LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042422.D
Acq On : 19 Jul 2024 23:07
Operator : JC/MD
Sample : P3238-07ME
Misc : 5.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF0ME

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\SFAMXLM070324WMA.M
Title : VOC Analysis

Signal : TIC: VX042422.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	37	rBV	32964	47251	6.99%	0.885%
2	1.368	43	46	58	rVB	66049	83854	12.40%	1.570%
3	1.648	89	92	102	rVB	45023	54028	7.99%	1.012%
4	2.184	179	180	181	rVB	332	121	0.02%	0.002%
5	2.300	192	199	211	rBV	130270	204157	30.19%	3.822%
6	2.495	229	231	233	rBV	329	272	0.04%	0.005%
7	2.611	248	250	254	rBV	180	148	0.02%	0.003%
8	2.788	275	279	286	rVB2	954	1686	0.25%	0.032%
9	2.867	288	292	293	rBV	134	156	0.02%	0.003%
10	2.947	297	305	315	rVB	3023	7264	1.07%	0.136%
11	3.081	325	327	329	rBV	195	130	0.02%	0.002%
12	3.123	332	334	337	rVV2	186	204	0.03%	0.004%
13	3.172	341	342	345	rVB	243	166	0.02%	0.003%
14	3.306	362	364	367	rVB2	137	134	0.02%	0.003%
15	3.337	367	369	372	rBV2	118	148	0.02%	0.003%
16	3.544	402	403	406	rBV	209	150	0.02%	0.003%
17	3.678	424	425	428	rBV	131	129	0.02%	0.002%
18	3.928	463	466	467	rBV	166	127	0.02%	0.002%
19	4.080	489	491	494	rVB2	130	123	0.02%	0.002%
20	4.117	494	497	499	rBV2	147	144	0.02%	0.003%
21	4.465	546	554	574	rBV	51777	154280	22.82%	2.889%
22	4.861	618	619	624	rBV	127	222	0.03%	0.004%
23	5.056	640	651	670	rBV	86160	264579	39.13%	4.954%
24	5.312	691	693	695	rBV2	145	164	0.02%	0.003%
25	5.403	703	708	712	rVB3	350	681	0.10%	0.013%
26	5.489	720	722	724	rVB	202	129	0.02%	0.002%
27	5.550	727	732	734	rBV3	345	386	0.06%	0.007%
28	5.696	754	756	757	rBV2	183	142	0.02%	0.003%
29	5.836	777	779	782	rVB	148	146	0.02%	0.003%
30	5.970	788	801	823	rBV2	228755	676173	100.00%	12.660%
31	6.361	863	865	866	rBV	159	124	0.02%	0.002%
32	6.428	874	876	879	rVB2	114	117	0.02%	0.002%
33	6.452	879	880	882	rBV2	123	117	0.02%	0.002%
34	6.556	895	897	901	rBV2	334	424	0.06%	0.008%
35	6.610	903	906	907	rBV2	117	124	0.02%	0.002%
36	6.763	921	931	945	rBV	212622	523648	77.44%	9.804%

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Sample : P3238-07ME
Misc : 5.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF0ME

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\SFAMXLM070324WMA.M
Title : VOC Analysis

37	7.013	970	972	973	rBV	140	134	0.02%	0.003%
38	7.068	979	981	984	rVB2	214	185	0.03%	0.003%
39	7.110	984	988	989	rBV2	1316	1290	0.19%	0.024%
40	7.208	1000	1004	1005	rBV2	363	358	0.05%	0.007%
41	7.305	1012	1020	1037	rBV	137223	303035	44.82%	5.674%
42	7.494	1050	1051	1054	rVB	317	185	0.03%	0.003%
43	7.592	1065	1067	1070	rBV	100	126	0.02%	0.002%
44	7.787	1096	1099	1100	rBV	198	152	0.02%	0.003%
45	7.958	1124	1127	1132	rVB4	471	752	0.11%	0.014%
46	8.000	1132	1134	1139	rVB3	210	219	0.03%	0.004%
47	8.068	1143	1145	1148	rBV2	161	133	0.02%	0.002%
48	8.104	1149	1151	1154	rVB2	121	112	0.02%	0.002%
49	8.324	1181	1187	1202	rVV	73441	126805	18.75%	2.374%
50	8.519	1215	1219	1223	rBV4	396	723	0.11%	0.014%
51	8.647	1234	1240	1257	rBV	333076	523346	77.40%	9.798%
52	8.952	1285	1290	1307	rBV	53408	82198	12.16%	1.539%
53	9.110	1313	1316	1318	rVV	164	147	0.02%	0.003%
54	9.183	1326	1328	1331	rBV	195	159	0.02%	0.003%
55	9.214	1331	1333	1336	rVB	234	164	0.02%	0.003%
56	9.275	1338	1343	1347	rBV3	1800	2748	0.41%	0.051%
57	9.384	1356	1361	1376	rBV	222844	335673	49.64%	6.285%
58	9.707	1410	1414	1418	rVB3	1352	2115	0.31%	0.040%
59	9.738	1418	1419	1425	rVB2	237	284	0.04%	0.005%
60	9.817	1428	1432	1433	rBV	224	215	0.03%	0.004%
61	9.951	1453	1454	1457	rBV	175	197	0.03%	0.004%
62	10.055	1465	1471	1486	rBV	426176	595702	88.10%	11.153%
63	10.317	1508	1514	1516	rBV3	453	638	0.09%	0.012%
64	10.488	1539	1542	1544	rBV2	174	181	0.03%	0.003%
65	10.512	1544	1546	1548	rVV	185	125	0.02%	0.002%
66	10.573	1554	1556	1559	rBV2	205	231	0.03%	0.004%
67	10.646	1566	1568	1570	rBV2	257	195	0.03%	0.004%
68	10.738	1580	1583	1586	rBV2	173	279	0.04%	0.005%
69	10.762	1586	1587	1591	rVV2	172	197	0.03%	0.004%
70	10.908	1610	1611	1613	rVB	308	147	0.02%	0.003%
71	10.945	1613	1617	1618	rBV	132	130	0.02%	0.002%
72	10.963	1618	1620	1622	rVV2	241	191	0.03%	0.004%
73	11.006	1625	1627	1628	rBV	257	176	0.03%	0.003%
74	11.189	1652	1657	1675	rBV	272062	357740	52.91%	6.698%
75	11.323	1677	1679	1681	rVB	283	187	0.03%	0.004%
76	11.634	1727	1730	1734	rBV	317	405	0.06%	0.008%

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Sample : P3238-07ME
Misc : 5.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF0ME

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\SFAMXLM070324WMA.M
Title : VOC Analysis

77	11.756	1748	1750	1752	rBB2	163	118	0.02%	0.002%
78	11.963	1782	1784	1788	rBV2	159	213	0.03%	0.004%
79	12.024	1788	1794	1802	rBV	397823	521622	77.14%	9.766%
80	12.207	1822	1824	1826	rVB	240	146	0.02%	0.003%
81	12.317	1837	1842	1855	rBV	349950	454447	67.21%	8.508%
82	12.603	1887	1889	1892	rBV2	171	160	0.02%	0.003%
83	12.670	1898	1900	1905	rBV	185	261	0.04%	0.005%
84	12.762	1911	1915	1919	rVB3	353	468	0.07%	0.009%
85	12.829	1923	1926	1931	rVB2	133	232	0.03%	0.004%
86	12.884	1933	1935	1938	rVB	252	197	0.03%	0.004%
87	13.176	1982	1983	1985	rBV	144	113	0.02%	0.002%
88	13.432	2024	2025	2028	rBV	196	140	0.02%	0.003%
89	13.457	2028	2029	2032	rVV	229	148	0.02%	0.003%
90	13.536	2040	2042	2043	rVB2	255	121	0.02%	0.002%
91	13.621	2053	2056	2057	rBV2	209	198	0.03%	0.004%
92	13.688	2065	2067	2068	rBV	168	112	0.02%	0.002%
93	13.774	2079	2081	2083	rBV2	134	185	0.03%	0.003%
94	13.884	2097	2099	2101	rBV2	171	176	0.03%	0.003%
95	14.012	2118	2120	2123	rVV2	235	176	0.03%	0.003%
96	14.036	2123	2124	2126	rVB2	167	120	0.02%	0.002%
97	14.127	2136	2139	2143	rBV2	775	1212	0.18%	0.023%
98	14.201	2148	2151	2154	rBV2	220	293	0.04%	0.005%
99	14.670	2226	2228	2229	rVB	268	135	0.02%	0.003%
100	15.609	2380	2382	2383	rBV2	507	296	0.04%	0.006%

Sum of corrected areas: 5341116

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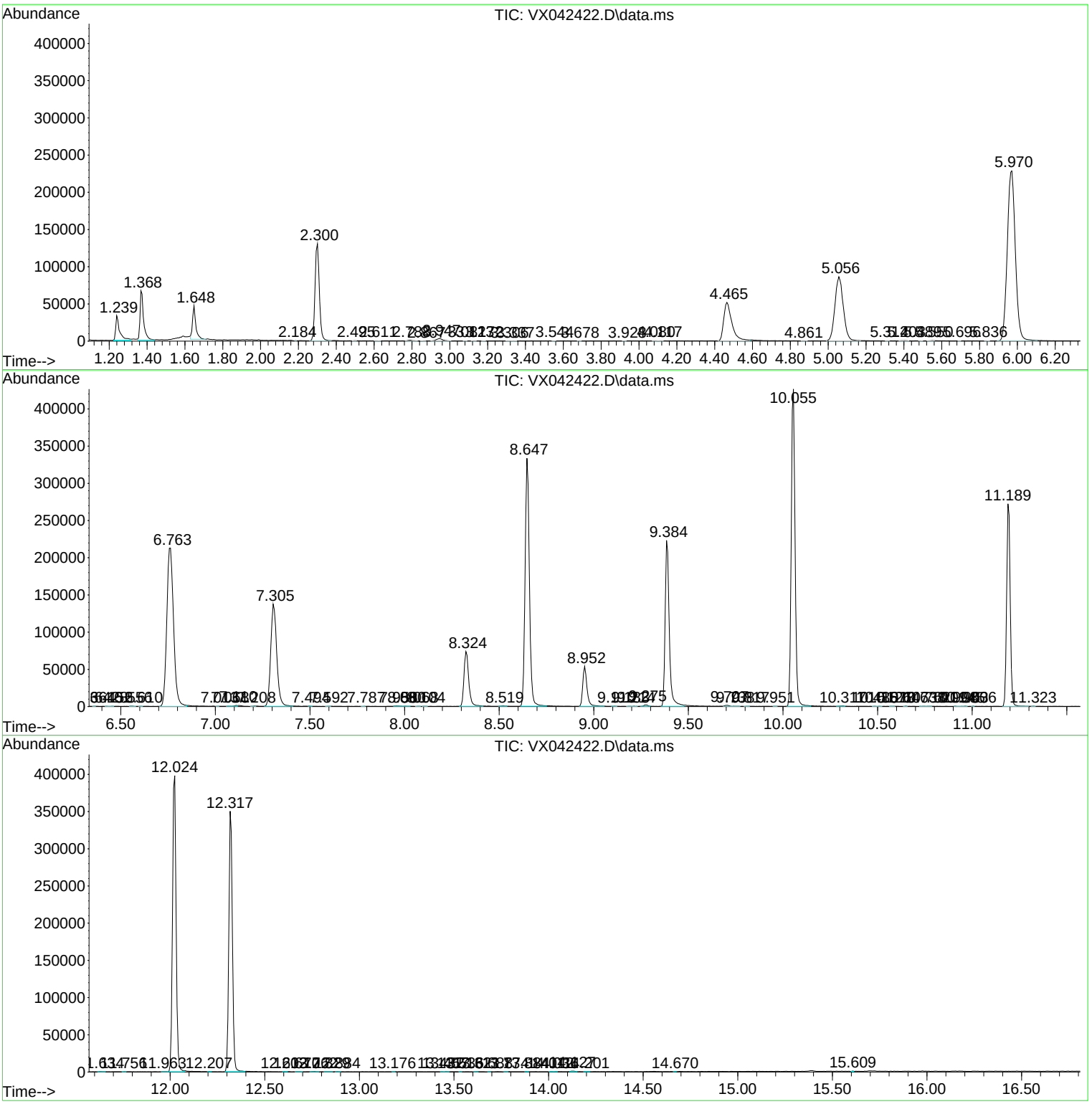
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF0ME

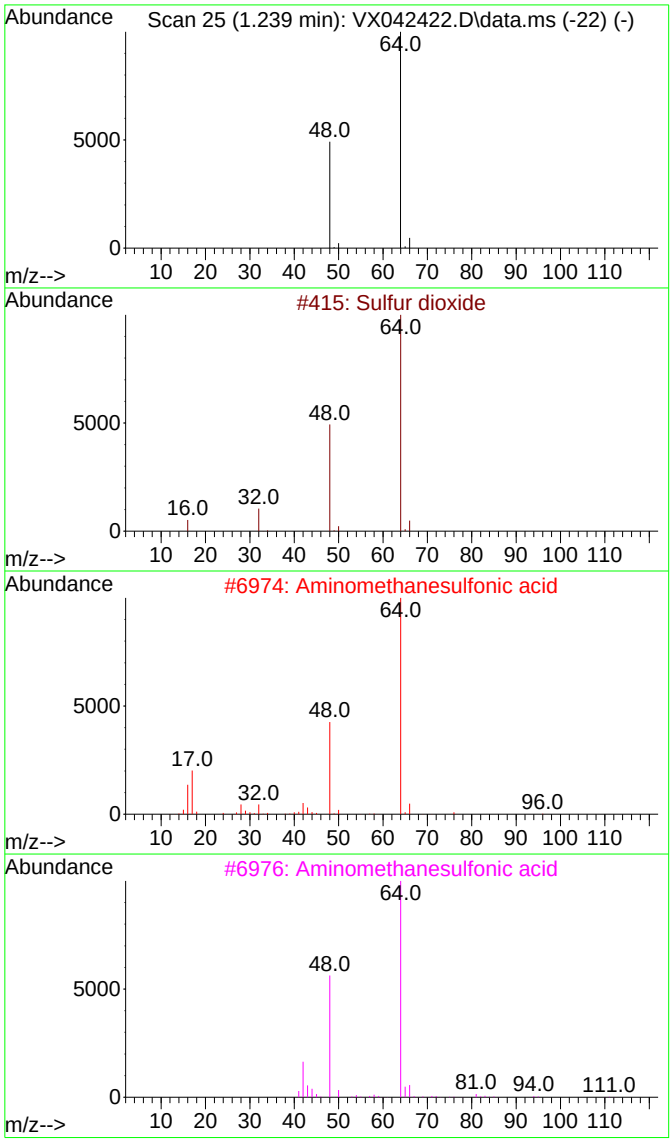
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

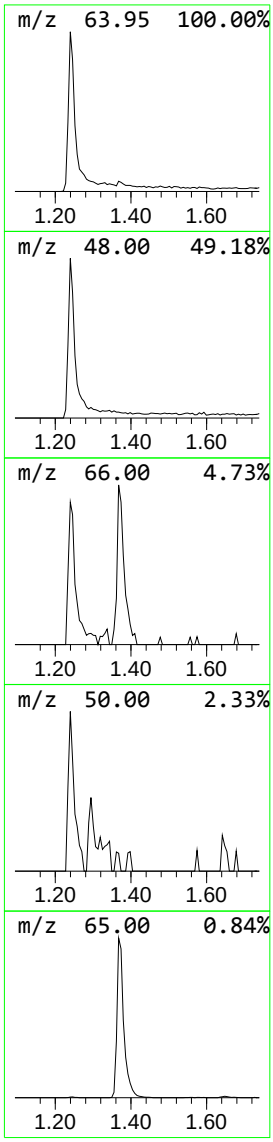
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	4.51 ug/L	47251	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.239	4.5	ug/L	47251	1	6.763	523648	50.0