

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
 Data File : VX044694.D
 Acq On : 22 Jan 2025 14:10
 Operator : JC/MD
 Sample : Q1130-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 JNLA7

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

Signal : TIC: VX044694.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	40	rBV2	27850	46551	3.74%	0.510%
2	1.368	42	46	56	rVB	170970	182196	14.62%	1.997%
3	1.563	74	78	79	rBV2	4171	5709	0.46%	0.063%
4	1.660	89	94	105	rVB	102963	141538	11.36%	1.551%
5	1.868	126	128	130	rBV3	958	679	0.05%	0.007%
6	2.300	193	199	208	rBV	219490	350853	28.16%	3.845%
7	2.373	208	211	215	rVV	5971	8886	0.71%	0.097%
8	2.416	215	218	224	rVB2	2899	4957	0.40%	0.054%
9	2.526	229	236	238	rBV4	1396	2910	0.23%	0.032%
10	2.660	255	258	259	rBV3	465	445	0.04%	0.005%
11	2.788	275	279	280	rBV4	797	1054	0.08%	0.012%
12	2.934	296	303	316	rVB2	13464	32448	2.60%	0.356%
13	3.446	379	387	394	rBV5	2570	6573	0.53%	0.072%
14	3.514	396	398	401	rVB3	572	564	0.05%	0.006%
15	3.739	431	435	438	rBV3	597	716	0.06%	0.008%
16	3.788	442	443	447	rVV3	544	606	0.05%	0.007%
17	3.879	454	458	460	rVV3	354	565	0.05%	0.006%
18	3.928	464	466	469	rBV3	566	698	0.06%	0.008%
19	4.135	496	500	503	rBV3	508	771	0.06%	0.008%
20	4.318	526	530	533	rBV2	609	919	0.07%	0.010%
21	4.440	543	550	563	rBV	80736	234489	18.82%	2.570%
22	5.044	637	649	667	rVV	161716	493426	39.60%	5.408%
23	5.166	667	669	670	rVV2	584	501	0.04%	0.005%
24	5.202	673	675	679	rBV2	754	762	0.06%	0.008%
25	5.385	698	705	706	rBV4	950	1572	0.13%	0.017%
26	5.556	728	733	735	rVV5	969	1527	0.12%	0.017%
27	5.617	741	743	748	rVB4	401	629	0.05%	0.007%
28	5.958	787	799	826	rBV2	403764	1246025	100.00%	13.656%
29	6.342	855	862	873	rVB3	4986	15377	1.23%	0.169%
30	6.598	901	904	906	rBV2	467	599	0.05%	0.007%
31	6.653	912	913	916	rBV2	593	614	0.05%	0.007%
32	6.751	920	929	954	rBV	282257	709660	56.95%	7.777%
33	6.928	956	958	963	rVB4	1035	1129	0.09%	0.012%
34	7.299	1010	1019	1034	rBV	256777	564550	45.31%	6.187%
35	7.568	1062	1063	1065	rBV2	683	462	0.04%	0.005%
36	7.647	1071	1076	1086	rBV3	2766	6654	0.53%	0.073%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Stop Thrs : 0

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Max Peaks: 100

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

37	7.799	1095	1101	1112	rBV	39072	77681	6.23%	0.851%
38	7.988	1131	1132	1137	rVB3	520	445	0.04%	0.005%
39	8.055	1140	1143	1147	rBV2	547	543	0.04%	0.006%
40	8.244	1171	1174	1175	rBV2	776	823	0.07%	0.009%
41	8.318	1180	1186	1204	rVV	190143	320961	25.76%	3.517%
42	8.476	1210	1212	1216	rVB4	528	674	0.05%	0.007%
43	8.543	1216	1223	1232	rBV	16736	31877	2.56%	0.349%
44	8.641	1233	1239	1260	rBV	593039	983692	78.95%	10.781%
45	8.946	1284	1289	1303	rBV	133452	208522	16.73%	2.285%
46	9.128	1317	1319	1322	rBV3	499	522	0.04%	0.006%
47	9.238	1333	1337	1346	rBV	23288	35611	2.86%	0.390%
48	9.336	1347	1353	1355	rVV4	2261	4452	0.36%	0.049%
49	9.378	1355	1360	1374	rVV	303957	462698	37.13%	5.071%
50	9.482	1374	1377	1387	rVV	16443	28896	2.32%	0.317%
51	9.592	1391	1395	1400	rVB4	2362	4226	0.34%	0.046%
52	9.695	1408	1412	1417	rVB3	4128	5177	0.42%	0.057%
53	9.848	1433	1437	1440	rVB2	435	708	0.06%	0.008%
54	9.909	1442	1447	1455	rVV	40332	53512	4.29%	0.586%
55	10.049	1464	1470	1486	rBV	566868	810574	65.05%	8.883%
56	10.250	1500	1503	1505	rVB4	742	773	0.06%	0.008%
57	10.275	1505	1507	1510	rBV4	485	613	0.05%	0.007%
58	10.384	1522	1525	1526	rBV2	589	584	0.05%	0.006%
59	10.421	1529	1531	1533	rBV2	460	492	0.04%	0.005%
60	10.506	1544	1545	1548	rBV3	459	532	0.04%	0.006%
61	10.750	1580	1585	1587	rBV4	400	533	0.04%	0.006%
62	10.823	1594	1597	1600	rVB3	782	1062	0.09%	0.012%
63	10.854	1600	1602	1604	rBV	668	695	0.06%	0.008%
64	11.189	1651	1657	1672	rVV	421100	557085	44.71%	6.105%
65	11.287	1672	1673	1677	rVV3	568	704	0.06%	0.008%
66	11.335	1679	1681	1682	rBV2	673	504	0.04%	0.006%
67	11.591	1722	1723	1727	rVB3	568	568	0.05%	0.006%
68	11.634	1727	1730	1733	rBV3	469	632	0.05%	0.007%
69	11.658	1733	1734	1738	rBV3	465	565	0.05%	0.006%
70	11.707	1738	1742	1746	rVB5	1207	1789	0.14%	0.020%
71	11.762	1746	1751	1752	rBV3	597	969	0.08%	0.011%
72	11.860	1764	1767	1769	rBV2	495	576	0.05%	0.006%
73	11.896	1771	1773	1775	rBV	441	598	0.05%	0.007%
74	12.018	1788	1793	1808	rBV	551378	682209	54.75%	7.477%
75	12.317	1836	1842	1851	rBV	592151	755564	60.64%	8.280%
76	12.542	1877	1879	1883	rVB2	705	808	0.06%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

77	12.573	1883	1884	1890	rBV3	415	658	0.05%	0.007%
78	12.756	1909	1914	1918	rBV4	720	1266	0.10%	0.014%
79	12.811	1918	1923	1926	rBV5	487	722	0.06%	0.008%
80	12.902	1936	1938	1940	rBV2	700	692	0.06%	0.008%
81	13.164	1977	1981	1983	rVB3	374	507	0.04%	0.006%
82	13.237	1991	1993	1996	rBV3	576	538	0.04%	0.006%
83	13.658	2059	2062	2065	rVB3	558	581	0.05%	0.006%
84	13.798	2082	2085	2088	rBV4	381	540	0.04%	0.006%
85	14.121	2137	2138	2142	rVB3	839	958	0.08%	0.010%
86	14.298	2166	2167	2171	rVB4	644	764	0.06%	0.008%
87	14.445	2189	2191	2198	rVV5	839	1106	0.09%	0.012%
88	14.518	2201	2203	2206	rVB3	602	522	0.04%	0.006%
89	14.615	2214	2219	2223	rBV3	617	909	0.07%	0.010%
90	14.652	2223	2225	2231	rVB4	642	925	0.07%	0.010%
91	14.701	2231	2233	2237	rBV3	523	995	0.08%	0.011%
92	14.859	2258	2259	2262	rVB2	571	441	0.04%	0.005%
93	14.914	2264	2268	2269	rBV3	583	492	0.04%	0.005%
94	15.146	2304	2306	2309	rBV2	485	559	0.04%	0.006%
95	15.286	2326	2329	2335	rBV6	469	1124	0.09%	0.012%
96	15.329	2335	2336	2339	rVV3	459	497	0.04%	0.005%
97	15.396	2344	2347	2351	rVB5	670	889	0.07%	0.010%
98	15.566	2373	2375	2378	rBV4	681	738	0.06%	0.008%
99	15.682	2392	2394	2396	rBV4	502	617	0.05%	0.007%
100	16.243	2483	2486	2487	rBV3	623	605	0.05%	0.007%

Sum of corrected areas: 9124708

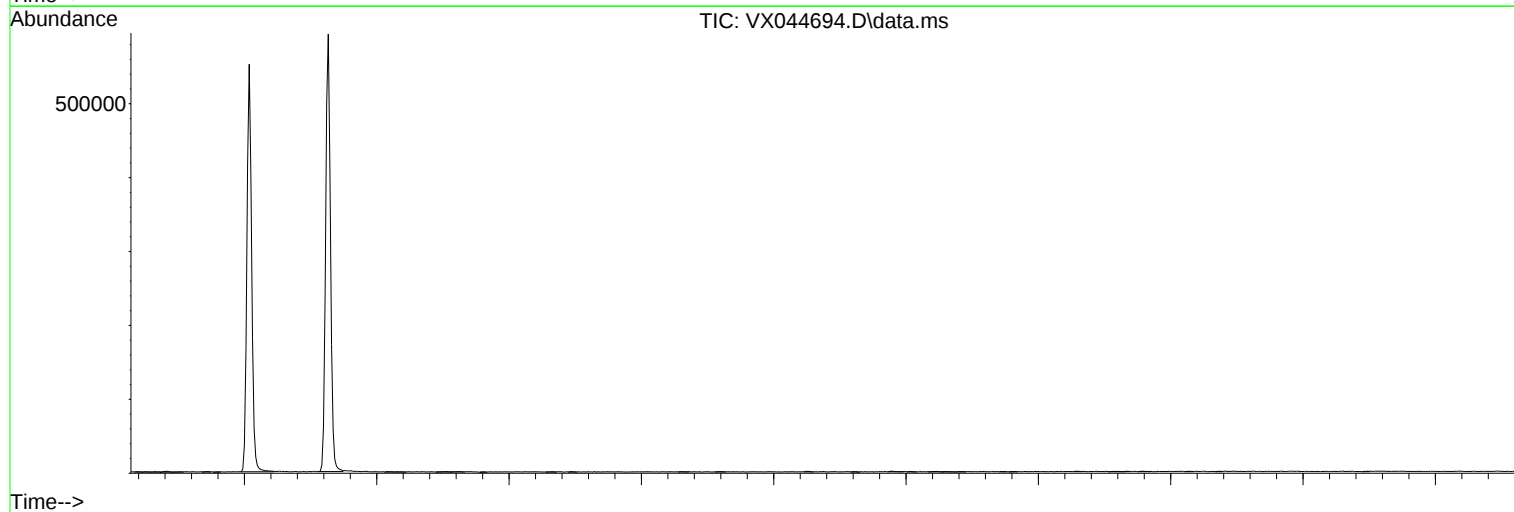
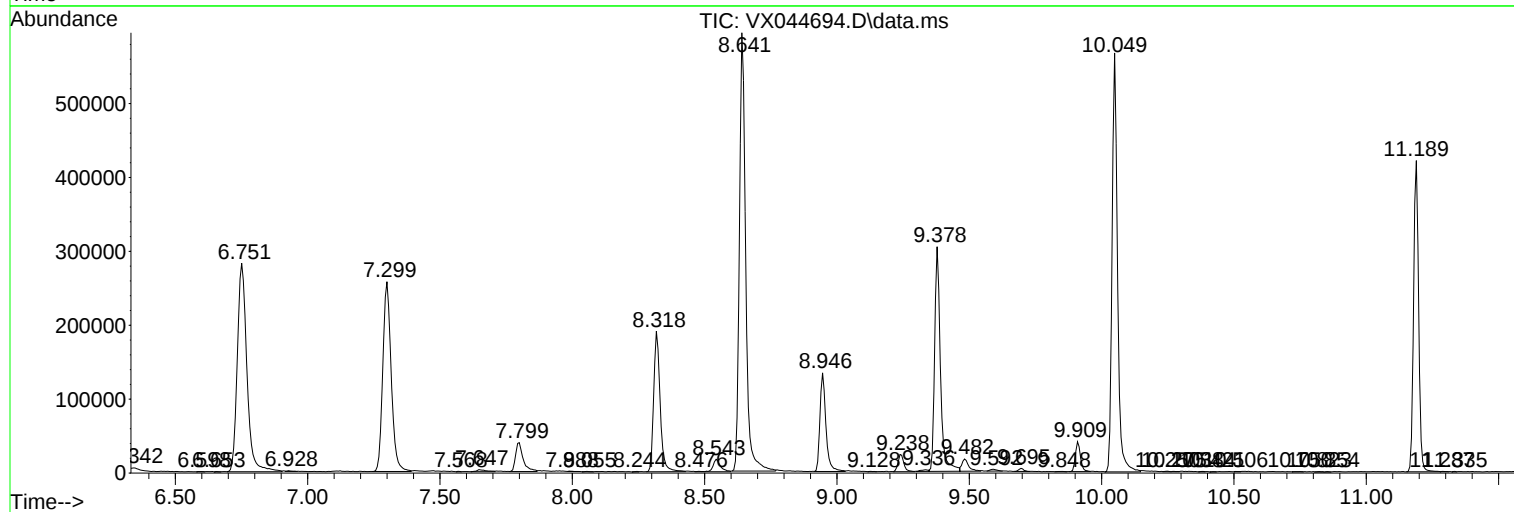
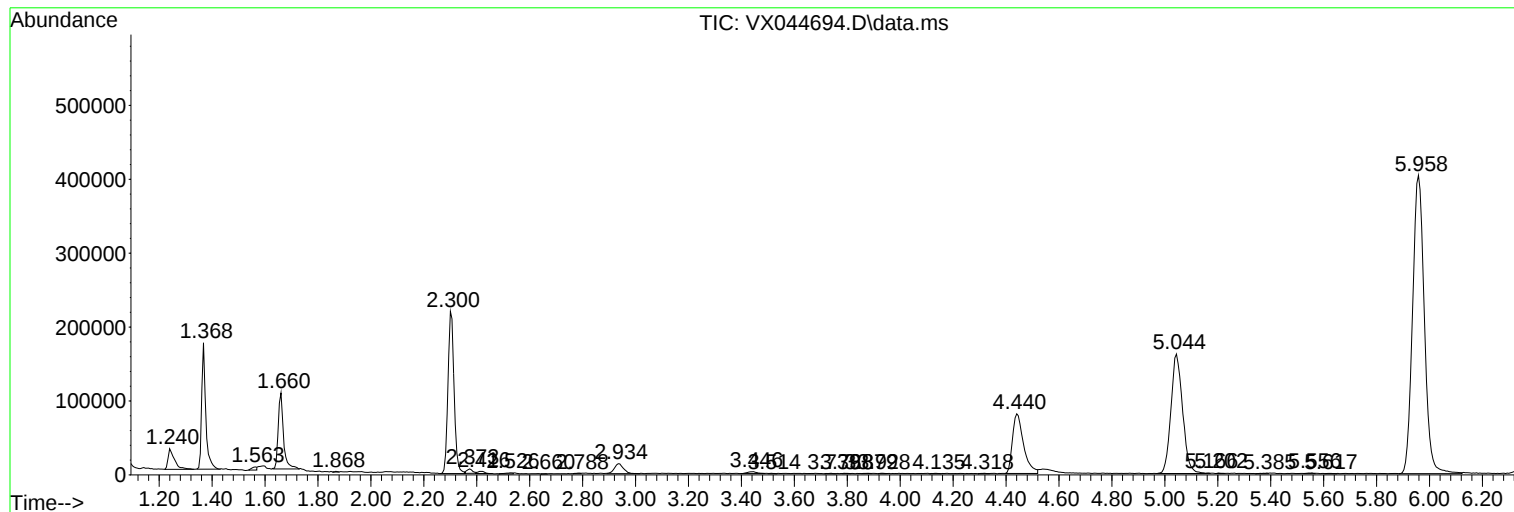
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012125WMA.M
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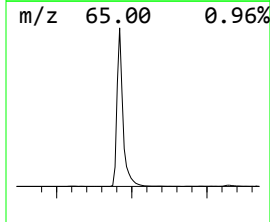
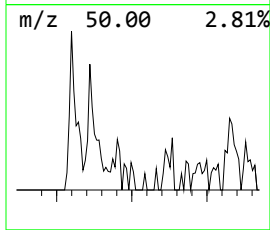
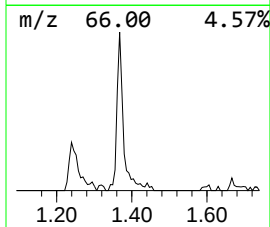
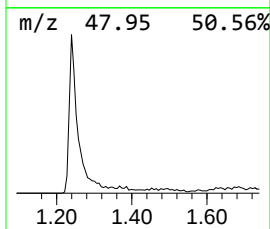
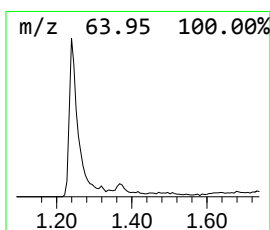
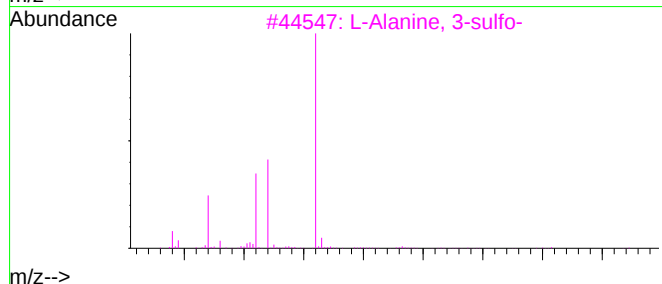
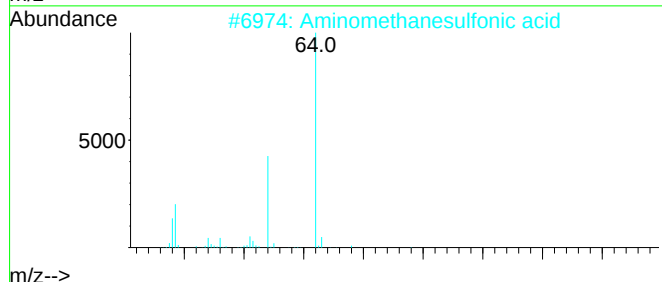
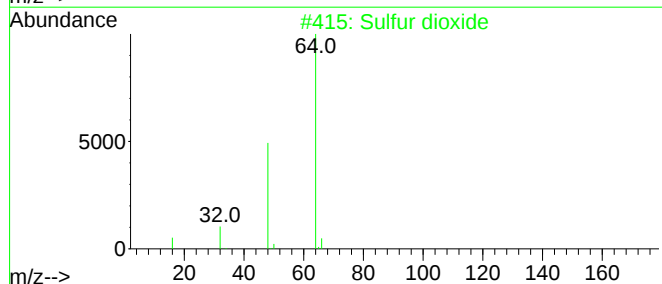
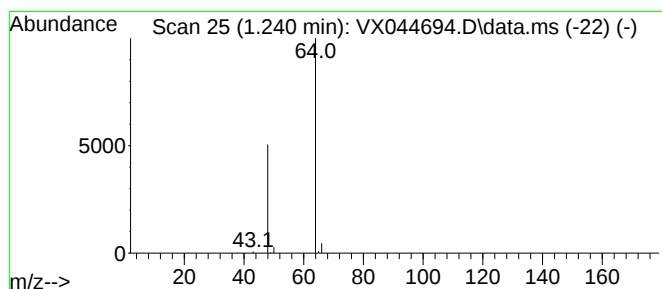
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.28 ug/L	46551	1,4-Difluorobenzene	6.751

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012125WMA.M
Quant Title : VOC Analysis

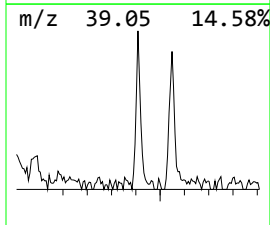
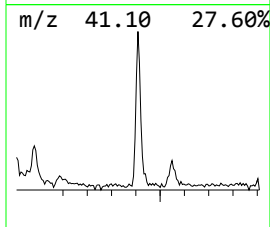
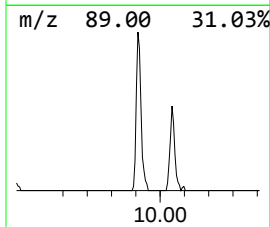
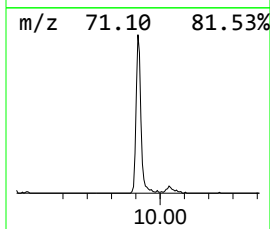
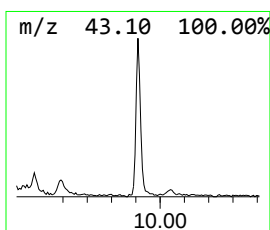
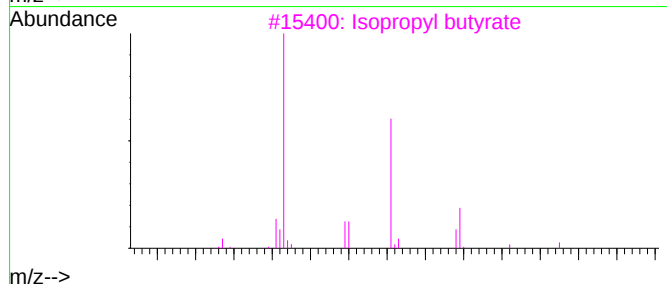
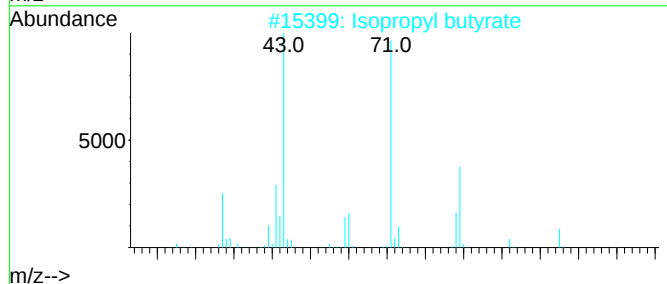
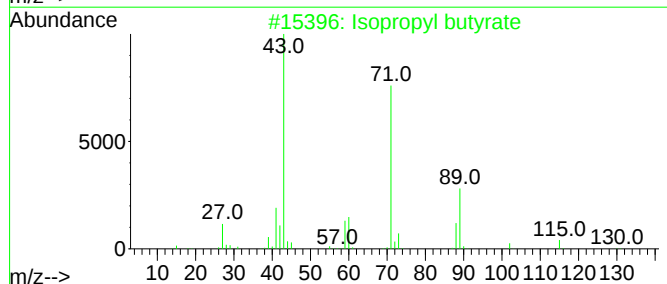
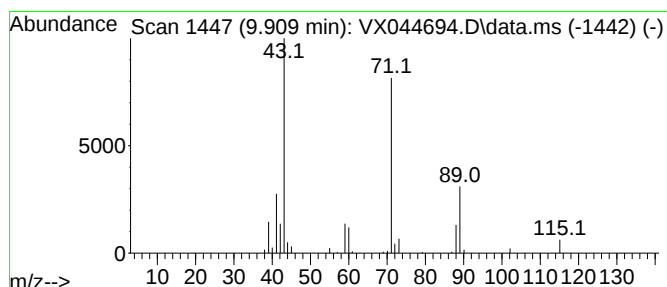
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.909	3.30 ug/L	53512	Chlorobenzene-d5	10.049

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.3	ug/L	46551	1	6.751	709660	50.0
Isopropyl butyrate	9.909	3.3	ug/L	53512	2	10.049	810574	50.0