

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
 Data File : VW030148.D
 Acq On : 19 Sep 2024 15:22
 Operator : SY/MD
 Sample : P4083-12
 Misc : 5.41g/10mL/MSVOA_W/SOIL/B
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4ELO

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
 Title : SFAM01.0

Signal : TIC: VW030148.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.259	59	61	65	rVB2	763	818	0.07%	0.011%
2	2.369	71	79	97	rVB	59349	144980	11.81%	1.889%
3	2.704	132	134	138	rVB5	733	767	0.06%	0.010%
4	2.783	145	147	149	rVB3	519	308	0.03%	0.004%
5	2.899	157	166	182	rBV	41774	128001	10.43%	1.668%
6	3.125	202	203	207	rBV2	403	426	0.03%	0.006%
7	3.179	209	212	214	rVB2	480	562	0.05%	0.007%
8	3.204	214	216	218	rBV2	270	213	0.02%	0.003%
9	3.283	226	229	230	rBV2	331	326	0.03%	0.004%
10	3.393	241	247	255	rVV4	1381	3311	0.27%	0.043%
11	3.490	262	263	265	rBV2	216	188	0.02%	0.002%
12	3.588	277	279	281	rBV2	371	358	0.03%	0.005%
13	3.692	294	296	298	rBV	228	243	0.02%	0.003%
14	3.716	298	300	302	rBV2	357	315	0.03%	0.004%
15	3.893	325	329	332	rBV2	161	260	0.02%	0.003%
16	4.021	339	350	362	rBV	138991	412263	33.59%	5.372%
17	4.131	362	368	387	rVB	28117	88307	7.19%	1.151%
18	4.313	395	398	400	rBV	293	338	0.03%	0.004%
19	4.393	402	411	419	rBV	5163	16426	1.34%	0.214%
20	4.533	431	434	440	rVB3	342	618	0.05%	0.008%
21	4.691	455	460	464	rVB3	218	392	0.03%	0.005%
22	4.783	471	475	479	rBV2	229	300	0.02%	0.004%
23	4.923	487	498	513	rBV2	9792	36101	2.94%	0.470%
24	5.106	524	528	529	rBV	235	244	0.02%	0.003%
25	5.185	538	541	545	rVB2	158	184	0.01%	0.002%
26	5.350	564	568	571	rVB2	262	366	0.03%	0.005%
27	5.374	571	572	574	rBV	274	218	0.02%	0.003%
28	5.472	586	588	591	rVB	240	199	0.02%	0.003%
29	5.527	591	597	598	rBV2	241	336	0.03%	0.004%
30	5.746	631	633	634	rBV	429	367	0.03%	0.005%
31	5.795	634	641	644	rBV4	1165	2424	0.20%	0.032%
32	5.935	657	664	673	rVV5	1687	5335	0.43%	0.070%
33	6.002	673	675	678	rVB	195	188	0.02%	0.002%
34	6.313	724	726	731	rVB2	207	219	0.02%	0.003%
35	6.545	761	764	768	rBV2	140	258	0.02%	0.003%
36	6.654	781	782	788	rVB	328	307	0.03%	0.004%

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Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Title : SFAM01.0

37	6.819	808	809	813	rBV2	176	217	0.02%	0.003%
38	7.081	841	852	861	rBV	28187	79598	6.49%	1.037%
39	7.173	863	867	882	rVV	12730	36527	2.98%	0.476%
40	7.270	882	883	886	rVB2	368	288	0.02%	0.004%
41	7.423	907	908	911	rVB2	292	218	0.02%	0.003%
42	7.484	914	918	920	rBV2	195	206	0.02%	0.003%
43	7.520	920	924	925	rBV2	233	304	0.02%	0.004%
44	7.532	925	926	930	rVV3	262	331	0.03%	0.004%
45	7.648	933	945	960	rBV	209682	526137	42.87%	6.856%
46	7.947	991	994	997	rVB2	160	213	0.02%	0.003%
47	8.179	1030	1032	1035	rVB2	129	177	0.01%	0.002%
48	8.276	1038	1048	1066	rVV2	423158	1227365	100.00%	15.995%
49	8.422	1070	1072	1075	rVB2	383	262	0.02%	0.003%
50	8.471	1078	1080	1084	rVB	229	234	0.02%	0.003%
51	8.538	1088	1091	1093	rVB3	276	245	0.02%	0.003%
52	8.569	1093	1096	1099	rBV3	322	529	0.04%	0.007%
53	8.697	1111	1117	1126	rBV5	908	2305	0.19%	0.030%
54	8.843	1132	1141	1160	rBV	445489	885125	72.12%	11.535%
55	9.081	1171	1180	1185	rBV5	1233	2711	0.22%	0.035%
56	9.276	1202	1212	1221	rBV	275287	563848	45.94%	7.348%
57	9.343	1221	1223	1228	rVB4	1191	1709	0.14%	0.022%
58	9.380	1228	1229	1231	rBV2	301	205	0.02%	0.003%
59	9.459	1240	1242	1248	rVB3	304	555	0.05%	0.007%
60	9.623	1267	1269	1273	rBV	191	217	0.02%	0.003%
61	9.660	1273	1275	1277	rVV2	488	480	0.04%	0.006%
62	9.684	1277	1279	1286	rVB	458	597	0.05%	0.008%
63	9.745	1286	1289	1290	rBV	258	188	0.02%	0.002%
64	9.855	1304	1307	1310	rBV2	232	304	0.02%	0.004%
65	9.959	1319	1324	1325	rVB2	234	273	0.02%	0.004%
66	10.032	1327	1336	1350	rBV	127972	236295	19.25%	3.079%
67	10.142	1352	1354	1357	rVB2	293	241	0.02%	0.003%
68	10.203	1362	1364	1368	rBV2	459	506	0.04%	0.007%
69	10.318	1376	1383	1392	rBV	527062	936036	76.26%	12.198%
70	10.501	1406	1413	1417	rBV7	873	1972	0.16%	0.026%
71	10.575	1417	1425	1437	rVV	74668	130475	10.63%	1.700%
72	10.703	1440	1446	1451	rVB2	8170	15179	1.24%	0.198%
73	10.806	1460	1463	1467	rBV3	245	467	0.04%	0.006%
74	10.873	1472	1474	1475	rBV2	334	261	0.02%	0.003%
75	10.922	1475	1482	1499	rBV	115210	203074	16.55%	2.646%
76	11.074	1504	1507	1511	rVB5	1116	1621	0.13%	0.021%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
 Title : SFAM01.0

77	11.129	1514	1516	1518	rVB3	323	260	0.02%	0.003%
78	11.178	1522	1524	1527	rVB4	579	554	0.05%	0.007%
79	11.215	1528	1530	1535	rBV4	848	856	0.07%	0.011%
80	11.257	1535	1537	1539	rBV3	517	676	0.06%	0.009%
81	11.318	1545	1547	1549	rBV3	548	526	0.04%	0.007%
82	11.513	1578	1579	1581	rVB2	325	231	0.02%	0.003%
83	11.629	1590	1598	1608	rBV	452728	758741	61.82%	9.888%
84	11.843	1628	1633	1637	rVB7	2402	4364	0.36%	0.057%
85	11.971	1650	1654	1656	rBV5	787	1048	0.09%	0.014%
86	12.025	1659	1663	1669	rVB6	1816	3114	0.25%	0.041%
87	12.074	1669	1671	1674	rBV4	321	348	0.03%	0.005%
88	12.117	1674	1678	1684	rBV6	1866	3437	0.28%	0.045%
89	12.178	1686	1688	1689	rBV	619	448	0.04%	0.006%
90	12.330	1707	1713	1716	rBV6	3287	7474	0.61%	0.097%
91	12.440	1724	1731	1742	rBV10	10429	35374	2.88%	0.461%
92	12.599	1754	1757	1765	rVB5	4868	10147	0.83%	0.132%
93	12.690	1765	1772	1780	rBV	141328	241280	19.66%	3.144%
94	12.879	1796	1803	1807	rBV9	5425	13001	1.06%	0.169%
95	12.970	1808	1818	1823	rBV9	17097	60976	4.97%	0.795%
96	13.196	1851	1855	1861	rVB4	11674	22590	1.84%	0.294%
97	13.379	1880	1885	1891	rBV6	12884	37175	3.03%	0.484%
98	13.556	1908	1914	1921	rVB	211269	355017	28.93%	4.626%
99	13.848	1957	1962	1969	rVB	183118	296288	24.14%	3.861%
100	15.318	2200	2203	2210	rVB2	64781	115696	9.43%	1.508%

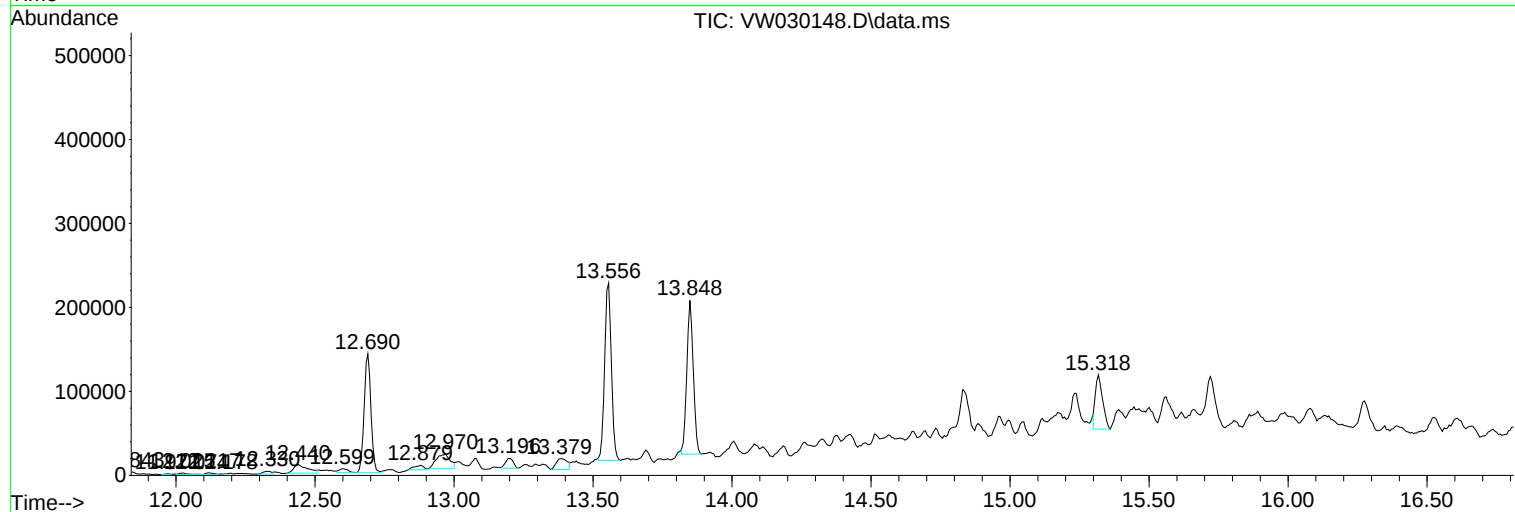
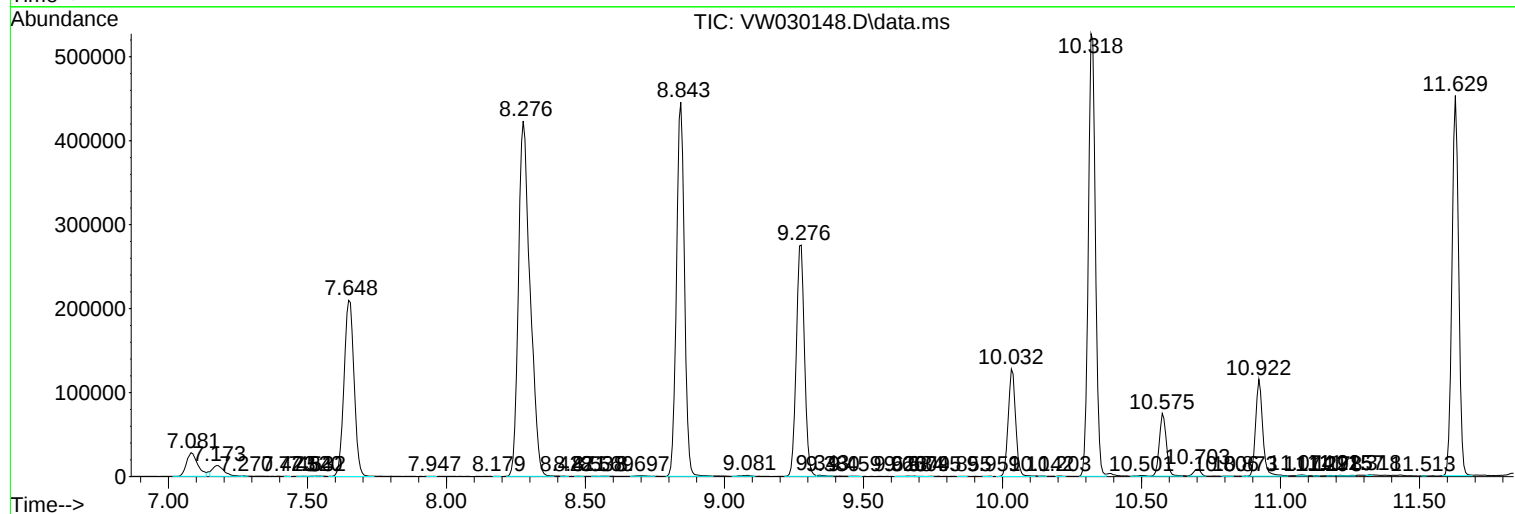
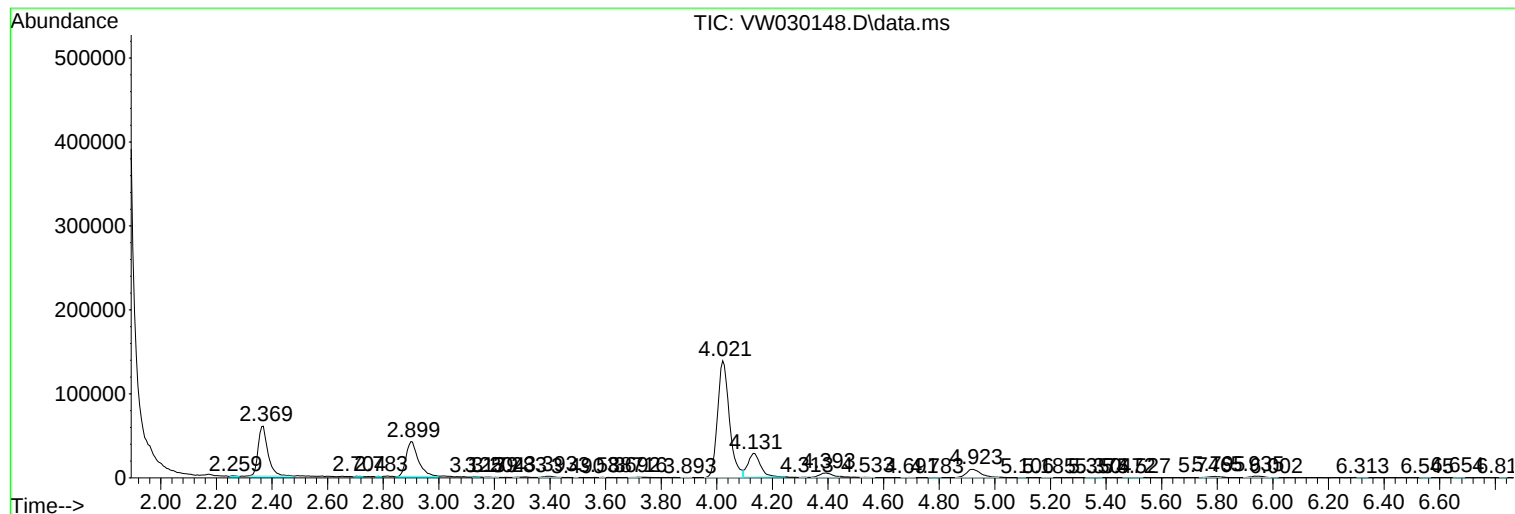
Sum of corrected areas: 7673582

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_W
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A4ELO

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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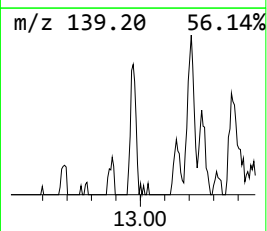
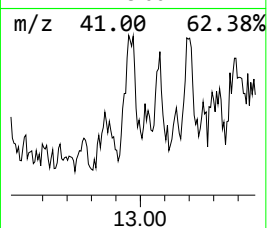
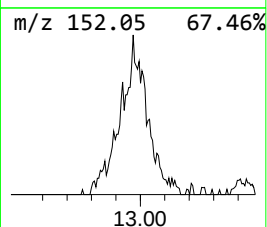
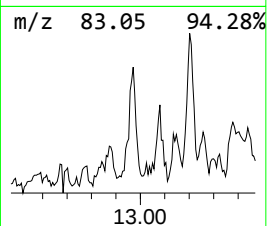
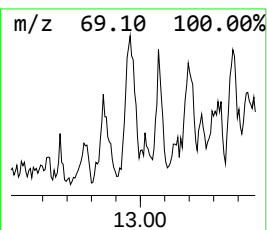
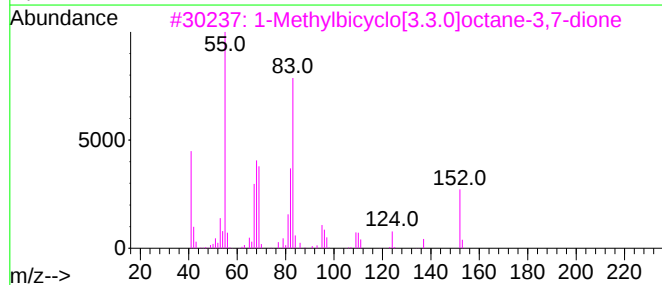
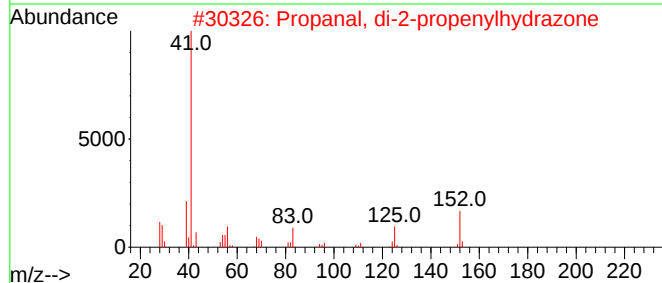
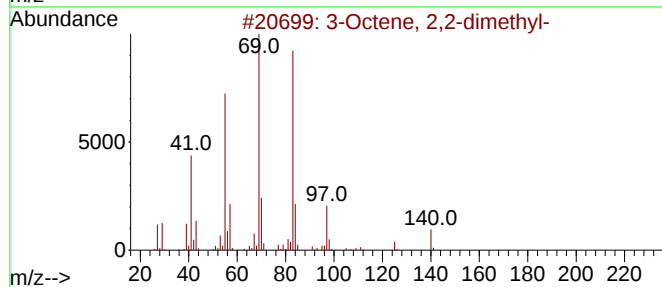
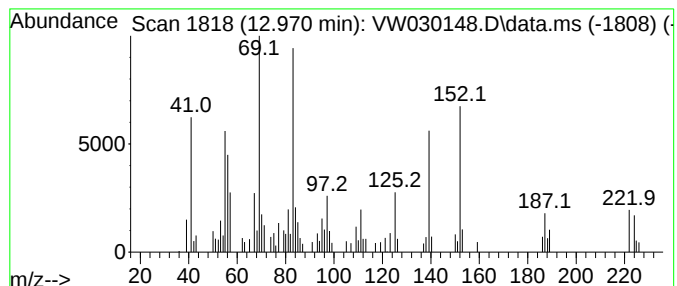
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.970	4.29 ug/L	60976	1,4-Dichlorobenzene-d4	13.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	46
2		Propanal, di-2-propenylhydrazone	152	C9H16N2	075268-09-6	30
3		1-Methylbicyclo[3.3.0]octane-3,7...	152	C9H12O2	021170-08-1	25
4		2-Acetyl-4,4-dimethyl-cyclopent-...	152	C9H12O2	081979-96-6	25
5		4-Nonene, 2,3,3-trimethyl-, (E)-	168	C12H24	063830-67-1	22



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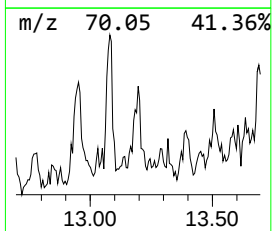
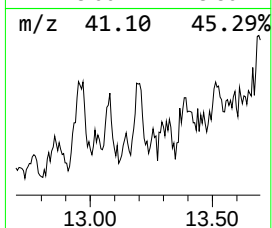
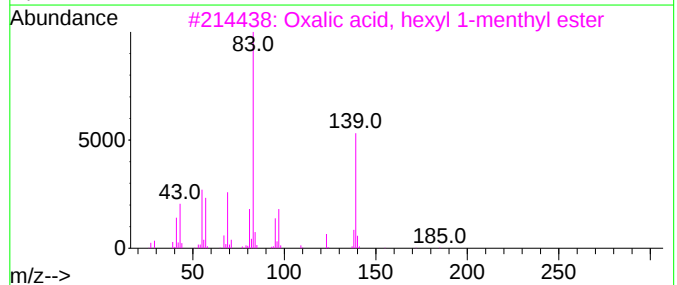
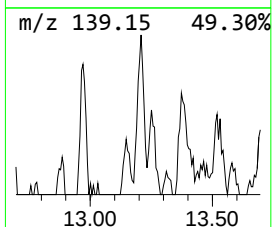
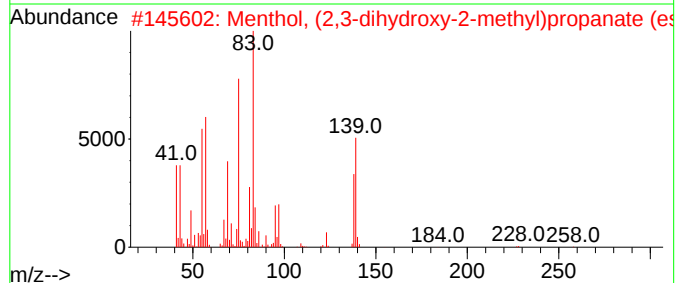
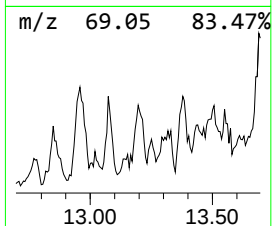
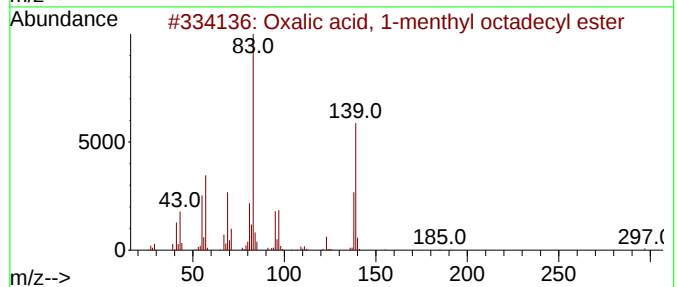
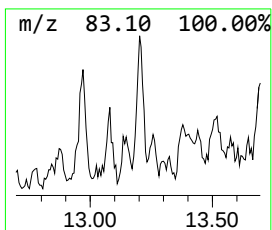
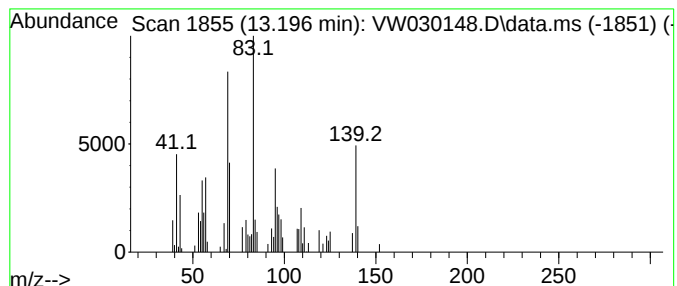
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.196	1.59 ug/L	22590	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, 1-menthyl octadecyl...	480	C30H56O4	1000314-98-5	35
2			Menthol, (2,3-dihydroxy-2-methyl...	258	C14H26O4	1010127-79-6	27
3			Oxalic acid, hexyl 1-menthyl ester	312	C18H32O4	1000314-97-4	27
4			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	27
5			Oxalic acid, hexadecyl 1-menthyl...	452	C28H52O4	1000314-98-3	27



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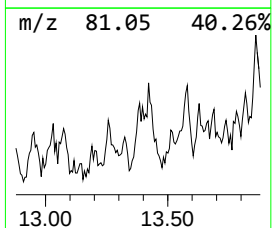
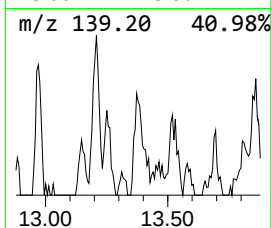
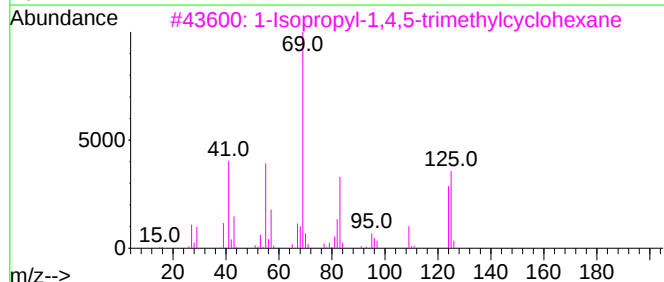
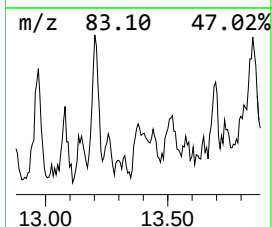
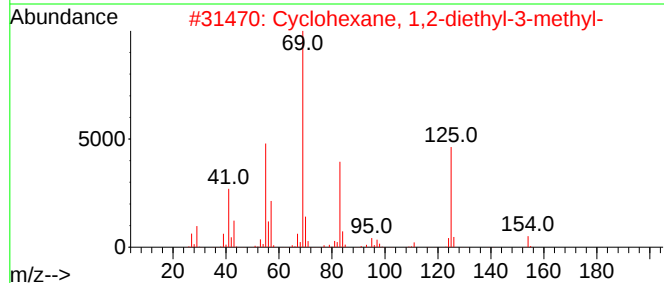
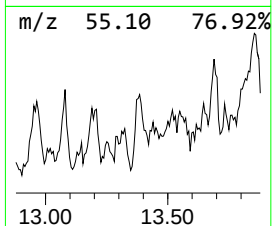
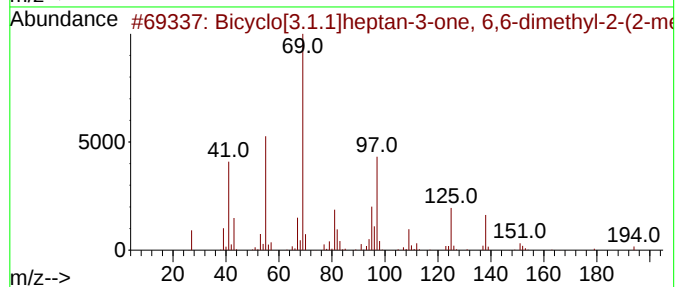
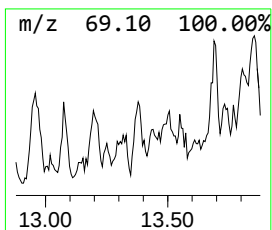
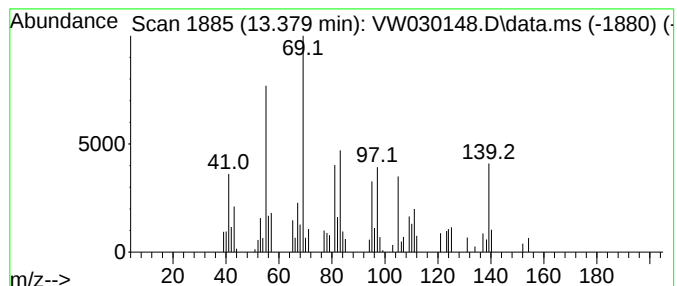
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.379	2.62 ug/L	37175	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	38
2			Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	38
3			1-Isopropyl-1,4,5-trimethylcyclo...	168	C12H24	219783-06-9	35
4			4-Butyl-cyclohexanone	154	C10H18O	061203-82-5	30
5			Cyclohexane, 1-ethyl-2-propyl-	154	C11H22	062238-33-9	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
Data File : VW030148.D
Acq On : 19 Sep 2024 15:22
Operator : SY/MD
Sample : P4083-12
Misc : 5.41g/10mL/MSVOA_W/SOIL/B
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4ELO

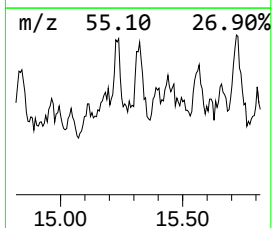
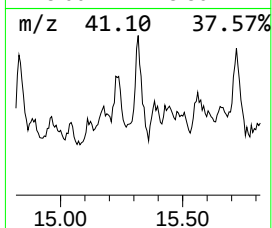
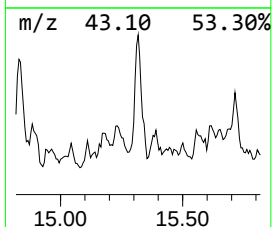
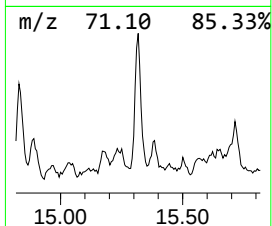
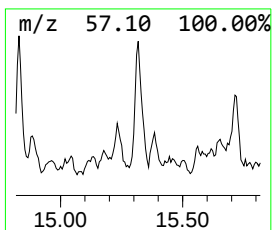
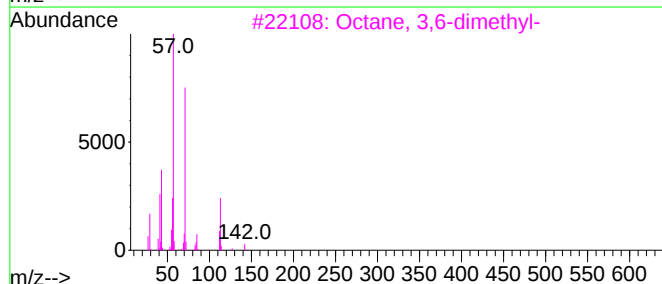
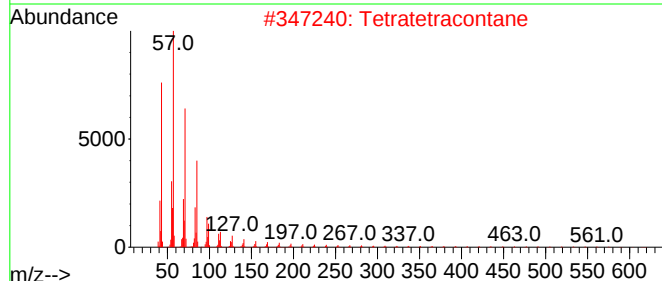
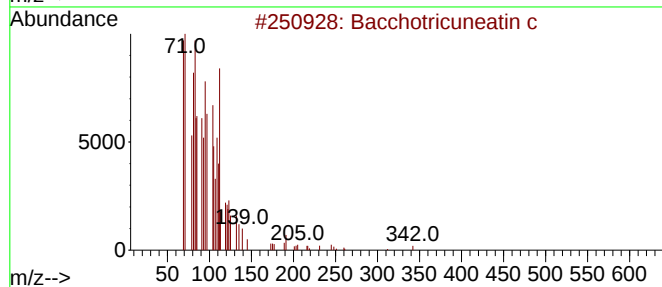
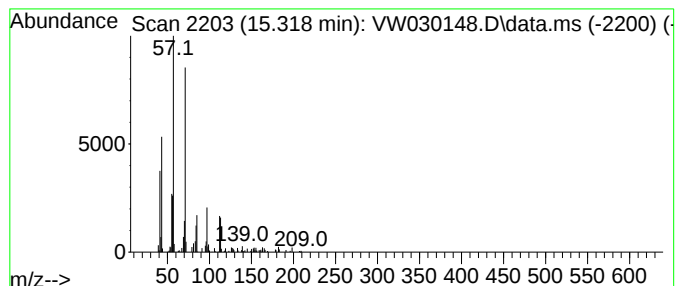
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Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Bacchotricuneatin c Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	8.15 ug/L	115696	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bacchotricuneatin c	342	C20H22O5	066563-30-2	86
2			Tetratetracontane	619	C44H90	007098-22-8	72
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	64
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
Data File : VW030148.D
Acq On : 19 Sep 2024 15:22
Operator : SY/MD
Sample : P4083-12
Misc : 5.41g/10mL/MSVOA_W/SOIL/B
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4ELO

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	12.970	4.3	ug/L	60976	3	13.556	355017	25.0
unknown-01	13.196	1.6	ug/L	22590	3	13.556	355017	25.0
unknown-02	13.379	2.6	ug/L	37175	3	13.556	355017	25.0
Bacchotricuneat...	15.318	8.2	ug/L	115696	3	13.556	355017	25.0