LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100319\
Data File : VU034921.D
Acq On : 03 Oct 2019 18:06
Operator : JC/SP
Sample : K5058-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBAM2

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_U\METHOD\SOMULM100319WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.325	56	73	89	rBV	338012	1434497	83.85%	9.624%
2	1.395	91	95	103	rVB	246002	278259	16.26%	1.867%
3	1.672	176	181	192	rVB	177843	214393	12.53%	1.438%
4	2.257	354	363	373	rBV	368598	558896	32.67%	3.750%
5	2.309	374	379	392	rVB	53899	81644	4.77%	0.548%
6	2.463	417	427	440	rBV	69607	116166	6.79%	0.779%
7	3.784	827	838	848	rBV5	4290	8045	0.47%	0.054%
8	3.881	864	868	875	rVB2	466	501	0.03%	0.003%
9	3.936	875	885	887	rBV	461	647	0.04%	0.004%
10	4.151	926	952	976	rBV	158814	436839	25.53%	2.931%
11	4.624	1081	1099	1125	rBV	270276	650273	38.01%	4.363%
12	4.849	1167	1169	1170	rBV3	673	310	0.02%	0.002%
13	4.955	1199	1202	1204	rVV2	545	398	0.02%	0.003%
14	4.968	1204	1206	1212	rVV3	889	764	0.04%	0.005%
15	5.096	1244	1246	1248	rVB2	512	244	0.01%	0.002%
16	5.138	1256	1259	1262	rBV3	357	340	0.02%	0.002%
17	5.186	1270	1274	1277	rBV2	310	266	0.02%	0.002%
18	5.202	1277	1279	1283	rVB	386	244	0.01%	0.002%
19	5.318	1291	1315	1345	rBV2	575167	1710828	100.00%	11.478%
20	5.585	1394	1398	1400	rBV4	717	538	0.03%	0.004%
21	5.717	1437	1439	1445	rVB4	384	273	0.02%	0.002%
22	5.784	1452	1460	1466	rBV6	1841	2760	0.16%	0.019%
23	5.865	1471	1485	1511	rBV	508814	1016161	59.40%	6.817%
24	6.308	1603	1623	1646	rBV	380667	809753	47.33%	5.433%
25	6.749	1757	1760	1761	rBV	429	278	0.02%	0.002%
26	6.804	1770	1777	1781	rBV3	627	743	0.04%	0.005%
27	6.845	1787	1790	1792	rBV3	528	349	0.02%	0.002%
28	7.045	1850	1852	1855	rVB2	792	438	0.03%	0.003%
29	7.090	1860	1866	1869	rVB3	415	380	0.02%	0.003%
30	7.112	1869	1873	1877	rBV4	381	377	0.02%	0.003%
31	7.141	1877	1882	1885	rVB4	383	442	0.03%	0.003%
32	7.164	1885	1889	1890	rBV	739	391	0.02%	0.003%
33	7.205	1890	1902	1929	rBV	204745	389856	22.79%	2.616%
34	7.450	1970	1978	1992	rVB5	4530	8172	0.48%	0.055%

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Instrument : MSVOA_U
ClientSampleId : DBAM2

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_U\METHOD\SOMULM100319WMA.M
Title : VOC Analysis

35	7.543	1992	2007	2048	rBV	779562	1408471	82.33%	9.449%
36	7.749	2063	2071	2085	rVB	16994	29208	1.71%	0.196%
37	7.829	2085	2096	2120	rBV	134436	251992	14.73%	1.691%
38	8.048	2160	2164	2166	rBV3	496	420	0.02%	0.003%
39	8.080	2168	2174	2187	rVB7	3960	7237	0.42%	0.049%
40	8.160	2187	2199	2206	rBV2	2678	5001	0.29%	0.034%
41	8.215	2210	2216	2220	rBV5	1351	1517	0.09%	0.010%
42	8.238	2220	2223	2225	rVB3	528	267	0.02%	0.002%
43	8.289	2228	2239	2279	rBV	477288	980204	57.29%	6.576%
44	8.617	2339	2341	2348	rVB6	780	637	0.04%	0.004%
45	8.668	2354	2357	2359	rBV2	494	359	0.02%	0.002%
46	8.739	2377	2379	2383	rBV2	300	233	0.01%	0.002%
47	8.894	2424	2427	2430	rBV3	469	327	0.02%	0.002%
48	8.929	2430	2438	2445	rBV6	2485	4483	0.26%	0.030%
49	8.974	2446	2452	2459	rVB7	2351	3804	0.22%	0.026%
50	9.067	2468	2481	2521	rBV	745636	1279313	74.78%	8.583%
51	9.234	2526	2533	2543	rVB3	5671	9254	0.54%	0.062%
52	9.299	2550	2553	2555	rBV3	913	624	0.04%	0.004%
53	9.324	2555	2561	2562	rVV6	2726	3054	0.18%	0.020%
54	9.357	2564	2571	2584	rVB2	11512	23249	1.36%	0.156%
55	9.447	2594	2599	2600	rBV3	762	554	0.03%	0.004%
56	9.456	2600	2602	2606	rVB2	1150	715	0.04%	0.005%
57	9.492	2611	2613	2617	rVV4	481	302	0.02%	0.002%
58	9.543	2625	2629	2630	rBV2	369	256	0.01%	0.002%
59	9.623	2652	2654	2656	rBV3	427	227	0.01%	0.002%
60	9.636	2656	2658	2662	rVB2	458	276	0.02%	0.002%
61	9.717	2681	2683	2686	rVB	532	258	0.02%	0.002%
62	9.762	2686	2697	2711	rBV2	9801	18122	1.06%	0.122%
63	9.877	2731	2733	2734	rBV	585	238	0.01%	0.002%
64	9.910	2740	2743	2747	rBV4	394	386	0.02%	0.003%
65	9.942	2748	2753	2755	rVV	494	414	0.02%	0.003%
66	10.074	2792	2794	2797	rVV2	399	251	0.01%	0.002%
67	10.144	2813	2816	2821	rVV3	705	640	0.04%	0.004%
68	10.302	2858	2865	2870	rBV5	406	519	0.03%	0.003%
69	10.337	2870	2876	2880	rBV3	606	622	0.04%	0.004%
70	10.408	2886	2898	2925	rBV	538436	875344	51.16%	5.873%
71	10.591	2946	2955	2965	rVB7	2837	4778	0.28%	0.032%

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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBAM2

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_U\METHOD\SOMULM100319WMA.M
Title : VOC Analysis

72	10.649	2969	2973	2975	rBV2	376	328	0.02%	0.002%
73	10.665	2975	2978	2979	rBV3	485	215	0.01%	0.001%
74	10.710	2990	2992	2994	rBV2	465	245	0.01%	0.002%
75	10.755	3000	3006	3008	rBV4	1034	1027	0.06%	0.007%
76	10.887	3044	3047	3049	rBV2	296	218	0.01%	0.001%
77	11.012	3080	3086	3097	rVB6	1435	2302	0.13%	0.015%
78	11.135	3110	3124	3131	rBV7	2468	4309	0.25%	0.029%
79	11.215	3144	3149	3153	rVB3	474	483	0.03%	0.003%
80	11.315	3178	3180	3183	rBV3	440	257	0.02%	0.002%
81	11.347	3188	3190	3194	rVB3	358	225	0.01%	0.002%
82	11.395	3202	3205	3213	rVB6	1912	2432	0.14%	0.016%
83	11.459	3213	3225	3251	rBV	635387	1099174	64.25%	7.374%
84	11.836	3330	3342	3362	rBV	683972	1148494	67.13%	7.705%
85	12.418	3519	3523	3526	rBV3	620	559	0.03%	0.004%
86	12.498	3546	3548	3551	rBV3	484	241	0.01%	0.002%
87	12.610	3579	3583	3584	rBV3	727	378	0.02%	0.003%
88	12.713	3613	3615	3619	rBV3	378	331	0.02%	0.002%
89	12.752	3624	3627	3628	rBV3	466	240	0.01%	0.002%
90	12.784	3633	3637	3638	rBV3	510	424	0.02%	0.003%
91	12.906	3672	3675	3677	rVB3	799	466	0.03%	0.003%
92	13.083	3725	3730	3732	rBV3	1253	1179	0.07%	0.008%
93	13.247	3775	3781	3786	rBV4	767	853	0.05%	0.006%
94	13.299	3791	3797	3798	rBV4	605	582	0.03%	0.004%
95	13.363	3814	3817	3818	rBV	471	235	0.01%	0.002%
96	13.385	3822	3824	3827	rVB3	693	367	0.02%	0.002%
97	13.450	3842	3844	3846	rVB3	578	262	0.02%	0.002%
98	13.668	3909	3912	3914	rVB4	596	276	0.02%	0.002%
99	13.707	3922	3924	3926	rBV3	480	298	0.02%	0.002%
100	13.970	4000	4006	4008	rBV4	974	1095	0.06%	0.007%

Sum of corrected areas: 14905516

LSC Report - Integrated Chromatogram

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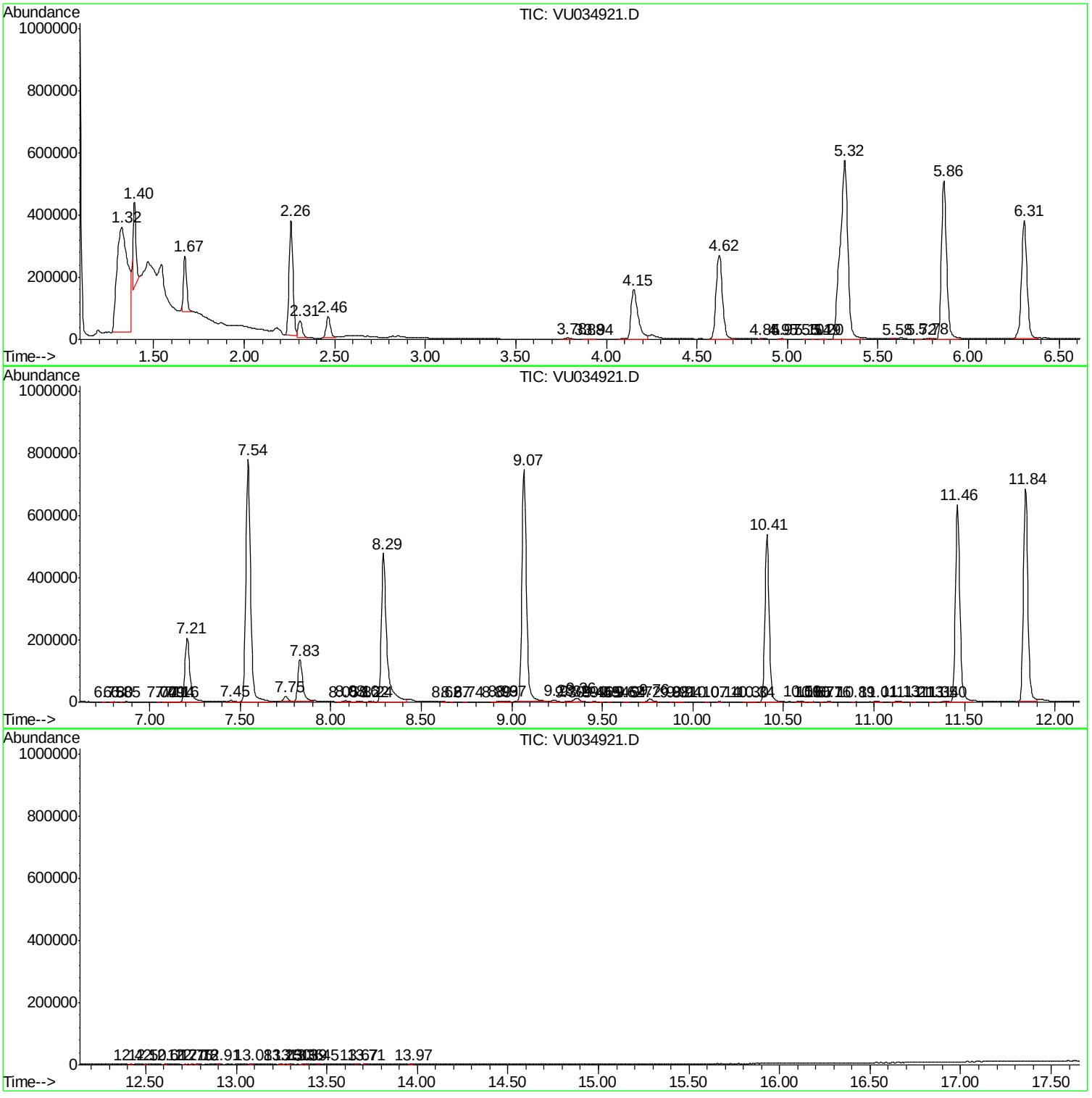
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBAM2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100319WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100319\
Data File : VU034921.D
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Operator : JC/SP
Sample : K5058-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBAM2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100319WMA.M
Quant Title : VOC Analysis

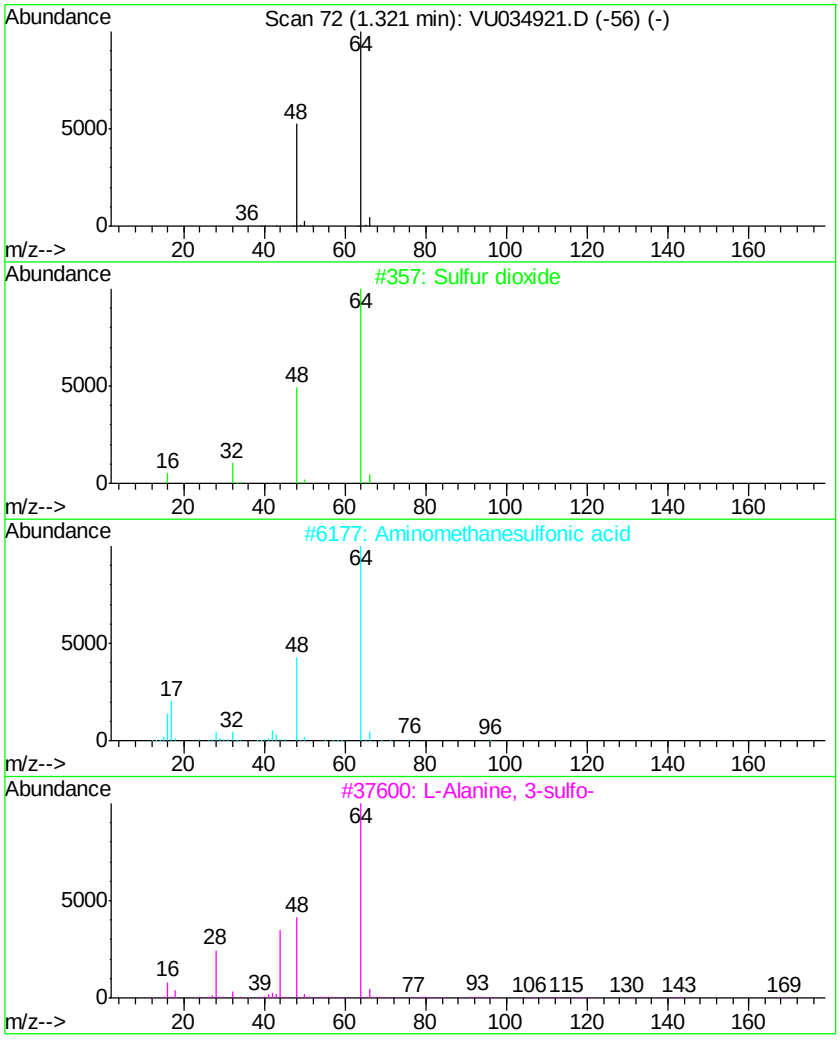
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

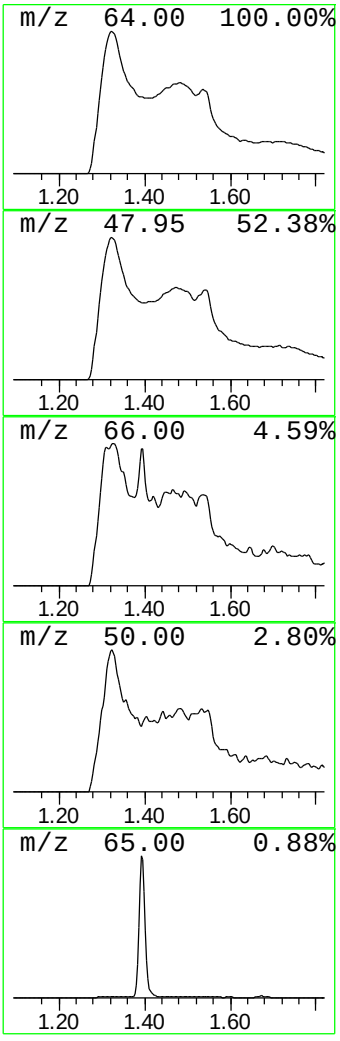
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	70.58 ug/L	1434500	1,4-Difluorobenzene	5.86

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

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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.32	70.6	ug/L	1434500	1	5.86	1016160	50.0