LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042477.D
Acq On : 23 Jul 2024 17:17
Operator : JC/MD
Sample : P3264-18ME
Misc : 5.89g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM6ME

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: VX042477.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	21	25	27	rBV	23476	27747	4.55%	0.540%
2	1.367	43	46	50	rBV	23898	42613	6.99%	0.830%
3	1.593	71	83	84	rBV5	4582	12390	2.03%	0.241%
4	1.648	86	92	96	rBV3	14275	30745	5.05%	0.599%
5	2.282	189	196	212	rBV	76766	149389	24.52%	2.909%
6	2.648	254	256	259	rBV	192	237	0.04%	0.005%
7	2.721	259	268	273	rVV	6856	13644	2.24%	0.266%
8	2.776	274	277	285	rVB3	1654	3307	0.54%	0.064%
9	2.946	297	305	315	rVV2	3258	7865	1.29%	0.153%
10	3.105	329	331	334	rVB2	190	237	0.04%	0.005%
11	4.489	549	558	576	rBV	32987	116891	19.19%	2.276%
12	4.910	625	627	630	rVB3	182	213	0.03%	0.004%
13	4.940	630	632	636	rVB2	170	232	0.04%	0.005%
14	5.056	639	651	668	rBV2	68881	215228	35.33%	4.191%
15	5.385	703	705	707	rBV2	252	270	0.04%	0.005%
16	5.409	707	709	714	rVB2	227	261	0.04%	0.005%
17	5.550	726	732	733	rBV3	227	349	0.06%	0.007%
18	5.964	790	800	814	rBV2	195697	563554	92.50%	10.974%
19	6.568	896	899	905	rVB2	136	193	0.03%	0.004%
20	6.757	921	930	946	rBV	190545	470725	77.26%	9.166%
21	7.110	983	988	997	rBV6	1122	2709	0.44%	0.053%
22	7.220	1000	1006	1012	rBV3	629	1368	0.22%	0.027%
23	7.305	1012	1020	1039	rBV	127604	290884	47.75%	5.664%
24	7.494	1045	1051	1052	rBV2	284	285	0.05%	0.006%
25	7.726	1086	1089	1090	rVV2	166	191	0.03%	0.004%
26	7.848	1106	1109	1112	rBV2	170	200	0.03%	0.004%
27	7.964	1123	1128	1129	rBV3	771	1205	0.20%	0.023%
28	8.324	1181	1187	1204	rBV	68764	122269	20.07%	2.381%
29	8.494	1212	1215	1216	rBV2	268	276	0.05%	0.005%
30	8.513	1216	1218	1220	rVV2	313	262	0.04%	0.005%
31	8.604	1229	1233	1234	rBV2	164	229	0.04%	0.004%
32	8.647	1234	1240	1250	rBV	329389	527384	86.56%	10.269%
33	8.951	1285	1290	1303	rBV	50456	80866	13.27%	1.575%
34	9.110	1313	1316	1317	rVB2	208	202	0.03%	0.004%
35	9.275	1339	1343	1351	rVB2	4771	7596	1.25%	0.148%
36	9.336	1351	1353	1357	rBV2	117	178	0.03%	0.003%

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Misc : 5.89g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : A4CM6ME

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	9.390	1357	1362	1383	rBV	167372	331671	54.44%	6.458%
38	9.622	1399	1400	1405	rVV2	283	269	0.04%	0.005%
39	9.714	1411	1415	1425	rVB5	1078	2660	0.44%	0.052%
40	9.787	1425	1427	1429	rBV2	343	342	0.06%	0.007%
41	10.006	1460	1463	1465	rVV2	162	184	0.03%	0.004%
42	10.055	1465	1471	1492	rVV	437274	609242	100.00%	11.863%
43	10.207	1494	1496	1500	rVV4	624	792	0.13%	0.015%
44	10.268	1504	1506	1508	rVB3	287	244	0.04%	0.005%
45	10.305	1508	1512	1518	rBV4	672	1402	0.23%	0.027%
46	10.396	1522	1527	1530	rBV2	201	320	0.05%	0.006%
47	10.646	1566	1568	1570	rBV3	400	386	0.06%	0.008%
48	10.805	1589	1594	1596	rBV2	152	241	0.04%	0.005%
49	10.969	1618	1621	1627	rVV3	861	1377	0.23%	0.027%
50	11.195	1652	1658	1672	rBV	273288	354470	58.18%	6.902%
51	11.305	1674	1676	1680	rVB3	359	495	0.08%	0.010%
52	11.457	1698	1701	1703	rBV2	298	365	0.06%	0.007%
53	11.488	1703	1706	1712	rVB2	466	776	0.13%	0.015%
54	11.634	1728	1730	1733	rBV2	153	230	0.04%	0.004%
55	11.725	1742	1745	1746	rBV2	152	168	0.03%	0.003%
56	11.750	1747	1749	1750	rBV2	299	172	0.03%	0.003%
57	11.890	1769	1772	1773	rBV2	155	172	0.03%	0.003%
58	11.981	1784	1787	1789	rBV3	1147	1449	0.24%	0.028%
59	12.024	1789	1794	1811	rVB	455356	578754	95.00%	11.270%
60	12.225	1823	1827	1835	rVB4	923	1633	0.27%	0.032%
61	12.323	1837	1843	1855	rBV	372005	498543	81.83%	9.708%
62	12.573	1882	1884	1888	rVB2	200	275	0.05%	0.005%
63	12.609	1888	1890	1892	rBV2	174	182	0.03%	0.004%
64	12.762	1911	1915	1919	rBV2	809	1181	0.19%	0.023%
65	12.872	1929	1933	1941	rVV2	4133	6118	1.00%	0.119%
66	13.030	1957	1959	1965	rVB3	238	310	0.05%	0.006%
67	13.079	1965	1967	1970	rVB2	162	188	0.03%	0.004%
68	13.115	1970	1973	1980	rBV2	227	503	0.08%	0.010%
69	13.402	2016	2020	2027	rVB3	3571	4838	0.79%	0.094%
70	13.499	2033	2036	2040	rVB2	146	249	0.04%	0.005%
71	13.597	2049	2052	2055	rBV3	243	247	0.04%	0.005%
72	13.658	2060	2062	2063	rBV	152	163	0.03%	0.003%
73	13.682	2063	2066	2071	rVB2	1077	1620	0.27%	0.032%
74	13.725	2071	2073	2075	rBV	292	210	0.03%	0.004%
75	13.780	2075	2082	2089	rVV3	1517	3162	0.52%	0.062%
76	13.829	2089	2090	2093	rVB	342	169	0.03%	0.003%

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CM6ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Title : VOC Analysis

77	13.926	2104	2106	2108	rBV2	173	170	0.03%	0.003%
78	13.969	2112	2113	2117	rVV2	273	228	0.04%	0.004%
79	14.133	2135	2140	2144	rBV	2392	3448	0.57%	0.067%
80	14.170	2144	2146	2150	rVB3	457	408	0.07%	0.008%
81	14.207	2150	2152	2154	rVB	192	184	0.03%	0.004%
82	14.426	2185	2188	2192	rBV4	1683	1949	0.32%	0.038%
83	14.493	2197	2199	2201	rVB	391	296	0.05%	0.006%
84	14.548	2201	2208	2209	rBV2	1843	3277	0.54%	0.064%
85	14.646	2221	2224	2228	rBV2	586	628	0.10%	0.012%
86	14.786	2246	2247	2250	rVV2	378	322	0.05%	0.006%
87	14.883	2259	2263	2266	rVB5	1359	1669	0.27%	0.032%
88	15.146	2302	2306	2309	rBV5	1122	1799	0.30%	0.035%
89	15.225	2317	2319	2321	rBV2	420	326	0.05%	0.006%
90	15.322	2333	2335	2336	rBV2	253	215	0.04%	0.004%
91	15.395	2342	2347	2352	rBV2	2658	4413	0.72%	0.086%
92	15.652	2385	2389	2391	rBV3	433	657	0.11%	0.013%
93	15.700	2393	2397	2407	rVB3	1741	4132	0.68%	0.080%
94	15.859	2421	2423	2424	rBV	588	397	0.07%	0.008%
95	15.956	2434	2439	2447	rBV4	2414	4296	0.71%	0.084%
96	16.176	2474	2475	2478	rBV3	335	413	0.07%	0.008%
97	16.566	2534	2539	2546	rBV3	2709	5180	0.85%	0.101%
98	16.615	2546	2547	2550	rVB2	448	290	0.05%	0.006%
99	16.664	2552	2555	2562	rVB6	1457	2642	0.43%	0.051%
100	16.724	2563	2565	2566	rBV	306	191	0.03%	0.004%

Sum of corrected areas: 5135496

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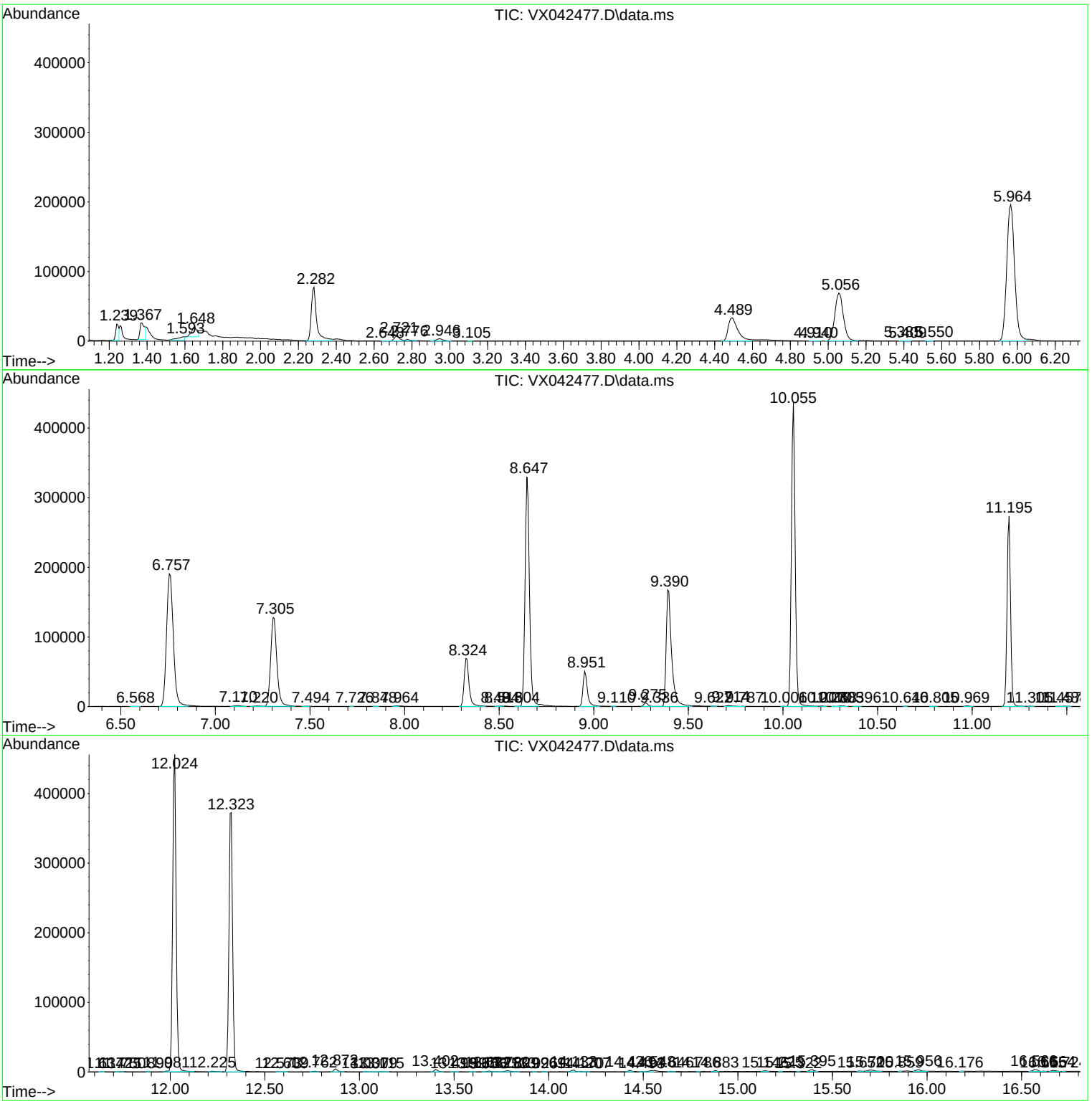
Instrument :
MSVOA_X
ClientSampleId :
A4CM6ME

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
ClientSampleId :
A4CM6ME

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

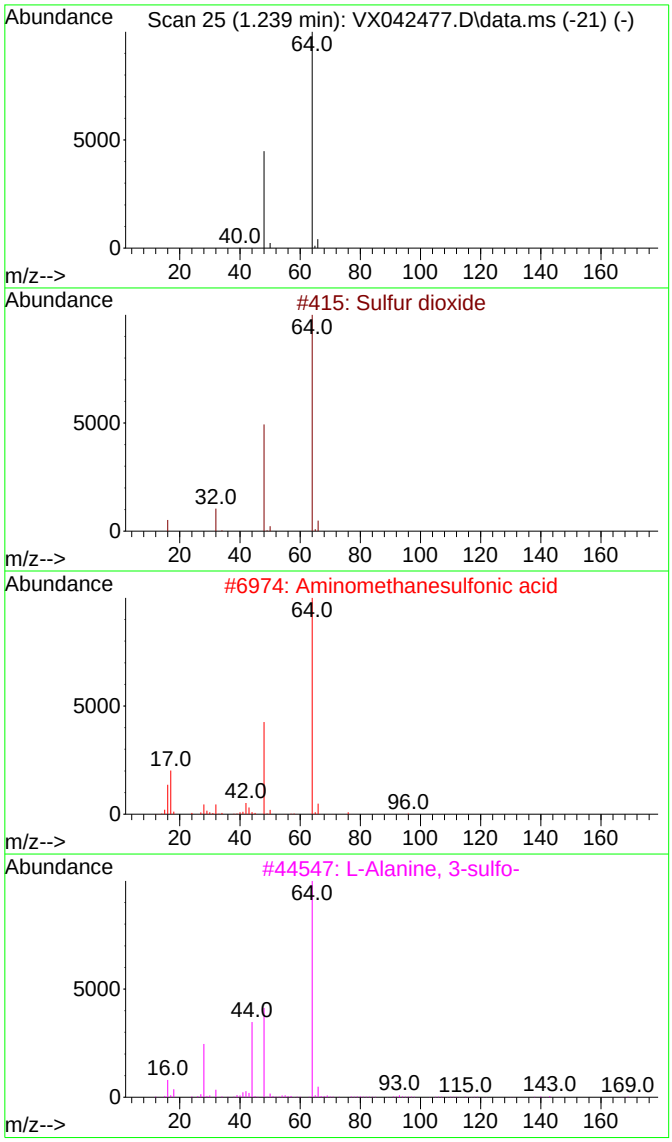
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

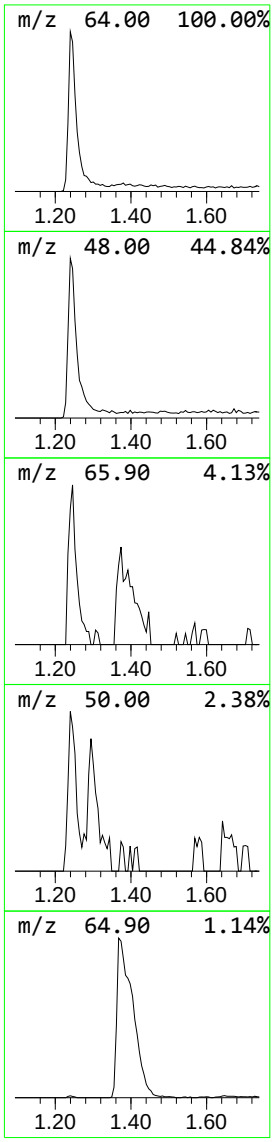
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	2.95 ug/L	27747	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	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	3.0	ug/L	27747	1	6.763	470725	50.0