LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
Data File : VV033891.D
Acq On : 26 Jan 2024 17:08
Operator : SY/MD
Sample : P1252-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS1

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_V\Method\SFAMVLM011024WMA.M
Title : VOC Analysis

Signal : TIC: VV033891.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	32	39	52	rBV	56802	63047	7.93%	0.916%
2	1.282	67	75	102	rBV3	302233	433032	54.50%	6.291%
3	1.529	146	152	167	rVB	85147	104581	13.16%	1.519%
4	2.060	308	317	347	rVB	183983	283612	35.69%	4.120%
5	2.243	366	374	381	rBV2	1452	2416	0.30%	0.035%
6	2.346	404	406	411	rVB2	305	250	0.03%	0.004%
7	2.449	430	438	450	rVB3	2282	3906	0.49%	0.057%
8	2.507	451	456	459	rBV2	156	172	0.02%	0.002%
9	2.603	483	486	489	rVV	162	111	0.01%	0.002%
10	2.700	507	516	532	rVB4	6016	10909	1.37%	0.158%
11	2.921	580	585	587	rBV2	150	162	0.02%	0.002%
12	3.114	642	645	651	rBV2	152	157	0.02%	0.002%
13	3.320	704	709	711	rBV	229	203	0.03%	0.003%
14	3.394	729	732	735	rBV2	171	127	0.02%	0.002%
15	3.468	751	755	757	rBV	204	155	0.02%	0.002%
16	3.510	765	768	772	rVB	168	117	0.01%	0.002%
17	3.716	829	832	834	rBV	167	134	0.02%	0.002%
18	3.812	845	862	903	rBV2	279927	794590	100.00%	11.543%
19	4.249	982	998	1028	rBV	110893	283202	35.64%	4.114%
20	4.391	1038	1042	1044	rVB3	452	259	0.03%	0.004%
21	4.516	1079	1081	1084	rBV	214	134	0.02%	0.002%
22	4.535	1085	1087	1089	rVB	370	175	0.02%	0.003%
23	4.552	1089	1092	1096	rBB2	299	169	0.02%	0.002%
24	4.674	1126	1130	1134	rVB2	219	177	0.02%	0.003%
25	4.696	1134	1137	1140	rBV	234	186	0.02%	0.003%
26	4.847	1182	1184	1189	rBV2	128	110	0.01%	0.002%
27	4.957	1202	1218	1261	rBV2	268508	713657	89.81%	10.368%
28	5.191	1289	1291	1292	rBV	293	129	0.02%	0.002%
29	5.252	1308	1310	1314	rVB2	372	202	0.03%	0.003%
30	5.272	1314	1316	1317	rBV	333	150	0.02%	0.002%
31	5.339	1333	1337	1340	rBV2	305	243	0.03%	0.004%
32	5.375	1345	1348	1353	rVB2	304	265	0.03%	0.004%
33	5.407	1353	1358	1363	rBV3	321	397	0.05%	0.006%
34	5.449	1368	1371	1373	rBV	200	126	0.02%	0.002%
35	5.481	1378	1381	1385	rBV	209	135	0.02%	0.002%
36	5.535	1386	1398	1419	rBV	253093	510225	64.21%	7.412%

LSC Area Percent Report

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Data File : VV033891.D
Acq On : 26 Jan 2024 17:08
Operator : SY/MD
Sample : P1252-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS1

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_V\Method\SFAMVLM011024WMA.M
Title : VOC Analysis

37	5.844	1482	1494	1514	rVB7	8221	18331	2.31%	0.266%
38	5.931	1514	1521	1525	rVB2	343	435	0.05%	0.006%
39	5.989	1525	1539	1570	rBV	156519	322049	40.53%	4.679%
40	6.127	1579	1582	1584	rBV	219	131	0.02%	0.002%
41	6.156	1589	1591	1598	rVB3	688	590	0.07%	0.009%
42	6.191	1599	1602	1604	rBV2	221	125	0.02%	0.002%
43	6.230	1610	1614	1616	rBV	235	201	0.03%	0.003%
44	6.416	1664	1672	1674	rBV2	304	438	0.06%	0.006%
45	6.693	1755	1758	1761	rBV	138	116	0.01%	0.002%
46	6.789	1786	1788	1790	rBV	239	168	0.02%	0.002%
47	6.850	1798	1807	1811	rBV2	203	367	0.05%	0.005%
48	6.915	1817	1827	1853	rBV	89340	167560	21.09%	2.434%
49	7.243	1918	1929	1954	rBV	320159	564751	71.07%	8.204%
50	7.555	2017	2026	2057	rBV	62326	110803	13.94%	1.610%
51	7.731	2079	2081	2086	rVB3	348	253	0.03%	0.004%
52	7.831	2108	2112	2113	rBV	146	111	0.01%	0.002%
53	7.867	2120	2123	2125	rBV2	187	126	0.02%	0.002%
54	8.024	2163	2172	2208	rBV	197422	358172	45.08%	5.203%
55	8.301	2256	2258	2261	rBV3	191	117	0.01%	0.002%
56	8.786	2397	2409	2453	rBV	377665	629310	79.20%	9.142%
57	9.002	2473	2476	2479	rBV3	194	131	0.02%	0.002%
58	9.069	2493	2497	2500	rBV	260	220	0.03%	0.003%
59	9.294	2563	2567	2573	rBV2	200	235	0.03%	0.003%
60	9.416	2603	2605	2612	rVB2	148	135	0.02%	0.002%
61	9.873	2743	2747	2753	rBV2	238	276	0.03%	0.004%
62	9.902	2753	2756	2763	rVB2	274	260	0.03%	0.004%
63	9.979	2776	2780	2782	rBV	192	144	0.02%	0.002%
64	10.021	2790	2793	2797	rBV	176	137	0.02%	0.002%
65	10.153	2822	2834	2857	rBV	216595	340856	42.90%	4.952%
66	10.275	2869	2872	2874	rVB	197	119	0.01%	0.002%
67	10.381	2902	2905	2908	rVB2	300	186	0.02%	0.003%
68	10.419	2914	2917	2921	rVB	298	230	0.03%	0.003%
69	10.448	2922	2926	2929	rBV2	185	142	0.02%	0.002%
70	10.468	2930	2932	2935	rBV	206	142	0.02%	0.002%
71	10.648	2984	2988	2992	rBV2	195	215	0.03%	0.003%
72	10.699	3001	3004	3007	rBV	202	127	0.02%	0.002%
73	10.786	3026	3031	3038	rVB	273	373	0.05%	0.005%
74	10.860	3051	3054	3057	rBV2	175	163	0.02%	0.002%
75	10.956	3082	3084	3090	rVB	200	154	0.02%	0.002%
76	11.133	3136	3139	3144	rBV3	318	310	0.04%	0.005%

LSC Area Percent Report

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Data File : VV033891.D
Acq On : 26 Jan 2024 17:08
Operator : SY/MD
Sample : P1252-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS1

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_V\Method\SFAMVLM011024WMA.M
Title : VOC Analysis

77	11.185	3144	3155	3181	rBV	398950	617485	77.71%	8.971%
78	11.368	3210	3212	3215	rVB2	248	112	0.01%	0.002%
79	11.455	3236	3239	3242	rBV	154	130	0.02%	0.002%
80	11.561	3258	3272	3288	rBV	334091	523086	65.83%	7.599%
81	11.699	3312	3315	3321	rVB2	553	501	0.06%	0.007%
82	11.728	3321	3324	3328	rVB3	178	128	0.02%	0.002%
83	12.410	3530	3536	3541	rBV2	263	384	0.05%	0.006%
84	12.622	3598	3602	3604	rBV	174	155	0.02%	0.002%
85	13.030	3726	3729	3733	rVB2	262	184	0.02%	0.003%
86	13.210	3779	3785	3793	rBV2	926	1093	0.14%	0.016%
87	13.262	3798	3801	3804	rBV	176	132	0.02%	0.002%
88	13.448	3852	3859	3868	rBV2	6667	9611	1.21%	0.140%
89	13.689	3927	3934	3941	rVB5	1531	2083	0.26%	0.030%
90	13.754	3951	3954	3958	rVB	365	269	0.03%	0.004%
91	13.821	3972	3975	3978	rBV2	208	201	0.03%	0.003%
92	13.905	3997	4001	4003	rBV	316	239	0.03%	0.003%
93	13.937	4009	4011	4014	rBV2	224	150	0.02%	0.002%
94	14.040	4040	4043	4045	rBV2	258	200	0.03%	0.003%
95	14.127	4068	4070	4073	rVV2	286	157	0.02%	0.002%
96	14.143	4073	4075	4080	rVB2	419	227	0.03%	0.003%
97	14.214	4094	4097	4099	rBV2	197	130	0.02%	0.002%
98	14.294	4119	4122	4124	rBV2	152	113	0.01%	0.002%
99	15.387	4461	4462	4468	rBV3	291	252	0.03%	0.004%
100	15.702	4558	4560	4562	rBV2	430	153	0.02%	0.002%

Sum of corrected areas: 6883506

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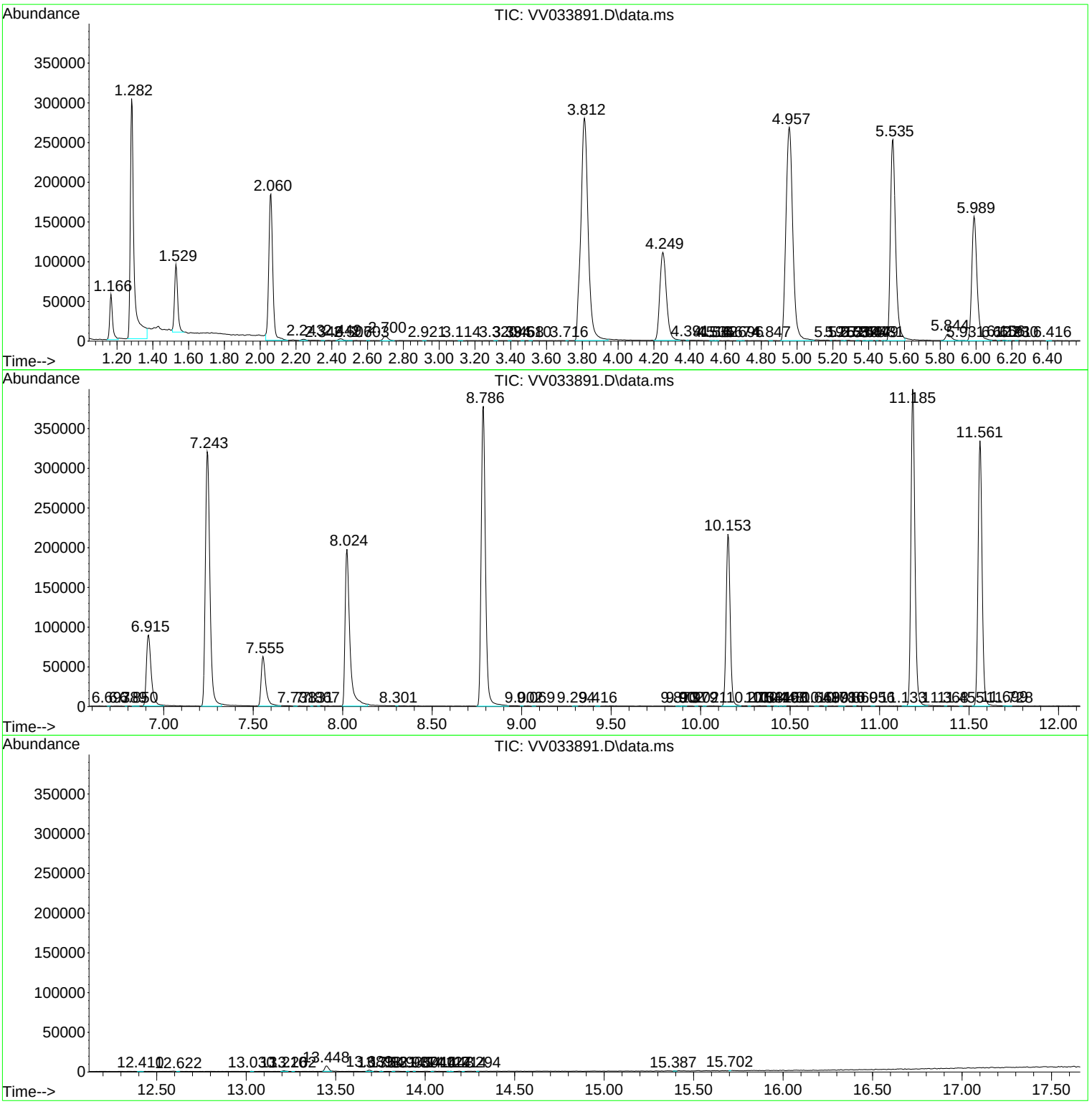
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS1

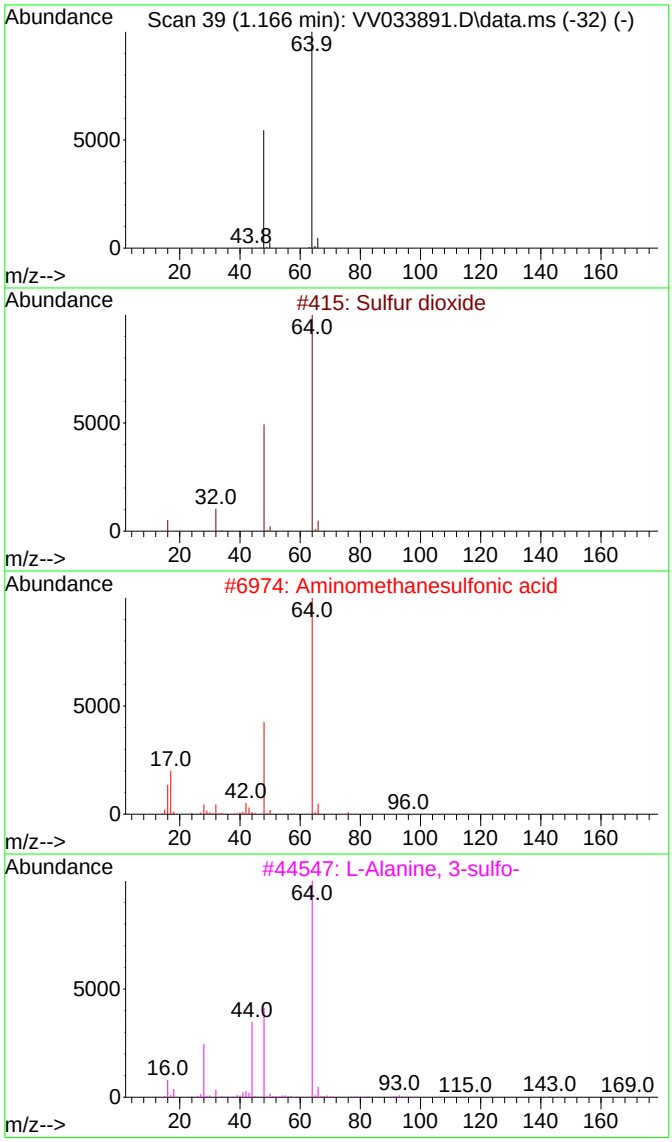
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

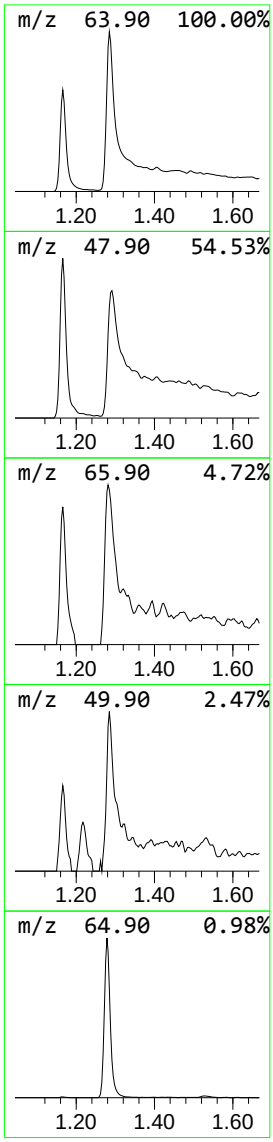
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	6.18 ug/L	63047	1,4-Difluorobenzene	5.535

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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012624\
Data File : VV033891.D
Acq On : 26 Jan 2024 17:08
Operator : SY/MD
Sample : P1252-03
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMS1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.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	1.166	6.2	ug/L	63047	1	5.535	510225	50.0