LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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	1.488	37	46	75	rBV	998608	2344120	65.98%	12.062%
2	1.610	79	84	96	rVB	220178	285081	8.02%	1.467%
3	1.929	176	183	200	rVB	147349	211628	5.96%	1.089%
4	2.588	376	388	403	rBV	286583	470109	13.23%	2.419%
5	2.826	445	462	492	rBV3	26859	99591	2.80%	0.512%
6	3.234	572	589	617	rBV3	18592	66778	1.88%	0.344%
7	4.038	821	839	853	rBV3	23420	60109	1.69%	0.309%
8	4.671	1018	1036	1068	rBV2	230238	696308	19.60%	3.583%
9	5.102	1154	1170	1190	rBV	231854	519042	14.61%	2.671%
10	5.758	1349	1374	1386	rBV2	485059	1277974	35.97%	6.576%
11	6.279	1522	1536	1558	rBV	349483	652776	18.37%	3.359%
12	6.719	1659	1673	1691	rBV	305431	585483	16.48%	3.013%
13	6.944	1725	1743	1765	rBV	399046	786893	22.15%	4.049%
14	7.362	1861	1873	1889	rBV2	60242	111783	3.15%	0.575%
15	7.539	1913	1928	1936	rBV	114134	204371	5.75%	1.052%
16	7.591	1936	1944	1966	rVB	130613	227771	6.41%	1.172%
17	7.739	1974	1990	2006	rBV	100634	188623	5.31%	0.971%
18	7.922	2033	2047	2059	rBV	575299	982865	27.67%	5.058%
19	7.993	2059	2069	2086	rVB	238617	401287	11.30%	2.065%
20	8.202	2122	2134	2153	rBV	83133	142521	4.01%	0.733%
21	8.655	2259	2275	2307	rBV	739669	1373146	38.65%	7.066%
22	9.436	2503	2518	2539	rBV	521285	874079	24.60%	4.498%
23	9.587	2557	2565	2580	rVB	37812	60375	1.70%	0.311%
24	10.275	2766	2779	2800	rBV	387107	765799	21.56%	3.941%
25	10.771	2915	2933	2944	rBV	247517	407651	11.47%	2.098%
26	10.951	2982	2989	3000	rVB3	29615	43674	1.23%	0.225%
27	11.044	3000	3018	3036	rBV	2140843	3552569	100.00%	18.281%
28	11.131	3037	3045	3052	rBV2	58176	82115	2.31%	0.423%
29	11.205	3061	3068	3075	rBV3	51473	70115	1.97%	0.361%
30	11.246	3075	3081	3091	rVB3	41006	60694	1.71%	0.312%
31	11.346	3103	3112	3123	rVB4	30021	45993	1.29%	0.237%
32	11.825	3245	3261	3276	rBV	537577	857218	24.13%	4.411%
33	12.205	3366	3379	3394	rBV	565334	924591	26.03%	4.758%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

Sum of corrected areas: 19433132

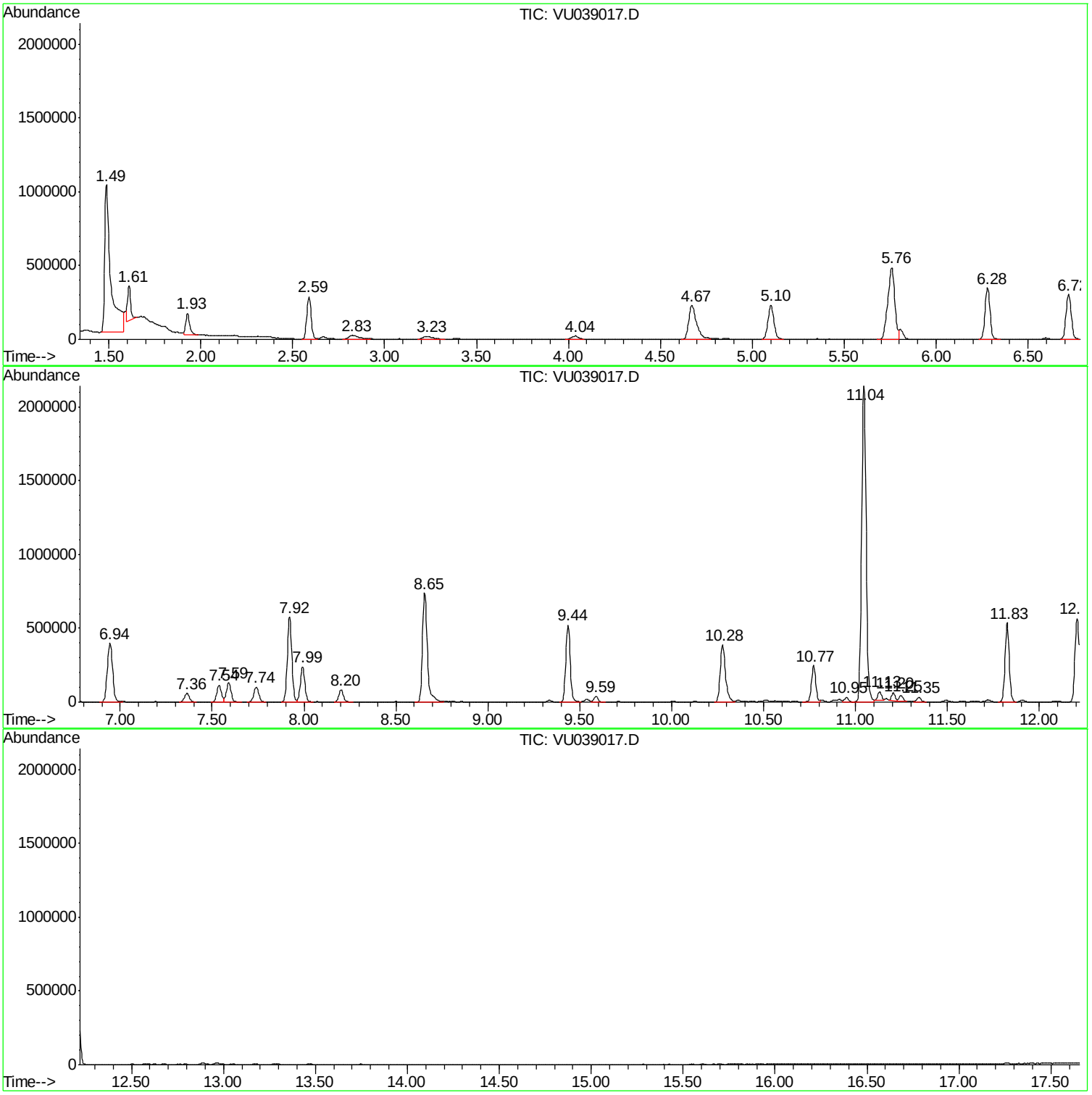
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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 : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

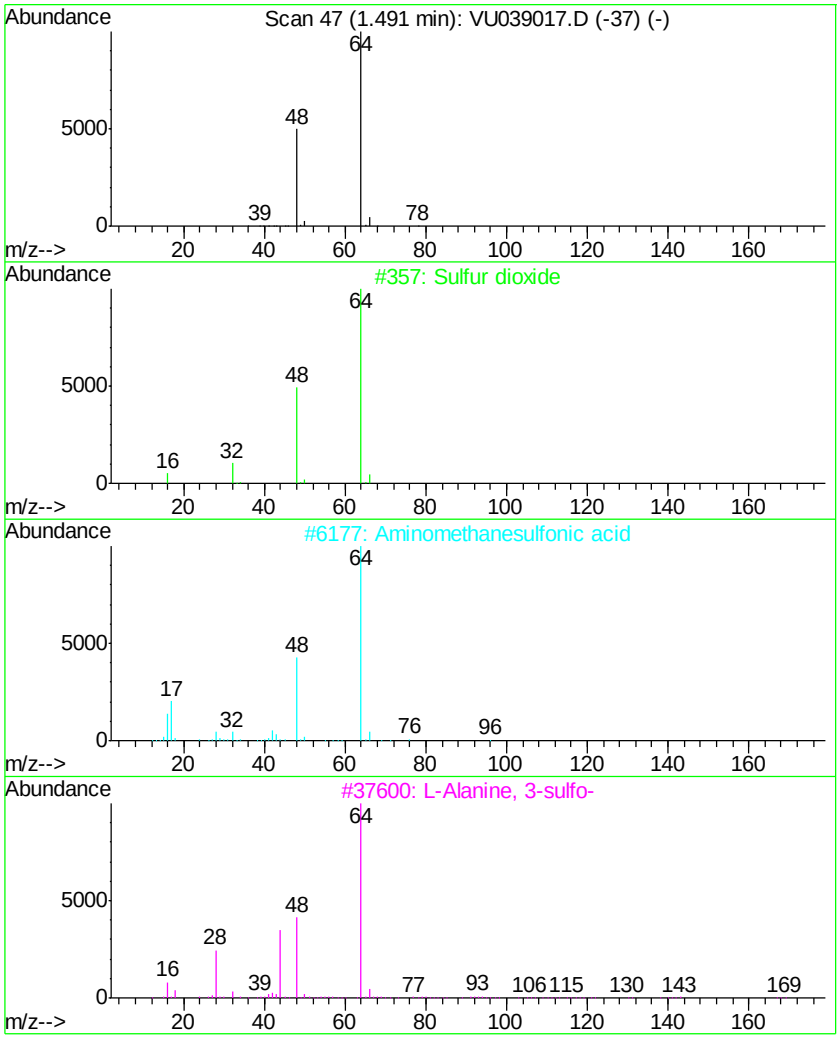
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

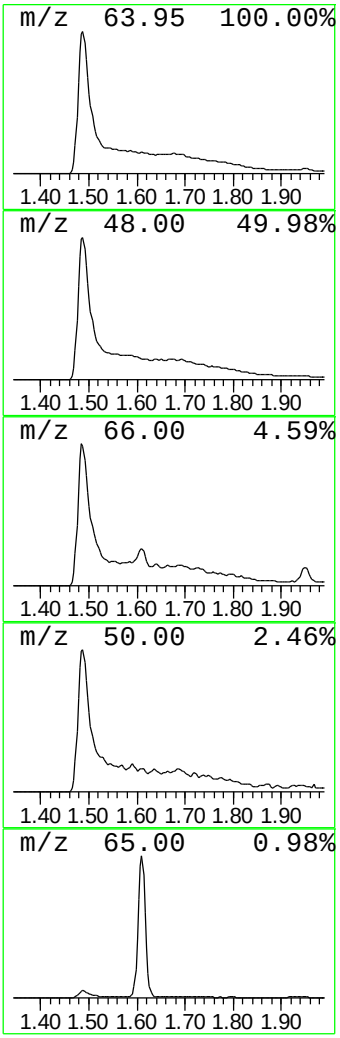
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	17.96 ug/L	2344120	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

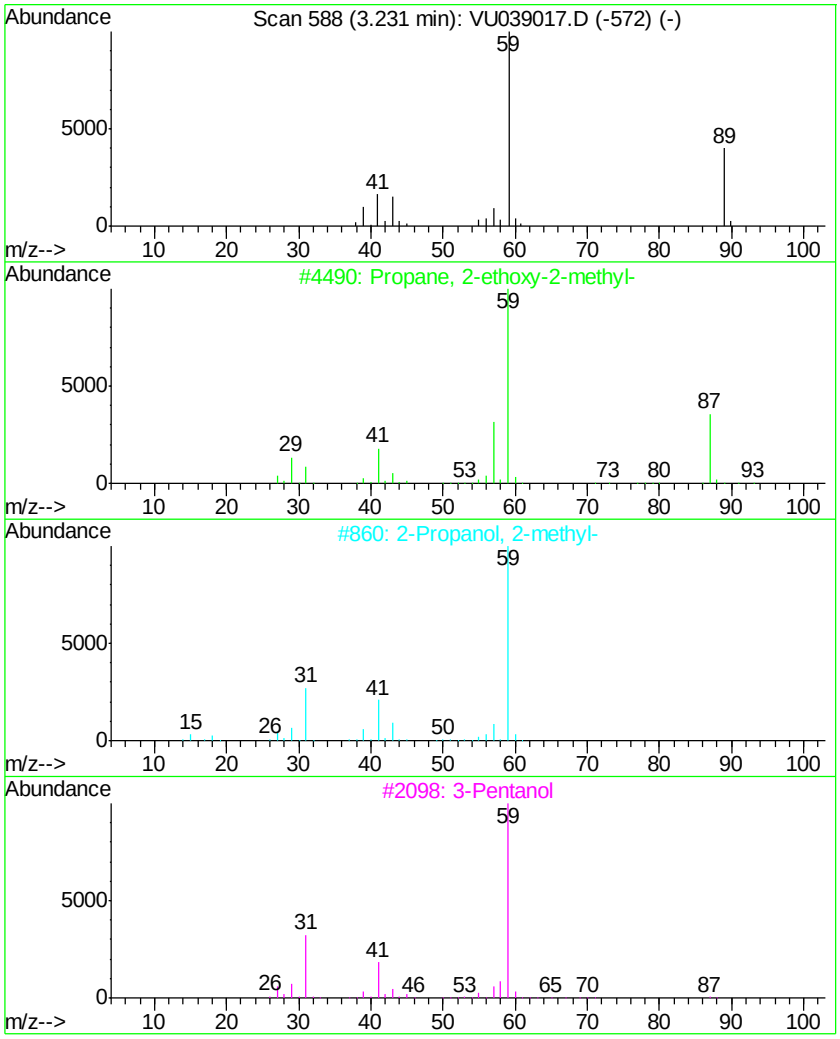
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

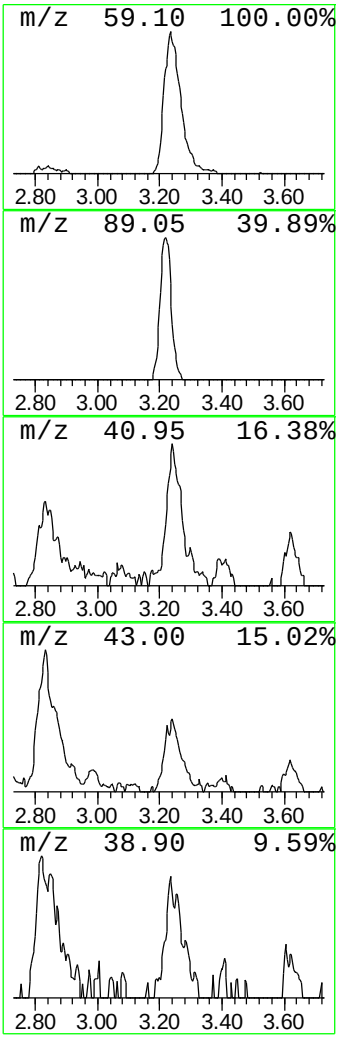
****

Peak Number 2 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	0.51 ug/L	66778	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	42
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
3	3-Pentanol	88	C5H12O	000584-02-1	36
4	1,2-Butanediol	90	C4H10O2	000584-03-2	36
5	1,2-Butanediol	90	C4H10O2	000584-03-2	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

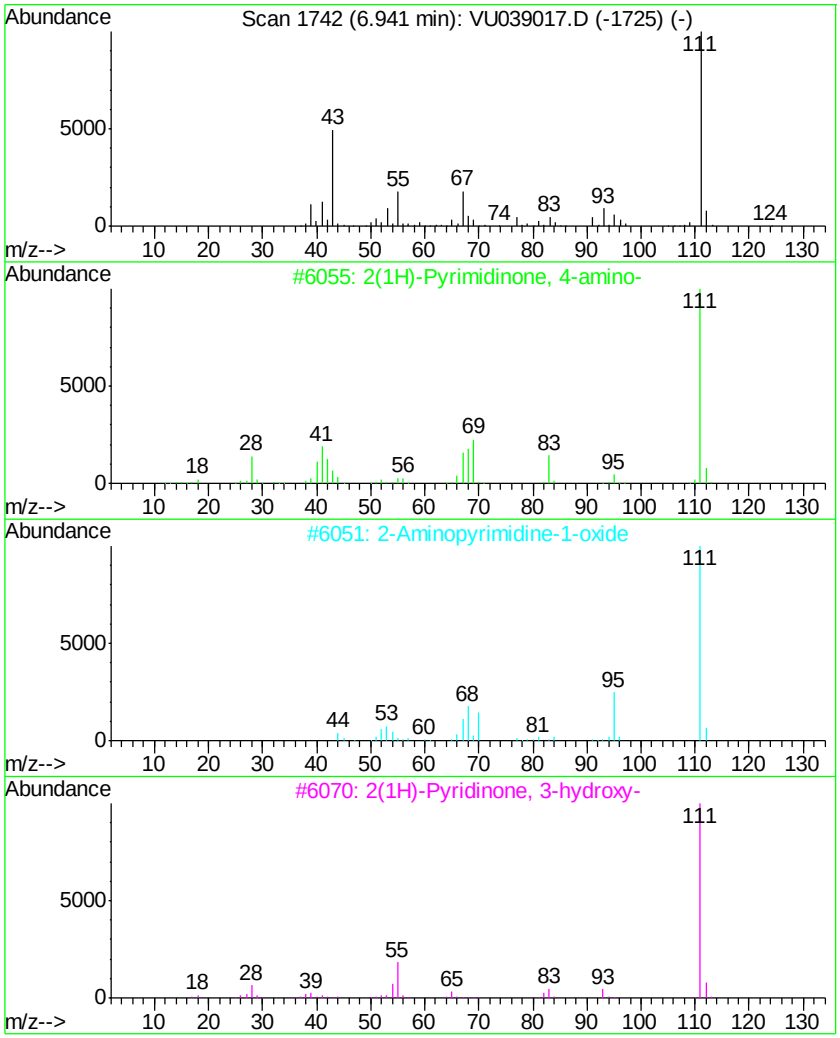
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

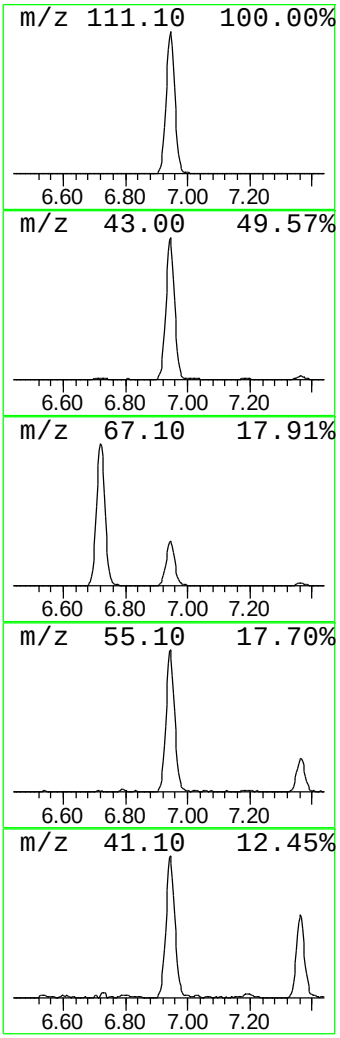
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	6.03 ug/L	786893	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	64
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	59
3	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	53
4	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
5	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

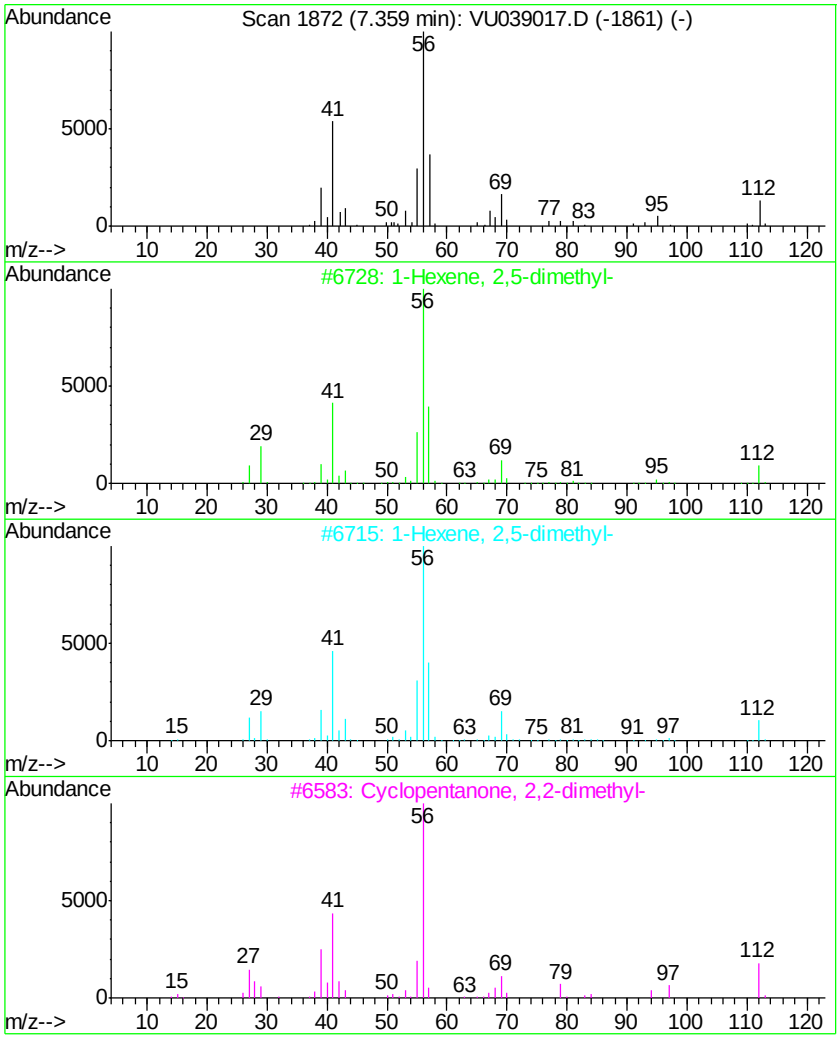
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

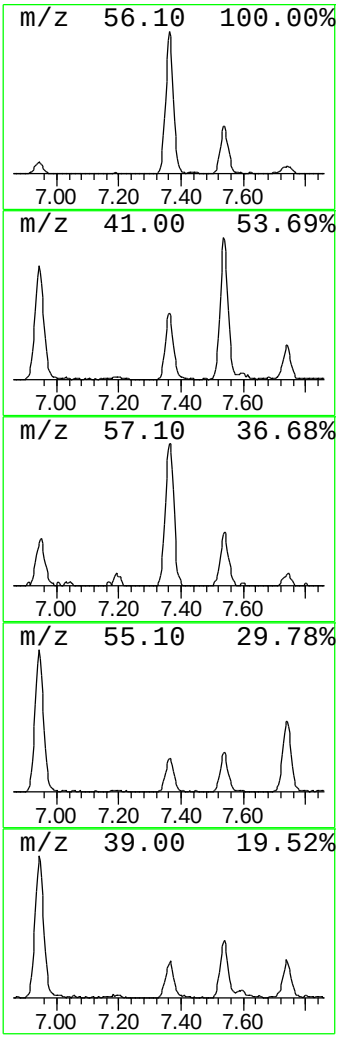
****

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	0.86 ug/L	111783	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	86
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	80
3	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	80
4	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	72
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

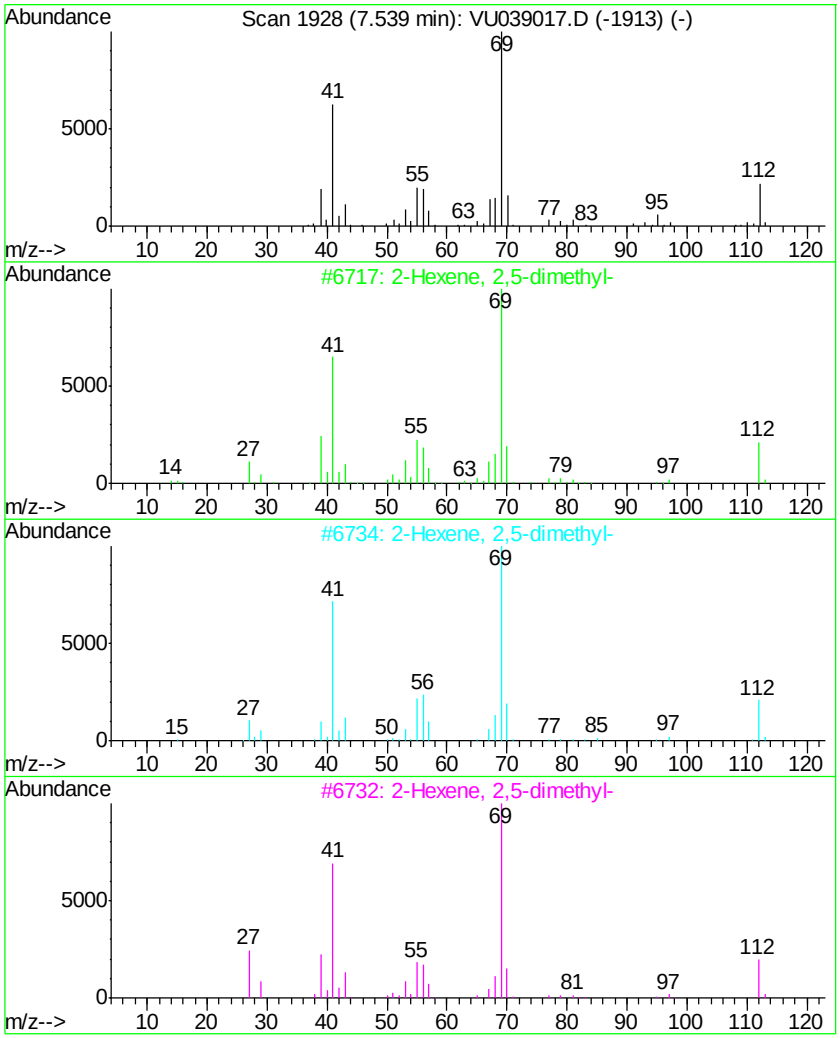
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

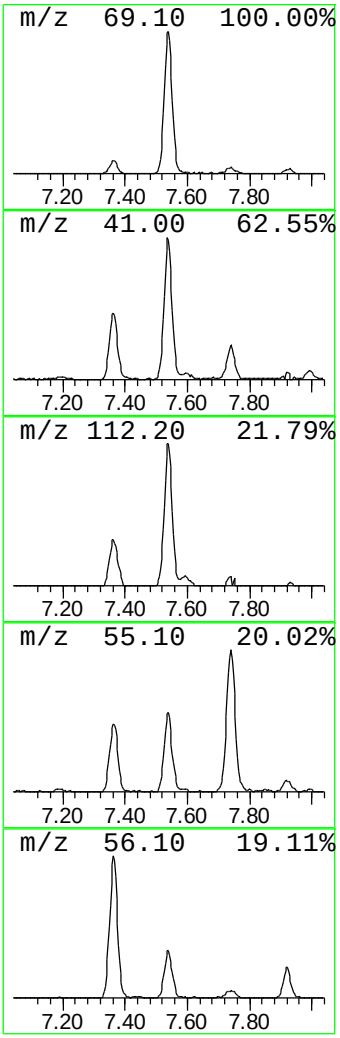
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	1.57 ug/L	204371	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	94
2	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90
3	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90
4	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90
5	3-Hexene, 2,5-dimethyl-, (E)-	112	C8H16	000692-70-6	86





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

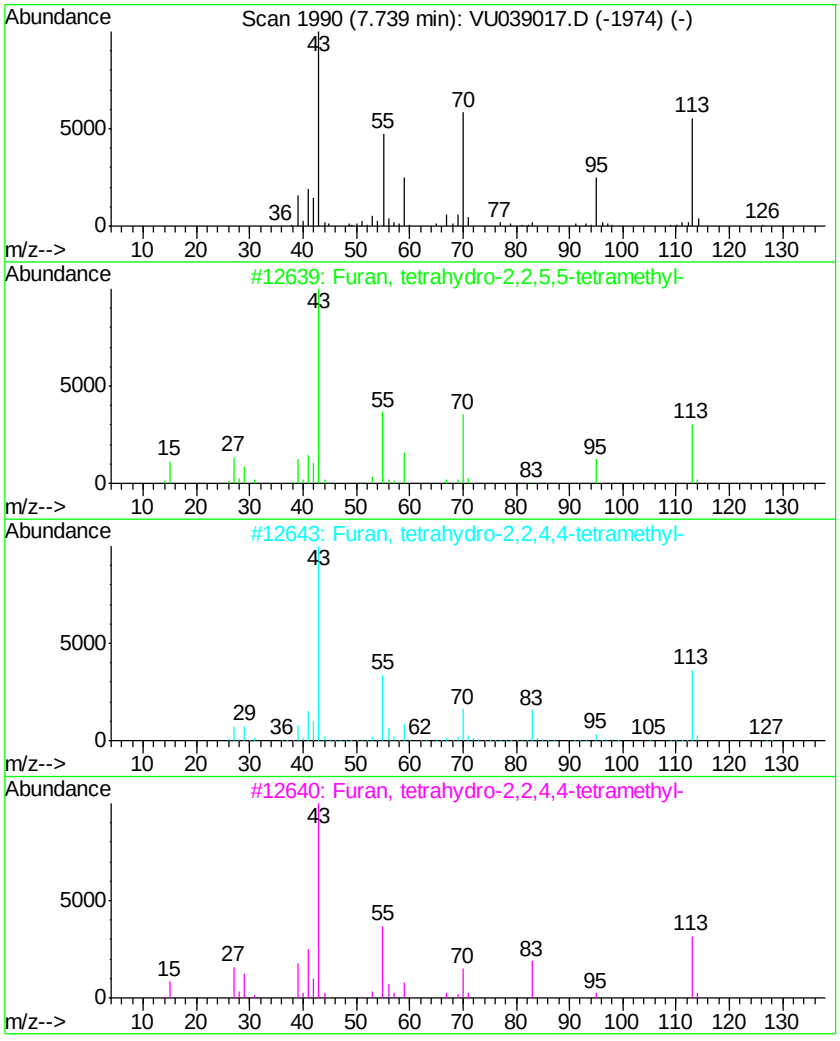
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

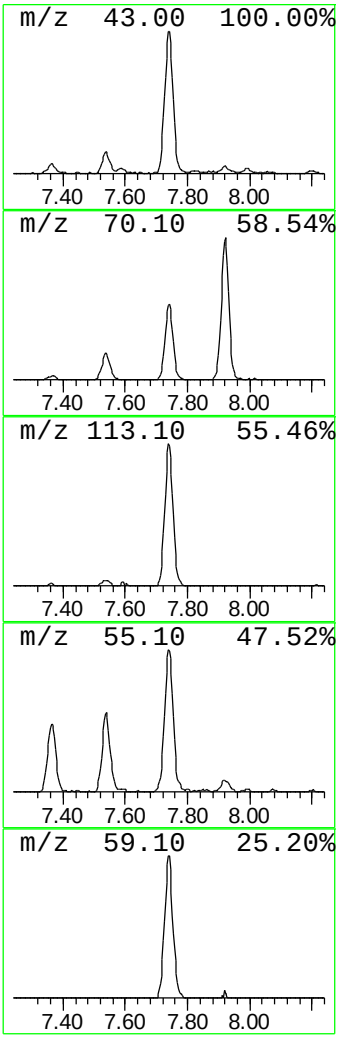
****

Peak Number 7 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	1.44 ug/L	188623	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-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	42
4	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	38
5	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

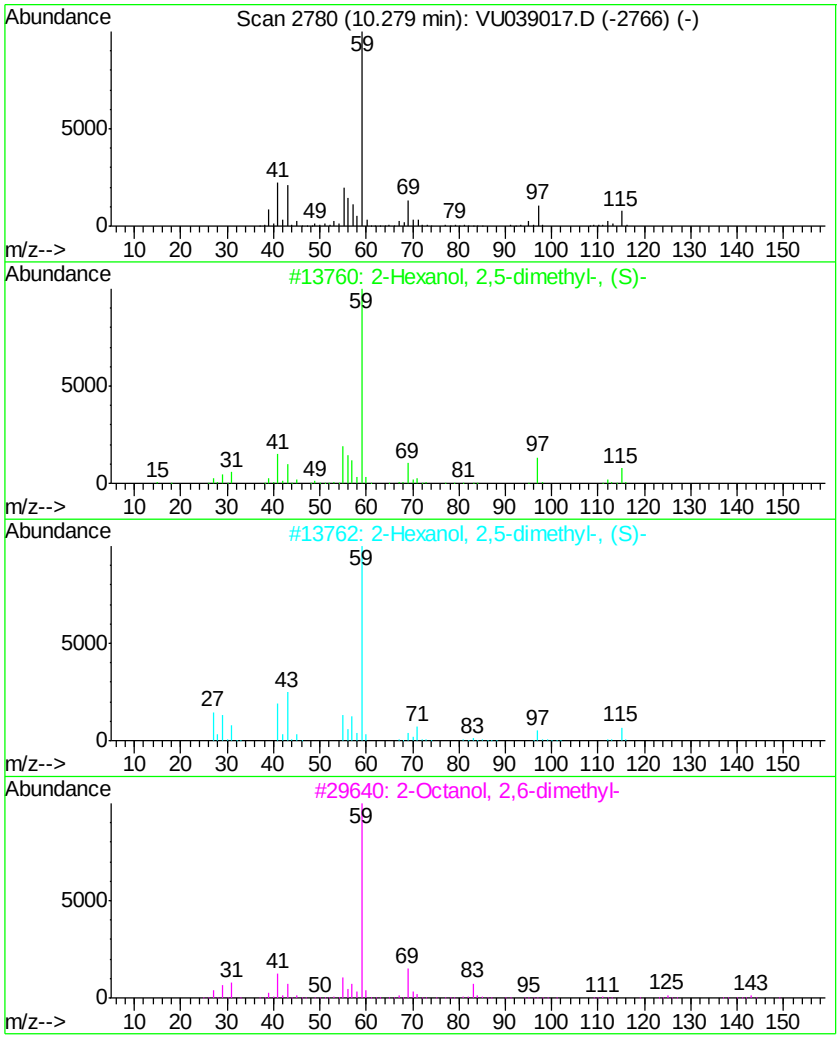
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

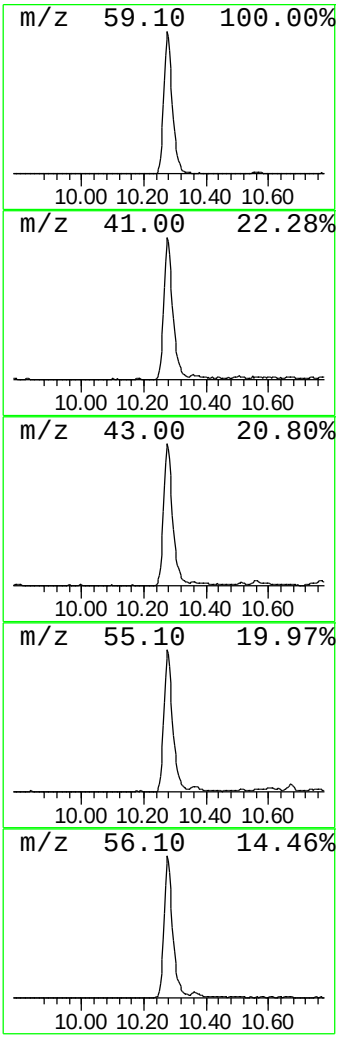
****

Peak Number 8 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	4.38 ug/L	765799	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	90
2	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	47
5	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

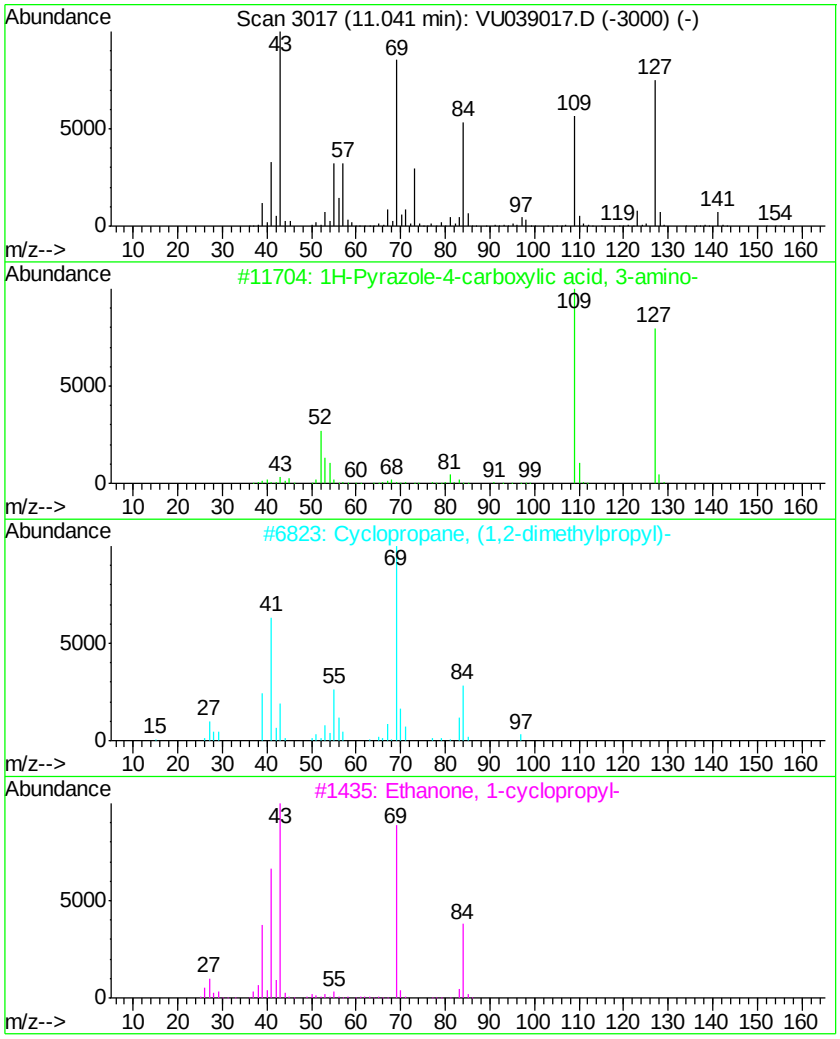
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

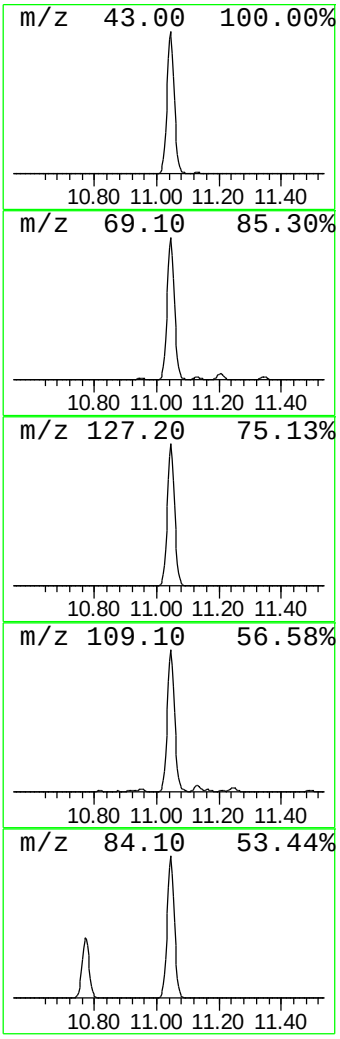
****

Peak Number 9 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	20.72 ug/L	3552570	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
2	Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
4	Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
5	1-Piperidinamine, N-[1-(ethylazo...	184	C9H20N4	059856-64-3	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039017.D
Acq On : 22 Jun 2020 20:24
Operator : SY/MD
Sample : L3061-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ3

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.49	18.0	ug/L	2344120	1	6.28	652776	5.0
unknown-01	3.23	0.5	ug/L	66778	1	6.28	652776	5.0
2(1H)-Pyrimidinon...	6.94	6.0	ug/L	786893	1	6.28	652776	5.0
(DEL) Alkane: Str...	7.36	0.9	ug/L	111783	1	6.28	652776	5.0
(DEL) Alkane: Str...	7.54	1.6	ug/L	204371	1	6.28	652776	5.0
Furan, tetrahydro...	7.74	1.4	ug/L	188623	1	6.28	652776	5.0
2-Hexanol, 2,5-di...	10.28	4.4	ug/L	765799	2	9.44	874079	5.0
unknown-02	11.04	20.7	ug/L	3552570	3	11.83	857218	5.0