LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025384.D
Acq On : 29 Nov 2021 20:52
Operator : JC/MD
Sample : M4837-10 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20930

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\82X111721W.M
Title : SW846 8260

Signal : TIC: VX025384.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	55	60	66	rBV	18020	20727	2.38%	0.354%
2	2.056	153	159	172	rBV	510571	760972	87.32%	13.013%
3	2.532	230	237	244	rBV	10433	18845	2.16%	0.322%
4	3.861	442	455	478	rBV	341576	871470	100.00%	14.902%
5	5.391	694	706	718	rBV	71573	211102	24.22%	3.610%
6	5.556	722	733	747	rVV	124463	348083	39.94%	5.952%
7	5.958	786	799	818	rBV	75252	207495	23.81%	3.548%
8	6.763	920	931	943	rBV	191360	450799	51.73%	7.709%
9	7.208	996	1004	1030	rBV	159490	337782	38.76%	5.776%
10	8.653	1234	1241	1249	rBV	385380	614889	70.56%	10.515%
11	9.238	1331	1337	1351	rBV	22315	39398	4.52%	0.674%
12	9.567	1385	1391	1410	rBV	75444	191980	22.03%	3.283%
13	10.055	1465	1471	1484	rVB	398941	530104	60.83%	9.065%
14	10.579	1552	1557	1565	rBV	81899	107290	12.31%	1.835%
15	10.659	1565	1570	1578	rVB3	6553	11983	1.38%	0.205%
16	11.085	1634	1640	1652	rVB	310142	403042	46.25%	6.892%
17	11.658	1729	1734	1746	rBV	5855	9560	1.10%	0.163%
18	12.024	1789	1794	1803	rVB	398096	490883	56.33%	8.394%
19	12.219	1821	1826	1839	rBV	121361	160719	18.44%	2.748%
20	12.414	1854	1858	1863	rVB	9803	11565	1.33%	0.198%
21	12.585	1881	1886	1902	rBV	31402	49296	5.66%	0.843%

Sum of corrected areas: 5847984

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Instrument :
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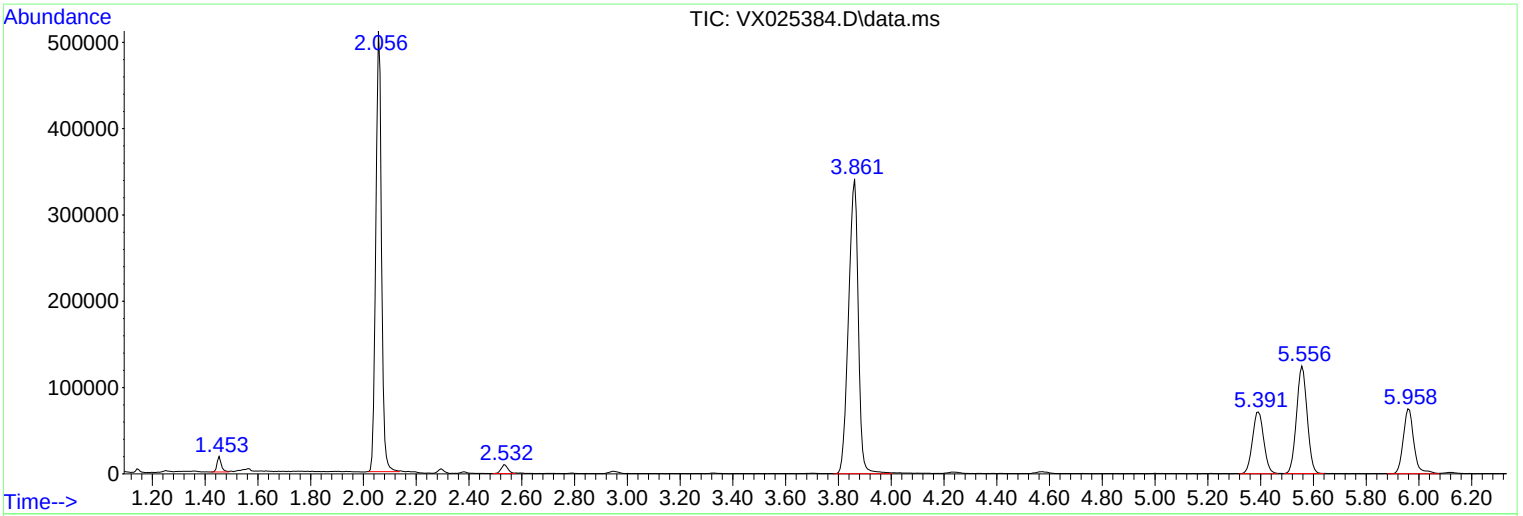
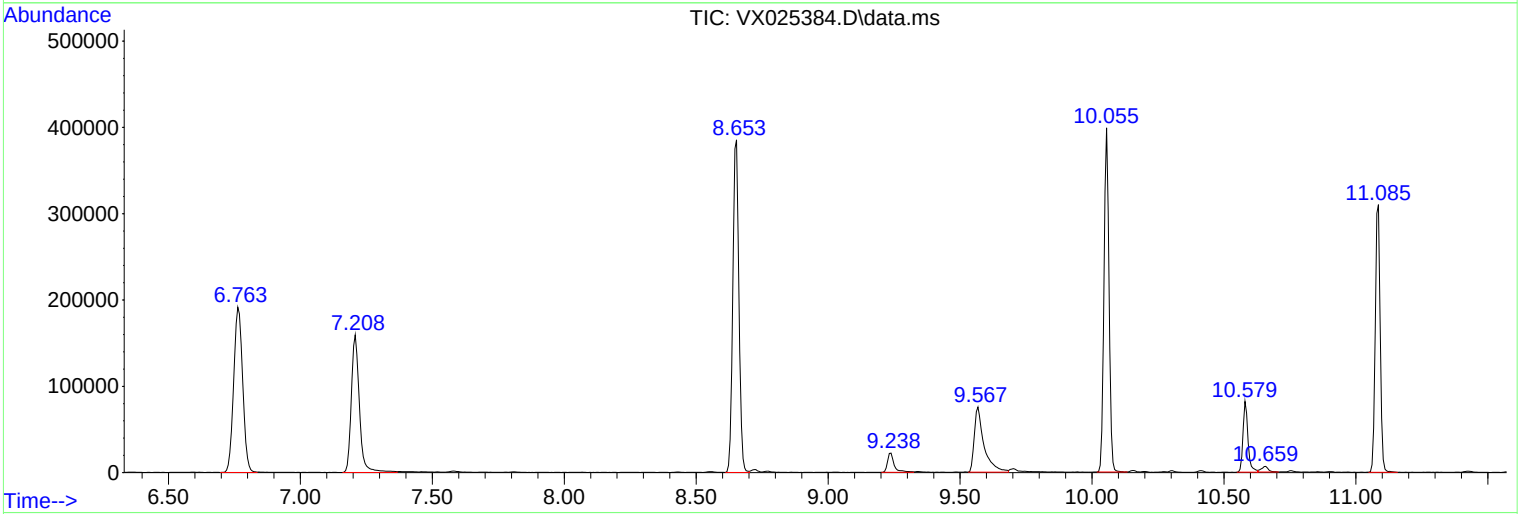
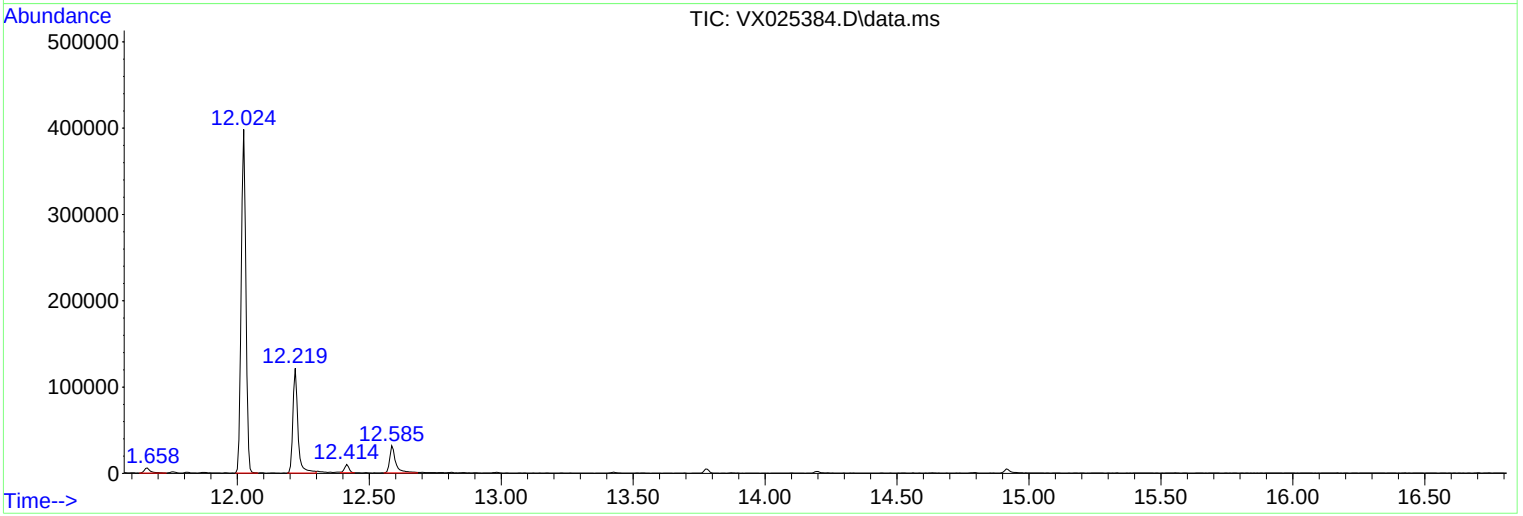
ClientSampleId :
20930

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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







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Data File : VX025384.D
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Quant Title : SW846 8260

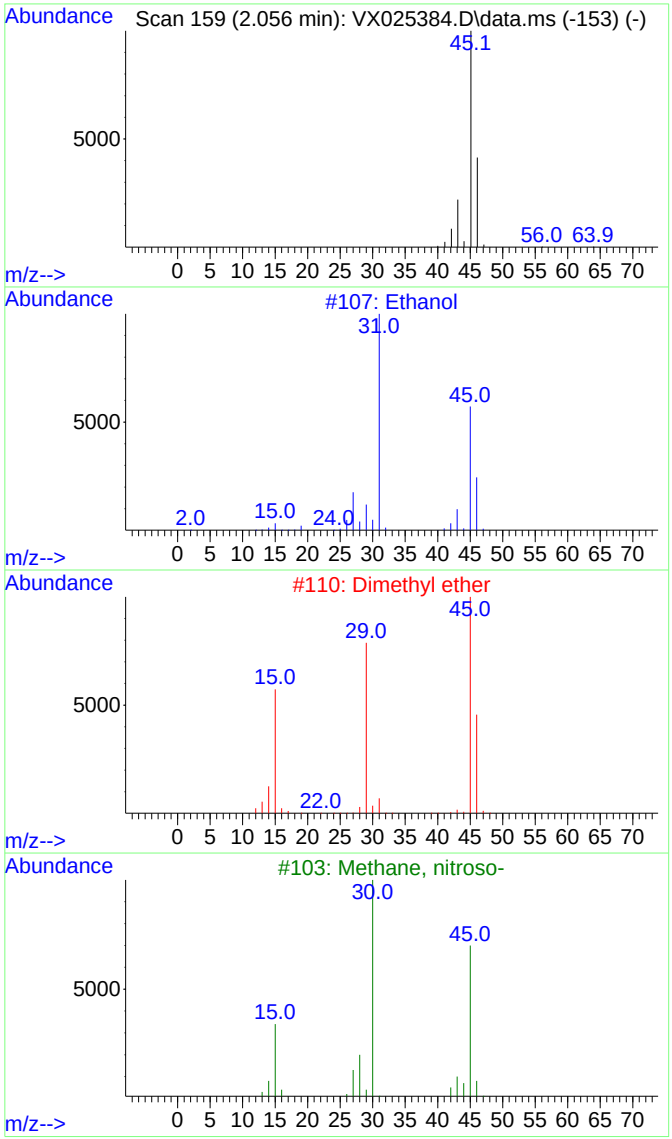
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

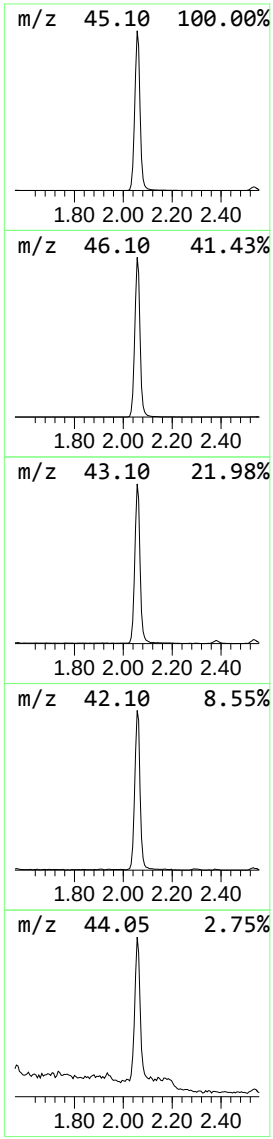
****

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	109.31 ug/l	760972	Pentafluorobenzene	5.556

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	Oxalic acid	90	C2H2O4	000144-62-7	4





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Data File : VX025384.D
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Operator : JC/MD
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20930

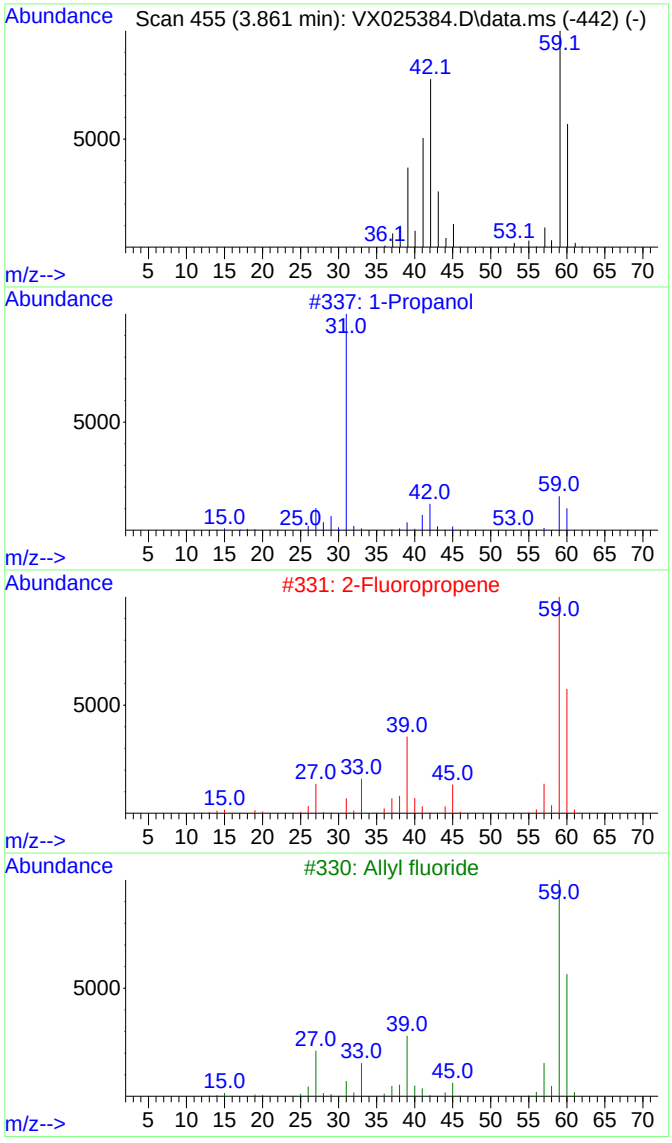
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

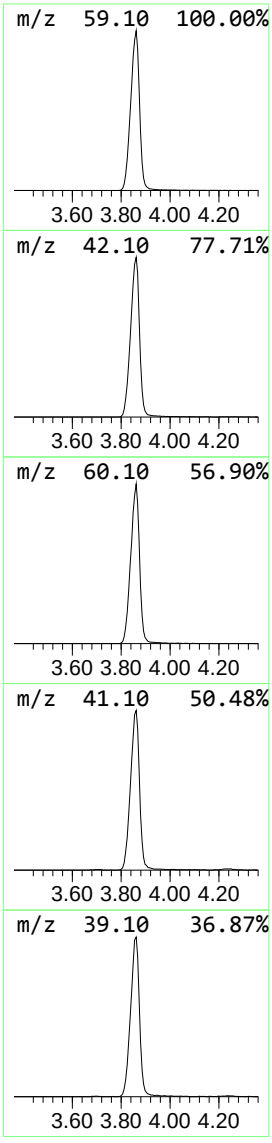
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.861	125.18 ug/l	871470	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	2-Fluoropropene	60	C3H5F	001184-60-7	49
3	Allyl fluoride	60	C3H5F	000818-92-8	47
4	Cyclopropane	42	C3H6	000075-19-4	16
5	Acetaldoxime	59	C2H5NO	000107-29-9	7





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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
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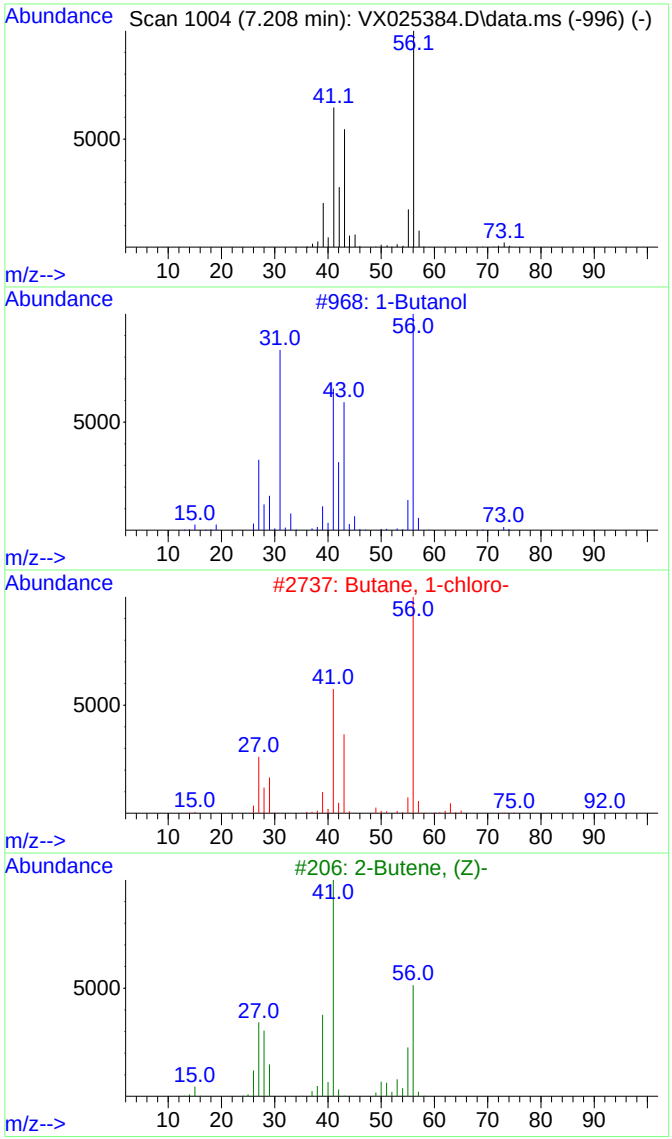
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

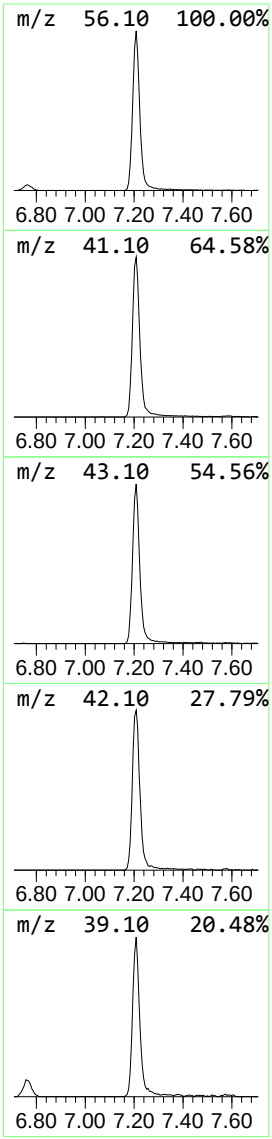
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	37.46 ug/l	337782	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
3	2-Butene, (Z)-	56	C4H8	000590-18-1	9
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20930

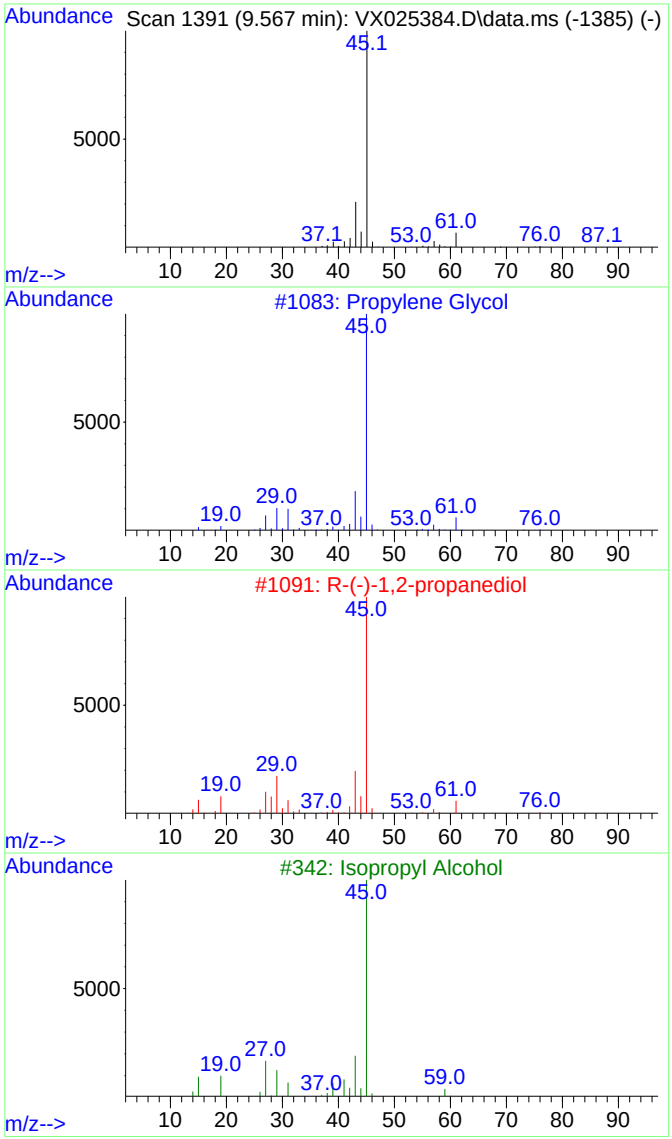
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

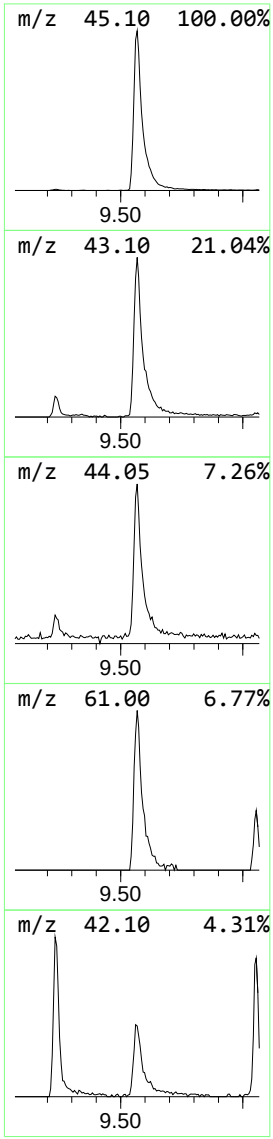
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.567	18.11 ug/l	191980	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20930

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

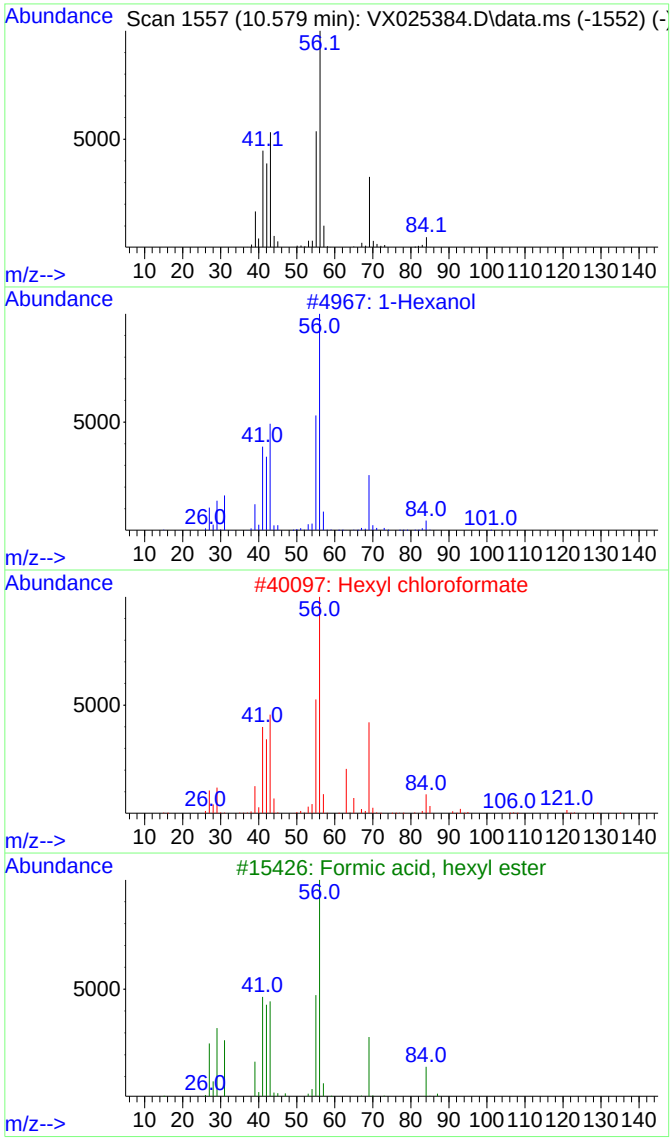
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

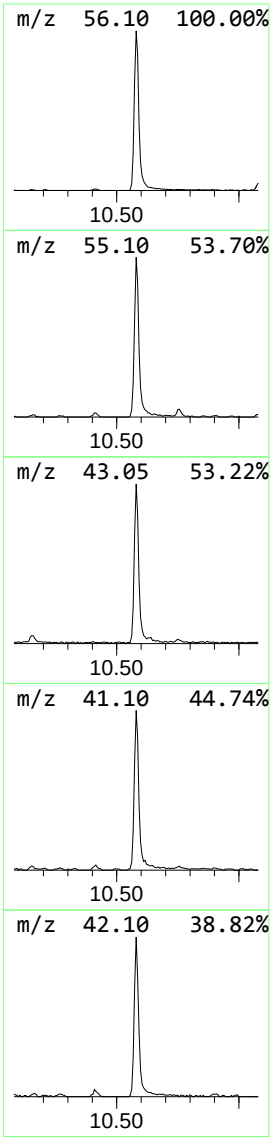
****

Peak Number 5 1-Hexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.579	10.12 ug/l	107290	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
3	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
4	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	78
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	59





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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20930

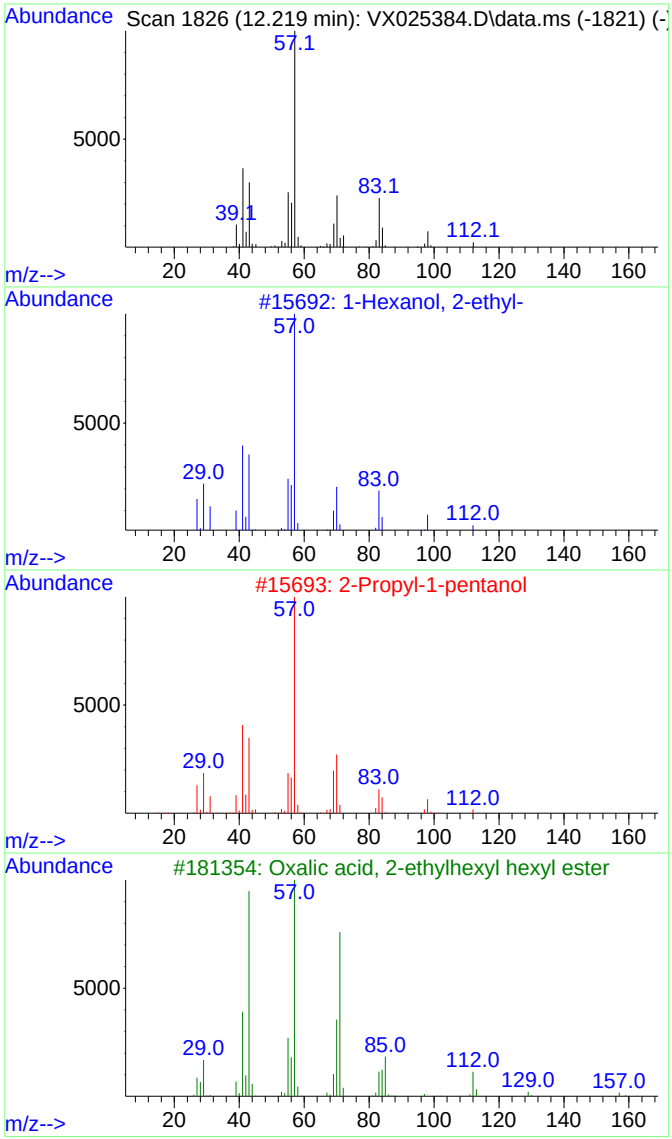
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

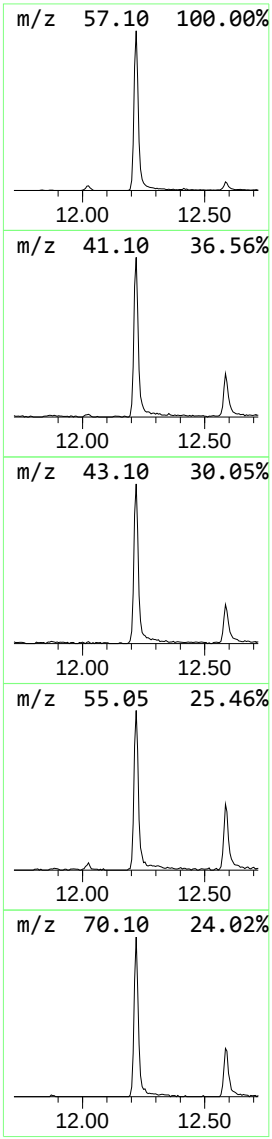
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	16.37 ug/l	160719	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	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	53
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53





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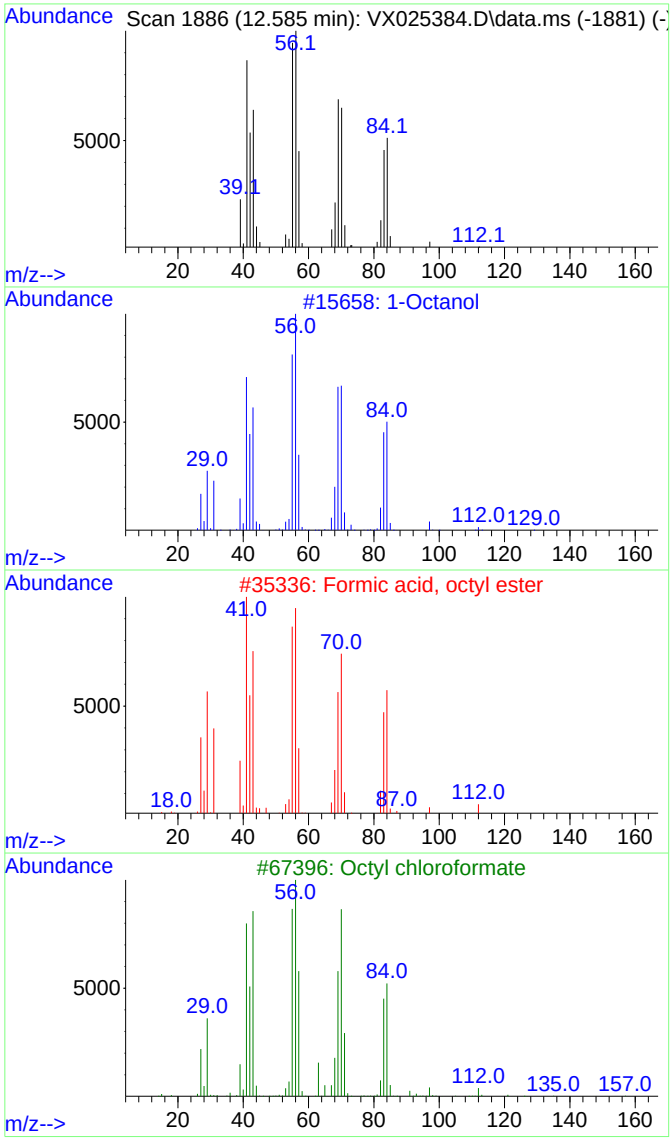
Quant Title : SW846 8260

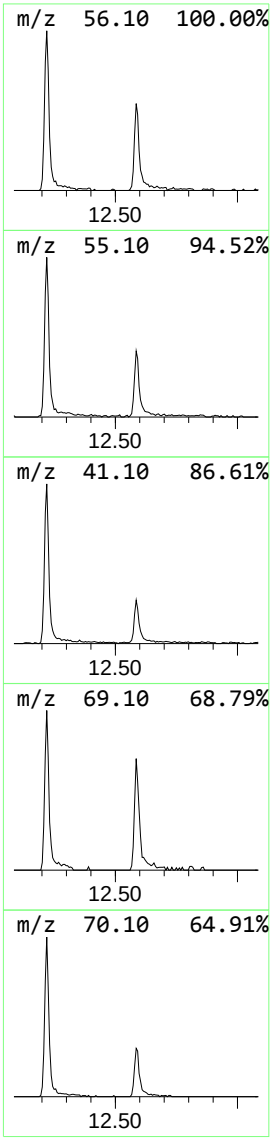
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Octanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	5.02 ug/l	49296	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	91
2	Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3	Octyl chloroformate	192	C9H17ClO2	007452-59-7	86
4	1-Nonanol	144	C9H20O	000143-08-8	72
5	Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	64





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	109.3	ug/l	760972	1	5.556	348083	50.0
1-Propanol	3.861	125.2	ug/l	871470	1	5.556	348083	50.0
1-Butanol	7.208	37.5	ug/l	337782	2	6.763	450799	50.0
Propylene Glycol	9.567	18.1	ug/l	191980	3	10.055	530104	50.0
1-Hexanol	10.579	10.1	ug/l	107290	3	10.055	530104	50.0
1-Hexanol, 2-et...	12.219	16.4	ug/l	160719	4	12.024	490883	50.0
1-Octanol	12.585	5.0	ug/l	49296	4	12.024	490883	50.0