LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU080918\
Data File : VU025987.D
Acq On : 09 Aug 2018 11:24
Operator : MD/SY
Sample : J4361-17
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A4ZD5

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	0.670	20	25	29	rBV2	304	309	0.00%	0.001%
2	0.985	119	123	128	rVB3	457	390	0.01%	0.001%
3	1.021	128	134	137	rBV3	391	512	0.01%	0.002%
4	1.085	137	154	178	rBV	1053803	1236054	18.67%	4.068%
5	1.201	185	190	205	rVB	44992	47643	0.72%	0.157%
6	1.291	212	218	223	rBV	37788	38102	0.58%	0.125%
7	1.326	223	229	243	rVB	116155	129733	1.96%	0.427%
8	1.397	244	251	265	rVB	171577	176733	2.67%	0.582%
9	1.629	311	323	330	rBV	639799	836870	12.64%	2.754%
10	1.876	391	400	416	rVB	140543	195557	2.95%	0.644%
11	2.182	490	495	504	rBV7	3156	4564	0.07%	0.015%
12	2.268	510	522	533	rBV2	344896	649591	9.81%	2.138%
13	2.336	533	543	574	rVV	4330122	6619921	100.00%	21.789%
14	2.471	575	585	609	rVB	111686	183479	2.77%	0.604%
15	2.616	622	630	642	rVB2	7883	12929	0.20%	0.043%
16	2.699	647	656	667	rVB2	5511	9844	0.15%	0.032%
17	2.783	679	682	687	rBV3	347	271	0.00%	0.001%
18	2.841	688	700	709	rVV4	3375	6656	0.10%	0.022%
19	2.995	729	748	775	rBV2	722298	1810456	27.35%	5.959%
20	3.143	790	794	795	rBV3	566	390	0.01%	0.001%
21	3.352	854	859	861	rBV2	344	378	0.01%	0.001%
22	3.439	882	886	889	rVV5	661	630	0.01%	0.002%
23	3.509	905	908	910	rBV	374	282	0.00%	0.001%
24	3.850	1011	1014	1021	rVB2	460	533	0.01%	0.002%
25	4.008	1061	1063	1068	rBV3	402	368	0.01%	0.001%
26	4.056	1074	1078	1079	rBV	430	294	0.00%	0.001%
27	4.175	1099	1115	1147	rBV	112034	301469	4.55%	0.992%
28	4.394	1181	1183	1188	rVB3	426	320	0.00%	0.001%
29	4.522	1218	1223	1225	rBV2	374	296	0.00%	0.001%
30	4.548	1225	1231	1233	rBV6	871	967	0.01%	0.003%
31	4.654	1243	1264	1289	rBV4	289448	944341	14.27%	3.108%
32	4.763	1295	1298	1306	rBV7	730	848	0.01%	0.003%
33	4.918	1328	1346	1362	rBV2	86545	213340	3.22%	0.702%
34	5.136	1395	1414	1435	rBV	184002	428753	6.48%	1.411%

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

35	5.339	1452	1477	1489	rBV2	453348	1339972	20.24%	4.410%
36	5.407	1490	1498	1520	rVB	145733	299391	4.52%	0.985%
37	5.535	1533	1538	1541	rBV3	457	528	0.01%	0.002%
38	5.651	1569	1574	1576	rBV3	306	314	0.00%	0.001%
39	5.709	1590	1592	1596	rVB3	461	302	0.00%	0.001%
40	5.802	1616	1621	1626	rVB2	251	293	0.00%	0.001%
41	5.889	1633	1648	1665	rBV	364975	719158	10.86%	2.367%
42	5.995	1680	1681	1688	rVB5	684	649	0.01%	0.002%
43	6.046	1691	1697	1706	rVB6	1772	2798	0.04%	0.009%
44	6.188	1725	1741	1757	rBV9	7829	15496	0.23%	0.051%
45	6.255	1759	1762	1765	rBV3	412	345	0.01%	0.001%
46	6.332	1770	1786	1800	rBV	304209	607068	9.17%	1.998%
47	6.416	1800	1812	1835	rVB2	205757	421634	6.37%	1.388%
48	6.519	1841	1844	1850	rVB5	586	541	0.01%	0.002%
49	6.551	1850	1854	1857	rBV3	405	282	0.00%	0.001%
50	6.615	1863	1874	1895	rBV2	30715	62749	0.95%	0.207%
51	6.760	1907	1919	1929	rVB4	1588	2872	0.04%	0.009%
52	6.882	1940	1957	1976	rBV	27718	54957	0.83%	0.181%
53	7.046	1999	2008	2027	rVB4	6947	14581	0.22%	0.048%
54	7.230	2051	2065	2071	rBV	187568	325903	4.92%	1.073%
55	7.271	2072	2078	2092	rVB	178415	299106	4.52%	0.984%
56	7.464	2123	2138	2157	rBV	308146	548284	8.28%	1.805%
57	7.567	2157	2170	2181	rVV	658001	1121127	16.94%	3.690%
58	7.638	2181	2192	2215	rVB	604146	1038581	15.69%	3.418%
59	7.850	2247	2258	2278	rBV	138961	250342	3.78%	0.824%
60	7.940	2279	2286	2295	rVB10	1848	3238	0.05%	0.011%
61	8.069	2313	2326	2346	rBV	187173	321150	4.85%	1.057%
62	8.181	2349	2361	2372	rBV	54215	107226	1.62%	0.353%
63	8.313	2391	2402	2432	rVB	395737	652754	9.86%	2.148%
64	8.480	2439	2454	2468	rBV2	178512	300608	4.54%	0.989%
65	8.590	2474	2488	2512	rBV	141568	245974	3.72%	0.810%
66	9.017	2616	2621	2624	rVB2	366	366	0.01%	0.001%
67	9.091	2630	2644	2666	rBV	541218	885746	13.38%	2.915%
68	9.255	2683	2695	2705	rBV3	5285	8333	0.13%	0.027%
69	9.381	2721	2734	2755	rBV	453123	693032	10.47%	2.281%
70	9.689	2827	2830	2835	rBV3	386	392	0.01%	0.001%
71	9.795	2849	2863	2895	rBV	316158	494716	7.47%	1.628%

LSC Area Percent Report

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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Title : VOC Analysis

72	9.959	2909	2914	2923	rVV4	1998	2924	0.04%	0.010%
73	10.017	2930	2932	2936	rVB	423	288	0.00%	0.001%
74	10.168	2969	2979	2990	rBV2	4677	7260	0.11%	0.024%
75	10.246	3000	3003	3009	rBV2	271	286	0.00%	0.001%
76	10.313	3021	3024	3028	rVB3	638	449	0.01%	0.001%
77	10.435	3049	3062	3087	rVV2	453488	1002693	15.15%	3.300%
78	10.615	3106	3118	3126	rBV4	13774	25963	0.39%	0.085%
79	10.657	3127	3131	3144	rVB4	7288	10690	0.16%	0.035%
80	10.770	3163	3166	3177	rBV5	1121	1555	0.02%	0.005%
81	10.911	3207	3210	3216	rBV2	430	554	0.01%	0.002%
82	10.975	3222	3230	3231	rBV4	3189	3403	0.05%	0.011%
83	11.011	3232	3241	3253	rVB	41604	67806	1.02%	0.223%
84	11.152	3273	3285	3305	rVV	725198	1076102	16.26%	3.542%
85	11.393	3358	3360	3362	rBV2	526	308	0.00%	0.001%
86	11.426	3363	3370	3377	rVB5	3266	4748	0.07%	0.016%
87	11.487	3377	3389	3413	rBV2	587325	1408867	21.28%	4.637%
88	11.599	3422	3424	3428	rBV3	434	330	0.00%	0.001%
89	11.696	3442	3454	3467	rBV2	17837	29404	0.44%	0.097%
90	11.863	3493	3506	3530	rBV	670110	1084042	16.38%	3.568%
91	12.245	3622	3625	3628	rBV2	369	286	0.00%	0.001%
92	12.361	3658	3661	3669	rVV4	443	436	0.01%	0.001%
93	12.480	3690	3698	3713	rVB2	3975	7484	0.11%	0.025%
94	12.660	3738	3754	3776	rVB	98896	162066	2.45%	0.533%
95	12.892	3820	3826	3832	rBV4	1784	2166	0.03%	0.007%
96	12.956	3842	3846	3847	rBV2	501	304	0.00%	0.001%
97	13.223	3920	3929	3942	rBV3	48392	73498	1.11%	0.242%
98	13.509	4010	4018	4028	rVB5	3182	4818	0.07%	0.016%
99	13.731	4084	4087	4089	rBV2	766	545	0.01%	0.002%
100	13.991	4155	4168	4193	rBV	435869	709650	10.72%	2.336%

Sum of corrected areas: 30382556

LSC Report - Integrated Chromatogram

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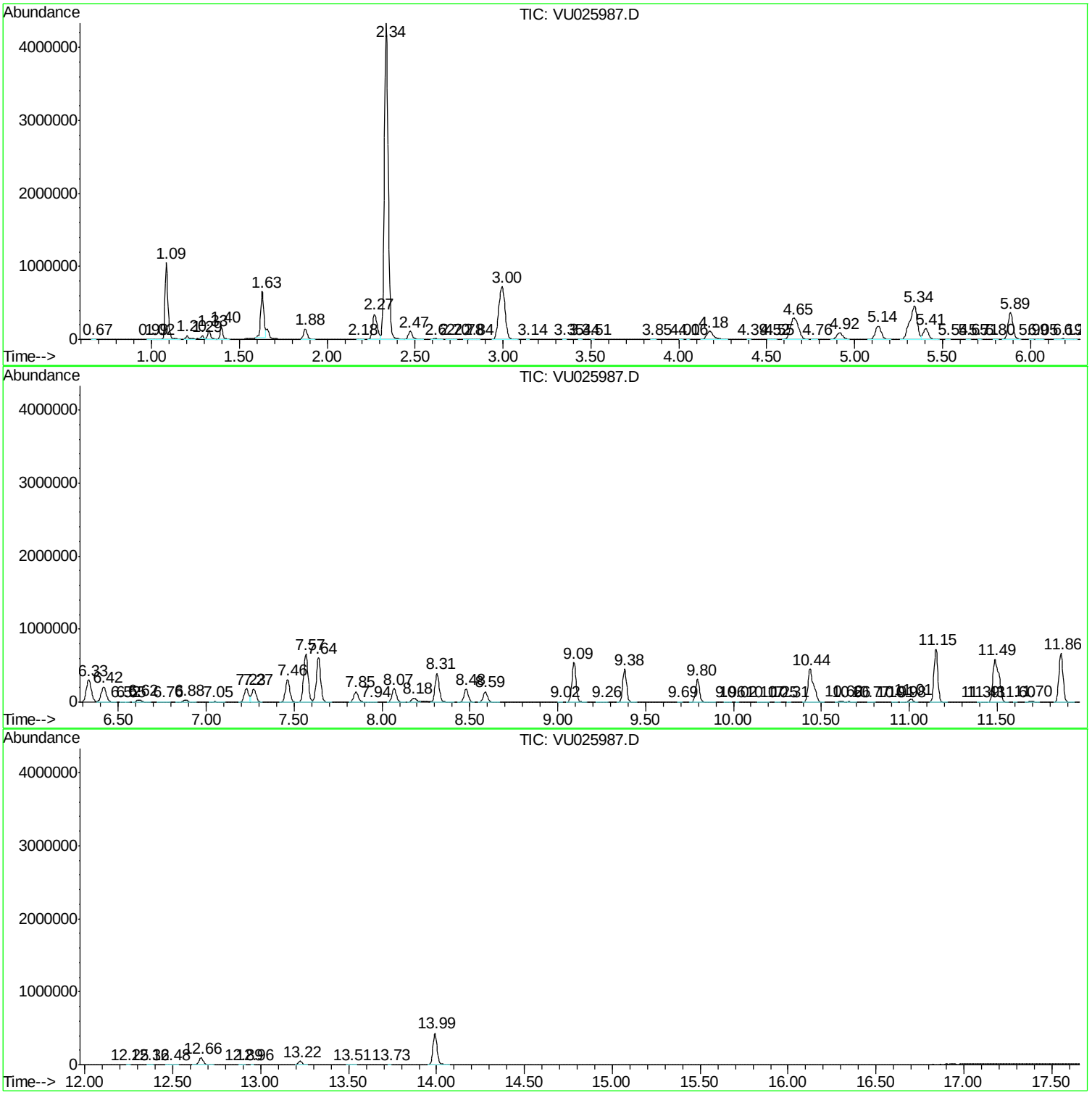
Instrument : MSVOA_U
ClientSampleId : A4ZD5

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\VU080918\
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Quant Title : VOC Analysis

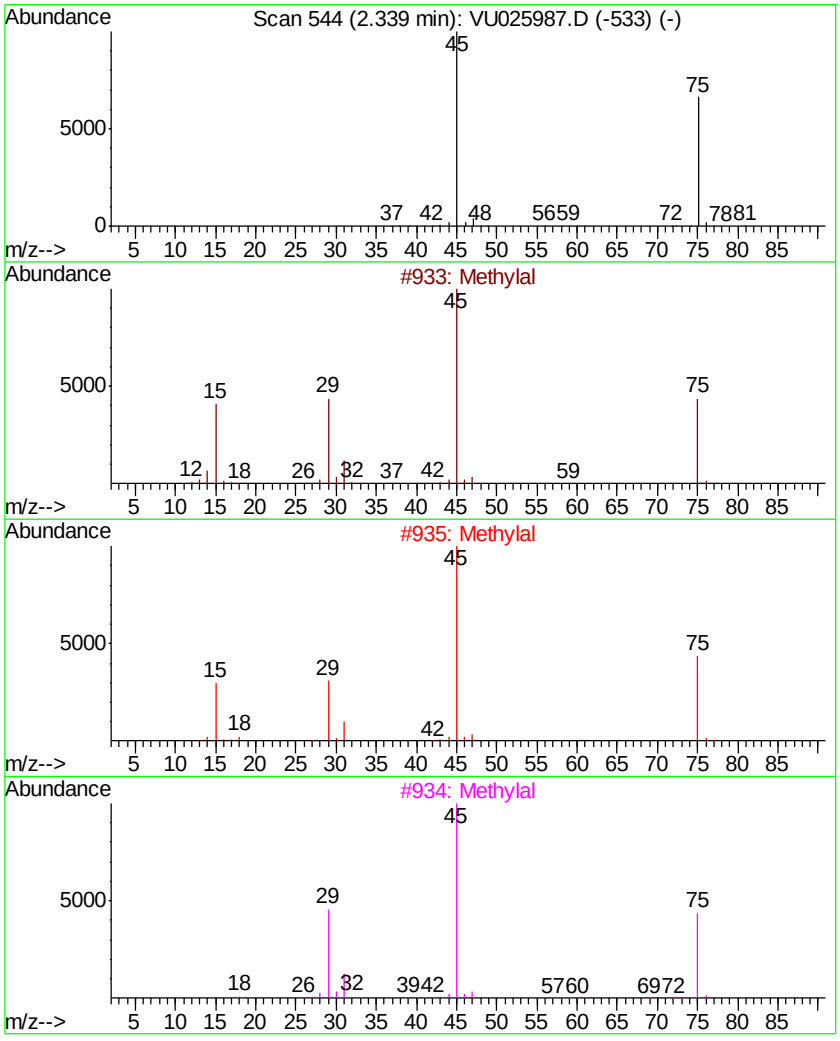
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

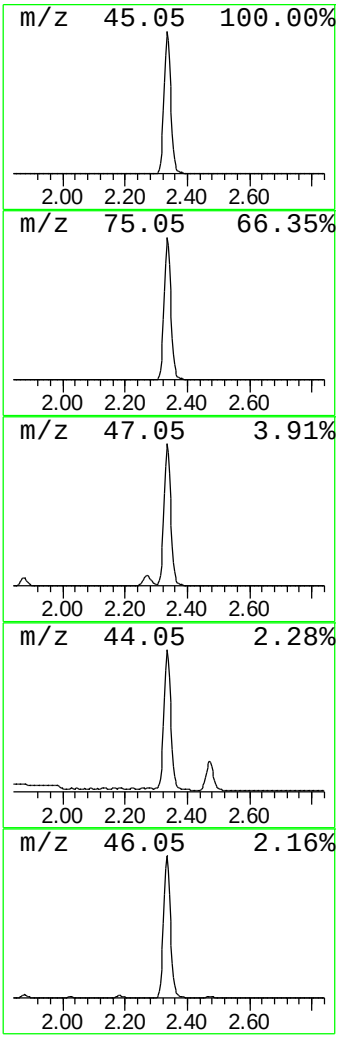
****

Peak Number 2 Methylal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	460.26 ug/L	6619920	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





Library Search Compound Report

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ClientSampleId : A4ZD5

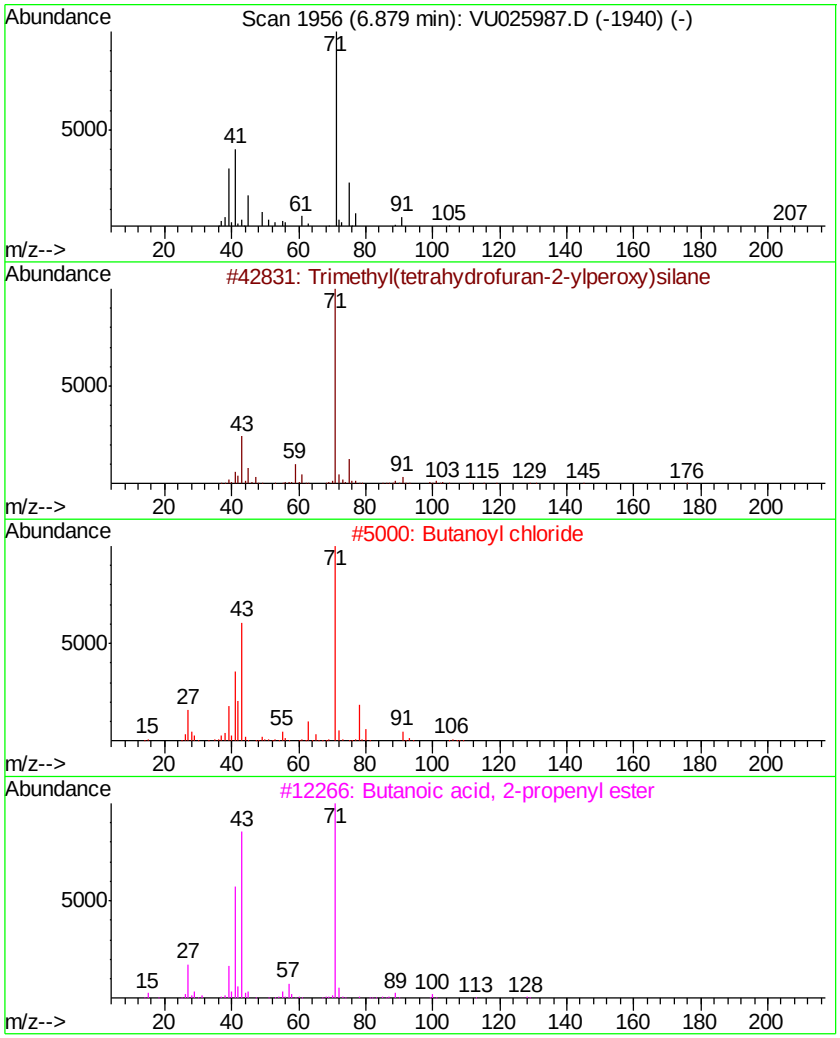
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM080918WMA.M
Quant Title : VOC Analysis

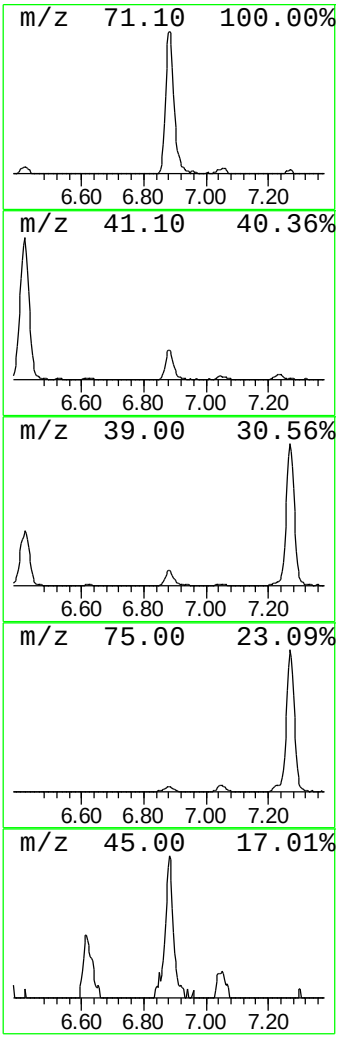
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Trimethyl(tetrahydrofuran-2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	3.82 ug/L	54957	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trimethyl(tetrahydrofuran-2-ylpe...	176	C7H16O3Si	1000368-50-8	64
2	Butanoyl chloride	106	C4H7ClO	000141-75-3	36
3	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	28
4	3-Methoxy-1-pentene	100	C6H12O	014092-18-3	10
5	Hexaborane	76	B6H10	023777-80-2	9





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ClientSampleId : A4ZD5

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

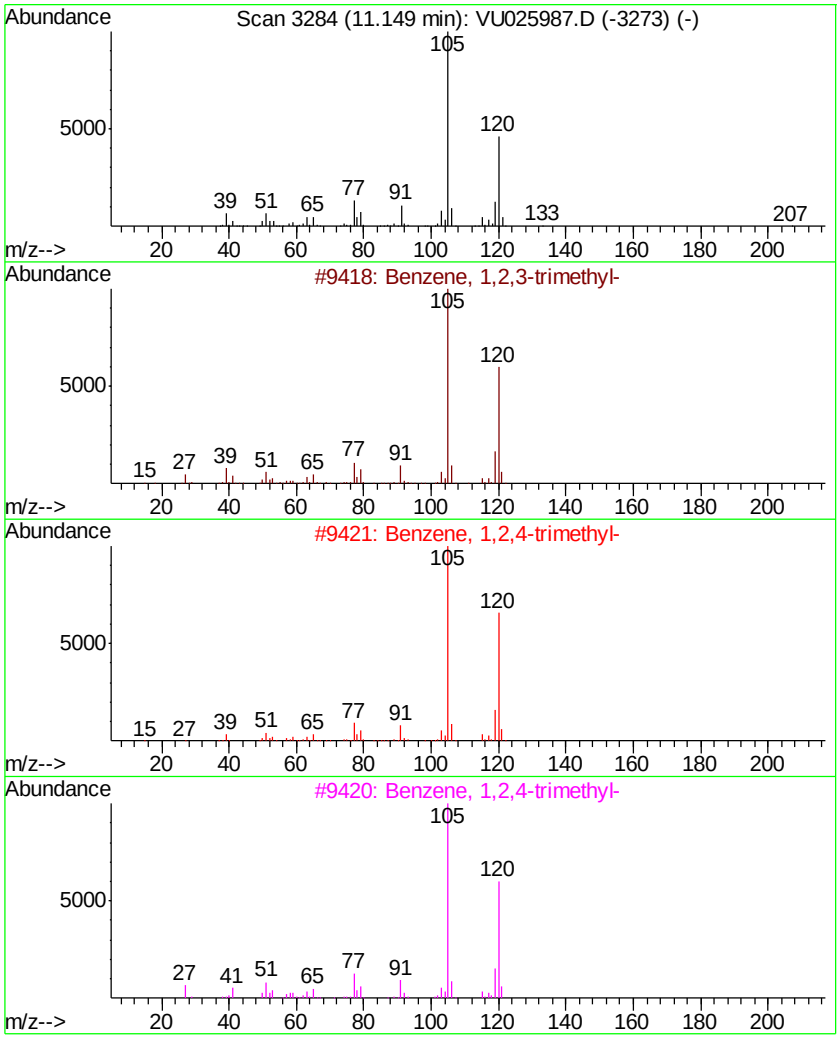
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

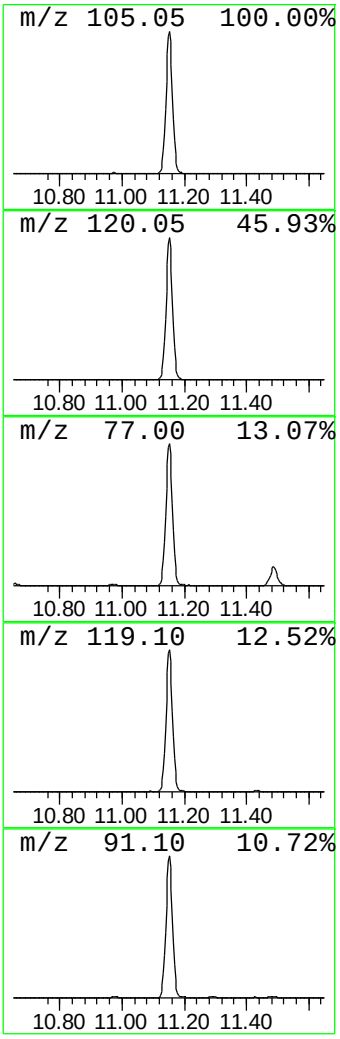
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	38.19 ug/L	1076100	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	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4	Mesitylene	120	C9H12	000108-67-8	94
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93





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ClientSampleId : A4ZD5

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

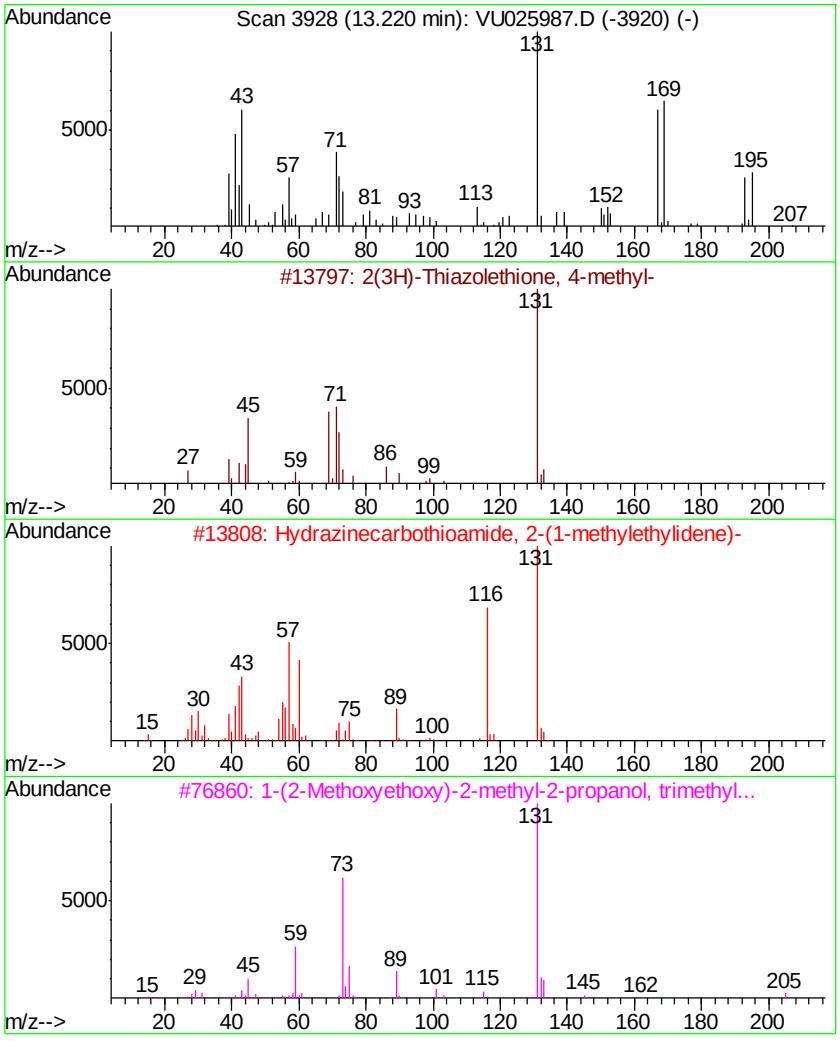
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

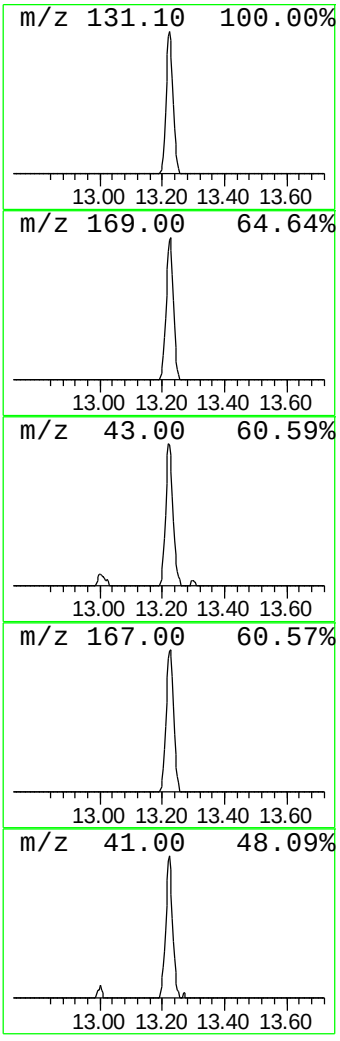
****

Peak Number 7 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.22	2.61 ug/L	73498	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Thiazolethione, 4-methyl-	131	C4H5NS2	005685-06-3	38
2	Hydrazinecarbothioamide, 2-(1-me...	131	C4H9N3S	001752-30-3	14
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	220	C10H24O3Si	1000364-20-4	10
4	2-Oxazolidinethione, 4,4-dimethyl-	131	C5H9NOS	054013-55-7	10
5	Diethyl 3,6,9,12-tetraoxatetrade...	322	C14H26O8	1000366-84-2	10





Tentatively Identified Compound (LSC) summary

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ClientSampleId : A4ZD5

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	460.3	ug/L	6619920	1	5.89	719158	50.0
Trimethyl(tetrahy...	6.88	3.8	ug/L	54957	1	5.89	719158	50.0
Benzene, 1,2,3-tr...	11.15	38.2	ug/L	1076100	3	11.49	1408870	50.0
unknown-01	13.22	2.6	ug/L	73498	3	11.49	1408870	50.0