LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061919\
Data File : VU032878.D
Acq On : 19 Jun 2019 23:19
Operator : JC/SP
Sample : K3414-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR060419WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.389	86	93	101	rBV	43576	45358	2.31%	0.752%
2	1.479	112	121	142	rBV	70964	186726	9.49%	3.095%
3	1.675	175	182	197	rVB	39226	52385	2.66%	0.868%
4	2.263	356	365	379	rBV	80387	121325	6.17%	2.011%
5	2.633	471	480	492	rBV	14617	34323	1.74%	0.569%
6	4.234	957	978	1017	rBV	25130	139132	7.07%	2.306%
7	4.640	1088	1104	1128	rBV	61301	152533	7.75%	2.528%
8	5.328	1293	1318	1339	rBV2	124262	333314	16.95%	5.524%
9	5.877	1477	1489	1508	rBV	113584	219027	11.14%	3.630%
10	6.324	1595	1628	1653	rBV3	92066	263498	13.40%	4.367%
11	7.221	1895	1907	1923	rBV	42614	75516	3.84%	1.252%
12	7.559	2000	2012	2025	rBV	152554	268561	13.65%	4.451%
13	7.845	2090	2101	2117	rBV	28066	49381	2.51%	0.818%
14	8.167	2187	2201	2236	rBV5	55826	234908	11.94%	3.893%
15	8.315	2237	2247	2281	rVV	219375	452608	23.01%	7.501%
16	8.463	2283	2293	2310	rVB2	60974	107061	5.44%	1.774%
17	9.083	2475	2486	2504	rBV	171495	287081	14.60%	4.758%
18	9.694	2659	2676	2721	rBV	878890	1966964	100.00%	32.598%
19	10.147	2808	2817	2832	rVB2	33112	49829	2.53%	0.826%
20	10.427	2893	2904	2918	rBV	65868	108024	5.49%	1.790%
21	11.022	3075	3089	3106	rBV	110849	211974	10.78%	3.513%
22	11.479	3220	3231	3250	rVB	195761	309708	15.75%	5.133%
23	11.855	3334	3348	3364	rBV	179249	287766	14.63%	4.769%
24	12.221	3453	3462	3495	rBV2	29538	76926	3.91%	1.275%

Sum of corrected areas: 6033928

LSC Report - Integrated Chromatogram

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Data File : VU032878.D
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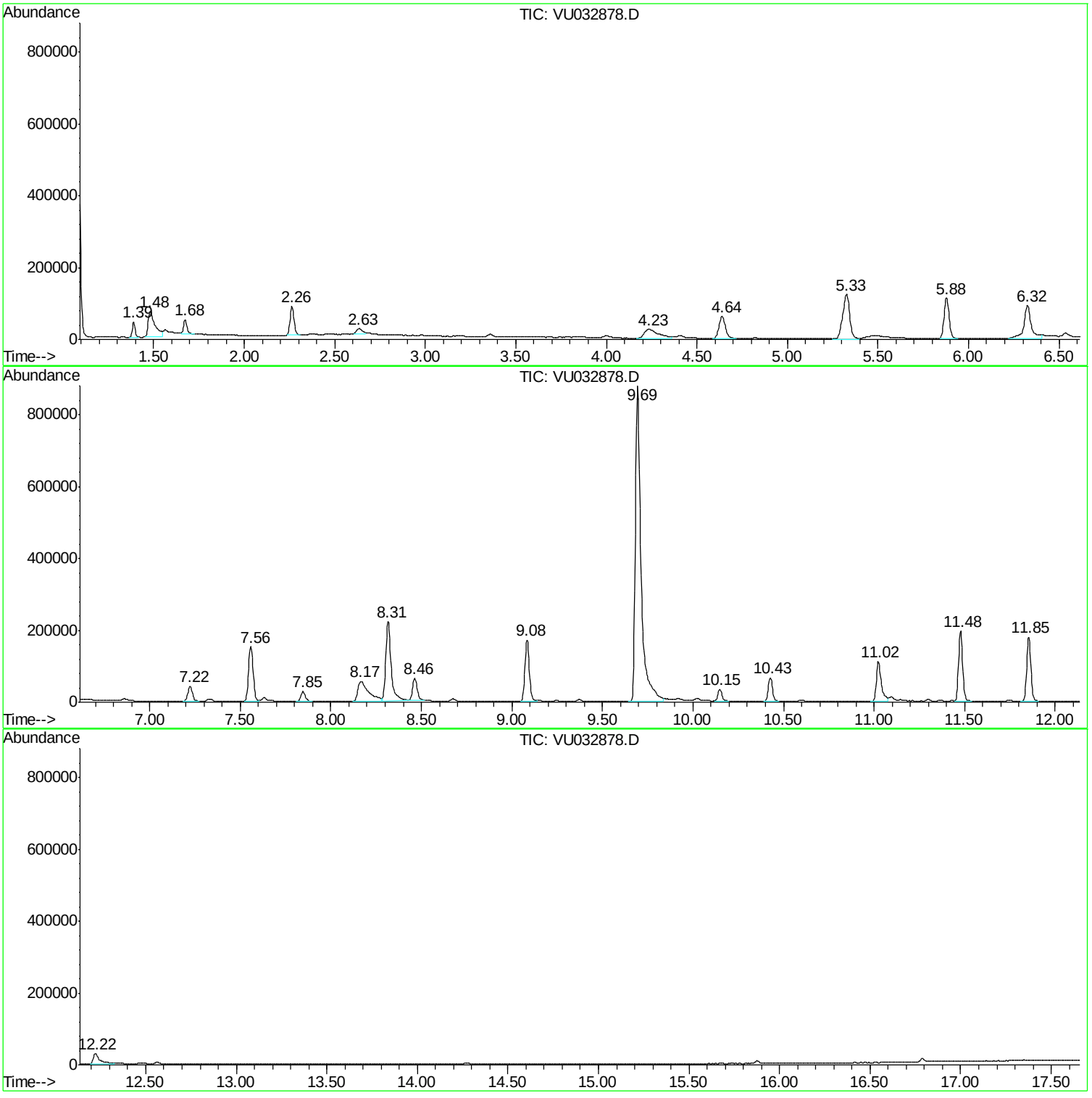
Operator : JC/SP
Sample : K3414-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061919\
Data File : VU032878.D
Acq On : 19 Jun 2019 23:19
Operator : JC/SP
Sample : K3414-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

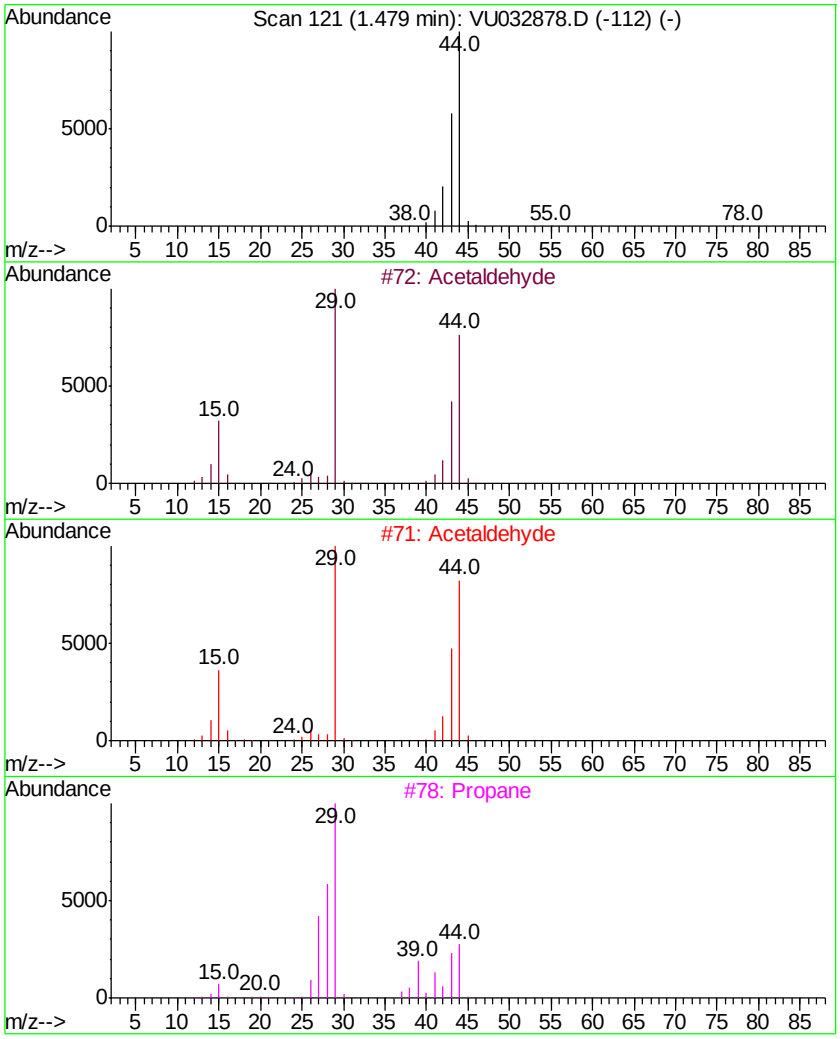
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

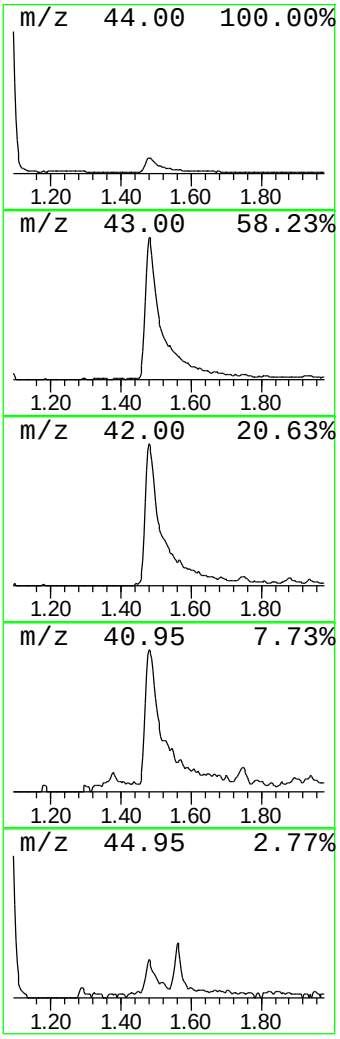
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	4.26 ug/L	186726	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	9
2	Acetaldehyde	44	C2H4O	000075-07-0	9
3	Propane	44	C3H8	000074-98-6	5
4	Ethylene oxide	44	C2H4O	000075-21-8	5
5	Ethylene oxide	44	C2H4O	000075-21-8	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061919\
Data File : VU032878.D
Acq On : 19 Jun 2019 23:19
Operator : JC/SP
Sample : K3414-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

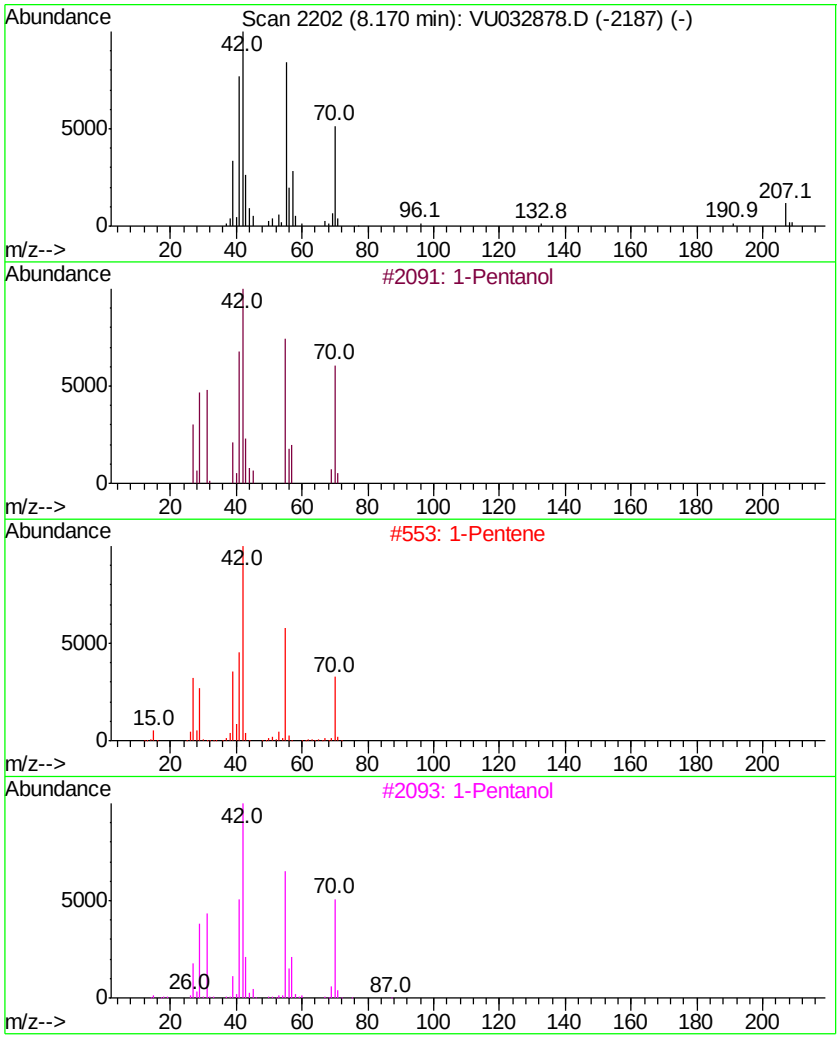
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

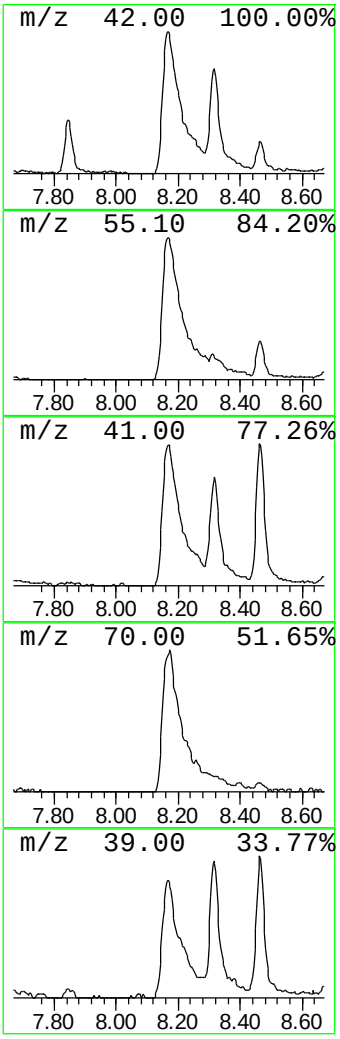
****

Peak Number 3 1-Pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	4.09 ug/L	234908	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	72
2	1-Pentene	70	C5H10	000109-67-1	64
3	1-Pentanol	88	C5H12O	000071-41-0	64
4	1-Pentene	70	C5H10	000109-67-1	58
5	1-Pentanol	88	C5H12O	000071-41-0	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061919\
Data File : VU032878.D
Acq On : 19 Jun 2019 23:19
Operator : JC/SP
Sample : K3414-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

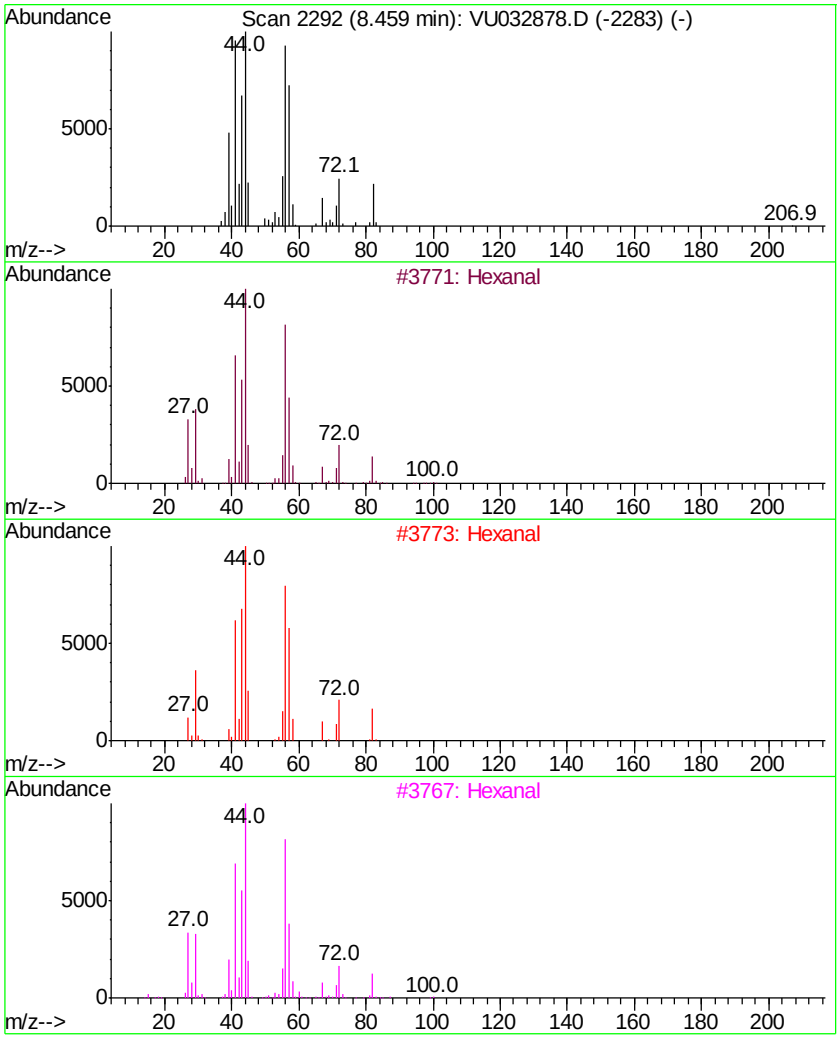
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

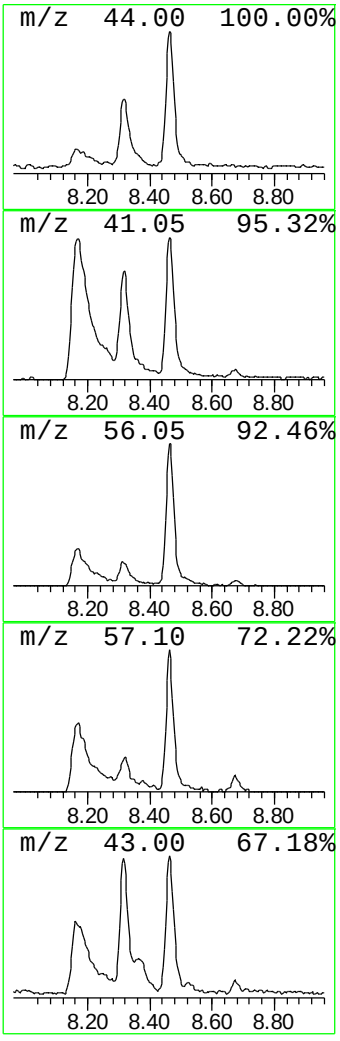
****

Peak Number 4 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	1.86 ug/L	107061	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	72
2	Hexanal	100	C6H12O	000066-25-1	64
3	Hexanal	100	C6H12O	000066-25-1	64
4	Hexanal	100	C6H12O	000066-25-1	59
5	Butanal	72	C4H8O	000123-72-8	25





Library Search Compound Report

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Data File : VU032878.D
Acq On : 19 Jun 2019 23:19
Operator : JC/SP
Sample : K3414-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

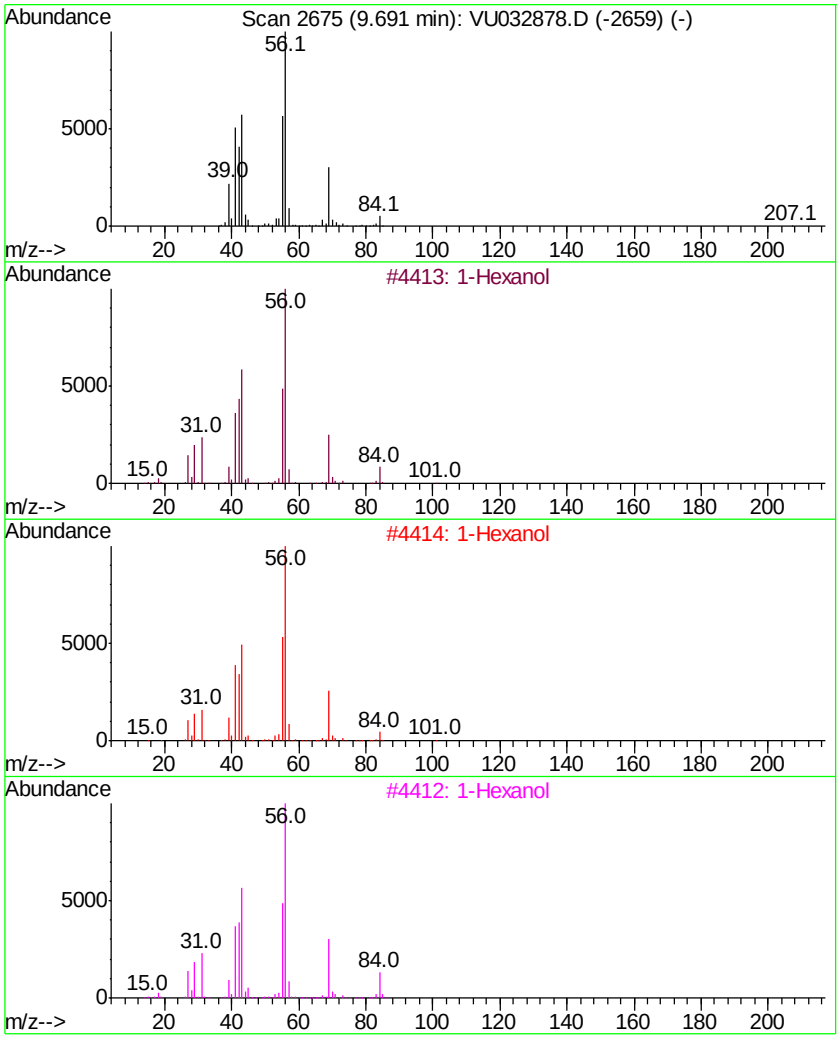
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

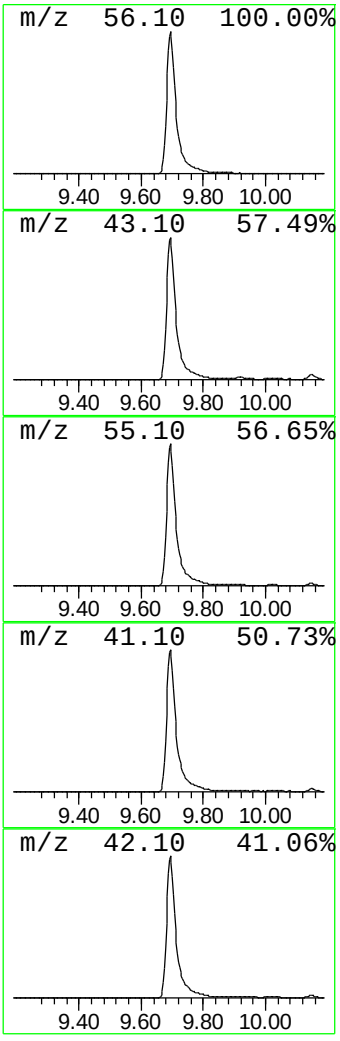
****

Peak Number 5 1-Hexanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	34.26 ug/L	1966960	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	90
2	1-Hexanol	102	C6H14O	000111-27-3	83
3	1-Hexanol	102	C6H14O	000111-27-3	78
4	Cyclobutane, butyl-	112	C8H16	013152-44-8	78
5	1-Hexanol	102	C6H14O	000111-27-3	78





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Acq On : 19 Jun 2019 23:19
Operator : JC/SP
Sample : K3414-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

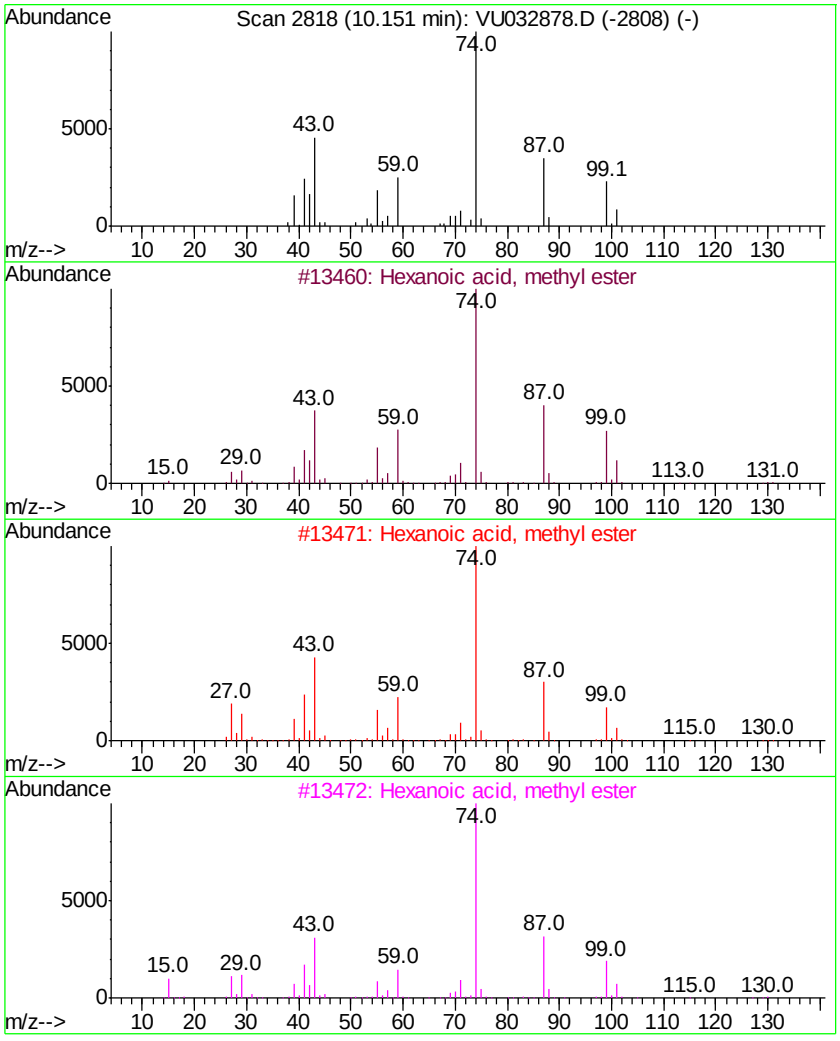
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

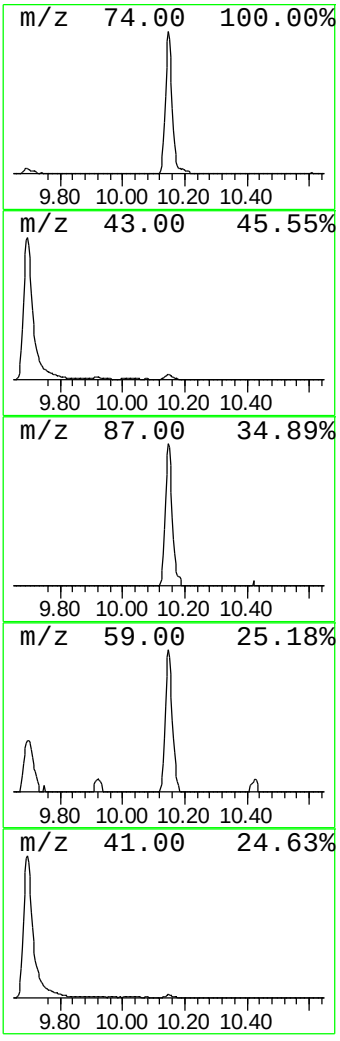
****

Peak Number 6 Hexanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	0.87 ug/L	49829	Chlorobenzene-d5	9.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	90
2	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	72
3	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	72
4	Methyl valerate	116	C6H12O2	000624-24-8	59
5	Methyl valerate	116	C6H12O2	000624-24-8	59





Library Search Compound Report

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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

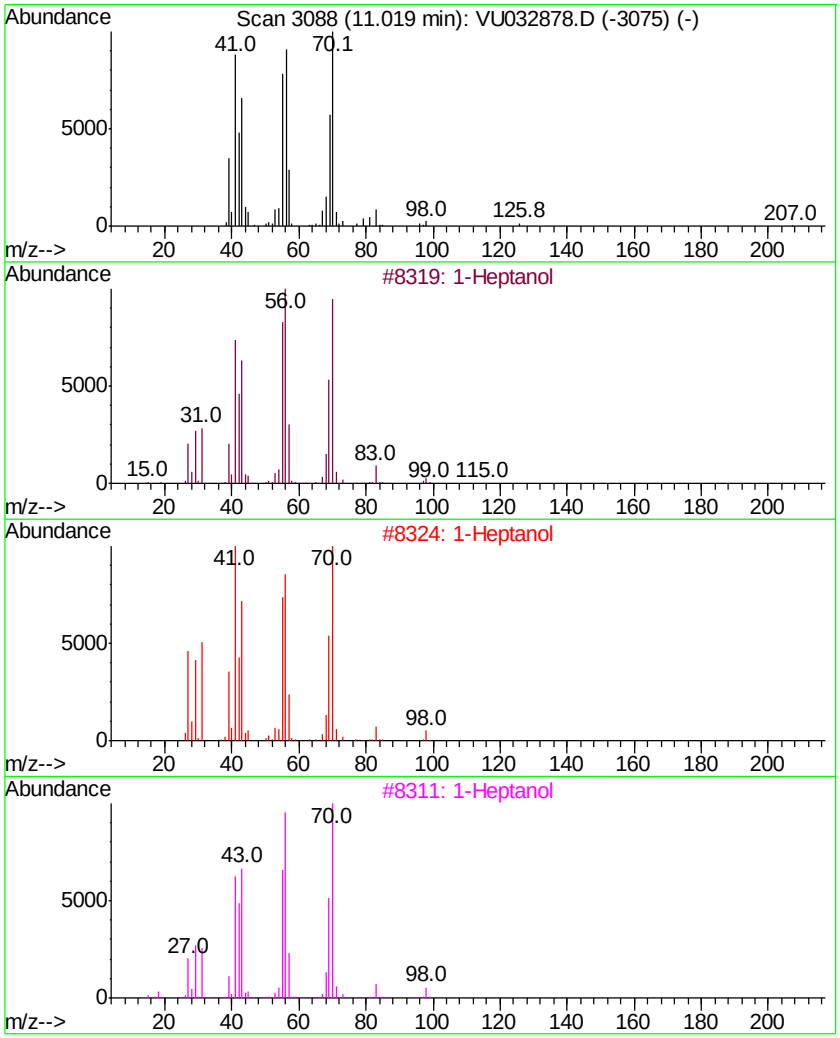
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

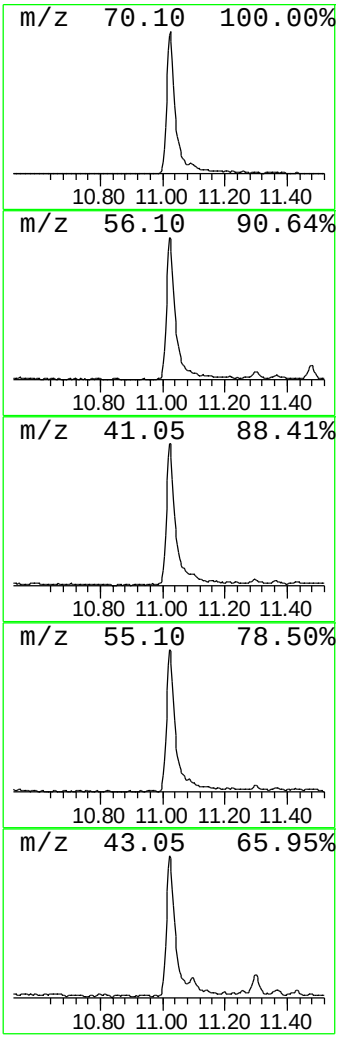
****

Peak Number 7 1-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	3.42 ug/L	211974	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol	116	C7H16O	000111-70-6	90
2	1-Heptanol	116	C7H16O	000111-70-6	90
3	1-Heptanol	116	C7H16O	000111-70-6	80
4	1-Heptanol	116	C7H16O	000111-70-6	78
5	Formic acid, heptyl ester	144	C8H16O2	000112-23-2	74





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ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GALM0

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

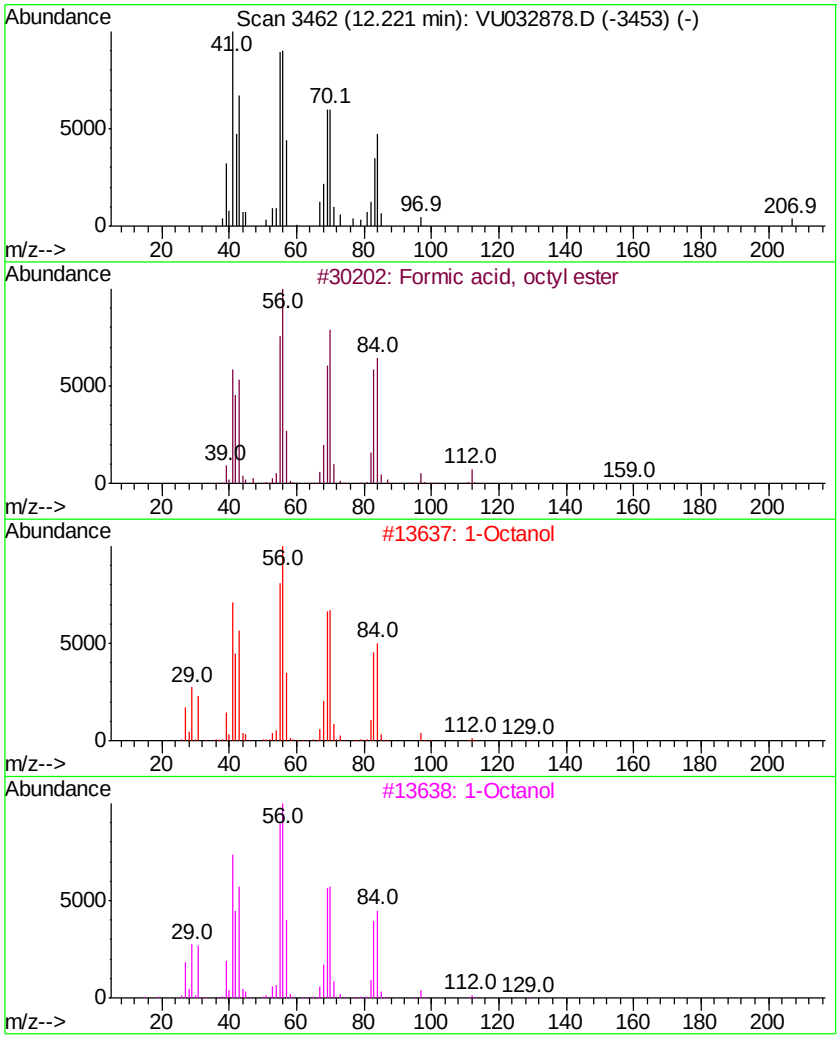
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

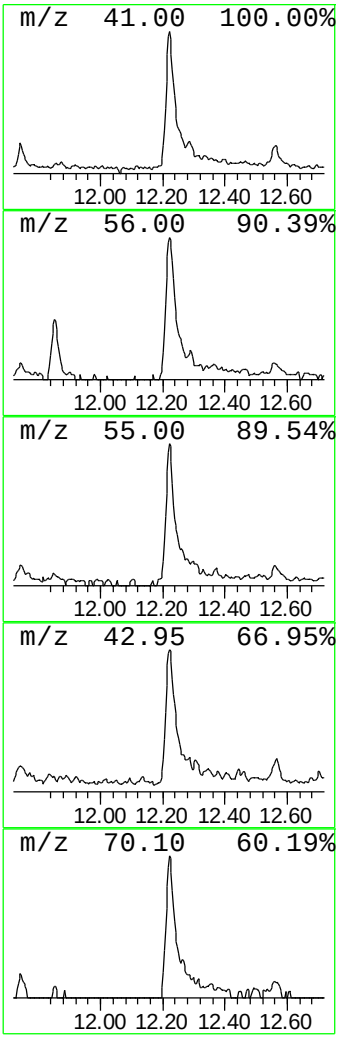
****

Peak Number 8 Formic acid, octyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.22	1.24 ug/L	76926	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
2	1-Octanol	130	C8H18O	000111-87-5	90
3	1-Octanol	130	C8H18O	000111-87-5	90
4	Octyl chloroformate	192	C9H17ClO2	007452-59-7	90
5	1-Octanol	130	C8H18O	000111-87-5	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061919\
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Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	1.48	4.3	ug/L	186726	1	5.88	219027	5.0
1-Pentanol	8.17	4.1	ug/L	234908	2	9.08	287081	5.0
Hexanal	8.46	1.9	ug/L	107061	2	9.08	287081	5.0
1-Hexanol	9.69	34.3	ug/L	1966960	2	9.08	287081	5.0
Hexanoic acid, me...	10.15	0.9	ug/L	49829	2	9.08	287081	5.0
1-Heptanol	11.02	3.4	ug/L	211974	3	11.48	309708	5.0
Formic acid, octy...	12.22	1.2	ug/L	76926	3	11.48	309708	5.0