LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042412.D
Acq On : 19 Jul 2024 19:15
Operator : JC/MD
Sample : P3238-15ME
Misc : 4.93g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BZ5ME

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: VX042412.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	40001	44587	6.31%	0.794%
2	1.368	43	46	64	rVB	37029	87994	12.46%	1.568%
3	1.648	89	92	95	rBV	15943	22761	3.22%	0.406%
4	2.282	190	196	213	rBV	117381	216237	30.61%	3.853%
5	2.648	253	256	258	rBV2	281	338	0.05%	0.006%
6	2.715	262	267	274	rBV	9550	18597	2.63%	0.331%
7	2.947	297	305	318	rBV	6533	17199	2.43%	0.306%
8	3.276	357	359	362	rVB	188	165	0.02%	0.003%
9	3.337	367	369	372	rBV3	253	367	0.05%	0.007%
10	3.398	376	379	381	rBV	221	247	0.03%	0.004%
11	3.520	397	399	401	rVB	144	104	0.01%	0.002%
12	3.550	401	404	406	rBV2	152	196	0.03%	0.003%
13	3.587	409	410	412	rBV	191	145	0.02%	0.003%
14	3.648	418	420	423	rBV2	128	139	0.02%	0.002%
15	3.892	458	460	462	rVB	155	114	0.02%	0.002%
16	3.940	464	468	469	rBV	179	115	0.02%	0.002%
17	4.007	476	479	483	rBV2	190	362	0.05%	0.006%
18	4.056	486	487	490	rVV	173	123	0.02%	0.002%
19	4.099	492	494	498	rVV	164	221	0.03%	0.004%
20	4.245	515	518	519	rBV2	138	137	0.02%	0.002%
21	4.379	537	540	543	rBV2	180	218	0.03%	0.004%
22	4.489	548	558	577	rBV	38223	139781	19.79%	2.491%
23	5.056	638	651	669	rBV	84333	264646	37.46%	4.715%
24	5.257	682	684	687	rVB2	278	258	0.04%	0.005%
25	5.336	693	697	699	rBV2	161	183	0.03%	0.003%
26	5.397	699	707	709	rBV4	476	1134	0.16%	0.020%
27	5.452	714	716	717	rBV	184	166	0.02%	0.003%
28	5.477	719	720	722	rBV	152	124	0.02%	0.002%
29	5.544	727	731	733	rBV2	482	624	0.09%	0.011%
30	5.641	744	747	750	rBV2	147	205	0.03%	0.004%
31	5.769	767	768	771	rBV2	160	170	0.02%	0.003%
32	5.964	789	800	819	rBV2	248197	706437	100.00%	12.587%
33	6.202	838	839	842	rVB	208	152	0.02%	0.003%
34	6.367	863	866	867	rVV	244	225	0.03%	0.004%
35	6.379	867	868	875	rVB4	400	680	0.10%	0.012%
36	6.543	891	895	899	rBV2	282	516	0.07%	0.009%

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BZ5ME

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	6.757	921	930	952	rBV	223258	537064	76.02%	9.569%
38	7.110	984	988	996	rVB3	1165	2491	0.35%	0.044%
39	7.306	1012	1020	1045	rBV	138979	309296	43.78%	5.511%
40	7.684	1081	1082	1084	rBV	157	110	0.02%	0.002%
41	7.769	1093	1096	1100	rBV2	141	193	0.03%	0.003%
42	7.970	1123	1129	1134	rBV5	572	1438	0.20%	0.026%
43	8.043	1139	1141	1142	rVB2	203	125	0.02%	0.002%
44	8.183	1162	1164	1167	rBV2	212	229	0.03%	0.004%
45	8.324	1181	1187	1202	rBV	77040	133802	18.94%	2.384%
46	8.464	1209	1210	1212	rVB2	271	195	0.03%	0.003%
47	8.488	1212	1214	1215	rBV	162	161	0.02%	0.003%
48	8.647	1232	1240	1256	rBV	367506	582448	82.45%	10.378%
49	8.952	1285	1290	1309	rBV	55020	86135	12.19%	1.535%
50	9.275	1339	1343	1346	rBV3	820	980	0.14%	0.017%
51	9.391	1357	1362	1379	rBV	165761	321977	45.58%	5.737%
52	9.708	1410	1414	1422	rVB5	1651	3196	0.45%	0.057%
53	9.897	1443	1445	1447	rBV	158	129	0.02%	0.002%
54	9.976	1456	1458	1461	rBV2	137	152	0.02%	0.003%
55	10.055	1465	1471	1491	rVV	444961	620130	87.78%	11.049%
56	10.311	1508	1513	1518	rVB2	640	1106	0.16%	0.020%
57	10.439	1532	1534	1536	rBV2	115	112	0.02%	0.002%
58	10.482	1539	1541	1542	rBV2	199	123	0.02%	0.002%
59	10.555	1549	1553	1558	rVB2	138	281	0.04%	0.005%
60	10.622	1562	1564	1566	rBV	238	188	0.03%	0.003%
61	10.640	1566	1567	1576	rVB3	349	775	0.11%	0.014%
62	10.707	1576	1578	1580	rBV2	189	206	0.03%	0.004%
63	10.970	1617	1621	1626	rVB2	1465	1896	0.27%	0.034%
64	11.195	1652	1658	1669	rBV	261937	350554	49.62%	6.246%
65	11.311	1674	1677	1682	rBV3	785	1114	0.16%	0.020%
66	11.567	1718	1719	1721	rBV	174	106	0.02%	0.002%
67	11.628	1726	1729	1732	rBV3	270	382	0.05%	0.007%
68	11.658	1732	1734	1737	rBV2	117	108	0.02%	0.002%
69	11.695	1738	1740	1742	rBV2	115	119	0.02%	0.002%
70	11.750	1747	1749	1752	rBV2	243	256	0.04%	0.005%
71	11.902	1772	1774	1777	rBV2	178	128	0.02%	0.002%
72	11.982	1781	1787	1788	rBV4	1532	1819	0.26%	0.032%
73	12.024	1788	1794	1802	rVV	455050	583670	82.62%	10.400%
74	12.195	1820	1822	1824	rBV	221	220	0.03%	0.004%
75	12.232	1824	1828	1834	rVB4	1352	2453	0.35%	0.044%
76	12.317	1837	1842	1858	rBV	384110	514309	72.80%	9.164%

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Instrument :
MSVOA_X
ClientSampleId :
A4BZ5ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
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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	12.591	1886	1887	1891	rVB	193	201	0.03%	0.004%
78	12.622	1891	1892	1894	rBV	210	129	0.02%	0.002%
79	12.652	1894	1897	1899	rBV2	145	186	0.03%	0.003%
80	12.707	1905	1906	1908	rBV	180	107	0.02%	0.002%
81	12.762	1911	1915	1920	rVB2	1264	1735	0.25%	0.031%
82	12.811	1920	1923	1924	rBV	180	187	0.03%	0.003%
83	12.872	1928	1933	1940	rBV2	5646	7815	1.11%	0.139%
84	13.042	1958	1961	1963	rVB2	283	341	0.05%	0.006%
85	13.286	1998	2001	2003	rBV	128	156	0.02%	0.003%
86	13.329	2005	2008	2010	rBV2	155	185	0.03%	0.003%
87	13.408	2016	2021	2026	rBV3	4039	6137	0.87%	0.109%
88	13.591	2049	2051	2052	rBV2	329	243	0.03%	0.004%
89	13.682	2063	2066	2067	rBV3	630	692	0.10%	0.012%
90	13.743	2074	2076	2078	rBV2	132	109	0.02%	0.002%
91	13.780	2078	2082	2090	rBV	1429	2359	0.33%	0.042%
92	13.939	2107	2108	2109	rBV2	190	112	0.02%	0.002%
93	14.018	2119	2121	2122	rBV	301	173	0.02%	0.003%
94	14.067	2127	2129	2130	rBV	174	128	0.02%	0.002%
95	14.134	2135	2140	2144	rVB	1491	2081	0.29%	0.037%
96	14.170	2144	2146	2148	rBV2	180	197	0.03%	0.004%
97	14.237	2154	2157	2159	rBV3	182	196	0.03%	0.003%
98	14.426	2185	2188	2195	rBV2	1671	2283	0.32%	0.041%
99	14.481	2195	2197	2198	rVB	336	183	0.03%	0.003%
100	16.493	2525	2527	2530	rBV2	567	696	0.10%	0.012%

Sum of corrected areas: 5612474

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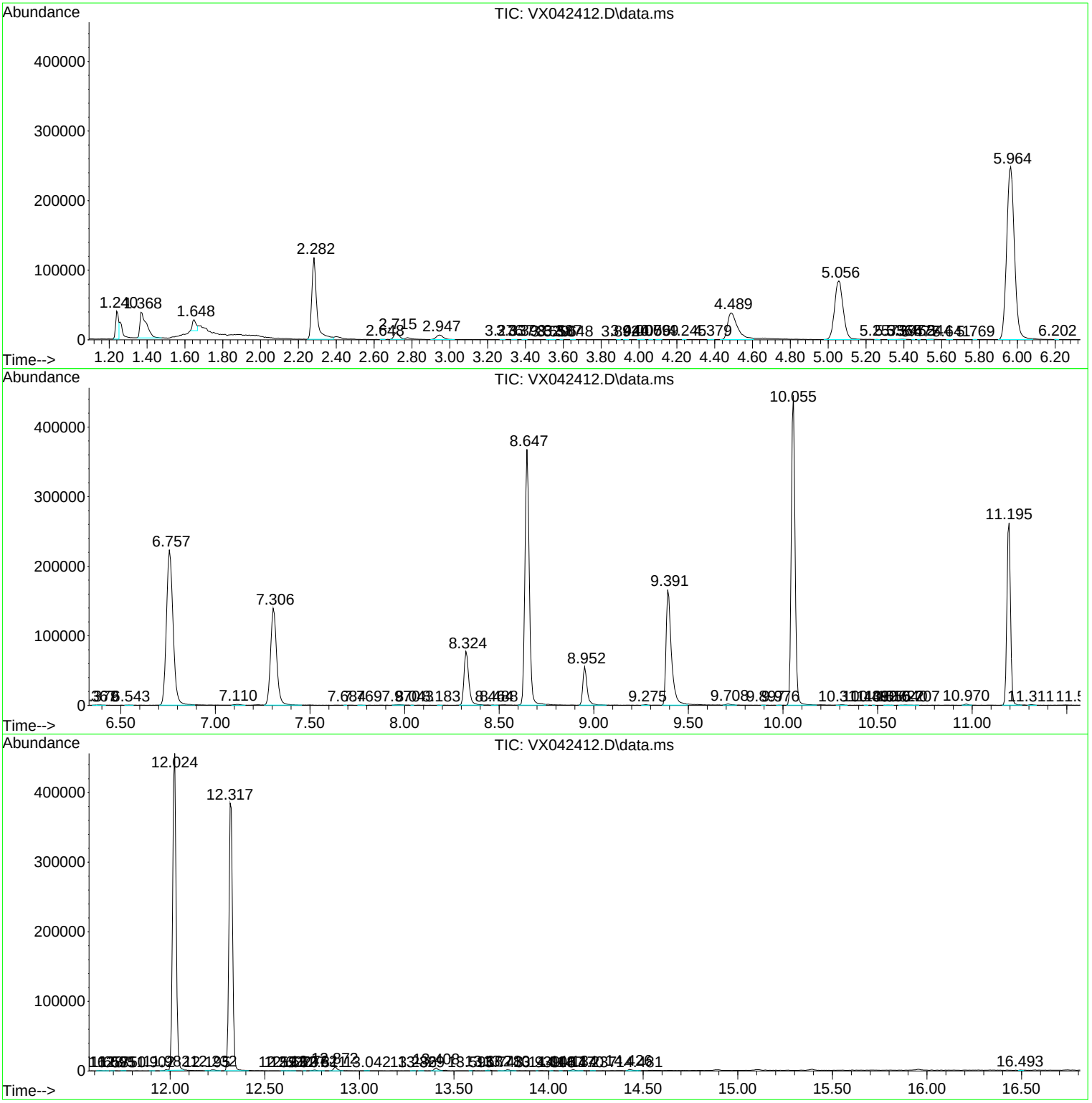
Instrument :
MSVOA_X
ClientSampleId :
A4BZ5ME

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 : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BZ5ME

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

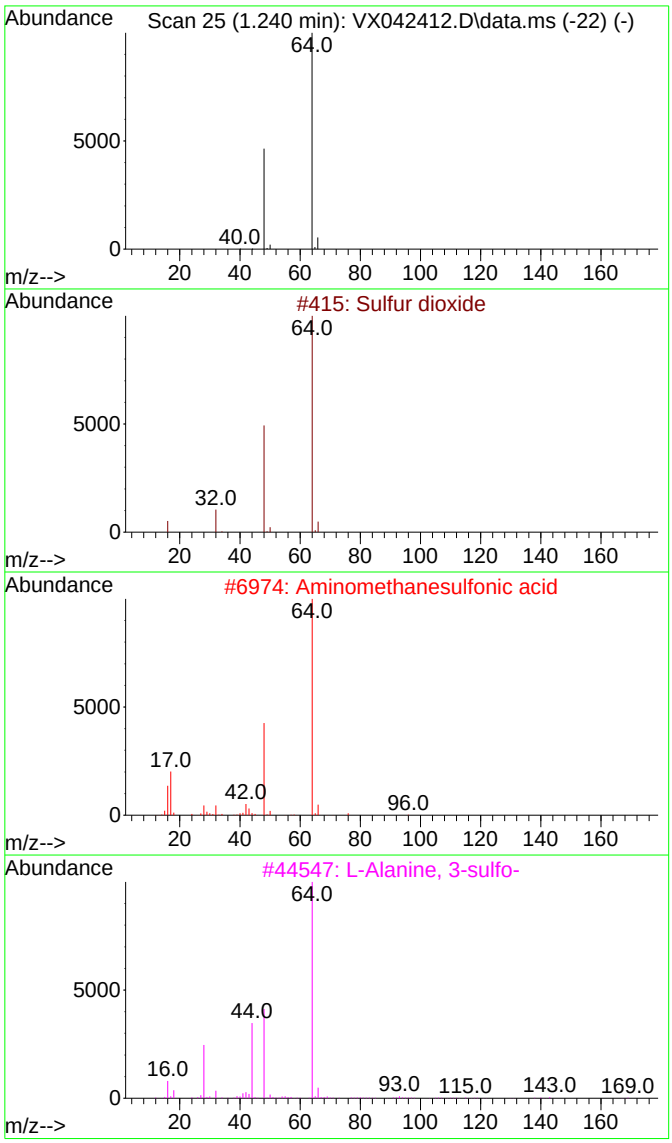
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

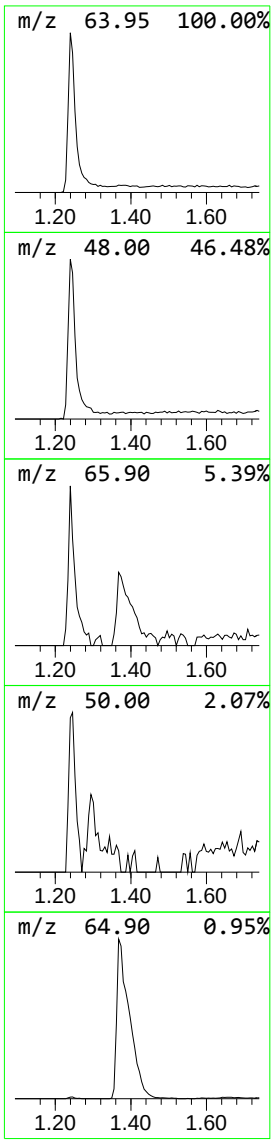
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	4.15 ug/L	44587	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	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Tentatively Identified Compound (LSC) summary

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Instrument :
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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.240	4.2	ug/L	44587	1	6.757	537064	50.0