

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
 Data File : VW029964.D
 Acq On : 20 Aug 2024 17:20
 Operator : SY/MD
 Sample : P3626-22
 Misc : 5.96g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCYE4

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: VW029964.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	52	53	59	rBV4	823	927	0.12%	0.014%
2	2.363	72	78	93	rVB	40115	97357	12.97%	1.502%
3	2.509	97	102	106	rBV2	5646	11870	1.58%	0.183%
4	2.899	158	166	181	rBV	31523	96264	12.83%	1.485%
5	3.393	240	247	255	rBV2	11943	26791	3.57%	0.413%
6	3.728	296	302	304	rBV6	723	1326	0.18%	0.020%
7	3.832	314	319	320	rBV3	626	723	0.10%	0.011%
8	4.021	338	350	363	rBV	67781	231105	30.80%	3.565%
9	4.137	363	369	387	rVB	24117	76373	10.18%	1.178%
10	4.393	407	411	416	rBV5	649	1175	0.16%	0.018%
11	4.460	419	422	425	rBV4	696	810	0.11%	0.012%
12	4.679	452	458	460	rBV2	2160	3576	0.48%	0.055%
13	4.929	488	499	508	rBV4	5026	19897	2.65%	0.307%
14	5.777	631	638	639	rBV5	1785	2736	0.36%	0.042%
15	5.911	656	660	661	rBV3	722	781	0.10%	0.012%
16	6.045	679	682	684	rBV	523	545	0.07%	0.008%
17	6.118	688	694	696	rBV4	628	1108	0.15%	0.017%
18	6.258	714	717	720	rBV3	586	892	0.12%	0.014%
19	6.356	729	733	737	rVV3	410	687	0.09%	0.011%
20	6.411	737	742	743	rVV4	449	558	0.07%	0.009%
21	6.508	756	758	761	rBV3	503	547	0.07%	0.008%
22	6.594	769	772	773	rBV3	476	564	0.08%	0.009%
23	6.899	814	822	834	rVV8	3140	10400	1.39%	0.160%
24	7.088	845	853	878	rVV2	19630	74690	9.95%	1.152%
25	7.258	880	881	886	rVV4	1181	2029	0.27%	0.031%
26	7.648	935	945	961	rVV	132271	330508	44.04%	5.098%
27	7.776	964	966	970	rVB5	680	1028	0.14%	0.016%
28	8.002	1000	1003	1009	rBV4	392	747	0.10%	0.012%
29	8.276	1038	1048	1064	rBV2	239668	729279	97.18%	11.249%
30	8.551	1083	1093	1102	rVV6	4095	11205	1.49%	0.173%
31	8.709	1110	1119	1129	rBV2	12077	28728	3.83%	0.443%
32	8.843	1132	1141	1153	rBV	352961	706151	94.10%	10.892%
33	8.977	1162	1163	1167	rBV2	513	677	0.09%	0.010%
34	9.148	1189	1191	1195	rVB3	726	804	0.11%	0.012%
35	9.270	1203	1211	1222	rBV	177529	361037	48.11%	5.569%
36	9.404	1227	1233	1247	rVV	31665	66183	8.82%	1.021%

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

37	9.904	1314	1315	1319	rVB3	722	530	0.07%	0.008%
38	10.032	1327	1336	1345	rBV	83229	154892	20.64%	2.389%
39	10.148	1351	1355	1356	rBV4	1249	1436	0.19%	0.022%
40	10.319	1373	1383	1391	rBV	304532	575977	76.75%	8.884%
41	10.422	1398	1400	1405	rVB4	1351	1765	0.24%	0.027%
42	10.502	1410	1413	1418	rVB4	1196	1937	0.26%	0.030%
43	10.575	1418	1425	1439	rBV	52358	98457	13.12%	1.519%
44	10.697	1439	1445	1450	rBV2	7061	13851	1.85%	0.214%
45	10.861	1465	1472	1474	rVB6	900	1681	0.22%	0.026%
46	10.922	1474	1482	1495	rBV	77637	142759	19.02%	2.202%
47	11.068	1499	1506	1521	rVB2	303553	492375	65.61%	7.595%
48	11.209	1527	1529	1534	rVB6	1223	1810	0.24%	0.028%
49	11.270	1537	1539	1542	rVV4	631	762	0.10%	0.012%
50	11.337	1546	1550	1552	rBV5	509	580	0.08%	0.009%
51	11.556	1583	1586	1590	rBV4	786	1515	0.20%	0.023%
52	11.629	1590	1598	1607	rBV	439664	750425	100.00%	11.575%
53	11.788	1622	1624	1627	rBV3	666	825	0.11%	0.013%
54	11.843	1627	1633	1644	rVV	22835	49406	6.58%	0.762%
55	11.940	1646	1649	1655	rVB6	2692	4798	0.64%	0.074%
56	12.020	1657	1662	1669	rBV2	8736	15352	2.05%	0.237%
57	12.148	1681	1683	1690	rBV5	656	1330	0.18%	0.021%
58	12.245	1695	1699	1704	rVB4	848	1319	0.18%	0.020%
59	12.337	1708	1714	1721	rBV2	10841	18475	2.46%	0.285%
60	12.465	1731	1735	1739	rVV3	2924	4955	0.66%	0.076%
61	12.507	1739	1742	1750	rVB5	1743	3262	0.43%	0.050%
62	12.599	1750	1757	1763	rBV2	9643	15989	2.13%	0.247%
63	12.690	1764	1772	1779	rBV	130129	214553	28.59%	3.309%
64	12.751	1779	1782	1786	rVB3	1006	1257	0.17%	0.019%
65	12.867	1798	1801	1802	rBV2	462	507	0.07%	0.008%
66	12.928	1802	1811	1817	rVV7	2672	5332	0.71%	0.082%
67	13.038	1824	1829	1833	rBV3	2827	4611	0.61%	0.071%
68	13.099	1834	1839	1843	rVV4	3163	5596	0.75%	0.086%
69	13.153	1843	1848	1853	rVV2	28198	47534	6.33%	0.733%
70	13.208	1853	1857	1863	rVV	20878	36324	4.84%	0.560%
71	13.282	1864	1869	1875	rVB6	7427	14945	1.99%	0.231%
72	13.391	1882	1887	1892	rBV4	9366	16472	2.20%	0.254%
73	13.464	1895	1899	1907	rBV9	1497	4322	0.58%	0.067%
74	13.550	1907	1913	1925	rVV	296075	491325	65.47%	7.578%
75	13.641	1925	1928	1936	rVB3	4161	6834	0.91%	0.105%
76	13.708	1936	1939	1942	rBV4	1126	1599	0.21%	0.025%

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 Title : SFAM01.0

77	13.848	1955	1962	1969	rBV	185760	306491	40.84%	4.728%
78	13.940	1975	1977	1981	rVB4	773	1116	0.15%	0.017%
79	14.019	1985	1990	1993	rBV5	1498	2872	0.38%	0.044%
80	14.068	1993	1998	2009	rVB3	11142	21160	2.82%	0.326%
81	14.214	2019	2022	2024	rBV4	661	839	0.11%	0.013%
82	14.324	2034	2040	2047	rBV4	7335	13013	1.73%	0.201%
83	14.403	2051	2053	2055	rBV2	786	554	0.07%	0.009%
84	14.519	2067	2072	2076	rVB6	1602	3240	0.43%	0.050%
85	14.550	2076	2077	2080	rVB2	665	510	0.07%	0.008%
86	14.592	2080	2084	2085	rBV3	599	688	0.09%	0.011%
87	14.684	2097	2099	2101	rBV3	598	558	0.07%	0.009%
88	14.848	2121	2126	2131	rVV6	2058	4034	0.54%	0.062%
89	14.885	2131	2132	2137	rVB3	950	857	0.11%	0.013%
90	14.946	2137	2142	2148	rBV5	2276	4072	0.54%	0.063%
91	15.074	2162	2163	2167	rBV4	598	766	0.10%	0.012%
92	15.171	2175	2179	2182	rBV6	1342	2305	0.31%	0.036%
93	15.245	2187	2191	2196	rVB5	2030	2975	0.40%	0.046%
94	15.470	2225	2228	2229	rBV3	1959	1949	0.26%	0.030%
95	15.751	2273	2274	2276	rBV	787	554	0.07%	0.009%
96	15.842	2284	2289	2294	rBV6	1487	2778	0.37%	0.043%
97	15.952	2303	2307	2308	rBV3	1384	1501	0.20%	0.023%
98	16.031	2316	2320	2323	rVB5	800	1178	0.16%	0.018%
99	16.409	2380	2382	2385	rBV4	656	559	0.07%	0.009%
100	16.476	2390	2393	2394	rBV3	774	830	0.11%	0.013%

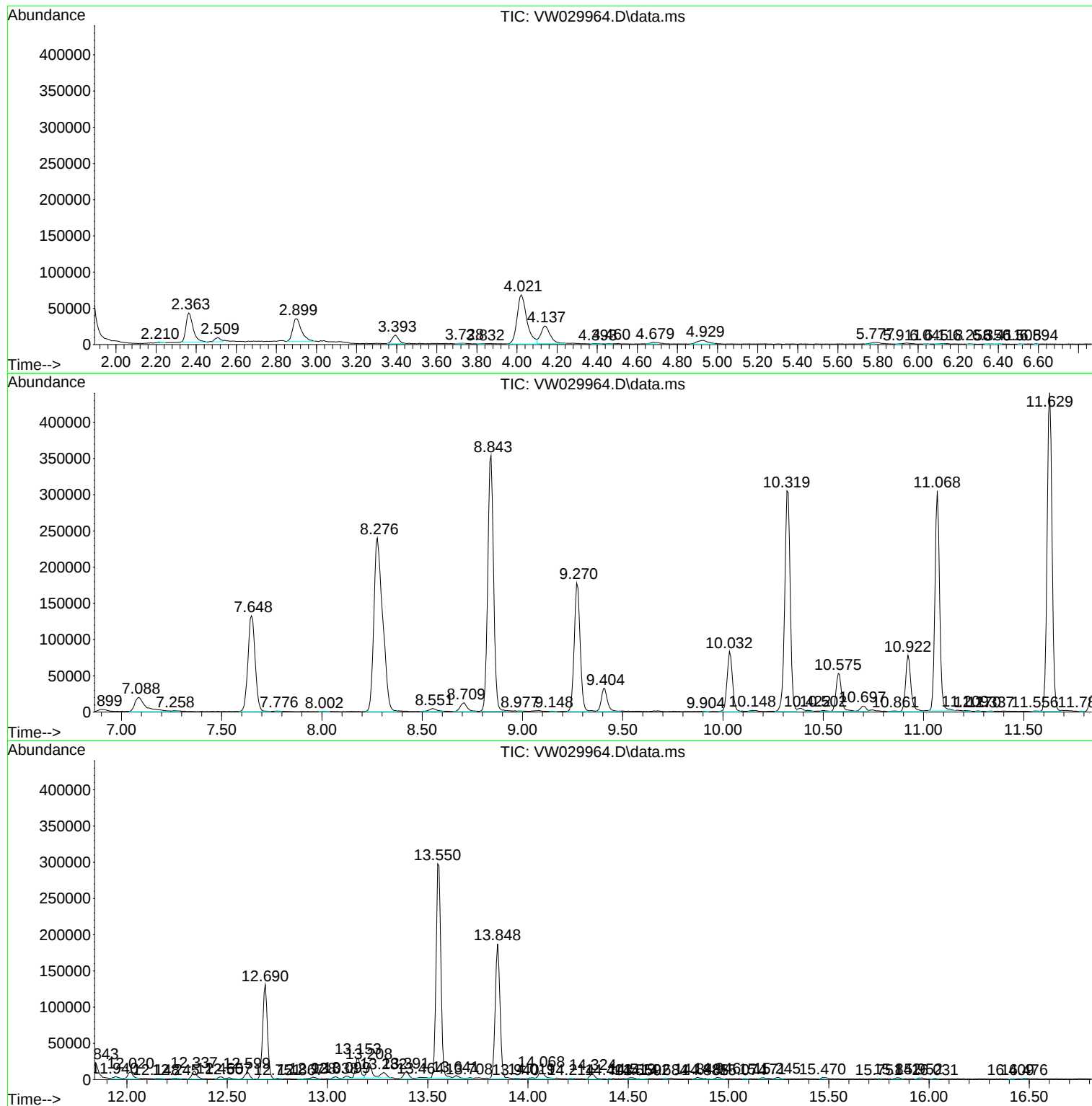
Sum of corrected areas: 6483151

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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
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Instrument :
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DCYE4

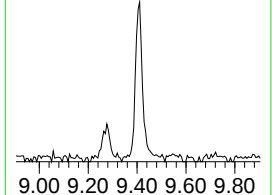
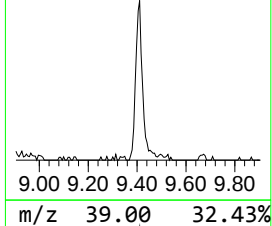
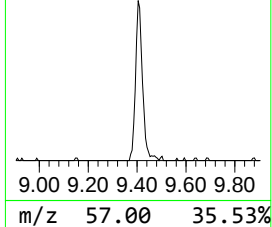
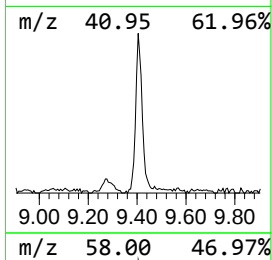
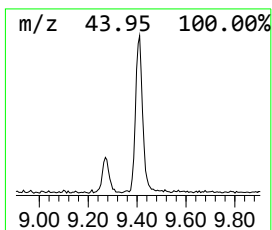
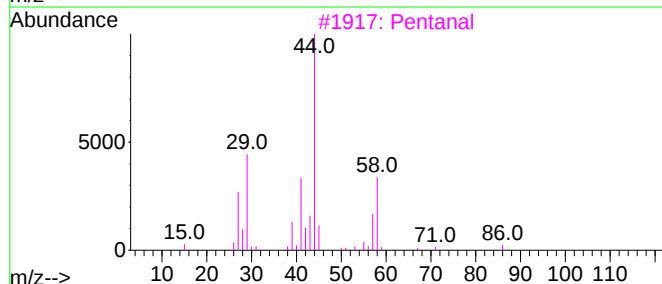
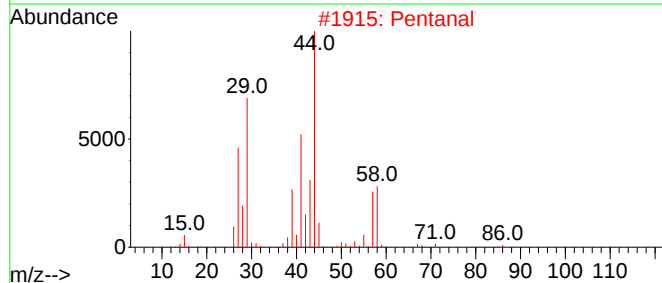
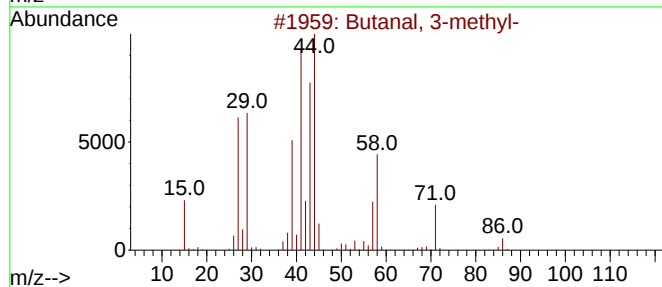
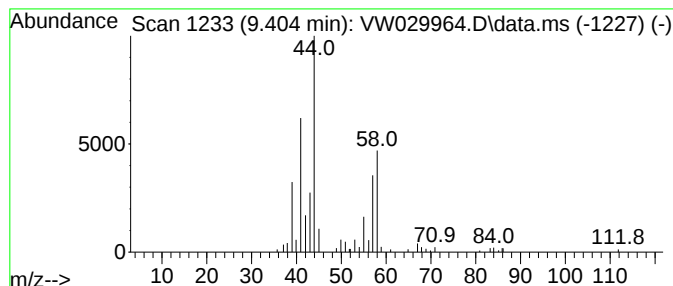
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Butanal, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.404	2.34 ug/L	66183	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	87
2			Pentanal	86	C5H10O	000110-62-3	78
3			Pentanal	86	C5H10O	000110-62-3	78
4			Pentanal	86	C5H10O	000110-62-3	72
5			Butanal, 3-methyl-	86	C5H10O	000590-86-3	56



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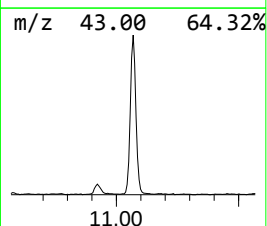
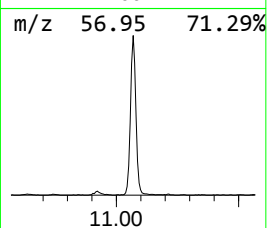
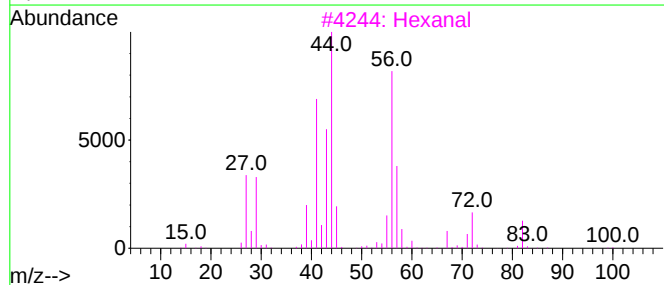
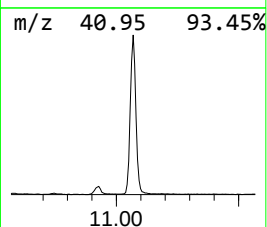
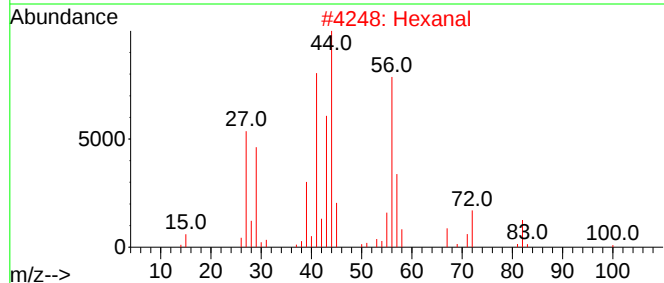
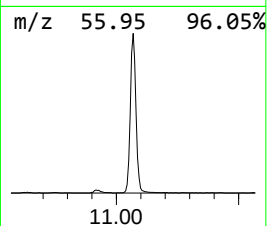
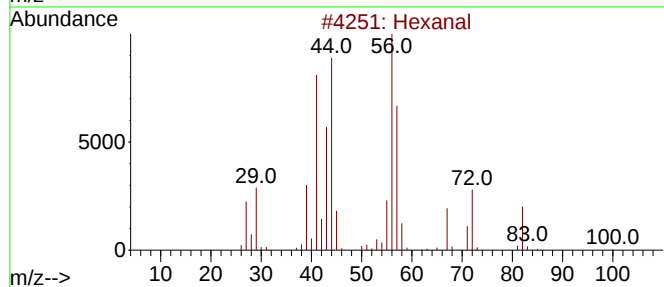
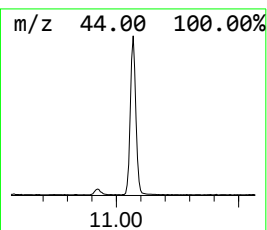
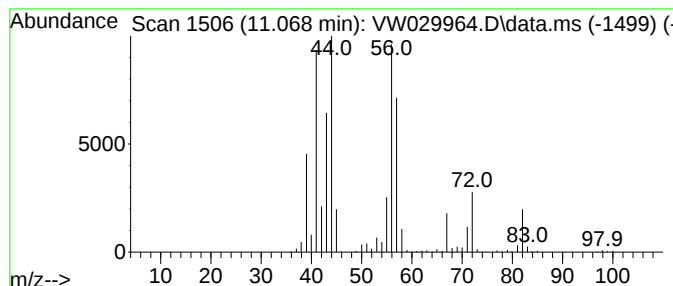
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.069	16.40 ug/L	492375	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	95
2	Hexanal			100	C6H12O	000066-25-1	81
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	59



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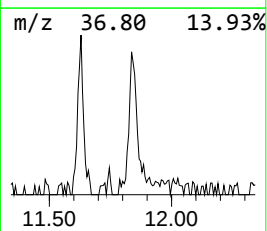
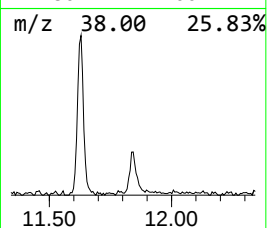
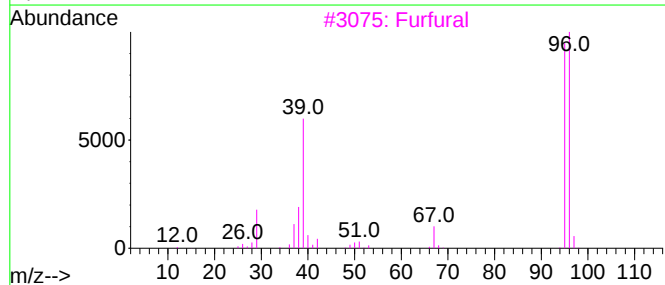
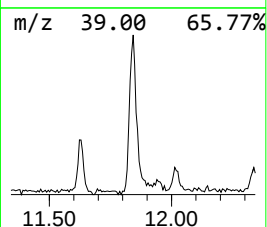
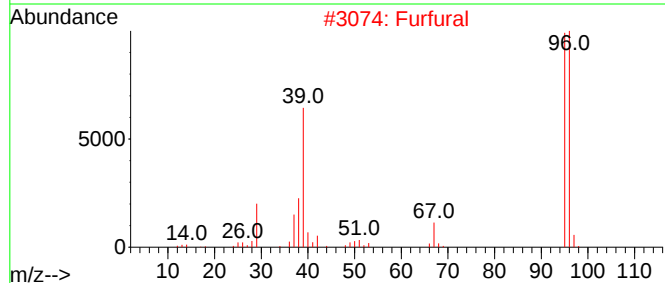
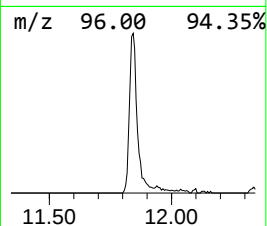
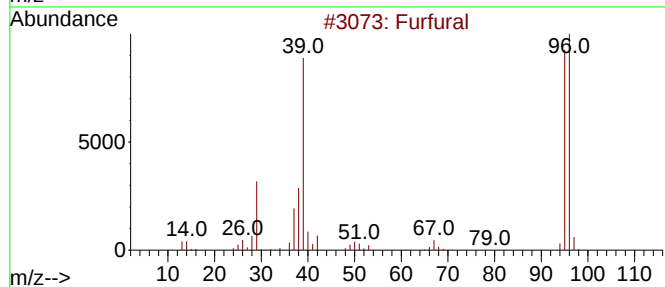
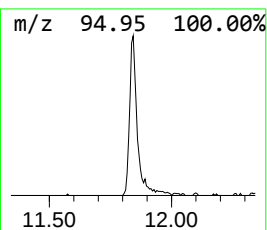
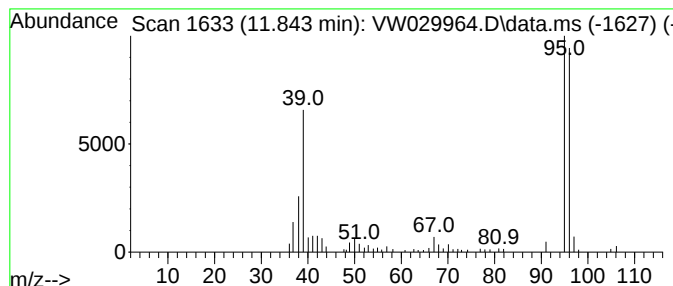
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Furfural Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.843	1.65 ug/L	49406	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	91
3			Furfural	96	C5H4O2	000098-01-1	91
4			3-Furaldehyde	96	C5H4O2	000498-60-2	90
5			1H-Imidazole, 1,4-dimethyl-	96	C5H8N2	006338-45-0	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
Data File : VW029964.D
Acq On : 20 Aug 2024 17:20
Operator : SY/MD
Sample : P3626-22
Misc : 5.96g/10mL/MSVOA_W/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYE4

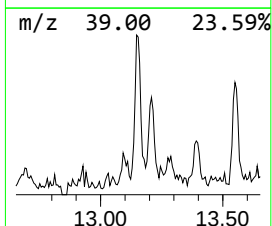
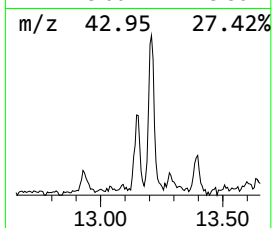
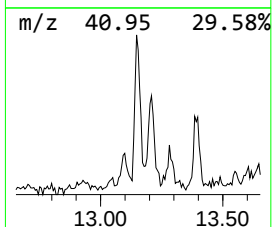
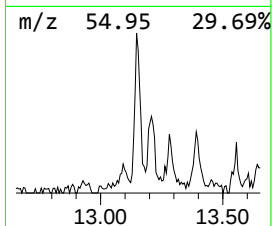
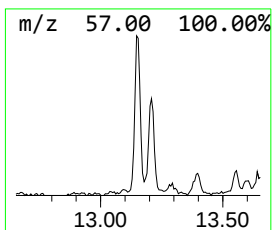
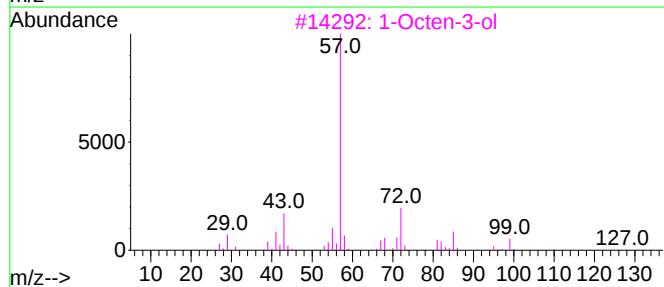
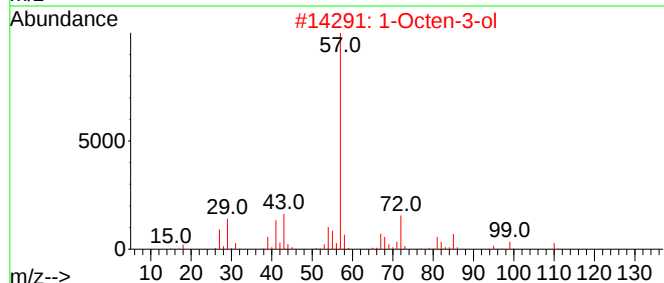
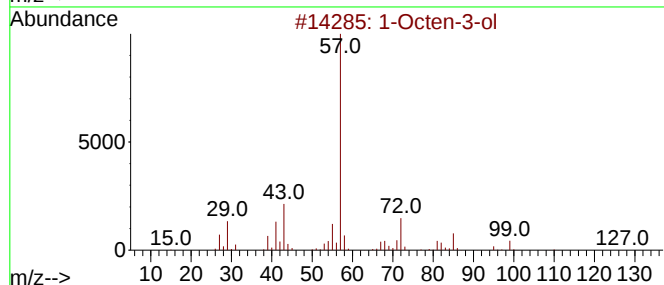
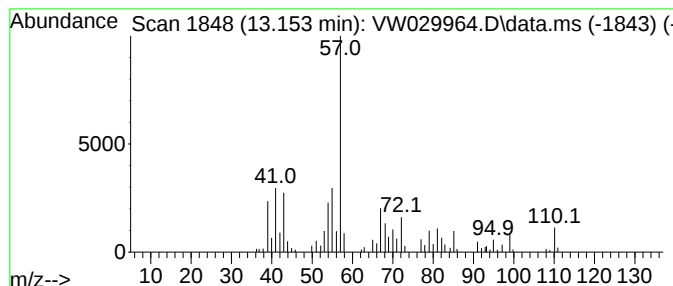
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Quant Title : SFAM01.0

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

Peak Number 5 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.153	2.42 ug/L	47534	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octen-3-ol	128	C8H16O	003391-86-4	43
2			1-Octen-3-ol	128	C8H16O	003391-86-4	40
3			1-Octen-3-ol	128	C8H16O	003391-86-4	38
4			2-Octen-1-ol, (Z)-	128	C8H16O	026001-58-1	37
5			1,7-Octadien-3-ol	126	C8H14O	030385-19-4	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
Data File : VW029964.D
Acq On : 20 Aug 2024 17:20
Operator : SY/MD
Sample : P3626-22
Misc : 5.96g/10mL/MSVOA_W/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYE4

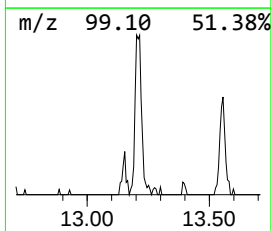
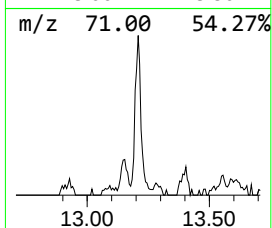
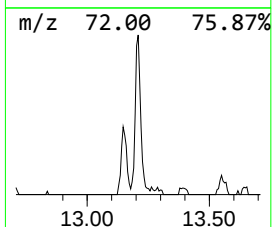
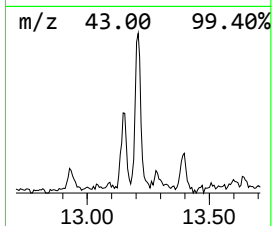
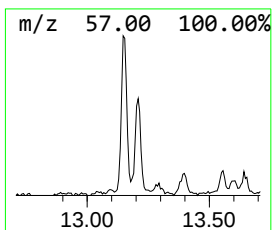
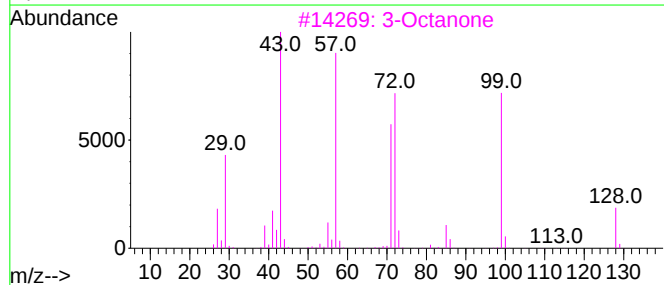
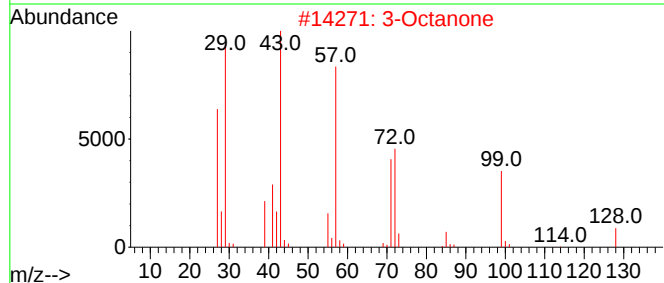
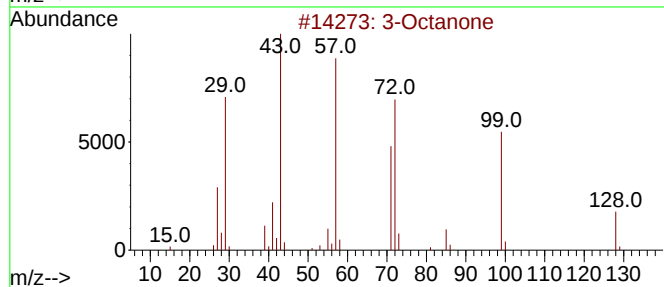
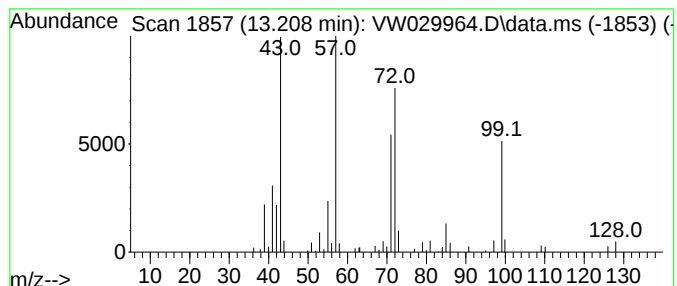
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Quant Title : SFAM01.0

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

Peak Number 6 3-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	1.85 ug/L	36324	1,4-Dichlorobenzene-d4	13.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octanone	128	C8H16O	000106-68-3	78
2		3-Octanone	128	C8H16O	000106-68-3	74
3		3-Octanone	128	C8H16O	000106-68-3	64
4		Butanal, 2-ethyl-	100	C6H12O	000097-96-1	47
5		Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082024\
Data File : VW029964.D
Acq On : 20 Aug 2024 17:20
Operator : SY/MD
Sample : P3626-22
Misc : 5.96g/10mL/MSVOA_W/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYE4

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
Butanal, 3-methyl-	9.404	2.3	ug/L	66183	1	8.843	706151	25.0
Hexanal	11.069	16.4	ug/L	492375	2	11.629	750425	25.0
Furfural	11.843	1.6	ug/L	49406	2	11.629	750425	25.0
unknown-01	13.153	2.4	ug/L	47534	3	13.556	491325	25.0
3-Octanone	13.208	1.9	ug/L	36324	3	13.556	491325	25.0