

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012125\
 Data File : VX044685.D
 Acq On : 21 Jan 2025 16:55
 Operator : JC/MD
 Sample : PB166134TB 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VLEB134

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: VX044685.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	38	rBV	35219	52337	4.00%	0.529%
2	1.368	43	46	59	rVV	155207	197122	15.08%	1.992%
3	1.648	89	92	97	rBV	33903	45362	3.47%	0.458%
4	2.294	192	198	209	rBV	261746	424959	32.52%	4.294%
5	2.386	209	213	222	rVB	9208	16890	1.29%	0.171%
6	2.892	294	296	297	rBV2	863	617	0.05%	0.006%
7	2.940	297	304	315	rVV	9969	26634	2.04%	0.269%
8	3.434	379	385	390	rBV3	3486	7330	0.56%	0.074%
9	3.532	399	401	402	rBV2	551	326	0.02%	0.003%
10	3.575	402	408	417	rVV2	9935	23701	1.81%	0.239%
11	3.879	455	458	459	rBV2	569	458	0.04%	0.005%
12	4.013	477	480	482	rBV4	667	869	0.07%	0.009%
13	4.172	504	506	507	rBV2	426	330	0.03%	0.003%
14	4.215	510	513	514	rBV2	484	497	0.04%	0.005%
15	4.300	523	527	530	rVB5	604	860	0.07%	0.009%
16	4.337	530	533	534	rBV2	365	378	0.03%	0.004%
17	4.391	541	542	544	rBV2	668	627	0.05%	0.006%
18	4.458	545	553	577	rVV	64054	228996	17.52%	2.314%
19	4.867	619	620	622	rBV2	533	391	0.03%	0.004%
20	4.946	631	633	637	rBV4	640	890	0.07%	0.009%
21	5.044	638	649	669	rVV	168666	523325	40.04%	5.288%
22	5.379	702	704	707	rBV4	948	973	0.07%	0.010%
23	5.489	721	722	726	rVB2	487	454	0.03%	0.005%
24	5.617	741	743	746	rVB2	614	451	0.03%	0.005%
25	5.647	746	748	752	rBV3	549	799	0.06%	0.008%
26	5.794	770	772	773	rVB2	700	411	0.03%	0.004%
27	5.806	773	774	776	rBV2	446	322	0.02%	0.003%
28	5.855	780	782	784	rBV3	422	435	0.03%	0.004%
29	5.958	787	799	820	rBV2	430629	1306906	100.00%	13.206%
30	6.220	838	842	844	rBV3	796	1014	0.08%	0.010%
31	6.348	855	863	877	rBV3	8369	25865	1.98%	0.261%
32	6.653	912	913	919	rVB3	798	1127	0.09%	0.011%
33	6.751	919	929	953	rBV	283356	734787	56.22%	7.425%
34	7.013	970	972	973	rBV2	462	337	0.03%	0.003%
35	7.074	978	982	984	rBV4	494	844	0.06%	0.009%
36	7.299	1011	1019	1038	rBV	264947	602828	46.13%	6.092%

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Instrument :
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 ClientSampleId :
 VLEB134

Integration Parameters: LSCINT.P

Integrator: RTE

Smoother: 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

37	7.580	1063	1065	1069	rVB3	629	977	0.07%	0.010%
38	7.659	1074	1078	1083	rBV	2944	5995	0.46%	0.061%
39	7.799	1095	1101	1120	rBV	106067	220726	16.89%	2.230%
40	8.183	1162	1164	1165	rBV2	532	315	0.02%	0.003%
41	8.220	1168	1170	1171	rBV	518	333	0.03%	0.003%
42	8.318	1180	1186	1203	rBV	196876	347368	26.58%	3.510%
43	8.549	1218	1224	1233	rBV	26540	49451	3.78%	0.500%
44	8.647	1233	1240	1265	rVB	578295	1031149	78.90%	10.420%
45	8.945	1284	1289	1308	rBV2	159408	279449	21.38%	2.824%
46	9.171	1325	1326	1328	rVB2	880	425	0.03%	0.004%
47	9.189	1328	1329	1331	rBV	501	357	0.03%	0.004%
48	9.244	1333	1338	1347	rVV	41031	62163	4.76%	0.628%
49	9.384	1356	1361	1373	rBV	269556	439374	33.62%	4.440%
50	9.482	1373	1377	1384	rVB	56233	83110	6.36%	0.840%
51	9.580	1389	1393	1405	rVB	34904	56597	4.33%	0.572%
52	9.909	1442	1447	1462	rBV	122719	175536	13.43%	1.774%
53	10.049	1465	1470	1487	rVV	571248	834862	63.88%	8.436%
54	10.287	1502	1509	1510	rBV6	1426	2244	0.17%	0.023%
55	10.403	1526	1528	1530	rBV2	366	376	0.03%	0.004%
56	10.646	1564	1568	1579	rVB	8005	14710	1.13%	0.149%
57	10.817	1594	1596	1599	rBV4	791	994	0.08%	0.010%
58	10.909	1609	1611	1612	rVB2	438	320	0.02%	0.003%
59	11.189	1651	1657	1670	rVV	443920	576885	44.14%	5.829%
60	11.299	1673	1675	1680	rVV4	882	1370	0.10%	0.014%
61	11.360	1683	1685	1688	rVB4	562	536	0.04%	0.005%
62	11.415	1692	1694	1698	rVB3	569	505	0.04%	0.005%
63	11.457	1698	1701	1703	rBV2	932	1180	0.09%	0.012%
64	11.591	1721	1723	1726	rBV3	331	359	0.03%	0.004%
65	11.646	1729	1732	1734	rVB3	565	624	0.05%	0.006%
66	11.683	1734	1738	1740	rBV2	551	832	0.06%	0.008%
67	11.707	1740	1742	1744	rBV3	568	498	0.04%	0.005%
68	11.750	1747	1749	1750	rBV2	693	434	0.03%	0.004%
69	11.793	1755	1756	1758	rBV	537	355	0.03%	0.004%
70	11.896	1768	1773	1776	rBV5	601	1141	0.09%	0.012%
71	11.969	1780	1785	1788	rBV5	1137	1404	0.11%	0.014%
72	12.018	1788	1793	1810	rBV	544611	688226	52.66%	6.955%
73	12.317	1836	1842	1849	rBV	621421	768284	58.79%	7.764%
74	12.488	1866	1870	1872	rBV4	582	738	0.06%	0.007%
75	12.542	1876	1879	1882	rBV4	488	554	0.04%	0.006%
76	12.707	1904	1906	1908	rBV3	476	373	0.03%	0.004%

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 ClientSampleId :
 VLEB134

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_X\Method\SFAMXML012125WMA.M
 Title : VOC Analysis

77	12.756	1912	1914	1918	rBV3	749	1040	0.08%	0.011%
78	12.792	1918	1920	1921	rVB2	595	337	0.03%	0.003%
79	12.817	1921	1924	1926	rBV3	349	436	0.03%	0.004%
80	12.859	1929	1931	1932	rBV	517	361	0.03%	0.004%
81	12.896	1934	1937	1939	rBV3	864	893	0.07%	0.009%
82	12.975	1948	1950	1951	rVB	780	407	0.03%	0.004%
83	13.006	1951	1955	1957	rBV5	780	1157	0.09%	0.012%
84	13.042	1960	1961	1964	rBV3	581	662	0.05%	0.007%
85	13.097	1969	1970	1972	rBV2	443	360	0.03%	0.004%
86	13.146	1976	1978	1980	rVV	735	632	0.05%	0.006%
87	13.280	1998	2000	2006	rBV4	484	794	0.06%	0.008%
88	13.323	2006	2007	2012	rVB3	439	442	0.03%	0.004%
89	13.469	2029	2031	2035	rVB4	442	570	0.04%	0.006%
90	13.591	2048	2051	2052	rBV2	486	614	0.05%	0.006%
91	13.750	2075	2077	2079	rVV2	650	487	0.04%	0.005%
92	13.792	2080	2084	2086	rVB3	964	1189	0.09%	0.012%
93	13.847	2091	2093	2096	rVB3	603	594	0.05%	0.006%
94	14.384	2179	2181	2183	rBV2	704	402	0.03%	0.004%
95	14.566	2209	2211	2213	rBV	544	375	0.03%	0.004%
96	14.652	2222	2225	2228	rBV4	352	555	0.04%	0.006%
97	14.694	2231	2232	2235	rBV2	456	514	0.04%	0.005%
98	14.890	2263	2264	2267	rBV2	563	490	0.04%	0.005%
99	15.725	2399	2401	2404	rBV2	740	758	0.06%	0.008%
100	16.694	2558	2560	2561	rBV	641	409	0.03%	0.004%

Sum of corrected areas: 9896059

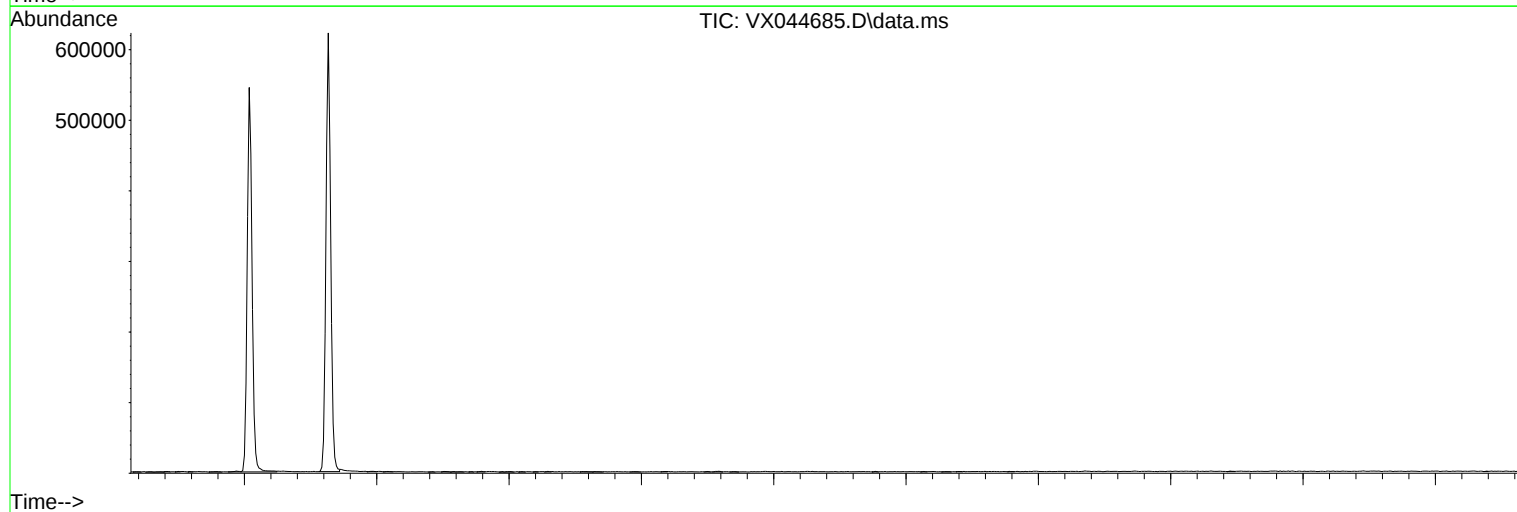
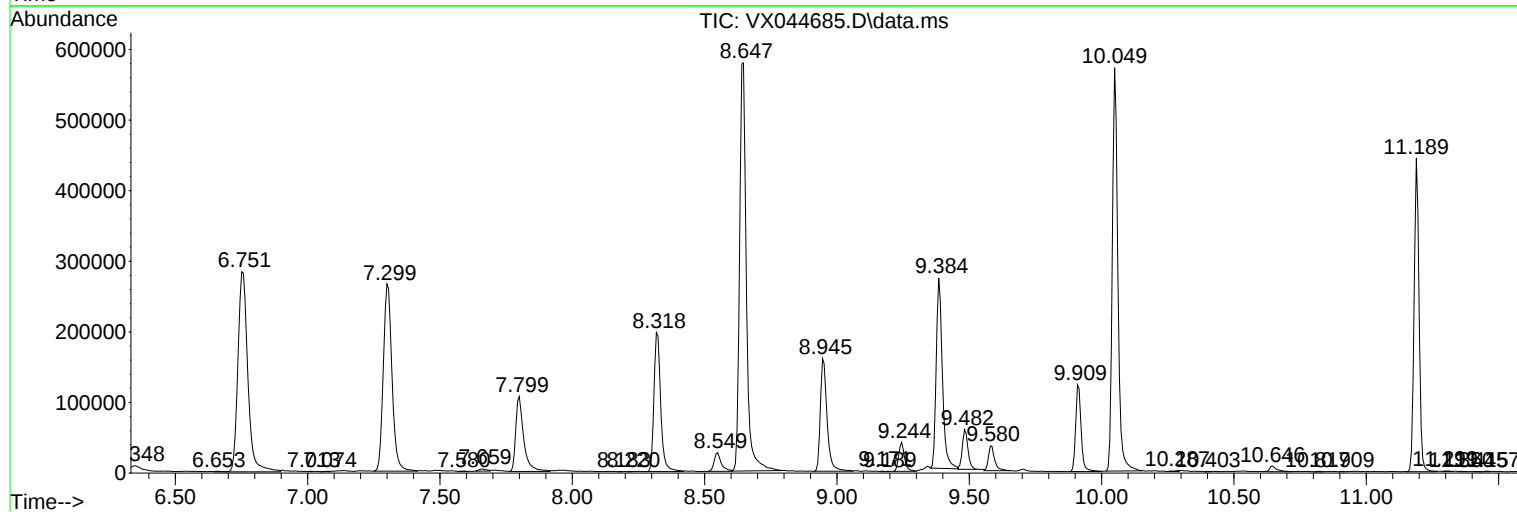
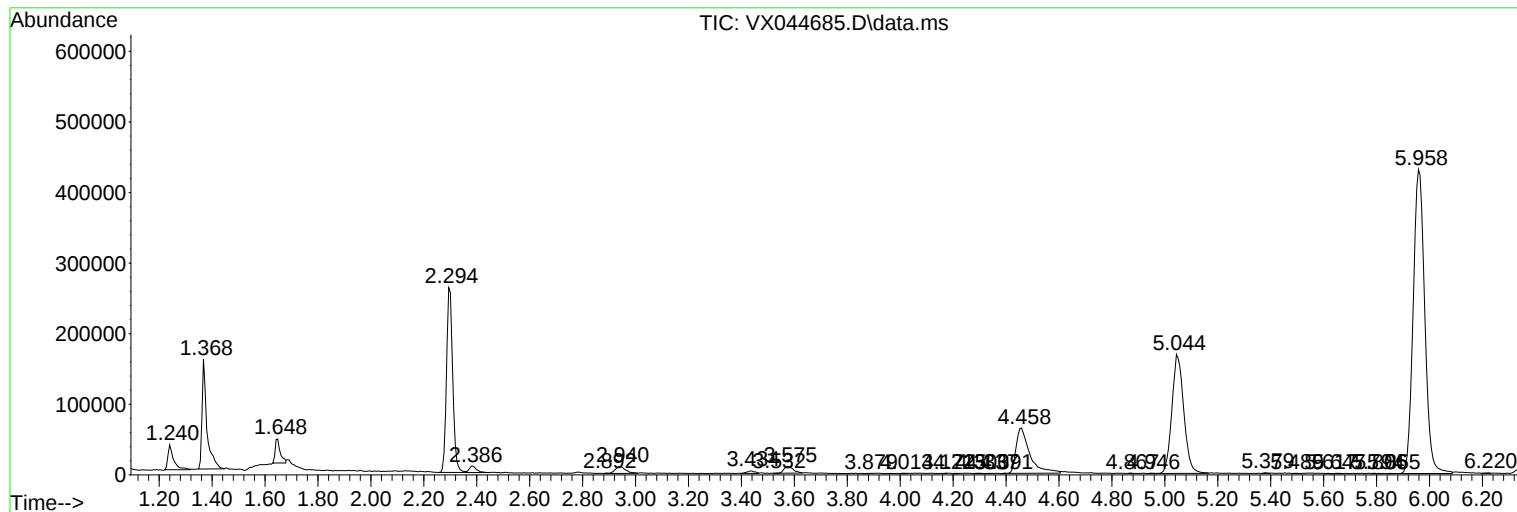
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VLEB134

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012125\
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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012125WMA.M
Quant Title : VOC Analysis

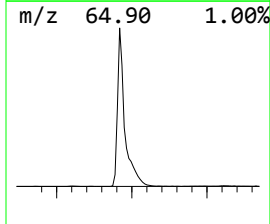
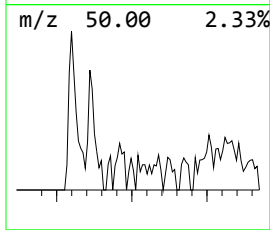
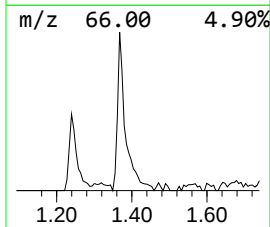
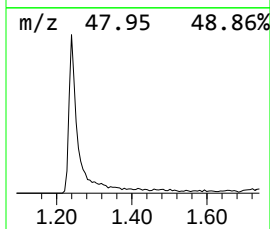
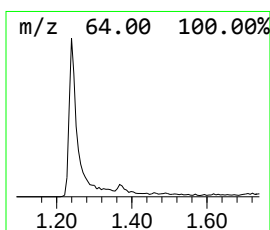
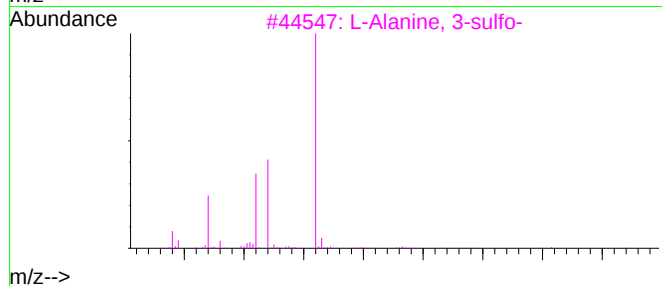
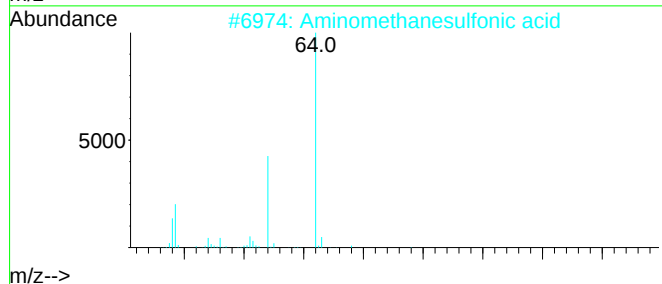
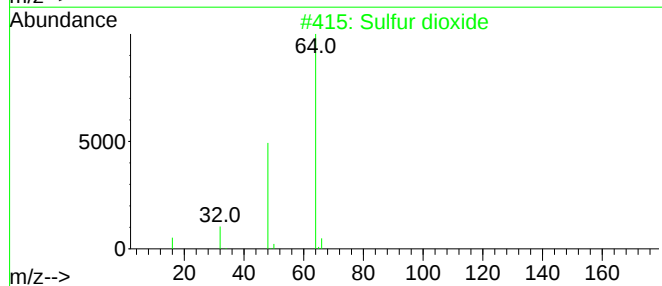
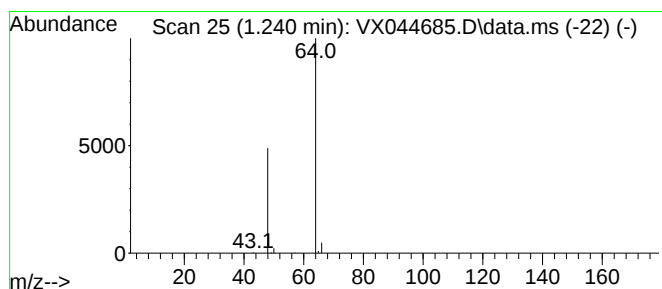
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.56 ug/L	52337	1,4-Difluorobenzene	6.757

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	Sulfur dioxide	64	O2S	007446-09-5	5



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

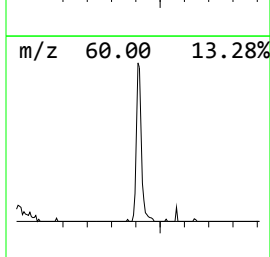
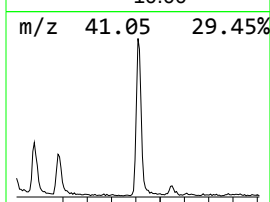
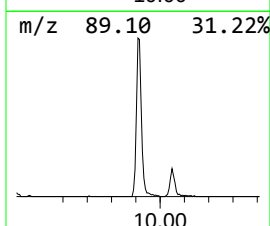
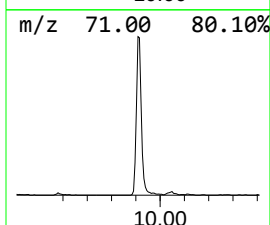
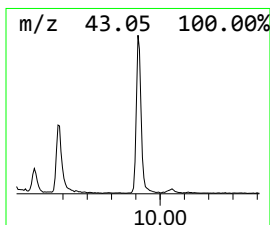
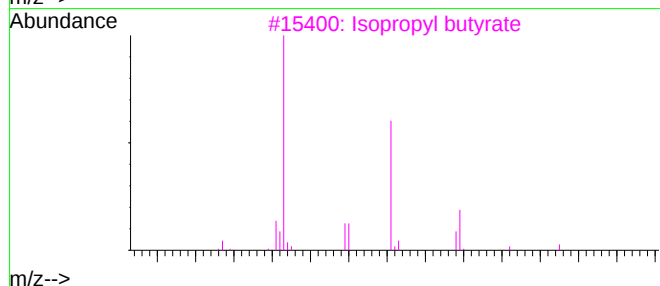
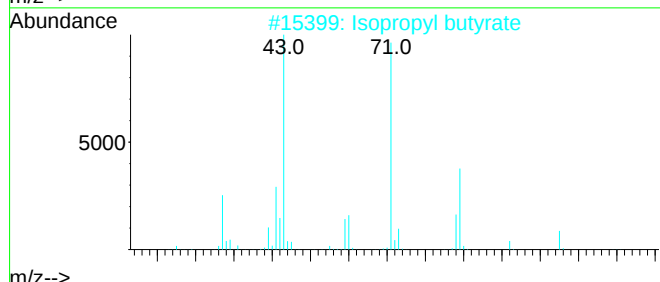
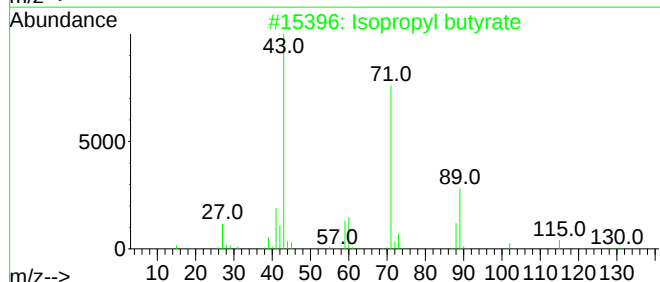
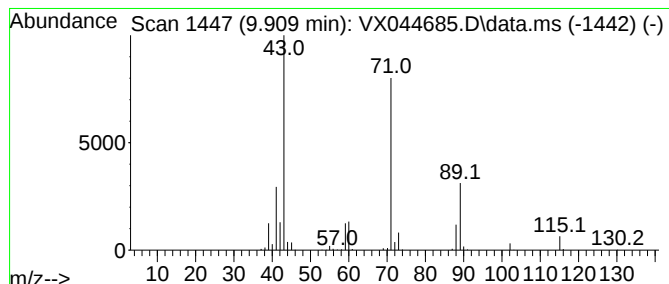
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.909	10.51 ug/L	175536	Chlorobenzene-d5	10.049

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	97
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	80
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78



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Instrument :
MSVOA_X
ClientSampleId :
VLEB134

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	3.6	ug/L	52337	1	6.757	734787	50.0
Isopropyl butyrate	9.909	10.5	ug/L	175536	2	10.049	834862	50.0