

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW070224\
 Data File : VW029442.D
 Acq On : 02 Jul 2024 14:19
 Operator : SY/MD
 Sample : P3088-14RE
 Misc : 4.94g/10mL/MSVOA_W/SOIL/B
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4D02RE

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\SFAMWLM061824SMA.M
 Title : SFAM01.0

Signal : TIC: VW029442.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	72	78	90	rVB	47220	106968	18.62%	4.001%
2	2.899	160	166	183	rVB	35595	102757	17.89%	3.843%
3	3.399	241	248	254	rVB3	3039	7213	1.26%	0.270%
4	4.021	340	350	363	rBV	71846	217082	37.80%	8.119%
5	4.430	416	417	420	rVB2	740	457	0.08%	0.017%
6	4.533	431	434	435	rBV3	318	301	0.05%	0.011%
7	4.606	439	446	450	rBV4	1937	4876	0.85%	0.182%
8	4.923	486	498	503	rBV4	4839	16004	2.79%	0.599%
9	5.088	522	525	527	rBV3	334	485	0.08%	0.018%
10	5.265	552	554	556	rBV2	375	297	0.05%	0.011%
11	5.417	577	579	582	rVB2	375	371	0.06%	0.014%
12	5.454	582	585	586	rBV2	328	398	0.07%	0.015%
13	5.655	613	618	620	rBV4	606	968	0.17%	0.036%
14	5.716	626	628	630	rVB	459	260	0.05%	0.010%
15	5.801	637	642	644	rBV2	599	768	0.13%	0.029%
16	5.941	657	665	667	rBV4	1924	4292	0.75%	0.161%
17	6.057	680	684	685	rBV2	281	422	0.07%	0.016%
18	6.118	691	694	695	rBV2	354	355	0.06%	0.013%
19	6.423	742	744	745	rVB	376	257	0.04%	0.010%
20	6.478	749	753	756	rBV4	336	499	0.09%	0.019%
21	6.582	767	770	772	rVB2	529	583	0.10%	0.022%
22	6.612	772	775	777	rBV2	555	621	0.11%	0.023%
23	6.728	792	794	797	rVB3	492	470	0.08%	0.018%
24	6.758	797	799	801	rBV	250	268	0.05%	0.010%
25	6.819	807	809	813	rVB2	472	509	0.09%	0.019%
26	6.953	828	831	832	rVB2	411	404	0.07%	0.015%
27	6.972	832	834	836	rVB3	588	509	0.09%	0.019%
28	6.990	836	837	839	rBV	395	363	0.06%	0.014%
29	7.014	839	841	844	rVB4	449	350	0.06%	0.013%
30	7.081	845	852	860	rBV	8070	25943	4.52%	0.970%
31	7.356	895	897	899	rVB2	446	406	0.07%	0.015%
32	7.380	899	901	904	rBV3	540	670	0.12%	0.025%
33	7.533	925	926	927	rBV	557	239	0.04%	0.009%
34	7.648	936	945	956	rBV	114089	275488	47.97%	10.303%
35	7.770	964	965	970	rVB3	813	961	0.17%	0.036%
36	7.844	975	977	979	rVV3	556	385	0.07%	0.014%

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Integrator: RTE

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 Title : SFAM01.0

37	7.886	982	984	986	rVV	340	290	0.05%	0.011%
38	7.911	986	988	990	rVB	625	505	0.09%	0.019%
39	7.935	990	992	995	rBV3	323	430	0.07%	0.016%
40	7.965	995	997	1000	rVB3	469	527	0.09%	0.020%
41	8.148	1023	1027	1028	rVB2	573	495	0.09%	0.019%
42	8.276	1037	1048	1066	rBV2	180919	574338	100.00%	21.480%
43	8.502	1084	1085	1088	rVB2	503	308	0.05%	0.012%
44	8.532	1088	1090	1093	rVB2	497	435	0.08%	0.016%
45	8.575	1093	1097	1099	rBV3	587	920	0.16%	0.034%
46	8.612	1102	1103	1105	rVB2	534	283	0.05%	0.011%
47	8.642	1105	1108	1111	rVB3	555	808	0.14%	0.030%
48	8.673	1111	1113	1114	rBV	346	374	0.07%	0.014%
49	8.843	1132	1141	1151	rBV	150408	301782	52.54%	11.286%
50	9.008	1166	1168	1171	rVB3	498	362	0.06%	0.014%
51	9.057	1171	1176	1177	rBV2	1248	1712	0.30%	0.064%
52	9.191	1196	1198	1199	rBV	604	381	0.07%	0.014%
53	9.209	1199	1201	1202	rVV2	379	238	0.04%	0.009%
54	9.276	1203	1212	1222	rVV	139194	283560	49.37%	10.605%
55	9.544	1252	1256	1258	rBV3	625	823	0.14%	0.031%
56	9.612	1265	1267	1270	rBV3	291	268	0.05%	0.010%
57	9.721	1282	1285	1286	rVB2	472	400	0.07%	0.015%
58	9.752	1286	1290	1295	rBV6	493	879	0.15%	0.033%
59	9.837	1301	1304	1306	rBV3	720	739	0.13%	0.028%
60	9.892	1309	1313	1316	rVB4	1068	1812	0.32%	0.068%
61	9.971	1325	1326	1329	rVB2	346	261	0.05%	0.010%
62	10.032	1330	1336	1344	rVV	24408	46253	8.05%	1.730%
63	10.197	1361	1363	1365	rVB	351	262	0.05%	0.010%
64	10.246	1365	1371	1372	rBV4	938	1679	0.29%	0.063%
65	10.325	1376	1384	1392	rBV	122306	227467	39.61%	8.507%
66	10.581	1420	1426	1435	rVB	17415	33281	5.79%	1.245%
67	10.703	1440	1446	1452	rVB2	8639	15584	2.71%	0.583%
68	10.861	1470	1472	1475	rVB3	503	365	0.06%	0.014%
69	11.026	1495	1499	1503	rBV5	2048	3339	0.58%	0.125%
70	11.629	1588	1598	1606	rBV	83436	153268	26.69%	5.732%
71	11.770	1618	1621	1622	rBV3	394	418	0.07%	0.016%
72	12.032	1662	1664	1665	rBV3	358	235	0.04%	0.009%
73	12.160	1683	1685	1688	rBV	549	768	0.13%	0.029%
74	12.343	1711	1715	1716	rBV2	425	507	0.09%	0.019%
75	12.465	1731	1735	1741	rVB5	1674	2804	0.49%	0.105%
76	12.599	1749	1757	1763	rBV	16972	28959	5.04%	1.083%

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Integration Parameters: LSCINT.P

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 Title : SFAM01.0

77	12.690	1765	1772	1779	rVV	41499	69258	12.06%	2.590%
78	12.757	1782	1783	1792	rVB5	794	1545	0.27%	0.058%
79	12.922	1808	1810	1813	rBV2	1109	1362	0.24%	0.051%
80	13.117	1837	1842	1845	rBV4	1568	2609	0.45%	0.098%
81	13.190	1845	1854	1858	rBV	3539	7893	1.37%	0.295%
82	13.294	1866	1871	1880	rVB5	2004	4070	0.71%	0.152%
83	13.404	1883	1889	1894	rVB3	5288	9382	1.63%	0.351%
84	13.471	1897	1900	1905	rVB5	3556	5772	1.00%	0.216%
85	13.556	1909	1914	1918	rBV	27438	43623	7.60%	1.631%
86	13.849	1956	1962	1968	rBV2	22752	39556	6.89%	1.479%
87	14.056	1992	1996	2003	rBV2	6622	11097	1.93%	0.415%
88	14.324	2037	2040	2045	rVB4	2240	3515	0.61%	0.131%
89	14.385	2048	2050	2052	rBV2	674	545	0.09%	0.020%
90	14.513	2068	2071	2076	rVB3	3862	6014	1.05%	0.225%
91	14.794	2114	2117	2121	rBV4	733	1168	0.20%	0.044%
92	14.928	2135	2139	2141	rBV4	553	838	0.15%	0.031%
93	15.050	2155	2159	2160	rBV2	539	636	0.11%	0.024%
94	15.098	2166	2167	2169	rVB2	778	453	0.08%	0.017%
95	15.172	2177	2179	2180	rBV2	568	498	0.09%	0.019%
96	15.470	2226	2228	2230	rBV2	754	763	0.13%	0.029%
97	15.793	2280	2281	2284	rVB2	691	481	0.08%	0.018%
98	16.549	2404	2405	2408	rVB2	604	400	0.07%	0.015%
99	16.586	2408	2411	2413	rBV2	912	770	0.13%	0.029%
100	16.738	2434	2436	2437	rBV2	446	286	0.05%	0.011%

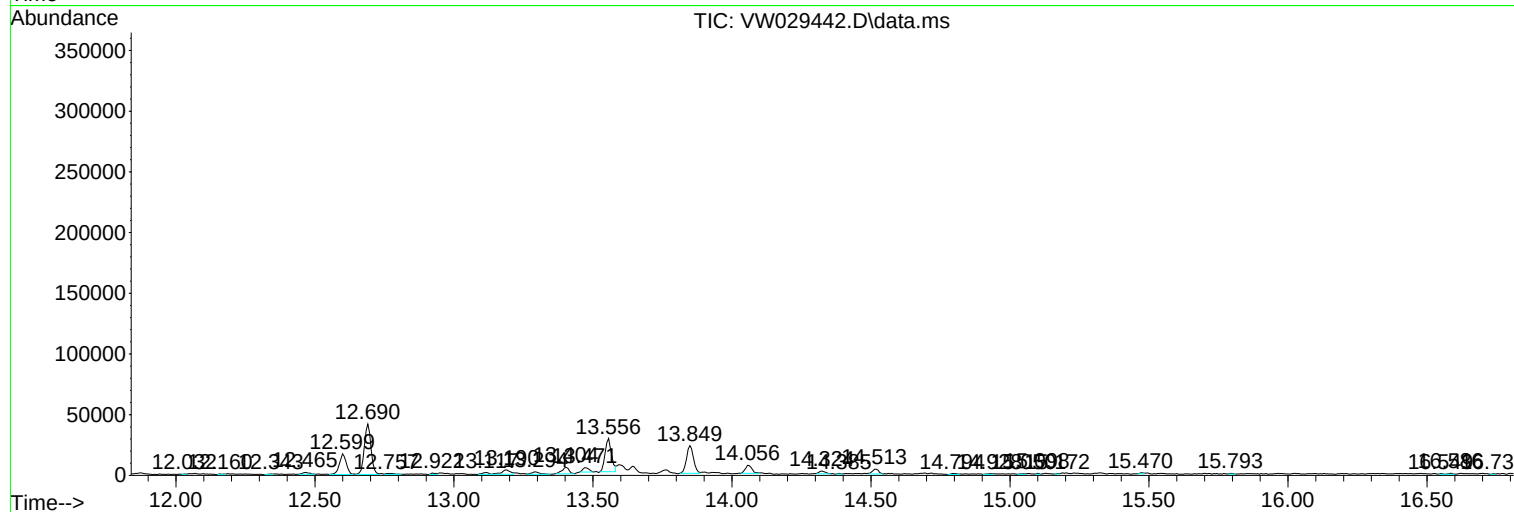
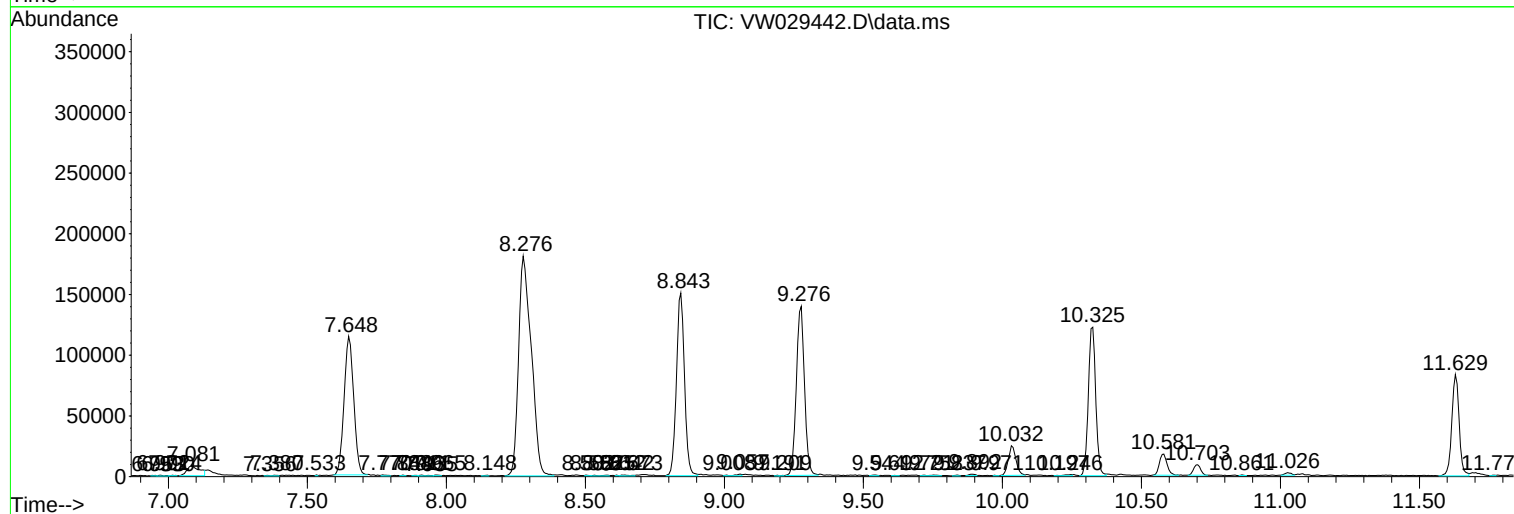
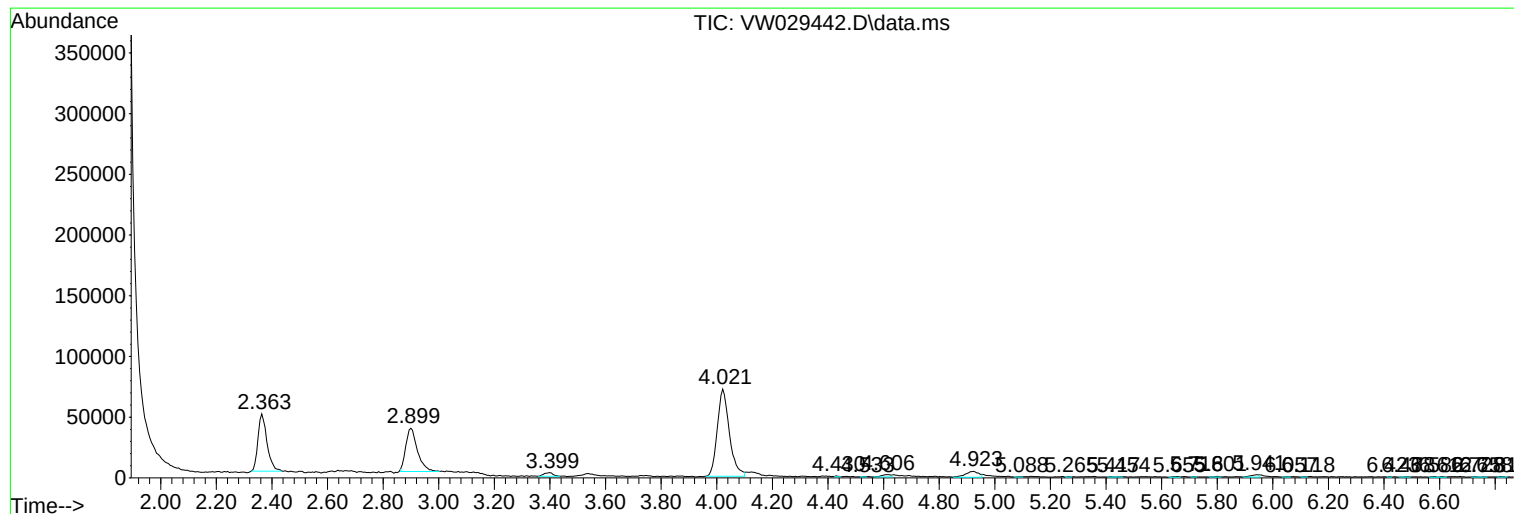
Sum of corrected areas: 2673852

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4D02RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.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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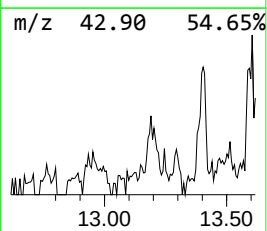
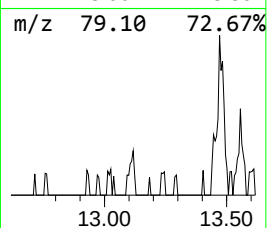
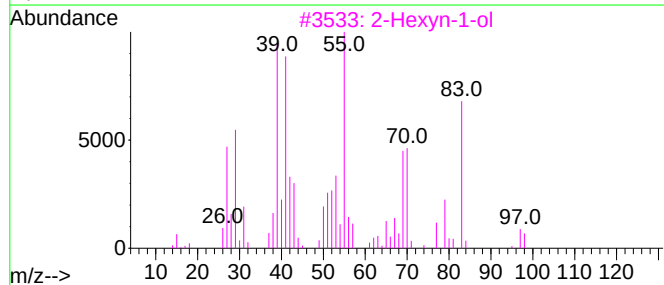
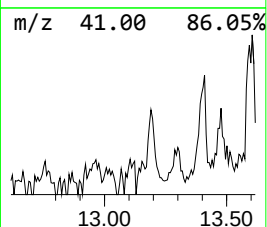
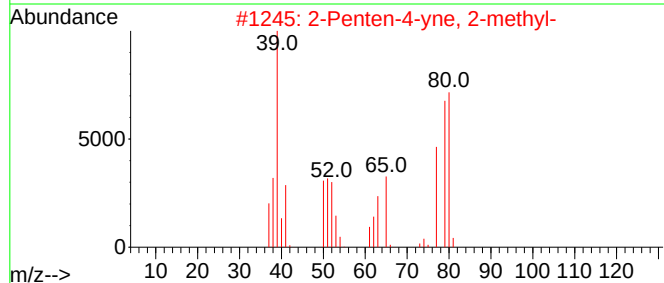
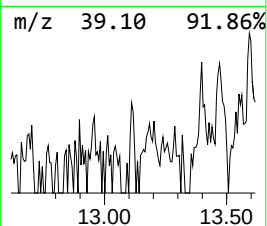
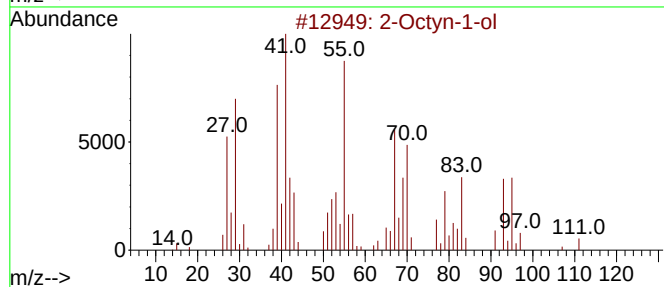
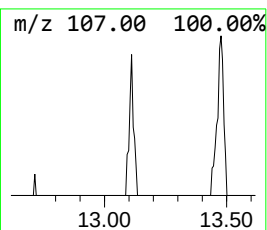
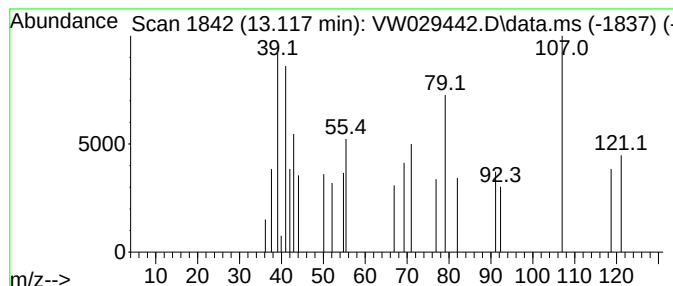
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-01 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.117	1.50 ug/L	2609	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octyn-1-ol	126	C8H14O	020739-58-6	37
2			2-Penten-4-yne, 2-methyl-	80	C6H8	001595-53-5	25
3			2-Hexyn-1-ol	98	C6H10O	000764-60-3	25
4			1-Cyclohexene-1-methanol	112	C7H12O	004845-04-9	23
5			5-Nonynoic acid	154	C9H14O2	056630-34-3	23



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A4D02RE

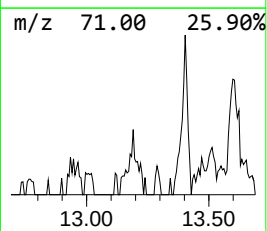
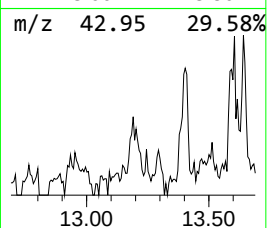
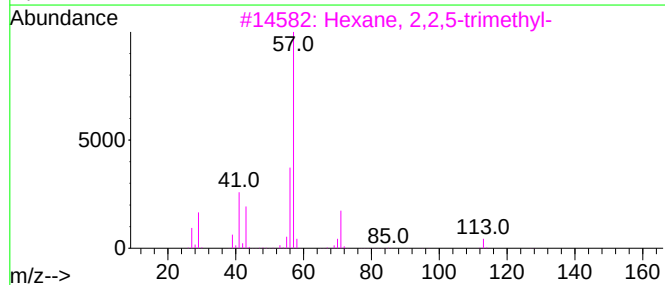
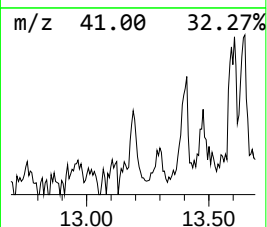
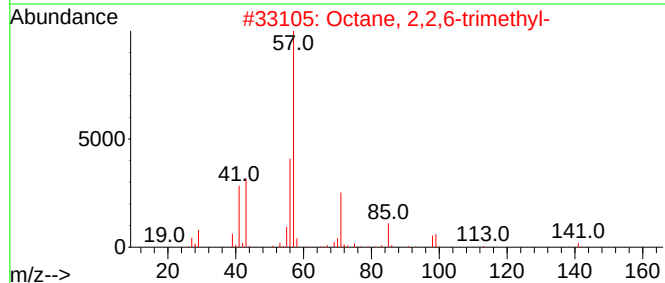
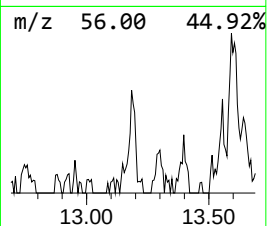
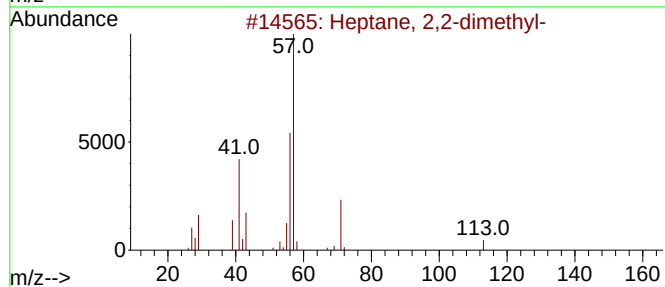
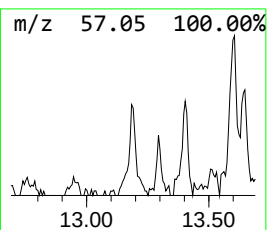
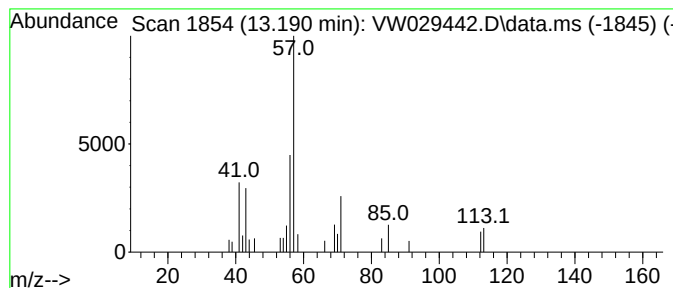
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	4.52 ug/L	7893	1,4-Dichlorobenzene-d4	13.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	50
2		Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	50
3		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	50
4		Heptane, 5-ethyl-2,2,3-trimethyl-	170	C12H26	062199-06-8	50
5		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	50



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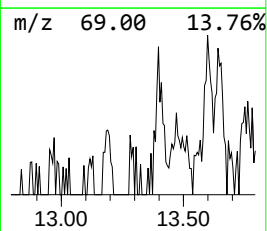
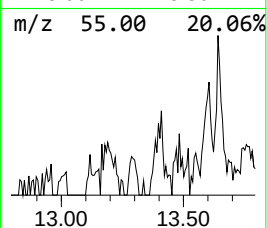
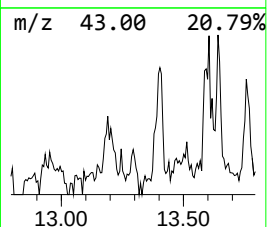
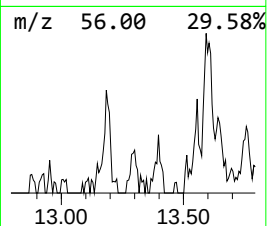
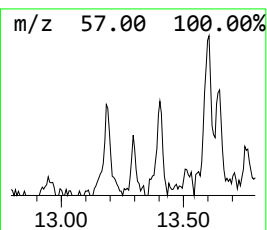
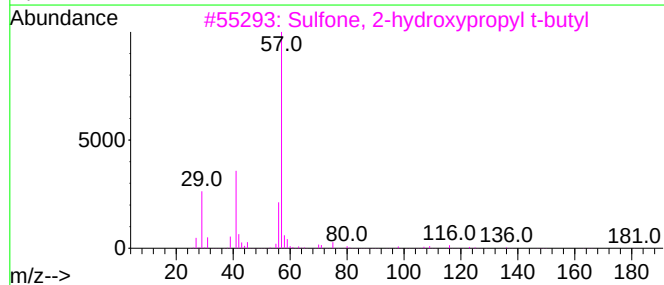
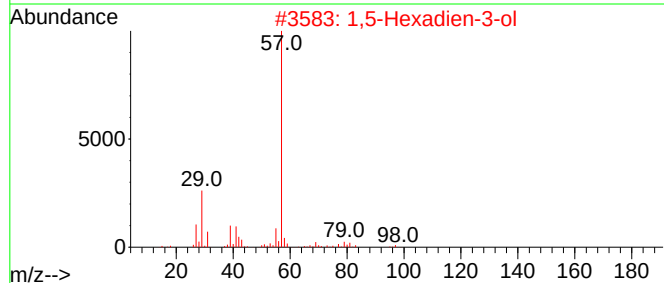
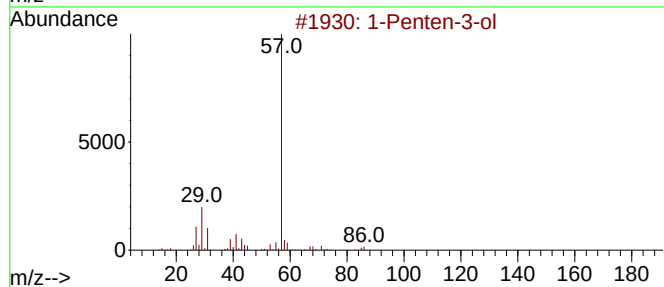
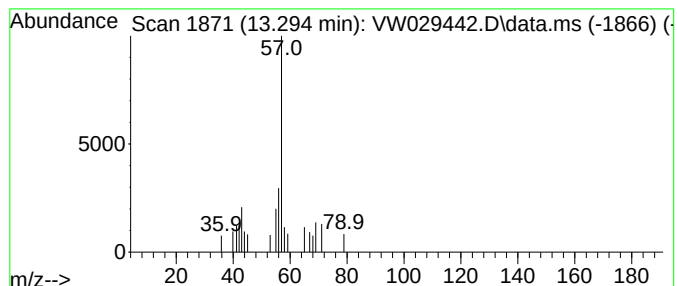
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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

Peak Number 7 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.294	2.33 ug/L	4070	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Penten-3-ol	86	C5H10O	000616-25-1	9
2			1,5-Hexadien-3-ol	98	C6H10O	000924-41-4	9
3			Sulfone, 2-hydroxypropyl t-butyl	180	C7H16O3S	154619-05-3	9
4			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	9
5			Azetidine	57	C3H7N	000503-29-7	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW070224\
Data File : VW029442.D
Acq On : 02 Jul 2024 14:19
Operator : SY/MD
Sample : P3088-14RE
Misc : 4.94g/10mL/MSVOA_W/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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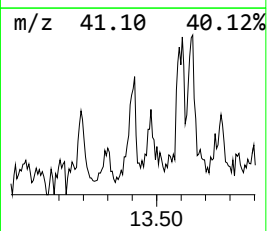
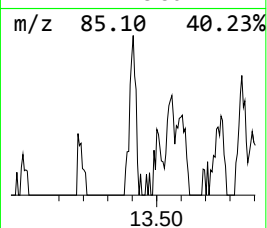
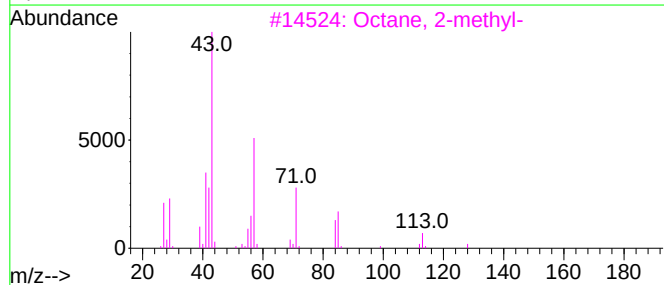
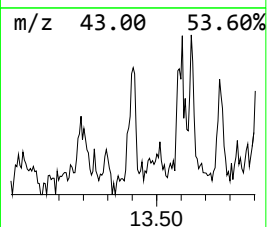
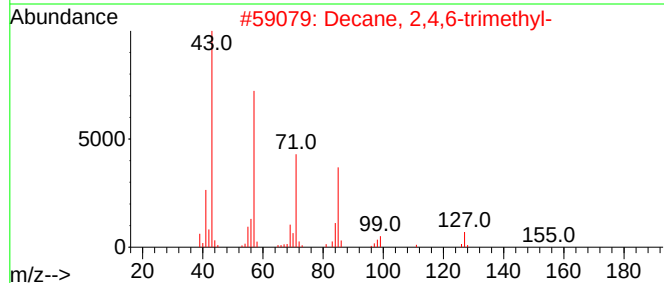
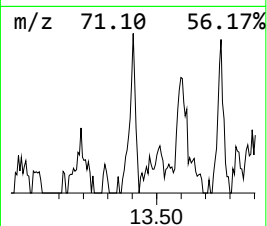
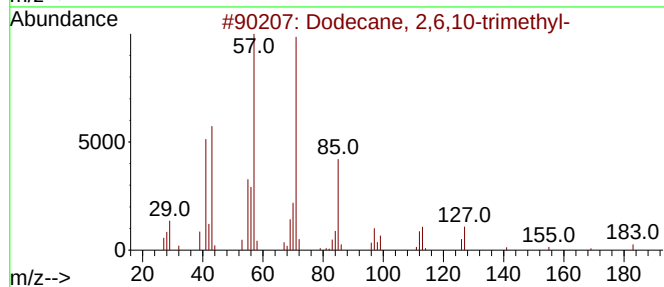
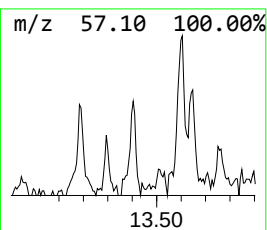
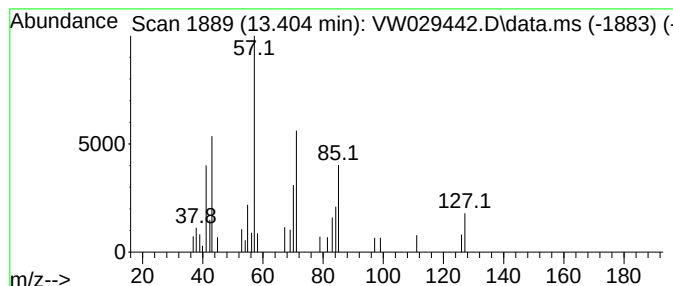
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Quant Title : SFAM01.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.403	5.38 ug/L	9382	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	53
2			Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	50
3			Octane, 2-methyl-	128	C9H20	003221-61-2	50
4			Nonane, 5-(1-methylpropyl)-	184	C13H28	062185-54-0	50
5			Nonane, 5-butyl-	184	C13H28	017312-63-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW070224\
Data File : VW029442.D
Acq On : 02 Jul 2024 14:19
Operator : SY/MD
Sample : P3088-14RE
Misc : 4.94g/10mL/MSVOA_W/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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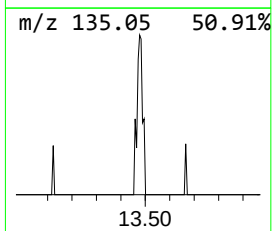
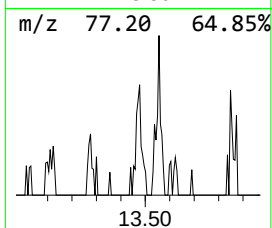
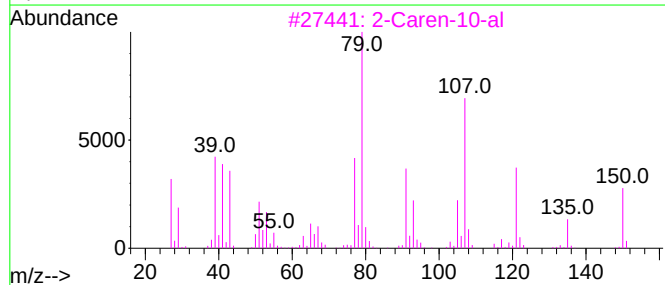
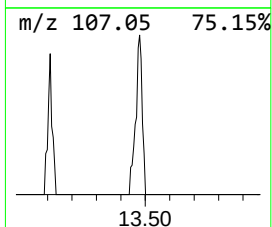
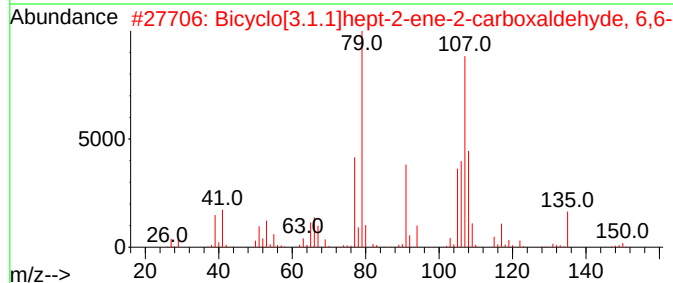
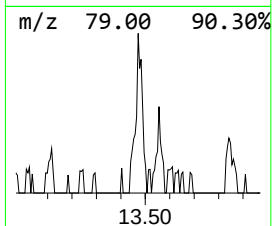
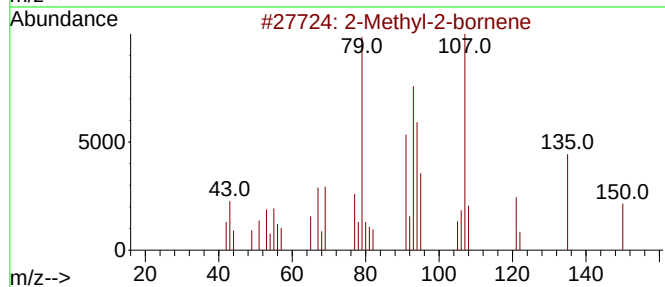
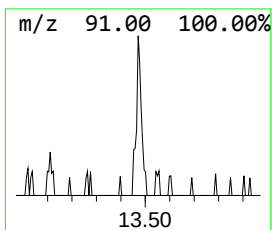
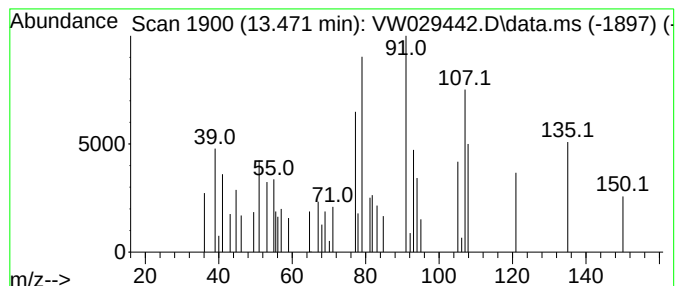
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Quant Title : SFAM01.0

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

Peak Number 9 2-Methyl-2-bornene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.471	3.31 ug/L	5772	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-2-bornene	150	C11H18	072540-93-3	59
2			Bicyclo[3.1.1]hept-2-ene-2-carbo...	150	C10H14O	000564-94-3	53
3			2-Caren-10-al	150	C10H14O	1000151-85-9	49
4			Propionic acid, 2,3-dihydroxy-3-...	182	C9H10O4	1000303-10-7	47
5			Benzenemethanol, .alpha.-2-prope...	148	C10H12O	000936-58-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW070224\
Data File : VW029442.D
Acq On : 02 Jul 2024 14:19
Operator : SY/MD
Sample : P3088-14RE
Misc : 4.94g/10mL/MSVOA_W/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4D02RE

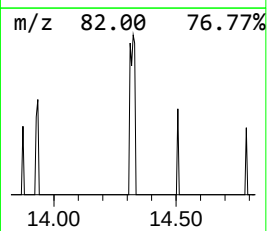
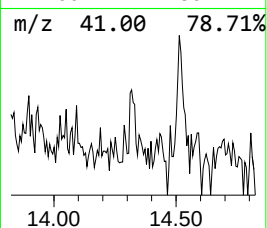
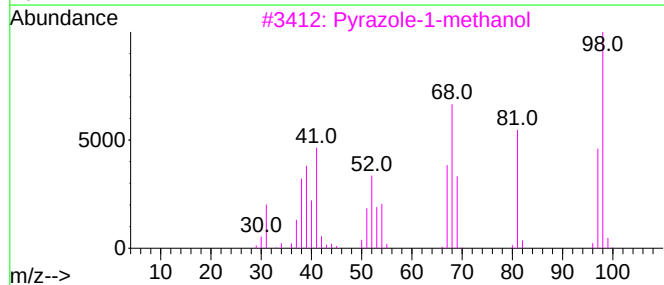
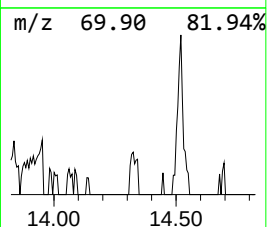
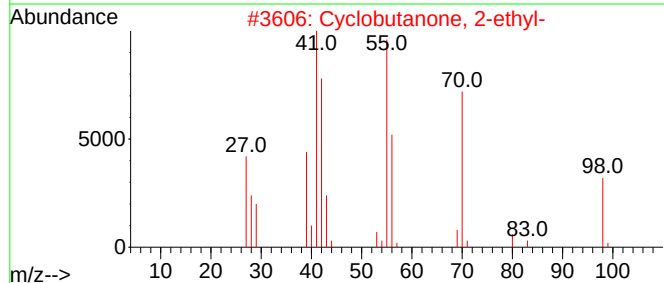
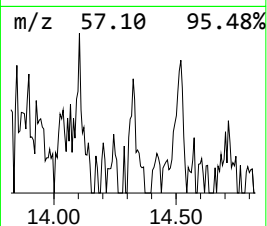
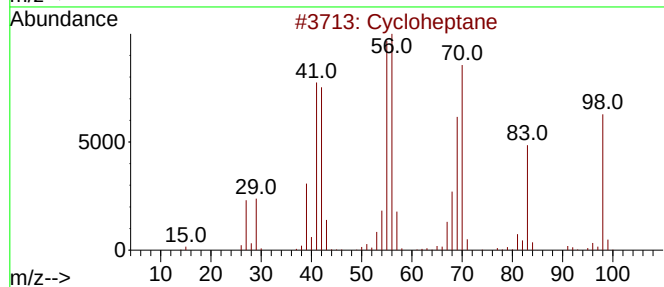
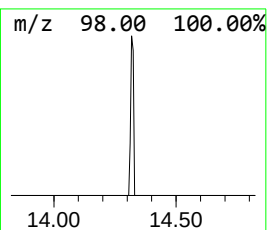
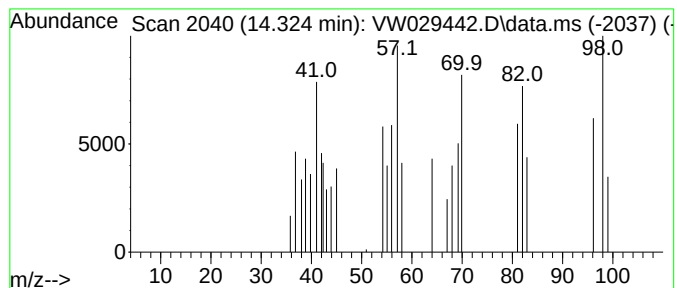
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Quant Title : SFAM01.0

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

Peak Number 11 (DEL) Alkane: Cyclic14.324 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.324	2.01 ug/L	3515	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloheptane	98	C7H14	000291-64-5	10
2			Cyclobutanone, 2-ethyl-	98	C6H10O	010374-14-8	10
3			Pyrazole-1-methanol	98	C4H6N2O	001120-82-7	10
4			1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	9
5			1H-Tetrazaborole, 4,5-dihydro-1,...	98	C2H7BN4	006982-51-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW070224\
Data File : VW029442.D
Acq On : 02 Jul 2024 14:19
Operator : SY/MD
Sample : P3088-14RE
Misc : 4.94g/10mL/MSVOA_W/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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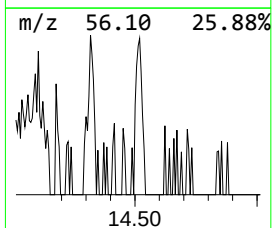
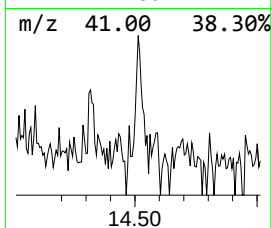
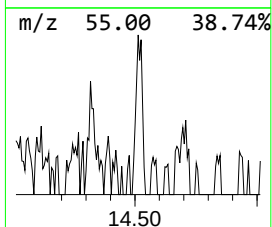
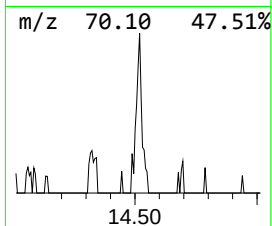
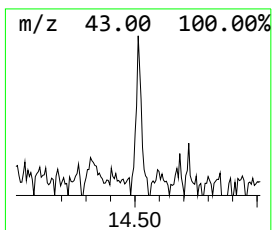
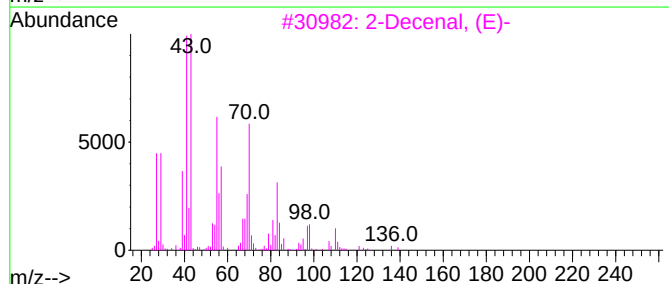
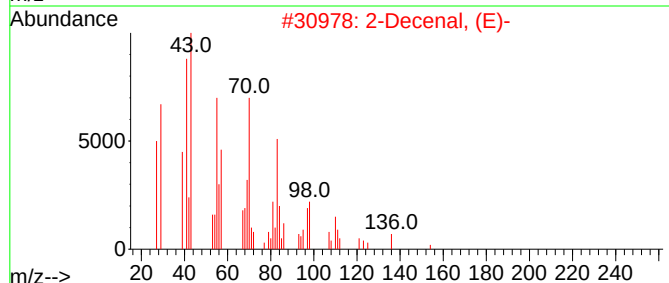
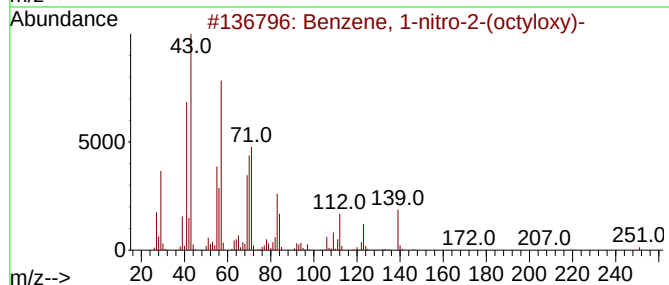
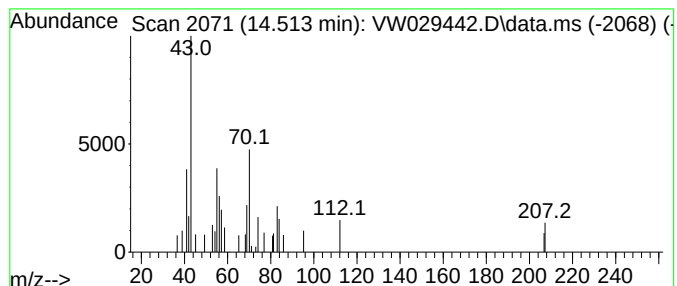
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Quant Title : SFAM01.0

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

Peak Number 12 Benzene, 1-nitro-2-(octyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.513	3.45 ug/L	6014	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-nitro-2-(octyloxy)-	251	C14H21NO3	037682-29-4	50
2			2-Decenal, (E)-	154	C10H18O	003913-81-3	47
3			2-Decenal, (E)-	154	C10H18O	003913-81-3	40
4			Bromoacetic acid, decyl ester	278	C12H23BrO2	005436-93-1	37
5			Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW070224\
Data File : VW029442.D
Acq On : 02 Jul 2024 14:19
Operator : SY/MD
Sample : P3088-14RE
Misc : 4.94g/10mL/MSVOA_W/SOIL/B
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4D02RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	13.117	1.5	ug/L	2609	3	13.556	43623	25.0
(DEL) Alkane: S...	13.190	4.5	ug/L	7893	3	13.556	43623	25.0
unknown-02	13.294	2.3	ug/L	4070	3	13.556	43623	25.0
(DEL) Alkane: S...	13.403	5.4	ug/L	9382	3	13.556	43623	25.0
2-Methyl-2-bornene	13.471	3.3	ug/L	5772	3	13.556	43623	25.0
(DEL) Alkane: C...	14.324	2.0	ug/L	3515	3	13.556	43623	25.0
Benzene, 1-nitr...	14.513	3.5	ug/L	6014	3	13.556	43623	25.0