LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081418\
Data File : VU026097.D
Acq On : 14 Aug 2018 13:28
Operator : MD/SY
Sample : J4451-22
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZL2

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	0.622	7	10	15	rBV3	406	407	0.01%	0.002%
2	0.760	49	53	57	rVV2	349	323	0.01%	0.001%
3	1.085	138	154	178	rBV	923701	1048689	28.13%	4.056%
4	1.201	184	190	205	rBV	44126	46489	1.25%	0.180%
5	1.291	212	218	223	rBV	40026	38242	1.03%	0.148%
6	1.326	223	229	243	rVB	116381	126170	3.38%	0.488%
7	1.397	244	251	264	rBV	125231	131593	3.53%	0.509%
8	1.628	311	323	330	rBV	484970	641253	17.20%	2.480%
9	1.876	390	400	417	rBV	140533	199585	5.35%	0.772%
10	2.268	510	522	533	rBV2	292755	572666	15.36%	2.215%
11	2.336	533	543	573	rVV	2415763	3727812	100.00%	14.417%
12	2.471	575	585	613	rVB	115061	195997	5.26%	0.758%
13	2.616	622	630	639	rVB2	5658	10030	0.27%	0.039%
14	2.661	642	644	648	rBV2	542	346	0.01%	0.001%
15	2.696	648	655	670	rVB4	4254	7623	0.20%	0.029%
16	2.757	670	674	676	rBV3	475	362	0.01%	0.001%
17	2.834	687	698	715	rVB2	5274	11498	0.31%	0.044%
18	2.995	729	748	776	rBV2	729701	1831060	49.12%	7.082%
19	3.230	818	821	825	rVB2	514	359	0.01%	0.001%
20	3.288	834	839	845	rVB3	495	516	0.01%	0.002%
21	3.368	861	864	872	rBV2	350	393	0.01%	0.002%
22	3.442	883	887	888	rBV	495	402	0.01%	0.002%
23	3.908	1026	1032	1038	rVB	400	366	0.01%	0.001%
24	3.966	1048	1050	1056	rVB2	377	324	0.01%	0.001%
25	4.175	1098	1115	1144	rBV2	93302	256134	6.87%	0.991%
26	4.394	1181	1183	1190	rVV3	480	499	0.01%	0.002%
27	4.558	1231	1234	1238	rBV4	600	500	0.01%	0.002%
28	4.657	1243	1265	1292	rBV4	263991	875196	23.48%	3.385%
29	4.915	1327	1345	1366	rBV2	90593	221513	5.94%	0.857%
30	5.133	1395	1413	1435	rVV	208662	479591	12.87%	1.855%
31	5.230	1441	1443	1447	rBV2	423	344	0.01%	0.001%
32	5.339	1450	1477	1489	rBV2	380211	1139632	30.57%	4.408%
33	5.403	1490	1497	1515	rVB	149608	302087	8.10%	1.168%
34	5.722	1588	1596	1600	rVB4	527	710	0.02%	0.003%

LSC Area Percent Report

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Sample : J4451-22
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZL2

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

35	5.886	1633	1647	1671	rBV	323172	637470	17.10%	2.465%
36	6.043	1693	1696	1697	rBV	551	319	0.01%	0.001%
37	6.188	1729	1741	1753	rBV5	12052	23654	0.63%	0.091%
38	6.332	1769	1786	1800	rBV	263614	521719	14.00%	2.018%
39	6.416	1800	1812	1834	rVB	212167	435421	11.68%	1.684%
40	6.615	1862	1874	1891	rBV	29120	56982	1.53%	0.220%
41	6.750	1912	1916	1917	rBV2	778	554	0.01%	0.002%
42	6.882	1938	1957	1975	rBV3	28735	58570	1.57%	0.227%
43	7.046	1999	2008	2024	rVB3	5115	8446	0.23%	0.033%
44	7.230	2052	2065	2071	rBV	159620	275673	7.40%	1.066%
45	7.271	2072	2078	2096	rVB	175290	292171	7.84%	1.130%
46	7.394	2113	2116	2119	rBV3	552	407	0.01%	0.002%
47	7.461	2124	2137	2156	rBV	331219	585173	15.70%	2.263%
48	7.567	2157	2170	2181	rVV	545739	940710	25.23%	3.638%
49	7.638	2181	2192	2217	rVB	634966	1084644	29.10%	4.195%
50	7.850	2247	2258	2278	rBV	116293	205455	5.51%	0.795%
51	7.940	2278	2286	2299	rVV7	5137	9542	0.26%	0.037%
52	8.069	2314	2326	2347	rBV	185547	317933	8.53%	1.230%
53	8.184	2350	2362	2375	rBV2	33567	91223	2.45%	0.353%
54	8.313	2393	2402	2426	rVB	324738	550610	14.77%	2.129%
55	8.477	2441	2453	2472	rVB	204180	350180	9.39%	1.354%
56	8.590	2474	2488	2509	rBV	144269	246835	6.62%	0.955%
57	8.815	2554	2558	2559	rBV2	499	384	0.01%	0.001%
58	8.998	2610	2615	2617	rBV2	357	365	0.01%	0.001%
59	9.091	2631	2644	2666	rVV	477063	792922	21.27%	3.067%
60	9.226	2681	2686	2687	rBV2	505	417	0.01%	0.002%
61	9.249	2689	2693	2705	rVB5	1638	2585	0.07%	0.010%
62	9.381	2722	2734	2753	rBV	452901	712474	19.11%	2.755%
63	9.525	2776	2779	2783	rBV3	427	495	0.01%	0.002%
64	9.686	2826	2829	2835	rVB	525	437	0.01%	0.002%
65	9.718	2835	2839	2841	rBV	544	463	0.01%	0.002%
66	9.795	2851	2863	2888	rBV	338882	526790	14.13%	2.037%
67	9.959	2907	2914	2920	rBV7	2264	3001	0.08%	0.012%
68	10.085	2948	2953	2959	rVB2	396	509	0.01%	0.002%
69	10.168	2970	2979	2985	rBV5	1596	2281	0.06%	0.009%
70	10.435	3049	3062	3086	rBV2	405880	918055	24.63%	3.551%
71	10.615	3107	3118	3125	rBV3	9701	18887	0.51%	0.073%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081418\
Data File : VU026097.D
Acq On : 14 Aug 2018 13:28
Operator : MD/SY
Sample : J4451-22
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZL2

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	10.773	3161	3167	3176	rVV4	1369	2069	0.06%	0.008%
73	10.979	3222	3231	3232	rBV3	2527	3197	0.09%	0.012%
74	11.008	3232	3240	3253	rVB	28498	46039	1.24%	0.178%
75	11.088	3262	3265	3271	rVB4	535	381	0.01%	0.001%
76	11.152	3271	3285	3302	rBV	725258	1100875	29.53%	4.258%
77	11.258	3315	3318	3320	rBV2	567	349	0.01%	0.001%
78	11.284	3323	3326	3329	rBV2	633	557	0.01%	0.002%
79	11.377	3348	3355	3358	rBV2	389	509	0.01%	0.002%
80	11.426	3361	3370	3376	rVB5	1506	2370	0.06%	0.009%
81	11.487	3376	3389	3413	rBV2	536829	1345924	36.10%	5.205%
82	11.644	3436	3438	3440	rBV2	555	342	0.01%	0.001%
83	11.696	3441	3454	3466	rVV3	14013	25693	0.69%	0.099%
84	11.863	3493	3506	3532	rBV	582005	936277	25.12%	3.621%
85	12.004	3547	3550	3553	rBV3	672	417	0.01%	0.002%
86	12.483	3690	3699	3709	rVB3	2625	3821	0.10%	0.015%
87	12.618	3738	3741	3742	rBV	822	420	0.01%	0.002%
88	12.660	3742	3754	3767	rVB	91722	148343	3.98%	0.574%
89	12.888	3822	3825	3832	rVB3	1108	1026	0.03%	0.004%
90	12.995	3855	3858	3866	rVB5	1014	1166	0.03%	0.005%
91	13.223	3920	3929	3941	rVB2	21747	30695	0.82%	0.119%
92	13.319	3955	3959	3966	rBV2	494	508	0.01%	0.002%
93	13.351	3966	3969	3974	rBV2	505	426	0.01%	0.002%
94	13.512	4013	4019	4027	rVB6	1729	2270	0.06%	0.009%
95	13.747	4086	4092	4102	rVB3	719	1270	0.03%	0.005%
96	13.847	4120	4123	4128	rBV	453	392	0.01%	0.002%
97	13.991	4156	4168	4197	rBV	390602	657229	17.63%	2.542%
98	14.114	4203	4206	4210	rVB2	1121	663	0.02%	0.003%
99	14.207	4231	4235	4236	rBV2	681	426	0.01%	0.002%
100	15.785	4724	4726	4730	rBV2	718	454	0.01%	0.002%

Sum of corrected areas: 25856575

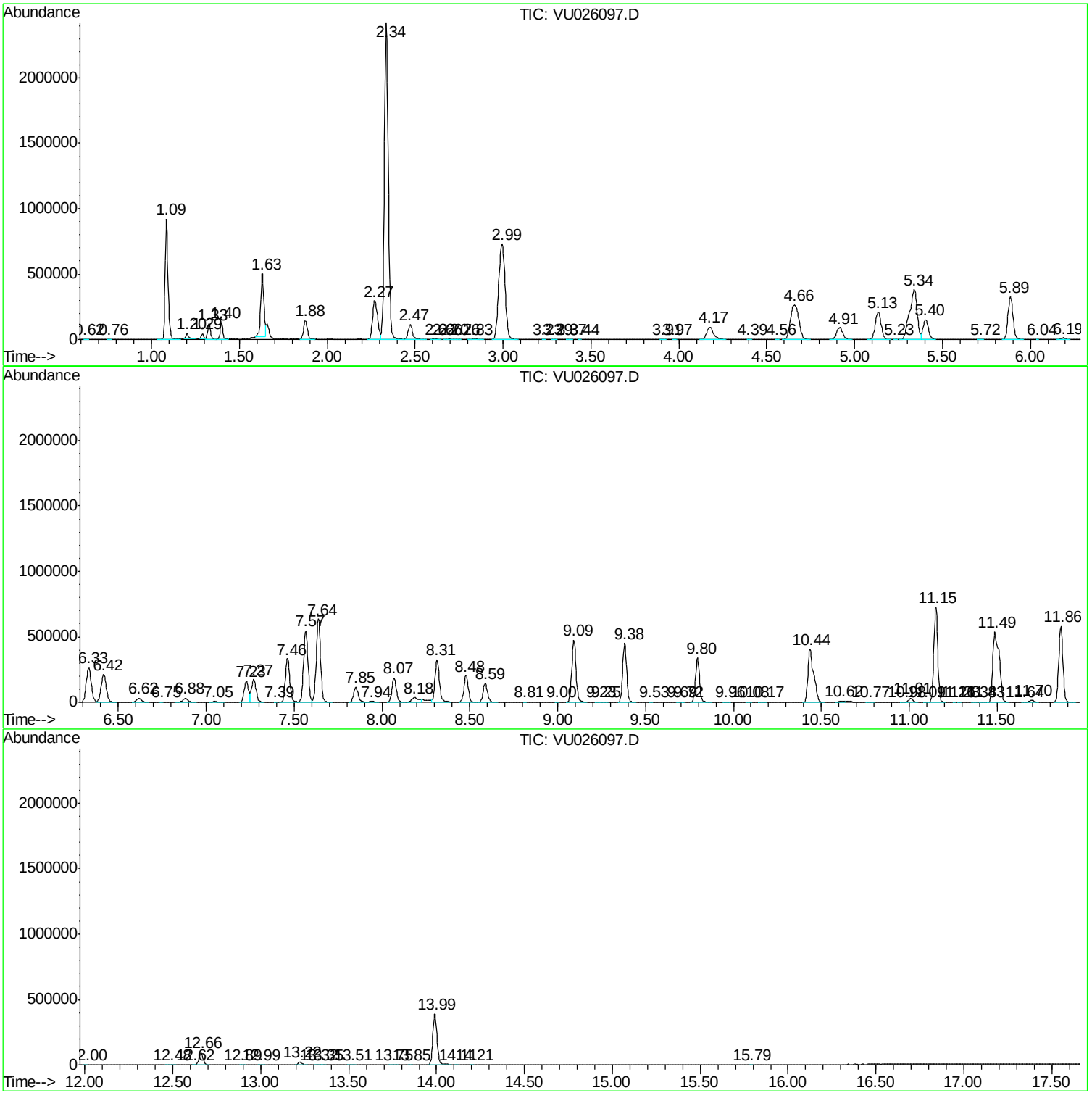
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081418\
Data File : VU026097.D
Acq On : 14 Aug 2018 13:28
Operator : MD/SY
Sample : J4451-22
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZL2

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081418\
Data File : VU026097.D
Acq On : 14 Aug 2018 13:28
Operator : MD/SY
Sample : J4451-22
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZL2

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

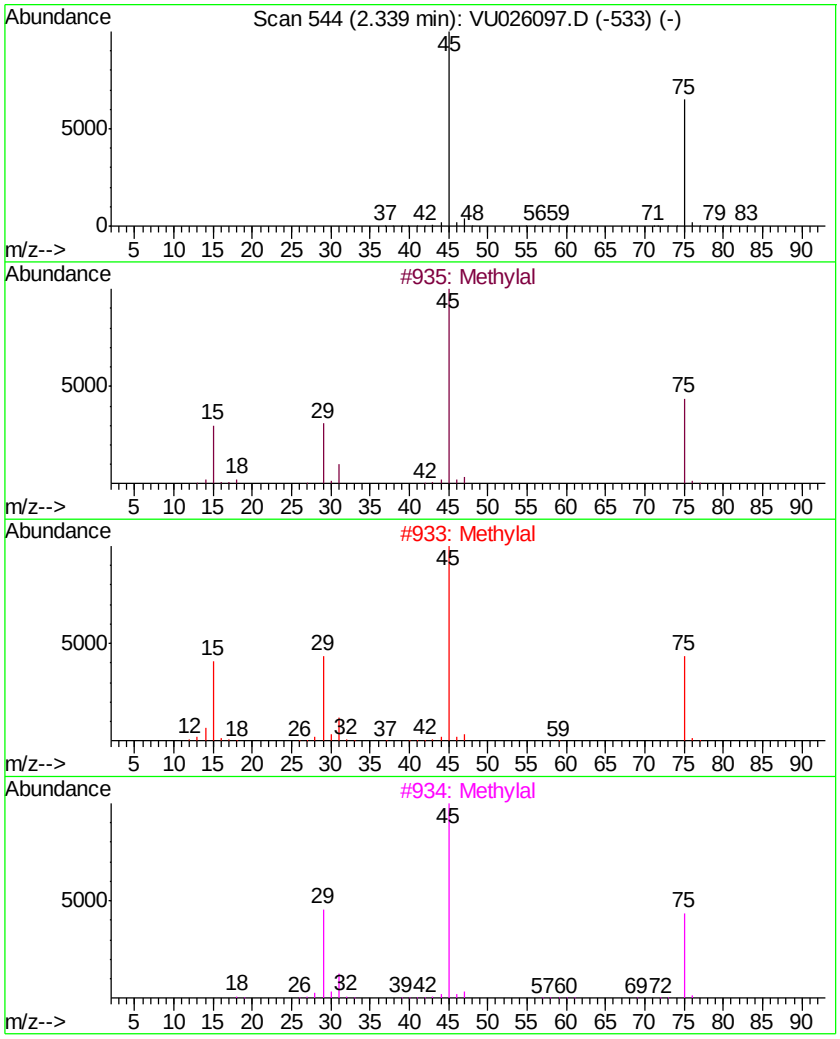
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

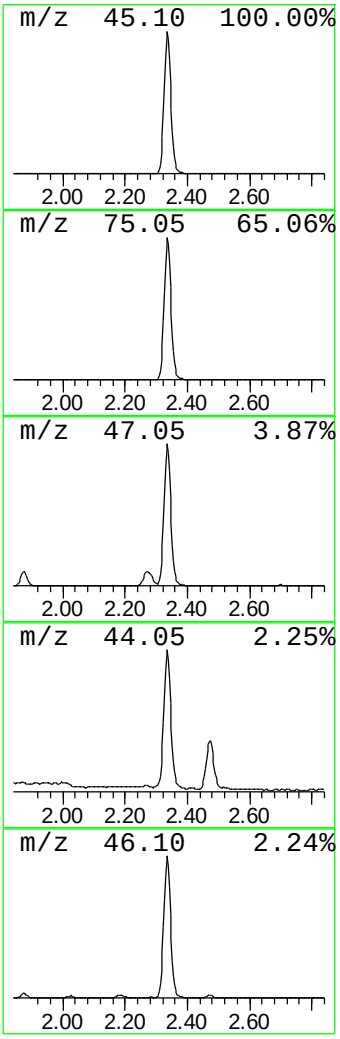
****

Peak Number 2 Methylal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	292.39 ug/L	3727810	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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Data File : VU026097.D
Acq On : 14 Aug 2018 13:28
Operator : MD/SY
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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZL2

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

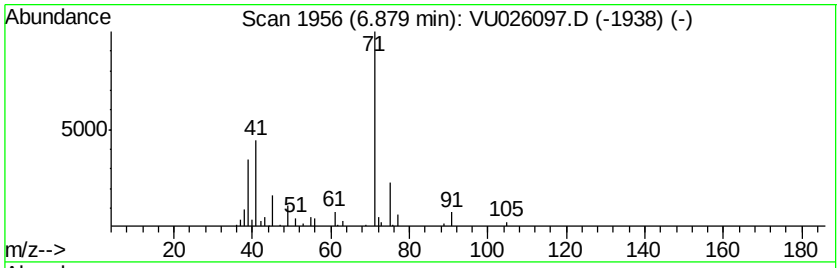
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

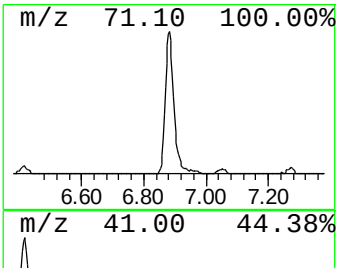
****

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	4.59 ug/L	58570	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethyl(tetrahydrofuran-2-ylpe...	176	C7H16O3Si	1000368-50-8	38
2	3-Penten-2-ol	86	C5H10O	001569-50-2	33
3	Butanoyl chloride	106	C4H7ClO	000141-75-3	33
4	2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	33
5	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	28





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ClientSampleId : A4ZL2

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

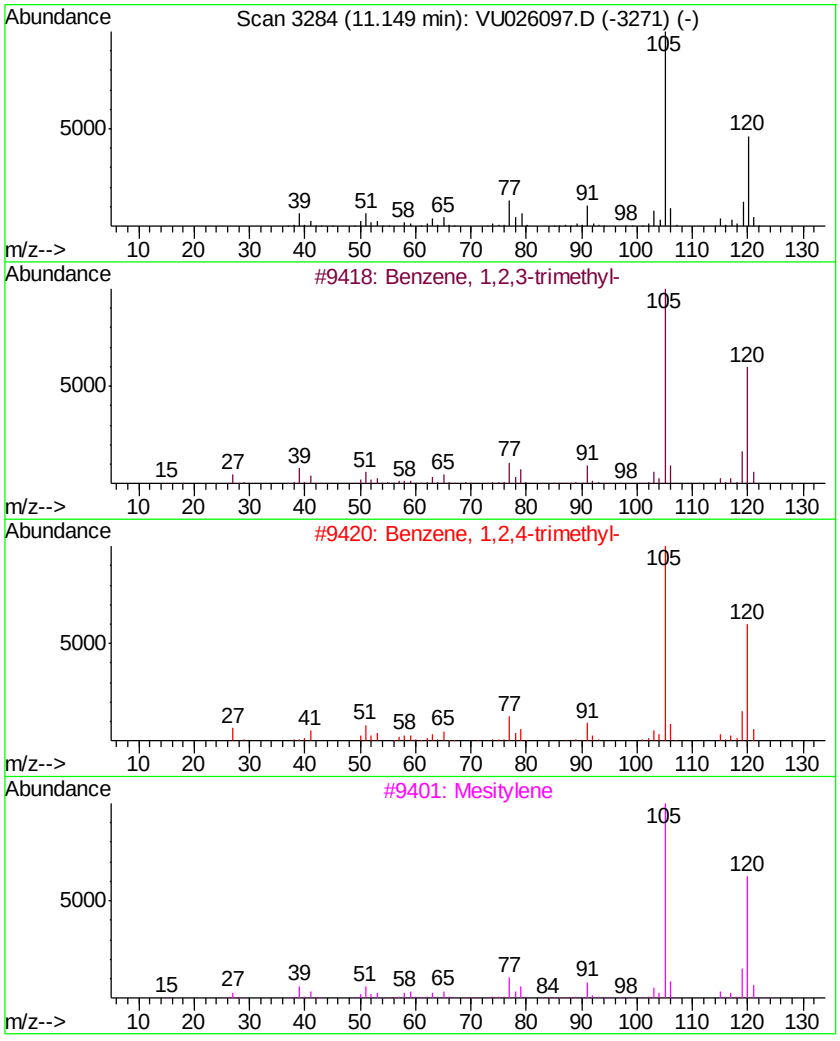
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

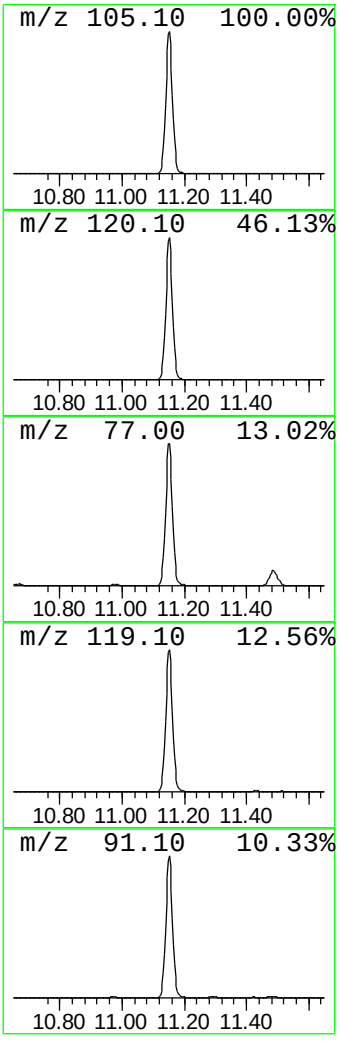
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	40.90 ug/L	1100880	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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081418\
Data File : VU026097.D
Acq On : 14 Aug 2018 13:28
Operator : MD/SY
Sample : J4451-22
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ClientSampleId : A4ZL2

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	292.4	ug/L	3727810	1	5.89	637470	50.0
unknown-01	6.88	4.6	ug/L	58570	1	5.89	637470	50.0
Benzene, 1,2,3-tr...	11.15	40.9	ug/L	1100880	3	11.49	1345920	50.0