LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039018.D
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

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\SOMUTR062220WMA.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	1.610	75	84	93	rBV	214409	276281	5.60%	1.686%
2	1.928	176	183	200	rVB2	145082	228416	4.63%	1.394%
3	2.587	375	388	404	rBV	289837	486473	9.86%	2.970%
4	2.819	446	460	495	rBV	14842	62306	1.26%	0.380%
5	3.234	571	589	614	rBV4	24096	85920	1.74%	0.524%
6	3.909	779	799	827	rBV	2061748	4933679	100.00%	30.116%
7	4.671	1018	1036	1074	rBV2	270317	751914	15.24%	4.590%
8	4.854	1079	1093	1118	rVB	28653	82018	1.66%	0.501%
9	5.099	1153	1169	1190	rBV	233037	515136	10.44%	3.145%
10	5.758	1350	1374	1408	rBV2	481509	1264070	25.62%	7.716%
11	6.279	1521	1536	1553	rBV	347581	654319	13.26%	3.994%
12	6.719	1658	1673	1691	rBV	307873	593198	12.02%	3.621%
13	6.944	1726	1743	1757	rBV2	89482	179634	3.64%	1.097%
14	7.590	1934	1944	1962	rVB	126994	222799	4.52%	1.360%
15	7.742	1976	1991	2011	rVB	82958	152990	3.10%	0.934%
16	7.922	2032	2047	2062	rBV	559385	964135	19.54%	5.885%
17	8.201	2119	2134	2145	rBV	85308	142185	2.88%	0.868%
18	8.658	2260	2276	2315	rBV	833740	1570995	31.84%	9.590%
19	9.436	2504	2518	2533	rBV	518697	857306	17.38%	5.233%
20	10.278	2763	2780	2799	rBV2	67822	143807	2.91%	0.878%
21	10.770	2921	2933	2951	rVB	247246	396267	8.03%	2.419%
22	11.044	3003	3018	3031	rBV2	75196	133322	2.70%	0.814%
23	11.825	3247	3261	3277	rBV	502953	796514	16.14%	4.862%
24	12.204	3365	3379	3396	rBV	551249	888380	18.01%	5.423%

Sum of corrected areas: 16382064

LSC Report - Integrated Chromatogram

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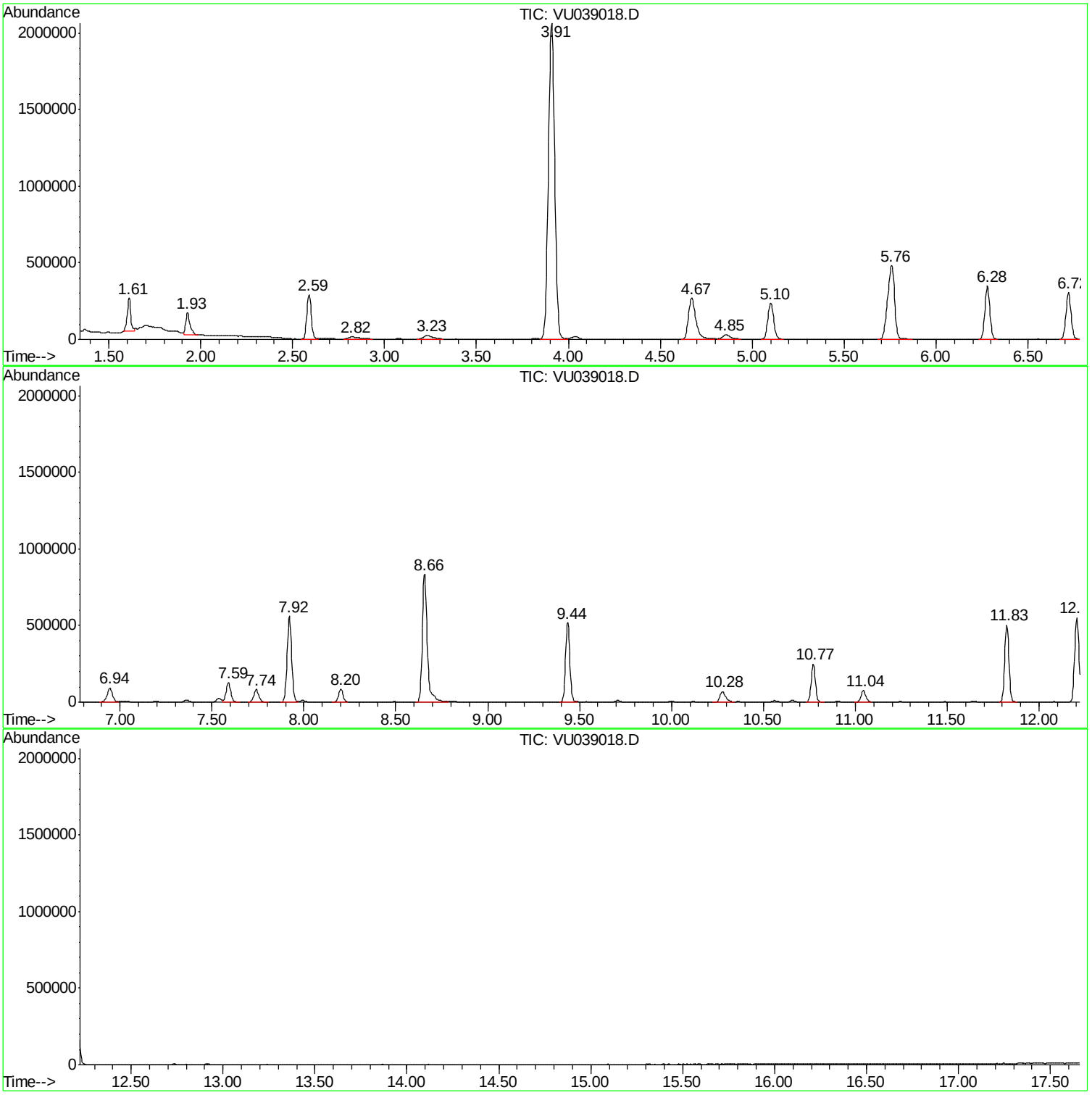
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039018.D
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

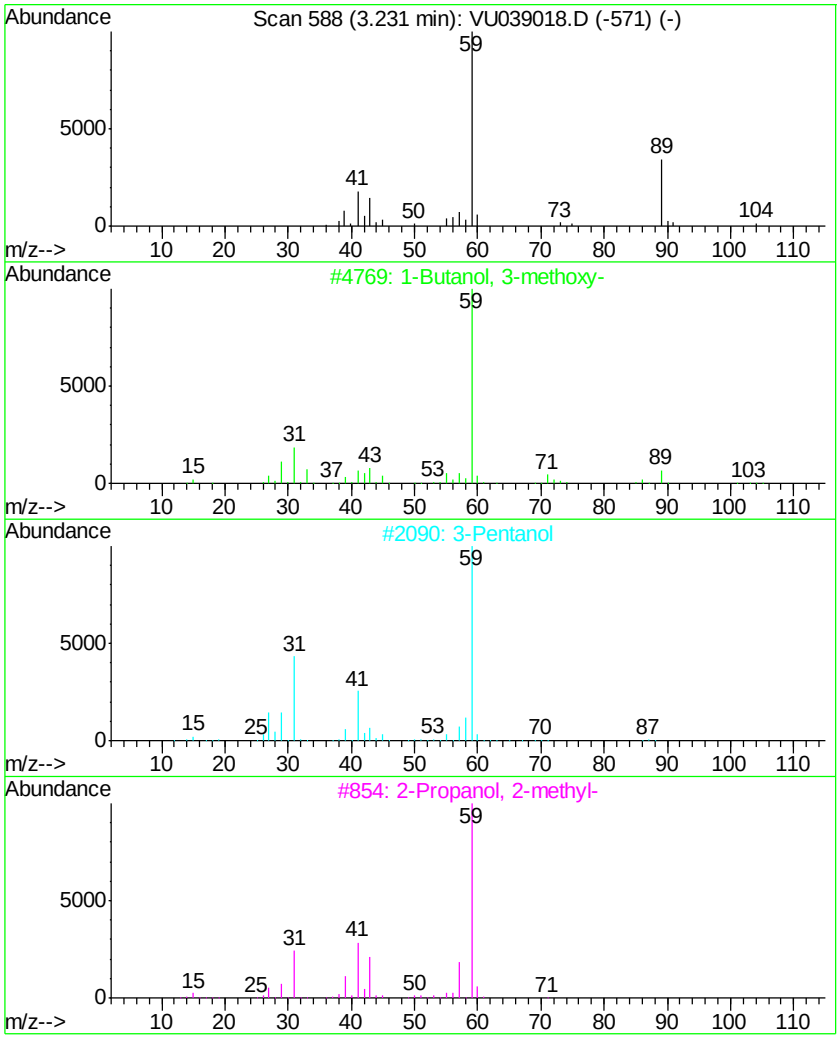
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

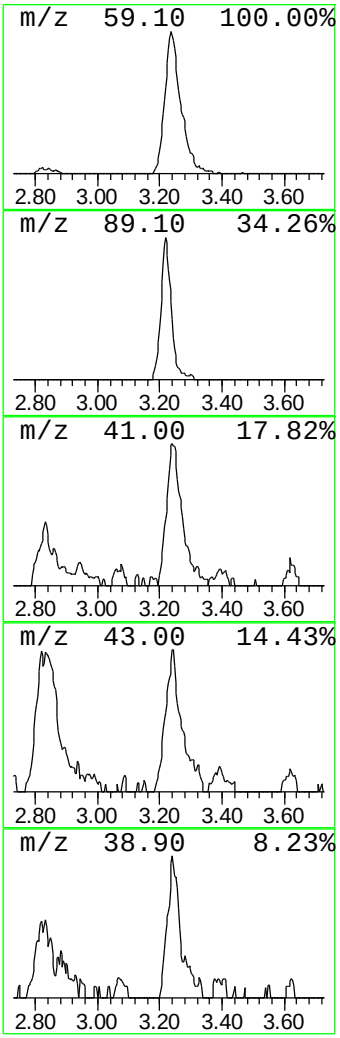
****

Peak Number 1 1-Butanol, 3-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	0.66 ug/L	85920	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	64
2	3-Pentanol	88	C5H12O	000584-02-1	45
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	45
4	3-Pentanol	88	C5H12O	000584-02-1	45
5	1,2-Butanediol	90	C4H10O2	000584-03-2	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039018.D
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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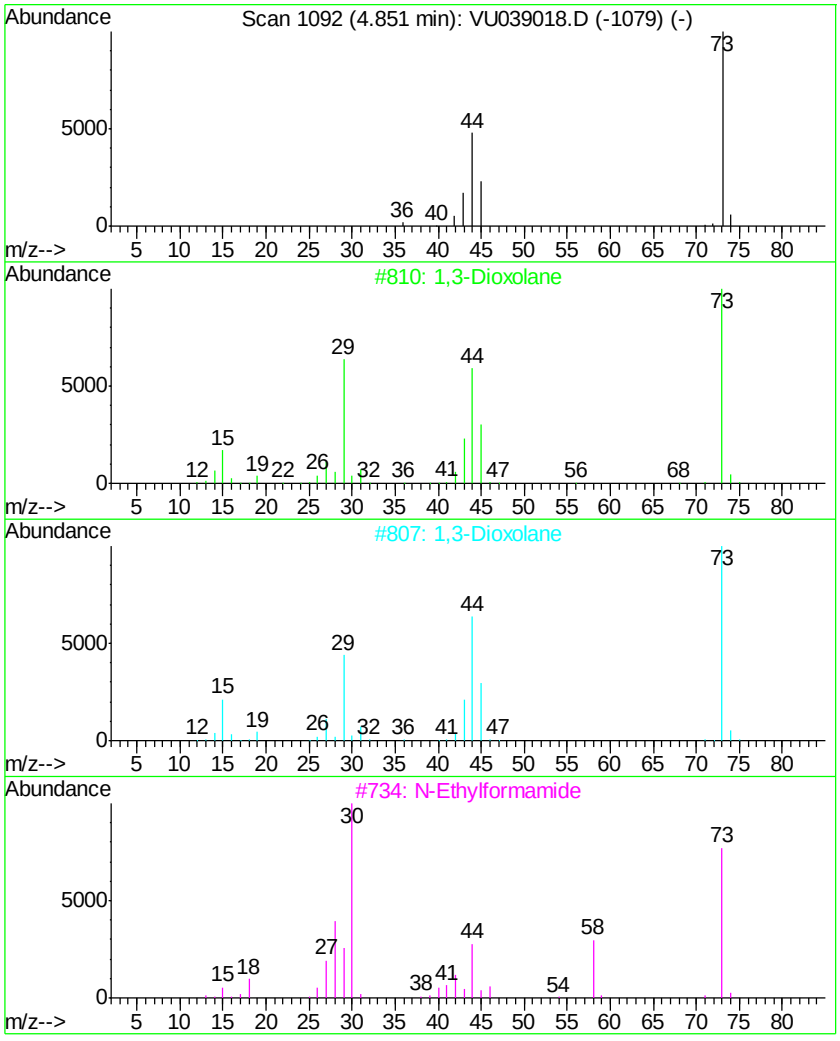
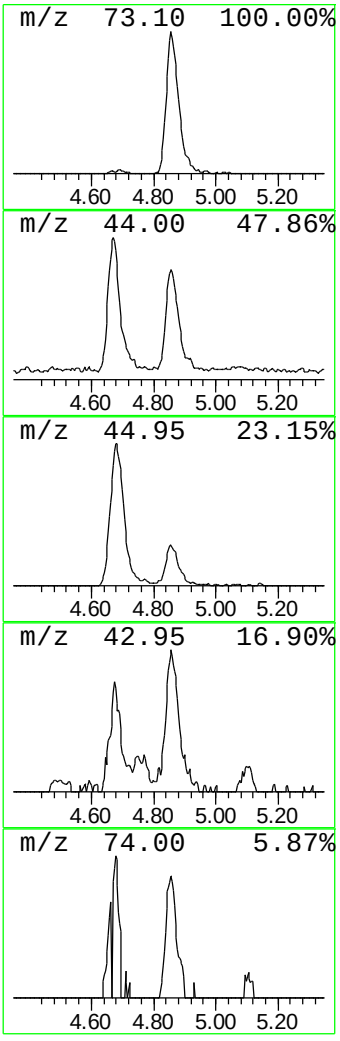
Peak Number 2 1,3-Dioxolane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	0.63 ug/L	82018	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane	74	C3H6O2	000646-06-0	86
2	1,3-Dioxolane	74	C3H6O2	000646-06-0	86
3	N-Ethylformamide	73	C3H7NO	000627-45-2	5
4	Guanidine, methyl-	73	C2H7N3	000471-29-4	5
5	Ethylene oxide	44	C2H4O	000075-21-8	3





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039018.D
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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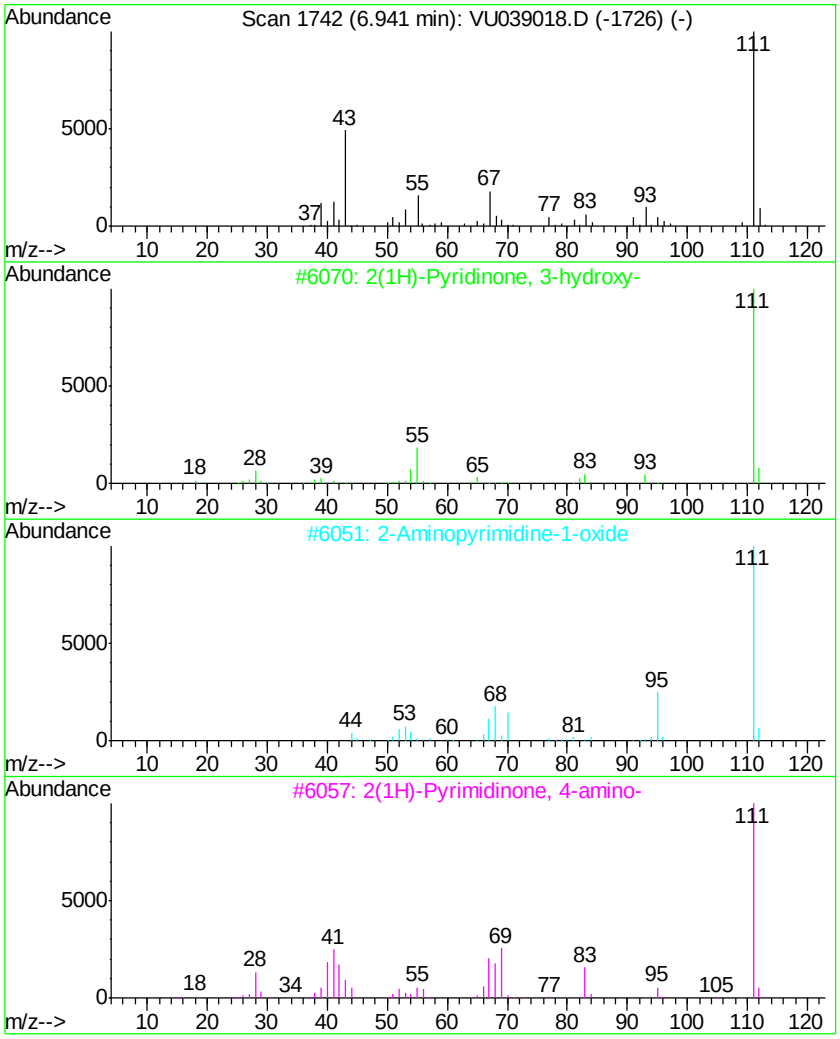
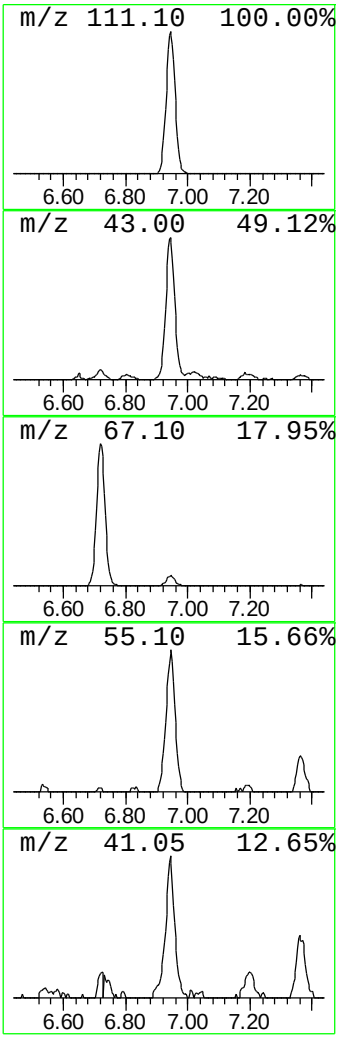
Peak Number 3 2(1H)-Pyridinone, 3-hydroxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	1.37 ug/L	179634	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	59
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	59
3	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
4	Bruceantin	548	C28H36O11	041451-75-6	45
5	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039018.D
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

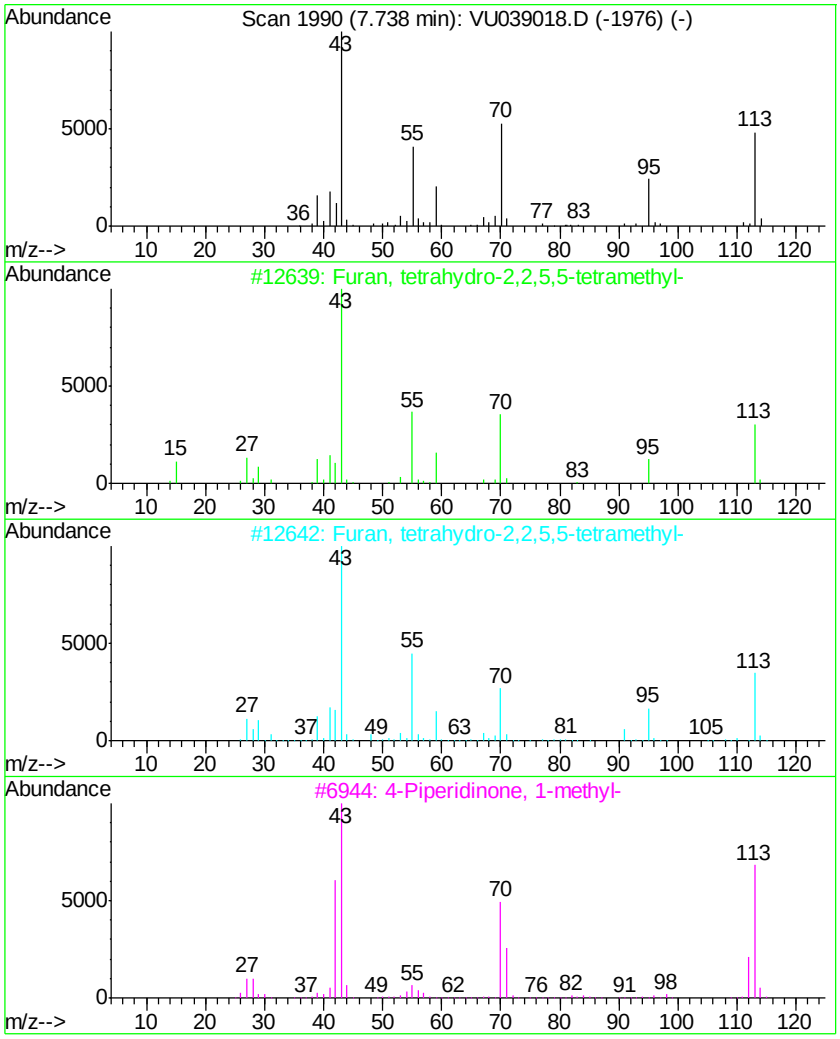
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

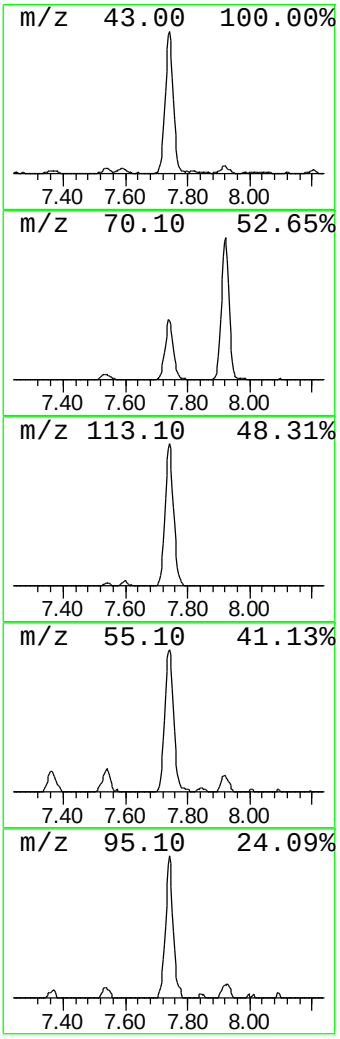
****

Peak Number 5 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	1.17 ug/L	152990	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	72
3	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	52
4	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	42
5	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	38





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Data File : VU039018.D
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

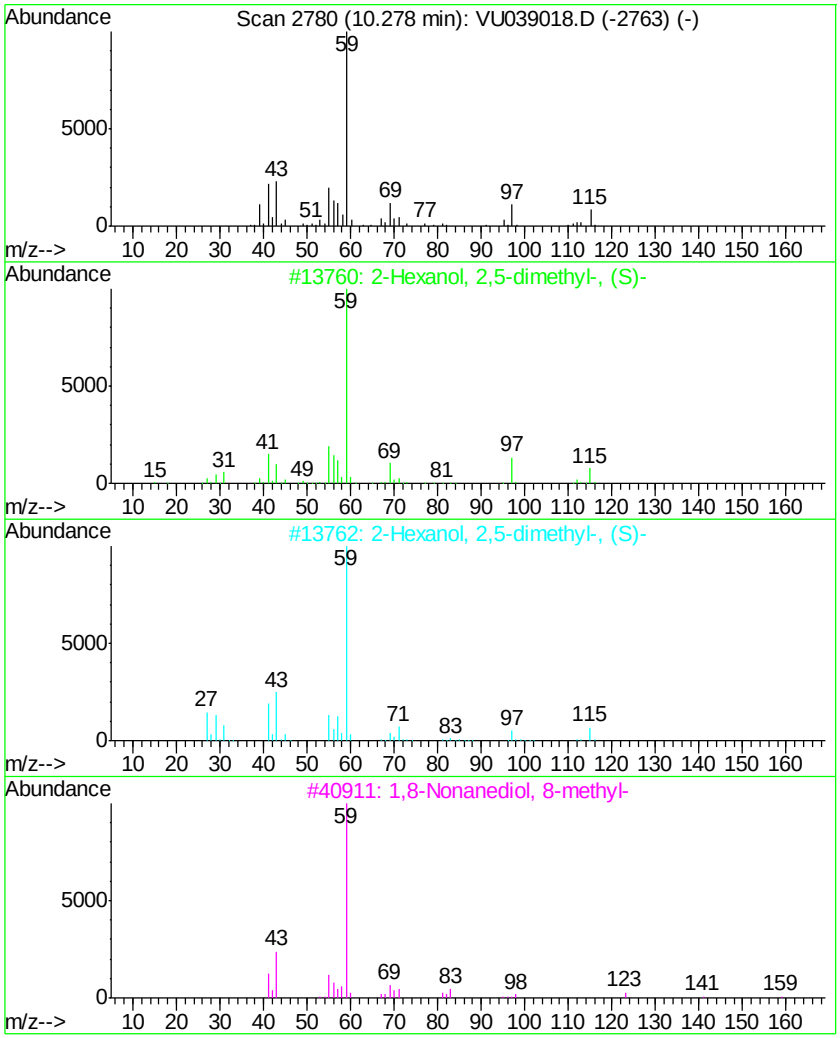
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

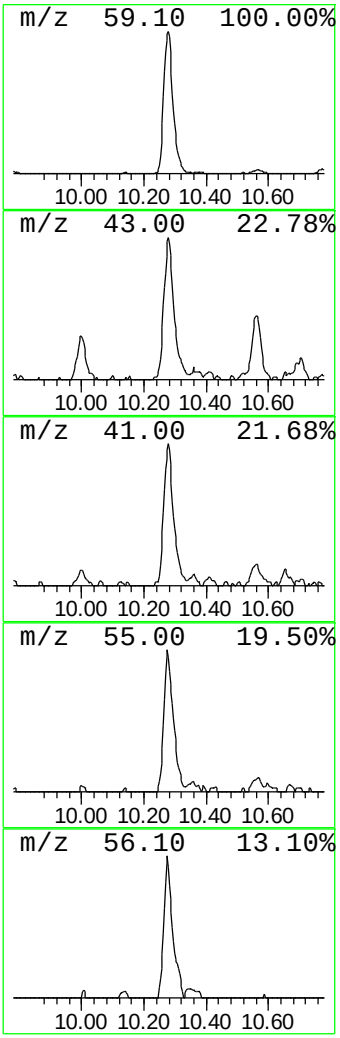
****

Peak Number 6 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	0.84 ug/L	143807	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	83
2	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	64
4	2-Heptanol, 2-methyl-	130	C8H18O	000625-25-2	59
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039018.D
Acq On : 22 Jun 2020 20:48
Operator : SY/MD
Sample : L3061-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

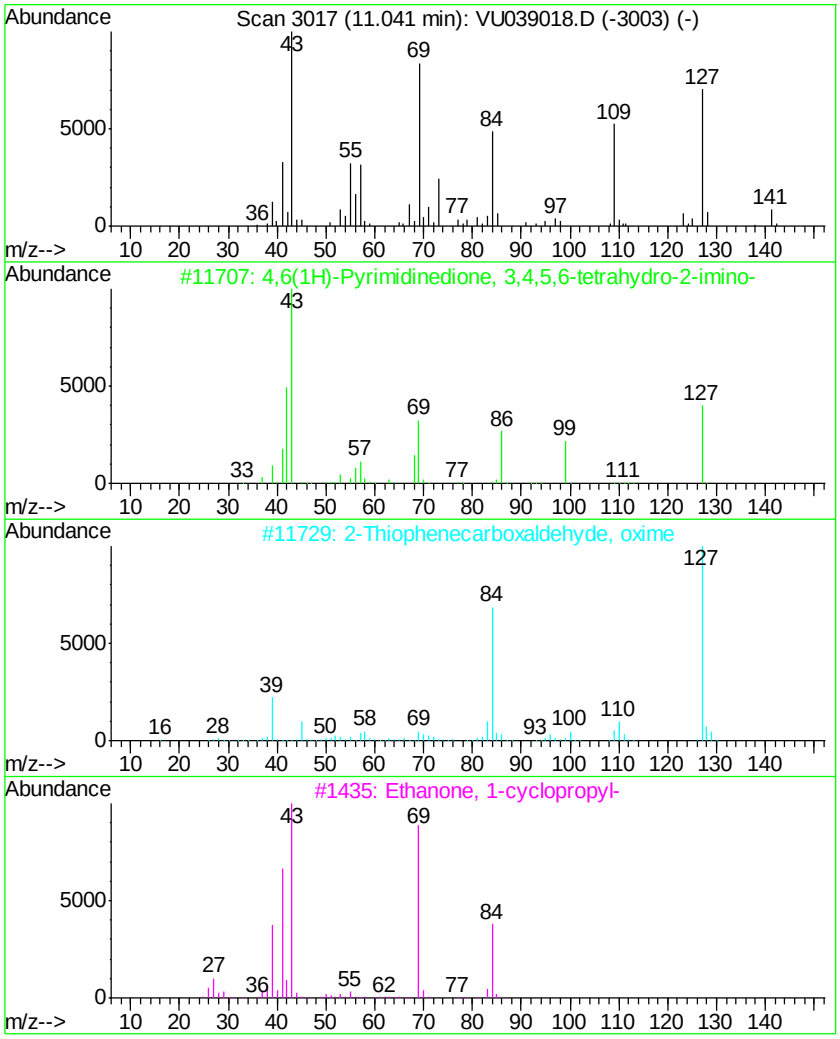
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

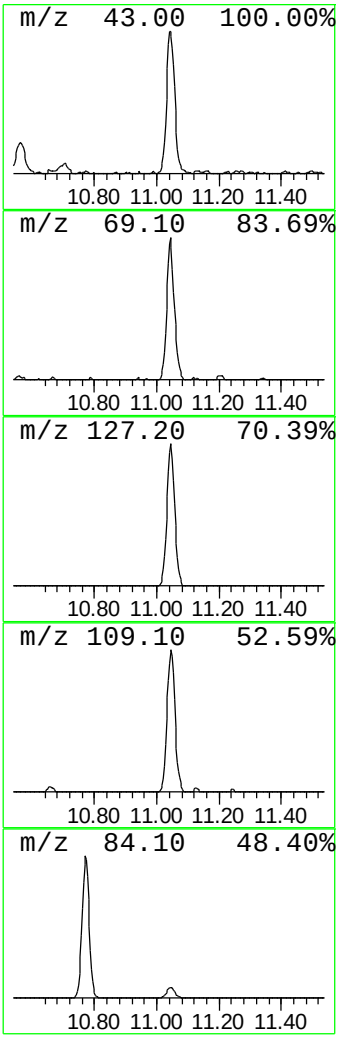
****

Peak Number 7 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	0.84 ug/L	133322	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6(1H)-Pyrimidinedione, 3,4,5,6...	127	C4H5N3O2	004425-67-6	43
2	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
4	Pentane, 3-methylene-	84	C6H12	000760-21-4	27
5	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27





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
1-Butanol, 3-meth...	3.23	0.7	ug/L	85920	1	6.28	654319	5.0
1,3-Dioxolane	4.85	0.6	ug/L	82018	1	6.28	654319	5.0
2(1H)-Pyridinone,...	6.94	1.4	ug/L	179634	1	6.28	654319	5.0
Furan, tetrahydro...	7.74	1.2	ug/L	152990	1	6.28	654319	5.0
2-Hexanol, 2,5-di...	10.28	0.8	ug/L	143807	2	9.44	857306	5.0
unknown-01	11.04	0.8	ug/L	133322	3	11.82	796514	5.0