

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
 Data File : VX036939.D
 Acq On : 11 Aug 2023 14:27
 Operator : JC/MD
 Sample : 03960-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 230809051-02-VOA

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_X\Method\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX036939.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.057	150	159	169	rBV	47249	76701	3.75%	0.768%
2	2.380	204	212	228	rBV	259163	442500	21.61%	4.433%
3	2.532	228	237	249	rVV2	54568	111604	5.45%	1.118%
4	2.959	297	307	327	rBV	717961	1555391	75.95%	15.581%
5	3.849	446	453	468	rBV2	23486	62204	3.04%	0.623%
6	4.568	554	571	585	rBV2	634338	2048002	100.00%	20.515%
7	5.001	631	642	671	rBV2	182498	590305	28.82%	5.913%
8	5.391	694	706	719	rBV	86280	254703	12.44%	2.551%
9	5.556	721	733	750	rVB	136647	393015	19.19%	3.937%
10	5.958	788	799	808	rBV2	90534	243526	11.89%	2.439%
11	6.239	837	845	855	rVB3	11245	31818	1.55%	0.319%
12	6.641	900	911	921	rBV	7788	20960	1.02%	0.210%
13	6.763	921	931	946	rVV	230216	539521	26.34%	5.404%
14	7.208	996	1004	1025	rBV	74043	171315	8.36%	1.716%
15	8.415	1194	1202	1212	rBV	22720	42625	2.08%	0.427%
16	8.574	1220	1228	1234	rBV2	14169	26597	1.30%	0.266%
17	8.647	1234	1240	1247	rBV	475769	739654	36.12%	7.409%
18	8.720	1247	1252	1257	rVB2	17774	29025	1.42%	0.291%
19	10.055	1460	1471	1484	rBV	497257	706576	34.50%	7.078%
20	10.195	1490	1494	1500	rBV2	21524	33343	1.63%	0.334%
21	10.299	1507	1511	1519	rVB2	21649	34792	1.70%	0.349%
22	10.640	1563	1567	1570	rVV	20204	29977	1.46%	0.300%
23	11.079	1634	1639	1646	rBV	416173	529825	25.87%	5.307%
24	11.506	1704	1709	1714	rVB	21266	27674	1.35%	0.277%
25	11.884	1765	1771	1780	rVB3	16703	26826	1.31%	0.269%
26	12.018	1787	1793	1802	rBV	508621	666626	32.55%	6.678%
27	12.104	1802	1807	1811	rVV2	25831	36910	1.80%	0.370%
28	12.518	1872	1875	1882	rBV3	16429	26427	1.29%	0.265%
29	12.902	1927	1938	1943	rBV	107669	148883	7.27%	1.491%
30	12.963	1943	1948	1952	rVB3	13961	21874	1.07%	0.219%
31	13.164	1977	1981	1986	rBV2	17697	26900	1.31%	0.269%
32	13.475	2027	2032	2034	rBV3	22569	33196	1.62%	0.333%
33	13.512	2034	2038	2044	rVV	67485	91895	4.49%	0.921%
34	13.591	2044	2051	2057	rVV2	35643	57170	2.79%	0.573%
35	13.658	2057	2062	2070	rVV	21633	33640	1.64%	0.337%
36	13.774	2077	2081	2087	rVB	54460	70921	3.46%	0.710%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_X\Method\82X072123W.M
Title : SW846 8260

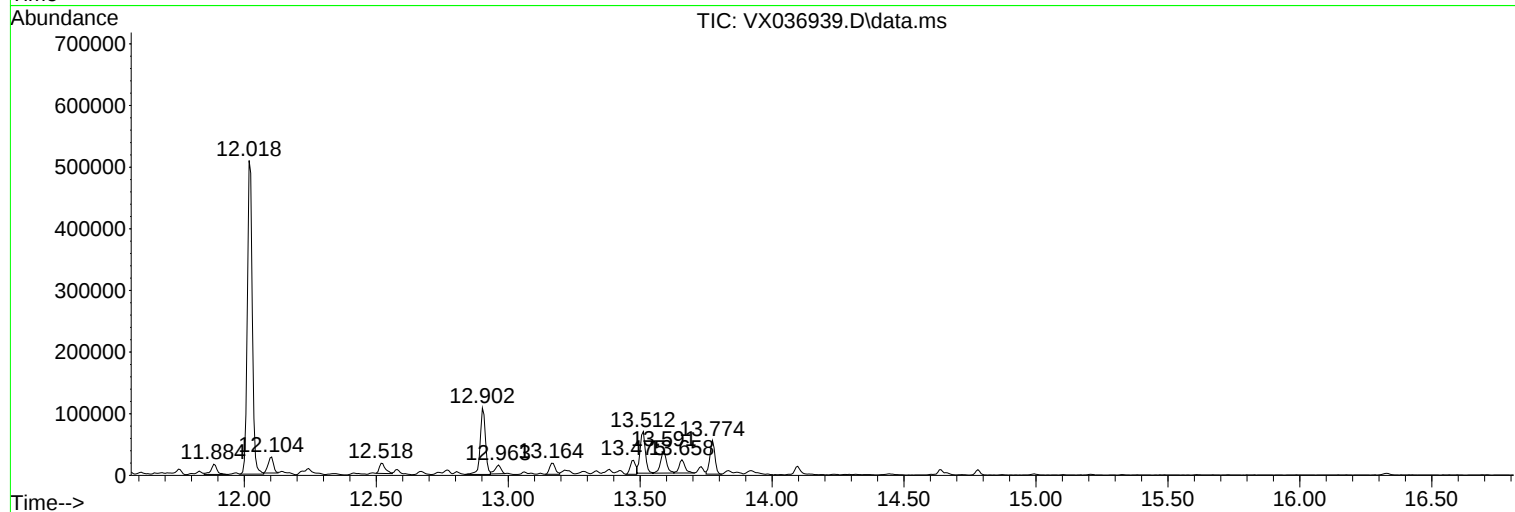
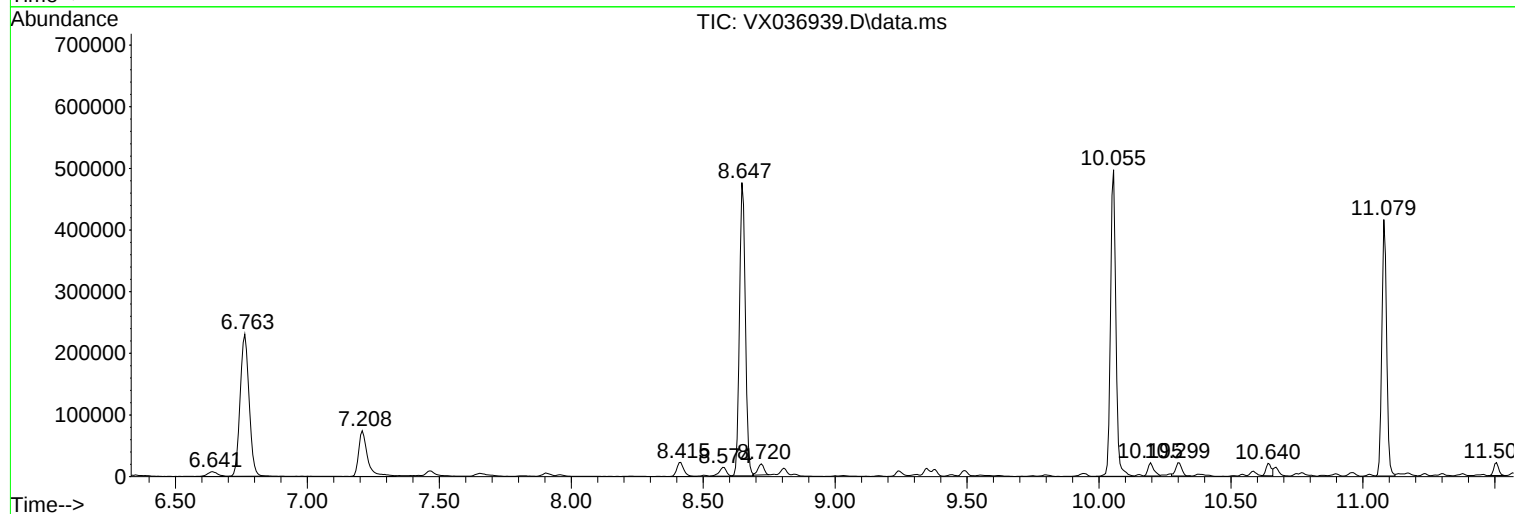
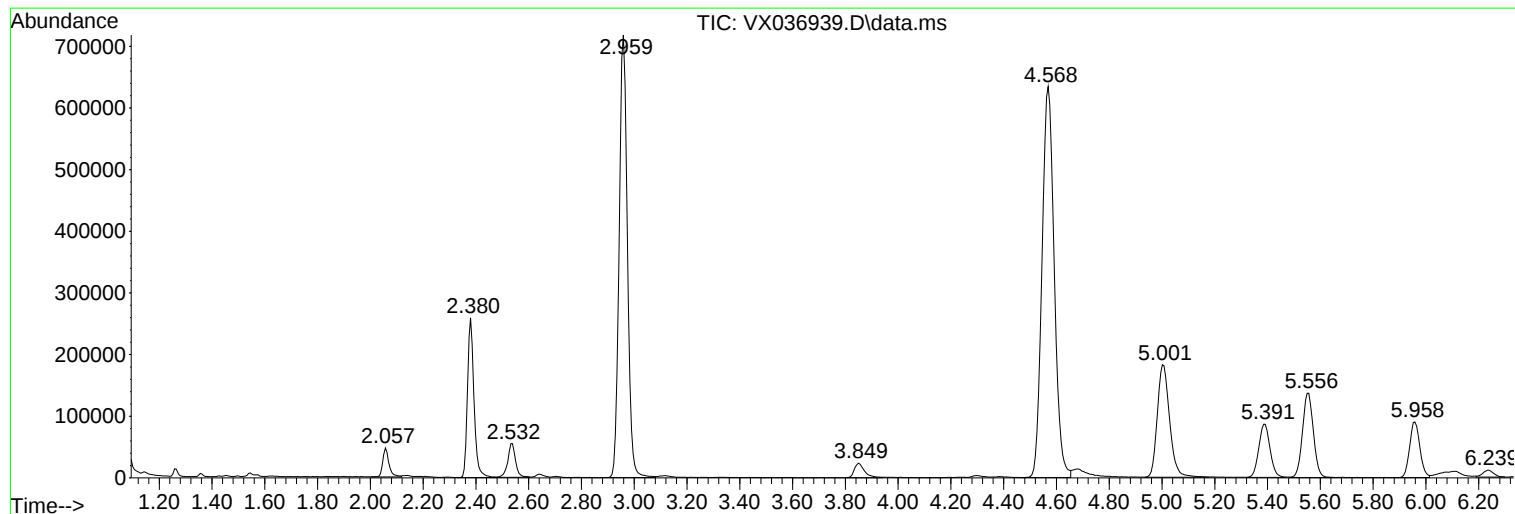
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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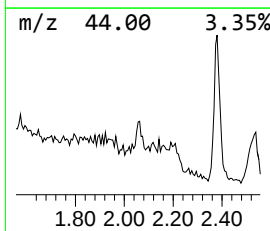
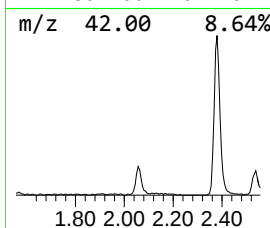
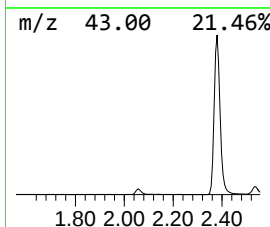
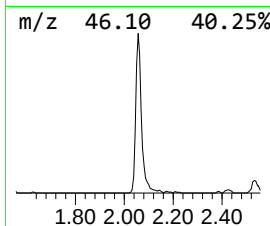
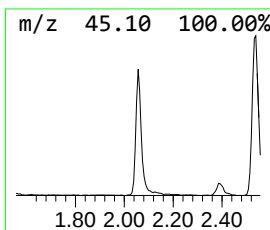
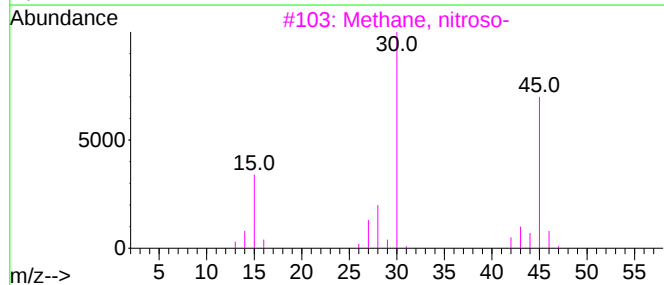
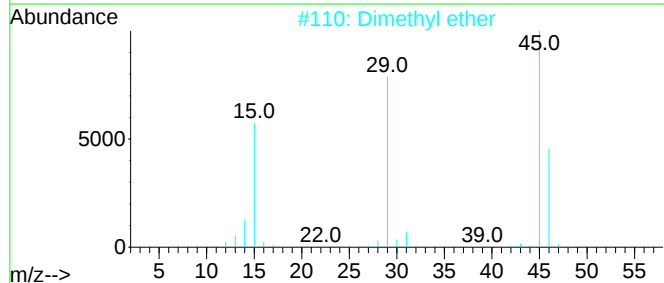
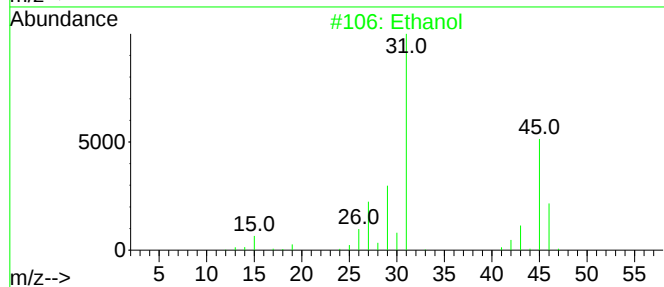
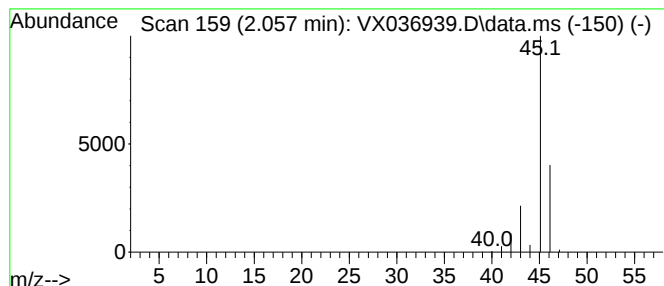
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	9.76 ug/l	76701	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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Instrument :
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230809051-02-VOA

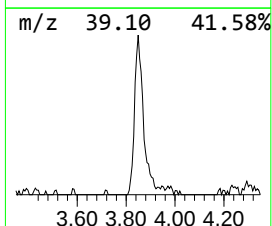
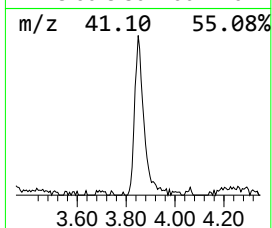
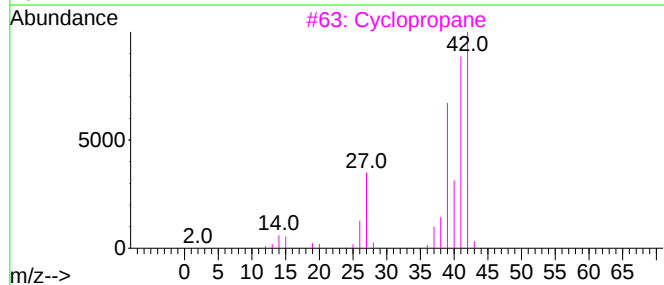
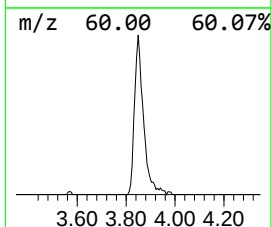
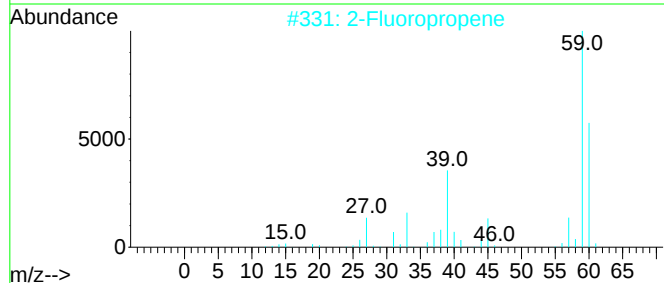
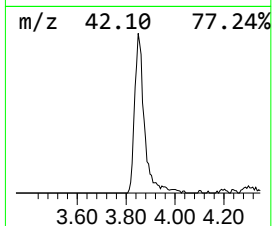
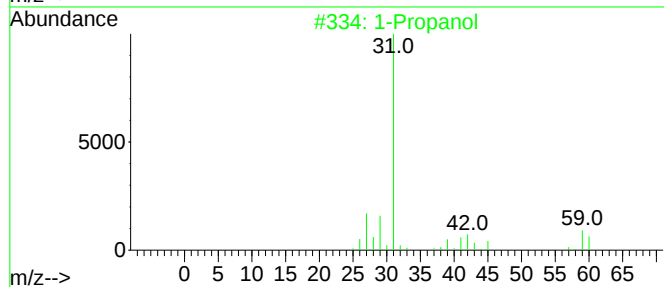
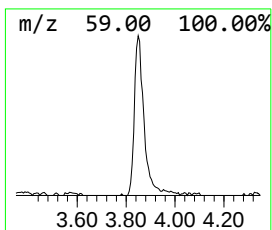
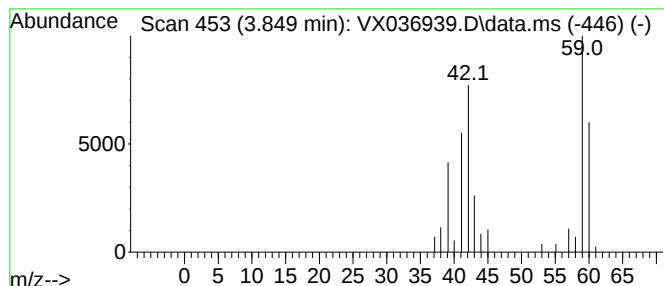
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.849	7.91 ug/l	62204	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	59
2	2-Fluoropropene			60	C3H5F	001184-60-7	58
3	Cyclopropane			42	C3H6	000075-19-4	35
4	Allyl fluoride			60	C3H5F	000818-92-8	32
5	Propene			42	C3H6	000115-07-1	9



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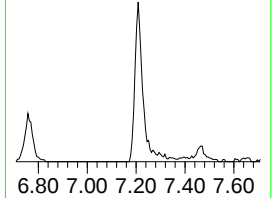
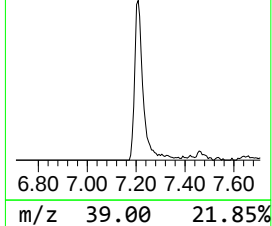
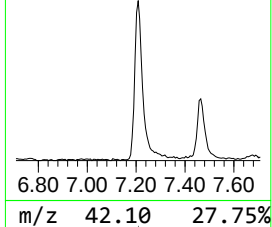
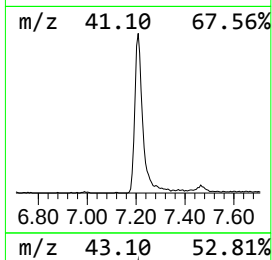
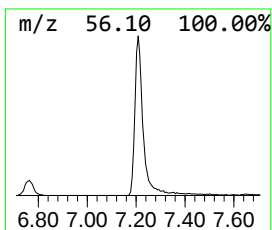
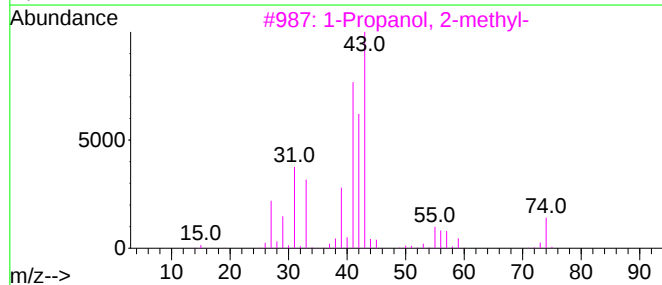
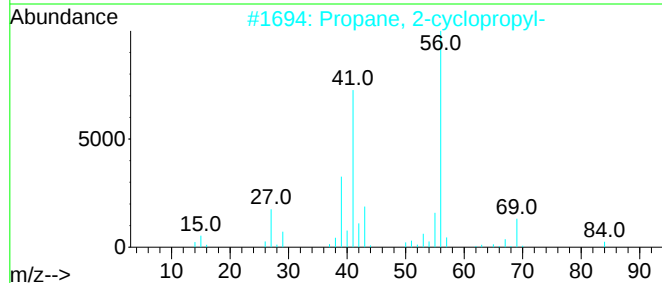
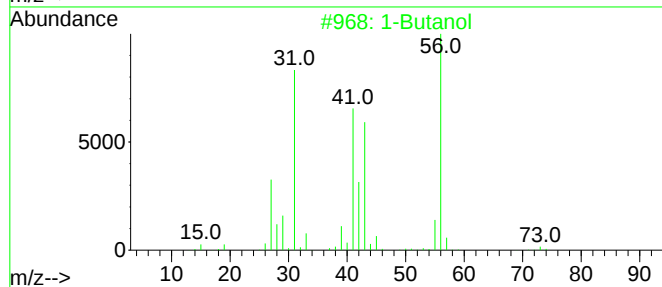
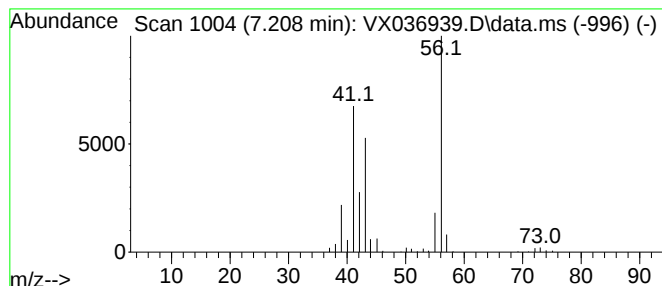
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	15.88 ug/l	171315	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	90
2	Propane, 2-cyclopropyl-		84	C6H12	003638-35-5	36
3	1-Propanol, 2-methyl-		74	C4H10O	000078-83-1	9
4	Formic acid, butyl ester		102	C5H10O2	000592-84-7	9
5	Oxetane, 2,3,4-trimethyl-, (2.al...		100	C6H12O	032347-12-9	9



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MSVOA_X
ClientSampleId :
230809051-02-VOA

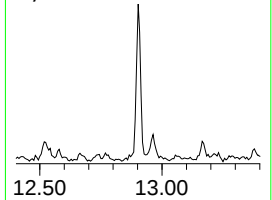
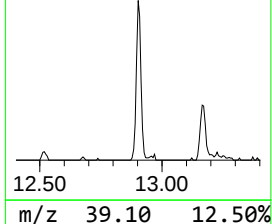
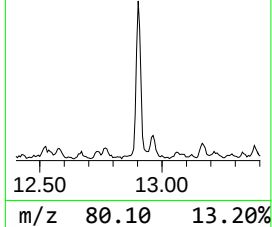
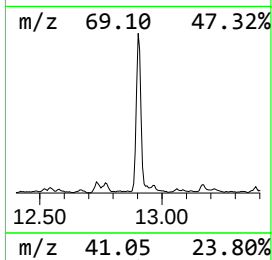
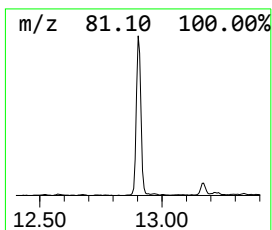
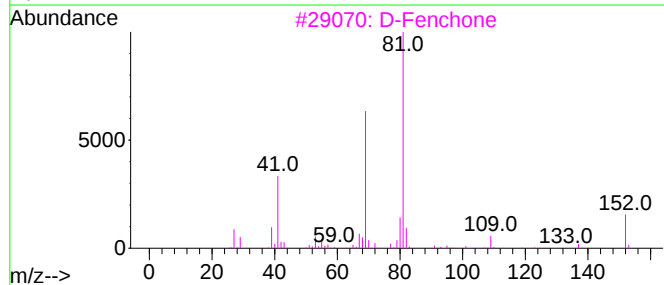
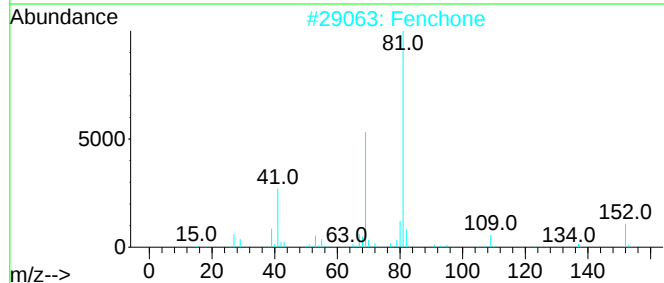
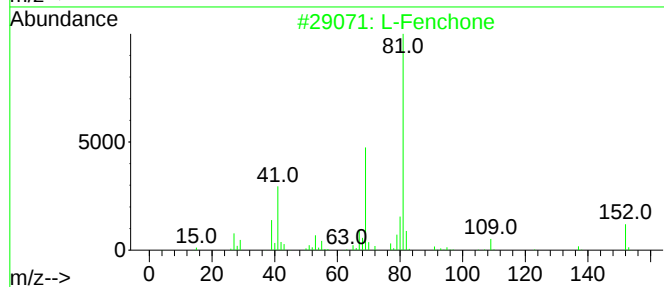
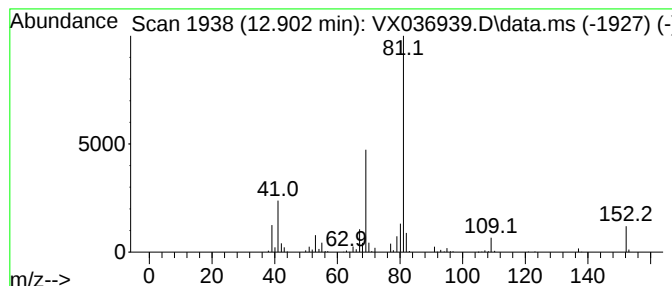
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Quant Title : SW846 8260

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

Peak Number 4 L-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	11.17 ug/l	148883	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		L-Fenchone	152	C10H16O	007787-20-4	95
2		Fenchone	152	C10H16O	001195-79-5	95
3		D-Fenchone	152	C10H16O	004695-62-9	94
4		2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	64
5		2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	53



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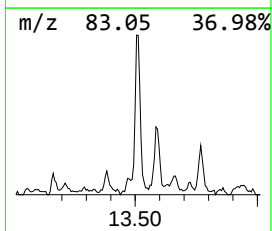
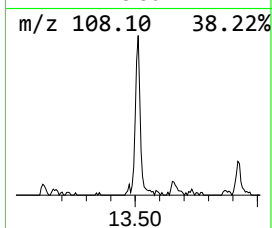
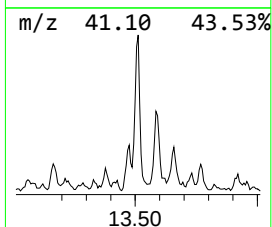
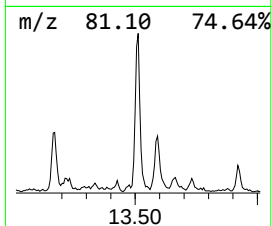
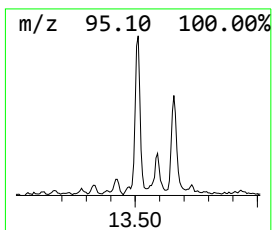
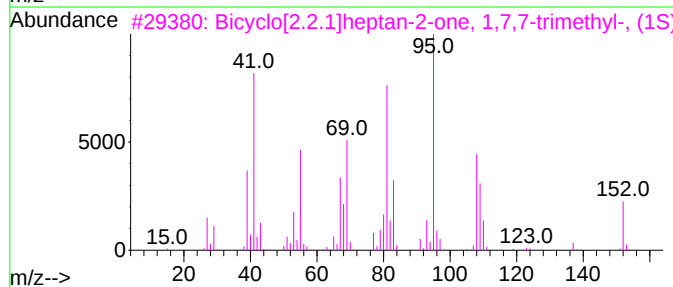
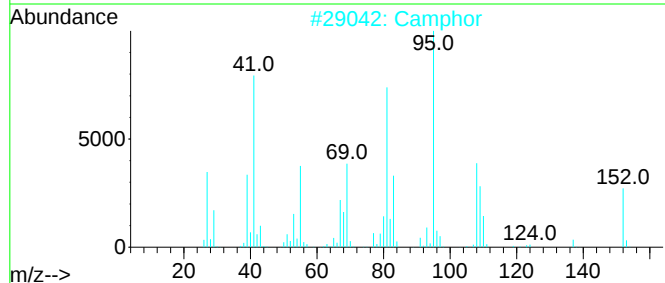
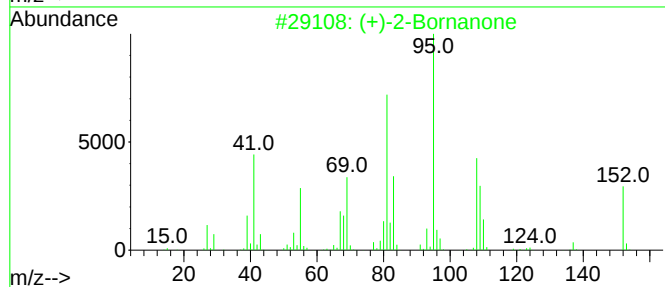
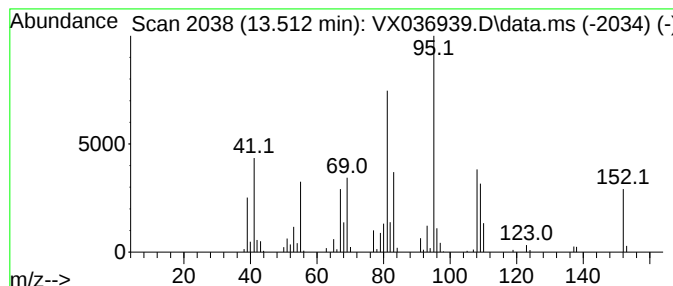
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TIC Integration Parameters: LSCINT.P

Peak Number 5 (+)-2-Bornanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.512	6.89 ug/l	91895	1,4-Dichlorobenzene-d4	12.024	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
2	Camphor	152	C10H16O	000076-22-2	97
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	46
5	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081123\
Data File : VX036939.D
Acq On : 11 Aug 2023 14:27
Operator : JC/MD
Sample : 03960-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230809051-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.057	9.8	ug/l	76701	1	5.556	393015	50.0
1-Propanol	3.849	7.9	ug/l	62204	1	5.556	393015	50.0
1-Butanol	7.208	15.9	ug/l	171315	2	6.763	539521	50.0
L-Fenchone	12.902	11.2	ug/l	148883	4	12.024	666626	50.0
(+)-2-Bornanone	13.512	6.9	ug/l	91895	4	12.024	666626	50.0