LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU030420\
Data File : VU037061.D
Acq On : 05 Mar 2020 00:51
Operator : JC/MD
Sample : L1780-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DG5

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	1.482	35	44	56	rBV	43212	90823	0.03%	0.014%
2	1.610	78	84	93	rBV	144714	149831	0.05%	0.022%
3	1.919	172	180	199	rVB	126761	172329	0.06%	0.026%
4	2.588	375	388	403	rBV2	221594	395785	0.13%	0.059%
5	2.658	404	410	420	rVV4	4677	7928	0.00%	0.001%
6	2.703	420	424	433	rVB3	877	923	0.00%	0.000%
7	2.793	439	452	468	rBV2	25094	52381	0.02%	0.008%
8	2.909	484	488	493	rBV4	380	424	0.00%	0.000%
9	2.928	493	494	499	rVB2	468	219	0.00%	0.000%
10	3.009	516	519	523	rBV2	369	287	0.00%	0.000%
11	3.063	531	536	539	rBV4	718	683	0.00%	0.000%
12	3.080	539	541	544	rVB3	513	225	0.00%	0.000%
13	3.102	546	548	551	rBV2	420	262	0.00%	0.000%
14	3.163	555	567	579	rBV3	18306	35959	0.01%	0.005%
15	3.211	579	582	585	rBV2	1730	1503	0.00%	0.000%
16	3.385	625	636	648	rBV4	6924	13258	0.00%	0.002%
17	3.613	700	707	709	rBV	258	275	0.00%	0.000%
18	3.732	742	744	750	rVV3	432	487	0.00%	0.000%
19	3.899	787	796	797	rBV2	460	506	0.00%	0.000%
20	4.353	930	937	939	rBV2	190	259	0.00%	0.000%
21	4.424	951	959	961	rBV2	234	324	0.00%	0.000%
22	4.568	990	1004	1020	rVV2	39159	96007	0.03%	0.014%
23	4.671	1020	1036	1060	rBV	103561	272447	0.09%	0.041%
24	4.851	1077	1092	1110	rBV3	18102	41869	0.01%	0.006%
25	4.941	1116	1120	1123	rBV3	335	229	0.00%	0.000%
26	4.986	1128	1134	1139	rBV3	349	522	0.00%	0.000%
27	5.102	1151	1170	1190	rBV	184341	409674	0.13%	0.061%
28	5.192	1196	1198	1204	rVB2	494	470	0.00%	0.000%
29	5.330	1230	1241	1243	rBV5	606	825	0.00%	0.000%
30	5.427	1248	1271	1286	rBV2	20205	45414	0.01%	0.007%
31	5.559	1304	1312	1316	rBV2	174	279	0.00%	0.000%
32	5.848	1355	1402	1411	rBV8	77142525	308440711	100.00%	46.048%
33	6.285	1530	1538	1555	rVB	386332	704244	0.23%	0.105%
34	6.520	1606	1611	1615	rVB3	317	351	0.00%	0.000%

LSC Area Percent Report

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Sample : L1780-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DG5

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

35	6.575	1615	1628	1639	rBV3	15912	30030	0.01%	0.004%
36	6.726	1659	1675	1691	rBV	274755	527891	0.17%	0.079%
37	6.870	1718	1720	1728	rVB3	532	523	0.00%	0.000%
38	6.948	1740	1744	1749	rVB3	332	290	0.00%	0.000%
39	7.002	1753	1761	1772	rVV3	3950	7124	0.00%	0.001%
40	7.086	1785	1787	1793	rVB	369	296	0.00%	0.000%
41	7.124	1793	1799	1802	rBV3	336	433	0.00%	0.000%
42	7.208	1817	1825	1835	rVB4	3609	6157	0.00%	0.001%
43	7.382	1876	1879	1881	rBV	359	236	0.00%	0.000%
44	7.436	1889	1896	1905	rVV6	1643	3070	0.00%	0.000%
45	7.594	1932	1945	1960	rBV	143937	246296	0.08%	0.037%
46	7.706	1972	1980	1987	rBV3	2014	3135	0.00%	0.000%
47	7.745	1987	1992	2002	rVB4	1707	2207	0.00%	0.000%
48	7.819	2011	2015	2019	rBV2	728	817	0.00%	0.000%
49	7.925	2034	2048	2063	rVV	552927	935338	0.30%	0.140%
50	7.996	2063	2070	2081	rVB2	14122	21756	0.01%	0.003%
51	8.108	2102	2105	2110	rBV2	206	233	0.00%	0.000%
52	8.205	2122	2135	2150	rBV2	100557	168546	0.05%	0.025%
53	8.366	2181	2185	2187	rBV2	537	408	0.00%	0.000%
54	8.494	2216	2225	2238	rVB3	1524	2398	0.00%	0.000%
55	8.546	2238	2241	2245	rBV2	269	223	0.00%	0.000%
56	8.610	2257	2261	2265	rBV2	322	301	0.00%	0.000%
57	8.665	2265	2278	2309	rBV	307467	563258	0.18%	0.084%
58	8.906	2348	2353	2358	rVB2	436	403	0.00%	0.000%
59	9.018	2385	2388	2390	rVV2	403	252	0.00%	0.000%
60	9.031	2390	2392	2396	rVV2	326	220	0.00%	0.000%
61	9.111	2411	2417	2421	rBV2	230	334	0.00%	0.000%
62	9.179	2434	2438	2441	rBV2	241	238	0.00%	0.000%
63	9.275	2465	2468	2473	rVB3	468	277	0.00%	0.000%
64	9.304	2473	2477	2480	rBV	263	224	0.00%	0.000%
65	9.497	2507	2537	2544	rBV7	81672728	235293289	76.28%	35.128%
66	10.189	2749	2752	2753	rBV2	434	271	0.00%	0.000%
67	10.382	2810	2812	2816	rVB3	561	316	0.00%	0.000%
68	10.439	2828	2830	2833	rBV	406	303	0.00%	0.000%
69	10.542	2860	2862	2867	rVB3	535	396	0.00%	0.000%
70	10.597	2877	2879	2883	rVB3	445	238	0.00%	0.000%
71	10.658	2896	2898	2902	rBV2	260	220	0.00%	0.000%

LSC Area Percent Report

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ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DG5

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

72	10.774	2922	2934	2960	rVB	341411	578998	0.19%	0.086%
73	10.902	2969	2974	2976	rBV4	924	800	0.00%	0.000%
74	11.002	2997	3005	3017	rBV2	13295	20445	0.01%	0.003%
75	11.118	3032	3041	3049	rVB3	6573	9596	0.00%	0.001%
76	11.333	3104	3108	3109	rBV	354	246	0.00%	0.000%
77	11.484	3153	3155	3158	rVB3	482	287	0.00%	0.000%
78	11.500	3158	3160	3167	rVB2	275	250	0.00%	0.000%
79	11.568	3178	3181	3186	rVB2	298	221	0.00%	0.000%
80	11.764	3228	3242	3253	rBV	2352941	3693164	1.20%	0.551%
81	11.864	3253	3273	3290	rVB2	47533691	78371187	25.41%	11.700%
82	12.070	3334	3337	3344	rVB8	1456	1595	0.00%	0.000%
83	12.102	3344	3347	3348	rBV2	507	224	0.00%	0.000%
84	12.237	3368	3389	3405	rBV	23533661	37786573	12.25%	5.641%
85	12.507	3470	3473	3479	rBV2	291	367	0.00%	0.000%
86	12.989	3617	3623	3633	rVB5	2456	3541	0.00%	0.001%
87	13.172	3677	3680	3685	rVB3	700	549	0.00%	0.000%
88	13.240	3692	3701	3707	rVB8	1339	2323	0.00%	0.000%
89	13.803	3871	3876	3878	rBV3	346	383	0.00%	0.000%
90	13.870	3884	3897	3912	rBV	349986	553140	0.18%	0.083%
91	14.002	3935	3938	3940	rBV3	384	254	0.00%	0.000%
92	14.118	3966	3974	3985	rBV2	4024	5482	0.00%	0.001%
93	14.246	4010	4014	4018	rBV4	299	345	0.00%	0.000%
94	14.288	4024	4027	4034	rBV2	272	285	0.00%	0.000%
95	14.362	4041	4050	4060	rBV2	17420	25982	0.01%	0.004%
96	14.651	4135	4140	4141	rBV2	373	352	0.00%	0.000%
97	14.680	4146	4149	4150	rBV	452	255	0.00%	0.000%
98	14.764	4172	4175	4176	rBV	466	245	0.00%	0.000%
99	15.857	4512	4515	4519	rBV3	624	548	0.00%	0.000%
100	16.047	4569	4574	4583	rVB6	2666	3846	0.00%	0.001%

Sum of corrected areas: 669817143

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU030420\
Data File : VU037061.D
Acq On : 05 Mar 2020 00:51
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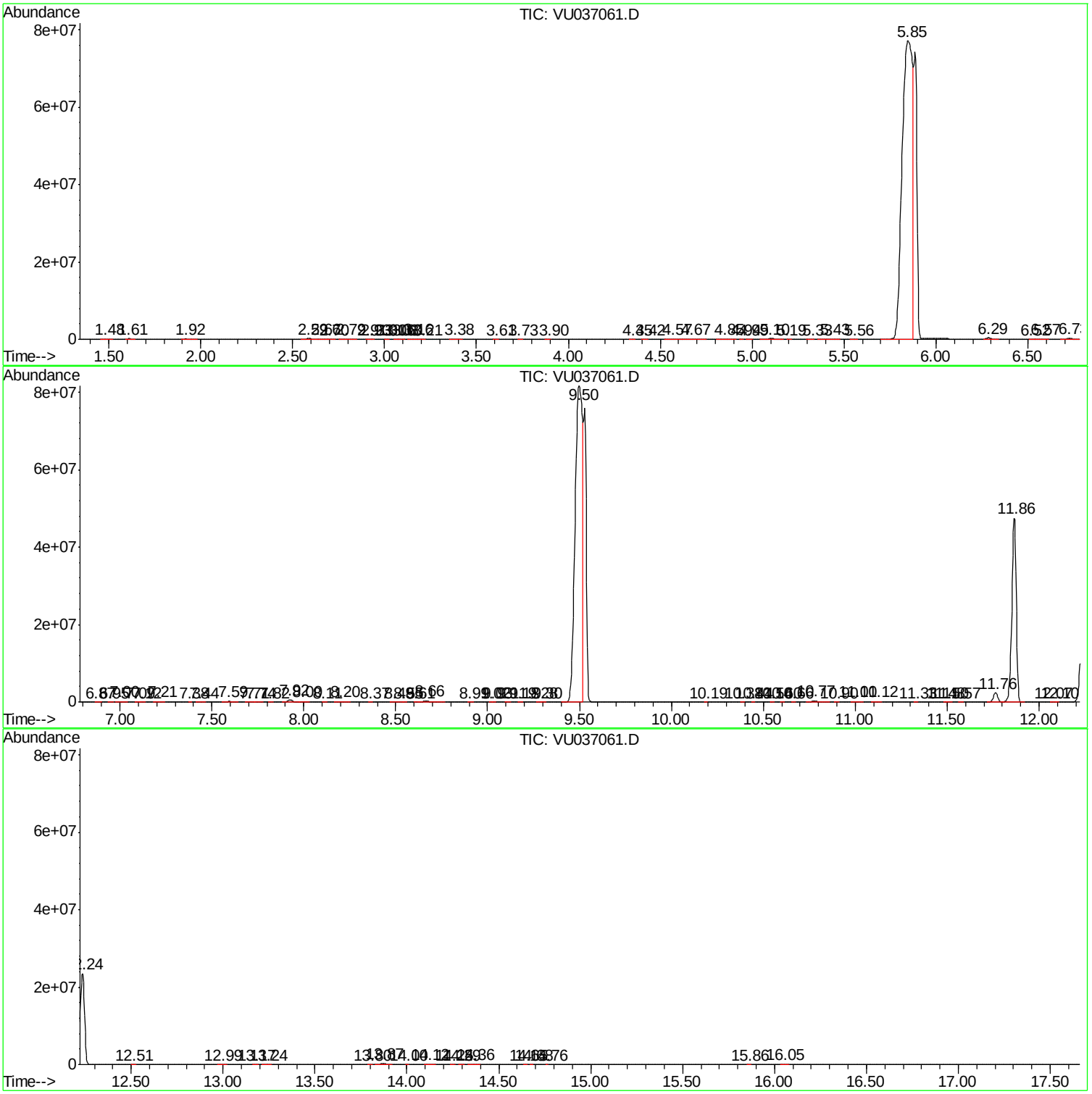
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DG5

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 Title : VOC Analysis

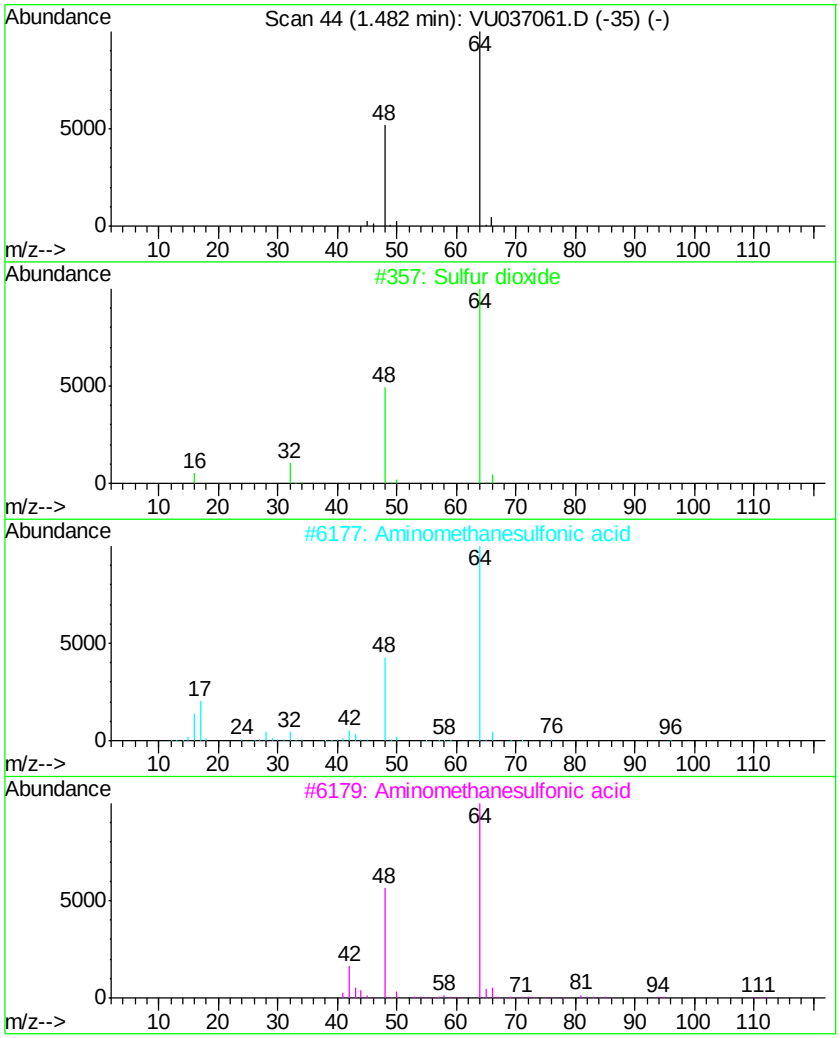
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

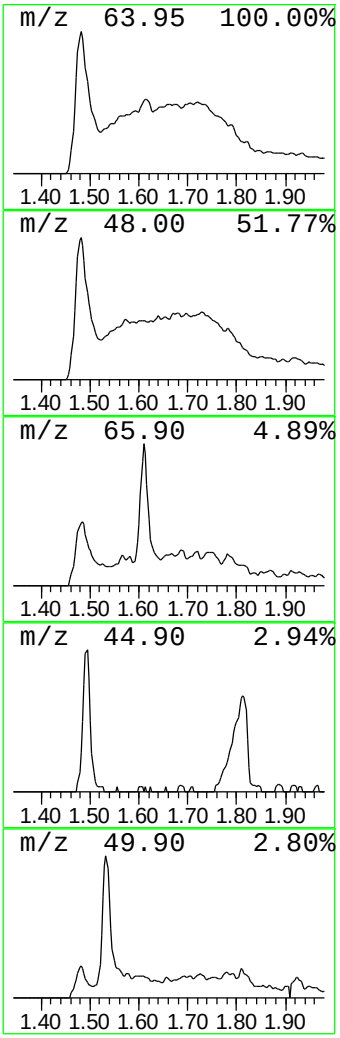
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	6.45 ug/L	90823	1,4-Difluorobenzene	6.29

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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU030420\
Data File : VU037061.D
Acq On : 05 Mar 2020 00:51
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ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DG5

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

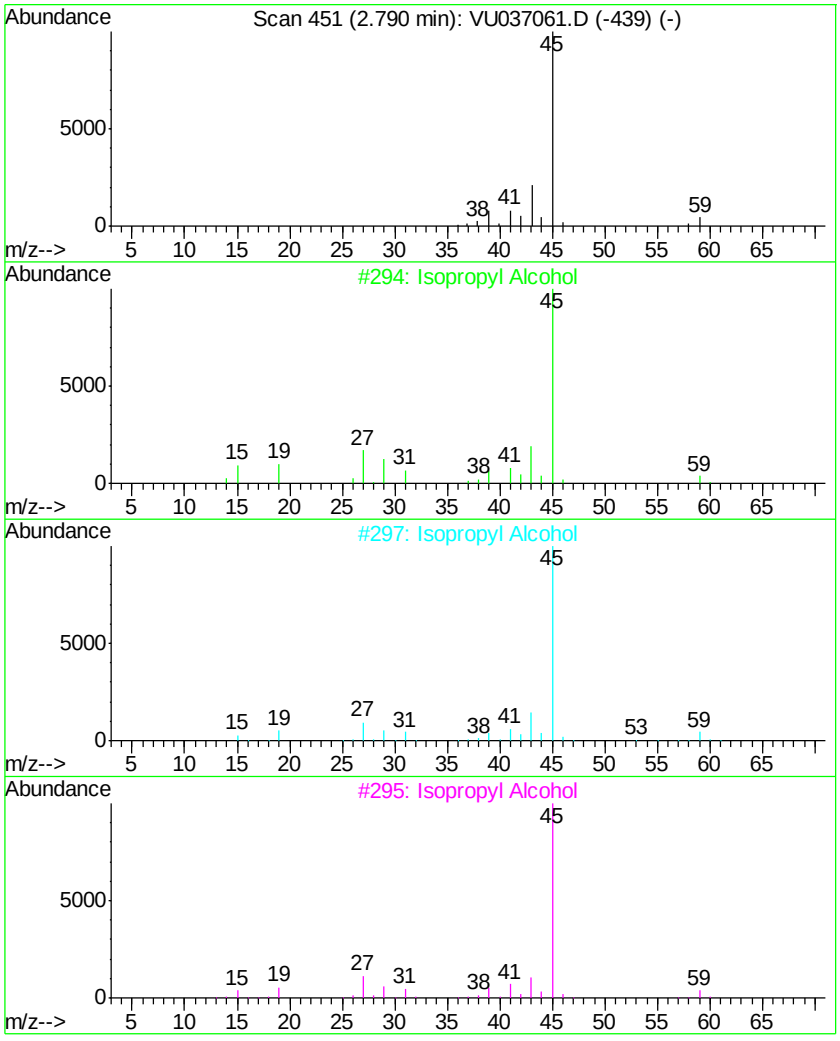
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

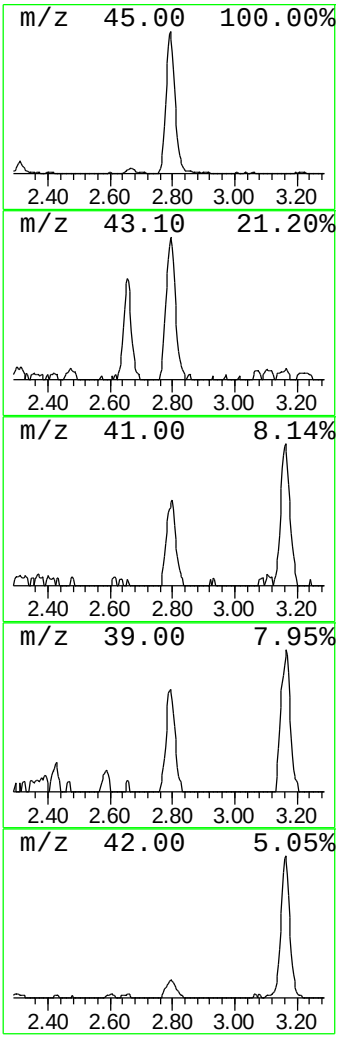
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	3.72 ug/L	52381	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Ethylamine	45	C2H7N	000075-04-7	4





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Instrument : MSVOA_U
ClientSampleId : C0DG5

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

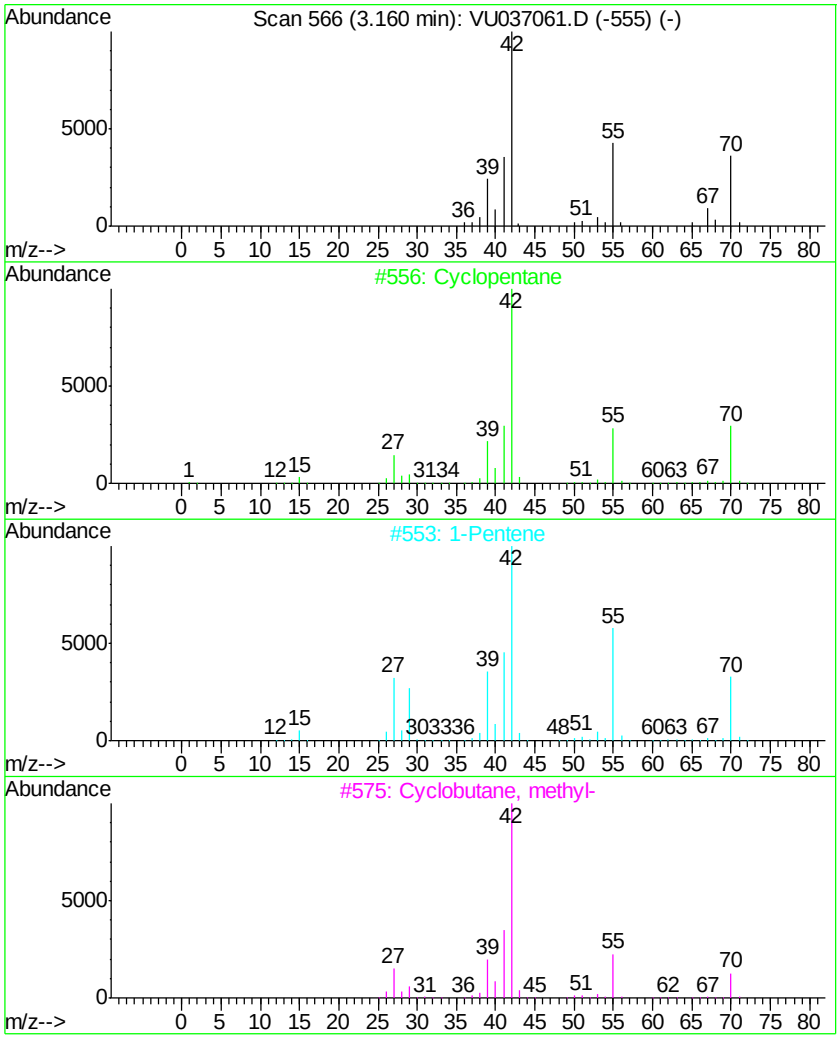
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

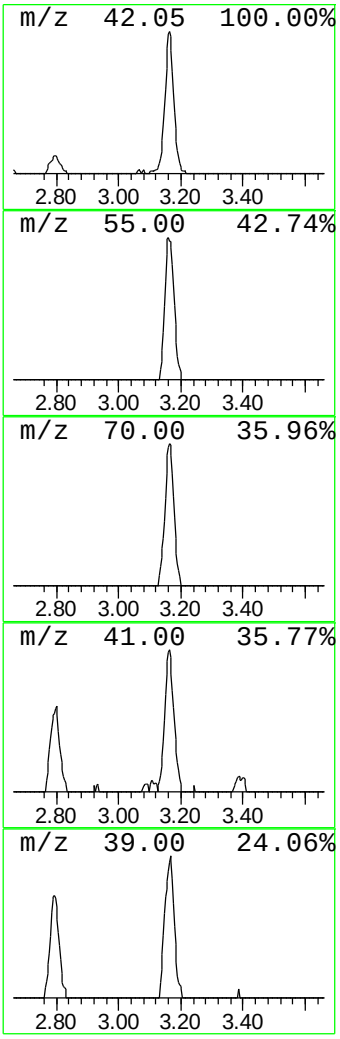
****

Peak Number 3 (DEL) Alkane: Cyclic3.16 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.16	2.55 ug/L	35959	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	1-Pentene	70	C5H10	000109-67-1	78
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4	1-Pentene	70	C5H10	000109-67-1	72
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	72





Library Search Compound Report

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ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DG5

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

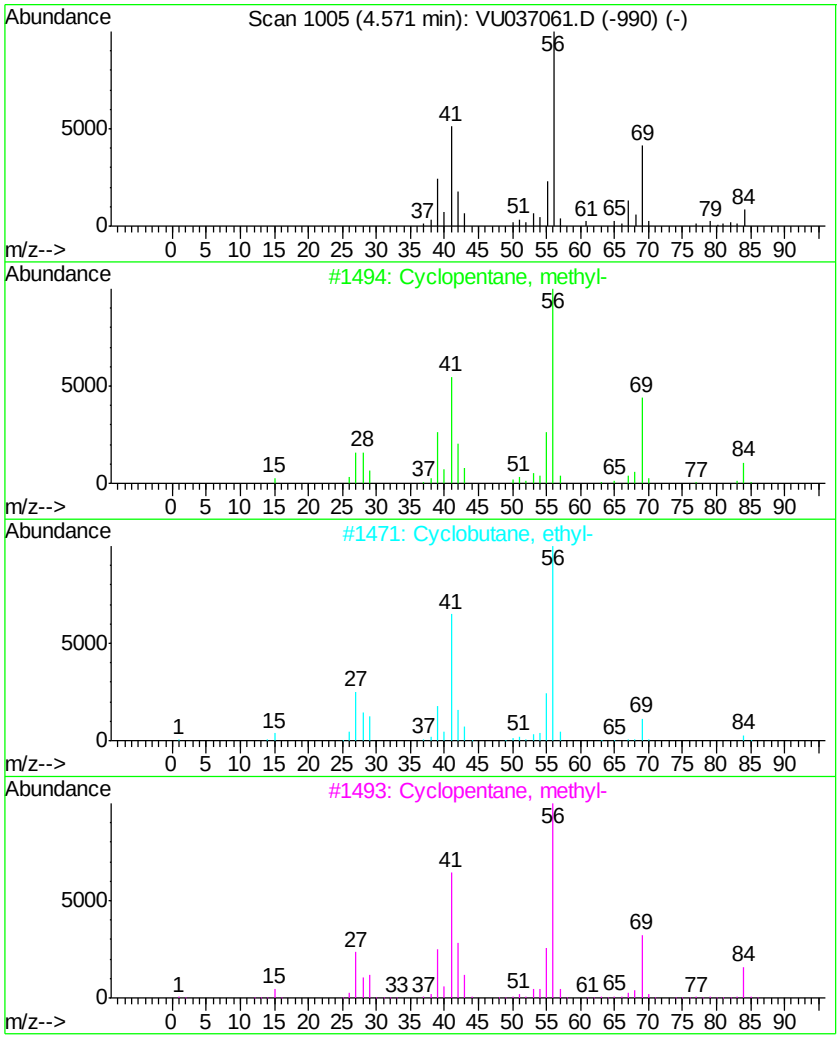
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

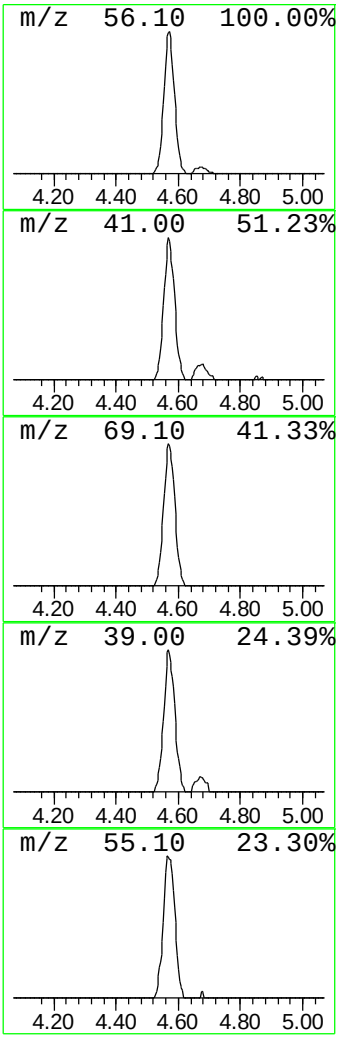
****

Peak Number 4 (DEL) Alkane: Cyclic4.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	6.82 ug/L	96007	1,4-Difluorobenzene	6.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	72





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Sample : L1780-09
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ALS Vial : 33 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0DG5

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

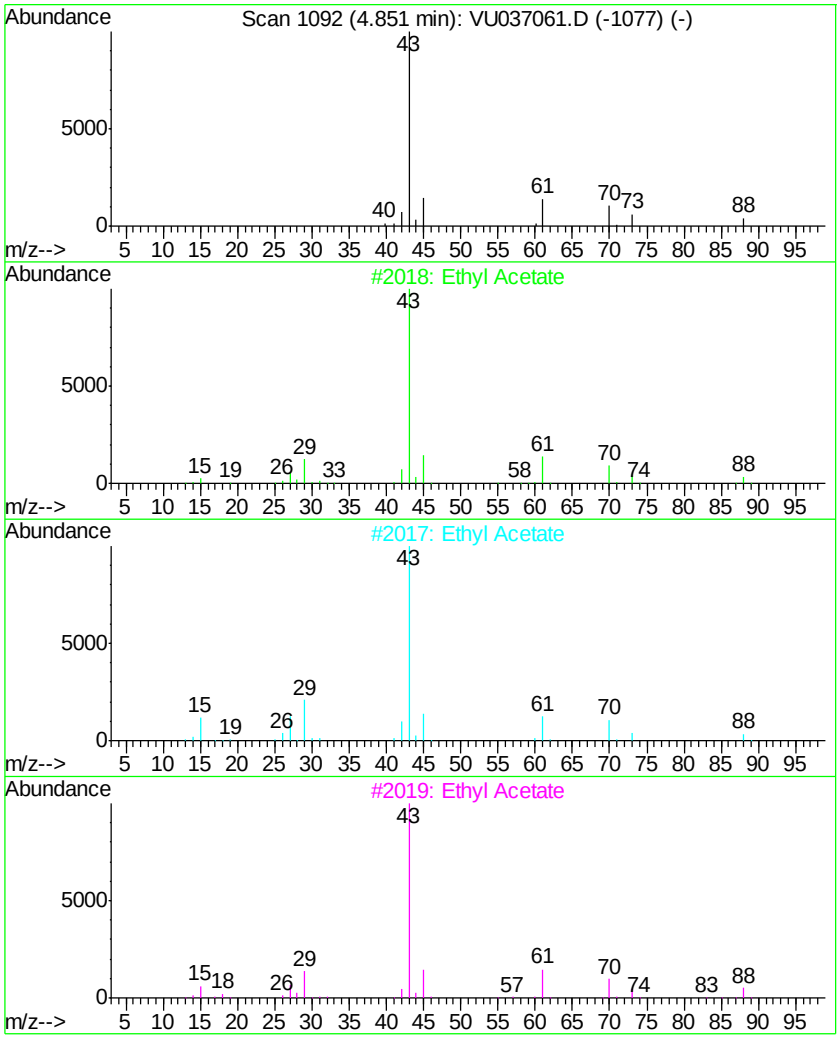
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

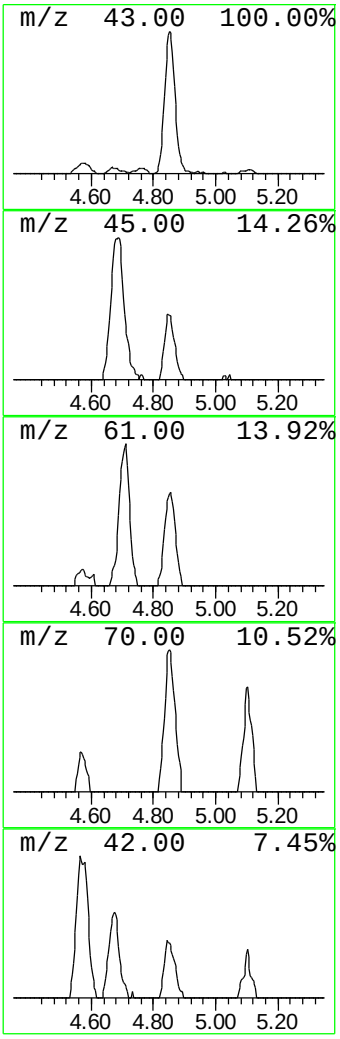
****

Peak Number 5 Ethyl Acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	2.97 ug/L	41869	1,4-Difluorobenzene	6.29

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	83
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU030420\
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Instrument : MSVOA_U
ClientSampleId : C0DG5

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	6.5	ug/L	90823	1	6.29	704244	50.0
Isopropyl Alcohol	2.79	3.7	ug/L	52381	1	6.29	704244	50.0
(DEL) Alkane: Cyc...	3.16	2.5	ug/L	35959	1	6.29	704244	50.0
(DEL) Alkane: Cyc...	4.57	6.8	ug/L	96007	1	6.29	704244	50.0
Ethyl Acetate	4.85	3.0	ug/L	41869	1	6.29	704244	50.0