

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU040920\
 Data File : VU037670.D
 Acq On : 10 Apr 2020 14:08
 Operator : JC/MD
 Sample : L2189-02 10X
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFS80

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\SOMULM040920WMA.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	1.610	77	84	93	rBV	271872	284253	12.13%	1.319%
2	1.903	167	175	188	rVB	209422	281717	12.02%	1.307%
3	2.584	373	387	405	rBV2	392817	686635	29.29%	3.186%
4	2.803	447	455	470	rVB	7225	15965	0.68%	0.074%
5	2.919	486	491	496	rBV5	838	1098	0.05%	0.005%
6	3.070	531	538	547	rVB6	1483	2699	0.12%	0.013%
7	3.218	569	584	603	rVB2	34551	85245	3.64%	0.395%
8	3.382	626	635	643	rBV10	2028	3566	0.15%	0.017%
9	3.559	686	690	694	rBV3	703	748	0.03%	0.003%
10	3.713	732	738	741	rBV5	763	806	0.03%	0.004%
11	3.906	779	798	818	rBV	243005	575583	24.55%	2.670%
12	4.038	821	839	853	rVV3	7992	20463	0.87%	0.095%
13	4.215	889	894	896	rVB3	691	526	0.02%	0.002%
14	4.282	913	915	920	rBV4	585	521	0.02%	0.002%
15	4.324	923	928	933	rVB5	976	929	0.04%	0.004%
16	4.356	933	938	944	rVB4	519	685	0.03%	0.003%
17	4.404	947	953	956	rBV4	709	822	0.04%	0.004%
18	4.440	961	964	970	rVB2	508	580	0.02%	0.003%
19	4.475	970	975	978	rBV3	703	688	0.03%	0.003%
20	4.543	991	996	1000	rVV4	688	587	0.03%	0.003%
21	4.665	1015	1034	1060	rBV	254961	618601	26.39%	2.870%
22	4.835	1083	1087	1089	rBV3	882	832	0.04%	0.004%
23	5.035	1143	1149	1151	rBV4	563	568	0.02%	0.003%
24	5.099	1152	1169	1190	rVV	350180	780737	33.30%	3.622%
25	5.253	1215	1217	1222	rVB4	779	589	0.03%	0.003%
26	5.350	1228	1247	1266	rBV	1043583	2344344	100.00%	10.876%
27	5.758	1351	1374	1401	rBV2	781437	2062802	87.99%	9.570%
28	6.002	1446	1450	1455	rBV5	560	650	0.03%	0.003%
29	6.031	1455	1459	1462	rVB3	920	795	0.03%	0.004%
30	6.070	1464	1471	1475	rBV6	1312	1531	0.07%	0.007%
31	6.144	1488	1494	1497	rBV3	668	801	0.03%	0.004%
32	6.279	1519	1536	1559	rBV	674122	1249843	53.31%	5.799%
33	6.417	1573	1579	1583	rVB4	868	797	0.03%	0.004%
34	6.517	1605	1610	1612	rBV2	750	778	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040920WMA.M
 Title : VOC Analysis

35	6.555	1613	1622	1641	rVB2	5023	11881	0.51%	0.055%
36	6.719	1656	1673	1695	rBV	505244	966819	41.24%	4.485%
37	6.899	1725	1729	1731	rBV3	630	628	0.03%	0.003%
38	6.948	1731	1744	1756	rVB2	36139	71242	3.04%	0.331%
39	7.176	1812	1815	1817	rVV4	750	528	0.02%	0.002%
40	7.208	1817	1825	1834	rVB7	5109	8691	0.37%	0.040%
41	7.362	1862	1873	1882	rBV2	7621	13117	0.56%	0.061%
42	7.536	1916	1927	1932	rBV4	14848	24614	1.05%	0.114%
43	7.591	1933	1944	1962	rVB	311085	540054	23.04%	2.506%
44	7.742	1974	1991	2003	rVB	32898	62111	2.65%	0.288%
45	7.819	2003	2015	2024	rBV5	2993	5835	0.25%	0.027%
46	7.919	2031	2046	2064	rBV	973572	1665410	71.04%	7.726%
47	7.993	2064	2069	2085	rVB6	4516	7239	0.31%	0.034%
48	8.160	2116	2121	2122	rBV3	628	622	0.03%	0.003%
49	8.202	2122	2134	2149	rBV	228810	375740	16.03%	1.743%
50	8.298	2162	2164	2171	rVB4	683	548	0.02%	0.003%
51	8.494	2216	2225	2232	rBV4	2595	4459	0.19%	0.021%
52	8.571	2238	2249	2256	rBV7	4236	6681	0.28%	0.031%
53	8.655	2262	2275	2301	rBV	862165	1477794	63.04%	6.856%
54	8.809	2320	2323	2332	rVB6	964	1043	0.04%	0.005%
55	9.337	2482	2487	2495	rVB7	1174	1169	0.05%	0.005%
56	9.436	2504	2518	2537	rBV	967644	1583154	67.53%	7.345%
57	9.539	2543	2550	2559	rVV7	3372	5222	0.22%	0.024%
58	9.587	2560	2565	2576	rVV6	2981	3645	0.16%	0.017%
59	9.710	2597	2603	2611	rVB4	3353	4011	0.17%	0.019%
60	9.780	2616	2625	2630	rBV5	1163	1684	0.07%	0.008%
61	9.931	2666	2672	2677	rBV4	770	977	0.04%	0.005%
62	10.118	2723	2730	2741	rVB5	4245	7452	0.32%	0.035%
63	10.275	2762	2779	2796	rBV	295651	489462	20.88%	2.271%
64	10.497	2843	2848	2853	rBV4	2491	3573	0.15%	0.017%
65	10.562	2861	2868	2879	rVB2	10279	14052	0.60%	0.065%
66	10.655	2890	2897	2899	rBV7	1529	1681	0.07%	0.008%
67	10.716	2912	2916	2919	rBV4	697	558	0.02%	0.003%
68	10.771	2919	2933	2948	rBV	701507	1132371	48.30%	5.254%
69	10.906	2962	2975	2985	rBV6	4671	10099	0.43%	0.047%
70	11.044	3006	3018	3033	rVB	412322	692552	29.54%	3.213%
71	11.205	3063	3068	3069	rBV3	1846	1430	0.06%	0.007%

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72	11.247	3076	3081	3084	rBV6	1477	1563	0.07%	0.007%
73	11.304	3095	3099	3106	rVB5	1347	1793	0.08%	0.008%
74	11.346	3106	3112	3116	rVB5	1218	1328	0.06%	0.006%
75	11.430	3134	3138	3141	rBV2	802	566	0.02%	0.003%
76	11.484	3145	3155	3161	rBV6	3053	4919	0.21%	0.023%
77	11.639	3190	3203	3207	rBV6	3109	5676	0.24%	0.026%
78	11.726	3225	3230	3237	rVV6	1811	2566	0.11%	0.012%
79	11.764	3237	3242	3248	rVB6	1724	2101	0.09%	0.010%
80	11.825	3248	3261	3277	rBV	1021180	1625956	69.36%	7.543%
81	11.912	3282	3288	3295	rBV7	1928	2415	0.10%	0.011%
82	12.108	3338	3349	3359	rVB6	19991	32573	1.39%	0.151%
83	12.205	3364	3379	3394	rVV	982655	1578684	67.34%	7.324%
84	12.732	3538	3543	3547	rBV5	711	823	0.04%	0.004%
85	12.796	3560	3563	3572	rVB5	1414	1451	0.06%	0.007%
86	12.886	3581	3591	3604	rBV	19044	30261	1.29%	0.140%
87	12.944	3605	3609	3614	rVV6	1826	2279	0.10%	0.011%
88	12.989	3618	3623	3631	rVB6	3676	5044	0.22%	0.023%
89	13.311	3719	3723	3726	rBV3	701	669	0.03%	0.003%
90	13.349	3732	3735	3744	rVB8	1292	1266	0.05%	0.006%
91	13.809	3875	3878	3880	rBV3	1000	761	0.03%	0.004%
92	13.867	3889	3896	3904	rVB7	1818	2235	0.10%	0.010%
93	13.941	3917	3919	3925	rBV4	608	593	0.03%	0.003%
94	14.115	3964	3973	3982	rBV2	4383	7633	0.33%	0.035%
95	14.195	3993	3998	4002	rBV5	1202	1254	0.05%	0.006%
96	14.356	4045	4048	4049	rBV2	854	538	0.02%	0.002%
97	14.623	4123	4131	4141	rVB2	6167	10347	0.44%	0.048%
98	14.722	4156	4162	4169	rVV8	1152	1865	0.08%	0.009%
99	14.832	4194	4196	4200	rBV5	1204	921	0.04%	0.004%
100	14.992	4243	4246	4249	rBV2	872	554	0.02%	0.003%

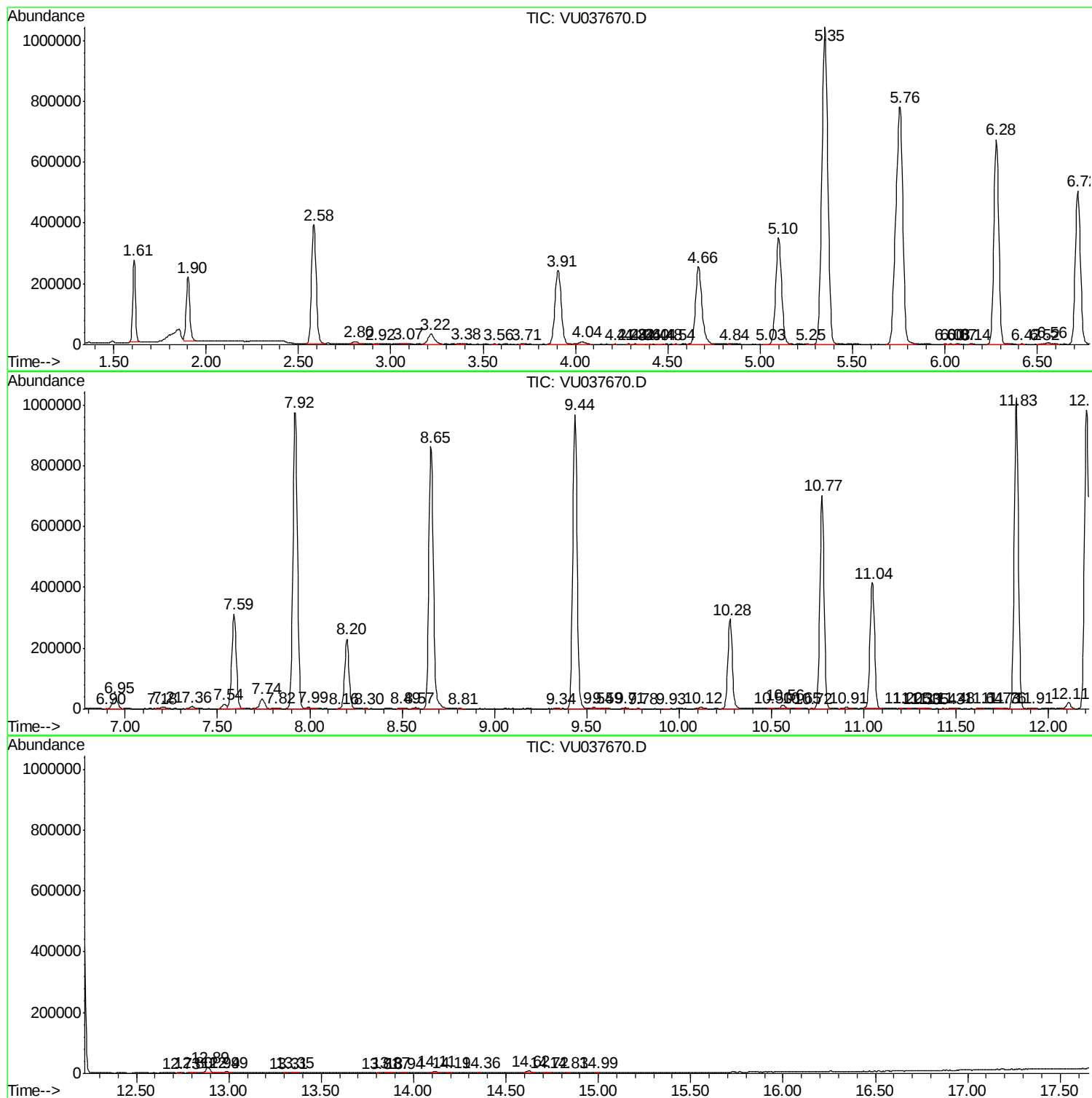
Sum of corrected areas: 21554566

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Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040920WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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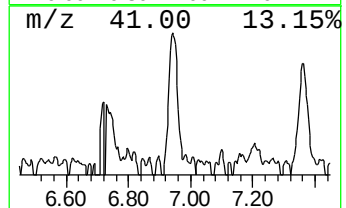
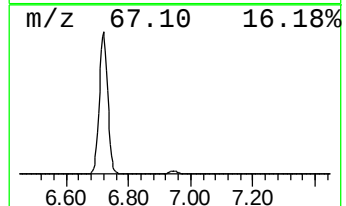
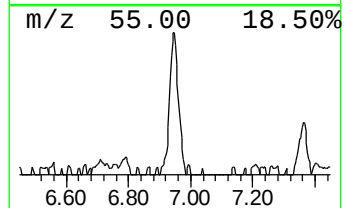
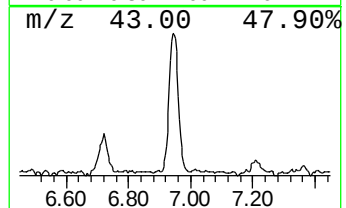
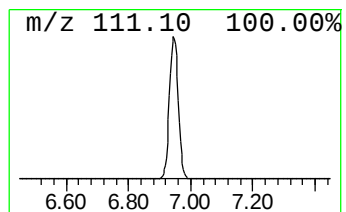
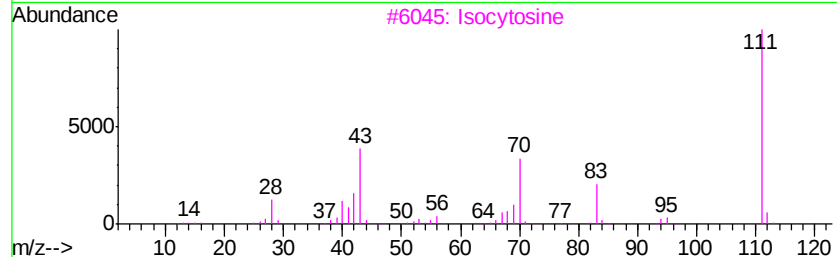
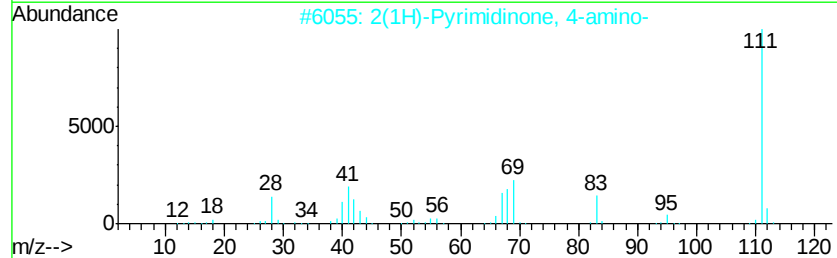
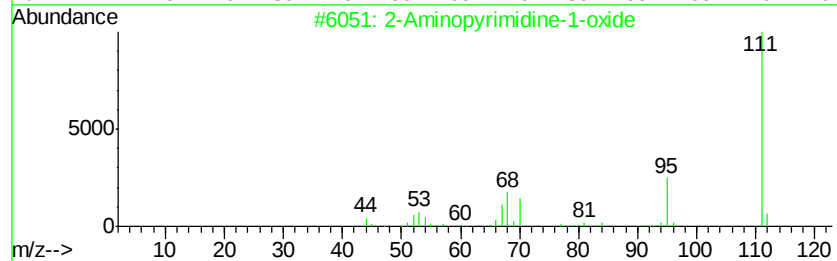
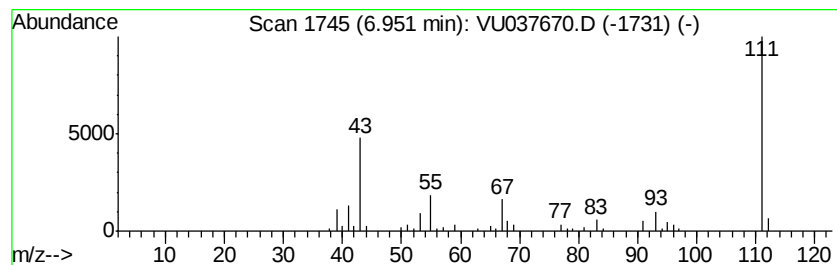
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040920WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Aminopyrimidine-1-oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	2.85 ug/L	71242	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	64
2		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	59
3		Isocytosine	111	C4H5N3O	000108-53-2	42
4		2,4-Diamino-1,3,5-triazine	111	C3H5N5	000504-08-5	40
5		2(1H)-Pyridinone, 5-hydroxy-	111	C5H5N2O	005154-01-8	39



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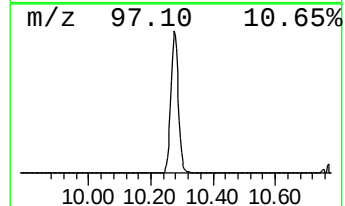
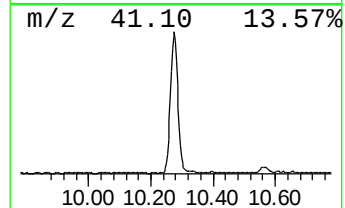
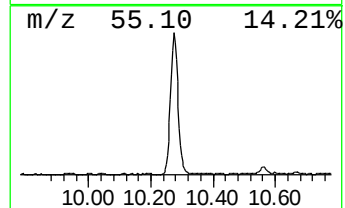
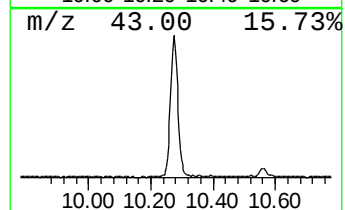
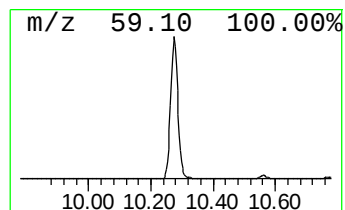
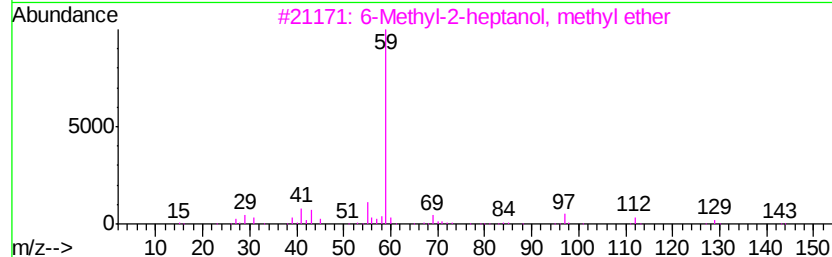
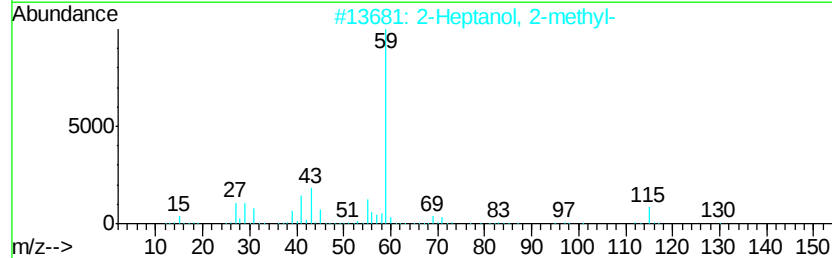
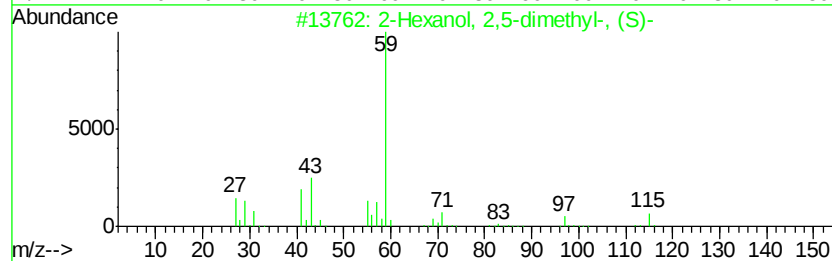
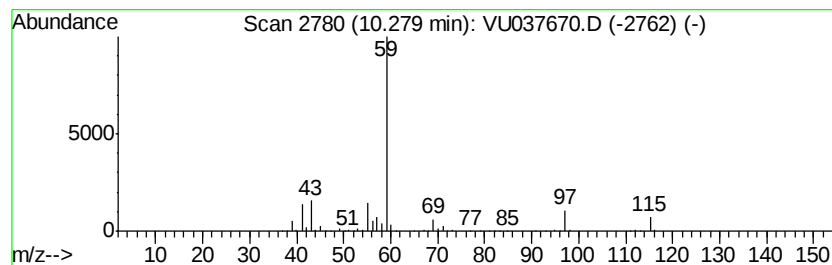
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Quant Title : VOC Analysis

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

Peak Number 4 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.28	15.46 ug/L	489462	Chlorobenzene-d5	9.44		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	78	
2	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	72	
3	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	64	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	64	
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	64	



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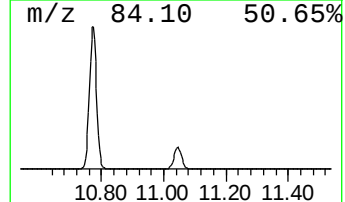
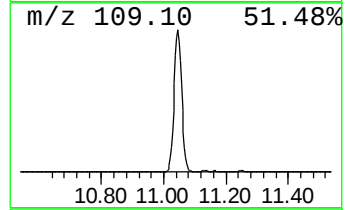
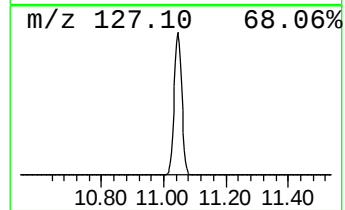
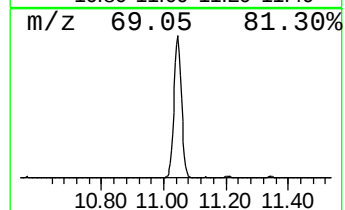
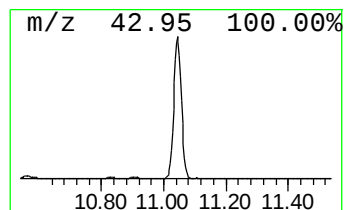
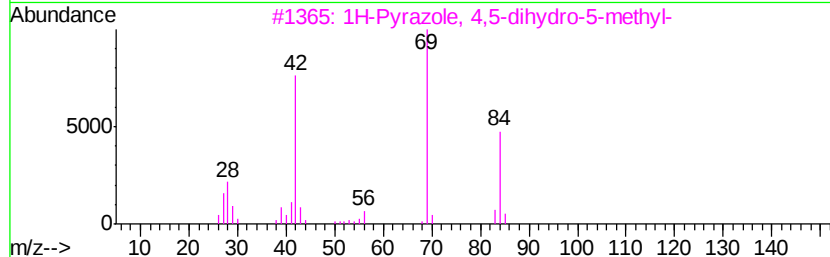
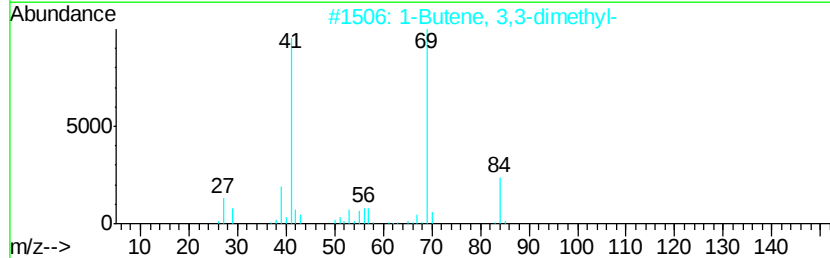
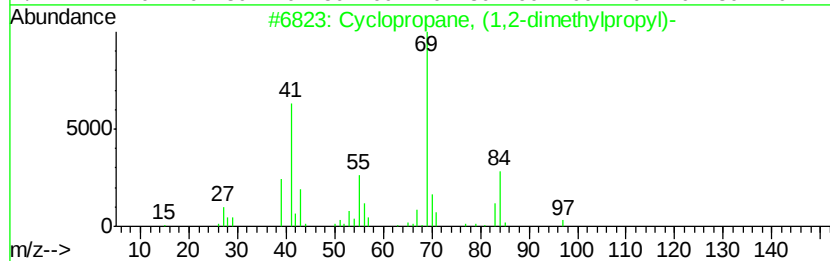
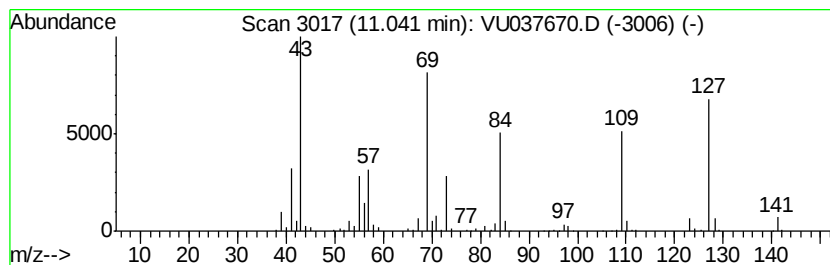
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Cyclic11.04 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	21.30 ug/L	692552	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	35
2		1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	35
3		1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	35
4		Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	35
5		Hexanal, 3,3-dimethyl-	128	C8H16O	055320-57-5	35



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU040920\
Data File : VU037670.D
Acq On : 10 Apr 2020 14:08
Operator : JC/MD
Sample : L2189-02 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFS80

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040920WMA.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
2-Aminopyrimidine...	6.95	2.9	ug/L	71242	1	6.28	1249840	50.0
2-Hexanol, 2,5-di...	10.28	15.5	ug/L	489462	2	9.44	1583150	50.0
(DEL) Alkane: Cyc...	11.04	21.3	ug/L	692552	3	11.83	1625960	50.0