LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU030420\
Data File : VU037058.D
Acq On : 04 Mar 2020 23:41
Operator : JC/MD
Sample : L1780-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DF9

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\SOMULM022420WMA.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	1.478	35	43	55	rBV2	26294	54636	0.03%	0.009%
2	1.610	78	84	95	rVB	139996	150793	0.09%	0.025%
3	1.919	172	180	196	rVB	119257	162678	0.10%	0.027%
4	2.588	375	388	402	rBV	201790	332105	0.20%	0.054%
5	2.655	403	409	422	rVB	6284	10455	0.01%	0.002%
6	2.793	438	452	472	rBV	31417	65167	0.04%	0.011%
7	3.076	531	540	553	rBV5	2704	4772	0.00%	0.001%
8	3.125	553	555	557	rVV	515	301	0.00%	0.000%
9	3.163	558	567	576	rVV4	3488	7494	0.00%	0.001%
10	3.224	576	586	601	rVB4	2731	6604	0.00%	0.001%
11	3.379	629	634	636	rBV3	883	849	0.00%	0.000%
12	3.462	657	660	667	rVB2	294	301	0.00%	0.000%
13	3.594	697	701	711	rVB2	373	401	0.00%	0.000%
14	3.729	737	743	744	rBV	743	557	0.00%	0.000%
15	3.809	761	768	772	rBV2	244	248	0.00%	0.000%
16	4.018	830	833	841	rVB3	433	458	0.00%	0.000%
17	4.195	881	888	891	rBV2	208	291	0.00%	0.000%
18	4.388	945	948	955	rBV2	212	250	0.00%	0.000%
19	4.571	988	1005	1020	rBV3	27286	64942	0.04%	0.011%
20	4.668	1020	1035	1060	rBV	101806	236785	0.15%	0.039%
21	4.848	1076	1091	1107	rBV	28296	60813	0.04%	0.010%
22	4.977	1127	1131	1134	rBV	288	234	0.00%	0.000%
23	5.125	1153	1177	1204	rBV2	540541	1447874	0.89%	0.237%
24	5.263	1217	1220	1223	rVB	378	244	0.00%	0.000%
25	5.285	1223	1227	1229	rBV3	467	326	0.00%	0.000%
26	5.317	1233	1237	1241	rBV4	726	848	0.00%	0.000%
27	5.369	1250	1253	1256	rVB2	493	303	0.00%	0.000%
28	5.424	1256	1270	1282	rBV4	14315	32557	0.02%	0.005%
29	5.488	1288	1290	1293	rBV3	402	272	0.00%	0.000%
30	5.562	1301	1313	1323	rBV4	2665	5742	0.00%	0.001%
31	5.620	1328	1331	1339	rVB3	812	890	0.00%	0.000%
32	5.658	1339	1343	1344	rBV3	728	469	0.00%	0.000%
33	5.819	1354	1393	1432	rBV2	32319430	67291555	41.44%	11.018%
34	6.282	1525	1537	1553	rVB	345378	643863	0.40%	0.105%

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ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DF9

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Title : VOC Analysis

35	6.523	1608	1612	1615	rVB2	283	235	0.00%	0.000%
36	6.571	1615	1627	1638	rBV5	11240	21682	0.01%	0.004%
37	6.723	1660	1674	1689	rBV	246625	481205	0.30%	0.079%
38	7.009	1757	1763	1768	rVB4	2002	2695	0.00%	0.000%
39	7.134	1792	1802	1812	rBV3	4367	7139	0.00%	0.001%
40	7.208	1816	1825	1835	rVB3	2799	4664	0.00%	0.001%
41	7.350	1863	1869	1871	rBV2	302	270	0.00%	0.000%
42	7.436	1887	1896	1897	rBV4	938	1133	0.00%	0.000%
43	7.594	1931	1945	1959	rBV	130035	223547	0.14%	0.037%
44	7.713	1973	1982	1991	rVB5	1924	3172	0.00%	0.001%
45	7.771	1995	2000	2005	rBV2	247	282	0.00%	0.000%
46	7.925	2033	2048	2062	rBV	494721	841870	0.52%	0.138%
47	7.996	2063	2070	2081	rVV2	8227	13583	0.01%	0.002%
48	8.079	2092	2096	2100	rVB3	425	396	0.00%	0.000%
49	8.205	2121	2135	2152	rBV	95157	154676	0.10%	0.025%
50	8.346	2176	2179	2185	rBV2	251	266	0.00%	0.000%
51	8.417	2197	2201	2207	rVB2	193	273	0.00%	0.000%
52	8.452	2207	2212	2214	rBV2	309	353	0.00%	0.000%
53	8.497	2216	2226	2238	rVB5	2158	3956	0.00%	0.001%
54	8.575	2242	2250	2259	rVB4	7866	12870	0.01%	0.002%
55	8.661	2264	2277	2305	rBV	320670	544434	0.34%	0.089%
56	8.832	2321	2330	2340	rVB2	7313	11548	0.01%	0.002%
57	9.041	2393	2395	2400	rVB	280	233	0.00%	0.000%
58	9.073	2400	2405	2410	rBV	253	353	0.00%	0.000%
59	9.488	2506	2534	2570	rVV3	66749970	129173640	79.55%	21.151%
60	9.684	2592	2595	2597	rBV3	424	266	0.00%	0.000%
61	9.822	2636	2638	2642	rVB2	398	243	0.00%	0.000%
62	9.919	2665	2668	2672	rVB3	434	279	0.00%	0.000%
63	10.121	2721	2731	2732	rBV3	701	740	0.00%	0.000%
64	10.147	2737	2739	2745	rVB2	322	338	0.00%	0.000%
65	10.198	2751	2755	2757	rBV2	282	250	0.00%	0.000%
66	10.311	2780	2790	2807	rBV2	19066	30662	0.02%	0.005%
67	10.491	2843	2846	2848	rVV	365	248	0.00%	0.000%
68	10.613	2881	2884	2888	rBV2	452	322	0.00%	0.000%
69	10.639	2888	2892	2895	rVV	250	248	0.00%	0.000%
70	10.774	2922	2934	2955	rVV2	336669	682650	0.42%	0.112%
71	10.909	2969	2976	2982	rVB5	1286	1749	0.00%	0.000%

LSC Area Percent Report

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Sample : L1780-05
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 30 Sample Multiplier: 1

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ClientSampleId : C0DF9

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\SOMULM022420WMA.M
Title : VOC Analysis

72	11.002	2994	3005	3016	rVB2	27414	41868	0.03%	0.007%
73	11.070	3017	3026	3030	rBV5	732	1018	0.00%	0.000%
74	11.115	3030	3040	3050	rVB	12827	18934	0.01%	0.003%
75	11.169	3054	3057	3062	rVB2	331	231	0.00%	0.000%
76	11.378	3118	3122	3127	rVB2	262	307	0.00%	0.000%
77	11.488	3151	3156	3161	rVB	743	635	0.00%	0.000%
78	11.655	3200	3208	3219	rVB3	2665	3813	0.00%	0.001%
79	11.767	3226	3243	3256	rBV	15575438	25356079	15.61%	4.152%
80	11.877	3256	3277	3293	rVB3	77456031	157327048	96.89%	25.761%
81	12.256	3370	3395	3409	rBV4	77445037	162384297	100.00%	26.589%
82	12.703	3526	3534	3545	rBV6	3256	5172	0.00%	0.001%
83	12.922	3593	3602	3611	rBV6	5000	7713	0.00%	0.001%
84	12.989	3611	3623	3635	rBV2	169569	267417	0.16%	0.044%
85	13.169	3667	3679	3688	rBV3	47030	109820	0.07%	0.018%
86	13.234	3688	3699	3723	rVV	603387	985978	0.61%	0.161%
87	13.349	3725	3735	3748	rVB	114959	185784	0.11%	0.030%
88	13.597	3803	3812	3822	rBV2	9672	15379	0.01%	0.003%
89	13.680	3834	3838	3844	rVB4	694	771	0.00%	0.000%
90	13.725	3850	3852	3854	rBV2	488	231	0.00%	0.000%
91	13.880	3882	3900	3922	rBV	29123005	46462197	28.61%	7.608%
92	14.115	3967	3973	3986	rVB2	5994	8611	0.01%	0.001%
93	14.182	3992	3994	3997	rBV2	410	270	0.00%	0.000%
94	14.365	4035	4051	4074	rBV	8877840	13915484	8.57%	2.279%
95	14.709	4156	4158	4164	rVB3	514	272	0.00%	0.000%
96	14.764	4164	4175	4190	rBV2	49420	80792	0.05%	0.013%
97	14.886	4204	4213	4215	rBV5	1806	2961	0.00%	0.000%
98	15.295	4338	4340	4345	rBV2	411	378	0.00%	0.000%
99	15.455	4374	4390	4404	rVB	165516	296980	0.18%	0.049%
100	16.047	4562	4574	4588	rBV	264525	434919	0.27%	0.071%

Sum of corrected areas: 610723906

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU030420\
Data File : VU037058.D
Acq On : 04 Mar 2020 23:41
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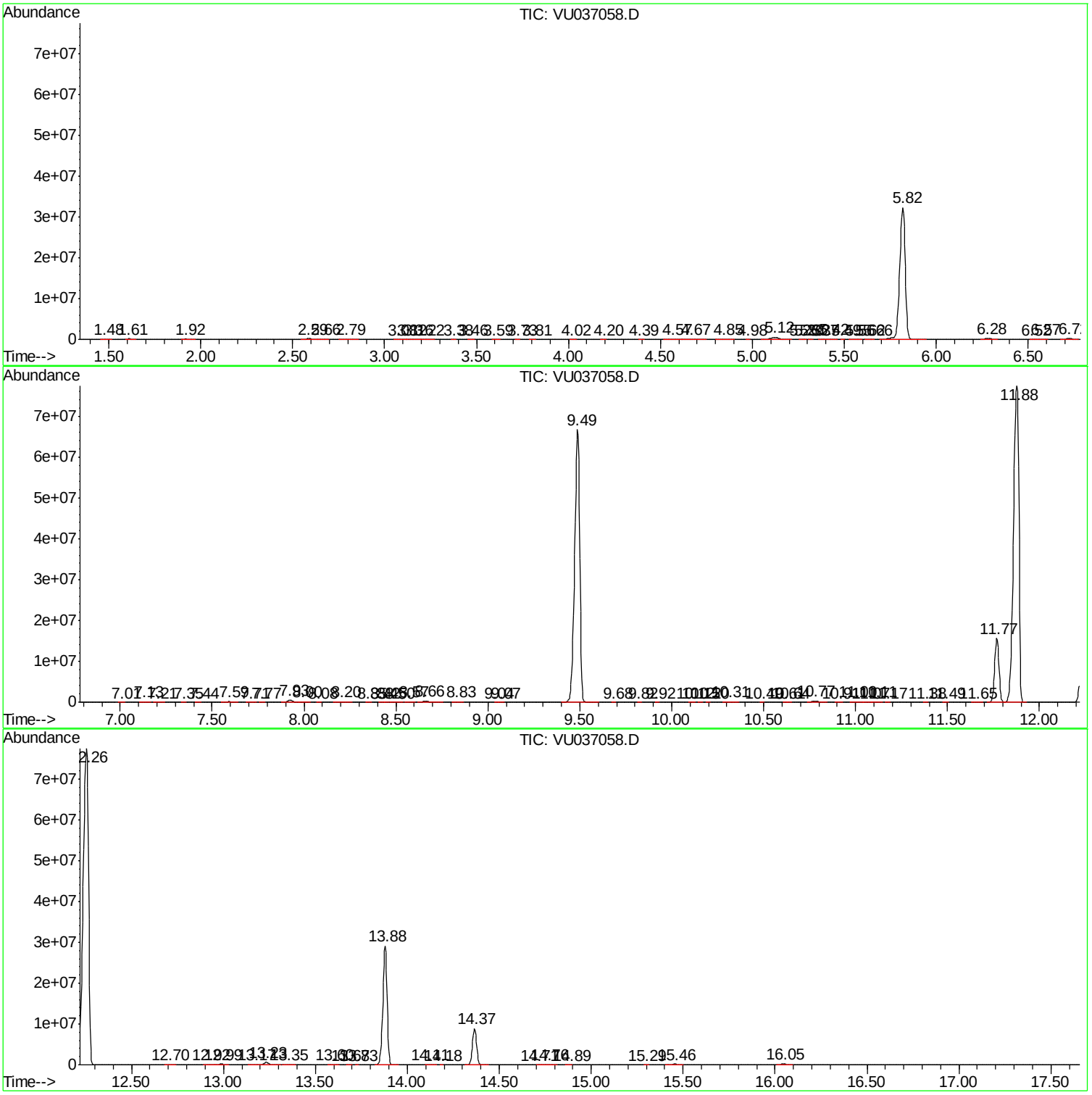
Sample : L1780-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DF9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

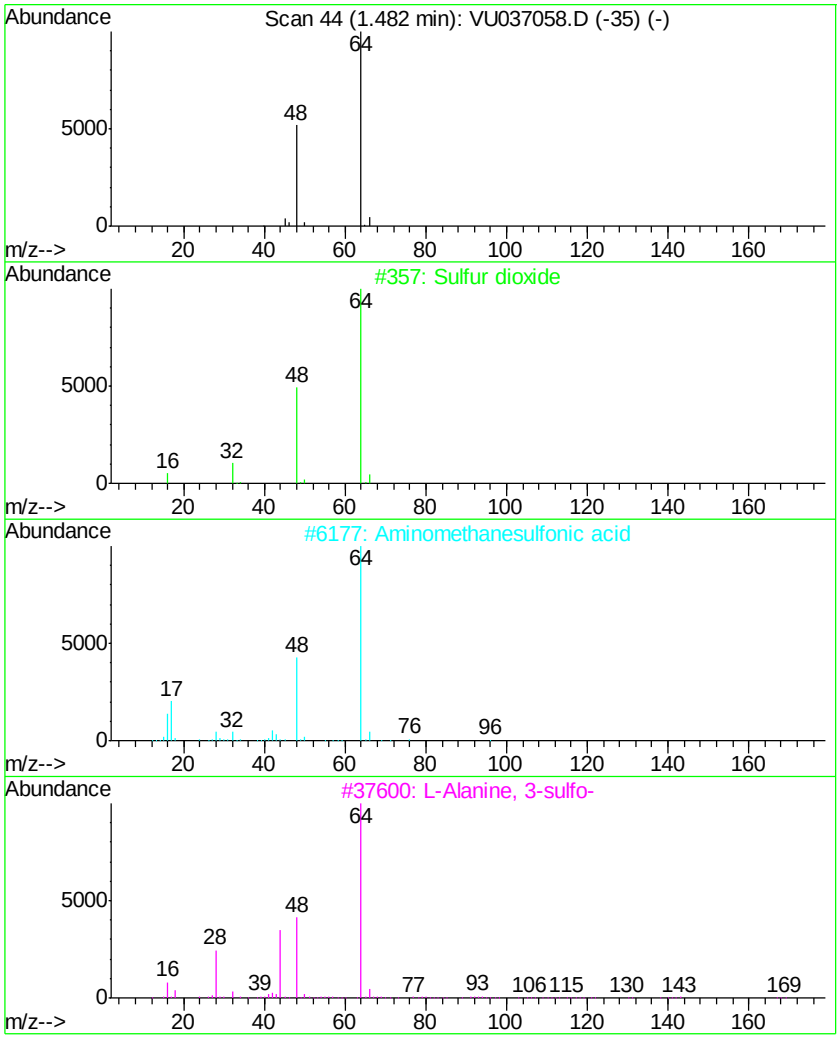
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

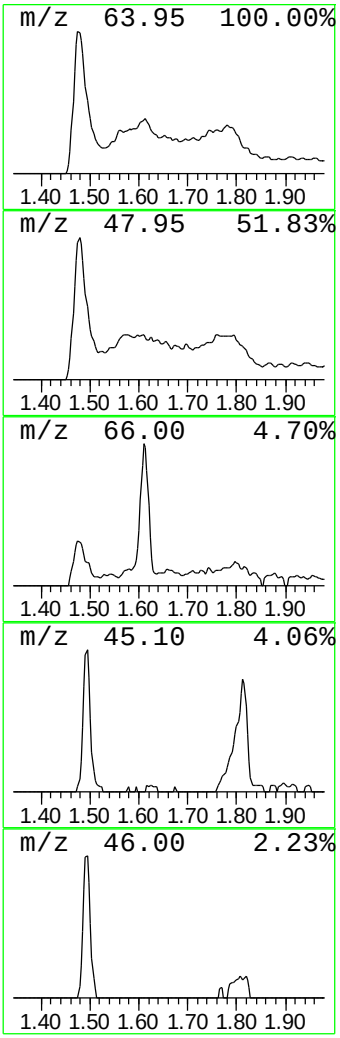
****

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	4.24 ug/L	54636	1,4-Difluorobenzene	6.28

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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU030420\
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Acq On : 04 Mar 2020 23:41
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ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DF9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

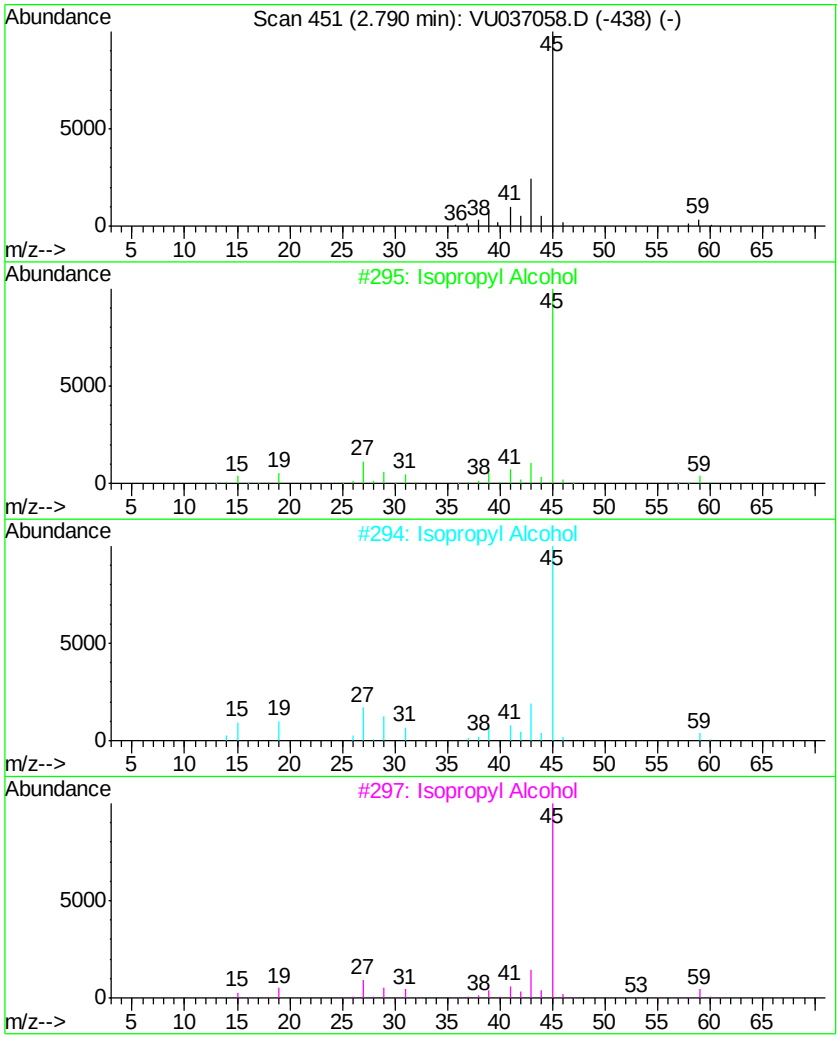
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

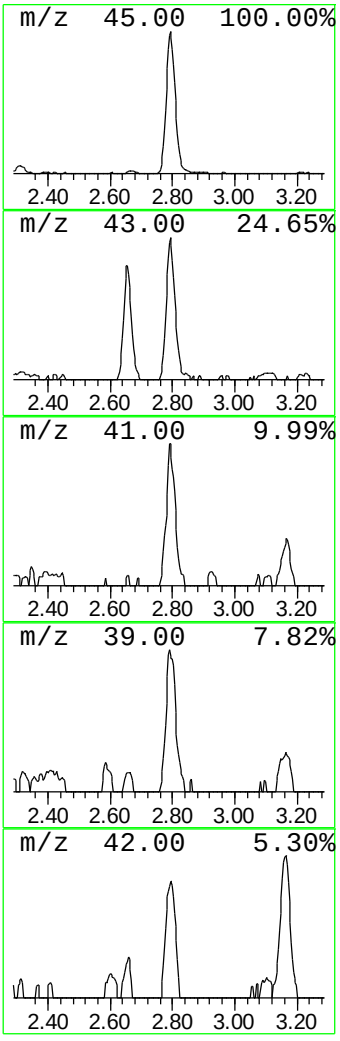
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	5.06 ug/L	65167	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40





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Instrument : MSVOA_U
ClientSampleId : C0DF9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

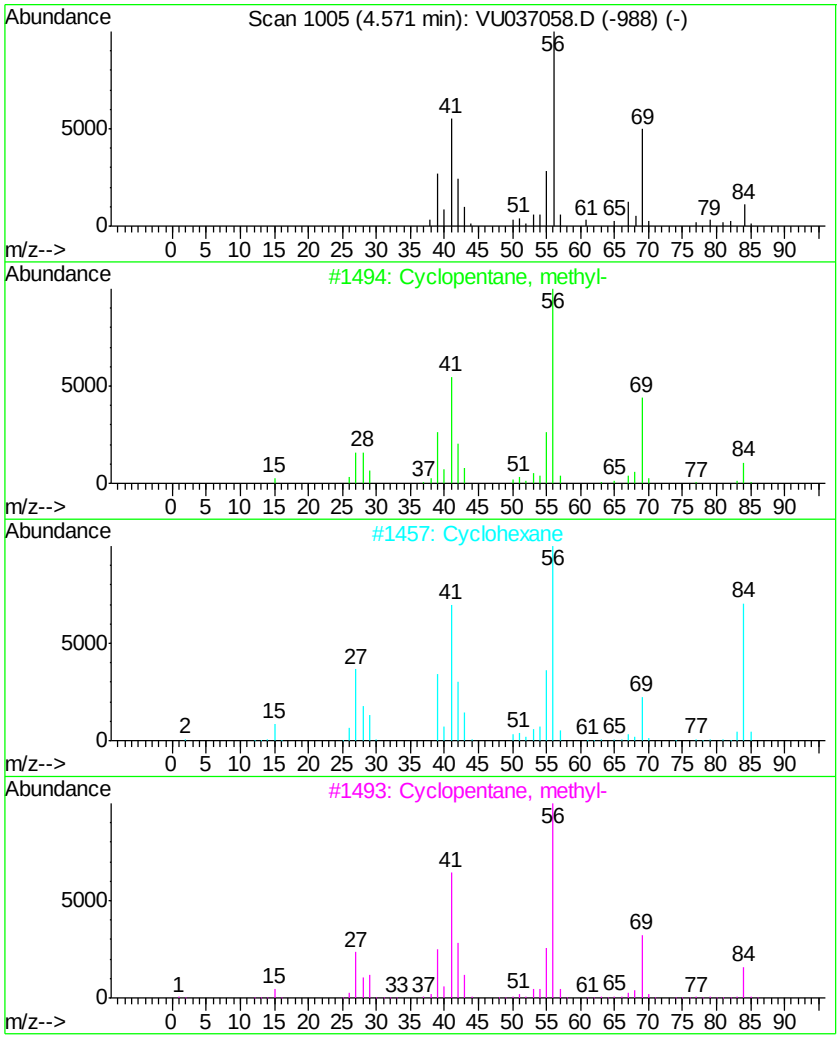
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

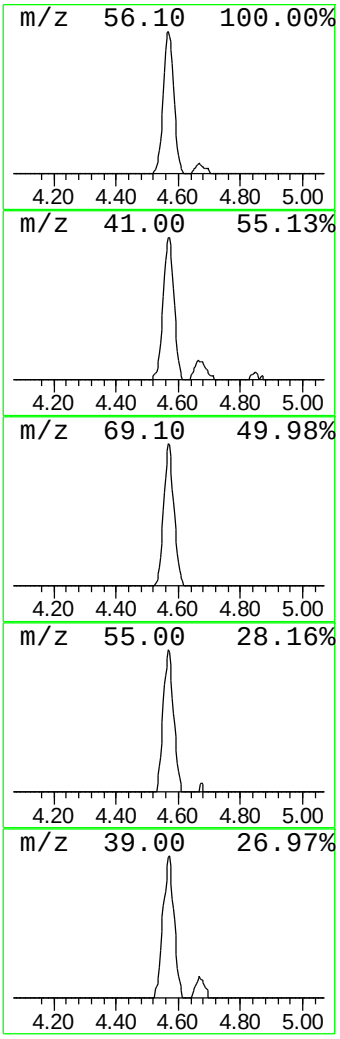
****

Peak Number 3 (DEL) Alkane: Cyclic4.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	5.04 ug/L	64942	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclohexane	84	C6H12	000110-82-7	80
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4	Cyclohexane	84	C6H12	000110-82-7	72
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72





Library Search Compound Report

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ALS Vial : 30 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DF9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

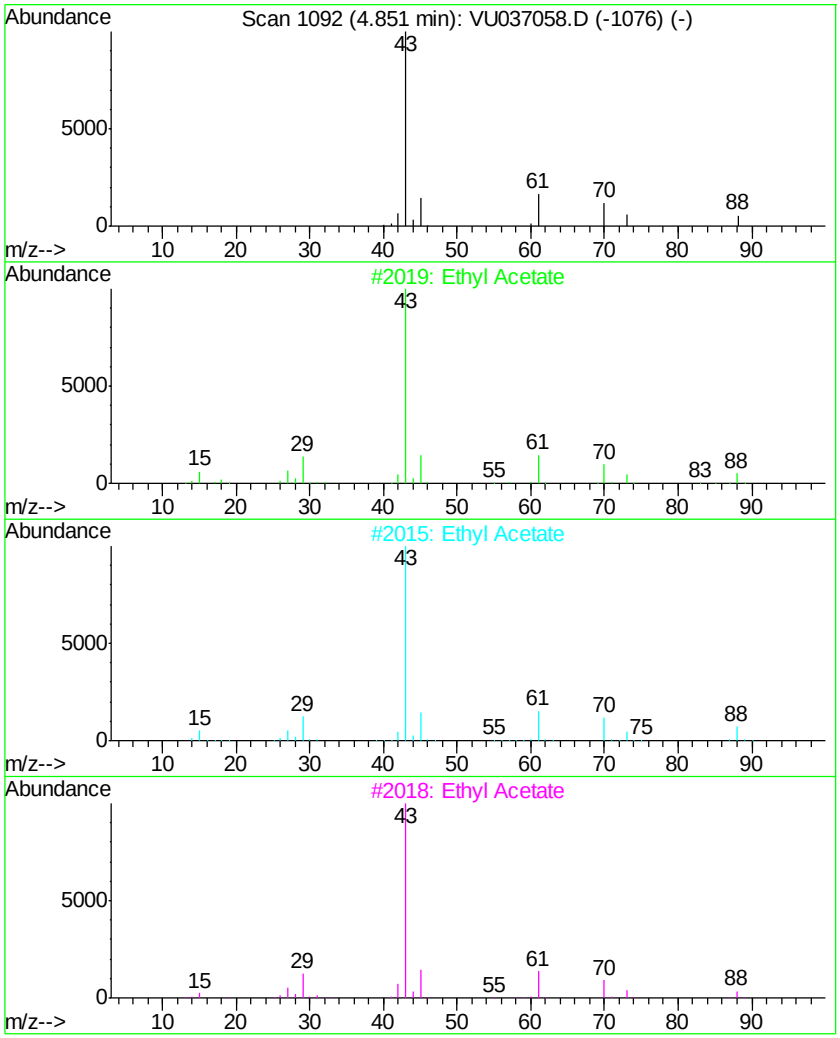
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

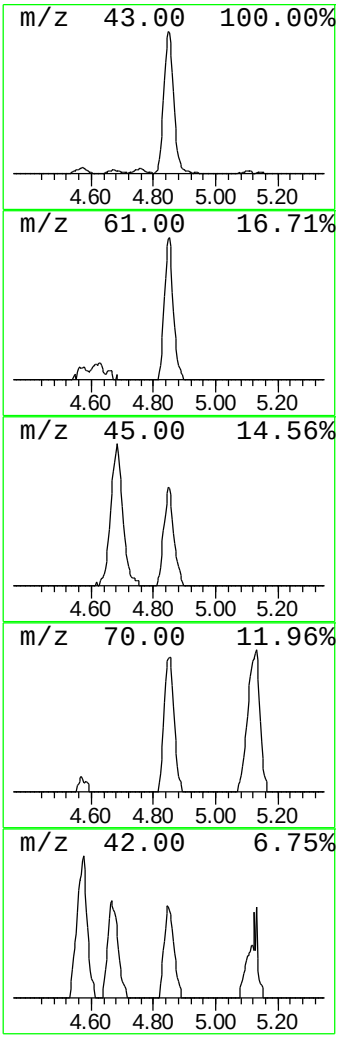
****

Peak Number 4 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	4.72 ug/L	60813	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2	Ethyl Acetate	88	C4H8O2	000141-78-6	90
3	Ethyl Acetate	88	C4H8O2	000141-78-6	90
4	Ethyl Acetate	88	C4H8O2	000141-78-6	90
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9





Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_U
ClientSampleId : C0DF9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
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	1.48	4.2	ug/L	54636	1	6.28	643863	50.0
Isopropyl Alcohol	2.79	5.1	ug/L	65167	1	6.28	643863	50.0
(DEL) Alkane: Cyc...	4.57	5.0	ug/L	64942	1	6.28	643863	50.0
Ethyl Acetate	4.85	4.7	ug/L	60813	1	6.28	643863	50.0