LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101022\
Data File : VX032024.D
Acq On : 10 Oct 2022 19:46
Operator : JC/MD
Sample : N4987-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1678

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\82X100622W.M
Title : SW846 8260

Signal : TIC: VX032024.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.416	52	54	55	rBV	13169621	9184210	59.69%	20.813%
2	2.172	156	178	193	rBV	2892877	15387245	100.00%	34.870%
3	2.288	193	197	208	rVV	217188	487696	3.17%	1.105%
4	2.386	208	213	230	rVB	99394	221383	1.44%	0.502%
5	4.233	503	516	536	rBV	1792083	4881237	31.72%	11.062%
6	5.385	693	705	720	rVB2	66614	193380	1.26%	0.438%
7	5.550	722	732	744	rBV	75598	216485	1.41%	0.491%
8	5.836	766	779	791	rBV	806676	2214494	14.39%	5.018%
9	5.958	791	799	808	rVB	77630	202343	1.32%	0.459%
10	6.623	895	908	921	rBV	150206	470895	3.06%	1.067%
11	6.757	922	930	940	rVV	121203	330147	2.15%	0.748%
12	6.873	940	949	968	rVB	541053	1303282	8.47%	2.953%
13	7.251	994	1011	1040	rBV	725468	2390390	15.53%	5.417%
14	7.574	1058	1064	1072	rBV	99745	193684	1.26%	0.439%
15	8.647	1233	1240	1248	rBV	398211	619605	4.03%	1.404%
16	10.055	1465	1471	1484	rVB2	321524	587988	3.82%	1.332%
17	10.311	1507	1513	1523	rBV2	160120	250797	1.63%	0.568%
18	11.079	1634	1639	1645	rBV	322103	406164	2.64%	0.920%
19	12.024	1790	1794	1800	rVB	366109	476334	3.10%	1.079%
20	12.219	1821	1826	1837	rBV	2424704	3041100	19.76%	6.892%
21	12.311	1837	1841	1852	rVB4	79416	171498	1.11%	0.389%
22	14.640	2213	2223	2232	rVB	135588	184360	1.20%	0.418%
23	16.085	2452	2460	2475	rBV2	327256	713167	4.63%	1.616%

Sum of corrected areas: 44127884

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Instrument :
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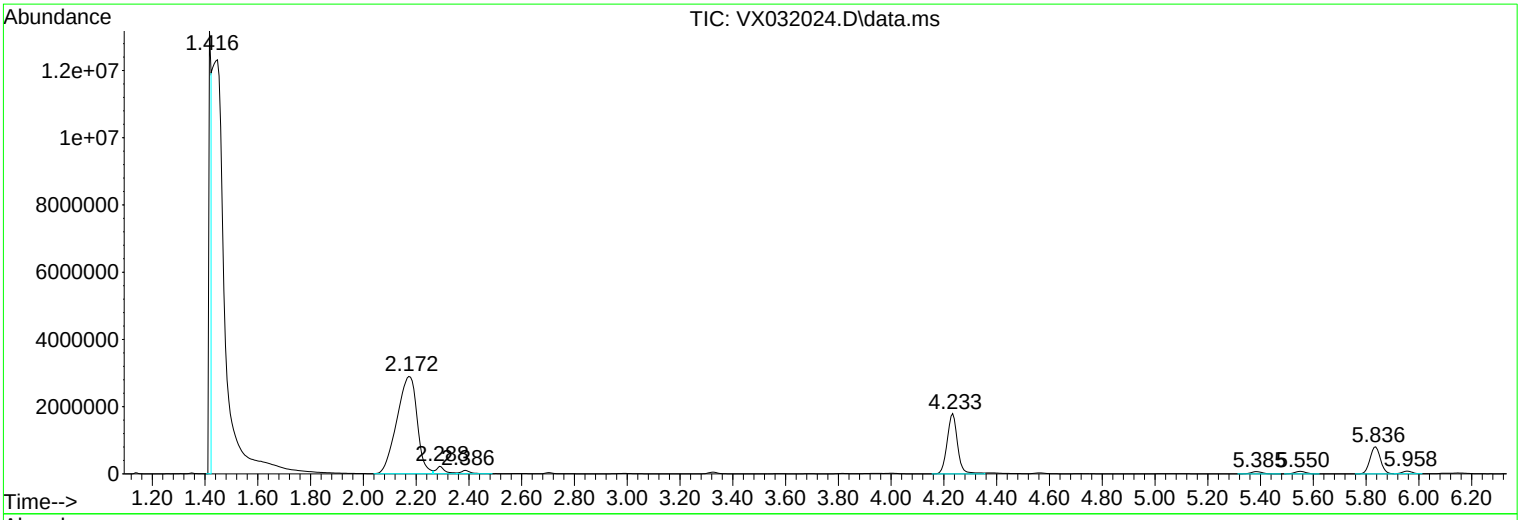
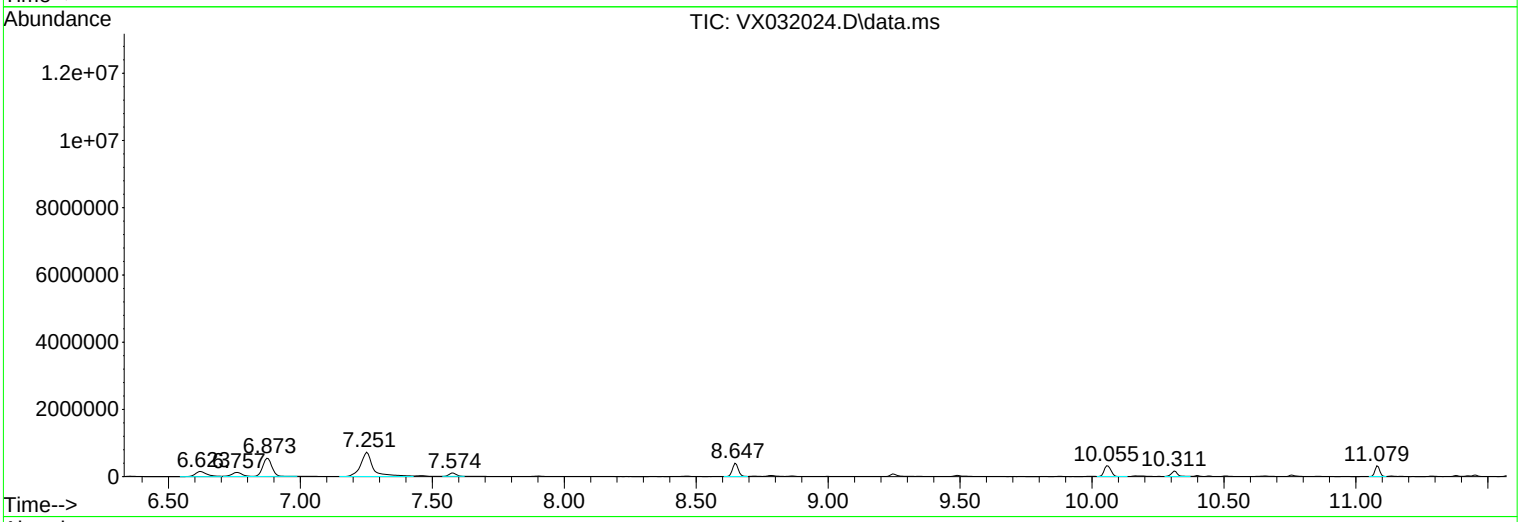
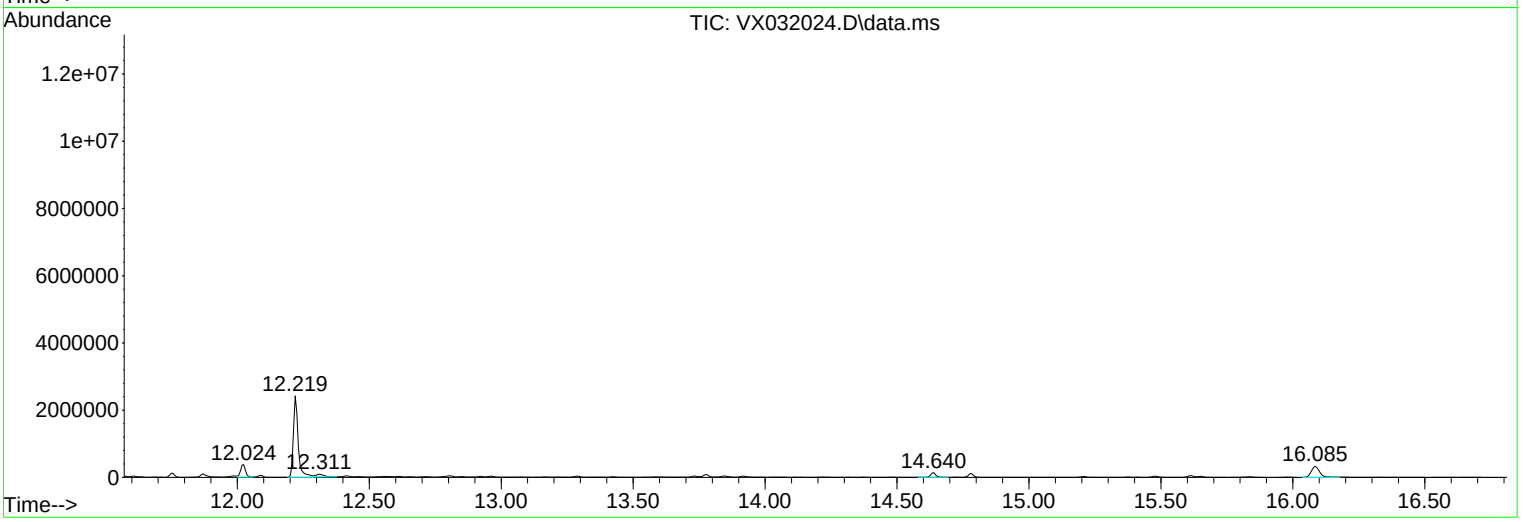
ClientSampleId :
AUD-1678

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

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







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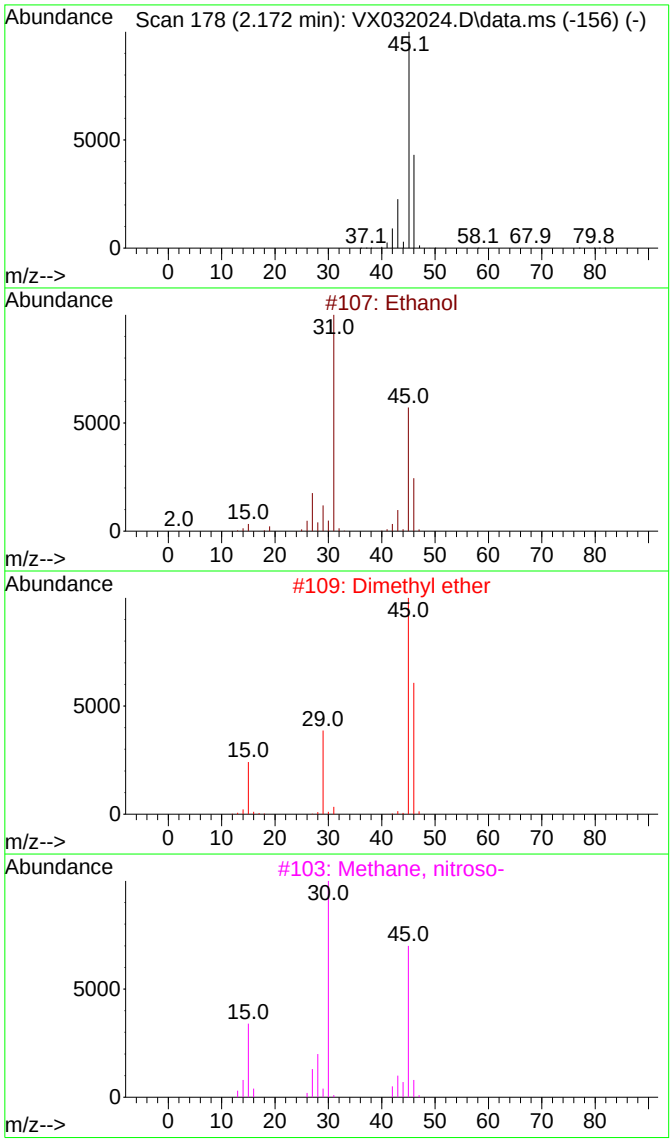
Quant Title : SW846 8260

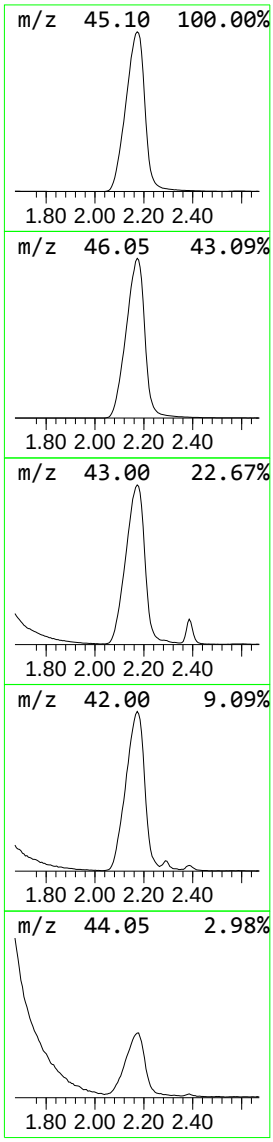
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.172	3553.88 ug/l	15387200	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
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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Data File : VX032024.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1678

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

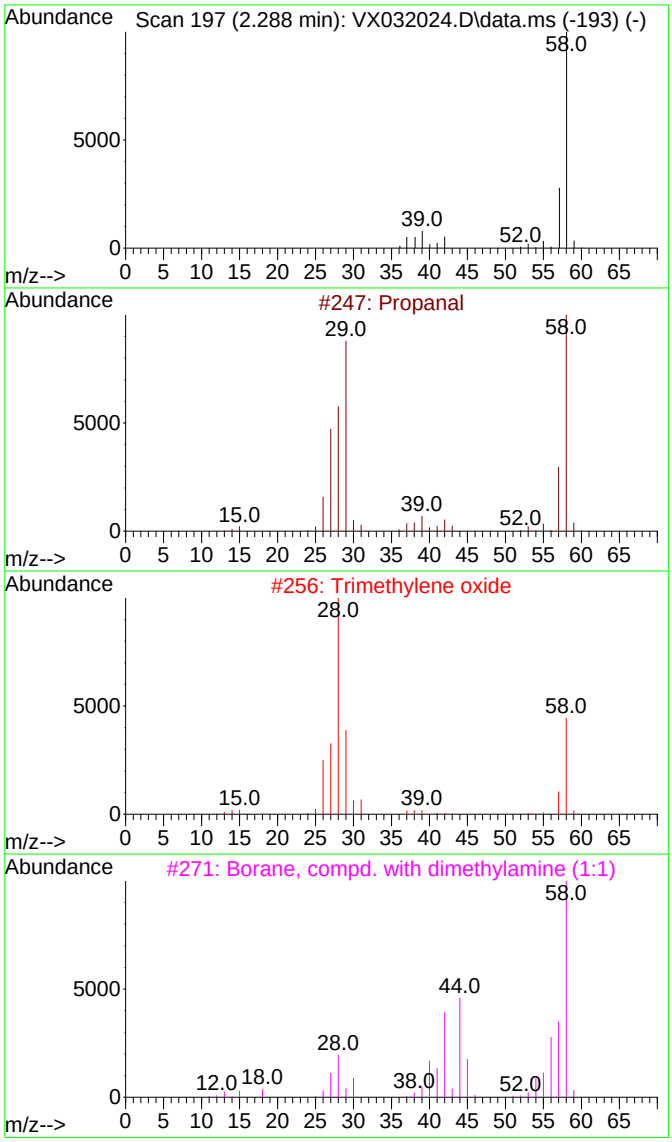
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

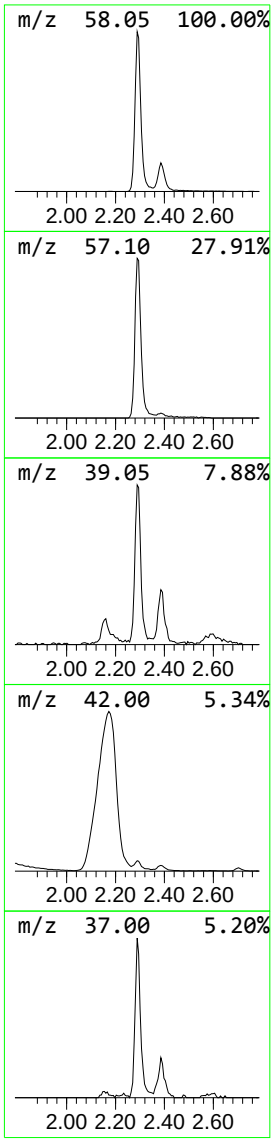
****

Peak Number 3 Propanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.288	112.64 ug/l	487696	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	7
4	Propylene oxide	58	C3H6O	000075-56-9	7
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5





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Instrument :
MSVOA_X
ClientSampleId :
AUD-1678

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

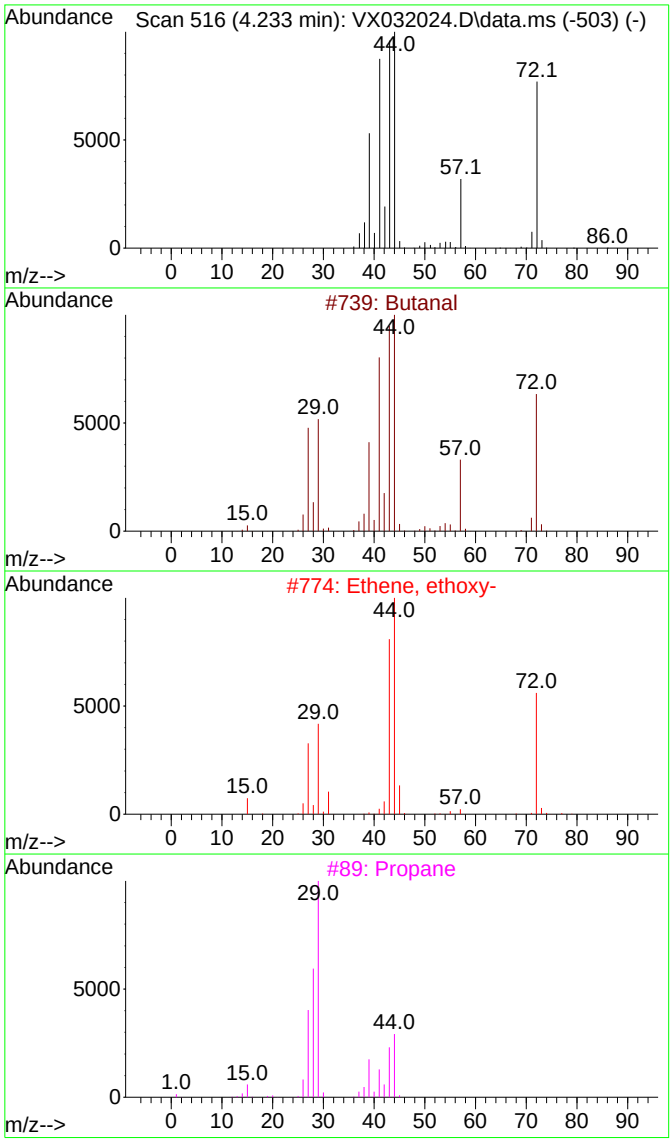
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

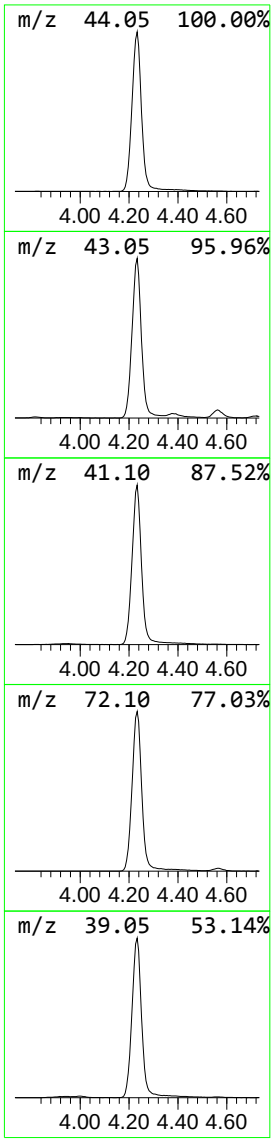
****

Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	1127.38 ug/l	4881240	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propane	44	C3H8	000074-98-6	47
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1678

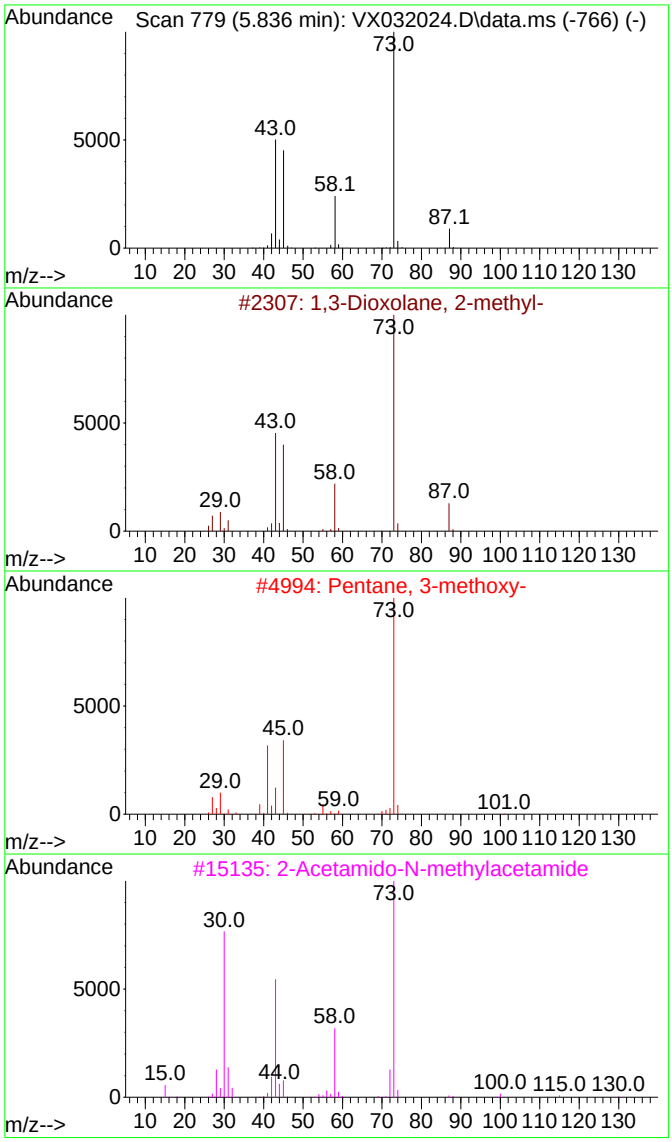
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

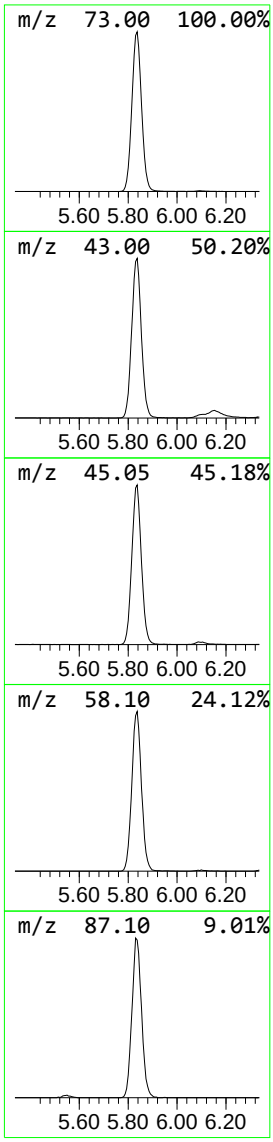
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dioxolane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.836	511.47 ug/l	2214490	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
3	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1678

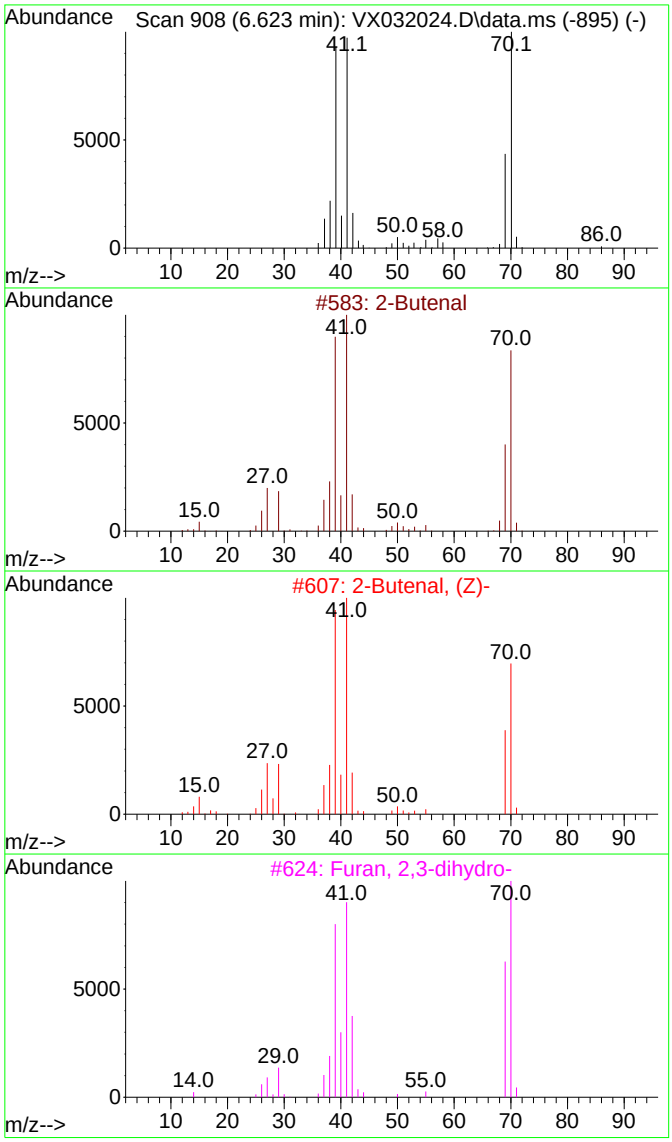
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

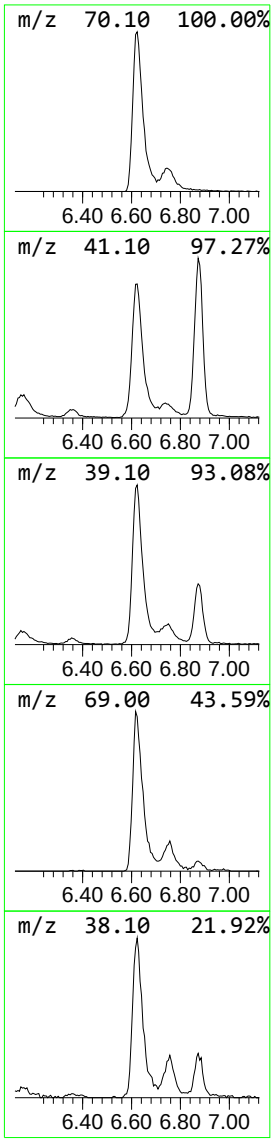
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Butenal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.623	71.32 ug/l	470895	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal	70	C4H6O	004170-30-3	94
2	2-Butenal, (Z)-	70	C4H6O	015798-64-8	91
3	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	91
4	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	91
5	2-Butenal, (E)-	70	C4H6O	000123-73-9	87





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

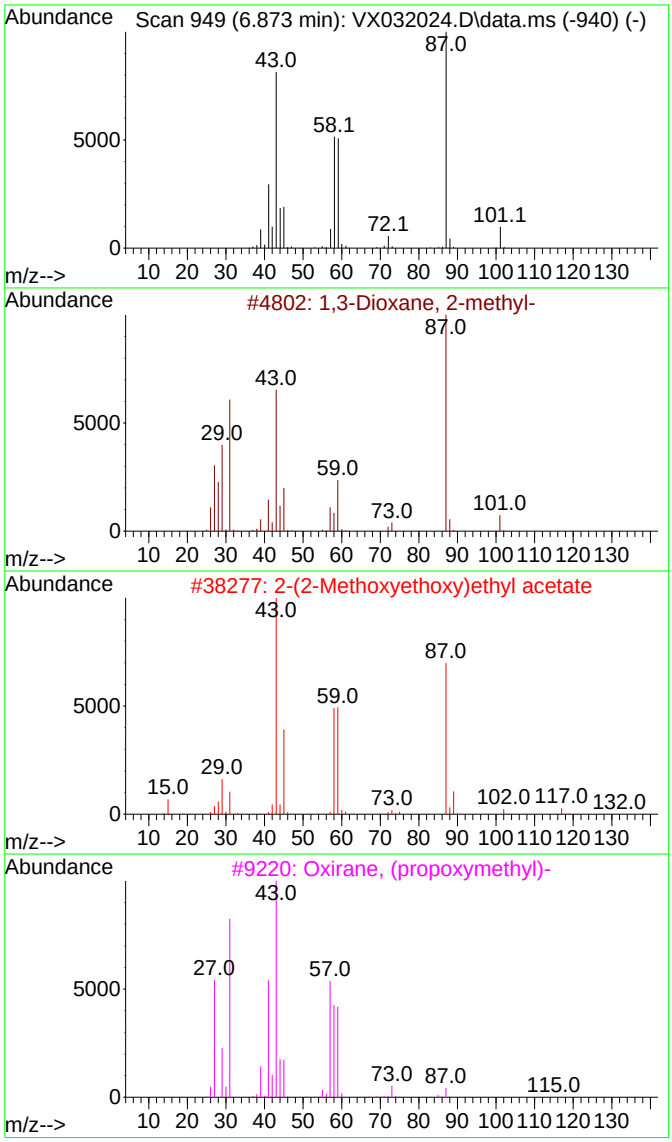
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

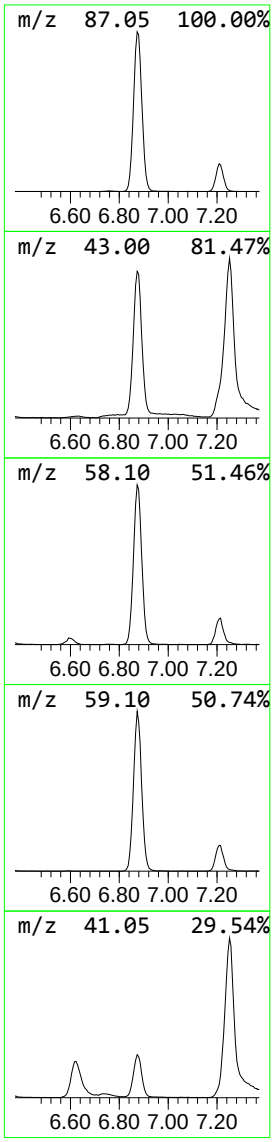
****

Peak Number 7 1,3-Dioxane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	197.38 ug/l	1303280	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	53
2	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
3	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	38
4	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	37





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Quant Title : SW846 8260

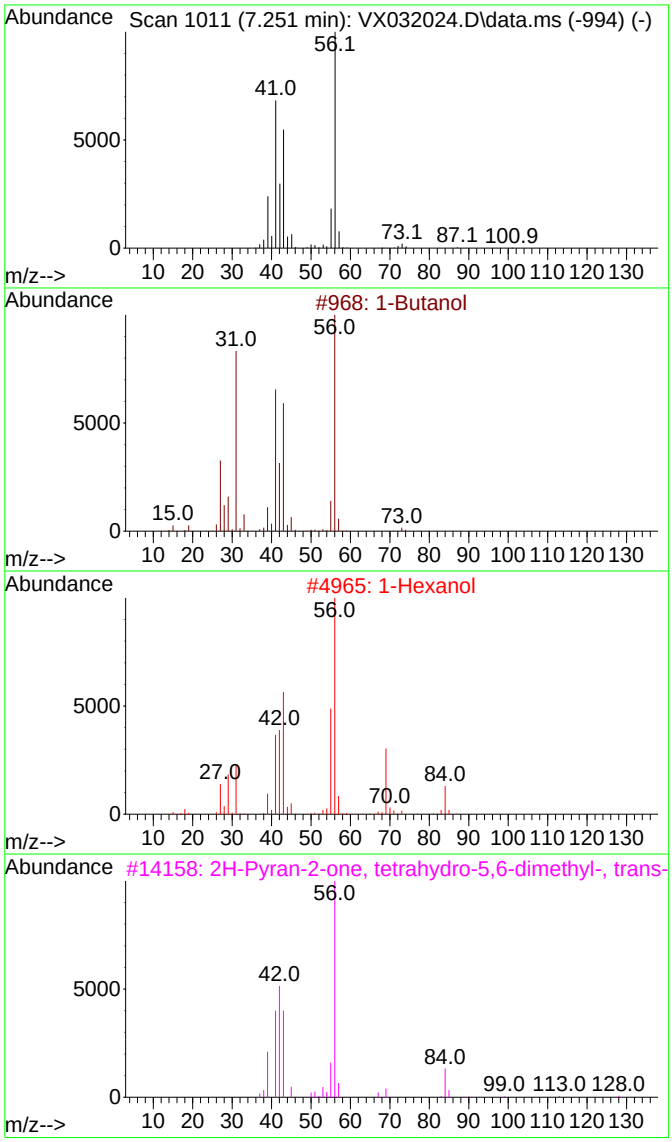
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

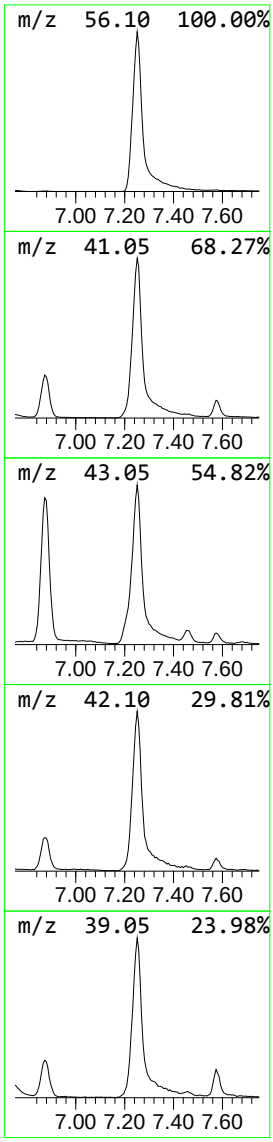
****

Peak Number 8 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.251	362.02 ug/l	2390390	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	1-Hexanol	102	C6H14O	000111-27-3	43
3	2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	38
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
5	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	23





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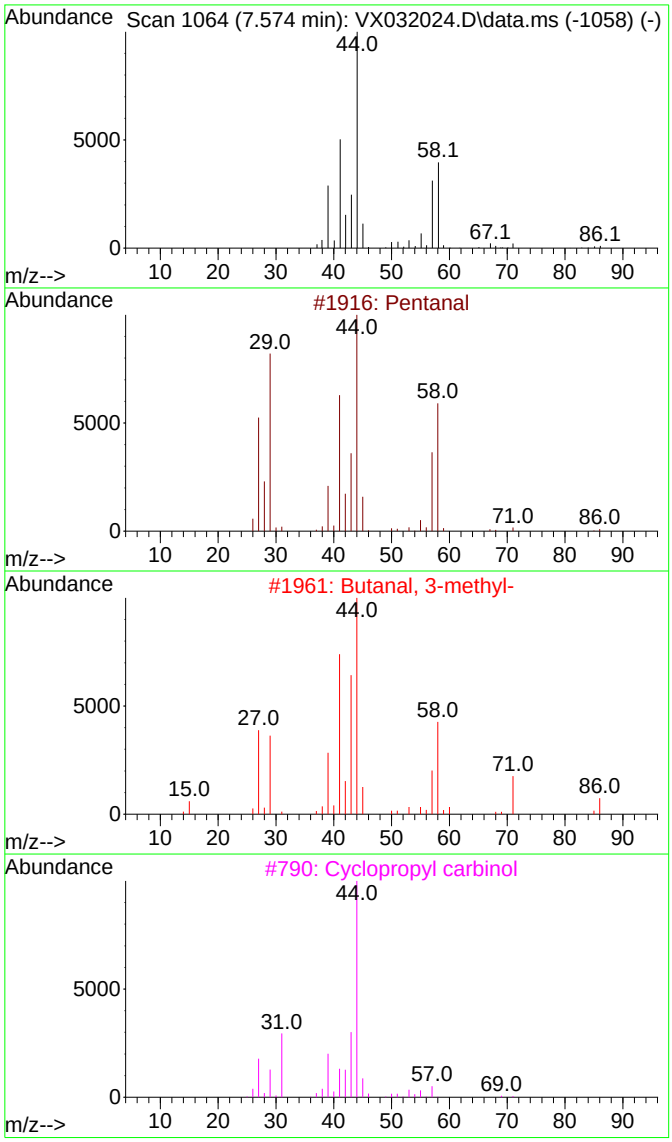
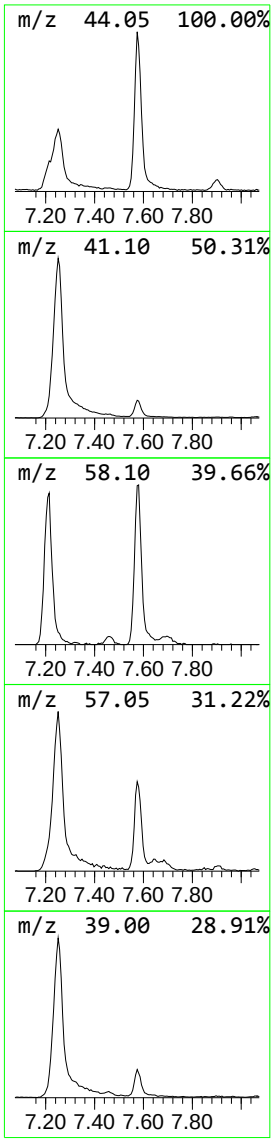
Peak Number 9 Pentanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.574	29.33 ug/l	193684	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	91
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	42
4	Ethanol, 2-(2-propenyloxy)-	102	C5H10O2	000111-45-5	12
5	Ethylene oxide	44	C2H4O	000075-21-8	9





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MSVOA_X
ClientSampleId :
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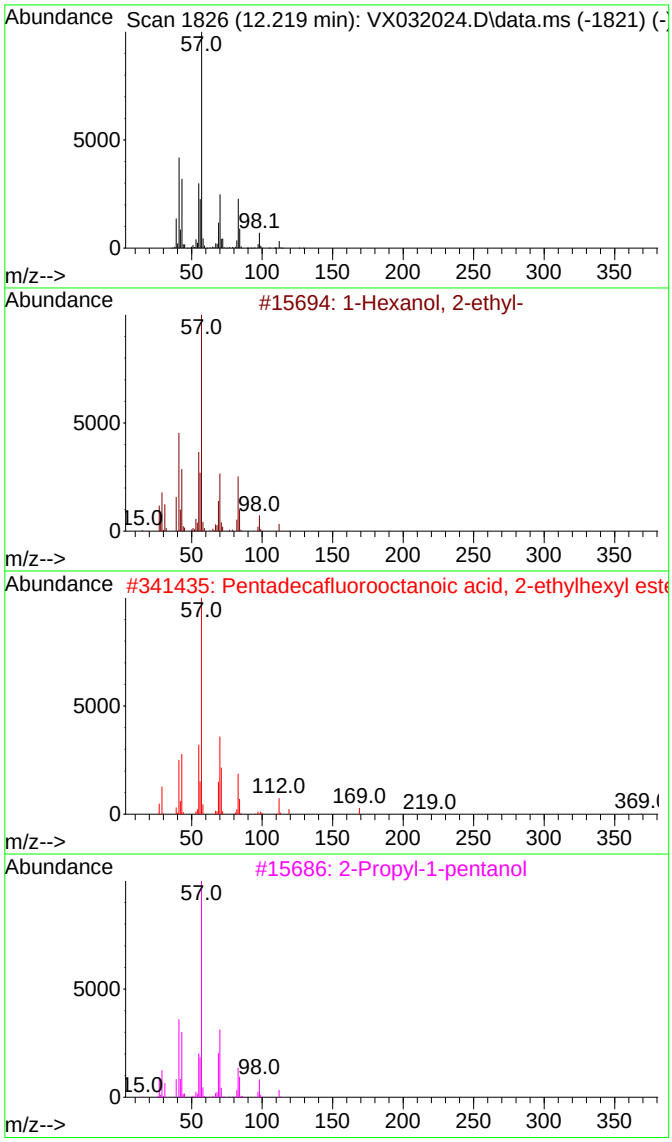
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

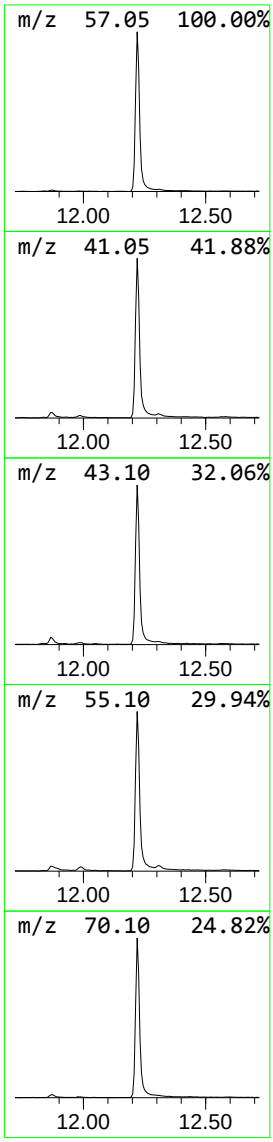
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	319.22 ug/l	3041100	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	90
2	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45





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TIC Integration Parameters: LSCINT.P

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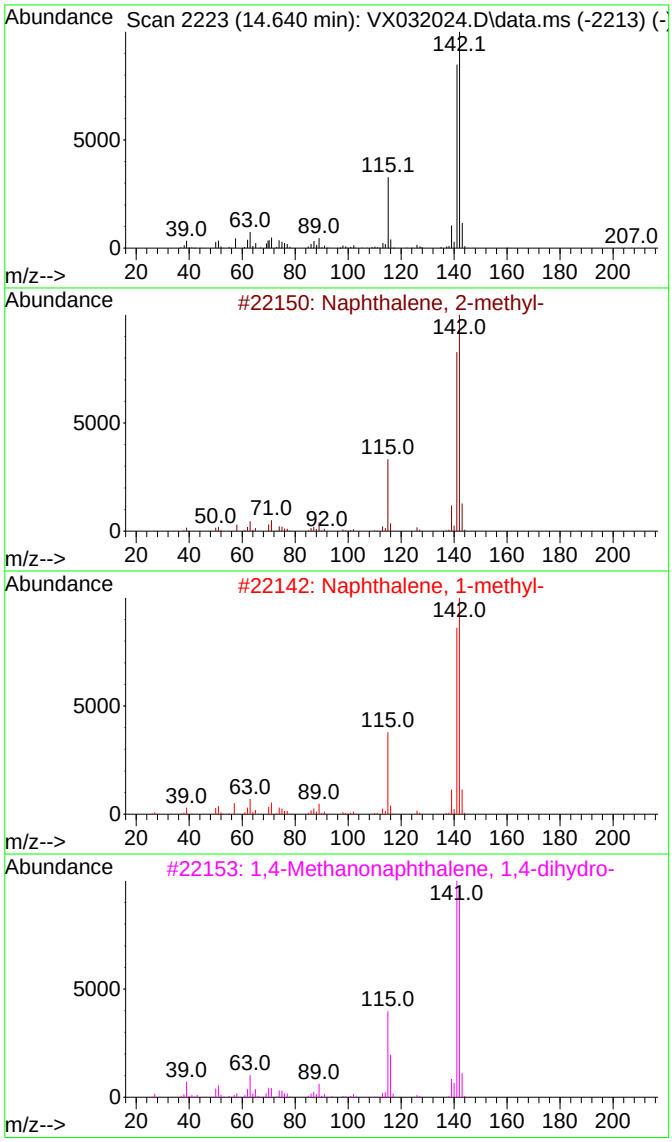
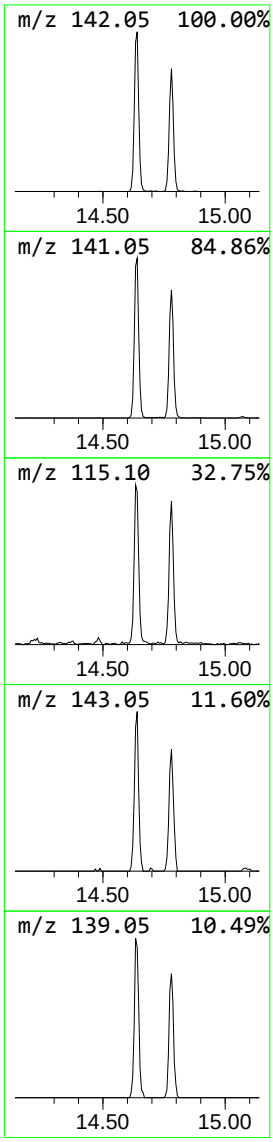
Peak Number 11 Naphthalene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	19.35 ug/l	184360	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101022\
Data File : VX032024.D
Acq On : 10 Oct 2022 19:46
Operator : JC/MD
Sample : N4987-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1678

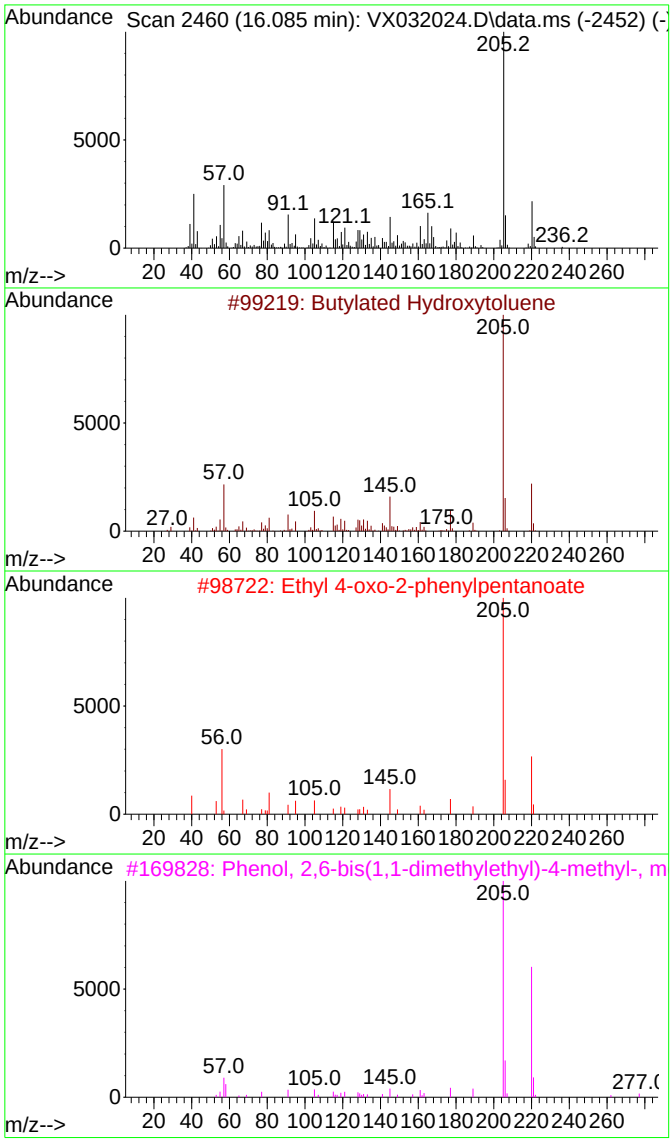
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

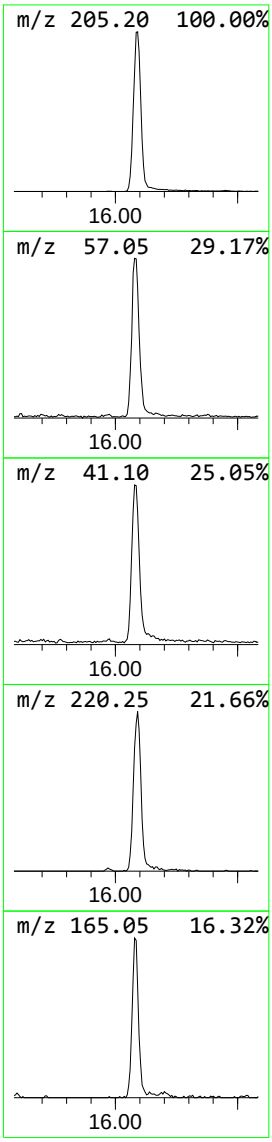
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Butylated Hydroxytoluene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.085	74.86 ug/l	713167	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
2	Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	91
3	Phenol, 2,6-bis(1,1-dimethylethy...	277	C17H27NO2	001918-11-2	83
4	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	70
5	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101022\
Data File : VX032024.D
Acq On : 10 Oct 2022 19:46
Operator : JC/MD
Sample : N4987-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1678

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100622W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	2.172	3553.9	ug/l	15387200	1	5.550	216485	50.0
Propanal	2.288	112.6	ug/l	487696	1	5.550	216485	50.0
Butanal	4.233	1127.4	ug/l	4881240	1	5.550	216485	50.0
1,3-Dioxolane, ...	5.836	511.5	ug/l	2214490	1	5.550	216485	50.0
2-Butenal	6.623	71.3	ug/l	470895	2	6.757	330147	50.0
1,3-Dioxane, 2-...	6.873	197.4	ug/l	1303280	2	6.757	330147	50.0
1-Butanol	7.251	362.0	ug/l	2390390	2	6.757	330147	50.0
Pentanal	7.574	29.3	ug/l	193684	2	6.757	330147	50.0
1-Hexanol, 2-et...	12.219	319.2	ug/l	3041100	4	12.024	476334	50.0
Naphthalene, 1-...	14.640	19.4	ug/l	184360	4	12.024	476334	50.0
Butylated Hydro...	16.085	74.9	ug/l	713167	4	12.024	476334	50.0