LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030143.D
Acq On : 20 Jul 2022 19:32
Operator : JC/MD
Sample : N3775-01 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

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\82X071222W.M
Title : SW846 8260

Signal : TIC: VX030143.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	69	rBV	846605	996972	100.00%	12.336%
2	1.563	71	78	80	rVB7	7861	14281	1.43%	0.177%
3	2.063	155	160	166	rBV	9835	16502	1.66%	0.204%
4	5.391	694	706	722	rBV	107144	317039	31.80%	3.923%
5	5.562	722	734	747	rVB	186012	536904	53.85%	6.643%
6	5.836	768	779	791	rBV2	37238	105752	10.61%	1.309%
7	5.964	791	800	816	rVB	129808	336867	33.79%	4.168%
8	6.769	923	932	944	rBV	313696	754007	75.63%	9.330%
9	8.653	1234	1241	1248	rBV	636419	987068	99.01%	12.214%
10	8.720	1248	1252	1260	rVB	71707	113968	11.43%	1.410%
11	10.055	1464	1471	1480	rBV	626854	844701	84.73%	10.452%
12	11.085	1634	1640	1649	rBV	457959	584728	58.65%	7.235%
13	12.024	1788	1794	1803	rBV	620438	741380	74.36%	9.173%
14	13.695	2062	2068	2074	rBV2	28709	41307	4.14%	0.511%
15	14.048	2116	2126	2132	rBV4	122131	269879	27.07%	3.339%
16	14.109	2132	2136	2147	rVB2	272114	387512	38.87%	4.795%
17	14.225	2147	2155	2158	rBV4	95695	191080	19.17%	2.364%
18	14.329	2166	2172	2176	rBV2	256166	473923	47.54%	5.864%
19	14.371	2176	2179	2182	rVV2	95852	170520	17.10%	2.110%
20	14.402	2182	2184	2201	rVB2	98787	186090	18.67%	2.303%
21	15.493	2358	2363	2368	rVB7	7701	11295	1.13%	0.140%

Sum of corrected areas: 8081775

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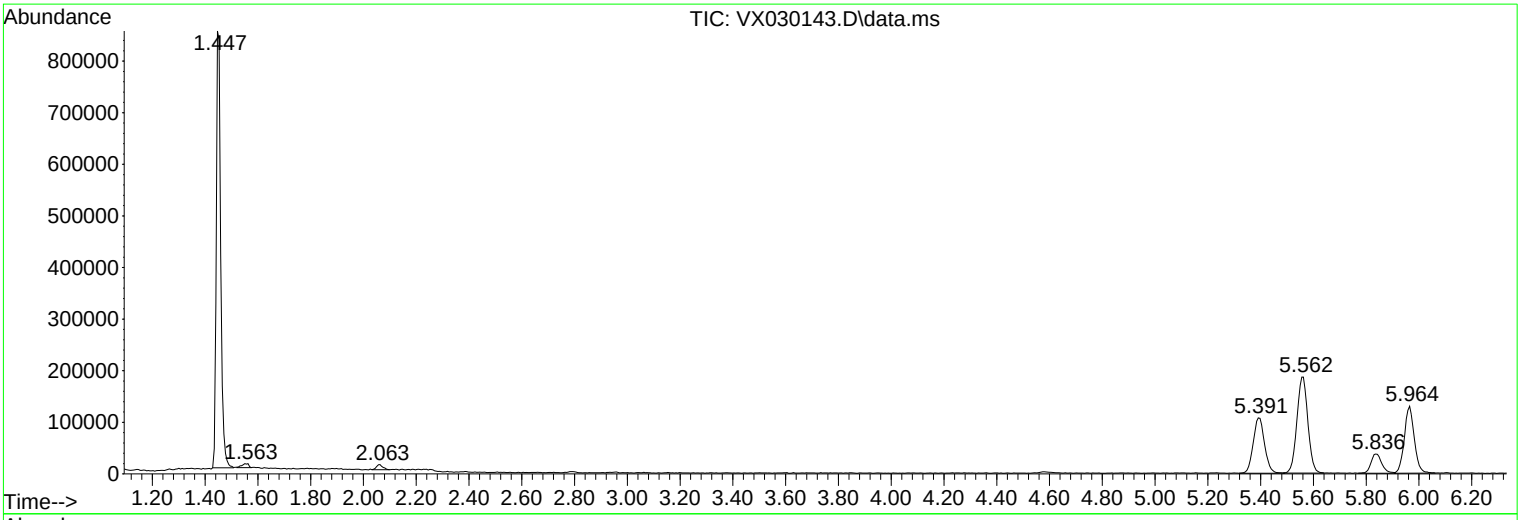
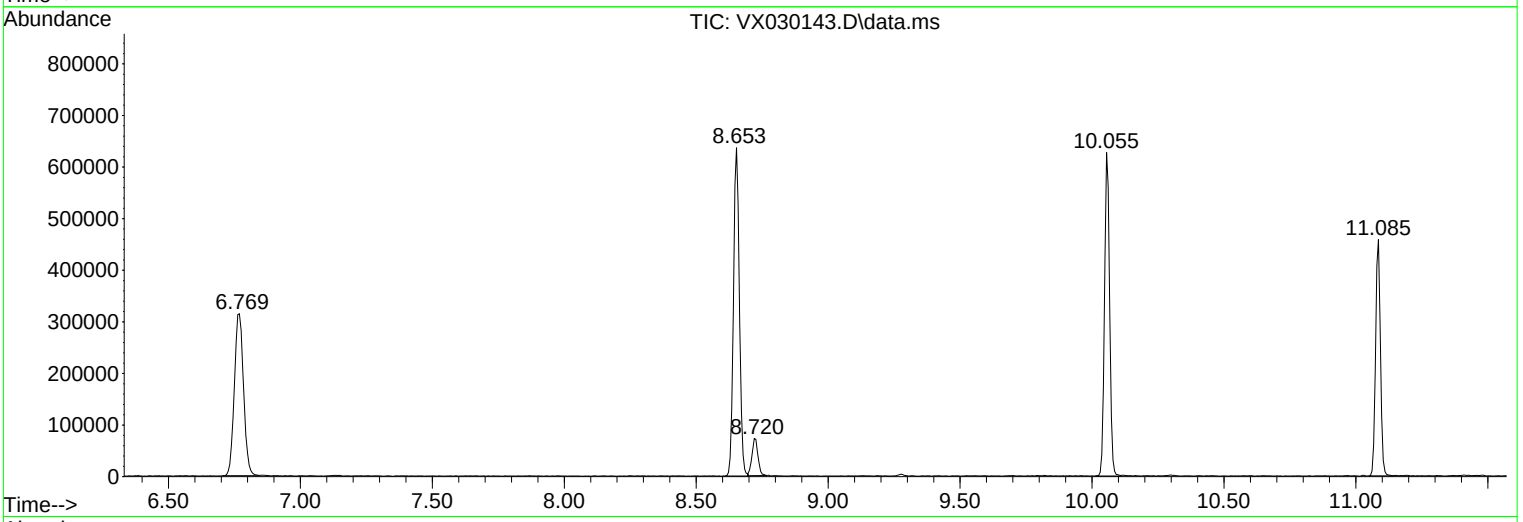
Sample : N3775-01 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

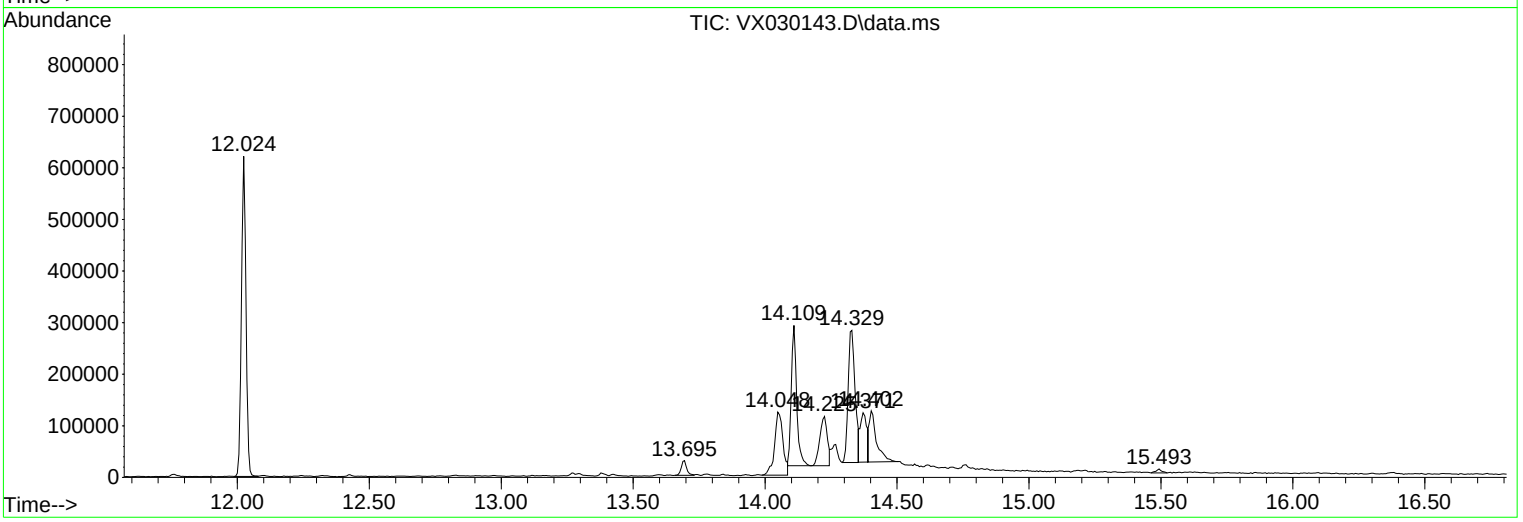
Instrument :
MSVOA_X
ClientSampleId :
M-R-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030143.D
Acq On : 20 Jul 2022 19:32
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

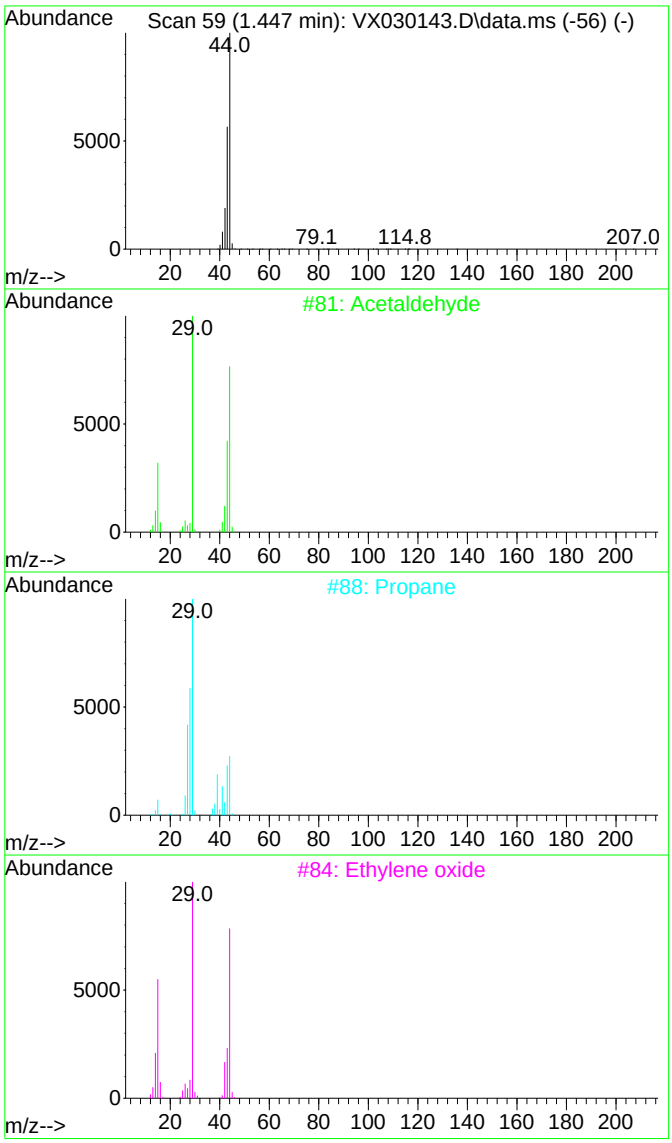
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

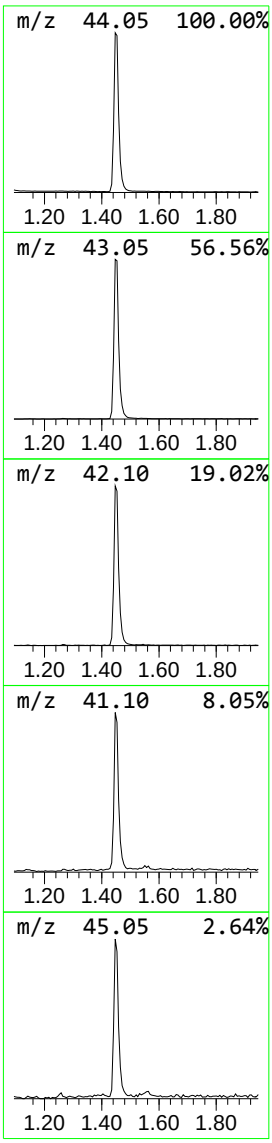
****

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	92.84 ug/l	996972	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Carbon dioxide	44	CO2	000124-38-9	3
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





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Data File : VX030143.D
Acq On : 20 Jul 2022 19:32
Operator : JC/MD
Sample : N3775-01 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

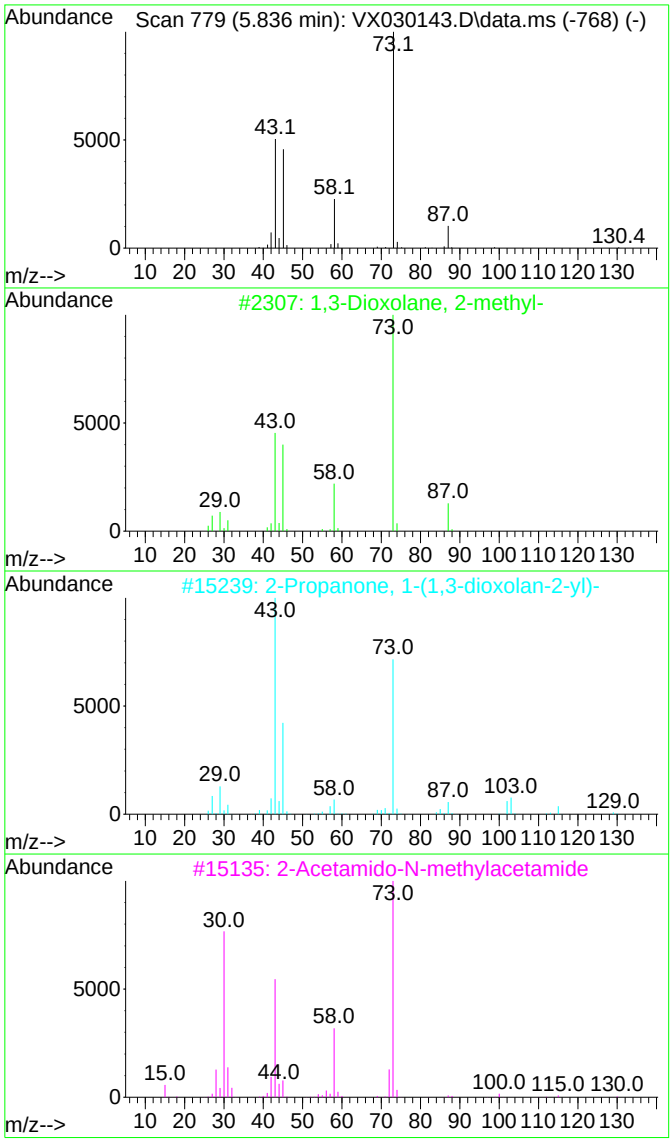
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

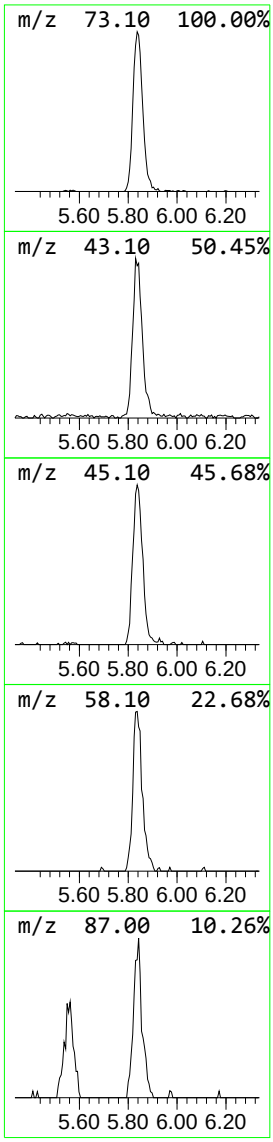
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,3-Dioxolane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.836	9.85 ug/l	105752	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2	2-Propanone, 1-(1,3-dioxolan-2-yl)-	130	C6H10O3	000767-04-4	53
3	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	49
4	Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	36
5	(3S)-3-Pyrrolidinol	87	C4H9NO	100243-39-8	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030143.D
Acq On : 20 Jul 2022 19:32
Operator : JC/MD
Sample : N3775-01 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

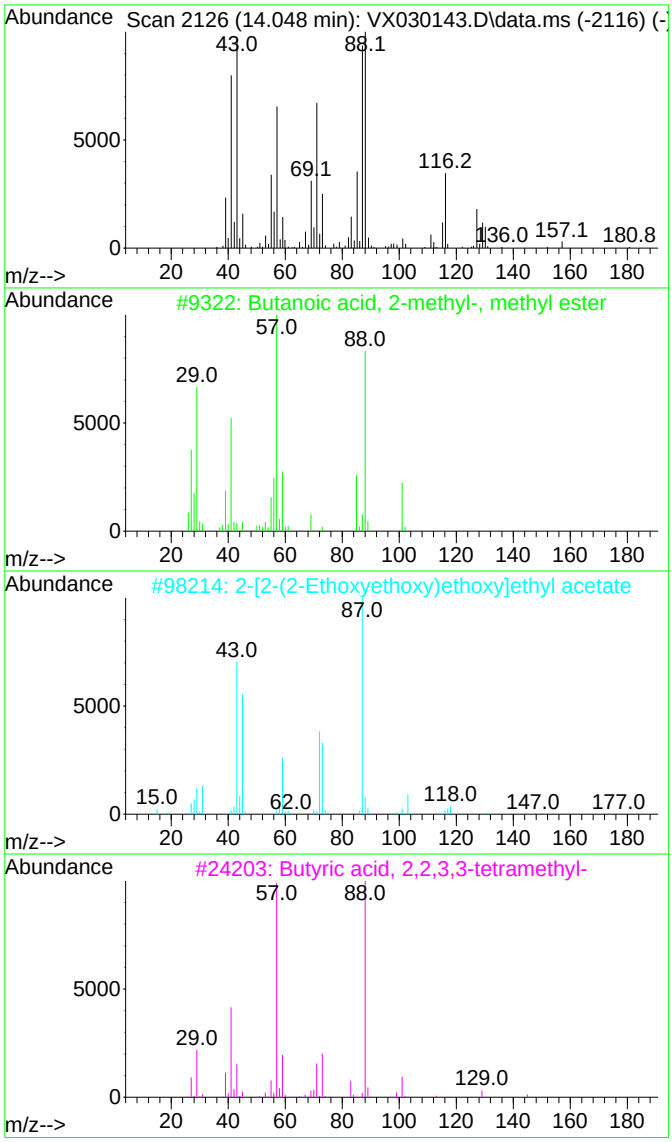
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

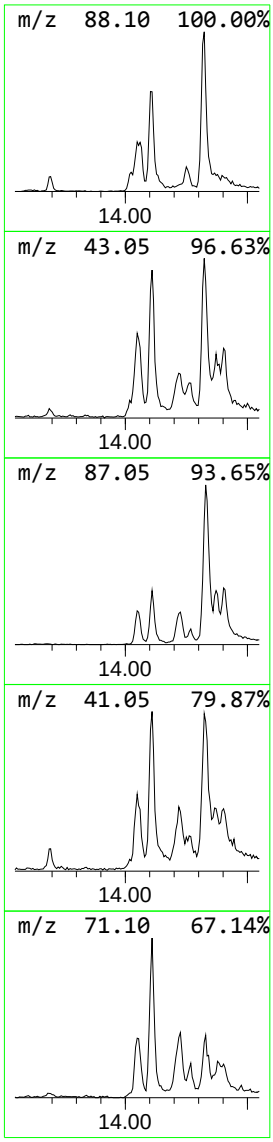
****

Peak Number 3 unknown14.048 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.048	18.20 ug/l	269879	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	27
2	2-[2-(2-Ethoxyethoxy)ethoxy]ethy...	220	C10H20O5	1000351-93-2	27
3	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	27
4	Trimethylsilyl 20-acetoxy-3,6,9,...	454	C19H38O10Si	1000366-93-4	22
5	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030143.D
Acq On : 20 Jul 2022 19:32
Operator : JC/MD
Sample : N3775-01 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

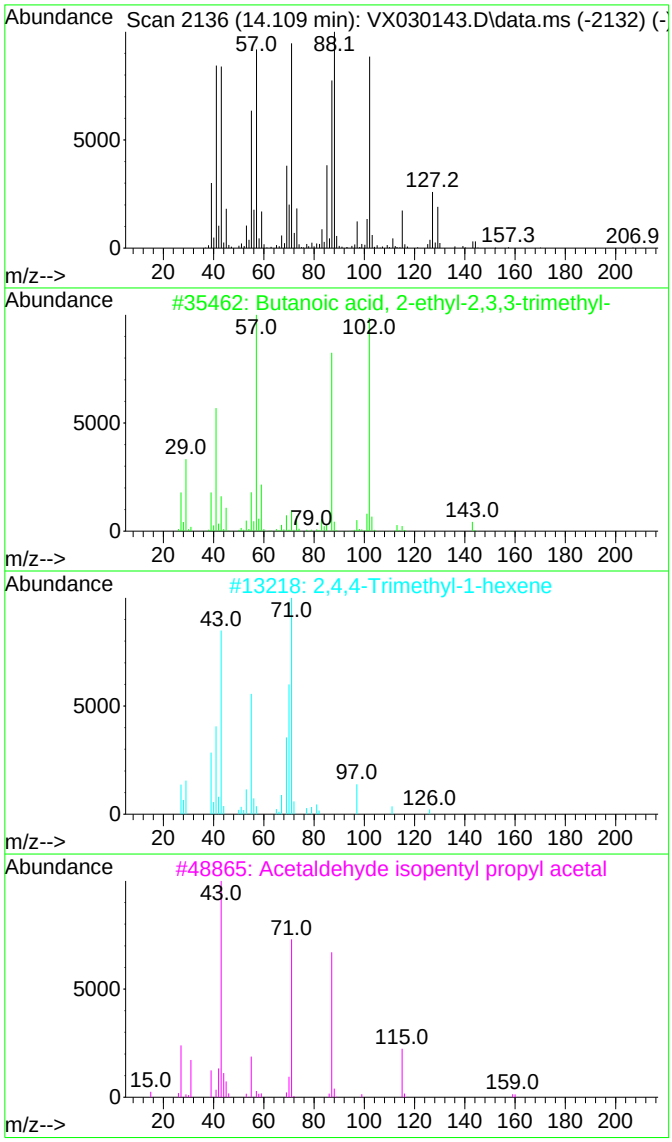
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

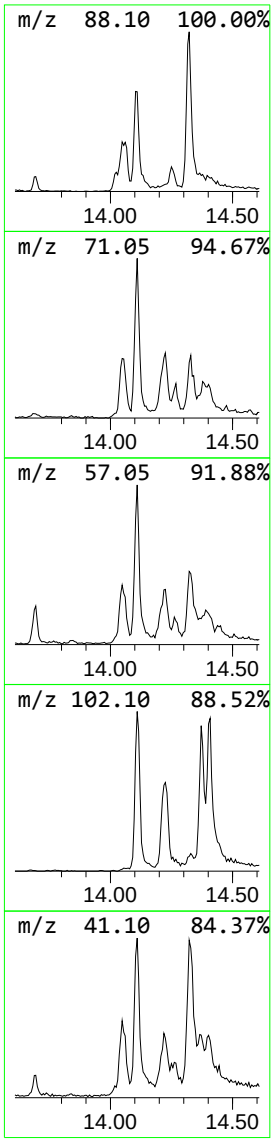
****

Peak Number 4 unknown14.109 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.109	26.13 ug/l	387512	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-2,3,3-tri...	158	C9H18O2	038541-67-2	27
2	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	25
3	Acetaldehyde isopentyl propyl ac...	174	C10H22O2	1000431-62-2	22
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	18
5	Butanoic acid, 3-methyl-, ethyl ...	130	C7H14O2	000108-64-5	15





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030143.D
Acq On : 20 Jul 2022 19:32
Operator : JC/MD
Sample : N3775-01 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

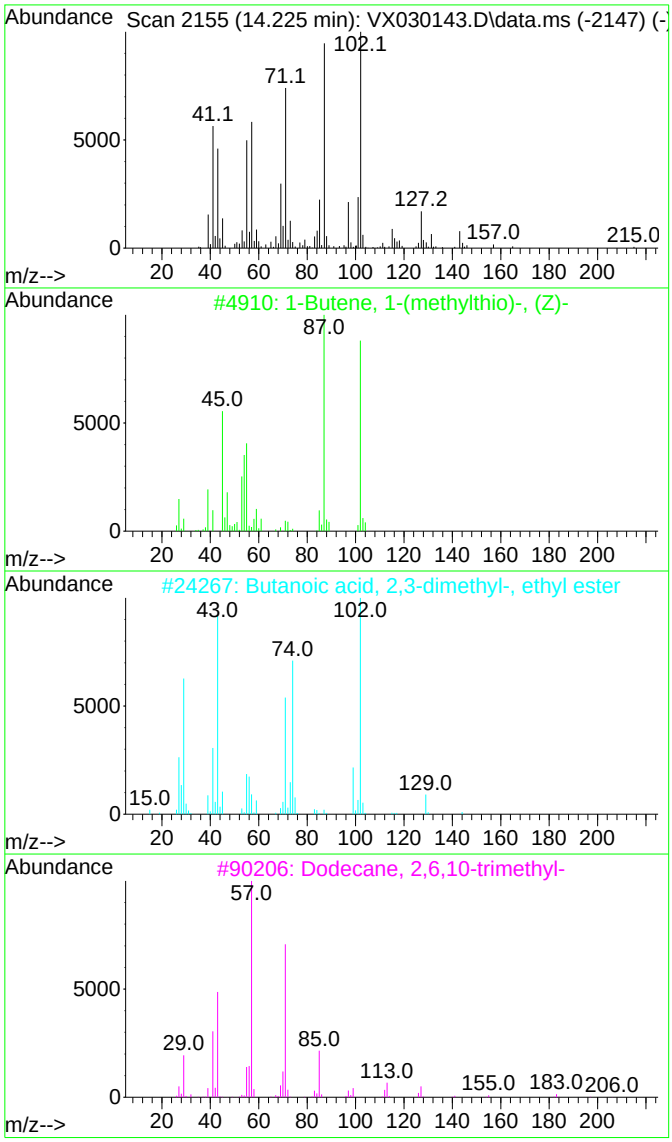
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

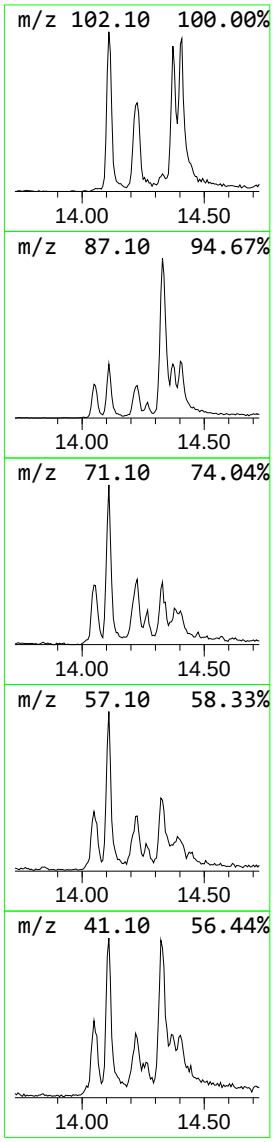
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown14.225 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.225	12.89 ug/l	191080	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	38
2	Butanoic acid, 2,3-dimethyl-, et...	144	C8H16O2	054004-42-1	22
3	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	14
4	5-Hydroxy-2,2-dimethylhexan-3-one	144	C8H16O2	173343-33-4	14
5	Sulfurous acid, pentyl undecyl e...	306	C16H34O3S	1000309-14-4	14





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
Data File : VX030143.D
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Operator : JC/MD
Sample : N3775-01 200X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

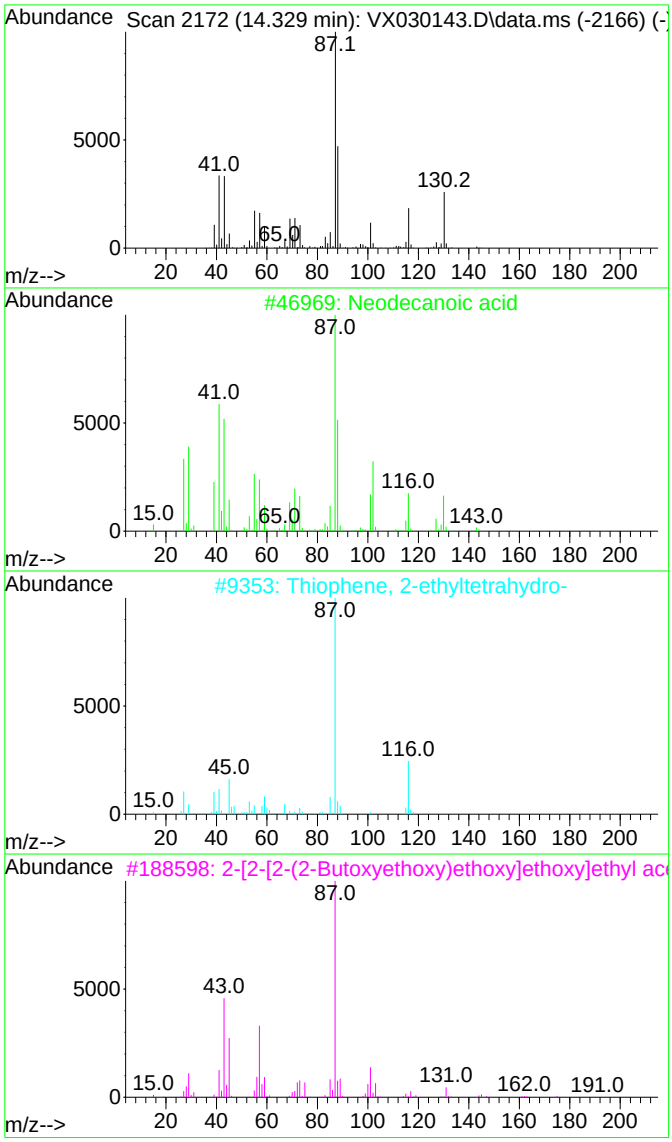
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

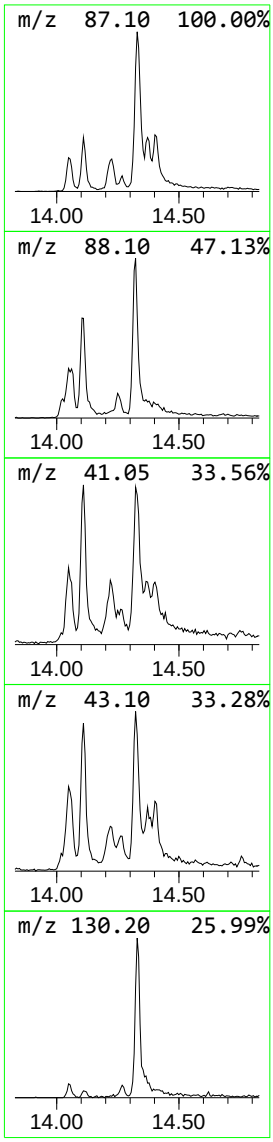
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown14.329 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	31.96 ug/l	473923	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neodecanoic acid	172	C10H20O2	026896-20-8	43
2	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	43
3	2-[2-[2-(2-Butoxyethoxy)ethoxy]e...	292	C14H28O6	1000351-93-9	43
4	3-Pentanol, 2,3,4-trimethyl-	130	C8H18O	003054-92-0	37
5	Thiophane, propyl-	130	C7H14S	001551-34-4	37





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

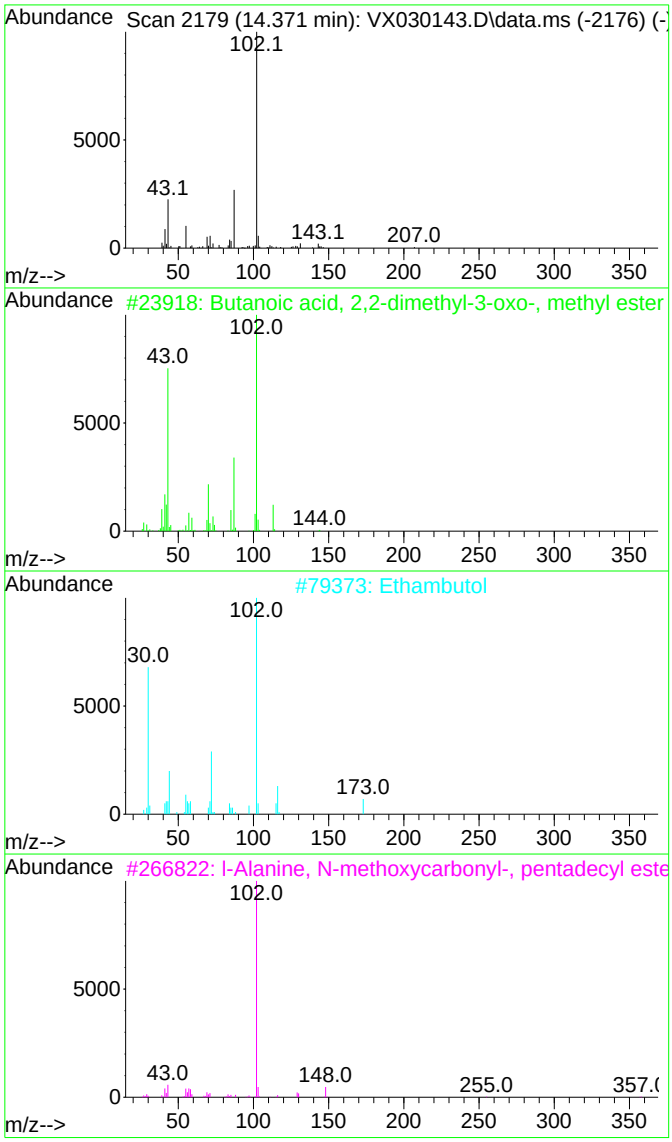
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

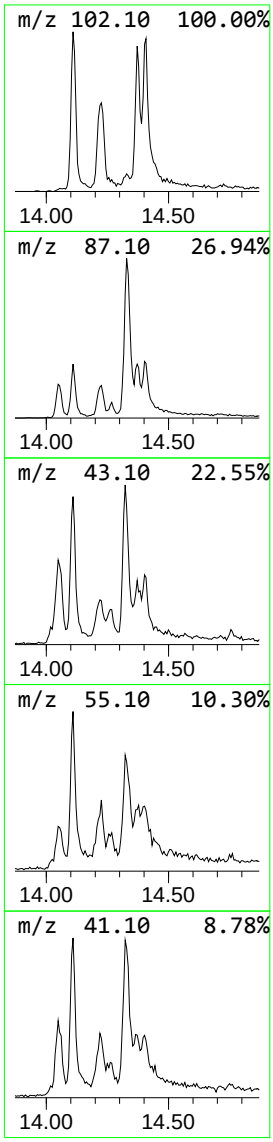
****

Peak Number 7 unknown14.371 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.371	11.50 ug/l	170520	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2,2-dimethyl-3-ox...	144	C7H12O3	038923-57-8	39
2	Ethambutol	204	C10H24N2O2	000074-55-5	36
3	l-Alanine, N-methoxycarbonyl-, p...	357	C20H39NO4	1000313-38-3	33
4	l-Alanine, N-methoxycarbonyl-, o...	399	C23H45NO4	1000313-38-6	33
5	l-Alanine, N-methoxycarbonyl-, t...	343	C19H37NO4	1000313-38-2	33





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Instrument :
MSVOA_X
ClientSampleId :
M-R-1

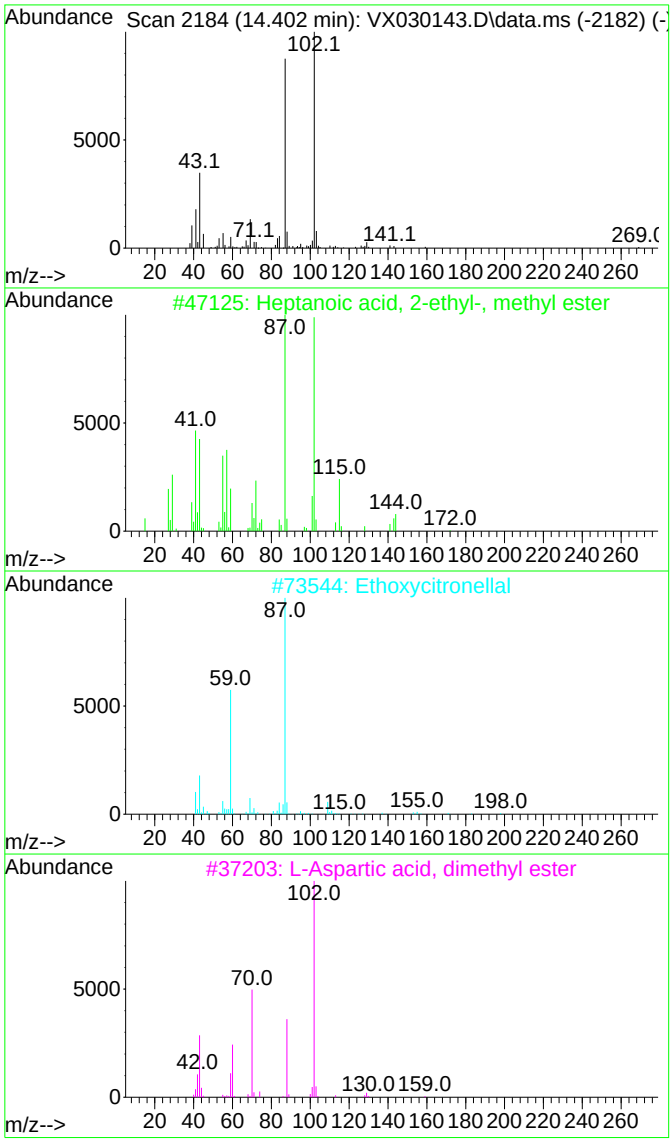
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

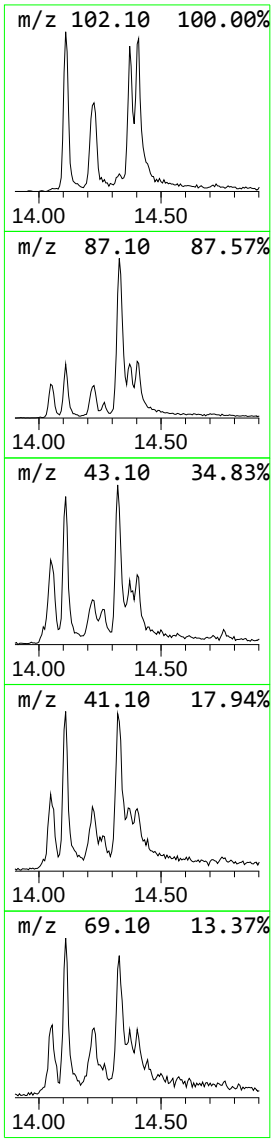
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptanoic acid, 2-ethyl-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.402	12.55 ug/l	186090	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid, 2-ethyl-, methyl...	172	C10H20O2	000816-63-7	56
2	Ethoxycitronellal	198	C12H22O2	1000132-02-6	32
3	L-Aspartic acid, dimethyl ester	161	C6H11NO4	006384-18-5	25
4	2-[2-[2-[2-[2-[2-[2-(2-Acetyl...	498	C22H42O12	1010351-90-5	25
5	Arachidamide, N-ethyl-	339	C22H45NO	1000420-44-1	25





Tentatively Identified Compound (LSC) summary

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M-R-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.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 #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
Acetaldehyde	1.447	92.8	ug/l	996972	1	5.556	536904	50.0
1,3-Dioxolane, ...	5.836	9.8	ug/l	105752	1	5.556	536904	50.0
unknown14.048	14.048	18.2	ug/l	269879	4	12.024	741380	50.0
unknown14.109	14.109	26.1	ug/l	387512	4	12.024	741380	50.0
unknown14.225	14.225	12.9	ug/l	191080	4	12.024	741380	50.0
unknown14.329	14.329	32.0	ug/l	473923	4	12.024	741380	50.0
unknown14.371	14.371	11.5	ug/l	170520	4	12.024	741380	50.0
Heptanoic acid,...	14.402	12.6	ug/l	186090	4	12.024	741380	50.0