

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
 Data File : VV027164.D
 Acq On : 02 Aug 2022 11:28
 Operator : SY/MD
 Sample : N3956-04DL 4X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EXF03DL

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: VV027164.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	44	rBV	6153852	6176613	32.83%	12.651%
2	1.198	44	49	74	rVV	294791	338901	1.80%	0.694%
3	1.304	75	82	100	rVB	330250	346083	1.84%	0.709%
4	1.564	155	163	173	rBV	264601	297644	1.58%	0.610%
5	2.060	309	317	322	rBV3	31397	44084	0.23%	0.090%
6	2.105	322	331	343	rVB	536081	757051	4.02%	1.551%
7	2.394	419	421	426	rBV4	800	615	0.00%	0.001%
8	2.471	441	445	446	rBV2	1048	838	0.00%	0.002%
9	2.507	449	456	459	rBV3	6780	8499	0.05%	0.017%
10	2.654	500	502	509	rVB5	2463	2366	0.01%	0.005%
11	2.728	522	525	530	rVB3	524	365	0.00%	0.001%
12	2.812	548	551	555	rBV2	465	428	0.00%	0.001%
13	2.970	597	600	604	rBV2	496	360	0.00%	0.001%
14	3.127	645	649	653	rVB2	528	410	0.00%	0.001%
15	3.188	654	668	680	rBV3	1770	4187	0.02%	0.009%
16	3.442	743	747	750	rBV3	458	304	0.00%	0.001%
17	3.696	822	826	830	rVB2	433	352	0.00%	0.001%
18	3.728	830	836	841	rVB3	487	462	0.00%	0.001%
19	3.879	872	883	914	rBV	168938	498201	2.65%	1.020%
20	4.214	984	987	994	rVB3	696	818	0.00%	0.002%
21	4.262	997	1002	1006	rBV4	436	370	0.00%	0.001%
22	4.342	1007	1027	1068	rBV	374001	950659	5.05%	1.947%
23	4.693	1134	1136	1140	rVB4	646	418	0.00%	0.001%
24	4.780	1160	1163	1167	rBV4	479	398	0.00%	0.001%
25	4.931	1203	1210	1212	rBV2	486	518	0.00%	0.001%
26	5.043	1227	1245	1253	rBV2	865883	2185866	11.62%	4.477%
27	5.404	1354	1357	1358	rBV	872	605	0.00%	0.001%
28	5.468	1373	1377	1379	rBV4	632	410	0.00%	0.001%
29	5.613	1410	1422	1459	rBV	703572	1450549	7.71%	2.971%
30	5.892	1496	1509	1536	rBV2	114607	265037	1.41%	0.543%
31	6.011	1544	1546	1549	rBV4	878	420	0.00%	0.001%
32	6.066	1549	1563	1579	rBV	494229	1028252	5.46%	2.106%
33	6.375	1644	1659	1690	rBV	226798	470134	2.50%	0.963%
34	6.600	1725	1729	1732	rBV5	472	375	0.00%	0.001%
35	6.641	1732	1742	1746	rBV7	2814	4788	0.03%	0.010%
36	6.715	1758	1765	1766	rBV4	2333	2278	0.01%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Stop Thrs : 0

Peak Location: TOP

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

37	6.895	1804	1821	1839	rBV	1521197	2773769	14.74%	5.681%
38	6.982	1839	1848	1874	rVB	298598	552922	2.94%	1.132%
39	7.239	1919	1928	1938	rBV10	2379	5107	0.03%	0.010%
40	7.313	1939	1951	1969	rBV	1011144	1799251	9.56%	3.685%
41	7.407	1969	1980	2018	rVB	1162612	2089634	11.11%	4.280%
42	7.619	2037	2046	2072	rVB	190734	332470	1.77%	0.681%
43	7.796	2092	2101	2117	rVB7	9270	17911	0.10%	0.037%
44	7.924	2138	2141	2143	rBV2	854	478	0.00%	0.001%
45	8.011	2152	2168	2183	rBV	11381313	18816108	100.00%	38.538%
46	8.085	2183	2191	2224	rVB	645621	1218071	6.47%	2.495%
47	8.452	2298	2305	2318	rVB5	7966	15603	0.08%	0.032%
48	8.628	2349	2360	2376	rVV2	12658	27038	0.14%	0.055%
49	8.760	2398	2401	2404	rBV3	647	420	0.00%	0.001%
50	8.780	2405	2407	2410	rVB2	764	354	0.00%	0.001%
51	8.850	2414	2429	2464	rBV	1060652	1772504	9.42%	3.630%
52	9.075	2493	2499	2506	rBV8	3058	5145	0.03%	0.011%
53	9.194	2532	2536	2539	rBV2	577	496	0.00%	0.001%
54	9.255	2551	2555	2556	rBV2	529	307	0.00%	0.001%
55	9.288	2558	2565	2578	rVB7	2085	3991	0.02%	0.008%
56	9.384	2585	2595	2610	rBV	26417	45581	0.24%	0.093%
57	9.474	2621	2623	2627	rVB3	626	383	0.00%	0.001%
58	9.522	2633	2638	2640	rBV4	927	629	0.00%	0.001%
59	9.554	2640	2648	2651	rBV4	1447	2001	0.01%	0.004%
60	9.751	2707	2709	2717	rVB3	474	467	0.00%	0.001%
61	10.079	2807	2811	2814	rBV4	1098	967	0.01%	0.002%
62	10.165	2834	2838	2841	rBV3	543	402	0.00%	0.001%
63	10.214	2841	2853	2883	rVV	774532	1205808	6.41%	2.470%
64	10.416	2913	2916	2919	rBV2	513	365	0.00%	0.001%
65	10.677	2994	2997	3002	rVB3	506	507	0.00%	0.001%
66	10.754	3014	3021	3025	rBV3	525	572	0.00%	0.001%
67	10.831	3038	3045	3049	rBV5	1930	2575	0.01%	0.005%
68	10.850	3049	3051	3057	rVB4	1352	1067	0.01%	0.002%
69	10.927	3072	3075	3079	rBV2	337	371	0.00%	0.001%
70	10.963	3079	3086	3097	rVV8	2492	4522	0.02%	0.009%
71	11.030	3104	3107	3113	rVB4	813	688	0.00%	0.001%
72	11.172	3139	3151	3163	rBV	46614	81608	0.43%	0.167%
73	11.246	3163	3174	3203	rVV	1012187	1546001	8.22%	3.166%
74	11.542	3260	3266	3273	rBV7	1890	2963	0.02%	0.006%
75	11.622	3278	3291	3324	rBV	980992	1637048	8.70%	3.353%
76	12.017	3411	3414	3417	rBV	389	320	0.00%	0.001%

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 Title : VOC Analysis

77	12.091	3430	3437	3441	rBV3	779	1206	0.01%	0.002%
78	12.365	3517	3522	3527	rBV4	589	689	0.00%	0.001%
79	12.410	3533	3536	3542	rVB3	360	341	0.00%	0.001%
80	12.738	3634	3638	3641	rBV3	405	368	0.00%	0.001%
81	12.824	3657	3665	3672	rBV4	2013	2882	0.02%	0.006%
82	13.143	3759	3764	3767	rBV3	418	500	0.00%	0.001%
83	13.188	3775	3778	3780	rBV2	511	319	0.00%	0.001%
84	13.259	3792	3800	3801	rBV	494	589	0.00%	0.001%
85	13.419	3848	3850	3854	rVV3	465	377	0.00%	0.001%
86	13.522	3878	3882	3884	rBV3	489	386	0.00%	0.001%
87	13.574	3896	3898	3903	rVB3	549	369	0.00%	0.001%
88	13.603	3903	3907	3911	rBV	774	754	0.00%	0.002%
89	13.783	3960	3963	3968	rVB2	614	462	0.00%	0.001%
90	13.808	3969	3971	3974	rBV3	657	410	0.00%	0.001%
91	13.876	3986	3992	3994	rBV3	498	490	0.00%	0.001%
92	13.908	3995	4002	4008	rBV5	1736	2384	0.01%	0.005%
93	14.066	4047	4051	4054	rBV2	372	364	0.00%	0.001%
94	14.120	4064	4068	4070	rBV2	542	484	0.00%	0.001%
95	14.326	4128	4132	4136	rBV2	570	673	0.00%	0.001%
96	14.683	4241	4243	4246	rBV2	483	320	0.00%	0.001%
97	14.892	4305	4308	4312	rBV4	549	383	0.00%	0.001%
98	14.972	4327	4333	4341	rVB5	1944	2816	0.01%	0.006%
99	15.008	4341	4344	4348	rBV3	550	444	0.00%	0.001%
100	15.156	4388	4390	4395	rBV4	736	498	0.00%	0.001%

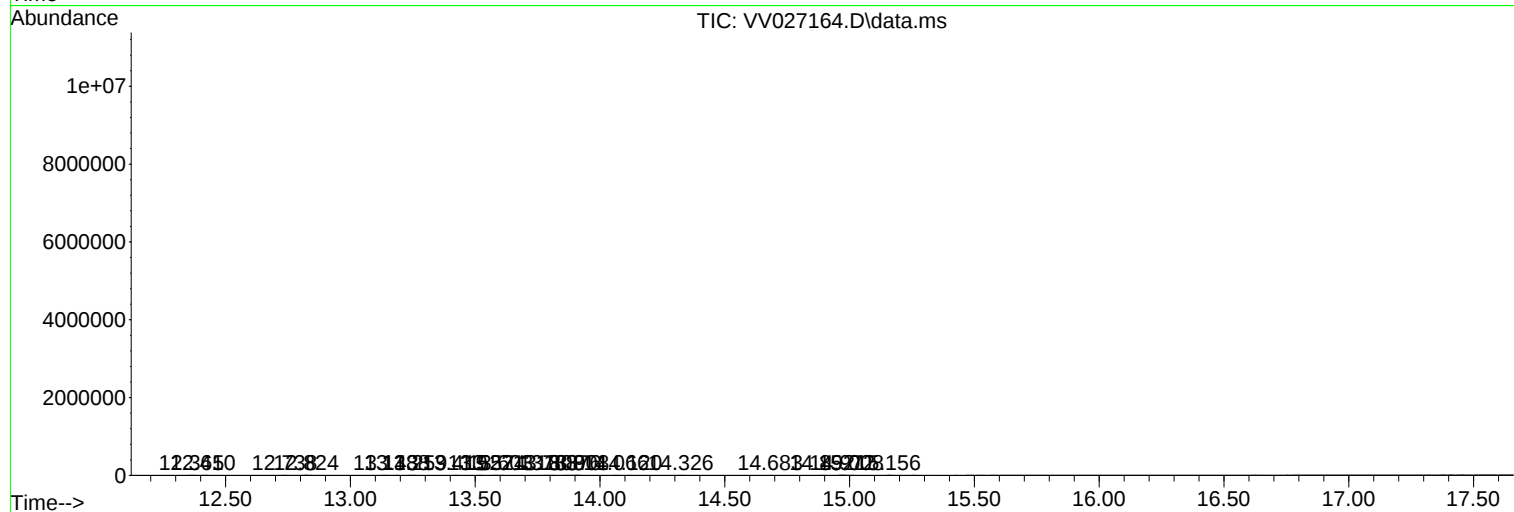
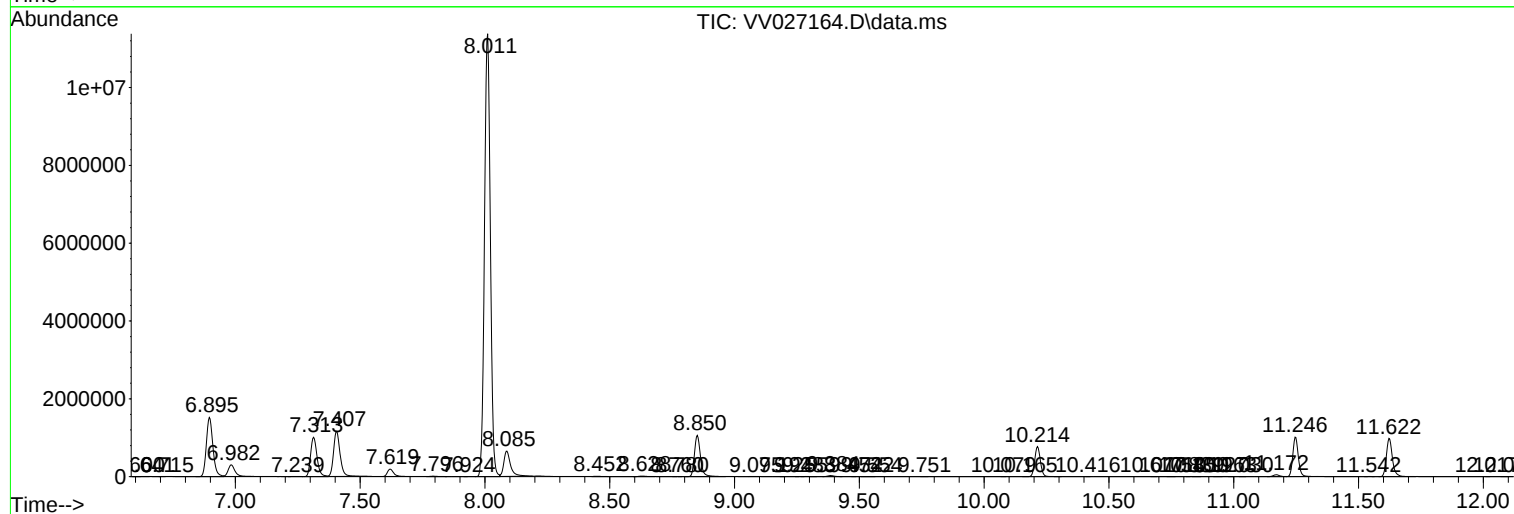
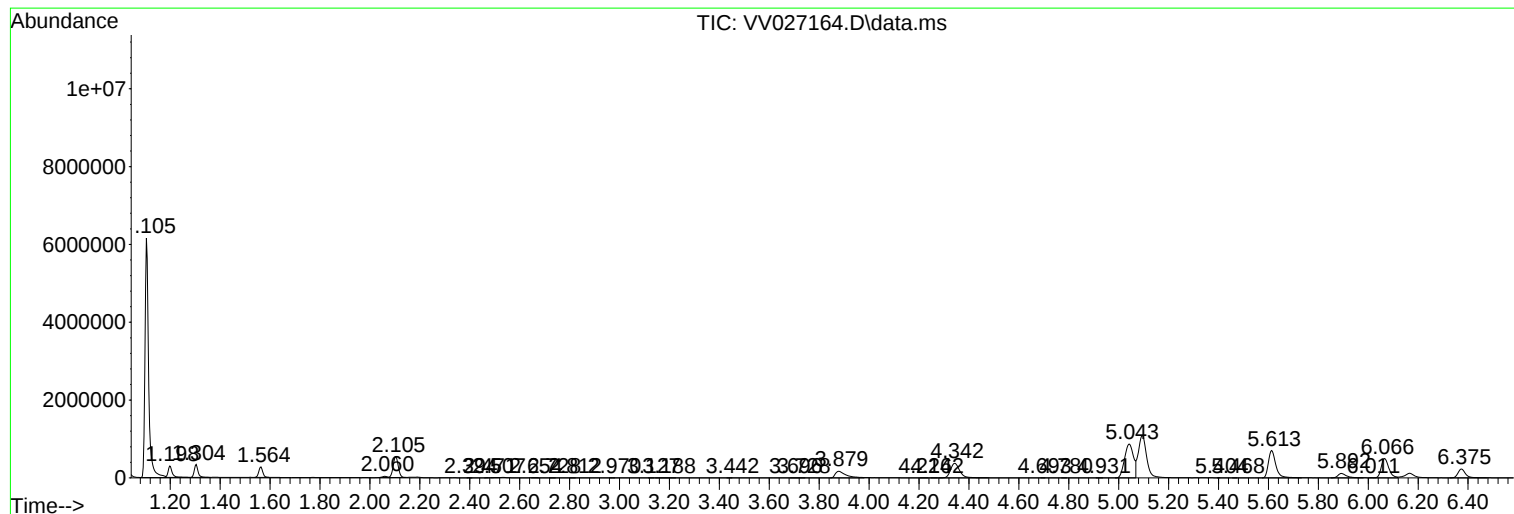
Sum of corrected areas: 48824590

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF03DL

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



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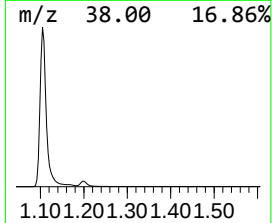
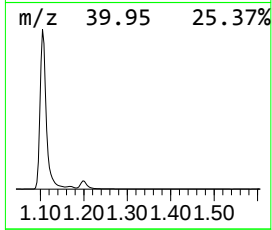
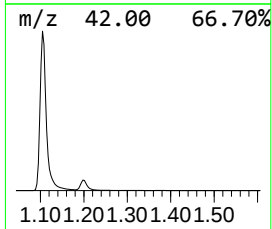
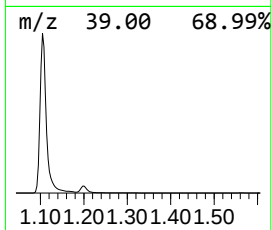
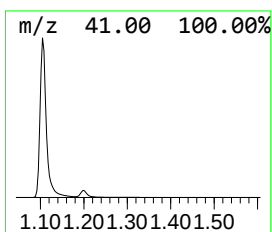
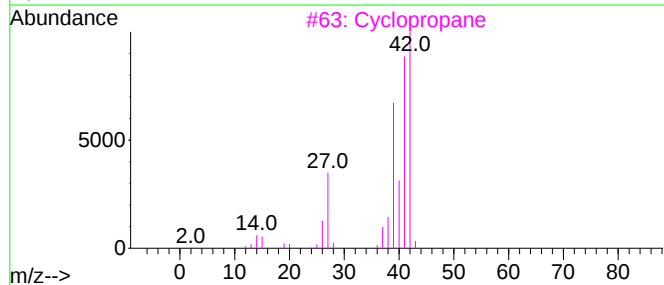
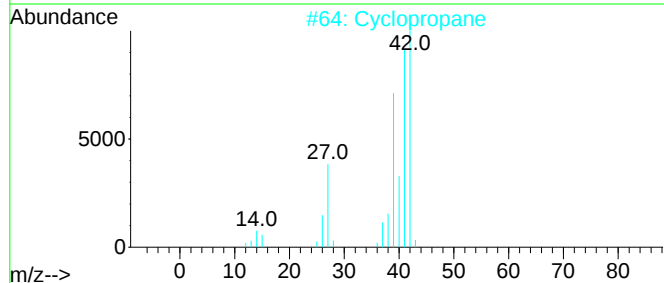
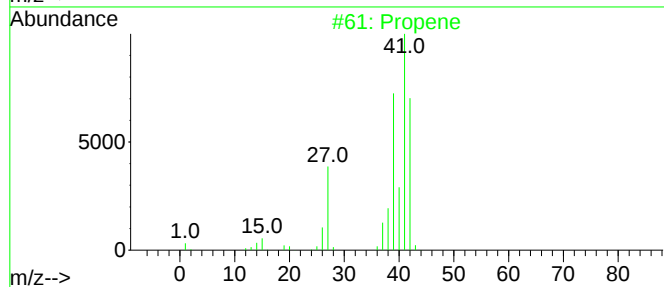
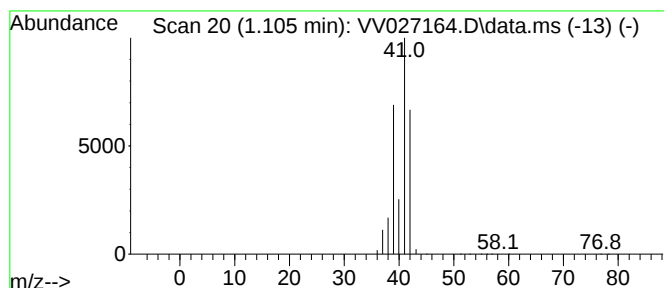
Instrument :
MSVOA_V
ClientSampleId :
EXF03DL

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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.105	212.91 ug/L	6176610	1,4-Difluorobenzene	5.613	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Cyclopropane	42	C3H6	000075-19-4	86
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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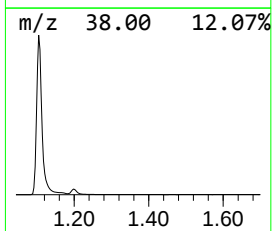
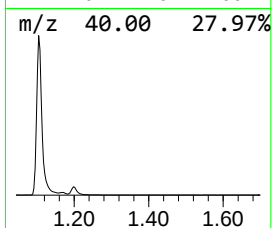
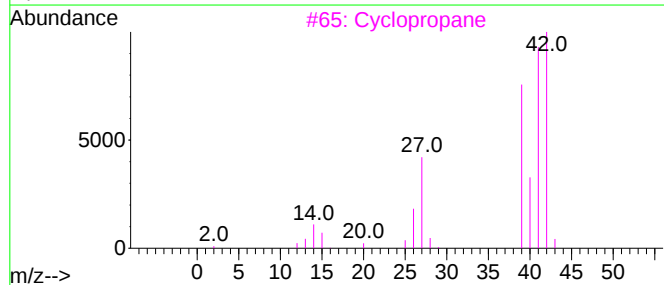
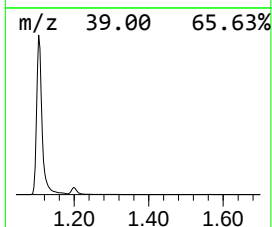
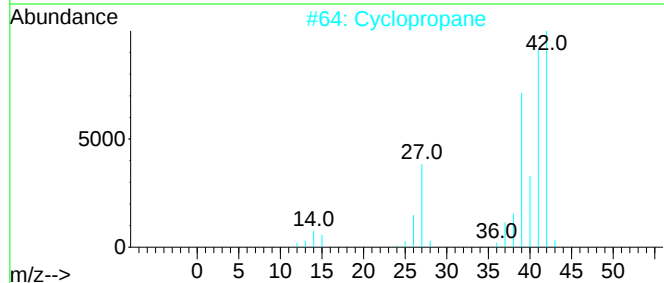
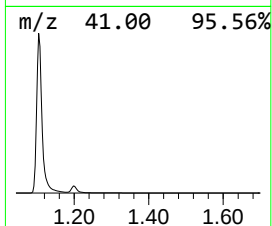
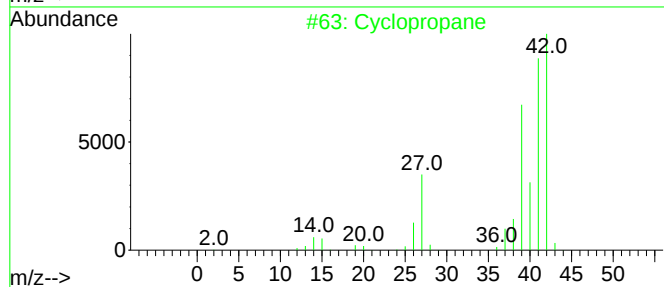
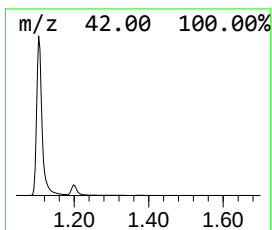
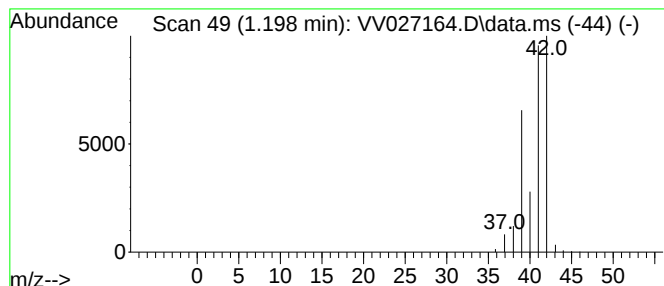
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080122WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic1.198 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.198	11.68 ug/L	338901	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane	42	C3H6	000075-19-4	90
2			Cyclopropane	42	C3H6	000075-19-4	86
3			Cyclopropane	42	C3H6	000075-19-4	72
4			Propene	42	C3H6	000115-07-1	9
5			Propene	42	C3H6	000115-07-1	4



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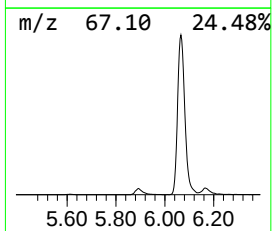
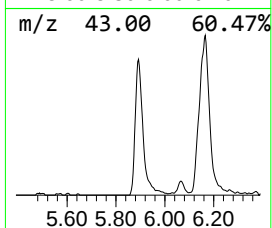
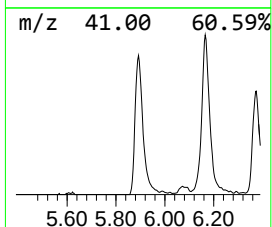
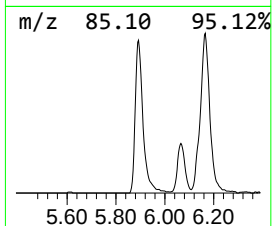
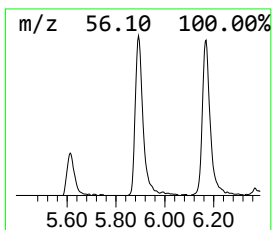
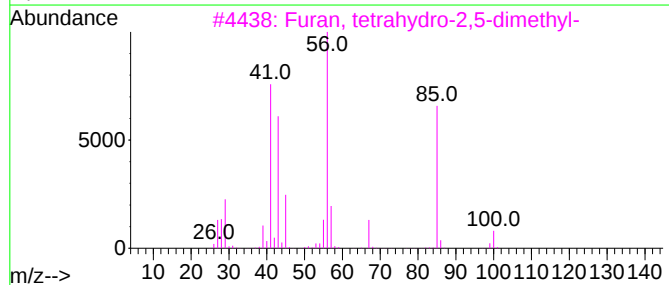
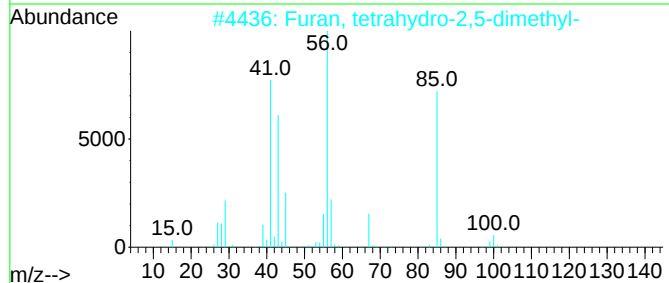
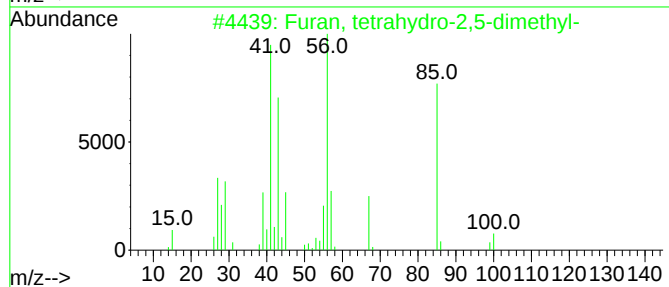
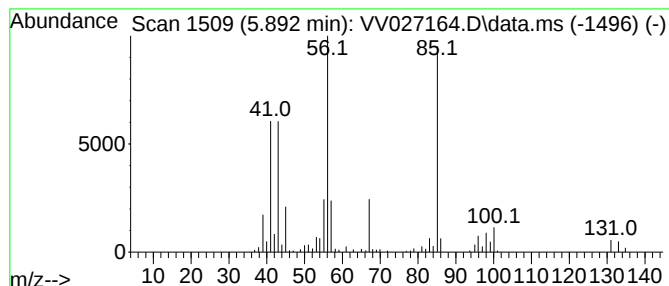
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080122WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Furan, tetrahydro-2,5-dimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.892	9.14 ug/L	265037	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	90
2			Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	90
3			Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	83
4			Furan, tetrahydro-2,5-dimethyl-,...	100	C6H12O	038484-59-2	72
5			Furan, tetrahydro-2,5-dimethyl-,...	100	C6H12O	002144-41-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027164.D
Acq On : 02 Aug 2022 11:28
Operator : SY/MD
Sample : N3956-04DL 4X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF03DL

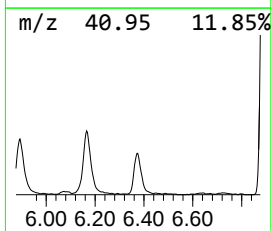
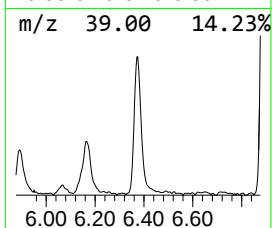
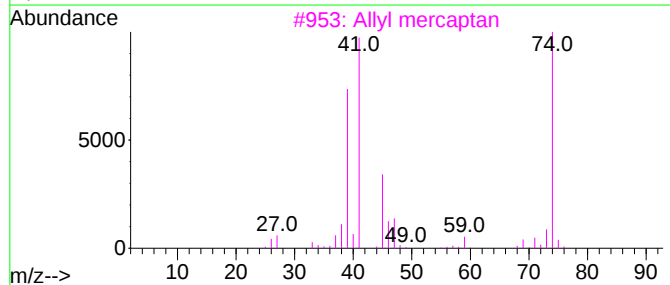
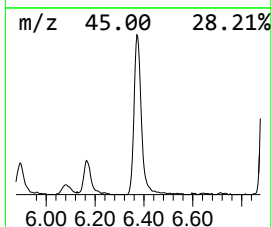
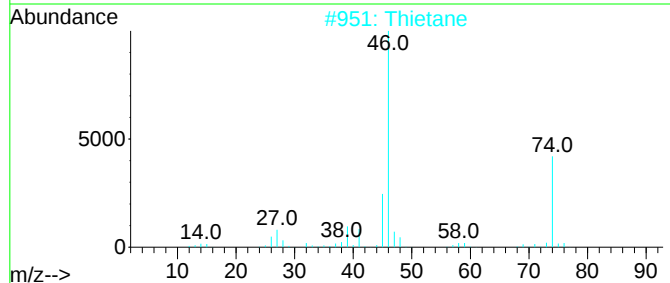
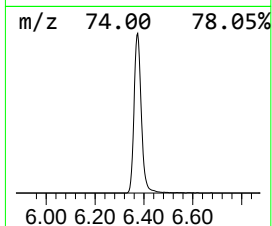
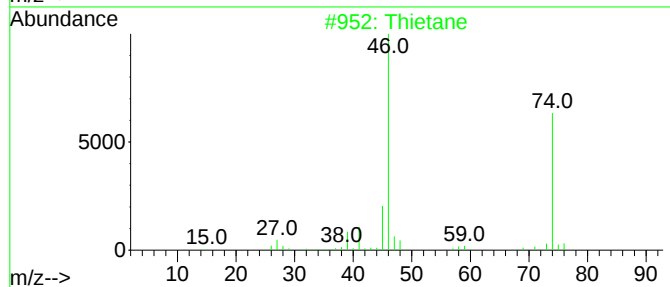
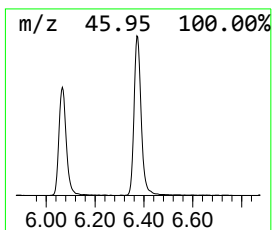
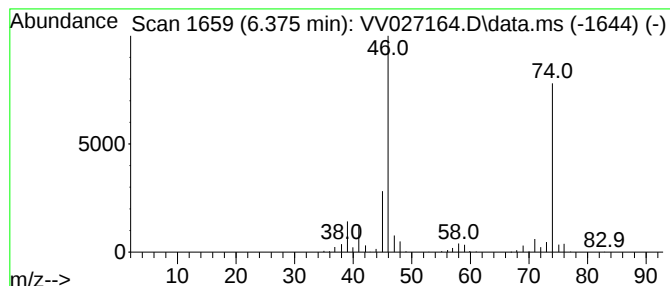
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Quant Title : VOC Analysis

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

Peak Number 4 Thietane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.375	16.21 ug/L	470134	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thietane	74	C3H6S	000287-27-4	91
2			Thietane	74	C3H6S	000287-27-4	91
3			Allyl mercaptan	74	C3H6S	000870-23-5	32
4			Thiirane, methyl-	74	C3H6S	001072-43-1	25
5			Thiirane, methyl-	74	C3H6S	001072-43-1	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027164.D
Acq On : 02 Aug 2022 11:28
Operator : SY/MD
Sample : N3956-04DL 4X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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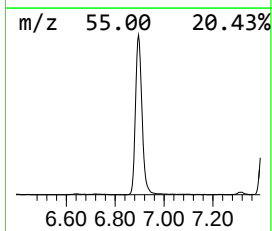
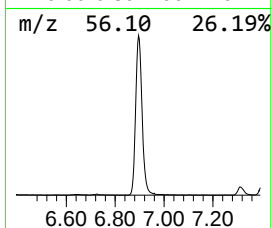
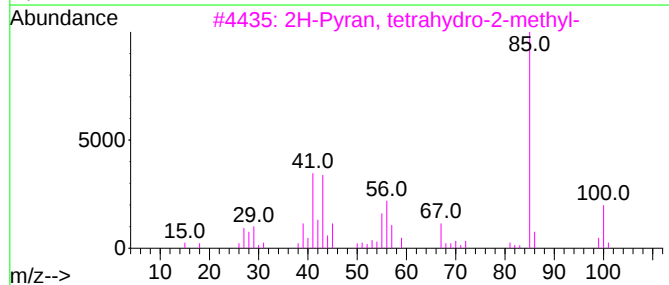
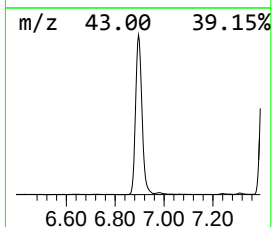
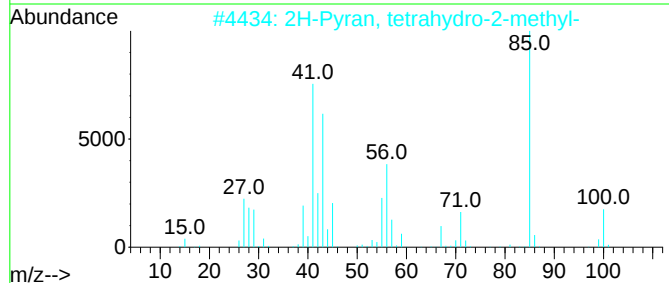
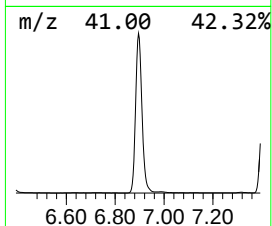
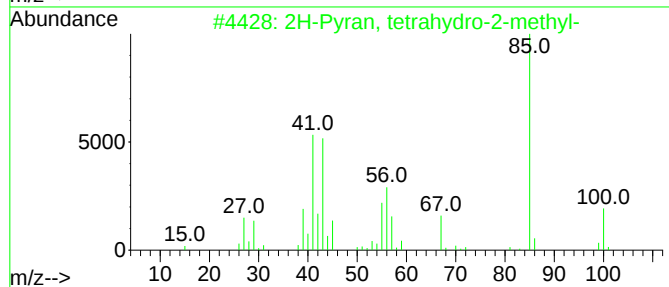
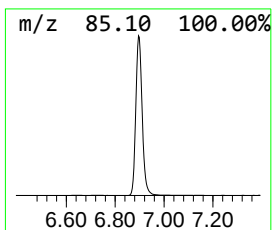
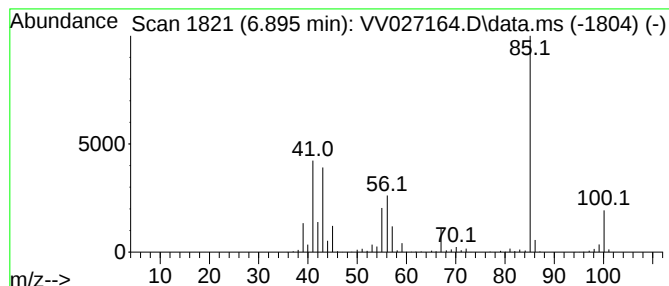
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Quant Title : VOC Analysis

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

Peak Number 5 2H-Pyran, tetrahydro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.895	95.61 ug/L	2773770	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	97		
2	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	91		
3	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	91		
4	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	83		
5	1-Methoxy-3-methyl-2-butene	100	C6H12O	022093-99-8	68		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027164.D
Acq On : 02 Aug 2022 11:28
Operator : SY/MD
Sample : N3956-04DL 4X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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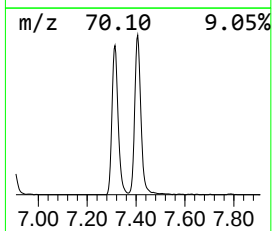
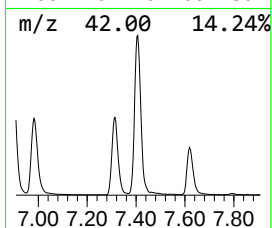
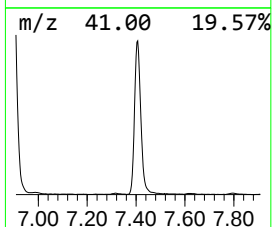
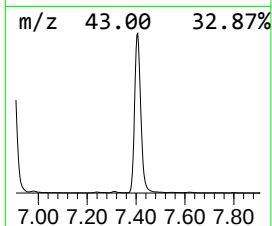
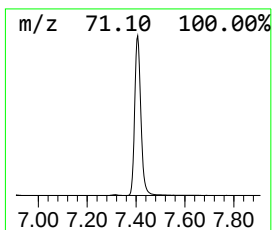
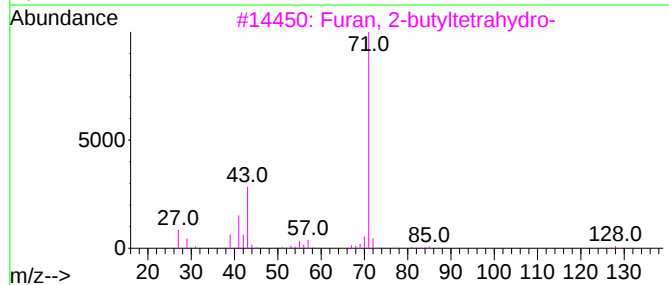
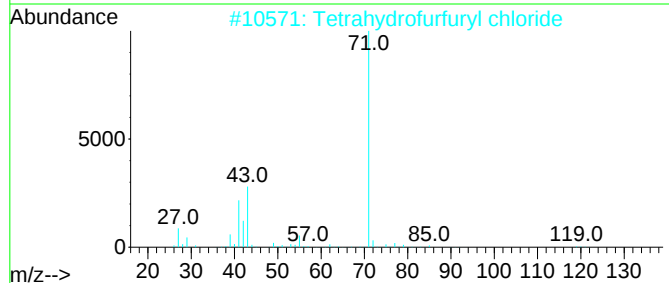
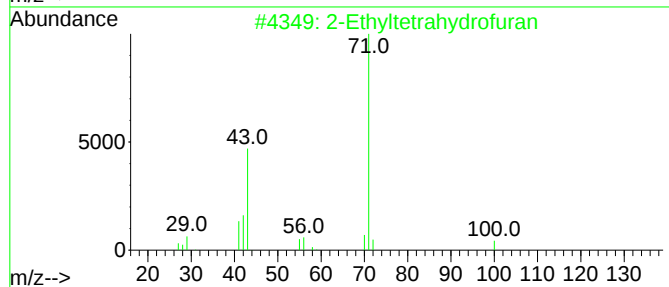
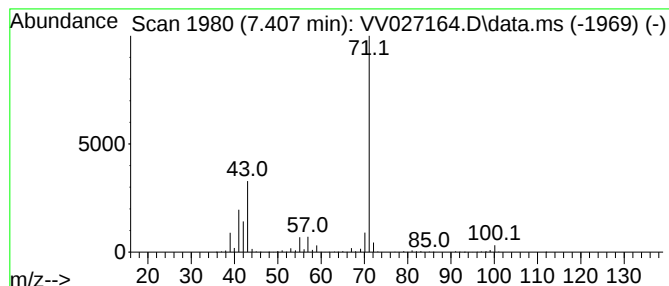
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Quant Title : VOC Analysis

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

Peak Number 7 2-Ethyltetrahydrofuran Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.407	58.95 ug/L	2089630	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyltetrahydrofuran			100	C6H12O	1010431-64-0	86
2	Tetrahydrofurfuryl chloride			120	C5H9ClO	003003-84-7	64
3	Furan, 2-butyltetrahydro-			128	C8H16O	001004-29-1	64
4	Butanoic acid, 2-propenyl ester			128	C7H12O2	002051-78-7	56
5	Tetrahydrofurfuryl chloride			120	C5H9ClO	003003-84-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027164.D
Acq On : 02 Aug 2022 11:28
Operator : SY/MD
Sample : N3956-04DL 4X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF03DL

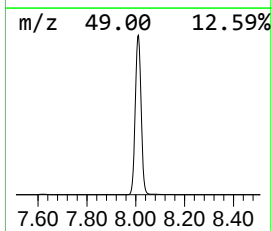
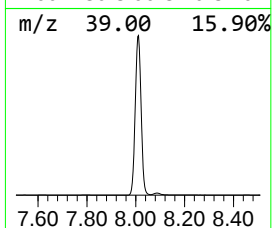
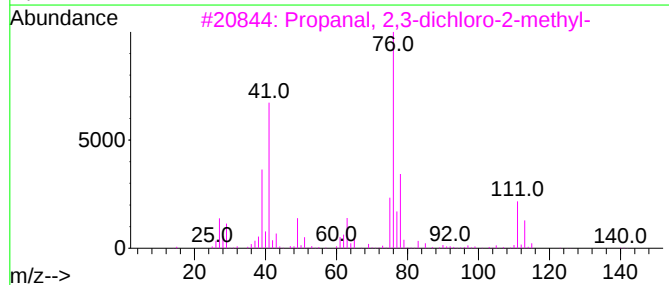
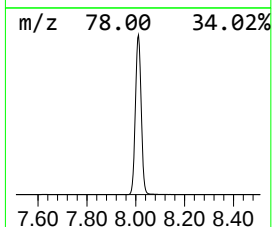
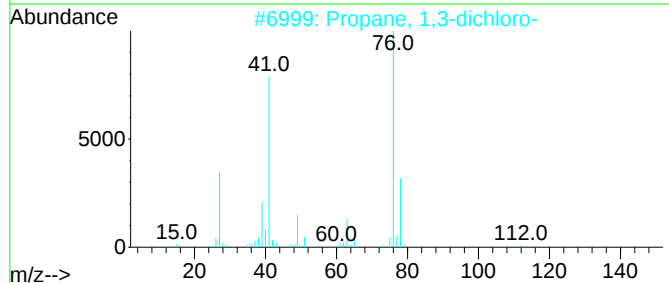
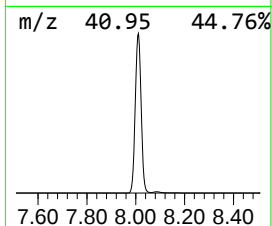
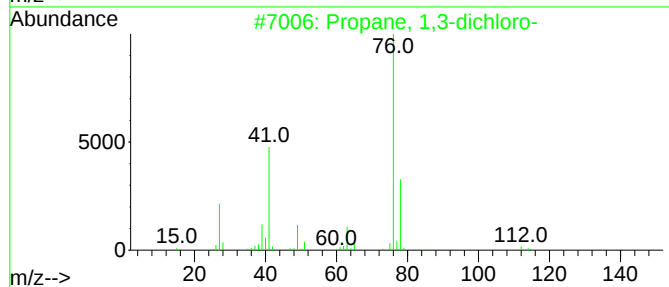
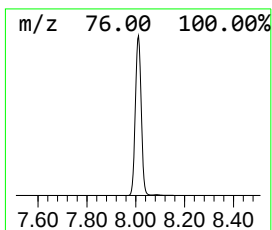
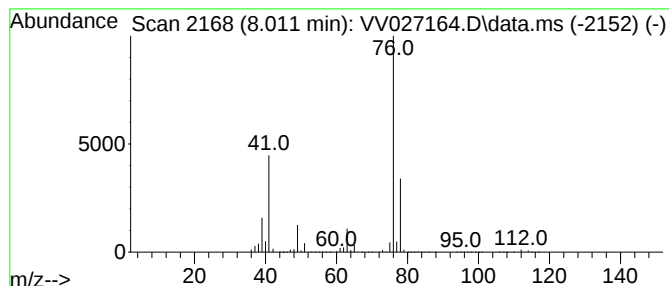
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Quant Title : VOC Analysis

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

Peak Number 8 Propane, 1,3-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.011	530.78 ug/L	18816100	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,3-dichloro-		112	C3H6Cl2	000142-28-9	94	
2	Propane, 1,3-dichloro-		112	C3H6Cl2	000142-28-9	90	
3	Propanal, 2,3-dichloro-2-methyl-		140	C4H6Cl2O	010141-22-7	74	
4	Propane, 1,3-dichloro-		112	C3H6Cl2	000142-28-9	15	
5	Thiourea		76	CH4N2S	000062-56-6	9	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027164.D
Acq On : 02 Aug 2022 11:28
Operator : SY/MD
Sample : N3956-04DL 4X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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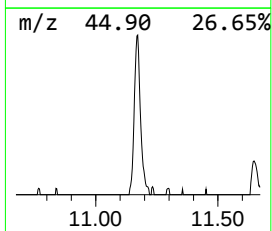
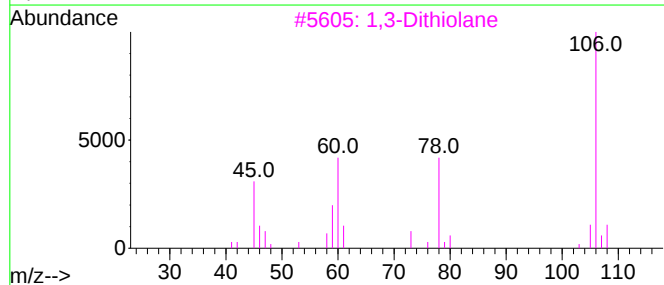
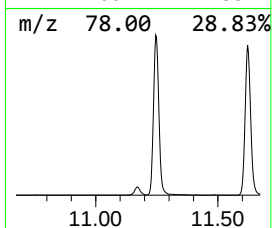
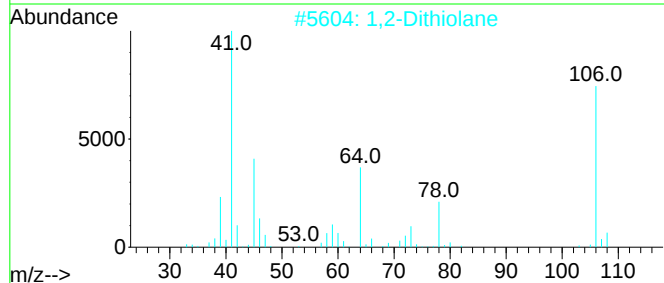
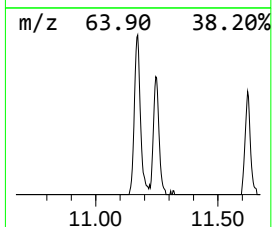
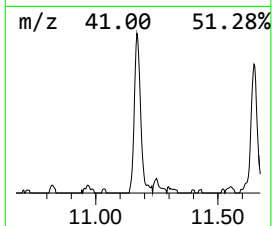
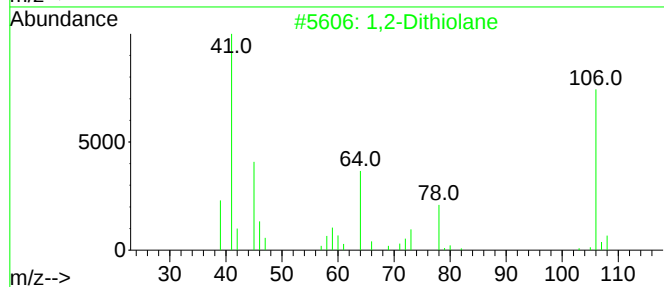
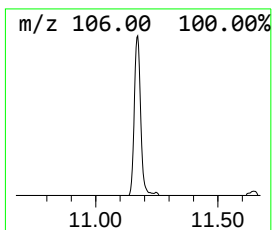
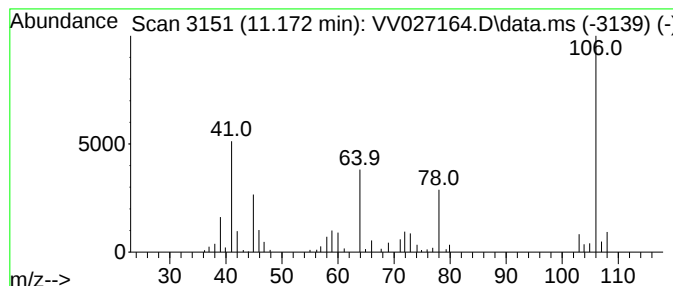
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Quant Title : VOC Analysis

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

Peak Number 9 1,2-Dithiolane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.172	2.64 ug/L	81608	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dithiolane	106	C3H6S2	000557-22-2	95
2			1,2-Dithiolane	106	C3H6S2	000557-22-2	94
3			1,3-Dithiolane	106	C3H6S2	004829-04-3	16
4			3-Mercaptopropionic acid	106	C3H6O2S	000107-96-0	10
5			Carbonothioic dihydrazide	106	CH6N4S	002231-57-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV080122\
Data File : VV027164.D
Acq On : 02 Aug 2022 11:28
Operator : SY/MD
Sample : N3956-04DL 4X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXF03DL

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	212.9	ug/L	6176610	1	5.613	1450550	50.0
(DEL) Alkane: C...	1.198	11.7	ug/L	338901	1	5.613	1450550	50.0
Furan, tetrahyd...	5.892	9.1	ug/L	265037	1	5.613	1450550	50.0
Thietane	6.375	16.2	ug/L	470134	1	5.613	1450550	50.0
2H-Pyran, tetra...	6.895	95.6	ug/L	2773770	1	5.613	1450550	50.0
2-Ethyltetrahyd...	7.407	59.0	ug/L	2089630	2	8.850	1772500	50.0
Propane, 1,3-di...	8.011	530.8	ug/L	18816100	2	8.850	1772500	50.0
1,2-Dithiolane	11.172	2.6	ug/L	81608	3	11.249	1546000	50.0