LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042414.D
Acq On : 19 Jul 2024 20:01
Operator : JC/MD
Sample : P3238-17ME
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C04ME

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: VX042414.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	27	rBV	34047	37759	6.89%	0.891%
2	1.373	43	47	59	rBV	22042	52411	9.56%	1.237%
3	1.629	86	89	90	rBV	17771	19161	3.50%	0.452%
4	2.282	190	196	212	rBV	80257	143236	26.13%	3.380%
5	2.648	254	256	259	rBV3	247	247	0.05%	0.006%
6	2.721	259	268	274	rBV	15361	31384	5.73%	0.741%
7	2.946	297	305	316	rBV	6592	16737	3.05%	0.395%
8	3.050	320	322	323	rBV2	186	129	0.02%	0.003%
9	3.068	323	325	329	rBV2	187	165	0.03%	0.004%
10	3.147	337	338	341	rVB2	121	114	0.02%	0.003%
11	3.172	341	342	345	rVB	127	119	0.02%	0.003%
12	3.202	345	347	349	rBV2	193	214	0.04%	0.005%
13	3.336	362	369	376	rBV4	506	1291	0.24%	0.030%
14	3.440	384	386	389	rVB	176	167	0.03%	0.004%
15	3.477	389	392	398	rVB2	95	168	0.03%	0.004%
16	3.580	403	409	410	rBV2	197	305	0.06%	0.007%
17	3.714	427	431	434	rBV2	159	233	0.04%	0.005%
18	3.885	456	459	460	rBV2	156	134	0.02%	0.003%
19	4.159	502	504	507	rVV2	135	129	0.02%	0.003%
20	4.275	522	523	526	rBV2	123	129	0.02%	0.003%
21	4.373	538	539	541	rBV	156	114	0.02%	0.003%
22	4.489	550	558	578	rBV	25675	94745	17.29%	2.236%
23	5.056	640	651	672	rBV	59478	183212	33.43%	4.323%
24	5.281	686	688	690	rBV	153	121	0.02%	0.003%
25	5.391	704	706	707	rBV	321	188	0.03%	0.004%
26	5.482	718	721	723	rVB2	124	158	0.03%	0.004%
27	5.537	727	730	731	rBV	332	330	0.06%	0.008%
28	5.647	745	748	751	rVB2	115	196	0.04%	0.005%
29	5.684	751	754	755	rBV2	120	127	0.02%	0.003%
30	5.714	757	759	762	rBV2	155	185	0.03%	0.004%
31	5.964	789	800	822	rBV2	172033	493211	89.99%	11.638%
32	6.202	838	839	841	rBV	343	165	0.03%	0.004%
33	6.251	845	847	850	rVB2	206	196	0.04%	0.005%
34	6.537	892	894	895	rBV	184	109	0.02%	0.003%
35	6.555	895	897	899	rVB2	169	135	0.02%	0.003%
36	6.757	920	930	953	rBV	194533	473781	86.44%	11.180%

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Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C04ME

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	7.110	984	988	990	rBV3	731	1006	0.18%	0.024%
38	7.214	1001	1005	1007	rBV3	614	826	0.15%	0.019%
39	7.305	1012	1020	1035	rBV	95813	215833	39.38%	5.093%
40	7.488	1048	1050	1051	rBV	320	194	0.04%	0.005%
41	7.610	1067	1070	1072	rBV2	142	205	0.04%	0.005%
42	7.708	1083	1086	1087	rBV2	123	136	0.02%	0.003%
43	7.744	1090	1092	1094	rBV2	157	161	0.03%	0.004%
44	7.988	1131	1132	1133	rBV	346	144	0.03%	0.003%
45	8.256	1173	1176	1177	rBV2	147	157	0.03%	0.004%
46	8.323	1182	1187	1200	rBV	50280	87962	16.05%	2.076%
47	8.482	1211	1213	1216	rBV2	188	137	0.02%	0.003%
48	8.512	1216	1218	1219	rBV	291	155	0.03%	0.004%
49	8.567	1225	1227	1230	rBV	163	184	0.03%	0.004%
50	8.646	1234	1240	1248	rBV	252073	396194	72.29%	9.349%
51	8.951	1285	1290	1306	rBV	36496	58478	10.67%	1.380%
52	9.171	1324	1326	1327	rVV	158	120	0.02%	0.003%
53	9.280	1339	1344	1350	rVB3	435	794	0.14%	0.019%
54	9.390	1357	1362	1379	rBV	106025	217764	39.73%	5.139%
55	9.707	1410	1414	1421	rVB	2242	3418	0.62%	0.081%
56	9.799	1427	1429	1431	rBV2	136	123	0.02%	0.003%
57	10.012	1462	1464	1465	rBV	143	115	0.02%	0.003%
58	10.055	1465	1471	1489	rBV	395776	548092	100.00%	12.933%
59	10.305	1509	1512	1520	rBV4	804	1468	0.27%	0.035%
60	10.469	1536	1539	1540	rBV	282	203	0.04%	0.005%
61	10.597	1556	1560	1561	rBV2	128	129	0.02%	0.003%
62	10.646	1566	1568	1571	rVB	423	429	0.08%	0.010%
63	10.744	1582	1584	1586	rBV	214	166	0.03%	0.004%
64	10.762	1586	1587	1590	rBV	164	149	0.03%	0.004%
65	10.805	1590	1594	1595	rBV2	195	176	0.03%	0.004%
66	10.829	1595	1598	1600	rVB3	203	208	0.04%	0.005%
67	10.878	1604	1606	1607	rBV	381	204	0.04%	0.005%
68	10.945	1614	1617	1619	rBV2	481	497	0.09%	0.012%
69	11.012	1626	1628	1630	rVB	215	158	0.03%	0.004%
70	11.091	1638	1641	1645	rBV2	167	222	0.04%	0.005%
71	11.195	1652	1658	1669	rBV	182412	244750	44.65%	5.775%
72	11.311	1674	1677	1680	rBV2	552	587	0.11%	0.014%
73	11.396	1687	1691	1692	rBV2	247	209	0.04%	0.005%
74	11.445	1697	1699	1700	rBV	191	147	0.03%	0.003%
75	11.518	1710	1711	1714	rVB	254	185	0.03%	0.004%
76	11.750	1746	1749	1752	rBV2	494	763	0.14%	0.018%

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Sample : P3238-17ME
Misc : 5.07g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : A4C04ME

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	11.835	1762	1763	1766	rVB2	225	155	0.03%	0.004%
78	11.871	1766	1769	1771	rVB2	141	155	0.03%	0.004%
79	11.896	1771	1773	1774	rBV	151	114	0.02%	0.003%
80	11.932	1776	1779	1782	rBV3	564	656	0.12%	0.015%
81	12.024	1788	1794	1807	rBB	400192	517049	94.34%	12.201%
82	12.231	1823	1828	1832	rBV4	1037	1424	0.26%	0.034%
83	12.323	1837	1843	1851	rBV	266788	355833	64.92%	8.397%
84	12.688	1902	1903	1905	rBV2	299	177	0.03%	0.004%
85	12.762	1911	1915	1919	rVB	1003	1443	0.26%	0.034%
86	12.877	1929	1934	1941	rVB2	2115	3692	0.67%	0.087%
87	12.932	1941	1943	1944	rBV	270	132	0.02%	0.003%
88	13.085	1966	1968	1970	rBV2	144	134	0.02%	0.003%
89	13.255	1995	1996	1997	rBV	214	104	0.02%	0.002%
90	13.383	2016	2017	2018	rBV	294	164	0.03%	0.004%
91	13.554	2043	2045	2046	rBV2	188	135	0.02%	0.003%
92	13.597	2049	2052	2057	rVV2	421	573	0.10%	0.014%
93	13.688	2062	2067	2074	rBV5	714	1676	0.31%	0.040%
94	13.786	2077	2083	2088	rVV4	1569	2973	0.54%	0.070%
95	14.042	2123	2125	2126	rBV	340	170	0.03%	0.004%
96	14.170	2144	2146	2148	rBV2	499	390	0.07%	0.009%
97	14.212	2151	2153	2155	rBV2	547	532	0.10%	0.013%
98	14.438	2185	2190	2192	rBV4	1110	1926	0.35%	0.045%
99	14.932	2268	2271	2275	rBV4	1762	2522	0.46%	0.060%
100	16.243	2481	2486	2490	rBV3	6134	11597	2.12%	0.274%

Sum of corrected areas: 4237779

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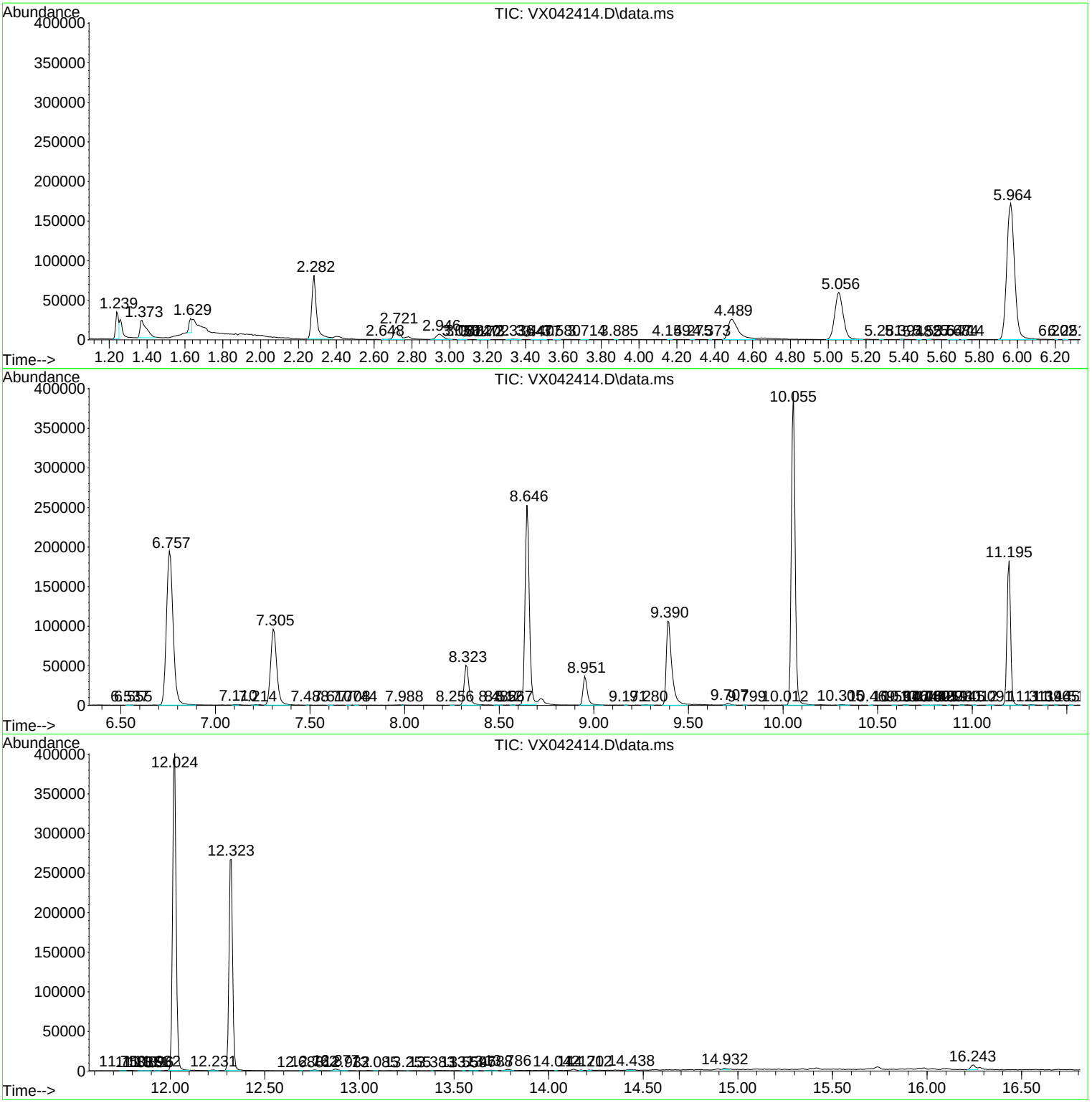
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C04ME

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 : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C04ME

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

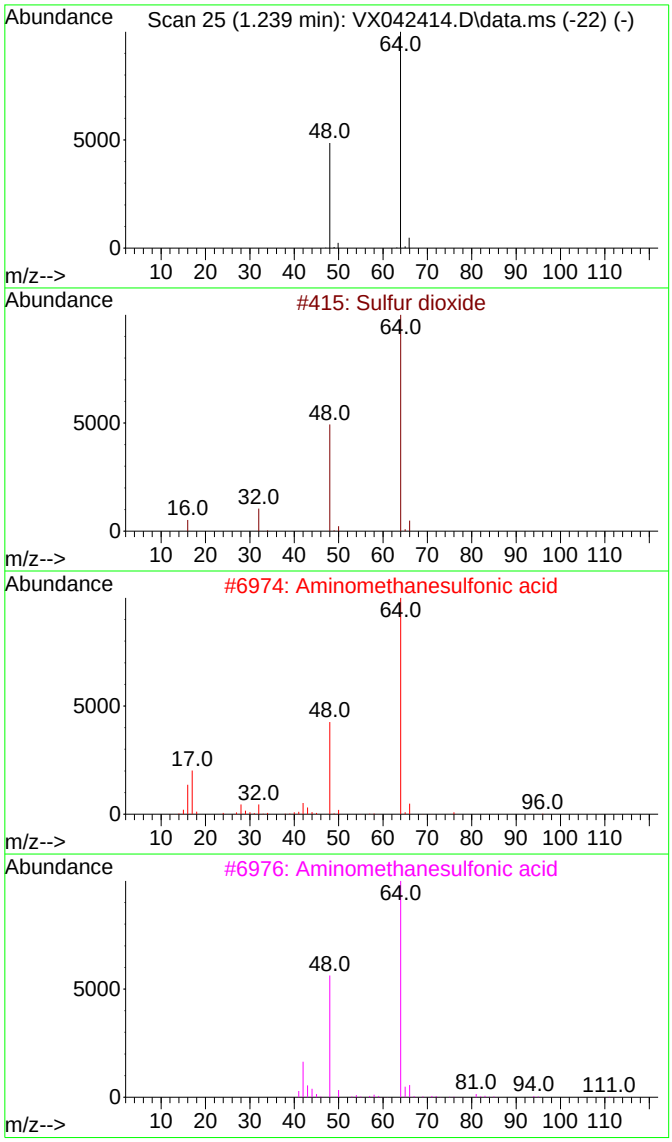
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

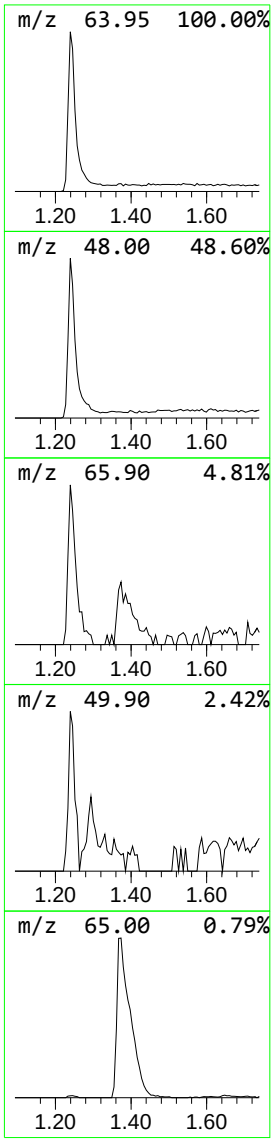
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	3.98 ug/L	37759	1,4-Difluorobenzene	6.757

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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Instrument :
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ClientSampleId :
A4C04ME

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	4.0	ug/L	37759	1	6.757	473781	50.0