LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012224\
Data File : VV033792.D
Acq On : 22 Jan 2024 10:37
Operator : SY/MD
Sample : VV0122MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK220

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: VV033792.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	31	39	51	rBV	67501	80010	9.09%	1.130%
2	1.278	67	74	90	rBV	117840	138093	15.69%	1.951%
3	1.510	141	146	164	rVB	100544	130129	14.79%	1.838%
4	2.053	305	315	333	rVB	222043	328005	37.28%	4.633%
5	2.179	350	354	363	rVB5	1488	1864	0.21%	0.026%
6	2.236	364	372	382	rVB4	1090	1902	0.22%	0.027%
7	2.442	430	436	442	rVV4	704	927	0.11%	0.013%
8	2.494	450	452	455	rVB	231	107	0.01%	0.002%
9	2.539	463	466	467	rBV2	218	121	0.01%	0.002%
10	2.558	468	472	478	rVB3	585	657	0.07%	0.009%
11	2.847	560	562	566	rVB2	267	144	0.02%	0.002%
12	2.953	584	595	597	rBV2	182	263	0.03%	0.004%
13	3.121	643	647	651	rVB2	202	149	0.02%	0.002%
14	3.368	718	724	731	rBV2	178	254	0.03%	0.004%
15	3.780	844	852	893	rBV	49246	136228	15.48%	1.924%
16	4.037	929	932	936	rVB3	508	399	0.05%	0.006%
17	4.240	980	995	1020	rBV	136315	346940	39.43%	4.901%
18	4.436	1054	1056	1058	rBV2	254	141	0.02%	0.002%
19	4.484	1067	1071	1075	rVB2	342	270	0.03%	0.004%
20	4.545	1088	1090	1093	rVB	185	104	0.01%	0.001%
21	4.564	1093	1096	1097	rBV	197	115	0.01%	0.002%
22	4.690	1132	1135	1140	rBV2	183	236	0.03%	0.003%
23	4.828	1174	1178	1183	rBV2	181	218	0.02%	0.003%
24	4.950	1199	1216	1246	rBV2	332492	879892	100.00%	12.429%
25	5.375	1343	1348	1352	rBV2	207	199	0.02%	0.003%
26	5.529	1383	1396	1436	rBV	278801	580065	65.92%	8.194%
27	5.834	1482	1491	1503	rVB6	1755	3781	0.43%	0.053%
28	5.921	1512	1518	1522	rBV3	709	927	0.11%	0.013%
29	5.940	1522	1524	1525	rVV3	534	229	0.03%	0.003%
30	5.982	1525	1537	1569	rVV	188289	392322	44.59%	5.542%
31	6.191	1600	1602	1604	rVV2	316	128	0.01%	0.002%
32	6.252	1619	1621	1626	rVB	241	134	0.02%	0.002%
33	6.355	1650	1653	1655	rVB	173	117	0.01%	0.002%
34	6.368	1655	1657	1660	rBV	140	108	0.01%	0.002%
35	6.580	1720	1723	1724	rBV	172	115	0.01%	0.002%
36	6.590	1724	1726	1728	rVV	221	141	0.02%	0.002%

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Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK220

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	6.908	1814	1825	1858	rBV	115091	216137	24.56%	3.053%
38	7.239	1916	1928	1956	rBV	411364	724314	82.32%	10.231%
39	7.548	2015	2024	2056	rBV	76011	140095	15.92%	1.979%
40	7.751	2085	2087	2092	rVB2	280	215	0.02%	0.003%
41	7.876	2122	2126	2128	rVB2	295	223	0.03%	0.003%
42	7.902	2128	2134	2140	rBV2	189	295	0.03%	0.004%
43	7.928	2140	2142	2146	rVB	189	149	0.02%	0.002%
44	7.956	2146	2151	2153	rBV	153	141	0.02%	0.002%
45	8.024	2163	2172	2220	rBV	178644	368206	41.85%	5.201%
46	8.326	2264	2266	2268	rBV	237	107	0.01%	0.002%
47	8.445	2298	2303	2307	rBV	195	253	0.03%	0.004%
48	8.780	2396	2407	2436	rBV	428616	707772	80.44%	9.998%
49	9.079	2497	2500	2502	rBV2	219	157	0.02%	0.002%
50	9.329	2571	2578	2581	rBV	146	146	0.02%	0.002%
51	9.410	2597	2603	2605	rBV	154	153	0.02%	0.002%
52	9.487	2622	2627	2629	rBV	268	307	0.03%	0.004%
53	9.526	2636	2639	2644	rBV3	356	323	0.04%	0.005%
54	9.683	2683	2688	2691	rBV2	135	142	0.02%	0.002%
55	9.760	2709	2712	2715	rBV2	137	123	0.01%	0.002%
56	9.818	2726	2730	2735	rVB2	136	131	0.01%	0.002%
57	9.879	2741	2749	2755	rVB3	581	891	0.10%	0.013%
58	10.008	2783	2789	2794	rBV2	170	209	0.02%	0.003%
59	10.098	2813	2817	2821	rBV	169	144	0.02%	0.002%
60	10.153	2821	2834	2856	rBV	239810	385000	43.76%	5.438%
61	10.288	2873	2876	2879	rBV	145	114	0.01%	0.002%
62	10.326	2883	2888	2896	rVB3	356	479	0.05%	0.007%
63	10.439	2920	2923	2930	rVB2	114	111	0.01%	0.002%
64	10.484	2930	2937	2943	rBV3	672	1063	0.12%	0.015%
65	10.709	3004	3007	3008	rBV	349	219	0.02%	0.003%
66	10.738	3013	3016	3019	rBV2	235	157	0.02%	0.002%
67	10.767	3021	3025	3026	rBV2	218	135	0.02%	0.002%
68	10.818	3039	3041	3045	rVB2	338	172	0.02%	0.002%
69	10.857	3045	3053	3055	rBV3	560	628	0.07%	0.009%
70	11.043	3108	3111	3114	rBV	130	102	0.01%	0.001%
71	11.127	3129	3137	3143	rBV5	1065	1495	0.17%	0.021%
72	11.185	3143	3155	3175	rBV	476068	746085	84.79%	10.539%
73	11.558	3260	3271	3293	rBV	434382	694903	78.98%	9.816%
74	11.741	3323	3328	3332	rVB2	233	218	0.02%	0.003%
75	11.879	3367	3371	3373	rBV2	156	135	0.02%	0.002%
76	12.124	3444	3447	3452	rBV2	153	129	0.01%	0.002%

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Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK220

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	12.300	3498	3502	3509	rBV2	184	235	0.03%	0.003%
78	12.352	3514	3518	3521	rBV	115	105	0.01%	0.001%
79	12.593	3585	3593	3604	rVB4	1471	1982	0.23%	0.028%
80	12.738	3633	3638	3642	rBV2	168	164	0.02%	0.002%
81	12.850	3670	3673	3677	rVB	173	116	0.01%	0.002%
82	13.204	3776	3783	3794	rBV4	4154	6440	0.73%	0.091%
83	13.307	3813	3815	3818	rBV	226	118	0.01%	0.002%
84	13.371	3831	3835	3840	rVB3	275	218	0.02%	0.003%
85	13.397	3840	3843	3847	rVB2	240	178	0.02%	0.003%
86	13.445	3847	3858	3880	rBV	23960	41393	4.70%	0.585%
87	13.612	3907	3910	3914	rVB2	243	152	0.02%	0.002%
88	13.686	3924	3933	3943	rBV3	5007	7691	0.87%	0.109%
89	13.857	3984	3986	3991	rVB2	257	176	0.02%	0.002%
90	13.898	3995	3999	4004	rBV2	274	242	0.03%	0.003%
91	13.950	4012	4015	4017	rBV	219	143	0.02%	0.002%
92	13.982	4022	4025	4032	rVB2	844	831	0.09%	0.012%
93	14.188	4085	4089	4090	rBV	243	168	0.02%	0.002%
94	14.223	4097	4100	4103	rBV3	226	222	0.03%	0.003%
95	14.316	4126	4129	4133	rBV2	248	205	0.02%	0.003%
96	14.480	4177	4180	4186	rVB3	296	225	0.03%	0.003%
97	14.776	4269	4272	4275	rBV2	226	155	0.02%	0.002%
98	14.975	4330	4334	4338	rBV3	437	380	0.04%	0.005%
99	15.088	4367	4369	4373	rBV5	308	205	0.02%	0.003%
100	15.281	4425	4429	4432	rBV4	443	383	0.04%	0.005%

Sum of corrected areas: 7079339

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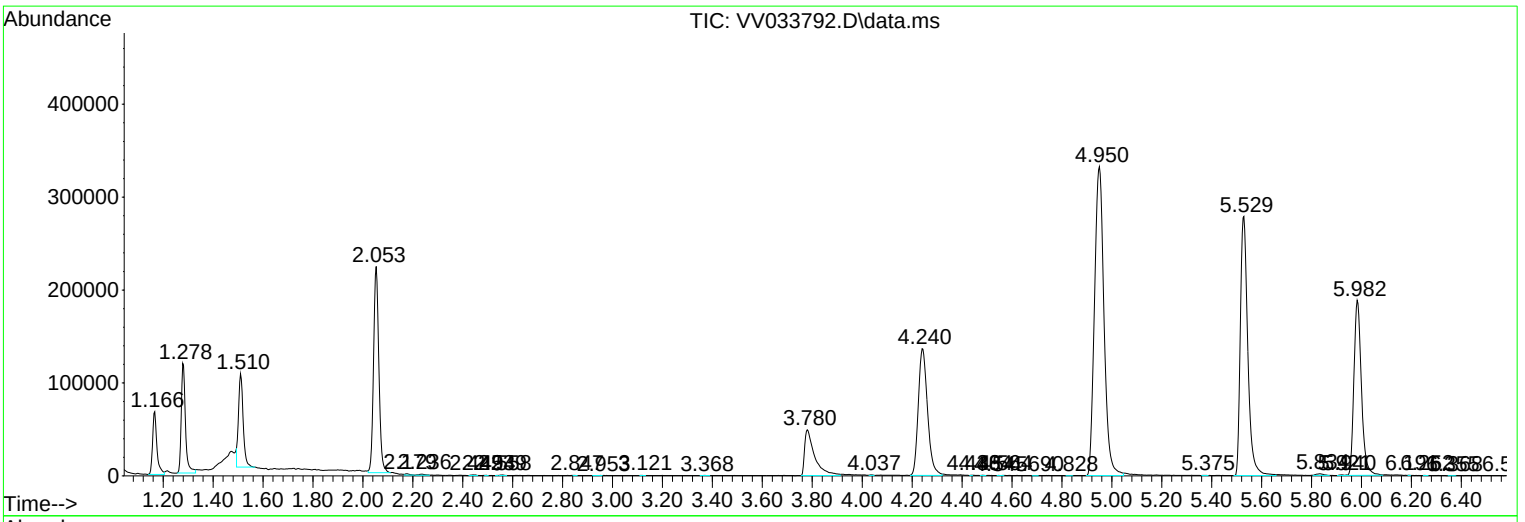
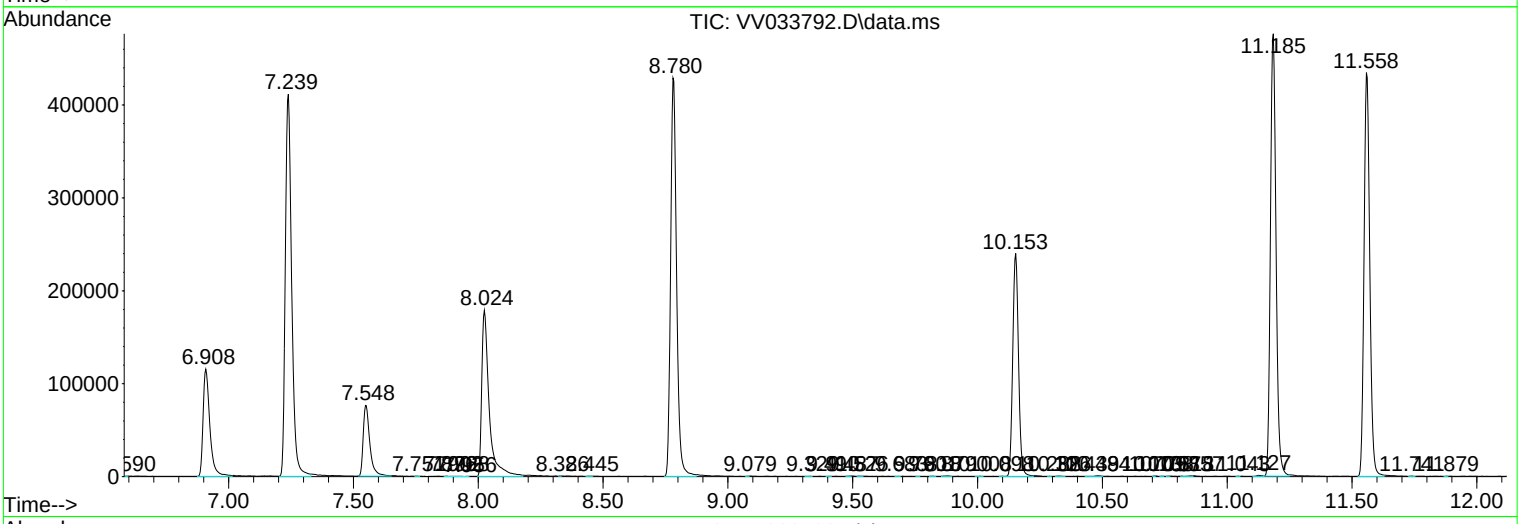
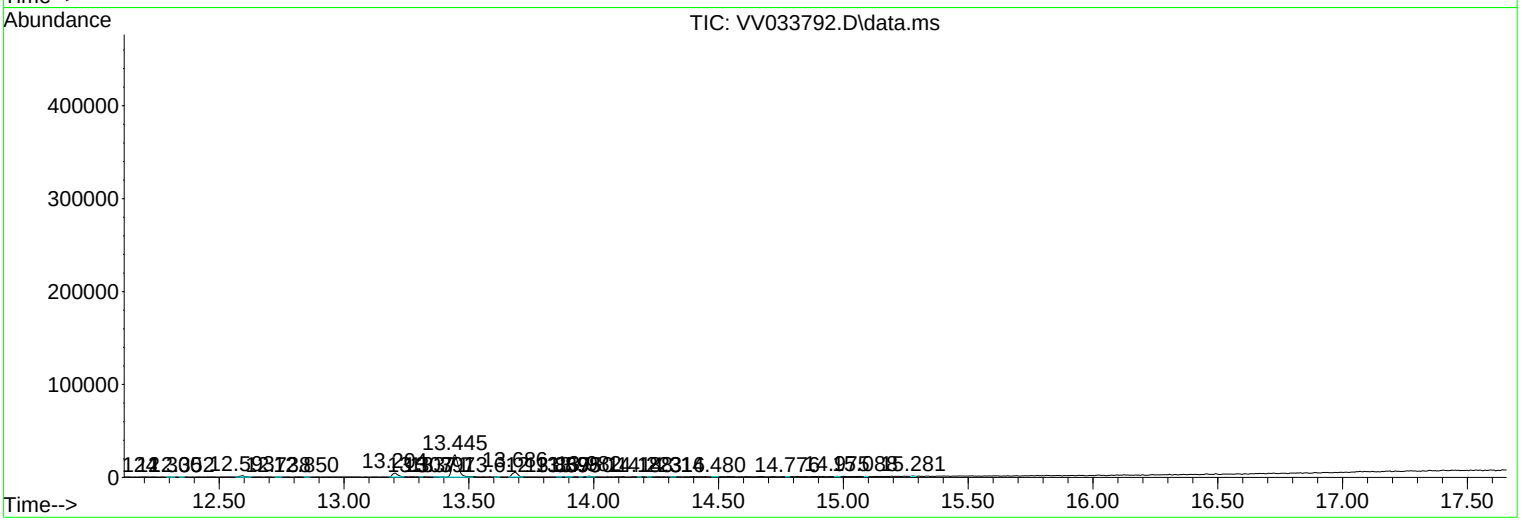
Instrument :
MSVOA_V
ClientSampleId :
VBLK220

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







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Instrument :
MSVOA_V
ClientSampleId :
VBLK220

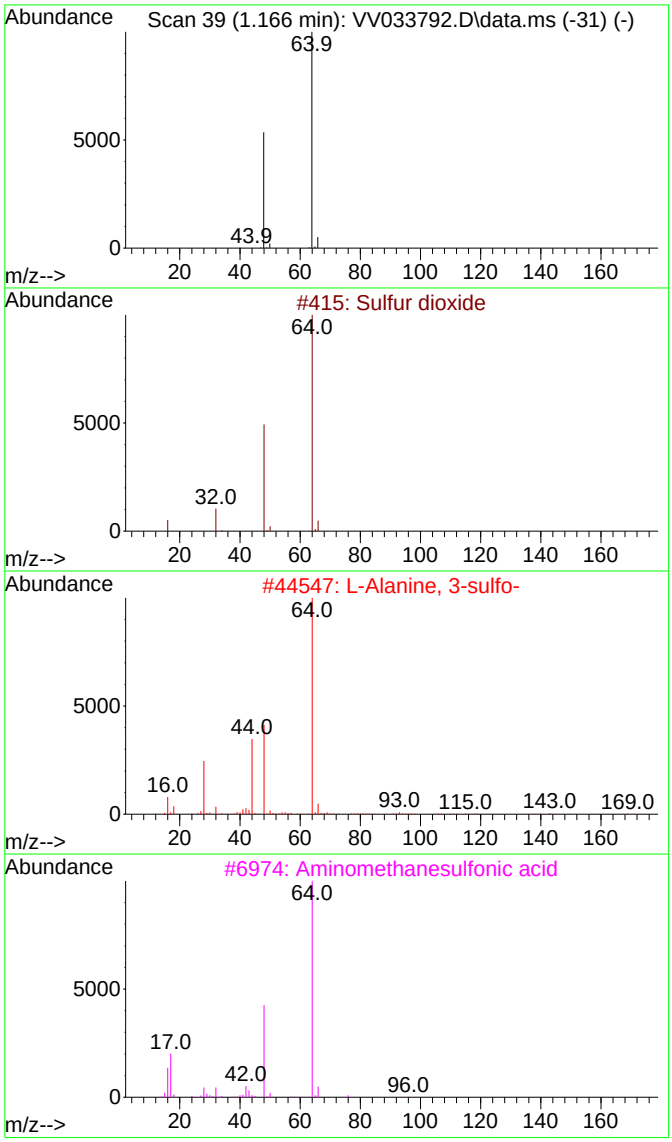
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

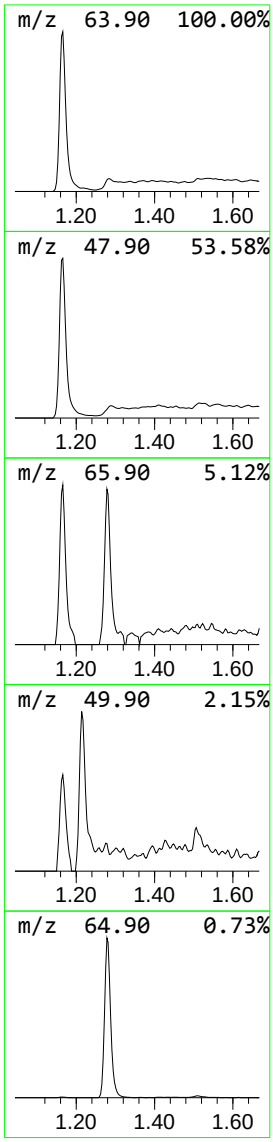
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.166	6.90 ug/L	80010	1,4-Difluorobenzene	5.529

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





Tentatively Identified Compound (LSC) summary

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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	6.9	ug/L	80010	1	5.529	580065	50.0