LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU032820\
Data File : VU037451.D
Acq On : 29 Mar 2020 06:11
Operator : JC/MD
Sample : L2001-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

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\SOMUTR032820WMA.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	1.607	75	83	93	rBV	48586	53691	3.83%	0.955%
2	1.925	173	182	190	rBV	41437	52033	3.71%	0.926%
3	2.584	377	387	404	rVB	76329	123770	8.83%	2.202%
4	3.009	509	519	533	rBV	20592	52228	3.73%	0.929%
5	3.819	761	771	786	rVB10	10057	24777	1.77%	0.441%
6	4.739	1042	1057	1087	rBV2	24077	106981	7.63%	1.904%
7	5.102	1157	1170	1193	rVB2	72220	193732	13.82%	3.447%
8	5.751	1356	1372	1389	rBV2	155302	339100	24.19%	6.034%
9	6.279	1523	1536	1552	rBV	120528	238271	17.00%	4.240%
10	6.726	1651	1675	1698	rBV2	96972	251547	17.95%	4.476%
11	7.594	1936	1945	1958	rVB2	51654	87236	6.22%	1.552%
12	7.706	1971	1980	1993	rVB2	17597	32464	2.32%	0.578%
13	7.922	2035	2047	2059	rVB	166511	280647	20.02%	4.994%
14	8.205	2126	2135	2148	rBV2	32688	54543	3.89%	0.971%
15	8.536	2221	2238	2264	rBV4	51289	207874	14.83%	3.699%
16	8.677	2271	2282	2312	rVB	219234	420845	30.02%	7.488%
17	9.015	2380	2387	2397	rVB3	12904	19091	1.36%	0.340%
18	9.436	2508	2518	2539	rVB	164758	279273	19.92%	4.969%
19	10.041	2693	2706	2750	rBV	602299	1401759	100.00%	24.942%
20	10.481	2832	2843	2855	rBV	57282	85136	6.07%	1.515%
21	10.639	2871	2892	2895	rBV5	15743	33376	2.38%	0.594%
22	10.777	2925	2935	2950	rVB	65446	103658	7.39%	1.844%
23	11.362	3105	3117	3130	rBV2	108318	194673	13.89%	3.464%
24	11.825	3247	3261	3285	rBV3	236561	470265	33.55%	8.368%
25	12.082	3332	3341	3360	rBV	73211	137958	9.84%	2.455%
26	12.208	3369	3380	3391	rVB	160776	258821	18.46%	4.605%
27	12.565	3482	3491	3505	rBV2	54506	96277	6.87%	1.713%
28	14.703	4149	4156	4169	rVB6	12927	20000	1.43%	0.356%

Sum of corrected areas: 5620026

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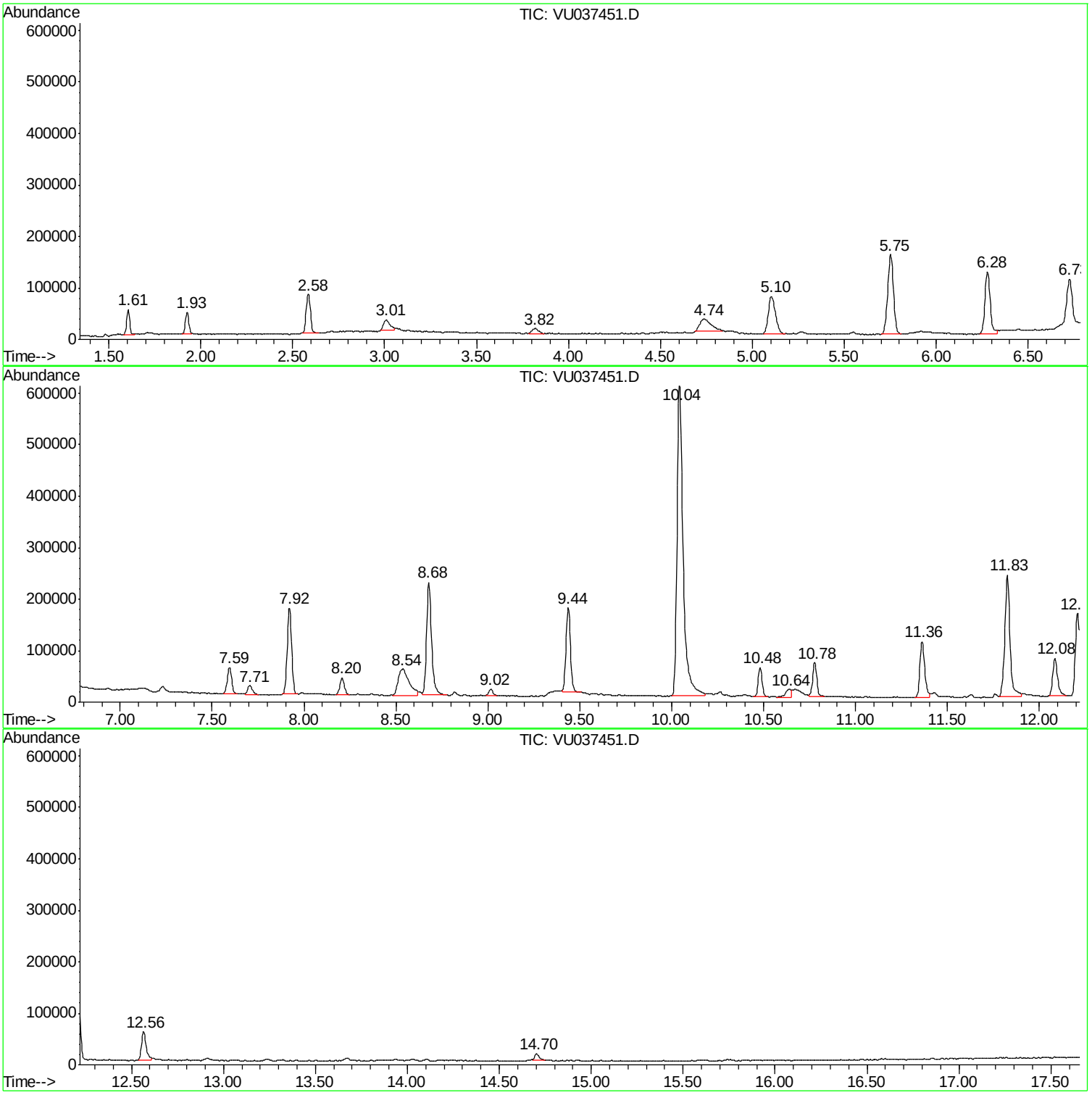
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Data File : VU037451.D
Acq On : 29 Mar 2020 06:11
Operator : JC/MD
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Quant Title : TRACE VOA SOM01.0

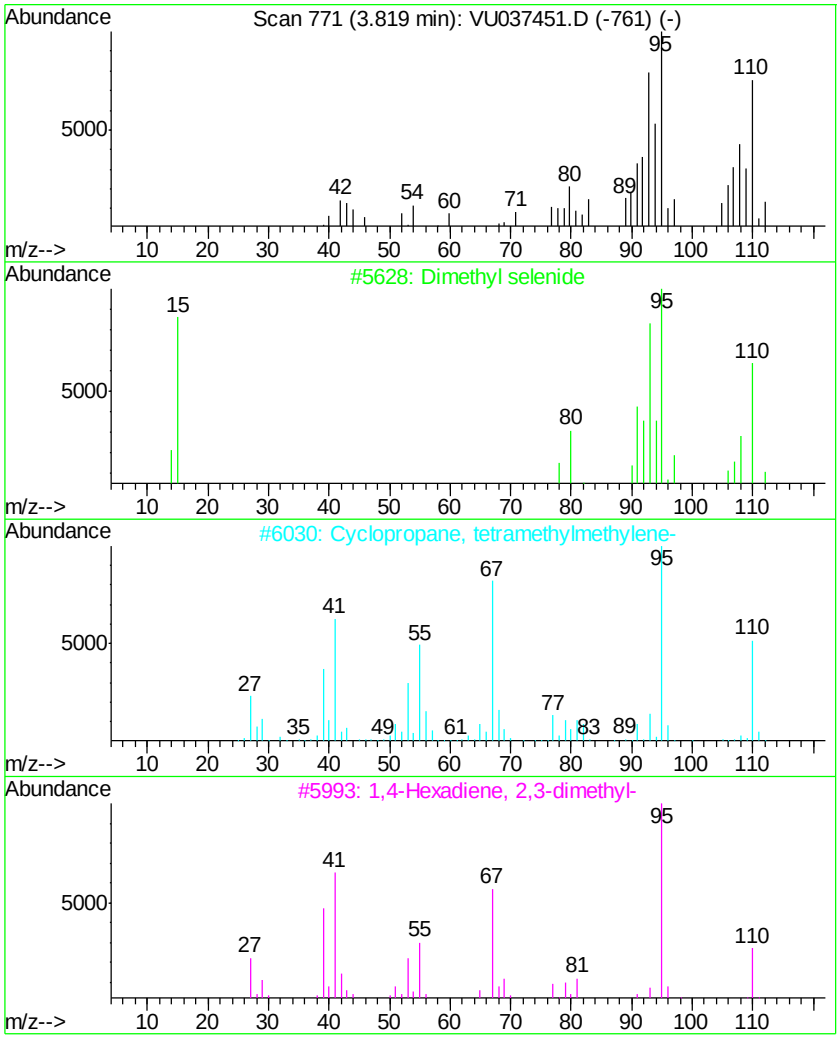
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

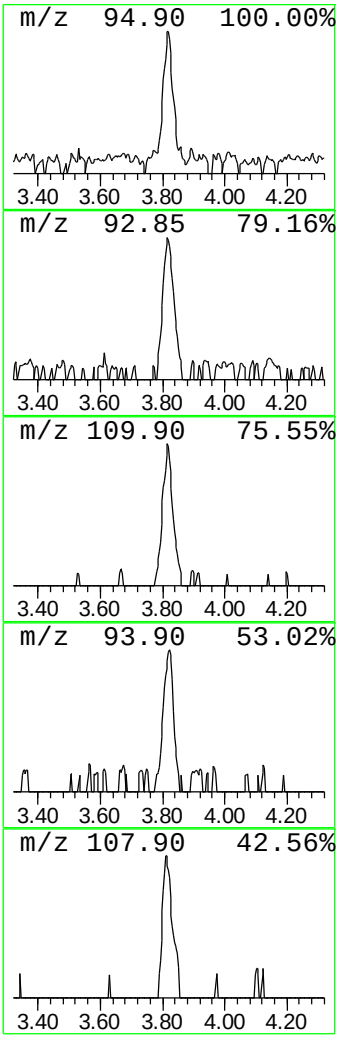
****

Peak Number 1 Dimethyl selenide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.82	0.52 ug/L	24777	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl selenide	110	C2H6Se	000593-79-3	74
2	Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	30
3	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	27
4	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	27
5	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	27





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Data File : VU037451.D
Acq On : 29 Mar 2020 06:11
Operator : JC/MD
Sample : L2001-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

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

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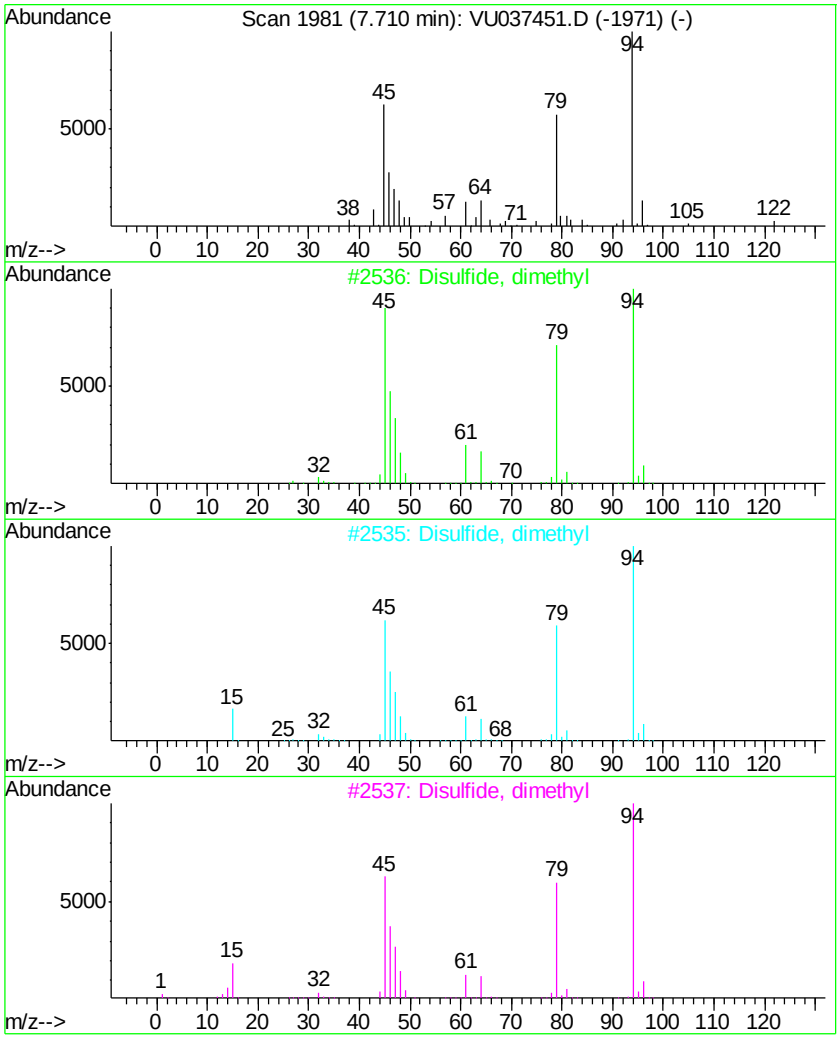
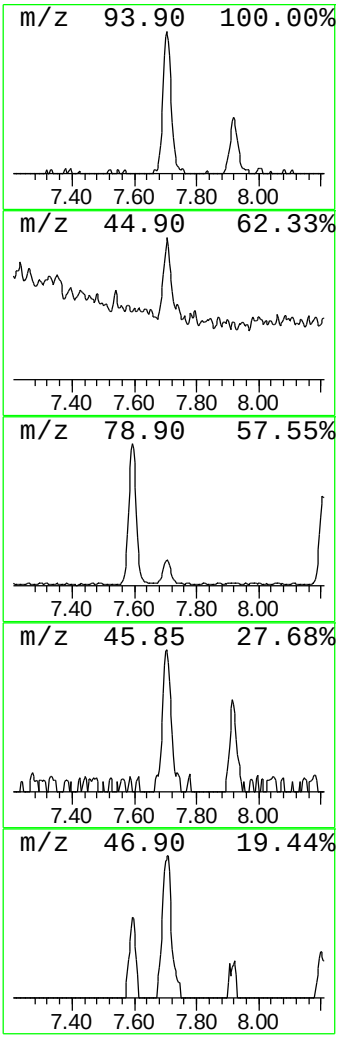
Peak Number 3 Disulfide, dimethyl Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	0.68 ug/L	32464	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
4	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU032820\
Data File : VU037451.D
Acq On : 29 Mar 2020 06:11
Operator : JC/MD
Sample : L2001-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

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

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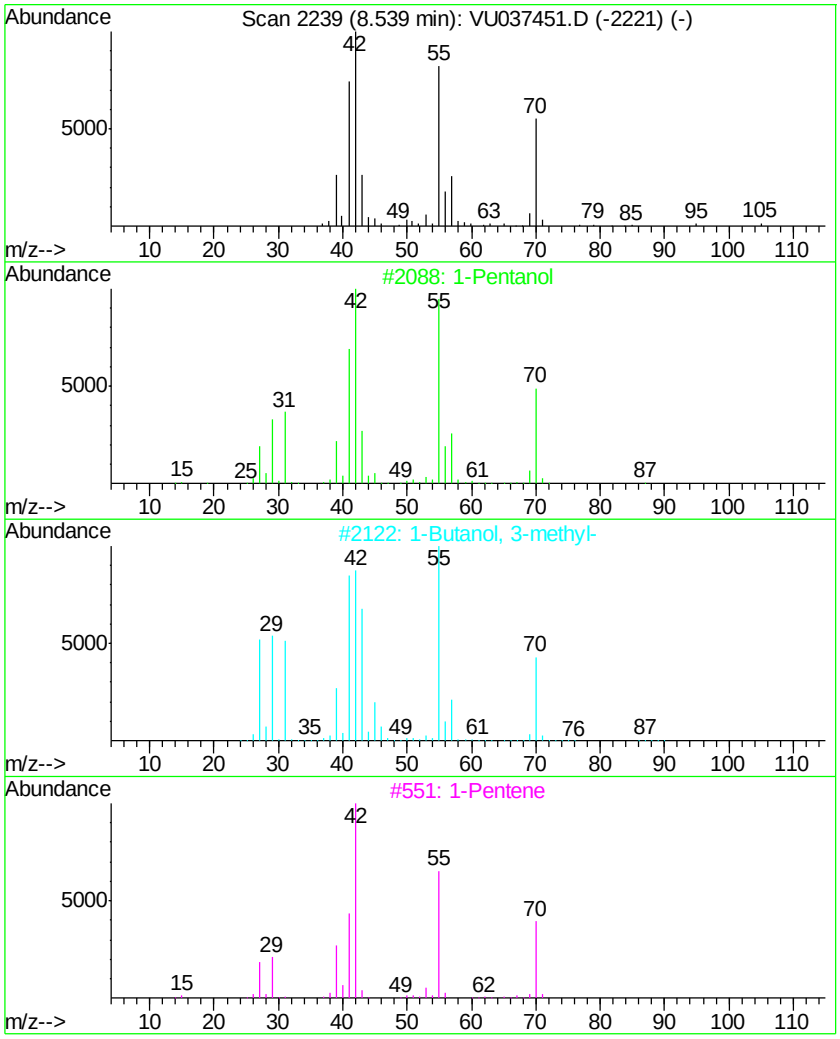
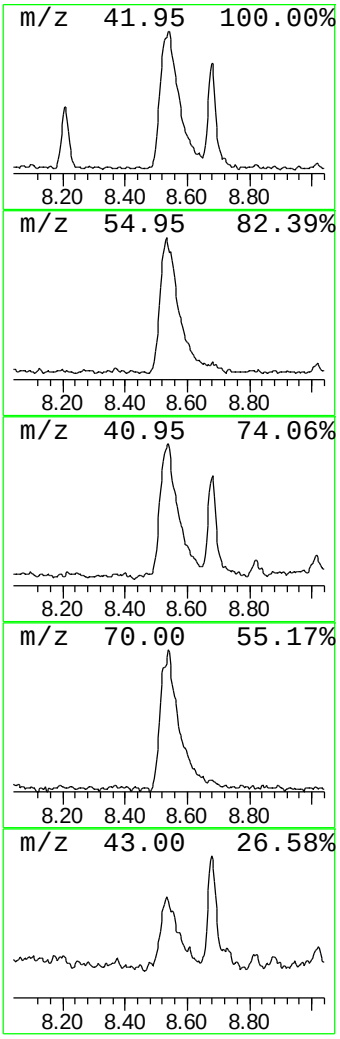
Peak Number 4 1-Pentanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.54	3.72 ug/L	207874	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	83
2	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	78
3	1-Pentene	70	C5H10	000109-67-1	72
4	1-Pentanol	88	C5H12O	000071-41-0	64
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU032820\
Data File : VU037451.D
Acq On : 29 Mar 2020 06:11
Operator : JC/MD
Sample : L2001-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

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

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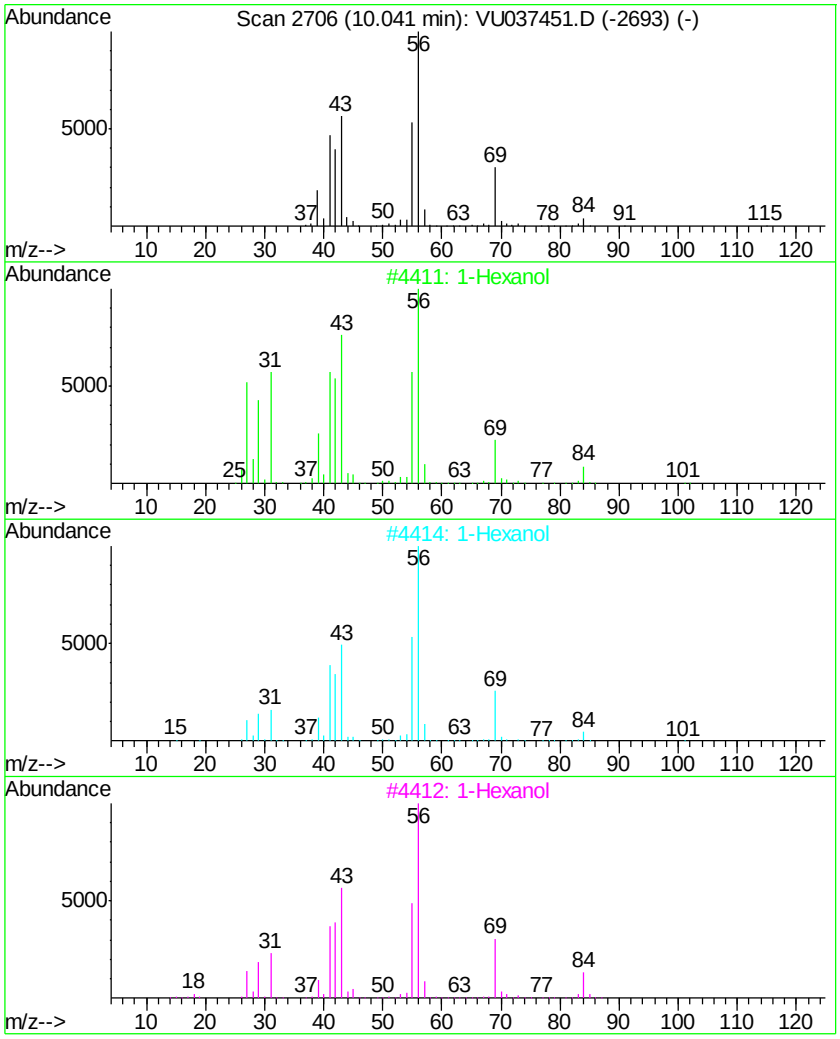
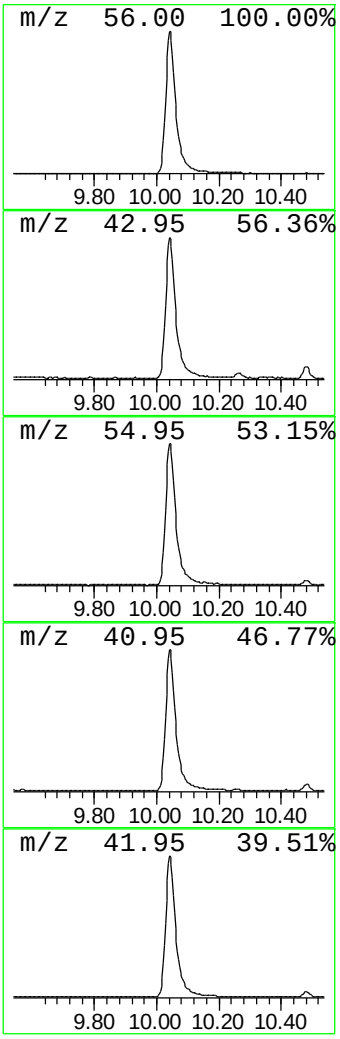
Peak Number 5 1-Hexanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.04	25.10 ug/L	1401760	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	1-Hexanol	102	C6H14O	000111-27-3	83
3	1-Hexanol	102	C6H14O	000111-27-3	78
4	1-Hexanol	102	C6H14O	000111-27-3	72
5	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU032820\
Data File : VU037451.D
Acq On : 29 Mar 2020 06:11
Operator : JC/MD
Sample : L2001-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

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

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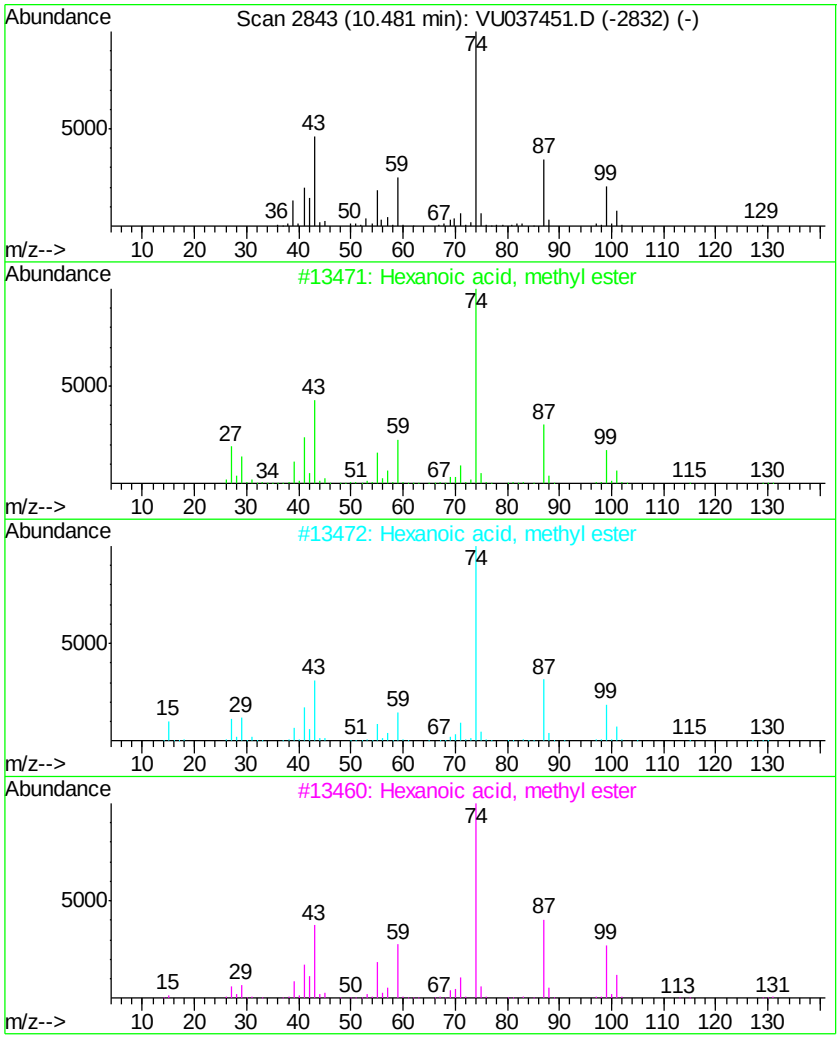
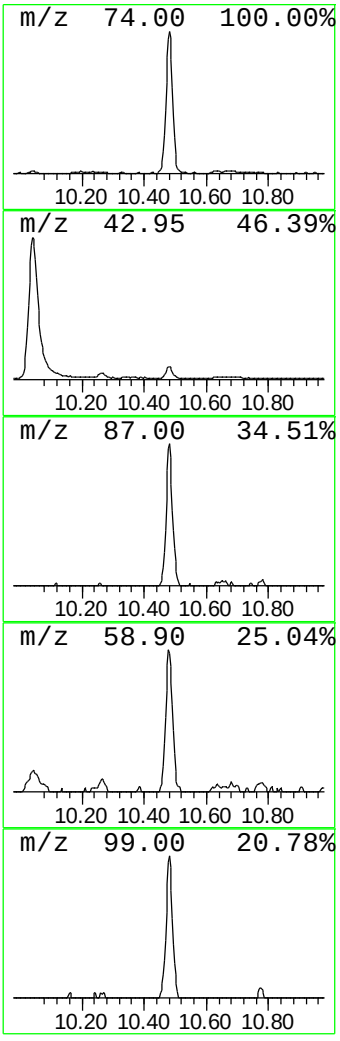
Peak Number 6 Hexanoic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.48	1.52 ug/L	85136	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	72
2	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	64
3	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	64
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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Operator : JC/MD
Sample : L2001-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

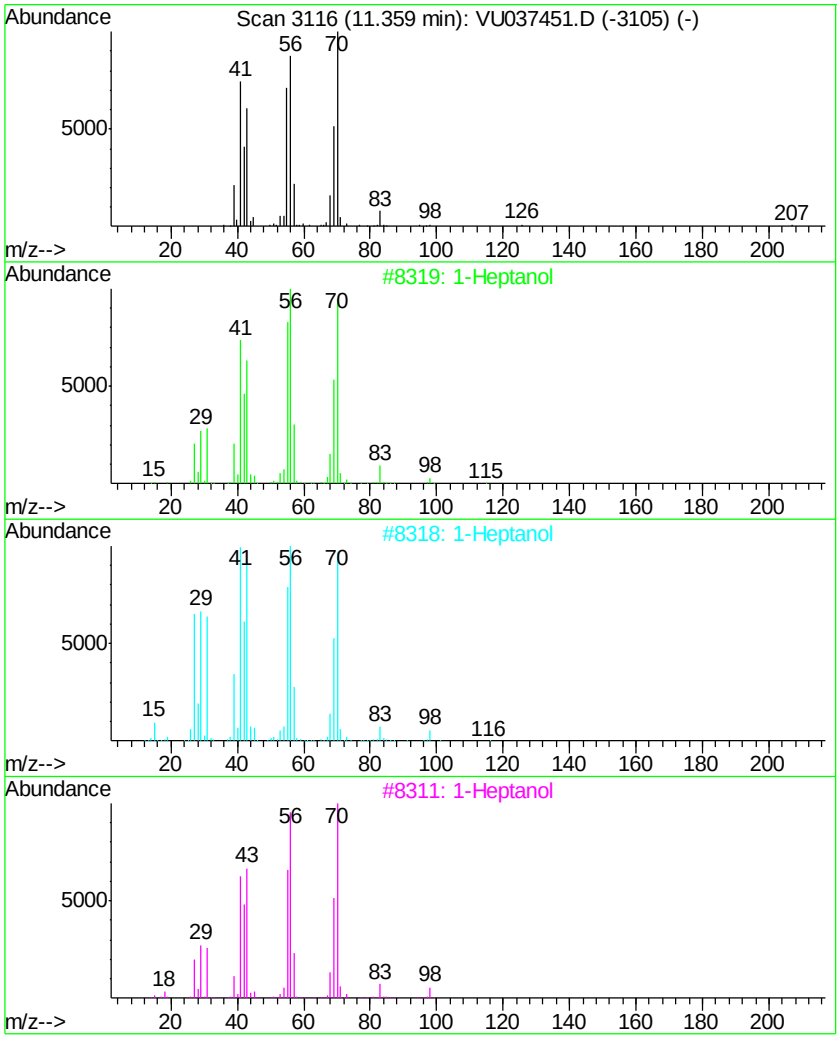
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

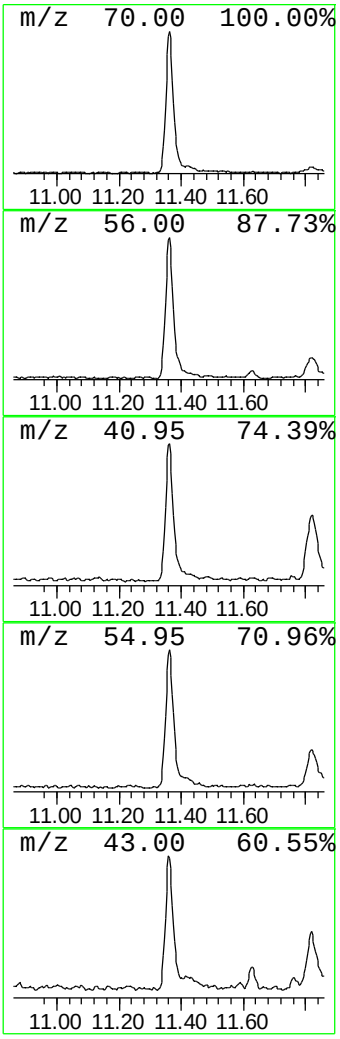
****

Peak Number 7 1-Heptanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.36	2.07 ug/L	194673	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol	116	C7H16O	000111-70-6	83
2	1-Heptanol	116	C7H16O	000111-70-6	83
3	1-Heptanol	116	C7H16O	000111-70-6	80
4	1-Heptanol	116	C7H16O	000111-70-6	80
5	Formic acid, heptyl ester	144	C8H16O2	000112-23-2	78





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ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

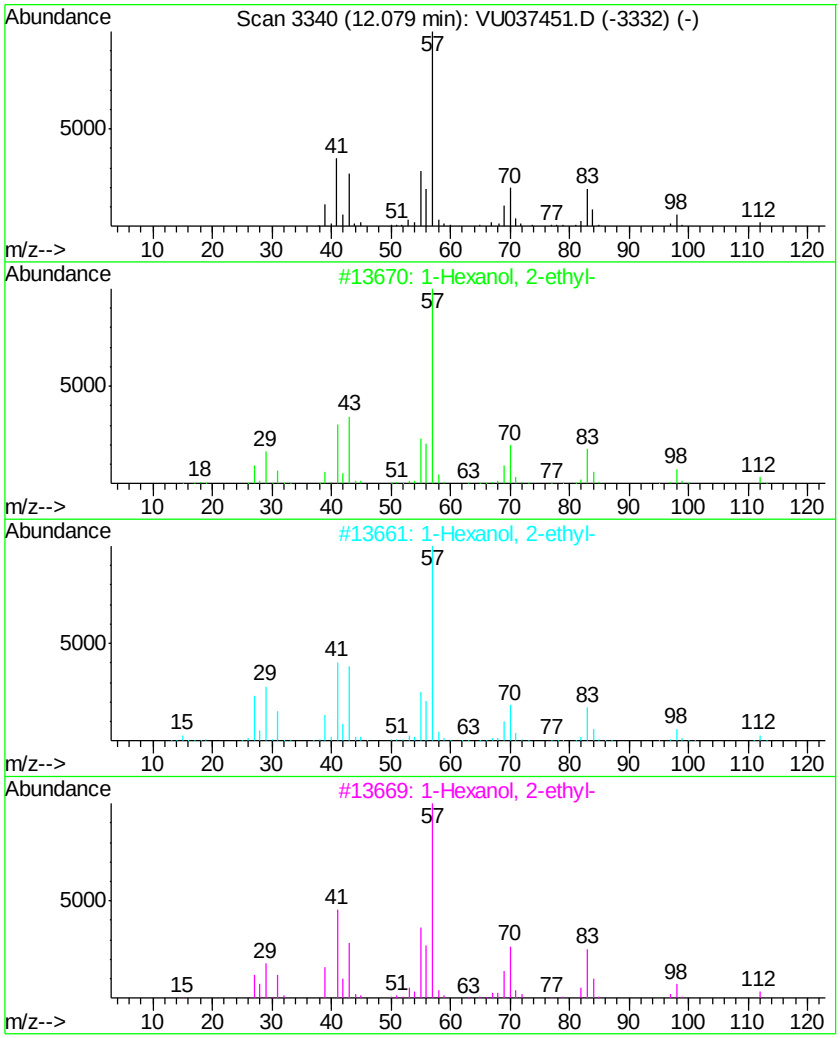
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

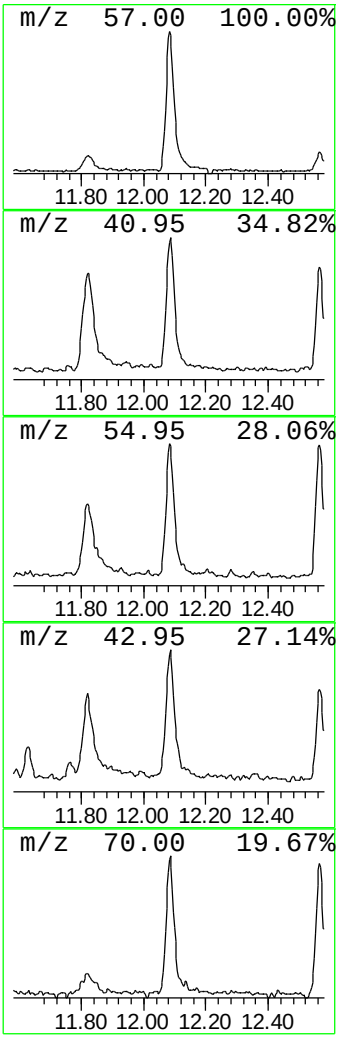
****

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	1.47 ug/L	137958	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53





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ClientSampleId : GAWF5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR032820WMA.M
Quant Title : TRACE VOA SOM01.0

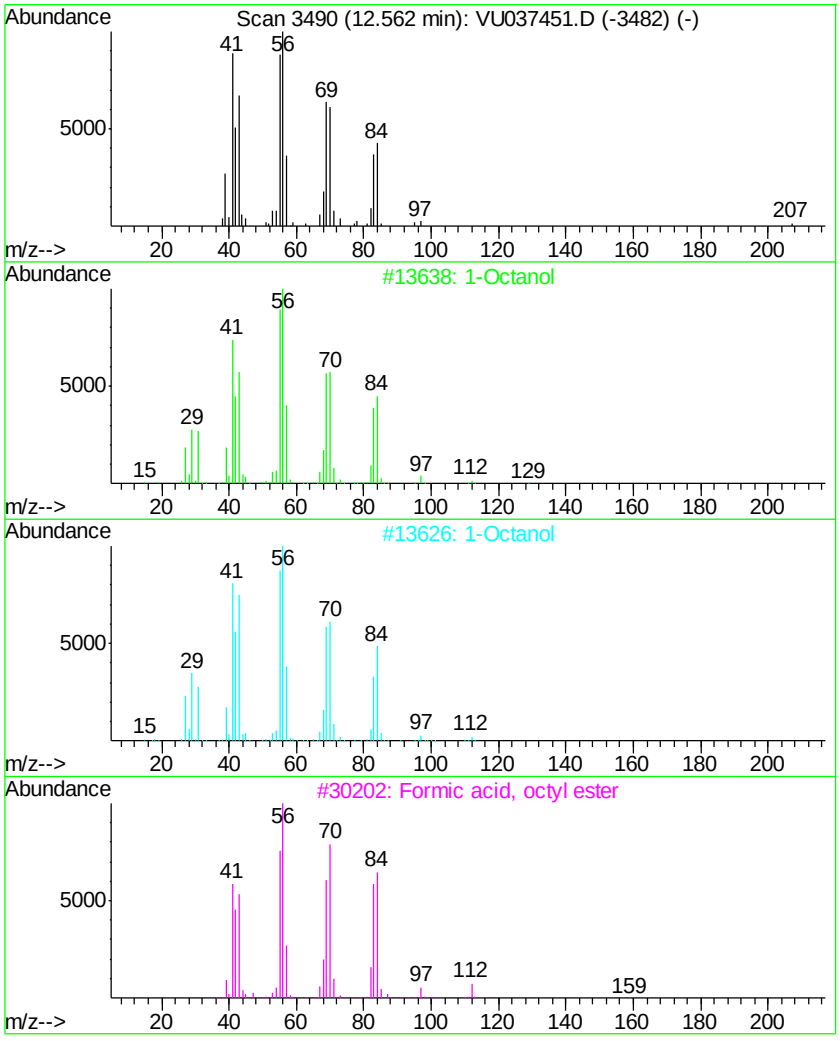
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

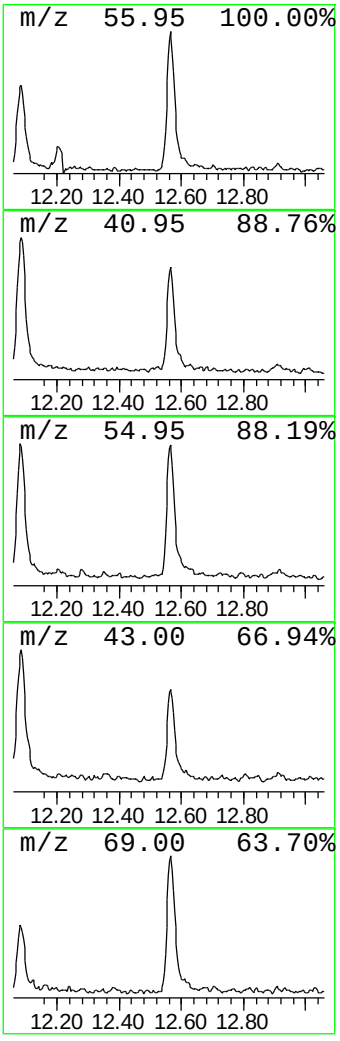
****

Peak Number 9 1-Octanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	1.02 ug/L	96277	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol	130	C8H18O	000111-87-5	90
2	1-Octanol	130	C8H18O	000111-87-5	90
3	Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
4	1-Octanol	130	C8H18O	000111-87-5	90
5	1-Octanol	130	C8H18O	000111-87-5	72





Tentatively Identified Compound (LSC) summary

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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
Dimethyl selenide	3.82	0.5	ug/L	24777	1	6.28	238271	5.0
Disulfide, dimethyl	7.71	0.7	ug/L	32464	1	6.28	238271	5.0
1-Pentanol	8.54	3.7	ug/L	207874	2	9.44	279273	5.0
1-Hexanol	10.04	25.1	ug/L	1401760	2	9.44	279273	5.0
Hexanoic acid, me...	10.48	1.5	ug/L	85136	2	9.44	279273	5.0
1-Heptanol	11.36	2.1	ug/L	194673	3	11.83	470265	5.0
1-Hexanol, 2-ethyl-	12.08	1.5	ug/L	137958	3	11.83	470265	5.0
1-Octanol	12.56	1.0	ug/L	96277	3	11.83	470265	5.0