

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042427.D
 Acq On : 20 Jul 2024 01:02
 Operator : JC/MD
 Sample : P3298-16 100X
 Misc : 4.38g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB76

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042427.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	40	rBV2	26633	38868	5.64%	0.727%
2	1.368	43	46	58	rVB	59492	74489	10.81%	1.394%
3	1.648	89	92	103	rVB	48451	62802	9.11%	1.175%
4	2.300	192	199	212	rBV	120641	194173	28.18%	3.634%
5	2.502	230	232	235	rVB2	307	333	0.05%	0.006%
6	2.709	263	266	270	rBV3	212	359	0.05%	0.007%
7	2.758	273	274	275	rBV	284	115	0.02%	0.002%
8	2.788	275	279	285	rVB2	892	1458	0.21%	0.027%
9	2.941	297	304	314	rVB2	2521	5968	0.87%	0.112%
10	3.056	321	323	325	rVB	162	137	0.02%	0.003%
11	3.087	325	328	330	rBV2	140	149	0.02%	0.003%
12	3.197	342	346	348	rVV2	122	176	0.03%	0.003%
13	3.221	348	350	353	rVB2	138	140	0.02%	0.003%
14	3.313	360	365	367	rVB2	184	261	0.04%	0.005%
15	3.349	367	371	372	rBV2	164	181	0.03%	0.003%
16	3.361	372	373	376	rBV	162	129	0.02%	0.002%
17	3.398	376	379	382	rBV2	123	187	0.03%	0.004%
18	3.477	389	392	395	rVB	138	199	0.03%	0.004%
19	3.501	395	396	398	rBV	161	128	0.02%	0.002%
20	3.526	398	400	404	rVV2	109	142	0.02%	0.003%
21	3.575	406	408	410	rVB2	146	137	0.02%	0.003%
22	3.599	410	412	413	rBV	228	159	0.02%	0.003%
23	3.733	432	434	436	rVB2	157	132	0.02%	0.002%
24	3.971	469	473	474	rBV2	181	184	0.03%	0.003%
25	4.209	508	512	515	rBV2	181	196	0.03%	0.004%
26	4.257	518	520	523	rVB2	112	109	0.02%	0.002%
27	4.282	523	524	527	rBV	201	140	0.02%	0.003%
28	4.343	532	534	536	rBV2	197	168	0.02%	0.003%
29	4.465	546	554	570	rBV	48923	147019	21.33%	2.752%
30	4.709	593	594	598	rVB2	396	369	0.05%	0.007%
31	4.776	603	605	607	rVB2	286	206	0.03%	0.004%
32	4.885	619	623	624	rBV2	156	198	0.03%	0.004%
33	4.904	624	626	629	rVV	114	157	0.02%	0.003%
34	4.952	632	634	636	rBV2	169	139	0.02%	0.003%
35	5.062	639	652	670	rVV	86706	266845	38.72%	4.995%
36	5.257	683	684	686	rBV2	223	159	0.02%	0.003%

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37	5.288	686	689	690	rVB2	206	190	0.03%	0.004%
38	5.373	702	703	704	rBV	172	109	0.02%	0.002%
39	5.550	729	732	733	rBV	220	170	0.02%	0.003%
40	5.794	769	772	774	rBV2	218	219	0.03%	0.004%
41	5.867	782	784	786	rBV2	136	162	0.02%	0.003%
42	5.964	789	800	816	rBV2	237691	689159	100.00%	12.899%
43	6.342	860	862	865	rBV	102	125	0.02%	0.002%
44	6.379	865	868	869	rVV	304	236	0.03%	0.004%
45	6.410	869	873	874	rVB2	133	152	0.02%	0.003%
46	6.477	880	884	885	rVB2	104	122	0.02%	0.002%
47	6.495	885	887	889	rBV2	117	137	0.02%	0.003%
48	6.562	896	898	901	rVB2	152	117	0.02%	0.002%
49	6.763	921	931	952	rBV	203455	495896	71.96%	9.282%
50	7.117	984	989	996	rVB7	1203	2996	0.43%	0.056%
51	7.220	1000	1006	1010	rBV3	391	863	0.13%	0.016%
52	7.306	1012	1020	1035	rBV	137037	306368	44.46%	5.734%
53	7.690	1081	1083	1085	rBV2	187	185	0.03%	0.003%
54	7.726	1087	1089	1091	rBV	231	200	0.03%	0.004%
55	7.854	1109	1110	1114	rBV2	104	150	0.02%	0.003%
56	7.928	1120	1122	1123	rBV	147	124	0.02%	0.002%
57	7.958	1123	1127	1128	rBV3	388	450	0.07%	0.008%
58	8.043	1139	1141	1144	rBV2	182	171	0.02%	0.003%
59	8.080	1146	1147	1150	rBV	104	136	0.02%	0.003%
60	8.324	1181	1187	1204	rBV	74617	127616	18.52%	2.389%
61	8.513	1214	1218	1220	rBV2	567	712	0.10%	0.013%
62	8.647	1233	1240	1257	rBV	351539	551833	80.07%	10.329%
63	8.952	1285	1290	1302	rBV	54279	82995	12.04%	1.553%
64	9.171	1324	1326	1329	rBV	140	118	0.02%	0.002%
65	9.263	1340	1341	1342	rBV	219	136	0.02%	0.003%
66	9.385	1356	1361	1374	rBV	217412	328134	47.61%	6.142%
67	9.580	1392	1393	1395	rVB2	435	190	0.03%	0.004%
68	9.702	1410	1413	1419	rVB3	1287	1666	0.24%	0.031%
69	9.775	1423	1425	1428	rBV2	161	157	0.02%	0.003%
70	9.866	1438	1440	1442	rBV2	247	186	0.03%	0.003%
71	9.891	1442	1444	1446	rBV2	124	140	0.02%	0.003%
72	10.055	1465	1471	1488	rVV	417948	580323	84.21%	10.862%
73	10.244	1499	1502	1503	rBV2	366	344	0.05%	0.006%
74	10.421	1529	1531	1532	rBV	148	150	0.02%	0.003%
75	10.470	1537	1539	1541	rVB2	145	110	0.02%	0.002%
76	10.506	1541	1545	1548	rBV	186	198	0.03%	0.004%

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77	10.695	1574	1576	1580	rVB2	152	167	0.02%	0.003%
78	10.732	1580	1582	1584	rBV2	166	148	0.02%	0.003%
79	10.915	1610	1612	1615	rBV2	179	185	0.03%	0.003%
80	10.976	1619	1622	1624	rVV	154	164	0.02%	0.003%
81	11.189	1652	1657	1666	rBV	276062	361410	52.44%	6.765%
82	11.457	1699	1701	1703	rBV2	129	131	0.02%	0.002%
83	11.549	1713	1716	1717	rBV	162	127	0.02%	0.002%
84	11.628	1728	1729	1733	rVB2	187	185	0.03%	0.003%
85	12.018	1788	1793	1803	rBV	393136	518928	75.30%	9.713%
86	12.226	1825	1827	1829	rBV	211	162	0.02%	0.003%
87	12.317	1837	1842	1858	rBV	379218	487588	70.75%	9.126%
88	12.610	1886	1890	1891	rBV2	163	202	0.03%	0.004%
89	12.756	1912	1914	1918	rBV	414	352	0.05%	0.007%
90	13.110	1970	1972	1976	rVV	174	132	0.02%	0.002%
91	13.244	1991	1994	1995	rVB	281	183	0.03%	0.003%
92	13.634	2056	2058	2059	rBV	169	128	0.02%	0.002%
93	13.969	2111	2113	2116	rBV	179	210	0.03%	0.004%
94	13.994	2116	2117	2120	rVB	189	201	0.03%	0.004%
95	14.036	2122	2124	2126	rVB	314	188	0.03%	0.004%
96	14.079	2127	2131	2133	rBV2	153	236	0.03%	0.004%
97	14.128	2136	2139	2143	rVB2	703	973	0.14%	0.018%
98	14.280	2161	2164	2165	rBV	193	211	0.03%	0.004%
99	14.640	2221	2223	2225	rBV	203	211	0.03%	0.004%
100	14.890	2263	2264	2265	rBV	281	129	0.02%	0.002%

Sum of corrected areas: 5342707

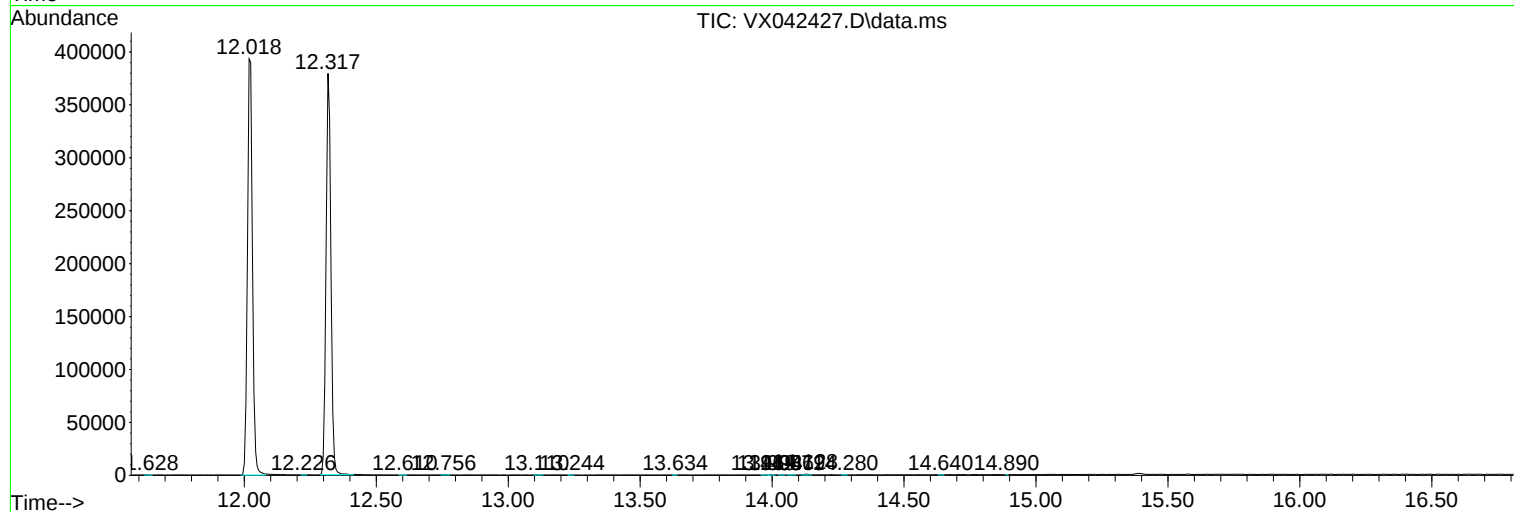
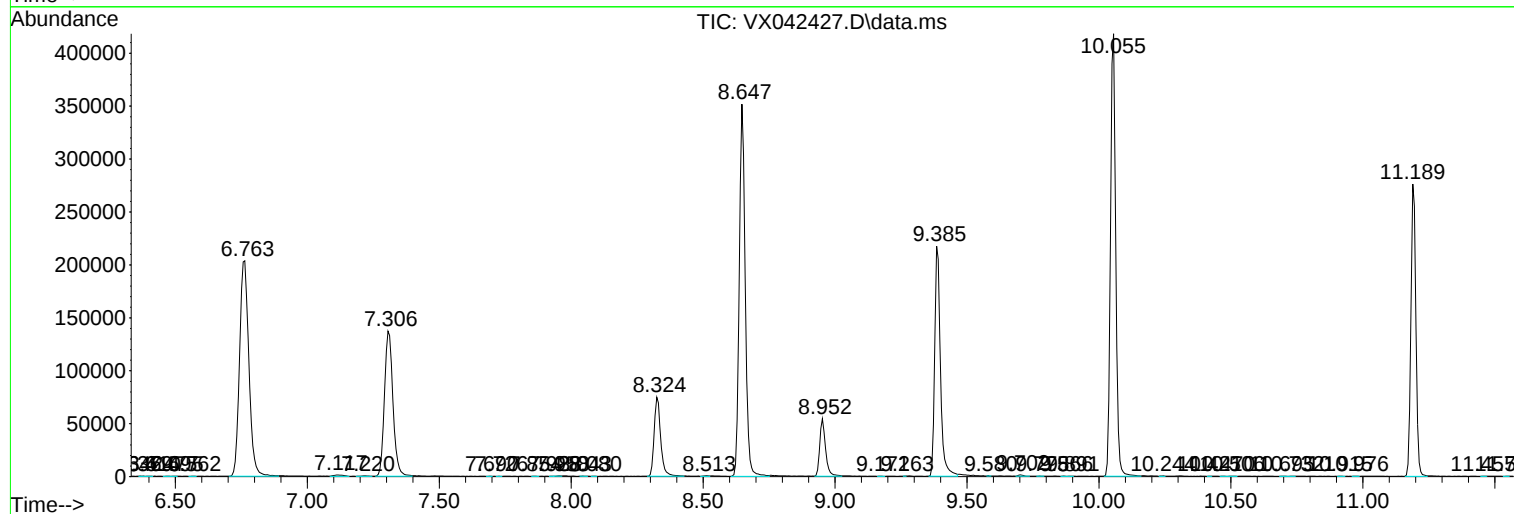
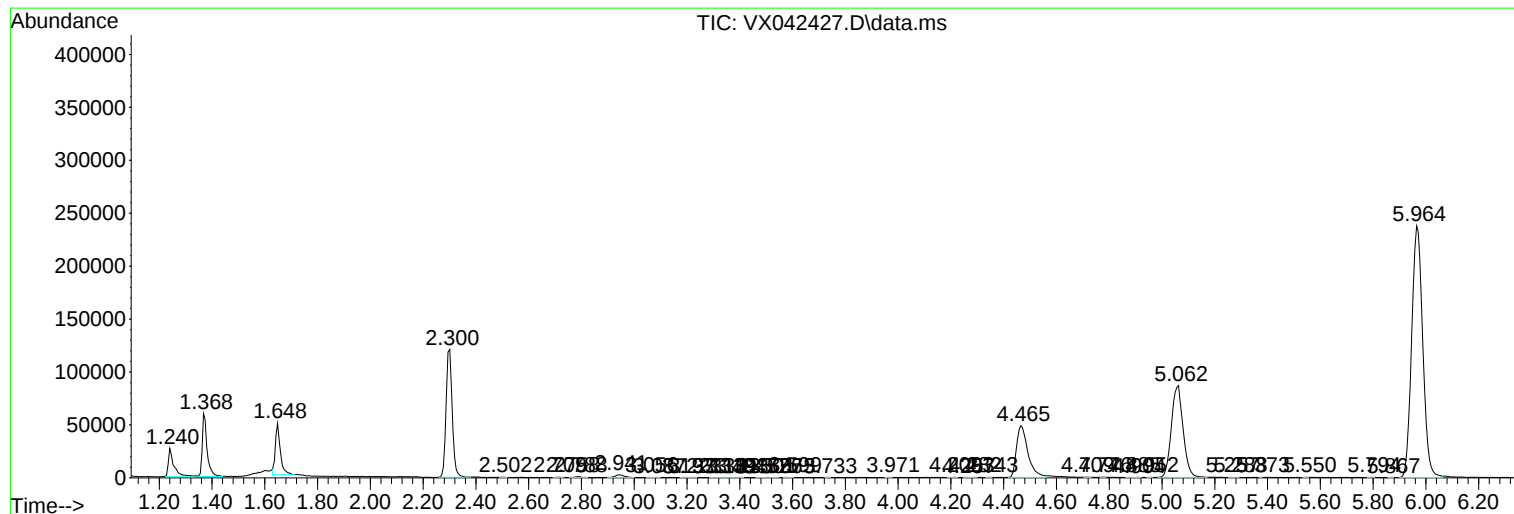
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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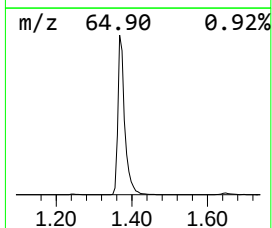
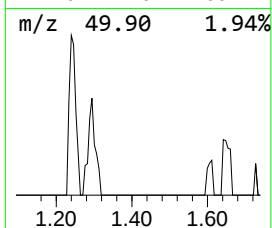
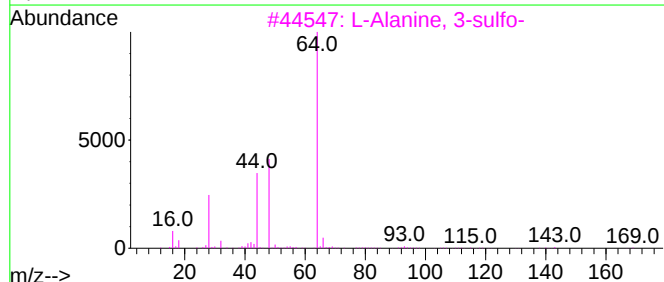
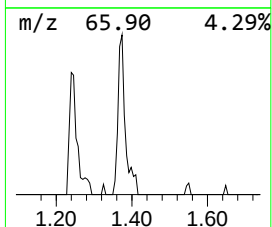
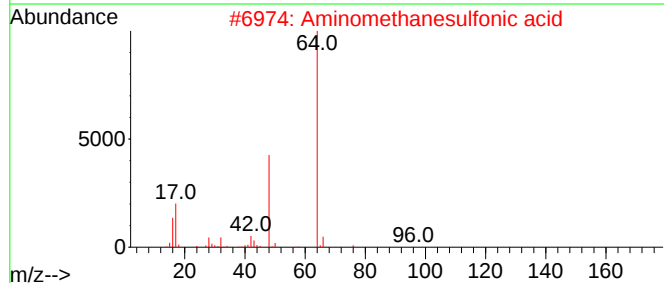
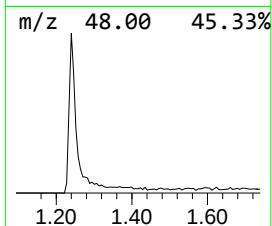
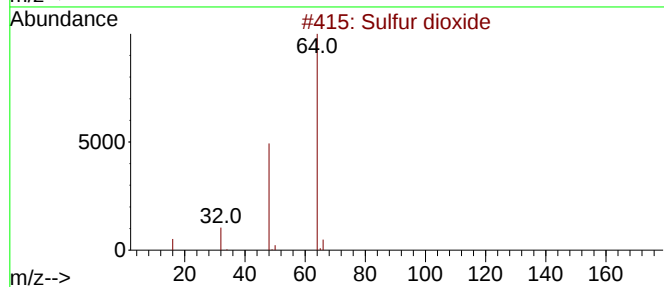
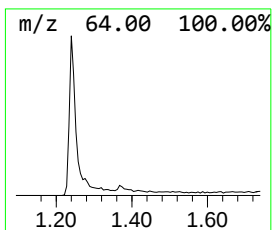
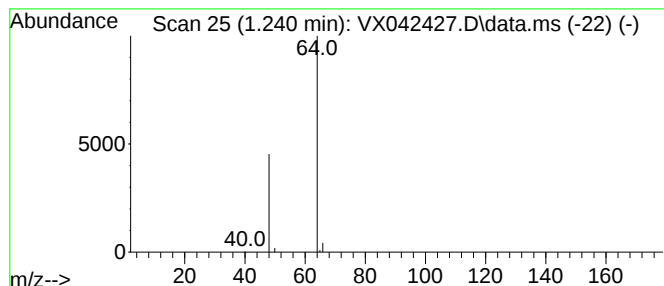
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.92 ug/L	38868	1,4-Difluorobenzene	6.763

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	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.9	ug/L	38868	1	6.763	495896	50.0