

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
 Data File : VX031413.D
 Acq On : 16 Sep 2022 16:26
 Operator : JC/MD
 Sample : N4671-01 5X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EFF-WW

Integration Parameters: RTEINT3.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_X\Method\624X091622W.M

Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

Signal : TIC: VX031413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.123	161	170	186	rVB2	13828	62598	2.17%	1.057%
2	2.294	193	198	206	rBV	25606	41458	1.44%	0.700%
3	2.386	206	213	230	rBV	1711554	2878351	100.00%	48.615%
4	2.575	234	244	264	rBV	379675	1261445	43.83%	21.306%
5	2.947	296	305	315	rBV2	13839	33385	1.16%	0.564%
6	4.233	503	516	529	rBV2	15417	41286	1.43%	0.697%
7	4.903	614	626	640	rBV2	29771	85084	2.96%	1.437%
8	5.964	790	800	815	rVB2	36063	97250	3.38%	1.643%
9	6.610	898	906	923	rBV	118048	297197	10.33%	5.020%
10	6.763	923	931	944	rVB	67808	162807	5.66%	2.750%
11	8.653	1234	1241	1244	rBV	164821	284229	9.87%	4.801%
12	9.622	1395	1400	1406	rBV	21895	34932	1.21%	0.590%
13	10.055	1466	1471	1483	rVB	135367	184383	6.41%	3.114%
14	11.085	1634	1640	1647	rBV	122661	160897	5.59%	2.718%
15	12.219	1821	1826	1843	rBV	167636	295388	10.26%	4.989%

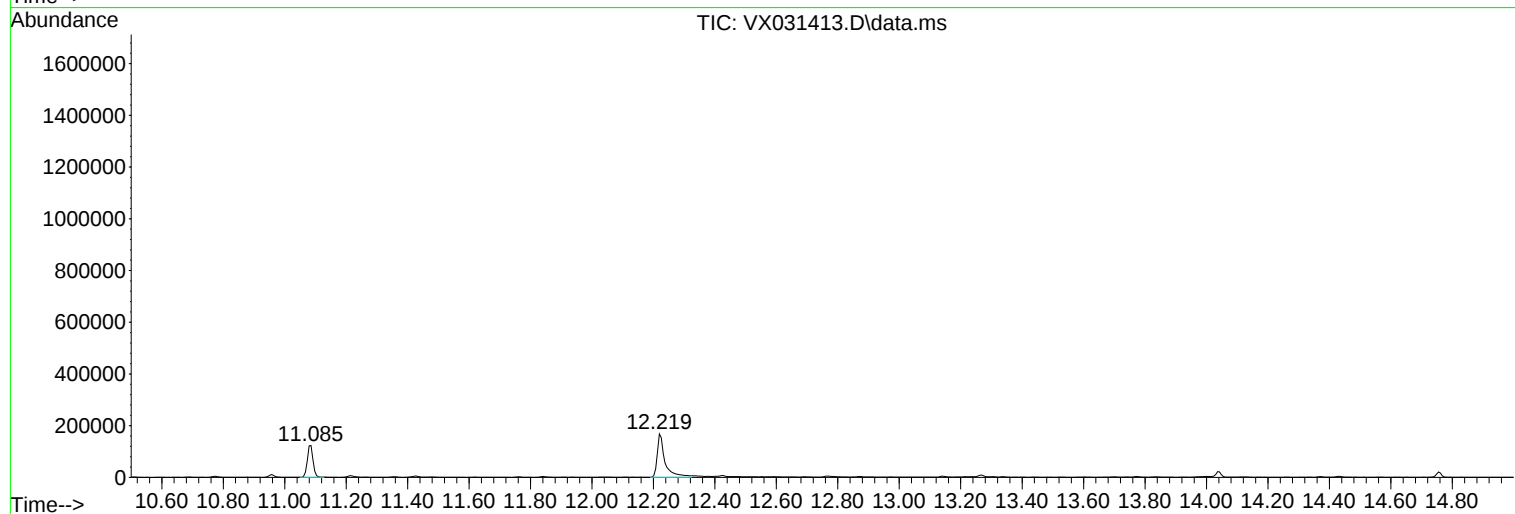
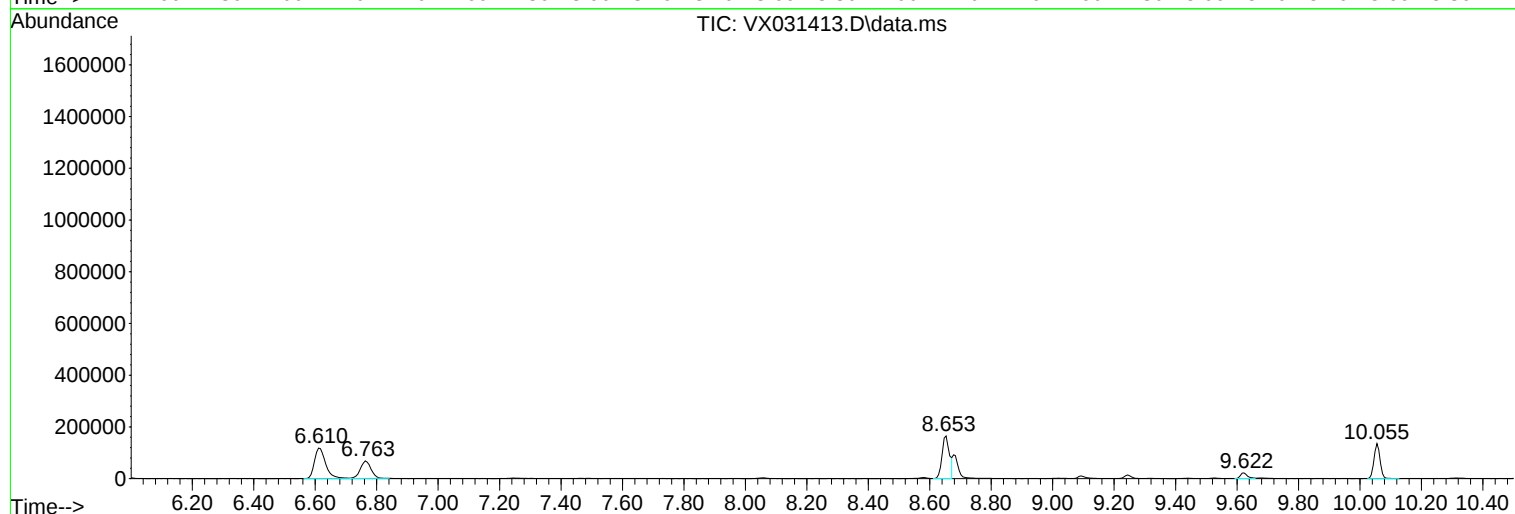
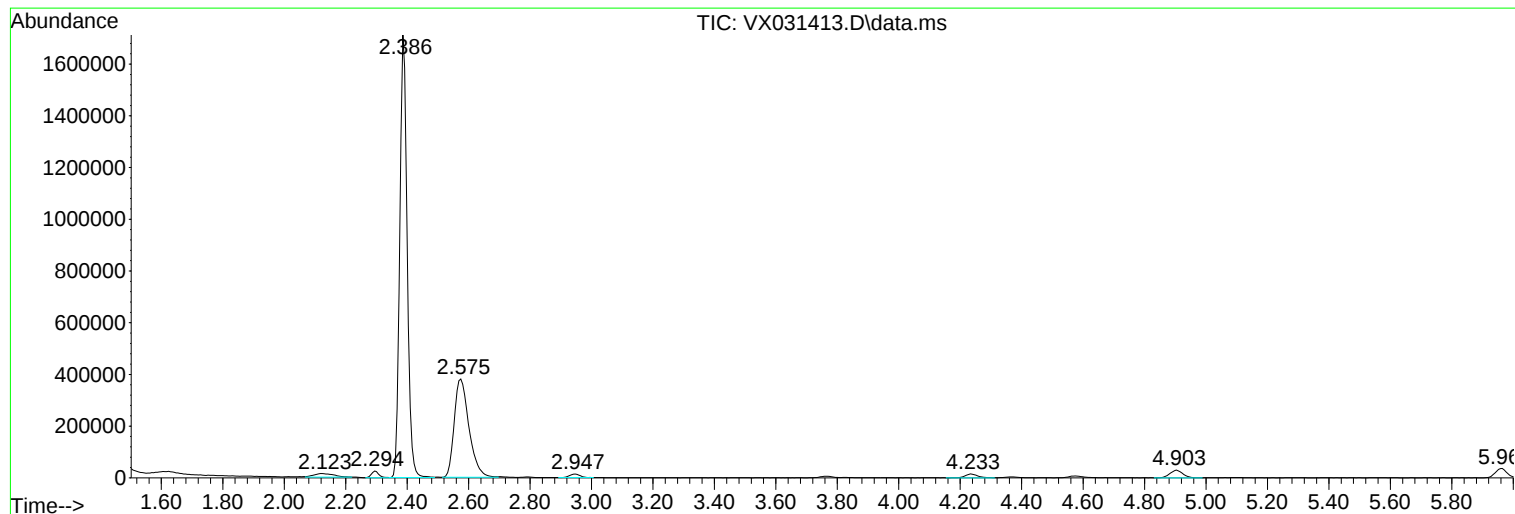
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\624X091622W.M
Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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



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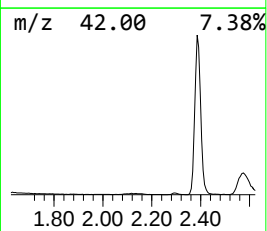
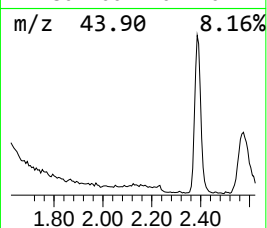
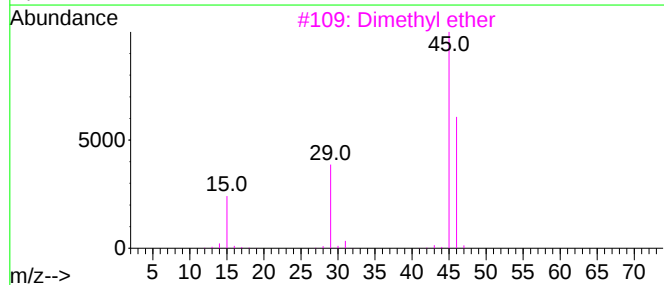
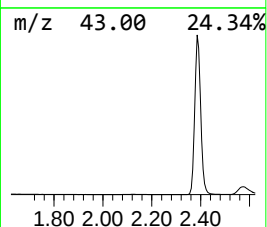
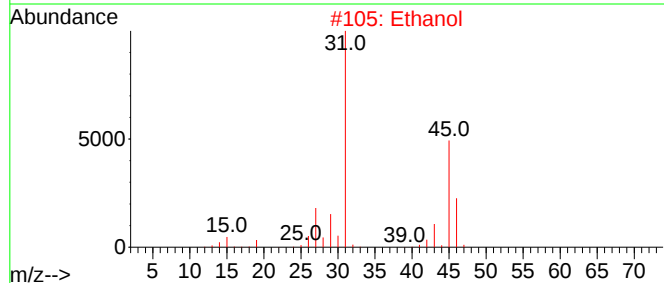
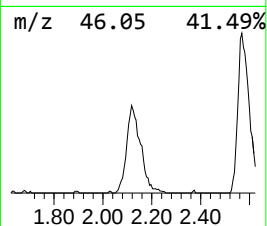
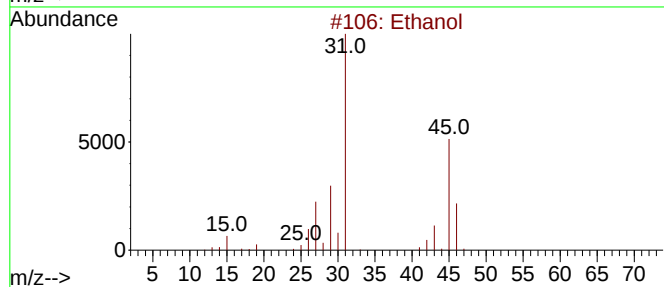
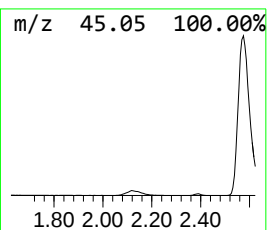
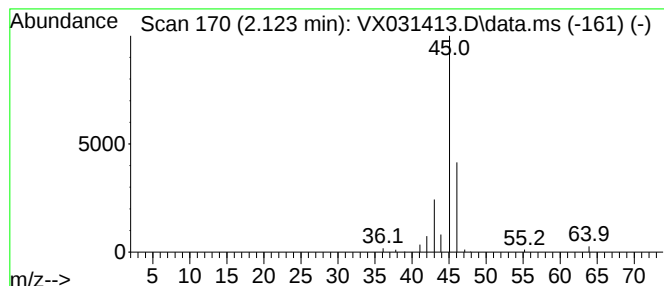
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 1 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.123	22.07 ug/l	62598	Bromochloromethane	4.903

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	56
2	Ethanol			46	C2H6O	000064-17-5	43
3	Dimethyl ether			46	C2H6O	000115-10-6	9
4	Dimethyl ether			46	C2H6O	000115-10-6	9
5	Ethanol			46	C2H6O	000064-17-5	9



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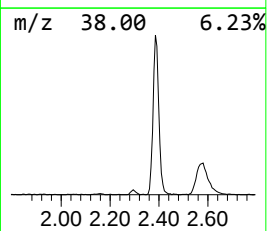
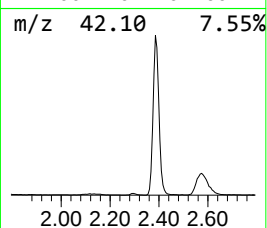
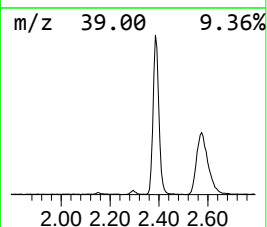
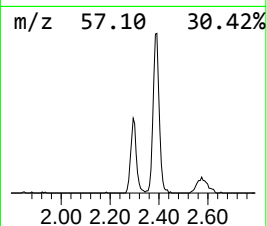
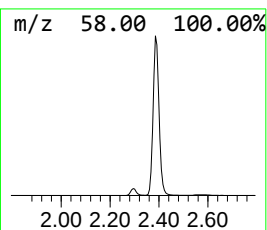
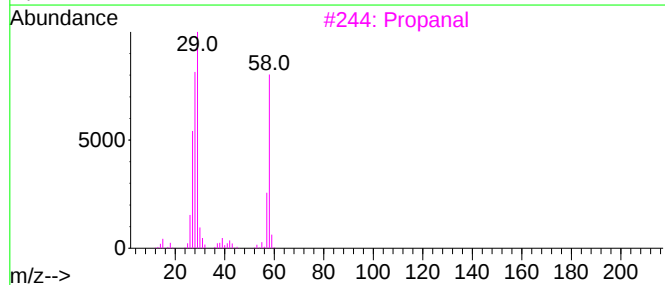
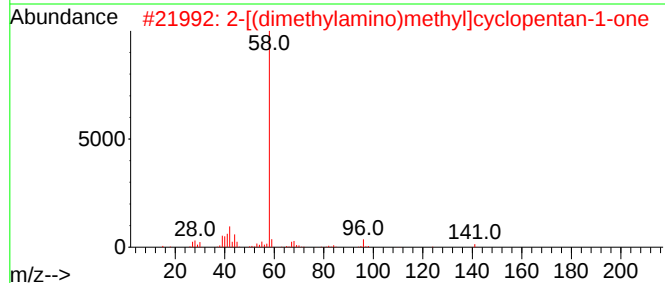
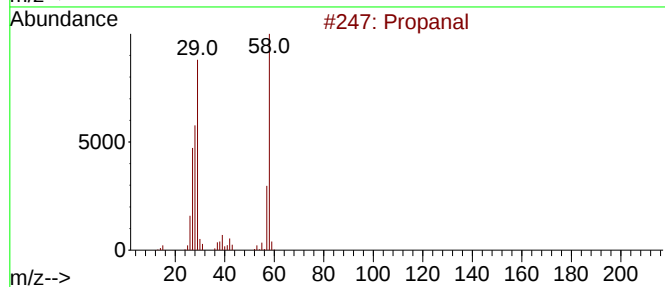
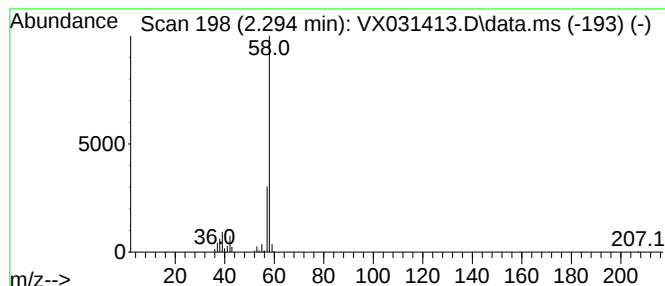
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 2 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	14.62 ug/l	41458	Bromochloromethane	4.903

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	72
2			2-[(dimethylamino)methyl]cyclope...	141	C8H15NO	006947-99-5	40
3			Propanal	58	C3H6O	000123-38-6	39
4			Propanal	58	C3H6O	000123-38-6	38
5			2,3 Methylene dioxymethcathinone	207	C11H13NO3	1010386-29-7	9



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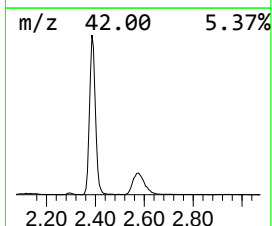
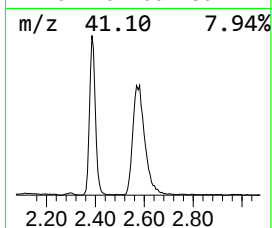
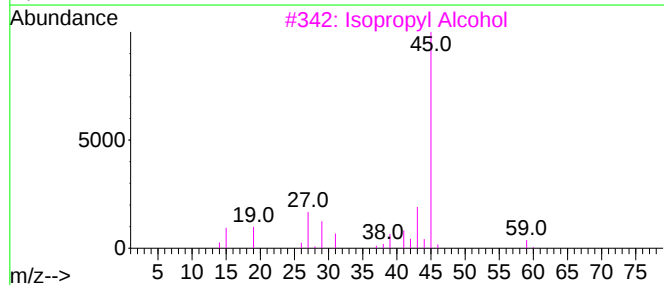
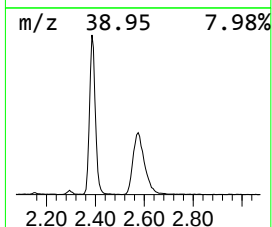
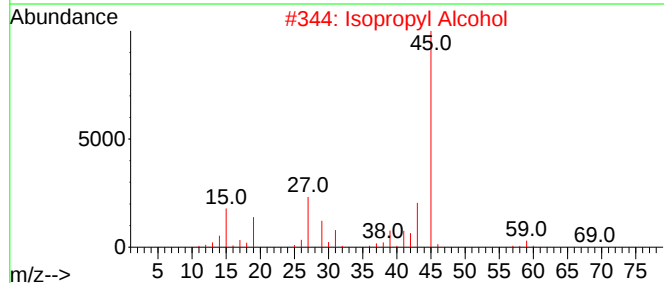
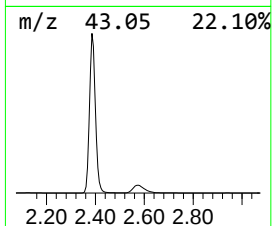
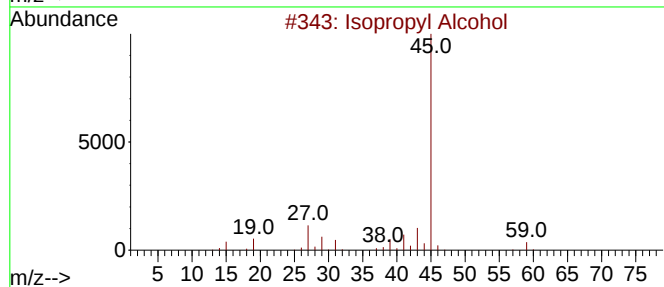
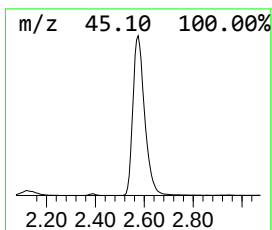
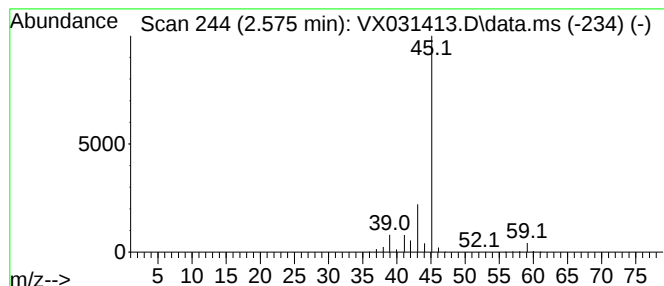
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.575	444.78 ug/l	1261450	Bromochloromethane	4.903

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	64



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MSVOA_X
ClientSampleId :
EFF-WW

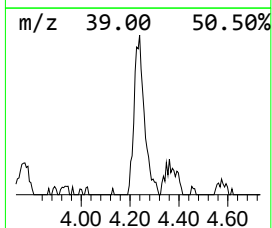
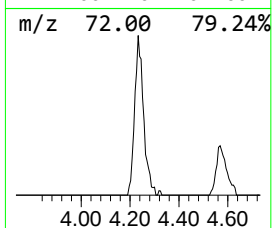
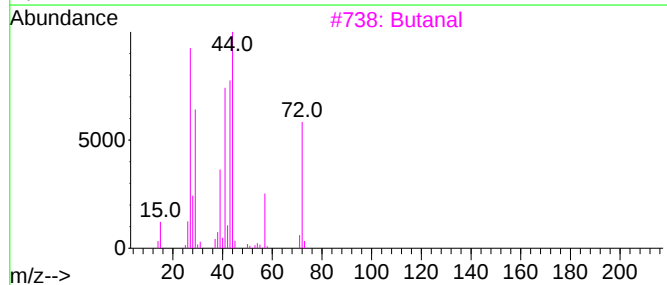
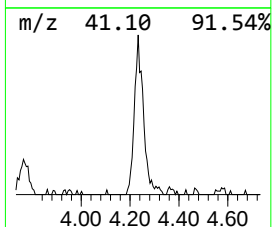
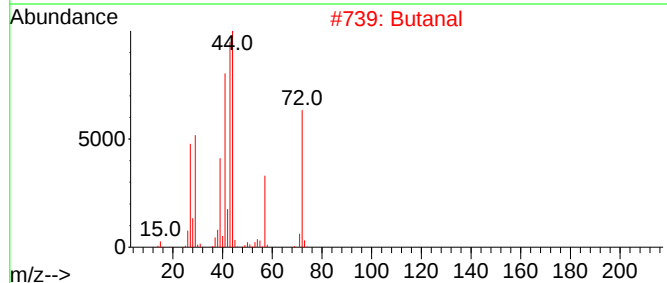
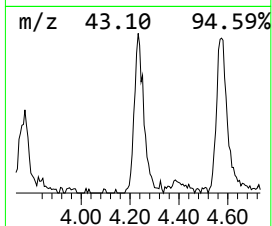
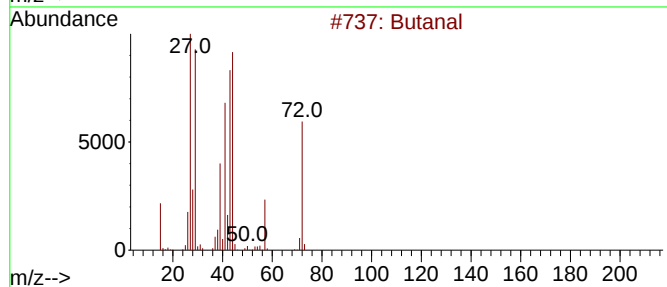
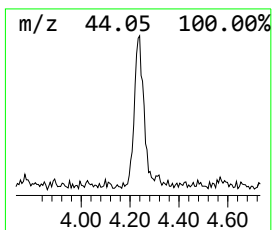
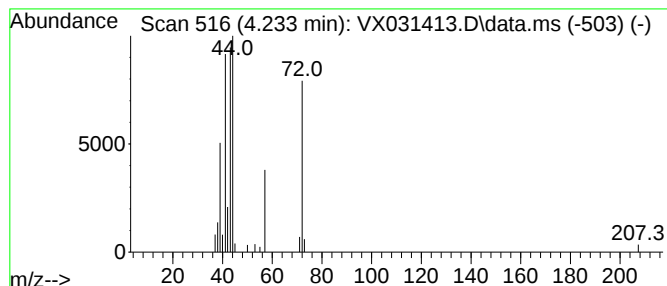
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	14.56 ug/l	41286	Bromochloromethane	4.903

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal			72	C4H8O	000123-72-8	91
2	Butanal			72	C4H8O	000123-72-8	91
3	Butanal			72	C4H8O	000123-72-8	72
4	Butanal			72	C4H8O	000123-72-8	59
5	Butanal			72	C4H8O	000123-72-8	53



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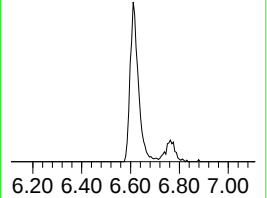
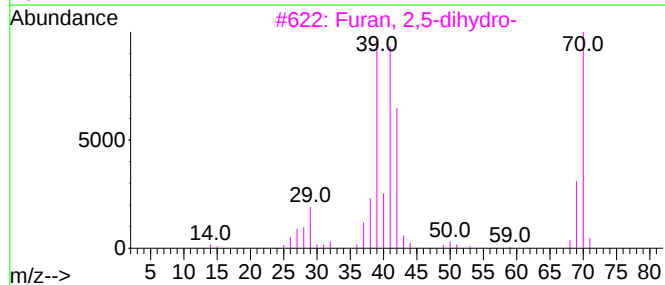
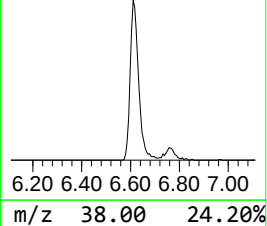
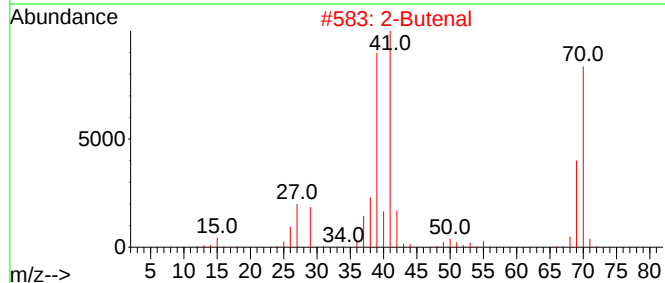
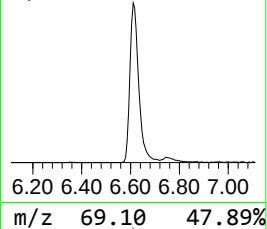
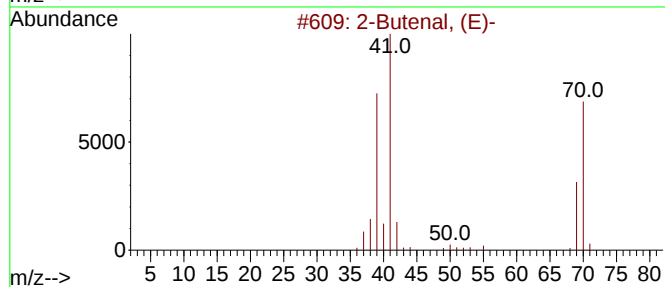
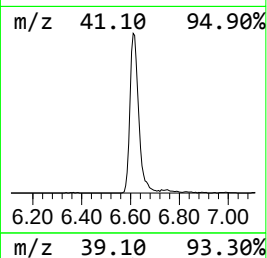
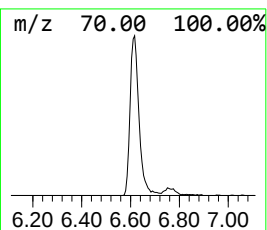
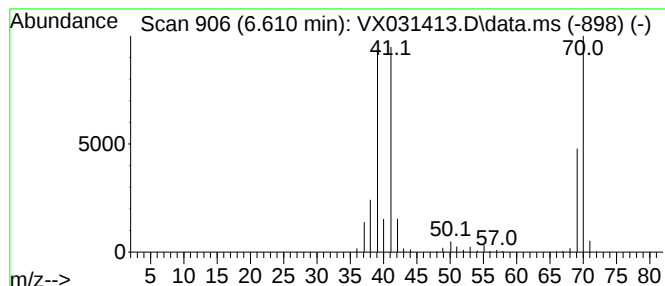
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Butenal, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.610	54.76 ug/l	297197	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal, (E)-	70	C4H6O	000123-73-9	91
2			2-Butenal	70	C4H6O	004170-30-3	91
3			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	90
4			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	90
5			2-Butenal, (Z)-	70	C4H6O	015798-64-8	83



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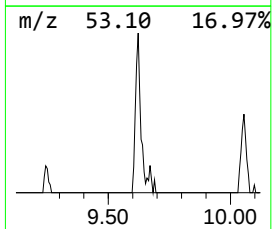
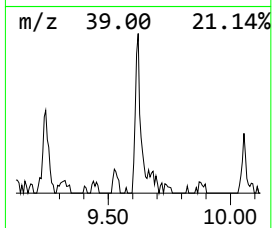
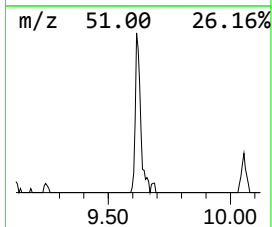
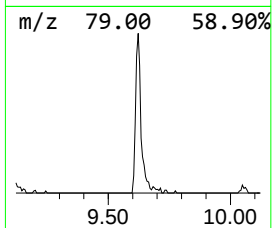
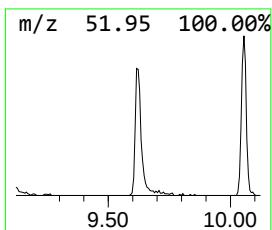
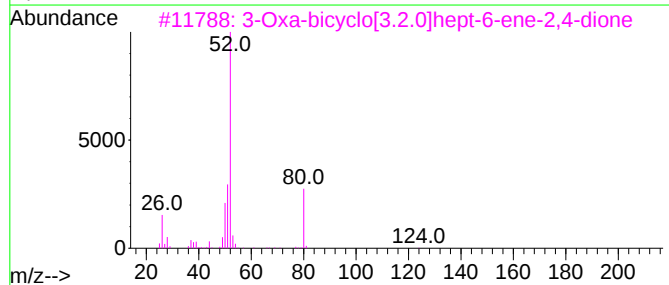
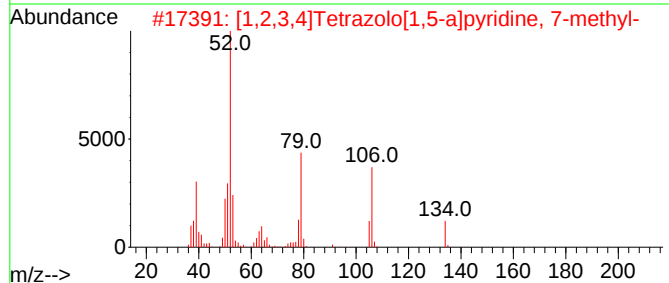
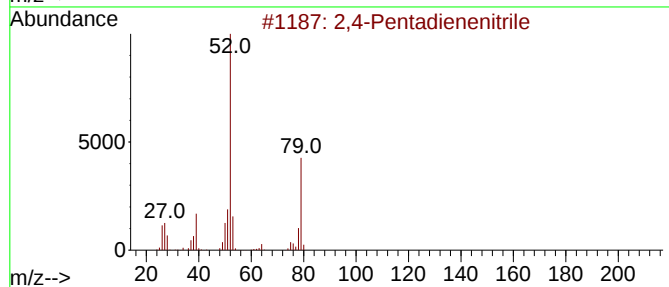
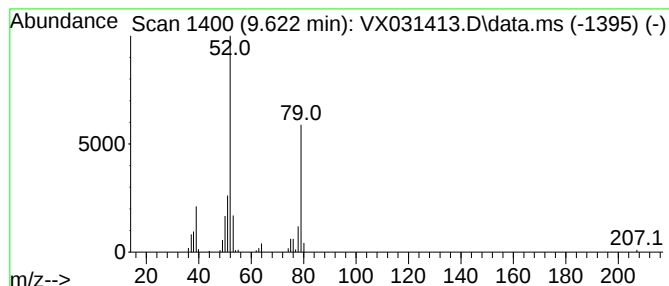
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 6 2,4-Pentadienenitrile Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.622	5.68 ug/l	34932	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Pentadienenitrile	79	C5H5N	001615-70-9	94
2			[1,2,3,4]Tetrazolo[1,5-a]pyridin...	134	C6H6N4	1000338-33-1	78
3			3-Oxa-bicyclo[3.2.0]hept-6-ene-2...	124	C6H4O3	113647-99-7	72
4			[1,2,3,4]Tetrazolo[1,5-a]pyridin...	134	C6H6N4	1000338-32-9	64
5			s-Triazolo[4,3-a]pyridine, 6-met...	133	C7H7N3	004919-09-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031413.D
Acq On : 16 Sep 2022 16:26
Operator : JC/MD
Sample : N4671-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EFF-WW

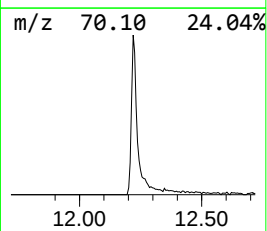
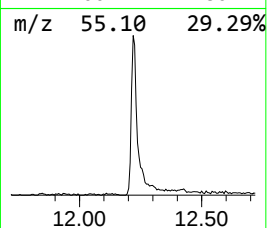
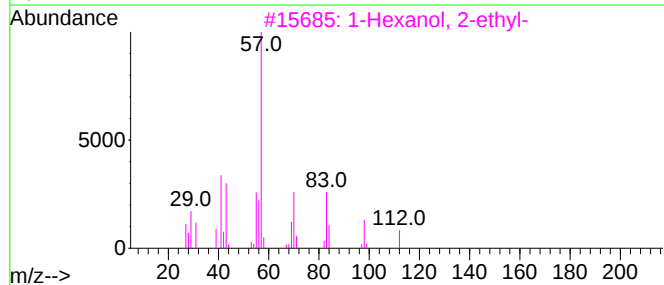
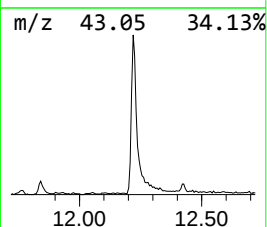
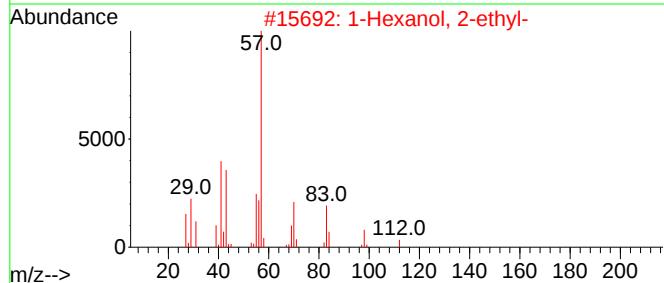
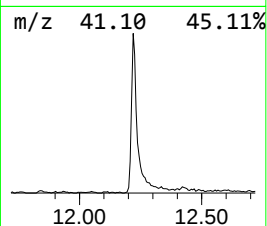
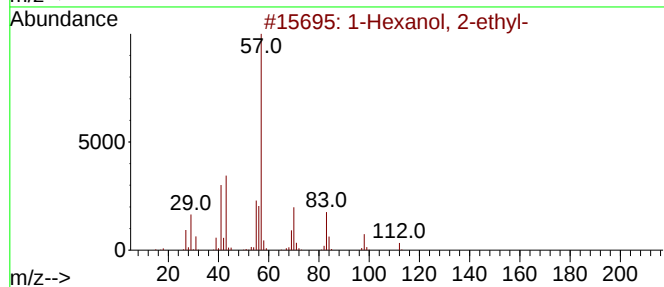
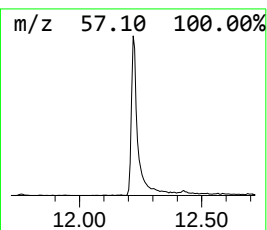
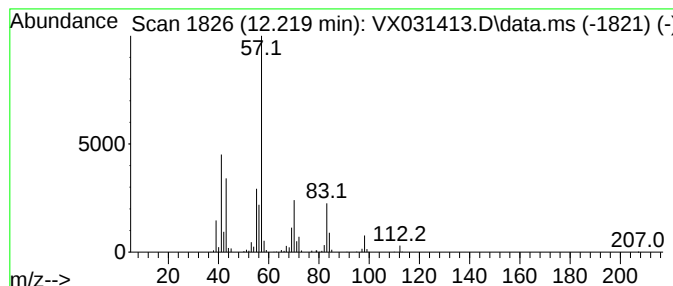
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	48.06 ug/l	295388	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	80
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031413.D
Acq On : 16 Sep 2022 16:26
Operator : JC/MD
Sample : N4671-01 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EFF-WW

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\624X091622W.M
Quant Title : METHOD 624 VOLATILE ORGANIC 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
Ethanol	2.123	22.1	ug/l	62598	1	4.903	85084	30.0
Propanal	2.294	14.6	ug/l	41458	1	4.903	85084	30.0
Isopropyl Alcohol	2.575	444.8	ug/l	1261450	1	4.903	85084	30.0
Butanal	4.233	14.6	ug/l	41286	1	4.903	85084	30.0
2-Butenal, (E)-	6.610	54.8	ug/l	297197	2	6.763	162807	30.0
2,4-Pentadienen...	9.622	5.7	ug/l	34932	3	10.055	184383	30.0
1-Hexanol, 2-et...	12.219	48.1	ug/l	295388	3	10.055	184383	30.0