LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042573.D
Acq On : 25 Jul 2024 17:45
Operator : JC/MD
Sample : P3334-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E20F0

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: VX042573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	19	rVB	2483	4152	0.88%	0.108%
2	1.240	21	25	37	rBV	38934	49290	10.44%	1.287%
3	1.368	43	46	58	rVB	35287	46343	9.82%	1.210%
4	1.575	72	80	82	rBV4	2328	5574	1.18%	0.146%
5	1.648	88	92	101	rVB	32620	43332	9.18%	1.132%
6	1.935	137	139	142	rVB3	693	728	0.15%	0.019%
7	2.294	192	198	210	rBV	84159	135141	28.63%	3.529%
8	2.392	210	214	218	rVB2	1137	1883	0.40%	0.049%
9	2.496	228	231	232	rBV	212	189	0.04%	0.005%
10	2.569	237	243	250	rVB	1228	2130	0.45%	0.056%
11	2.648	253	256	260	rBV2	165	303	0.06%	0.008%
12	2.788	273	279	286	rVV2	1112	2403	0.51%	0.063%
13	2.849	286	289	293	rVB2	136	218	0.05%	0.006%
14	2.886	293	295	298	rBV	157	166	0.04%	0.004%
15	2.947	298	305	315	rBV	2673	6797	1.44%	0.177%
16	3.044	319	321	324	rVB	115	136	0.03%	0.004%
17	3.093	324	329	336	rBV3	1713	3376	0.72%	0.088%
18	3.349	369	371	374	rVB	139	139	0.03%	0.004%
19	3.441	385	386	391	rVV2	212	184	0.04%	0.005%
20	3.532	398	401	404	rBV2	129	168	0.04%	0.004%
21	3.904	459	462	464	rBV	187	213	0.05%	0.006%
22	3.971	470	473	474	rBV	153	159	0.03%	0.004%
23	4.007	477	479	481	rBV2	149	157	0.03%	0.004%
24	4.111	492	496	497	rBV2	125	150	0.03%	0.004%
25	4.477	546	556	581	rBV2	60405	207165	43.89%	5.410%
26	4.660	584	586	591	rVB2	139	177	0.04%	0.005%
27	4.873	618	621	622	rBV	204	195	0.04%	0.005%
28	4.940	629	632	635	rVB2	116	139	0.03%	0.004%
29	5.056	640	651	668	rBV	64620	191392	40.55%	4.998%
30	5.306	689	692	693	rBV2	149	160	0.03%	0.004%
31	5.397	704	707	708	rVV2	235	169	0.04%	0.004%
32	5.544	729	731	733	rBV2	162	154	0.03%	0.004%
33	5.971	790	801	819	rBV2	160127	471962	100.00%	12.325%
34	6.214	839	841	844	rVB	225	157	0.03%	0.004%
35	6.245	844	846	848	rVB	327	225	0.05%	0.006%
36	6.263	848	849	853	rBV	168	176	0.04%	0.005%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042573.D
Acq On : 25 Jul 2024 17:45
Operator : JC/MD
Sample : P3334-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20F0

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	6.763	921	931	947	rBV	139312	334274	70.83%	8.729%
38	7.129	983	991	1002	rBV	38441	87539	18.55%	2.286%
39	7.306	1012	1020	1040	rBV	95517	216409	45.85%	5.651%
40	7.964	1119	1128	1129	rBV3	492	929	0.20%	0.024%
41	8.324	1182	1187	1201	rVV	46272	78773	16.69%	2.057%
42	8.421	1201	1203	1206	rVB	176	138	0.03%	0.004%
43	8.507	1214	1217	1220	rBV3	251	390	0.08%	0.010%
44	8.647	1234	1240	1249	rBV	225918	363765	77.08%	9.499%
45	8.830	1268	1270	1272	rVB2	287	222	0.05%	0.006%
46	8.866	1274	1276	1279	rVB2	206	177	0.04%	0.005%
47	8.952	1285	1290	1299	rBV	33939	50092	10.61%	1.308%
48	9.092	1310	1313	1314	rBV2	118	136	0.03%	0.004%
49	9.110	1314	1316	1319	rVB2	147	153	0.03%	0.004%
50	9.275	1339	1343	1347	rVB2	1430	2019	0.43%	0.053%
51	9.385	1356	1361	1374	rBV	155161	237382	50.30%	6.199%
52	9.610	1395	1398	1400	rVB	270	204	0.04%	0.005%
53	10.055	1465	1471	1488	rBV	279574	378415	80.18%	9.882%
54	10.208	1492	1496	1499	rVB2	561	899	0.19%	0.023%
55	10.244	1499	1502	1503	rBV2	200	230	0.05%	0.006%
56	10.311	1507	1513	1517	rBV3	908	1405	0.30%	0.037%
57	10.378	1523	1524	1528	rVB2	158	150	0.03%	0.004%
58	10.647	1566	1568	1576	rVB2	461	696	0.15%	0.018%
59	10.750	1583	1585	1588	rVB2	158	147	0.03%	0.004%
60	10.793	1588	1592	1593	rBV	134	159	0.03%	0.004%
61	10.964	1618	1620	1624	rBV2	283	328	0.07%	0.009%
62	11.189	1652	1657	1670	rVV	195514	261756	55.46%	6.835%
63	11.281	1670	1672	1674	rVB2	180	148	0.03%	0.004%
64	11.311	1674	1677	1681	rBV2	431	561	0.12%	0.015%
65	11.451	1697	1700	1704	rBV3	332	424	0.09%	0.011%
66	11.598	1721	1724	1729	rBV2	116	196	0.04%	0.005%
67	11.756	1747	1750	1754	rVB3	457	614	0.13%	0.016%
68	11.976	1784	1786	1789	rBV3	188	172	0.04%	0.004%
69	12.024	1789	1794	1803	rBV	244410	308998	65.47%	8.069%
70	12.177	1817	1819	1822	rBV2	198	167	0.04%	0.004%
71	12.219	1822	1826	1833	rBV2	4308	6401	1.36%	0.167%
72	12.317	1837	1842	1856	rBV	241757	313067	66.33%	8.175%
73	12.792	1916	1920	1922	rVV	175	179	0.04%	0.005%
74	13.116	1970	1973	1976	rBV2	92	139	0.03%	0.004%
75	13.786	2080	2083	2087	rBB2	233	343	0.07%	0.009%
76	13.963	2110	2112	2115	rBV2	177	200	0.04%	0.005%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042573.D
Acq On : 25 Jul 2024 17:45
Operator : JC/MD
Sample : P3334-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20F0

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

77	14.006	2115	2119	2121	rVV2	211	194	0.04%	0.005%
78	14.219	2152	2154	2157	rVB	188	179	0.04%	0.005%
79	14.439	2189	2190	2195	rVV	190	239	0.05%	0.006%
80	14.500	2198	2200	2204	rVB3	170	210	0.04%	0.005%
81	14.585	2211	2214	2215	rVV2	209	186	0.04%	0.005%
82	14.603	2215	2217	2220	rVB3	122	151	0.03%	0.004%
83	14.664	2224	2227	2229	rBV2	304	282	0.06%	0.007%
84	14.810	2246	2251	2253	rBV2	240	354	0.08%	0.009%
85	14.945	2270	2273	2274	rBV3	148	144	0.03%	0.004%
86	15.024	2284	2286	2288	rVB3	209	161	0.03%	0.004%
87	15.164	2308	2309	2311	rBV2	278	181	0.04%	0.005%
88	15.213	2313	2317	2318	rBV2	189	273	0.06%	0.007%
89	15.316	2332	2334	2337	rVB3	208	212	0.04%	0.006%
90	15.383	2342	2345	2348	rBV3	355	581	0.12%	0.015%
91	15.554	2371	2373	2379	rBV3	214	348	0.07%	0.009%
92	15.615	2381	2383	2384	rBV	199	165	0.03%	0.004%
93	15.658	2388	2390	2392	rBV	271	188	0.04%	0.005%
94	15.749	2403	2405	2408	rVB4	302	290	0.06%	0.008%
95	15.957	2437	2439	2440	rVB	210	147	0.03%	0.004%
96	16.066	2455	2457	2459	rBV2	165	151	0.03%	0.004%
97	16.207	2478	2480	2481	rBV	212	154	0.03%	0.004%
98	16.402	2509	2512	2513	rBV3	218	183	0.04%	0.005%
99	16.639	2549	2551	2553	rBV2	194	196	0.04%	0.005%
100	16.664	2553	2555	2558	rVB3	339	402	0.09%	0.010%

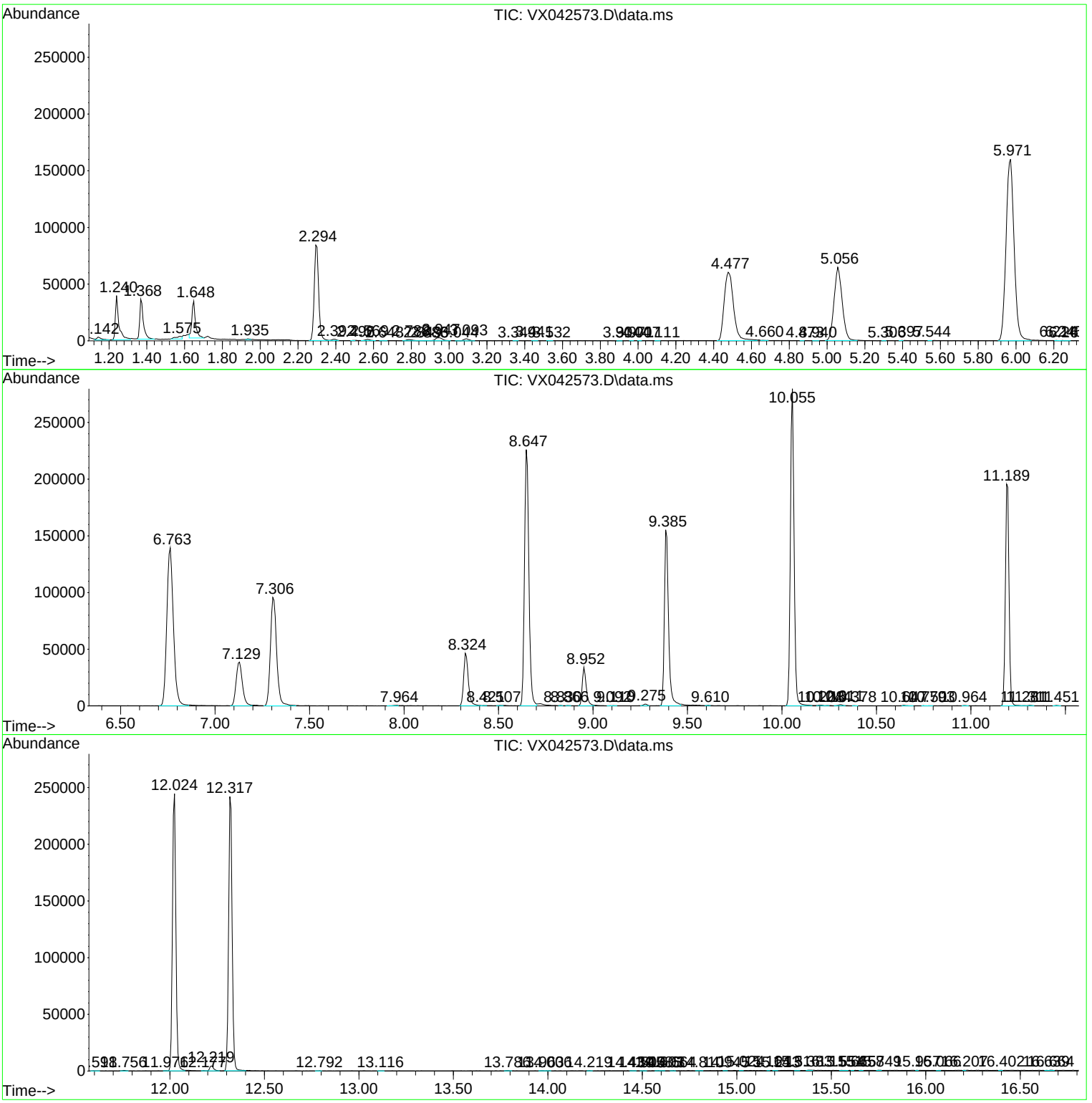
Sum of corrected areas: 3829369

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042573.D
Acq On : 25 Jul 2024 17:45
Operator : JC/MD
Sample : P3334-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20F0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042573.D
Acq On : 25 Jul 2024 17:45
Operator : JC/MD
Sample : P3334-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20F0

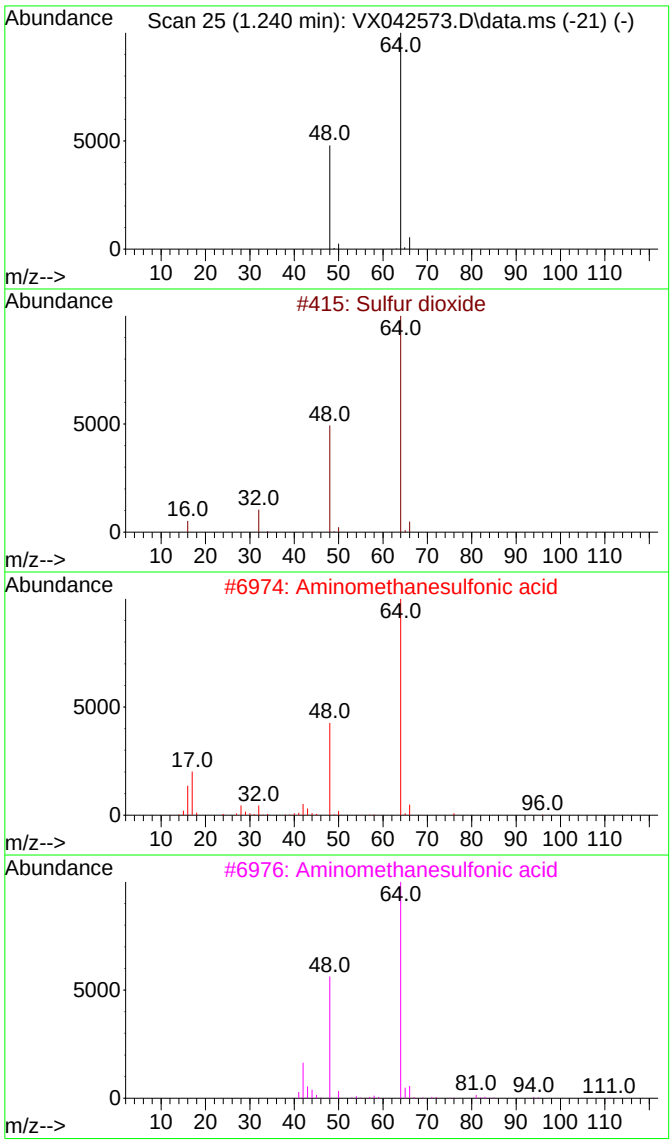
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

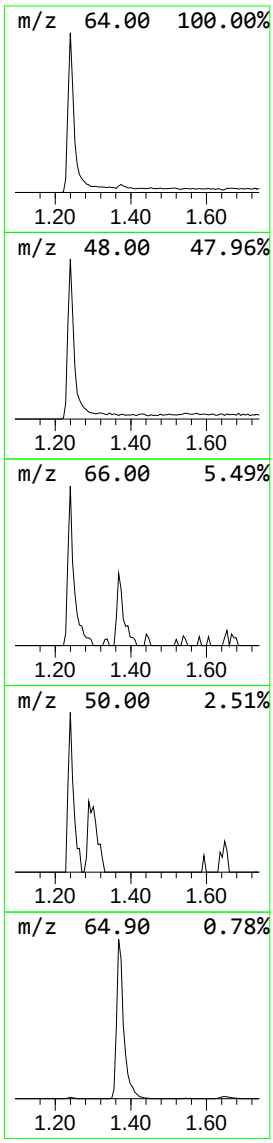
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	7.37 ug/L	49290	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	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042573.D
Acq On : 25 Jul 2024 17:45
Operator : JC/MD
Sample : P3334-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20F0

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	7.4	ug/L	49290	1	6.763	334274	50.0