LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042429.D
Acq On : 20 Jul 2024 01:48
Operator : JC/MD
Sample : P3313-01 100X
Misc : 6.39g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHJB8

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: VX042429.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	37	rBV2	23121	34725	5.09%	0.658%
2	1.368	43	46	57	rVB	56308	72445	10.61%	1.373%
3	1.648	88	92	103	rVB	46158	66910	9.80%	1.268%
4	2.294	192	198	210	rBV	128772	205945	30.16%	3.904%
5	2.441	220	222	225	rBV2	127	126	0.02%	0.002%
6	2.495	229	231	234	rBV3	233	272	0.04%	0.005%
7	2.569	238	243	244	rBV3	349	472	0.07%	0.009%
8	2.623	249	252	254	rBB2	103	121	0.02%	0.002%
9	2.666	257	259	262	rVB	216	202	0.03%	0.004%
10	2.709	262	266	267	rBV2	221	242	0.04%	0.005%
11	2.782	274	278	288	rVB3	2288	4802	0.70%	0.091%
12	2.940	297	304	314	rBV	10122	24855	3.64%	0.471%
13	3.062	322	324	327	rVB	185	173	0.03%	0.003%
14	3.136	334	336	339	rVB	139	147	0.02%	0.003%
15	3.349	368	371	372	rBV	153	113	0.02%	0.002%
16	3.532	400	401	403	rBV	152	114	0.02%	0.002%
17	3.959	470	471	475	rVB2	159	198	0.03%	0.004%
18	4.044	483	485	486	rBV	154	122	0.02%	0.002%
19	4.111	494	496	499	rVB2	157	168	0.02%	0.003%
20	4.245	517	518	521	rBV2	153	127	0.02%	0.002%
21	4.343	529	534	537	rBV2	146	200	0.03%	0.004%
22	4.379	537	540	545	rBV	170	306	0.04%	0.006%
23	4.465	545	554	570	rBV	49754	151177	22.14%	2.866%
24	4.849	615	617	619	rVB2	221	187	0.03%	0.004%
25	4.867	619	620	622	rBV	235	156	0.02%	0.003%
26	5.056	639	651	668	rBV	86303	266969	39.10%	5.060%
27	5.214	675	677	678	rVB2	319	201	0.03%	0.004%
28	5.294	688	690	692	rVB	141	124	0.02%	0.002%
29	5.367	700	702	704	rBV	136	155	0.02%	0.003%
30	5.483	720	721	725	rBV	130	149	0.02%	0.003%
31	5.562	731	734	736	rBV2	171	199	0.03%	0.004%
32	5.794	769	772	773	rBV	164	151	0.02%	0.003%
33	5.879	782	786	787	rBV2	149	180	0.03%	0.003%
34	5.964	789	800	819	rBV2	233360	682751	100.00%	12.942%
35	6.251	846	847	849	rBV2	135	110	0.02%	0.002%
36	6.379	864	868	872	rVB2	315	475	0.07%	0.009%

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Instrument : MSVOA_X
ClientSampleId : BHJB8

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

37	6.495	885	887	890	rVB2	121	113	0.02%	0.002%
38	6.757	921	930	952	rVV	203049	495009	72.50%	9.383%
39	7.110	982	988	996	rVB5	1194	3027	0.44%	0.057%
40	7.306	1012	1020	1036	rBV	137915	304737	44.63%	5.776%
41	7.470	1046	1047	1049	rBV2	238	177	0.03%	0.003%
42	7.592	1065	1067	1072	rVB	133	117	0.02%	0.002%
43	7.732	1088	1090	1091	rBV	257	154	0.02%	0.003%
44	7.873	1112	1113	1115	rBV	141	124	0.02%	0.002%
45	7.952	1123	1126	1127	rBV2	537	546	0.08%	0.010%
46	8.031	1136	1139	1142	rBV3	192	302	0.04%	0.006%
47	8.153	1157	1159	1162	rBV2	167	140	0.02%	0.003%
48	8.238	1171	1173	1176	rBV2	136	120	0.02%	0.002%
49	8.324	1181	1187	1203	rBV	74821	126287	18.50%	2.394%
50	8.525	1214	1220	1221	rBV3	306	533	0.08%	0.010%
51	8.647	1231	1240	1256	rBV	330664	529301	77.52%	10.033%
52	8.952	1285	1290	1303	rBV	51684	80714	11.82%	1.530%
53	9.147	1320	1322	1325	rVV2	196	210	0.03%	0.004%
54	9.183	1326	1328	1334	rVV2	198	300	0.04%	0.006%
55	9.348	1350	1355	1356	rBV	182	292	0.04%	0.006%
56	9.384	1356	1361	1381	rBV	216788	331759	48.59%	6.289%
57	9.701	1408	1413	1417	rBV2	2074	2934	0.43%	0.056%
58	9.762	1422	1423	1426	rBV	157	122	0.02%	0.002%
59	9.878	1440	1442	1445	rVV2	142	112	0.02%	0.002%
60	10.055	1465	1471	1485	rBV	402516	563662	82.56%	10.684%
61	10.195	1492	1494	1497	rVB3	376	388	0.06%	0.007%
62	10.281	1505	1508	1510	rBV2	193	182	0.03%	0.003%
63	10.311	1510	1513	1515	rBV2	399	517	0.08%	0.010%
64	10.646	1566	1568	1572	rVB2	150	150	0.02%	0.003%
65	10.713	1575	1579	1582	rBV	123	167	0.02%	0.003%
66	10.823	1595	1597	1599	rBB2	138	127	0.02%	0.002%
67	10.854	1599	1602	1604	rBV2	108	137	0.02%	0.003%
68	10.939	1614	1616	1618	rVB2	137	121	0.02%	0.002%
69	10.963	1618	1620	1622	rBV2	213	186	0.03%	0.004%
70	11.049	1630	1634	1635	rBV2	105	134	0.02%	0.003%
71	11.116	1642	1645	1649	rBV2	167	333	0.05%	0.006%
72	11.189	1652	1657	1668	rBV	278893	360122	52.75%	6.826%
73	11.287	1671	1673	1674	rBV2	241	228	0.03%	0.004%
74	11.348	1681	1683	1685	rVB2	166	161	0.02%	0.003%
75	11.366	1685	1686	1687	rBV	270	134	0.02%	0.003%
76	11.439	1697	1698	1700	rBV	209	141	0.02%	0.003%

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

77	11.469	1702	1703	1706	rBV	169	121	0.02%	0.002%
78	11.585	1719	1722	1725	rVB2	155	196	0.03%	0.004%
79	11.628	1727	1729	1735	rVB3	283	397	0.06%	0.008%
80	11.805	1756	1758	1761	rBV	150	204	0.03%	0.004%
81	11.933	1778	1779	1781	rBV	123	121	0.02%	0.002%
82	11.975	1784	1786	1788	rVB	161	124	0.02%	0.002%
83	12.018	1788	1793	1806	rBV	376223	493134	72.23%	9.348%
84	12.317	1837	1842	1855	rBV	351951	457291	66.98%	8.668%
85	12.652	1896	1897	1900	rBV	182	166	0.02%	0.003%
86	12.762	1909	1915	1919	rBV3	351	606	0.09%	0.011%
87	12.878	1931	1934	1935	rBV	184	163	0.02%	0.003%
88	13.012	1954	1956	1958	rBV2	131	120	0.02%	0.002%
89	13.256	1995	1996	1999	rBV	158	119	0.02%	0.002%
90	13.311	2003	2005	2006	rBV	204	185	0.03%	0.004%
91	13.640	2055	2059	2062	rVB	205	298	0.04%	0.006%
92	13.750	2076	2077	2080	rVB	136	128	0.02%	0.002%
93	13.786	2080	2083	2084	rBV	224	234	0.03%	0.004%
94	13.932	2105	2107	2108	rBV2	163	145	0.02%	0.003%
95	14.097	2132	2134	2136	rBV2	253	214	0.03%	0.004%
96	14.127	2136	2139	2143	rVV2	772	982	0.14%	0.019%
97	14.207	2150	2152	2154	rVB2	265	180	0.03%	0.003%
98	14.414	2185	2186	2188	rBV2	212	186	0.03%	0.004%
99	14.463	2192	2194	2196	rBV	219	185	0.03%	0.004%
100	14.664	2226	2227	2230	rBV3	293	261	0.04%	0.005%

Sum of corrected areas: 5275549

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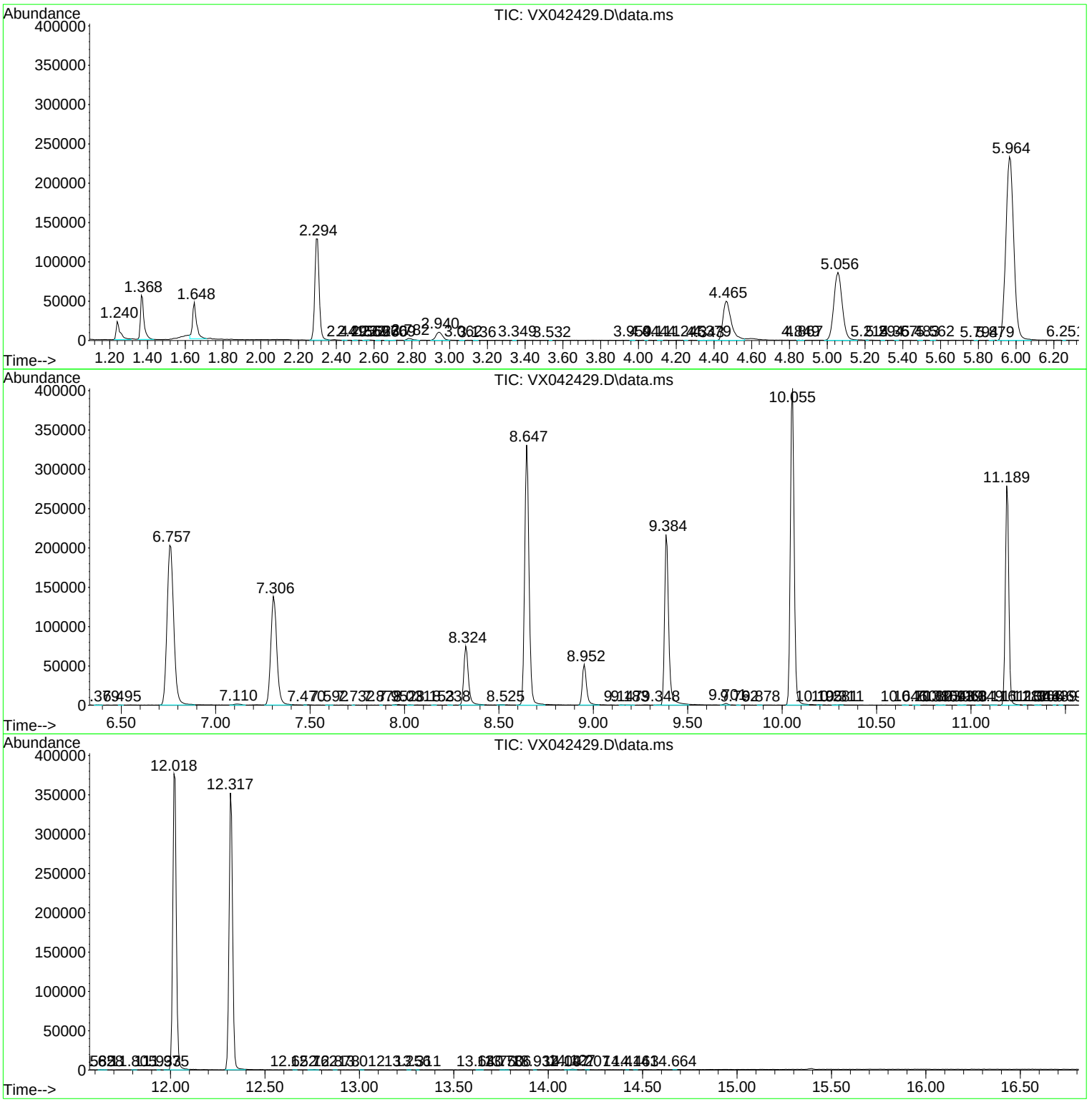
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
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BHJB8

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

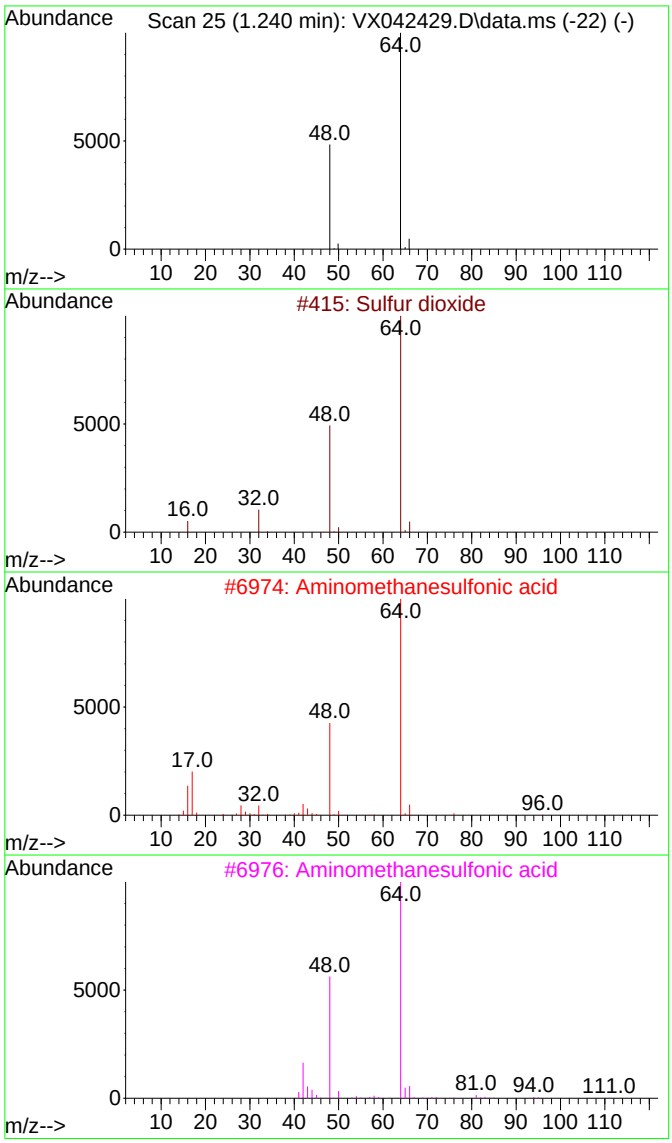
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

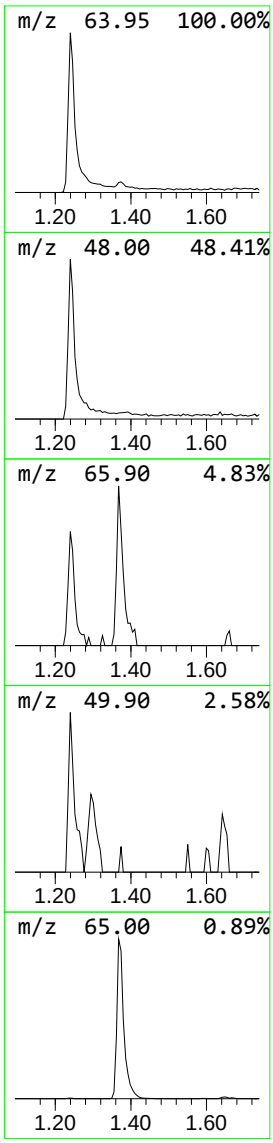
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.51 ug/L	34725	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	Sulfur dioxide	64	O2S	007446-09-5	5





Tentatively Identified Compound (LSC) summary

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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	3.5	ug/L	34725	1	6.763	495009	50.0