

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101122\
 Data File : VV028518.D
 Acq On : 11 Oct 2022 13:06
 Operator : SY/MD
 Sample : N5079-02
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFYZ9

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\SFAMVLM100722WMA.M
 Title : VOC Analysis

Signal : TIC: VV028518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	75	82	101	rBV	160479	168839	4.71%	1.148%
2	1.565	157	163	182	rVB	125607	145533	4.06%	0.989%
3	2.105	322	331	348	rVB	262375	380760	10.63%	2.589%
4	2.947	588	593	598	rBV6	612	819	0.02%	0.006%
5	3.021	612	616	617	rBV	618	445	0.01%	0.003%
6	3.069	629	631	636	rVB2	659	437	0.01%	0.003%
7	3.095	636	639	640	rBV3	350	203	0.01%	0.001%
8	3.185	653	667	685	rBV	46831	100012	2.79%	0.680%
9	3.285	685	698	716	rVV2	18156	41828	1.17%	0.284%
10	3.539	774	777	779	rBV2	343	257	0.01%	0.002%
11	3.738	834	839	840	rBV2	497	409	0.01%	0.003%
12	3.806	857	860	864	rBV	484	316	0.01%	0.002%
13	3.899	879	889	925	rBV	53908	225578	6.30%	1.534%
14	4.343	1013	1027	1052	rBV	194168	487401	13.60%	3.314%
15	4.593	1098	1105	1106	rBV4	1848	1970	0.05%	0.013%
16	4.674	1124	1130	1134	rBV5	1029	1208	0.03%	0.008%
17	4.896	1197	1199	1203	rBV	325	273	0.01%	0.002%
18	4.953	1213	1217	1220	rVB3	415	372	0.01%	0.003%
19	5.040	1227	1244	1276	rBV2	495405	1308914	36.53%	8.899%
20	5.378	1346	1349	1351	rBV3	786	449	0.01%	0.003%
21	5.516	1388	1392	1394	rBV2	322	257	0.01%	0.002%
22	5.613	1410	1422	1450	rBV	319147	652227	18.20%	4.434%
23	5.912	1507	1515	1521	rBV10	3040	5438	0.15%	0.037%
24	6.066	1549	1563	1593	rBV	275918	583418	16.28%	3.966%
25	6.310	1627	1639	1657	rBV	113893	237913	6.64%	1.617%
26	6.638	1738	1741	1743	rBV2	388	213	0.01%	0.001%
27	6.677	1750	1753	1755	rBV2	390	242	0.01%	0.002%
28	6.751	1764	1776	1789	rBV3	13708	27745	0.77%	0.189%
29	6.854	1806	1808	1812	rVB	331	207	0.01%	0.001%
30	6.931	1820	1832	1839	rBV2	49941	86804	2.42%	0.590%
31	6.982	1840	1848	1871	rVB	171518	316608	8.84%	2.153%
32	7.133	1883	1895	1916	rVB2	79483	157589	4.40%	1.071%
33	7.310	1938	1950	1978	rBV	595971	1051692	29.35%	7.150%
34	7.616	2035	2045	2073	rBV	116601	218694	6.10%	1.487%
35	7.793	2098	2100	2103	rBV2	624	290	0.01%	0.002%
36	7.863	2117	2122	2125	rBV3	762	682	0.02%	0.005%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
 Title : VOC Analysis

37	7.915	2133	2138	2139	rBV2	1255	854	0.02%	0.006%
38	7.995	2161	2163	2167	rVB2	413	205	0.01%	0.001%
39	8.024	2169	2172	2178	rVB3	538	486	0.01%	0.003%
40	8.085	2178	2191	2227	rBV	297639	631345	17.62%	4.292%
41	8.522	2324	2327	2329	rBV3	326	258	0.01%	0.002%
42	8.574	2340	2343	2347	rVB3	697	408	0.01%	0.003%
43	8.703	2379	2383	2385	rVB3	526	277	0.01%	0.002%
44	8.725	2385	2390	2391	rBV2	303	208	0.01%	0.001%
45	8.754	2391	2399	2409	rBV7	3936	6435	0.18%	0.044%
46	8.847	2416	2428	2455	rBV	460705	798020	22.27%	5.425%
47	9.120	2511	2513	2514	rBV	531	232	0.01%	0.002%
48	9.146	2514	2521	2523	rBV5	918	1020	0.03%	0.007%
49	9.291	2564	2566	2570	rBV2	493	256	0.01%	0.002%
50	9.352	2580	2585	2588	rBV2	500	388	0.01%	0.003%
51	9.423	2605	2607	2612	rVB2	540	344	0.01%	0.002%
52	9.452	2612	2616	2621	rVB2	319	355	0.01%	0.002%
53	9.497	2627	2630	2634	rBV3	528	491	0.01%	0.003%
54	9.542	2640	2644	2645	rBV2	547	297	0.01%	0.002%
55	9.587	2655	2658	2662	rVV4	573	389	0.01%	0.003%
56	9.612	2662	2666	2669	rVB2	698	565	0.02%	0.004%
57	9.632	2669	2672	2677	rVB2	726	449	0.01%	0.003%
58	9.661	2677	2681	2682	rBV	303	209	0.01%	0.001%
59	9.725	2689	2701	2727	rBV	636259	1095321	30.57%	7.447%
60	10.018	2780	2792	2811	rBV4	13107	35082	0.98%	0.239%
61	10.207	2841	2851	2878	rVB	366241	591689	16.51%	4.023%
62	10.474	2920	2934	2958	rBV	2167114	3583045	100.00%	24.360%
63	10.696	2997	3003	3005	rBV3	1279	1332	0.04%	0.009%
64	10.728	3011	3013	3015	rBV2	468	215	0.01%	0.001%
65	10.767	3020	3025	3026	rBV	621	453	0.01%	0.003%
66	10.847	3047	3050	3051	rBV	716	390	0.01%	0.003%
67	10.915	3069	3071	3075	rBV3	700	680	0.02%	0.005%
68	10.960	3083	3085	3087	rBV2	503	315	0.01%	0.002%
69	10.998	3095	3097	3101	rBV2	311	224	0.01%	0.002%
70	11.091	3113	3126	3136	rBV8	7410	15956	0.45%	0.108%
71	11.172	3145	3151	3156	rBV7	2365	2910	0.08%	0.020%
72	11.239	3161	3172	3196	rBV	484381	773276	21.58%	5.257%
73	11.458	3236	3240	3241	rBV2	410	241	0.01%	0.002%
74	11.516	3254	3258	3260	rBV3	1736	1216	0.03%	0.008%
75	11.616	3277	3289	3308	rBV	566323	901964	25.17%	6.132%
76	11.828	3353	3355	3358	rVV2	453	210	0.01%	0.001%

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 Title : VOC Analysis

77	11.863	3363	3366	3371	rVV3	616	424	0.01%	0.003%
78	11.956	3393	3395	3399	rVV2	641	373	0.01%	0.003%
79	12.079	3430	3433	3435	rBV3	668	376	0.01%	0.003%
80	12.143	3446	3453	3461	rVB5	5179	7746	0.22%	0.053%
81	12.313	3491	3506	3517	rBV	22544	37298	1.04%	0.254%
82	12.593	3588	3593	3598	rBV6	1306	1529	0.04%	0.010%
83	12.673	3614	3618	3622	rVB3	414	411	0.01%	0.003%
84	12.699	3622	3626	3627	rBV3	605	482	0.01%	0.003%
85	12.882	3680	3683	3685	rVB2	530	280	0.01%	0.002%
86	12.898	3685	3688	3690	rBV2	386	211	0.01%	0.001%
87	13.017	3722	3725	3729	rVB3	573	455	0.01%	0.003%
88	13.082	3743	3745	3748	rBV2	518	345	0.01%	0.002%
89	13.204	3780	3783	3785	rBV	336	223	0.01%	0.002%
90	13.278	3804	3806	3808	rBV	384	216	0.01%	0.001%
91	13.294	3808	3811	3815	rVB3	576	444	0.01%	0.003%
92	13.355	3827	3830	3833	rBV2	633	489	0.01%	0.003%
93	13.419	3847	3850	3852	rBV	530	284	0.01%	0.002%
94	13.435	3852	3855	3857	rBV2	615	345	0.01%	0.002%
95	13.641	3915	3919	3923	rVV3	576	616	0.02%	0.004%
96	13.680	3929	3931	3933	rBV2	532	283	0.01%	0.002%
97	13.796	3965	3967	3970	rVB3	417	226	0.01%	0.002%
98	14.374	4142	4147	4150	rBV4	730	720	0.02%	0.005%
99	14.397	4151	4154	4155	rBV2	466	280	0.01%	0.002%
100	14.911	4310	4314	4316	rBV	1096	731	0.02%	0.005%

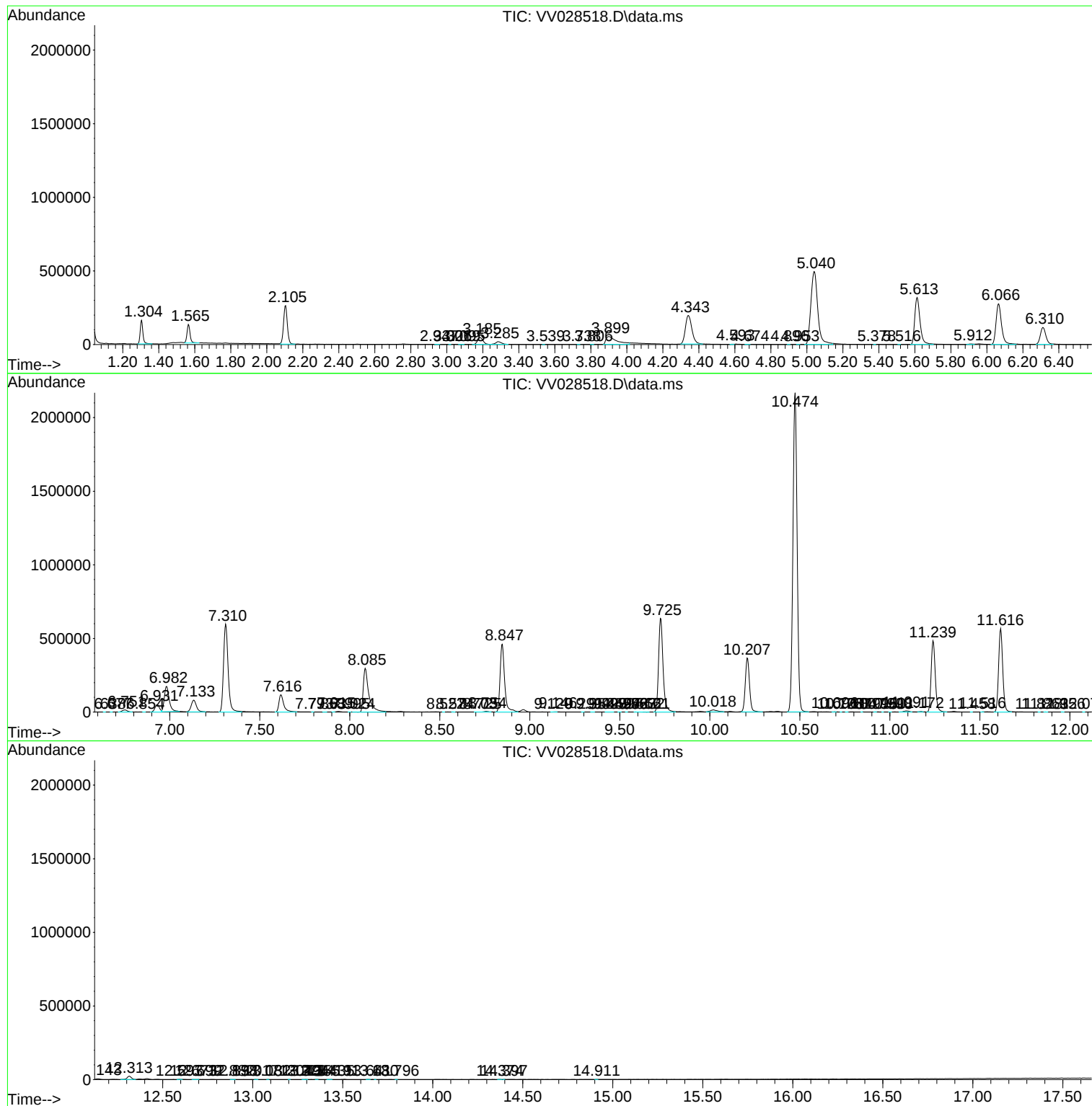
Sum of corrected areas: 14708839

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101122\
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Instrument :
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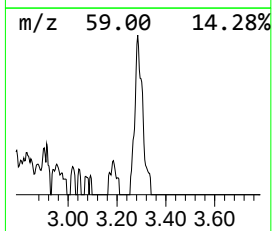
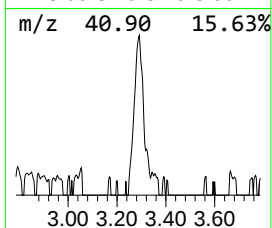
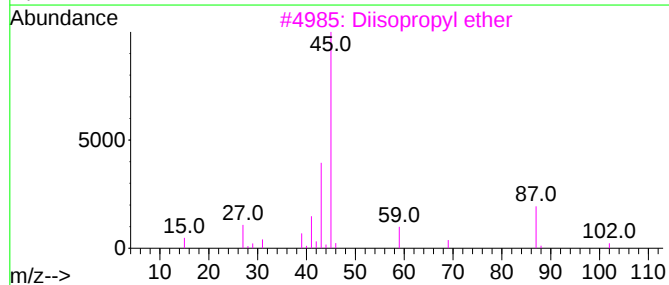
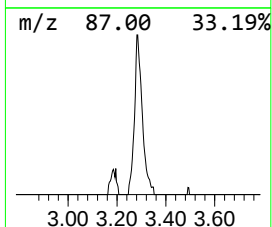
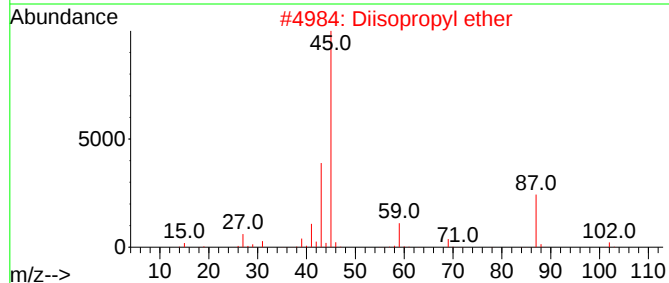
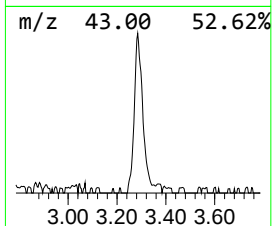
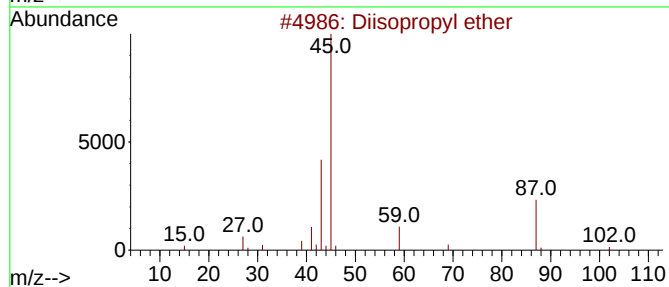
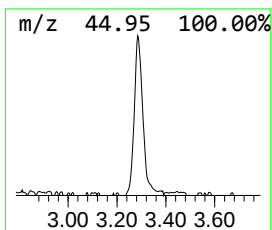
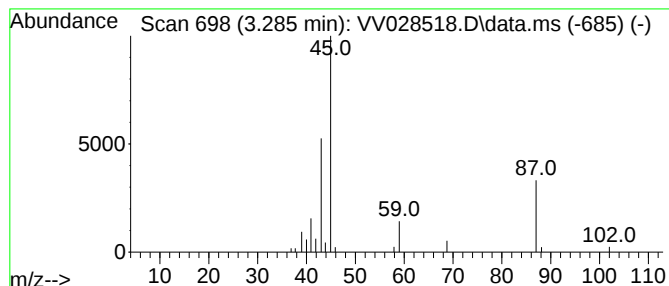
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Diisopropyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.285	3.21 ug/L	41828	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl ether	102	C6H14O	000108-20-3	91
2			Diisopropyl ether	102	C6H14O	000108-20-3	90
3			Diisopropyl ether	102	C6H14O	000108-20-3	86
4			Diisopropyl ether	102	C6H14O	000108-20-3	83
5			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	83



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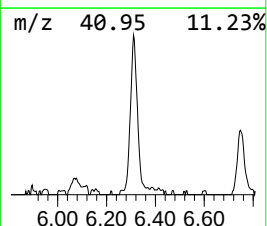
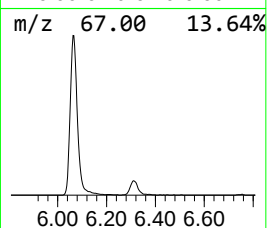
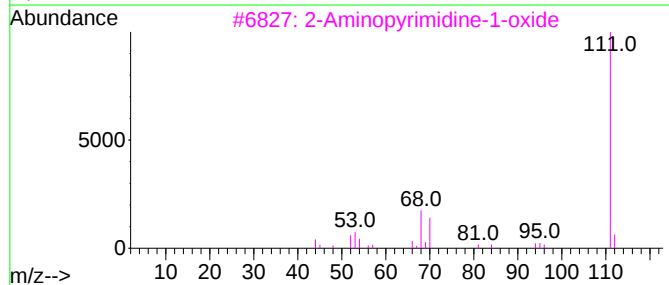
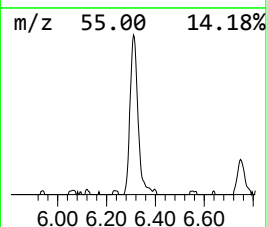
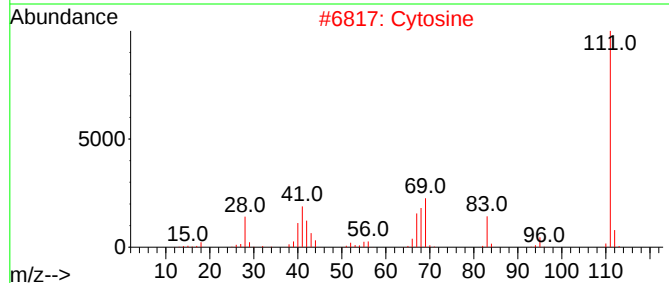
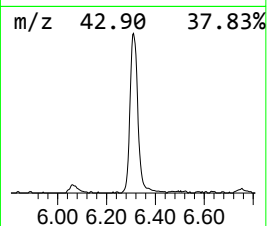
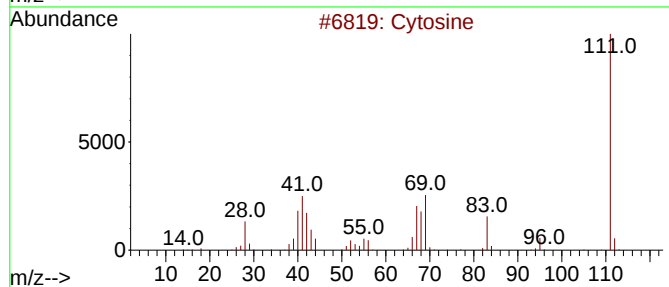
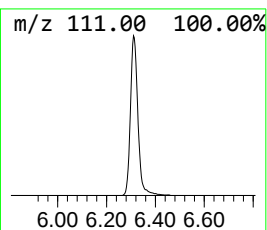
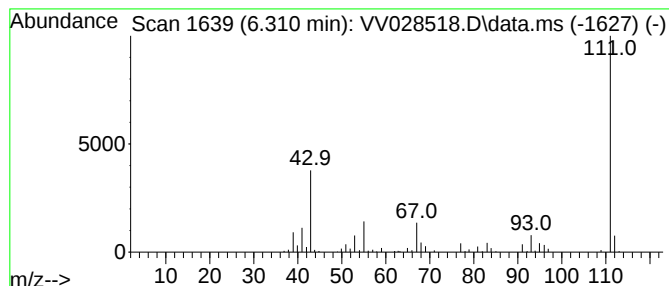
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Cytosine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.310	18.24 ug/L	237913	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cytosine	111	C4H5N3O	000071-30-7	64
2			Cytosine	111	C4H5N3O	000071-30-7	64
3			2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	59
4			Cyclopentene-1-carboxamide	111	C6H9NO	1000423-09-9	45
5			2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	42



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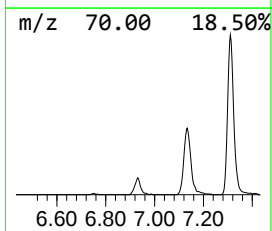
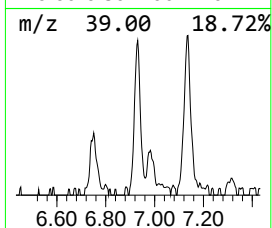
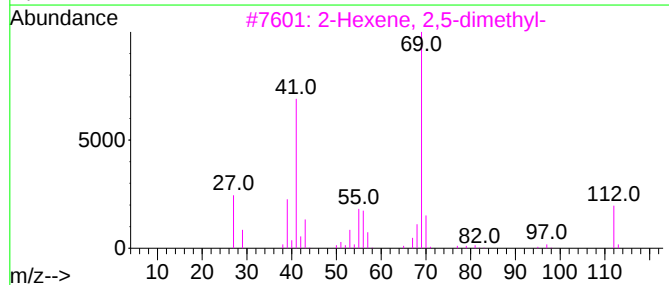
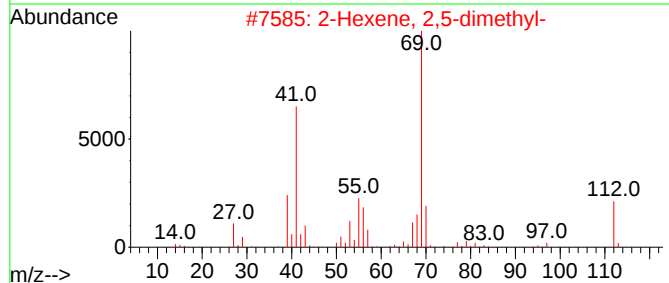
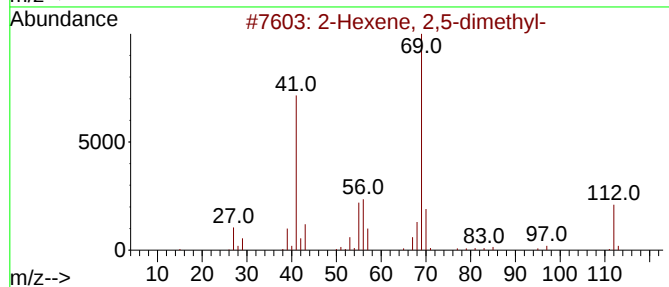
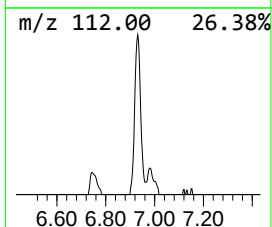
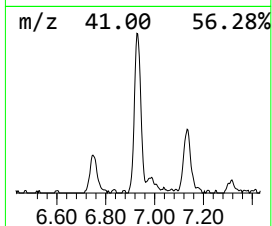
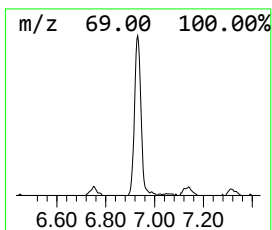
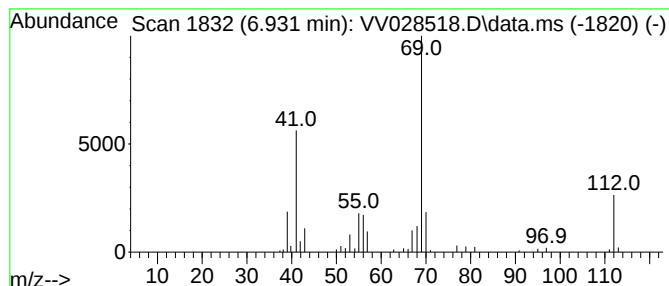
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.931	6.65 ug/L	86804	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 2,5-dimethyl-			112	C8H16	003404-78-2	91
2	2-Hexene, 2,5-dimethyl-			112	C8H16	003404-78-2	91
3	2-Hexene, 2,5-dimethyl-			112	C8H16	003404-78-2	91
4	2-Hexene, 2,5-dimethyl-			112	C8H16	003404-78-2	91
5	3-Heptene, 2-methyl-, (E)-			112	C8H16	000692-96-6	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101122\
Data File : VV028518.D
Acq On : 11 Oct 2022 13:06
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

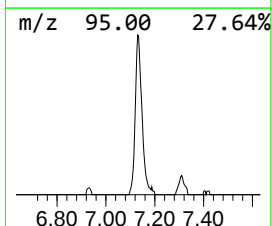
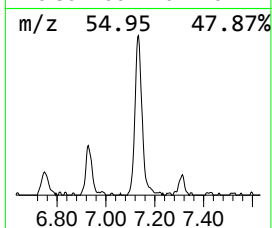
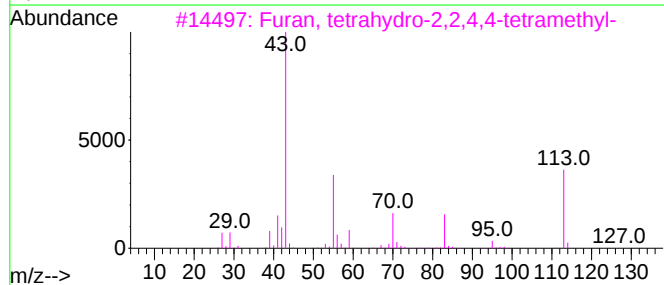
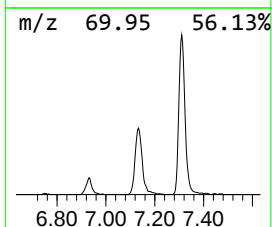
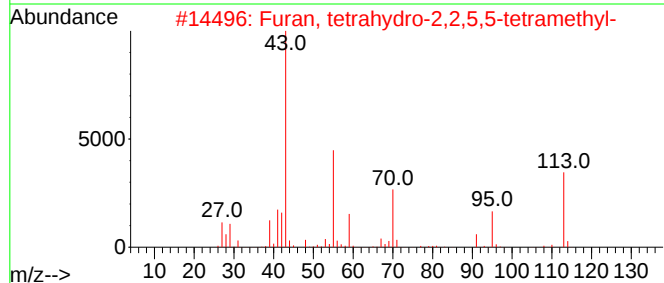
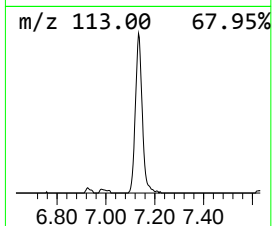
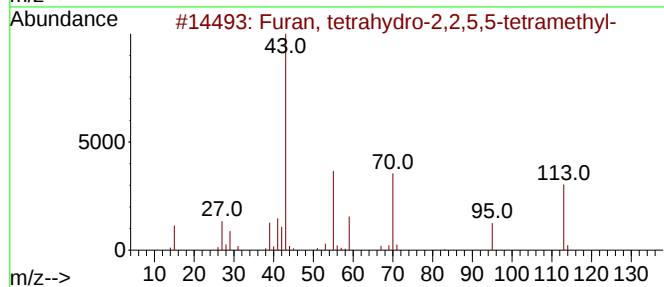
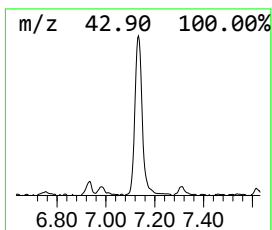
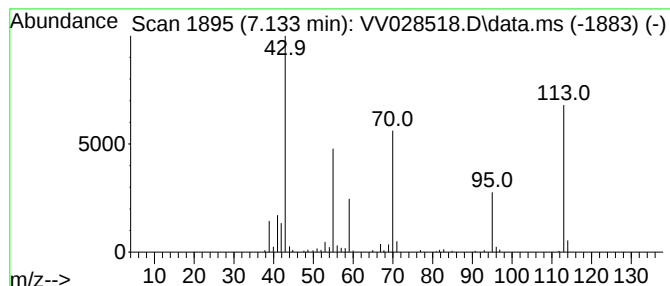
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Quant Title : VOC Analysis

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

Peak Number 5 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.133	12.08 ug/L	157589	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	72
3			Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
4			4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
5			1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101122\
Data File : VV028518.D
Acq On : 11 Oct 2022 13:06
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

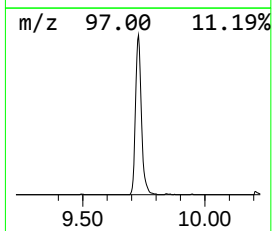
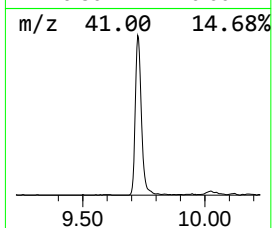
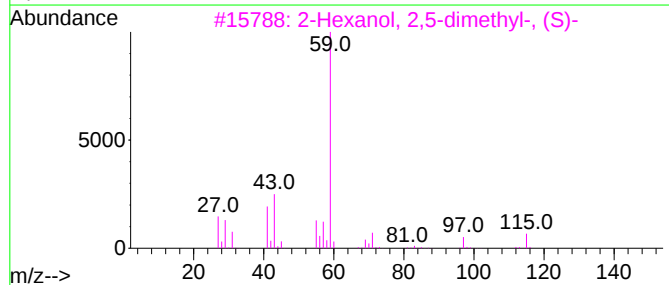
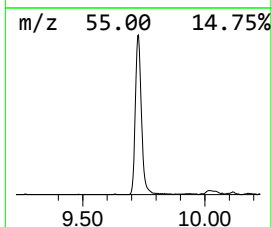
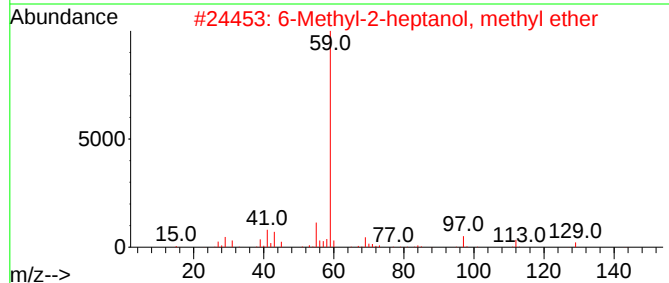
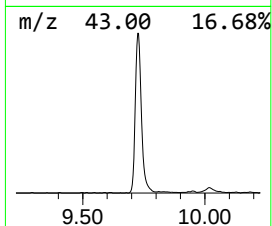
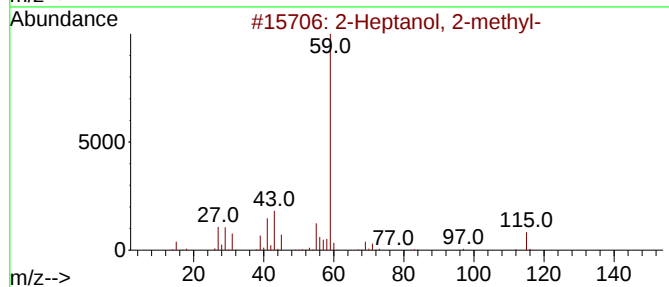
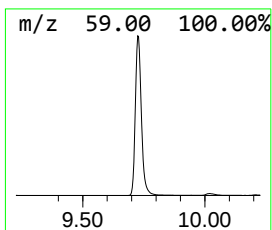
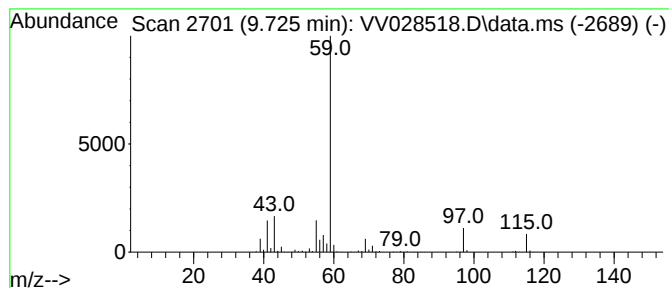
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Quant Title : VOC Analysis

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

Peak Number 6 2-Heptanol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.725	68.63 ug/L	1095320	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	72
2			6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	72
3			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	64
4			2-Decanol, methyl ether	172	C11H24O	1000333-83-9	64
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101122\
Data File : VV028518.D
Acq On : 11 Oct 2022 13:06
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

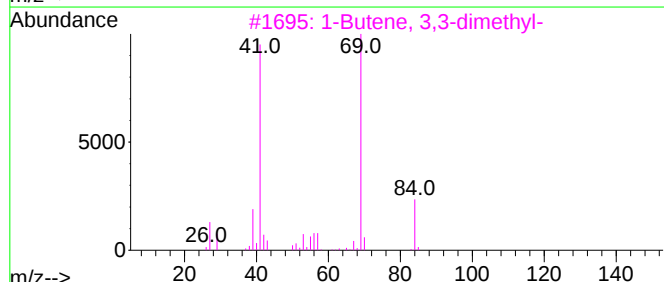
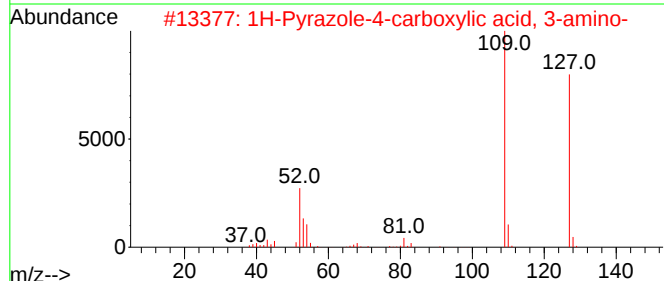
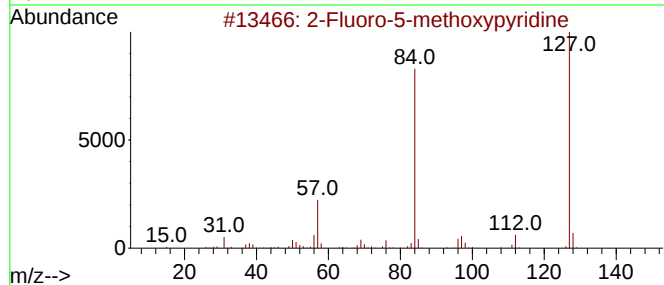
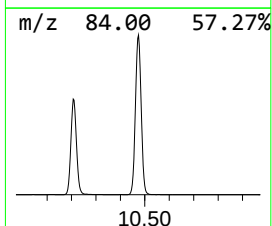
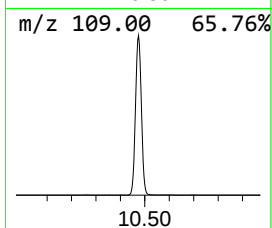
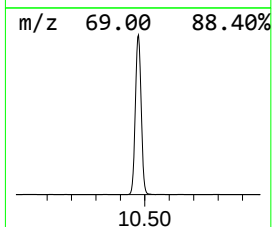
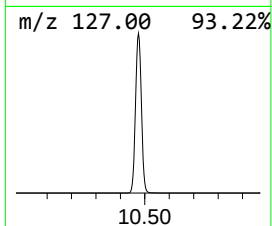
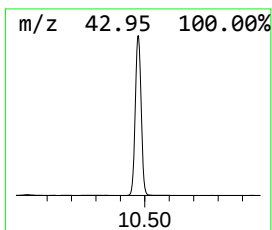
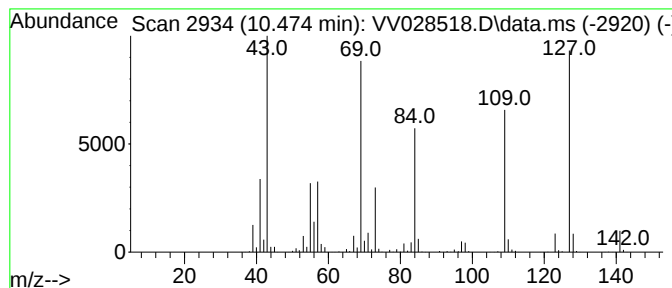
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.474	231.68 ug/L	3583050	1,4-Dichlorobenzene-d4	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluoro-5-methoxypyridine		127	C6H6FNO	136888-79-4	35	
2	1H-Pyrazole-4-carboxylic acid, 3...		127	C4H5N3O2	041680-34-6	35	
3	1-Butene, 3,3-dimethyl-		84	C6H12	000558-37-2	30	
4	Cyclopropane, (1,2-dimethylpropyl)-		112	C8H16	006976-27-8	27	
5	Pentane, 2-chloro-4-methyl-		120	C6H13Cl	025346-32-1	27	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101122\
Data File : VV028518.D
Acq On : 11 Oct 2022 13:06
Operator : SY/MD
Sample : N5079-02
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFYZ9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM100722WMA.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
Diisopropyl ether	3.285	3.2	ug/L	41828	1	5.613	652227	50.0
Cytosine	6.310	18.2	ug/L	237913	1	5.613	652227	50.0
(DEL) Alkane: S...	6.931	6.7	ug/L	86804	1	5.613	652227	50.0
Furan, tetrahyd...	7.133	12.1	ug/L	157589	1	5.613	652227	50.0
2-Heptanol, 2-m...	9.725	68.6	ug/L	1095320	2	8.847	798020	50.0
unknown-01	10.474	231.7	ug/L	3583050	3	11.239	773276	50.0