LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042475.D
Acq On : 23 Jul 2024 16:30
Operator : JC/MD
Sample : P3264-15ME
Misc : 5.03g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM1ME

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: VX042475.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	23285	29216	4.59%	0.554%
2	2.270	189	194	211	rBV	73195	138543	21.75%	2.629%
3	2.721	261	268	286	rBV	22381	55406	8.70%	1.051%
4	3.129	333	335	336	rBV2	109	103	0.02%	0.002%
5	3.172	338	342	344	rVB2	129	184	0.03%	0.003%
6	3.294	360	362	363	rBV	200	106	0.02%	0.002%
7	3.337	367	369	373	rVB2	165	202	0.03%	0.004%
8	3.410	378	381	388	rVB4	258	443	0.07%	0.008%
9	3.587	406	410	411	rBV2	489	467	0.07%	0.009%
10	3.849	446	453	462	rVB3	1304	3492	0.55%	0.066%
11	3.977	471	474	476	rBV2	97	127	0.02%	0.002%
12	4.154	501	503	508	rVB	155	159	0.02%	0.003%
13	4.391	540	542	544	rVB2	151	110	0.02%	0.002%
14	4.416	544	546	548	rBV	326	247	0.04%	0.005%
15	4.495	551	559	581	rBV	35661	132613	20.82%	2.517%
16	5.056	639	651	666	rBV2	76146	241948	37.98%	4.592%
17	5.318	691	694	695	rBV2	155	144	0.02%	0.003%
18	5.385	701	705	711	rBV4	291	607	0.10%	0.012%
19	5.525	726	728	729	rBV	156	97	0.02%	0.002%
20	5.544	729	731	733	rBV	356	392	0.06%	0.007%
21	5.763	765	767	769	rBV2	125	147	0.02%	0.003%
22	5.964	789	800	817	rBV2	221823	631632	99.16%	11.987%
23	6.391	866	870	871	rBV2	348	528	0.08%	0.010%
24	6.604	904	905	911	rVB2	174	206	0.03%	0.004%
25	6.665	911	915	916	rBV	321	361	0.06%	0.007%
26	6.757	921	930	955	rVV	223856	548839	86.16%	10.415%
27	7.117	984	989	994	rVB3	1048	2319	0.36%	0.044%
28	7.226	1002	1007	1012	rBV4	606	1345	0.21%	0.026%
29	7.306	1012	1020	1042	rVB	127865	287259	45.10%	5.451%
30	7.604	1068	1069	1071	rBV	180	135	0.02%	0.003%
31	7.659	1076	1078	1081	rVV	246	193	0.03%	0.004%
32	7.897	1115	1117	1118	rBV	141	94	0.01%	0.002%
33	7.976	1123	1130	1132	rBV4	838	1823	0.29%	0.035%
34	8.165	1158	1161	1162	rVB2	163	158	0.02%	0.003%
35	8.324	1182	1187	1203	rBV	66505	116374	18.27%	2.208%
36	8.464	1209	1210	1212	rBV2	246	128	0.02%	0.002%

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM1ME

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	8.513	1216	1218	1219	rBV	399	193	0.03%	0.004%
38	8.647	1234	1240	1250	rBV	313128	506552	79.52%	9.613%
39	8.909	1280	1283	1285	rBV3	1002	1048	0.16%	0.020%
40	8.952	1285	1290	1302	rVV	48510	75714	11.89%	1.437%
41	9.275	1338	1343	1349	rVB	5796	8880	1.39%	0.169%
42	9.397	1357	1363	1381	rBV	139352	320039	50.24%	6.073%
43	9.714	1410	1415	1421	rBV4	847	1628	0.26%	0.031%
44	9.775	1424	1425	1426	rBV	275	126	0.02%	0.002%
45	9.842	1434	1436	1437	rVB	203	103	0.02%	0.002%
46	9.860	1437	1439	1442	rBV2	173	170	0.03%	0.003%
47	10.055	1465	1471	1486	rBV	451132	636986	100.00%	12.088%
48	10.275	1505	1507	1508	rBV	194	153	0.02%	0.003%
49	10.305	1508	1512	1515	rBV4	718	1220	0.19%	0.023%
50	10.427	1530	1532	1533	rBV2	191	122	0.02%	0.002%
51	10.653	1563	1569	1571	rBV3	437	765	0.12%	0.015%
52	10.884	1602	1607	1617	rBV4	1442	3374	0.53%	0.064%
53	10.970	1617	1621	1628	rVB3	972	1717	0.27%	0.033%
54	11.061	1632	1636	1641	rBV3	527	812	0.13%	0.015%
55	11.195	1652	1658	1672	rBV	252482	338957	53.21%	6.432%
56	11.396	1689	1691	1692	rVB	239	123	0.02%	0.002%
57	11.439	1692	1698	1701	rBV4	2678	3711	0.58%	0.070%
58	11.482	1702	1705	1713	rVB2	3552	5508	0.86%	0.105%
59	11.628	1726	1729	1731	rBV2	215	251	0.04%	0.005%
60	11.683	1736	1738	1740	rBV	155	186	0.03%	0.004%
61	11.713	1740	1743	1744	rBV	387	334	0.05%	0.006%
62	11.744	1745	1748	1752	rBV3	878	1112	0.17%	0.021%
63	11.829	1760	1762	1763	rBV2	185	105	0.02%	0.002%
64	11.908	1773	1775	1776	rBV2	192	146	0.02%	0.003%
65	11.933	1776	1779	1785	rVV4	3451	5461	0.86%	0.104%
66	12.024	1789	1794	1808	rVB	486784	617969	97.01%	11.727%
67	12.219	1824	1826	1831	rVB3	450	575	0.09%	0.011%
68	12.262	1831	1833	1837	rBV2	189	166	0.03%	0.003%
69	12.323	1837	1843	1850	rBV	355951	477275	74.93%	9.057%
70	12.421	1857	1859	1865	rVB5	1182	1616	0.25%	0.031%
71	12.555	1879	1881	1883	rVB	226	153	0.02%	0.003%
72	12.579	1883	1885	1886	rBV2	198	141	0.02%	0.003%
73	12.677	1897	1901	1902	rBV	242	275	0.04%	0.005%
74	12.762	1912	1915	1921	rVB2	991	1471	0.23%	0.028%
75	12.823	1923	1925	1927	rVB2	173	101	0.02%	0.002%
76	12.859	1927	1931	1940	rBV4	5877	11486	1.80%	0.218%

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM1ME

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	13.067	1964	1965	1969	rBV	176	157	0.02%	0.003%
78	13.158	1977	1980	1984	rBV2	718	819	0.13%	0.016%
79	13.225	1987	1991	1994	rVB3	600	721	0.11%	0.014%
80	13.262	1994	1997	2001	rBV4	574	746	0.12%	0.014%
81	13.347	2010	2011	2014	rBV	153	137	0.02%	0.003%
82	13.402	2016	2020	2027	rVV	6932	8897	1.40%	0.169%
83	13.481	2031	2033	2039	rVB3	271	334	0.05%	0.006%
84	13.591	2049	2051	2056	rBV2	337	285	0.04%	0.005%
85	13.652	2059	2061	2062	rBV	304	161	0.03%	0.003%
86	13.689	2064	2067	2072	rVV3	1005	1416	0.22%	0.027%
87	13.731	2072	2074	2078	rVV2	756	671	0.11%	0.013%
88	13.786	2079	2083	2089	rVB3	1573	2575	0.40%	0.049%
89	13.890	2096	2100	2104	rBV4	3151	4557	0.72%	0.086%
90	13.939	2104	2108	2114	rVB4	1386	2589	0.41%	0.049%
91	13.993	2114	2117	2120	rBV2	714	824	0.13%	0.016%
92	14.036	2122	2124	2128	rVB	678	579	0.09%	0.011%
93	14.128	2135	2139	2145	rVB	2319	2978	0.47%	0.057%
94	14.426	2186	2188	2192	rBV2	723	821	0.13%	0.016%
95	14.457	2192	2193	2196	rVB2	1012	589	0.09%	0.011%
96	14.749	2240	2241	2244	rBV3	408	491	0.08%	0.009%
97	15.176	2307	2311	2319	rVB5	3282	5183	0.81%	0.098%
98	15.389	2343	2346	2354	rVB4	2446	4089	0.64%	0.078%
99	15.524	2364	2368	2371	rVB5	1588	2161	0.34%	0.041%
100	15.950	2435	2438	2448	rVB3	2729	4803	0.75%	0.091%

Sum of corrected areas: 5269454

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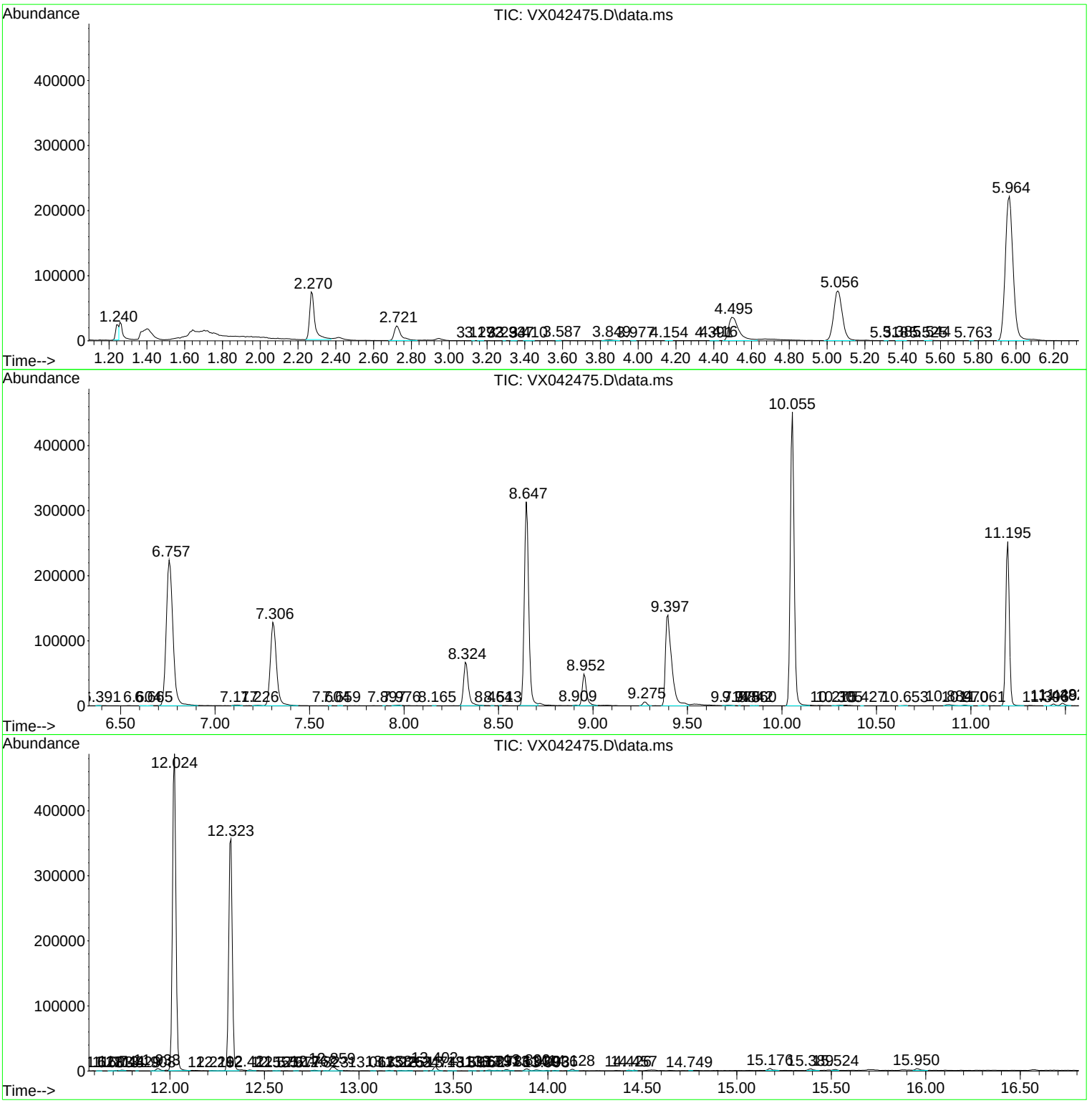
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM1ME

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 :
A4CM1ME

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

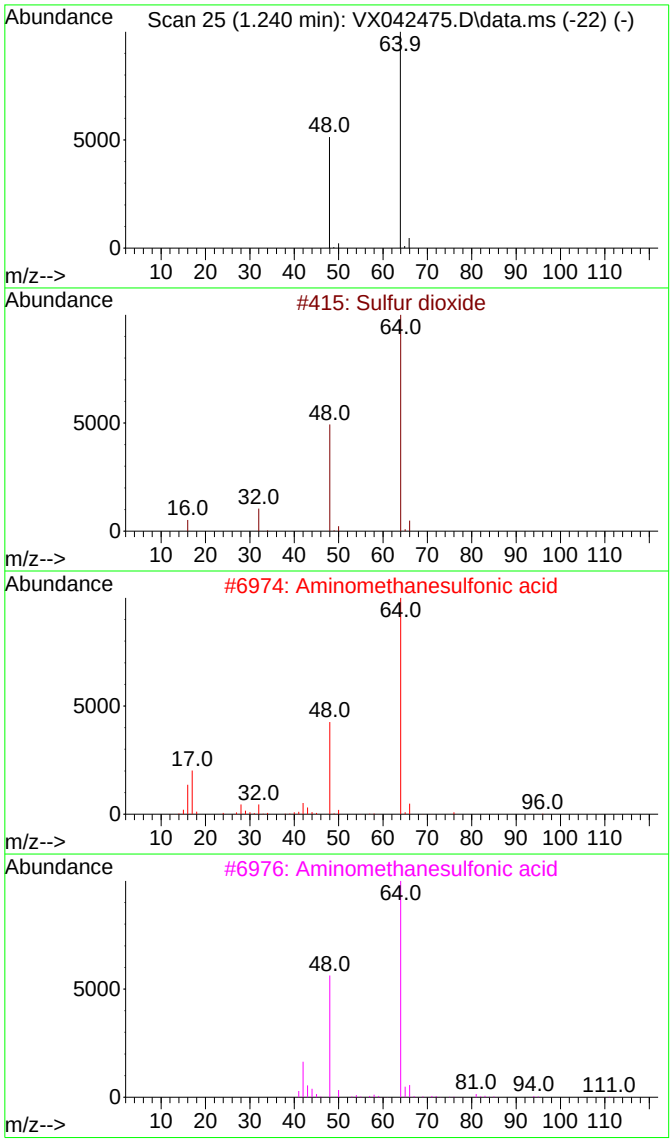
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

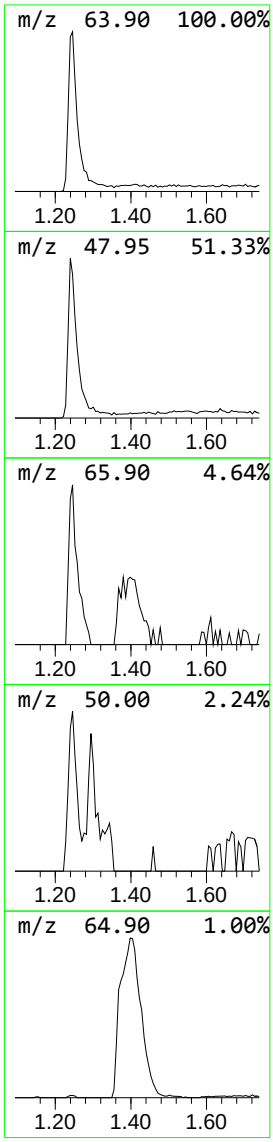
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	2.66 ug/L	29216	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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9





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	1.240	2.7	ug/L	29216	1	6.757	548839	50.0