LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020224\
Data File : VX040079.D
Acq On : 02 Feb 2024 12:12
Operator : JC/MD
Sample : P1284-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1142

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\82X013024W.M
Title : SW846 8260

Signal : TIC: VX040079.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	71	rBV	647482	744293	8.04%	3.512%
2	2.056	152	159	171	rBV	83138	140891	1.52%	0.665%
3	2.239	183	189	192	rBV	105543	163645	1.77%	0.772%
4	2.294	192	198	207	rVV	5972727	9262980	100.00%	43.707%
5	2.380	207	212	232	rVV	370890	733731	7.92%	3.462%
6	3.331	358	368	380	rBV	41408	97118	1.05%	0.458%
7	3.891	438	460	477	rBV	1116426	3487906	37.65%	16.457%
8	4.233	506	516	533	rBV	292131	760033	8.21%	3.586%
9	4.556	561	569	583	rBV	77334	214619	2.32%	1.013%
10	5.385	695	705	717	rVB3	57971	169934	1.83%	0.802%
11	5.550	722	732	750	rVB	99637	281784	3.04%	1.330%
12	5.952	789	798	811	rBV	71506	187269	2.02%	0.884%
13	6.763	922	931	945	rVB	161287	385436	4.16%	1.819%
14	7.208	996	1004	1013	rBV	61367	143283	1.55%	0.676%
15	8.647	1234	1240	1249	rBV	340434	526220	5.68%	2.483%
16	10.055	1462	1471	1484	rBV2	362840	591178	6.38%	2.789%
17	10.506	1539	1545	1554	rBV	73425	99756	1.08%	0.471%
18	10.683	1569	1574	1580	rVB	146042	184710	1.99%	0.872%
19	10.768	1582	1588	1596	rBV2	76502	114713	1.24%	0.541%
20	11.079	1634	1639	1645	rBV	303771	389661	4.21%	1.839%
21	11.152	1645	1651	1661	rVB	241383	311278	3.36%	1.469%
22	11.567	1713	1719	1723	rBV	78718	106856	1.15%	0.504%
23	11.951	1778	1782	1785	rBV	124604	170324	1.84%	0.804%
24	11.988	1785	1788	1791	rVV	297313	393498	4.25%	1.857%
25	12.018	1791	1793	1802	rVB	395926	501037	5.41%	2.364%
26	12.219	1818	1826	1837	rBV	624832	911568	9.84%	4.301%
27	12.951	1941	1946	1952	rBV	91769	119807	1.29%	0.565%

Sum of corrected areas: 21193528

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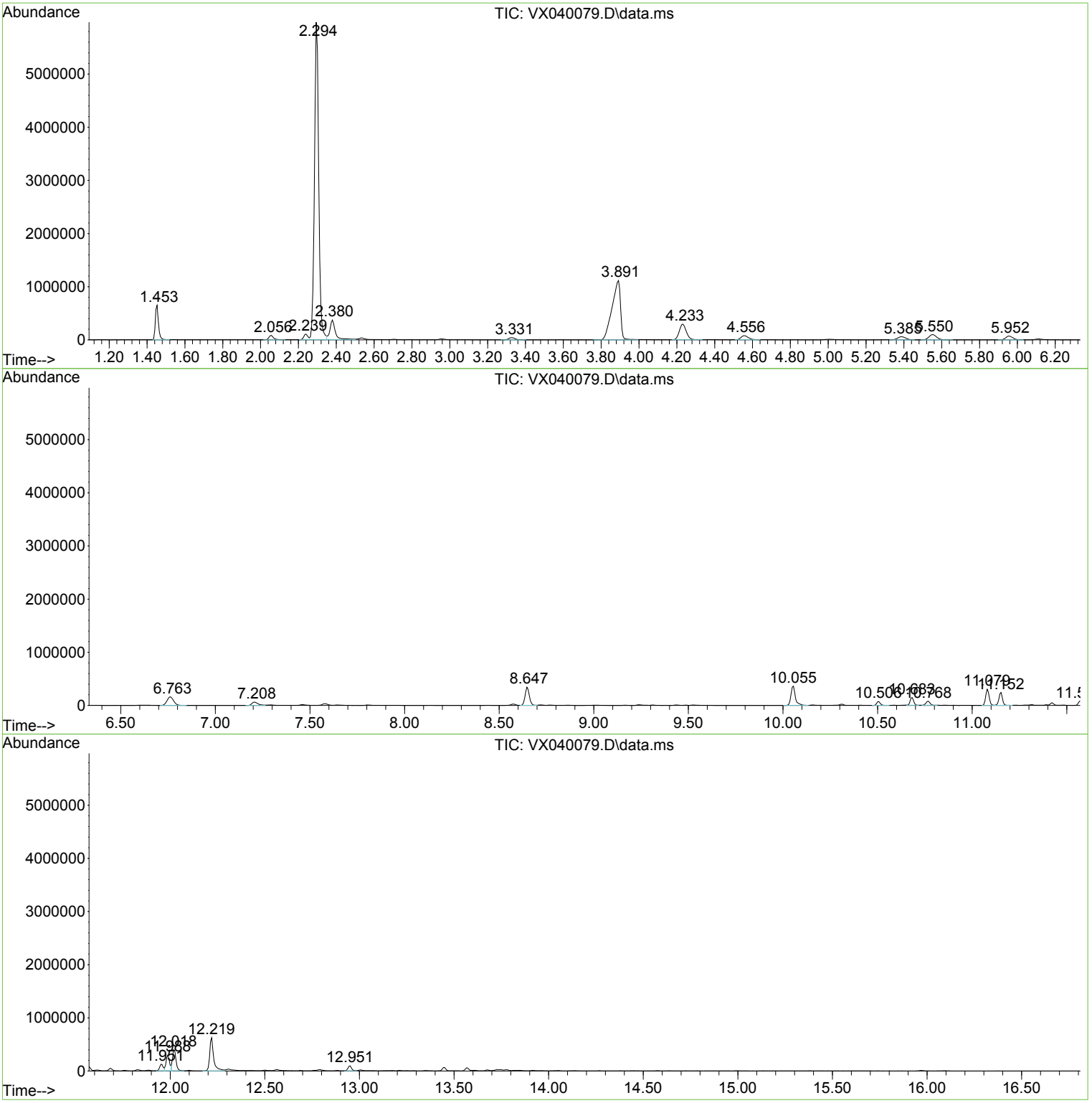
MSVOA_X
ClientSampleId :
1142

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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



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Data File : VX040079.D
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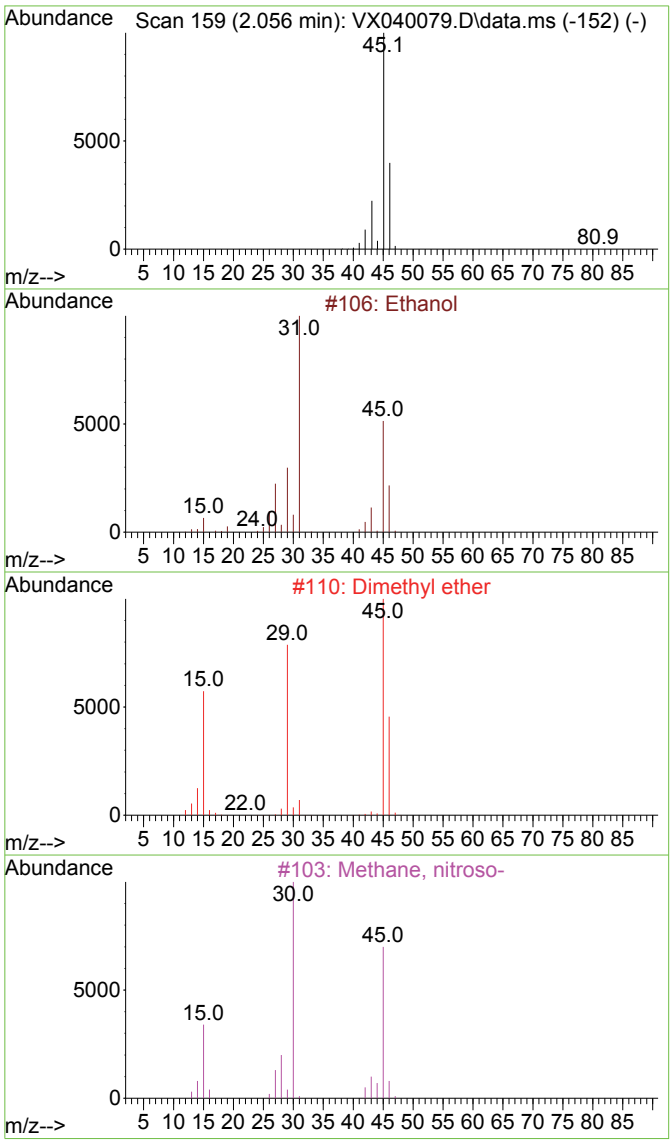
Quant Title : SW846 8260

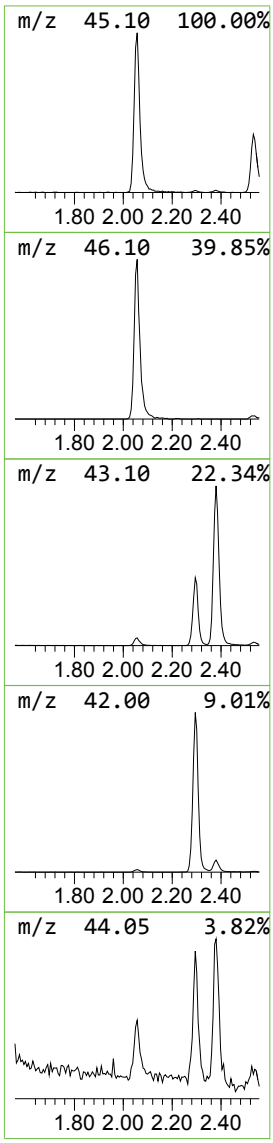
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	25.00 ug/l	140891	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	90
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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Instrument :
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ClientSampleId :
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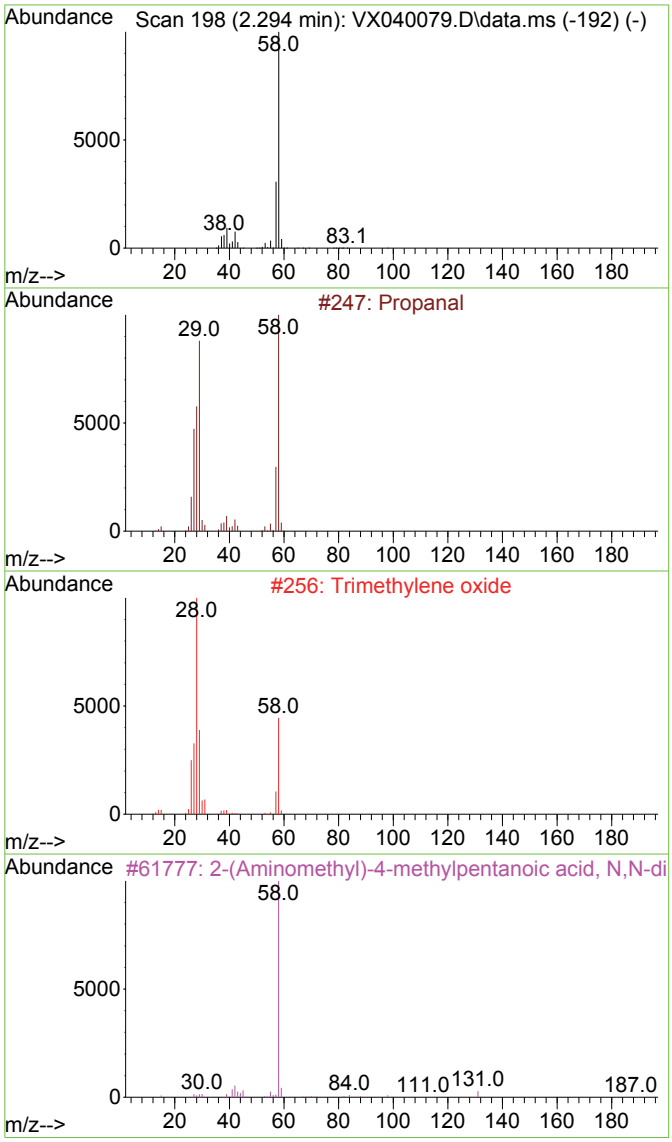
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

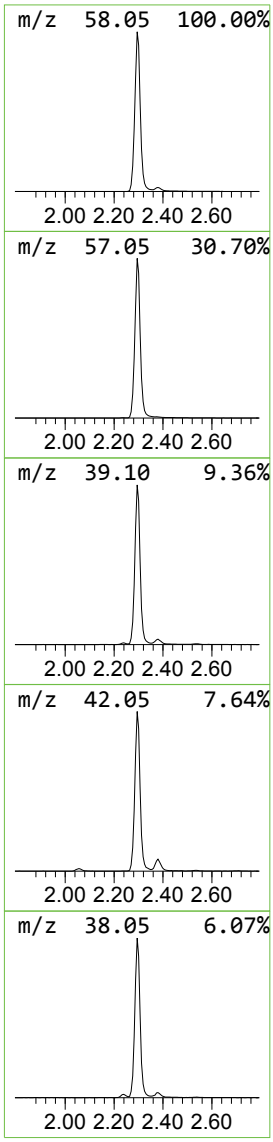
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	1643.63 ug/l	9262980	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	72
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
4	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
5	Propylene oxide	58	C3H6O	000075-56-9	7





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Instrument :
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ClientSampleId :
1142

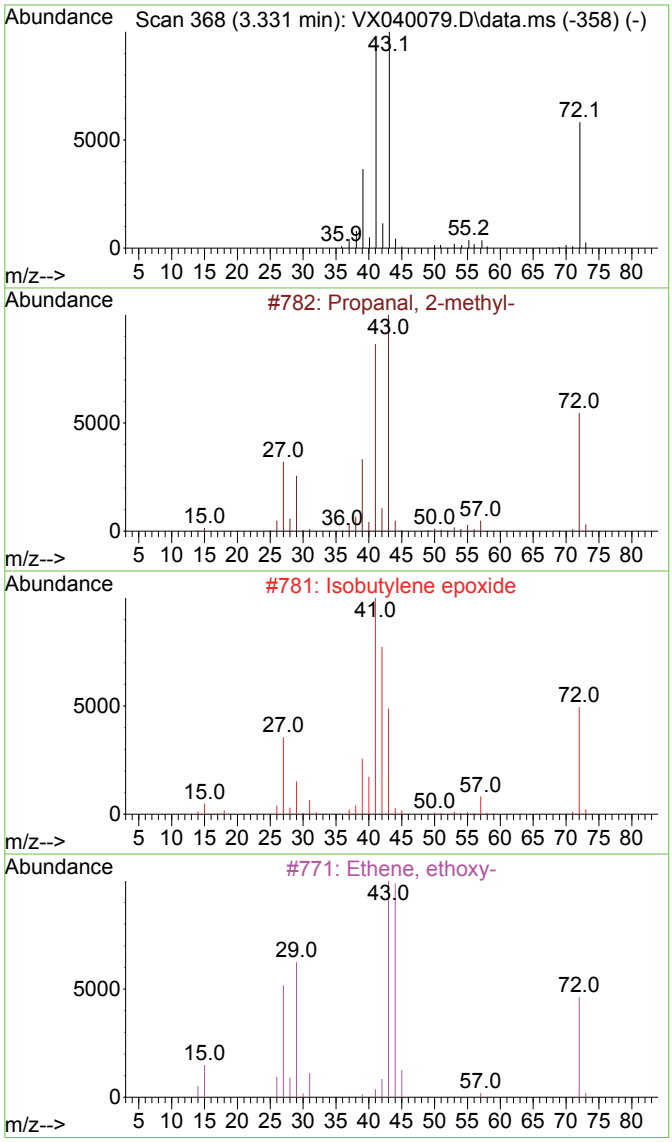
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

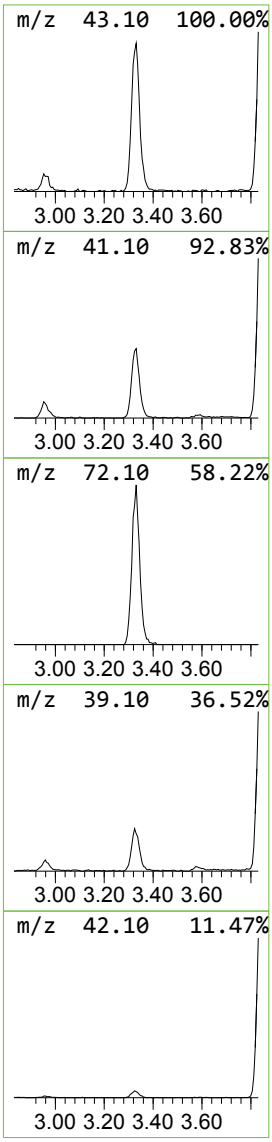
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanal, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.331	17.23 ug/l	97118	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91
2	Isobutylene epoxide	72	C4H8O	000558-30-5	53
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	42
4	Butanal	72	C4H8O	000123-72-8	42
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	37





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Operator : JC/MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1142

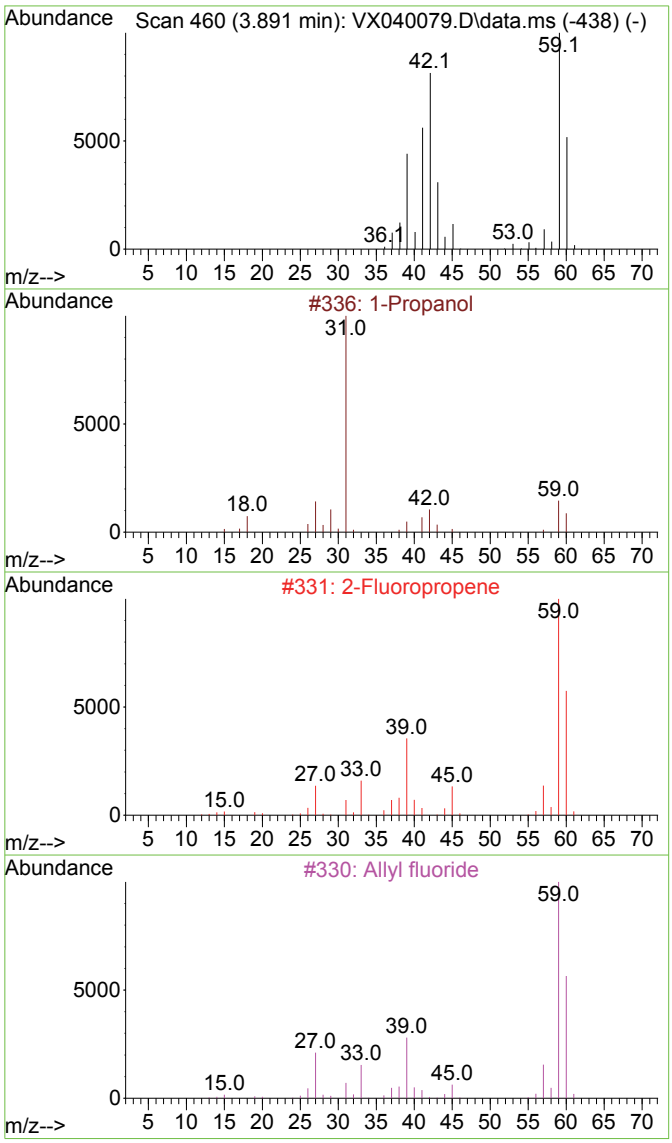
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

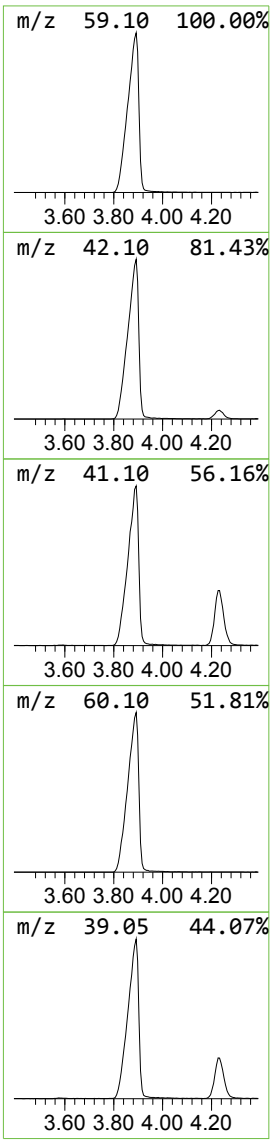
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.891	618.90 ug/l	3487910	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	59
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	25
5	Propene	42	C3H6	000115-07-1	25





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1142

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

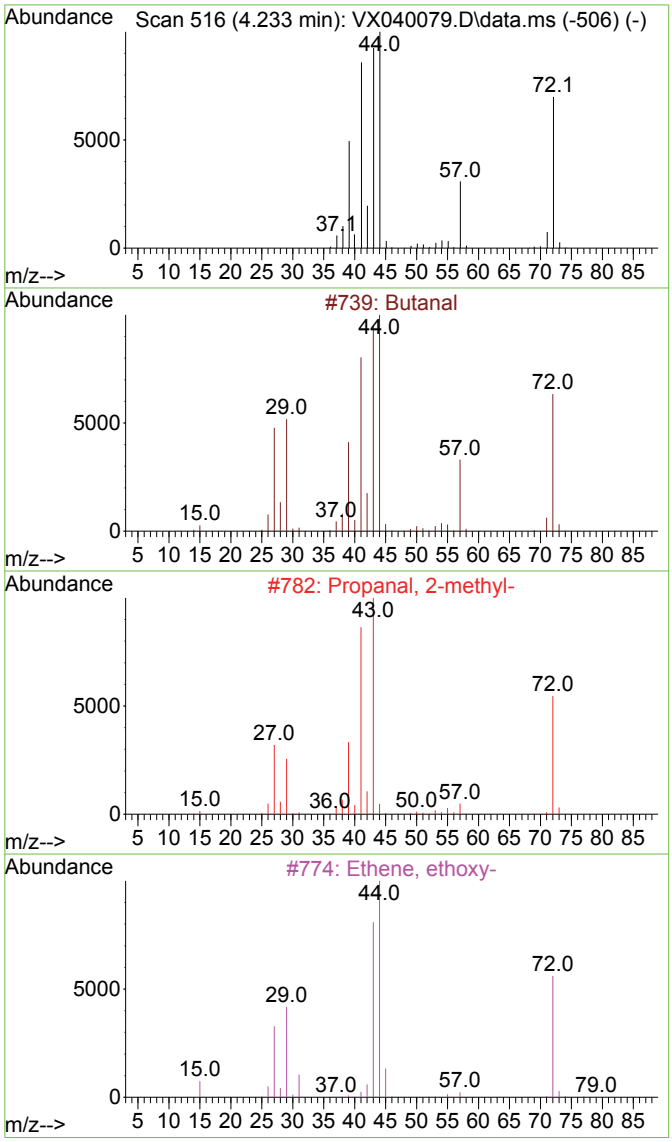
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

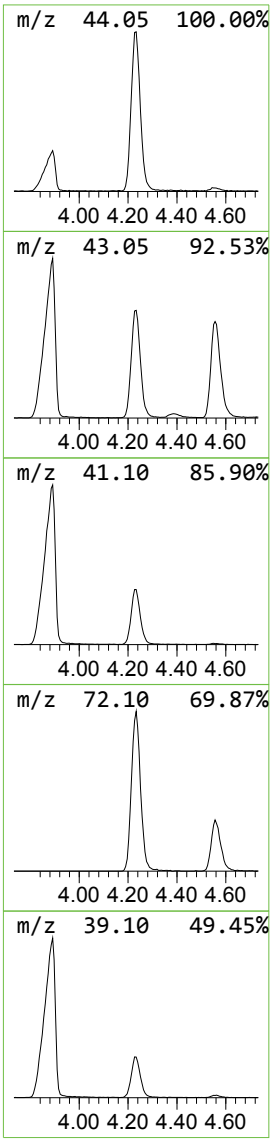
****

Peak Number 6 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	134.86 ug/l	760033	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
4	Methacrolein	70	C4H6O	000078-85-3	27
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	17





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1142

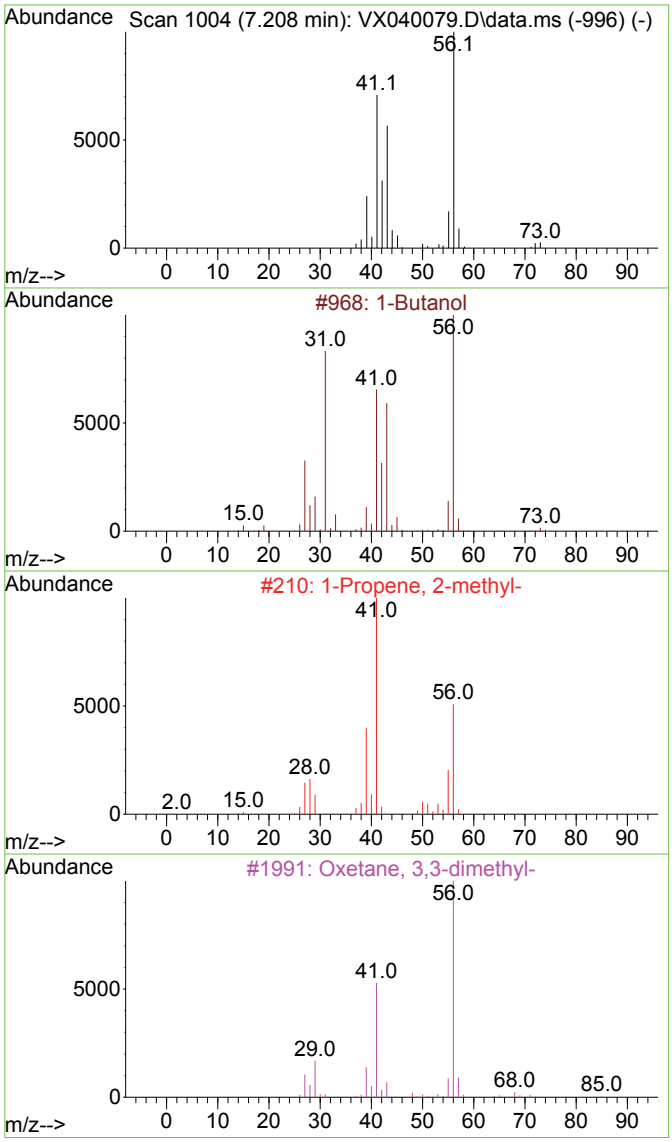
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

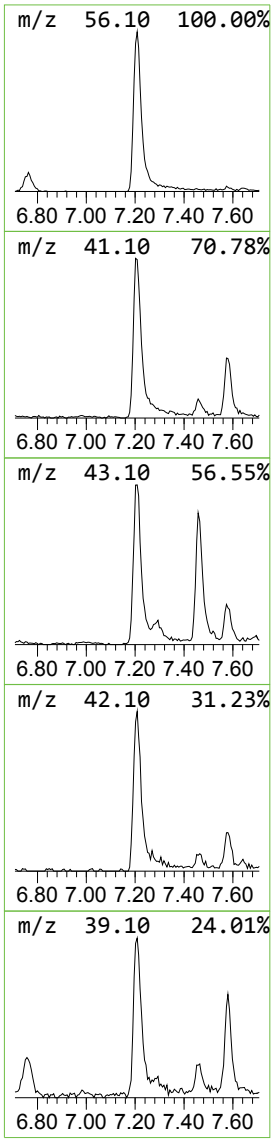
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	18.59 ug/l	143283	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	50
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	38
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
5	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9





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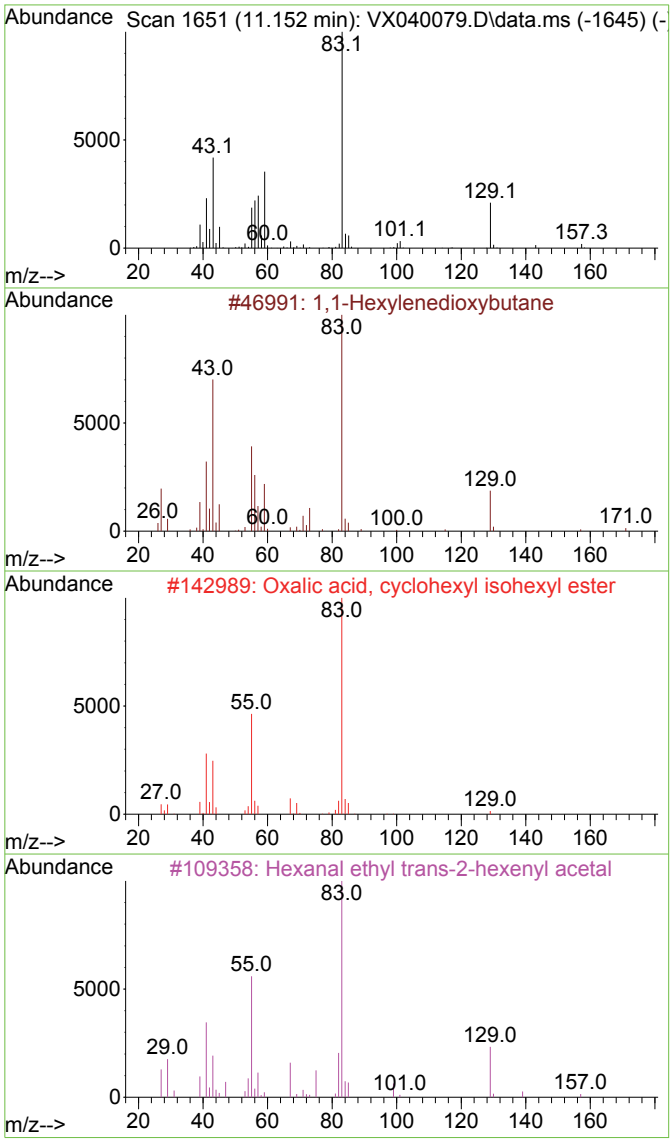
Quant Title : SW846 8260

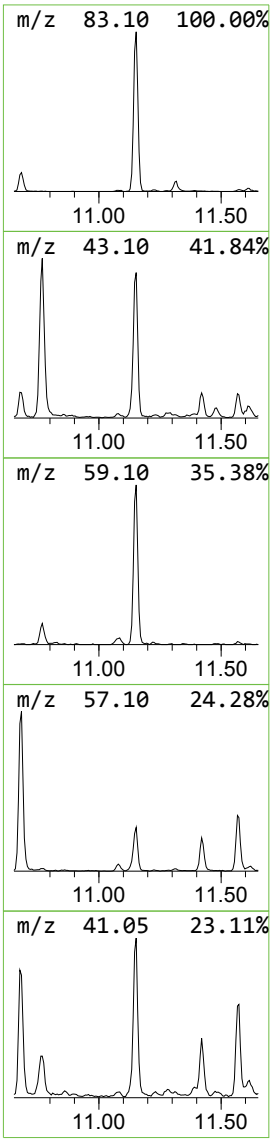
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,1-Hexylenedioxybutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.152	31.06 ug/l	311278	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	78
2	Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	43
3	Hexanal ethyl trans-2-hexenyl ac...	228	C14H28O2	1000431-42-6	40
4	Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	38
5	n-Butyl tiglate	156	C9H16O2	007785-66-2	33





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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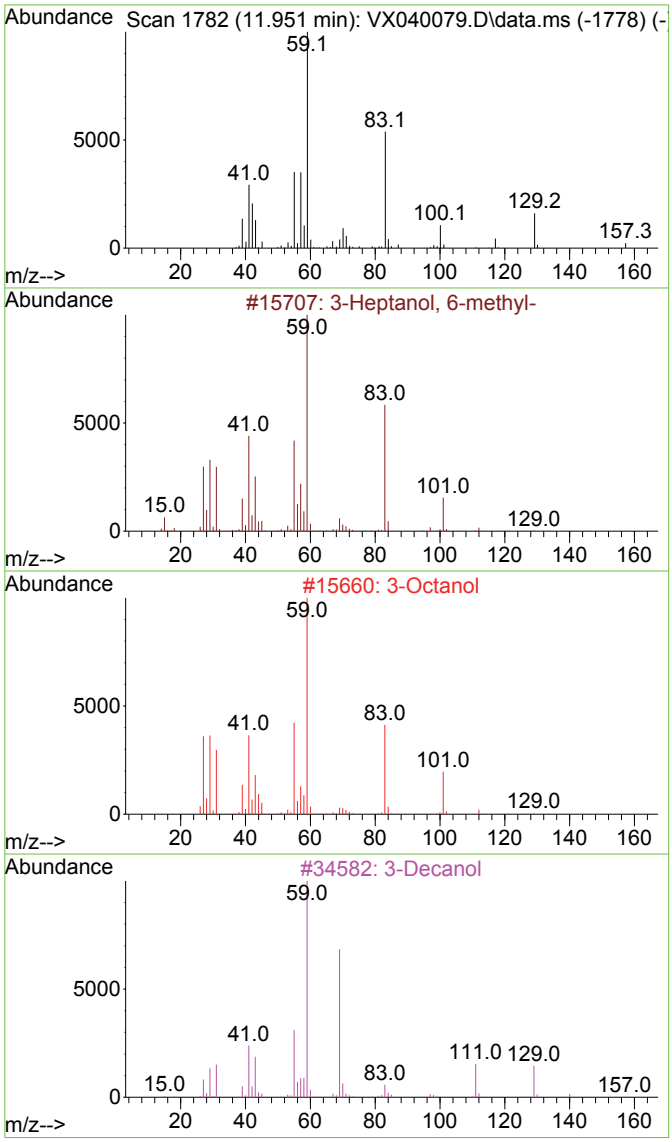
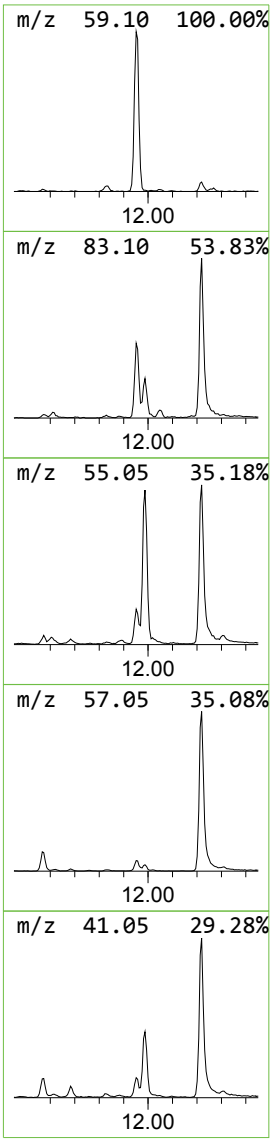
****
Peak Number 9 3-Heptanol, 6-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	17.00 ug/l	170324	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	53
2	3-Octanol	130	C8H18O	000589-98-0	53
3	3-Decanol	158	C10H22O	001565-81-7	50
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	42
5	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	37





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ClientSampleId :
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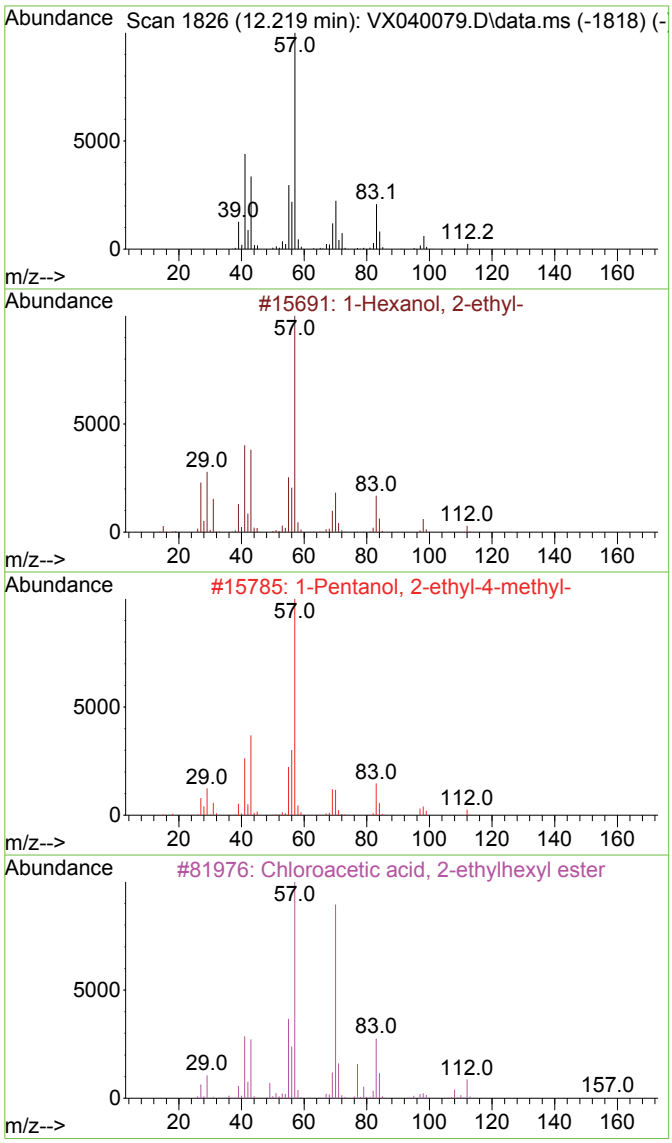
Quant Title : SW846 8260

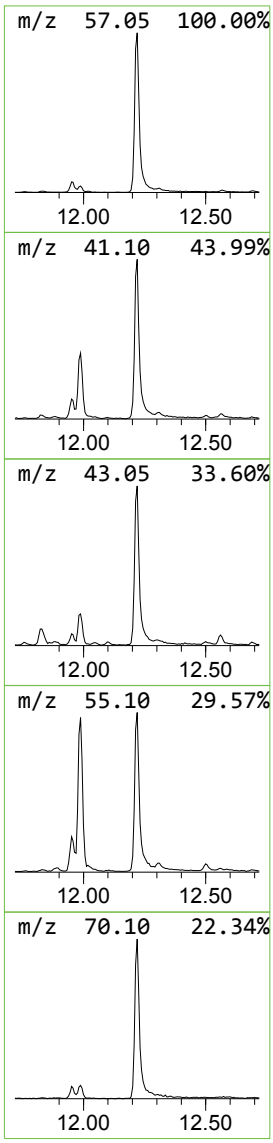
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	90.97 ug/l	911568	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	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47





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	2.056	25.0	ug/l	140891	1	5.550	281784	50.0
Propanal	2.294	1643.6	ug/l	9262980	1	5.550	281784	50.0
Propanal, 2-met...	3.331	17.2	ug/l	97118	1	5.550	281784	50.0
1-Propanol	3.891	618.9	ug/l	3487910	1	5.550	281784	50.0
Butanal	4.233	134.9	ug/l	760033	1	5.550	281784	50.0
1-Butanol	7.208	18.6	ug/l	143283	2	6.763	385436	50.0
1,1-Hexylenedio...	11.152	31.1	ug/l	311278	4	12.024	501037	50.0
3-Heptanol, 6-m...	11.951	17.0	ug/l	170324	4	12.024	501037	50.0
1-Hexanol, 2-et...	12.219	91.0	ug/l	911568	4	12.024	501037	50.0