LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042582.D
Acq On : 25 Jul 2024 21:14
Operator : JC/MD
Sample : P3334-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E20E8

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: VX042582.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	33	rBV	22552	28742	1.77%	0.447%
2	1.374	43	47	56	rVB2	35263	48311	2.97%	0.752%
3	1.581	70	81	82	rBV3	2679	6571	0.40%	0.102%
4	1.599	82	84	86	rVV3	3294	4362	0.27%	0.068%
5	1.648	88	92	100	rVB	31507	42161	2.60%	0.656%
6	1.971	144	145	151	rBV3	326	385	0.02%	0.006%
7	2.221	184	186	188	rVB2	199	138	0.01%	0.002%
8	2.246	188	190	193	rVB	196	223	0.01%	0.003%
9	2.300	193	199	209	rBV	78122	128789	7.93%	2.003%
10	2.398	209	215	218	rVV2	949	1730	0.11%	0.027%
11	2.453	222	224	228	rVB	144	213	0.01%	0.003%
12	2.502	230	232	235	rBV	260	328	0.02%	0.005%
13	2.538	235	238	240	rVB	157	169	0.01%	0.003%
14	2.569	240	243	245	rBV2	233	245	0.02%	0.004%
15	2.788	274	279	284	rBV2	929	1631	0.10%	0.025%
16	2.861	289	291	294	rBV2	117	167	0.01%	0.003%
17	2.947	299	305	314	rVV	1120	2573	0.16%	0.040%
18	3.087	321	328	338	rVV	18676	34852	2.15%	0.542%
19	3.184	342	344	345	rBV	141	146	0.01%	0.002%
20	3.258	352	356	358	rVB	120	139	0.01%	0.002%
21	3.587	406	410	411	rBV	149	142	0.01%	0.002%
22	3.605	411	413	420	rVB3	217	392	0.02%	0.006%
23	3.703	428	429	431	rVB	232	142	0.01%	0.002%
24	3.721	431	432	435	rBV	205	225	0.01%	0.004%
25	3.818	447	448	451	rBV	100	138	0.01%	0.002%
26	4.111	495	496	499	rBV2	156	153	0.01%	0.002%
27	4.172	499	506	507	rBV2	115	216	0.01%	0.003%
28	4.221	512	514	517	rBV2	100	136	0.01%	0.002%
29	4.379	538	540	543	rBV2	187	269	0.02%	0.004%
30	4.483	546	557	580	rBV2	579415	1624059	100.00%	25.264%
31	4.806	608	610	614	rVB4	216	266	0.02%	0.004%
32	4.849	616	617	621	rBV2	170	185	0.01%	0.003%
33	4.928	628	630	633	rBV2	198	261	0.02%	0.004%
34	5.056	639	651	667	rBV	56547	175804	10.82%	2.735%
35	5.196	672	674	677	rVV3	238	289	0.02%	0.004%
36	5.257	682	684	687	rBV2	135	138	0.01%	0.002%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042582.D
Acq On : 25 Jul 2024 21:14
Operator : JC/MD
Sample : P3334-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E20E8

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	5.330	694	696	697	rBV	210	137	0.01%	0.002%
38	5.532	725	729	730	rBV	152	167	0.01%	0.003%
39	5.568	730	735	736	rBV2	183	263	0.02%	0.004%
40	5.964	789	800	819	rBV2	147049	435760	26.83%	6.779%
41	6.135	827	828	830	rVB	202	148	0.01%	0.002%
42	6.245	843	846	849	rVB2	115	173	0.01%	0.003%
43	6.653	908	913	914	rBV	198	226	0.01%	0.004%
44	6.763	922	931	947	rBV	140500	341432	21.02%	5.311%
45	6.922	956	957	958	rBV	322	139	0.01%	0.002%
46	7.007	970	971	974	rVB2	197	181	0.01%	0.003%
47	7.123	980	990	1013	rBV	599635	1310010	80.66%	20.379%
48	7.312	1013	1021	1036	rVB	87105	196076	12.07%	3.050%
49	7.495	1045	1051	1053	rBV3	281	362	0.02%	0.006%
50	7.702	1083	1085	1090	rVB2	139	191	0.01%	0.003%
51	7.836	1104	1107	1109	rBV	115	156	0.01%	0.002%
52	7.964	1122	1128	1131	rBV2	424	730	0.04%	0.011%
53	8.080	1145	1147	1152	rVB2	146	205	0.01%	0.003%
54	8.324	1182	1187	1201	rBV	39172	69527	4.28%	1.082%
55	8.519	1215	1219	1221	rBV2	369	546	0.03%	0.008%
56	8.647	1234	1240	1250	rBV	213787	341645	21.04%	5.315%
57	8.897	1280	1281	1284	rBV	127	139	0.01%	0.002%
58	8.952	1285	1290	1302	rVV	30101	45459	2.80%	0.707%
59	9.068	1307	1309	1313	rBV2	103	162	0.01%	0.003%
60	9.275	1340	1343	1348	rBV3	1248	1514	0.09%	0.024%
61	9.336	1350	1353	1354	rBV	175	161	0.01%	0.003%
62	9.385	1356	1361	1381	rBV	149869	236598	14.57%	3.681%
63	9.781	1422	1426	1428	rBV	185	311	0.02%	0.005%
64	9.817	1430	1432	1434	rVV	161	134	0.01%	0.002%
65	10.055	1465	1471	1487	rVV	293200	399002	24.57%	6.207%
66	10.208	1493	1496	1497	rBV	293	330	0.02%	0.005%
67	10.311	1510	1513	1519	rVB3	498	746	0.05%	0.012%
68	10.531	1548	1549	1552	rVV	152	173	0.01%	0.003%
69	10.598	1556	1560	1561	rBV	147	213	0.01%	0.003%
70	10.653	1565	1569	1572	rVV3	326	447	0.03%	0.007%
71	10.683	1573	1574	1580	rVB2	189	317	0.02%	0.005%
72	10.793	1591	1592	1595	rBV2	132	160	0.01%	0.002%
73	11.189	1652	1657	1672	rVB	186179	250520	15.43%	3.897%
74	11.317	1675	1678	1683	rVB2	356	375	0.02%	0.006%
75	11.372	1686	1687	1692	rVB	150	138	0.01%	0.002%
76	11.415	1692	1694	1699	rBV2	122	142	0.01%	0.002%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042582.D
Acq On : 25 Jul 2024 21:14
Operator : JC/MD
Sample : P3334-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20E8

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	11.738	1745	1747	1749	rBV	145	156	0.01%	0.002%
78	11.762	1749	1751	1756	rVB2	235	307	0.02%	0.005%
79	11.976	1784	1786	1788	rBV	205	182	0.01%	0.003%
80	12.018	1788	1793	1807	rBV	268387	355376	21.88%	5.528%
81	12.219	1821	1826	1837	rBV2	4789	7094	0.44%	0.110%
82	12.317	1837	1842	1855	rBV	248621	320539	19.74%	4.986%
83	12.457	1863	1865	1867	rVB2	203	145	0.01%	0.002%
84	13.244	1992	1994	1997	rVV2	139	139	0.01%	0.002%
85	13.494	2030	2035	2036	rBV2	128	161	0.01%	0.003%
86	13.786	2082	2083	2085	rVB	241	153	0.01%	0.002%
87	14.103	2133	2135	2138	rVV	159	158	0.01%	0.002%
88	14.134	2138	2140	2143	rVB	212	189	0.01%	0.003%
89	14.243	2156	2158	2159	rBV	258	201	0.01%	0.003%
90	14.481	2195	2197	2200	rBV2	172	207	0.01%	0.003%
91	14.609	2216	2218	2221	rBV2	201	292	0.02%	0.005%
92	14.707	2232	2234	2236	rBV2	268	238	0.01%	0.004%
93	14.768	2242	2244	2247	rBV3	179	212	0.01%	0.003%
94	15.152	2306	2307	2308	rBV	330	154	0.01%	0.002%
95	15.310	2331	2333	2336	rBV3	254	231	0.01%	0.004%
96	15.390	2341	2346	2355	rVV5	791	1565	0.10%	0.024%
97	15.457	2355	2357	2358	rVB2	276	148	0.01%	0.002%
98	15.475	2358	2360	2364	rVB2	276	267	0.02%	0.004%
99	16.304	2494	2496	2499	rBV4	272	222	0.01%	0.003%
100	16.584	2541	2542	2545	rVB	252	154	0.01%	0.002%

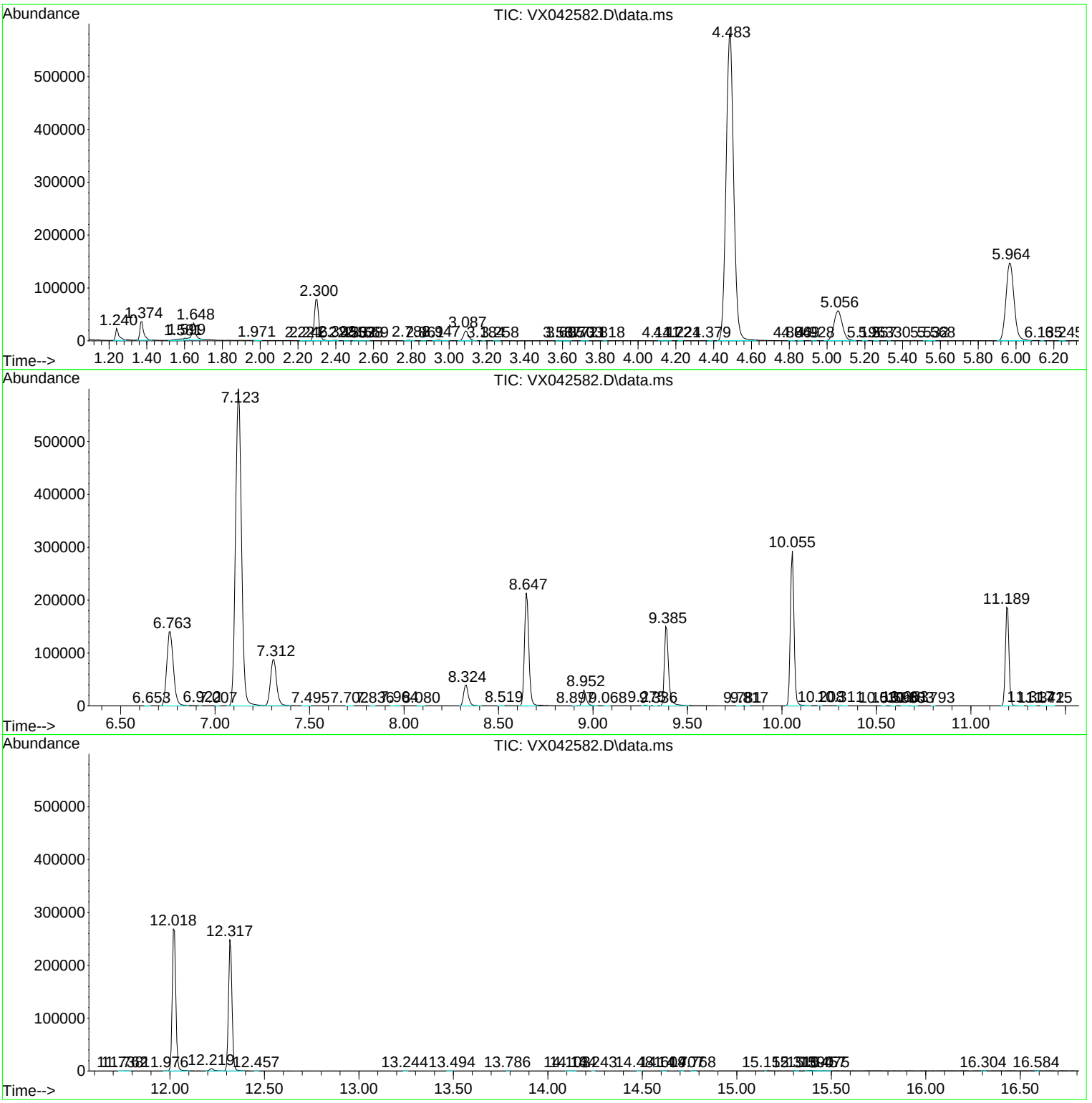
Sum of corrected areas: 6428295

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042582.D
Acq On : 25 Jul 2024 21:14
Operator : JC/MD
Sample : P3334-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20E8

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 : VX042582.D
Acq On : 25 Jul 2024 21:14
Operator : JC/MD
Sample : P3334-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20E8

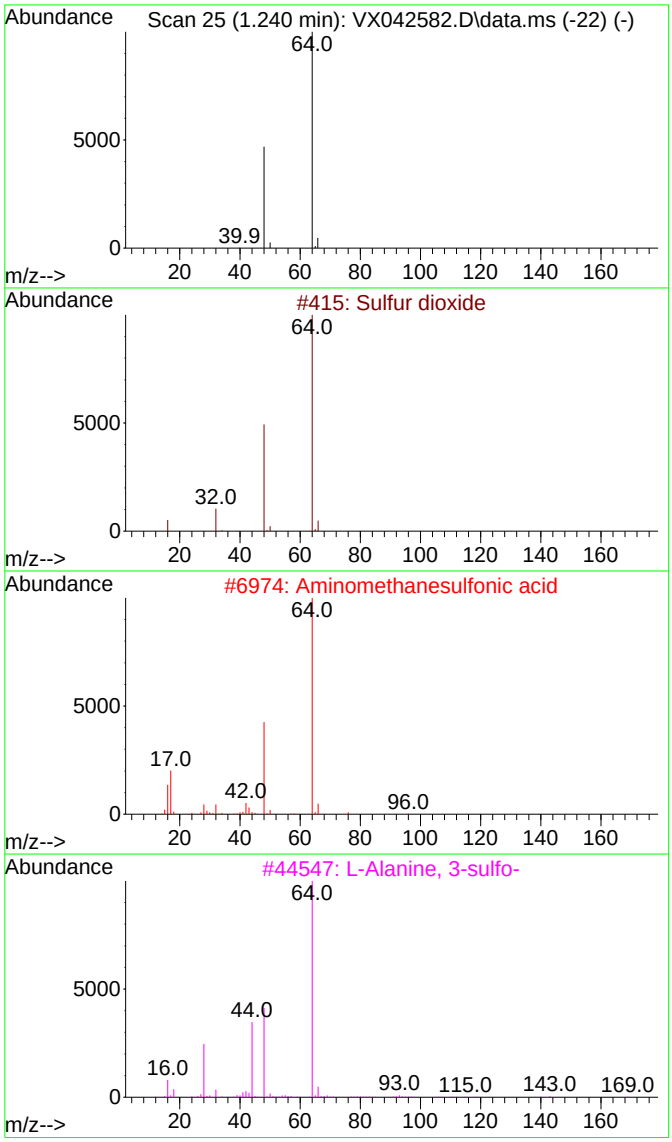
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

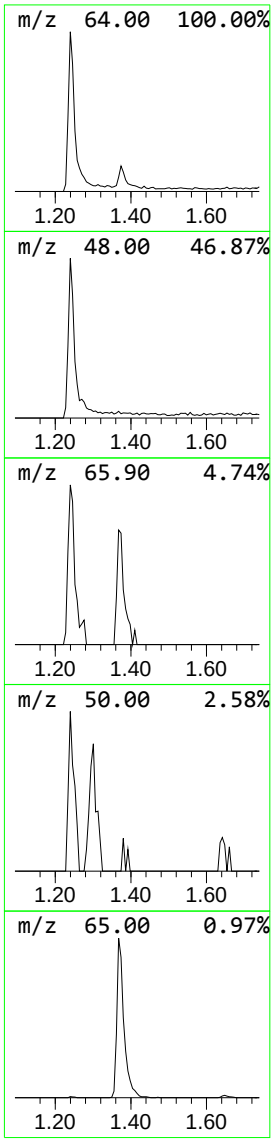
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	4.21 ug/L	28742	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	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042582.D
Acq On : 25 Jul 2024 21:14
Operator : JC/MD
Sample : P3334-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20E8

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	28742	1	6.763	341432	50.0