

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
 Data File : VX044693.D
 Acq On : 22 Jan 2025 12:40
 Operator : JC/MD
 Sample : Q1131-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 JNLE5

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: VX044693.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	33	rBV2	15276	27587	4.12%	0.559%
2	1.368	43	46	62	rVB	63996	110506	16.49%	2.239%
3	1.496	64	67	71	rVB	11904	14298	2.13%	0.290%
4	1.550	73	76	78	rBV3	3664	4905	0.73%	0.099%
5	1.648	89	92	97	rBV	13942	21043	3.14%	0.426%
6	2.294	192	198	209	rVB	112569	174861	26.09%	3.543%
7	2.392	211	214	218	rBV5	865	1202	0.18%	0.024%
8	2.501	228	232	234	rVV5	645	981	0.15%	0.020%
9	2.575	236	244	250	rVV3	869	2162	0.32%	0.044%
10	2.709	262	266	272	rVB7	930	2213	0.33%	0.045%
11	2.782	276	278	280	rVB3	782	630	0.09%	0.013%
12	2.837	285	287	289	rVB3	684	437	0.07%	0.009%
13	2.940	296	304	310	rBV3	3556	8697	1.30%	0.176%
14	2.989	310	312	315	rVB3	684	868	0.13%	0.018%
15	3.135	333	336	337	rBV2	366	458	0.07%	0.009%
16	3.312	363	365	369	rVB2	398	466	0.07%	0.009%
17	3.428	377	384	395	rBV3	5292	12430	1.85%	0.252%
18	3.587	405	410	411	rBV4	365	390	0.06%	0.008%
19	3.916	462	464	467	rBV4	642	886	0.13%	0.018%
20	4.257	516	520	521	rBV2	764	958	0.14%	0.019%
21	4.458	545	553	568	rBV	57226	190418	28.41%	3.858%
22	4.721	594	596	597	rBV	610	416	0.06%	0.008%
23	4.794	606	608	611	rBV3	370	371	0.06%	0.008%
24	5.044	638	649	665	rBV	82792	261922	39.08%	5.307%
25	5.288	688	689	692	rBV3	503	402	0.06%	0.008%
26	5.678	752	753	756	rBV2	381	352	0.05%	0.007%
27	5.763	764	767	772	rBV5	676	1410	0.21%	0.029%
28	5.958	788	799	818	rBV3	221543	670244	100.00%	13.581%
29	6.232	842	844	845	rVB2	546	331	0.05%	0.007%
30	6.269	848	850	853	rVB3	782	647	0.10%	0.013%
31	6.580	899	901	904	rVB3	489	375	0.06%	0.008%
32	6.629	904	909	911	rBV4	554	1028	0.15%	0.021%
33	6.751	921	929	953	rBV	181510	464165	69.25%	9.405%
34	7.104	985	987	988	rBV2	757	584	0.09%	0.012%
35	7.299	1011	1019	1036	rBV	135380	307418	45.87%	6.229%
36	7.635	1072	1074	1076	rBV2	564	583	0.09%	0.012%

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Integrator: RTE

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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	7.921	1120	1121	1124	rBV2	532	481	0.07%	0.010%
38	7.952	1124	1126	1130	rVV3	710	989	0.15%	0.020%
39	8.214	1166	1169	1170	rBV3	432	459	0.07%	0.009%
40	8.317	1181	1186	1200	rBV	89237	162961	24.31%	3.302%
41	8.574	1225	1228	1229	rBV2	581	485	0.07%	0.010%
42	8.641	1233	1239	1256	rBV	291743	510497	76.17%	10.344%
43	8.945	1284	1289	1302	rBV	59211	102330	15.27%	2.073%
44	9.275	1338	1343	1349	rVB4	1452	2706	0.40%	0.055%
45	9.329	1349	1352	1354	rBV3	523	675	0.10%	0.014%
46	9.390	1356	1362	1382	rBV	161087	362468	54.08%	7.344%
47	9.701	1411	1413	1415	rBV2	399	327	0.05%	0.007%
48	9.756	1421	1422	1426	rVB3	473	355	0.05%	0.007%
49	9.811	1429	1431	1435	rVB2	509	541	0.08%	0.011%
50	9.860	1438	1439	1443	rVB	524	508	0.08%	0.010%
51	9.994	1460	1461	1464	rBV2	527	588	0.09%	0.012%
52	10.049	1465	1470	1484	rVV	310129	478817	71.44%	9.702%
53	10.207	1492	1496	1497	rBV3	876	1090	0.16%	0.022%
54	10.293	1506	1510	1511	rBV3	794	1036	0.15%	0.021%
55	10.311	1511	1513	1515	rVV2	758	667	0.10%	0.014%
56	10.518	1545	1547	1552	rBV3	512	808	0.12%	0.016%
57	10.610	1560	1562	1565	rBV2	466	541	0.08%	0.011%
58	10.756	1583	1586	1587	rBV2	609	661	0.10%	0.013%
59	10.799	1590	1593	1594	rBV3	490	388	0.06%	0.008%
60	11.030	1629	1631	1634	rBV2	368	464	0.07%	0.009%
61	11.079	1636	1639	1640	rVV2	483	613	0.09%	0.012%
62	11.110	1642	1644	1646	rBV	576	388	0.06%	0.008%
63	11.189	1652	1657	1666	rBV	241634	322527	48.12%	6.535%
64	11.835	1761	1763	1766	rVB3	438	366	0.05%	0.007%
65	11.872	1766	1769	1770	rBV3	540	435	0.06%	0.009%
66	12.018	1788	1793	1806	rBV	264689	354512	52.89%	7.183%
67	12.183	1816	1820	1821	rBV3	453	531	0.08%	0.011%
68	12.225	1825	1827	1829	rBV3	625	674	0.10%	0.014%
69	12.317	1837	1842	1853	rBV	242409	321668	47.99%	6.518%
70	12.481	1867	1869	1871	rBV2	751	734	0.11%	0.015%
71	12.628	1891	1893	1897	rVB2	624	629	0.09%	0.013%
72	12.670	1897	1900	1901	rBV2	447	333	0.05%	0.007%
73	12.689	1901	1903	1906	rVV3	466	396	0.06%	0.008%
74	12.719	1906	1908	1909	rVV	516	342	0.05%	0.007%
75	12.762	1911	1915	1917	rVB4	815	958	0.14%	0.019%
76	12.780	1917	1918	1923	rBV3	494	632	0.09%	0.013%

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Integration Parameters: LSCINT.P

Integrator: RTE

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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	12.847	1926	1929	1931	rBV	443	489	0.07%	0.010%
78	12.920	1940	1941	1945	rBV2	461	577	0.09%	0.012%
79	12.957	1945	1947	1948	rVB	679	409	0.06%	0.008%
80	12.987	1948	1952	1954	rBV3	606	855	0.13%	0.017%
81	13.024	1956	1958	1959	rBV2	370	352	0.05%	0.007%
82	13.237	1990	1993	1994	rBV2	578	657	0.10%	0.013%
83	13.268	1996	1998	2001	rVV2	420	399	0.06%	0.008%
84	13.347	2009	2011	2015	rVB3	517	524	0.08%	0.011%
85	13.426	2021	2024	2026	rBV2	565	534	0.08%	0.011%
86	13.743	2075	2076	2080	rVB3	485	481	0.07%	0.010%
87	13.847	2091	2093	2096	rVB3	592	601	0.09%	0.012%
88	14.396	2182	2183	2186	rBV2	461	374	0.06%	0.008%
89	14.676	2227	2229	2230	rVB2	512	341	0.05%	0.007%
90	14.731	2236	2238	2239	rBV2	490	415	0.06%	0.008%
91	14.822	2251	2253	2256	rVB2	536	496	0.07%	0.010%
92	14.963	2274	2276	2278	rVB2	531	385	0.06%	0.008%
93	15.042	2288	2289	2291	rBV2	553	463	0.07%	0.009%
94	15.164	2307	2309	2312	rBV2	411	417	0.06%	0.008%
95	15.219	2316	2318	2320	rVB3	528	384	0.06%	0.008%
96	15.481	2358	2361	2362	rBV2	584	573	0.09%	0.012%
97	16.176	2473	2475	2476	rVB2	603	354	0.05%	0.007%
98	16.542	2533	2535	2537	rBV3	971	888	0.13%	0.018%
99	16.590	2541	2543	2544	rBV	814	584	0.09%	0.012%
100	16.700	2559	2561	2564	rBV5	521	526	0.08%	0.011%

Sum of corrected areas: 4935302

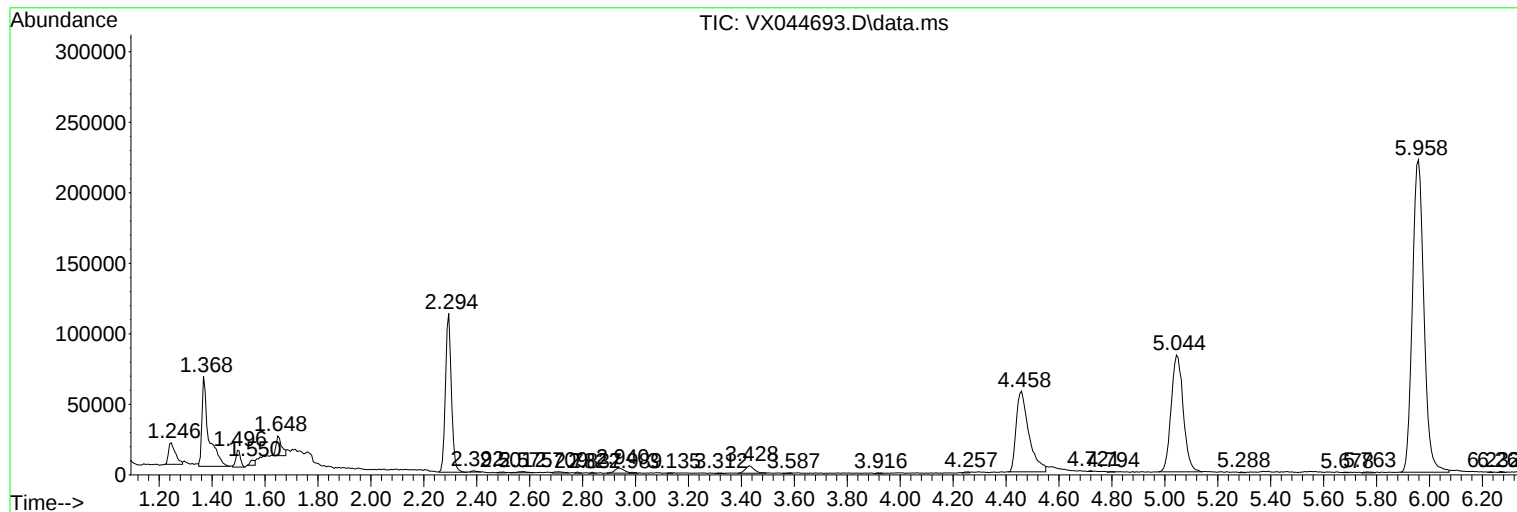
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012225\
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012125WMA.M
Quant Title : VOC Analysis

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
Quant Title : VOC Analysis

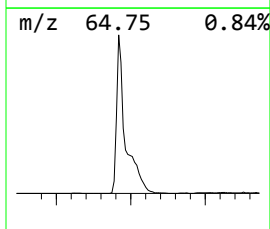
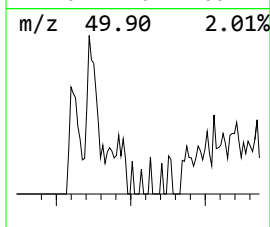
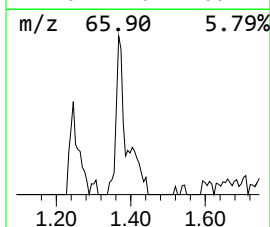
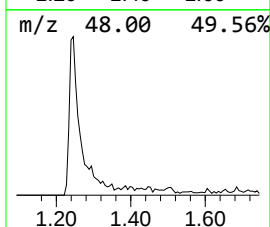
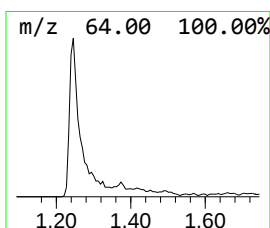
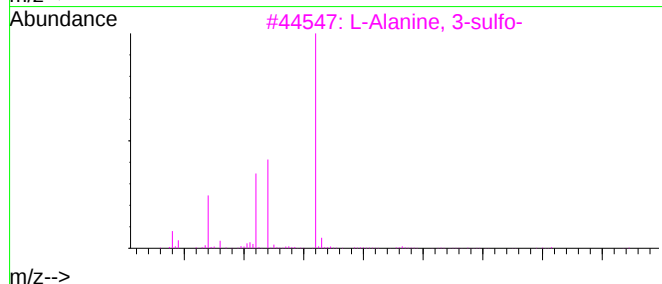
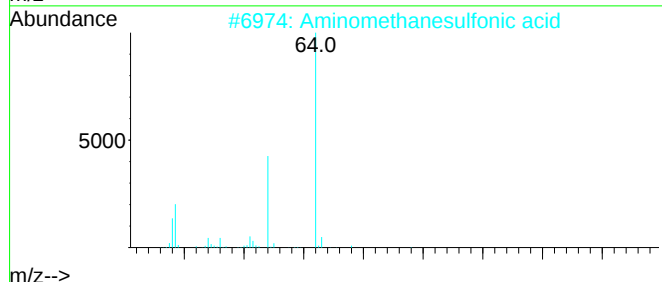
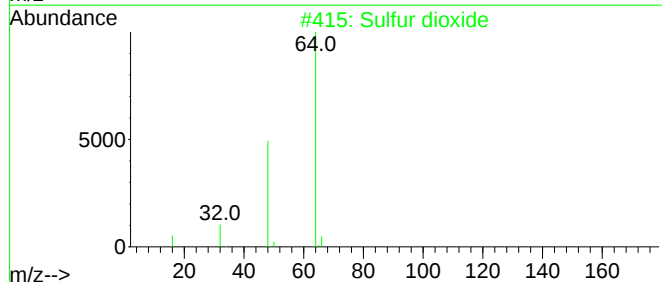
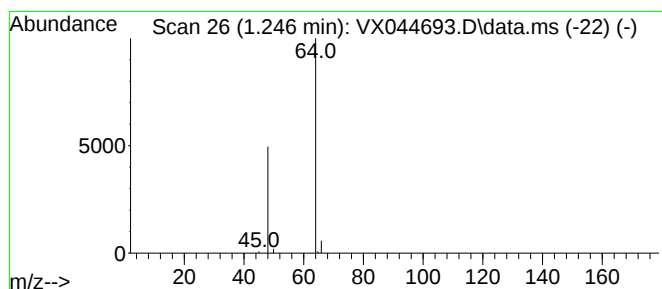
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	2.97 ug/L	27587	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	4



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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	1.246	3.0	ug/L	27587	1	6.751	464165	50.0