

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
 Data File : VX044692.D
 Acq On : 22 Jan 2025 12:08
 Operator : JC/MD
 Sample : VX0122WBL01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK752

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: VX044692.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	32	rBV2	15564	28422	4.14%	0.576%
2	1.368	43	46	61	rVB	71317	116529	16.97%	2.362%
3	1.648	90	92	97	rBV	14674	16486	2.40%	0.334%
4	2.294	192	198	211	rBV	140601	223105	32.50%	4.522%
5	2.489	228	230	236	rBV5	1020	1254	0.18%	0.025%
6	2.855	288	290	292	rBV	454	390	0.06%	0.008%
7	2.879	292	294	295	rVV	475	271	0.04%	0.005%
8	3.123	333	334	338	rBV2	460	370	0.05%	0.007%
9	3.257	355	356	358	rBV2	576	441	0.06%	0.009%
10	3.434	378	385	392	rVV4	7868	18194	2.65%	0.369%
11	3.556	402	405	408	rBV5	523	790	0.12%	0.016%
12	3.684	424	426	429	rBV3	415	532	0.08%	0.011%
13	3.849	452	453	454	rBV	485	324	0.05%	0.007%
14	4.129	498	499	504	rBV3	594	574	0.08%	0.012%
15	4.208	510	512	515	rBV2	441	660	0.10%	0.013%
16	4.355	534	536	539	rVB2	444	363	0.05%	0.007%
17	4.379	539	540	541	rBV	576	292	0.04%	0.006%
18	4.458	545	553	571	rBV	42473	142299	20.73%	2.884%
19	4.775	604	605	608	rVB2	413	295	0.04%	0.006%
20	4.910	624	627	630	rBV3	422	588	0.09%	0.012%
21	5.044	638	649	664	rBV	88874	267260	38.93%	5.417%
22	5.257	683	684	688	rVB	429	349	0.05%	0.007%
23	5.288	688	689	693	rVB2	527	492	0.07%	0.010%
24	5.324	693	695	696	rBV2	542	400	0.06%	0.008%
25	5.434	711	713	714	rVB2	465	254	0.04%	0.005%
26	5.458	714	717	718	rBV2	650	761	0.11%	0.015%
27	5.513	724	726	728	rBV	403	293	0.04%	0.006%
28	5.855	781	782	783	rBV	497	315	0.05%	0.006%
29	5.958	788	799	819	rBV2	228472	686503	100.00%	13.915%
30	6.336	855	861	863	rBV5	886	1647	0.24%	0.033%
31	6.751	920	929	950	rBV	184765	469408	68.38%	9.515%
32	7.123	982	990	996	rBV7	1525	4488	0.65%	0.091%
33	7.177	997	999	1000	rVV2	540	281	0.04%	0.006%
34	7.299	1011	1019	1036	rBV	137021	314411	45.80%	6.373%
35	7.726	1085	1089	1095	rBV4	375	806	0.12%	0.016%
36	7.799	1100	1101	1104	rBV	380	437	0.06%	0.009%

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 ClientSampleId :
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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

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	7.970	1128	1129	1132	rBV2	849	600	0.09%	0.012%
38	8.208	1164	1168	1170	rBV2	457	641	0.09%	0.013%
39	8.257	1170	1176	1180	rVV5	2728	4925	0.72%	0.100%
40	8.317	1181	1186	1204	rVB	94964	169861	24.74%	3.443%
41	8.555	1223	1225	1226	rVB	450	286	0.04%	0.006%
42	8.641	1232	1239	1266	rBV	303433	539729	78.62%	10.940%
43	8.945	1285	1289	1300	rBV	61306	103522	15.08%	2.098%
44	9.165	1323	1325	1326	rBV	323	256	0.04%	0.005%
45	9.244	1336	1338	1341	rVB2	813	744	0.11%	0.015%
46	9.281	1341	1344	1347	rBV4	666	879	0.13%	0.018%
47	9.390	1356	1362	1378	rBV	119275	258957	37.72%	5.249%
48	9.653	1403	1405	1406	rBV	605	423	0.06%	0.009%
49	9.915	1446	1448	1449	rVV2	400	264	0.04%	0.005%
50	9.933	1449	1451	1453	rVB2	715	529	0.08%	0.011%
51	10.049	1465	1470	1488	rBV	326678	502162	73.15%	10.179%
52	10.305	1510	1512	1513	rVB2	907	404	0.06%	0.008%
53	10.360	1518	1521	1524	rBV2	564	863	0.13%	0.017%
54	10.396	1524	1527	1528	rBV2	370	388	0.06%	0.008%
55	10.537	1548	1550	1551	rVB	478	339	0.05%	0.007%
56	10.555	1551	1553	1555	rBV3	802	806	0.12%	0.016%
57	10.604	1560	1561	1563	rVB3	567	261	0.04%	0.005%
58	10.640	1563	1567	1568	rBV3	638	1000	0.15%	0.020%
59	10.671	1570	1572	1575	rVV3	408	399	0.06%	0.008%
60	10.707	1575	1578	1581	rVB3	350	493	0.07%	0.010%
61	10.768	1586	1588	1590	rVV2	469	359	0.05%	0.007%
62	10.811	1594	1595	1597	rBV2	644	387	0.06%	0.008%
63	10.835	1597	1599	1600	rBV2	623	505	0.07%	0.010%
64	11.097	1640	1642	1645	rBV3	495	572	0.08%	0.012%
65	11.189	1652	1657	1668	rBV	224133	309102	45.03%	6.265%
66	11.536	1713	1714	1718	rBV2	261	274	0.04%	0.006%
67	11.573	1718	1720	1722	rVB2	405	289	0.04%	0.006%
68	11.603	1723	1725	1727	rBV	574	358	0.05%	0.007%
69	11.683	1736	1738	1741	rBV2	285	337	0.05%	0.007%
70	11.945	1777	1781	1784	rBV4	459	844	0.12%	0.017%
71	11.969	1784	1785	1788	rBV3	513	549	0.08%	0.011%
72	12.018	1788	1793	1806	rVV	275015	371930	54.18%	7.539%
73	12.256	1830	1832	1833	rBV	700	480	0.07%	0.010%
74	12.317	1837	1842	1850	rVV	263228	343908	50.10%	6.971%
75	12.518	1874	1875	1878	rBV2	672	482	0.07%	0.010%
76	12.622	1890	1892	1894	rVB2	564	475	0.07%	0.010%

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Instrument :
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 ClientSampleId :
 VBLK752

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

77	12.658	1896	1898	1901	rBV2	473	417	0.06%	0.008%
78	12.713	1905	1907	1911	rVB2	494	589	0.09%	0.012%
79	12.756	1911	1914	1917	rBV2	909	1296	0.19%	0.026%
80	12.804	1920	1922	1925	rBV2	457	526	0.08%	0.011%
81	12.939	1943	1944	1947	rBV2	599	567	0.08%	0.011%
82	12.975	1949	1950	1952	rVV2	329	268	0.04%	0.005%
83	13.097	1967	1970	1972	rBV	578	662	0.10%	0.013%
84	13.189	1984	1985	1989	rVB2	437	365	0.05%	0.007%
85	13.250	1994	1995	1999	rVB3	685	680	0.10%	0.014%
86	13.286	1999	2001	2002	rBV	643	421	0.06%	0.009%
87	13.329	2006	2008	2010	rBV2	462	473	0.07%	0.010%
88	13.536	2038	2042	2043	rBV2	379	441	0.06%	0.009%
89	13.567	2043	2047	2050	rBV2	443	459	0.07%	0.009%
90	13.713	2069	2071	2073	rBV3	280	281	0.04%	0.006%
91	13.774	2079	2081	2082	rBV2	388	326	0.05%	0.007%
92	13.792	2082	2084	2087	rVV3	500	636	0.09%	0.013%
93	13.969	2110	2113	2116	rVV3	368	425	0.06%	0.009%
94	14.042	2122	2125	2126	rBV2	587	556	0.08%	0.011%
95	14.127	2137	2139	2142	rVB2	884	864	0.13%	0.018%
96	14.158	2142	2144	2147	rVV	402	354	0.05%	0.007%
97	14.182	2147	2148	2153	rVB3	430	475	0.07%	0.010%
98	14.542	2205	2207	2209	rBV2	654	502	0.07%	0.010%
99	14.859	2256	2259	2260	rBV	759	821	0.12%	0.017%
100	16.511	2526	2530	2532	rBV3	921	1253	0.18%	0.025%

Sum of corrected areas: 4933523

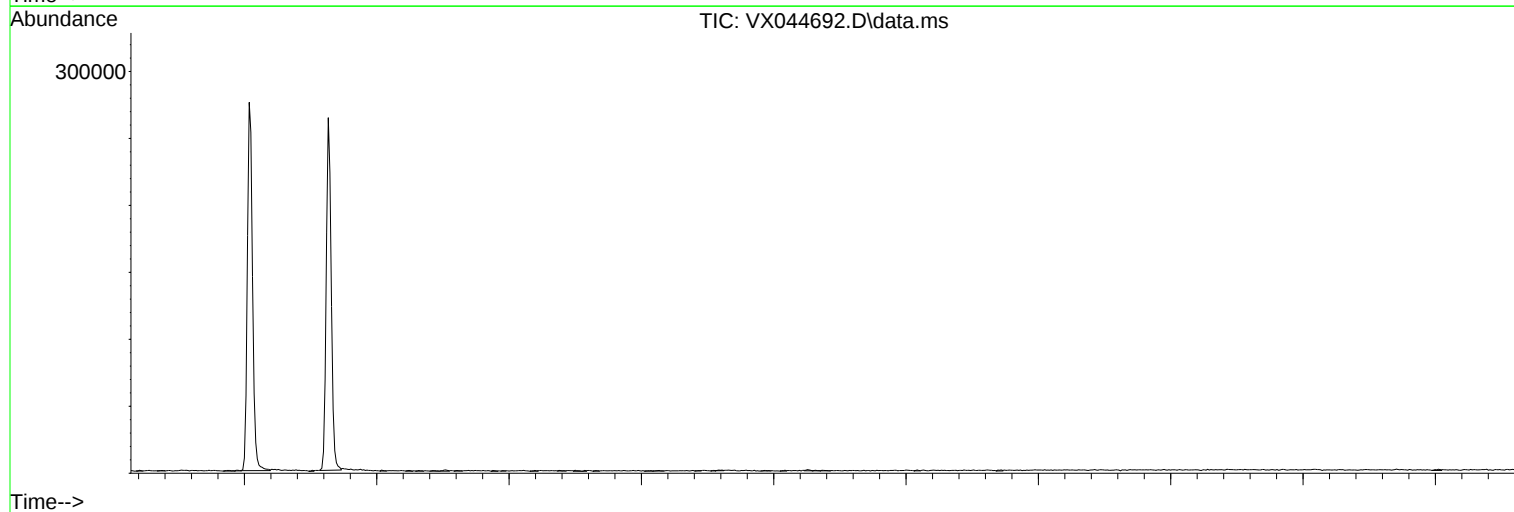
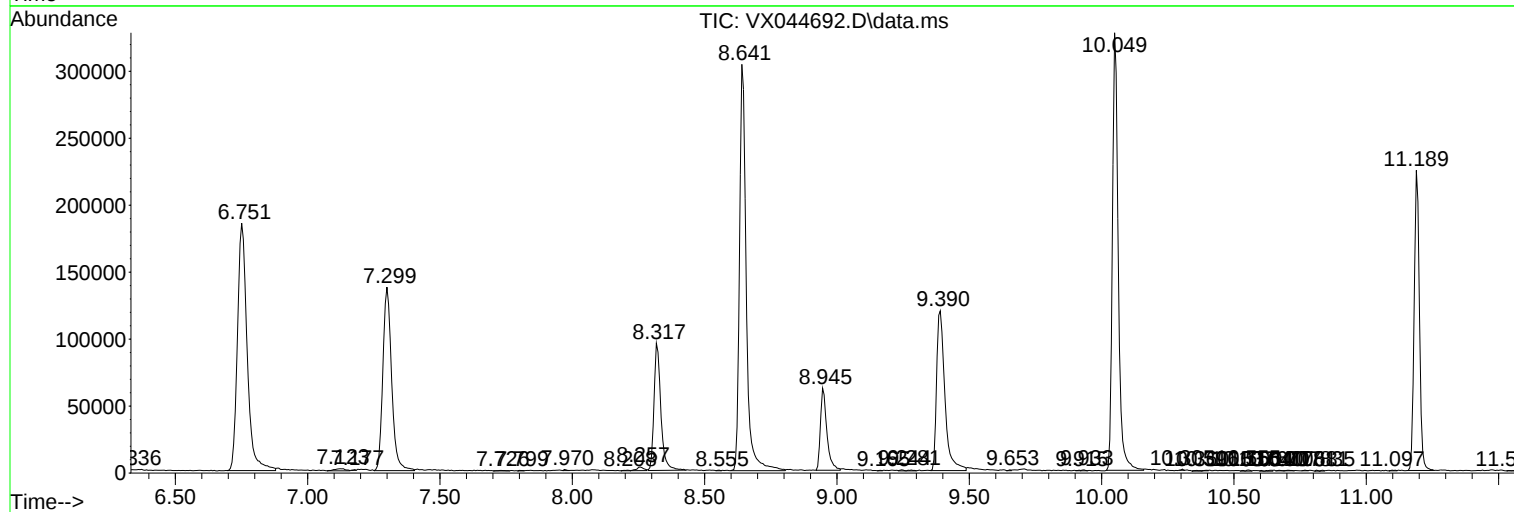
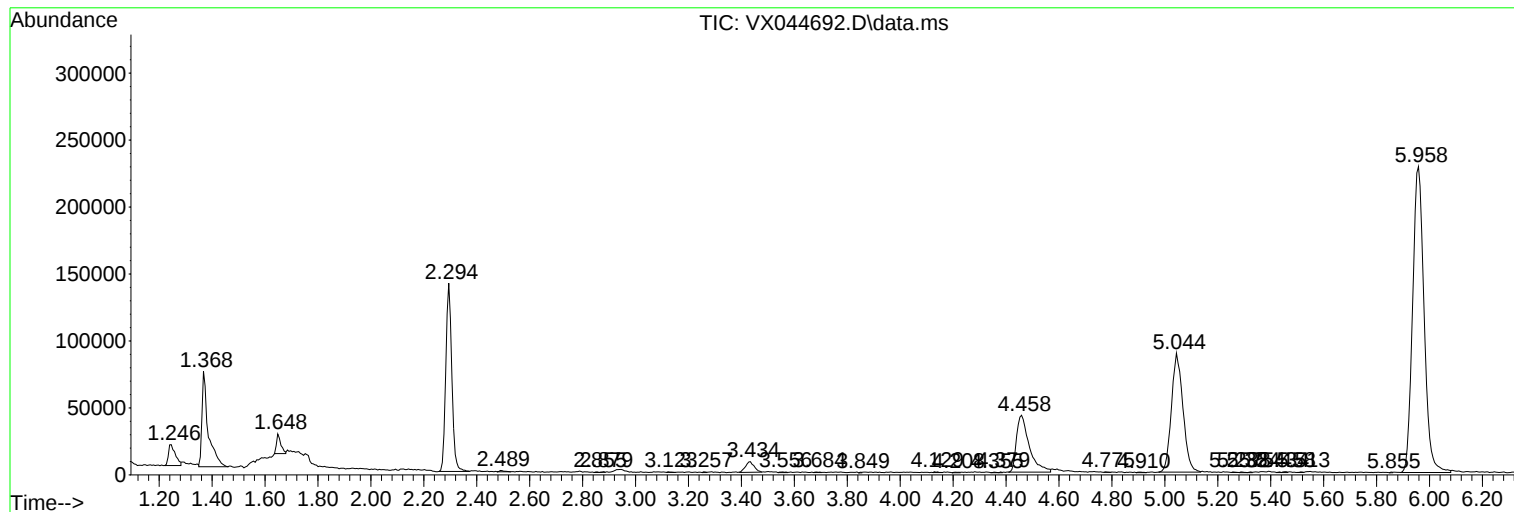
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ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VBLK752

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 Title : VOC Analysis

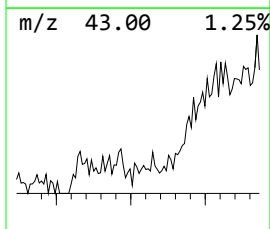
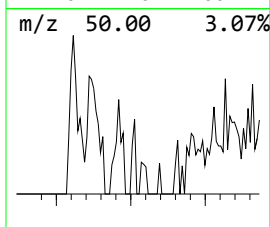
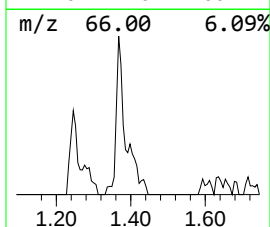
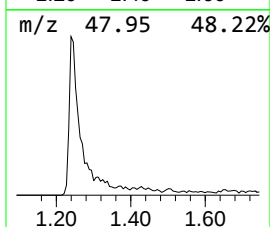
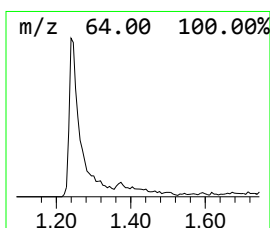
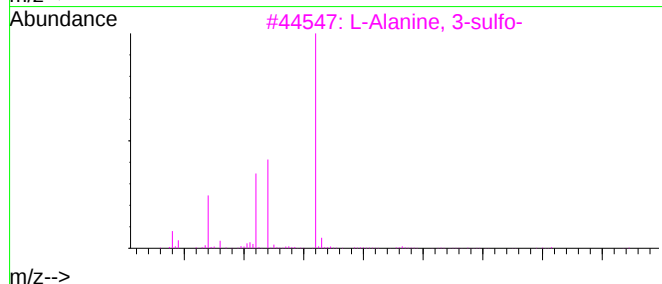
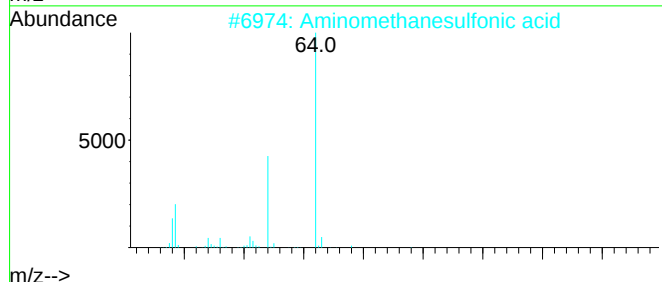
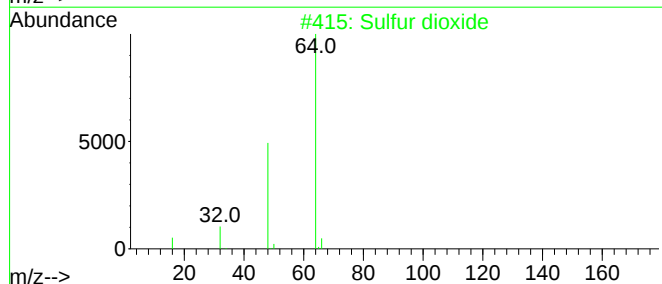
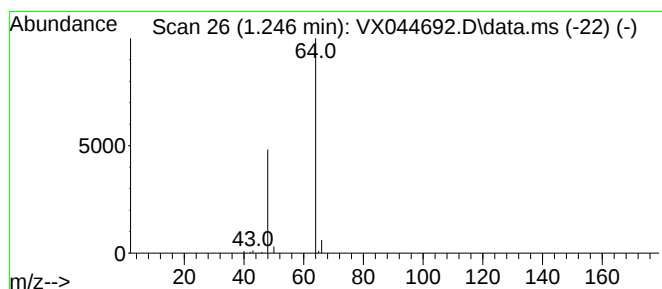
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	3.03 ug/L	28422	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	64
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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	3.0	ug/L	28422	1	6.751	469408	50.0