LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
Data File : VX025383.D
Acq On : 29 Nov 2021 20:28
Operator : JC/MD
Sample : M4837-08 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20928

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: VX025383.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	57	60	67	rBV	10027	11916	1.05%	0.179%
2	2.056	153	159	175	rBV	495917	763553	67.11%	11.444%
3	2.532	230	237	244	rBV	14737	28185	2.48%	0.422%
4	3.867	441	456	478	rBV	432513	1137748	100.00%	17.052%
5	5.391	695	706	720	rBV	72281	210067	18.46%	3.148%
6	5.556	720	733	749	rVB	123479	350976	30.85%	5.260%
7	5.958	788	799	808	rBV	75288	203483	17.88%	3.050%
8	6.763	921	931	948	rBV	190967	452302	39.75%	6.779%
9	7.208	995	1004	1022	rBV	233480	478470	42.05%	7.171%
10	8.647	1232	1240	1248	rBV	390863	624266	54.87%	9.356%
11	8.720	1248	1252	1257	rVB	13715	20610	1.81%	0.309%
12	9.232	1331	1336	1348	rBV	40623	65017	5.71%	0.974%
13	9.567	1385	1391	1409	rBV	86249	207226	18.21%	3.106%
14	10.055	1465	1471	1484	rBV	410932	547695	48.14%	8.208%
15	10.579	1552	1557	1565	rBV	148002	181480	15.95%	2.720%
16	10.652	1565	1569	1580	rVB3	8649	17318	1.52%	0.260%
17	11.079	1634	1639	1653	rVB	325741	424061	37.27%	6.356%
18	11.658	1729	1734	1739	rBV	9819	15186	1.33%	0.228%
19	12.024	1788	1794	1802	rBV	434200	532212	46.78%	7.976%
20	12.219	1821	1826	1839	rBV	141001	184059	16.18%	2.759%
21	12.414	1854	1858	1865	rVB	10262	12751	1.12%	0.191%
22	12.585	1880	1886	1903	rBV	57839	84951	7.47%	1.273%
23	13.426	2017	2024	2037	rBV	25068	43698	3.84%	0.655%
24	14.194	2145	2150	2166	rBV	28824	52156	4.58%	0.782%
25	14.920	2263	2269	2280	rBV2	11406	22916	2.01%	0.343%

Sum of corrected areas: 6672302

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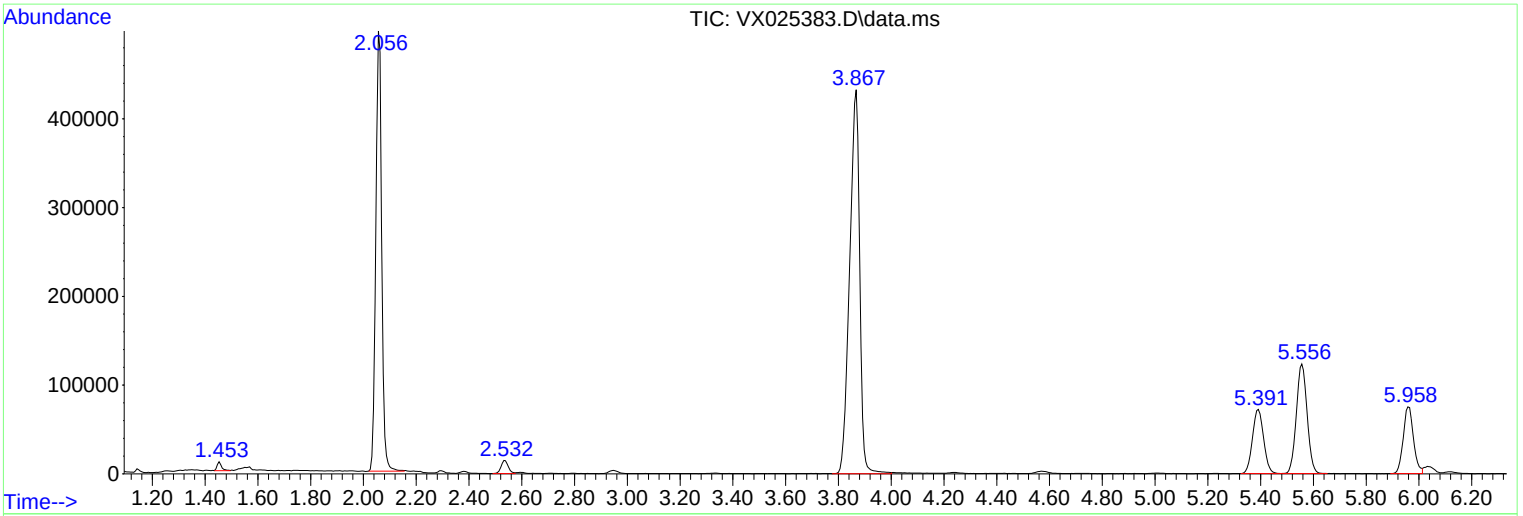
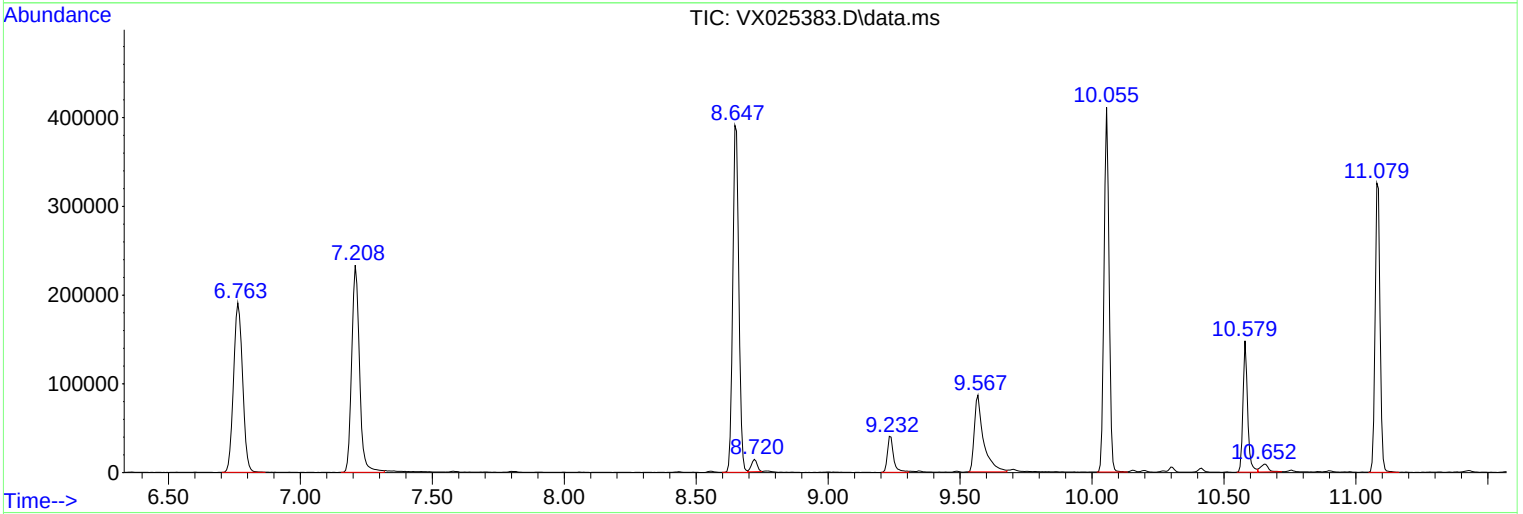
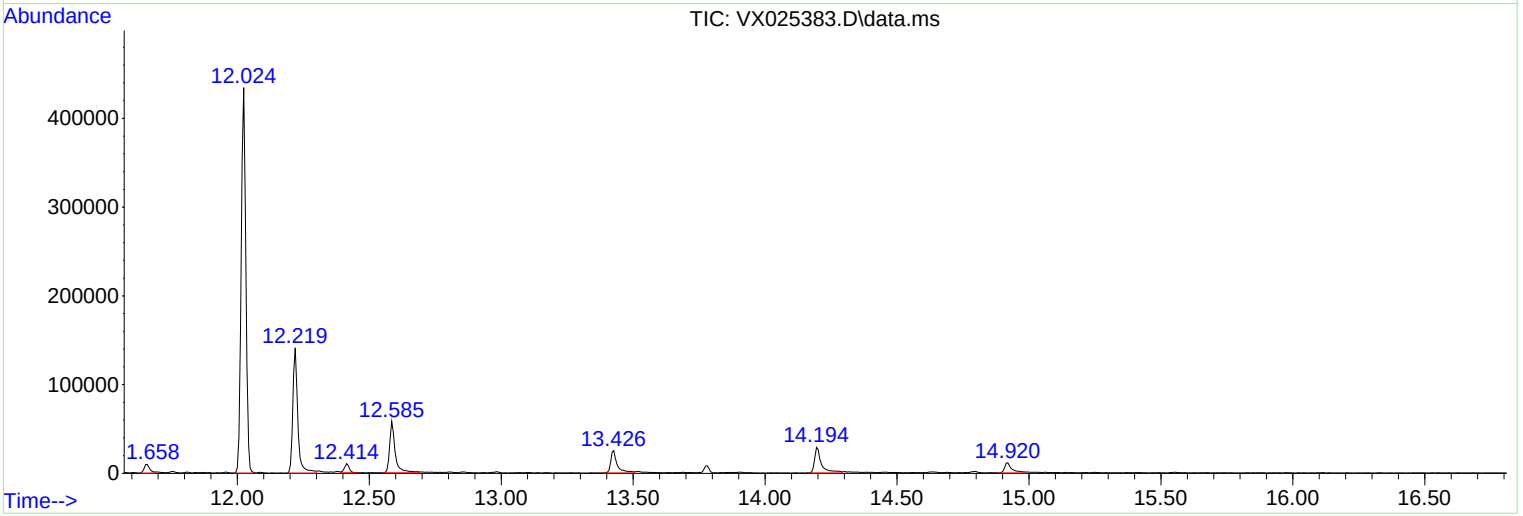
ClientSampleId :
20928

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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Quant Title : SW846 8260

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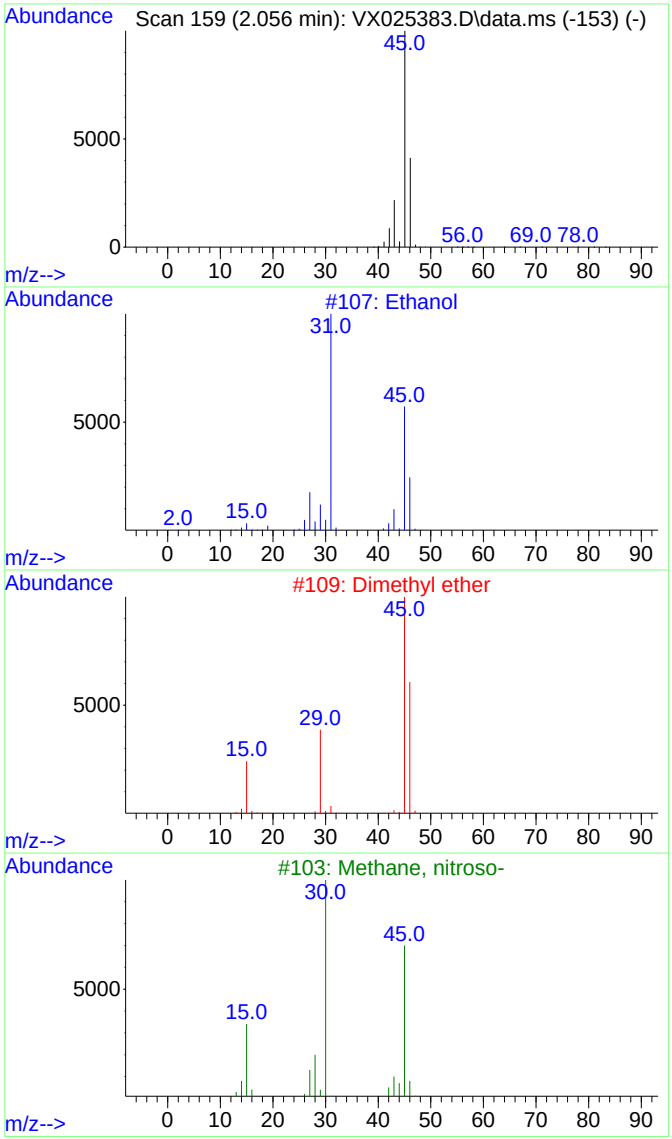
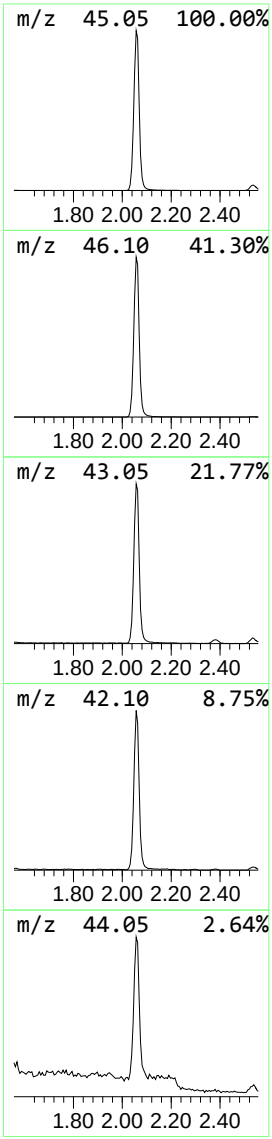
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	108.78 ug/l	763553	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
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 : VX025383.D
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Operator : JC/MD
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20928

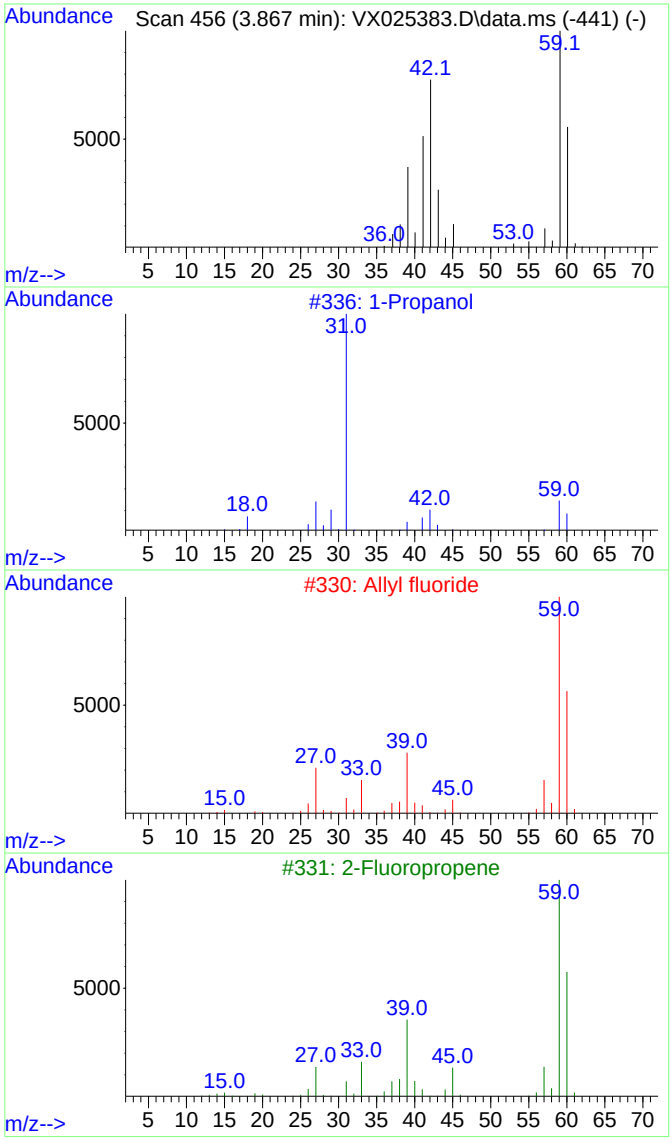
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

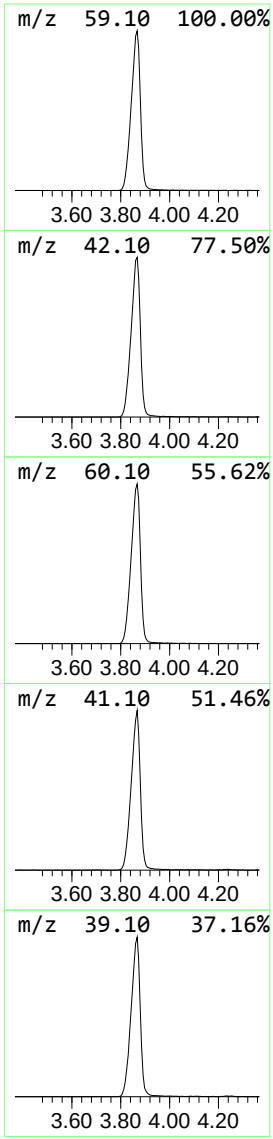
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.867	162.08 ug/l	1137750	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	Allyl fluoride	60	C3H5F	000818-92-8	47
3	2-Fluoropropene	60	C3H5F	001184-60-7	43
4	Cyclopropane	42	C3H6	000075-19-4	16
5	Formamidoxime	60	CH4N2O	000624-82-8	9





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Instrument :
MSVOA_X
ClientSampleId :
20928

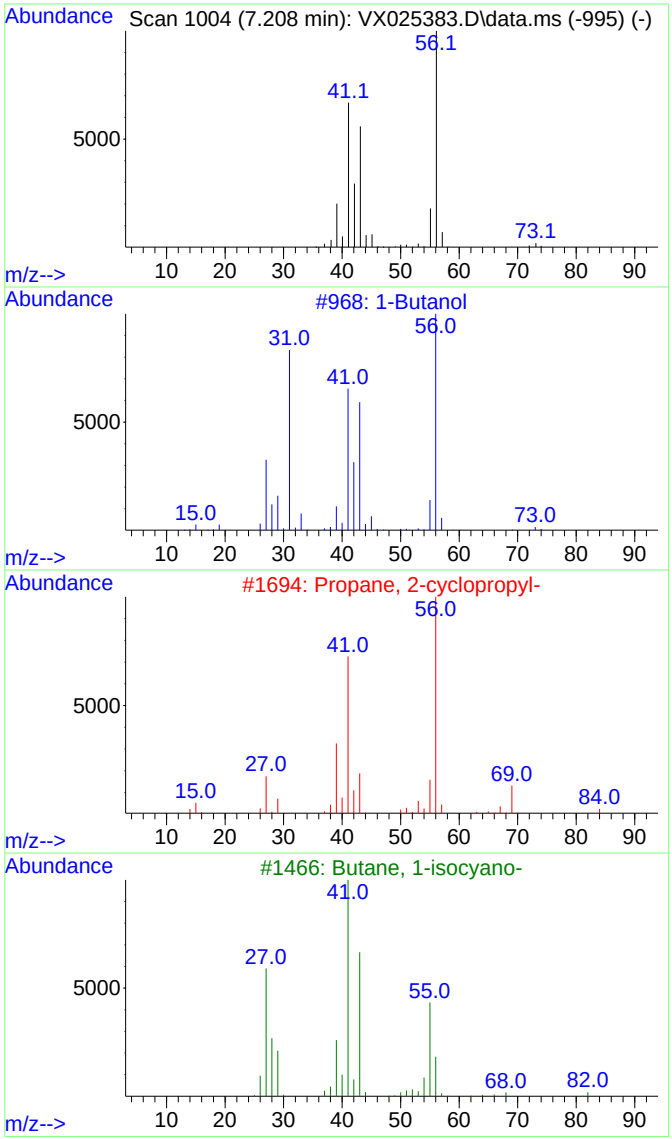
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

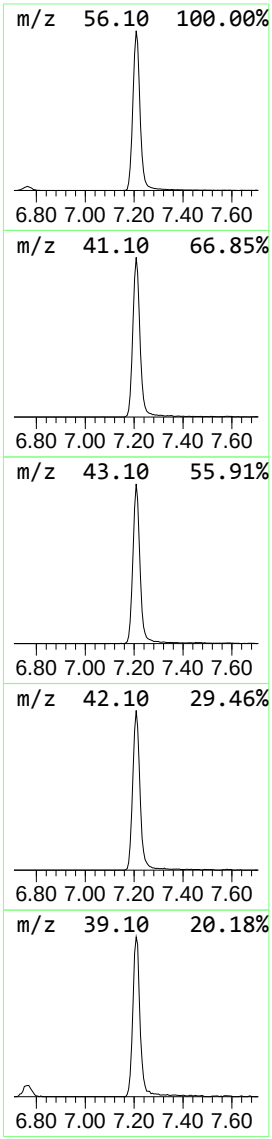
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	52.89 ug/l	478470	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
3	Butane, 1-isocyano-	83	C5H9N	002769-64-4	9
4	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9





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Operator : JC/MD
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20928

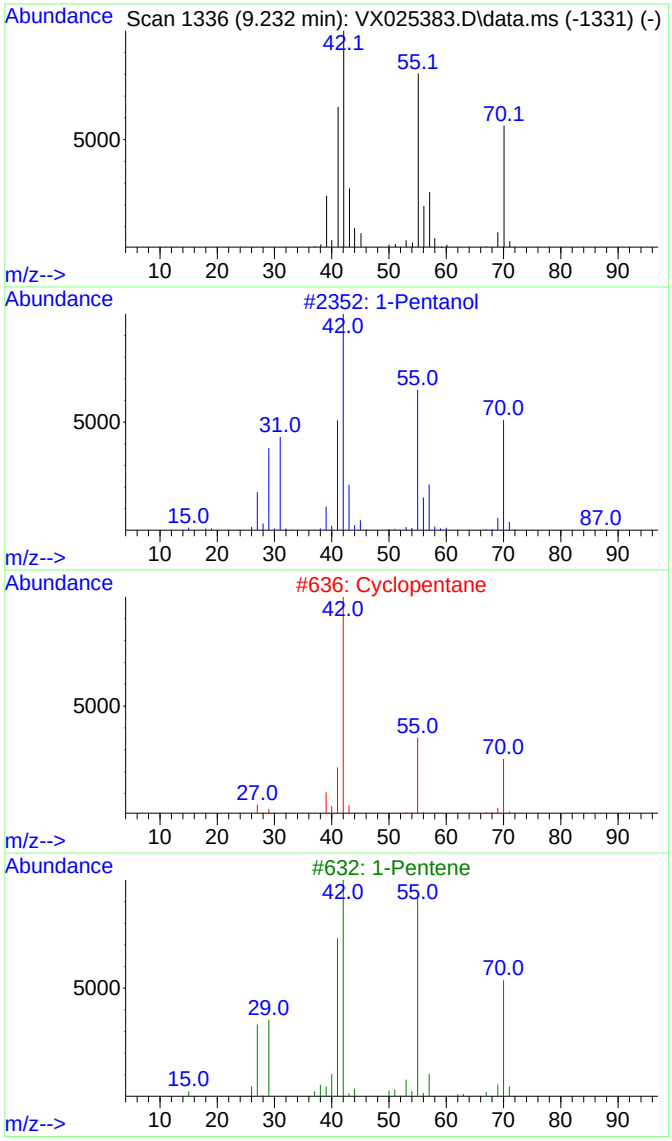
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

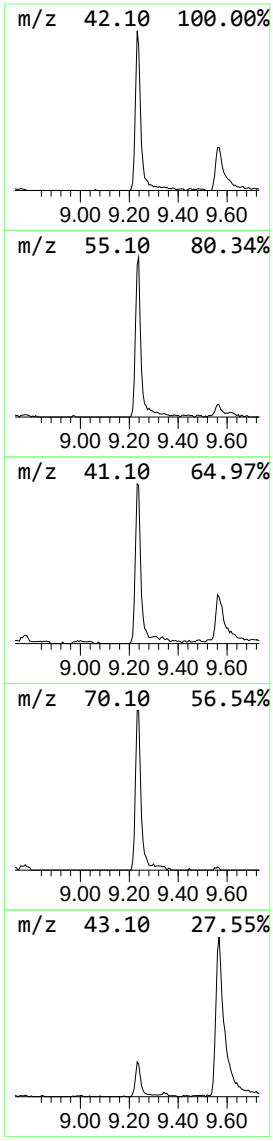
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Pentanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	5.94 ug/l	65017	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	Cyclopentane	70	C5H10	000287-92-3	64
3	1-Pentene	70	C5H10	000109-67-1	64
4	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	45
5	Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	40





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20928

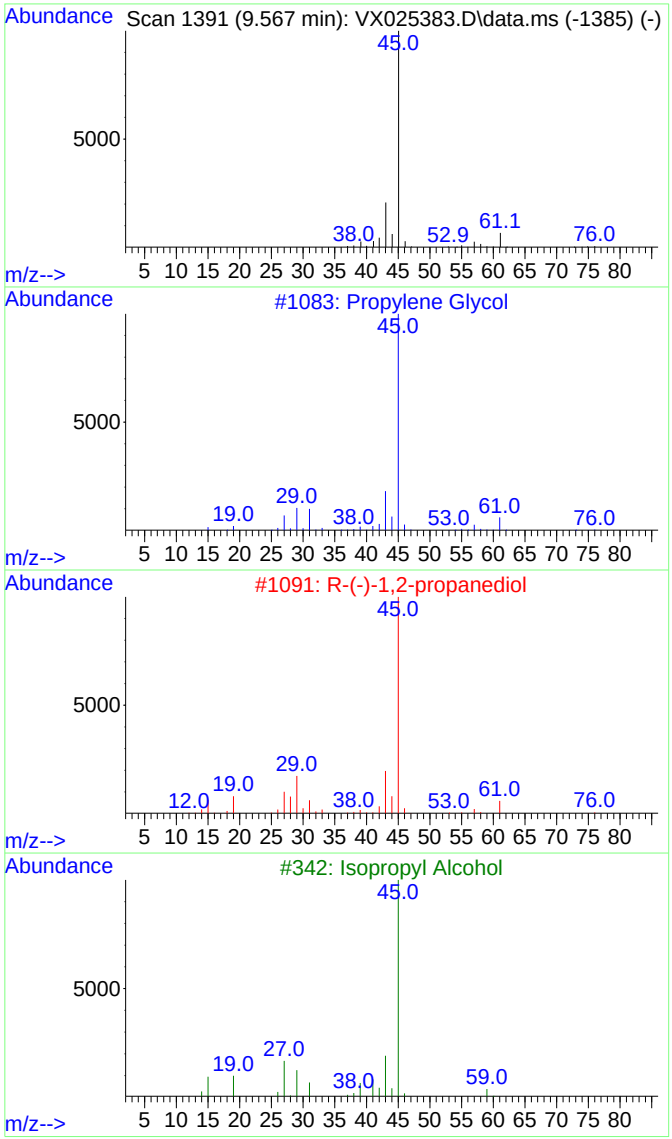
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

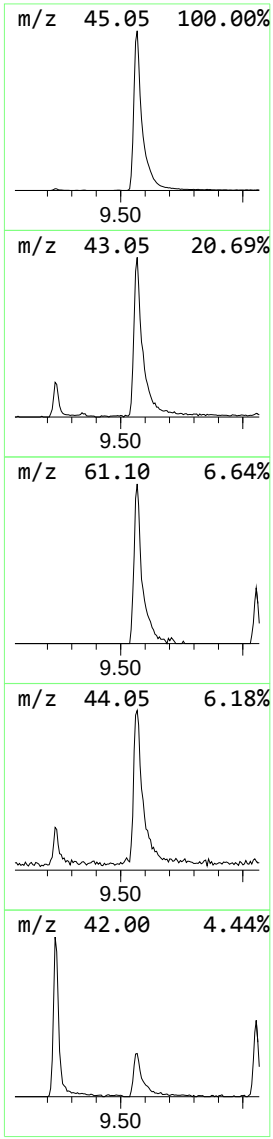
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.567	18.92 ug/l	207226	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	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12





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MSVOA_X
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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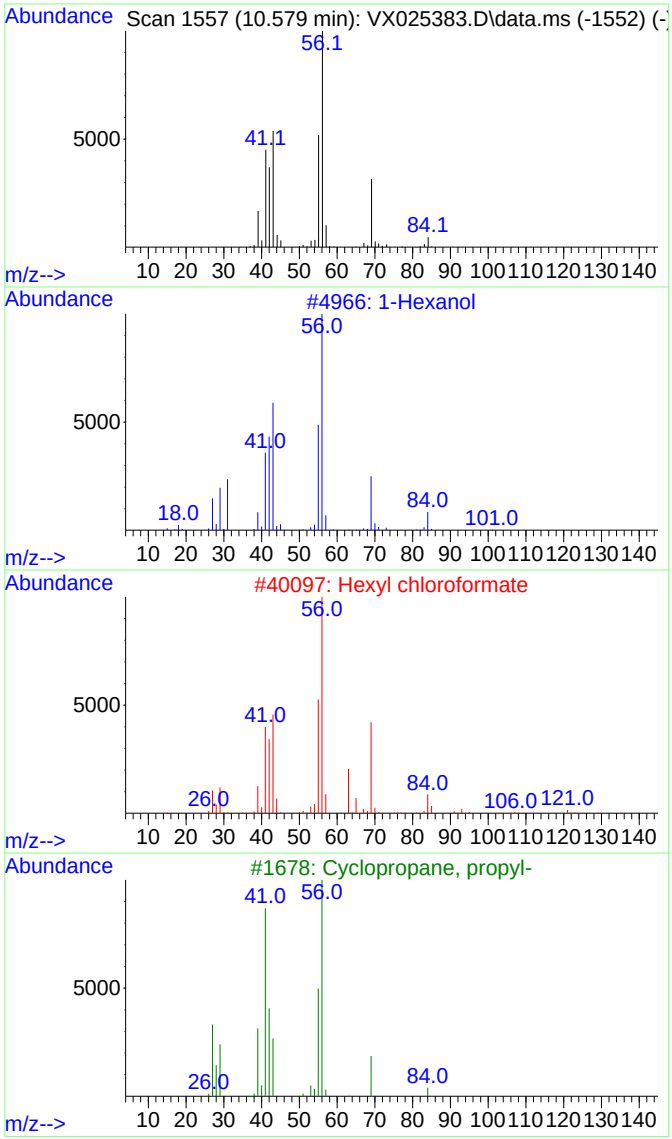
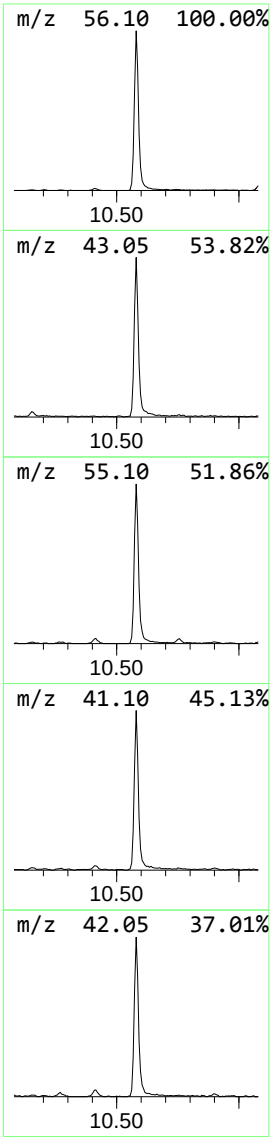
****
Peak Number 6 1-Hexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.579	16.57 ug/l	181480	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	74
3	Cyclopropane, propyl-	84	C6H12	002415-72-7	72
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	64





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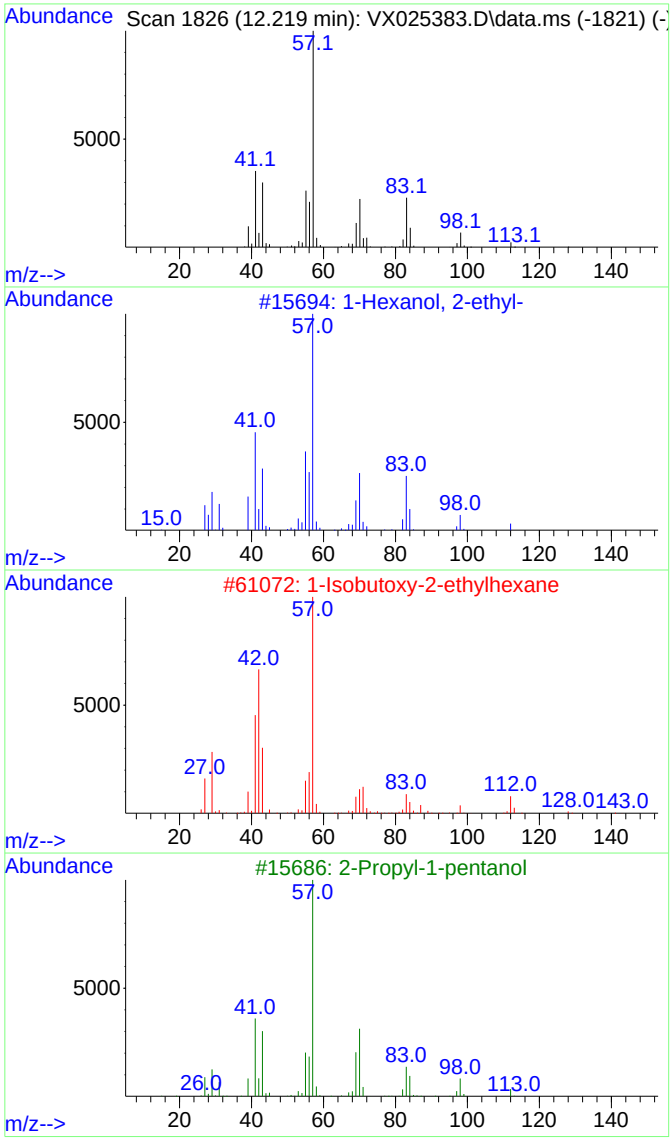
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

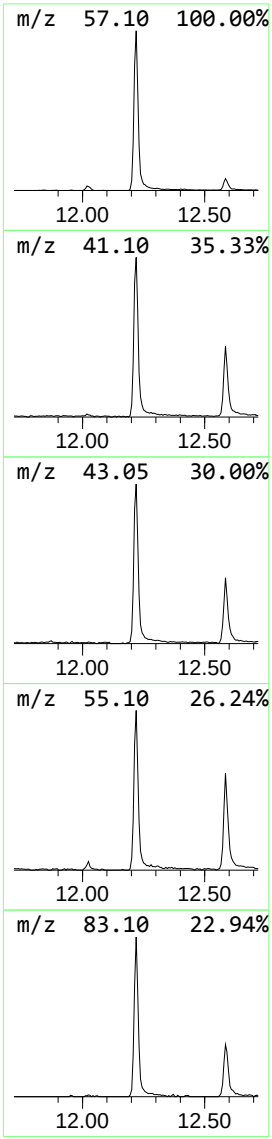
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	17.29 ug/l	184059	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-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	42





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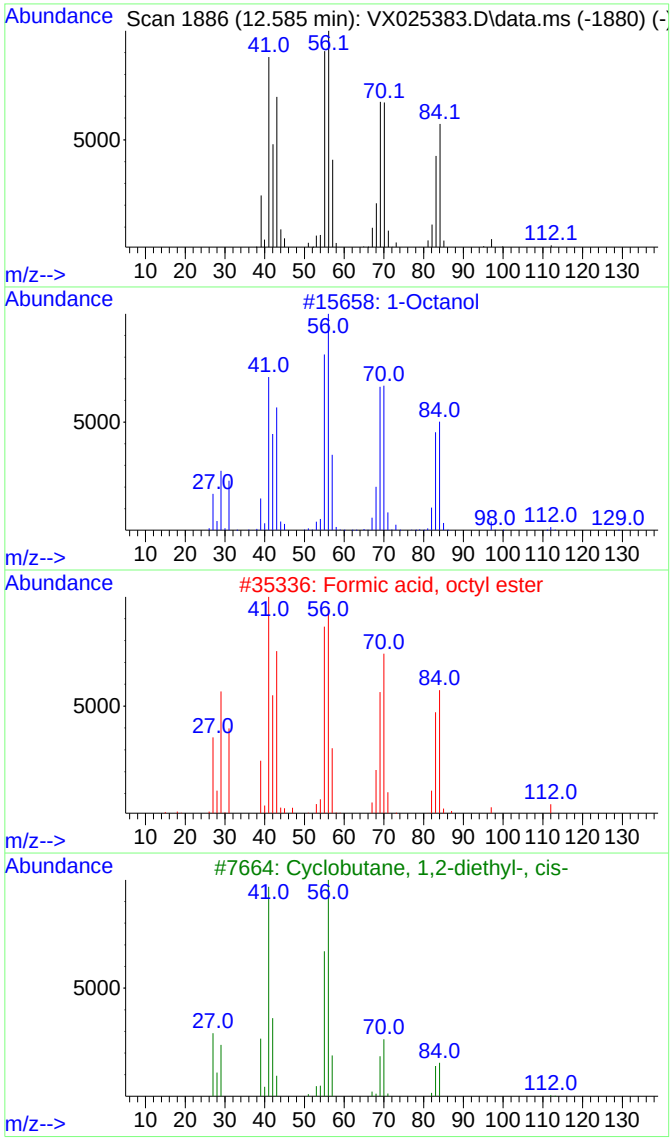
Quant Title : SW846 8260

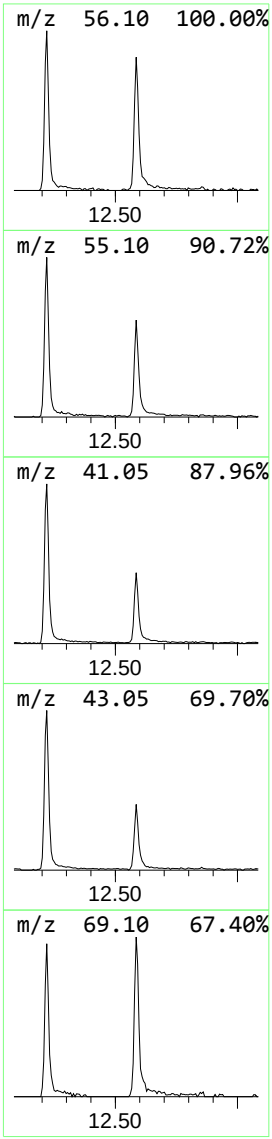
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	7.98 ug/l	84951	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	Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	64
4	Octyl chloroformate	192	C9H17ClO2	007452-59-7	64
5	1-Nonanol	144	C9H20O	000143-08-8	59





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	108.8	ug/l	763553	1	5.556	350976	50.0
1-Propanol	3.867	162.1	ug/l	1137750	1	5.556	350976	50.0
1-Butanol	7.208	52.9	ug/l	478470	2	6.763	452302	50.0
1-Pentanol	9.232	5.9	ug/l	65017	3	10.055	547695	50.0
Propylene Glycol	9.567	18.9	ug/l	207226	3	10.055	547695	50.0
1-Hexanol	10.579	16.6	ug/l	181480	3	10.055	547695	50.0
1-Hexanol, 2-et...	12.219	17.3	ug/l	184059	4	12.024	532212	50.0
1-Octanol	12.585	8.0	ug/l	84951	4	12.024	532212	50.0