

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
 Data File : VV022513.D
 Acq On : 02 Oct 2021 16:07
 Operator : SY/MD
 Sample : M3996-13DL 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F4A28DL

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_V\Method\SFAMVLM100121WMA.M

Title : VOC Analysis

Signal : TIC: VV022513.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.201	45	50	61	rVB2	48518	62034	9.08%	0.856%
2	1.307	76	83	95	rBV	221131	223812	32.77%	3.088%
3	1.564	156	163	174	rBV	90123	102477	15.01%	1.414%
4	1.632	176	184	198	rVB	243469	298330	43.69%	4.116%
5	1.806	230	238	252	rVB3	59923	93852	13.74%	1.295%
6	1.899	262	267	277	rVB	24087	30171	4.42%	0.416%
7	2.024	299	306	317	rVB	59382	81795	11.98%	1.129%
8	2.108	321	332	360	rVB	191533	299769	43.90%	4.136%
9	2.494	427	452	456	rBV5	30296	70021	10.25%	0.966%
10	2.761	523	535	556	rVB2	54662	112380	16.46%	1.550%
11	2.896	573	577	579	rBV2	276	194	0.03%	0.003%
12	2.944	579	592	606	rVB4	5003	10578	1.55%	0.146%
13	3.040	608	622	637	rVB4	10749	23153	3.39%	0.319%
14	3.159	646	659	668	rBV7	2991	6502	0.95%	0.090%
15	3.436	736	745	757	rBV3	6263	13130	1.92%	0.181%
16	3.764	833	847	864	rBV2	63541	158712	23.24%	2.190%
17	3.889	877	886	914	rBV2	45564	124599	18.25%	1.719%
18	4.349	1014	1029	1058	rBV2	108360	285992	41.88%	3.946%
19	4.551	1089	1092	1095	rBV2	621	491	0.07%	0.007%
20	4.677	1114	1131	1145	rBV3	38784	99028	14.50%	1.366%
21	4.912	1188	1204	1219	rBV6	7573	23541	3.45%	0.325%
22	5.047	1229	1246	1254	rBV2	278763	682880	100.00%	9.422%
23	5.490	1377	1384	1396	rBV4	3201	5802	0.85%	0.080%
24	5.619	1412	1424	1461	rBV	265043	557393	81.62%	7.690%
25	5.918	1507	1517	1536	rVB	19445	51628	7.56%	0.712%
26	6.072	1550	1565	1578	rBV	152204	321035	47.01%	4.429%
27	6.259	1618	1623	1626	rBV6	1073	1212	0.18%	0.017%
28	6.301	1631	1636	1643	rBV6	1004	1511	0.22%	0.021%
29	6.368	1647	1657	1667	rBV5	3823	7196	1.05%	0.099%
30	6.442	1676	1680	1681	rBV2	515	320	0.05%	0.004%
31	6.458	1682	1685	1688	rBV3	627	514	0.08%	0.007%
32	6.558	1702	1716	1719	rBV6	2956	5559	0.81%	0.077%
33	6.654	1733	1746	1761	rVB4	6665	15215	2.23%	0.210%
34	6.776	1771	1784	1800	rBV6	10049	23637	3.46%	0.326%
35	6.886	1816	1818	1820	rVB2	539	207	0.03%	0.003%
36	6.899	1820	1822	1825	rVB	437	196	0.03%	0.003%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
 Title : VOC Analysis

37	6.921	1827	1829	1832	rBV2	550	381	0.06%	0.005%
38	6.989	1837	1850	1872	rBV	81784	153963	22.55%	2.124%
39	7.262	1927	1935	1936	rBV4	1755	1926	0.28%	0.027%
40	7.317	1942	1952	1970	rBV	325207	558282	81.75%	7.703%
41	7.625	2039	2048	2068	rVB2	54341	94578	13.85%	1.305%
42	7.793	2095	2100	2108	rVB6	1902	2752	0.40%	0.038%
43	7.841	2109	2115	2125	rVV6	3632	5472	0.80%	0.075%
44	7.892	2129	2131	2134	rBV2	461	298	0.04%	0.004%
45	7.937	2142	2145	2146	rBV	381	189	0.03%	0.003%
46	7.979	2149	2158	2170	rVV2	21145	36261	5.31%	0.500%
47	8.050	2177	2180	2183	rVB2	483	321	0.05%	0.004%
48	8.092	2183	2193	2209	rBV	160613	286880	42.01%	3.958%
49	8.439	2300	2301	2305	rVV	385	215	0.03%	0.003%
50	8.458	2305	2307	2314	rVV3	286	257	0.04%	0.004%
51	8.510	2321	2323	2335	rBV4	713	911	0.13%	0.013%
52	8.628	2353	2360	2366	rBV2	939	1290	0.19%	0.018%
53	8.670	2371	2373	2375	rVB2	513	201	0.03%	0.003%
54	8.728	2382	2391	2408	rVB2	7870	13887	2.03%	0.192%
55	8.799	2409	2413	2417	rBV3	525	574	0.08%	0.008%
56	8.854	2418	2430	2452	rBV	387547	623883	91.36%	8.608%
57	9.018	2471	2481	2498	rVB	38276	61887	9.06%	0.854%
58	9.146	2510	2521	2533	rBV2	16662	28448	4.17%	0.392%
59	9.246	2548	2552	2555	rVB2	227	196	0.03%	0.003%
60	9.265	2555	2558	2560	rBV2	327	195	0.03%	0.003%
61	9.551	2638	2647	2660	rBV2	4364	6873	1.01%	0.095%
62	9.937	2759	2767	2777	rVB2	6683	10039	1.47%	0.139%
63	10.127	2820	2826	2837	rVB4	1811	2967	0.43%	0.041%
64	10.217	2838	2854	2876	rBV	204798	323655	47.40%	4.465%
65	10.358	2892	2898	2914	rVB3	5212	8386	1.23%	0.116%
66	10.452	2919	2927	2941	rBV3	6660	12623	1.85%	0.174%
67	10.542	2950	2955	2962	rBV5	2863	3496	0.51%	0.048%
68	10.699	3002	3004	3007	rVV	424	259	0.04%	0.004%
69	10.741	3008	3017	3029	rVV2	15663	23629	3.46%	0.326%
70	10.818	3037	3041	3043	rBV	330	278	0.04%	0.004%
71	10.918	3062	3072	3088	rVB	33986	52920	7.75%	0.730%
72	11.095	3122	3127	3136	rVB3	1061	1366	0.20%	0.019%
73	11.146	3136	3143	3144	rBV2	1193	1101	0.16%	0.015%
74	11.198	3153	3159	3165	rBV5	1049	1217	0.18%	0.017%
75	11.249	3165	3175	3195	rVV	395238	598427	87.63%	8.256%
76	11.336	3198	3202	3213	rVB3	5450	8050	1.18%	0.111%

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Title : VOC Analysis

77	11.538	3254	3265	3275	rBV5	5139	10703	1.57%	0.148%
78	11.625	3281	3292	3308	rVB	319009	506860	74.22%	6.993%
79	11.741	3326	3328	3330	rBV	381	214	0.03%	0.003%
80	11.786	3339	3342	3343	rBV2	820	469	0.07%	0.006%
81	11.818	3350	3352	3358	rBV2	752	656	0.10%	0.009%
82	11.988	3399	3405	3406	rBV2	309	224	0.03%	0.003%
83	12.046	3421	3423	3426	rVB3	554	341	0.05%	0.005%
84	12.088	3434	3436	3438	rBV	462	242	0.04%	0.003%
85	12.304	3499	3503	3506	rBV2	273	214	0.03%	0.003%
86	12.365	3517	3522	3526	rBV2	200	262	0.04%	0.004%
87	12.413	3531	3537	3538	rBV2	564	492	0.07%	0.007%
88	12.461	3549	3552	3554	rBV3	380	233	0.03%	0.003%
89	12.670	3615	3617	3619	rVV2	415	186	0.03%	0.003%
90	12.844	3668	3671	3675	rBV2	306	268	0.04%	0.004%
91	12.882	3679	3683	3685	rBV	700	581	0.09%	0.008%
92	13.300	3812	3813	3818	rBV	267	203	0.03%	0.003%
93	13.509	3874	3878	3881	rVV3	413	296	0.04%	0.004%
94	13.525	3881	3883	3886	rVV2	414	279	0.04%	0.004%
95	13.911	3999	4003	4006	rBV2	254	264	0.04%	0.004%
96	13.959	4014	4018	4024	rBV3	375	416	0.06%	0.006%
97	14.021	4033	4037	4038	rBV2	358	243	0.04%	0.003%
98	14.133	4067	4072	4073	rBV	268	194	0.03%	0.003%
99	14.458	4168	4173	4176	rBV2	481	440	0.06%	0.006%
100	14.529	4193	4195	4199	rBV2	368	349	0.05%	0.005%

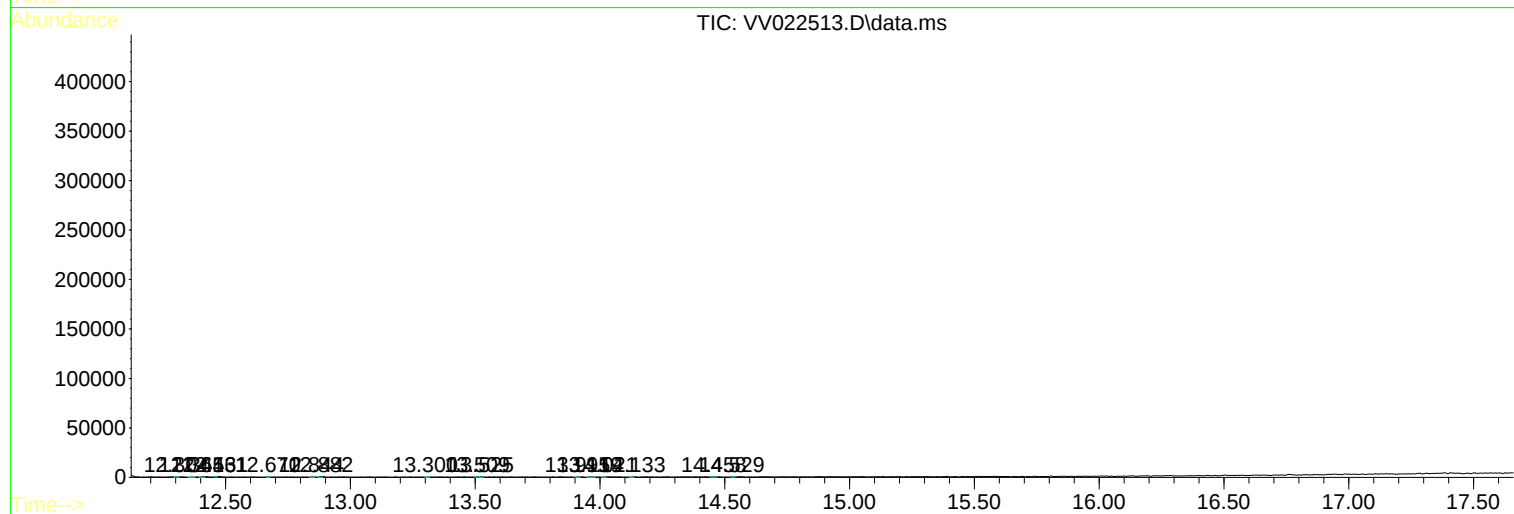
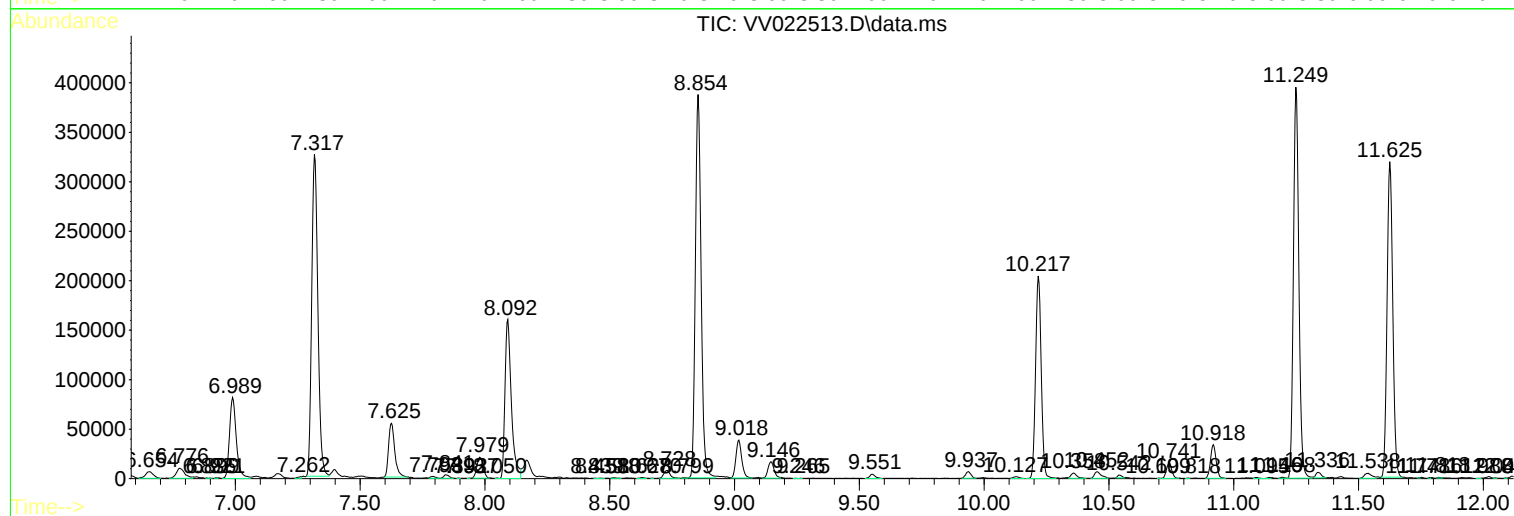
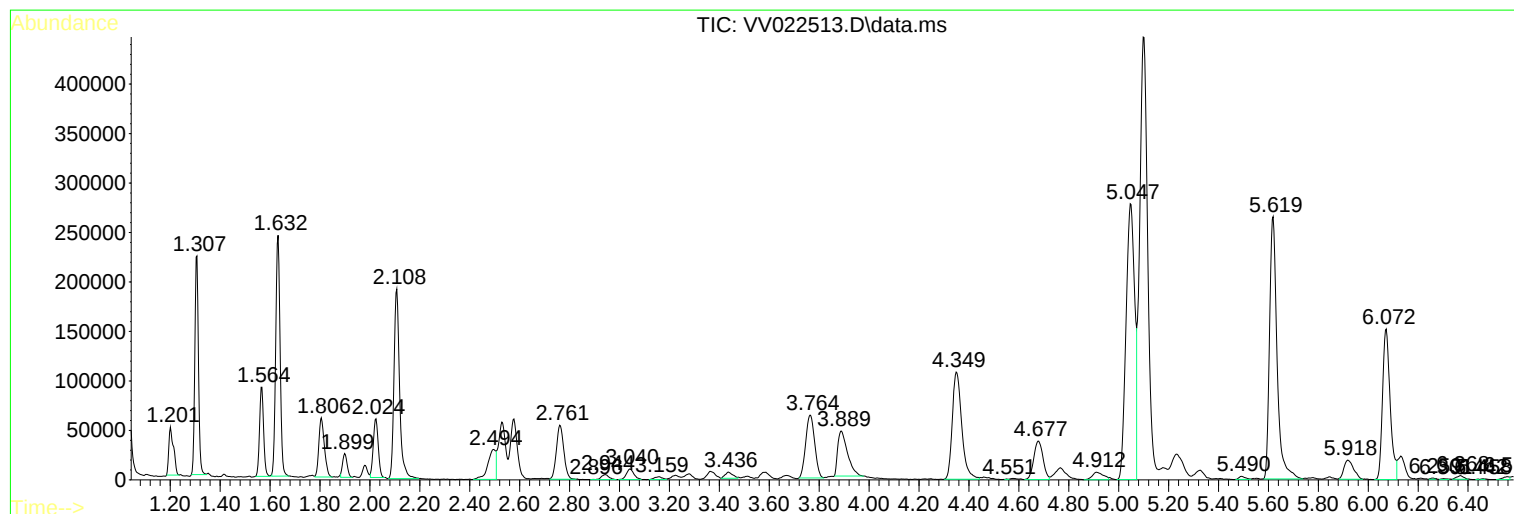
Sum of corrected areas: 7248028

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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F4A28DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
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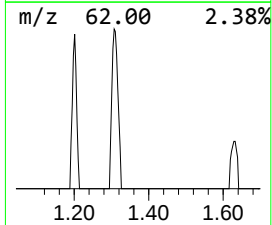
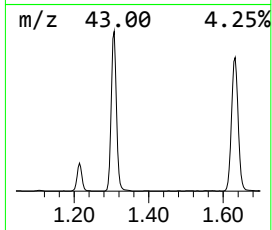
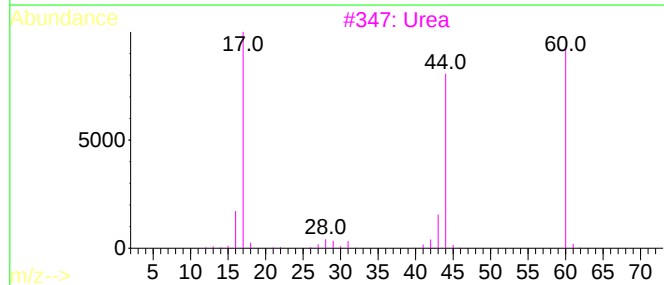
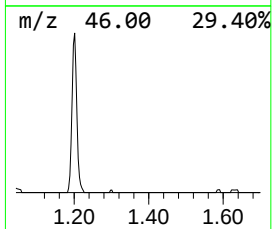
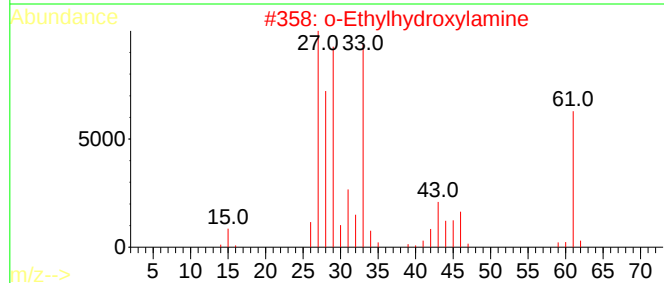
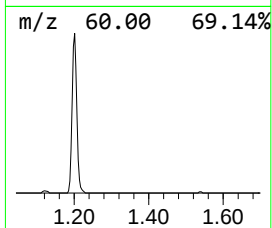
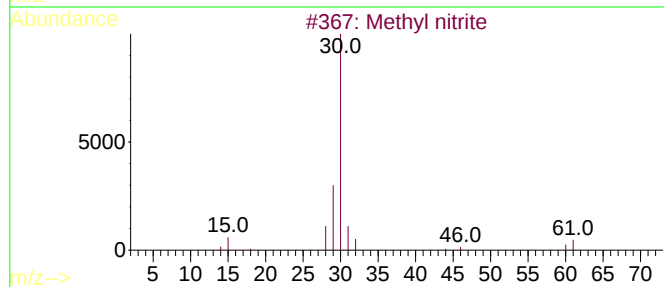
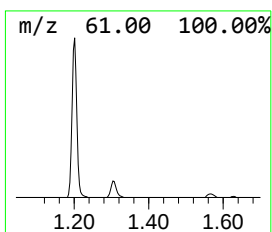
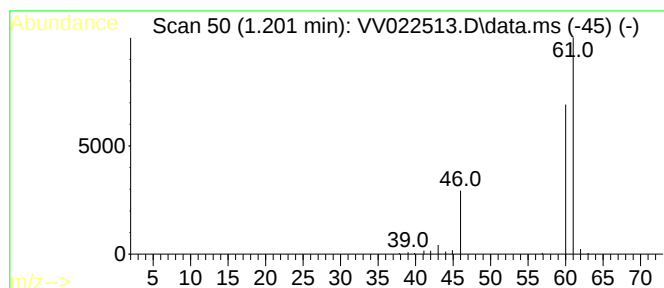
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.201	5.56 ug/L	62034	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
3			Urea	60	CH4N2O	000057-13-6	4
4			Thiirane	60	C2H4S	000420-12-2	4
5			Ethyne, chloro-	60	C2HCl	000593-63-5	4



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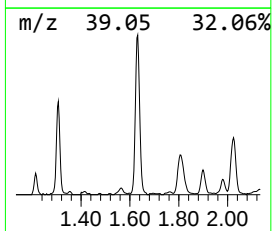
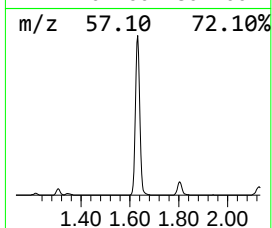
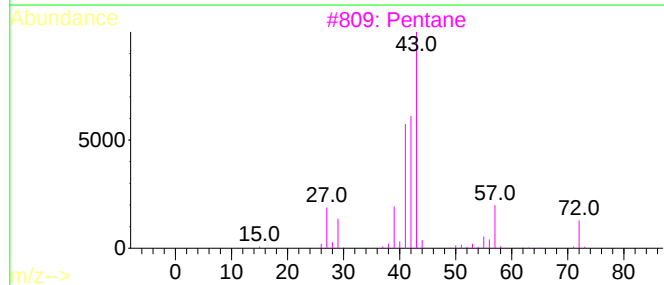
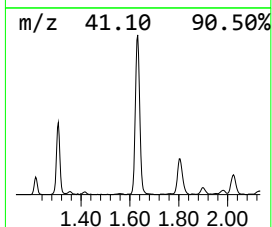
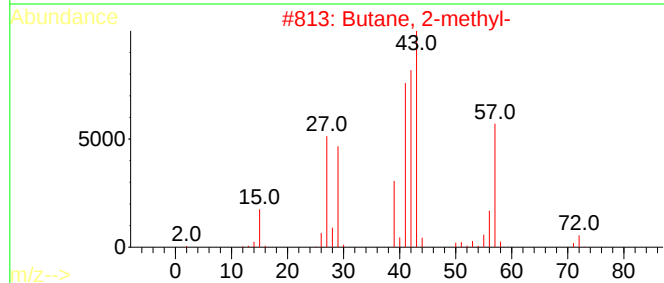
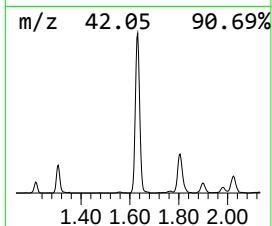
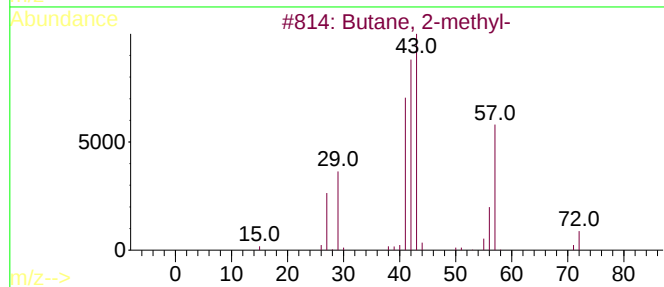
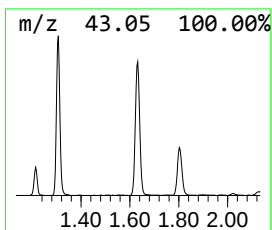
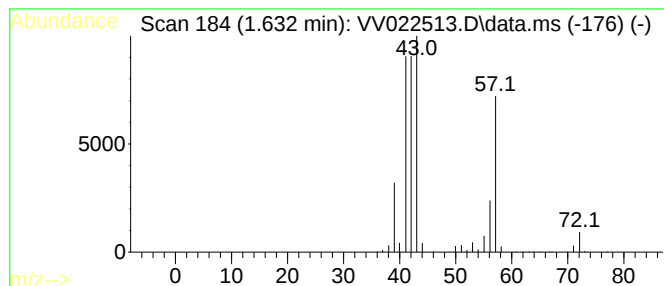
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.632	26.76 ug/L	298330	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	91
3		Pentane	72	C5H12	000109-66-0	47
4		3-Buten-1-ol	72	C4H8O	000627-27-0	28
5		3-Buten-1-ol	72	C4H8O	000627-27-0	9



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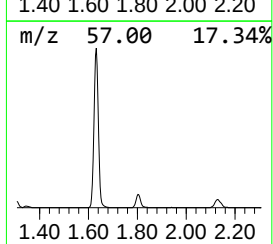
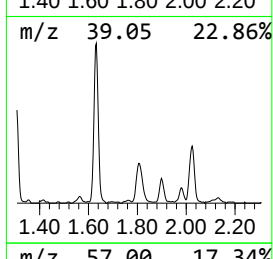
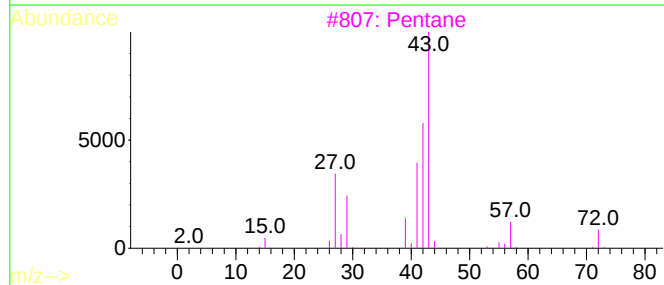
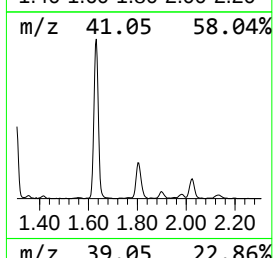
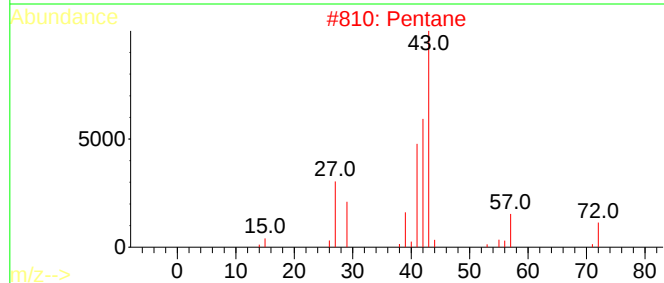
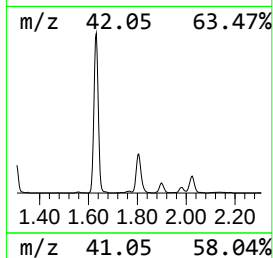
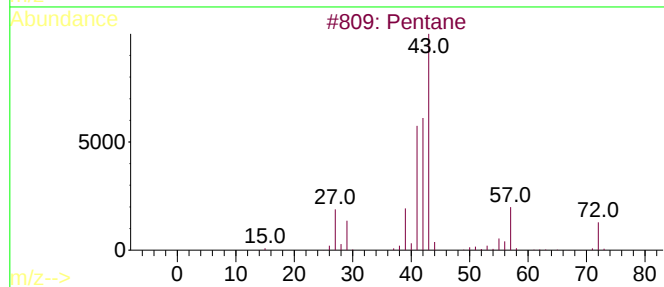
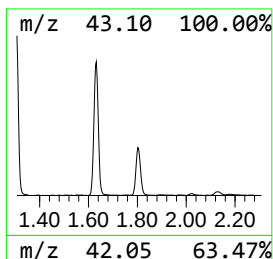
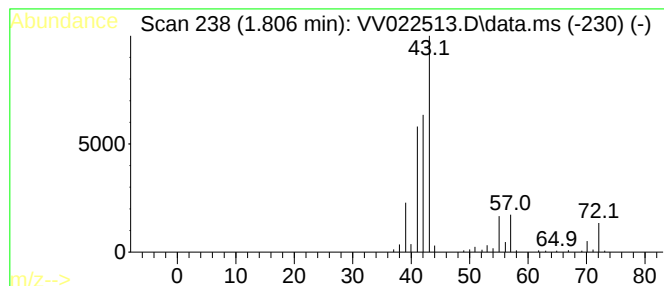
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.806	8.42 ug/L	93852	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	90
2	Pentane			72	C5H12	000109-66-0	80
3	Pentane			72	C5H12	000109-66-0	72
4	Pentane			72	C5H12	000109-66-0	64
5	Pentane			72	C5H12	000109-66-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
Data File : VV022513.D
Acq On : 02 Oct 2021 16:07
Operator : SY/MD
Sample : M3996-13DL 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F4A28DL

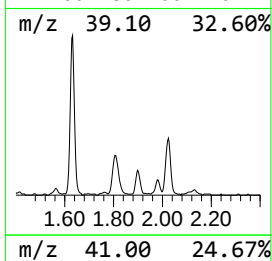
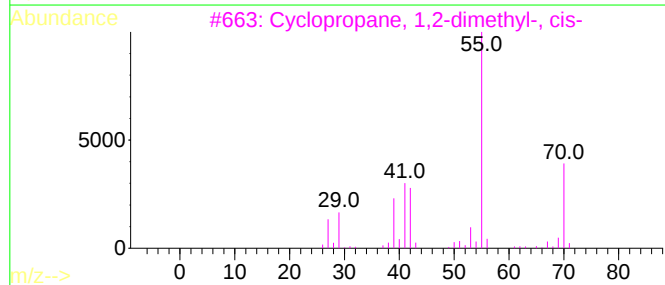
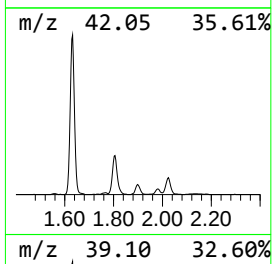
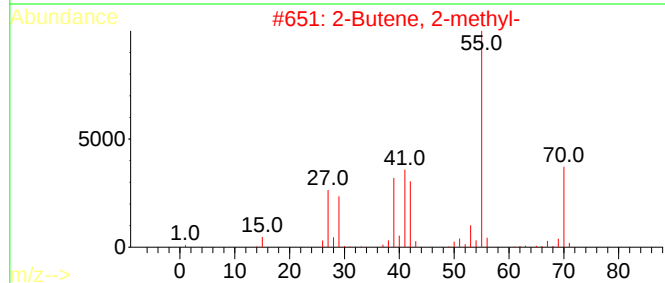
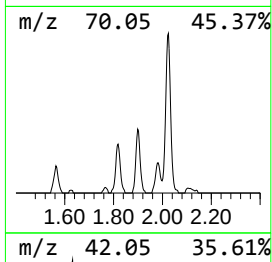
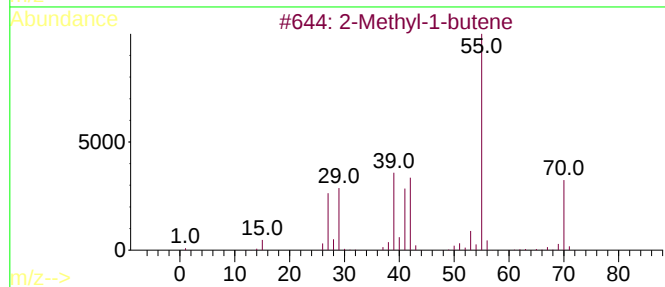
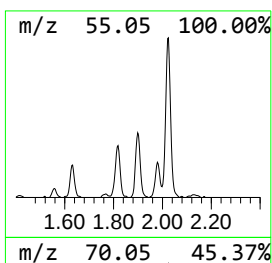
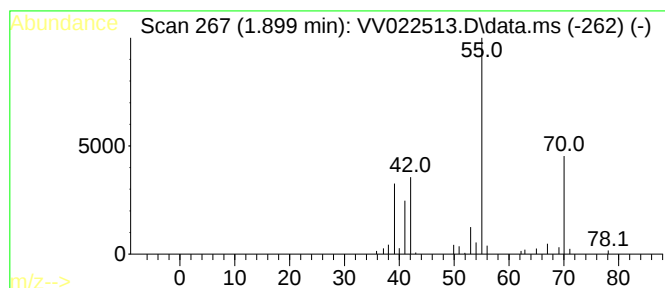
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.899	2.71 ug/L	30171	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Methyl-1-butene	70	C5H10	000563-46-2	86
2		2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
3		Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
4		2-Methyl-1-butene	70	C5H10	000563-46-2	86
5		2-Pentene, (Z)-	70	C5H10	000627-20-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
Data File : VV022513.D
Acq On : 02 Oct 2021 16:07
Operator : SY/MD
Sample : M3996-13DL 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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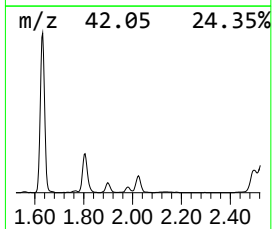
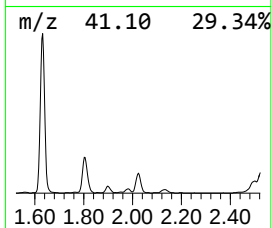
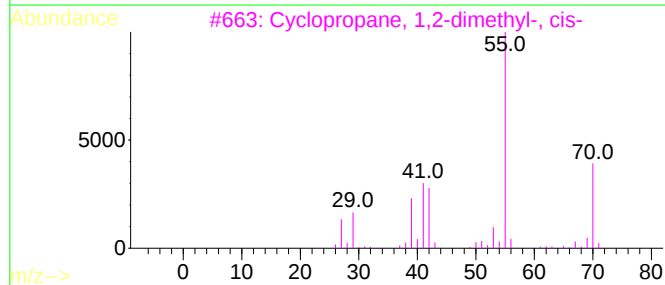
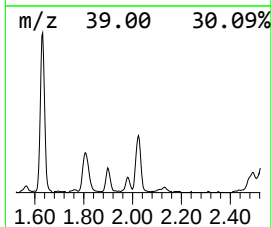
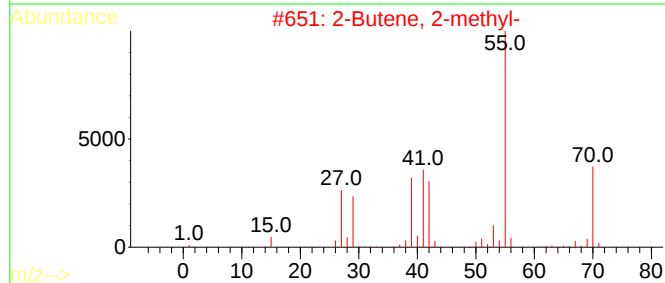
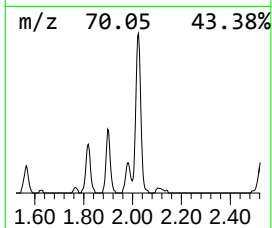
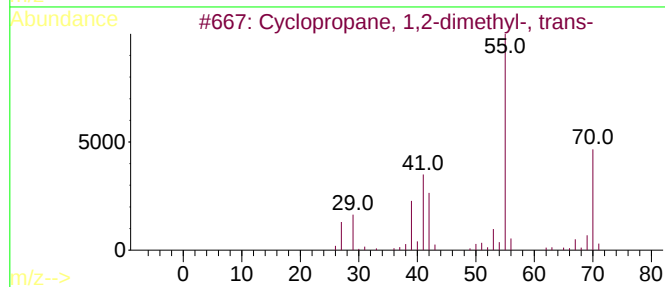
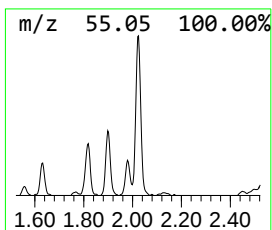
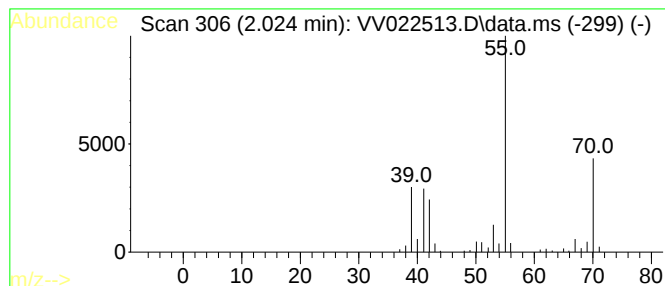
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Cyclic2.024 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.024	7.34 ug/L	81795	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
4			2-Pentene, (E)-	70	C5H10	000646-04-8	87
5			2-Methyl-1-butene	70	C5H10	000563-46-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
Data File : VV022513.D
Acq On : 02 Oct 2021 16:07
Operator : SY/MD
Sample : M3996-13DL 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F4A28DL

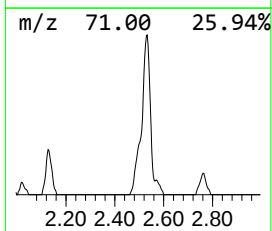
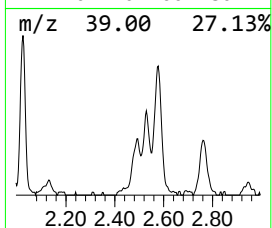
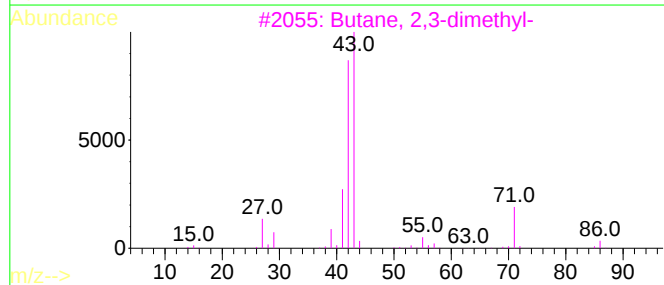
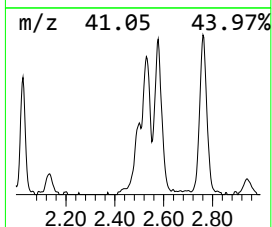
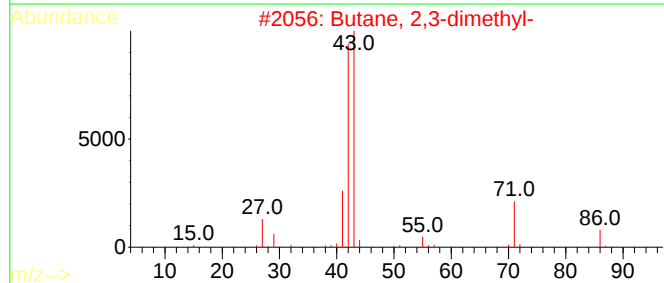
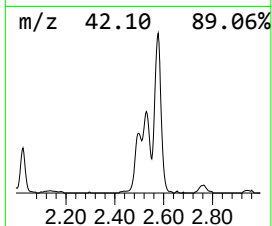
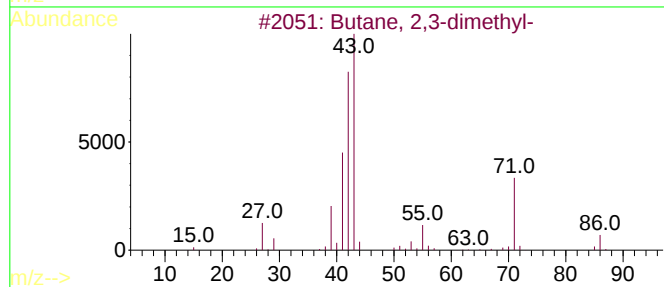
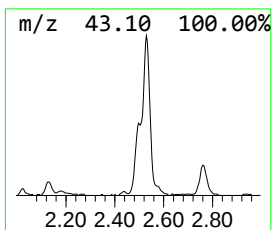
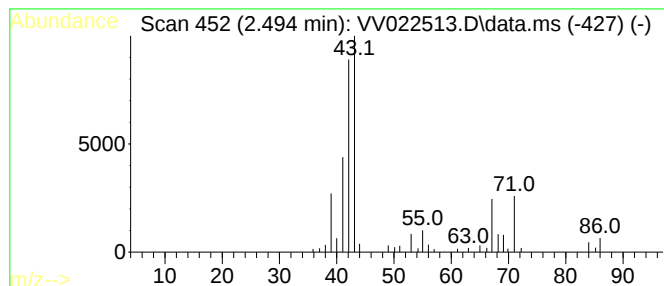
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.494	6.28 ug/L	70021	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	81
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	59
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	58
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
Data File : VV022513.D
Acq On : 02 Oct 2021 16:07
Operator : SY/MD
Sample : M3996-13DL 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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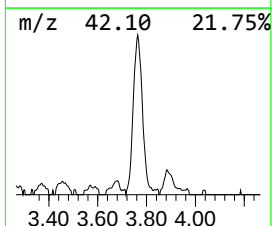
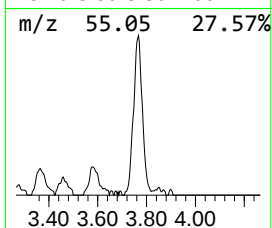
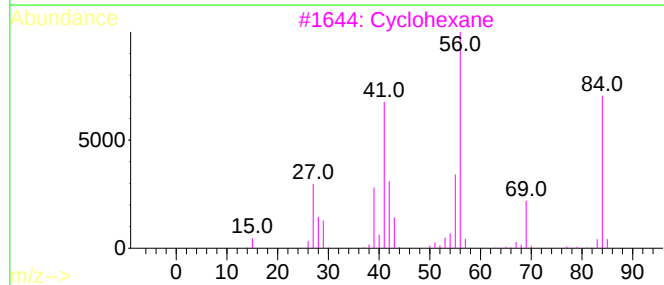
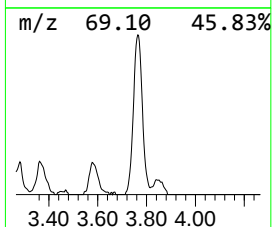
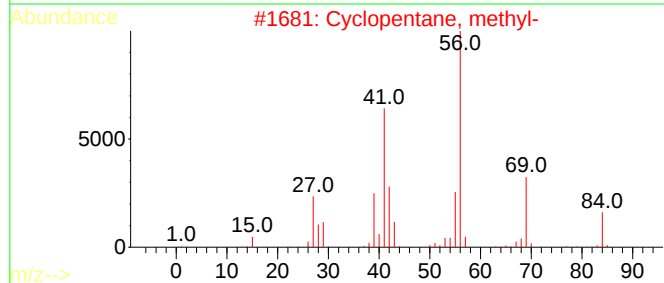
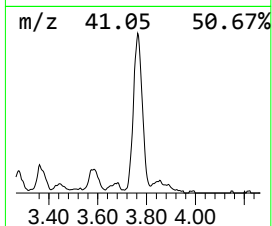
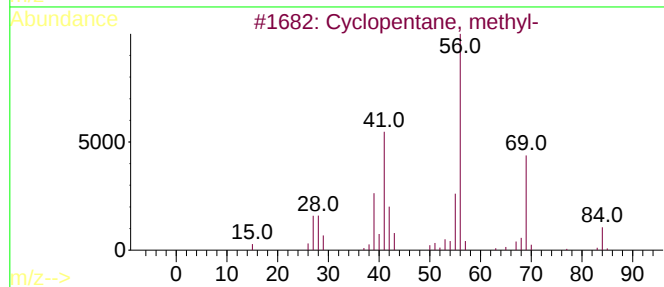
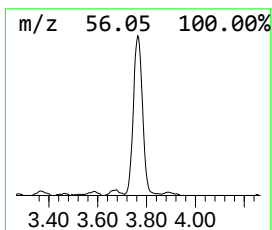
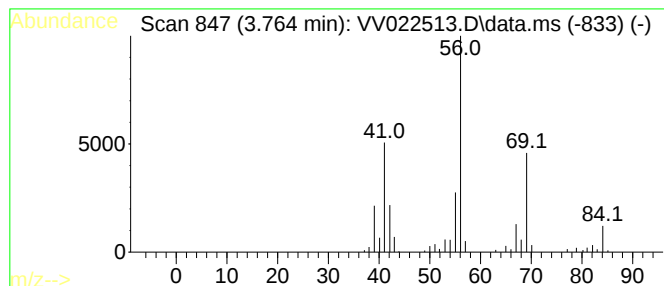
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 (DEL) Alkane: Cyclic3.764 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.764	14.24 ug/L	158712	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3			Cyclohexane	84	C6H12	000110-82-7	86
4			Cyclohexane	84	C6H12	000110-82-7	83
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100221\
Data File : VV022513.D
Acq On : 02 Oct 2021 16:07
Operator : SY/MD
Sample : M3996-13DL 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F4A28DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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(DEL) Alkane: S...	1.632	26.8	ug/L	298330	1	5.619	557393	50.0
(DEL) Alkane: S...	1.806	8.4	ug/L	93852	1	5.619	557393	50.0
(DEL) Alkane: S...	1.899	2.7	ug/L	30171	1	5.619	557393	50.0
(DEL) Alkane: C...	2.024	7.3	ug/L	81795	1	5.619	557393	50.0
(DEL) Alkane: S...	2.494	6.3	ug/L	70021	1	5.619	557393	50.0
(DEL) Alkane: C...	3.764	14.2	ug/L	158712	1	5.619	557393	50.0