

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
 Data File : VV027146.D
 Acq On : 01 Aug 2022 23:45
 Operator : SY/MD
 Sample : N3956-03DL 20X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EXF02DL

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\SFAMVLM080122WMA.M

Title : VOC Analysis

Signal : TIC: VV027146.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	13	20	48	rBV	2946369	3005534	100.00%	12.464%
2	1.304	75	82	102	rVB	364044	417091	13.88%	1.730%
3	1.555	153	160	171	rBV	184524	200220	6.66%	0.830%
4	2.098	319	329	343	rVB	675506	951046	31.64%	3.944%
5	2.285	381	387	394	rBV	5511	8426	0.28%	0.035%
6	2.500	445	454	467	rVB2	15904	27394	0.91%	0.114%
7	2.616	481	490	498	rBV	15712	29671	0.99%	0.123%
8	2.828	547	556	567	rBV7	3042	5910	0.20%	0.025%
9	3.031	610	619	621	rBV7	1014	1288	0.04%	0.005%
10	3.178	658	665	671	rBV5	925	1104	0.04%	0.005%
11	3.288	692	699	704	rBV7	2112	3198	0.11%	0.013%
12	3.375	721	726	729	rBV3	462	503	0.02%	0.002%
13	3.400	729	734	737	rBV3	608	625	0.02%	0.003%
14	3.500	762	765	770	rVV4	727	658	0.02%	0.003%
15	3.760	833	846	854	rBV5	1704	3568	0.12%	0.015%
16	3.822	854	865	869	rBV5	2824	5020	0.17%	0.021%
17	3.876	872	882	919	rBV	178789	533598	17.75%	2.213%
18	4.339	1010	1026	1058	rBV	409474	1025606	34.12%	4.253%
19	4.657	1123	1125	1127	rBV2	798	516	0.02%	0.002%
20	4.735	1143	1149	1153	rBV3	714	611	0.02%	0.003%
21	5.040	1222	1244	1253	rBV2	1027450	2576198	85.72%	10.683%
22	5.329	1329	1334	1336	rBV5	2560	2585	0.09%	0.011%
23	5.609	1409	1421	1455	rBV	718137	1466902	48.81%	6.083%
24	5.902	1495	1512	1535	rBV7	24631	94240	3.14%	0.391%
25	6.063	1550	1562	1590	rBV	552355	1148494	38.21%	4.763%
26	6.278	1625	1629	1634	rVB5	1009	888	0.03%	0.004%
27	6.374	1649	1659	1670	rBV3	9541	18565	0.62%	0.077%
28	6.635	1735	1740	1742	rBV4	1364	1340	0.04%	0.006%
29	6.902	1809	1823	1838	rBV2	80839	159389	5.30%	0.661%
30	6.982	1838	1848	1881	rVB	297631	544457	18.12%	2.258%
31	7.246	1924	1930	1935	rBV5	2060	2638	0.09%	0.011%
32	7.313	1939	1951	1965	rBV	1202361	2054468	68.36%	8.520%
33	7.391	1966	1975	1998	rVB2	177464	482876	16.07%	2.002%
34	7.619	2035	2046	2072	rBV	201657	360621	12.00%	1.495%
35	7.741	2082	2084	2089	rBV5	772	611	0.02%	0.003%
36	7.789	2089	2099	2118	rVB2	34345	65817	2.19%	0.273%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080122WMA.M
 Title : VOC Analysis

37	7.934	2141	2144	2148	rBV5	707	566	0.02%	0.002%
38	8.011	2152	2168	2182	rBV	98764	177607	5.91%	0.737%
39	8.088	2182	2192	2226	rVV	646397	1196084	39.80%	4.960%
40	8.448	2291	2304	2318	rVV3	22755	43092	1.43%	0.179%
41	8.548	2331	2335	2337	rBV4	780	590	0.02%	0.002%
42	8.635	2357	2362	2363	rBV2	1431	996	0.03%	0.004%
43	8.850	2410	2429	2432	rBV	1168887	1658051	55.17%	6.876%
44	9.143	2514	2520	2535	rVB2	12687	23874	0.79%	0.099%
45	9.297	2564	2568	2574	rBV6	1198	1516	0.05%	0.006%
46	9.387	2588	2596	2605	rBV5	5543	9112	0.30%	0.038%
47	9.448	2611	2615	2616	rBV	1056	674	0.02%	0.003%
48	9.548	2636	2646	2661	rBV	8930	15955	0.53%	0.066%
49	9.718	2695	2699	2704	rVB3	614	588	0.02%	0.002%
50	9.824	2725	2732	2739	rBV8	1466	2474	0.08%	0.010%
51	9.937	2765	2767	2774	rVB3	1068	895	0.03%	0.004%
52	9.992	2777	2784	2786	rBV5	1854	2003	0.07%	0.008%
53	10.082	2801	2812	2826	rBV3	26722	43700	1.45%	0.181%
54	10.214	2841	2853	2877	rBV	858978	1358727	45.21%	5.634%
55	10.361	2892	2899	2905	rVV9	3190	4468	0.15%	0.019%
56	10.410	2905	2914	2931	rVB4	18701	40820	1.36%	0.169%
57	10.545	2948	2956	2964	rBV3	8989	14088	0.47%	0.058%
58	10.686	2988	3000	3009	rBV4	11821	19010	0.63%	0.079%
59	10.747	3013	3019	3028	rVB4	2145	3026	0.10%	0.013%
60	10.824	3037	3043	3044	rBV2	917	669	0.02%	0.003%
61	10.921	3064	3073	3081	rBV3	3253	5088	0.17%	0.021%
62	10.956	3081	3084	3085	rBV2	1102	626	0.02%	0.003%
63	11.027	3098	3106	3115	rBV5	3214	4749	0.16%	0.020%
64	11.120	3131	3135	3140	rBV3	682	677	0.02%	0.003%
65	11.188	3150	3156	3163	rBV8	1598	1833	0.06%	0.008%
66	11.246	3163	3174	3187	rBV	1036217	1607574	53.49%	6.666%
67	11.400	3215	3222	3228	rVB8	2326	3112	0.10%	0.013%
68	11.525	3258	3261	3265	rBV5	1668	1583	0.05%	0.007%
69	11.622	3278	3291	3316	rBV	1162101	1839146	61.19%	7.627%
70	11.754	3330	3332	3338	rVB4	2452	1686	0.06%	0.007%
71	11.911	3377	3381	3388	rBV5	1818	2064	0.07%	0.009%
72	12.107	3437	3442	3447	rVV6	1795	1884	0.06%	0.008%
73	12.152	3453	3456	3463	rVB6	1575	1644	0.05%	0.007%
74	12.400	3519	3533	3545	rVV10	10991	20833	0.69%	0.086%
75	12.464	3548	3553	3560	rVB3	777	1032	0.03%	0.004%
76	12.532	3571	3574	3577	rBV3	1127	747	0.02%	0.003%

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 Title : VOC Analysis

77	12.583	3585	3590	3599	rVB8	1024	1621	0.05%	0.007%
78	12.718	3626	3632	3635	rBV4	701	776	0.03%	0.003%
79	12.747	3635	3641	3652	rVV2	6015	9112	0.30%	0.038%
80	12.818	3655	3663	3679	rVB3	26450	39480	1.31%	0.164%
81	12.882	3679	3683	3689	rBV6	1365	1451	0.05%	0.006%
82	13.049	3727	3735	3738	rBV3	1019	1145	0.04%	0.005%
83	13.156	3761	3768	3773	rBV8	2518	3588	0.12%	0.015%
84	13.204	3778	3783	3787	rVV6	1700	1845	0.06%	0.008%
85	13.268	3799	3803	3809	rVB7	1726	1981	0.07%	0.008%
86	13.480	3862	3869	3874	rBV7	4732	7188	0.24%	0.030%
87	13.631	3910	3916	3920	rBV3	682	821	0.03%	0.003%
88	13.789	3956	3965	3976	rVB5	8574	14528	0.48%	0.060%
89	13.853	3978	3985	3990	rBV6	3460	4050	0.13%	0.017%
90	13.901	3990	4000	4018	rVB2	100904	165899	5.52%	0.688%
91	14.024	4030	4038	4049	rVB3	13789	19886	0.66%	0.082%
92	14.503	4183	4187	4193	rVB5	644	707	0.02%	0.003%
93	14.548	4193	4201	4205	rBV5	1037	1344	0.04%	0.006%
94	14.641	4223	4230	4242	rVB4	2866	5190	0.17%	0.022%
95	14.692	4242	4246	4247	rBV2	1739	1207	0.04%	0.005%
96	14.818	4278	4285	4293	rVV3	2982	4426	0.15%	0.018%
97	14.966	4321	4331	4342	rBV2	75414	113156	3.76%	0.469%
98	15.226	4409	4412	4415	rVB4	1666	1073	0.04%	0.004%
99	15.799	4579	4590	4602	rBV	260032	398659	13.26%	1.653%
100	16.020	4657	4659	4662	rBV4	1485	944	0.03%	0.004%

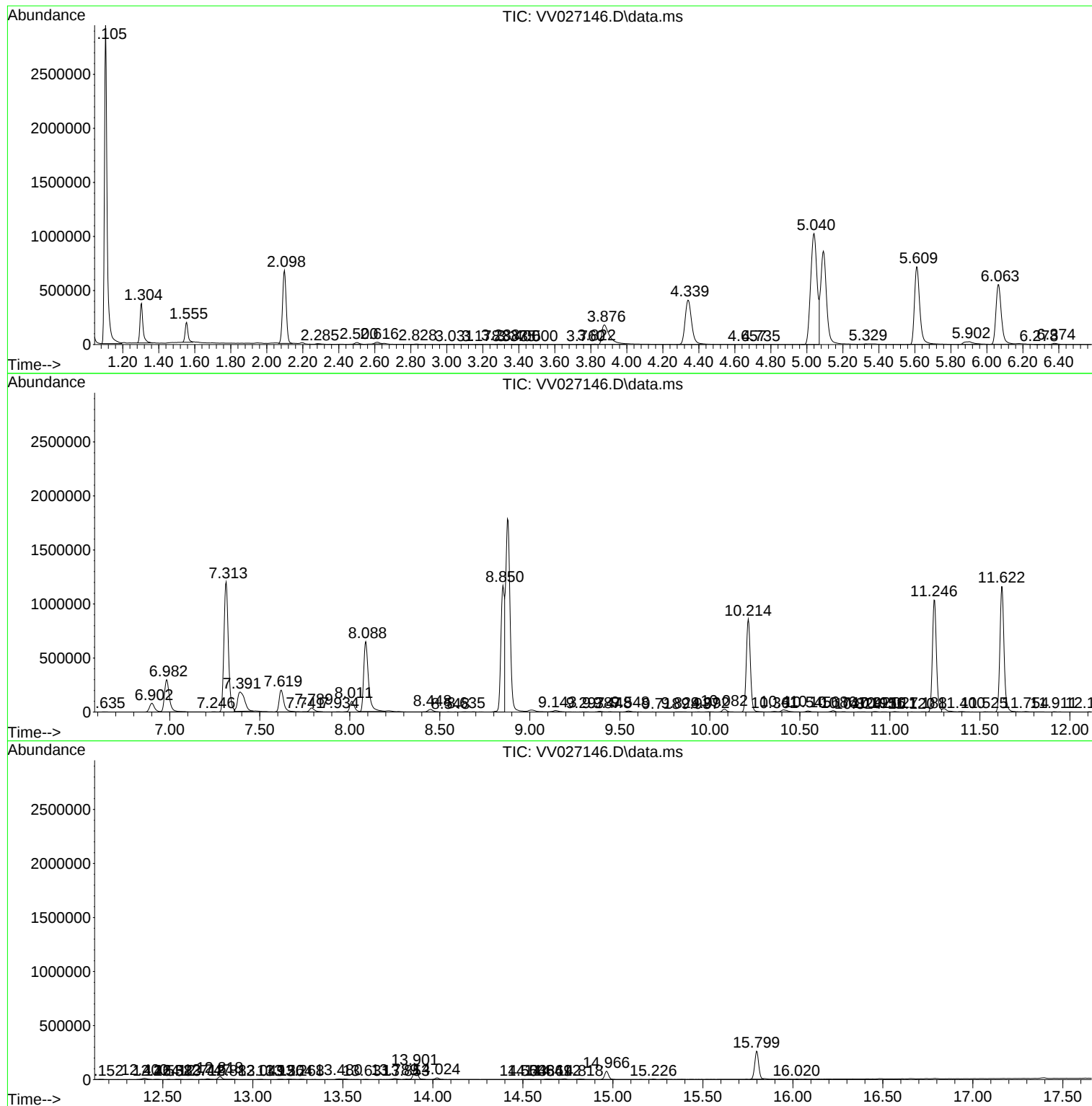
Sum of corrected areas: 24114616

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Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080122WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
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Instrument :
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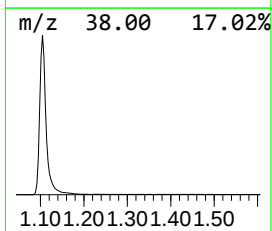
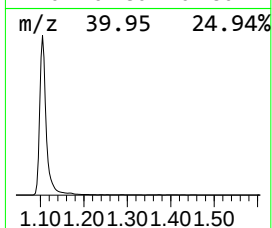
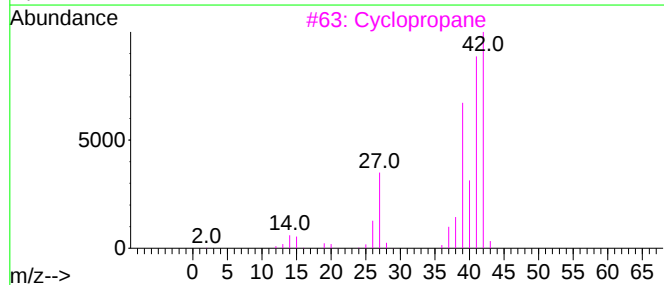
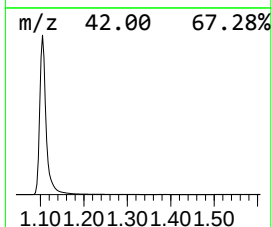
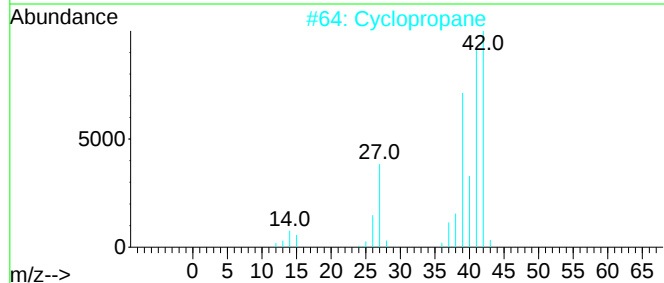
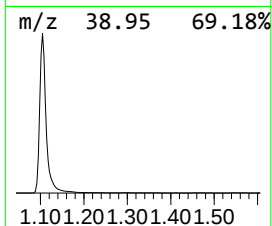
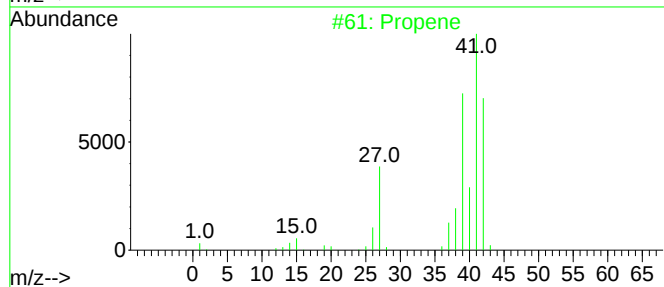
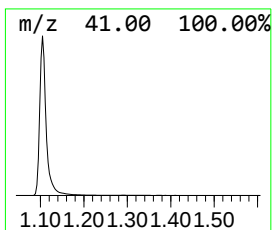
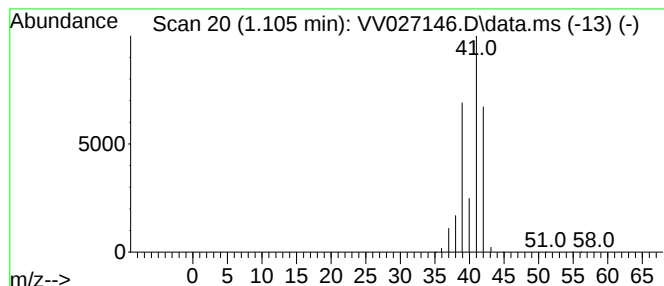
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080122WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.105	102.44 ug/L	3005530	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	86
2			Cyclopropane	42	C3H6	000075-19-4	80
3			Cyclopropane	42	C3H6	000075-19-4	72
4			Propene	42	C3H6	000115-07-1	47
5			Cyclopropene	40	C3H4	002781-85-3	16



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Instrument :
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ClientSampleId :
EXF02DL

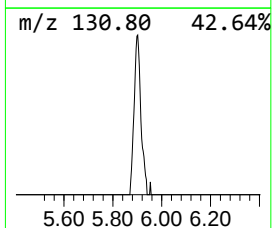
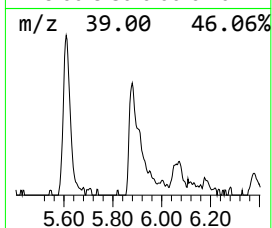
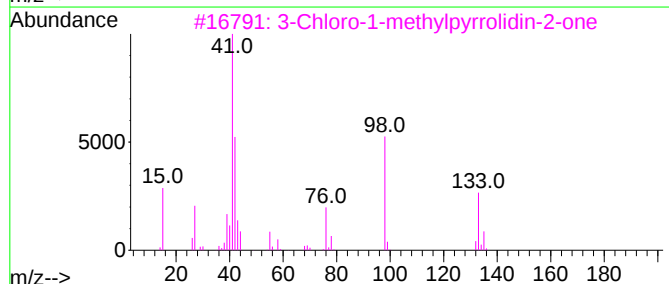
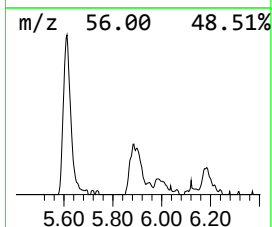
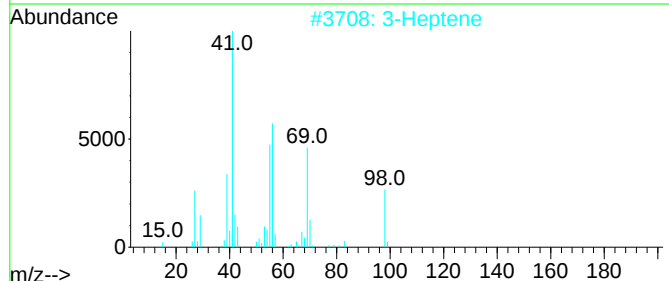
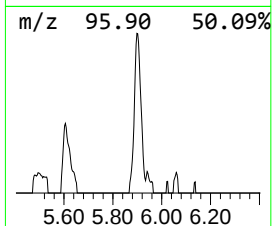
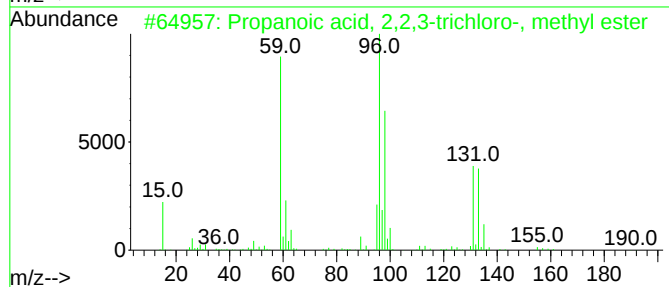
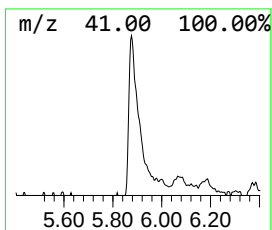
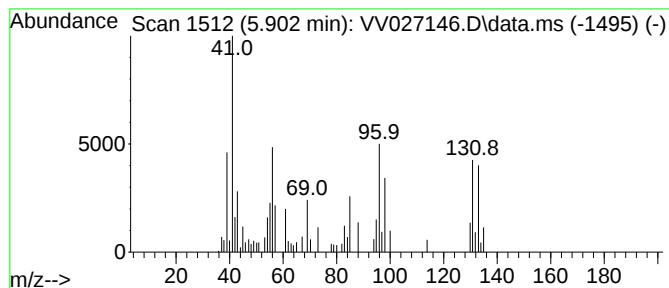
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080122WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.21 ug/L	94240	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	25
2			3-Heptene	98	C7H14	000592-78-9	10
3			3-Chloro-1-methylpyrrolidin-2-one	133	C5H8ClNO	1000487-04-2	9
4			3-Dimethylaminoacrylonitrile	96	C5H8N2	002407-68-3	9
5			3-(Chloromethyl)-4-methyl-4H-1,2...	131	C4H6ClN3	740056-61-5	9



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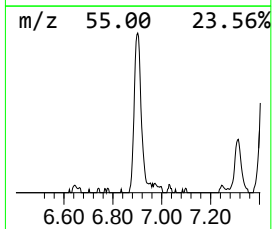
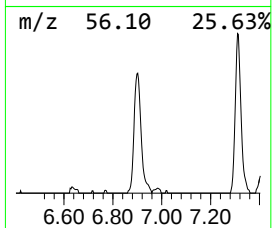
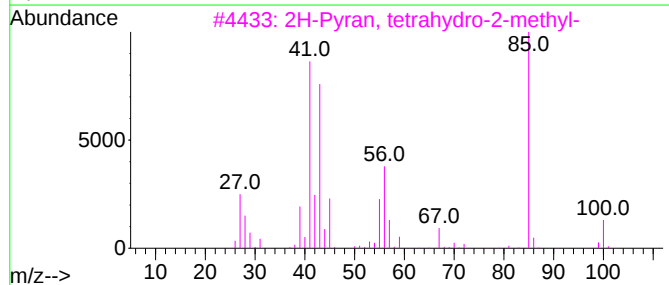
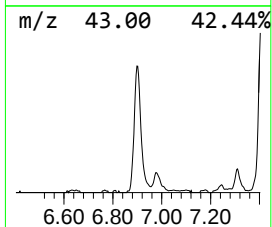
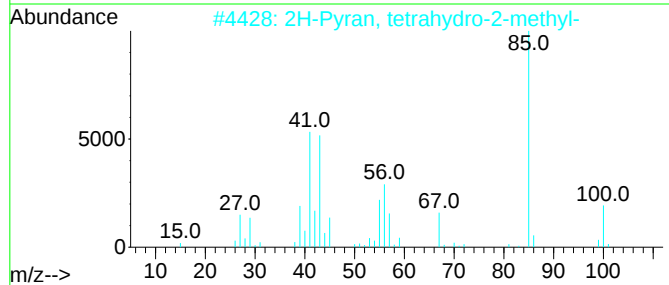
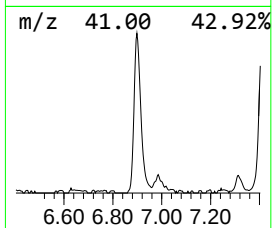
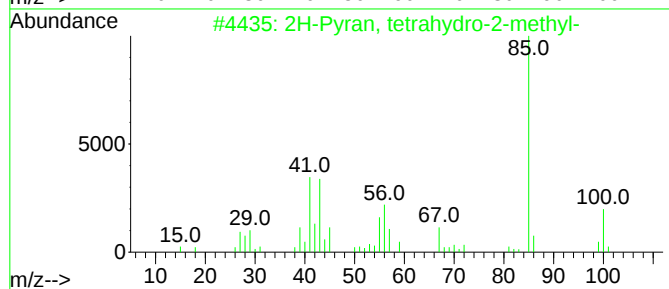
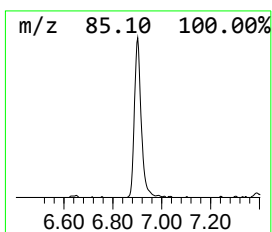
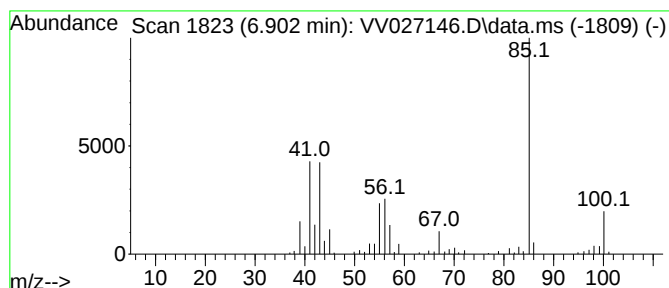
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ClientSampleId :
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Quant Title : VOC Analysis

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

Peak Number 3 2H-Pyran, tetrahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.902	5.43 ug/L	159389	1,4-Difluorobenzene	5.612	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	90
2	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	90
3	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	78
4	1-Methoxy-3-methyl-2-butene	100	C6H12O	022093-99-8	64
5	trans-1-Methoxy-3-methyl-1-butene	100	C6H12O	1000139-44-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027146.D
Acq On : 01 Aug 2022 23:45
Operator : SY/MD
Sample : N3956-03DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF02DL

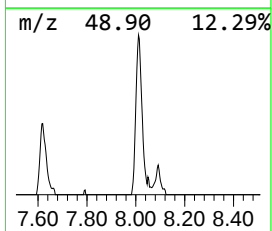
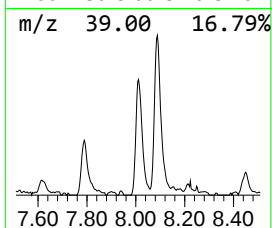
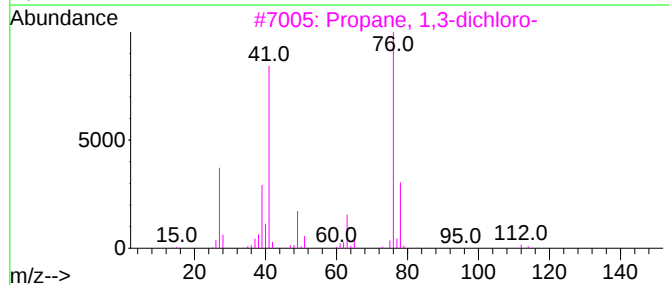
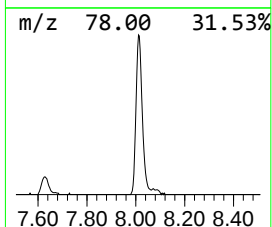
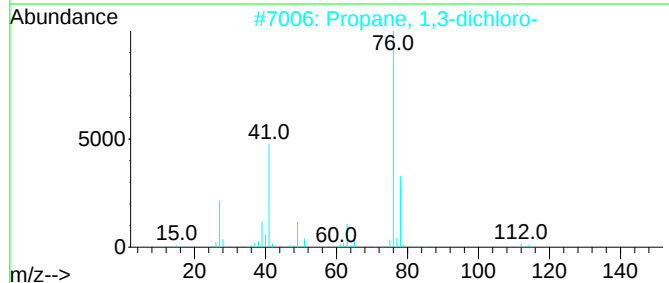
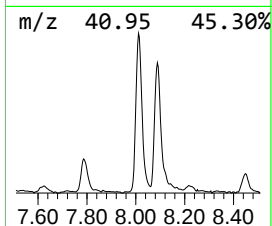
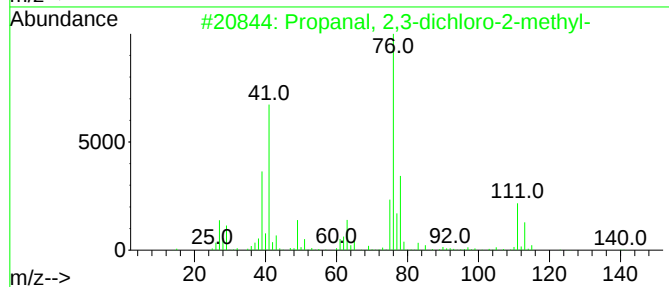
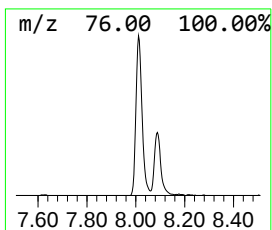
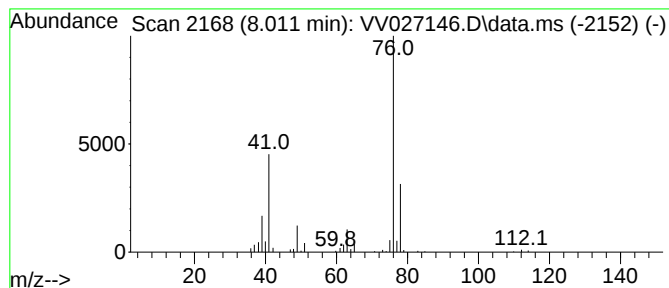
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Quant Title : VOC Analysis

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

Peak Number 5 Propanal, 2,3-dichloro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.011	5.36 ug/L	177607	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,3-dichloro-2-methyl-	140	C4H6Cl2O	010141-22-7	64
2			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	11
3			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	11
4			Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	11
5			Thiourea	76	CH4N2S	000062-56-6	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027146.D
Acq On : 01 Aug 2022 23:45
Operator : SY/MD
Sample : N3956-03DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF02DL

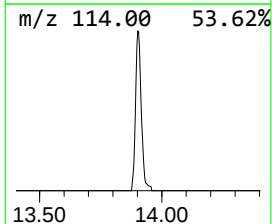
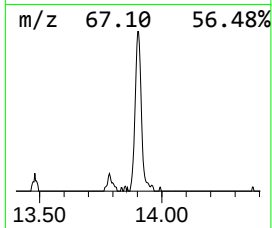
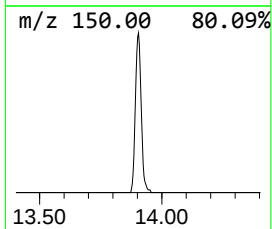
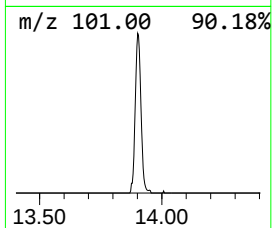
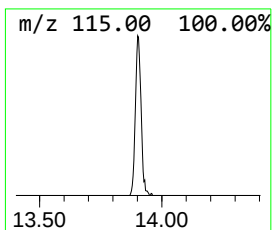
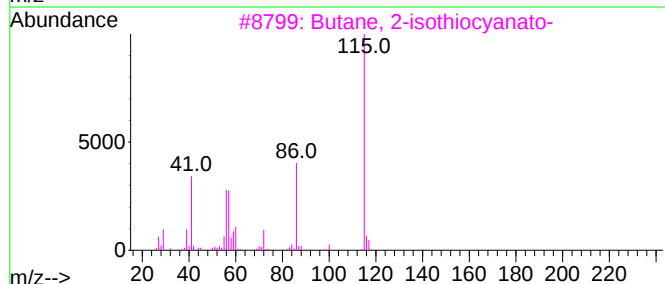
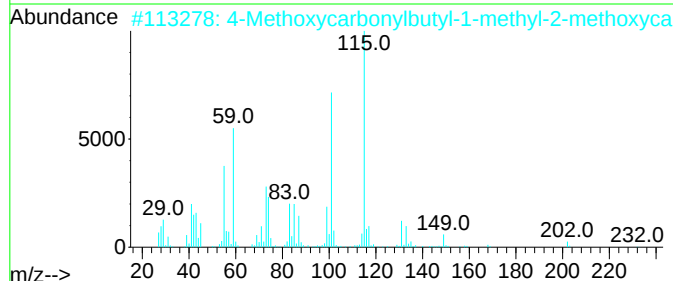
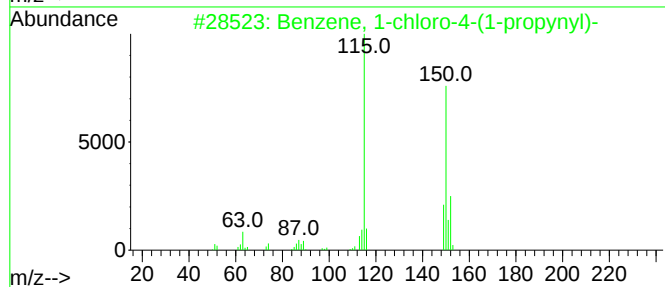
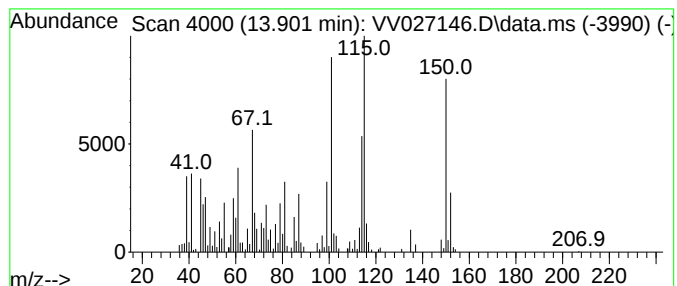
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.902	5.16 ug/L	165899	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-4-(1-propynyl)-	150	C9H7Cl	002809-65-6	43
2			4-Methoxycarbonylbutyl-1-methyl-...	232	C11H20O5	1000140-30-2	35
3			Butane, 2-isothiocyanato-	115	C5H9NS	004426-79-3	11
4			6H-Purin-6-one, 1,7-dihydro-7-me...	150	C6H6N4O	001006-08-2	11
5			[1,2,4]Triazole, 4-amino-3-(pyra...	150	C5H6N6	1000316-93-2	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027146.D
Acq On : 01 Aug 2022 23:45
Operator : SY/MD
Sample : N3956-03DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF02DL

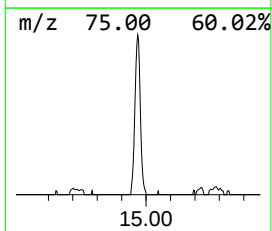
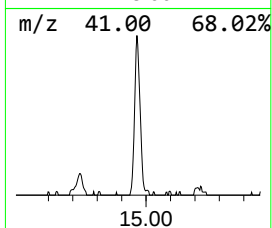
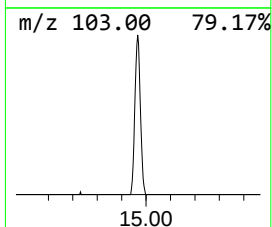
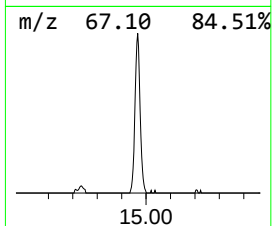
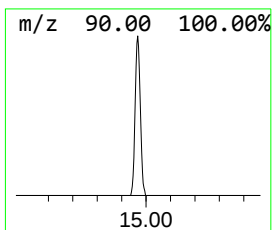
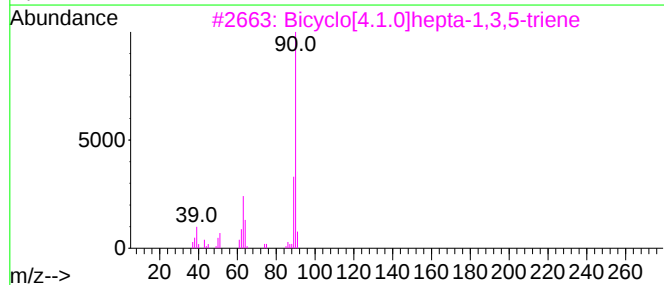
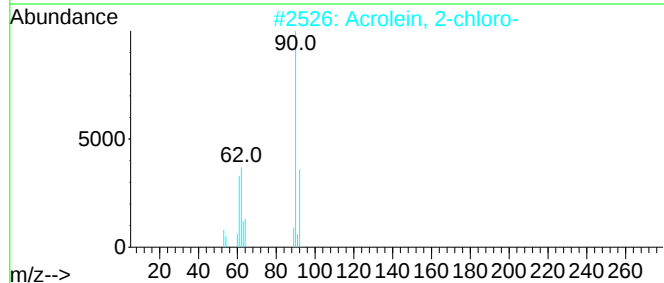
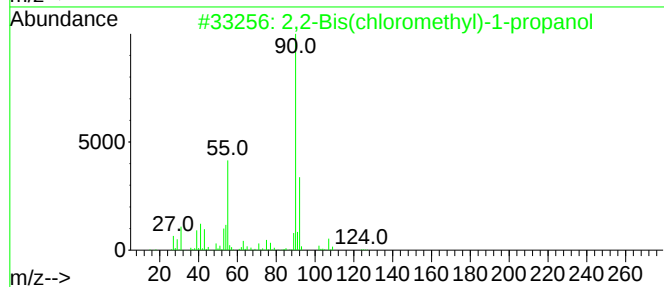
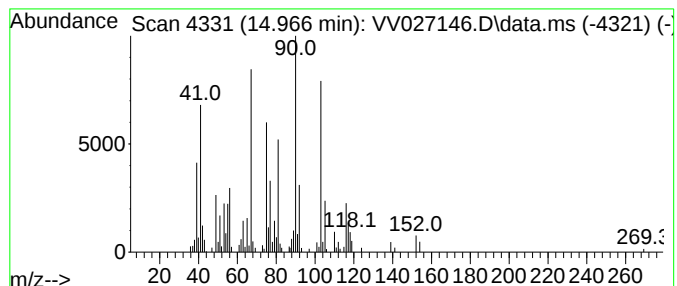
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Quant Title : VOC Analysis

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

Peak Number 7 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.966	3.52 ug/L	113156	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	38
2			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
3			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	35
4			2-Phenyl-3-(4-nitrophenyl)-oxirane	241	C14H11NO3	1000144-81-2	25
5			Borane, chloro(dimethylamino)ethyl-	119	C4H11BClN	001739-26-0	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027146.D
Acq On : 01 Aug 2022 23:45
Operator : SY/MD
Sample : N3956-03DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF02DL

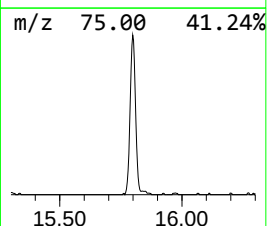
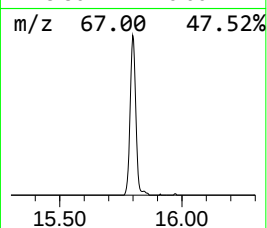
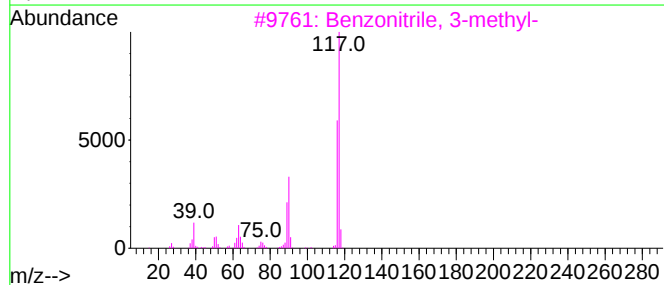
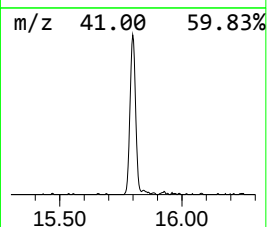
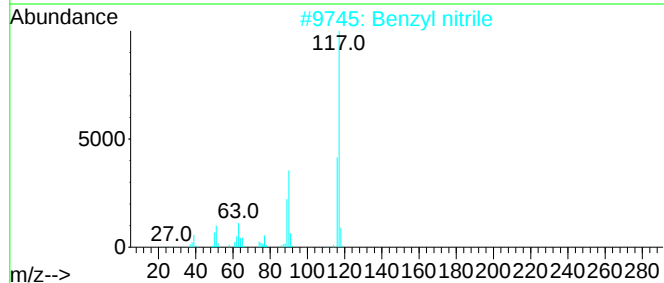
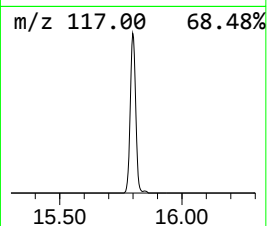
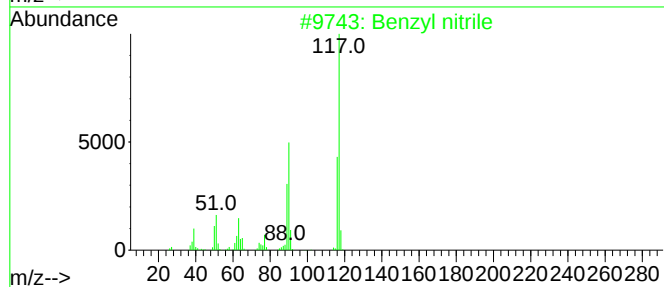
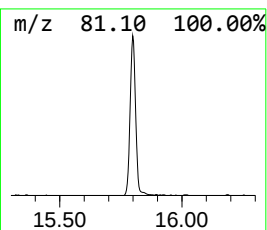
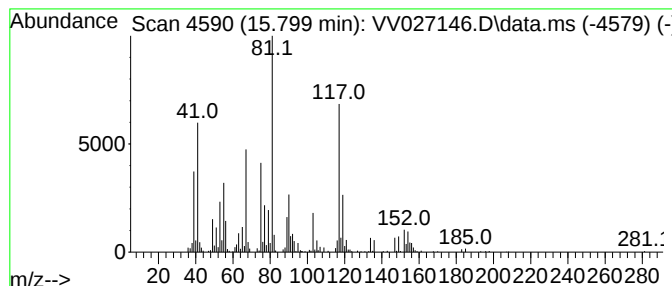
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Quant Title : VOC Analysis

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

Peak Number 8 unknown-04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.799	12.40 ug/L	398659	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl nitrile	117	C8H7N	000140-29-4	25
2			Benzyl nitrile	117	C8H7N	000140-29-4	25
3			Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	25
4			Indolizine	117	C8H7N	000274-40-8	25
5			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027146.D
Acq On : 01 Aug 2022 23:45
Operator : SY/MD
Sample : N3956-03DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF02DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080122WMA.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
(DEL) Alkane: S...	1.105	102.4	ug/L	3005530	1	5.612	1466900	50.0
unknown-01	5.902	3.2	ug/L	94240	1	5.612	1466900	50.0
2H-Pyran, tetra...	6.902	5.4	ug/L	159389	1	5.612	1466900	50.0
Propanal, 2,3-d...	8.011	5.4	ug/L	177607	2	8.850	1658050	50.0
unknown-02	13.902	5.2	ug/L	165899	3	11.249	1607570	50.0
unknown-03	14.966	3.5	ug/L	113156	3	11.249	1607570	50.0
unknown-04	15.799	12.4	ug/L	398659	3	11.249	1607570	50.0