

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122221\
 Data File : VW021614.D
 Acq On : 23 Dec 2021 15:31
 Operator : SY/VA
 Sample : M5174-13
 Misc : 6.63g/10.0mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GBC22

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\SFAMWLM120921SMA.M
 Title : SFAM01.0

Signal : TIC: VW021614.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	80	rVB2	29145	49760	18.86%	2.353%
2	2.501	92	98	114	rVB	27907	61526	23.32%	2.909%
3	2.812	142	149	155	rBV	41596	83088	31.50%	3.929%
4	2.879	156	160	170	rVB	16887	34019	12.90%	1.608%
5	3.019	176	183	194	rVB4	3825	9037	3.43%	0.427%
6	3.385	237	243	251	rVB4	1831	4111	1.56%	0.194%
7	3.458	251	255	258	rBV	129	255	0.10%	0.012%
8	3.714	292	297	299	rBV	964	1649	0.63%	0.078%
9	4.013	335	346	358	rBV2	30090	82409	31.24%	3.896%
10	4.147	359	368	387	rVB	14493	47260	17.91%	2.235%
11	4.385	397	407	419	rBB	1542	4670	1.77%	0.221%
12	4.684	449	456	465	rBV3	849	2357	0.89%	0.111%
13	4.915	482	494	507	rBV3	3165	11049	4.19%	0.522%
14	5.421	570	577	586	rVV3	1585	4288	1.63%	0.203%
15	5.793	628	638	648	rBV3	6613	21665	8.21%	1.024%
16	5.940	652	662	669	rBB3	2050	5454	2.07%	0.258%
17	6.080	682	685	688	rBV	97	163	0.06%	0.008%
18	6.232	707	710	713	rBV	128	172	0.07%	0.008%
19	6.421	739	741	746	rBB	145	218	0.08%	0.010%
20	6.903	812	820	827	rBV4	1072	2801	1.06%	0.132%
21	6.982	827	833	838	rBV4	596	1241	0.47%	0.059%
22	7.086	842	850	858	rBV	10691	30227	11.46%	1.429%
23	7.647	932	942	953	rBB	46739	114475	43.39%	5.413%
24	7.909	982	985	986	rBV	179	184	0.07%	0.009%
25	7.951	986	992	999	rVB3	869	2047	0.78%	0.097%
26	8.159	1022	1026	1030	rBB	490	529	0.20%	0.025%
27	8.275	1036	1045	1060	rBV2	82012	263808	100.00%	12.473%
28	8.561	1086	1092	1100	rVB7	1387	3666	1.39%	0.173%
29	8.701	1109	1115	1122	rBV5	1298	2874	1.09%	0.136%
30	8.842	1128	1138	1146	rBV	93211	184055	69.77%	8.702%
31	9.274	1201	1209	1216	rBV	60065	122364	46.38%	5.786%
32	9.409	1226	1231	1237	rBV2	1441	2680	1.02%	0.127%
33	9.512	1246	1248	1250	rVB	281	238	0.09%	0.011%
34	9.604	1260	1263	1268	rBB2	376	554	0.21%	0.026%
35	9.658	1268	1272	1277	rBB	231	360	0.14%	0.017%
36	9.750	1281	1287	1291	rBB2	358	680	0.26%	0.032%

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 Title : SFAM01.0

37	9.951	1315	1320	1326	rBB2	562	999	0.38%	0.047%
38	10.036	1327	1334	1340	rBV	29142	52462	19.89%	2.480%
39	10.323	1374	1381	1387	rBV	117160	198658	75.30%	9.393%
40	10.384	1387	1391	1399	rVB	12484	21601	8.19%	1.021%
41	10.500	1403	1410	1414	rBB4	1576	3245	1.23%	0.153%
42	10.579	1417	1423	1429	rBV	17361	30279	11.48%	1.432%
43	10.701	1441	1443	1449	rVB	985	1098	0.42%	0.052%
44	10.750	1449	1451	1456	rVB	419	711	0.27%	0.034%
45	10.859	1467	1469	1473	rBV	380	507	0.19%	0.024%
46	10.927	1473	1480	1491	rBV	42615	72551	27.50%	3.430%
47	11.030	1494	1497	1499	rBV	311	371	0.14%	0.018%
48	11.073	1499	1504	1510	rVB2	1904	3267	1.24%	0.154%
49	11.170	1518	1520	1524	rVB2	1105	1504	0.57%	0.071%
50	11.231	1525	1530	1535	rVB3	3675	6267	2.38%	0.296%
51	11.280	1535	1538	1541	rBV	234	283	0.11%	0.013%
52	11.329	1541	1546	1552	rVB4	721	1105	0.42%	0.052%
53	11.378	1552	1554	1555	rBV4	156	147	0.06%	0.007%
54	11.433	1559	1563	1568	rVB2	1007	1526	0.58%	0.072%
55	11.518	1571	1577	1580	rBB	399	659	0.25%	0.031%
56	11.561	1581	1584	1588	rBB	240	193	0.07%	0.009%
57	11.628	1588	1595	1604	rBV	110626	189139	71.70%	8.943%
58	11.731	1606	1612	1617	rBV	3804	6325	2.40%	0.299%
59	11.835	1621	1629	1634	rBV3	2272	5520	2.09%	0.261%
60	11.969	1649	1651	1654	rVB3	214	185	0.07%	0.009%
61	12.036	1659	1662	1663	rBV	162	159	0.06%	0.008%
62	12.140	1671	1679	1682	rBV3	1303	3021	1.15%	0.143%
63	12.243	1690	1696	1700	rVB6	833	1640	0.62%	0.078%
64	12.292	1700	1704	1707	rBV3	444	699	0.26%	0.033%
65	12.341	1707	1712	1717	rBV3	2062	4290	1.63%	0.203%
66	12.451	1727	1730	1733	rBV	390	476	0.18%	0.023%
67	12.530	1737	1743	1746	rBV3	438	845	0.32%	0.040%
68	12.603	1751	1755	1760	rBB4	1189	1853	0.70%	0.088%
69	12.688	1763	1769	1776	rBV	50264	83504	31.65%	3.948%
70	12.774	1779	1783	1789	rVB4	2541	4354	1.65%	0.206%
71	12.859	1792	1797	1802	rBV6	890	1573	0.60%	0.074%
72	12.932	1802	1809	1817	rBV7	1643	4169	1.58%	0.197%
73	13.042	1824	1827	1829	rBV	333	374	0.14%	0.018%
74	13.170	1844	1848	1856	rVB5	768	1658	0.63%	0.078%
75	13.255	1856	1862	1863	rBV2	1870	2717	1.03%	0.128%
76	13.554	1905	1911	1923	rBV	71800	119763	45.40%	5.663%

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 Title : SFAM01.0

77	13.652	1923	1927	1929	rVB4	835	1111	0.42%	0.053%
78	13.853	1953	1960	1968	rVB	55796	92742	35.16%	4.385%
79	14.066	1991	1995	1998	rBV2	2444	3318	1.26%	0.157%
80	14.200	2010	2017	2022	rBV5	1573	3076	1.17%	0.145%
81	14.261	2023	2027	2031	rVB3	767	887	0.34%	0.042%
82	14.328	2034	2038	2042	rVB5	1212	1794	0.68%	0.085%
83	14.383	2043	2047	2049	rBV2	1013	1214	0.46%	0.057%
84	14.505	2063	2067	2068	rBV2	586	790	0.30%	0.037%
85	14.682	2094	2096	2100	rBV	301	439	0.17%	0.021%
86	14.725	2100	2103	2108	rVB3	648	757	0.29%	0.036%
87	14.786	2108	2113	2122	rBV4	1961	4671	1.77%	0.221%
88	14.962	2138	2142	2143	rVB2	419	474	0.18%	0.022%
89	14.975	2143	2144	2146	rBV	325	284	0.11%	0.013%
90	14.999	2146	2148	2153	rVB3	573	657	0.25%	0.031%
91	15.060	2153	2158	2161	rBV4	696	1263	0.48%	0.060%
92	15.133	2168	2170	2171	rBV	302	237	0.09%	0.011%
93	15.176	2171	2177	2184	rVB5	808	1995	0.76%	0.094%
94	15.243	2184	2188	2190	rBV2	242	419	0.16%	0.020%
95	15.365	2204	2208	2212	rBV2	341	652	0.25%	0.031%
96	15.487	2222	2228	2234	rVB	7033	11938	4.53%	0.564%
97	15.852	2287	2288	2290	rBV	230	160	0.06%	0.008%
98	16.035	2316	2318	2319	rVV	215	149	0.06%	0.007%
99	16.358	2369	2371	2373	rBV	247	168	0.06%	0.008%
100	16.426	2380	2382	2383	rBV	200	155	0.06%	0.007%

Sum of corrected areas: 2114980

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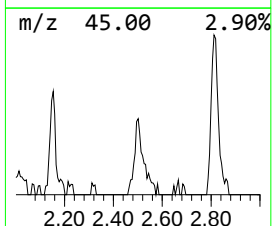
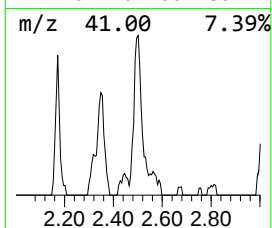
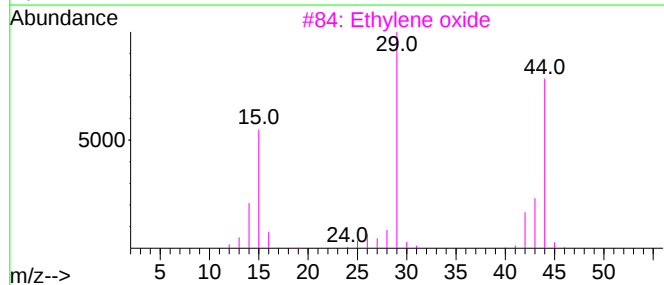
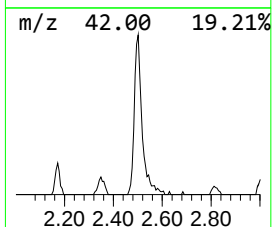
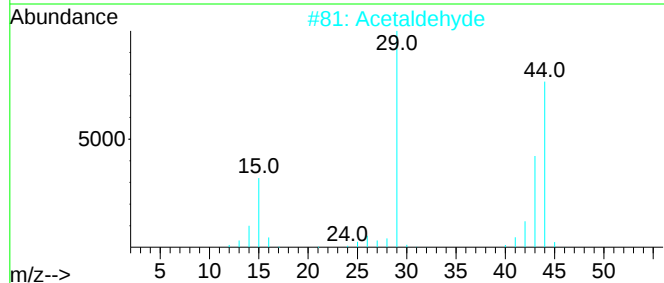
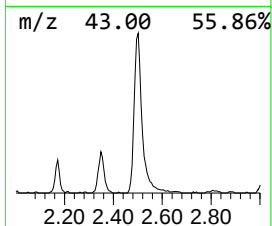
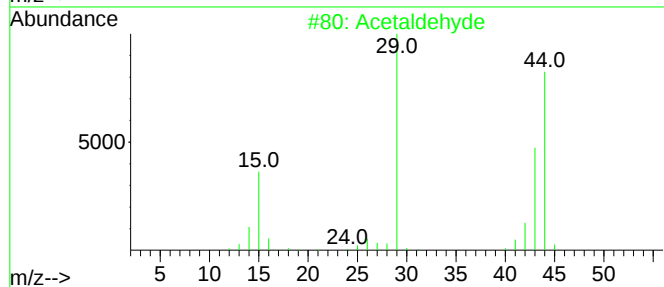
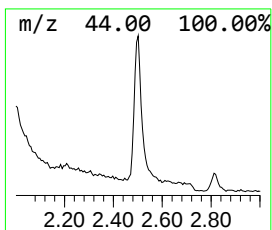
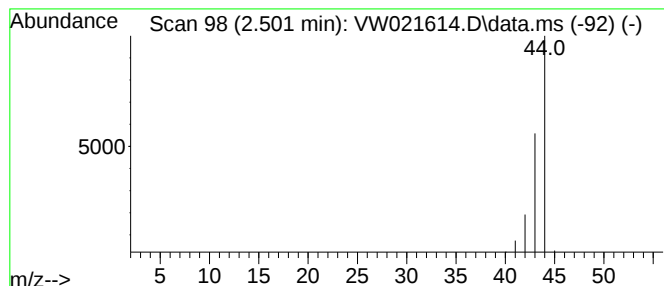
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.501	8.36 ug/L	61526	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Acetaldehyde	44	C2H4O	000075-07-0	74
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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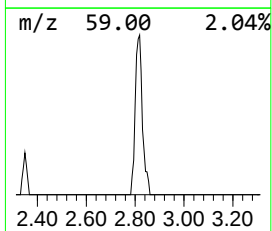
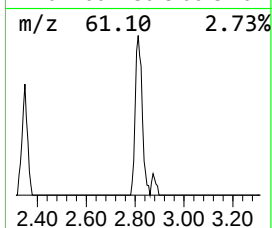
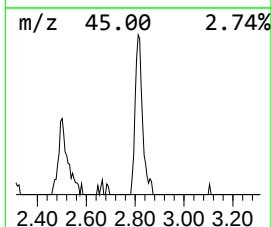
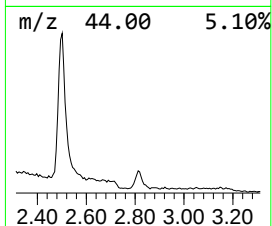
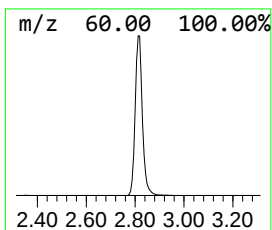
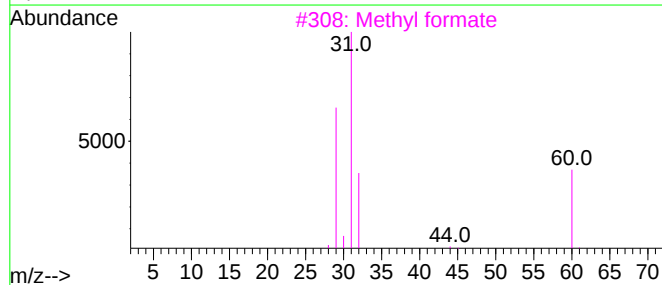
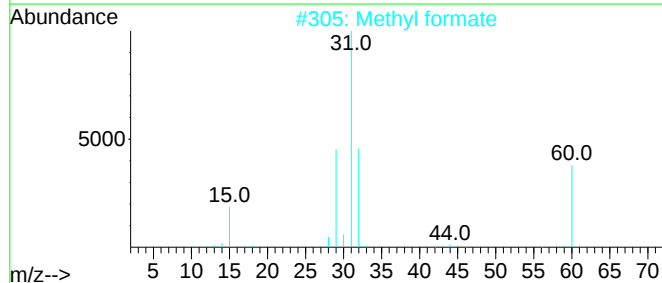
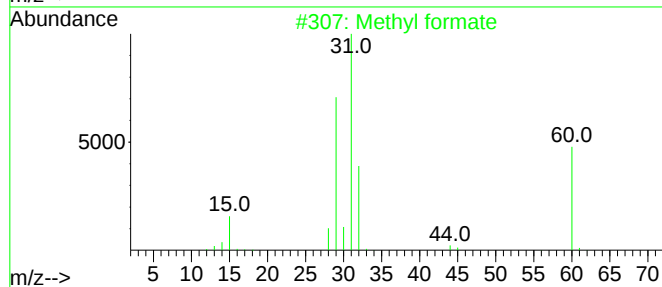
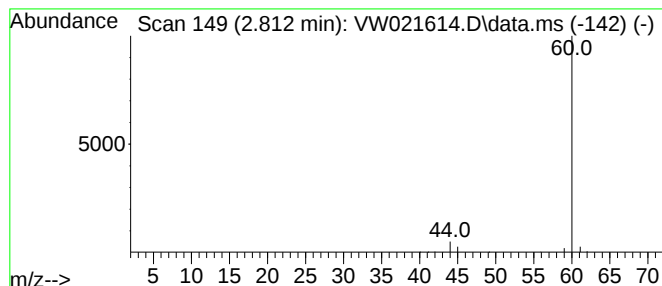
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.812	11.29 ug/L	83088	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl formate	60	C2H4O2	000107-31-3	7
2			Methyl formate	60	C2H4O2	000107-31-3	7
3			Methyl formate	60	C2H4O2	000107-31-3	5
4			Carbonyl sulfide	60	CO S	000463-58-1	5
5			Methyl formate	60	C2H4O2	000107-31-3	5



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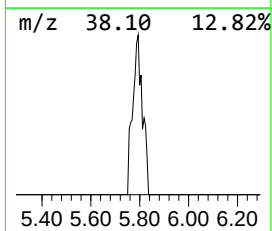
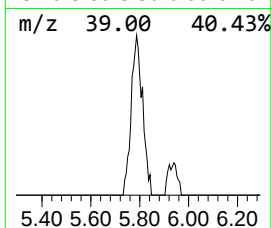
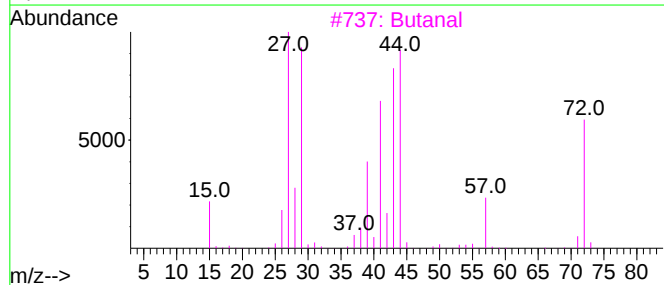
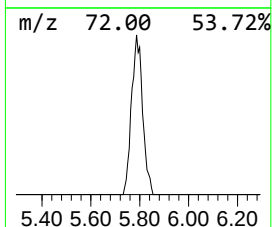
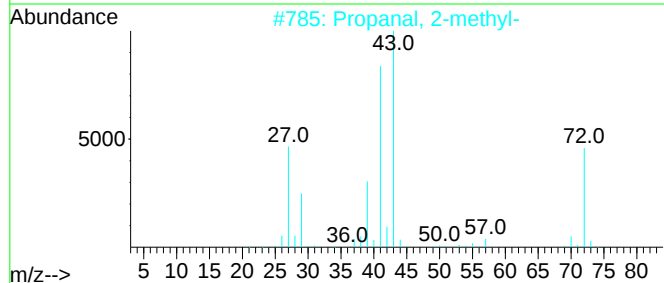
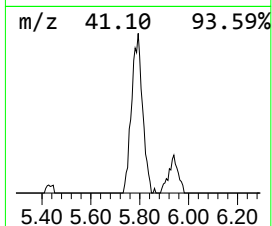
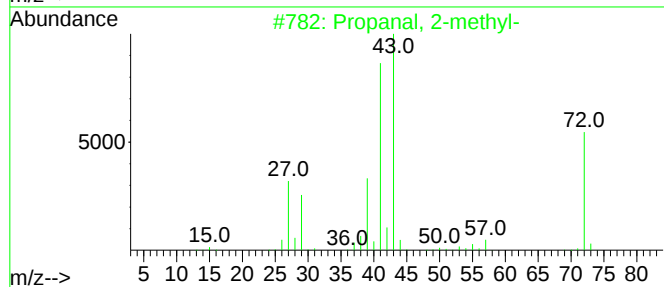
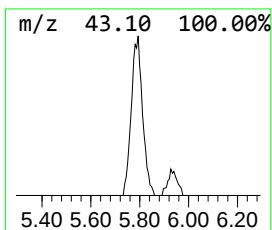
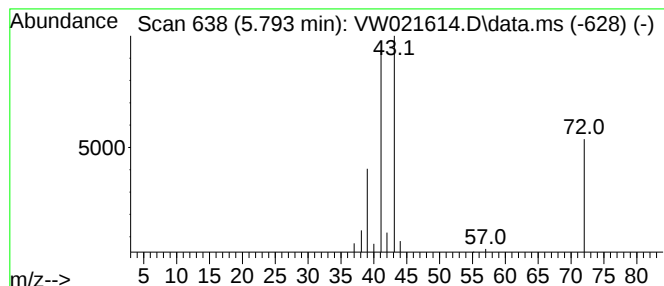
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Propanal, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.793	2.94 ug/L	21665	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91		
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	90		
3	Butanal	72	C4H8O	000123-72-8	72		
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	53		
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	50		



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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	2.501	8.4	ug/L	61526	1	8.842	184055	25.0
unknown-01	2.812	11.3	ug/L	83088	1	8.842	184055	25.0
Propanal, 2-met...	5.793	2.9	ug/L	21665	1	8.842	184055	25.0