

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
 Data File : VX044695.D
 Acq On : 22 Jan 2025 14:39
 Operator : JC/MD
 Sample : Q1131-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

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\SFAMXLM012125WMA.M
 Title : VOC Analysis

Signal : TIC: VX044695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	32	rBV	20071	32923	3.91%	0.543%
2	1.367	43	46	62	rVB	92425	137800	16.38%	2.271%
3	1.562	72	78	80	rBV6	5222	10904	1.30%	0.180%
4	1.648	89	92	99	rBV	23301	30995	3.68%	0.511%
5	2.294	192	198	212	rVB	143713	225331	26.78%	3.713%
6	2.422	217	219	223	rVB3	560	539	0.06%	0.009%
7	2.458	223	225	227	rBV3	358	377	0.04%	0.006%
8	2.507	230	233	236	rBV4	533	816	0.10%	0.013%
9	2.696	260	264	265	rBV2	442	552	0.07%	0.009%
10	2.788	276	279	281	rVB2	598	600	0.07%	0.010%
11	2.818	281	284	286	rVB2	637	647	0.08%	0.011%
12	2.843	286	288	291	rBV3	412	615	0.07%	0.010%
13	2.934	297	303	310	rBV4	2156	4435	0.53%	0.073%
14	3.086	325	328	330	rBV2	478	502	0.06%	0.008%
15	3.257	353	356	358	rBV3	433	418	0.05%	0.007%
16	3.428	376	384	394	rBV4	5259	13366	1.59%	0.220%
17	3.617	412	415	416	rBV	391	474	0.06%	0.008%
18	3.836	447	451	452	rBV3	534	701	0.08%	0.012%
19	3.855	452	454	460	rVB4	528	837	0.10%	0.014%
20	3.909	460	463	464	rBV2	559	459	0.05%	0.008%
21	4.452	545	552	567	rBV	52370	164006	19.49%	2.703%
22	5.043	639	649	667	rBV	105426	327934	38.97%	5.404%
23	5.226	677	679	682	rVB2	467	584	0.07%	0.010%
24	5.495	721	723	726	rBV4	401	560	0.07%	0.009%
25	5.543	729	731	732	rBV	672	430	0.05%	0.007%
26	5.775	768	769	775	rBV3	266	379	0.05%	0.006%
27	5.958	788	799	820	rVV2	281099	841433	100.00%	13.866%
28	6.330	858	860	861	rBV2	391	363	0.04%	0.006%
29	6.354	861	864	870	rVB4	805	1686	0.20%	0.028%
30	6.543	893	895	896	rBV	519	447	0.05%	0.007%
31	6.604	903	905	910	rVB3	479	515	0.06%	0.008%
32	6.665	913	915	917	rBV2	404	371	0.04%	0.006%
33	6.750	920	929	948	rBV	219647	558031	66.32%	9.196%
34	7.110	983	988	989	rBV4	1220	1564	0.19%	0.026%
35	7.299	1011	1019	1033	rBV	173837	386661	45.95%	6.372%
36	7.433	1040	1041	1044	rBV3	499	512	0.06%	0.008%

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Integrator: RTE

Smoothing : OFF

Sampling : 1

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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	7.610	1066	1070	1072	rBV3	439	663	0.08%	0.011%
38	7.744	1089	1092	1095	rVB3	907	814	0.10%	0.013%
39	8.031	1137	1139	1141	rBV2	461	496	0.06%	0.008%
40	8.146	1156	1158	1160	rVB	456	409	0.05%	0.007%
41	8.171	1160	1162	1163	rBV2	504	404	0.05%	0.007%
42	8.226	1169	1171	1173	rVB2	638	486	0.06%	0.008%
43	8.317	1180	1186	1202	rBV	120249	213957	25.43%	3.526%
44	8.640	1233	1239	1260	rBV	387795	664272	78.95%	10.946%
45	8.945	1284	1289	1302	rBV	84182	134237	15.95%	2.212%
46	9.171	1324	1326	1329	rVB3	402	434	0.05%	0.007%
47	9.384	1356	1361	1382	rVV	174437	313507	37.26%	5.166%
48	9.610	1397	1398	1401	rVB2	827	438	0.05%	0.007%
49	9.701	1409	1413	1421	rBV5	1870	3951	0.47%	0.065%
50	9.823	1430	1433	1434	rBV3	464	517	0.06%	0.009%
51	10.049	1465	1470	1491	rVV	408840	617250	73.36%	10.171%
52	10.219	1497	1498	1501	rVB2	678	437	0.05%	0.007%
53	10.305	1510	1512	1517	rBV4	437	565	0.07%	0.009%
54	10.439	1532	1534	1536	rVB3	619	517	0.06%	0.009%
55	10.609	1561	1562	1565	rBV3	356	385	0.05%	0.006%
56	10.737	1581	1583	1584	rVV2	576	360	0.04%	0.006%
57	10.945	1611	1617	1620	rBV3	387	758	0.09%	0.012%
58	11.000	1624	1626	1629	rBV3	397	500	0.06%	0.008%
59	11.109	1642	1644	1645	rVB	556	364	0.04%	0.006%
60	11.189	1651	1657	1668	rBV	289798	387668	46.07%	6.388%
61	11.402	1690	1692	1695	rVB3	540	518	0.06%	0.009%
62	11.457	1698	1701	1703	rBV4	509	698	0.08%	0.012%
63	11.518	1709	1711	1713	rBV2	322	376	0.04%	0.006%
64	11.560	1715	1718	1720	rBV2	402	474	0.06%	0.008%
65	11.615	1725	1727	1731	rBV5	372	448	0.05%	0.007%
66	11.646	1731	1732	1735	rVB2	507	389	0.05%	0.006%
67	11.743	1745	1748	1750	rBV2	521	474	0.06%	0.008%
68	11.762	1750	1751	1753	rBV2	638	364	0.04%	0.006%
69	11.969	1783	1785	1788	rVB3	418	433	0.05%	0.007%
70	12.018	1788	1793	1805	rBV	371083	487684	57.96%	8.036%
71	12.316	1837	1842	1850	rBV	356845	467134	55.52%	7.698%
72	12.536	1877	1878	1881	rVB	619	359	0.04%	0.006%
73	12.615	1887	1891	1892	rVB3	416	448	0.05%	0.007%
74	12.627	1892	1893	1895	rBV	433	373	0.04%	0.006%
75	12.762	1914	1915	1918	rVB	955	573	0.07%	0.009%
76	12.890	1934	1936	1939	rBV2	630	695	0.08%	0.011%

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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	13.152	1977	1979	1981	rBV3	598	488	0.06%	0.008%
78	13.444	2025	2027	2030	rBV3	367	457	0.05%	0.008%
79	13.658	2060	2062	2064	rBV2	497	409	0.05%	0.007%
80	13.749	2075	2077	2082	rVB	408	400	0.05%	0.007%
81	13.798	2082	2085	2087	rBV3	491	557	0.07%	0.009%
82	13.883	2095	2099	2101	rBV3	403	664	0.08%	0.011%
83	13.932	2105	2107	2110	rBV3	367	376	0.04%	0.006%
84	14.011	2117	2120	2122	rBV2	491	388	0.05%	0.006%
85	14.127	2136	2139	2145	rVB3	1129	1758	0.21%	0.029%
86	14.182	2145	2148	2149	rBV2	636	480	0.06%	0.008%
87	14.414	2184	2186	2190	rBV4	723	798	0.09%	0.013%
88	14.749	2239	2241	2243	rBV	680	560	0.07%	0.009%
89	14.779	2243	2246	2247	rBV2	310	407	0.05%	0.007%
90	14.840	2255	2256	2260	rBV2	642	711	0.08%	0.012%
91	14.938	2269	2272	2275	rBV3	641	979	0.12%	0.016%
92	15.182	2310	2312	2314	rVB2	752	751	0.09%	0.012%
93	15.206	2314	2316	2317	rBV	974	806	0.10%	0.013%
94	15.249	2321	2323	2325	rBV	744	450	0.05%	0.007%
95	15.517	2366	2367	2369	rBV2	742	480	0.06%	0.008%
96	15.712	2397	2399	2402	rBV4	529	537	0.06%	0.009%
97	15.779	2408	2410	2416	rBV4	582	933	0.11%	0.015%
98	16.035	2450	2452	2453	rBV2	508	369	0.04%	0.006%
99	16.468	2520	2523	2525	rVB2	569	634	0.08%	0.010%
100	16.706	2560	2562	2564	rVB3	686	475	0.06%	0.008%

Sum of corrected areas: 6068463

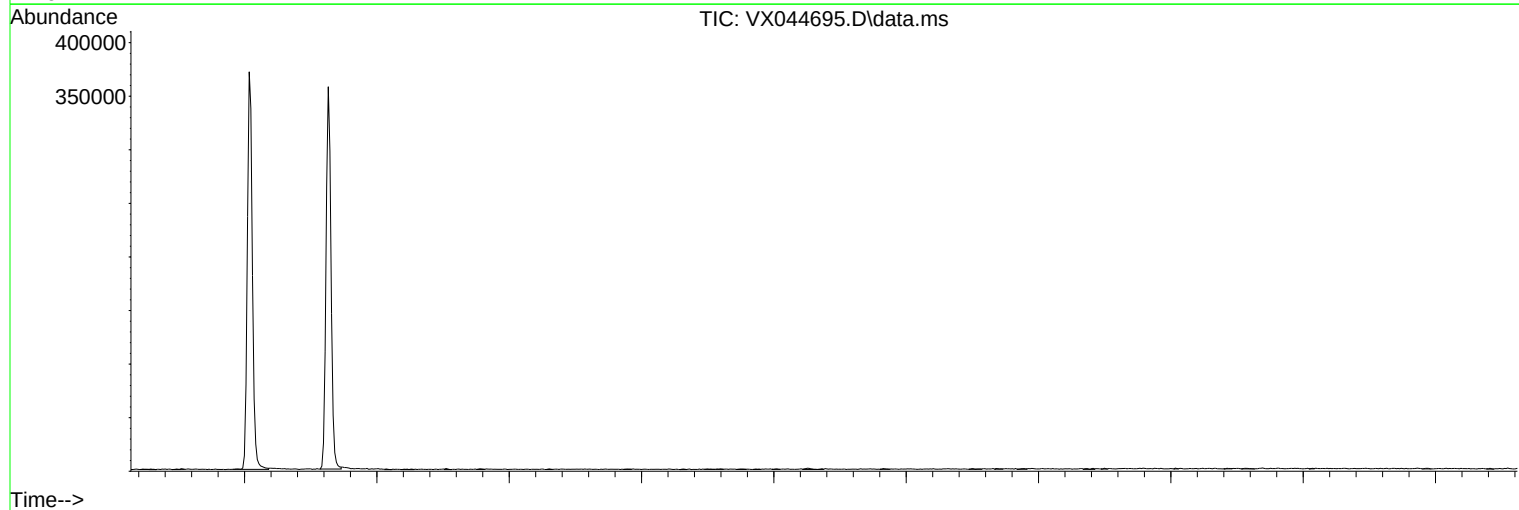
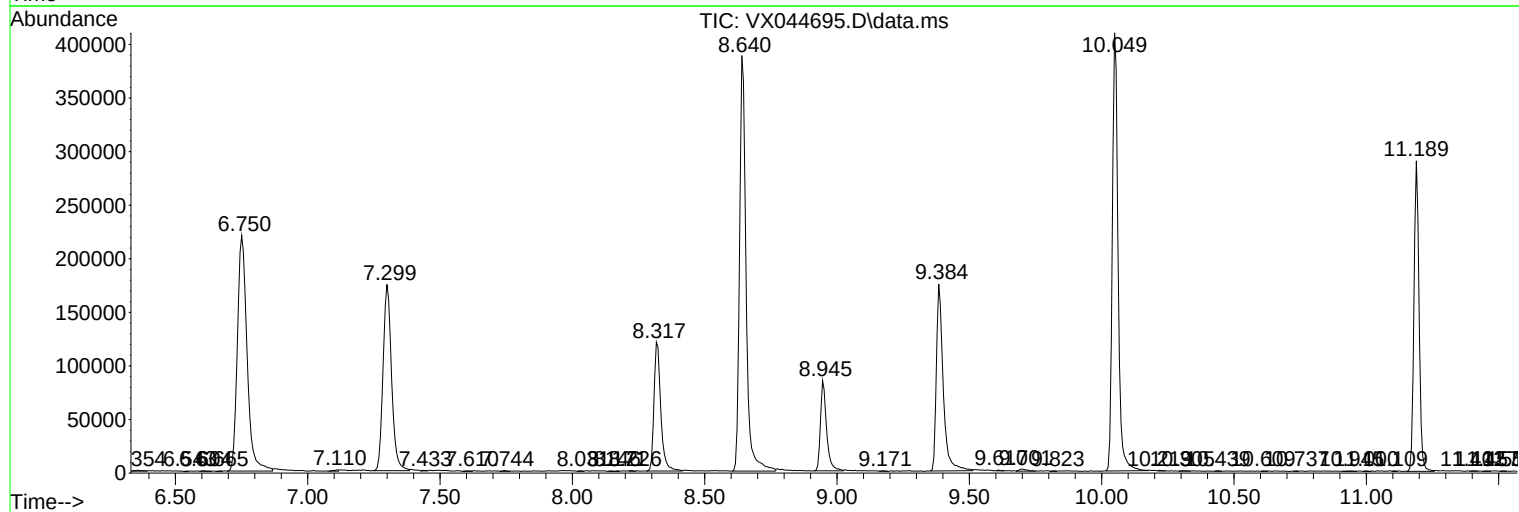
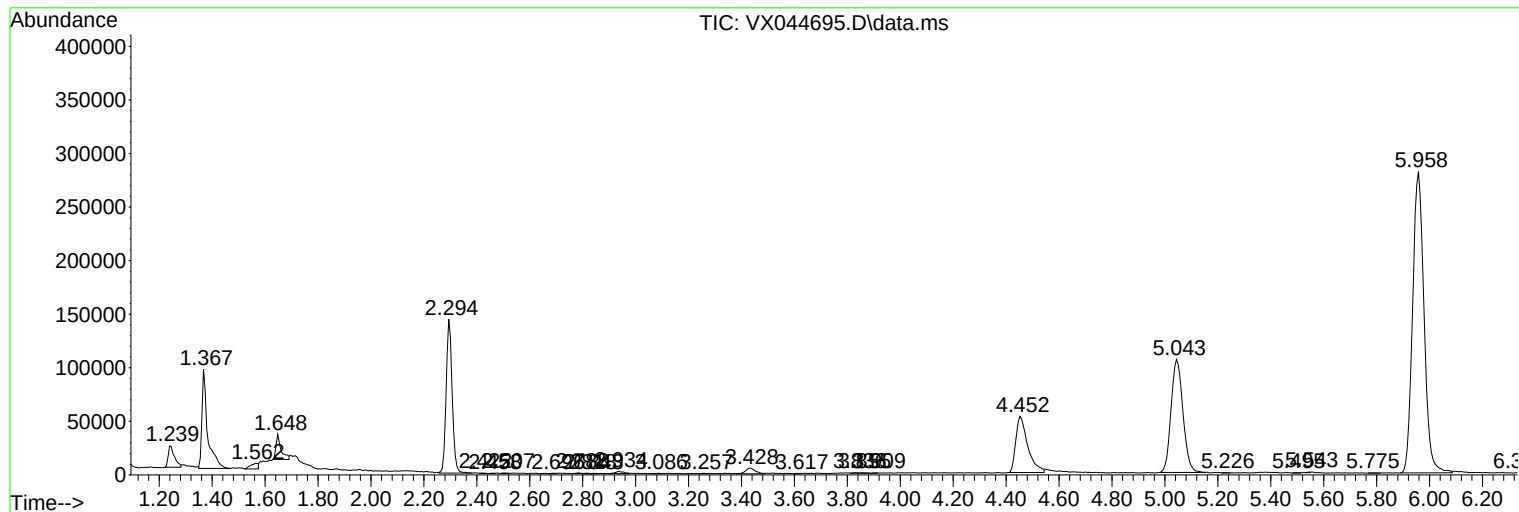
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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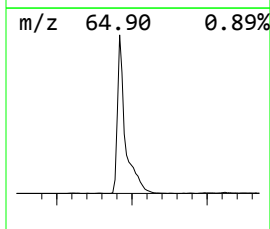
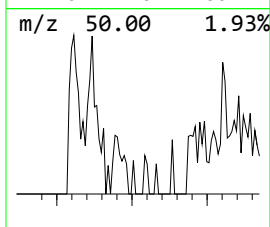
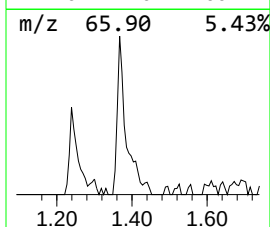
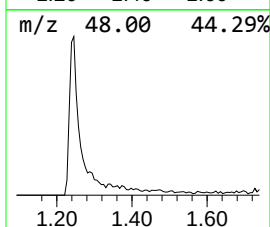
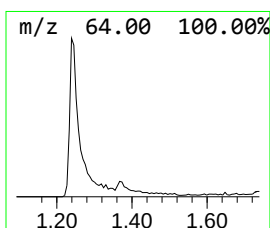
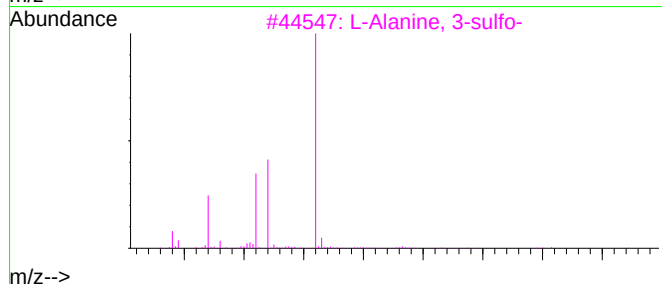
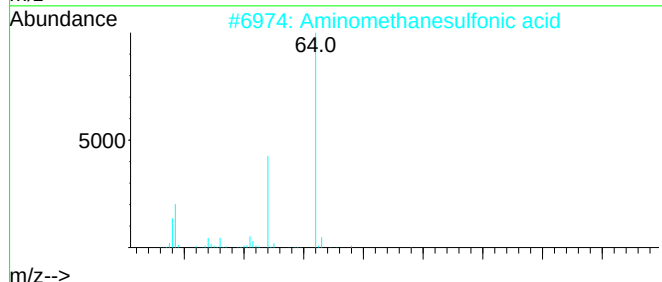
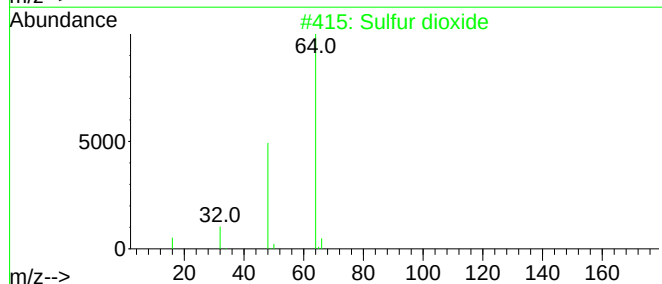
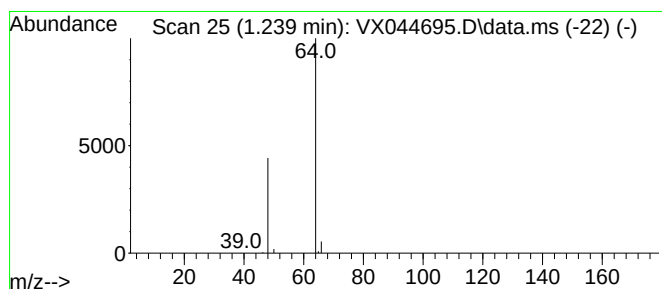
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	2.95 ug/L	32923	1,4-Difluorobenzene	6.750

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	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Sulfur dioxide	64	O2S	007446-09-5	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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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	1.239	3.0	ug/L	32923	1	6.750	558031	50.0