

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV031020\
 Data File : VV014826.D
 Acq On : 11 Mar 2020 01:06
 Operator : SY/MD
 Sample : L1840-22
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBET7

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_V\METHOD\SOMVLM030620WMA.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	1.222	35	41	50	rBV2	23446	23669	1.59%	0.177%
2	1.315	63	70	84	rVB	165564	177091	11.89%	1.327%
3	1.393	88	94	105	rBV	24657	33488	2.25%	0.251%
4	1.479	115	121	130	rVB	19859	21050	1.41%	0.158%
5	1.579	144	152	165	rVB	138063	166750	11.19%	1.250%
6	2.119	310	320	336	rBV	279119	403980	27.11%	3.028%
7	2.460	412	426	438	rBV2	8104	21766	1.46%	0.163%
8	2.627	476	478	481	rBV3	1318	819	0.05%	0.006%
9	2.762	516	520	525	rVB4	838	704	0.05%	0.005%
10	2.984	579	589	596	rVV3	4013	7283	0.49%	0.055%
11	3.248	668	671	675	rVB4	1057	741	0.05%	0.006%
12	3.425	723	726	732	rVB3	595	689	0.05%	0.005%
13	3.537	748	761	782	rBV3	22475	53826	3.61%	0.403%
14	3.730	805	821	848	rBV2	122785	342474	22.99%	2.567%
15	3.923	871	881	909	rBV	74441	250424	16.81%	1.877%
16	4.376	1007	1022	1047	rBV2	232666	580293	38.95%	4.349%
17	5.074	1221	1239	1275	rBV3	587797	1489955	100.00%	11.166%
18	5.270	1286	1300	1323	rBV3	37814	132067	8.86%	0.990%
19	5.473	1361	1363	1368	rVB3	1032	612	0.04%	0.005%
20	5.502	1368	1372	1375	rBV4	937	886	0.06%	0.007%
21	5.643	1400	1416	1437	rBV	543387	1059670	71.12%	7.941%
22	5.811	1465	1468	1471	rBV3	929	674	0.05%	0.005%
23	5.843	1475	1478	1484	rVB4	896	879	0.06%	0.007%
24	5.923	1497	1503	1506	rBV6	2475	2636	0.18%	0.020%
25	6.097	1536	1557	1583	rBV	334489	694910	46.64%	5.208%
26	6.618	1717	1719	1723	rVV3	1424	1147	0.08%	0.009%
27	7.010	1829	1841	1863	rVV	177315	322471	21.64%	2.417%
28	7.142	1879	1882	1885	rBV4	768	688	0.05%	0.005%
29	7.338	1929	1943	1961	rBV	722555	1271485	85.34%	9.529%
30	7.569	2012	2015	2020	rVB5	916	948	0.06%	0.007%
31	7.643	2025	2038	2060	rBV	141081	258997	17.38%	1.941%
32	7.962	2124	2137	2150	rBV3	9523	18712	1.26%	0.140%
33	8.116	2168	2185	2221	rBV	439711	931511	62.52%	6.981%
34	8.335	2245	2253	2267	rVB2	10883	21654	1.45%	0.162%

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 Title : VOC Analysis

35	8.428	2280	2282	2288	rVB7	1267	1177	0.08%	0.009%
36	8.727	2367	2375	2388	rBV6	3923	8093	0.54%	0.061%
37	8.875	2408	2421	2452	rBV	799743	1345804	90.33%	10.086%
38	9.058	2466	2478	2491	rBV2	16366	36214	2.43%	0.271%
39	9.161	2504	2510	2522	rVB9	5653	11297	0.76%	0.085%
40	9.225	2527	2530	2535	rVV6	782	765	0.05%	0.006%
41	9.267	2540	2543	2548	rVV4	761	598	0.04%	0.004%
42	9.408	2581	2587	2590	rBV4	1696	1993	0.13%	0.015%
43	9.527	2619	2624	2625	rBV3	910	821	0.06%	0.006%
44	9.566	2629	2636	2643	rBV7	1780	3058	0.21%	0.023%
45	9.621	2646	2653	2656	rBV6	1515	1566	0.11%	0.012%
46	9.691	2672	2675	2679	rBV4	984	954	0.06%	0.007%
47	9.740	2684	2690	2691	rBV3	1072	1121	0.08%	0.008%
48	9.749	2691	2693	2698	rVB4	813	622	0.04%	0.005%
49	9.836	2716	2720	2724	rBV5	1548	1443	0.10%	0.011%
50	9.968	2752	2761	2775	rVB8	4690	9840	0.66%	0.074%
51	10.045	2781	2785	2791	rVB5	1037	1130	0.08%	0.008%
52	10.129	2806	2811	2812	rBV4	990	849	0.06%	0.006%
53	10.167	2813	2823	2834	rBV	77326	125334	8.41%	0.939%
54	10.238	2834	2845	2860	rVB	511892	789139	52.96%	5.914%
55	10.354	2874	2881	2882	rBV5	2420	2310	0.16%	0.017%
56	10.450	2904	2911	2923	rVB4	6871	12063	0.81%	0.090%
57	10.527	2930	2935	2940	rBV5	3389	4291	0.29%	0.032%
58	10.723	2990	2996	3000	rVB6	1386	1416	0.10%	0.011%
59	10.859	3029	3038	3046	rBV5	8047	16385	1.10%	0.123%
60	10.936	3057	3062	3071	rVB6	2789	3216	0.22%	0.024%
61	11.016	3081	3087	3093	rBV6	1552	2046	0.14%	0.015%
62	11.125	3114	3121	3130	rVB9	4964	8550	0.57%	0.064%
63	11.270	3151	3166	3184	rBV	835815	1291521	86.68%	9.679%
64	11.431	3210	3216	3234	rVB5	6235	13688	0.92%	0.103%
65	11.524	3237	3245	3249	rBV4	14802	21369	1.43%	0.160%
66	11.646	3271	3283	3305	rBV	768596	1217211	81.69%	9.122%
67	11.855	3338	3348	3357	rVB	5977	10770	0.72%	0.081%
68	11.945	3366	3376	3387	rVB4	15115	26693	1.79%	0.200%
69	12.039	3401	3405	3406	rBV3	1277	851	0.06%	0.006%
70	12.116	3423	3429	3432	rVV5	1274	1257	0.08%	0.009%
71	12.270	3474	3477	3482	rBV5	942	921	0.06%	0.007%

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72	12.305	3482	3488	3491	rBV5	1441	1537	0.10%	0.012%
73	12.482	3536	3543	3554	rVB8	5058	9553	0.64%	0.072%
74	12.572	3564	3571	3580	rBV9	3170	5152	0.35%	0.039%
75	12.736	3617	3622	3624	rBV3	813	656	0.04%	0.005%
76	12.756	3624	3628	3632	rVB4	923	880	0.06%	0.007%
77	12.801	3635	3642	3649	rBV9	2251	2949	0.20%	0.022%
78	12.900	3662	3673	3676	rBV8	1201	1936	0.13%	0.015%
79	12.948	3683	3688	3694	rBV6	2099	2856	0.19%	0.021%
80	13.087	3728	3731	3735	rVB2	727	696	0.05%	0.005%
81	13.202	3764	3767	3773	rVB5	1067	910	0.06%	0.007%
82	13.248	3776	3781	3784	rBV5	725	654	0.04%	0.005%
83	13.289	3786	3794	3800	rBV9	1832	2769	0.19%	0.021%
84	13.402	3827	3829	3831	rVV4	1314	708	0.05%	0.005%
85	13.437	3832	3840	3852	rVB4	10124	17569	1.18%	0.132%
86	13.518	3862	3865	3866	rBV3	1242	624	0.04%	0.005%
87	13.530	3866	3869	3873	rVB4	1795	1234	0.08%	0.009%
88	13.765	3940	3942	3951	rVB6	1969	2049	0.14%	0.015%
89	14.045	4027	4029	4035	rVB4	1241	644	0.04%	0.005%
90	14.151	4060	4062	4065	rBV4	1061	683	0.05%	0.005%
91	14.219	4078	4083	4084	rBV3	1661	1282	0.09%	0.010%
92	14.302	4104	4109	4111	rBV4	1109	768	0.05%	0.006%
93	14.328	4114	4117	4121	rVB3	958	622	0.04%	0.005%
94	14.469	4156	4161	4163	rBV4	904	788	0.05%	0.006%
95	14.624	4203	4209	4214	rBV7	2948	4172	0.28%	0.031%
96	14.739	4243	4245	4249	rBV3	761	613	0.04%	0.005%
97	14.759	4249	4251	4254	rVB3	1132	610	0.04%	0.005%
98	15.315	4420	4424	4427	rBV3	1124	1145	0.08%	0.009%
99	15.418	4454	4456	4459	rBV3	1234	758	0.05%	0.006%
100	15.826	4575	4583	4591	rBV3	4168	7537	0.51%	0.056%

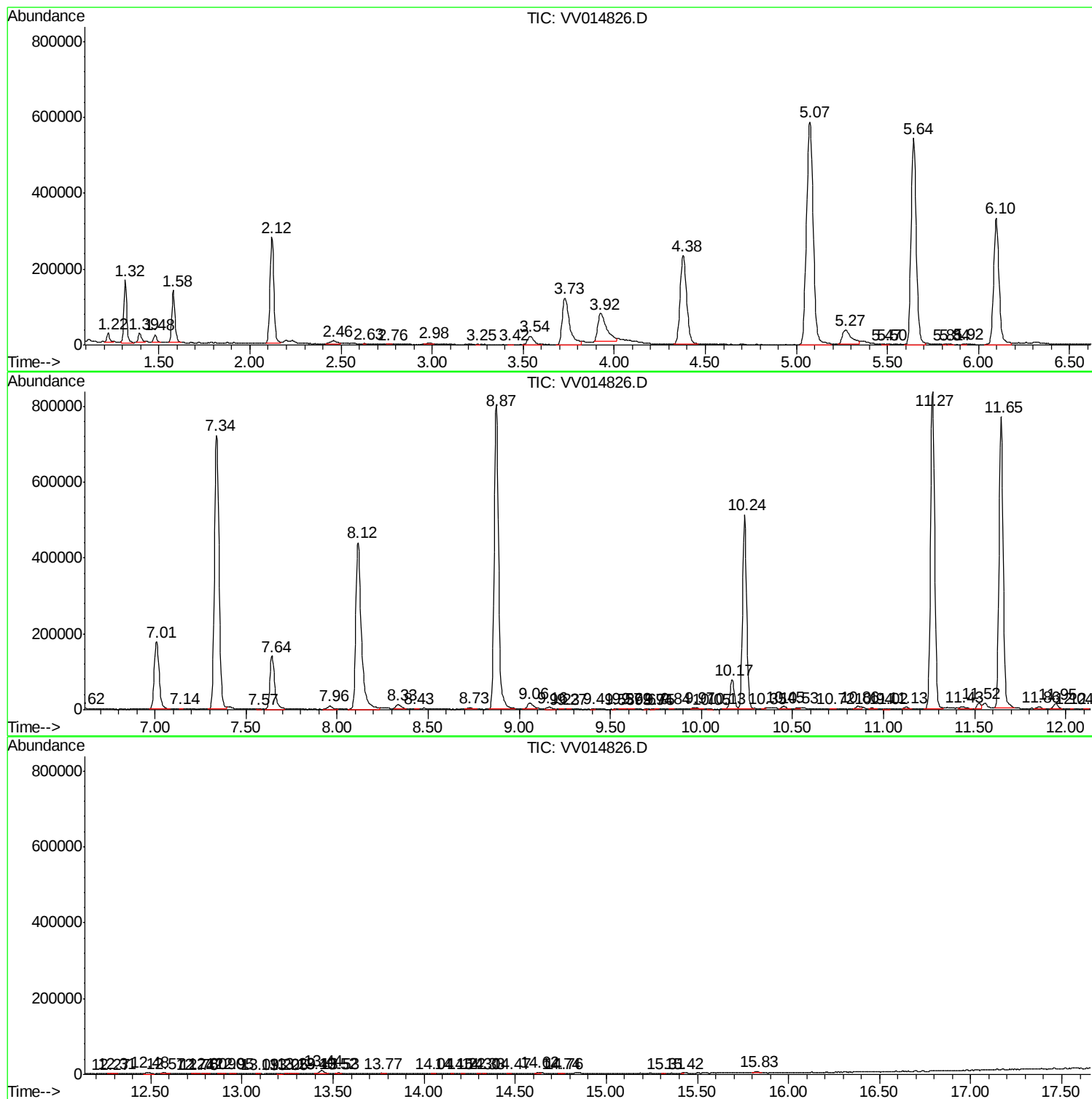
Sum of corrected areas: 13343679

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Instrument :
MSVOA_V
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

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



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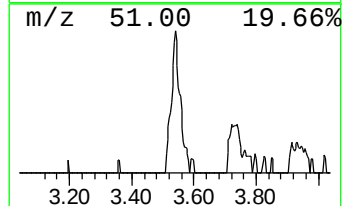
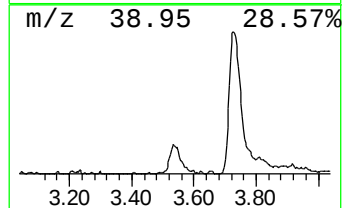
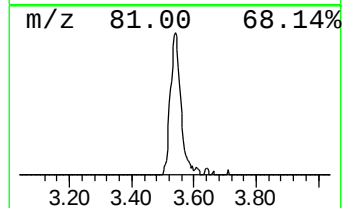
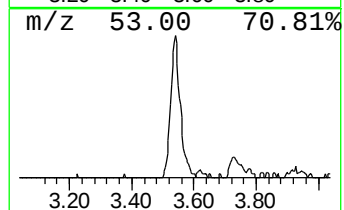
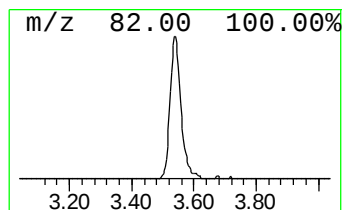
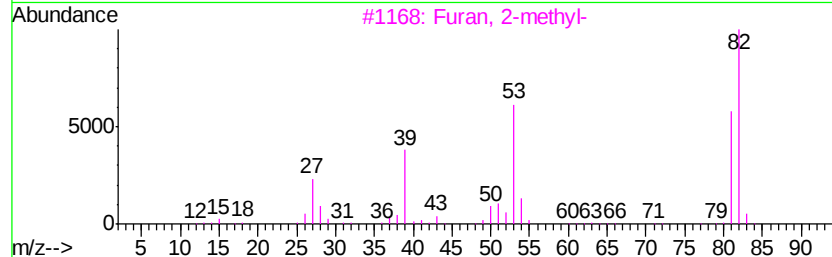
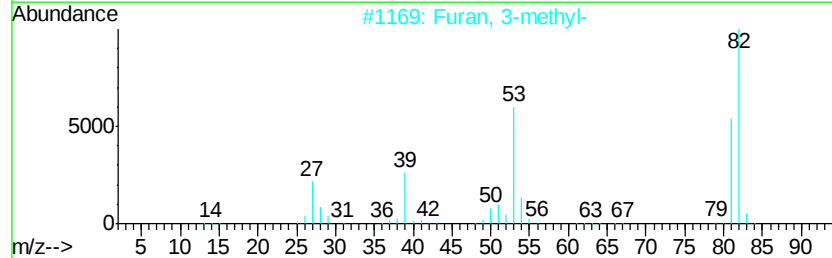
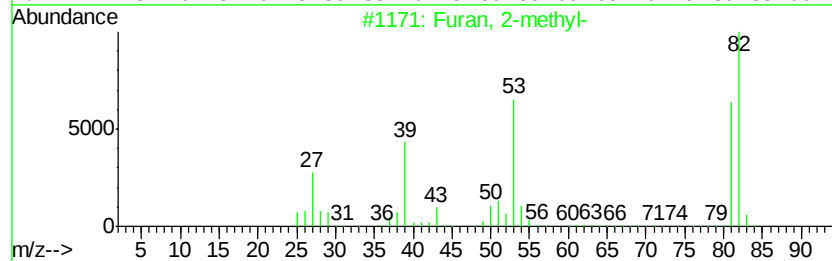
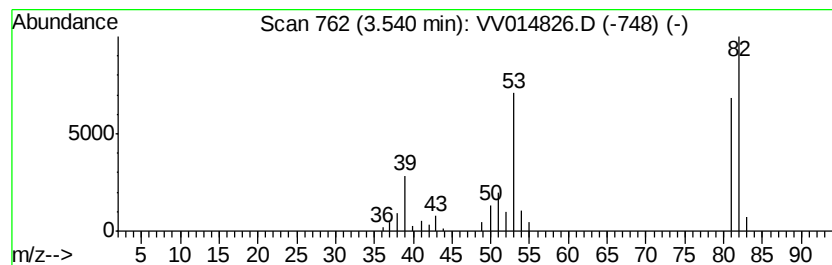
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Furan, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.54	2.54 ug/L	53826	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, 2-methyl-	82	C5H6O	000534-22-5	91
2		Furan, 3-methyl-	82	C5H6O	000930-27-8	90
3		Furan, 2-methyl-	82	C5H6O	000534-22-5	90
4		Furan, 2-methyl-	82	C5H6O	000534-22-5	86
5		Furan, 2-methyl-	82	C5H6O	000534-22-5	72



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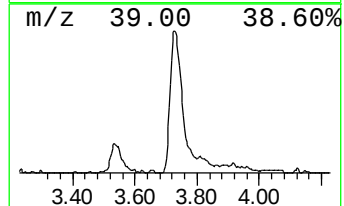
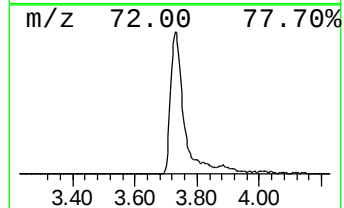
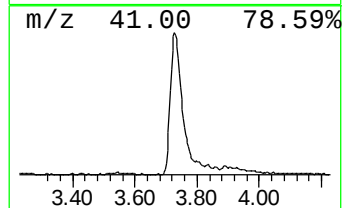
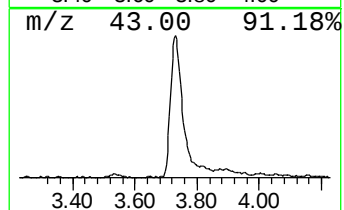
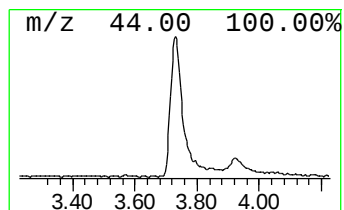
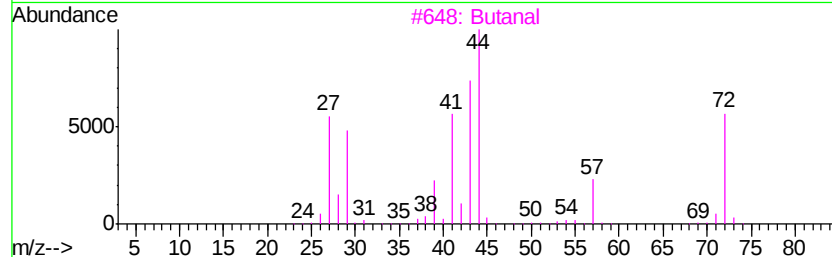
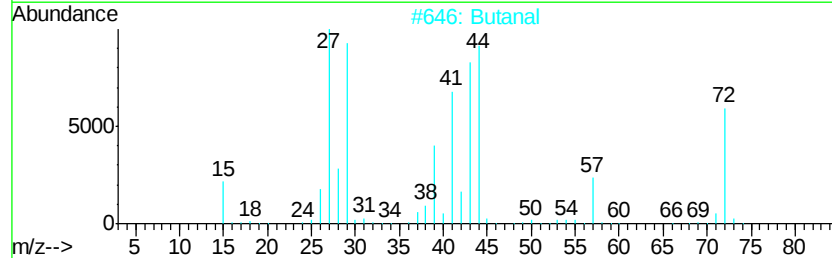
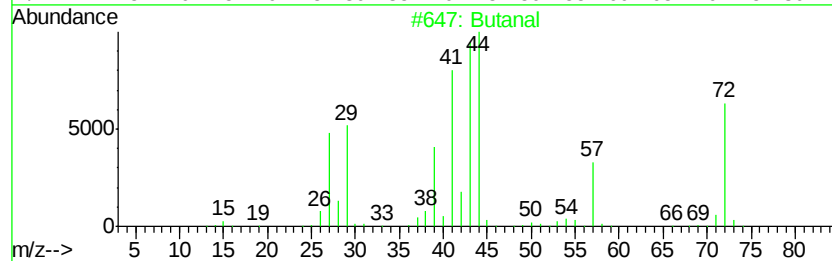
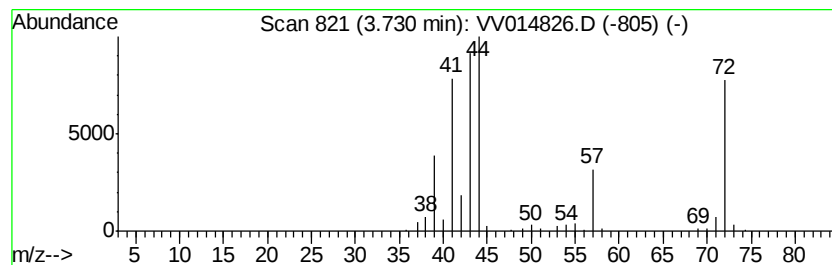
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Quant Title : VOC Analysis

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

Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	16.16 ug/L	342474	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	94
2		Butanal	72	C4H8O	000123-72-8	91
3		Butanal	72	C4H8O	000123-72-8	74
4		Butanal	72	C4H8O	000123-72-8	72
5		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43



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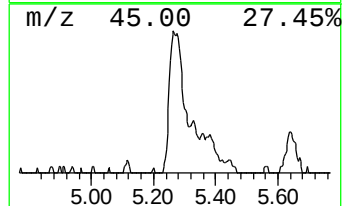
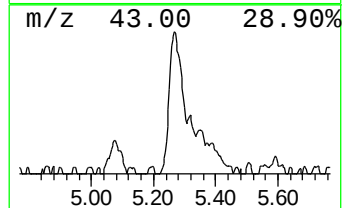
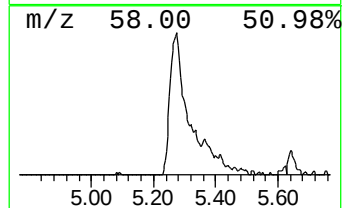
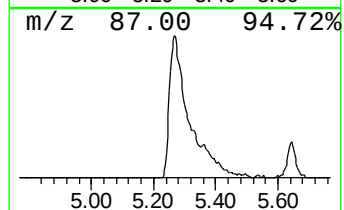
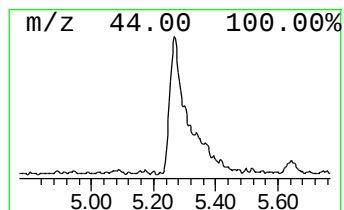
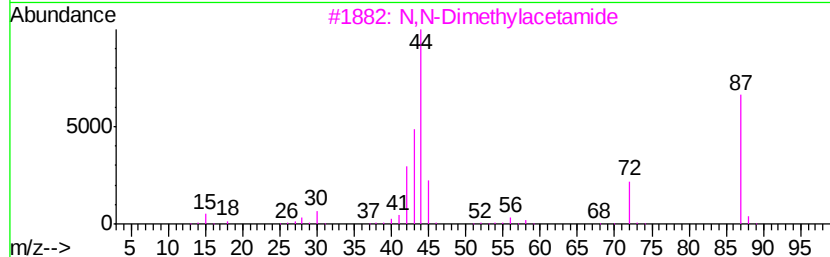
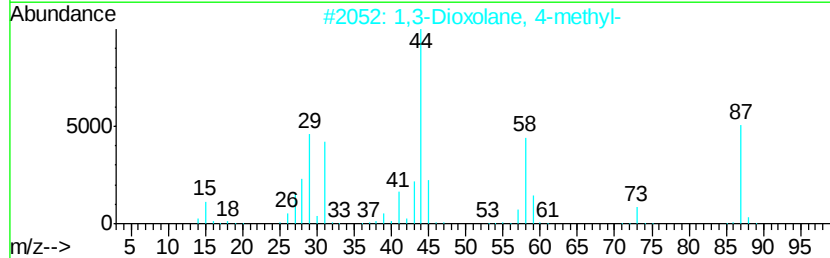
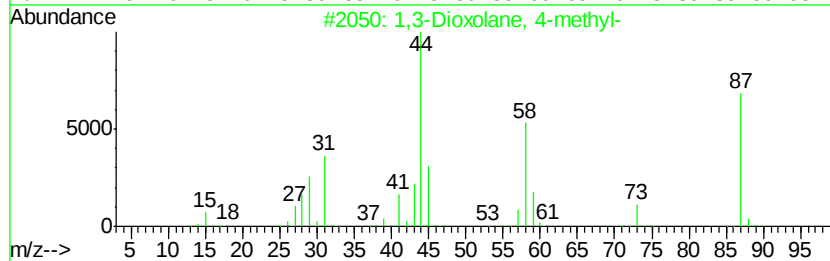
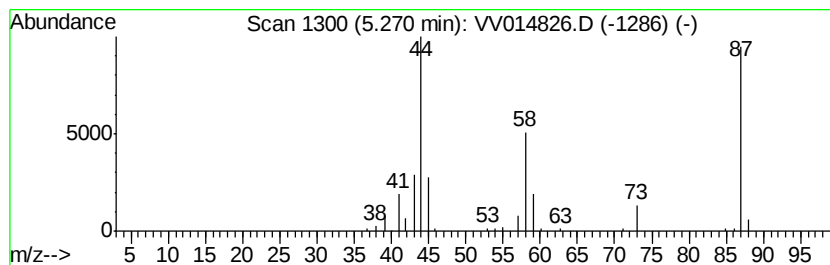
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Quant Title : VOC Analysis

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

Peak Number 3 1,3-Dioxolane, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	6.23 ug/L	132067	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 4-methyl-	88	C4H8O2	001072-47-5	74
2		1,3-Dioxolane, 4-methyl-	88	C4H8O2	001072-47-5	72
3		N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	59
4		N-Acetyl-L-alanine ethylamide	158	C7H14N2O2	024847-34-5	40
5		N-Acetyl-DL-alanine methylamide	144	C6H12N2O2	034276-27-2	36



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV031020\
Data File : VV014826.D
Acq On : 11 Mar 2020 01:06
Operator : SY/MD
Sample : L1840-22
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBET7

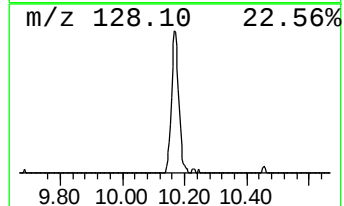
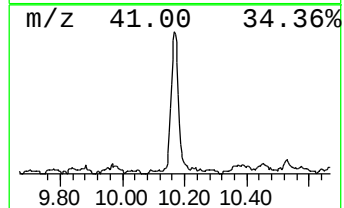
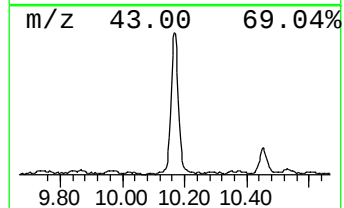
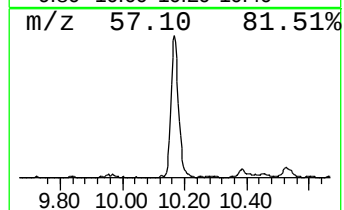
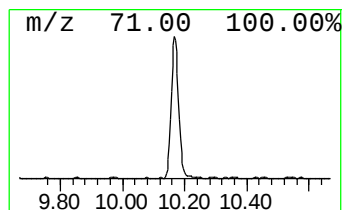
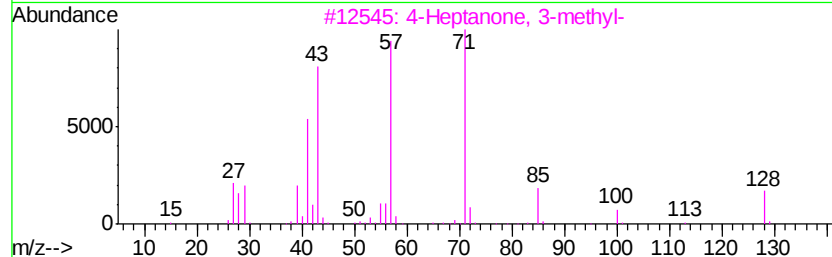
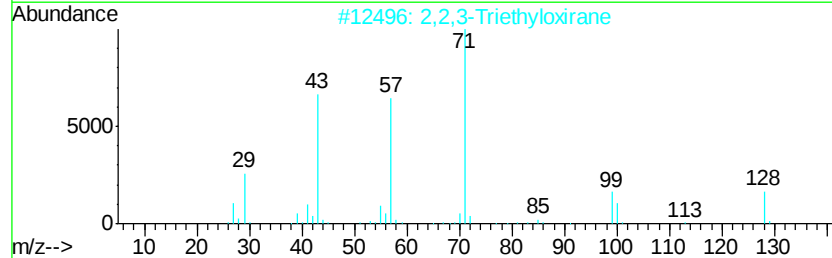
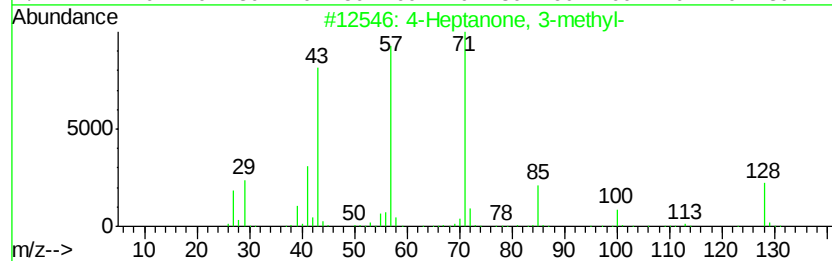
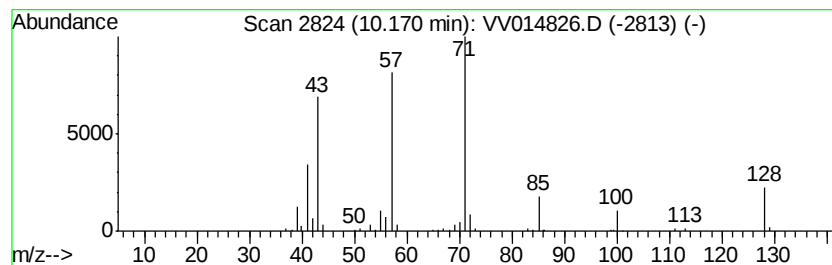
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Quant Title : VOC Analysis

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

Peak Number 5 4-Heptanone, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.17	4.85 ug/L	125334	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	95
2		2,2,3-Triethyloxirane	128	C8H16O	053229-40-6	87
3		4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	86
4		4-Octanone	128	C8H16O	000589-63-9	64
5		1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV031020\
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Instrument :
MSVOA_V
ClientSampleId :
DBET7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM030620WMA.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
Furan, 2-methyl-	3.54	2.5	ug/L	53826	1	5.64	1059670	50.0
Butanal	3.73	16.2	ug/L	342474	1	5.64	1059670	50.0
1,3-Dioxolane, 4-...	5.27	6.2	ug/L	132067	1	5.64	1059670	50.0
4-Heptanone, 3-me...	10.17	4.8	ug/L	125334	3	11.27	1291520	50.0