

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042415.D
 Acq On : 19 Jul 2024 20:25
 Operator : JC/MD
 Sample : P3238-18MERE
 Misc : 5.98g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CG8MERE

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: VX042415.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.245	22	26	27	rBV	30967	36414	5.20%	0.881%
2	1.373	43	47	49	rBV	16158	24317	3.47%	0.589%
3	2.282	190	196	212	rBV	48718	93651	13.37%	2.267%
4	2.617	249	251	255	rBV3	221	302	0.04%	0.007%
5	2.672	259	260	261	rBV	256	173	0.02%	0.004%
6	2.721	262	268	275	rBV	9831	20879	2.98%	0.505%
7	2.940	298	304	321	rVB	6187	16822	2.40%	0.407%
8	3.062	322	324	327	rBV2	214	150	0.02%	0.004%
9	3.087	327	328	329	rVB	157	57	0.01%	0.001%
10	3.105	329	331	332	rBV2	139	76	0.01%	0.002%
11	3.154	337	339	341	rBV2	215	163	0.02%	0.004%
12	3.190	343	345	346	rVB	169	83	0.01%	0.002%
13	3.208	346	348	350	rVB2	115	102	0.01%	0.002%
14	3.227	350	351	352	rBV	139	68	0.01%	0.002%
15	3.251	352	355	356	rBV2	52	61	0.01%	0.001%
16	3.276	356	359	360	rVB2	60	42	0.01%	0.001%
17	3.294	360	362	364	rBV2	96	81	0.01%	0.002%
18	3.410	380	381	385	rBV2	124	134	0.02%	0.003%
19	3.446	385	387	388	rBV	61	57	0.01%	0.001%
20	3.458	388	389	391	rVV2	91	53	0.01%	0.001%
21	3.550	402	404	405	rVB	58	28	0.00%	0.001%
22	3.574	405	408	409	rBV2	130	116	0.02%	0.003%
23	3.593	409	411	412	rVB	134	72	0.01%	0.002%
24	3.660	419	422	423	rBV	160	119	0.02%	0.003%
25	3.708	428	430	431	rVB	71	46	0.01%	0.001%
26	3.769	436	440	441	rBV2	90	100	0.01%	0.002%
27	3.812	446	447	448	rVB	75	28	0.00%	0.001%
28	3.867	454	456	457	rBV2	128	89	0.01%	0.002%
29	3.897	459	461	464	rBV2	90	65	0.01%	0.002%
30	3.940	466	468	470	rVB2	108	52	0.01%	0.001%
31	3.971	470	473	474	rBV2	112	127	0.02%	0.003%
32	4.007	476	479	480	rBV	107	138	0.02%	0.003%
33	4.038	480	484	487	rBV2	141	175	0.02%	0.004%
34	4.074	488	490	492	rBV	104	73	0.01%	0.002%
35	4.111	494	496	497	rBV	111	110	0.02%	0.003%
36	4.208	510	512	513	rBV	101	65	0.01%	0.002%

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

37	4.263	520	521	526	rVB2	118	160	0.02%	0.004%
38	4.300	526	527	530	rBV	140	108	0.02%	0.003%
39	4.349	533	535	536	rBV	149	82	0.01%	0.002%
40	4.422	546	547	548	rBV	172	91	0.01%	0.002%
41	4.495	551	559	575	rBV2	20868	73747	10.53%	1.785%
42	5.056	639	651	670	rBV	47184	150042	21.43%	3.632%
43	5.330	695	696	697	rBV	144	53	0.01%	0.001%
44	5.373	701	703	704	rBV2	322	216	0.03%	0.005%
45	5.556	726	733	738	rBV3	467	1117	0.16%	0.027%
46	5.690	754	755	757	rBV	136	101	0.01%	0.002%
47	5.885	785	787	790	rBV	142	147	0.02%	0.004%
48	5.958	790	799	816	rBV3	138559	401086	57.28%	9.709%
49	6.373	865	867	869	rBV2	276	248	0.04%	0.006%
50	6.659	912	914	915	rBV	239	185	0.03%	0.004%
51	6.757	921	930	945	rBV	252656	604594	86.34%	14.635%
52	7.110	984	988	991	rBV3	844	1157	0.17%	0.028%
53	7.165	995	997	998	rBV	247	193	0.03%	0.005%
54	7.226	1002	1007	1008	rBV3	449	690	0.10%	0.017%
55	7.305	1013	1020	1038	rVB	78407	175920	25.12%	4.258%
56	7.482	1048	1049	1050	rVB	228	83	0.01%	0.002%
57	7.653	1076	1077	1079	rVB	168	81	0.01%	0.002%
58	7.872	1111	1113	1115	rBV2	139	133	0.02%	0.003%
59	8.098	1148	1150	1151	rBV2	125	115	0.02%	0.003%
60	8.323	1181	1187	1199	rBV	39591	71905	10.27%	1.741%
61	8.647	1231	1240	1249	rBV	199956	324343	46.32%	7.851%
62	8.872	1275	1277	1280	rVB	249	233	0.03%	0.006%
63	8.951	1285	1290	1304	rVV	28220	46428	6.63%	1.124%
64	9.171	1324	1326	1331	rBV2	153	259	0.04%	0.006%
65	9.396	1357	1363	1383	rBV	82951	180747	25.81%	4.375%
66	9.707	1410	1414	1423	rVB4	2527	4292	0.61%	0.104%
67	10.055	1465	1471	1487	rBV	504114	700250	100.00%	16.951%
68	10.866	1602	1604	1606	rBV	133	118	0.02%	0.003%
69	10.969	1617	1621	1628	rBV3	1220	1859	0.27%	0.045%
70	11.195	1652	1658	1668	rBV	147349	199870	28.54%	4.838%
71	11.311	1675	1677	1681	rVB2	406	425	0.06%	0.010%
72	11.707	1740	1742	1743	rBV2	302	249	0.04%	0.006%
73	11.762	1746	1751	1755	rVV5	1030	2150	0.31%	0.052%
74	11.859	1765	1767	1771	rBV2	213	264	0.04%	0.006%
75	11.890	1771	1772	1773	rBV	261	111	0.02%	0.003%
76	11.939	1778	1780	1782	rVB2	319	198	0.03%	0.005%

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 Title : VOC Analysis

77	11.987	1783	1788	1789	rVV2	1402	1913	0.27%	0.046%
78	12.024	1789	1794	1808	rVB	517357	668133	95.41%	16.173%
79	12.225	1825	1827	1830	rBV3	850	836	0.12%	0.020%
80	12.280	1835	1836	1837	rBV	247	160	0.02%	0.004%
81	12.323	1837	1843	1851	rBV	218226	292205	41.73%	7.073%
82	12.567	1881	1883	1884	rBV	216	146	0.02%	0.004%
83	12.762	1911	1915	1919	rBV3	640	978	0.14%	0.024%
84	12.871	1929	1933	1939	rBV	5051	7463	1.07%	0.181%
85	13.262	1996	1997	2000	rVB2	234	213	0.03%	0.005%
86	13.402	2016	2020	2024	rBV6	3642	5985	0.85%	0.145%
87	13.530	2040	2041	2044	rBV2	127	92	0.01%	0.002%
88	13.591	2049	2051	2056	rVB2	412	494	0.07%	0.012%
89	13.640	2057	2059	2061	rVB	269	165	0.02%	0.004%
90	13.682	2061	2066	2071	rBV4	2068	3080	0.44%	0.075%
91	13.780	2078	2082	2090	rBV	2092	3188	0.46%	0.077%
92	13.969	2110	2113	2115	rBV2	423	511	0.07%	0.012%
93	13.993	2115	2117	2120	rVV	284	189	0.03%	0.005%
94	14.018	2120	2121	2122	rBV	189	85	0.01%	0.002%
95	14.127	2135	2139	2144	rBV	1151	1529	0.22%	0.037%
96	14.213	2151	2153	2154	rBV2	227	192	0.03%	0.005%
97	14.426	2185	2188	2197	rVB2	3108	4343	0.62%	0.105%

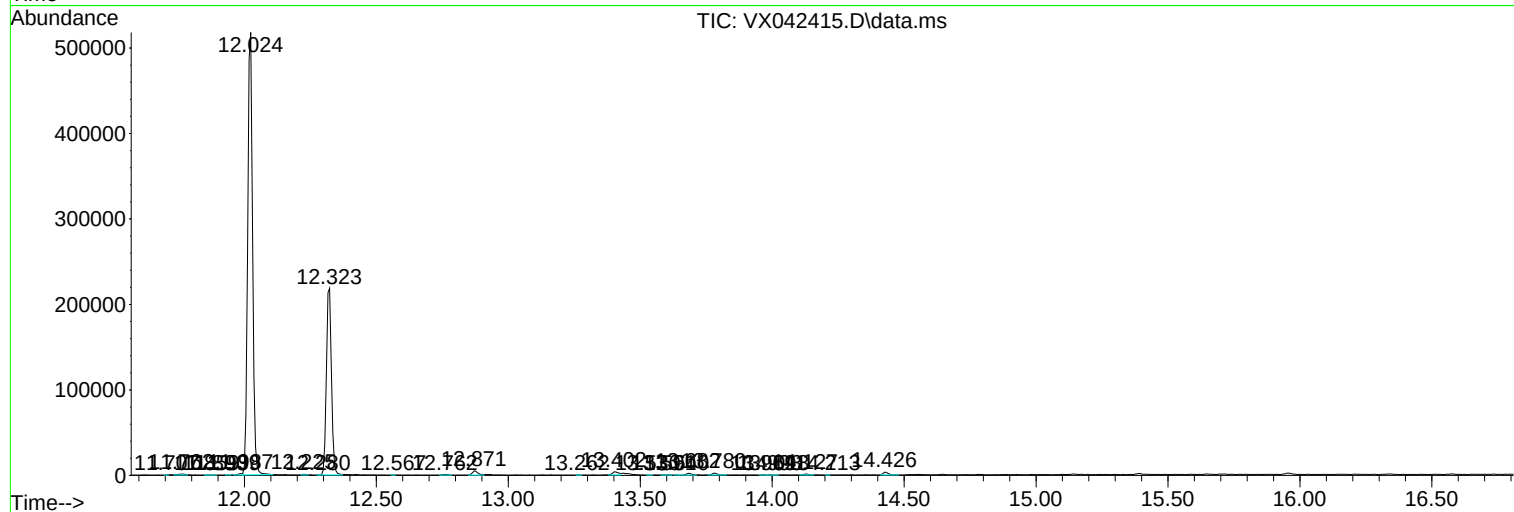
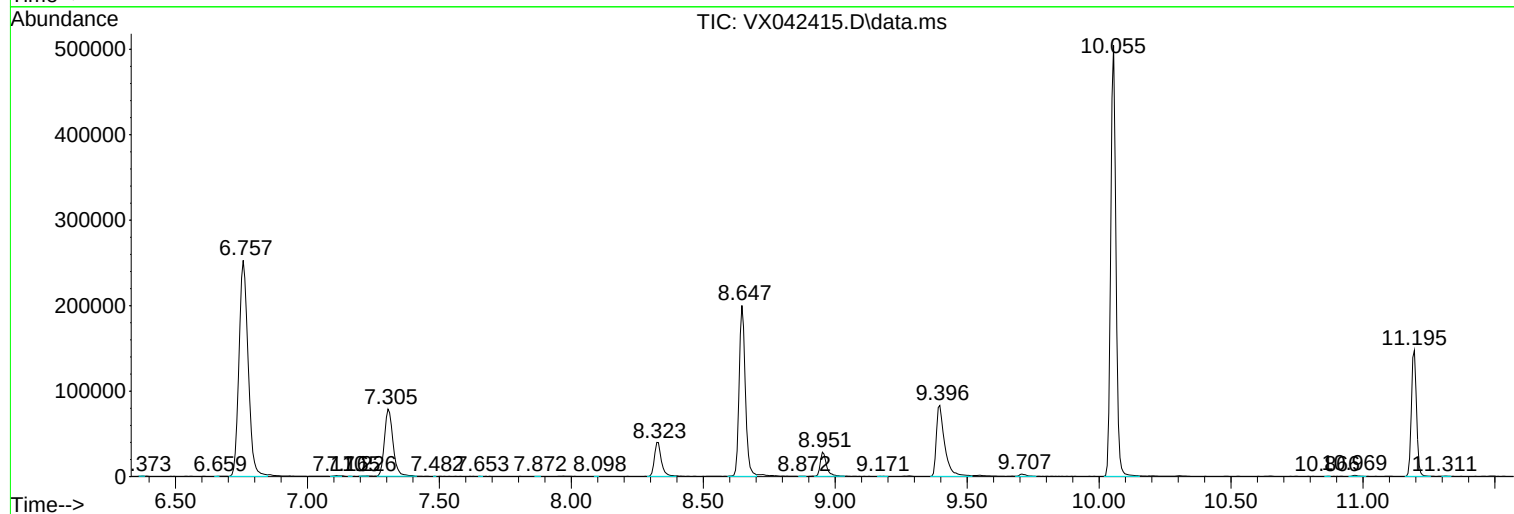
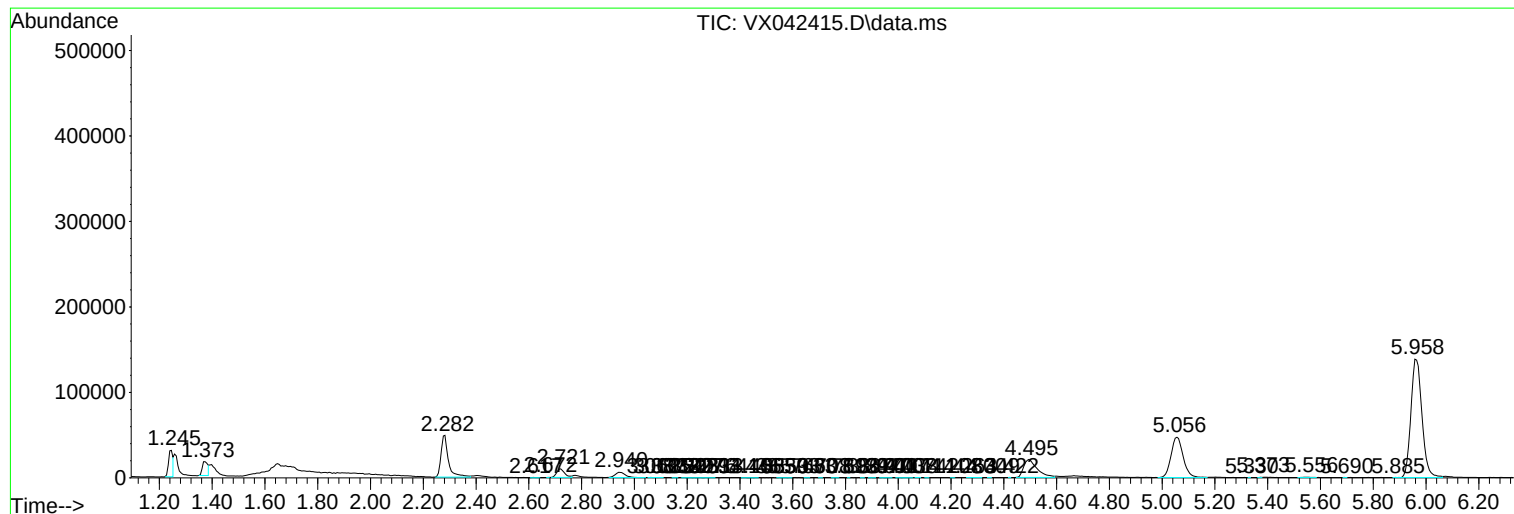
Sum of corrected areas: 4131038

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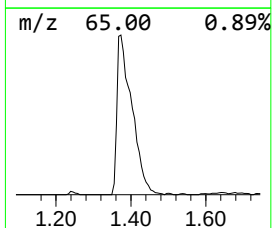
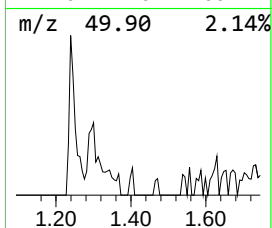
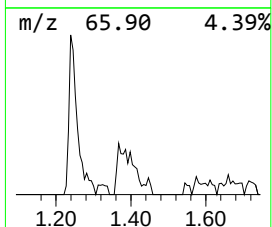
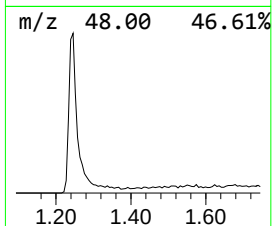
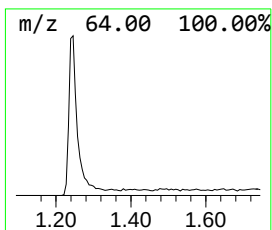
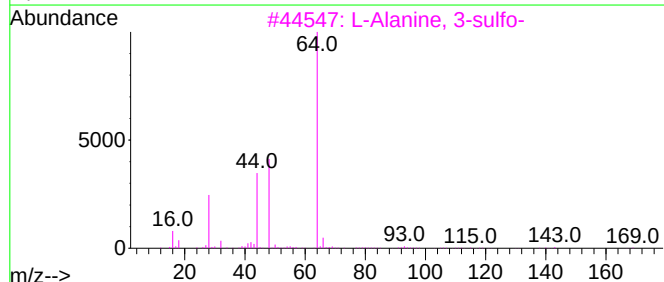
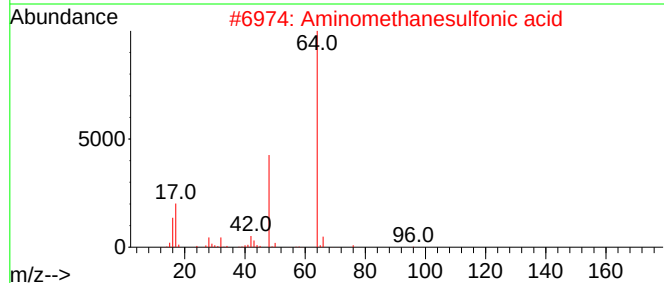
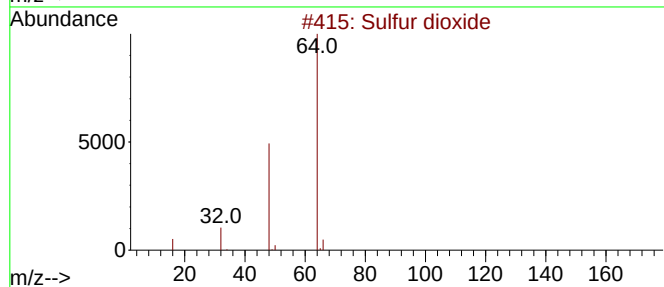
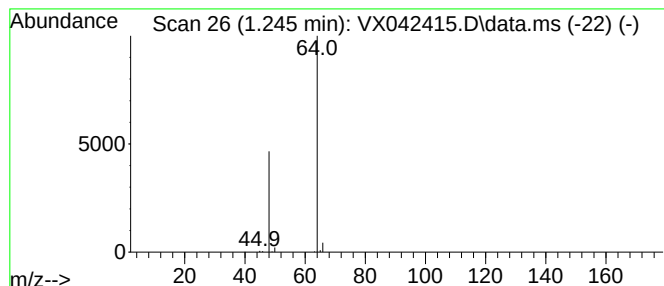
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.245	3.01 ug/L	36414	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			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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.245	3.0	ug/L	36414	1	6.757	604594	50.0