LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042476.D
Acq On : 23 Jul 2024 16:53
Operator : JC/MD
Sample : P3264-16ME
Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : A4CM3ME

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: VX042476.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	27	rBV	26244	30732	4.75%	0.570%
2	1.368	43	46	63	rVB	22116	63781	9.86%	1.183%
3	1.642	86	91	106	rVB2	17802	62467	9.65%	1.158%
4	2.282	190	196	212	rBV	78387	149797	23.15%	2.777%
5	2.526	234	236	239	rBV3	254	307	0.05%	0.006%
6	2.617	249	251	254	rVB3	194	162	0.03%	0.003%
7	2.721	261	268	273	rBV	10347	20576	3.18%	0.381%
8	2.941	298	304	318	rVB	3667	10001	1.55%	0.185%
9	3.075	324	326	327	rBV	153	142	0.02%	0.003%
10	3.105	329	331	333	rBV	117	143	0.02%	0.003%
11	3.514	397	398	400	rBV	178	144	0.02%	0.003%
12	3.599	409	412	414	rBV2	113	121	0.02%	0.002%
13	4.489	550	558	575	rBV2	39099	136361	21.07%	2.528%
14	5.056	638	651	669	rBV	76783	246344	38.07%	4.567%
15	5.349	697	699	702	rVB	219	176	0.03%	0.003%
16	5.385	702	705	706	rBV2	352	410	0.06%	0.008%
17	5.544	724	731	732	rBV2	446	747	0.12%	0.014%
18	5.635	743	746	749	rBV2	133	168	0.03%	0.003%
19	5.733	758	762	763	rBV2	160	127	0.02%	0.002%
20	5.964	787	800	829	rBV2	222404	647119	100.00%	11.998%
21	6.416	871	874	878	rVV2	110	131	0.02%	0.002%
22	6.537	892	894	898	rVB2	170	181	0.03%	0.003%
23	6.623	904	908	911	rVV2	148	216	0.03%	0.004%
24	6.757	921	930	945	rBV	216637	531780	82.18%	9.860%
25	7.111	982	988	997	rVB8	1349	3584	0.55%	0.066%
26	7.220	1000	1006	1007	rBV3	625	778	0.12%	0.014%
27	7.306	1012	1020	1040	rVV	127018	289575	44.75%	5.369%
28	7.495	1047	1051	1053	rVB3	283	406	0.06%	0.008%
29	7.519	1053	1055	1056	rBV2	203	161	0.02%	0.003%
30	7.556	1059	1061	1065	rVB2	192	215	0.03%	0.004%
31	7.598	1065	1068	1072	rBV2	165	321	0.05%	0.006%
32	7.665	1076	1079	1081	rBV2	152	178	0.03%	0.003%
33	7.793	1095	1100	1101	rBV2	109	150	0.02%	0.003%
34	7.903	1116	1118	1121	rBV2	123	154	0.02%	0.003%
35	7.958	1121	1127	1129	rBV4	715	1195	0.18%	0.022%
36	8.141	1156	1157	1160	rBV	194	186	0.03%	0.003%

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Misc : 5.86g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM3ME

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	8.324	1181	1187	1204	rBV	68397	121010	18.70%	2.244%
38	8.513	1214	1218	1219	rBV3	448	646	0.10%	0.012%
39	8.647	1234	1240	1249	rBV	331700	511090	78.98%	9.476%
40	8.952	1285	1290	1302	rBV	50161	77206	11.93%	1.431%
41	9.104	1313	1315	1319	rVB2	313	332	0.05%	0.006%
42	9.135	1319	1320	1323	rBV	222	154	0.02%	0.003%
43	9.275	1338	1343	1351	rVB2	5347	7915	1.22%	0.147%
44	9.391	1357	1362	1384	rBV	158373	324767	50.19%	6.021%
45	9.708	1411	1414	1417	rBV2	882	994	0.15%	0.018%
46	9.933	1449	1451	1454	rBV2	111	141	0.02%	0.003%
47	10.055	1465	1471	1490	rBV	440609	623830	96.40%	11.566%
48	10.305	1509	1512	1515	rBV	734	885	0.14%	0.016%
49	10.366	1520	1522	1523	rBV	227	128	0.02%	0.002%
50	10.543	1549	1551	1556	rVV	126	153	0.02%	0.003%
51	10.653	1565	1569	1572	rVB3	261	328	0.05%	0.006%
52	10.848	1599	1601	1603	rBV2	192	160	0.02%	0.003%
53	10.970	1618	1621	1630	rVB3	778	1490	0.23%	0.028%
54	11.043	1630	1633	1634	rBV2	195	198	0.03%	0.004%
55	11.073	1634	1638	1640	rBV2	131	182	0.03%	0.003%
56	11.195	1652	1658	1668	rVV	257584	343467	53.08%	6.368%
57	11.311	1673	1677	1683	rVB3	447	918	0.14%	0.017%
58	11.402	1690	1692	1693	rBV	161	129	0.02%	0.002%
59	11.427	1693	1696	1697	rBV2	157	132	0.02%	0.002%
60	11.488	1703	1706	1712	rVB3	498	843	0.13%	0.016%
61	11.622	1726	1728	1730	rBV2	151	145	0.02%	0.003%
62	11.713	1742	1743	1746	rBV2	171	163	0.03%	0.003%
63	11.750	1746	1749	1754	rVV4	448	766	0.12%	0.014%
64	11.854	1764	1766	1770	rBV	225	229	0.04%	0.004%
65	11.939	1775	1780	1781	rBV2	234	285	0.04%	0.005%
66	11.982	1781	1787	1789	rBV3	1295	1921	0.30%	0.036%
67	12.024	1789	1794	1803	rVV	462868	594270	91.83%	11.018%
68	12.225	1824	1827	1833	rVB3	623	885	0.14%	0.016%
69	12.317	1837	1842	1856	rVV	367616	483592	74.73%	8.966%
70	12.597	1885	1888	1889	rVV2	157	123	0.02%	0.002%
71	12.664	1897	1899	1900	rBV	260	150	0.02%	0.003%
72	12.768	1911	1916	1924	rVB3	796	1486	0.23%	0.028%
73	12.872	1927	1933	1941	rBV2	5028	7913	1.22%	0.147%
74	13.158	1979	1980	1985	rVB2	288	285	0.04%	0.005%
75	13.213	1985	1989	1991	rBV2	206	297	0.05%	0.006%
76	13.250	1993	1995	1997	rBV2	180	222	0.03%	0.004%

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Sample : P3264-16ME
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM3ME

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

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Peak separation: 5

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

77	13.298	2000	2003	2005	rBV2	104	137	0.02%	0.003%
78	13.402	2016	2020	2023	rBV2	3013	3770	0.58%	0.070%
79	13.573	2046	2048	2050	rVB2	200	121	0.02%	0.002%
80	13.603	2050	2053	2054	rBV	235	270	0.04%	0.005%
81	13.683	2061	2066	2075	rBV	3875	5467	0.84%	0.101%
82	13.750	2075	2077	2078	rVV2	434	369	0.06%	0.007%
83	13.780	2079	2082	2090	rVV3	1902	3258	0.50%	0.060%
84	13.841	2090	2092	2094	rVB	139	140	0.02%	0.003%
85	14.006	2117	2119	2126	rVB	217	399	0.06%	0.007%
86	14.060	2126	2128	2130	rBV	172	160	0.02%	0.003%
87	14.128	2133	2139	2143	rBV2	2466	3411	0.53%	0.063%
88	14.170	2143	2146	2149	rVB	1240	1416	0.22%	0.026%
89	14.347	2173	2175	2177	rBV	163	135	0.02%	0.003%
90	14.371	2177	2179	2182	rVV3	187	274	0.04%	0.005%
91	14.426	2184	2188	2198	rVB	8242	11390	1.76%	0.211%
92	14.646	2221	2224	2230	rBV4	623	1069	0.17%	0.020%
93	14.884	2258	2263	2267	rBV	7517	8933	1.38%	0.166%
94	14.944	2270	2273	2279	rVB4	2787	3806	0.59%	0.071%
95	15.140	2301	2305	2314	rVB	6454	8499	1.31%	0.158%
96	15.390	2342	2346	2351	rVB3	2576	3898	0.60%	0.072%
97	15.646	2385	2388	2391	rVB4	2338	2720	0.42%	0.050%
98	15.956	2435	2439	2448	rVB	7089	11163	1.73%	0.207%
99	16.572	2536	2540	2545	rVB2	5864	8874	1.37%	0.165%
100	16.676	2552	2557	2563	rBV6	2748	4984	0.77%	0.092%

Sum of corrected areas: 5393529

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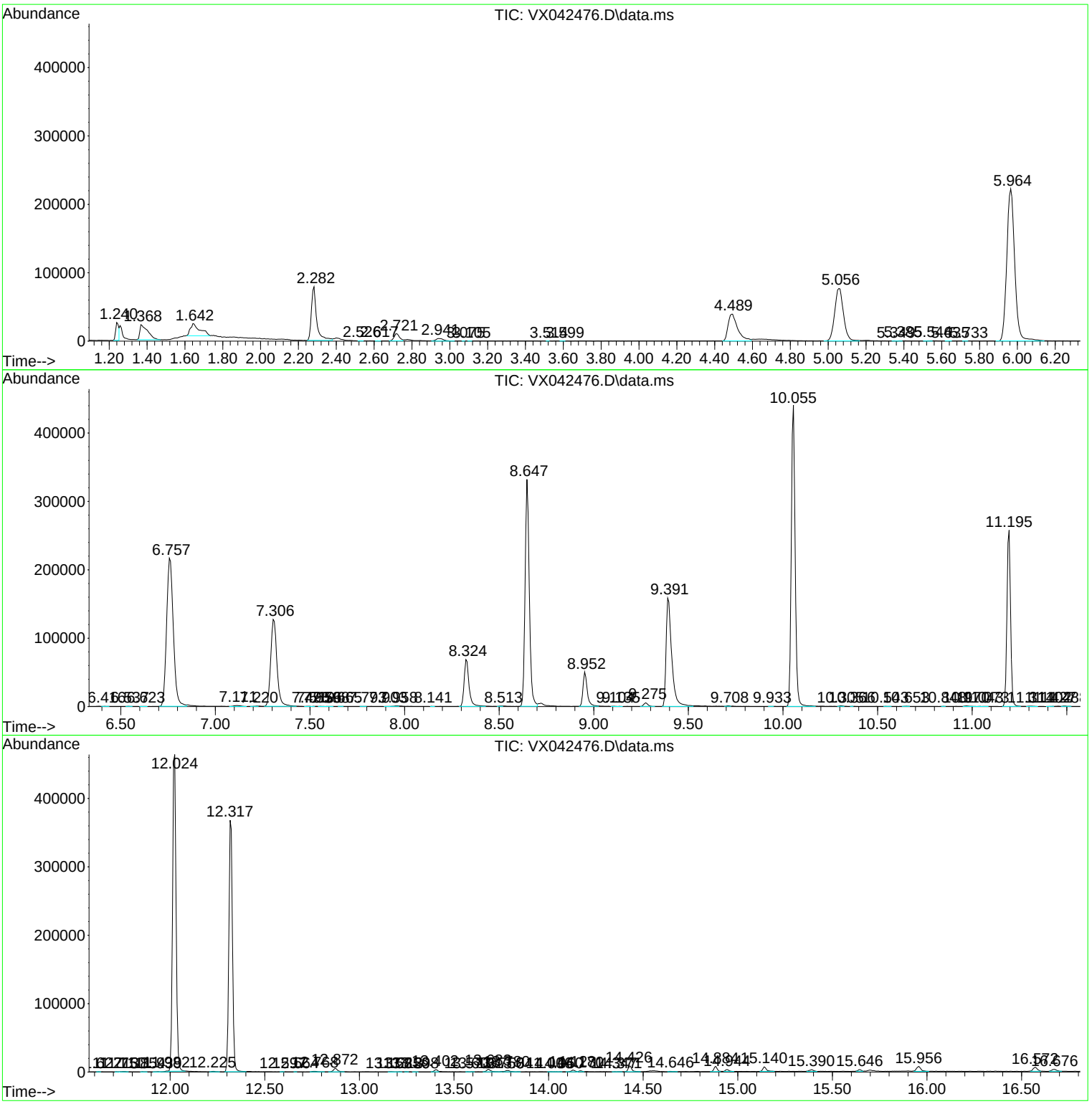
Instrument :
MSVOA_X
ClientSampleId :
A4CM3ME

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 : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM3ME

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

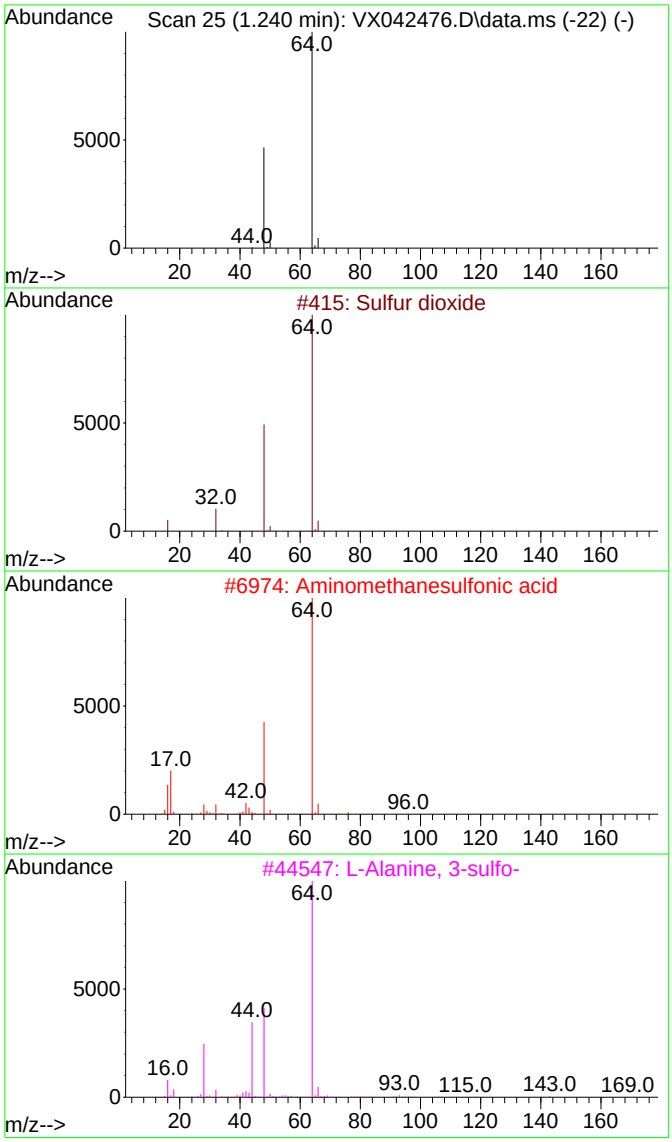
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

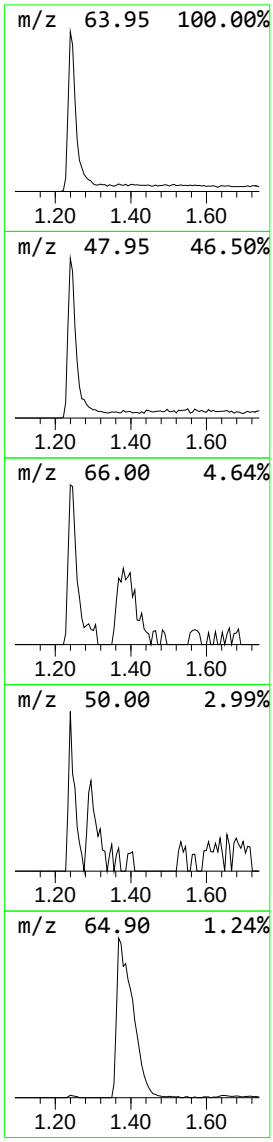
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	2.89 ug/L	30732	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	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
A4CM3ME

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	1.240	2.9	ug/L	30732	1	6.757	531780	50.0