

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW042823\
 Data File : VW025754.D
 Acq On : 28 Apr 2023 12:53
 Operator : SY/MD
 Sample : 02526-08
 Misc : 5.70g/10mL/MSVOA_W/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCCF2

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\SFAMWLM042723SMA.M
 Title : SFAM01.0

Signal : TIC: VW025754.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	91	rVB	73045	165671	3.13%	0.673%
2	2.497	94	100	122	rBV	345656	1210790	22.85%	4.919%
3	2.899	160	166	179	rVB	54015	143057	2.70%	0.581%
4	3.228	218	220	225	rVV6	1883	2132	0.04%	0.009%
5	3.393	243	247	248	rBV4	1591	1822	0.03%	0.007%
6	3.527	259	269	278	rBV	11263	32577	0.61%	0.132%
7	3.625	283	285	289	rVB5	1615	1493	0.03%	0.006%
8	3.728	293	302	317	rBV	65827	201471	3.80%	0.819%
9	4.021	339	350	357	rBV	166648	487188	9.19%	1.979%
10	4.112	357	365	395	rVB	1921832	5298433	100.00%	21.526%
11	4.387	403	410	417	rBV2	8079	22018	0.42%	0.089%
12	4.740	465	468	470	rBV3	1639	1653	0.03%	0.007%
13	4.917	487	497	508	rBV	18171	61834	1.17%	0.251%
14	5.137	527	533	534	rBV6	1647	2528	0.05%	0.010%
15	5.423	574	580	586	rVV6	2449	6249	0.12%	0.025%
16	5.789	628	640	653	rBV2	86030	282700	5.34%	1.149%
17	5.947	659	666	673	rVB6	5680	16322	0.31%	0.066%
18	6.039	677	681	685	rVB5	1233	1816	0.03%	0.007%
19	6.100	685	691	693	rBV7	2106	4107	0.08%	0.017%
20	6.283	716	721	725	rVB8	1636	2895	0.05%	0.012%
21	6.441	745	747	752	rVB6	1209	1997	0.04%	0.008%
22	6.520	756	760	764	rBV7	1199	2402	0.05%	0.010%
23	6.600	764	773	782	rBV8	2667	8553	0.16%	0.035%
24	6.911	815	824	830	rBV6	8636	28177	0.53%	0.114%
25	6.972	830	834	836	rBV5	1947	2953	0.06%	0.012%
26	7.081	843	852	858	rBV	59909	163960	3.09%	0.666%
27	7.167	858	866	881	rVB2	276934	751056	14.18%	3.051%
28	7.508	917	922	923	rBV5	1601	2290	0.04%	0.009%
29	7.648	935	945	963	rVB	243994	602185	11.37%	2.446%
30	7.874	979	982	985	rBV4	1394	1556	0.03%	0.006%
31	7.947	989	994	995	rBV5	1226	1904	0.04%	0.008%
32	8.026	1002	1007	1010	rVB7	1153	1625	0.03%	0.007%
33	8.063	1010	1013	1014	rBV3	1434	1592	0.03%	0.006%
34	8.142	1022	1026	1027	rBV4	1487	2206	0.04%	0.009%
35	8.276	1038	1048	1067	rBV2	485254	1570606	29.64%	6.381%
36	8.551	1081	1093	1107	rBV	378978	849143	16.03%	3.450%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
 Title : SFAM01.0

37	8.709	1111	1119	1128	rBV2	189531	418229	7.89%	1.699%
38	8.843	1133	1141	1152	rVB	537566	1068202	20.16%	4.340%
39	9.032	1165	1172	1175	rBV2	9717	18930	0.36%	0.077%
40	9.093	1176	1182	1191	rVB	39882	87315	1.65%	0.355%
41	9.276	1203	1212	1227	rBV2	364321	781081	14.74%	3.173%
42	9.422	1230	1236	1246	rVB5	8917	26309	0.50%	0.107%
43	9.666	1268	1276	1283	rVV9	4960	14862	0.28%	0.060%
44	9.758	1289	1291	1295	rVB5	1975	2320	0.04%	0.009%
45	9.886	1306	1312	1317	rVV8	2802	6279	0.12%	0.026%
46	10.032	1329	1336	1345	rBV	170600	312749	5.90%	1.271%
47	10.130	1346	1352	1360	rVB	20587	40067	0.76%	0.163%
48	10.209	1360	1365	1371	rBV2	15423	28923	0.55%	0.118%
49	10.325	1372	1384	1390	rVV	672365	1222187	23.07%	4.965%
50	10.386	1390	1394	1405	rVB2	37525	87966	1.66%	0.357%
51	10.575	1419	1425	1433	rBV	114743	198302	3.74%	0.806%
52	10.697	1442	1445	1450	rVB2	6660	10078	0.19%	0.041%
53	10.861	1463	1472	1478	rBV	2205388	3775743	71.26%	15.340%
54	10.922	1478	1482	1488	rVB	193635	314045	5.93%	1.276%
55	11.075	1502	1507	1516	rVB3	16840	33118	0.63%	0.135%
56	11.209	1527	1529	1534	rVB5	1778	2282	0.04%	0.009%
57	11.416	1559	1563	1567	rBV7	1193	2308	0.04%	0.009%
58	11.532	1579	1582	1583	rBV3	1316	1548	0.03%	0.006%
59	11.629	1590	1598	1608	rBV	680470	1162177	21.93%	4.722%
60	11.733	1608	1615	1622	rVB9	9599	22281	0.42%	0.091%
61	11.830	1627	1631	1645	rVB3	14939	41894	0.79%	0.170%
62	12.093	1671	1674	1680	rVB5	5136	9462	0.18%	0.038%
63	12.172	1680	1687	1693	rBV4	17250	39187	0.74%	0.159%
64	12.233	1693	1697	1702	rVB2	12373	18738	0.35%	0.076%
65	12.343	1711	1715	1719	rBV7	2556	4508	0.09%	0.018%
66	12.507	1739	1742	1743	rBV3	1490	1908	0.04%	0.008%
67	12.605	1749	1758	1763	rBV2	25488	50822	0.96%	0.206%
68	12.690	1765	1772	1779	rVV	291727	482199	9.10%	1.959%
69	12.751	1779	1782	1787	rVB5	4877	8324	0.16%	0.034%
70	12.867	1797	1801	1803	rBV5	3334	4708	0.09%	0.019%
71	12.940	1808	1813	1820	rVB5	10782	20509	0.39%	0.083%
72	13.099	1837	1839	1847	rVB6	4773	8479	0.16%	0.034%
73	13.196	1851	1855	1858	rBV5	6300	11299	0.21%	0.046%
74	13.251	1860	1864	1865	rBV2	15334	20766	0.39%	0.084%
75	13.397	1881	1888	1896	rBV6	9384	22865	0.43%	0.093%
76	13.470	1896	1900	1901	rBV3	4771	5731	0.11%	0.023%

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 Title : SFAM01.0

77	13.556	1907	1914	1925	rBV	683749	1121454	21.17%	4.556%
78	13.647	1925	1929	1934	rVB2	17086	28301	0.53%	0.115%
79	13.757	1942	1947	1948	rBV5	4018	6138	0.12%	0.025%
80	13.848	1955	1962	1974	rVB	547689	907121	17.12%	3.685%
81	14.013	1984	1989	1992	rBV6	2738	5495	0.10%	0.022%
82	14.062	1992	1997	2015	rVB	28192	65900	1.24%	0.268%
83	14.220	2015	2023	2028	rBV6	7050	15723	0.30%	0.064%
84	14.318	2033	2039	2045	rBV8	9474	19895	0.38%	0.081%
85	14.446	2058	2060	2065	rVB5	2411	3682	0.07%	0.015%
86	14.495	2065	2068	2069	rBV3	1628	1800	0.03%	0.007%
87	14.617	2085	2088	2092	rBV5	3376	5801	0.11%	0.024%
88	14.842	2123	2125	2126	rBV2	2544	1934	0.04%	0.008%
89	14.934	2139	2140	2141	rBV	2184	1499	0.03%	0.006%
90	15.068	2157	2162	2166	rBV8	5155	8756	0.17%	0.036%
91	15.177	2176	2180	2186	rVB8	3880	6016	0.11%	0.024%
92	15.287	2196	2198	2199	rBV2	1696	1519	0.03%	0.006%
93	15.360	2205	2210	2215	rVB	11315	20396	0.38%	0.083%
94	15.427	2217	2221	2226	rVV2	19344	34144	0.64%	0.139%
95	15.482	2226	2230	2237	rVB	9084	18430	0.35%	0.075%
96	15.543	2237	2240	2246	rBV8	2686	5069	0.10%	0.021%
97	15.781	2276	2279	2280	rBV3	2178	2269	0.04%	0.009%
98	15.879	2292	2295	2298	rBV4	1475	2225	0.04%	0.009%
99	16.031	2316	2320	2322	rBV5	1229	1617	0.03%	0.007%
100	16.433	2384	2386	2390	rVB5	2061	1508	0.03%	0.006%

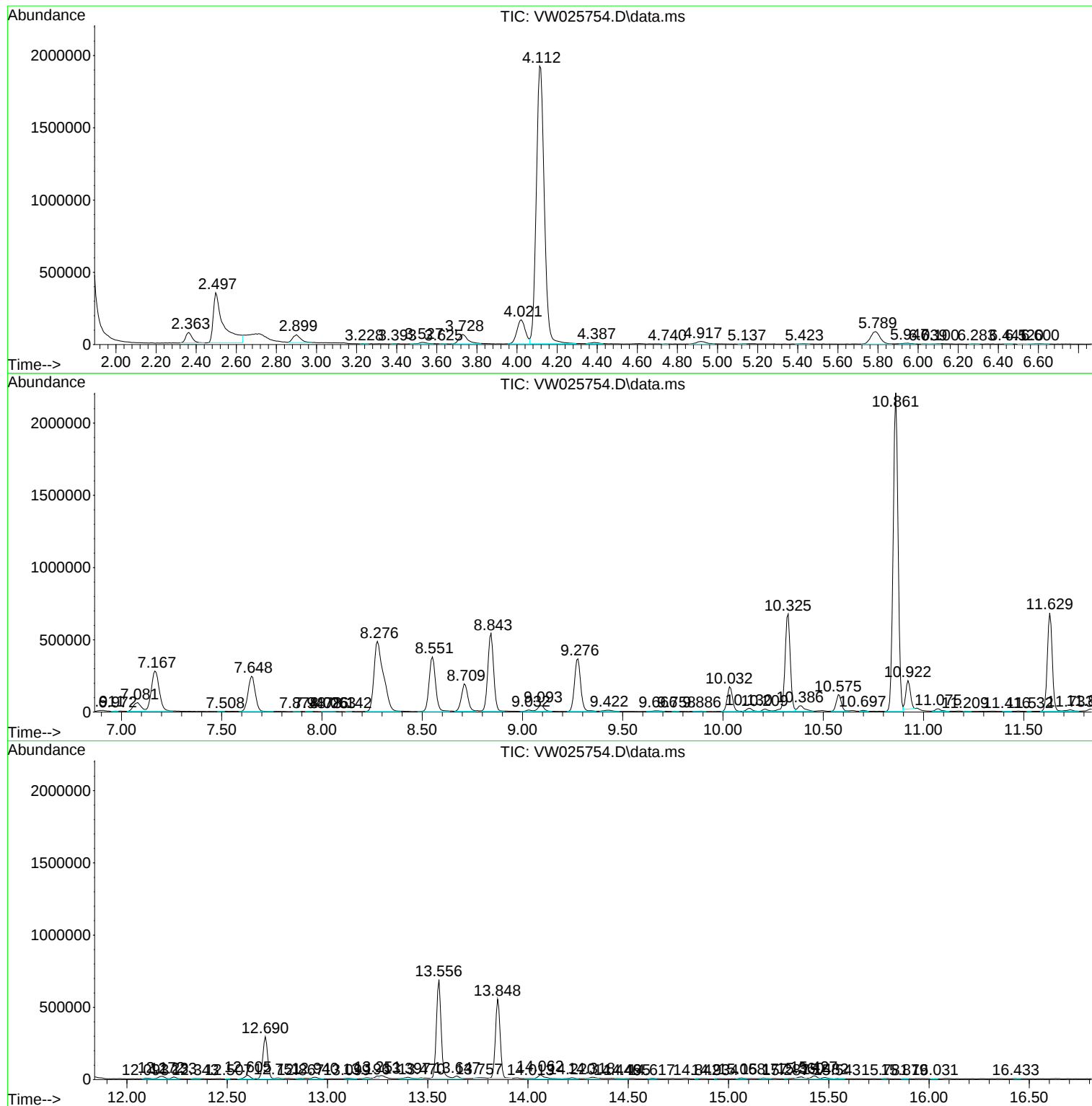
Sum of corrected areas: 24614353

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
Quant Title : SFAM01.0

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



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Instrument :
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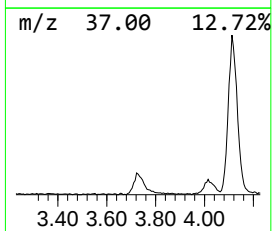
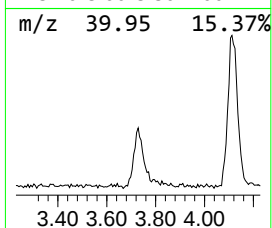
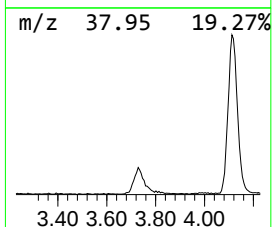
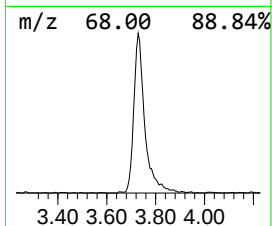
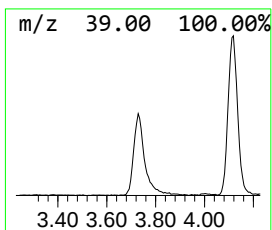
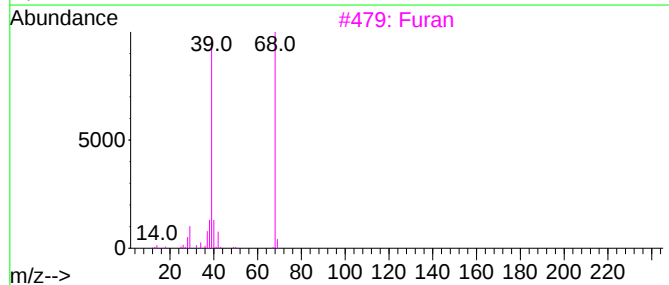
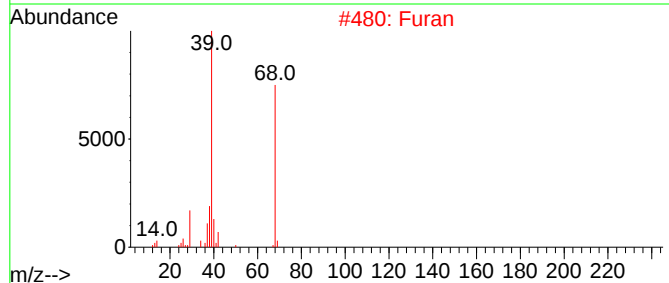
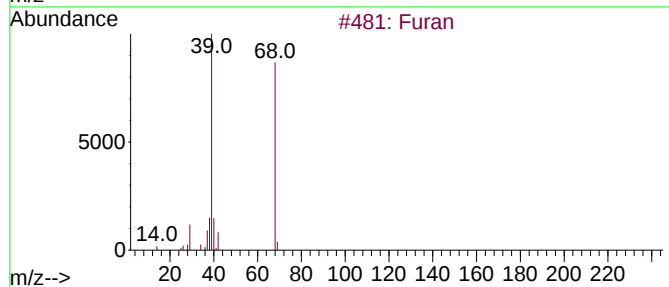
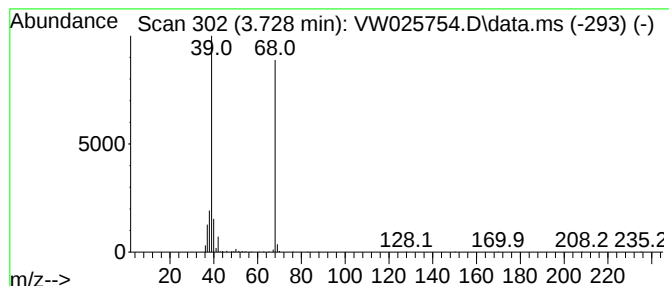
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Furan Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.728	4.72 ug/L	201471	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan			68	C4H4O	000110-00-9	90
2	Furan			68	C4H4O	000110-00-9	90
3	Furan			68	C4H4O	000110-00-9	83
4	2,5-Furandione, 3-methyl-			112	C5H4O3	000616-02-4	83
5	2H-Pyran-2-one			96	C5H4O2	000504-31-4	74



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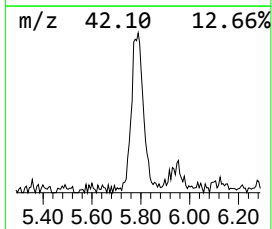
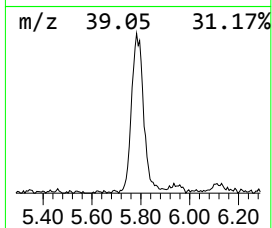
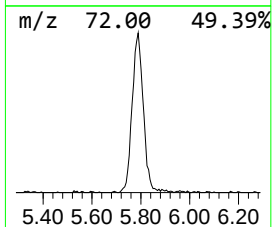
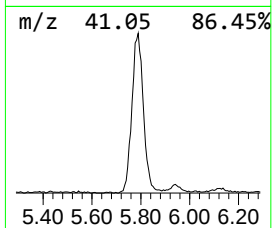
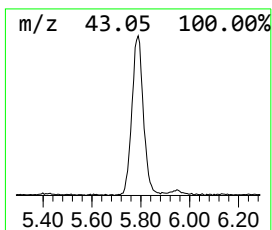
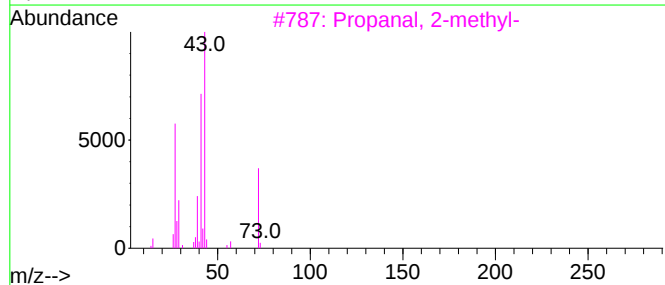
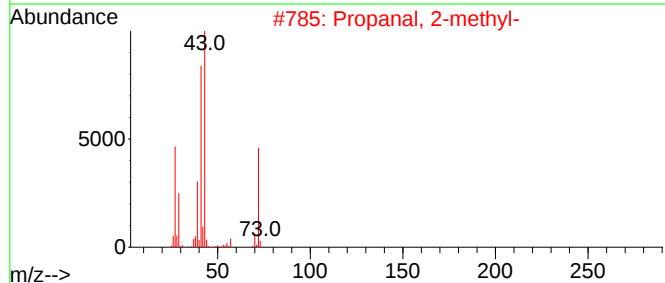
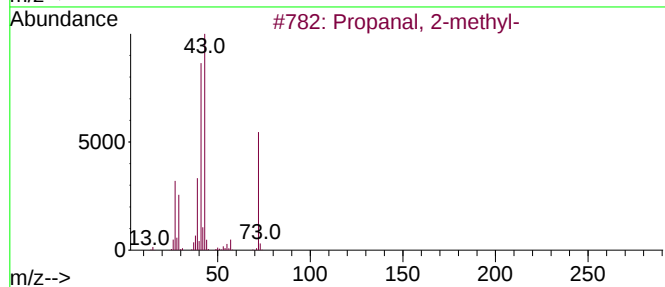
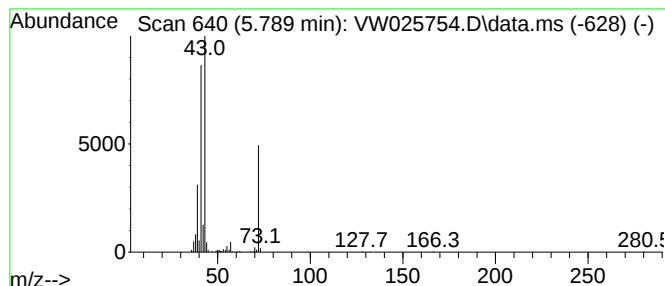
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Propanal, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.789	6.62 ug/L	282700	1,4-Difluorobenzene	8.843

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	Propanal, 2-methyl-		72	C4H8O	000078-84-2	86	
4	Propanal, 2-methyl-		72	C4H8O	000078-84-2	78	
5	Butanal		72	C4H8O	000123-72-8	40	



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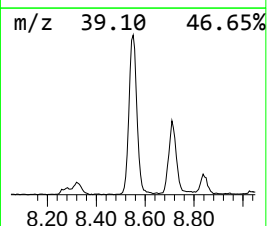
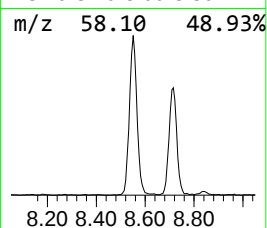
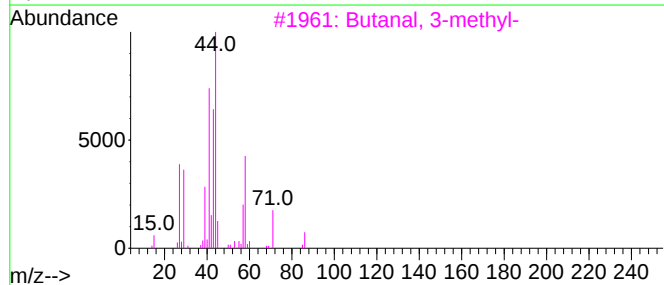
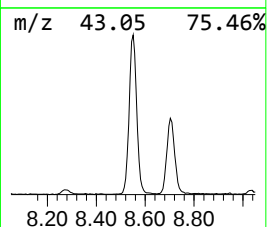
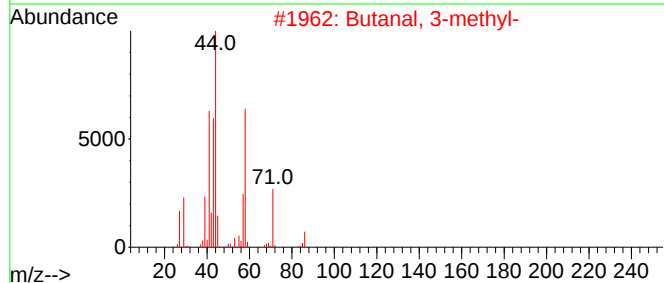
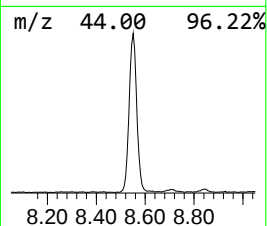
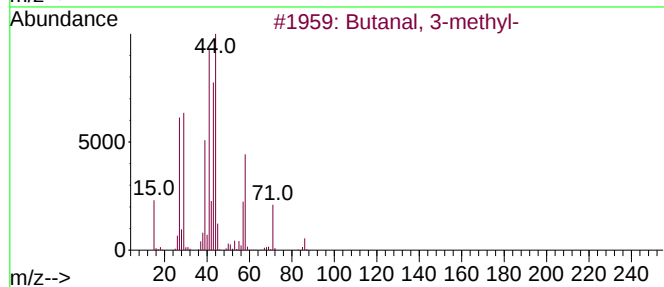
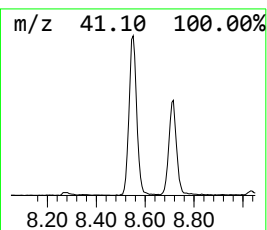
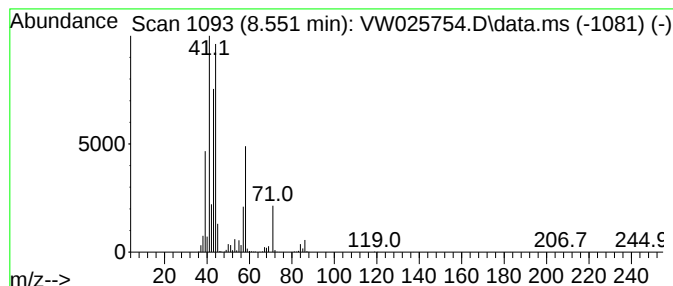
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Butanal, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	19.87 ug/L	849143	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	97
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	70
3			Butanal, 3-methyl-	86	C5H10O	000590-86-3	52
4			Pentanal	86	C5H10O	000110-62-3	46
5			Pentanal	86	C5H10O	000110-62-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW042823\
Data File : VW025754.D
Acq On : 28 Apr 2023 12:53
Operator : SY/MD
Sample : 02526-08
Misc : 5.70g/10mL/MSVOA_W/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCCF2

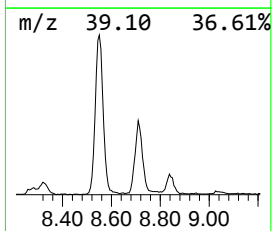
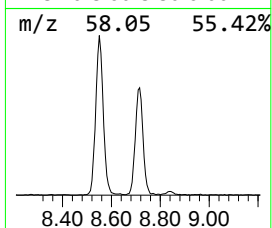
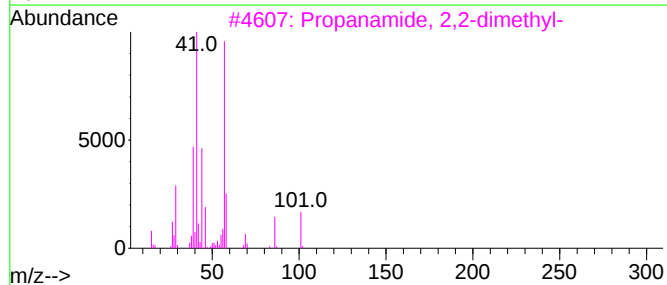
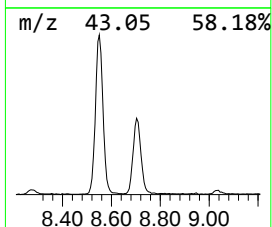
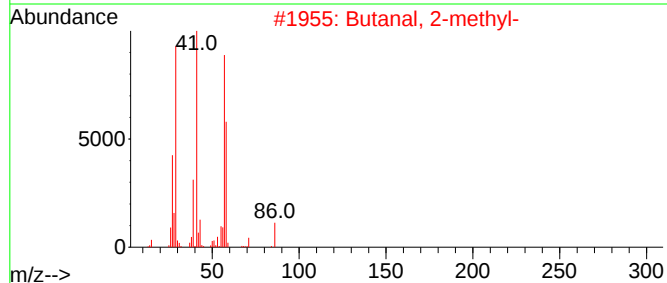
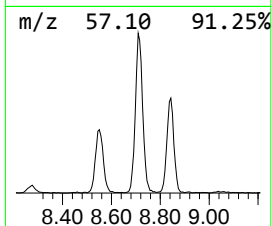
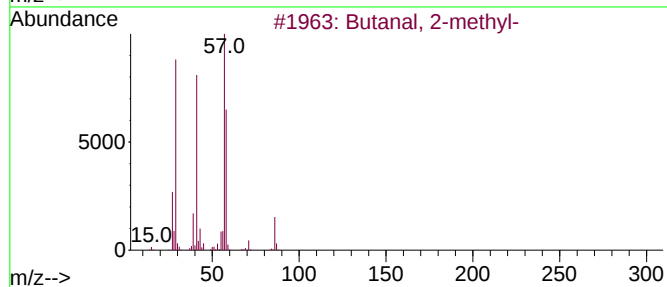
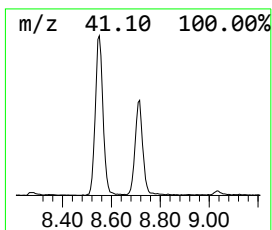
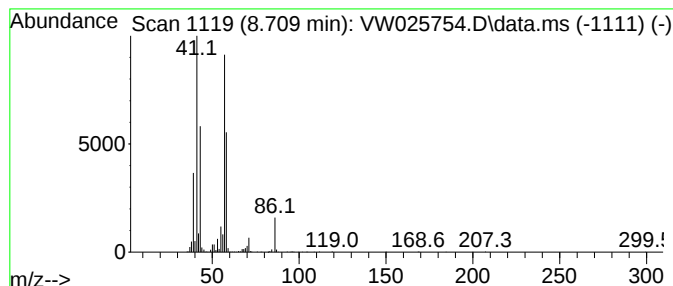
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Quant Title : SFAM01.0

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

Peak Number 5 Butanal, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.709	9.79 ug/L	418229	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 2-methyl-	86	C5H10O	000096-17-3	80
2			Butanal, 2-methyl-	86	C5H10O	000096-17-3	78
3			Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	50
4			1-Propen-2-ol, formate	86	C4H6O2	032978-00-0	46
5			n-Hexane	86	C6H14	000110-54-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW042823\
Data File : VW025754.D
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Sample : 02526-08
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
DCCF2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.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
Furan	3.728	4.7	ug/L	201471	1	8.843	1068200	25.0
Propanal, 2-met...	5.789	6.6	ug/L	282700	1	8.843	1068200	25.0
Butanal, 3-methyl-	8.551	19.9	ug/L	849143	1	8.843	1068200	25.0
Butanal, 2-methyl-	8.709	9.8	ug/L	418229	1	8.843	1068200	25.0