

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081023\
 Data File : VX036910.D
 Acq On : 10 Aug 2023 14:07
 Operator : JC/MD
 Sample : 03960-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 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: VX036910.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	39	rVB	13217	20316	1.09%	0.226%
2	2.056	154	159	169	rBV	37697	63170	3.40%	0.702%
3	2.379	206	212	229	rBV	216851	365203	19.66%	4.058%
4	2.538	229	238	245	rBV2	49549	95452	5.14%	1.061%
5	2.959	297	307	325	rBV	668495	1444907	77.78%	16.054%
6	3.849	446	453	466	rBV2	19944	53722	2.89%	0.597%
7	4.568	554	571	585	rBV2	566611	1857646	100.00%	20.639%
8	5.007	632	643	666	rBV2	164173	522426	28.12%	5.804%
9	5.391	695	706	719	rBV	78810	228848	12.32%	2.543%
10	5.556	721	733	747	rVB	126943	359224	19.34%	3.991%
11	5.958	787	799	809	rBV	83939	220159	11.85%	2.446%
12	6.239	835	845	856	rVB2	11223	31246	1.68%	0.347%
13	6.763	921	931	947	rVV	207703	491532	26.46%	5.461%
14	7.208	998	1004	1024	rBV	63527	151639	8.16%	1.685%
15	8.415	1195	1202	1210	rBV	20542	38493	2.07%	0.428%
16	8.574	1221	1228	1234	rBV2	13014	24117	1.30%	0.268%
17	8.647	1234	1240	1248	rBV	424279	674695	36.32%	7.496%
18	8.720	1248	1252	1258	rVV2	15603	24404	1.31%	0.271%
19	10.055	1461	1471	1484	rBV	454791	629094	33.87%	6.990%
20	10.195	1490	1494	1501	rBV2	18194	28444	1.53%	0.316%
21	10.305	1508	1512	1519	rVB	19478	30725	1.65%	0.341%
22	10.640	1563	1567	1570	rVV2	17433	25575	1.38%	0.284%
23	11.079	1634	1639	1646	rBV	357403	462952	24.92%	5.144%
24	11.506	1704	1709	1715	rVB	21017	28644	1.54%	0.318%
25	11.884	1765	1771	1780	rVB4	16762	27323	1.47%	0.304%
26	12.024	1788	1794	1802	rVV	422355	569052	30.63%	6.322%
27	12.103	1802	1807	1811	rVB2	21701	29888	1.61%	0.332%
28	12.524	1872	1876	1882	rBV2	15765	25474	1.37%	0.283%
29	12.902	1927	1938	1943	rBV	92180	131299	7.07%	1.459%
30	12.963	1943	1948	1952	rVB4	13132	20127	1.08%	0.224%
31	13.164	1977	1981	1986	rBV	17876	27439	1.48%	0.305%
32	13.475	2027	2032	2034	rBV2	21070	29768	1.60%	0.331%
33	13.512	2034	2038	2043	rVV	60091	84896	4.57%	0.943%
34	13.591	2044	2051	2058	rVV3	36480	61902	3.33%	0.688%
35	13.658	2058	2062	2070	rVV	20862	33657	1.81%	0.374%
36	13.774	2077	2081	2086	rVB	48698	65541	3.53%	0.728%

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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

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37	14.097	2125	2134	2141	rBV3	13840	21452	1.15%	0.238%
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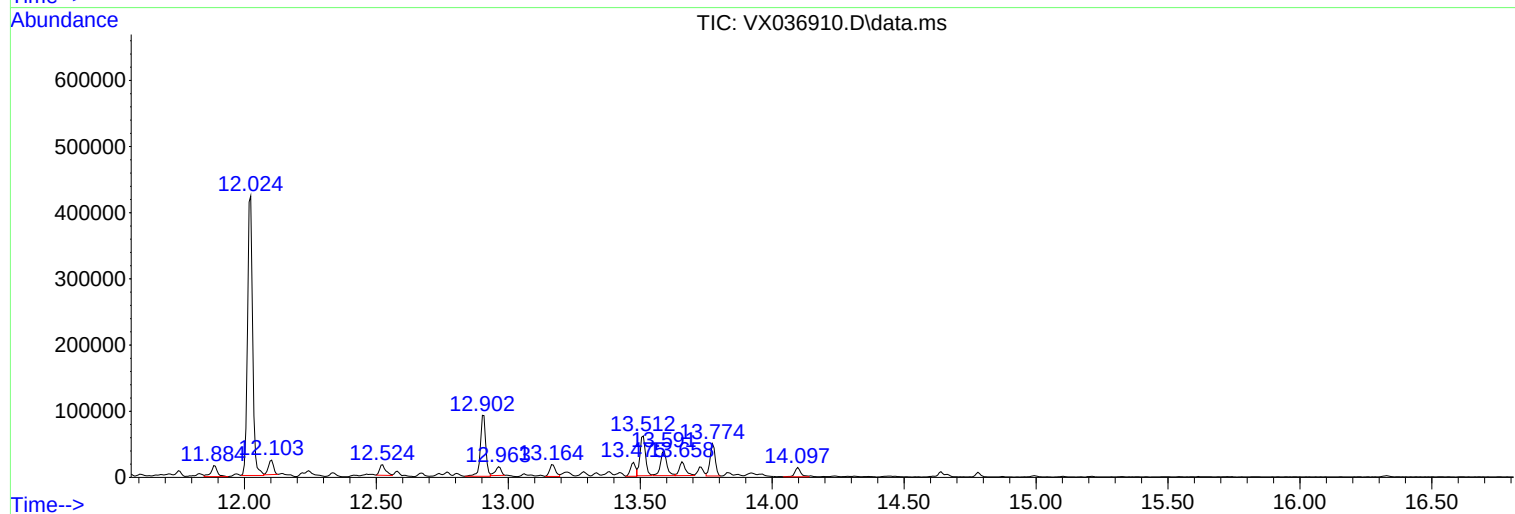
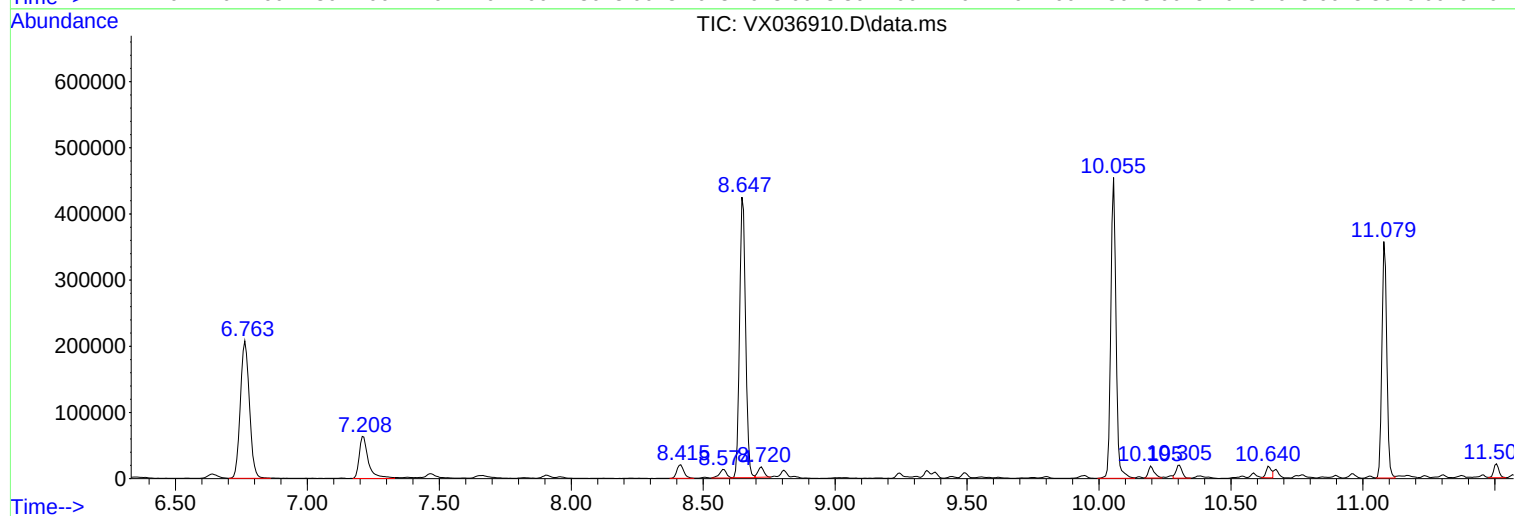
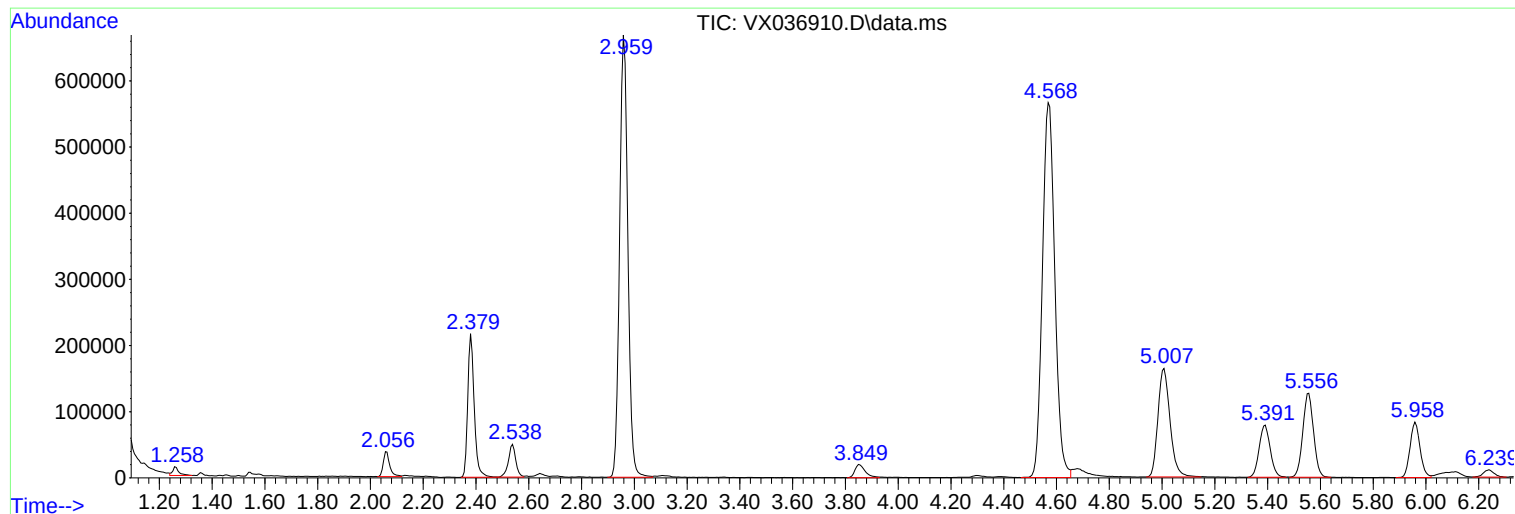
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Quant Title : SW846 8260

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



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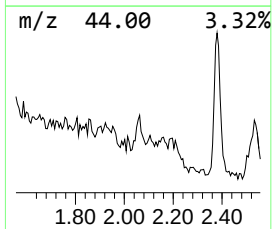
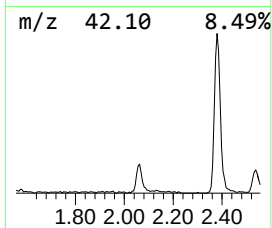
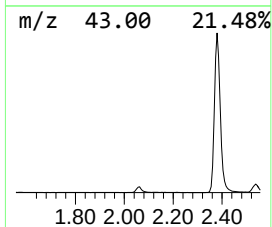
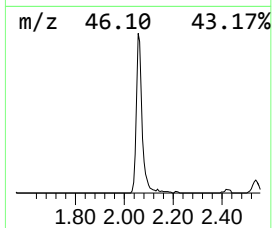
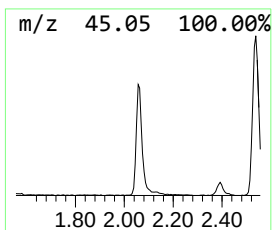
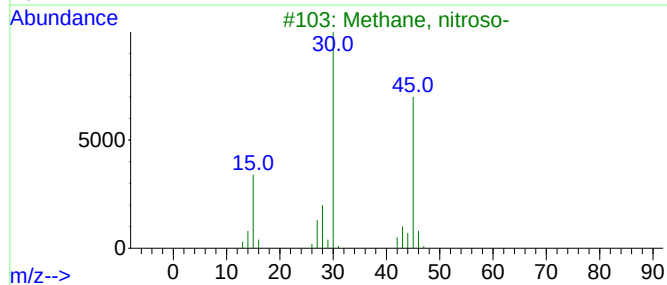
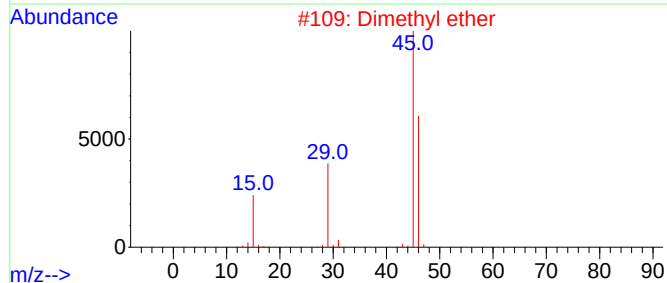
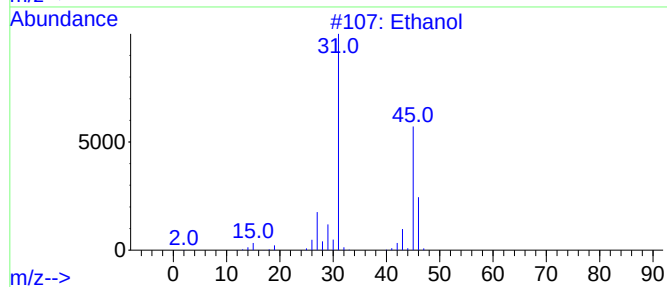
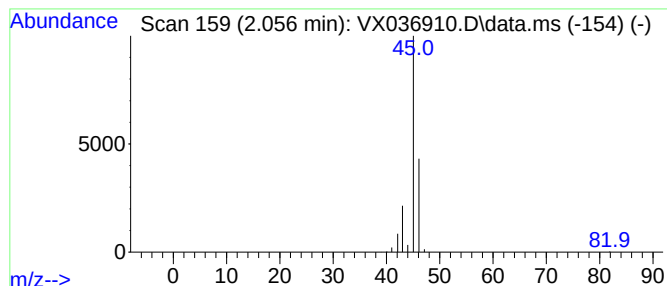
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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.
2.056	8.79 ug/l	63170	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			Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4



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ALS Vial : 10 Sample Multiplier: 1

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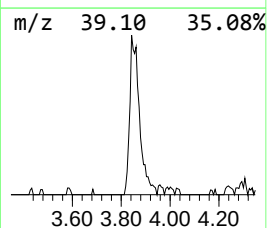
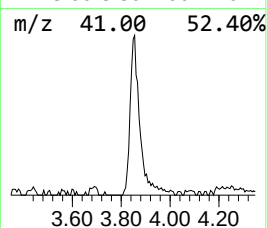
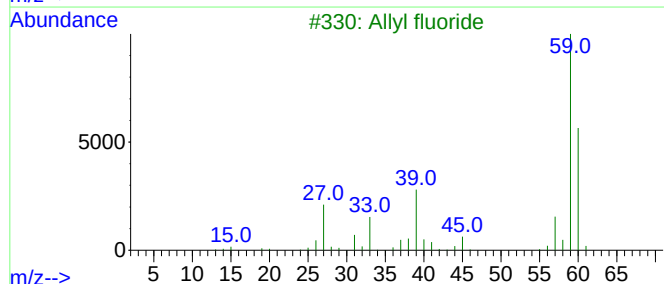
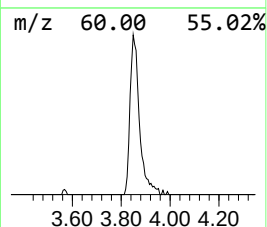
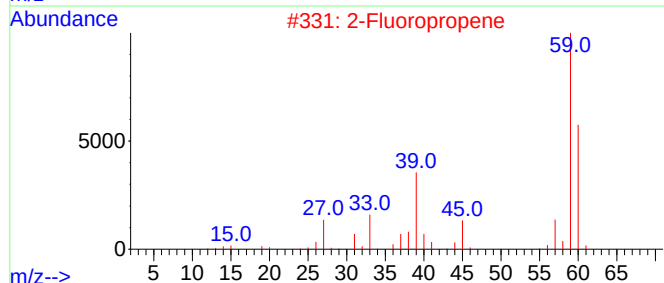
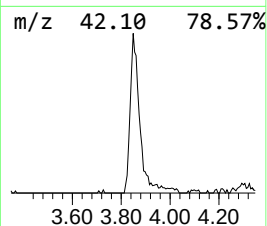
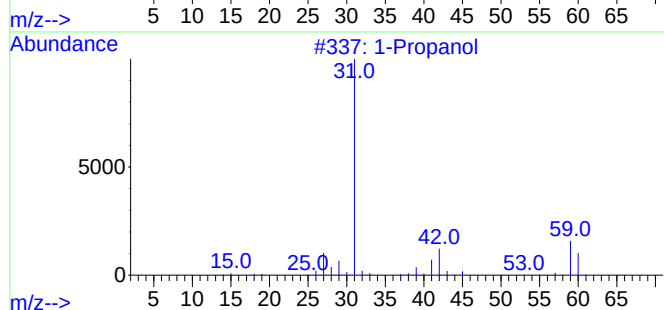
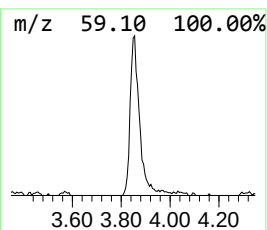
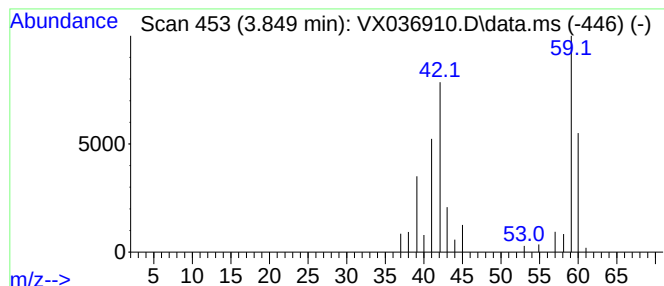
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.849	7.48 ug/l	53722	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	78
2	2-Fluoropropene			60	C3H5F	001184-60-7	49
3	Allyl fluoride			60	C3H5F	000818-92-8	47
4	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	9
5	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	9



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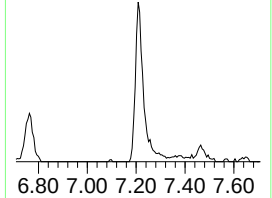
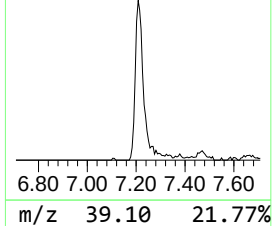
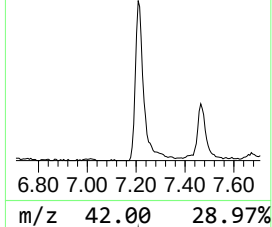
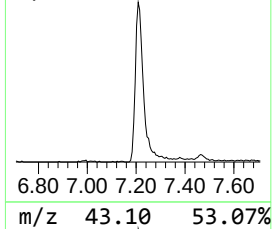
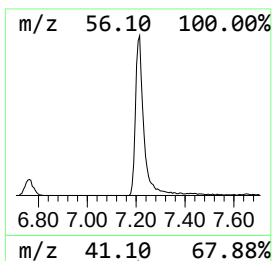
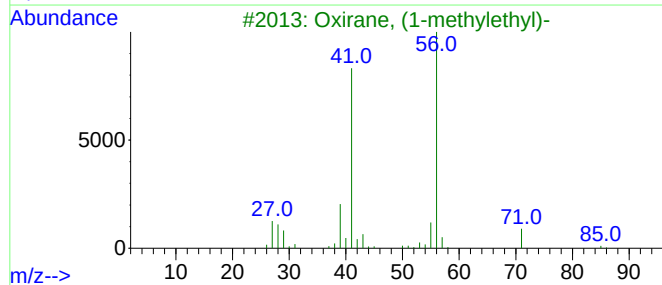
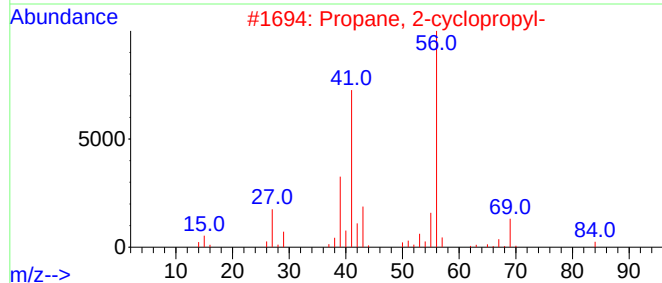
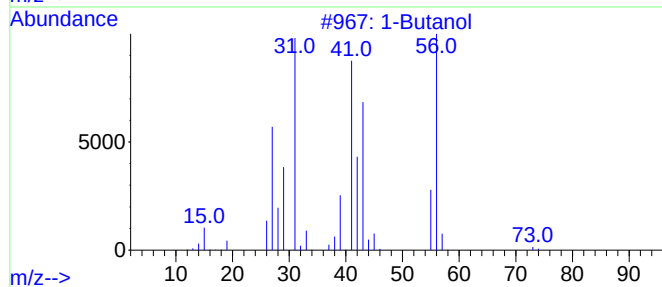
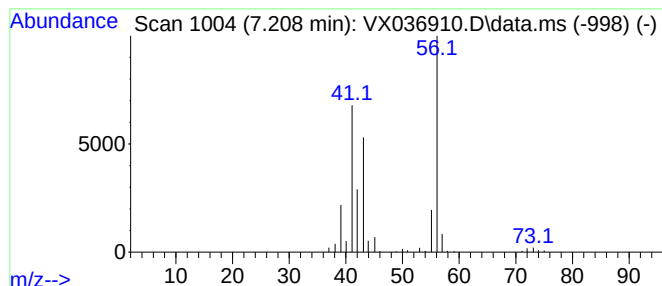
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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	15.43 ug/l	151639	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	91
2	Propane, 2-cyclopropyl-			84	C6H12	003638-35-5	38
3	Oxirane, (1-methylethyl)-			86	C5H10O	001438-14-8	9
4	Formic acid, butyl ester			102	C5H10O2	000592-84-7	9
5	2-Butene, (Z)-			56	C4H8	000590-18-1	9



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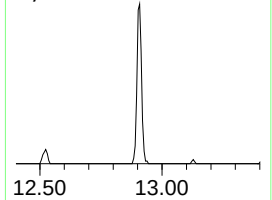
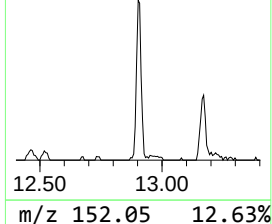
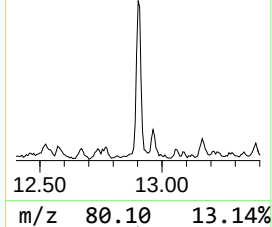
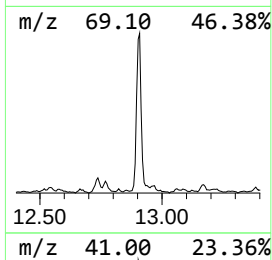
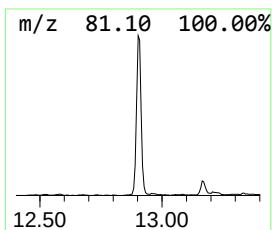
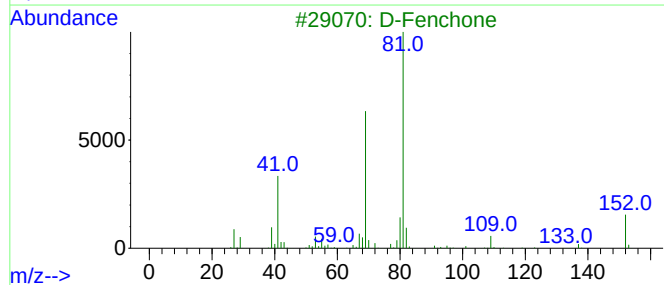
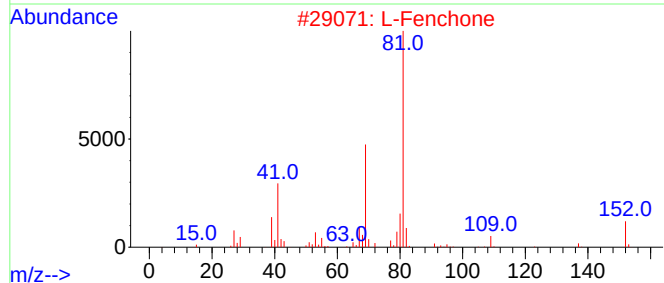
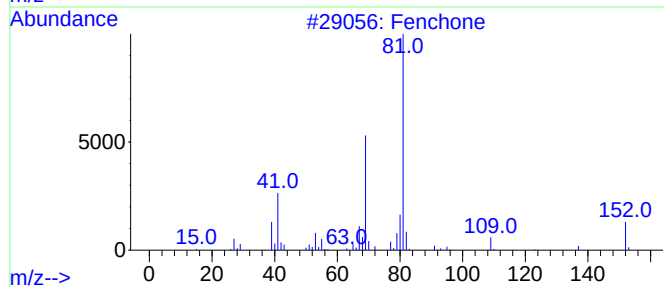
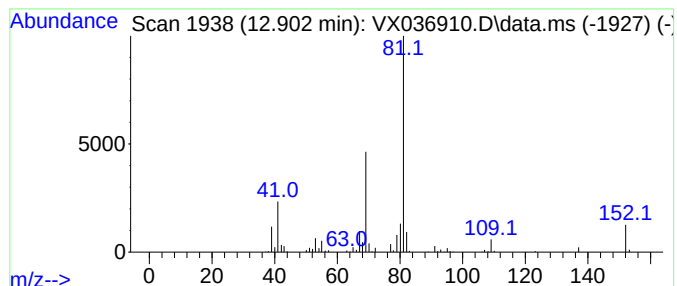
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	11.54 ug/l	131299	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	95
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	45
5			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42



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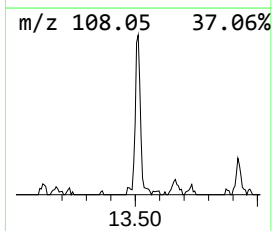
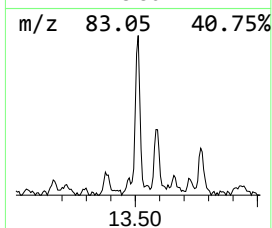
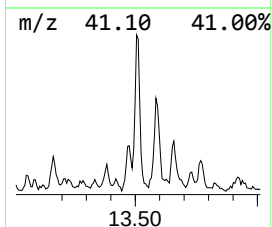
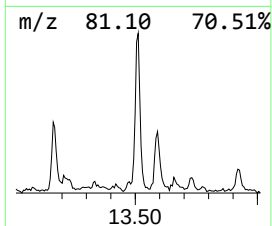
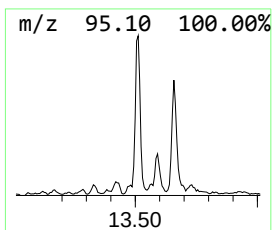
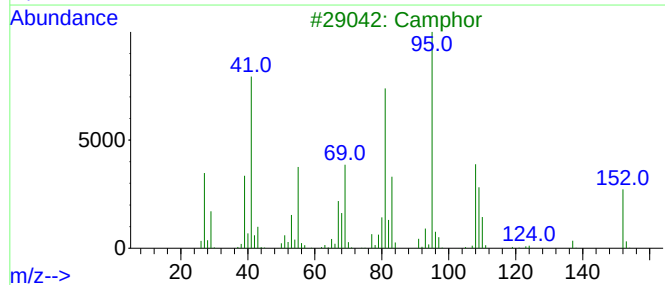
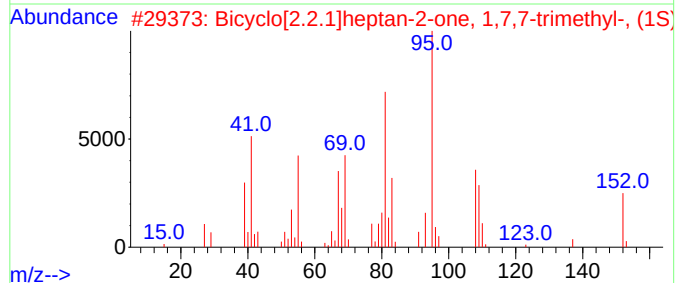
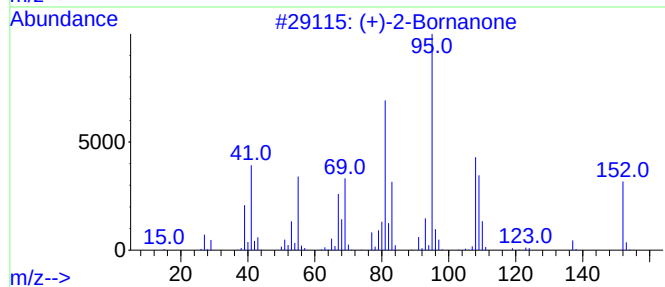
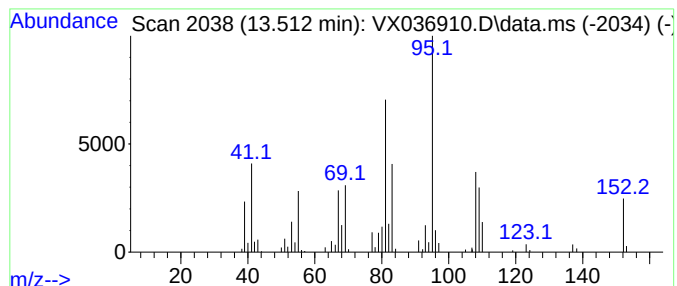
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.512	7.46 ug/l	84896	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	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
3	Camphor	152	C10H16O	000076-22-2	96
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	49
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081023\
Data File : VX036910.D
Acq On : 10 Aug 2023 14:07
Operator : JC/MD
Sample : 03960-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230809051-02-VOA

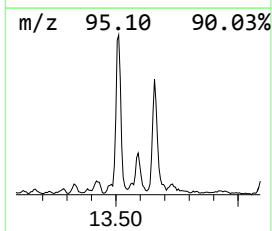
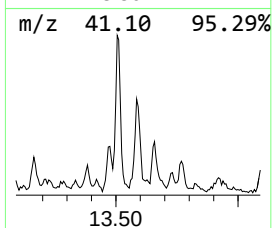
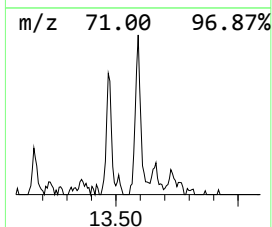
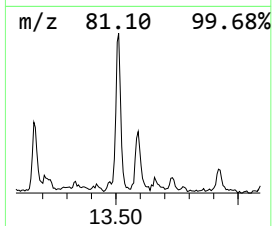
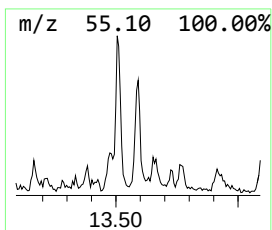
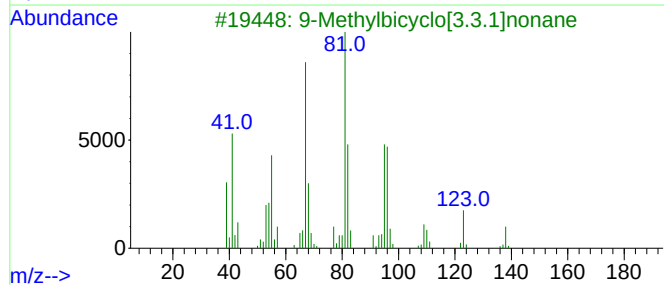
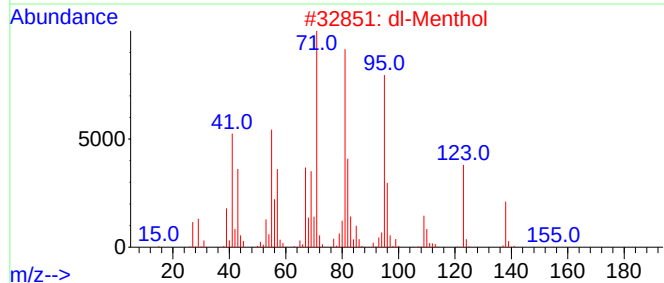
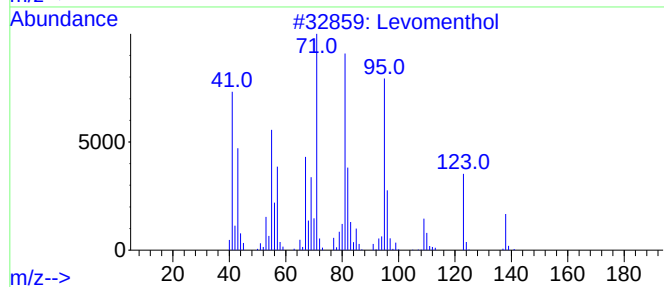
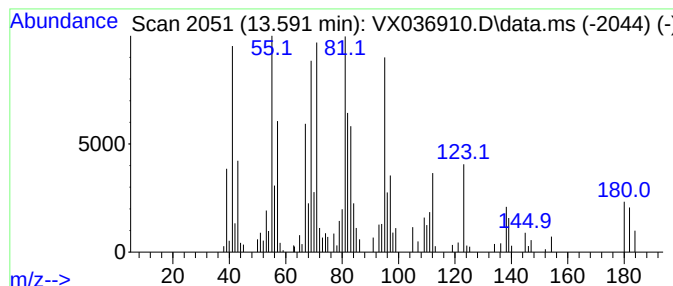
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Quant Title : SW846 8260

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

Peak Number 6 Levomenthol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	5.44 ug/l	61902	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Levomenthol	156	C10H20O	002216-51-5	58
2			dl-Menthol	156	C10H20O	000089-78-1	52
3			9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	42
4			cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	41
5			2-n-Octylfuran	180	C12H20O	004179-38-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081023\
Data File : VX036910.D
Acq On : 10 Aug 2023 14:07
Operator : JC/MD
Sample : 03960-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.056	8.8	ug/l	63170	1	5.556	359224	50.0
1-Propanol	3.849	7.5	ug/l	53722	1	5.556	359224	50.0
1-Butanol	7.208	15.4	ug/l	151639	2	6.763	491532	50.0
Fenchone	12.902	11.5	ug/l	131299	4	12.024	569052	50.0
(+)-2-Bornanone	13.512	7.5	ug/l	84896	4	12.024	569052	50.0
Levomenthol	13.591	5.4	ug/l	61902	4	12.024	569052	50.0