LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062320\
Data File : VU039046.D
Acq On : 23 Jun 2020 17:44
Operator : SY/MD
Sample : L3061-04DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1DL

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\SOMUTR062320WMA.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	1.614	77	85	96	rBV	170461	195557	11.55%	1.539%
2	1.932	175	184	199	rBV	142606	201504	11.90%	1.586%
3	2.594	378	390	405	rBV2	297698	528944	31.25%	4.163%
4	3.077	527	540	552	rVB3	19851	37628	2.22%	0.296%
5	3.910	778	799	823	rBV	375791	899921	53.16%	7.082%
6	4.035	824	838	853	rVB3	10447	28803	1.70%	0.227%
7	4.668	1016	1035	1064	rBV2	274793	809437	47.82%	6.370%
8	5.102	1151	1170	1200	rBV	232617	529132	31.26%	4.164%
9	5.758	1352	1374	1395	rBV2	491001	1273807	75.25%	10.025%
10	6.279	1521	1536	1554	rBV	356831	666434	39.37%	5.245%
11	6.720	1657	1673	1691	rBV	306890	596545	35.24%	4.695%
12	6.942	1725	1742	1761	rBV2	116896	233752	13.81%	1.840%
13	7.591	1933	1944	1960	rVB	160748	279379	16.50%	2.199%
14	7.739	1976	1990	2004	rBV3	42179	80093	4.73%	0.630%
15	7.919	2032	2046	2061	rBV	561597	964739	56.99%	7.592%
16	8.202	2119	2134	2152	rBV	106050	186693	11.03%	1.469%
17	8.655	2261	2275	2319	rBV	947899	1692827	100.00%	13.322%
18	9.433	2502	2517	2537	rBV	517078	854809	50.50%	6.727%
19	10.276	2767	2779	2799	rBV	57673	113837	6.72%	0.896%
20	10.771	2917	2933	2948	rBV	259782	418562	24.73%	3.294%
21	11.044	3002	3018	3038	rBV	271794	465806	27.52%	3.666%
22	11.822	3248	3260	3279	rBV	494871	787577	46.52%	6.198%
23	12.202	3365	3378	3395	rBV	530985	861051	50.86%	6.776%

Sum of corrected areas: 12706837

LSC Report - Integrated Chromatogram

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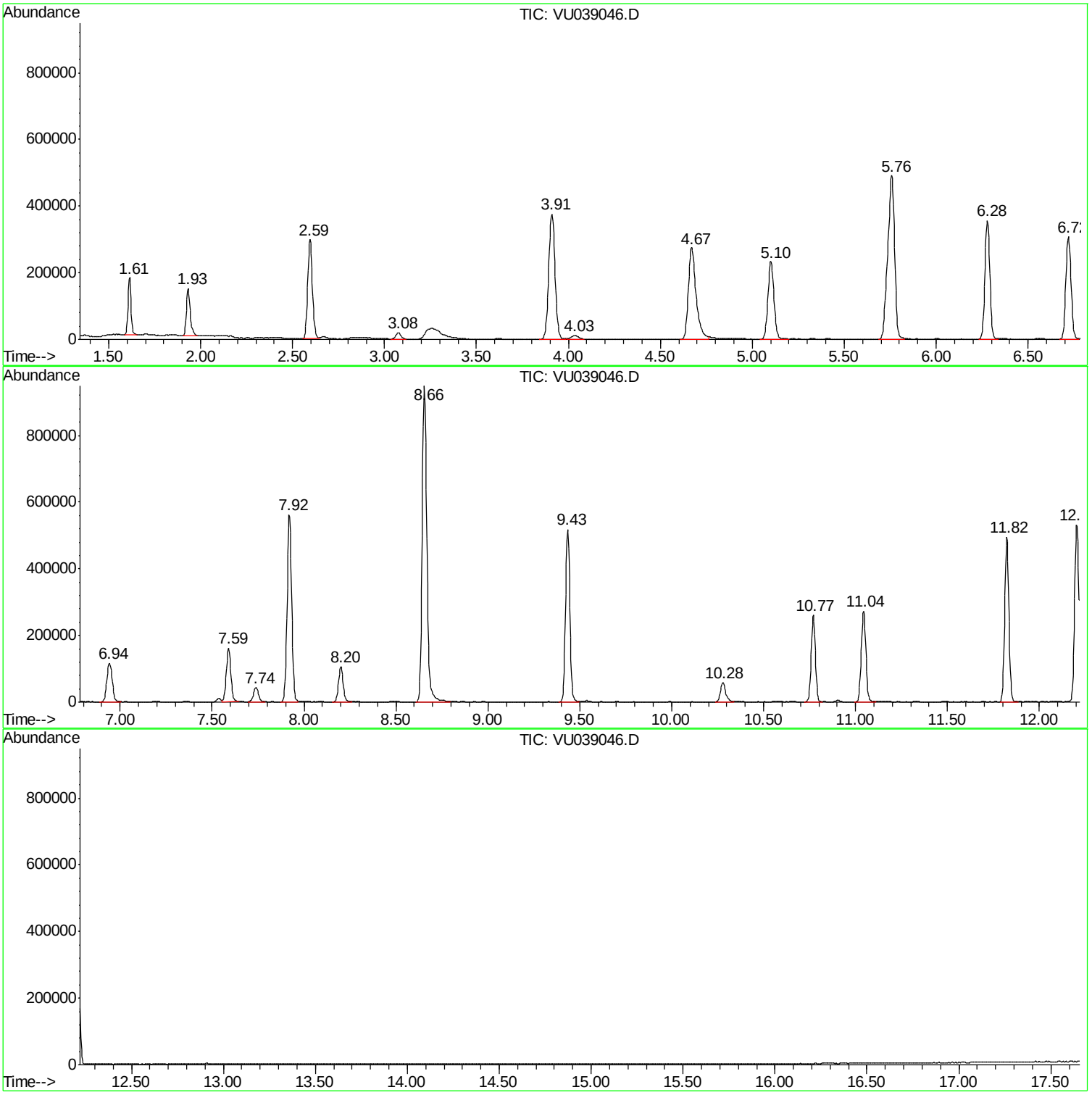
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

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Data File : VU039046.D
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ClientSampleId : BFXJ1DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

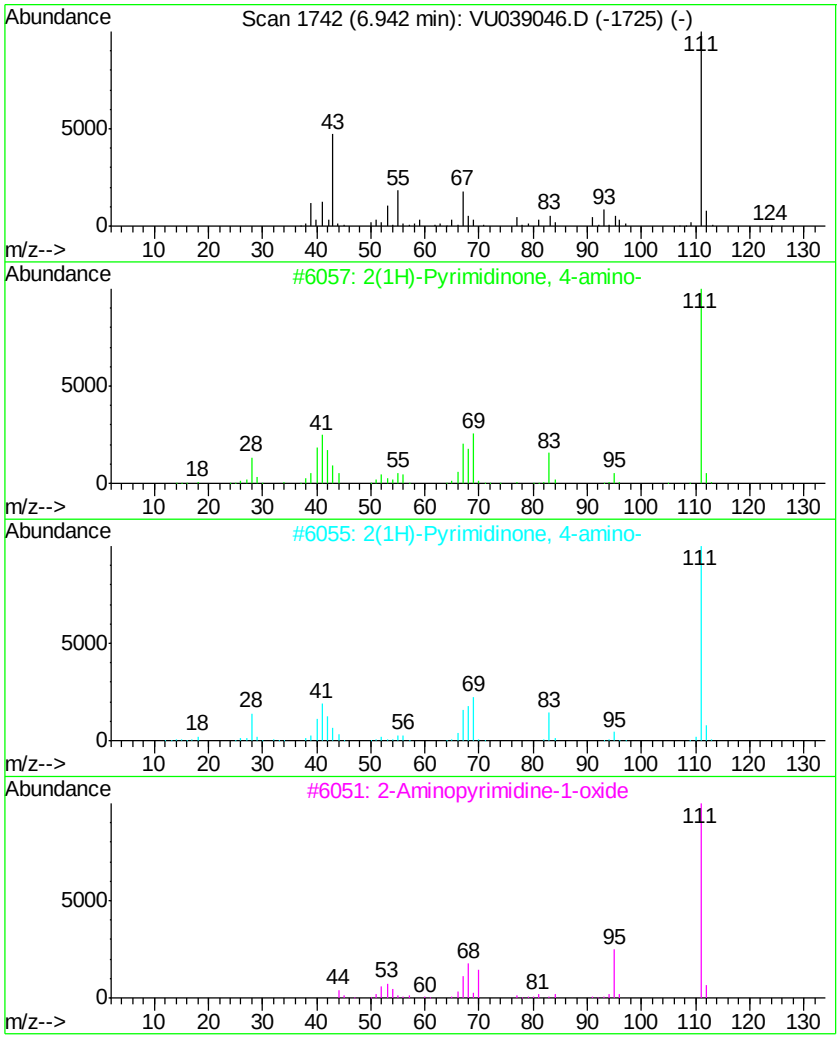
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

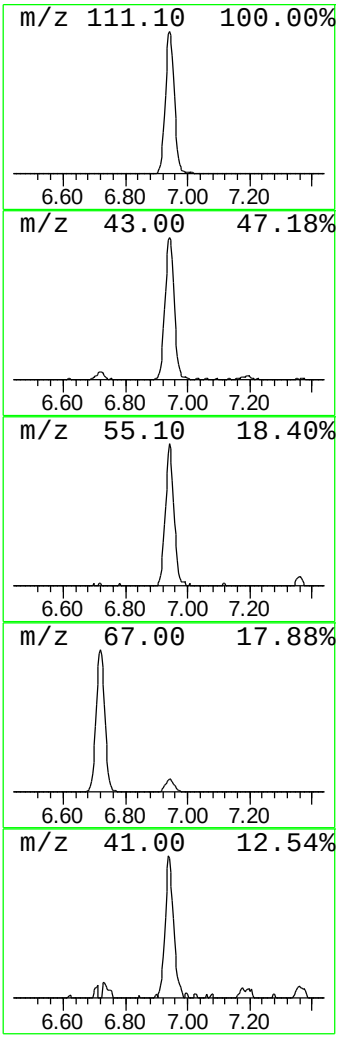
****

Peak Number 1 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	1.75 ug/L	233752	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	59
2	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	59
3	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	56
4	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	53
5	Bruceantin	548	C28H36O11	041451-75-6	50





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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1DL

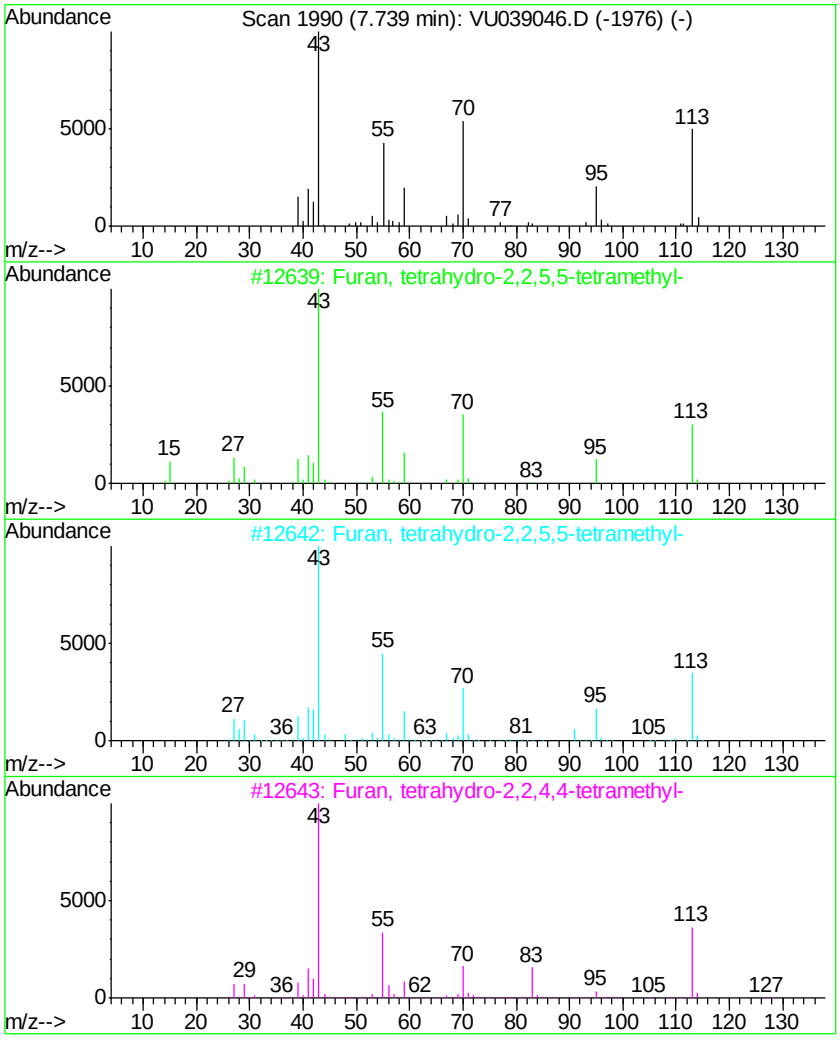
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

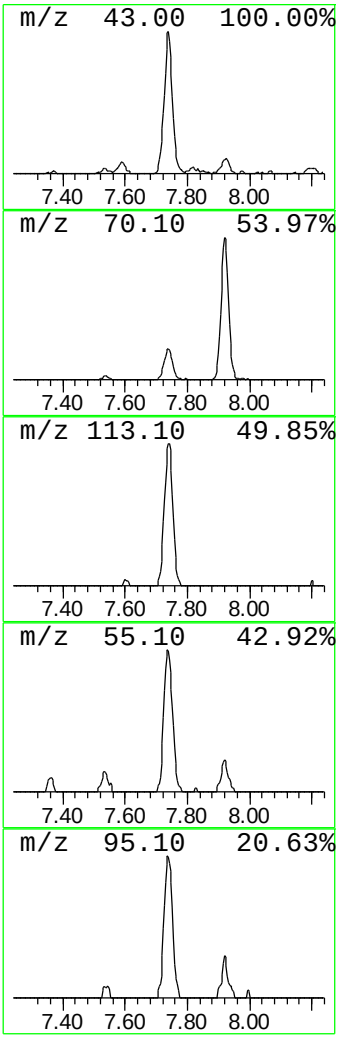
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	0.60 ug/L	80093	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	72
2	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	72
3	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
4	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
5	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	42





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Data File : VU039046.D
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Operator : SY/MD
Sample : L3061-04DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

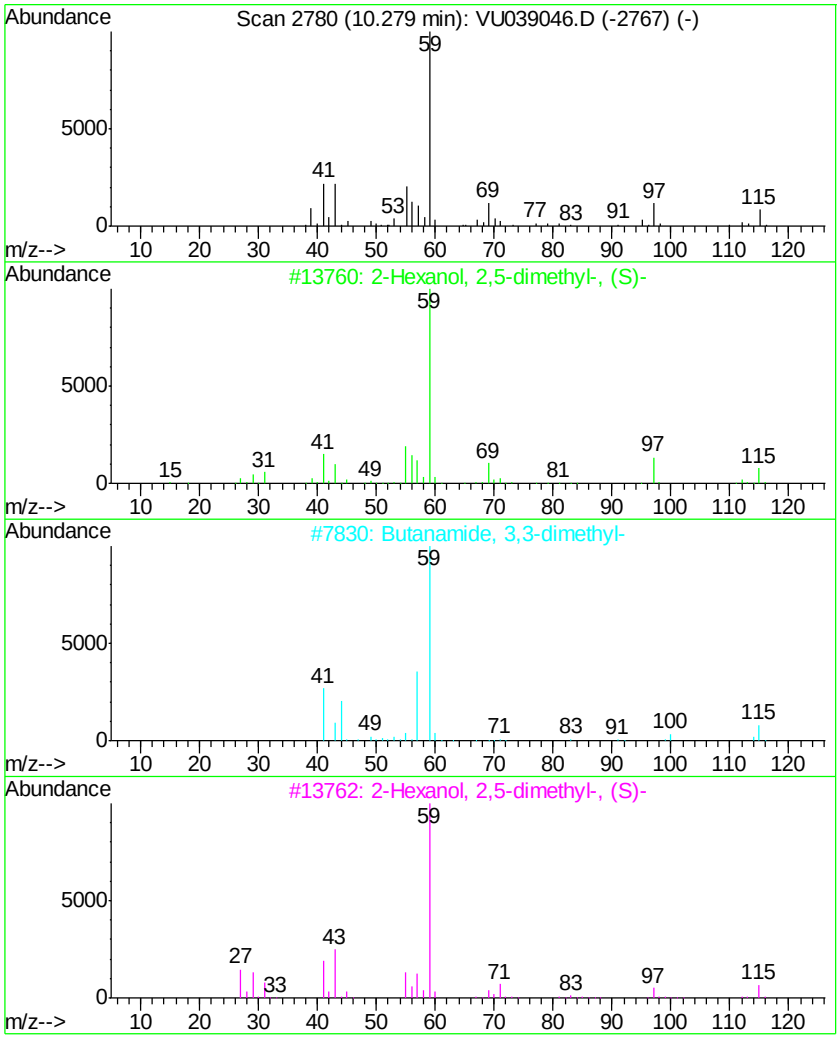
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

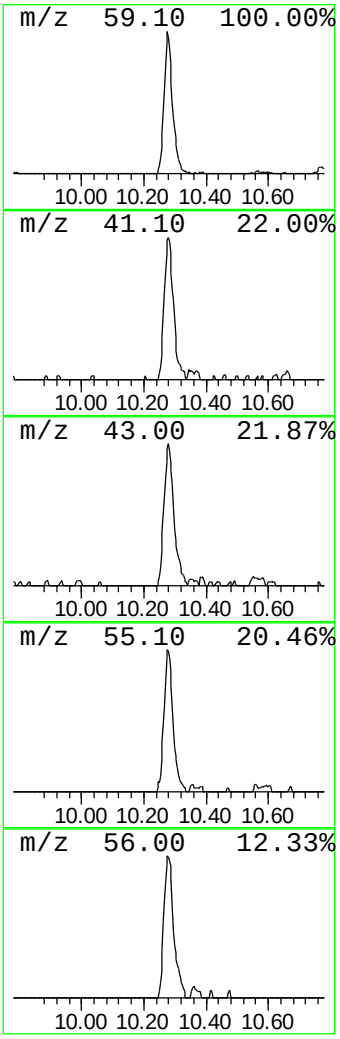
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	0.67 ug/L	113837	Chlorobenzene-d5	9.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90
2	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	52
3	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
5	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45





Library Search Compound Report

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Operator : SY/MD
Sample : L3061-04DL 5X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1DL

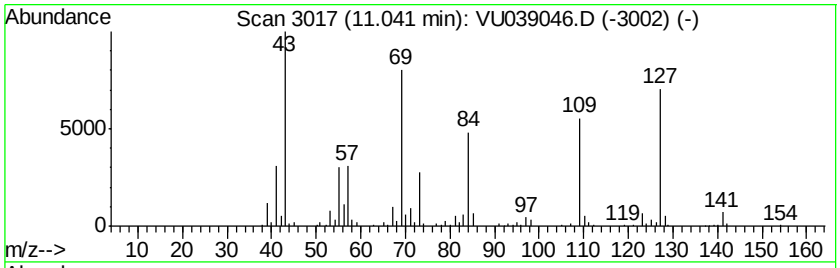
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

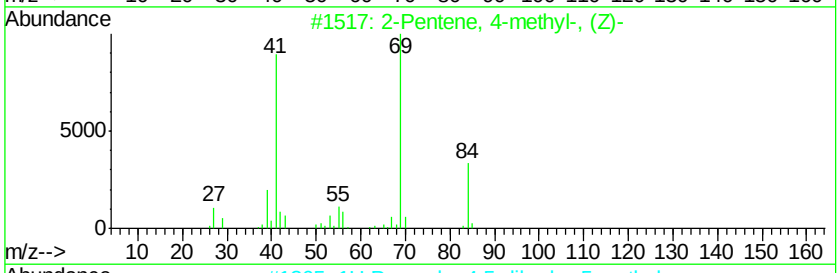
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

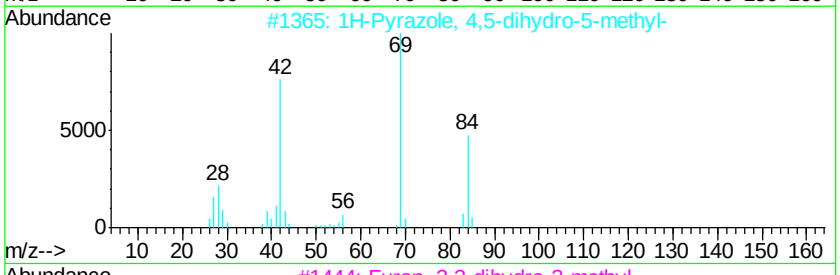
****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

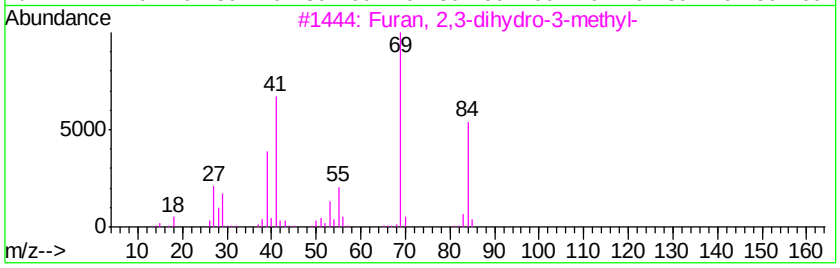
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	2.96 ug/L	465806	1,4-Dichlorobenzene-d4	11.82

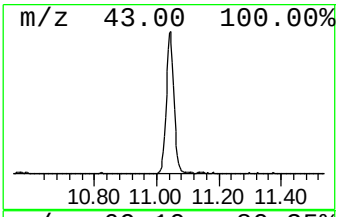
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	35
2	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	35
3	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	35
4	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	35
5	Formic acid, 4-methylpent-2-yl e...	130	C7H14O2	1000367-94-0	32

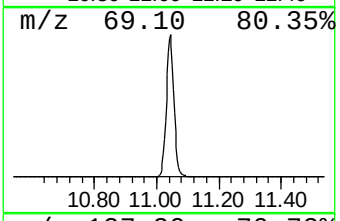


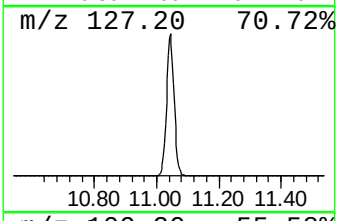


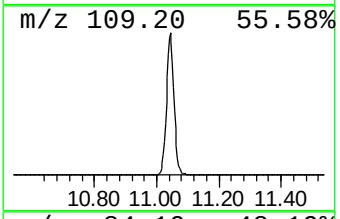


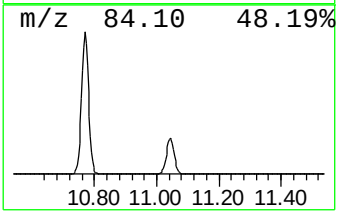












Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SOM01.0

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2(1H)-Pyrimidinon...	6.94	1.8	ug/L	233752	1	6.28	666434	5.0
Furan, tetrahydro...	7.74	0.6	ug/L	80093	1	6.28	666434	5.0
2-Hexanol, 2,5-di...	10.28	0.7	ug/L	113837	2	9.43	854809	5.0
(DEL) Alkane: Str...	11.04	3.0	ug/L	465806	3	11.82	787577	5.0