LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122121\
Data File : VX025951.D
Acq On : 21 Dec 2021 13:02
Operator : JC/MD
Sample : M5150-18DL 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : GBBX6DL

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\SFAMXLM122021WMA.M
Title : VOC Analysis

Signal : TIC: VX025951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	32	rBV2	18898	28781	4.52%	0.514%
2	1.367	43	46	54	rVB	76659	81139	12.74%	1.448%
3	1.666	91	95	103	rBV	69514	88163	13.85%	1.574%
4	2.306	194	200	209	rBV	124626	204425	32.10%	3.649%
5	2.465	222	226	227	rVB	288	334	0.05%	0.006%
6	2.507	230	233	236	rBV3	394	596	0.09%	0.011%
7	2.568	241	243	246	rVB2	281	303	0.05%	0.005%
8	2.703	263	265	272	rVB2	390	658	0.10%	0.012%
9	2.788	275	279	286	rVB2	1823	3089	0.49%	0.055%
10	2.843	286	288	291	rBV2	170	179	0.03%	0.003%
11	2.867	291	292	296	rVB2	239	209	0.03%	0.004%
12	2.904	296	298	299	rBV	287	209	0.03%	0.004%
13	2.946	302	305	316	rVB4	894	1759	0.28%	0.031%
14	3.093	327	329	335	rVB5	525	613	0.10%	0.011%
15	3.330	367	368	371	rVB2	240	202	0.03%	0.004%
16	3.391	375	378	380	rVV2	156	188	0.03%	0.003%
17	3.532	400	401	404	rBV	211	221	0.03%	0.004%
18	3.599	410	412	414	rVV	265	185	0.03%	0.003%
19	3.721	430	432	437	rVB2	181	204	0.03%	0.004%
20	3.818	445	448	453	rBV	246	451	0.07%	0.008%
21	3.879	456	458	461	rVB2	150	178	0.03%	0.003%
22	4.172	503	506	507	rBV2	220	187	0.03%	0.003%
23	4.239	515	517	520	rBV2	153	190	0.03%	0.003%
24	4.318	527	530	533	rBV	140	184	0.03%	0.003%
25	4.458	544	553	573	rBV	51215	164124	25.77%	2.929%
26	4.800	608	609	611	rBV	194	195	0.03%	0.003%
27	4.916	624	628	632	rVB2	198	314	0.05%	0.006%
28	4.964	632	636	638	rBV2	231	289	0.05%	0.005%
29	5.068	640	653	671	rVV	87143	262465	41.22%	4.684%
30	5.458	714	717	718	rBV	508	336	0.05%	0.006%
31	5.543	729	731	733	rBV2	194	209	0.03%	0.004%
32	5.763	765	767	770	rVB2	170	188	0.03%	0.003%
33	5.970	789	801	814	rBV2	211555	635833	99.85%	11.348%
34	6.214	839	841	844	rVB3	184	226	0.04%	0.004%
35	6.324	856	859	862	rBV2	166	237	0.04%	0.004%
36	6.525	890	892	895	rBV2	243	256	0.04%	0.005%

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GBBX6DL

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\SFAMXLM122021WMA.M
Title : VOC Analysis

37	6.580	898	901	903	rVB	257	193	0.03%	0.003%
38	6.616	905	907	910	rBV2	185	247	0.04%	0.004%
39	6.763	922	931	943	rBV	134115	316481	49.70%	5.649%
40	7.019	971	973	975	rVB2	339	343	0.05%	0.006%
41	7.049	975	978	980	rBV	244	224	0.04%	0.004%
42	7.129	982	991	1007	rVV	175837	386009	60.62%	6.889%
43	7.311	1013	1021	1035	rBV	135168	290289	45.59%	5.181%
44	7.440	1040	1042	1044	rBV	202	224	0.04%	0.004%
45	7.488	1048	1050	1052	rVB	357	276	0.04%	0.005%
46	7.726	1086	1089	1091	rBV2	187	197	0.03%	0.004%
47	7.787	1096	1099	1100	rBV	244	199	0.03%	0.004%
48	7.976	1128	1130	1133	rVB2	242	181	0.03%	0.003%
49	8.006	1133	1135	1137	rBV	175	195	0.03%	0.003%
50	8.220	1167	1170	1172	rBV	331	295	0.05%	0.005%
51	8.323	1181	1187	1199	rBV	99200	164790	25.88%	2.941%
52	8.476	1210	1212	1215	rBV3	212	273	0.04%	0.005%
53	8.653	1233	1241	1248	rBV	396144	636781	100.00%	11.365%
54	8.951	1284	1290	1299	rBV	66977	97016	15.24%	1.732%
55	9.281	1339	1344	1346	rBV4	1094	1195	0.19%	0.021%
56	9.384	1355	1361	1380	rBV	260126	387109	60.79%	6.909%
57	9.573	1390	1392	1395	rVB3	257	255	0.04%	0.005%
58	10.055	1465	1471	1488	rVB	362100	486730	76.44%	8.687%
59	10.201	1490	1495	1499	rBV2	387	617	0.10%	0.011%
60	10.305	1509	1512	1517	rVB4	883	1116	0.18%	0.020%
61	10.372	1521	1523	1525	rVB	279	214	0.03%	0.004%
62	10.396	1525	1527	1528	rBV	330	303	0.05%	0.005%
63	10.494	1542	1543	1547	rBV2	219	302	0.05%	0.005%
64	10.555	1549	1553	1556	rVB2	276	402	0.06%	0.007%
65	10.604	1556	1561	1562	rBV2	244	357	0.06%	0.006%
66	10.640	1565	1567	1574	rBV3	421	601	0.09%	0.011%
67	10.695	1574	1576	1579	rBV2	153	193	0.03%	0.003%
68	10.811	1592	1595	1599	rBV2	164	232	0.04%	0.004%
69	11.122	1642	1646	1650	rBV2	1799	2427	0.38%	0.043%
70	11.195	1652	1658	1666	rBV	289146	379007	59.52%	6.765%
71	11.280	1671	1672	1673	rBV	373	229	0.04%	0.004%
72	11.445	1698	1699	1702	rVV2	432	384	0.06%	0.007%
73	11.481	1702	1705	1707	rVV2	617	763	0.12%	0.014%
74	11.555	1714	1717	1720	rBV3	298	409	0.06%	0.007%
75	11.750	1746	1749	1753	rVB3	1567	2117	0.33%	0.038%
76	11.927	1775	1778	1783	rVB4	725	1169	0.18%	0.021%

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Instrument :
MSVOA_X
ClientSampleId :
GBBX6DL

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\SFAMXLM122021WMA.M
Title : VOC Analysis

77	12.024	1789	1794	1805	rVB	356563	444099	69.74%	7.926%
78	12.323	1837	1843	1850	rVV	393849	514854	80.85%	9.189%
79	12.378	1850	1852	1856	rVB3	771	702	0.11%	0.013%
80	12.658	1896	1898	1904	rBV3	306	339	0.05%	0.006%
81	13.036	1959	1960	1963	rBV	185	188	0.03%	0.003%
82	13.195	1984	1986	1989	rBV2	269	291	0.05%	0.005%
83	13.268	1996	1998	2000	rBV2	182	217	0.03%	0.004%
84	13.725	2072	2073	2077	rVV2	184	190	0.03%	0.003%
85	14.066	2125	2129	2131	rBV2	212	327	0.05%	0.006%
86	14.261	2158	2161	2163	rBV	206	198	0.03%	0.004%
87	14.524	2202	2204	2207	rBV2	216	226	0.04%	0.004%
88	14.688	2229	2231	2234	rVB	223	211	0.03%	0.004%
89	14.926	2268	2270	2271	rBV2	272	185	0.03%	0.003%
90	14.993	2279	2281	2284	rBV3	228	205	0.03%	0.004%
91	15.170	2308	2310	2312	rBV2	301	248	0.04%	0.004%
92	15.304	2328	2332	2333	rBV3	261	365	0.06%	0.007%
93	15.554	2371	2373	2376	rBV3	151	189	0.03%	0.003%
94	15.895	2425	2429	2430	rBV3	288	327	0.05%	0.006%
95	15.956	2437	2439	2441	rBV3	210	240	0.04%	0.004%
96	16.139	2465	2469	2471	rBV	279	404	0.06%	0.007%
97	16.188	2476	2477	2483	rVB2	346	425	0.07%	0.008%
98	16.237	2483	2485	2487	rBV2	243	189	0.03%	0.003%
99	16.340	2500	2502	2504	rBV3	246	189	0.03%	0.003%
100	16.517	2529	2531	2536	rBV2	267	389	0.06%	0.007%

Sum of corrected areas: 5602860

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Instrument :
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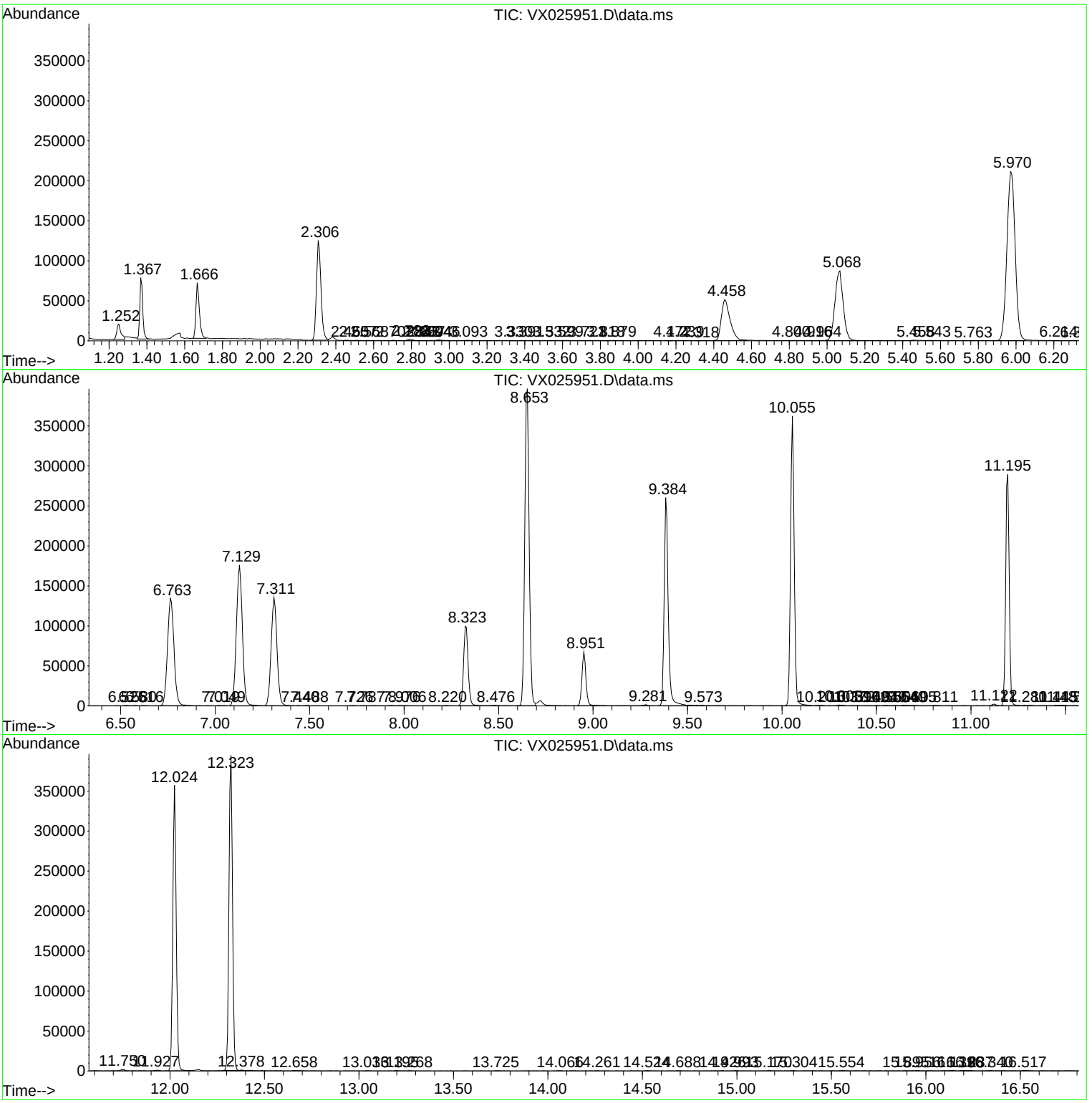
ClientSampleId :
GBBX6DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
Quant Title : VOC Analysis

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



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Quant Title : VOC Analysis

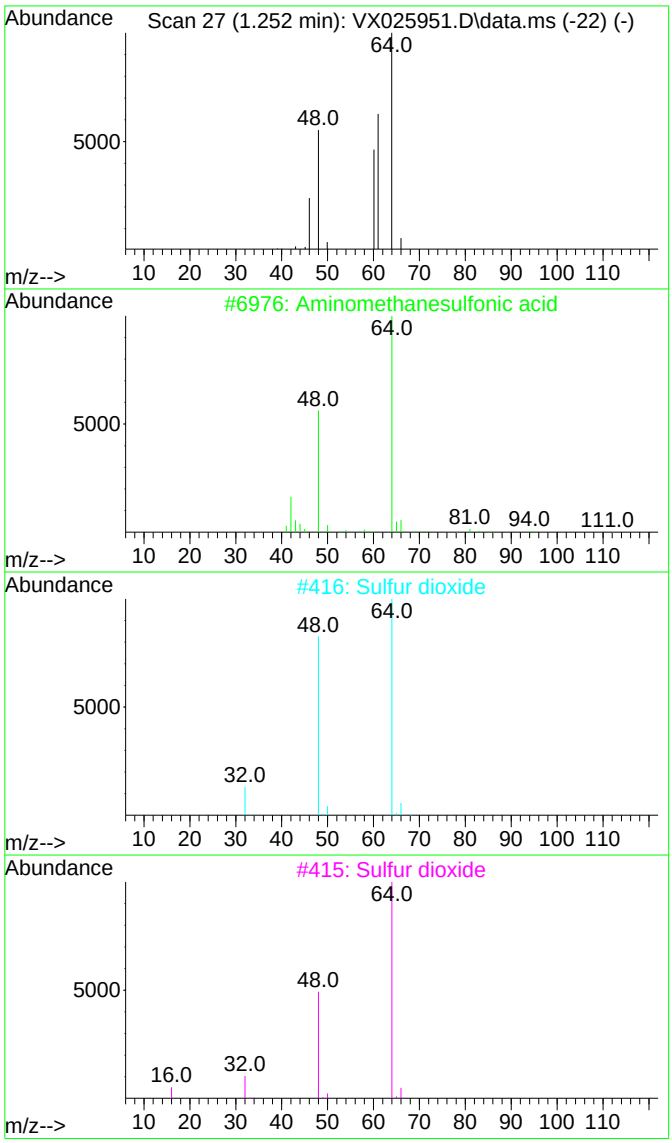
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

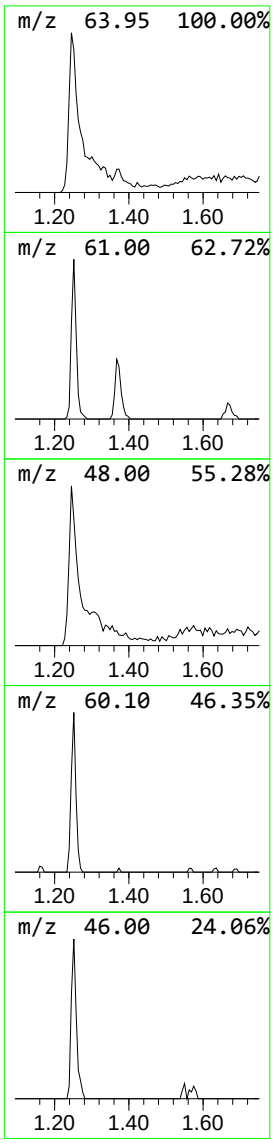
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	4.55 ug/L	28781	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	45
2	Sulfur dioxide	64	O2S	007446-09-5	45
3	Sulfur dioxide	64	O2S	007446-09-5	45
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	38
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\SFAMXLM122021WMA.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
unknown-01	1.252	4.5	ug/L	28781	1	6.763	316481	50.0