LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041408.D
Acq On : 07 May 2024 15:50
Operator : JC/MD
Sample : P2389-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

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\82X043024W.M
Title : SW846 8260

Signal : TIC: VX041408.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	68	rBV	923014	1326522	45.78%	10.620%
2	1.557	71	77	106	rVV	135320	730944	25.22%	5.852%
3	1.739	106	107	127	rVB3	14628	44287	1.53%	0.355%
4	2.154	164	175	187	rVB2	22643	84947	2.93%	0.680%
5	2.300	193	199	208	rBV	24410	45629	1.57%	0.365%
6	2.398	208	215	239	rVB	71138	170164	5.87%	1.362%
7	4.385	531	541	554	rBV	76507	242879	8.38%	1.944%
8	5.385	693	705	721	rBV	87212	257244	8.88%	2.059%
9	5.550	721	732	750	rVB	163622	470772	16.25%	3.769%
10	5.952	789	798	823	rVB	91189	251601	8.68%	2.014%
11	6.757	921	930	940	rBV	239180	582651	20.11%	4.665%
12	6.879	940	950	979	rVB	1118359	2897796	100.00%	23.199%
13	7.214	997	1005	1028	rBV	145562	369236	12.74%	2.956%
14	8.647	1234	1240	1250	rBV	400402	622170	21.47%	4.981%
15	9.000	1292	1298	1314	rBV	65603	107153	3.70%	0.858%
16	10.055	1465	1471	1486	rBV	425656	604501	20.86%	4.840%
17	10.988	1618	1624	1633	rBV	35980	58314	2.01%	0.467%
18	11.079	1633	1639	1649	rVV2	413024	543271	18.75%	4.349%
19	11.195	1653	1658	1669	rVB	38743	51973	1.79%	0.416%
20	11.689	1734	1739	1747	rBV	20555	29353	1.01%	0.235%
21	12.024	1789	1794	1803	rVB	458220	606732	20.94%	4.857%
22	12.219	1821	1826	1837	rBV	37502	60410	2.08%	0.484%
23	12.768	1911	1916	1927	rBV	1944855	2332264	80.48%	18.672%

Sum of corrected areas: 12490813

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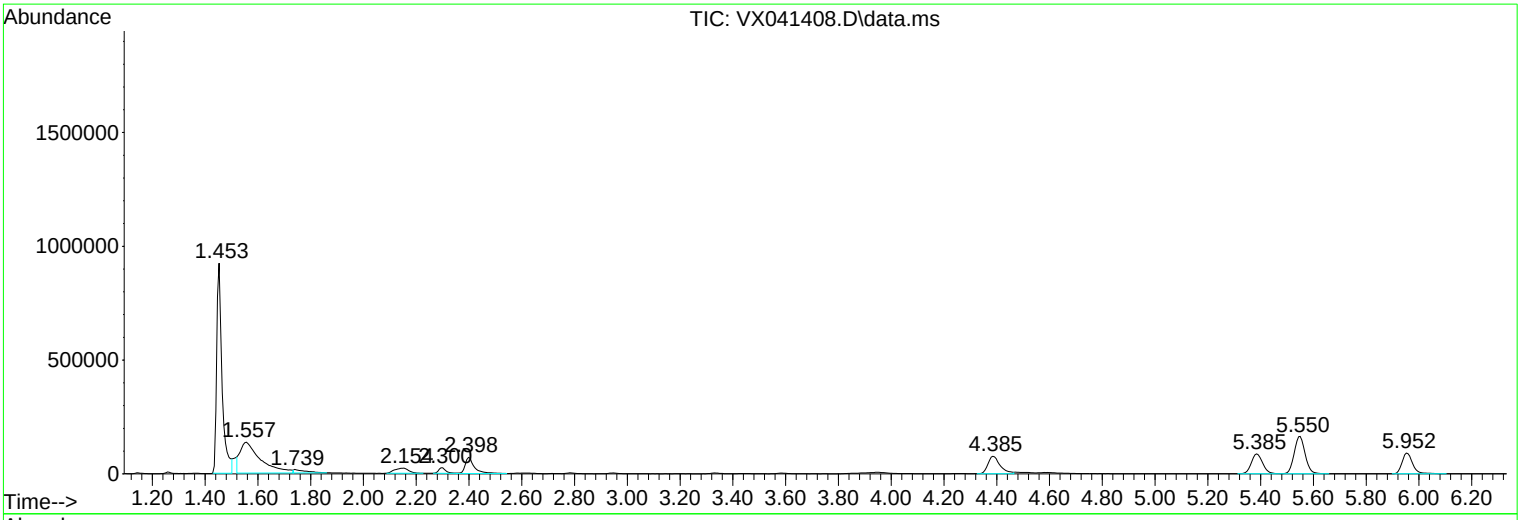
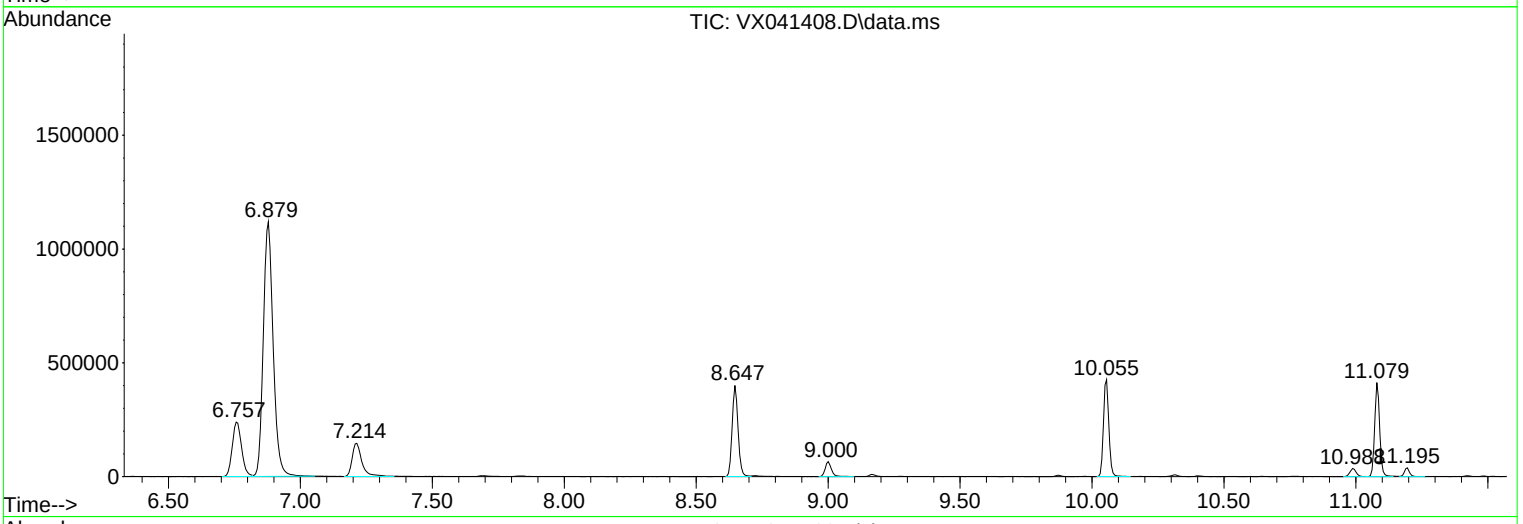
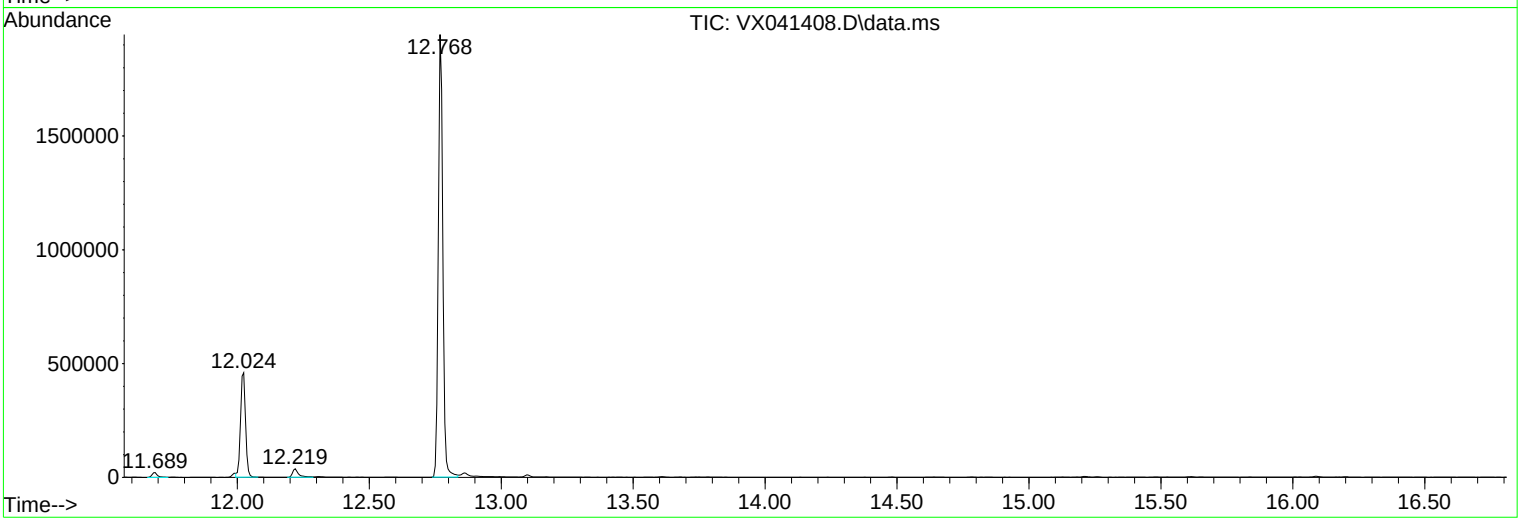
Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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







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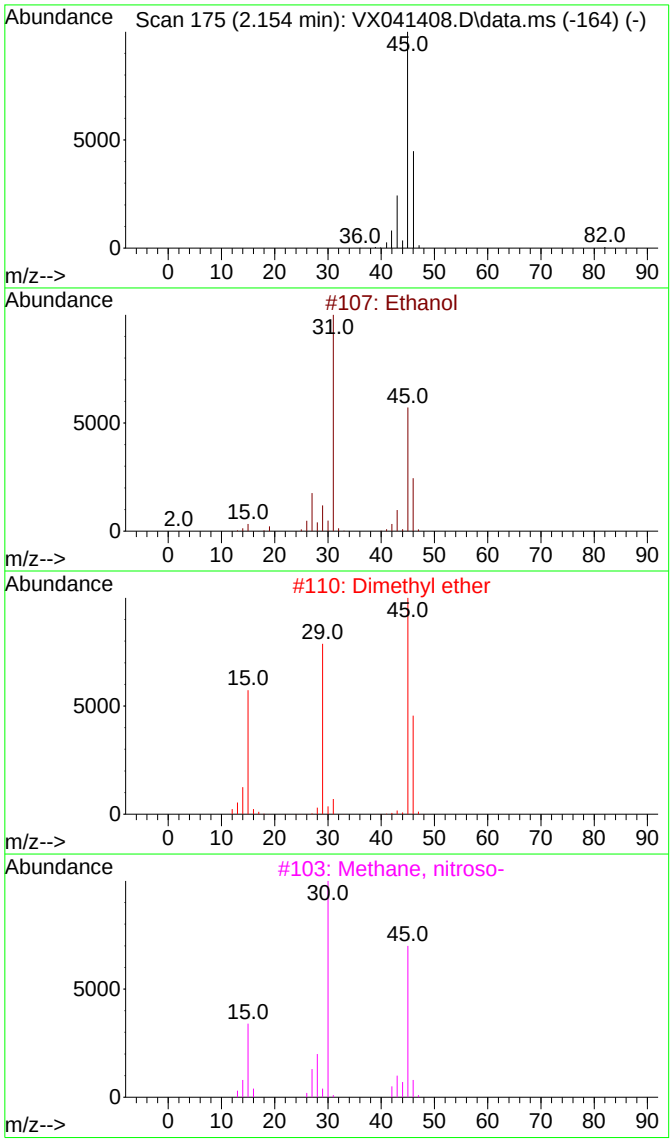
Quant Title : SW846 8260

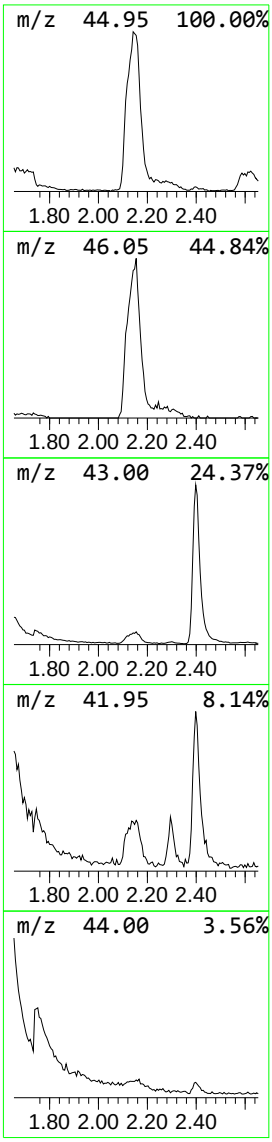
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.154	9.02 ug/l	84947	Pentafluorobenzene	5.550

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 : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

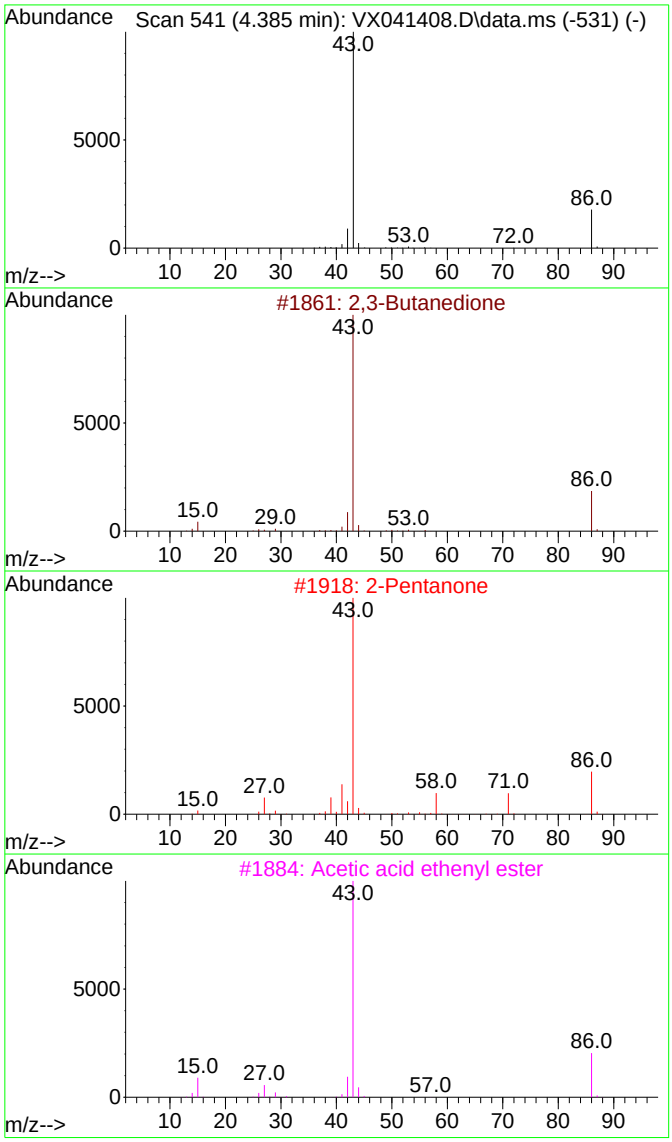
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

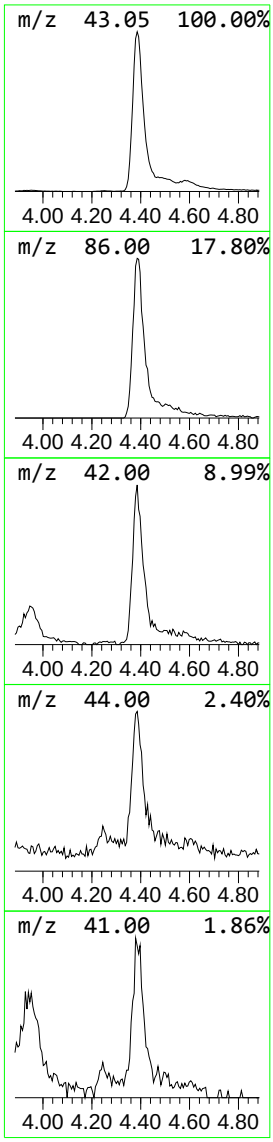
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,3-Butanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.385	25.80 ug/l	242879	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	80
2	2-Pentanone	86	C5H10O	000107-87-9	9
3	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9
4	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7
5	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	5





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

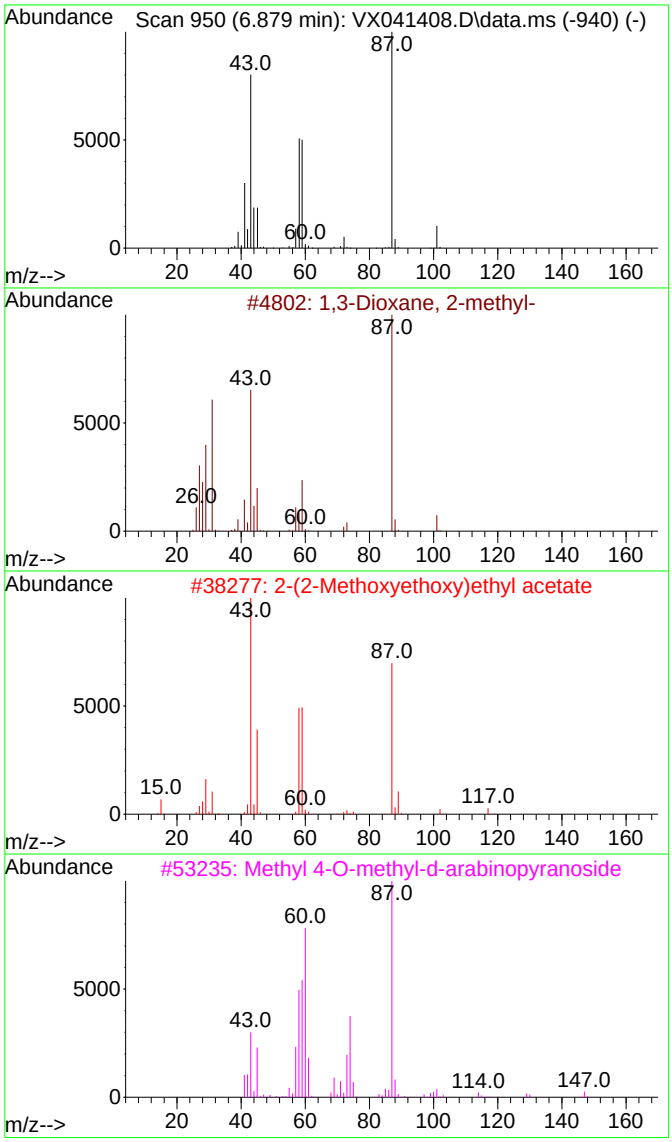
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

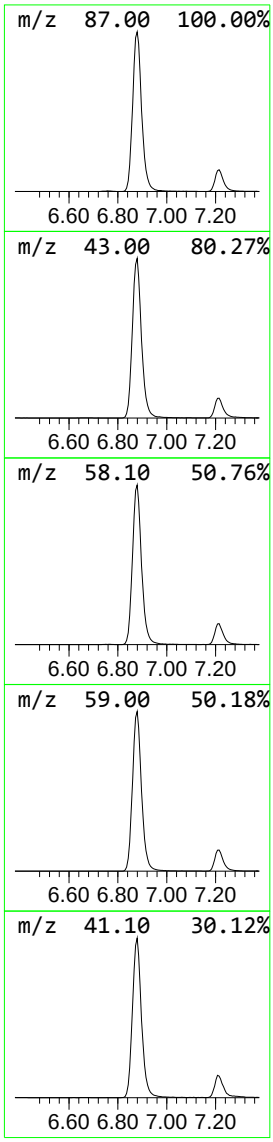
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	248.67 ug/l	2897800	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	50
2	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
5	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
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Instrument :
MSVOA_X
ClientSampleId :
1400

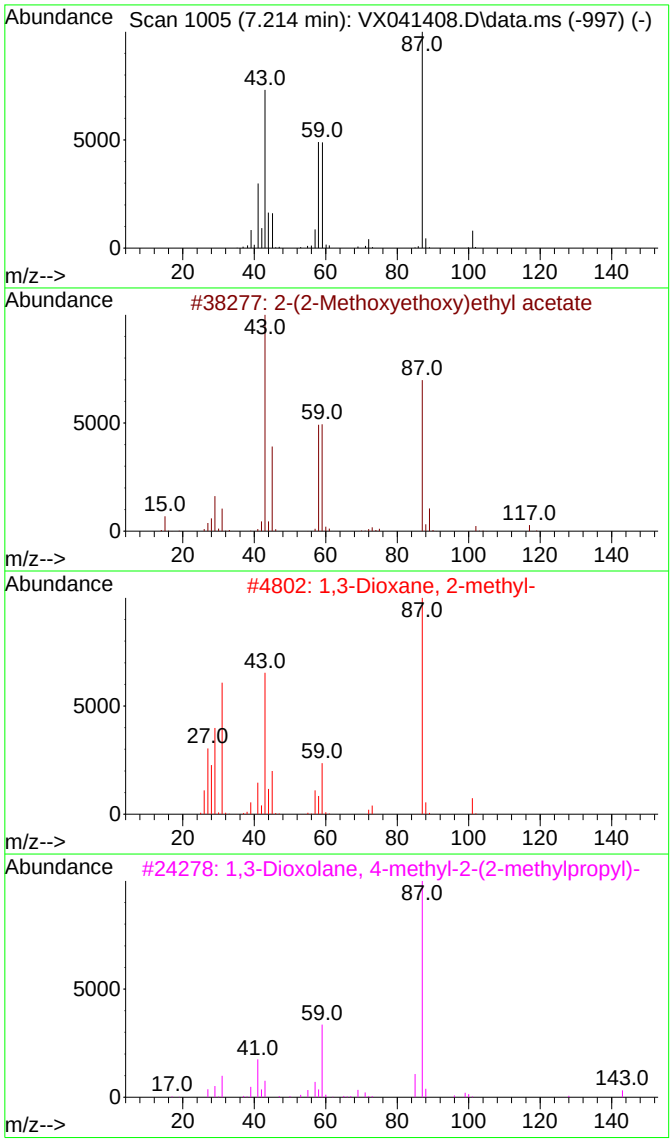
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

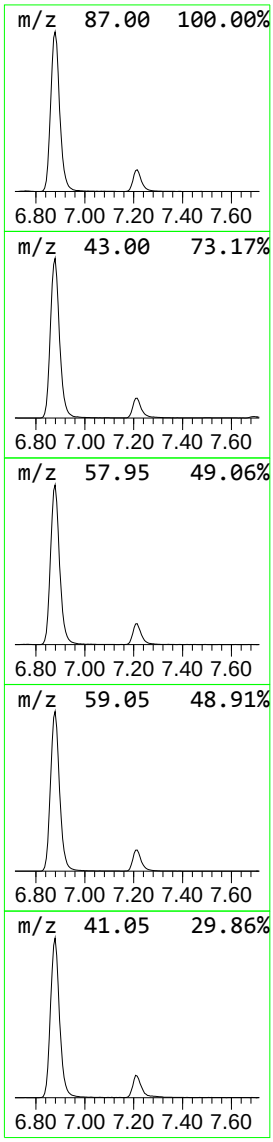
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	31.69 ug/l	369236	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	50
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	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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Operator : JC/MD
Sample : P2389-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

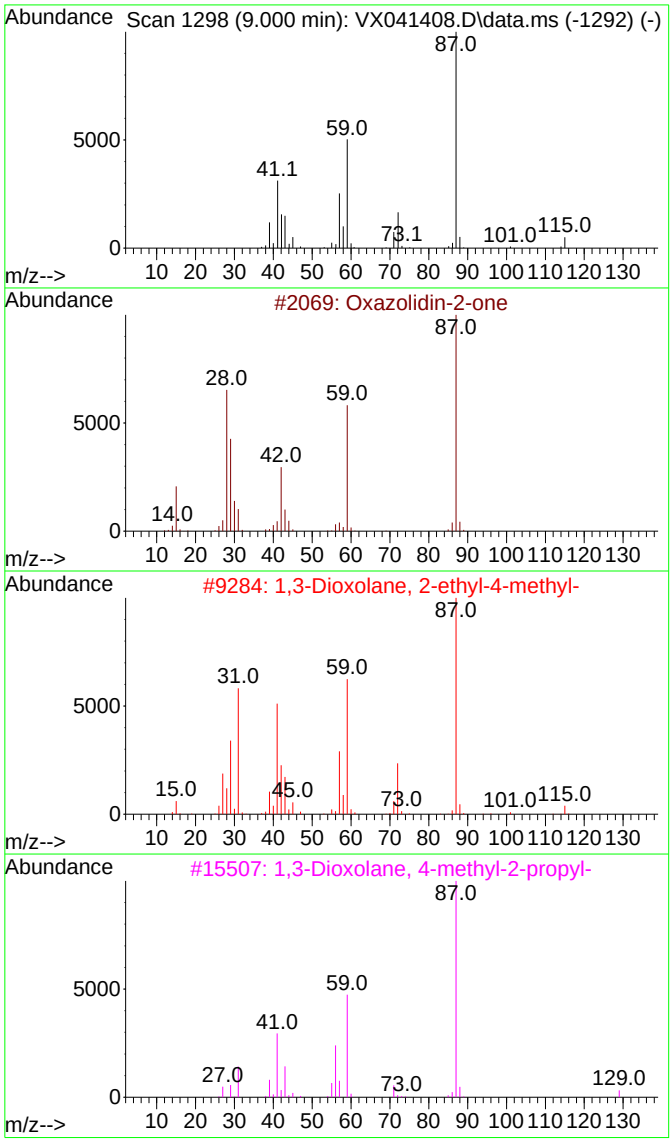
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

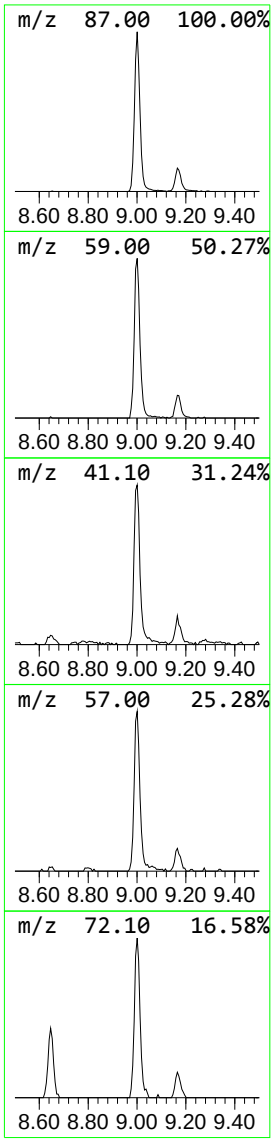
****

Peak Number 7 Oxazolidin-2-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	8.86 ug/l	107153	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
2	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	59
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
4	2-[2-[2-(2-Methoxyethoxy)ethoxy]...	250	C11H22O6	1000351-91-4	59
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	56





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1400

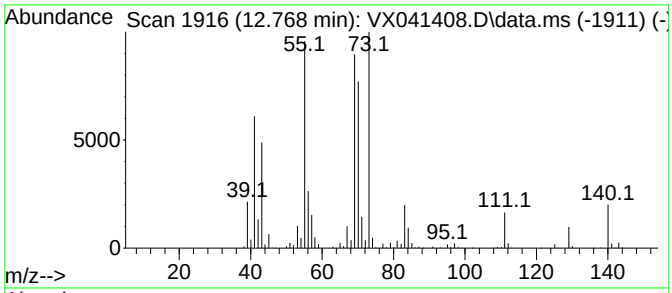
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

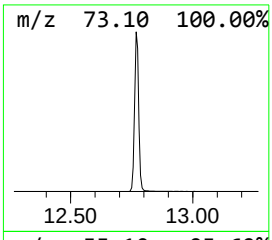
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

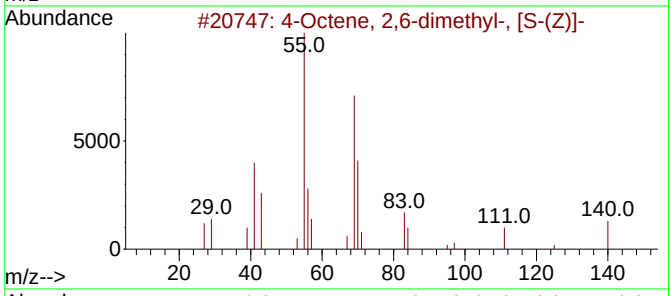
****
Peak Number 8 4-Octene, 2,6-dimethyl-, [S... Concentration Rank 2

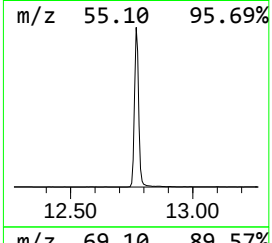
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	192.20 ug/l	2332260	1,4-Dichlorobenzene-d4	12.024

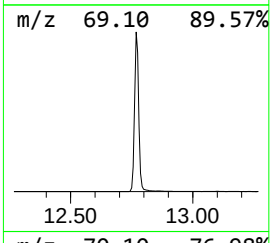
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Octene, 2,6-dimethyl-, [S-(Z)]-	140	C10H20	062960-77-4	74
2	Cyclohexane, 1,2,3-trimethyl-, (...	126	C9H18	001839-88-9	72
3	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	64
4	3-Octene, 4-ethyl-	140	C10H20	053966-51-1	62
5	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	58

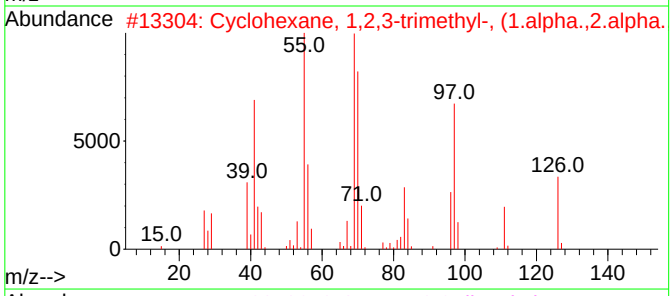


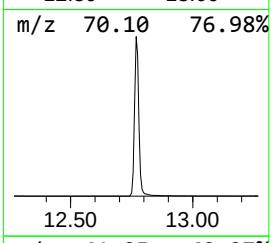


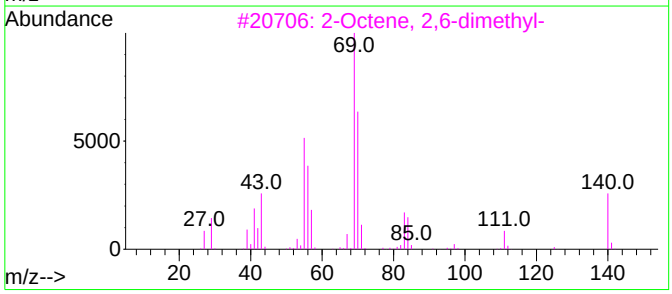


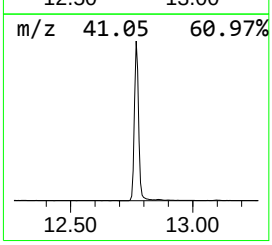












Tentatively Identified Compound (LSC) summary

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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	2.154	9.0	ug/l	84947	1	5.550	470772	50.0
2,3-Butanedione	4.385	25.8	ug/l	242879	1	5.550	470772	50.0
1,3-Dioxane, 2-...	6.879	248.7	ug/l	2897800	2	6.757	582651	50.0
2-(2-Methoxyeth...	7.214	31.7	ug/l	369236	2	6.757	582651	50.0
Oxazolidin-2-one	9.000	8.9	ug/l	107153	3	10.055	604501	50.0
4-Octene, 2,6-d...	12.768	192.2	ug/l	2332260	4	12.024	606732	50.0