

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061120\
 Data File : VU038791.D
 Acq On : 10 Jun 2020 21:30
 Operator : SY/MD
 Sample : L2915-19
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9E65

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.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	1.369	5	9	17	rBV4	7348	7151	0.33%	0.038%
2	1.613	77	85	94	rBV	274362	296739	13.58%	1.565%
3	1.928	175	183	199	rVB	209251	271011	12.40%	1.429%
4	2.215	269	272	276	rBV5	2203	2127	0.10%	0.011%
5	2.591	375	389	406	rBV	471084	812976	37.19%	4.287%
6	2.822	453	461	465	rBV3	4051	6267	0.29%	0.033%
7	3.079	532	541	550	rVB7	2161	4038	0.18%	0.021%
8	3.170	561	569	573	rBV4	802	837	0.04%	0.004%
9	3.224	573	586	588	rBV3	1518	2586	0.12%	0.014%
10	3.379	629	634	636	rBV3	724	542	0.02%	0.003%
11	3.723	734	741	744	rBV3	359	511	0.02%	0.003%
12	4.362	935	940	950	rVB2	398	524	0.02%	0.003%
13	4.475	969	975	979	rBV5	1009	1416	0.06%	0.007%
14	4.668	1019	1035	1073	rBV	228373	604009	27.63%	3.185%
15	4.848	1081	1091	1102	rVB	8393	17896	0.82%	0.094%
16	5.102	1152	1170	1189	rBV	391929	849752	38.88%	4.481%
17	5.279	1219	1225	1229	rVB2	640	791	0.04%	0.004%
18	5.311	1229	1235	1236	rBV3	1148	959	0.04%	0.005%
19	5.324	1236	1239	1246	rVB4	1551	1931	0.09%	0.010%
20	5.423	1260	1270	1281	rVB6	4955	10686	0.49%	0.056%
21	5.671	1334	1347	1354	rBV6	10229	21266	0.97%	0.112%
22	5.758	1354	1374	1411	rVB2	801956	2185753	100.00%	11.526%
23	6.060	1464	1468	1470	rBV3	702	466	0.02%	0.002%
24	6.279	1520	1536	1573	rBV	670618	1302232	59.58%	6.867%
25	6.571	1614	1627	1628	rBV6	10211	16557	0.76%	0.087%
26	6.719	1658	1673	1698	rBV	489507	957347	43.80%	5.048%
27	7.021	1760	1767	1769	rBV4	2422	2531	0.12%	0.013%
28	7.089	1782	1788	1789	rBV3	1518	1340	0.06%	0.007%
29	7.198	1817	1822	1823	rBV2	1883	1267	0.06%	0.007%
30	7.259	1832	1841	1850	rVB5	2629	4703	0.22%	0.025%
31	7.423	1887	1892	1894	rBV3	900	871	0.04%	0.005%
32	7.591	1928	1944	1967	rBV	277594	507776	23.23%	2.678%
33	7.710	1978	1981	1992	rVB5	2457	3030	0.14%	0.016%
34	7.816	2004	2014	2025	rVB3	4558	8313	0.38%	0.044%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
 Title : VOC Analysis

35	7.922	2032	2047	2080	rBV	928461	1713415	78.39%	9.035%
36	8.201	2120	2134	2148	rBV	191122	327085	14.96%	1.725%
37	8.333	2164	2175	2184	rVB3	17264	28841	1.32%	0.152%
38	8.394	2184	2194	2202	rBV3	4804	7133	0.33%	0.038%
39	8.488	2213	2223	2231	rBV3	5605	9536	0.44%	0.050%
40	8.655	2261	2275	2303	rBV	701608	1292162	59.12%	6.814%
41	8.944	2358	2365	2369	rBV4	1912	2477	0.11%	0.013%
42	8.992	2377	2380	2385	rVB	616	519	0.02%	0.003%
43	9.063	2396	2402	2411	rVB8	1277	1963	0.09%	0.010%
44	9.211	2440	2448	2459	rVB5	8027	12506	0.57%	0.066%
45	9.282	2463	2470	2474	rBV3	1268	1243	0.06%	0.007%
46	9.346	2479	2490	2501	rVB8	6702	11917	0.55%	0.063%
47	9.436	2504	2518	2552	rBV	957093	1670330	76.42%	8.808%
48	9.587	2558	2565	2567	rBV3	950	1089	0.05%	0.006%
49	9.700	2593	2600	2601	rBV3	2566	2332	0.11%	0.012%
50	9.793	2622	2629	2634	rBV5	1297	1798	0.08%	0.009%
51	9.845	2634	2645	2652	rVV3	25037	44632	2.04%	0.235%
52	9.890	2652	2659	2671	rVB5	24817	48916	2.24%	0.258%
53	9.980	2678	2687	2694	rBV9	2007	3563	0.16%	0.019%
54	10.057	2709	2711	2713	rBV3	784	466	0.02%	0.002%
55	10.118	2728	2730	2738	rVB4	801	707	0.03%	0.004%
56	10.198	2747	2755	2756	rBV3	1800	1700	0.08%	0.009%
57	10.288	2771	2783	2796	rBV5	52876	103563	4.74%	0.546%
58	10.381	2800	2812	2821	rVV4	46145	84687	3.87%	0.447%
59	10.439	2821	2830	2844	rVB3	51587	88401	4.04%	0.466%
60	10.594	2872	2878	2880	rBV5	1143	1340	0.06%	0.007%
61	10.619	2880	2886	2894	rVV5	5373	7868	0.36%	0.041%
62	10.661	2894	2899	2908	rVB6	6252	8518	0.39%	0.045%
63	10.771	2912	2933	2952	rBV	676095	1248976	57.14%	6.586%
64	10.861	2952	2961	2968	rVV2	36316	56876	2.60%	0.300%
65	10.906	2971	2975	2980	rVV6	14227	17771	0.81%	0.094%
66	10.951	2981	2989	3002	rVB7	29660	63901	2.92%	0.337%
67	11.025	3002	3012	3020	rBV2	12759	19593	0.90%	0.103%
68	11.079	3020	3029	3038	rBV3	36153	56798	2.60%	0.300%
69	11.272	3073	3089	3098	rBV6	14072	28621	1.31%	0.151%
70	11.333	3098	3108	3119	rBV3	44755	76711	3.51%	0.405%
71	11.404	3119	3130	3148	rVB8	42770	116127	5.31%	0.612%

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72	11.484	3152	3155	3156	rBV2	1308	680	0.03%	0.004%
73	11.533	3156	3170	3179	rBV6	29408	55263	2.53%	0.291%
74	11.594	3179	3189	3199	rBV6	28440	51615	2.36%	0.272%
75	11.671	3201	3213	3225	rBV5	42733	102197	4.68%	0.539%
76	11.822	3248	3260	3285	rVB	1076340	1803739	82.52%	9.511%
77	11.957	3292	3302	3310	rBV5	14437	23707	1.08%	0.125%
78	12.018	3313	3321	3332	rBV6	23471	52768	2.41%	0.278%
79	12.201	3368	3378	3398	rVB	1048820	1736343	79.44%	9.156%
80	12.381	3429	3434	3442	rBV7	9794	14261	0.65%	0.075%
81	12.767	3549	3554	3561	rBV9	4189	5342	0.24%	0.028%
82	13.346	3727	3734	3746	rVB9	7026	15007	0.69%	0.079%
83	13.809	3876	3878	3884	rVB7	2585	1803	0.08%	0.010%
84	13.841	3884	3888	3892	rBV7	2437	2784	0.13%	0.015%
85	13.934	3908	3917	3925	rVB10	4691	7757	0.35%	0.041%
86	14.114	3969	3973	3977	rBV4	1855	1863	0.09%	0.010%
87	14.266	4015	4020	4021	rBV3	2708	2096	0.10%	0.011%
88	14.391	4054	4059	4062	rBV4	1634	1687	0.08%	0.009%
89	14.468	4078	4083	4084	rBV4	2779	2462	0.11%	0.013%
90	14.600	4120	4124	4129	rBV5	1401	1570	0.07%	0.008%
91	14.825	4192	4194	4196	rVB3	1124	499	0.02%	0.003%
92	14.909	4218	4220	4227	rVB4	1364	1128	0.05%	0.006%
93	14.989	4239	4245	4247	rBV4	1655	1688	0.08%	0.009%
94	15.063	4263	4268	4275	rVB9	1932	2234	0.10%	0.012%
95	15.153	4293	4296	4298	rBV2	1168	645	0.03%	0.003%
96	15.253	4324	4327	4329	rBV2	721	519	0.02%	0.003%
97	15.298	4339	4341	4345	rVB2	1080	659	0.03%	0.003%
98	15.320	4345	4348	4350	rBV3	775	460	0.02%	0.002%
99	15.346	4352	4356	4357	rBV3	2334	1673	0.08%	0.009%
100	15.664	4451	4455	4459	rBV5	1351	1479	0.07%	0.008%

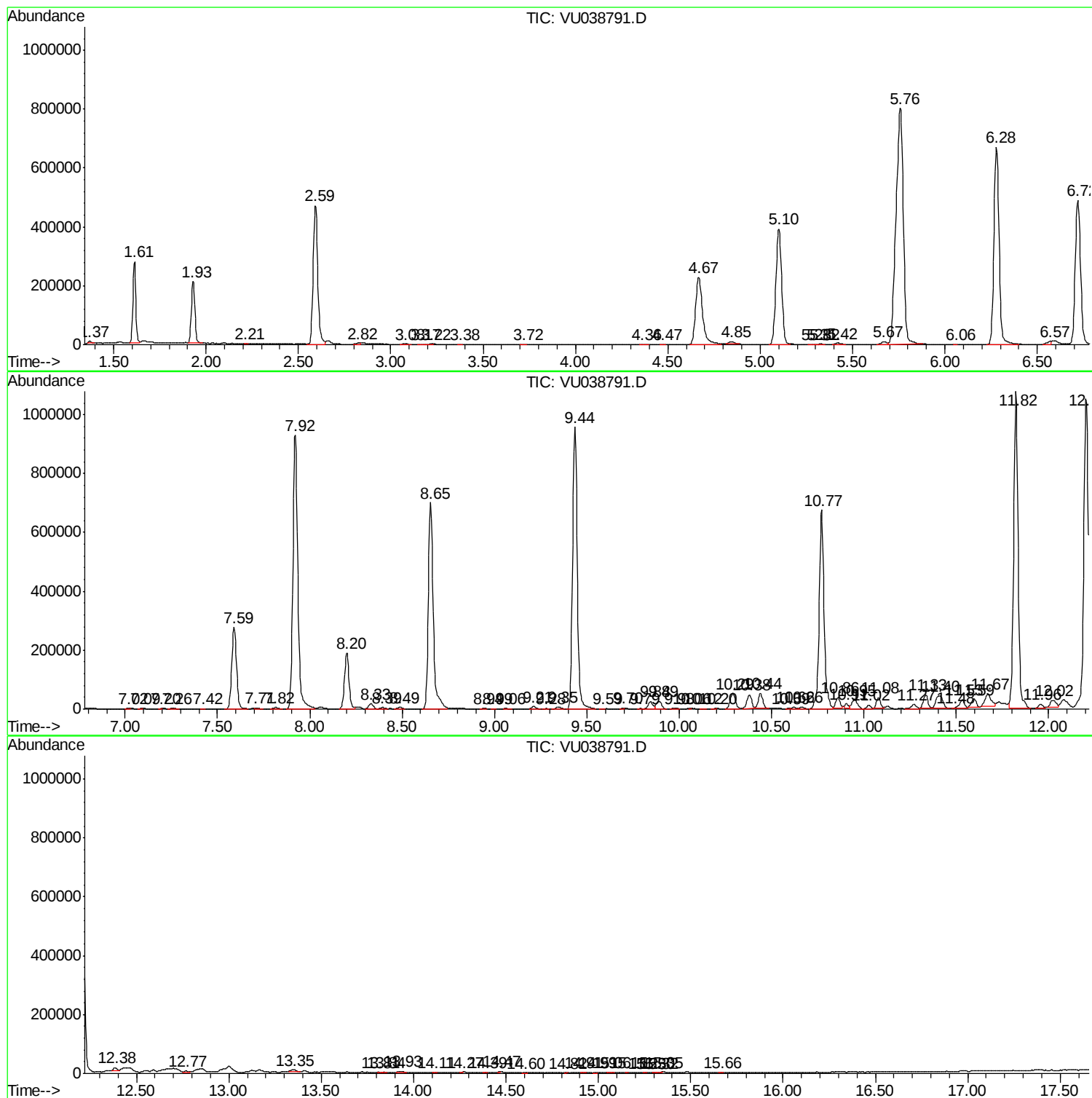
Sum of corrected areas: 18964210

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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



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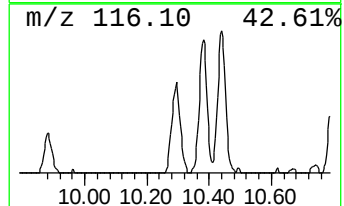
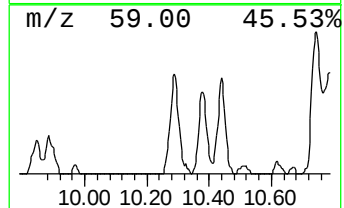
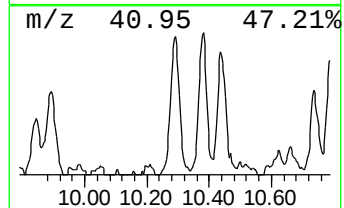
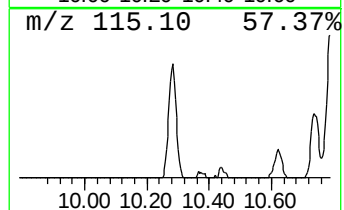
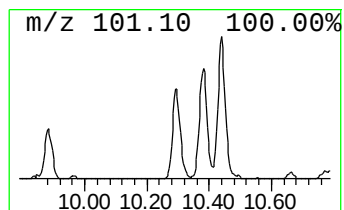
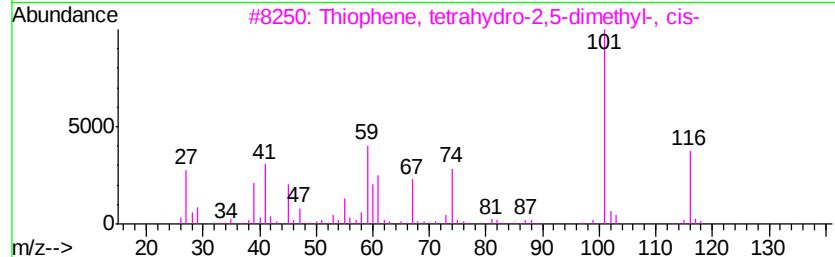
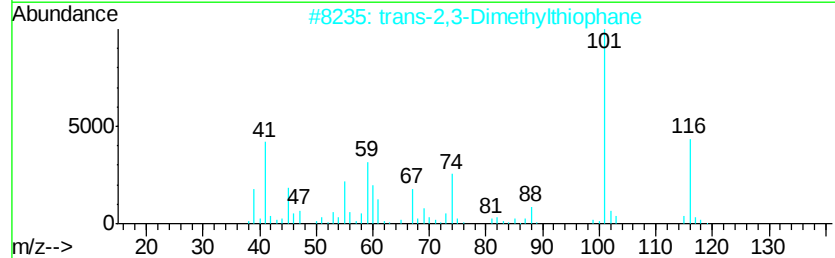
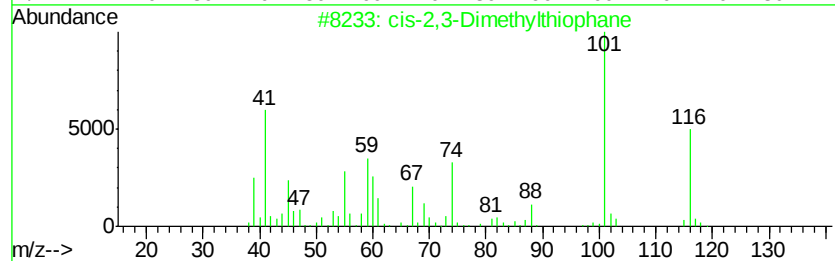
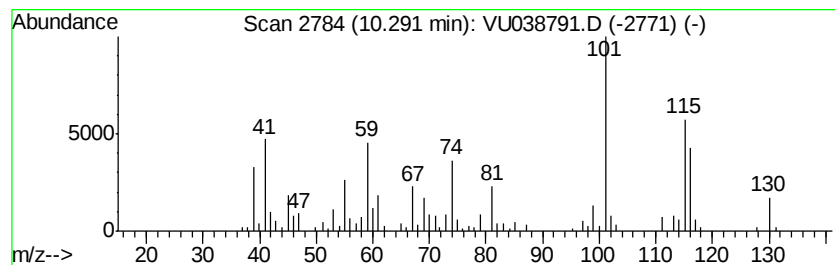
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 cis-2,3-Dimethylthiophane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.29	3.10 ug/L	103563	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	55
2		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	50
3		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-13-7	49
4		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	49
5		N-(1,3,4-Thiadiazol-2-yl)formamide	129	C3H3N3OS	026861-89-2	35



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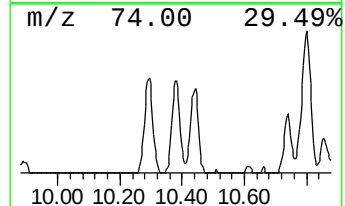
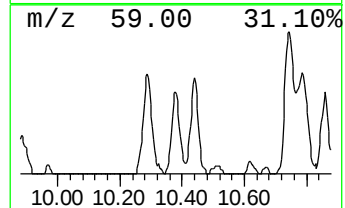
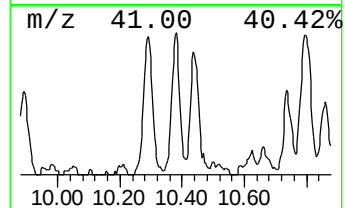
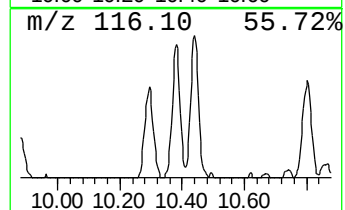
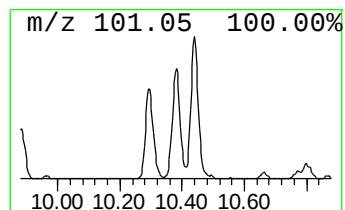
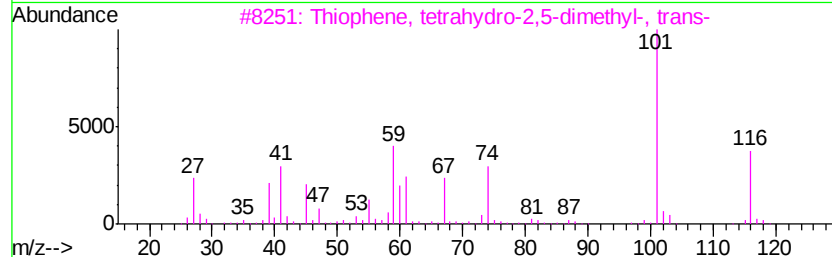
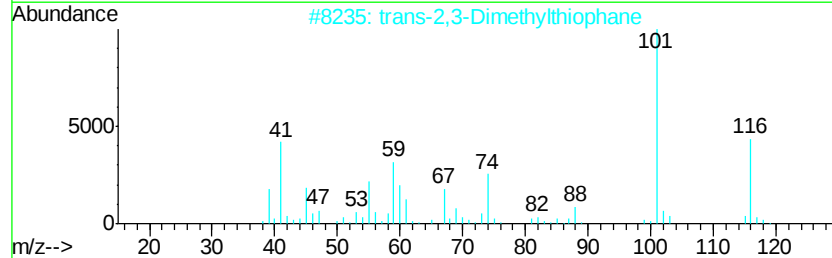
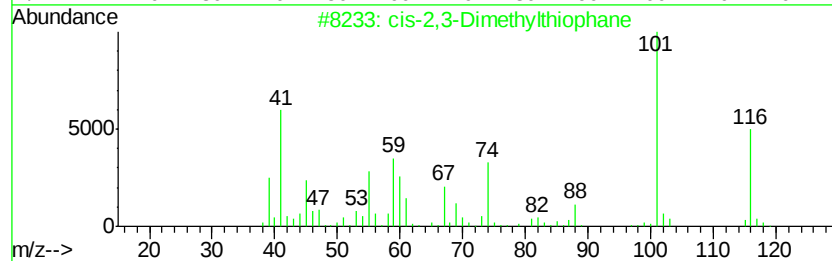
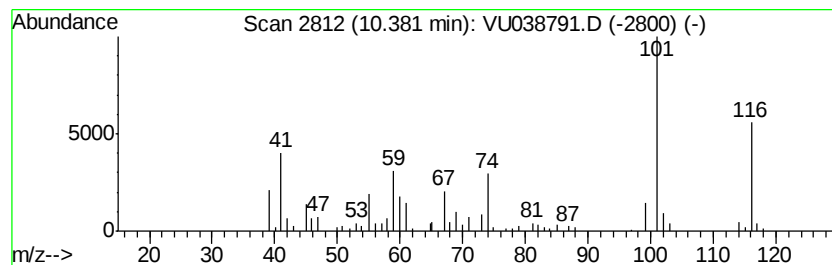
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Quant Title : VOC Analysis

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

Peak Number 3 trans-2,3-Dimethylthiophane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.54 ug/L	84687	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-2,3-Dimethylthiophane	116	C6H12S	005161-77-3	93
2		trans-2,3-Dimethylthiophane	116	C6H12S	005161-78-4	93
3		Thiophene, tetrahydro-2,5-dimeth...	116	C6H12S	005161-14-8	86
4		2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	81
5		Allylthiourea	116	C4H8N2S	000109-57-9	50



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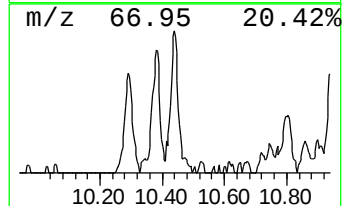
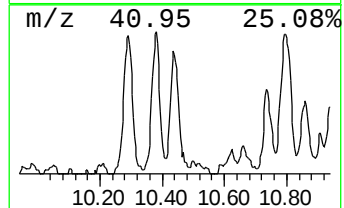
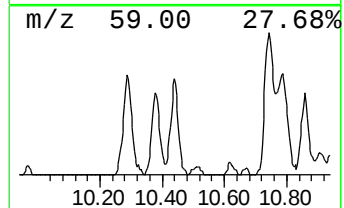
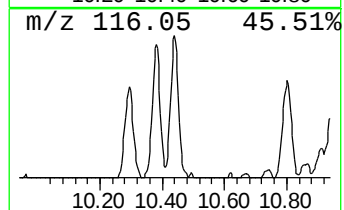
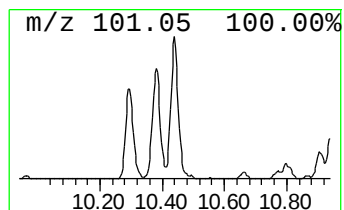
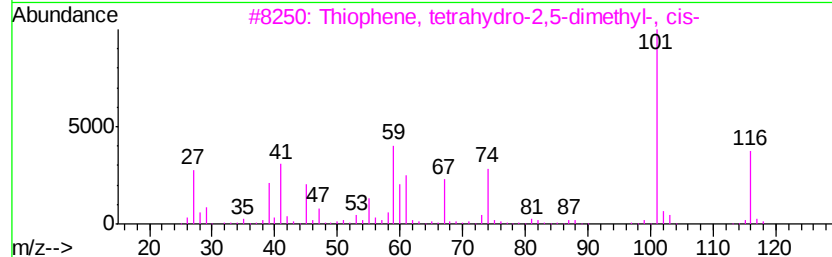
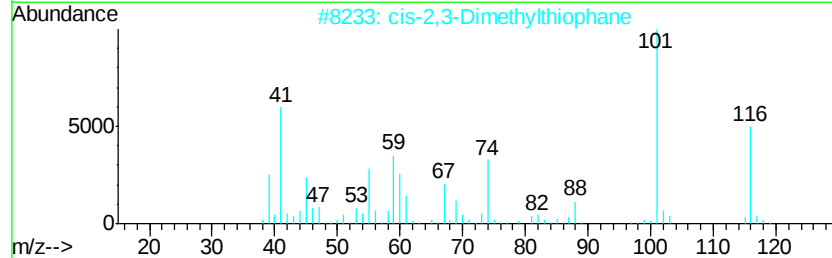
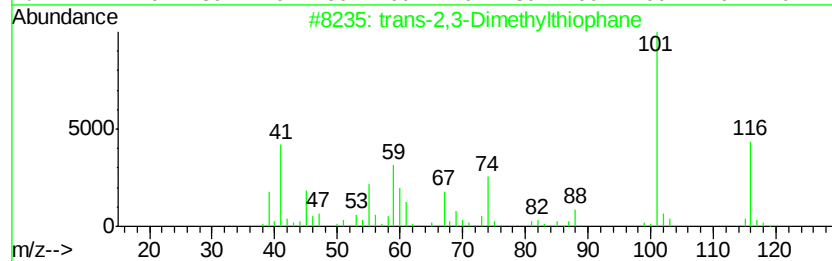
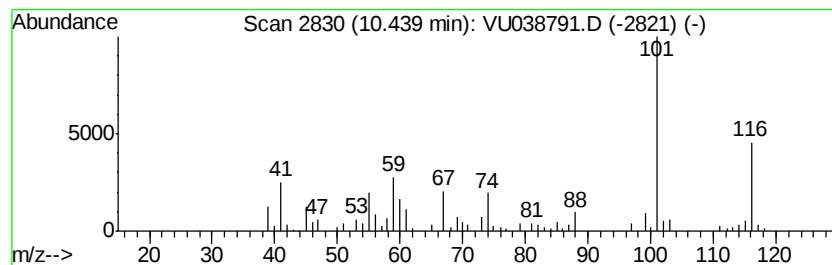
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Quant Title : VOC Analysis

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

Peak Number 4 Thiophene, tetrahydro-2,5-d... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.44	2.65 ug/L	88401	Chlorobenzene-d5	9.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Dimethylthiophane			116	C6H12S	005161-78-4	94
2	cis-2,3-Dimethylthiophane			116	C6H12S	005161-77-3	93
3	Thiophene, tetrahydro-2,5-dimeth...			116	C6H12S	005161-13-7	83
4	2H-Thiopyran, tetrahydro-2-methyl-			116	C6H12S	005161-16-0	81
5	Thiophene, tetrahydro-2,5-dimeth...			116	C6H12S	005161-14-8	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061120\
Data File : VU038791.D
Acq On : 10 Jun 2020 21:30
Operator : SY/MD
Sample : L2915-19
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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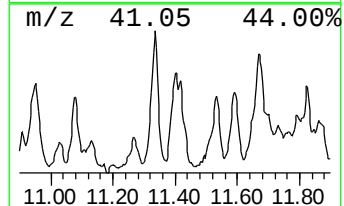
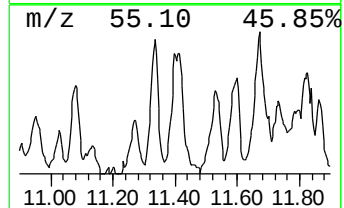
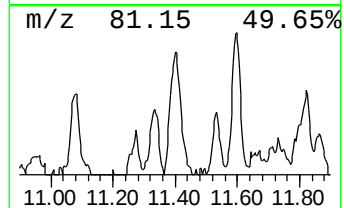
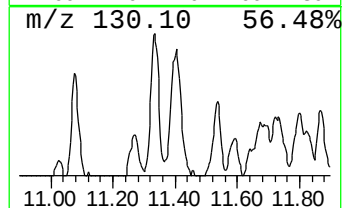
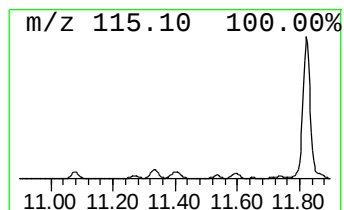
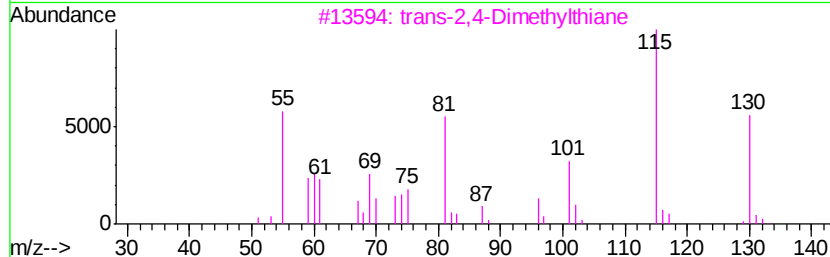
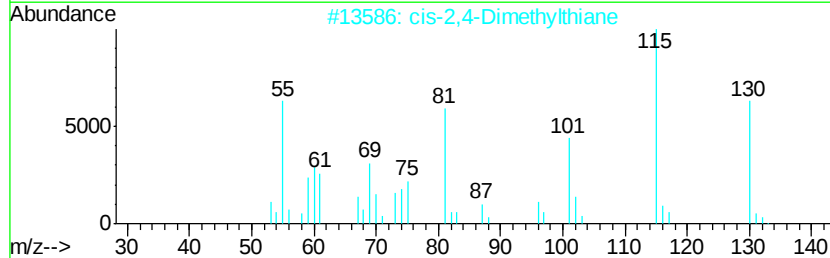
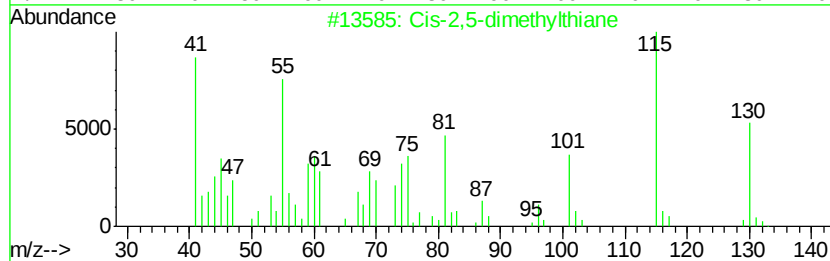
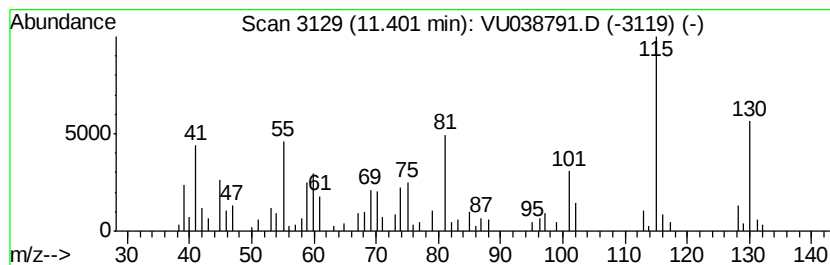
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	3.22 ug/L	116127	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cis-2,5-dimethylthiane	130	C7H14S	1000215-06-6	93
2		cis-2,4-Dimethylthiane	130	C7H14S	061568-43-2	81
3		trans-2,4-Dimethylthiane	130	C7H14S	061568-42-1	81
4		Cis-2,3-dimethylthiane	130	C7H14S	1000215-06-5	55
5		But-2-enyloxy-dimethyl-silane	130	C6H14OSi	1000145-63-6	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061120\
Data File : VU038791.D
Acq On : 10 Jun 2020 21:30
Operator : SY/MD
Sample : L2915-19
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9E65

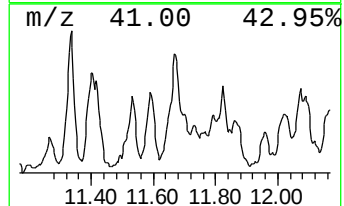
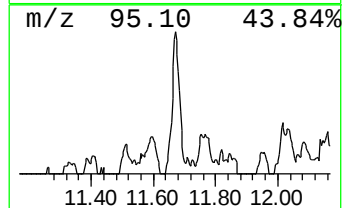
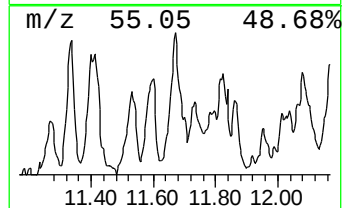
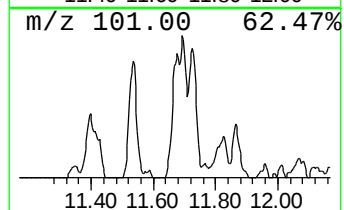
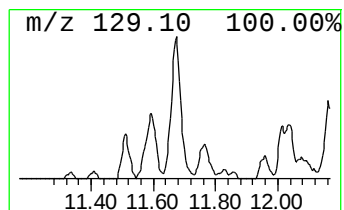
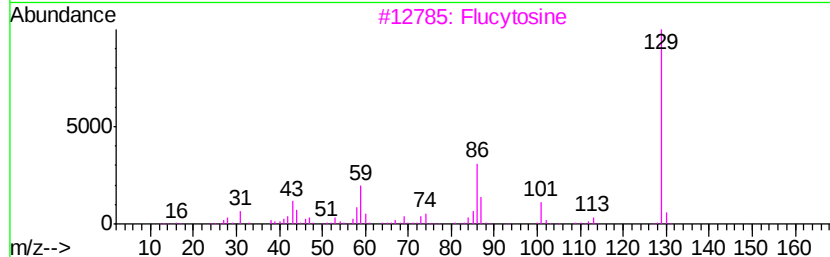
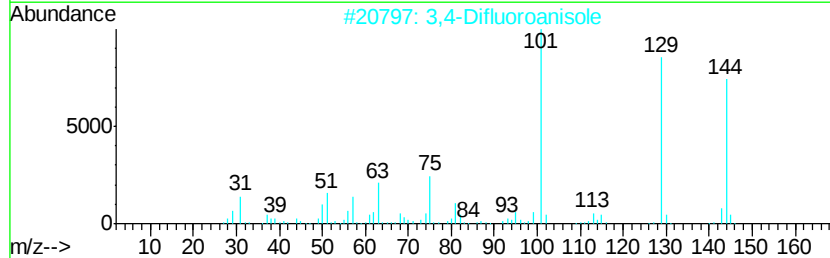
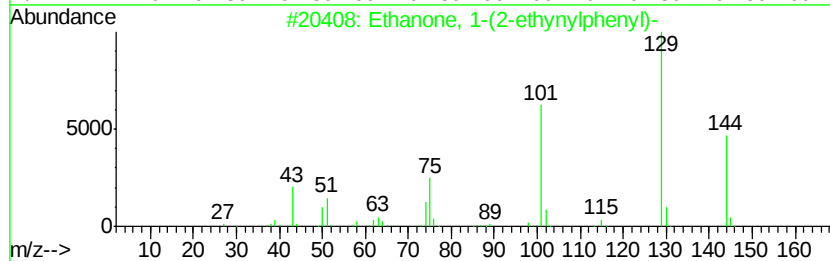
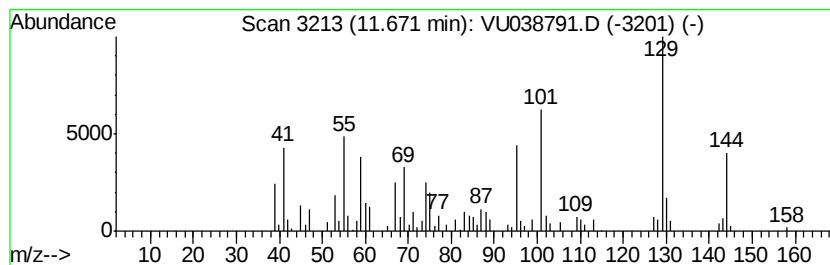
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.83 ug/L	102197	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(2-ethynylphenyl)-	144	C10H8O	104190-22-9	47
2		3,4-Difluoroanisole	144	C7H6F2O	115144-40-6	38
3		Flucytosine	129	C4H4FN3O	002022-85-7	38
4		N-(1,3,4-Thiadiazol-2-yl)formamide	129	C3H3N3OS	026861-89-2	35
5		3,4-Difluoroanisole	144	C7H6F2O	115144-40-6	35



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061120\
Data File : VU038791.D
Acq On : 10 Jun 2020 21:30
Operator : SY/MD
Sample : L2915-19
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9E65

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060820WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
cis-2,3-Dimethylt...	10.29	3.1	ug/L	103563	2	9.44	1670330	50.0
trans-2,3-Dimethy...	10.38	2.5	ug/L	84687	2	9.44	1670330	50.0
Thiophene, tetrah...	10.44	2.6	ug/L	88401	2	9.44	1670330	50.0
unknown-01	11.40	3.2	ug/L	116127	3	11.82	1803740	50.0
unknown-02	11.67	2.8	ug/L	102197	3	11.82	1803740	50.0