

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061923\
Data File : VX036206.D
Acq On : 19 Jun 2023 15:17
Operator : JC/MD
Sample : 03301-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1619

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\82X061623W.M

Title : SW846 8260

Signal : TIC: VX036206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	56	59	103	rBV	14747523	23529200	100.00%	70.975%
2	2.123	158	170	193	rVB	251054	1120302	4.76%	3.379%
3	4.227	506	515	530	rBV2	111722	312636	1.33%	0.943%
4	5.385	693	705	721	rBV2	119750	352722	1.50%	1.064%
5	5.549	721	732	748	rVV	200057	556163	2.36%	1.678%
6	5.958	789	799	810	rBV	156388	411813	1.75%	1.242%
7	6.763	922	931	950	rVB	318509	762608	3.24%	2.300%
8	8.646	1233	1240	1248	rBV	668162	1048306	4.46%	3.162%
9	10.055	1460	1471	1482	rBV	662172	923386	3.92%	2.785%
10	10.311	1507	1513	1524	rVB	1532495	2009428	8.54%	6.061%
11	11.079	1634	1639	1649	rBV	614531	774212	3.29%	2.335%
12	12.018	1781	1793	1801	rBV	656549	885558	3.76%	2.671%
13	12.219	1818	1826	1840	rBV2	225295	465151	1.98%	1.403%

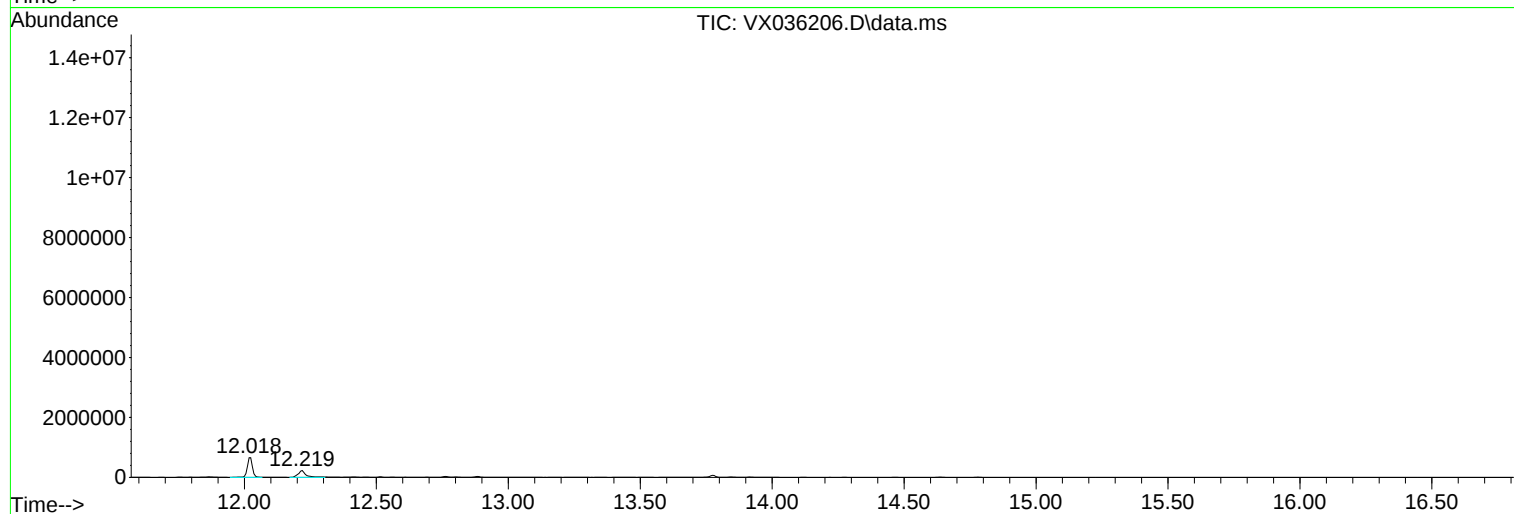
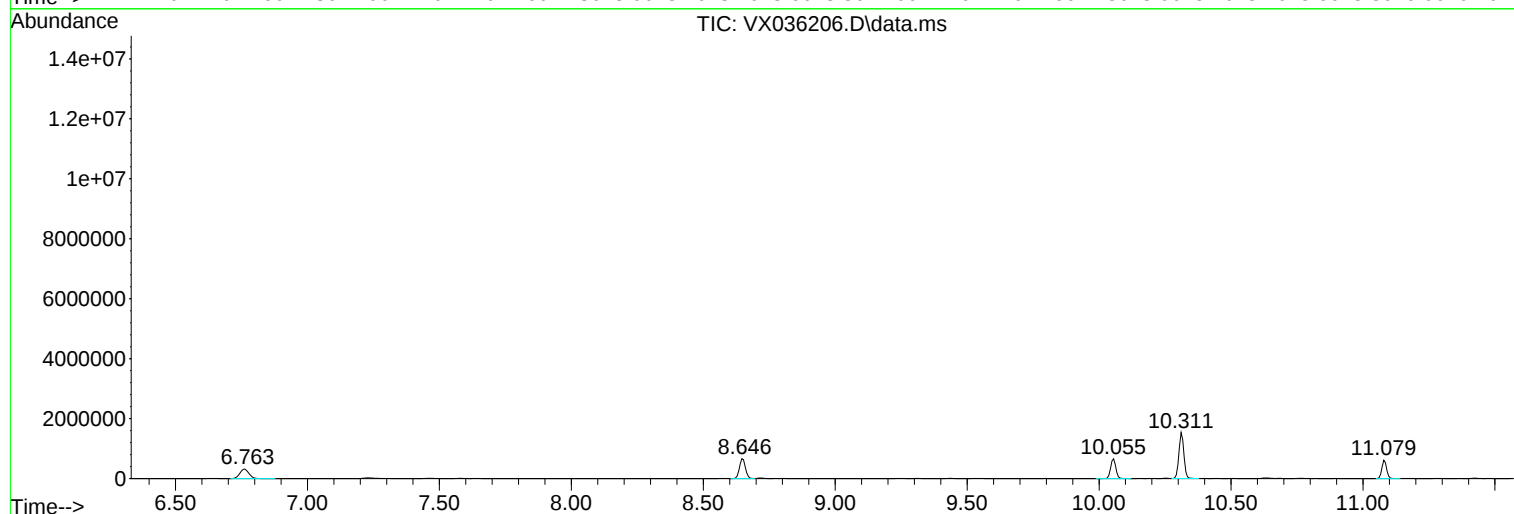
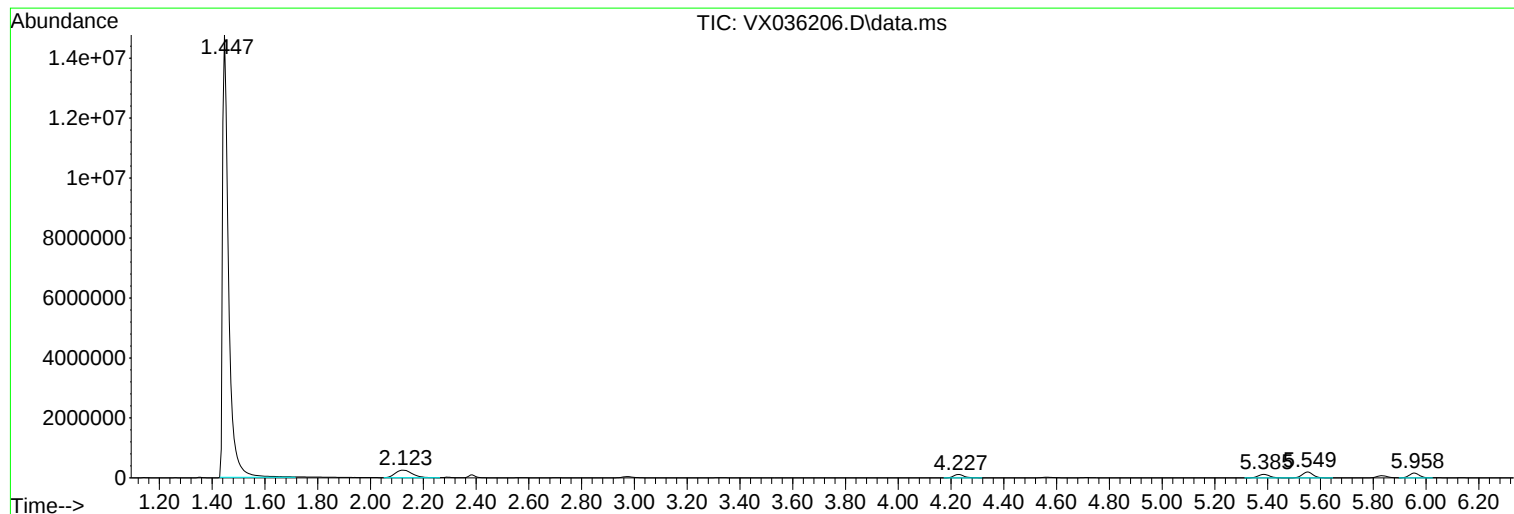
Sum of corrected areas: 33151485

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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



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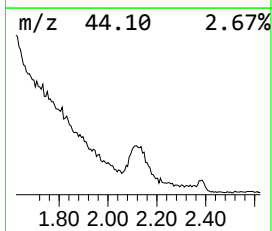
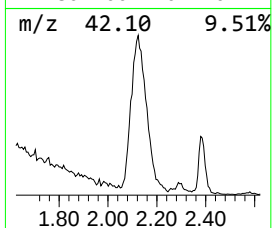
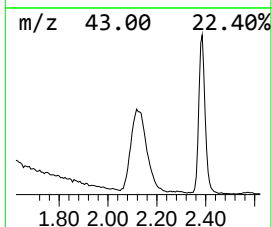
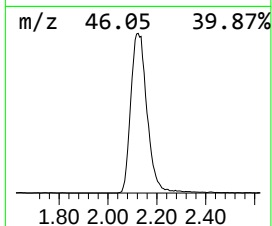
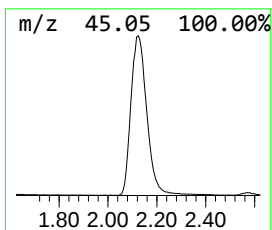
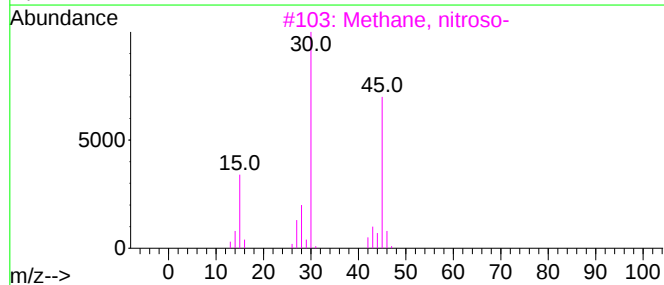
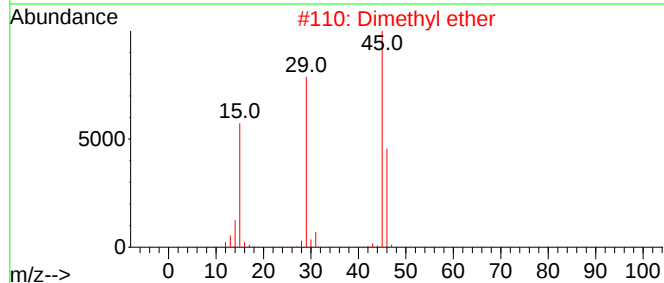
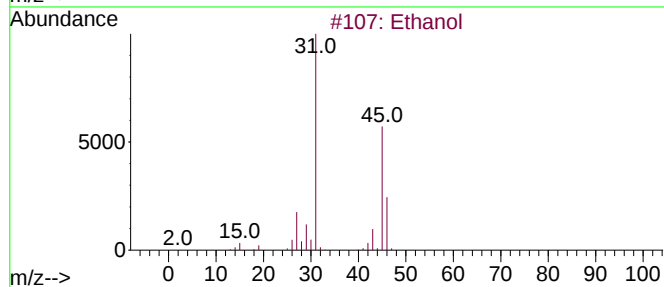
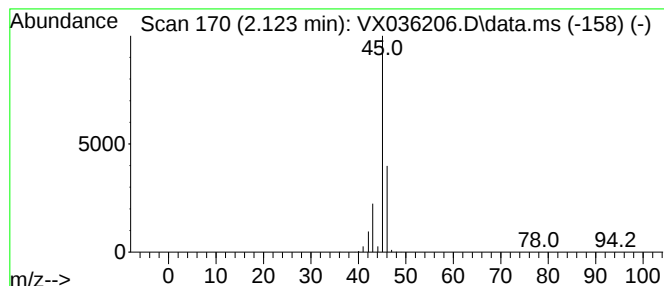
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061623W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.123	100.72 ug/l	1120300	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
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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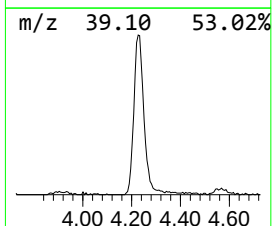
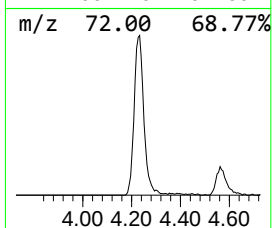
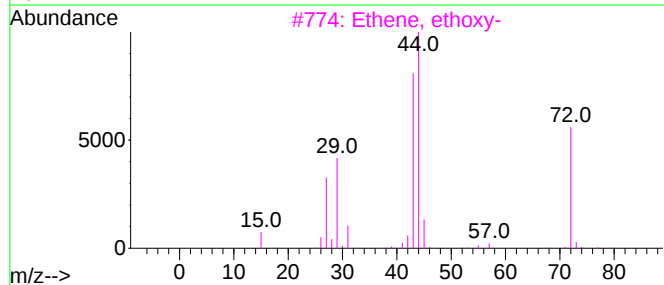
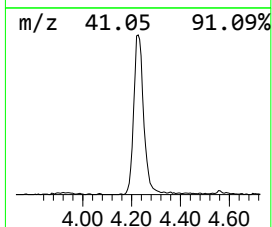
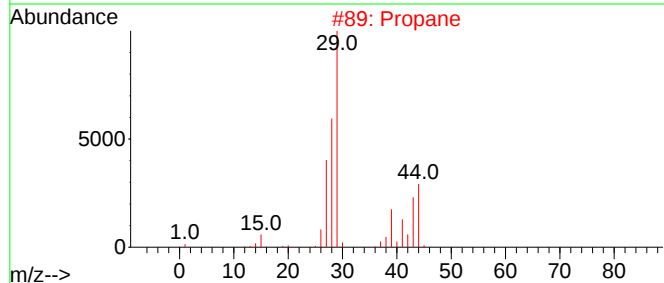
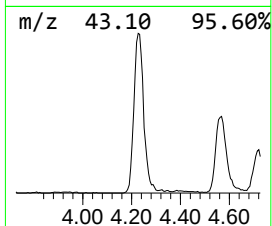
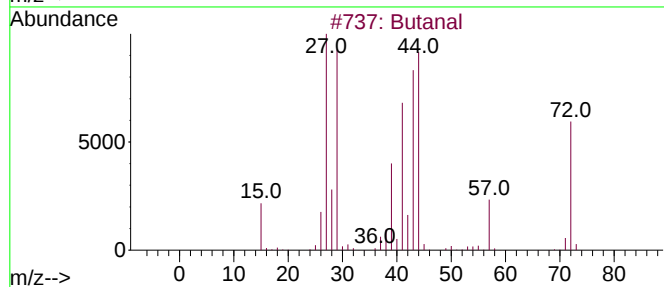
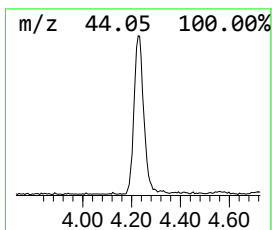
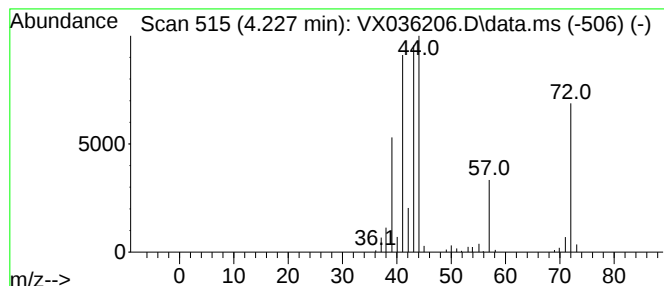
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Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	28.11 ug/l	312636	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	59
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5			Methacrolein	70	C4H6O	000078-85-3	27



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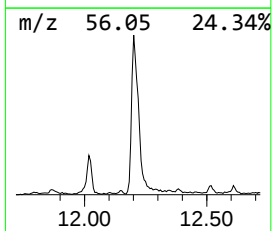
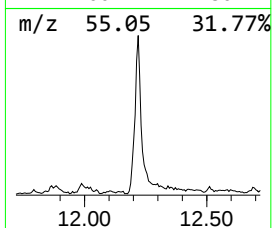
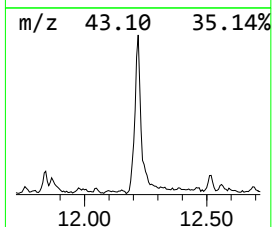
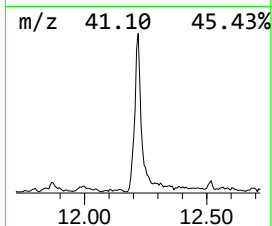
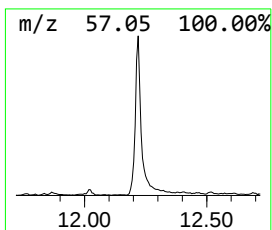
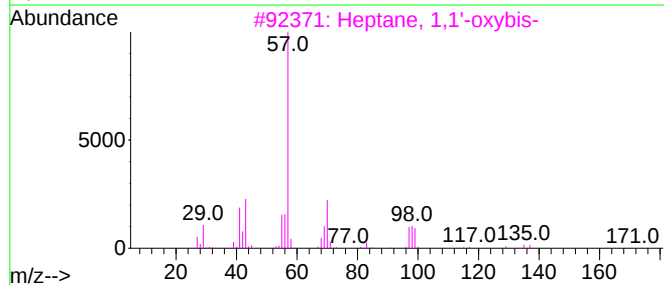
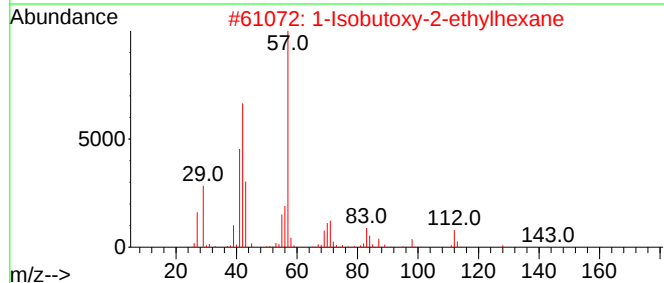
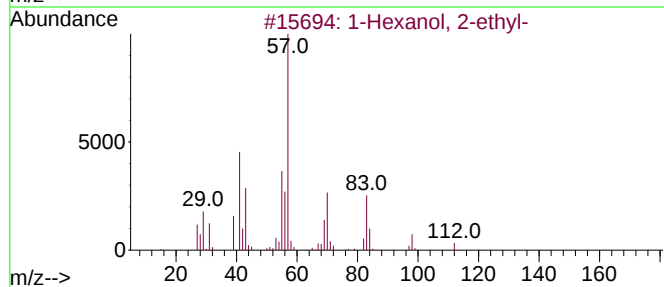
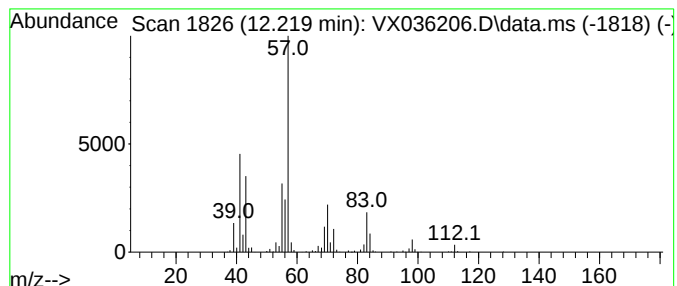
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	26.26 ug/l	465151	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47



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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	2.123	100.7	ug/l	1120300	1	5.556	556163	50.0
Butanal	4.227	28.1	ug/l	312636	1	5.556	556163	50.0
1-Hexanol, 2-et...	12.219	26.3	ug/l	465151	4	12.024	885558	50.0