LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032521\
Data File : VX021500.D
Acq On : 25 Mar 2021 20:36
Operator : JC/MD
Sample : M1776-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 107

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\82X032421W.M
Title : SW846 8260

Signal : TIC: VX021500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.617	1274	1280	1287	rBV	464075	731264	1.17%	1.055%
2	9.141	1350	1369	1373	rBV	19518306	62593938	100.00%	90.336%
3	11.930	1836	1843	1851	rBV	1522853	2284641	3.65%	3.297%
4	12.324	1904	1910	1913	rBV2	1329735	2943013	4.70%	4.247%
5	12.394	1919	1922	1938	rVB	381574	737366	1.18%	1.064%

Sum of corrected areas: 69290222

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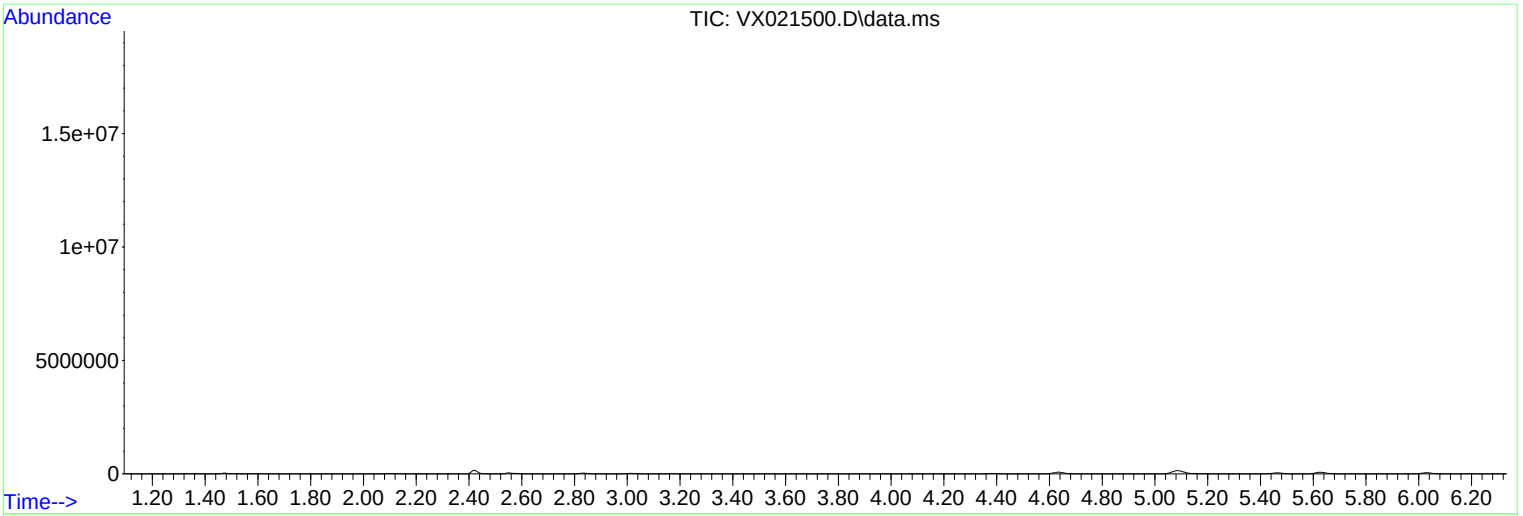
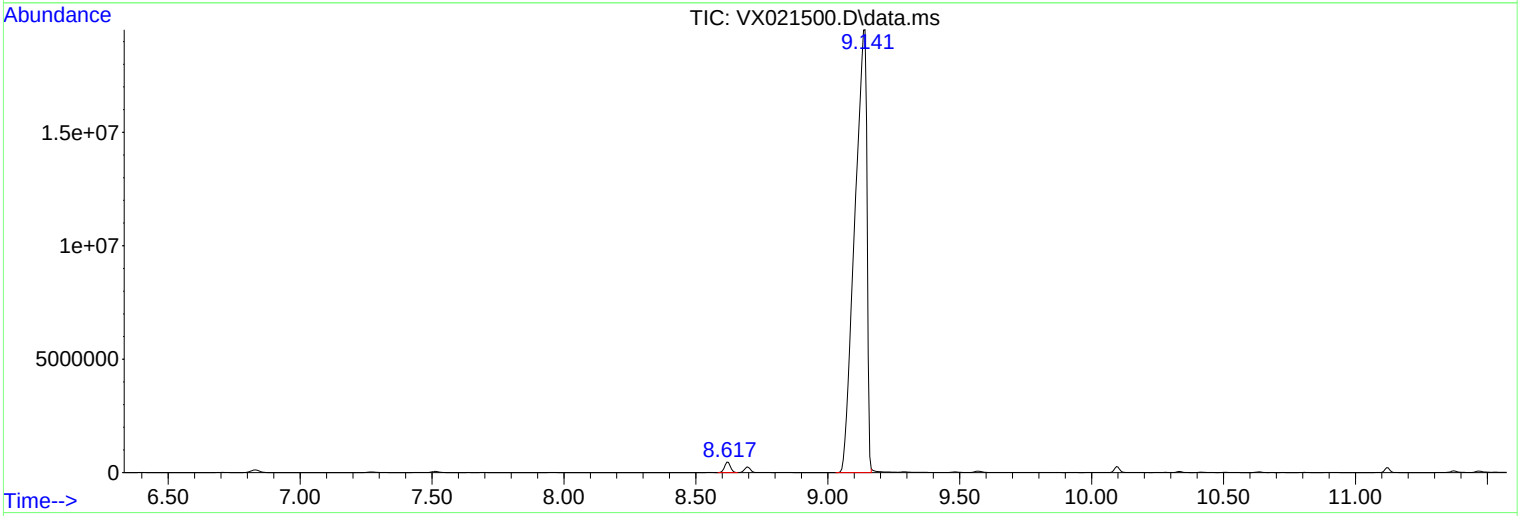
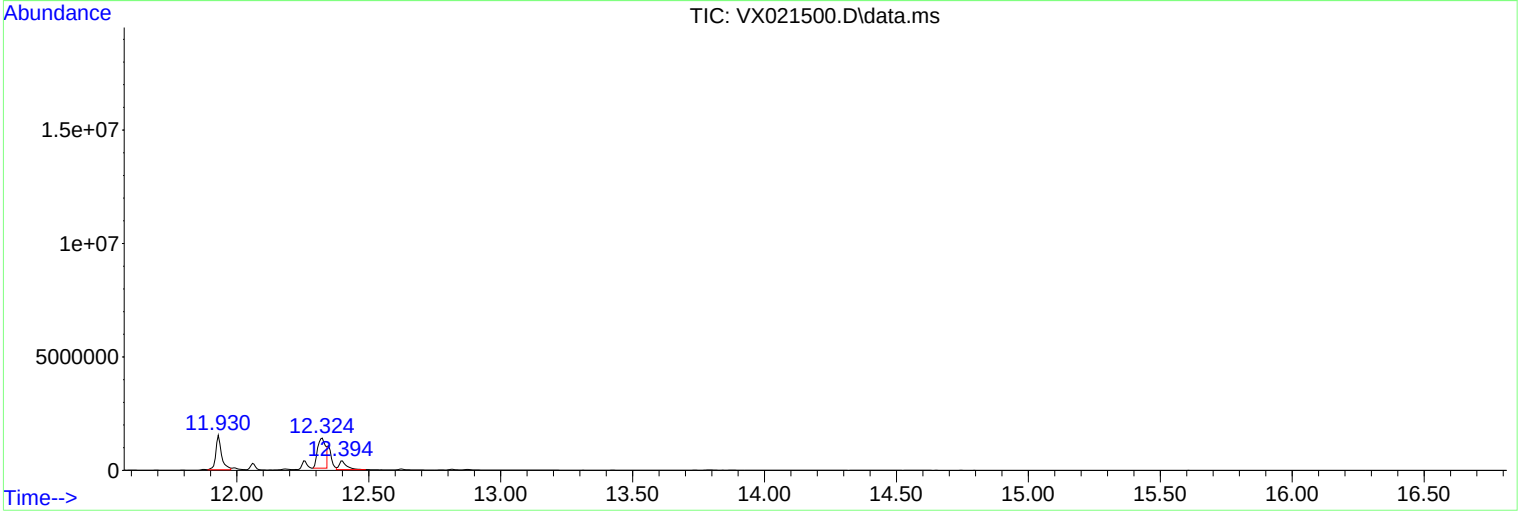
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Quant Title : SW846 8260

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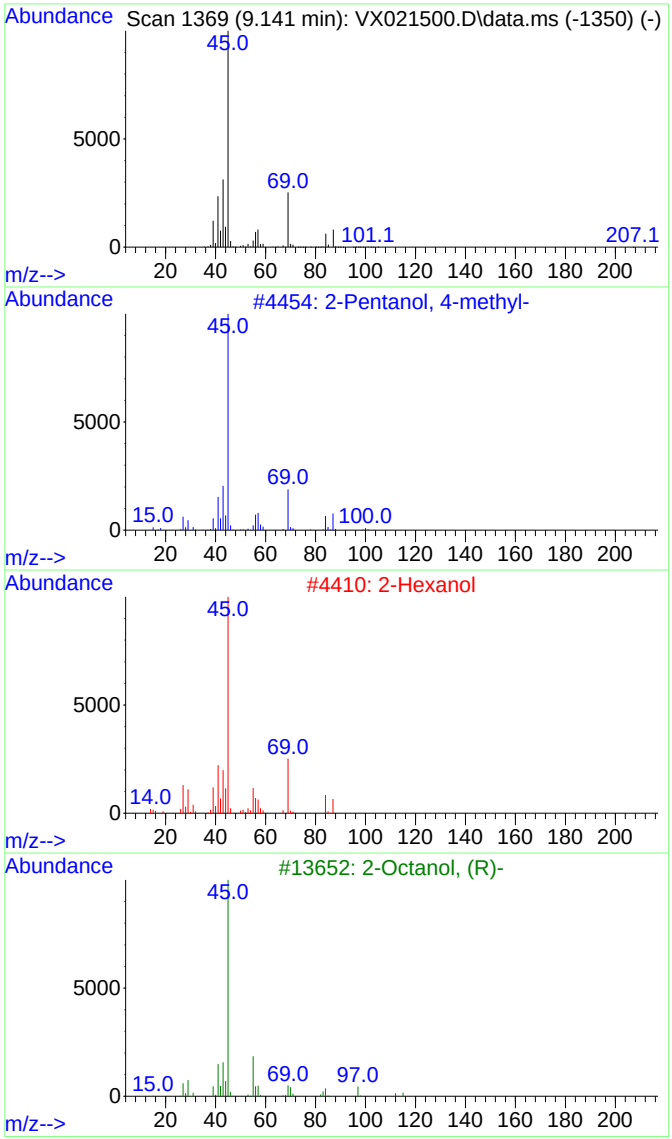
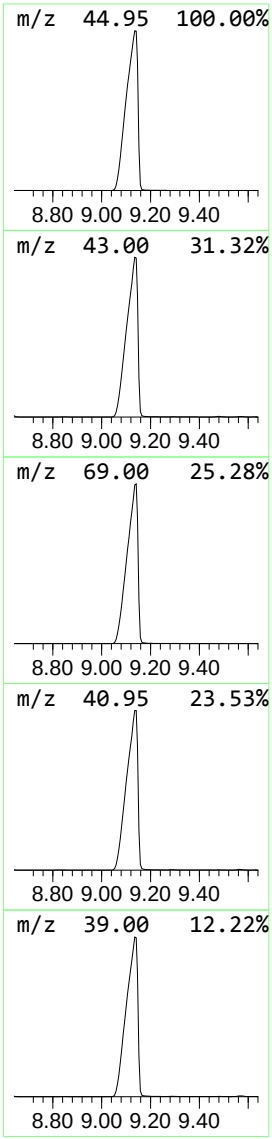
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanol, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.141	50.00 ug/l	62593900	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
2	2-Hexanol	102	C6H14O	000626-93-7	83
3	2-Octanol, (R)-	130	C8H18O	005978-70-1	78
4	2-Octanol	130	C8H18O	000123-96-6	78
5	2-Octanol, (S)-	130	C8H18O	006169-06-8	78





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Quant Title : SW846 8260

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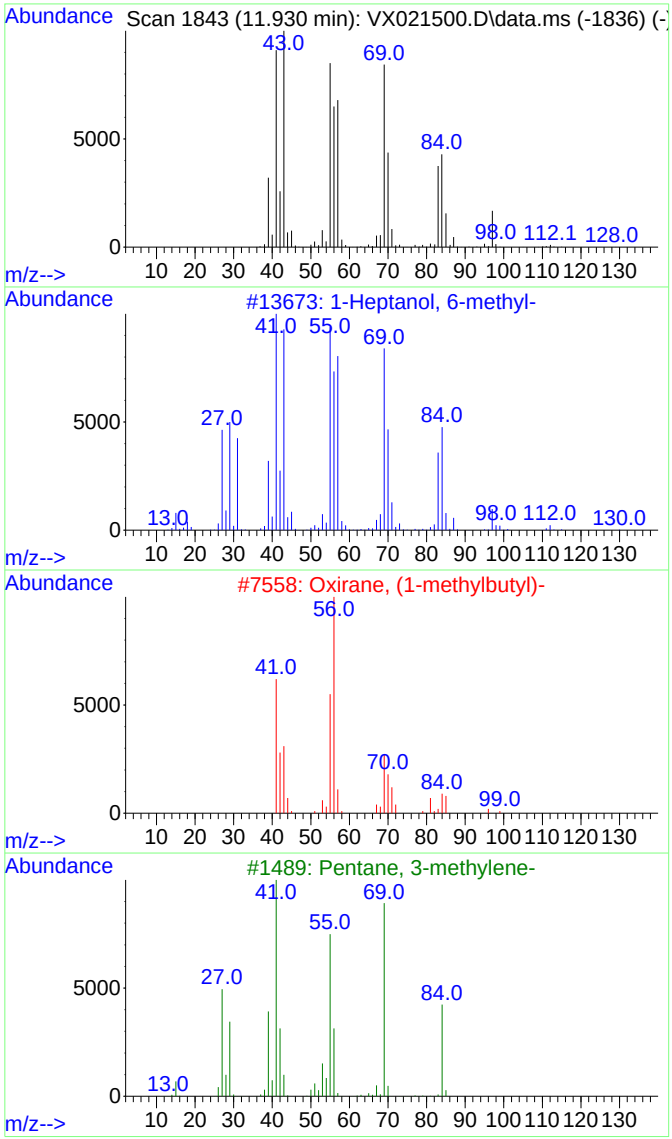
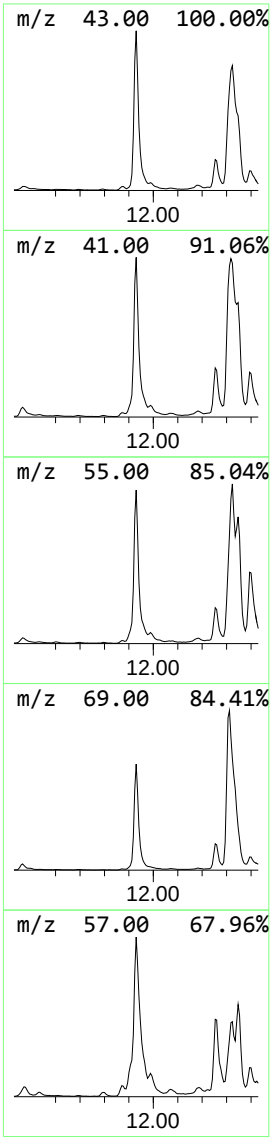
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Heptanol, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.930	50.00 ug/l	2284640	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	90
2	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	53
3	Pentane, 3-methylene-	84	C6H12	000760-21-4	52
4	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	50
5	1-Dodecene	168	C12H24	000112-41-4	47





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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 107

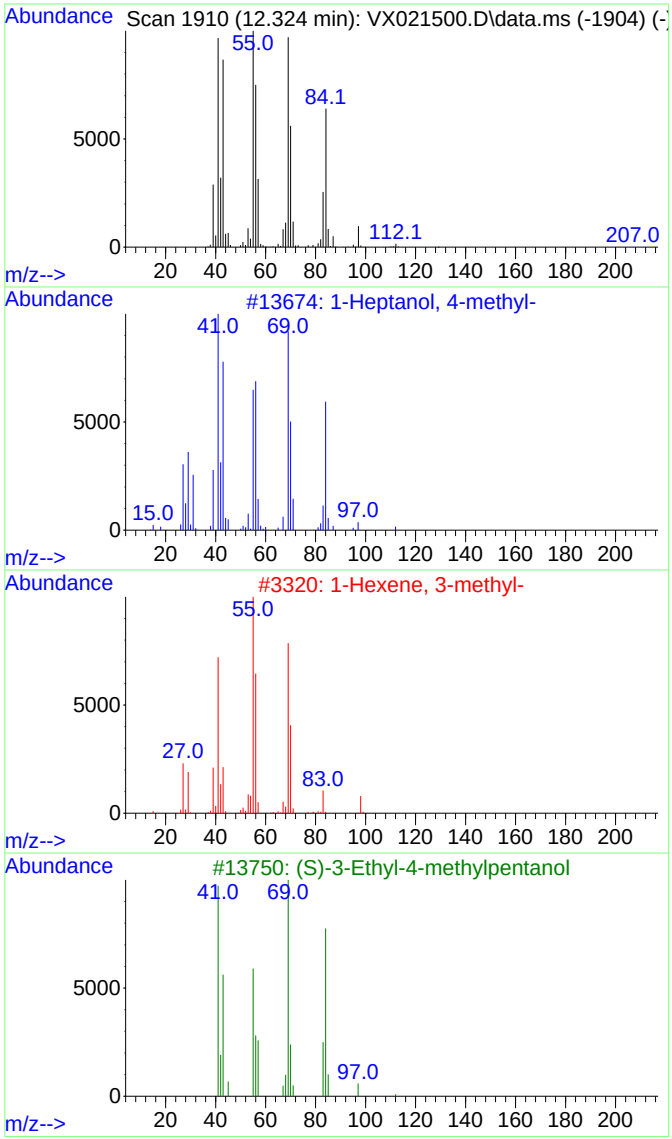
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

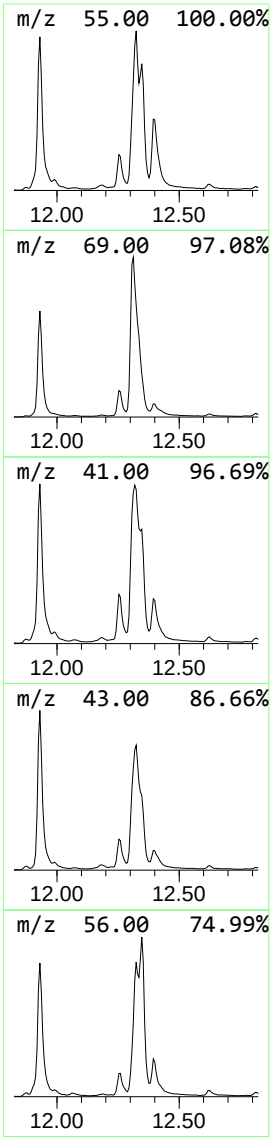
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Heptanol, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.324	64.41 ug/l	2943010	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	78
2	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	59
3	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	50
4	3-Octene, (E)-	112	C8H16	014919-01-8	49
5	Pentane, 3-methylene-	84	C6H12	000760-21-4	49





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

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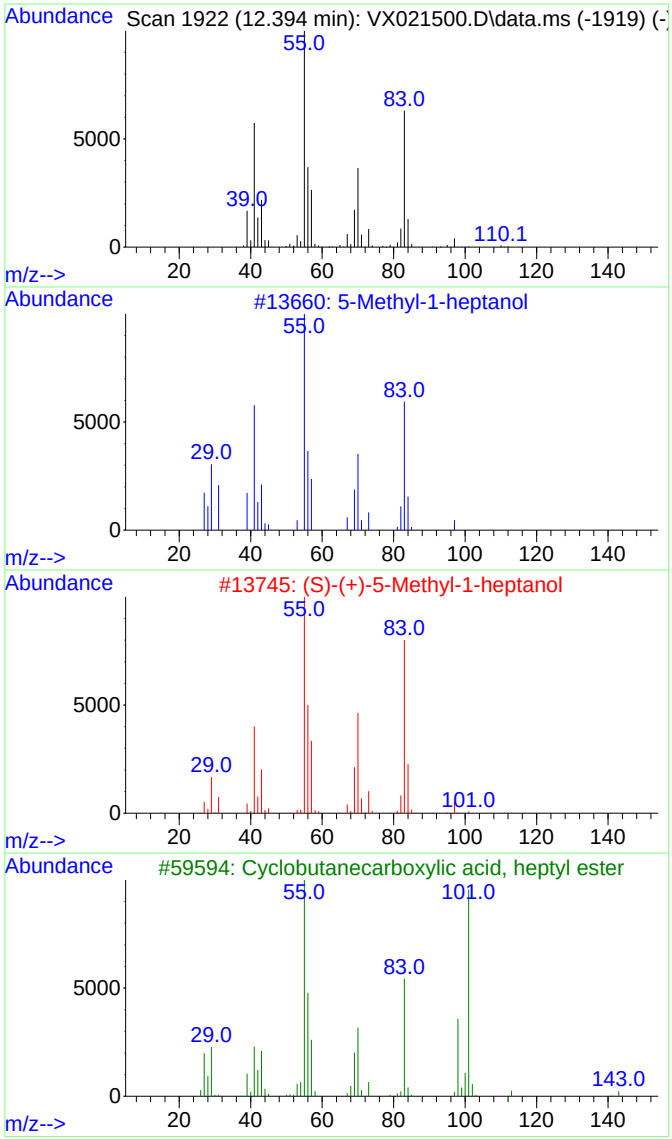
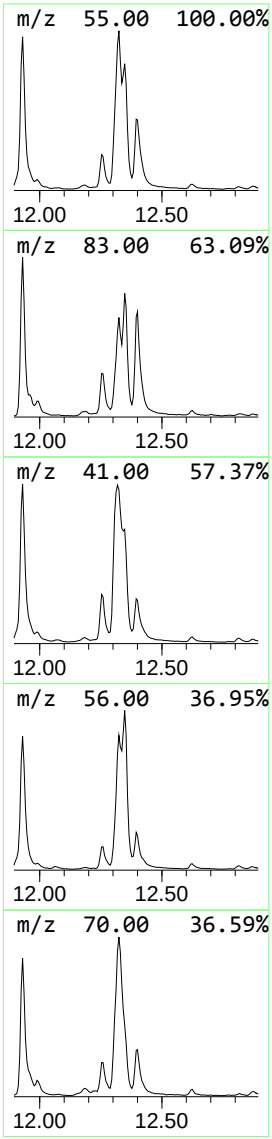
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 5-Methyl-1-heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.394	16.14 ug/l	737366	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-1-heptanol	130	C8H18O	007212-53-5	90
2	(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	86
3	Cyclobutanecarboxylic acid, hept...	198	C12H22O2	1000280-40-4	64
4	Cyclohexanone, 4-methyl-	112	C7H12O	000589-92-4	50
5	2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	50





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanol, 4-m...	9.141	50.0	ug/l	62593900	3	10.094	62593900	50.0
1-Heptanol, 6-m...	11.930	50.0	ug/l	2284640	4	12.059	2284640	50.0
1-Heptanol, 4-m...	12.324	64.4	ug/l	2943010	4	12.059	2284640	50.0
5-Methyl-1-hept...	12.394	16.1	ug/l	737366	4	12.059	2284640	50.0