

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081524\
 Data File : VW029908.D
 Acq On : 15 Aug 2024 16:19
 Operator : SY/MD
 Sample : P3626-03
 Misc : 6.16g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCYC7

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\SFAMWLM072424SMA.M
 Title : SFAM01.0

Signal : TIC: VW029908.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.174	41	47	49	rBV5	1138	2372	0.24%	0.028%
2	2.204	49	52	53	rBV3	1115	1057	0.11%	0.012%
3	2.369	71	79	95	rBV	47936	132300	13.47%	1.563%
4	2.503	95	101	111	rBV	16615	48586	4.95%	0.574%
5	2.899	159	166	182	rVB2	39695	115912	11.80%	1.369%
6	3.393	238	247	255	rBV2	12510	28541	2.91%	0.337%
7	4.021	336	350	361	rBV2	95220	335022	34.11%	3.958%
8	4.131	361	368	381	rVB	48360	141573	14.41%	1.672%
9	4.679	452	458	463	rBV4	1616	4058	0.41%	0.048%
10	4.917	486	497	522	rVB4	10795	52854	5.38%	0.624%
11	5.435	575	582	586	rBV6	619	1148	0.12%	0.014%
12	5.795	630	641	650	rBV5	3999	14009	1.43%	0.165%
13	5.935	657	664	665	rBV2	3947	6148	0.63%	0.073%
14	6.118	684	694	702	rBV6	2330	8372	0.85%	0.099%
15	6.606	768	774	776	rBV5	752	1258	0.13%	0.015%
16	6.776	800	802	808	rBV3	563	850	0.09%	0.010%
17	6.898	813	822	832	rBV4	6465	20382	2.08%	0.241%
18	7.081	842	852	861	rBV2	22708	73146	7.45%	0.864%
19	7.459	911	914	919	rBV5	671	785	0.08%	0.009%
20	7.648	934	945	956	rBV	162504	399766	40.70%	4.722%
21	7.825	972	974	977	rVB2	817	760	0.08%	0.009%
22	8.160	1023	1029	1031	rBV4	864	1449	0.15%	0.017%
23	8.276	1038	1048	1064	rBV2	307693	905493	92.19%	10.696%
24	8.392	1064	1067	1069	rVV3	853	1047	0.11%	0.012%
25	8.550	1085	1093	1103	rBV2	11332	27019	2.75%	0.319%
26	8.703	1111	1118	1128	rBV3	8979	23263	2.37%	0.275%
27	8.843	1131	1141	1151	rBV	446939	876292	89.22%	10.351%
28	9.270	1201	1211	1221	rBV	211081	438908	44.69%	5.185%
29	9.404	1227	1233	1243	rVB	46282	88774	9.04%	1.049%
30	9.556	1254	1258	1262	rVB6	736	1322	0.13%	0.016%
31	9.672	1274	1277	1283	rVB5	789	1470	0.15%	0.017%
32	9.880	1308	1311	1319	rVB6	761	1578	0.16%	0.019%
33	9.959	1319	1324	1326	rBV5	786	1040	0.11%	0.012%
34	10.032	1329	1336	1347	rBV	107344	196193	19.97%	2.318%
35	10.129	1349	1352	1353	rBV3	904	1136	0.12%	0.013%
36	10.239	1366	1370	1374	rVV7	843	1402	0.14%	0.017%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
 Title : SFAM01.0

37	10.318	1374	1383	1390	rVV	410440	739359	75.28%	8.734%
38	10.386	1390	1394	1404	rVV	12660	26731	2.72%	0.316%
39	10.501	1407	1413	1417	rVV4	3966	5488	0.56%	0.065%
40	10.575	1418	1425	1440	rVV	68513	126279	12.86%	1.492%
41	10.696	1440	1445	1450	rBV	4637	7901	0.80%	0.093%
42	10.739	1450	1452	1458	rVB5	1209	1846	0.19%	0.022%
43	10.855	1466	1471	1472	rBV5	848	1284	0.13%	0.015%
44	10.922	1474	1482	1498	rBV	92092	165094	16.81%	1.950%
45	11.068	1498	1506	1520	rBV	458802	733078	74.64%	8.660%
46	11.459	1568	1570	1574	rVB3	518	780	0.08%	0.009%
47	11.501	1574	1577	1581	rBV5	677	800	0.08%	0.009%
48	11.562	1583	1587	1590	rBV5	1647	2709	0.28%	0.032%
49	11.629	1590	1598	1609	rVV	596085	982194	100.00%	11.602%
50	11.836	1626	1632	1642	rBV2	25376	52744	5.37%	0.623%
51	11.946	1646	1650	1657	rVV6	2491	4772	0.49%	0.056%
52	12.013	1657	1661	1669	rVV	7991	13828	1.41%	0.163%
53	12.172	1682	1687	1692	rBV6	2402	4756	0.48%	0.056%
54	12.239	1695	1698	1703	rVB4	1512	2498	0.25%	0.030%
55	12.336	1707	1714	1725	rBV3	15789	28809	2.93%	0.340%
56	12.464	1730	1735	1740	rBV3	8583	15395	1.57%	0.182%
57	12.507	1740	1742	1749	rVB4	3991	5996	0.61%	0.071%
58	12.605	1751	1758	1764	rVB	4220	7280	0.74%	0.086%
59	12.690	1764	1772	1783	rBV	146069	249500	25.40%	2.947%
60	12.800	1788	1790	1795	rVB3	1113	1614	0.16%	0.019%
61	12.867	1795	1801	1803	rBV4	2193	3525	0.36%	0.042%
62	12.897	1804	1806	1809	rBV3	1034	1070	0.11%	0.013%
63	12.934	1809	1812	1821	rVB8	3643	9485	0.97%	0.112%
64	13.031	1821	1828	1834	rBV4	4632	9588	0.98%	0.113%
65	13.092	1834	1838	1844	rBV6	6104	12391	1.26%	0.146%
66	13.153	1844	1848	1853	rVB5	5021	7229	0.74%	0.085%
67	13.208	1853	1857	1860	rBV3	2116	3175	0.32%	0.038%
68	13.245	1860	1863	1866	rBV2	2787	4919	0.50%	0.058%
69	13.361	1879	1882	1883	rBV2	997	1068	0.11%	0.013%
70	13.391	1883	1887	1891	rVV4	9618	16556	1.69%	0.196%
71	13.446	1891	1896	1901	rVV4	18544	46509	4.74%	0.549%
72	13.489	1901	1903	1907	rVV	21752	30717	3.13%	0.363%
73	13.556	1907	1914	1924	rVB	434574	687184	69.96%	8.118%
74	13.708	1935	1939	1941	rBV4	1093	1103	0.11%	0.013%
75	13.751	1944	1946	1952	rVB6	910	1339	0.14%	0.016%
76	13.848	1955	1962	1970	rBV	243220	402347	40.96%	4.753%

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 Title : SFAM01.0

77	14.013	1983	1989	1992	rBV7	2190	4553	0.46%	0.054%
78	14.068	1992	1998	2008	rVB2	16646	31160	3.17%	0.368%
79	14.318	2034	2039	2047	rVV4	8293	15397	1.57%	0.182%
80	14.610	2083	2087	2092	rBV6	2531	4607	0.47%	0.054%
81	14.690	2095	2100	2101	rBV5	853	1405	0.14%	0.017%
82	14.799	2112	2118	2120	rVB6	804	1280	0.13%	0.015%
83	14.848	2122	2126	2135	rVV8	985	2211	0.23%	0.026%
84	14.946	2138	2142	2147	rVB5	3685	5866	0.60%	0.069%
85	15.080	2161	2164	2166	rVV3	806	1189	0.12%	0.014%
86	15.122	2169	2171	2174	rVV3	793	771	0.08%	0.009%
87	15.177	2174	2180	2188	rVV3	1716	5156	0.52%	0.061%
88	15.238	2188	2190	2191	rVV2	1285	1200	0.12%	0.014%
89	15.293	2195	2199	2201	rVB2	674	773	0.08%	0.009%
90	15.354	2206	2209	2210	rBV2	742	717	0.07%	0.008%
91	15.470	2226	2228	2234	rBV3	864	1551	0.16%	0.018%
92	15.757	2273	2275	2278	rVB5	1080	958	0.10%	0.011%
93	15.842	2283	2289	2296	rBV9	2294	5173	0.53%	0.061%
94	15.970	2305	2310	2312	rVB4	1210	1869	0.19%	0.022%
95	16.092	2327	2330	2333	rVB3	923	1131	0.12%	0.013%
96	16.183	2340	2345	2346	rVB4	768	796	0.08%	0.009%
97	16.208	2346	2349	2352	rBV4	531	817	0.08%	0.010%
98	16.256	2352	2357	2360	rVB5	542	1066	0.11%	0.013%
99	16.281	2360	2361	2364	rBV3	588	768	0.08%	0.009%
100	16.769	2437	2441	2444	rVB4	526	728	0.07%	0.009%

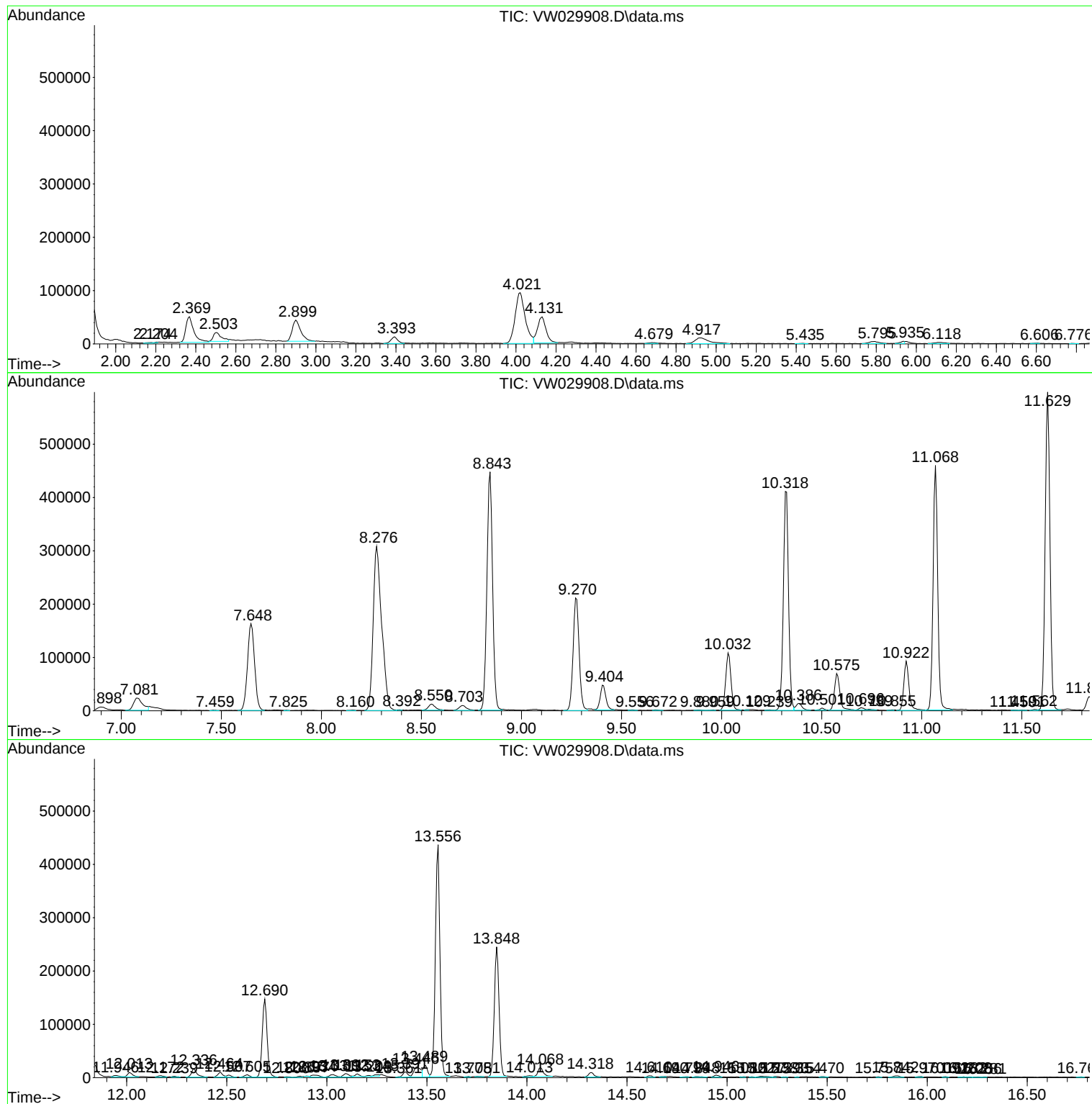
Sum of corrected areas: 8465367

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MSVOA_W
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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



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Instrument :
MSVOA_W
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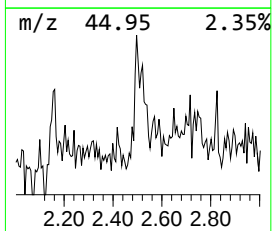
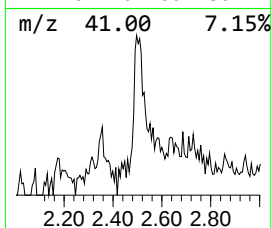
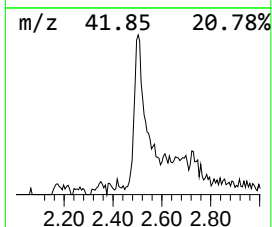
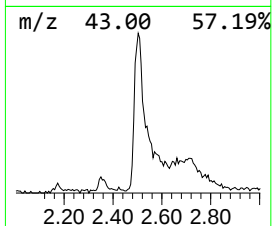
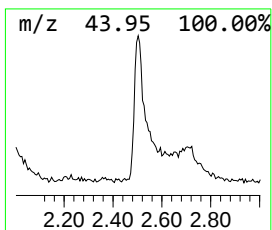
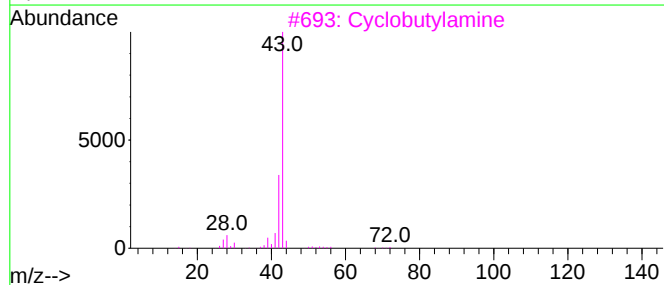
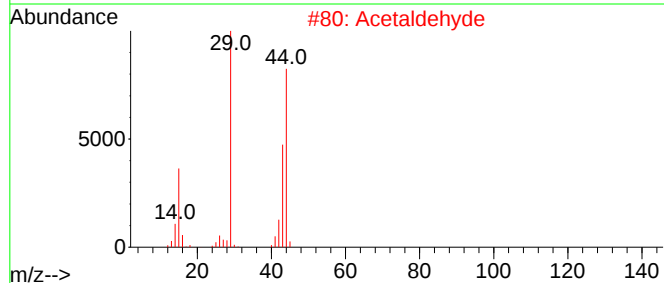
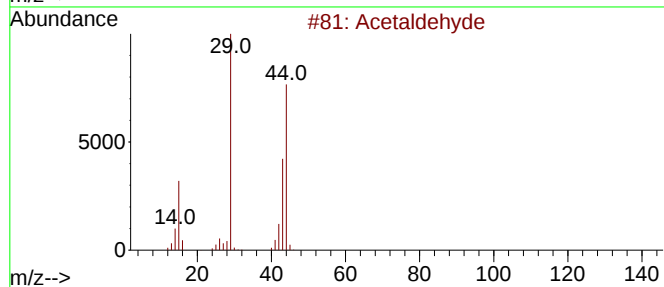
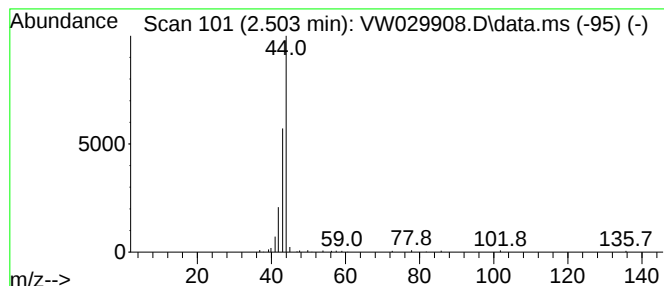
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.503	1.39 ug/L	48586	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Cyclobutylamine	71	C4H9N	002516-34-9	9
4			2-Propanamine	59	C3H9N	000075-31-0	9
5			Cyclobutanol	72	C4H8O	002919-23-5	7



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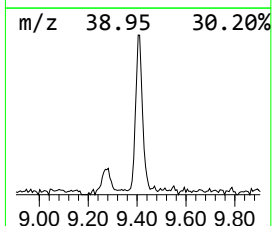
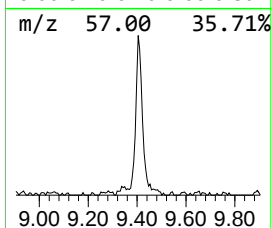
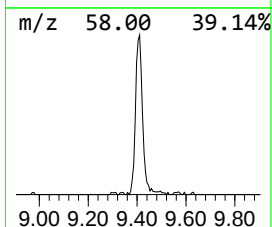
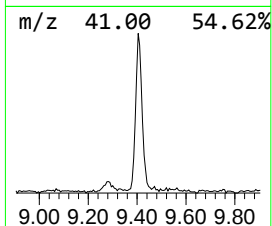
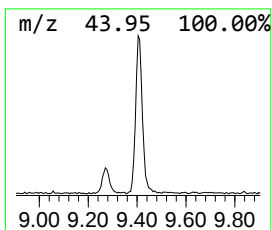
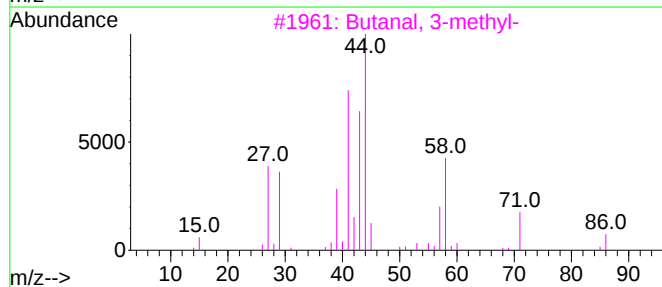
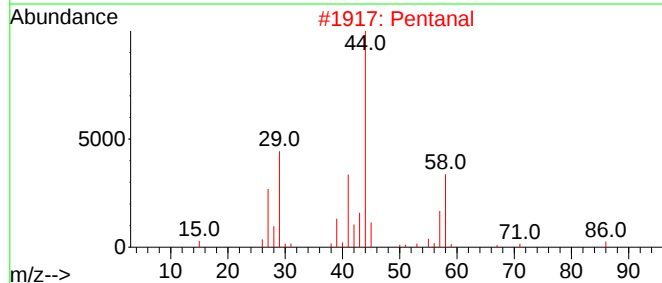
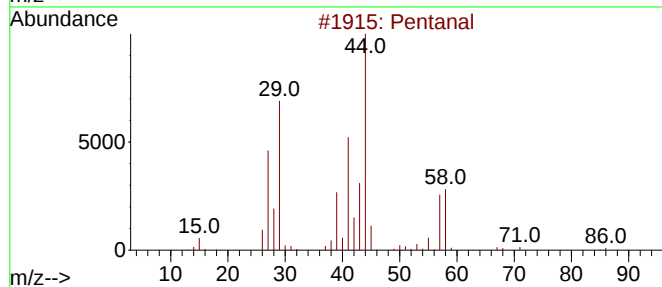
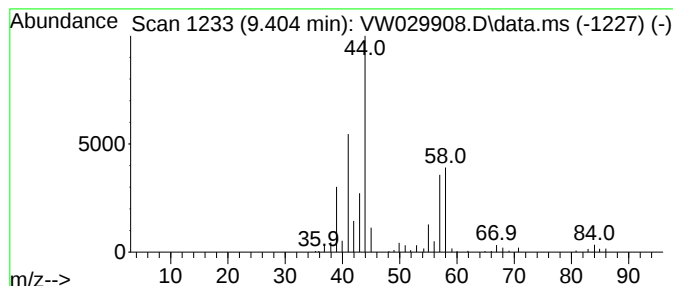
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.404	2.53 ug/L	88774	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	87
2	Pentanal			86	C5H10O	000110-62-3	78
3	Butanal, 3-methyl-			86	C5H10O	000590-86-3	64
4	Pentanal			86	C5H10O	000110-62-3	64
5	Butanal, 3-methyl-			86	C5H10O	000590-86-3	64



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MSVOA_W
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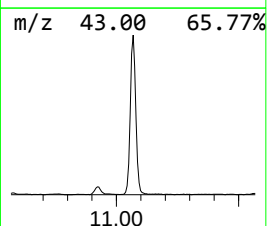
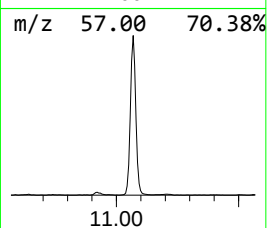
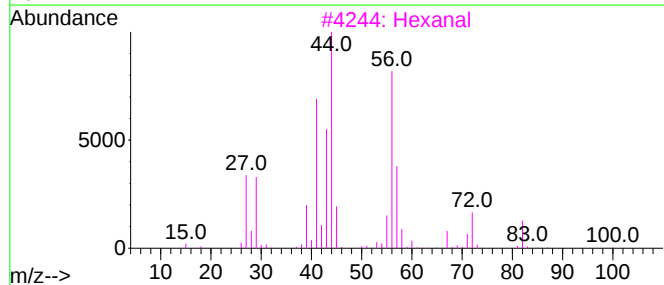
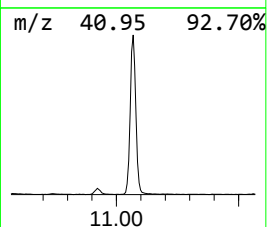
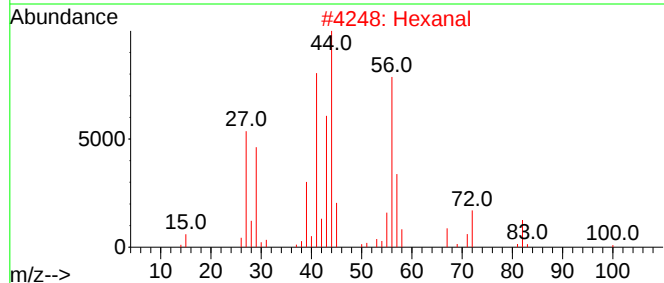
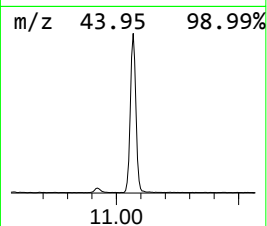
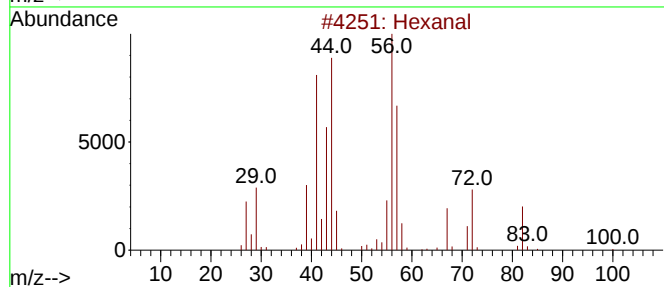
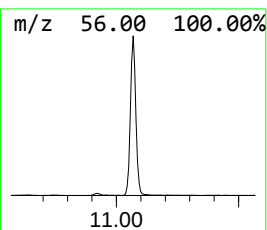
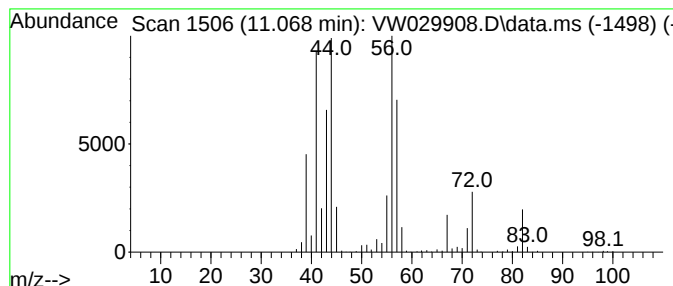
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.068	18.66 ug/L	733078	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	94
2	Hexanal			100	C6H12O	000066-25-1	81
3	Hexanal			100	C6H12O	000066-25-1	81
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081524\
Data File : VW029908.D
Acq On : 15 Aug 2024 16:19
Operator : SY/MD
Sample : P3626-03
Misc : 6.16g/10mL/MSVOA_W/SOIL/A
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYC7

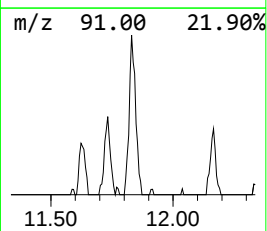
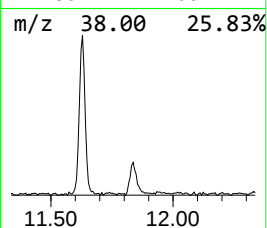
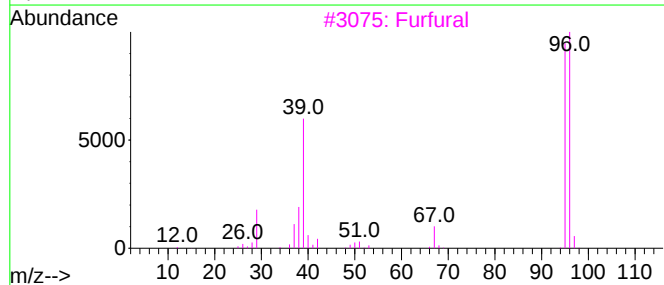
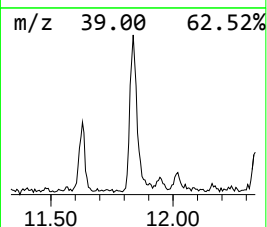
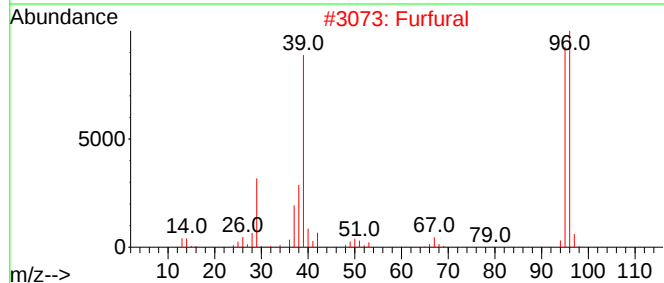
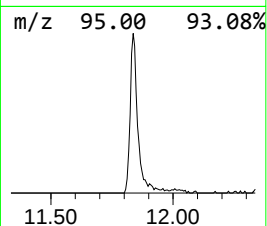
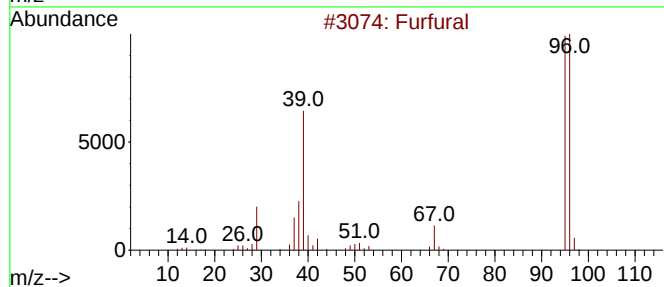
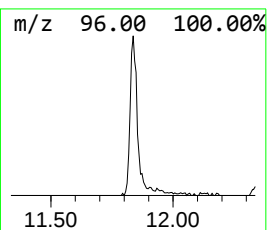
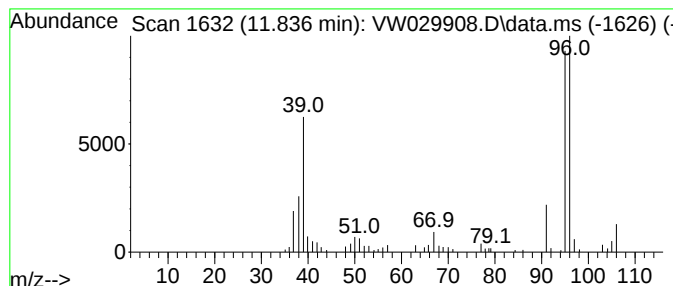
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Quant Title : SFAM01.0

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

Peak Number 6 Furfural Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.836	1.34 ug/L	52744	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furfural			96	C5H4O2	000098-01-1	91
2	Furfural			96	C5H4O2	000098-01-1	90
3	Furfural			96	C5H4O2	000098-01-1	87
4	3-Furaldehyde			96	C5H4O2	000498-60-2	78
5	2(1H)-Pyridinone			95	C5H5NO	000142-08-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081524\
Data File : VW029908.D
Acq On : 15 Aug 2024 16:19
Operator : SY/MD
Sample : P3626-03
Misc : 6.16g/10mL/MSVOA_W/SOIL/A
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYC7

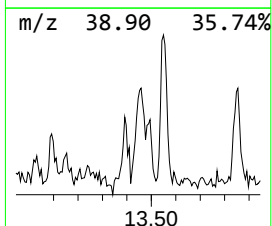
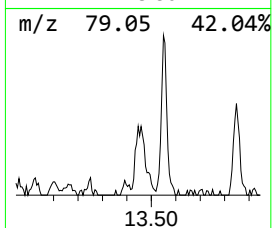
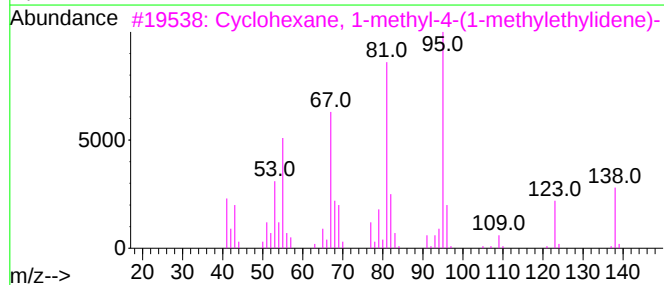
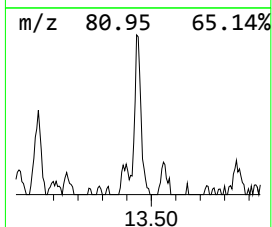
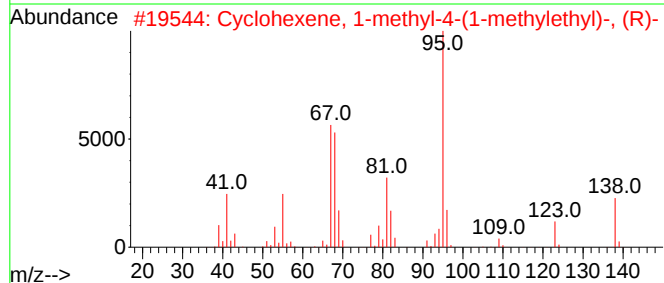
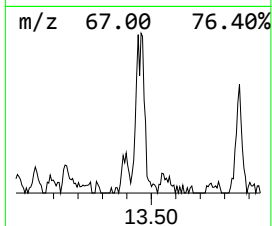
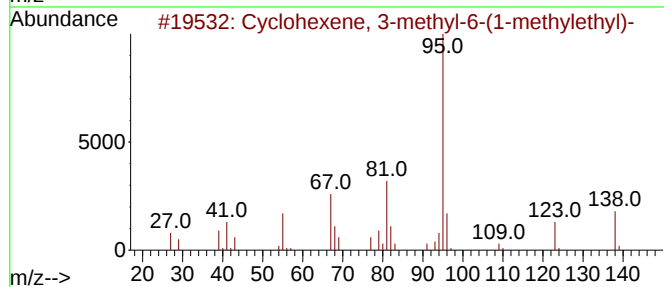
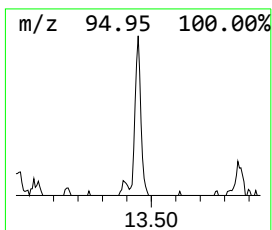
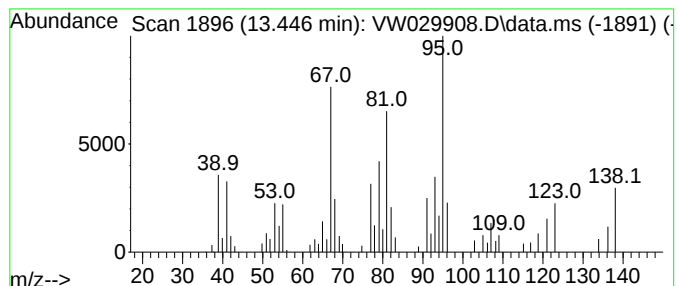
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Quant Title : SFAM01.0

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

Peak Number 7 Cyclohexene, 3-methyl-6-(1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.446	1.69 ug/L	46509	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	64
2			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	001195-31-9	64
3			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	60
4			Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	60
5			Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081524\
Data File : VW029908.D
Acq On : 15 Aug 2024 16:19
Operator : SY/MD
Sample : P3626-03
Misc : 6.16g/10mL/MSVOA_W/SOIL/A
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYC7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.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
unknown-01	2.503	1.4	ug/L	48586	1	8.843	876292	25.0
Pentanal	9.404	2.5	ug/L	88774	1	8.843	876292	25.0
Hexanal	11.068	18.7	ug/L	733078	2	11.629	982194	25.0
Furfural	11.836	1.3	ug/L	52744	2	11.629	982194	25.0
Cyclohexene, 3-...	13.446	1.7	ug/L	46509	3	13.556	687184	25.0