	182	99	183	78	184	24
185	15	186	18	187	25	188	24	189	51	190	31	191	45	192	45	193	99	194	139
195	249	196	197	197	93	198	25	199	18	200	74	201	50	202	25	203	16	204	13
205	40	206	33	207	43	208	39	209	235	210	134	211	114	212	24	213	11	214	9
215	11	216	4	217	2	218	4	219	18	220	19	221	75	222	48	223	149	224	51
225	89	226	537	227	113	228	18	229	6	230	2	231	2	232	2	233	7	234	5
235	6	236	6	237	46	238	270	239	175	240	86	241	32	242	8	243	5	244	1
245	Tr	246	1	247	3	248	5	249	12	250	6	251	22	252	4	253	3	254	5
255	88	256	32	257	6	258	1	259	1	260	Tr	261	Tr	262	1	263	1	264	3
265	5	266	90	267	21	268	5	269	85	270	15	271	2	272	1	273	1	274	1
277	Tr	279	Tr	280	1	281	1	282	4	283	6	284	999	285	173	286	28	287	3

Synonyms:

1.7-Hydroxy-1-methyl-8-methylenegibba-1,3,4a(10a)-triene-10-carboxylic acid #

Hit 8 : 5-[2-(2,3-Dihydro-1,4-benzodioxin-6-yl)ethenyl]-2-methoxyphenol
 C₁₇H₁₆O₄; MF: 583; RMF: 608; Prob 5.41%; CAS: 1257321-28-0; Lib: mainlib; ID: 243088.



Name: 5-[2-(2,3-Dihydro-1,4-benzodioxin-6-yl)ethenyl]-2-methoxyphenol

Formula: C₁₇H₁₆O₄

MW: 284 Exact Mass: 284.104858 CAS#: 1257321-28-0 NIST#: 434814 ID#: 243088 DB: mainlib

Other DBs: None

Contributor: V.A.Korolev, Moscow, Russia

InChIKey: QTDSJRSHKSGNJC-NSCUHMNNSA-N Non-stereo

10 largest peaks:

284 999 | 128 781 | 139 714 | 115 635 | 127 547 | 223 540 | 157 430 | 77 391 | 102 367 | 129 329 |

137 m/z Values and Intensities:

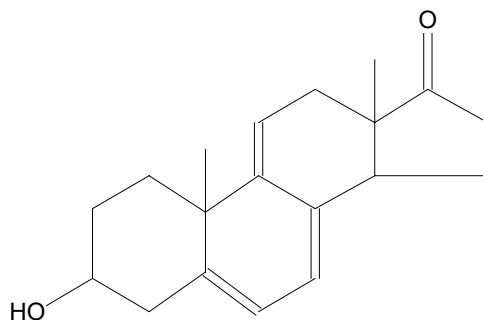
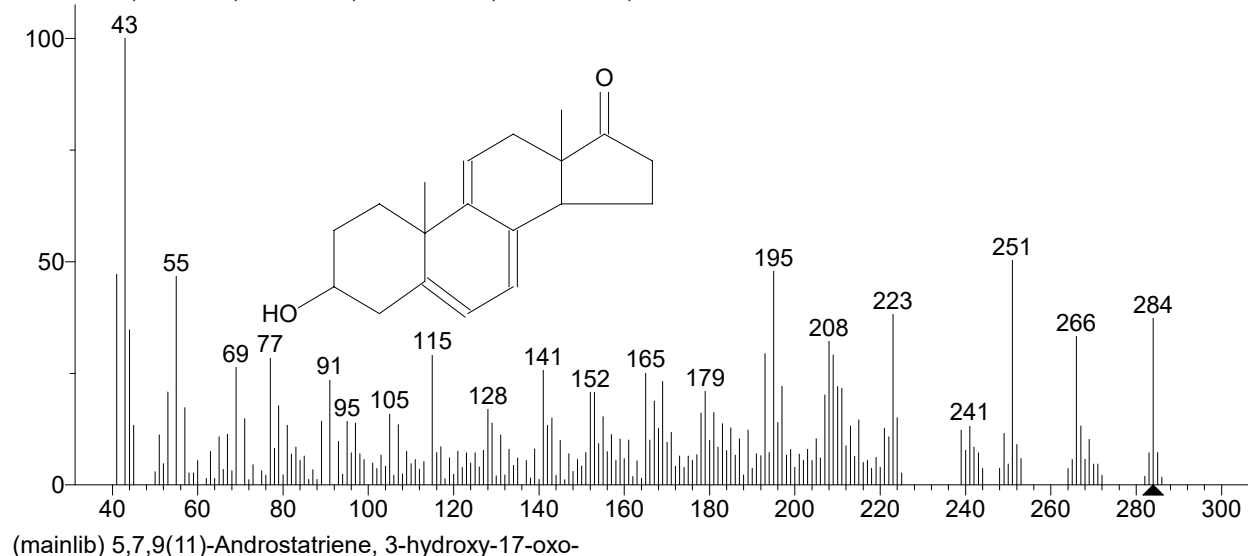
39	11	40	9	43	12	45	24	46	3	51	38	52	3	53	4	54	3	55	78
56	8	62	8	63	35	64	10	68	5	69	6	70	69	71	2	73	14	74	32
75	83	76	162	77	391	78	134	79	74	80	12	81	32	82	14	83	22	84	156
86	15	87	56	88	47	89	203	90	49	91	59	92	44	93	8	96	13	97	18
98	43	99	49	100	29	101	84	102	367	103	213	104	59	105	117	106	121	107	19
111	19	112	26	113	218	114	96	115	635	116	61	117	18	118	47	119	36	125	13
126	144	127	547	128	781	129	329	130	72	131	192	132	23	133	35	134	12	138	13

139 714	140 246	141 256	142 307	143 15	149 25	150 24	151 135	152 210	153 110
154 23	155 112	156 100	157 430	158 39	159 25	165 9	166 54	167 325	168 228
169 200	170 25	171 20	172 26	180 15	181 69	182 14	183 29	184 51	185 227
186 33	195 96	196 69	197 170	198 26	199 29	200 36	201 5	207 45	208 11
210 4	211 38	212 22	213 71	214 8	222 7	223 540	224 80	225 10	226 7
228 12	239 8	240 6	241 62	242 12	250 19	251 166	252 21	253 27	254 3
269 34	270 5	283 6	284 999	285 195	286 25	288 2			

Synonyms:

no synonyms.

Hit 9 : 5,7,9(11)-Androstatriene, 3-hydroxy-17-oxo-
C₁₉H₂₄O₂; MF: 575; RMF: 576; Prob 4.04%; Lib: mainlib; ID: 15194.



Name: 5,7,9(11)-Androstatriene, 3-hydroxy-17-oxo-
Formula: C₁₉H₂₄O₂
MW: 284 Exact Mass: 284.17763 NIST#: 251163 ID#: 15194 DB: mainlib
Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892
InChIKey: BFFKDUOHNSMWGF-UHFFFAOYSA-N Non-stereo

10 largest peaks:

43 999	251 502	195 478	41 470	55 466	223 382	284 372	44 346	266 333	208 321
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196 m/z Values and Intensities:

41 470	43 999	44 346	45 133	50 29	51 111	52 47	53 207	55 466	57 172
58 26	59 26	60 54	62 14	63 74	64 14	65 107	66 34	67 113	68 31
69 263	71 148	72 11	73 45	75 31	76 21	77 284	78 81	79 176	80 22
81 133	82 68	83 84	84 55	85 64	86 12	87 33	88 12	89 142	91 235
93 97	94 23	95 143	96 71	97 138	98 69	99 56	101 48	102 36	103 66
104 41	105 159	106 21	107 134	108 24	109 75	110 47	111 56	112 35	113 52
115 291	116 72	117 85	118 13	119 60	120 23	121 75	122 38	123 71	124 48
125 71	126 40	127 77	128 169	129 138	130 20	131 111	132 22	133 79	134 43

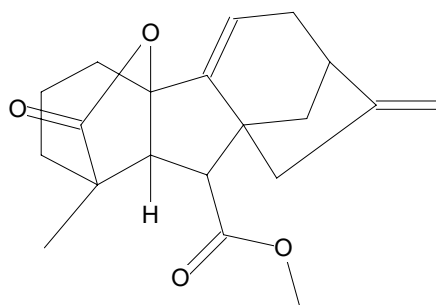
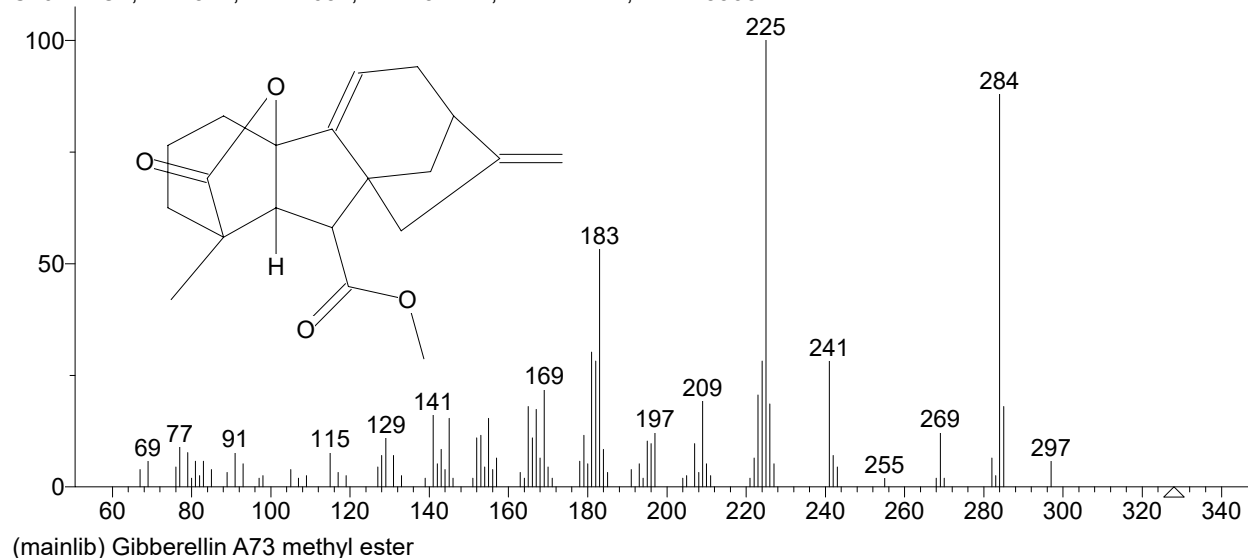
135	60		137	54		138	15		139	80		140	12		141	257		142	133		143	149		144	21		145	99	
146	11		147	69		148	30		149	56		150	42		151	72		152	208		153	208		154	92		155	152	
156	74		157	112		158	55		159	102		160	58		161	100		162	18		163	53		164	14		165	251	
166	100		167	187		168	126		169	231		170	95		171	117		172	41		173	64		174	39		175	64	
176	55		177	67		178	160		179	210		180	99		181	161		182	84		183	136		184	76		185	127	
186	66		187	103		188	22		189	122		190	37		191	69		192	65		193	293		194	72		195	478	
196	139		197	220		198	66		199	79		200	39		201	68		202	55		203	79		204	54		205	103	
206	60		207	201		208	321		209	290		210	219		211	216		212	87		213	131		214	63		215	145	
216	50		217	55		218	37		219	61		220	39		221	126		222	107		223	382		224	150		225	26	
239	122		240	77		241	133		242	84		243	71		244	36		248	37		249	115		250	46		251	502	
252	90		253	58		264	36		265	56		266	333		267	131		268	57		269	101		270	46		271	46	
272	21		282	19		283	71		284	372		285	72		286	17													

Synonyms:

1.3-Hydroxyandrosta-5,7,9(11)-trien-17-one #

Hit 10 : Gibberellin A73 methyl ester

C₂₀H₂₄O₄; MF: 571; RMF: 652; Prob 3.41%; Lib: mainlib; ID: 218595.



Name: Gibberellin A73 methyl ester

Formula: C₂₀H₂₄O₄

MW: 328 Exact Mass: 328.16746 NIST#: 440966 ID#: 218595 DB: mainlib

Contributor: The data for these pages was compiled and collated by Jake MacMillan, Paul Gaskin and Steve Croker.

Link to the data base: <http://www.plant-hormones.info/ga1info.htm>

InChIKey: HQSDLFRIZKDOEE-UHFFFAOYSA-N Non-stereo

10 largest peaks:

225 999 | 284 877 | 183 531 | 181 301 | 182 281 | 224 281 | 241 281 | 169 217 | 223 205 | 209 192 |

89 m/z Values and Intensities:

67	38	69	57	76	44	77	89	79	76	80	19	81	57	82	25	83	57	85	38
89	32	91	76	93	51	97	19	98	25	105	38	107	19	109	25	115	76	117	32
119	25	127	44	128	70	129	109	131	70	133	25	139	19	141	160	142	51	143	83
144	38	145	153	146	19	151	19	152	109	153	115	154	44	155	153	156	38	157	64
163	32	164	19	165	179	166	109	167	173	168	64	169	217	170	44	171	19	178	57
179	115	180	51	181	301	182	281	183	531	184	83	185	32	191	38	193	51	194	19
195	102	196	96	197	121	204	19	205	25	207	96	208	32	209	192	210	51	211	25

221 19 | 222 64 | 223 205 | 224 281 | 225 999 | 226 185 | 227 51 | 241 281 | 242 70 | 243 44 |
255 19 | 268 19 | 269 121 | 270 19 | 282 64 | 283 25 | 284 877 | 285 179 | 297 57 |
Synonyms:
no synonyms.