LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU081018\
Data File : VU026037.D
Acq On : 10 Aug 2018 12:36
Operator : MD/SY
Sample : J4401-23
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZG9

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\SOMULM080918WMA.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	0.609	3	6	12	rVB2	442	478	0.03%	0.002%
2	0.667	22	24	31	rVV3	302	360	0.02%	0.002%
3	0.802	61	66	69	rBV	311	347	0.02%	0.001%
4	1.085	139	154	175	rBV	889569	1019816	55.81%	4.399%
5	1.201	184	190	204	rBV	44104	46289	2.53%	0.200%
6	1.291	212	218	223	rBV	37053	35733	1.96%	0.154%
7	1.326	223	229	241	rVB	113853	126882	6.94%	0.547%
8	1.397	244	251	265	rVB	116112	121774	6.66%	0.525%
9	1.606	311	316	318	rBV2	26254	23577	1.29%	0.102%
10	1.632	318	324	329	rVV	142322	171563	9.39%	0.740%
11	1.661	329	333	344	rVB	97403	121803	6.67%	0.525%
12	1.876	390	400	411	rBV	140156	196318	10.74%	0.847%
13	2.185	489	496	505	rBV5	2931	5040	0.28%	0.022%
14	2.272	511	523	534	rBV2	277616	545412	29.85%	2.353%
15	2.336	534	543	566	rVB	549959	847055	46.36%	3.654%
16	2.471	574	585	607	rVB	122874	201451	11.02%	0.869%
17	2.571	613	616	618	rBV2	518	302	0.02%	0.001%
18	2.619	622	631	642	rVB2	3243	5778	0.32%	0.025%
19	2.696	646	655	666	rVB2	3894	6465	0.35%	0.028%
20	2.834	684	698	711	rVV2	5604	12751	0.70%	0.055%
21	2.995	729	748	774	rVV2	724322	1827240	100.00%	7.882%
22	3.127	785	789	796	rVB4	755	712	0.04%	0.003%
23	3.272	832	834	840	rVB2	355	291	0.02%	0.001%
24	3.522	908	912	917	rBV2	416	332	0.02%	0.001%
25	3.747	975	982	984	rBV	335	314	0.02%	0.001%
26	3.783	989	993	996	rBV2	424	431	0.02%	0.002%
27	4.175	1099	1115	1148	rBV	104391	284297	15.56%	1.226%
28	4.358	1167	1172	1175	rBV2	276	358	0.02%	0.002%
29	4.545	1226	1230	1234	rBV2	286	301	0.02%	0.001%
30	4.657	1245	1265	1291	rBV4	263237	869237	47.57%	3.750%
31	4.773	1299	1301	1305	rVB3	754	482	0.03%	0.002%
32	4.915	1328	1345	1365	rBV2	89067	215134	11.77%	0.928%
33	5.024	1375	1379	1380	rBV	394	290	0.02%	0.001%
34	5.136	1396	1414	1435	rVV	223566	514329	28.15%	2.219%

LSC Area Percent Report

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Sample : J4401-23
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZG9

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\SOMULM080918WMA.M
Title : VOC Analysis

35	5.339	1452	1477	1489	rVV2	380882	1147153	62.78%	4.949%
36	5.407	1490	1498	1522	rVV	145328	299760	16.41%	1.293%
37	5.603	1555	1559	1563	rVB3	414	383	0.02%	0.002%
38	5.638	1566	1570	1576	rVB3	341	293	0.02%	0.001%
39	5.789	1613	1617	1618	rBV2	477	299	0.02%	0.001%
40	5.886	1632	1647	1671	rBV	340525	673031	36.83%	2.903%
41	6.050	1693	1698	1707	rVB4	862	1358	0.07%	0.006%
42	6.114	1715	1718	1721	rVB2	413	315	0.02%	0.001%
43	6.143	1721	1727	1730	rBV2	373	361	0.02%	0.002%
44	6.188	1730	1741	1751	rBV6	5586	9651	0.53%	0.042%
45	6.333	1770	1786	1800	rBV	264734	532915	29.17%	2.299%
46	6.416	1800	1812	1833	rVB	208332	427148	23.38%	1.843%
47	6.615	1862	1874	1895	rVV3	29486	60225	3.30%	0.260%
48	6.696	1895	1899	1905	rVB4	642	753	0.04%	0.003%
49	6.750	1913	1916	1918	rBV2	445	325	0.02%	0.001%
50	6.882	1936	1957	1973	rBV	31278	62789	3.44%	0.271%
51	6.943	1973	1976	1980	rVV3	815	599	0.03%	0.003%
52	7.046	2001	2008	2012	rBV3	1040	1189	0.07%	0.005%
53	7.230	2052	2065	2071	rBV	159064	277793	15.20%	1.198%
54	7.271	2072	2078	2100	rVB	174867	295822	16.19%	1.276%
55	7.461	2124	2137	2158	rVV	402469	713844	39.07%	3.079%
56	7.567	2158	2170	2181	rVV	543406	936649	51.26%	4.041%
57	7.638	2181	2192	2211	rVB	611085	1048737	57.39%	4.524%
58	7.850	2247	2258	2277	rVB	116865	196073	10.73%	0.846%
59	7.940	2277	2286	2300	rBV4	7789	13844	0.76%	0.060%
60	8.069	2314	2326	2348	rBV	190342	317845	17.39%	1.371%
61	8.185	2348	2362	2383	rBV2	93300	241611	13.22%	1.042%
62	8.313	2392	2402	2427	rVB	367154	618931	33.87%	2.670%
63	8.480	2441	2454	2474	rVB	230672	391914	21.45%	1.691%
64	8.590	2476	2488	2507	rVB	144451	244982	13.41%	1.057%
65	8.696	2517	2521	2524	rVV3	578	444	0.02%	0.002%
66	8.712	2524	2526	2533	rVB3	356	325	0.02%	0.001%
67	8.834	2557	2564	2569	rBV2	457	566	0.03%	0.002%
68	9.091	2631	2644	2664	rVV	503615	817658	44.75%	3.527%
69	9.381	2720	2734	2752	rBV	463150	707497	38.72%	3.052%
70	9.535	2777	2782	2787	rBV2	556	763	0.04%	0.003%
71	9.615	2802	2807	2809	rBV3	524	503	0.03%	0.002%

LSC Area Percent Report

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Sample : J4401-23
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZG9

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\SOMULM080918WMA.M
Title : VOC Analysis

72	9.795	2851	2863	2882	rBV	397450	621833	34.03%	2.682%
73	9.956	2907	2913	2915	rBV4	2340	2146	0.12%	0.009%
74	10.217	2987	2994	2996	rBV2	460	477	0.03%	0.002%
75	10.313	3020	3024	3029	rBV3	711	530	0.03%	0.002%
76	10.435	3049	3062	3088	rVV2	430524	952538	52.13%	4.109%
77	10.612	3103	3117	3128	rBV3	27871	52514	2.87%	0.227%
78	10.773	3158	3167	3176	rBV3	1488	2466	0.13%	0.011%
79	10.882	3199	3201	3206	rVB2	521	346	0.02%	0.001%
80	10.979	3224	3231	3233	rBV3	2025	2538	0.14%	0.011%
81	11.011	3234	3241	3250	rVB2	11564	17875	0.98%	0.077%
82	11.152	3273	3285	3303	rVB	732020	1095362	59.95%	4.725%
83	11.291	3322	3328	3334	rBV4	862	1018	0.06%	0.004%
84	11.487	3376	3389	3413	rBV2	558971	1367706	74.85%	5.900%
85	11.638	3433	3436	3440	rVB3	585	466	0.03%	0.002%
86	11.699	3440	3455	3466	rBV5	5681	11488	0.63%	0.050%
87	11.863	3493	3506	3526	rBV	584515	936584	51.26%	4.040%
88	12.114	3580	3584	3589	rBV3	480	531	0.03%	0.002%
89	12.487	3690	3700	3708	rVB3	6444	10294	0.56%	0.044%
90	12.557	3718	3722	3726	rBV2	363	368	0.02%	0.002%
91	12.660	3742	3754	3768	rBV2	93043	150517	8.24%	0.649%
92	12.844	3807	3811	3815	rBV2	321	376	0.02%	0.002%
93	12.872	3818	3820	3824	rVV	406	304	0.02%	0.001%
94	13.223	3920	3929	3944	rVB2	20489	27970	1.53%	0.121%
95	13.509	4010	4018	4027	rBV6	3498	5259	0.29%	0.023%
96	13.991	4155	4168	4189	rBV	397342	669715	36.65%	2.889%
97	14.278	4252	4257	4260	rBV3	1258	1427	0.08%	0.006%
98	14.676	4379	4381	4383	rBV2	514	292	0.02%	0.001%
99	15.323	4580	4582	4585	rBV2	764	434	0.02%	0.002%
100	15.724	4705	4707	4711	rVB3	815	493	0.03%	0.002%

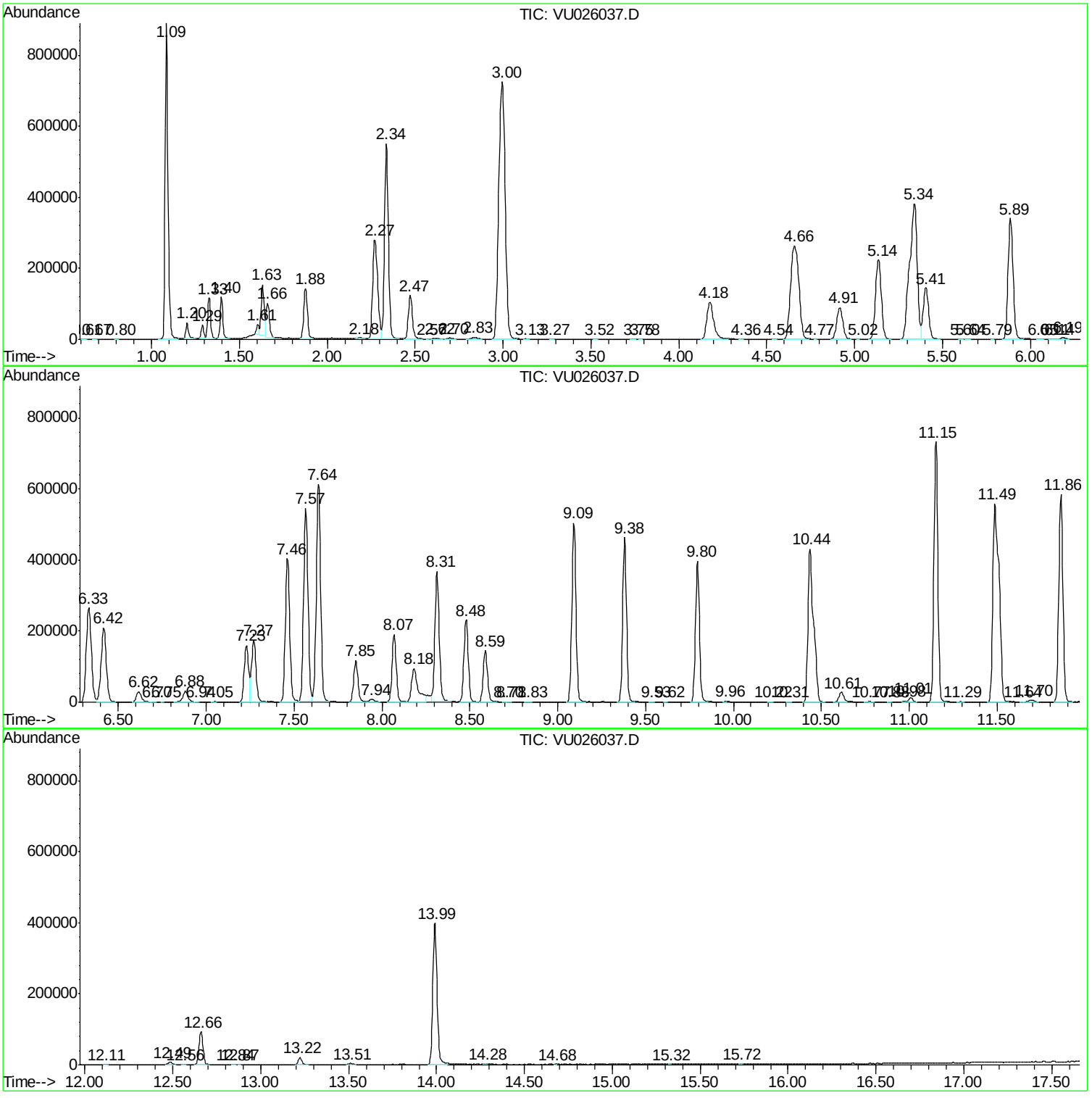
Sum of corrected areas: 23181157

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081018\
Data File : VU026037.D
Acq On : 10 Aug 2018 12:36
Operator : MD/SY
Sample : J4401-23
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZG9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081018\
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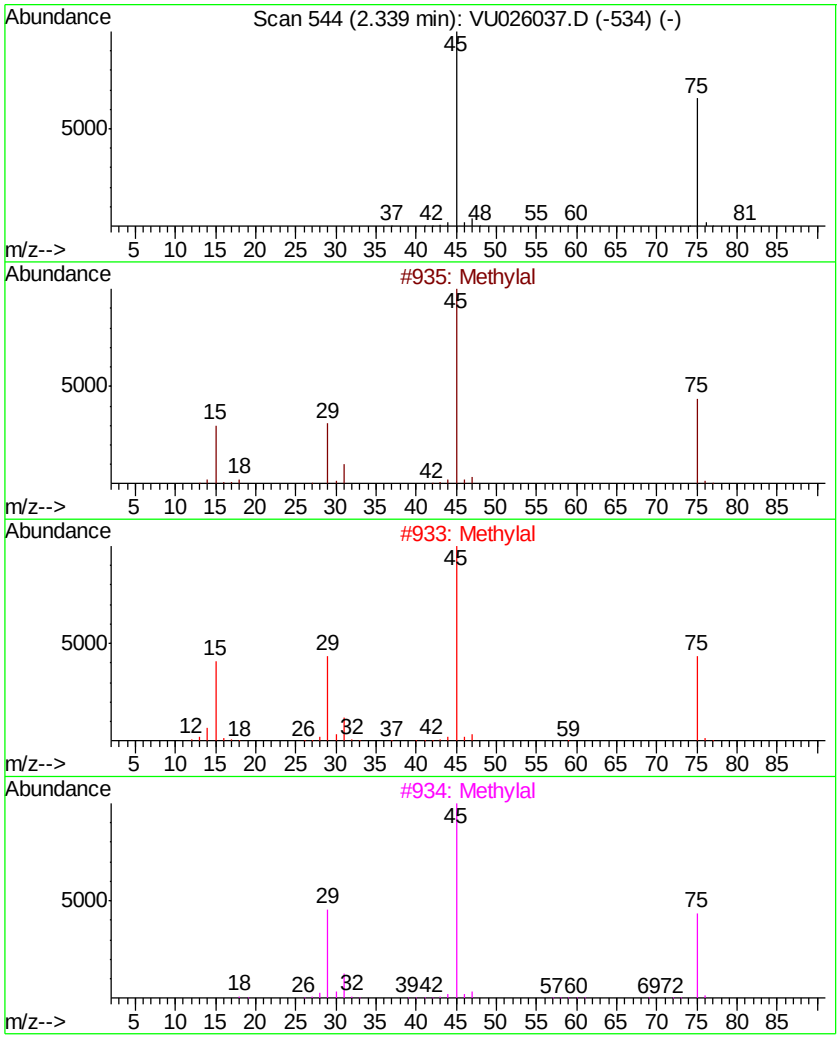
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

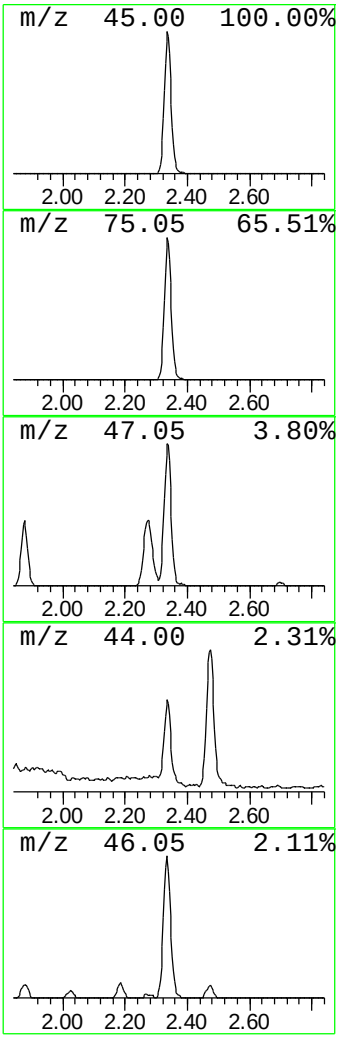
****

Peak Number 2 Methylal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	62.93 ug/L	847055	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylal	76	C3H8O2	000109-87-5	78
2	Methylal	76	C3H8O2	000109-87-5	78
3	Methylal	76	C3H8O2	000109-87-5	59
4	Methanamine, N,N-dimethyl-, N-oxide	75	C3H9NO	001184-78-7	9
5	Ethanethioamide	75	C2H5NS	000062-55-5	5





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Acq On : 10 Aug 2018 12:36
Operator : MD/SY
Sample : J4401-23
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ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZG9

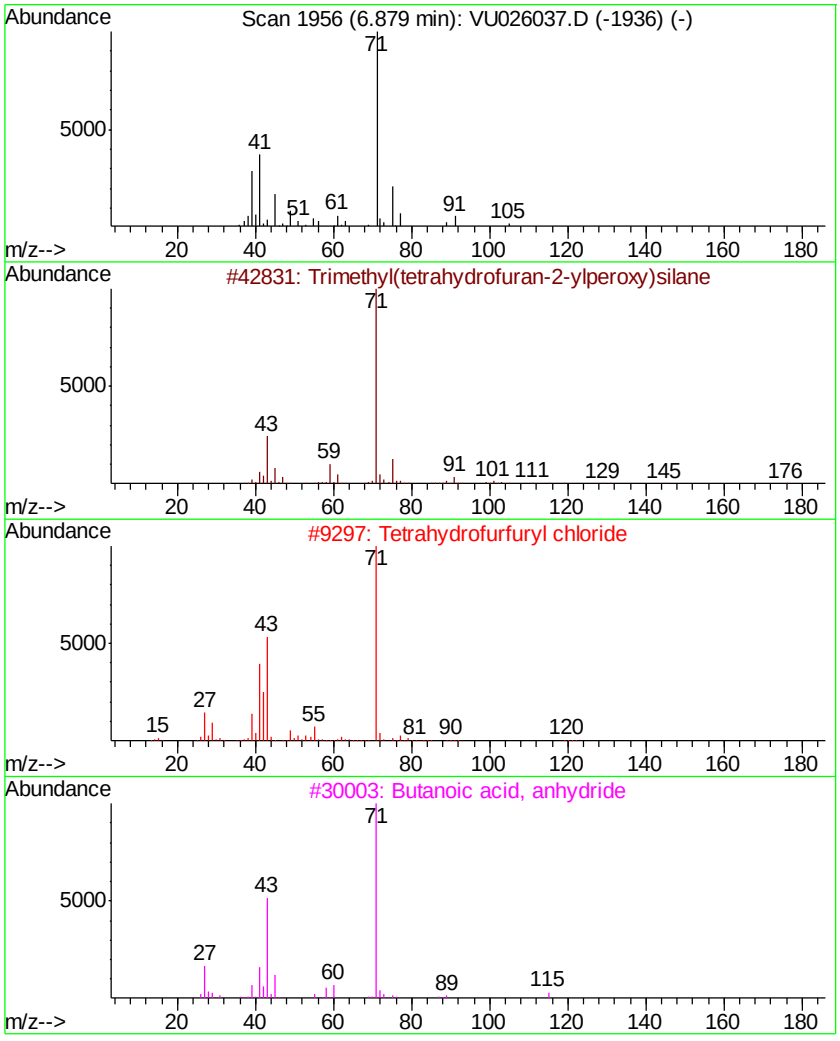
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Quant Title : VOC Analysis

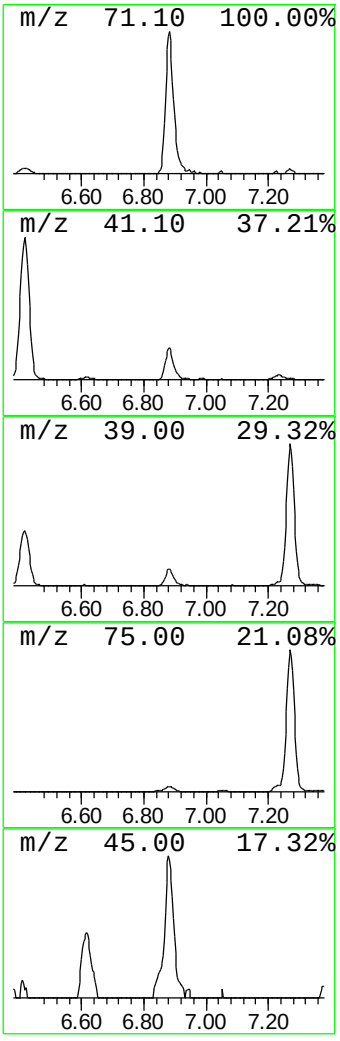
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Trimethyl(tetrahydrofuran-2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	4.66 ug/L	62789	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethyl(tetrahydrofuran-2-ylpe...	176	C7H16O3Si	1000368-50-8	72
2	Tetrahydrofurfuryl chloride	120	C5H9ClO	003003-84-7	40
3	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	36
4	Butanoyl chloride	106	C4H7ClO	000141-75-3	33
5	2-Propenoic acid, 2-methyl-, (te...	170	C9H14O3	002455-24-5	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081018\
Data File : VU026037.D
Acq On : 10 Aug 2018 12:36
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ClientSampleId : A4ZG9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Quant Title : VOC Analysis

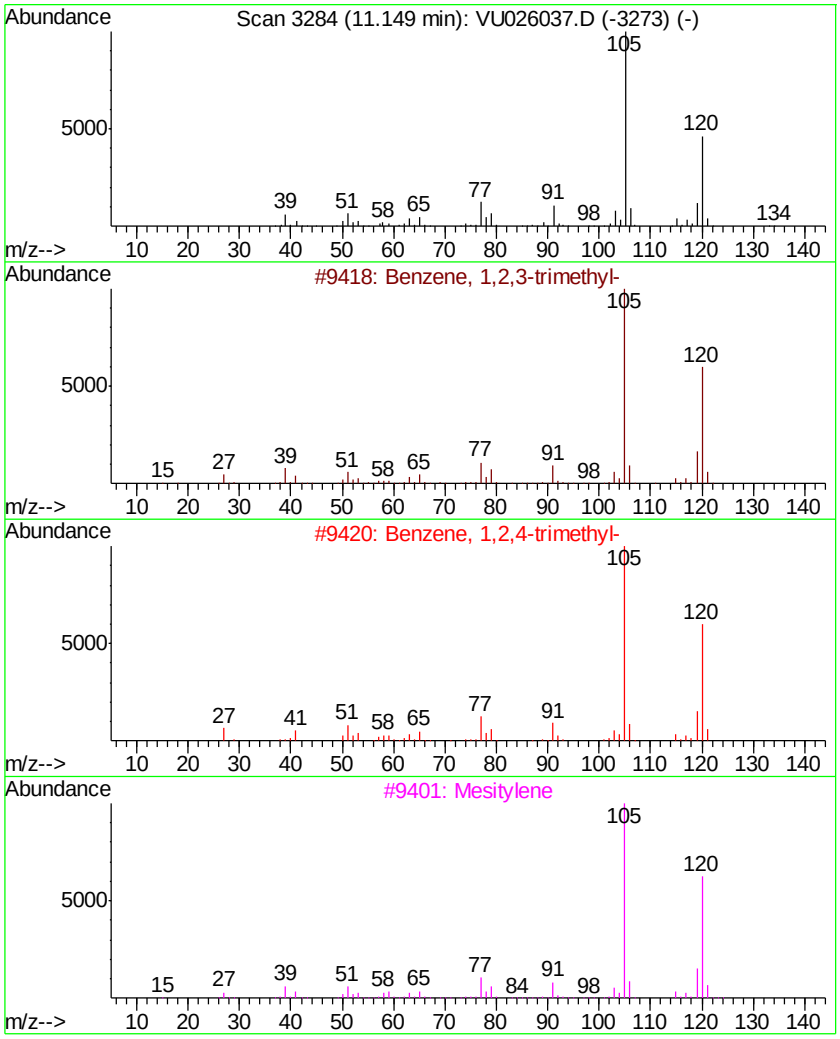
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

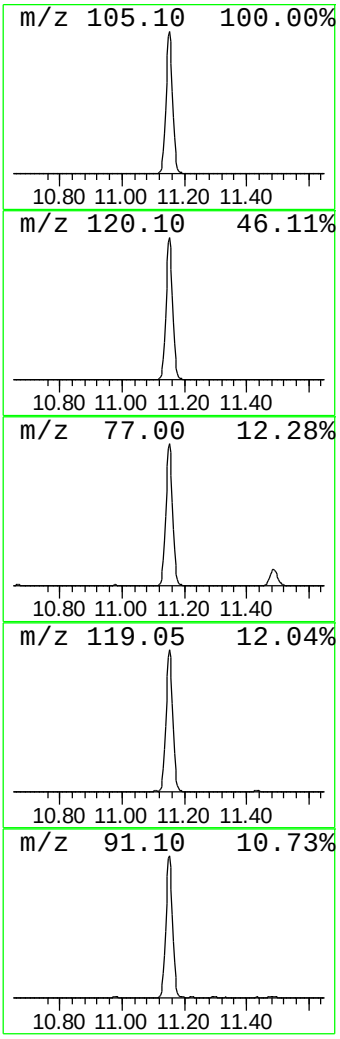
****

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	40.04 ug/L	1095360	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Tentatively Identified Compound (LSC) summary

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Data File : VU026037.D
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Operator : MD/SY
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ALS Vial : 4 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZG9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.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
Methylal	2.34	62.9	ug/L	847055	1	5.89	673031	50.0
Trimethyl(tetrahy...	6.88	4.7	ug/L	62789	1	5.89	673031	50.0
Benzene, 1,2,3-tr...	11.15	40.0	ug/L	1095360	3	11.49	1367710	50.0