

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082224\
 Data File : VW029991.D
 Acq On : 22 Aug 2024 16:37
 Operator : SY/MD
 Sample : P3673-13
 Misc : 4.39g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCYD9

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: VW029991.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	71	78	92	rBV	48610	111987	12.21%	1.390%
2	2.497	95	100	109	rBV	11181	25722	2.81%	0.319%
3	2.814	149	152	157	rVB	1779	3382	0.37%	0.042%
4	2.899	158	166	183	rVB	35281	106533	11.62%	1.322%
5	3.393	240	247	257	rVB2	6284	14648	1.60%	0.182%
6	3.533	267	270	271	rBV3	414	493	0.05%	0.006%
7	3.716	296	300	301	rVV2	273	318	0.03%	0.004%
8	3.735	301	303	309	rVB3	495	959	0.10%	0.012%
9	3.905	330	331	335	rVB3	364	357	0.04%	0.004%
10	4.021	337	350	359	rBV	87143	278111	30.33%	3.451%
11	4.119	360	366	382	rVB	53212	150107	16.37%	1.862%
12	4.271	389	391	393	rBV2	395	333	0.04%	0.004%
13	4.320	397	399	402	rVB	624	504	0.05%	0.006%
14	4.381	404	409	410	rBV2	1058	1426	0.16%	0.018%
15	4.673	447	457	466	rBV2	5022	14962	1.63%	0.186%
16	4.917	487	497	515	rBV3	7356	26653	2.91%	0.331%
17	5.789	631	640	648	rBV4	2549	8059	0.88%	0.100%
18	5.941	656	665	676	rVB4	3466	10535	1.15%	0.131%
19	6.118	687	694	707	rVB3	989	3182	0.35%	0.039%
20	6.899	811	822	832	rBV4	8296	24899	2.72%	0.309%
21	7.002	835	839	842	rVB3	626	1075	0.12%	0.013%
22	7.075	843	851	865	rBV	28886	91192	9.94%	1.131%
23	7.648	934	945	960	rVV	167408	409308	44.64%	5.079%
24	7.746	960	961	963	rVV2	400	368	0.04%	0.005%
25	7.776	963	966	971	rVV4	551	1031	0.11%	0.013%
26	8.276	1038	1048	1064	rBV2	308713	914807	99.76%	11.351%
27	8.551	1083	1093	1102	rVV2	6126	14832	1.62%	0.184%
28	8.618	1102	1104	1106	rVB3	466	376	0.04%	0.005%
29	8.703	1111	1118	1129	rBV	11499	27656	3.02%	0.343%
30	8.843	1132	1141	1151	rBV	428809	871362	95.02%	10.812%
31	8.984	1163	1164	1167	rVB3	346	306	0.03%	0.004%
32	9.051	1170	1175	1176	rBV2	741	946	0.10%	0.012%
33	9.270	1203	1211	1222	rBV	214967	443639	48.38%	5.505%
34	9.410	1226	1234	1246	rVB	49666	99311	10.83%	1.232%
35	9.672	1266	1277	1283	rBV5	888	2606	0.28%	0.032%
36	10.032	1321	1336	1347	rBV	104468	192401	20.98%	2.387%

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 Title : SFAM01.0

37	10.130	1347	1352	1353	rBV3	790	1039	0.11%	0.013%
38	10.154	1353	1356	1361	rVB4	1609	2441	0.27%	0.030%
39	10.215	1363	1366	1371	rVB2	289	406	0.04%	0.005%
40	10.325	1371	1384	1391	rBV	392835	721585	78.69%	8.953%
41	10.386	1391	1394	1406	rVB	6927	13589	1.48%	0.169%
42	10.502	1406	1413	1418	rBV6	1306	2568	0.28%	0.032%
43	10.575	1418	1425	1432	rBV	67795	120145	13.10%	1.491%
44	10.703	1440	1446	1451	rBV	11906	19734	2.15%	0.245%
45	10.861	1469	1472	1475	rVB2	507	617	0.07%	0.008%
46	10.922	1475	1482	1498	rBV	113612	202146	22.04%	2.508%
47	11.069	1499	1506	1528	rVB	323438	526015	57.36%	6.527%
48	11.398	1558	1560	1565	rVB4	316	476	0.05%	0.006%
49	11.459	1565	1570	1572	rBV3	293	481	0.05%	0.006%
50	11.562	1583	1587	1590	rBV3	565	914	0.10%	0.011%
51	11.629	1590	1598	1607	rBV	554179	916989	100.00%	11.378%
52	11.831	1625	1631	1644	rBV	35526	73205	7.98%	0.908%
53	11.946	1646	1650	1656	rVV4	5406	10394	1.13%	0.129%
54	12.014	1658	1661	1670	rVV3	4150	8026	0.88%	0.100%
55	12.087	1671	1673	1675	rVV2	874	801	0.09%	0.010%
56	12.172	1682	1687	1688	rBV5	499	621	0.07%	0.008%
57	12.233	1693	1697	1701	rBV4	1465	2247	0.25%	0.028%
58	12.337	1706	1714	1725	rBV2	21495	38499	4.20%	0.478%
59	12.465	1729	1735	1740	rBV4	3905	7214	0.79%	0.090%
60	12.599	1752	1757	1764	rVB	12803	21549	2.35%	0.267%
61	12.690	1764	1772	1779	rBV	167552	285397	31.12%	3.541%
62	12.818	1790	1793	1796	rVB2	431	491	0.05%	0.006%
63	12.928	1800	1811	1823	rBV4	6013	14415	1.57%	0.179%
64	13.044	1825	1830	1833	rBV3	2316	4036	0.44%	0.050%
65	13.093	1833	1838	1844	rBV4	4752	8422	0.92%	0.104%
66	13.154	1844	1848	1852	rVB4	3575	5204	0.57%	0.065%
67	13.208	1852	1857	1862	rBV2	20354	32906	3.59%	0.408%
68	13.269	1862	1867	1880	rVB3	14470	33453	3.65%	0.415%
69	13.391	1880	1887	1895	rBV2	14025	24355	2.66%	0.302%
70	13.464	1895	1899	1902	rBV3	3193	5550	0.61%	0.069%
71	13.556	1907	1914	1925	rVV	374097	608731	66.38%	7.553%
72	13.647	1925	1929	1935	rVB5	3083	5466	0.60%	0.068%
73	13.690	1935	1936	1937	rBV	464	332	0.04%	0.004%
74	13.757	1943	1947	1950	rBV6	799	1541	0.17%	0.019%
75	13.849	1955	1962	1975	rBV	233505	380084	41.45%	4.716%
76	13.983	1983	1984	1985	rBV	547	355	0.04%	0.004%

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 Title : SFAM01.0

77	14.013	1985	1989	1993	rVV3	2988	5146	0.56%	0.064%
78	14.068	1993	1998	2008	rVB3	20580	40179	4.38%	0.499%
79	14.184	2015	2017	2020	rBV4	368	477	0.05%	0.006%
80	14.214	2020	2022	2031	rVB4	753	1615	0.18%	0.020%
81	14.281	2031	2033	2034	rBV	585	387	0.04%	0.005%
82	14.318	2034	2039	2046	rBV2	10611	16330	1.78%	0.203%
83	14.513	2064	2071	2077	rVB6	1686	3845	0.42%	0.048%
84	14.598	2083	2085	2086	rBV	528	486	0.05%	0.006%
85	14.611	2086	2087	2089	rVV2	684	479	0.05%	0.006%
86	14.647	2091	2093	2094	rVV	826	706	0.08%	0.009%
87	14.684	2096	2099	2102	rVV3	1337	2234	0.24%	0.028%
88	14.714	2102	2104	2109	rVB4	1099	1075	0.12%	0.013%
89	14.848	2119	2126	2129	rBV5	2118	3477	0.38%	0.043%
90	14.946	2136	2142	2147	rBV3	6156	10285	1.12%	0.128%
91	15.171	2173	2179	2181	rBV4	1218	1890	0.21%	0.023%
92	15.251	2187	2192	2198	rVB7	1283	2130	0.23%	0.026%
93	15.330	2203	2205	2208	rBV2	258	348	0.04%	0.004%
94	15.360	2208	2210	2212	rBV2	410	430	0.05%	0.005%
95	15.385	2212	2214	2216	rVB2	703	488	0.05%	0.006%
96	15.476	2225	2229	2233	rBV2	1935	3331	0.36%	0.041%
97	15.659	2257	2259	2264	rVB3	454	613	0.07%	0.008%
98	15.842	2284	2289	2297	rVB5	2988	5188	0.57%	0.064%
99	15.952	2302	2307	2308	rBV2	912	1201	0.13%	0.015%
100	16.251	2354	2356	2358	rBV3	395	349	0.04%	0.004%

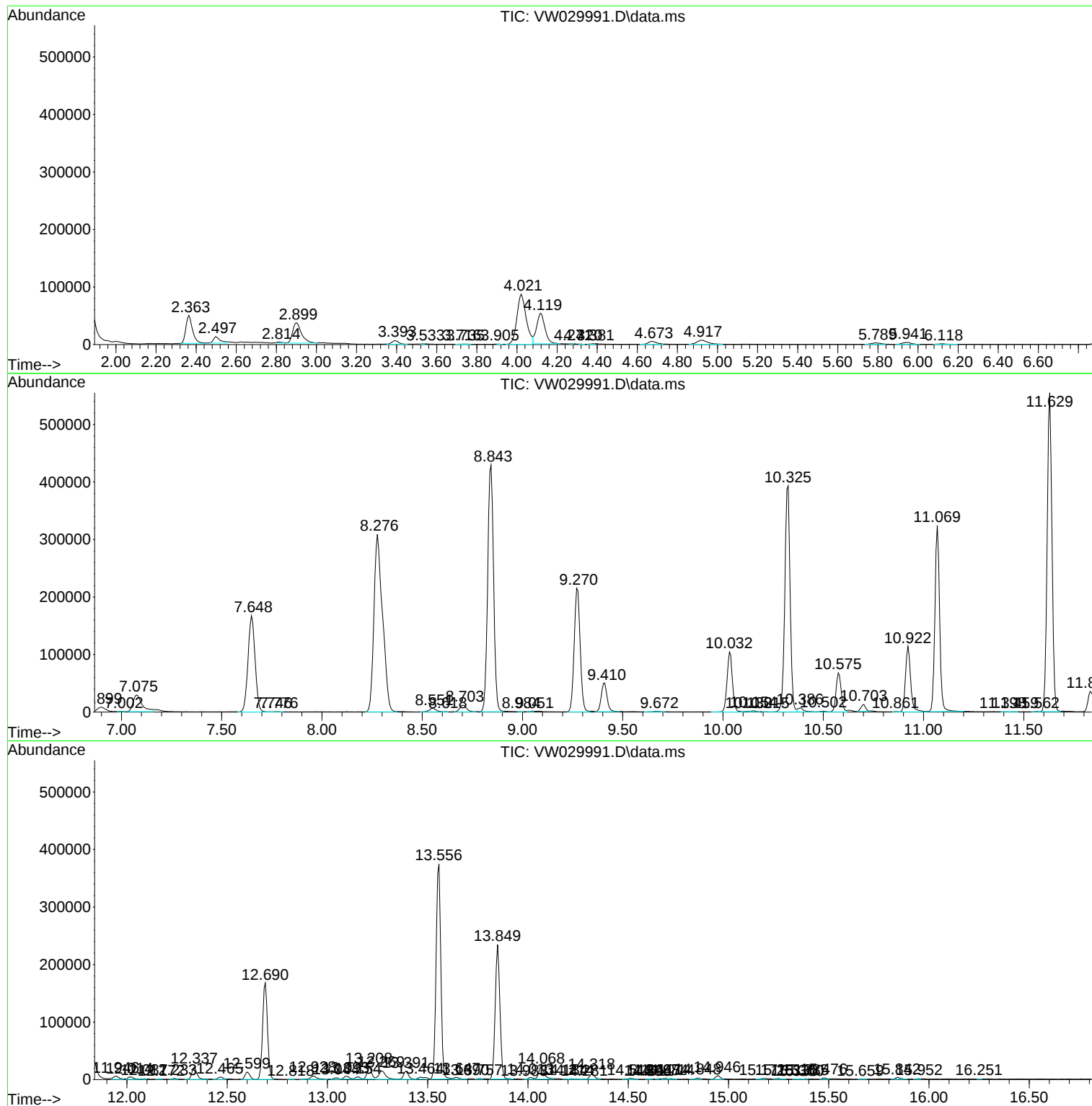
Sum of corrected areas: 8059514

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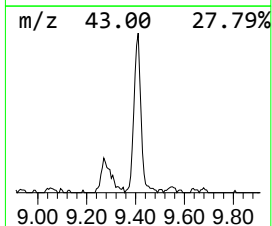
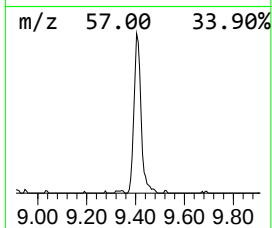
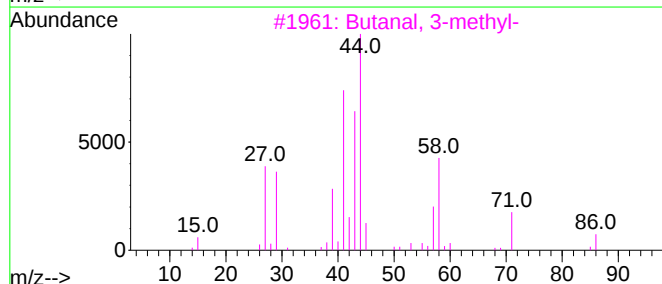
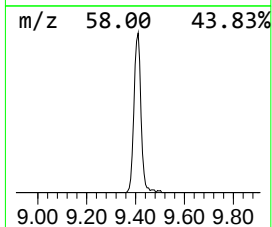
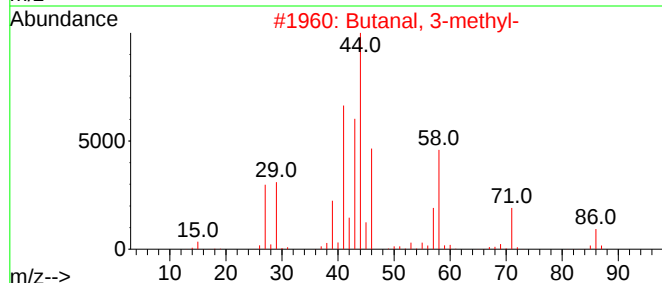
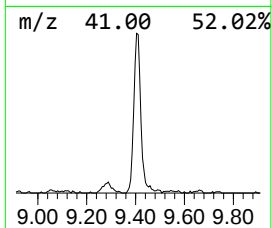
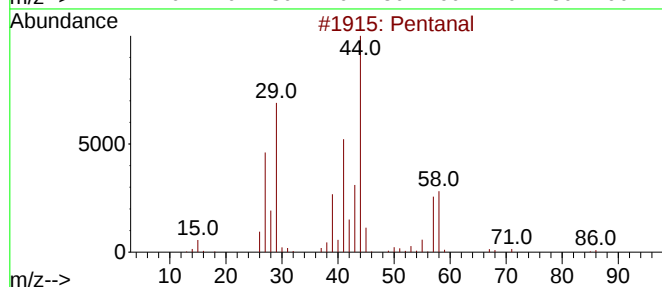
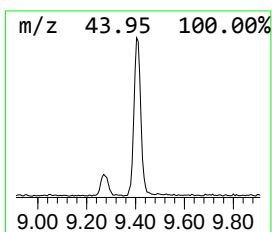
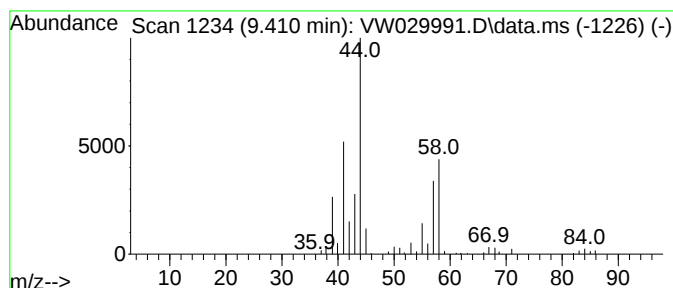
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	2.85 ug/L	99311	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	90
2	Butanal, 3-methyl-			86	C5H10O	000590-86-3	83
3	Butanal, 3-methyl-			86	C5H10O	000590-86-3	83
4	Pentanal			86	C5H10O	000110-62-3	78
5	Pentanal			86	C5H10O	000110-62-3	74



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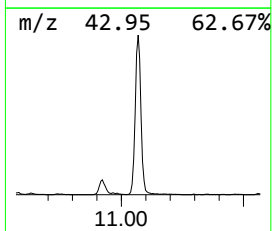
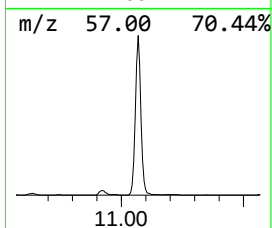
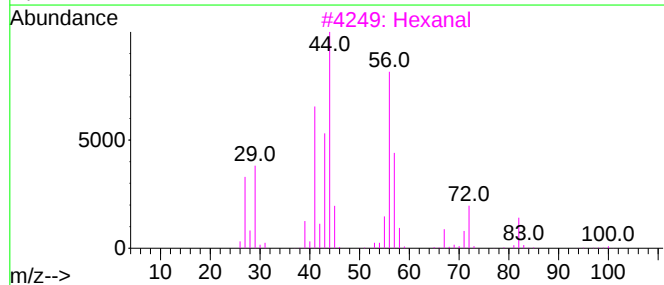
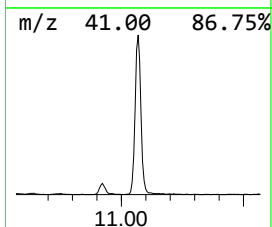
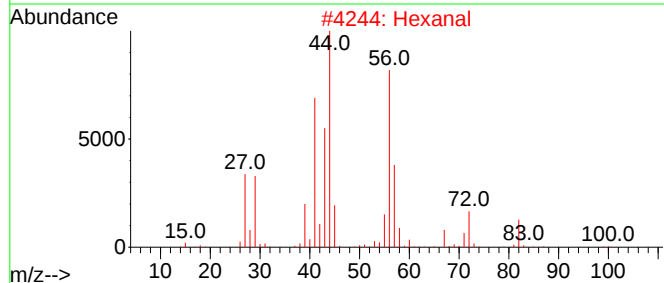
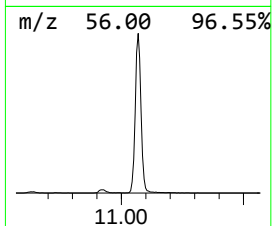
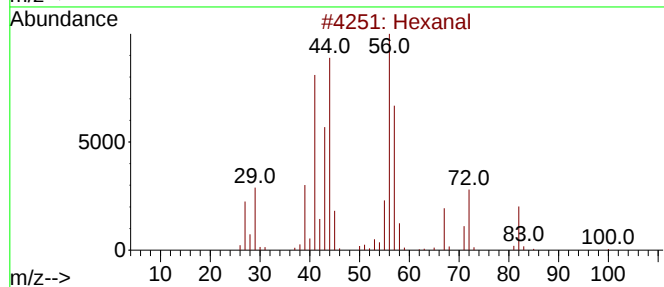
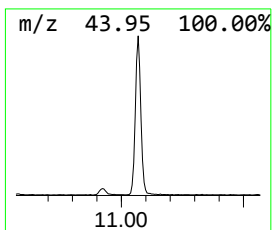
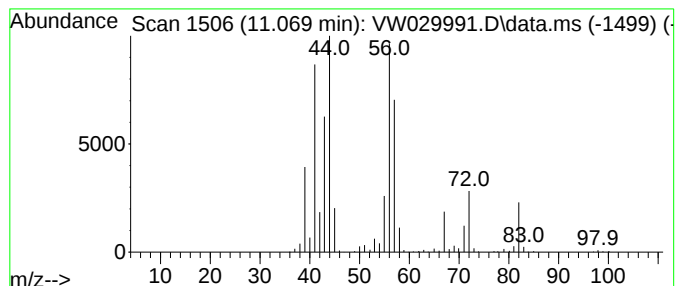
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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	14.34 ug/L	526015	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	87
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	59
5	Hexanal			100	C6H12O	000066-25-1	59



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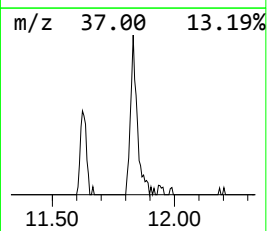
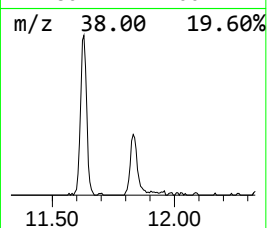
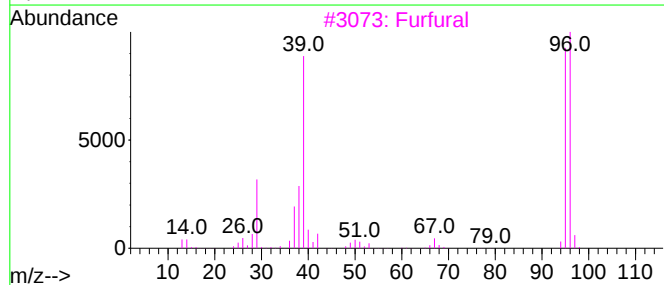
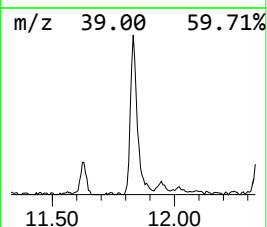
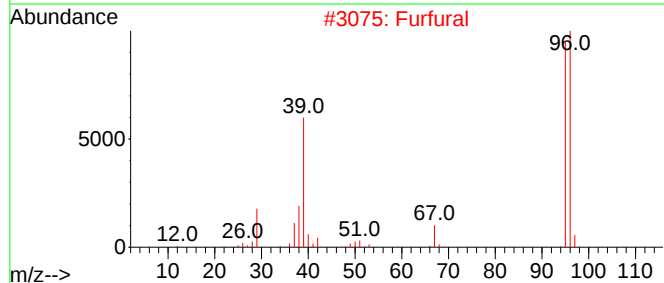
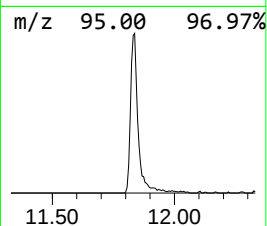
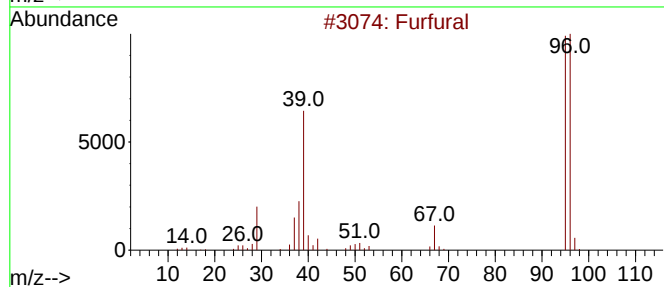
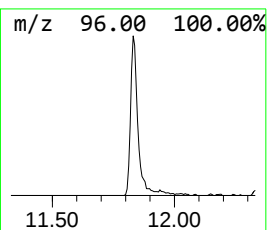
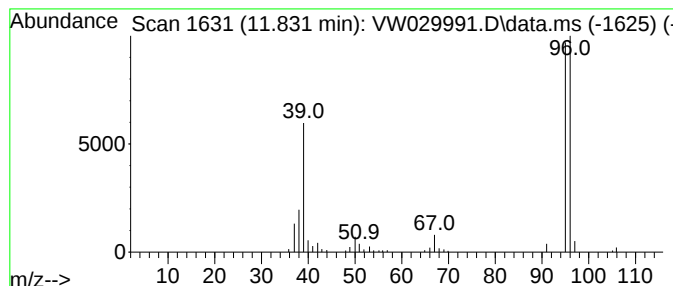
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Furfural Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.831	2.00 ug/L	73205	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furfural			96	C5H4O2	000098-01-1	96
2	Furfural			96	C5H4O2	000098-01-1	94
3	Furfural			96	C5H4O2	000098-01-1	91
4	Furfural			96	C5H4O2	000098-01-1	76
5	3(2H)-Pyridazinone			96	C4H4N2O	000504-30-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082224\
Data File : VW029991.D
Acq On : 22 Aug 2024 16:37
Operator : SY/MD
Sample : P3673-13
Misc : 4.39g/10mL/MSVOA_W/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYD9

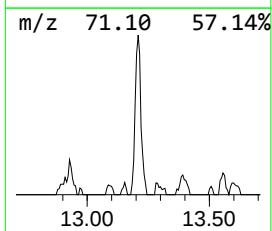
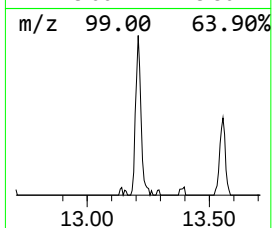
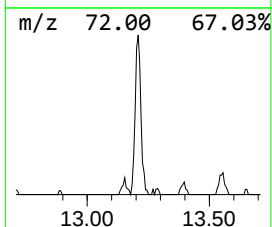
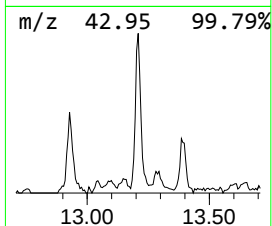
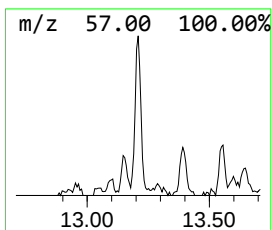
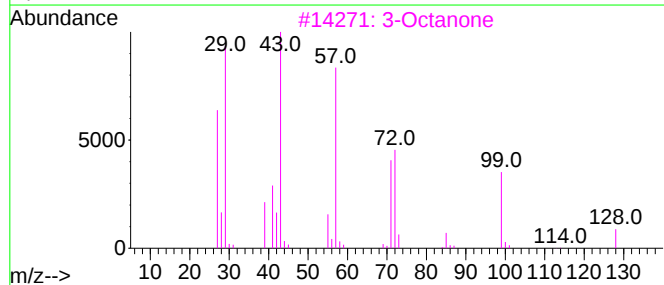
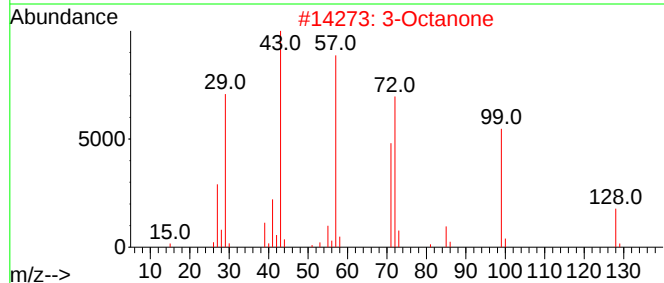
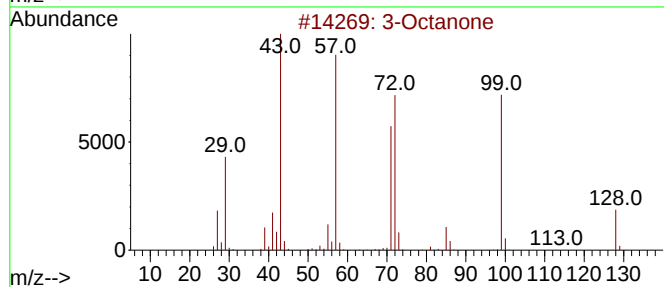
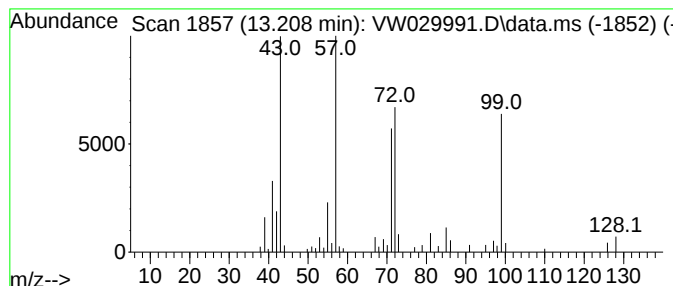
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Quant Title : SFAM01.0

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

Peak Number 5 3-Octanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	1.35 ug/L	32906	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone			128	C8H16O	000106-68-3	94
2	3-Octanone			128	C8H16O	000106-68-3	90
3	3-Octanone			128	C8H16O	000106-68-3	78
4	3-Heptanone, 5-methyl-			128	C8H16O	000541-85-5	53
5	4-Methylthiazole			99	C4H5NS	000693-95-8	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082224\
Data File : VW029991.D
Acq On : 22 Aug 2024 16:37
Operator : SY/MD
Sample : P3673-13
Misc : 4.39g/10mL/MSVOA_W/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYD9

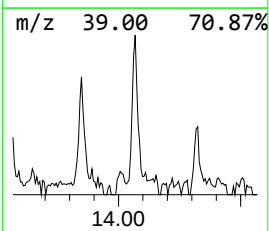
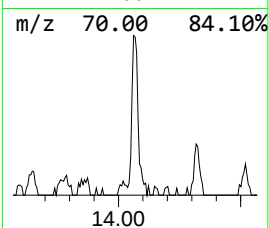
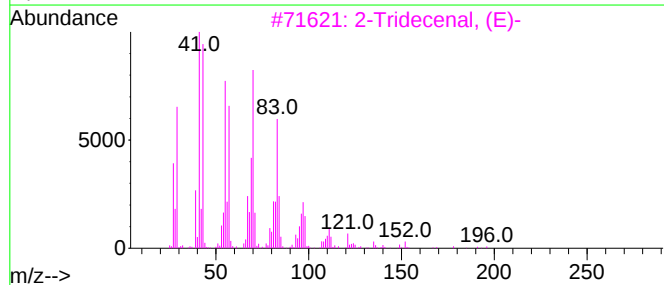
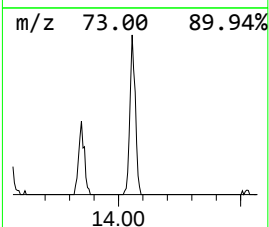
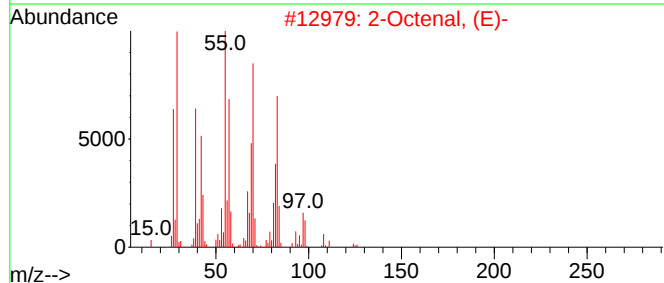
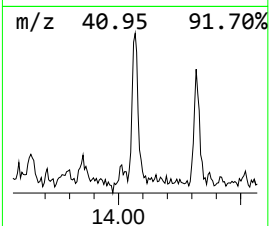
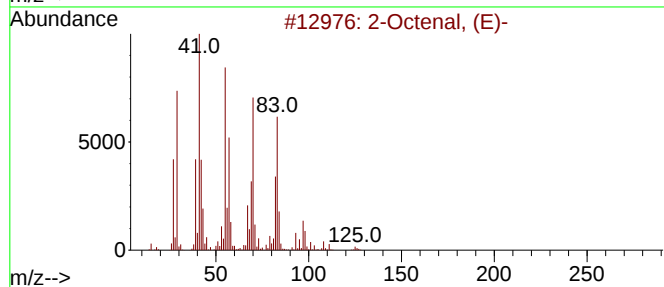
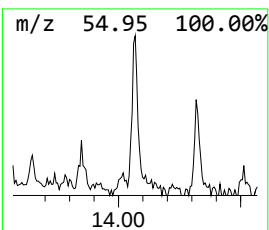
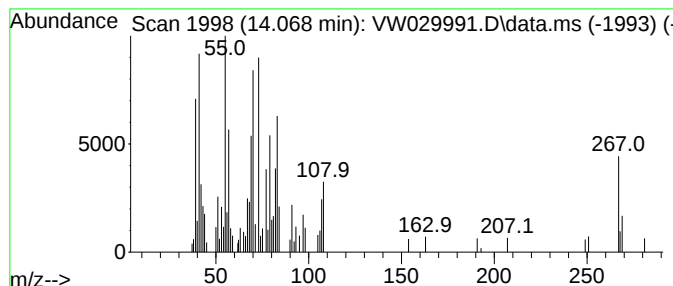
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Quant Title : SFAM01.0

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

Peak Number 7 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	1.65 ug/L	40179	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octenal, (E)-			126	C8H14O	002548-87-0	38
2	2-Octenal, (E)-			126	C8H14O	002548-87-0	38
3	2-Tridecenal, (E)-			196	C13H24O	007069-41-2	27
4	2-Dodecenal, (E)-			182	C12H22O	020407-84-5	27
5	2-Undecenal, E-			168	C11H20O	053448-07-0	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082224\
Data File : VW029991.D
Acq On : 22 Aug 2024 16:37
Operator : SY/MD
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Misc : 4.39g/10mL/MSVOA_W/SOIL/A
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCYD9

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
Pentanal	9.410	2.9	ug/L	99311	1	8.843	871362	25.0
Hexanal	11.069	14.3	ug/L	526015	2	11.629	916989	25.0
Furfural	11.831	2.0	ug/L	73205	2	11.629	916989	25.0
3-Octanone	13.208	1.4	ug/L	32906	3	13.556	608731	25.0
unknown-01	14.068	1.6	ug/L	40179	3	13.556	608731	25.0