LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042410.D
Acq On : 19 Jul 2024 18:29
Operator : JC/MD
Sample : P3238-08MERE
Misc : 5.32g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF3MERE

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: VX042410.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	36	rBV2	44400	78803	10.29%	1.738%
2	1.368	43	46	59	rVB	20988	46900	6.13%	1.034%
3	2.282	190	196	212	rBV	68219	124030	16.20%	2.736%
4	2.672	256	260	261	rBV3	240	330	0.04%	0.007%
5	2.715	261	267	274	rBV	22098	44722	5.84%	0.986%
6	2.947	298	305	313	rBV2	3164	8089	1.06%	0.178%
7	3.020	315	317	320	rVB	183	179	0.02%	0.004%
8	3.129	330	335	337	rBV2	233	223	0.03%	0.005%
9	3.331	361	368	369	rBV4	561	956	0.12%	0.021%
10	3.593	408	411	416	rBV4	319	614	0.08%	0.014%
11	3.763	437	439	442	rVB2	155	161	0.02%	0.004%
12	3.983	472	475	479	rBV2	185	309	0.04%	0.007%
13	4.080	489	491	497	rVB	211	248	0.03%	0.005%
14	4.489	550	558	576	rBV	21191	77381	10.11%	1.707%
15	4.940	630	632	636	rVB	203	183	0.02%	0.004%
16	5.056	639	651	667	rBV2	47028	150745	19.69%	3.325%
17	5.531	727	729	730	rBV	299	173	0.02%	0.004%
18	5.623	741	744	746	rBV2	188	186	0.02%	0.004%
19	5.647	746	748	753	rVB2	175	167	0.02%	0.004%
20	5.751	763	765	768	rBV2	126	153	0.02%	0.003%
21	5.964	789	800	822	rVV2	141042	406210	53.06%	8.959%
22	6.165	831	833	834	rBV	257	218	0.03%	0.005%
23	6.281	850	852	854	rBV2	214	175	0.02%	0.004%
24	6.367	862	866	867	rBV2	435	502	0.07%	0.011%
25	6.537	889	894	896	rVV3	224	353	0.05%	0.008%
26	6.623	906	908	911	rVB	227	274	0.04%	0.006%
27	6.647	911	912	914	rBV2	170	163	0.02%	0.004%
28	6.757	921	930	950	rBV	276905	662666	86.56%	14.616%
29	7.117	984	989	994	rBV3	732	1400	0.18%	0.031%
30	7.202	1000	1003	1004	rBV	473	411	0.05%	0.009%
31	7.306	1012	1020	1037	rBV	78481	176823	23.10%	3.900%
32	7.519	1053	1055	1057	rVB	278	184	0.02%	0.004%
33	7.629	1071	1073	1075	rVB2	200	151	0.02%	0.003%
34	7.738	1086	1091	1095	rVV3	377	736	0.10%	0.016%
35	7.793	1099	1100	1103	rVV	187	136	0.02%	0.003%
36	7.921	1119	1121	1123	rVB	202	138	0.02%	0.003%

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Instrument :
MSVOA_X
ClientSampleId :
A4BF3MERE

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	7.982	1123	1131	1134	rBV4	780	1794	0.23%	0.040%
38	8.080	1144	1147	1148	rBV2	138	145	0.02%	0.003%
39	8.165	1159	1161	1164	rBV2	234	194	0.03%	0.004%
40	8.324	1181	1187	1200	rBV	42594	75037	9.80%	1.655%
41	8.525	1218	1220	1224	rVB3	359	395	0.05%	0.009%
42	8.592	1228	1231	1233	rBV2	283	365	0.05%	0.008%
43	8.647	1234	1240	1257	rBV	210342	334256	43.66%	7.372%
44	8.842	1270	1272	1273	rVB	316	162	0.02%	0.004%
45	8.909	1281	1283	1285	rBV2	268	199	0.03%	0.004%
46	8.952	1285	1290	1305	rBV	28118	48355	6.32%	1.067%
47	9.153	1322	1323	1326	rBV	190	183	0.02%	0.004%
48	9.183	1326	1328	1332	rVV2	155	181	0.02%	0.004%
49	9.220	1332	1334	1337	rVV2	120	139	0.02%	0.003%
50	9.281	1339	1344	1348	rVV3	391	652	0.09%	0.014%
51	9.391	1357	1362	1381	rBV	87455	179630	23.46%	3.962%
52	9.726	1412	1417	1424	rBV4	812	1813	0.24%	0.040%
53	9.921	1448	1449	1452	rVB2	205	187	0.02%	0.004%
54	10.055	1465	1471	1481	rBV	554236	765541	100.00%	16.885%
55	10.244	1500	1502	1504	rVB2	319	197	0.03%	0.004%
56	10.311	1506	1513	1519	rBV3	990	1778	0.23%	0.039%
57	10.640	1562	1567	1569	rBV3	297	455	0.06%	0.010%
58	10.817	1592	1596	1600	rBV3	2767	3953	0.52%	0.087%
59	10.963	1614	1620	1625	rVV3	3221	5275	0.69%	0.116%
60	11.091	1636	1641	1646	rBV3	417	700	0.09%	0.015%
61	11.134	1646	1648	1649	rBV	139	137	0.02%	0.003%
62	11.195	1650	1658	1668	rVV	147462	207102	27.05%	4.568%
63	11.311	1674	1677	1681	rBV4	346	483	0.06%	0.011%
64	11.457	1699	1701	1702	rBV2	424	287	0.04%	0.006%
65	11.640	1729	1731	1733	rBV2	224	247	0.03%	0.005%
66	11.677	1736	1737	1740	rVV	244	152	0.02%	0.003%
67	11.713	1740	1743	1745	rVB2	207	191	0.02%	0.004%
68	11.762	1745	1751	1754	rBV5	600	1019	0.13%	0.022%
69	11.823	1760	1761	1764	rVB2	156	136	0.02%	0.003%
70	11.884	1769	1771	1774	rBV	163	166	0.02%	0.004%
71	11.982	1782	1787	1789	rBV3	2970	4163	0.54%	0.092%
72	12.024	1789	1794	1806	rVB	573676	744622	97.27%	16.423%
73	12.219	1823	1826	1837	rVB3	1987	3476	0.45%	0.077%
74	12.323	1837	1843	1855	rBV	226599	306413	40.03%	6.758%
75	12.573	1883	1884	1886	rVB	270	193	0.03%	0.004%
76	12.701	1902	1905	1907	rBV2	222	299	0.04%	0.007%

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Instrument :
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ClientSampleId :
A4BF3MERE

Integration Parameters: LSCINT.P
Integrator: RTE
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Title : VOC Analysis

77	12.731	1909	1910	1911	rVV	281	140	0.02%	0.003%
78	12.768	1911	1916	1919	rVB3	939	1439	0.19%	0.032%
79	12.872	1927	1933	1939	rBV	9881	13315	1.74%	0.294%
80	12.987	1950	1952	1953	rBV2	196	159	0.02%	0.004%
81	13.079	1966	1967	1972	rBV	416	482	0.06%	0.011%
82	13.256	1994	1996	2000	rBV3	109	153	0.02%	0.003%
83	13.402	2015	2020	2025	rBV5	5642	11548	1.51%	0.255%
84	13.682	2062	2066	2073	rVV4	1736	2919	0.38%	0.064%
85	13.786	2078	2083	2087	rBV3	862	1245	0.16%	0.027%
86	13.847	2092	2093	2099	rBV2	279	494	0.06%	0.011%
87	13.957	2107	2111	2116	rBV2	438	715	0.09%	0.016%
88	14.042	2123	2125	2126	rBV2	198	148	0.02%	0.003%
89	14.097	2132	2134	2135	rVB	354	196	0.03%	0.004%
90	14.127	2135	2139	2144	rBV2	1898	2432	0.32%	0.054%
91	14.170	2144	2146	2148	rBV2	381	454	0.06%	0.010%
92	14.249	2157	2159	2162	rBV2	233	294	0.04%	0.006%
93	14.426	2185	2188	2195	rBV	4963	7431	0.97%	0.164%
94	14.640	2221	2223	2226	rBV3	419	477	0.06%	0.011%
95	14.786	2244	2247	2249	rBV3	521	634	0.08%	0.014%
96	14.877	2260	2262	2263	rBV2	619	501	0.07%	0.011%
97	15.115	2294	2301	2305	rBV5	1532	4215	0.55%	0.093%
98	15.389	2343	2346	2351	rVB4	2102	3349	0.44%	0.074%
99	15.950	2435	2438	2447	rVB6	2582	4433	0.58%	0.098%
100	16.273	2489	2491	2497	rBV2	647	1043	0.14%	0.023%

Sum of corrected areas: 4533980

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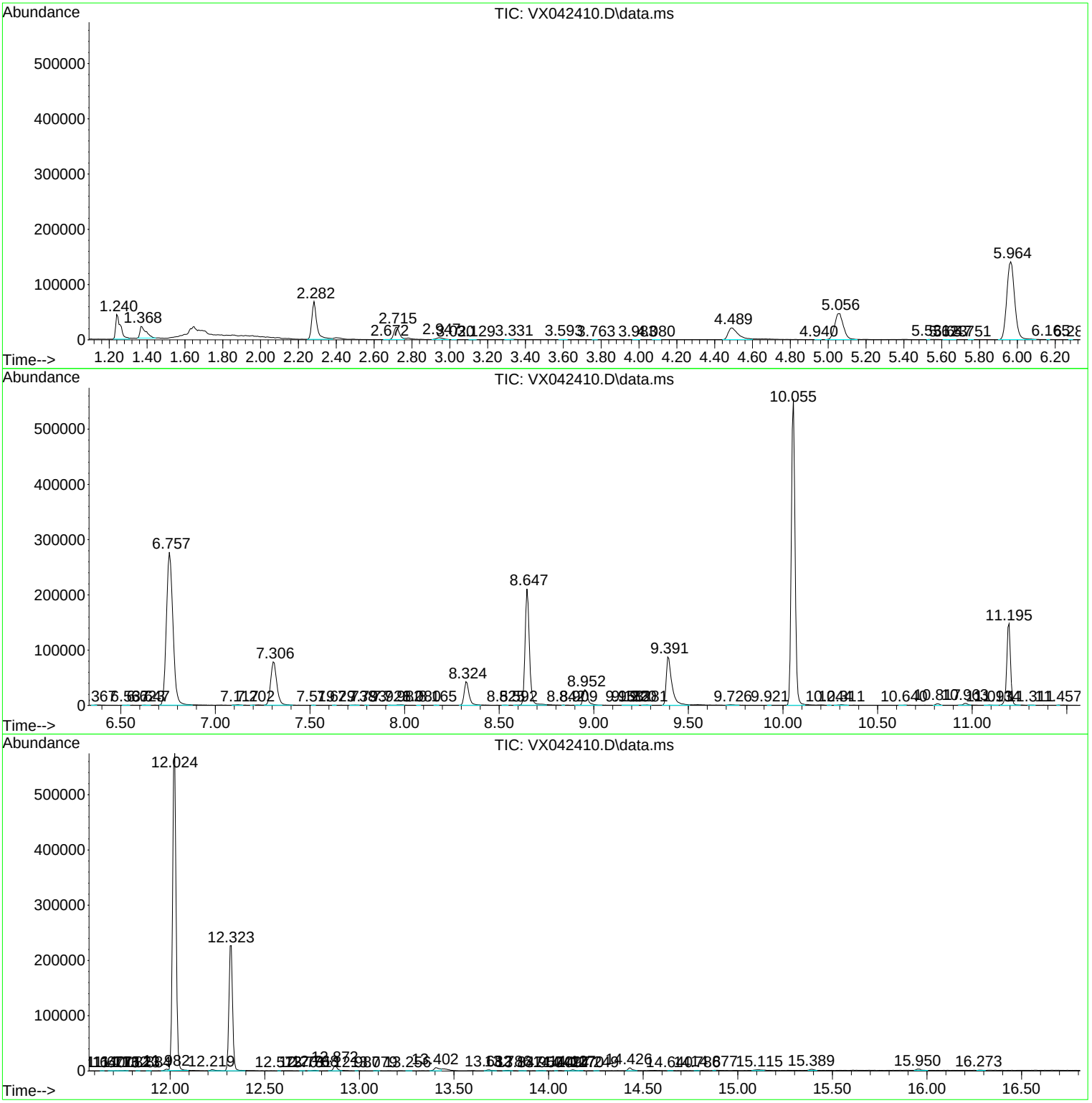
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
ClientSampleId :
A4BF3MERE

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

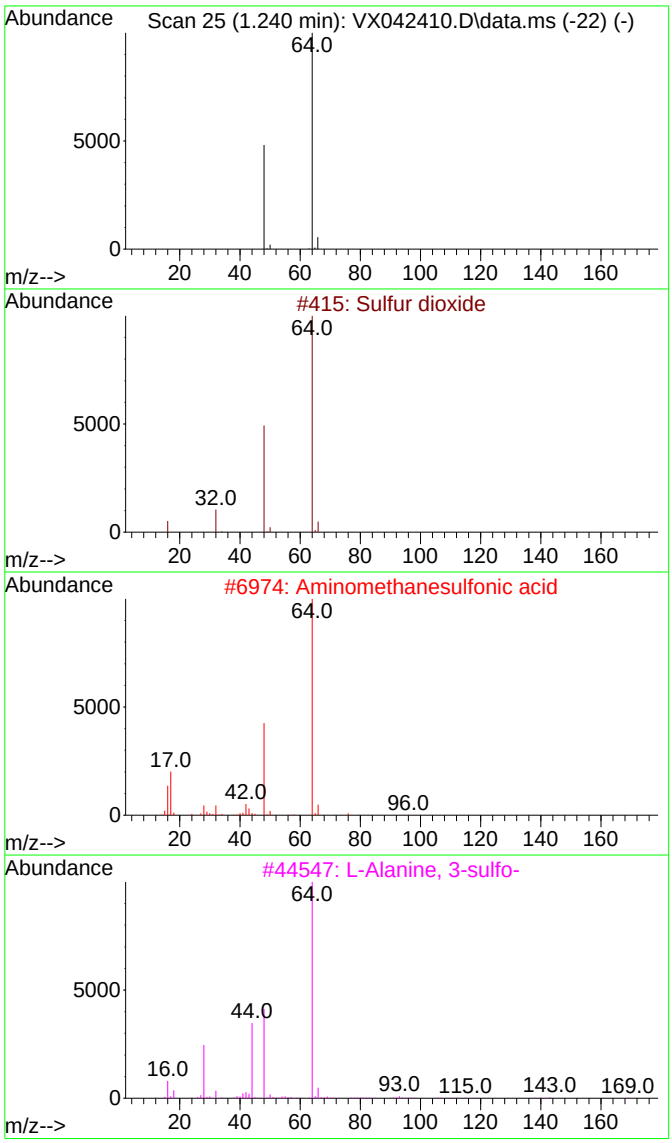
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

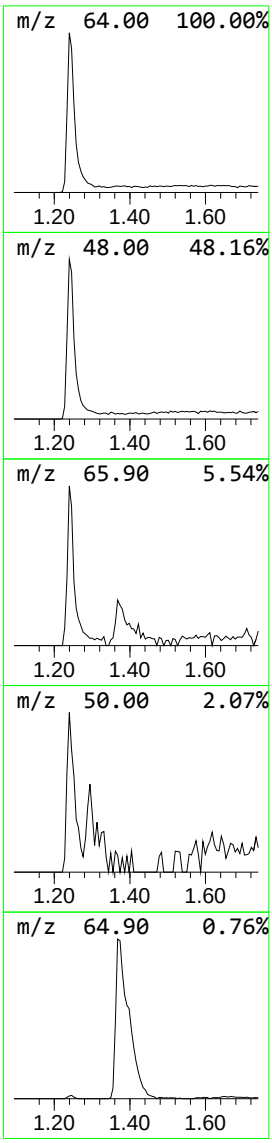
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	5.95 ug/L	78803	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	Sulfur dioxide	64	O2S	007446-09-5	4
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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	6.0	ug/L	78803	1	6.757	662666	50.0