

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012125\
 Data File : VX044688.D
 Acq On : 21 Jan 2025 18:03
 Operator : JC/MD
 Sample : Q1130-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 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\SFAMXML012125WMA.M
 Title : VOC Analysis

Signal : TIC: VX044688.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	39	rBV	33026	50878	3.77%	0.554%
2	1.368	43	46	61	rVB	151806	204379	15.16%	2.224%
3	1.648	89	92	95	rBV	36609	43909	3.26%	0.478%
4	2.294	192	198	213	rVB	223838	356036	26.41%	3.874%
5	2.495	229	231	233	rBV2	726	711	0.05%	0.008%
6	2.556	240	241	245	rVB4	636	527	0.04%	0.006%
7	2.593	245	247	248	rBV2	442	346	0.03%	0.004%
8	2.947	299	305	312	rVV2	4805	10128	0.75%	0.110%
9	3.020	315	317	319	rVB2	647	499	0.04%	0.005%
10	3.184	341	344	346	rBV2	483	551	0.04%	0.006%
11	3.245	352	354	355	rBV2	410	294	0.02%	0.003%
12	3.312	363	365	368	rBV3	706	949	0.07%	0.010%
13	3.440	378	386	393	rBV4	3426	8789	0.65%	0.096%
14	3.495	393	395	397	rVV3	579	519	0.04%	0.006%
15	3.532	399	401	404	rBV3	666	1006	0.07%	0.011%
16	3.642	418	419	422	rBV2	506	448	0.03%	0.005%
17	3.806	445	446	448	rBV	598	364	0.03%	0.004%
18	3.934	465	467	470	rVV4	601	512	0.04%	0.006%
19	3.983	473	475	477	rVB2	577	470	0.03%	0.005%
20	4.099	492	494	496	rBV2	508	544	0.04%	0.006%
21	4.184	504	508	509	rBV2	489	514	0.04%	0.006%
22	4.398	541	543	545	rBV3	506	365	0.03%	0.004%
23	4.459	545	553	574	rBV	65895	228136	16.92%	2.483%
24	5.050	636	650	668	rBV	166305	537275	39.85%	5.847%
25	5.385	703	705	706	rBV2	473	378	0.03%	0.004%
26	5.483	720	721	724	rBV3	515	399	0.03%	0.004%
27	5.696	754	756	758	rBV	318	260	0.02%	0.003%
28	5.733	761	762	764	rBV2	516	400	0.03%	0.004%
29	5.958	787	799	818	rBV2	445929	1348357	100.00%	14.673%
30	6.446	876	879	880	rBV3	585	574	0.04%	0.006%
31	6.751	920	929	949	rBV	297115	754395	55.95%	8.210%
32	7.165	996	997	1000	rBV3	598	727	0.05%	0.008%
33	7.299	1011	1019	1042	rBV	272639	621144	46.07%	6.759%
34	7.604	1066	1069	1071	rBV2	447	410	0.03%	0.004%
35	7.763	1093	1095	1097	rBV2	335	257	0.02%	0.003%
36	7.787	1097	1099	1100	rVB2	466	266	0.02%	0.003%

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

37	7.915	1118	1120	1123	rVB4	578	615	0.05%	0.007%
38	7.964	1125	1128	1129	rBV4	993	1272	0.09%	0.014%
39	8.007	1133	1135	1138	rBV4	626	656	0.05%	0.007%
40	8.318	1180	1186	1201	rBV	201586	356386	26.43%	3.878%
41	8.641	1233	1239	1258	rBV	601073	1054218	78.19%	11.472%
42	8.946	1284	1289	1302	rBV	141664	226049	16.76%	2.460%
43	9.177	1326	1327	1330	rVB3	544	313	0.02%	0.003%
44	9.208	1330	1332	1333	rBV	502	417	0.03%	0.005%
45	9.384	1356	1361	1376	rBV	258458	436265	32.36%	4.748%
46	9.701	1409	1413	1418	rBV2	3646	4788	0.36%	0.052%
47	9.769	1422	1424	1427	rVB3	392	275	0.02%	0.003%
48	9.860	1435	1439	1442	rBV4	549	771	0.06%	0.008%
49	9.970	1455	1457	1458	rVB	472	304	0.02%	0.003%
50	10.049	1465	1470	1491	rBV	574275	852872	63.25%	9.281%
51	10.421	1529	1531	1533	rBV2	320	360	0.03%	0.004%
52	10.640	1565	1567	1568	rBV2	588	320	0.02%	0.003%
53	10.774	1588	1589	1590	rBV	460	318	0.02%	0.003%
54	10.793	1590	1592	1596	rVV3	684	696	0.05%	0.008%
55	10.823	1596	1597	1600	rVV3	530	356	0.03%	0.004%
56	10.866	1602	1604	1607	rBV2	653	871	0.06%	0.009%
57	10.976	1619	1622	1624	rBV	644	694	0.05%	0.008%
58	11.110	1642	1644	1645	rVB2	595	387	0.03%	0.004%
59	11.122	1645	1646	1648	rBV	537	471	0.03%	0.005%
60	11.189	1652	1657	1665	rVV	444068	580531	43.05%	6.317%
61	11.421	1693	1695	1698	rBV3	450	463	0.03%	0.005%
62	11.445	1698	1699	1701	rBV	453	404	0.03%	0.004%
63	11.537	1713	1714	1716	rBV2	511	301	0.02%	0.003%
64	11.561	1716	1718	1721	rVV2	400	364	0.03%	0.004%
65	11.610	1725	1726	1728	rBV	413	313	0.02%	0.003%
66	11.665	1734	1735	1736	rBV	570	262	0.02%	0.003%
67	11.707	1740	1742	1745	rBV3	576	655	0.05%	0.007%
68	11.732	1745	1746	1748	rVB	488	298	0.02%	0.003%
69	11.768	1748	1752	1753	rBV4	792	976	0.07%	0.011%
70	11.817	1758	1760	1762	rBV3	384	467	0.03%	0.005%
71	11.969	1784	1785	1788	rVB2	570	436	0.03%	0.005%
72	12.018	1788	1793	1804	rBV	548553	695191	51.56%	7.565%
73	12.244	1828	1830	1833	rBV2	426	456	0.03%	0.005%
74	12.317	1837	1842	1857	rVV	631996	782479	58.03%	8.515%
75	12.469	1865	1867	1869	rVV2	637	433	0.03%	0.005%
76	12.488	1869	1870	1871	rVV	606	279	0.02%	0.003%

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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	12.524	1874	1876	1879	rBV3	291	297	0.02%	0.003%
78	12.567	1881	1883	1885	rBV2	367	298	0.02%	0.003%
79	12.731	1908	1910	1911	rBV2	379	258	0.02%	0.003%
80	12.853	1928	1930	1932	rBV2	313	275	0.02%	0.003%
81	12.920	1938	1941	1944	rVB4	453	491	0.04%	0.005%
82	12.969	1948	1949	1952	rVB	499	281	0.02%	0.003%
83	13.073	1965	1966	1969	rVB2	439	381	0.03%	0.004%
84	13.128	1972	1975	1977	rBV3	623	837	0.06%	0.009%
85	13.231	1990	1992	1994	rBV3	473	345	0.03%	0.004%
86	13.250	1994	1995	1997	rVV2	360	261	0.02%	0.003%
87	13.365	2011	2014	2015	rBV3	487	425	0.03%	0.005%
88	13.414	2019	2022	2023	rBV2	324	382	0.03%	0.004%
89	13.487	2032	2034	2035	rBV2	386	274	0.02%	0.003%
90	13.658	2060	2062	2065	rVB4	431	337	0.02%	0.004%
91	13.731	2072	2074	2075	rBV2	487	465	0.03%	0.005%
92	13.774	2079	2081	2082	rBV	476	257	0.02%	0.003%
93	13.993	2116	2117	2119	rBB	520	299	0.02%	0.003%
94	14.420	2185	2187	2190	rBV3	343	436	0.03%	0.005%
95	14.475	2195	2196	2197	rBV	657	366	0.03%	0.004%
96	14.493	2197	2199	2200	rVB	611	364	0.03%	0.004%
97	14.603	2215	2217	2218	rBV2	501	318	0.02%	0.003%
98	14.883	2261	2263	2265	rBV3	600	537	0.04%	0.006%
99	15.152	2305	2307	2309	rBV3	693	714	0.05%	0.008%
100	15.274	2325	2327	2328	rBV	801	687	0.05%	0.007%

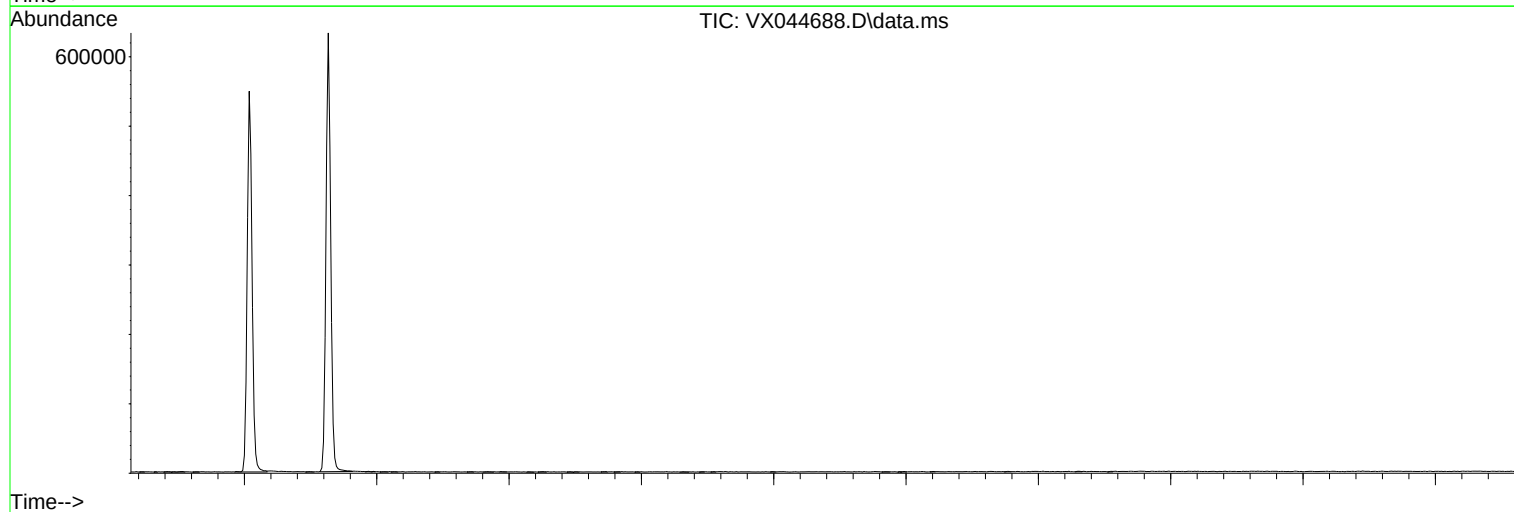
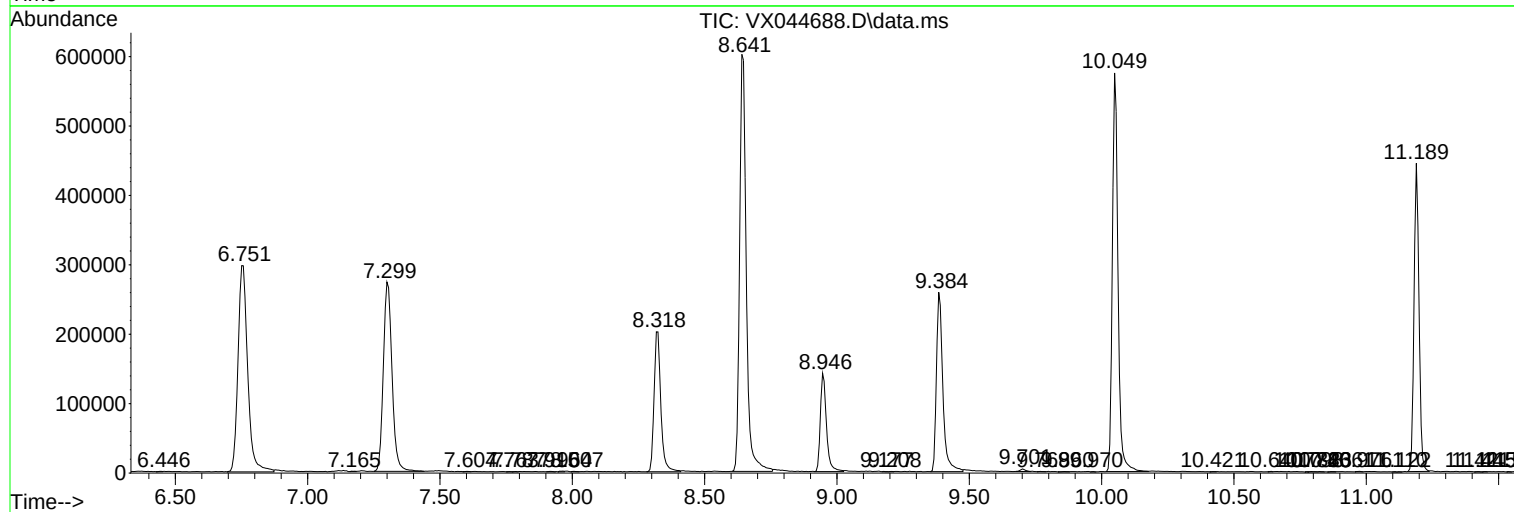
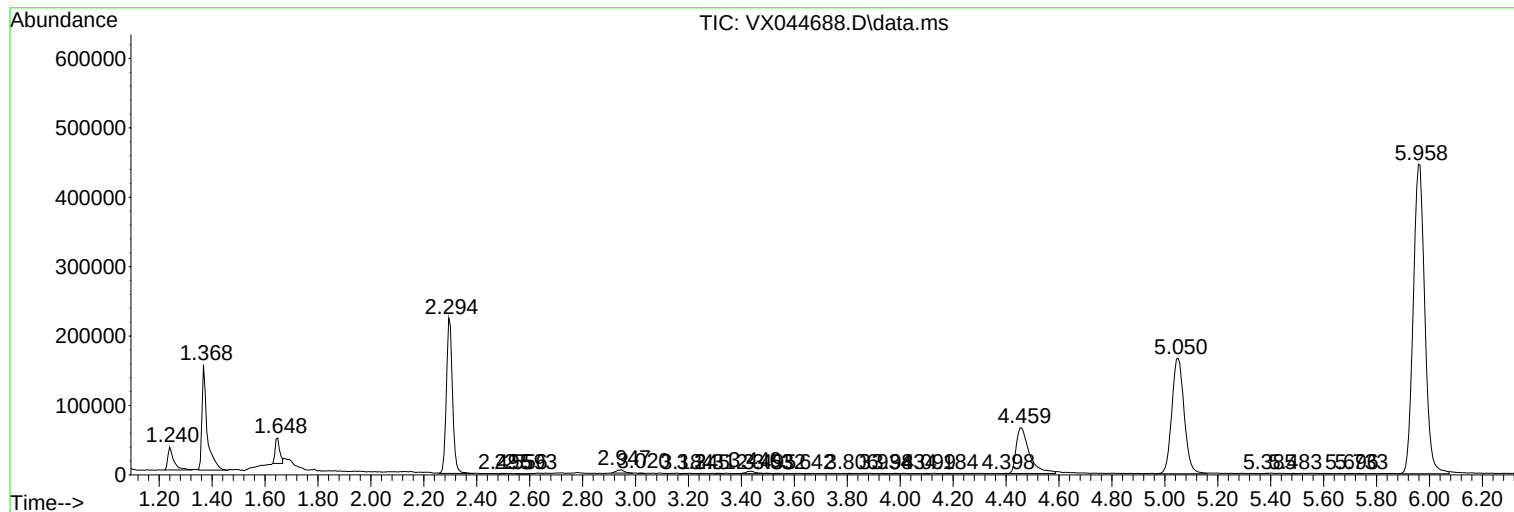
Sum of corrected areas: 9189283

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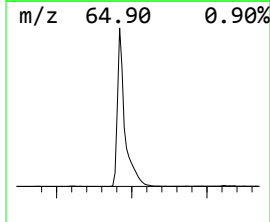
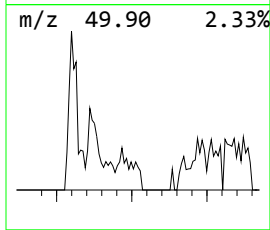
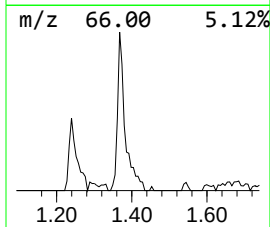
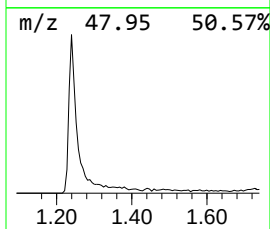
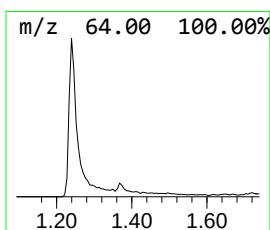
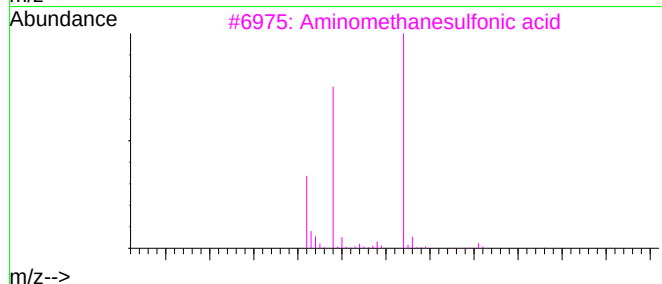
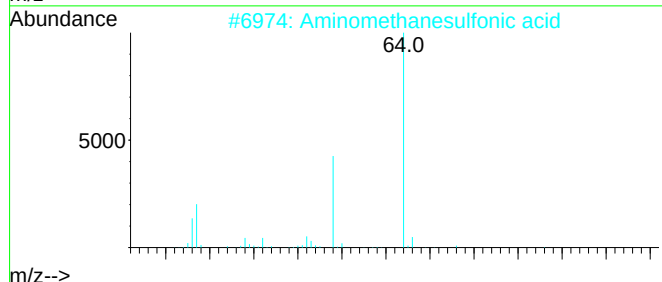
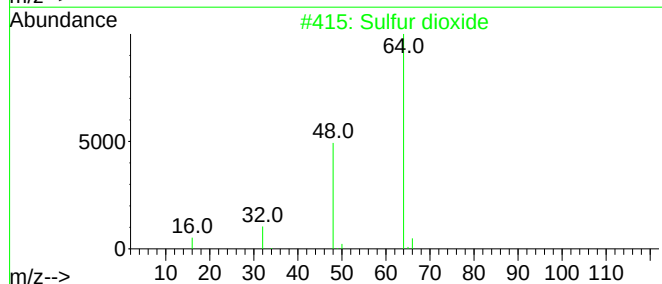
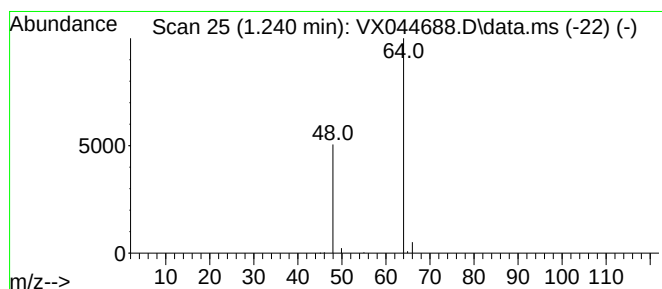
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.37 ug/L	50878	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	64
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.4	ug/L	50878	1	6.757	754395	50.0