

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
 Data File : VW029963.D
 Acq On : 20 Aug 2024 16:56
 Operator : SY/MD
 Sample : P3626-21
 Misc : 5.59g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCYC6

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: VW029963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.162	43	45	47	rBV3	697	858	0.12%	0.014%
2	2.363	72	78	89	rBV	37252	91898	12.94%	1.473%
3	2.509	95	102	119	rBV	18969	67050	9.44%	1.075%
4	2.899	160	166	184	rVB	31171	92458	13.02%	1.482%
5	3.228	217	220	222	rBV3	703	792	0.11%	0.013%
6	3.302	230	232	238	rVB6	965	1638	0.23%	0.026%
7	3.393	241	247	258	rVB2	4043	10981	1.55%	0.176%
8	3.734	299	303	308	rVB7	1036	1515	0.21%	0.024%
9	4.021	337	350	362	rBV2	66785	228515	32.17%	3.662%
10	4.137	363	369	385	rVB	29987	91331	12.86%	1.464%
11	4.387	407	410	411	rBV3	511	598	0.08%	0.010%
12	4.686	451	459	467	rBV4	2105	6384	0.90%	0.102%
13	4.923	489	498	511	rVV4	4898	19406	2.73%	0.311%
14	5.246	547	551	554	rBV3	711	868	0.12%	0.014%
15	5.405	575	577	581	rBV3	446	709	0.10%	0.011%
16	5.454	583	585	590	rVB2	469	599	0.08%	0.010%
17	5.588	605	607	611	rBV3	358	568	0.08%	0.009%
18	5.685	620	623	628	rBV5	349	647	0.09%	0.010%
19	5.789	632	640	641	rBV4	3133	5839	0.82%	0.094%
20	5.880	653	655	658	rVB4	594	586	0.08%	0.009%
21	5.941	658	665	666	rBV5	1255	2416	0.34%	0.039%
22	6.039	679	681	685	rBV4	603	712	0.10%	0.011%
23	6.118	688	694	698	rVV5	1643	3812	0.54%	0.061%
24	6.484	751	754	756	rBV2	493	594	0.08%	0.010%
25	6.905	813	823	836	rBV6	5577	18419	2.59%	0.295%
26	7.081	843	852	861	rBV	20936	62875	8.85%	1.008%
27	7.648	934	945	956	rBV	123207	313637	44.15%	5.026%
28	7.770	963	965	966	rBV	693	538	0.08%	0.009%
29	8.136	1020	1025	1027	rBV4	592	727	0.10%	0.012%
30	8.276	1036	1048	1062	rBV2	236899	702452	98.89%	11.258%
31	8.551	1084	1093	1103	rBV2	10123	25468	3.59%	0.408%
32	8.630	1104	1106	1108	rVB2	817	647	0.09%	0.010%
33	8.709	1111	1119	1128	rBV3	7594	18138	2.55%	0.291%
34	8.843	1132	1141	1157	rBV	349030	668436	94.10%	10.712%
35	9.038	1170	1173	1175	rBV3	571	825	0.12%	0.013%
36	9.270	1202	1211	1221	rBV	168048	344389	48.48%	5.519%

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

37	9.410	1227	1234	1242	rVB	25824	51053	7.19%	0.818%
38	9.563	1257	1259	1262	rVB3	821	793	0.11%	0.013%
39	9.648	1269	1273	1275	rBV5	516	904	0.13%	0.014%
40	9.764	1290	1292	1296	rVB4	660	635	0.09%	0.010%
41	9.813	1298	1300	1303	rVB3	518	538	0.08%	0.009%
42	9.892	1307	1313	1317	rVB6	1320	2180	0.31%	0.035%
43	10.032	1328	1336	1347	rBV	80144	148588	20.92%	2.381%
44	10.130	1350	1352	1355	rVB4	733	579	0.08%	0.009%
45	10.160	1355	1357	1359	rVB3	552	559	0.08%	0.009%
46	10.325	1374	1384	1390	rBV	298791	532333	74.94%	8.531%
47	10.386	1390	1394	1401	rVB	6112	12347	1.74%	0.198%
48	10.508	1408	1414	1417	rBV7	1125	2120	0.30%	0.034%
49	10.575	1419	1425	1432	rBV	51992	92026	12.95%	1.475%
50	10.697	1440	1445	1452	rVB	14513	25320	3.56%	0.406%
51	10.855	1465	1471	1476	rBV6	956	2087	0.29%	0.033%
52	10.922	1476	1482	1494	rVV	82629	145059	20.42%	2.325%
53	11.001	1494	1495	1497	rVV2	1455	987	0.14%	0.016%
54	11.069	1499	1506	1523	rVV	241587	391024	55.05%	6.267%
55	11.209	1527	1529	1532	rVB3	645	555	0.08%	0.009%
56	11.629	1590	1598	1609	rBV	427853	710358	100.00%	11.384%
57	11.843	1625	1633	1643	rBV	26615	57167	8.05%	0.916%
58	11.946	1646	1650	1657	rVV8	2568	5907	0.83%	0.095%
59	12.020	1660	1662	1670	rVB3	1482	2399	0.34%	0.038%
60	12.154	1681	1684	1686	rBV4	1069	1184	0.17%	0.019%
61	12.337	1708	1714	1727	rBV3	13449	24970	3.52%	0.400%
62	12.465	1727	1735	1748	rBV	38043	68611	9.66%	1.100%
63	12.599	1752	1757	1765	rVB	17902	30097	4.24%	0.482%
64	12.690	1765	1772	1783	rBV	125775	231409	32.58%	3.709%
65	12.818	1790	1793	1796	rVB4	526	569	0.08%	0.009%
66	12.867	1798	1801	1804	rBV4	808	863	0.12%	0.014%
67	12.897	1804	1806	1808	rBV3	781	907	0.13%	0.015%
68	12.940	1808	1813	1817	rVB6	2157	4125	0.58%	0.066%
69	13.044	1823	1830	1834	rBV6	1493	2940	0.41%	0.047%
70	13.093	1834	1838	1844	rVV5	3569	7543	1.06%	0.121%
71	13.147	1844	1847	1851	rVV4	2723	4579	0.64%	0.073%
72	13.208	1853	1857	1860	rVV4	3807	5796	0.82%	0.093%
73	13.269	1864	1867	1876	rVB5	4646	9717	1.37%	0.156%
74	13.397	1881	1888	1894	rBV4	14284	26561	3.74%	0.426%
75	13.464	1894	1899	1901	rBV3	8048	12369	1.74%	0.198%
76	13.556	1907	1914	1925	rVV	288312	468568	65.96%	7.509%

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 Title : SFAM01.0

77	13.641	1925	1928	1934	rVB7	1723	3622	0.51%	0.058%
78	13.849	1955	1962	1971	rVV	172038	281459	39.62%	4.511%
79	13.995	1982	1986	1987	rBV4	1723	2212	0.31%	0.035%
80	14.068	1992	1998	2008	rVV2	13948	27162	3.82%	0.435%
81	14.318	2032	2039	2050	rBV6	8309	16546	2.33%	0.265%
82	14.513	2066	2071	2075	rBV5	895	1678	0.24%	0.027%
83	14.556	2075	2078	2081	rVB4	563	668	0.09%	0.011%
84	14.684	2095	2099	2103	rBV3	2403	3651	0.51%	0.059%
85	14.775	2111	2114	2117	rBV4	827	988	0.14%	0.016%
86	14.848	2122	2126	2132	rVB6	1424	2466	0.35%	0.040%
87	14.946	2138	2142	2148	rBV4	2267	3777	0.53%	0.061%
88	15.074	2158	2163	2165	rBV3	865	1559	0.22%	0.025%
89	15.178	2177	2180	2181	rVV3	619	581	0.08%	0.009%
90	15.196	2181	2183	2185	rVV2	668	671	0.09%	0.011%
91	15.245	2188	2191	2195	rVV6	2529	3904	0.55%	0.063%
92	15.287	2195	2198	2204	rVB3	2685	4897	0.69%	0.078%
93	15.348	2207	2208	2212	rBV3	784	1037	0.15%	0.017%
94	15.470	2223	2228	2229	rBV4	1983	2434	0.34%	0.039%
95	15.842	2284	2289	2294	rBV6	1872	3114	0.44%	0.050%
96	15.946	2304	2306	2311	rVB4	881	1015	0.14%	0.016%
97	16.031	2317	2320	2322	rVB4	659	677	0.10%	0.011%
98	16.092	2329	2330	2334	rVV4	566	610	0.09%	0.010%
99	16.153	2337	2340	2344	rBV4	357	700	0.10%	0.011%
100	16.604	2410	2414	2421	rBV5	446	701	0.10%	0.011%

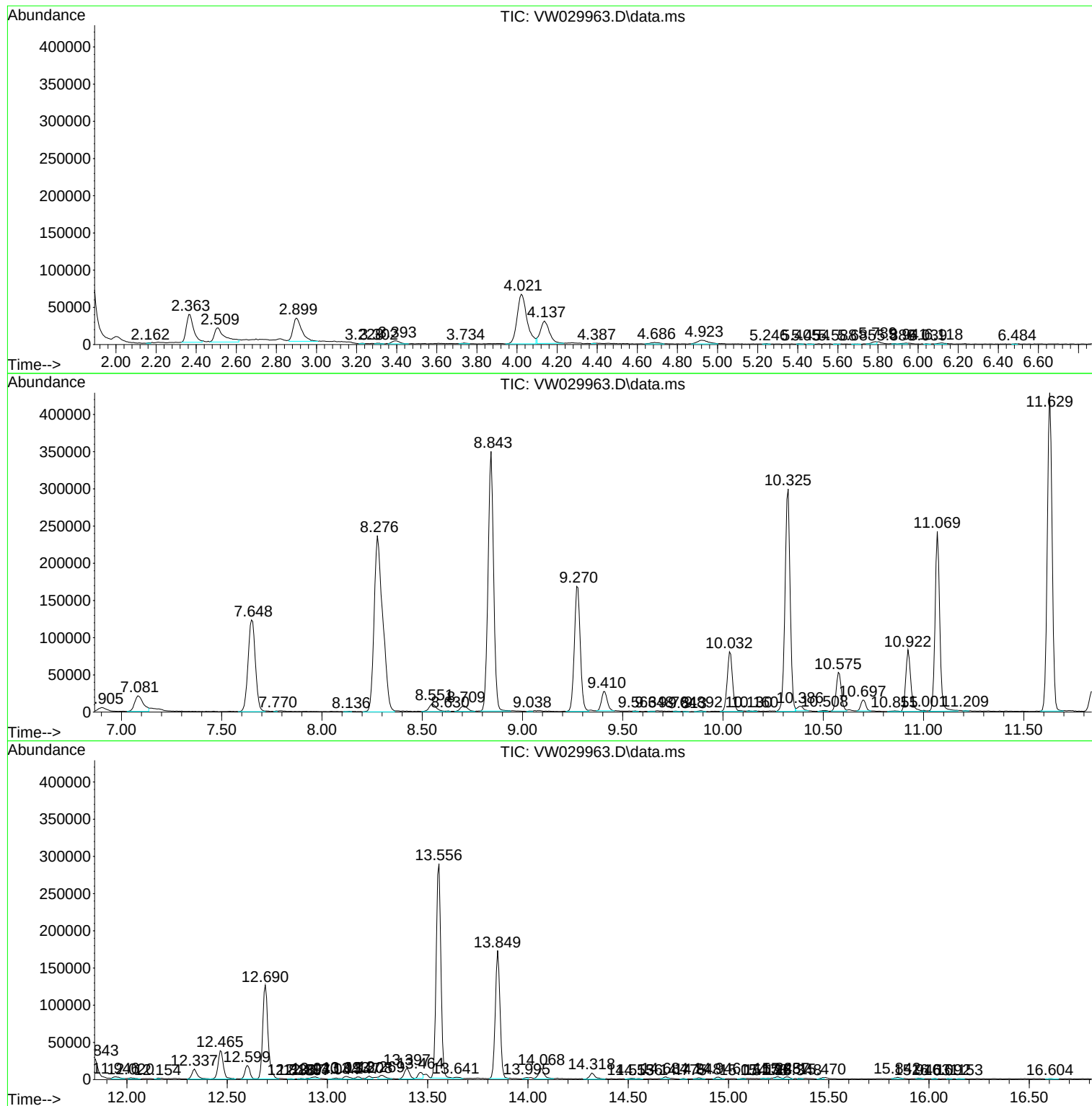
Sum of corrected areas: 6239780

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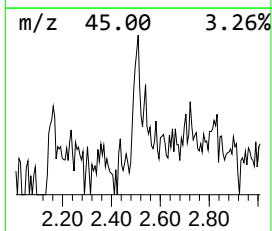
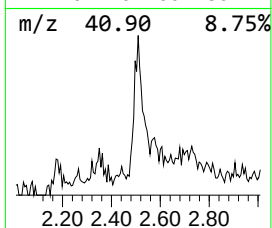
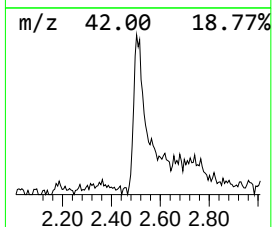
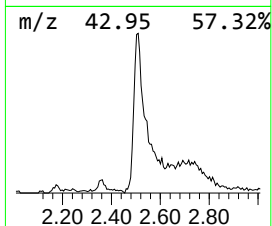
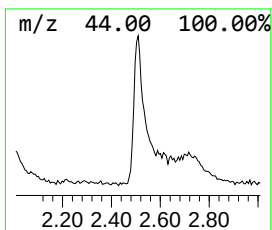
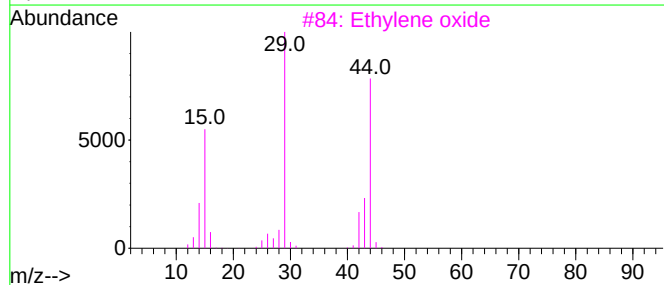
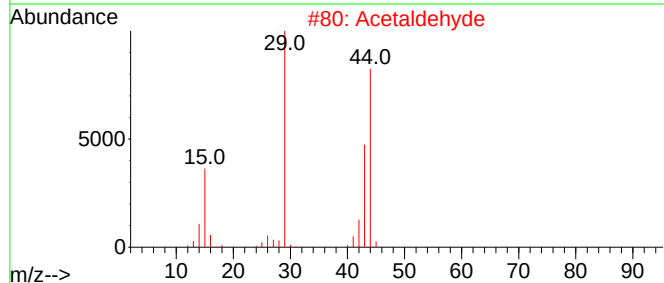
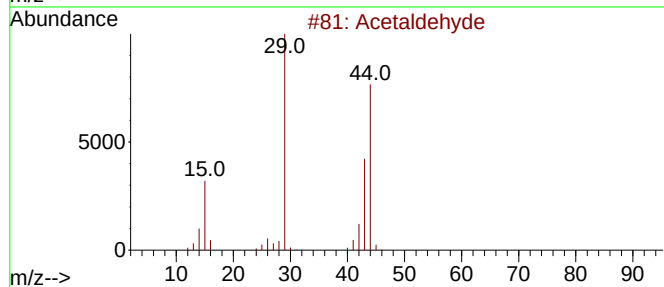
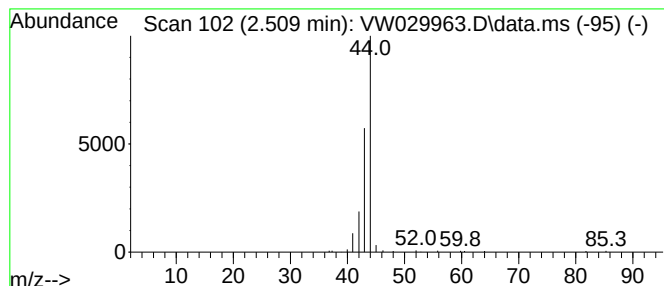
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.509	2.51 ug/L	67050	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Acetaldehyde	44	C2H4O	000075-07-0	56
3			Ethylene oxide	44	C2H4O	000075-21-8	9
4			Ethylene oxide	44	C2H4O	000075-21-8	7
5			Propane	44	C3H8	000074-98-6	5



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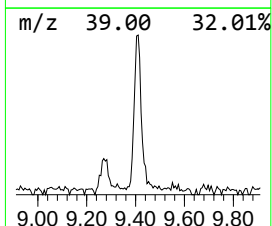
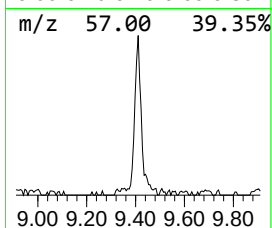
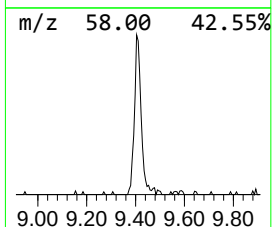
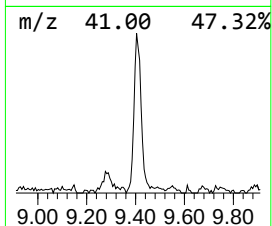
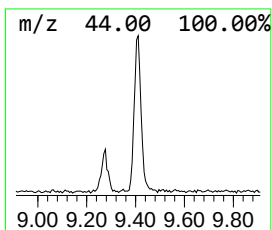
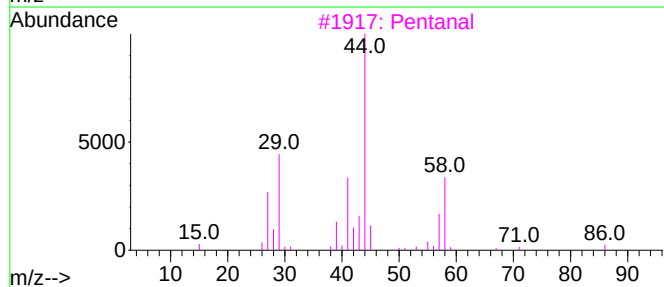
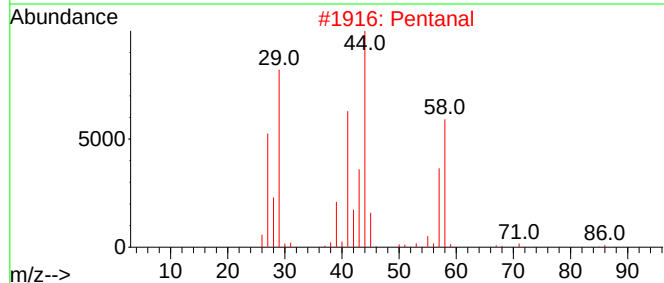
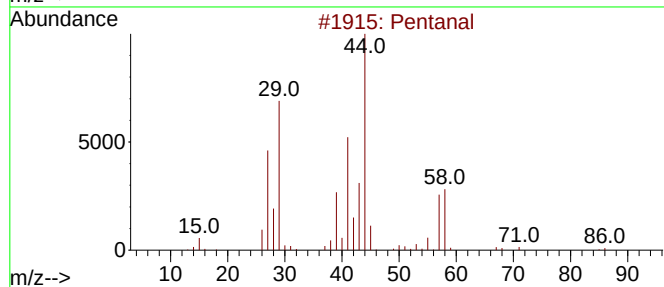
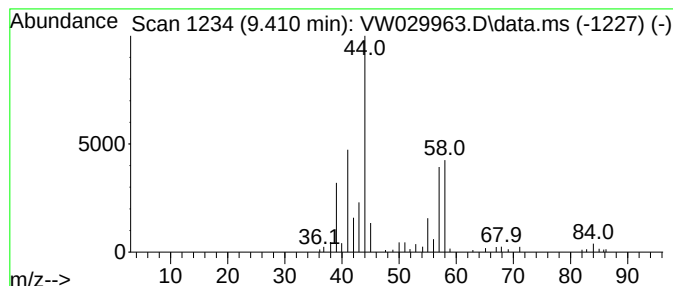
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	1.91 ug/L	51053	1,4-Difluorobenzene	8.843

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



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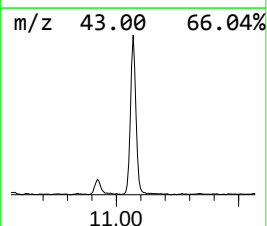
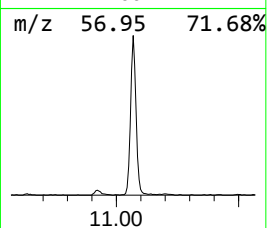
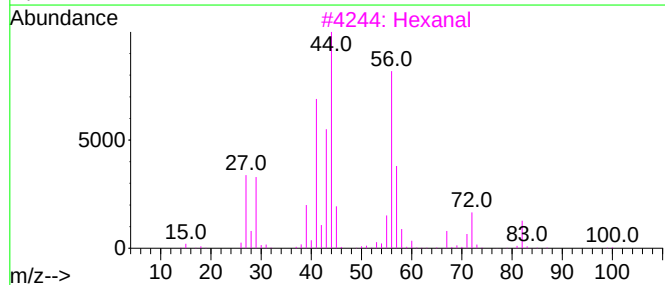
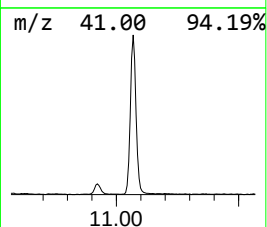
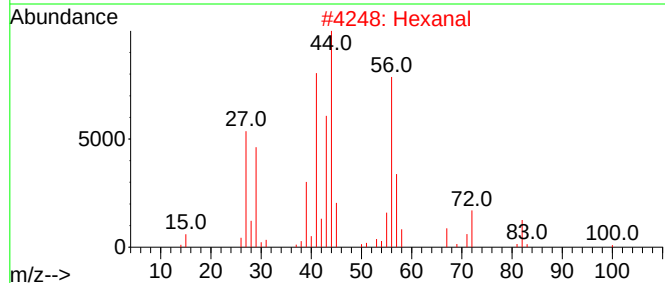
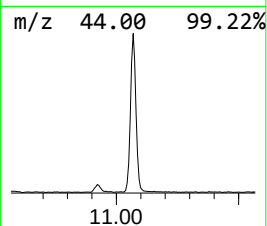
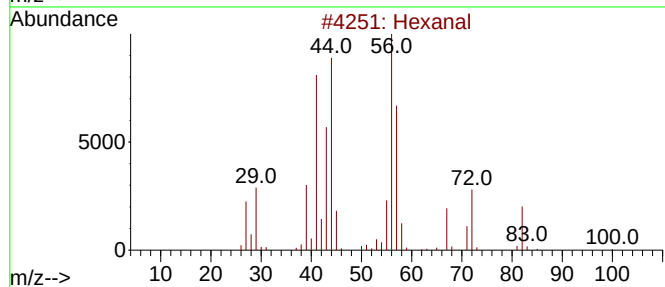
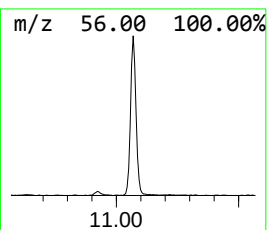
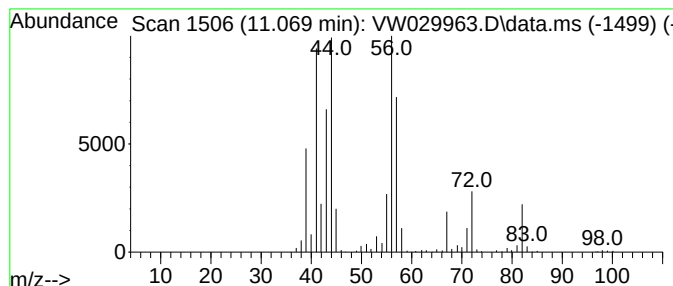
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.069	13.76 ug/L	391024	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	74
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
Data File : VW029963.D
Acq On : 20 Aug 2024 16:56
Operator : SY/MD
Sample : P3626-21
Misc : 5.59g/10mL/MSVOA_W/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYC6

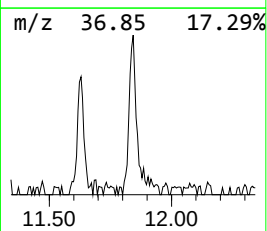
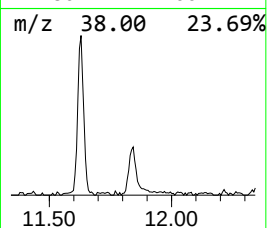
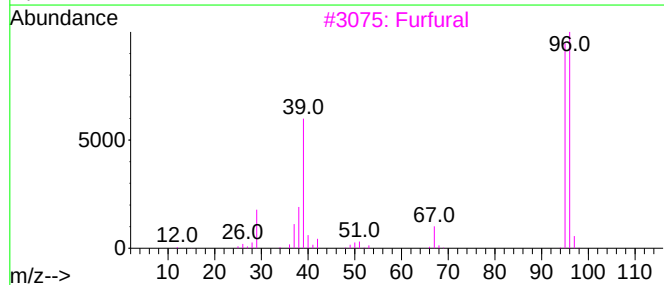
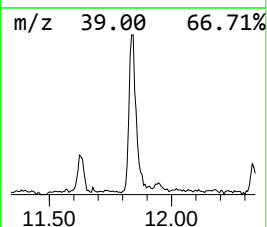
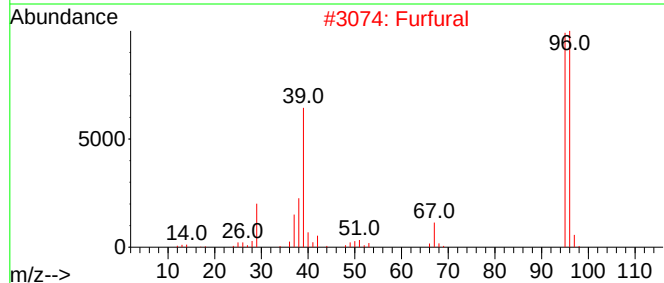
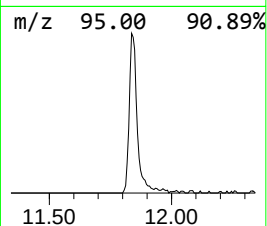
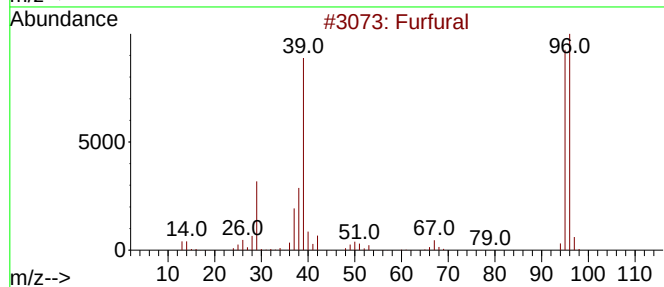
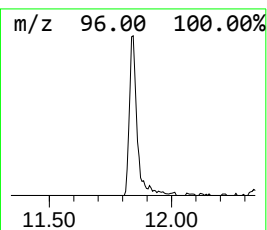
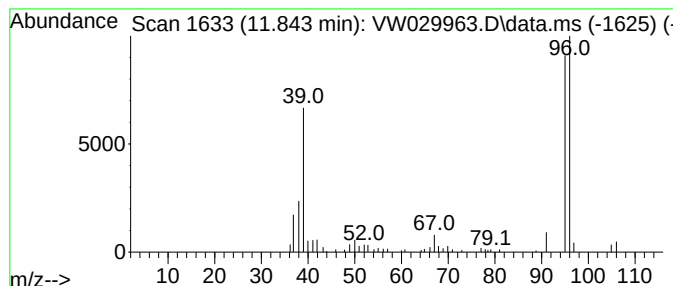
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Quant Title : SFAM01.0

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

Peak Number 5 Furfural Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.843	2.01 ug/L	57167	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furfural			96	C5H4O2	000098-01-1	95
2	Furfural			96	C5H4O2	000098-01-1	94
3	Furfural			96	C5H4O2	000098-01-1	64
4	Furfural			96	C5H4O2	000098-01-1	58
5	3(2H)-Pyridazinone			96	C4H4N2O	000504-30-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
Data File : VW029963.D
Acq On : 20 Aug 2024 16:56
Operator : SY/MD
Sample : P3626-21
Misc : 5.59g/10mL/MSVOA_W/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYC6

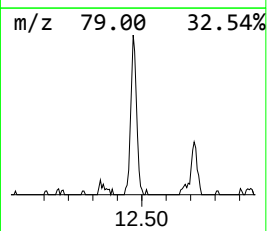
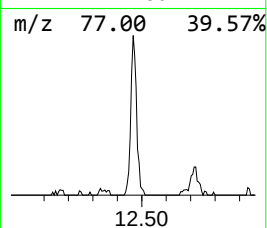
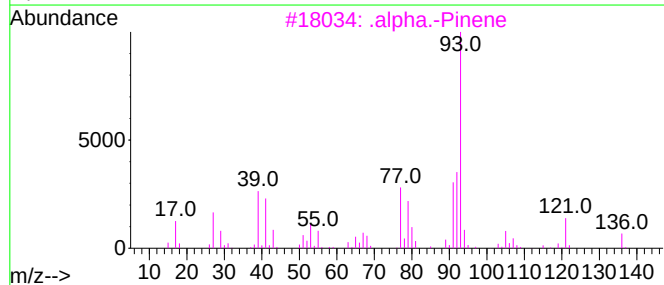
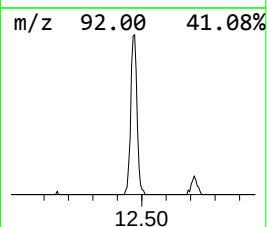
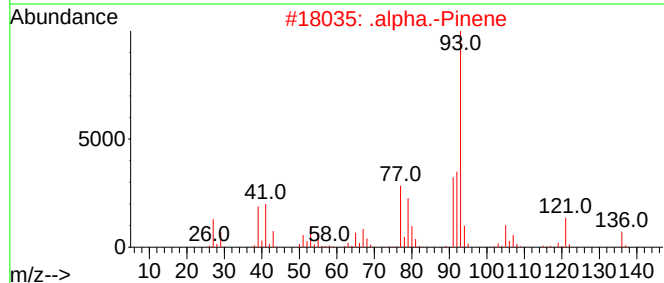
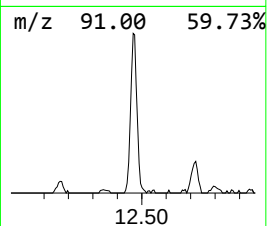
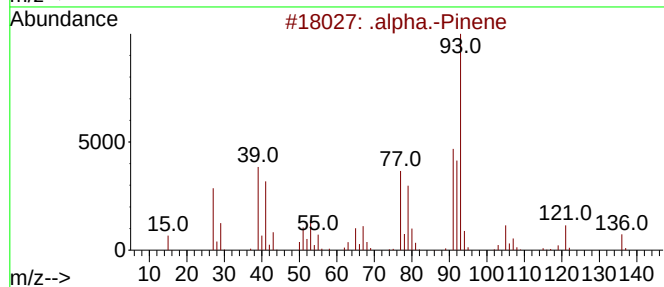
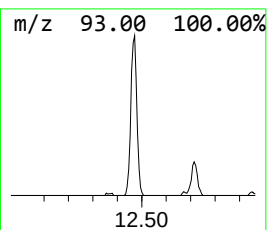
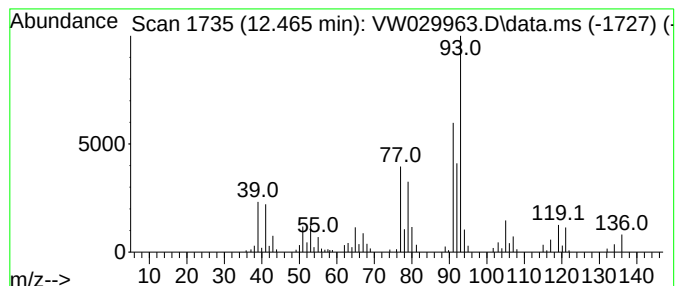
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Quant Title : SFAM01.0

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

Peak Number 6 .alpha.-Pinene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.465	2.41 ug/L	68611	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	alpha.-Pinene	136	C10H16	000080-56-8	93	
2	.	alpha.-Pinene	136	C10H16	000080-56-8	90	
3	.	alpha.-Pinene	136	C10H16	000080-56-8	86	
4	(1S)-2,6,6-Trimethylbicyclo[3.1...	136	C10H16	007785-26-4	81		
5	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	76		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
Data File : VW029963.D
Acq On : 20 Aug 2024 16:56
Operator : SY/MD
Sample : P3626-21
Misc : 5.59g/10mL/MSVOA_W/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYC6

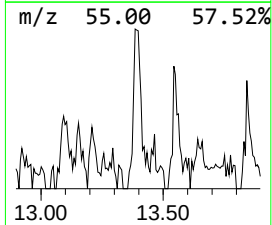
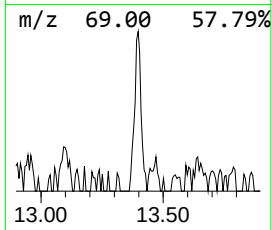
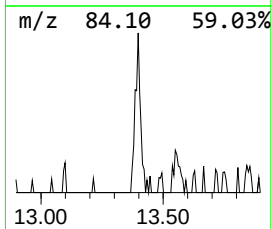
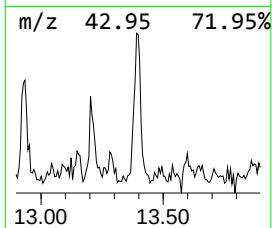
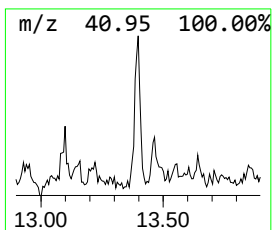
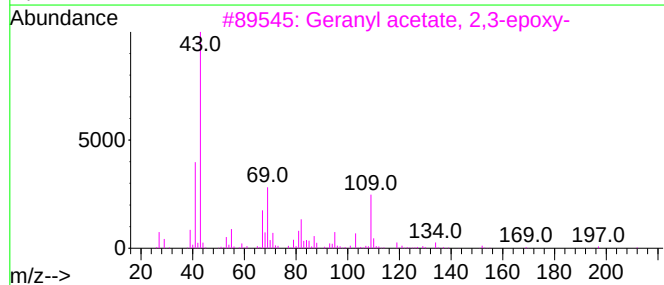
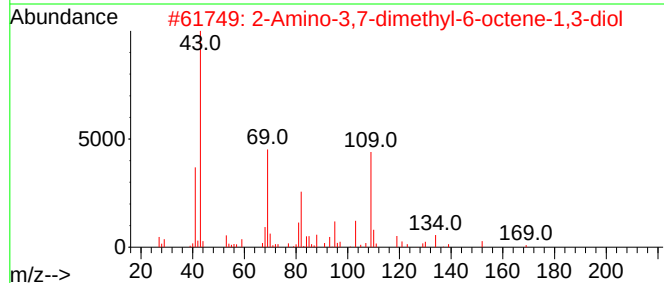
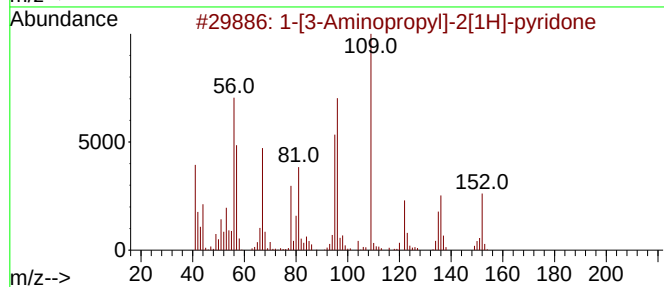
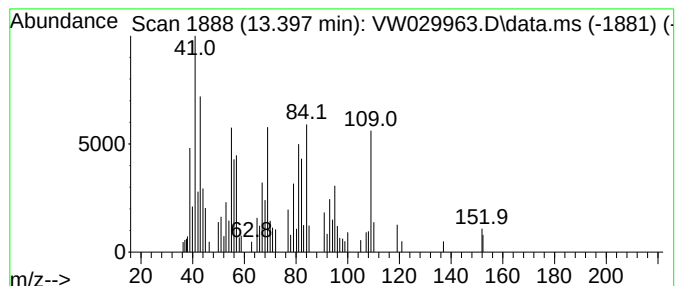
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Quant Title : SFAM01.0

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

Peak Number 8 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.397	1.42 ug/L	26561	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1		[3-Aminopropyl]-2[1H]-pyridone	152	C8H12N2O	102675-58-1	45
2	2		Amino-3,7-dimethyl-6-octene-1,...	187	C10H21NO2	1000432-16-0	27
3	3		Geranyl acetate, 2,3-epoxy-	212	C12H20O3	050727-95-2	27
4	4		2-Allyl-2-methyl-1,3-cyclopentan...	152	C9H12O2	026828-48-8	27
5	5		Pyridine, 4-methyl-, 1-oxide	109	C6H7NO	001003-67-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
Data File : VW029963.D
Acq On : 20 Aug 2024 16:56
Operator : SY/MD
Sample : P3626-21
Misc : 5.59g/10mL/MSVOA_W/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYC6

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
Acetaldehyde	2.509	2.5	ug/L	67050	1	8.843	668436	25.0
Pentanal	9.410	1.9	ug/L	51053	1	8.843	668436	25.0
Hexanal	11.069	13.8	ug/L	391024	2	11.629	710358	25.0
Furfural	11.843	2.0	ug/L	57167	2	11.629	710358	25.0
.alpha.-Pinene	12.465	2.4	ug/L	68611	2	11.629	710358	25.0
unknown-01	13.397	1.4	ug/L	26561	3	13.556	468568	25.0