

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW102021\
 Data File : VW020647.D
 Acq On : 20 Oct 2021 12:12
 Operator : SY/VA
 Sample : M4264-02
 Misc : 4.41g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GB7G7

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\SFAMWLM100821SMA.M
 Title : SFAM01.0

Signal : TIC: VW020647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.349	68	73	85	rVB	66475	108878	12.99%	1.644%
2	2.495	91	97	108	rVB	27001	51696	6.17%	0.780%
3	2.702	129	131	132	rBV2	667	366	0.04%	0.006%
4	2.879	154	160	173	rVB	23218	48159	5.75%	0.727%
5	3.026	179	184	191	rVB5	725	1738	0.21%	0.026%
6	3.141	199	203	204	rBV3	301	450	0.05%	0.007%
7	3.385	235	243	253	rVB2	5023	12151	1.45%	0.183%
8	3.525	264	266	267	rBV	311	241	0.03%	0.004%
9	3.727	294	299	308	rVB4	658	1566	0.19%	0.024%
10	3.836	314	317	320	rBV2	214	246	0.03%	0.004%
11	4.019	334	347	358	rBV2	94194	293125	34.98%	4.425%
12	4.129	358	365	379	rVV	19971	56276	6.72%	0.849%
13	4.263	379	387	396	rVB3	1347	4144	0.49%	0.063%
14	4.385	399	407	416	rBV3	1141	3922	0.47%	0.059%
15	4.446	416	417	420	rVB2	324	275	0.03%	0.004%
16	4.598	438	442	445	rBV3	231	436	0.05%	0.007%
17	4.684	450	456	465	rVB3	801	1930	0.23%	0.029%
18	4.922	485	495	503	rBV3	2610	8310	0.99%	0.125%
19	5.787	627	637	651	rBV3	2586	8383	1.00%	0.127%
20	5.940	657	662	670	rVB3	1102	2732	0.33%	0.041%
21	6.110	683	690	691	rBV3	653	981	0.12%	0.015%
22	6.903	809	820	831	rBV3	5264	15077	1.80%	0.228%
23	7.086	840	850	861	rBV	24269	68468	8.17%	1.034%
24	7.555	917	927	929	rBV2	253	522	0.06%	0.008%
25	7.647	932	942	956	rBV	134874	342627	40.89%	5.172%
26	8.275	1033	1045	1059	rBV2	275723	838005	100.00%	12.650%
27	8.549	1087	1090	1109	rVB5	7290	21117	2.52%	0.319%
28	8.707	1109	1116	1126	rVB3	3518	9366	1.12%	0.141%
29	8.842	1130	1138	1150	rBV	266737	524792	62.62%	7.922%
30	9.043	1165	1171	1176	rBV3	973	2180	0.26%	0.033%
31	9.146	1186	1188	1195	rVB3	228	413	0.05%	0.006%
32	9.274	1199	1209	1224	rBV	201583	407652	48.65%	6.154%
33	9.409	1224	1231	1244	rVV	42973	81621	9.74%	1.232%
34	9.512	1244	1248	1252	rVB2	400	642	0.08%	0.010%
35	9.659	1268	1272	1277	rBV4	423	677	0.08%	0.010%
36	9.915	1311	1314	1318	rBV3	176	283	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
 Title : SFAM01.0

37	10.037	1326	1334	1345	rBV	106549	188629	22.51%	2.847%
38	10.213	1359	1363	1368	rVB3	230	439	0.05%	0.007%
39	10.323	1372	1381	1388	rBV	370664	651750	77.77%	9.838%
40	10.384	1388	1391	1403	rVB	11807	21978	2.62%	0.332%
41	10.506	1405	1411	1416	rBV3	1221	1986	0.24%	0.030%
42	10.579	1416	1423	1430	rBV	68926	117532	14.03%	1.774%
43	10.628	1430	1431	1438	rVB3	2017	2697	0.32%	0.041%
44	10.701	1438	1443	1448	rBV	7981	13635	1.63%	0.206%
45	10.841	1461	1466	1469	rBV	180	274	0.03%	0.004%
46	10.927	1473	1480	1494	rBV	102206	173243	20.67%	2.615%
47	11.073	1496	1504	1519	rBV	509021	825806	98.54%	12.466%
48	11.414	1555	1560	1566	rVB5	815	1614	0.19%	0.024%
49	11.573	1582	1586	1588	rVV3	627	863	0.10%	0.013%
50	11.634	1588	1596	1605	rVV	330714	555393	66.28%	8.384%
51	11.713	1605	1609	1610	rBV3	812	845	0.10%	0.013%
52	11.841	1624	1630	1639	rVB4	5594	12144	1.45%	0.183%
53	11.945	1639	1647	1653	rBV3	6323	11937	1.42%	0.180%
54	12.012	1653	1658	1668	rVV	7439	13801	1.65%	0.208%
55	12.091	1670	1671	1677	rVV4	738	1173	0.14%	0.018%
56	12.170	1679	1684	1690	rVV5	1155	2527	0.30%	0.038%
57	12.237	1690	1695	1701	rVV3	1171	2163	0.26%	0.033%
58	12.335	1706	1711	1727	rVV	23186	39298	4.69%	0.593%
59	12.463	1727	1732	1735	rVV2	321	428	0.05%	0.006%
60	12.603	1747	1755	1763	rBV2	10759	18507	2.21%	0.279%
61	12.695	1763	1770	1776	rBV	127422	209751	25.03%	3.166%
62	12.756	1776	1780	1786	rVB3	1755	3036	0.36%	0.046%
63	12.798	1786	1787	1792	rVB2	338	278	0.03%	0.004%
64	12.877	1795	1800	1801	rBV2	236	413	0.05%	0.006%
65	13.048	1822	1828	1832	rBV4	2536	4671	0.56%	0.071%
66	13.097	1832	1836	1840	rVV2	5188	7856	0.94%	0.119%
67	13.207	1849	1854	1859	rVB3	1790	2801	0.33%	0.042%
68	13.274	1859	1865	1874	rVB7	2538	7252	0.87%	0.109%
69	13.396	1879	1885	1892	rBV2	24359	38530	4.60%	0.582%
70	13.475	1892	1898	1901	rBV4	1580	2593	0.31%	0.039%
71	13.554	1905	1911	1918	rBV	211842	344637	41.13%	5.202%
72	13.646	1922	1926	1934	rVB2	6176	10324	1.23%	0.156%
73	13.713	1934	1937	1940	rBV4	263	316	0.04%	0.005%
74	13.768	1942	1946	1947	rBV3	697	965	0.12%	0.015%
75	13.853	1953	1960	1967	rBV	182540	302394	36.08%	4.565%
76	14.017	1982	1987	1991	rBV3	4486	7157	0.85%	0.108%

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 Title : SFAM01.0

77	14.066	1991	1995	2005	rVB3	15224	26102	3.11%	0.394%
78	14.188	2012	2015	2018	rBV2	376	468	0.06%	0.007%
79	14.322	2030	2037	2043	rBV	17122	26705	3.19%	0.403%
80	14.389	2045	2048	2052	rVB4	1041	1471	0.18%	0.022%
81	14.517	2060	2069	2075	rBV4	1850	3915	0.47%	0.059%
82	14.621	2080	2086	2090	rBV4	2012	3583	0.43%	0.054%
83	14.725	2098	2103	2107	rVB3	1303	2167	0.26%	0.033%
84	14.792	2112	2114	2120	rVB4	230	296	0.04%	0.004%
85	14.877	2123	2128	2134	rVB4	674	1302	0.16%	0.020%
86	14.950	2134	2140	2146	rBV3	3187	6043	0.72%	0.091%
87	15.066	2155	2159	2161	rBV4	550	897	0.11%	0.014%
88	15.133	2166	2170	2172	rBV3	955	1358	0.16%	0.020%
89	15.176	2173	2177	2184	rVB4	2980	5167	0.62%	0.078%
90	15.249	2185	2189	2195	rBV4	917	1740	0.21%	0.026%
91	15.304	2196	2198	2199	rVB2	386	239	0.03%	0.004%
92	15.395	2203	2213	2220	rBV7	2023	5272	0.63%	0.080%
93	15.487	2223	2228	2232	rVV2	2857	5254	0.63%	0.079%
94	15.554	2236	2239	2245	rVB5	1136	1482	0.18%	0.022%
95	15.792	2274	2278	2283	rVB3	922	1640	0.20%	0.025%
96	15.846	2283	2287	2301	rVB5	2287	4954	0.59%	0.075%
97	15.962	2301	2306	2313	rVB3	1335	2673	0.32%	0.040%
98	16.017	2313	2315	2317	rBV2	316	256	0.03%	0.004%
99	16.096	2324	2328	2331	rVB3	311	307	0.04%	0.005%
100	16.359	2369	2371	2375	rVB3	279	295	0.04%	0.004%

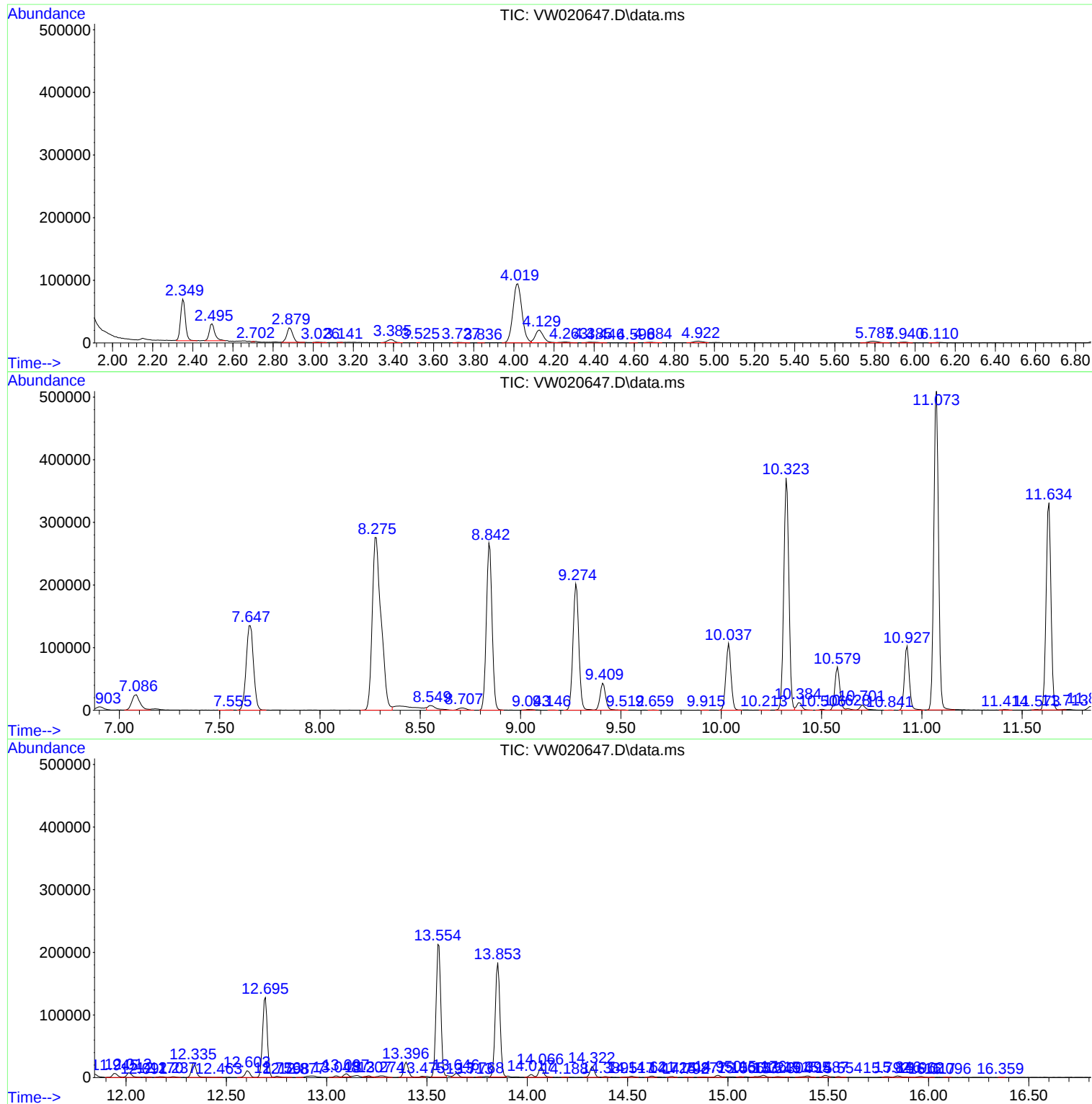
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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



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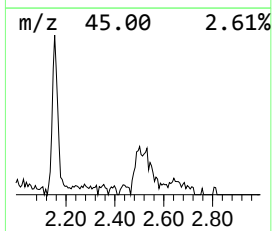
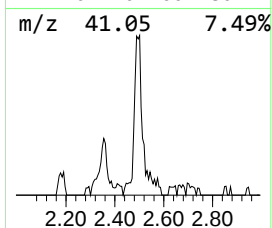
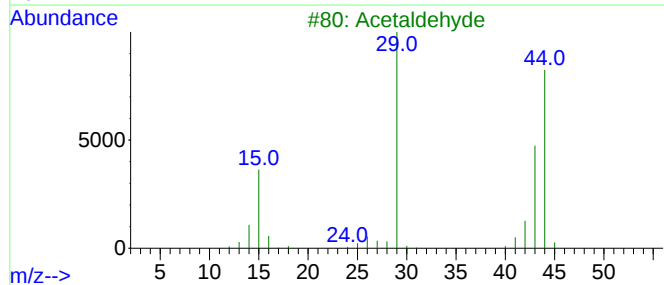
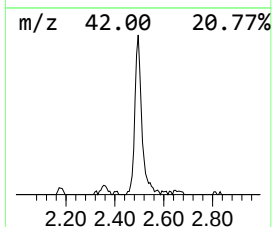
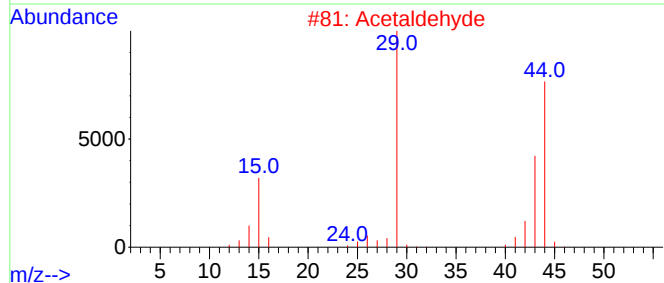
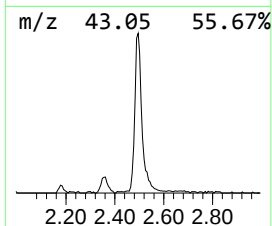
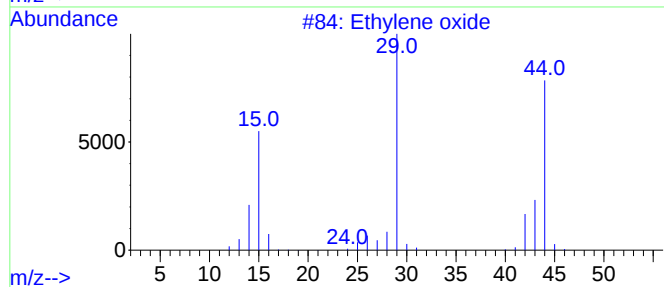
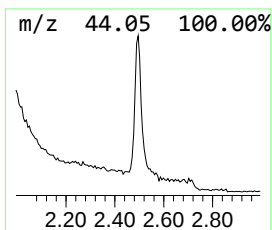
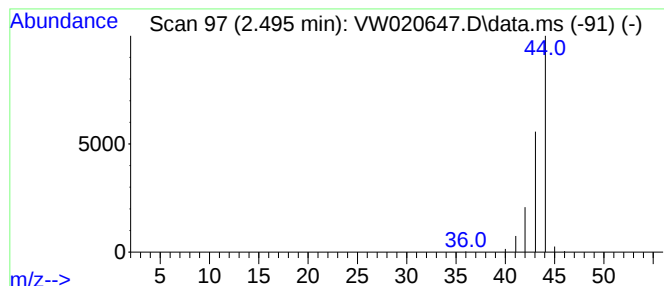
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.495	2.46 ug/L	51696	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene oxide	44	C2H4O	000075-21-8	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Acetaldehyde	44	C2H4O	000075-07-0	9
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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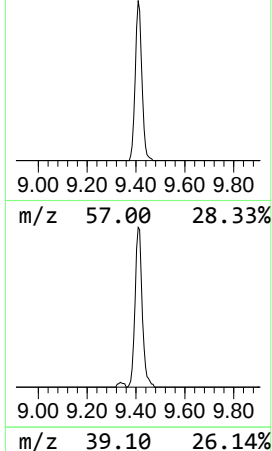
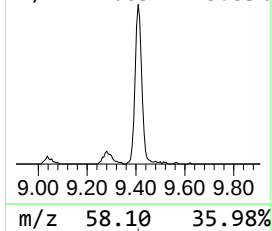
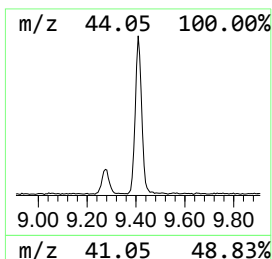
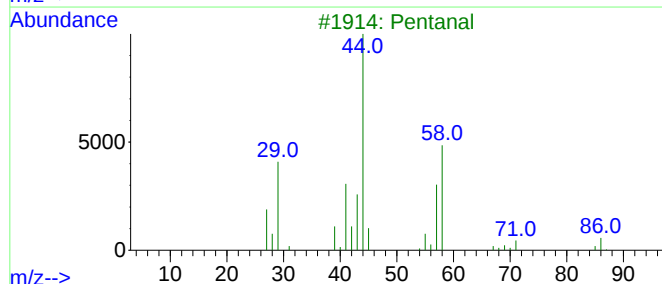
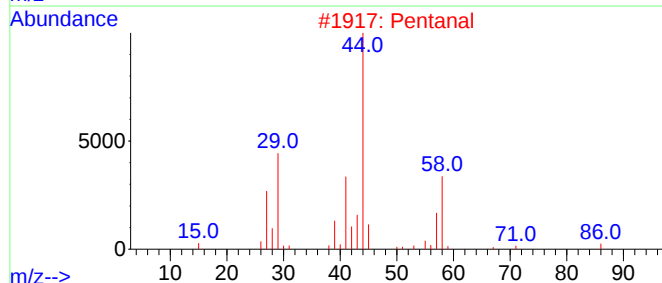
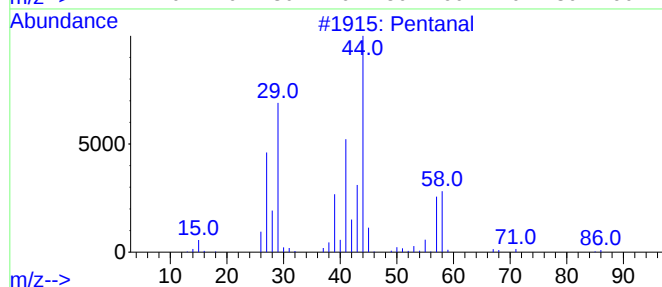
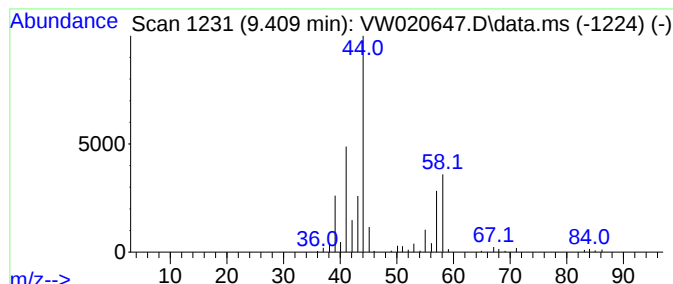
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.409	3.89 ug/L	81621	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	90
2	Pentanal			86	C5H10O	000110-62-3	74
3	Pentanal			86	C5H10O	000110-62-3	56
4	Butanal, 3-methyl-			86	C5H10O	000590-86-3	50
5	Pentanal			86	C5H10O	000110-62-3	49



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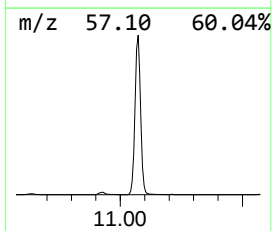
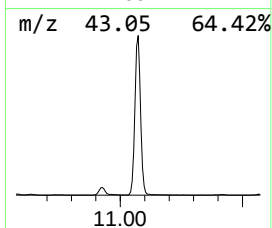
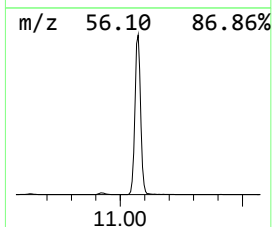
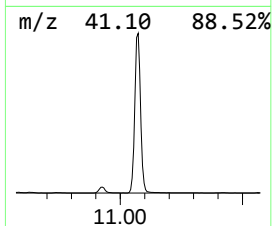
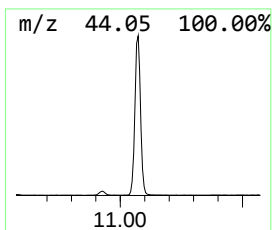
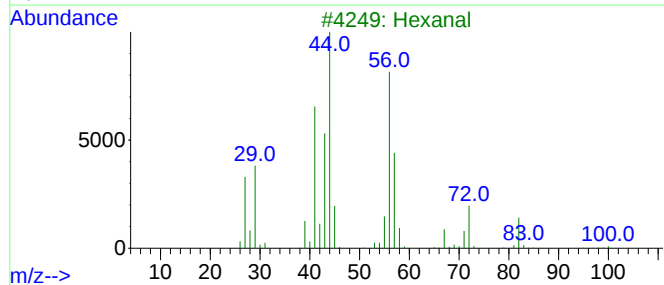
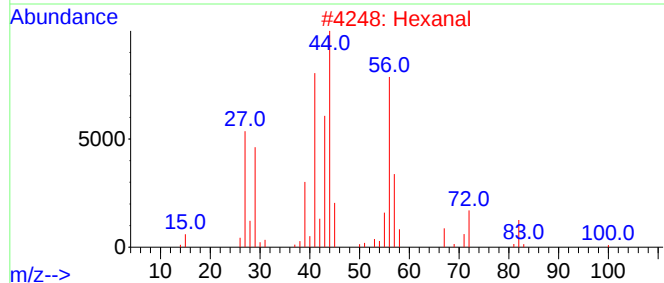
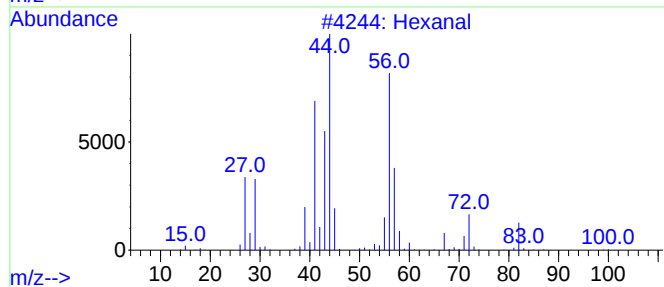
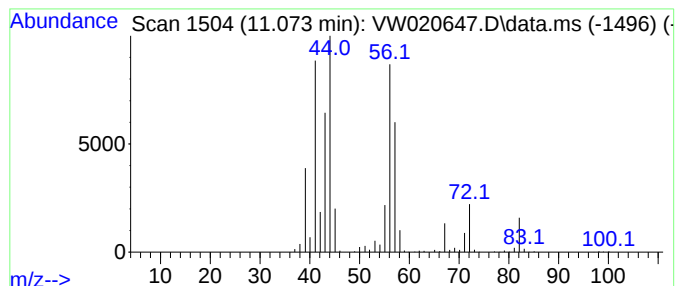
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	37.17 ug/L	825806	Chlorobenzene-d5	11.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	87
2	Hexanal			100	C6H12O	000066-25-1	80
3	Hexanal			100	C6H12O	000066-25-1	80
4	Hexanal			100	C6H12O	000066-25-1	72
5	Hexanal			100	C6H12O	000066-25-1	64



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GB7G7

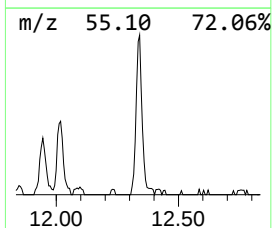
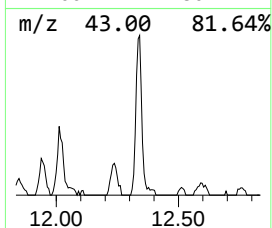
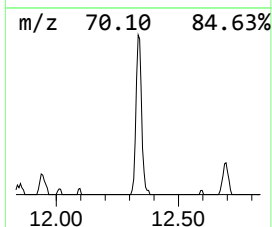
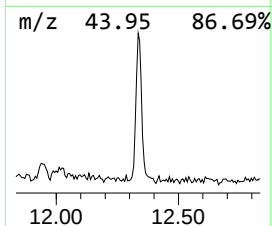
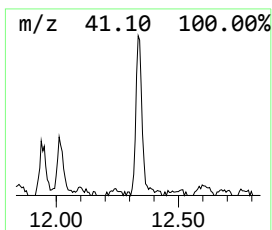
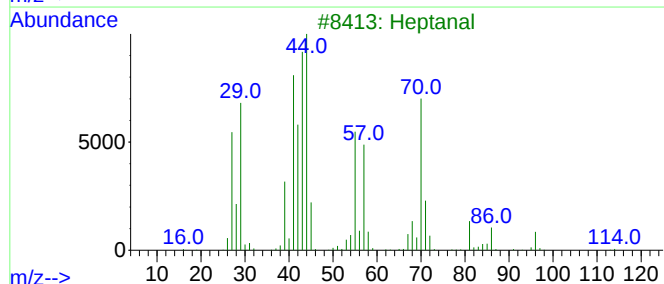
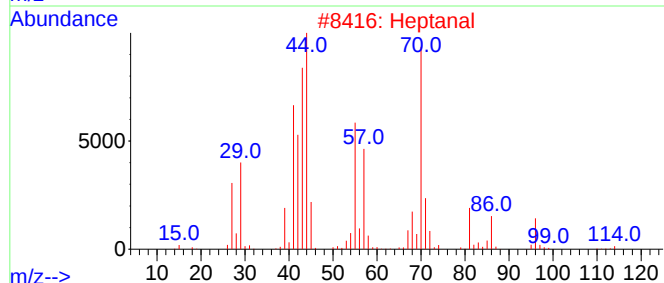
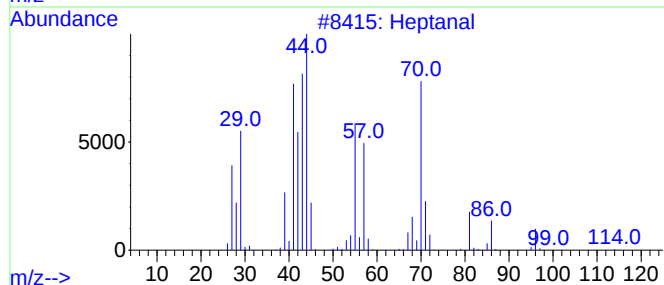
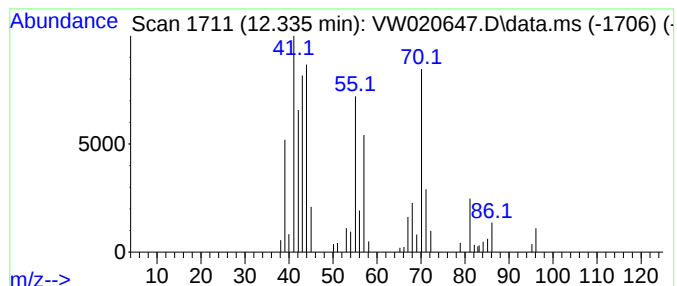
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Quant Title : SFAM01.0

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

Peak Number 5 Heptanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.335	1.77 ug/L	39298	Chlorobenzene-d5	11.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	86
2			Heptanal	114	C7H14O	000111-71-7	86
3			Heptanal	114	C7H14O	000111-71-7	78
4			Heptanal	114	C7H14O	000111-71-7	78
5			Heptanal	114	C7H14O	000111-71-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW102021\
Data File : VW020647.D
Acq On : 20 Oct 2021 12:12
Operator : SY/VA
Sample : M4264-02
Misc : 4.41g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GB7G7

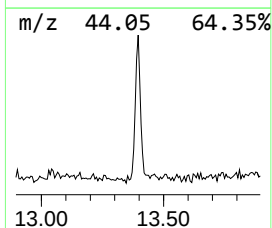
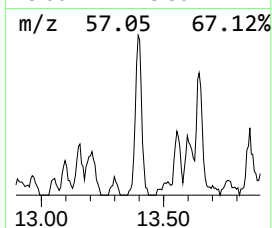
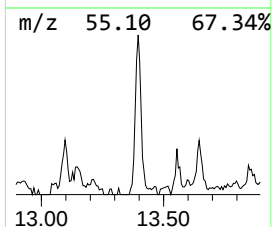
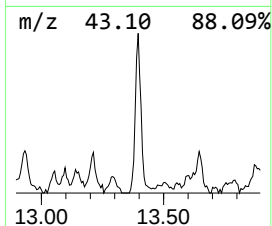
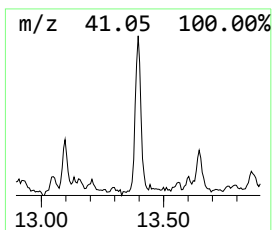
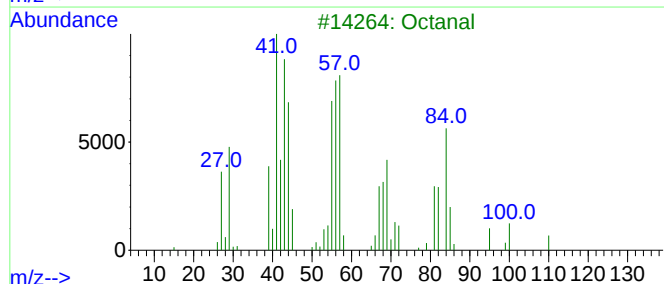
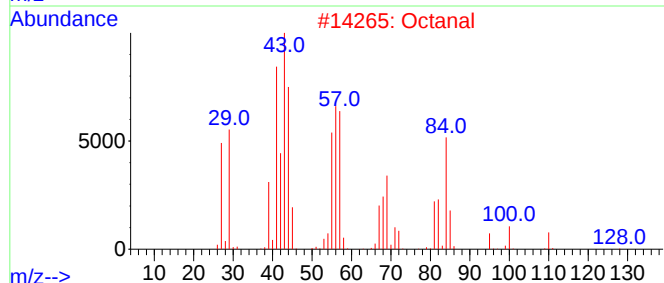
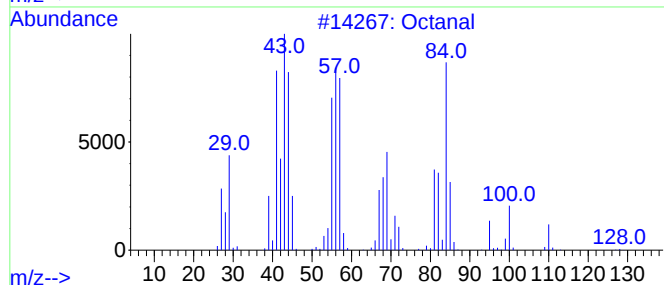
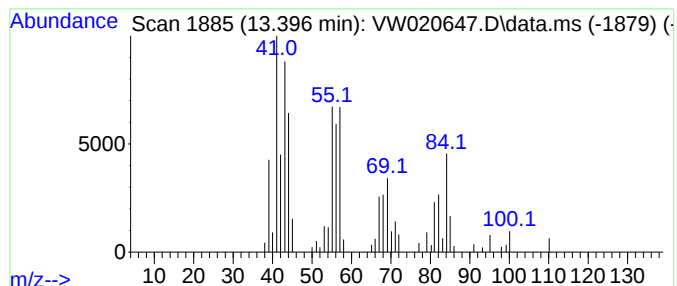
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Quant Title : SFAM01.0

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

Peak Number 7 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.396	2.79 ug/L	38530	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	83
2	Octanal			128	C8H16O	000124-13-0	74
3	Octanal			128	C8H16O	000124-13-0	74
4	Octanal			128	C8H16O	000124-13-0	52
5	2-Hexene, (Z)-			84	C6H12	007688-21-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW102021\
Data File : VW020647.D
Acq On : 20 Oct 2021 12:12
Operator : SY/VA
Sample : M4264-02
Misc : 4.41g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GB7G7

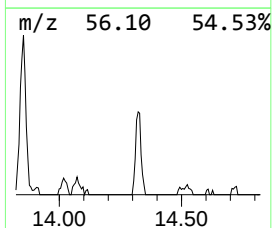
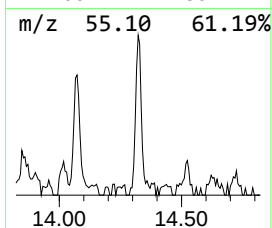
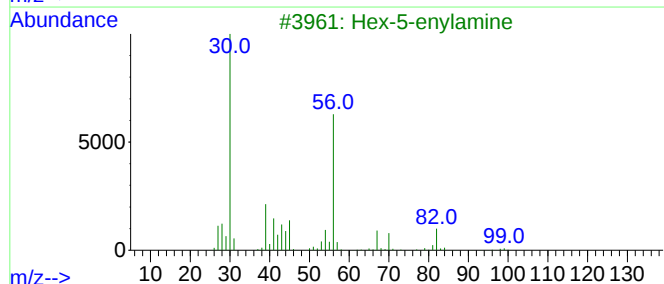
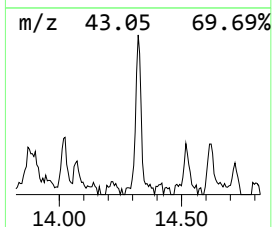
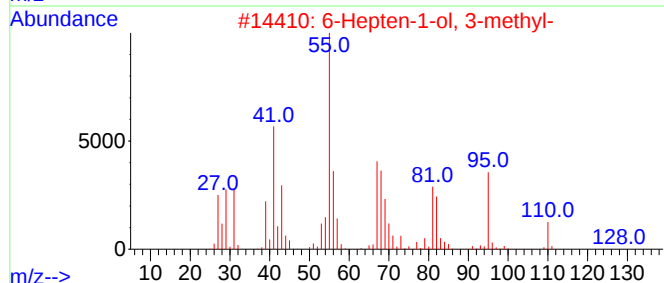
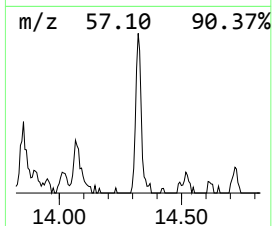
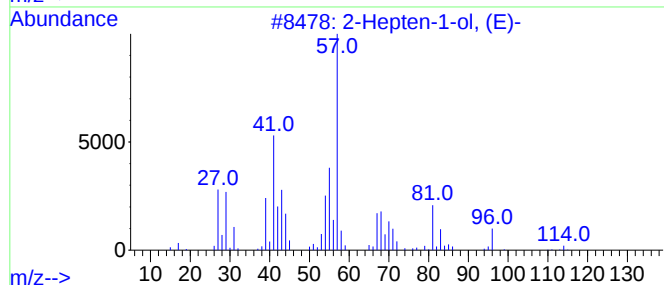
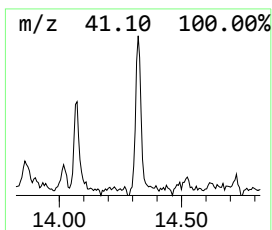
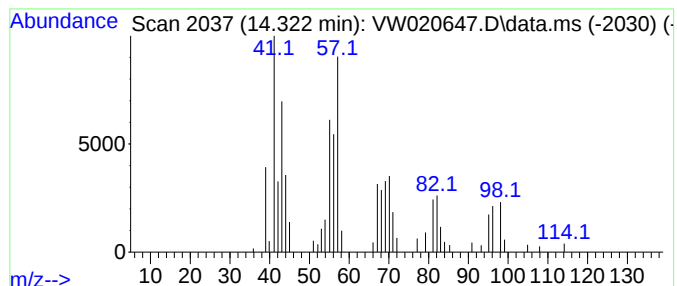
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Quant Title : SFAM01.0

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

Peak Number 9 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.322	1.94 ug/L	26705	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	45
2			6-Hepten-1-ol, 3-methyl-	128	C8H16O	004048-32-2	35
3			Hex-5-enylamine	99	C6H13N	034825-70-2	30
4			2-Heptene	98	C7H14	000592-77-8	30
5			(Z)-2-Heptene	98	C7H14	006443-92-1	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW102021\
Data File : VW020647.D
Acq On : 20 Oct 2021 12:12
Operator : SY/VA
Sample : M4264-02
Misc : 4.41g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GB7G7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.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	2.495	2.5	ug/L	51696	1	8.842	524792	25.0
Pentanal	9.409	3.9	ug/L	81621	1	8.842	524792	25.0
Hexanal	11.073	37.2	ug/L	825806	2	11.634	555393	25.0
Heptanal	12.335	1.8	ug/L	39298	2	11.634	555393	25.0
Octanal	13.396	2.8	ug/L	38530	3	13.554	344637	25.0
unknown-02	14.322	1.9	ug/L	26705	3	13.554	344637	25.0