

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071124\
 Data File : VW029530.D
 Acq On : 11 Jul 2024 15:34
 Operator : SY/MD
 Sample : P3178-10
 Misc : 5.49g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4BT5

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\SFAMWLM070824SMA.M
 Title : SFAM01.0

Signal : TIC: VW029530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	71	78	95	rBV	78740	193119	14.42%	2.130%
2	2.899	158	166	185	rBV	52726	162137	12.10%	1.788%
3	3.277	224	228	230	rBV3	549	974	0.07%	0.011%
4	3.387	243	246	250	rVV4	978	1463	0.11%	0.016%
5	3.710	297	299	301	rBV3	499	505	0.04%	0.006%
6	3.777	308	310	312	rBV3	508	553	0.04%	0.006%
7	3.801	312	314	317	rVB2	612	491	0.04%	0.005%
8	3.929	332	335	336	rBV2	548	431	0.03%	0.005%
9	4.021	338	350	366	rBV	147521	470615	35.13%	5.191%
10	4.332	397	401	404	rBV4	595	783	0.06%	0.009%
11	4.435	416	418	421	rVB3	711	716	0.05%	0.008%
12	4.923	485	498	510	rBV	41412	157490	11.76%	1.737%
13	5.118	527	530	531	rBV3	620	616	0.05%	0.007%
14	5.161	533	537	539	rVV4	1002	1438	0.11%	0.016%
15	5.252	550	552	555	rBV2	467	624	0.05%	0.007%
16	5.411	576	578	580	rVV2	456	503	0.04%	0.006%
17	5.490	589	591	595	rVB2	532	561	0.04%	0.006%
18	5.886	650	656	657	rVV5	372	571	0.04%	0.006%
19	5.941	657	665	676	rVB6	5194	16056	1.20%	0.177%
20	6.112	688	693	696	rBV3	375	436	0.03%	0.005%
21	6.325	726	728	730	rBV3	529	529	0.04%	0.006%
22	6.374	733	736	737	rBV	451	415	0.03%	0.005%
23	6.429	741	745	746	rBV2	462	480	0.04%	0.005%
24	6.496	755	756	759	rBV	454	466	0.03%	0.005%
25	6.661	781	783	786	rBV3	384	565	0.04%	0.006%
26	6.776	799	802	805	rBV2	432	556	0.04%	0.006%
27	6.831	807	811	812	rBV2	463	604	0.05%	0.007%
28	6.880	816	819	821	rBV3	346	491	0.04%	0.005%
29	6.929	821	827	832	rVB5	1316	2909	0.22%	0.032%
30	7.075	842	851	873	rBV	29754	99895	7.46%	1.102%
31	7.429	906	909	911	rVV3	334	430	0.03%	0.005%
32	7.471	914	916	919	rVB3	498	552	0.04%	0.006%
33	7.551	924	929	933	rBV3	484	979	0.07%	0.011%
34	7.648	933	945	959	rVV	226173	557936	41.65%	6.154%
35	7.752	959	962	966	rVV4	940	1725	0.13%	0.019%
36	7.788	966	968	971	rVV2	751	694	0.05%	0.008%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
 Title : SFAM01.0

37	7.813	971	972	975	rVV2	474	481	0.04%	0.005%
38	7.953	990	995	997	rVB5	354	658	0.05%	0.007%
39	8.045	1008	1010	1013	rVV3	422	446	0.03%	0.005%
40	8.276	1035	1048	1066	rBV2	461547	1339671	100.00%	14.777%
41	8.630	1104	1106	1109	rVB3	860	1063	0.08%	0.012%
42	8.666	1109	1112	1113	rBV2	426	463	0.03%	0.005%
43	8.715	1118	1120	1125	rVB4	700	908	0.07%	0.010%
44	8.843	1131	1141	1151	rBV	474416	942326	70.34%	10.394%
45	9.044	1170	1174	1176	rBV4	1313	1979	0.15%	0.022%
46	9.197	1196	1199	1201	rVB3	464	427	0.03%	0.005%
47	9.270	1201	1211	1222	rBV	307156	636476	47.51%	7.021%
48	9.422	1234	1236	1239	rVB2	395	441	0.03%	0.005%
49	9.502	1247	1249	1254	rVB2	593	559	0.04%	0.006%
50	9.544	1254	1256	1258	rBV2	637	567	0.04%	0.006%
51	9.654	1271	1274	1275	rBV3	547	664	0.05%	0.007%
52	9.745	1286	1289	1290	rBV2	564	519	0.04%	0.006%
53	9.770	1290	1293	1294	rVV2	499	425	0.03%	0.005%
54	9.861	1306	1308	1311	rBV3	402	553	0.04%	0.006%
55	9.934	1316	1320	1321	rBV2	415	491	0.04%	0.005%
56	10.032	1326	1336	1344	rBV	151345	270068	20.16%	2.979%
57	10.203	1360	1364	1367	rVB5	805	772	0.06%	0.009%
58	10.233	1367	1369	1373	rVB5	506	562	0.04%	0.006%
59	10.318	1375	1383	1391	rBV	609971	1081487	80.73%	11.929%
60	10.575	1418	1425	1434	rBV	89090	158977	11.87%	1.754%
61	10.703	1439	1446	1452	rVB2	5102	10246	0.76%	0.113%
62	10.770	1452	1457	1459	rVB4	557	917	0.07%	0.010%
63	10.843	1465	1469	1470	rBV2	861	1067	0.08%	0.012%
64	10.922	1475	1482	1497	rBV	109816	204588	15.27%	2.257%
65	11.178	1520	1524	1528	rVB4	1356	1951	0.15%	0.022%
66	11.215	1528	1530	1535	rBB3	669	756	0.06%	0.008%
67	11.404	1554	1561	1564	rBV4	842	1567	0.12%	0.017%
68	11.465	1568	1571	1573	rVB4	509	549	0.04%	0.006%
69	11.629	1588	1598	1609	rBV	525096	875743	65.37%	9.660%
70	11.837	1626	1632	1642	rVB5	3545	8921	0.67%	0.098%
71	12.013	1658	1661	1663	rBV3	637	737	0.06%	0.008%
72	12.050	1663	1667	1668	rBV3	463	582	0.04%	0.006%
73	12.160	1681	1685	1690	rVV5	2111	3710	0.28%	0.041%
74	12.202	1690	1692	1693	rVV	742	421	0.03%	0.005%
75	12.343	1712	1715	1717	rVV4	789	931	0.07%	0.010%
76	12.464	1731	1735	1739	rBV2	969	1686	0.13%	0.019%

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77	12.538	1744	1747	1749	rVV3	447	516	0.04%	0.006%
78	12.592	1750	1756	1765	rVV3	16103	33742	2.52%	0.372%
79	12.690	1765	1772	1778	rVV	177312	293515	21.91%	3.238%
80	12.757	1778	1783	1794	rVB3	4313	11470	0.86%	0.127%
81	12.879	1801	1803	1807	rVB4	1267	1436	0.11%	0.016%
82	12.958	1807	1816	1821	rBV5	4836	12975	0.97%	0.143%
83	13.013	1823	1825	1827	rVB2	1364	996	0.07%	0.011%
84	13.080	1833	1836	1837	rBV2	1107	1113	0.08%	0.012%
85	13.129	1841	1844	1845	rBV3	916	946	0.07%	0.010%
86	13.190	1846	1854	1861	rVB	28311	48556	3.62%	0.536%
87	13.269	1861	1867	1869	rBV	18431	29993	2.24%	0.331%
88	13.403	1880	1889	1895	rBV	43817	82514	6.16%	0.910%
89	13.470	1897	1900	1902	rVV3	4663	5847	0.44%	0.064%
90	13.513	1902	1907	1908	rVV4	11486	17874	1.33%	0.197%
91	13.556	1908	1914	1918	rVV	306871	493053	36.80%	5.439%
92	13.598	1918	1921	1932	rVB	70518	139921	10.44%	1.543%
93	13.757	1942	1947	1954	rVB3	26849	50544	3.77%	0.558%
94	13.848	1955	1962	1968	rBV	323698	533992	39.86%	5.890%
95	14.062	1993	1997	2001	rBV	12705	22100	1.65%	0.244%
96	14.324	2036	2040	2045	rVB5	7049	11770	0.88%	0.130%
97	14.495	2061	2068	2078	rVB3	5709	16936	1.26%	0.187%
98	14.684	2097	2099	2101	rBV3	2233	2337	0.17%	0.026%
99	15.232	2187	2189	2194	rVB6	4589	6411	0.48%	0.071%
100	15.397	2211	2216	2219	rBV5	6773	12452	0.93%	0.137%

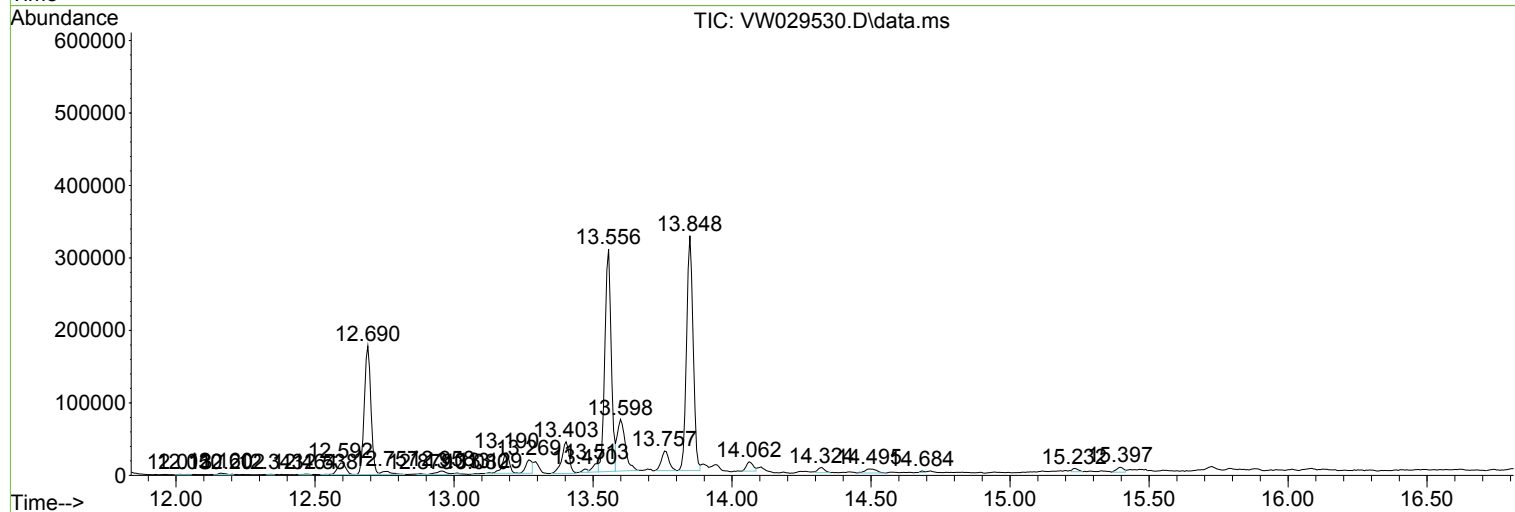
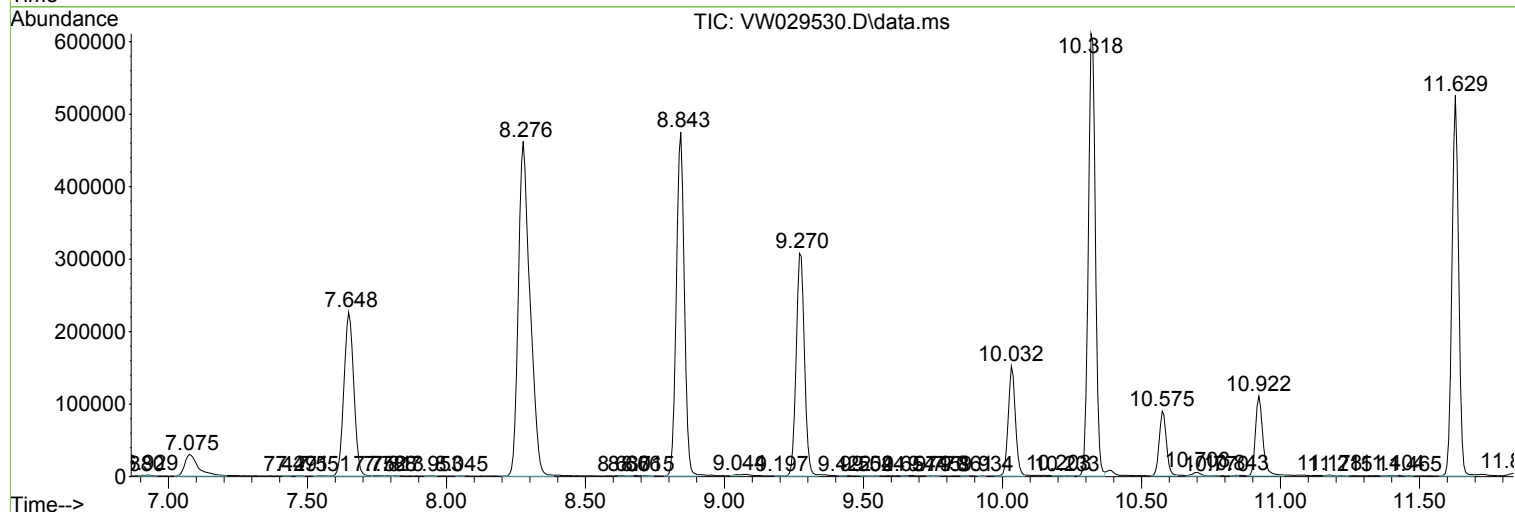
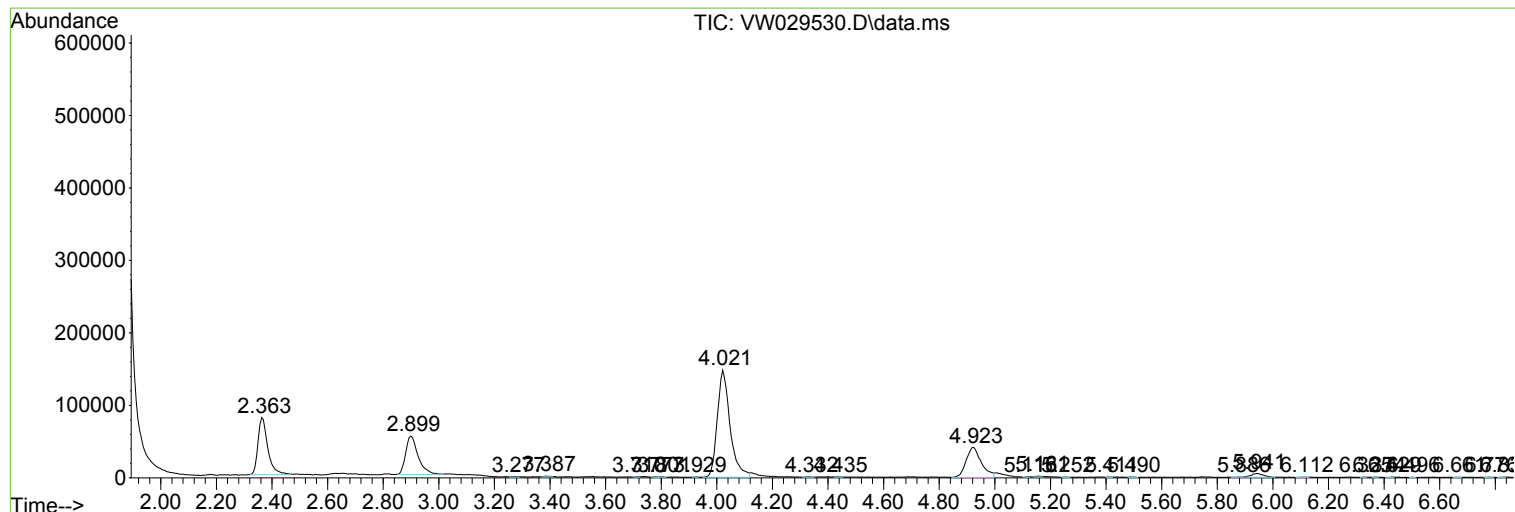
Sum of corrected areas: 9065672

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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



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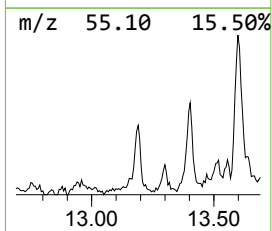
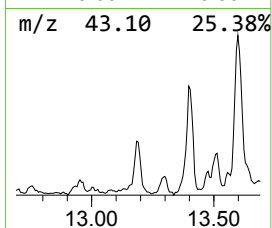
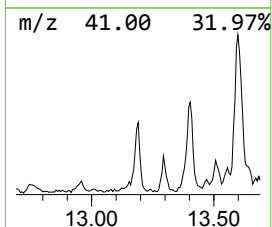
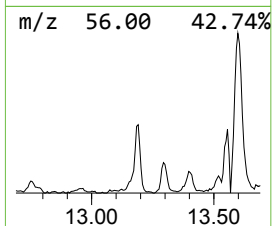
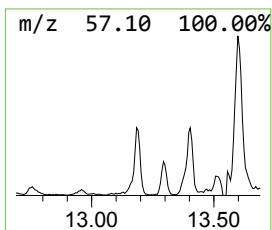
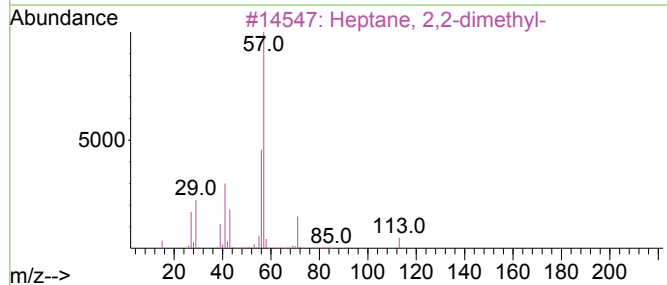
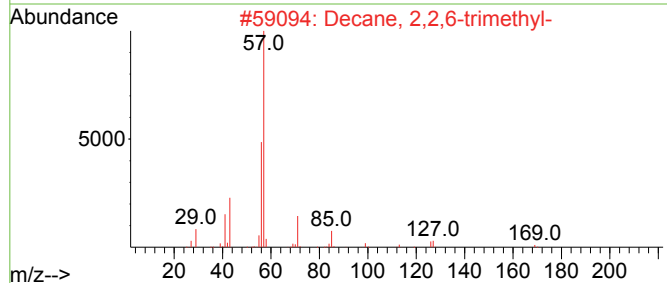
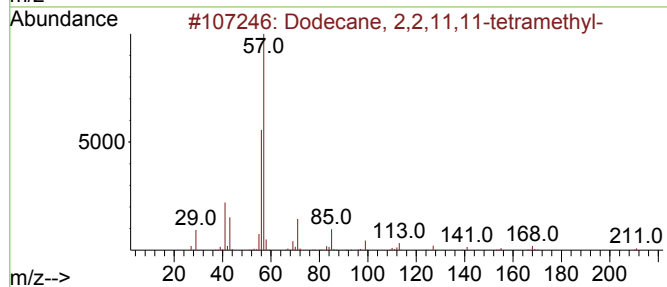
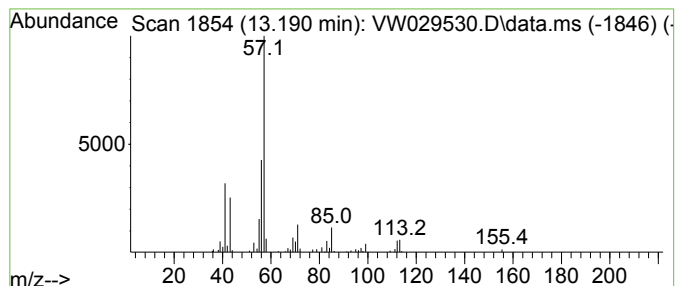
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	2.46 ug/L	48556	1,4-Dichlorobenzene-d4	13.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	72
2		Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	64
3		Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	59
4		Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	59
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53



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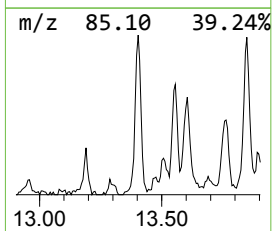
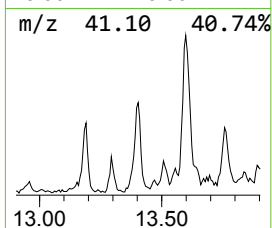
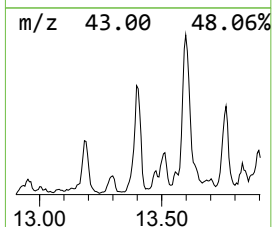
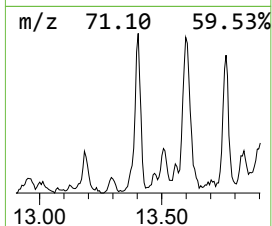
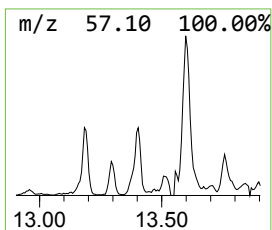
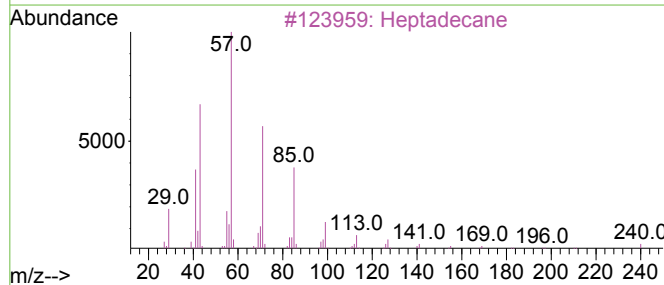
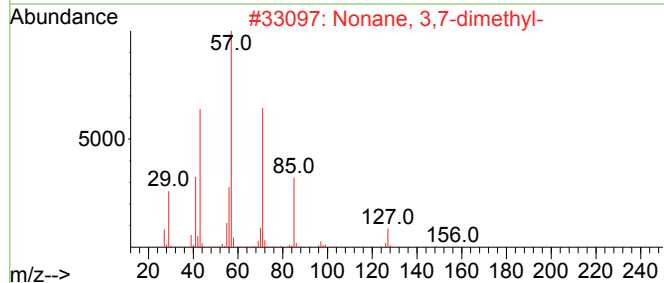
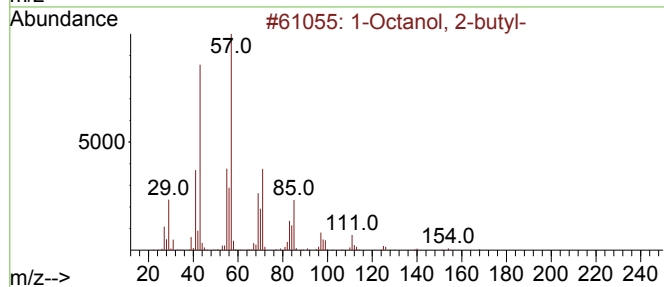
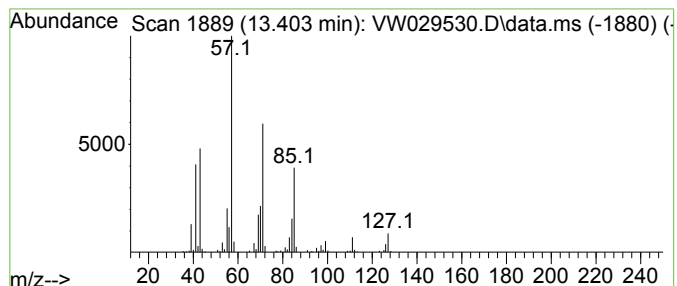
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 1-Octanol, 2-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.403	4.18 ug/L	82514	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	78
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
3			Heptadecane	240	C17H36	000629-78-7	64
4			Tridecane	184	C13H28	000629-50-5	64
5			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	59



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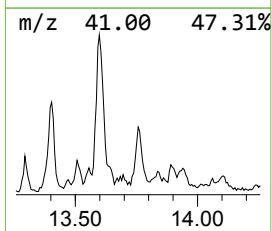
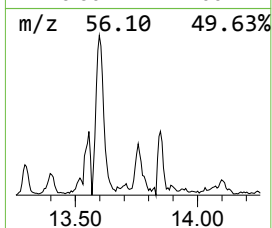
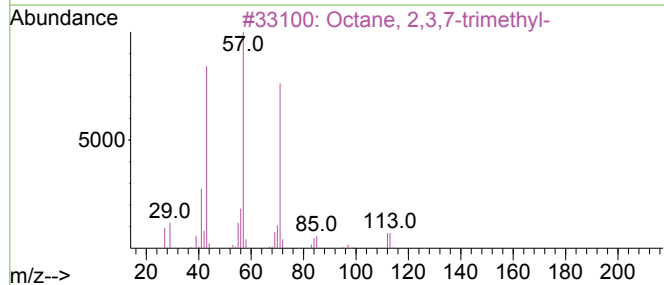
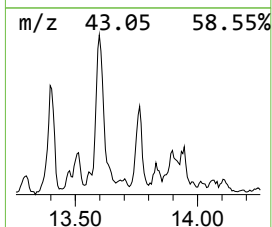
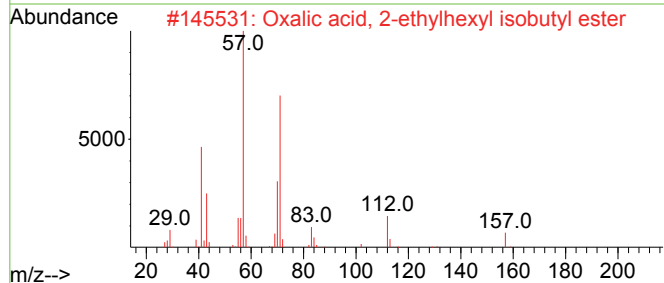
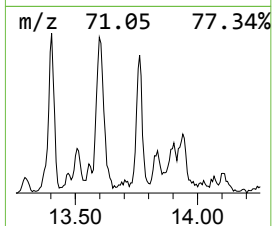
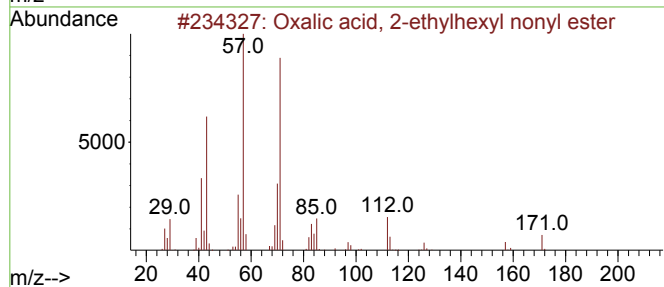
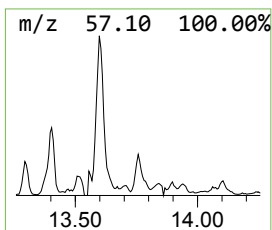
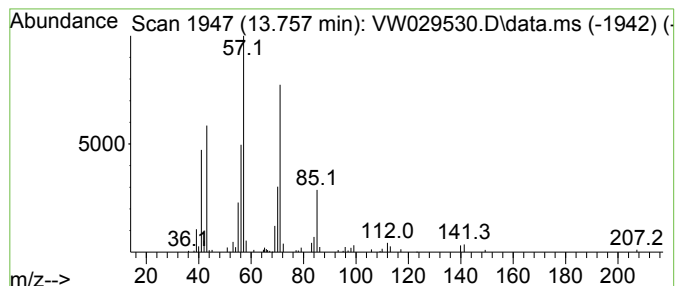
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 Oxalic acid, 2-ethylhexyl n... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	2.56 ug/L	50544	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, 2-ethylhexyl nonyl ...	328	C19H36O4	1000309-39-2	59
2			Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1010309-38-5	53
3			Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	53
4			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	53
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071124\
Data File : VW029530.D
Acq On : 11 Jul 2024 15:34
Operator : SY/MD
Sample : P3178-10
Misc : 5.49g/10mL/MSVOA_W/SOIL/A
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4BT5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM070824SMA.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...	13.190	2.5	ug/L	48556	3	13.556	493053	25.0
1-Octanol, 2-bu...	13.403	4.2	ug/L	82514	3	13.556	493053	25.0
Oxalic acid, 2-...	13.757	2.6	ug/L	50544	3	13.556	493053	25.0