LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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	73	84	92	rBV3	249502	349538	7.61%	1.650%
2	1.928	176	183	187	rBV	131760	170973	3.72%	0.807%
3	2.594	376	390	404	rBV3	451636	892499	19.43%	4.213%
4	2.813	446	458	478	rVB2	22885	55374	1.21%	0.261%
5	3.227	569	587	617	rBV	321747	837045	18.22%	3.951%
6	3.909	778	799	823	rBV	1932201	4593406	100.00%	21.683%
7	4.034	824	838	858	rVB3	55106	147797	3.22%	0.698%
8	4.668	1017	1035	1062	rBV	266502	747367	16.27%	3.528%
9	5.102	1154	1170	1190	rBV	223487	518962	11.30%	2.450%
10	5.758	1353	1374	1403	rBV2	482920	1264273	27.52%	5.968%
11	6.279	1520	1536	1554	rBV	342615	643188	14.00%	3.036%
12	6.719	1659	1673	1693	rBV	302024	583457	12.70%	2.754%
13	6.944	1725	1743	1767	rBV	640207	1259048	27.41%	5.943%
14	7.362	1860	1873	1886	rBV	48145	88298	1.92%	0.417%
15	7.539	1912	1928	1936	rBV	134601	243676	5.30%	1.150%
16	7.590	1936	1944	1959	rVB	166440	284535	6.19%	1.343%
17	7.738	1975	1990	2008	rBV2	205936	395266	8.61%	1.866%
18	7.922	2032	2047	2061	rBV	581773	990220	21.56%	4.674%
19	8.201	2121	2134	2150	rBV	107212	182413	3.97%	0.861%
20	8.655	2261	2275	2314	rBV	852029	1545082	33.64%	7.294%
21	9.436	2505	2518	2539	rBV	519048	885849	19.29%	4.182%
22	10.275	2765	2779	2798	rBV	229665	484634	10.55%	2.288%
23	10.770	2920	2933	2945	rBV	247232	396490	8.63%	1.872%
24	11.044	3004	3018	3037	rBV	1106800	1874617	40.81%	8.849%
25	11.825	3248	3261	3278	rVB	522750	836620	18.21%	3.949%
26	12.204	3366	3379	3395	rBV	565456	913413	19.89%	4.312%

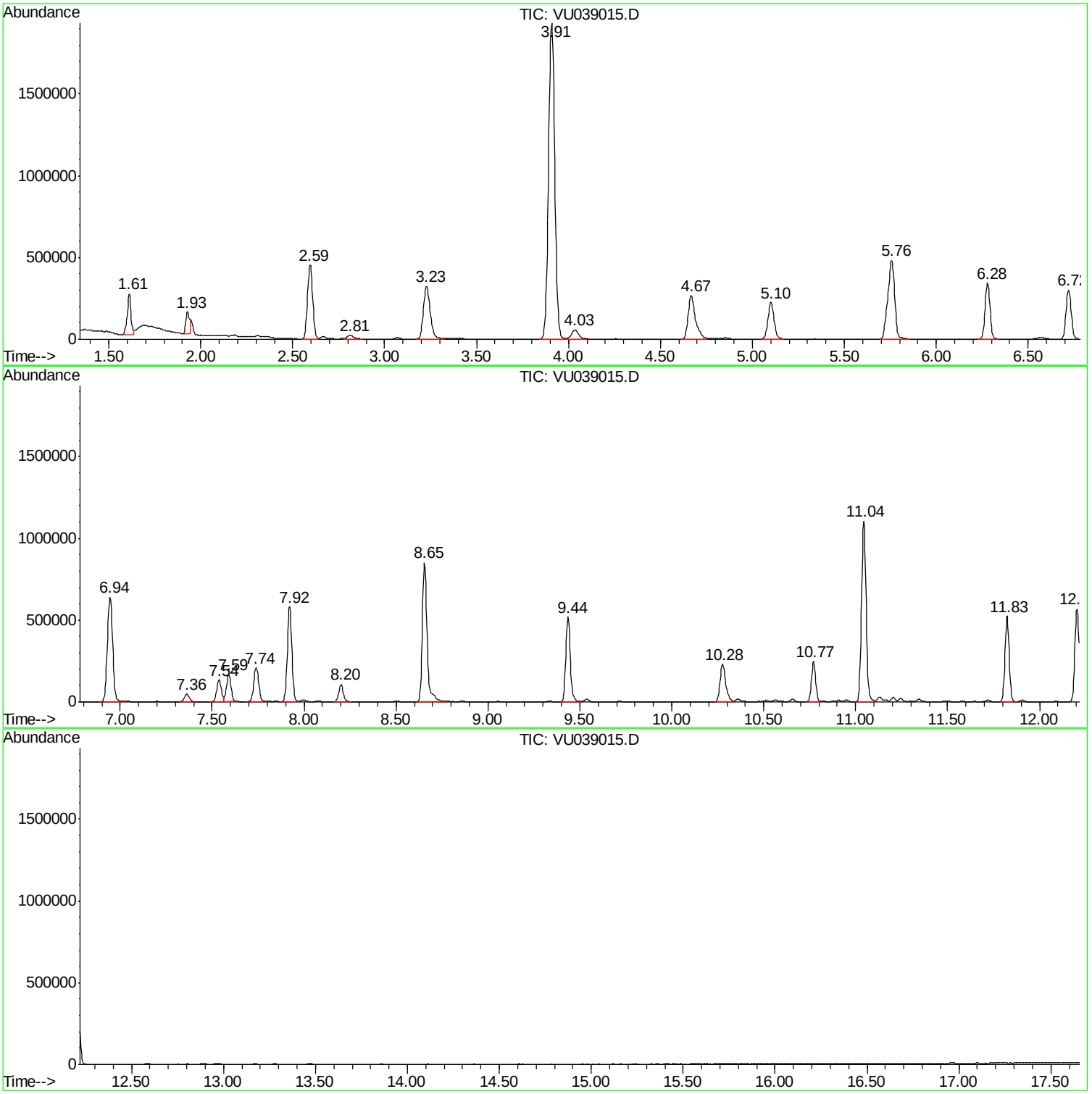
Sum of corrected areas: 21184040

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

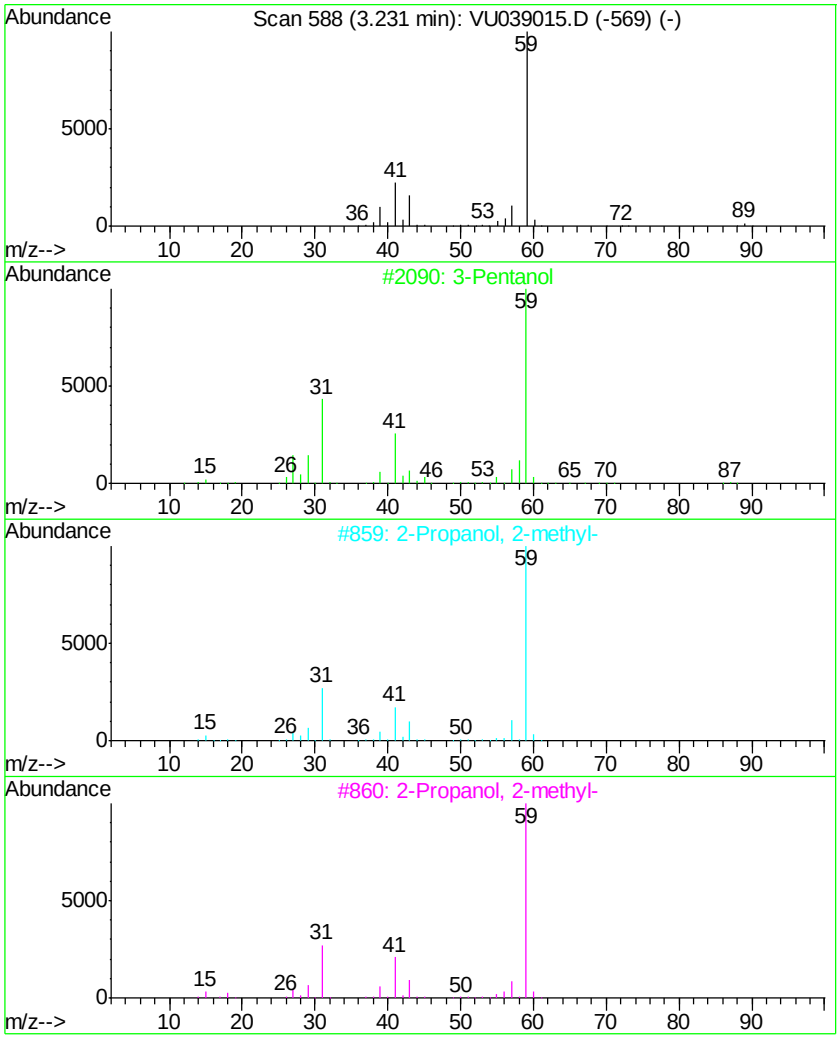
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

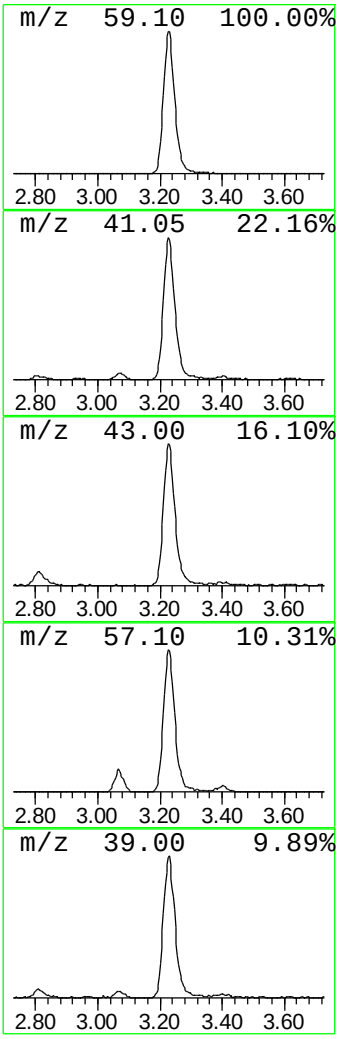
****

Peak Number 1 3-Pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	6.51 ug/L	837045	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol	88	C5H12O	000584-02-1	64
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	43
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

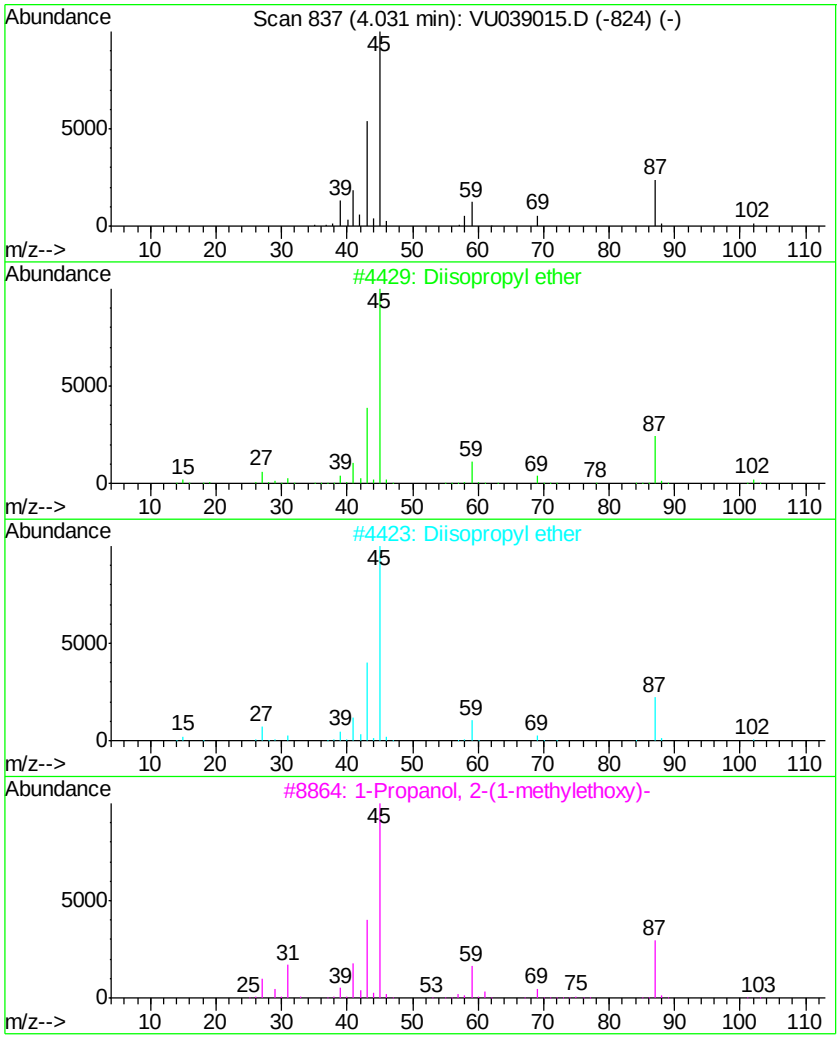
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

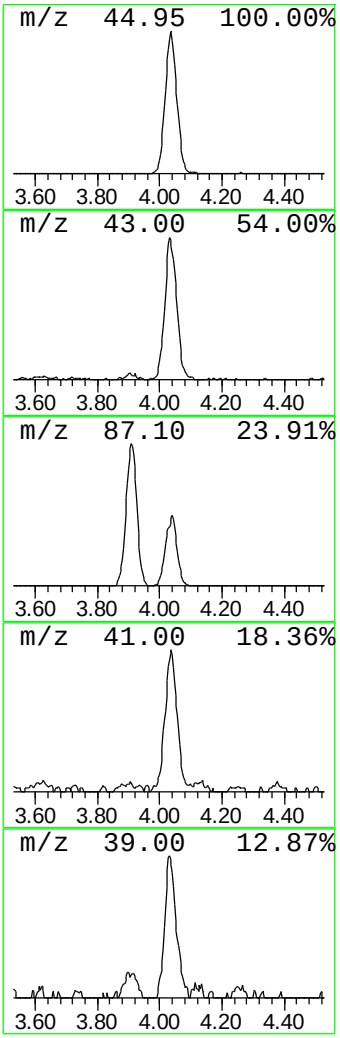
****

Peak Number 2 Diisopropyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	1.15 ug/L	147797	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl ether	102	C6H14O	000108-20-3	90
2	Diisopropyl ether	102	C6H14O	000108-20-3	78
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	78
4	Diisopropyl ether	102	C6H14O	000108-20-3	64
5	Ether, 2-chloro-1-methylethyl is...	136	C6H13ClO	098277-76-0	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

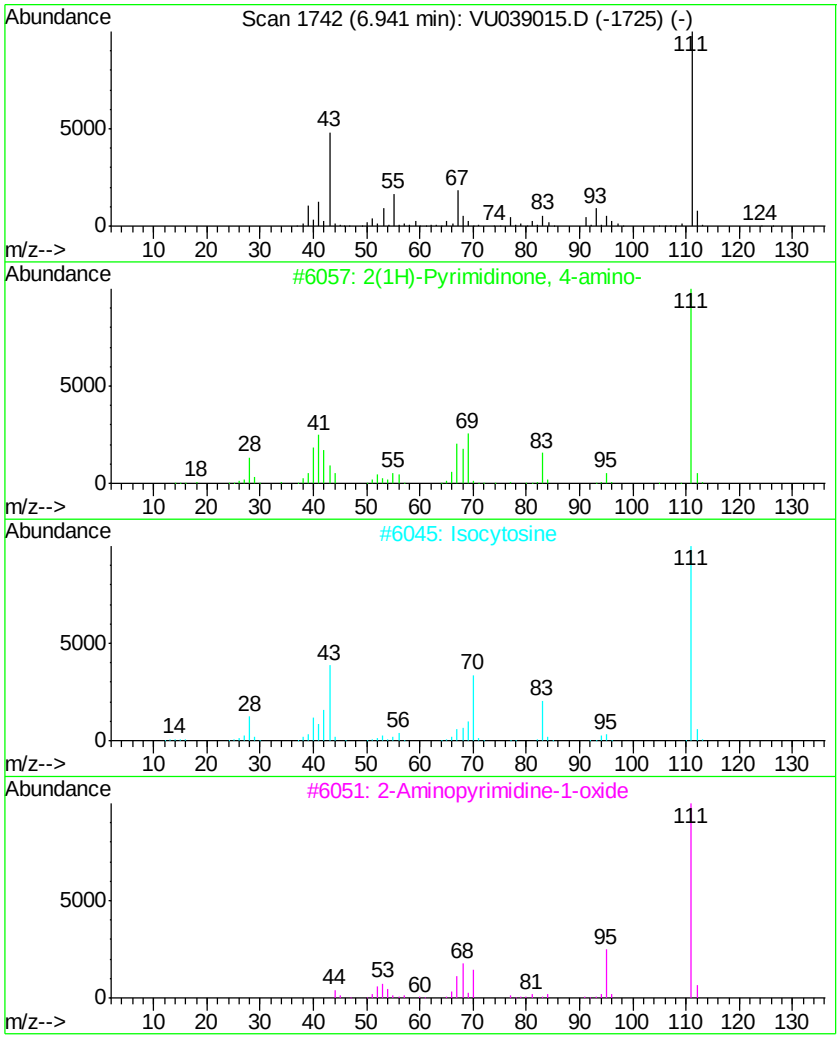
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

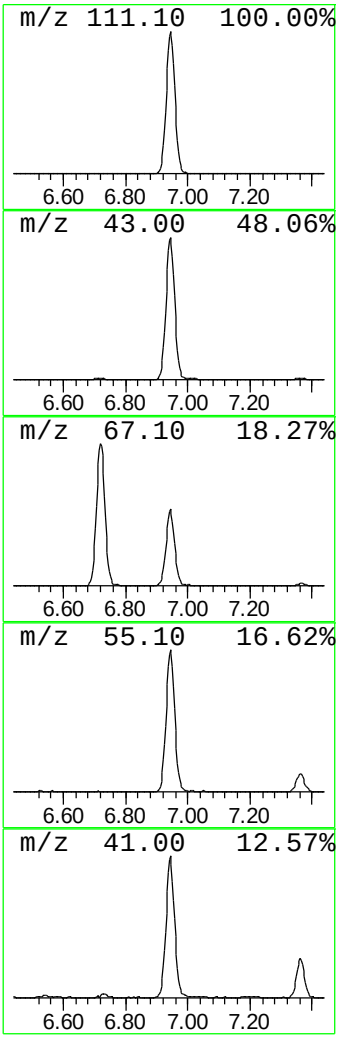
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	9.79 ug/L	1259050	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	Isocytosine	111	C4H5N3O	000108-53-2	58
3	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	56
4	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	42
5	2(1H)-Pyridinone, 5-hydroxy-	111	C5H5NO2	005154-01-8	39





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

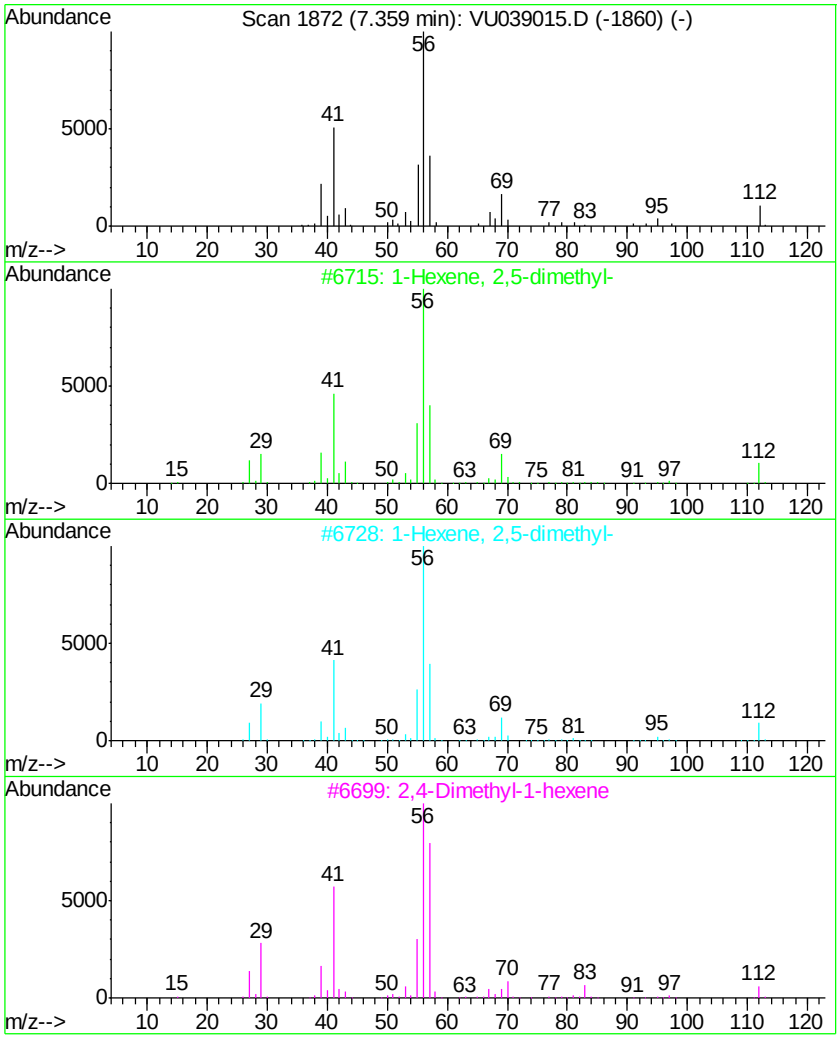
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

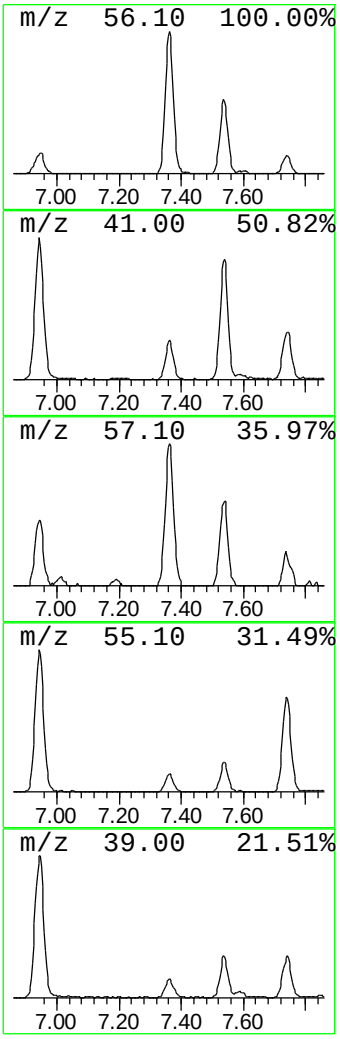
****

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	0.69 ug/L	88298	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	90
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	87
3	2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	80
4	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	72
5	2-Heptene, 5-methyl-	112	C8H16	022487-87-2	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

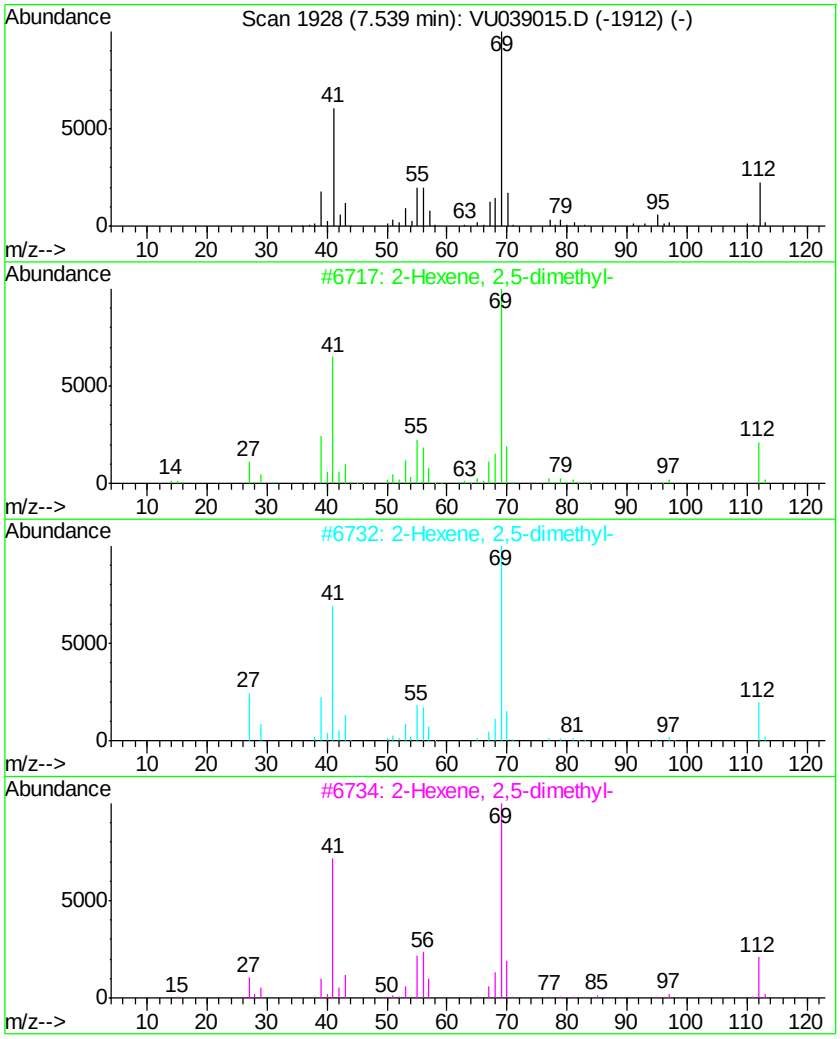
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

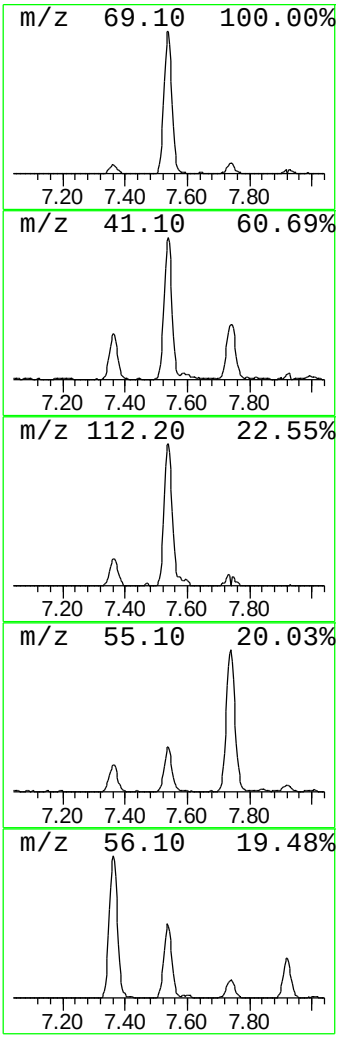
****

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	1.89 ug/L	243676	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	91
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-Heptene, 2-methyl-, (E)-	112	C8H16	000692-96-6	78





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

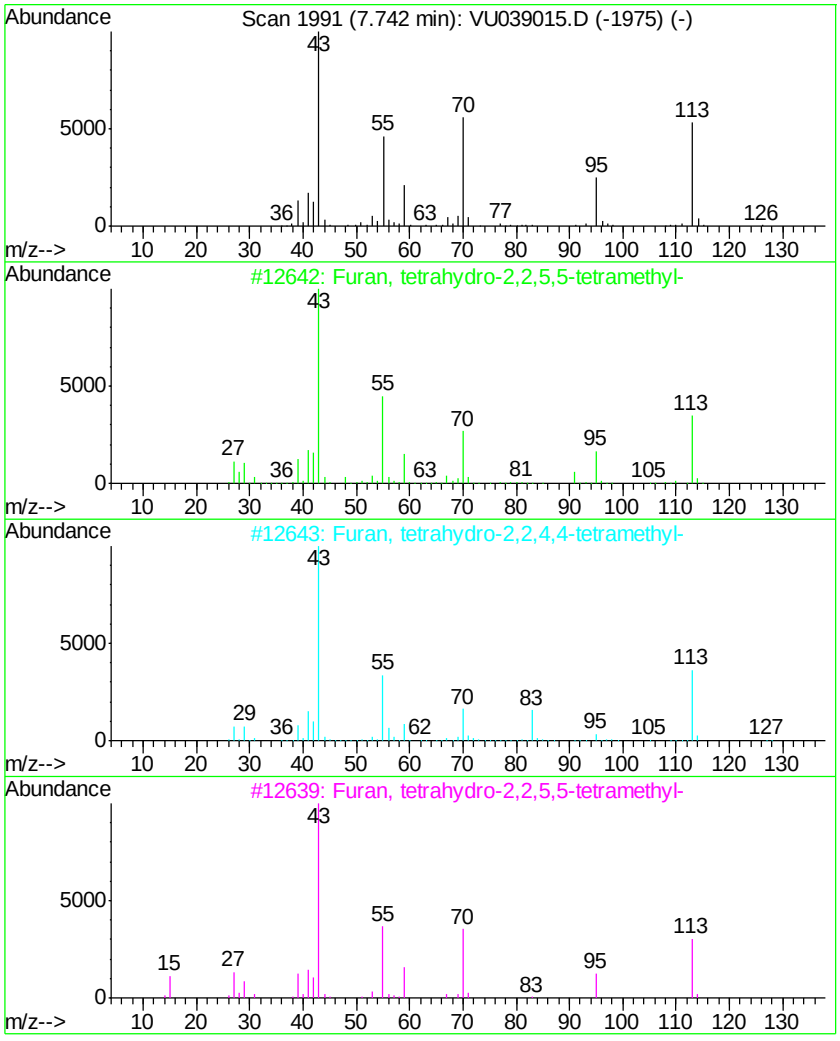
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

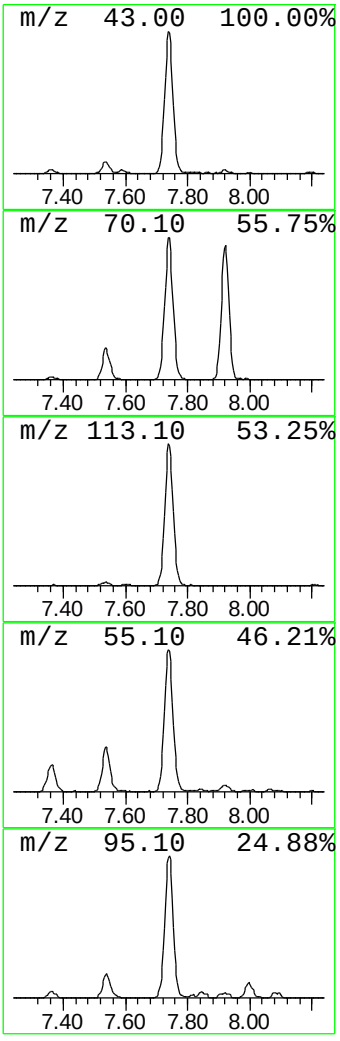
****

Peak Number 7 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	3.07 ug/L	395266	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-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	50
4	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
5	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

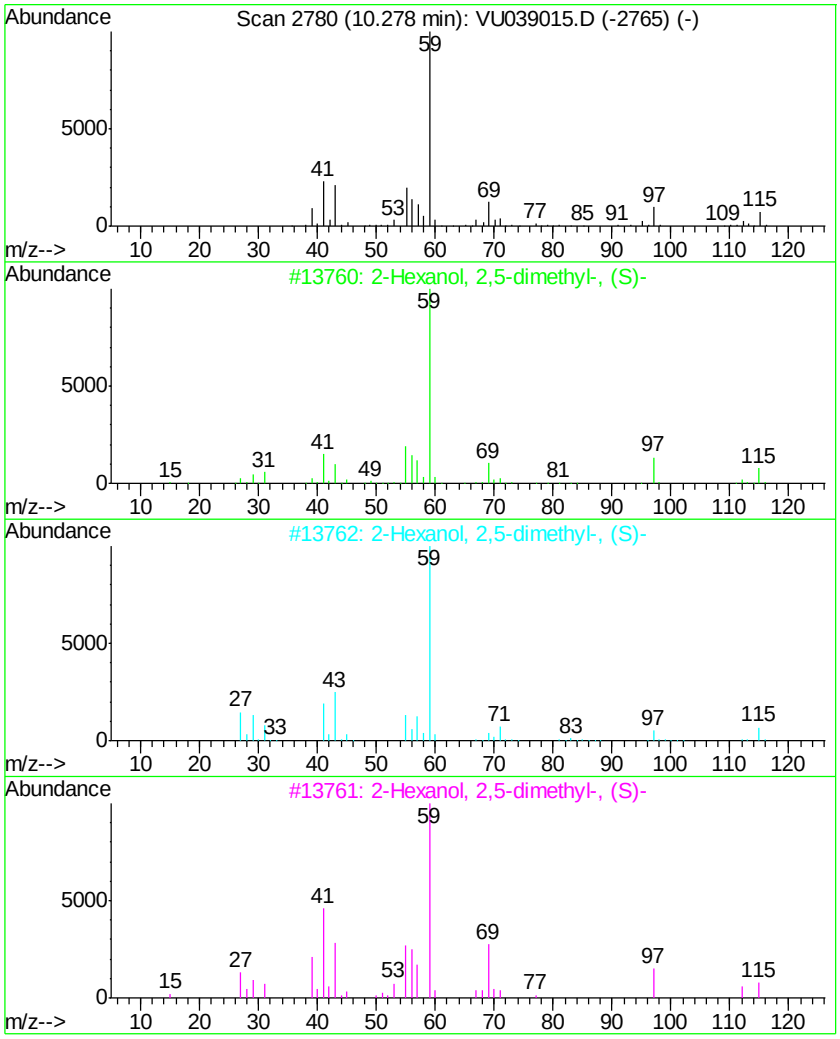
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

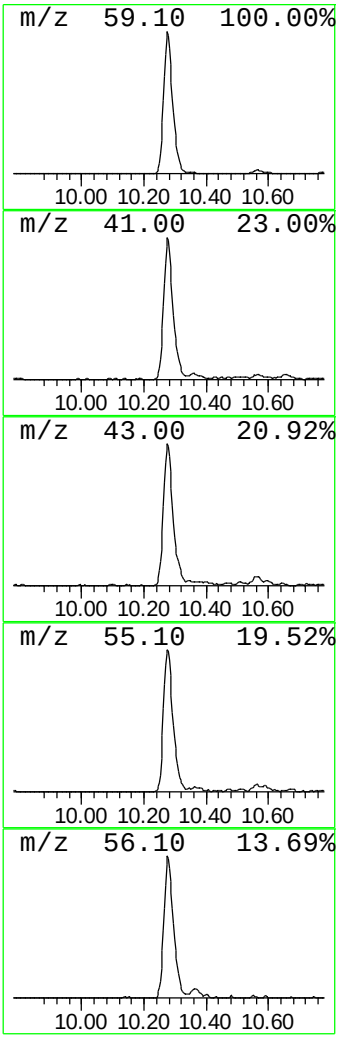
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.74 ug/L	484634	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-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	45
5	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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

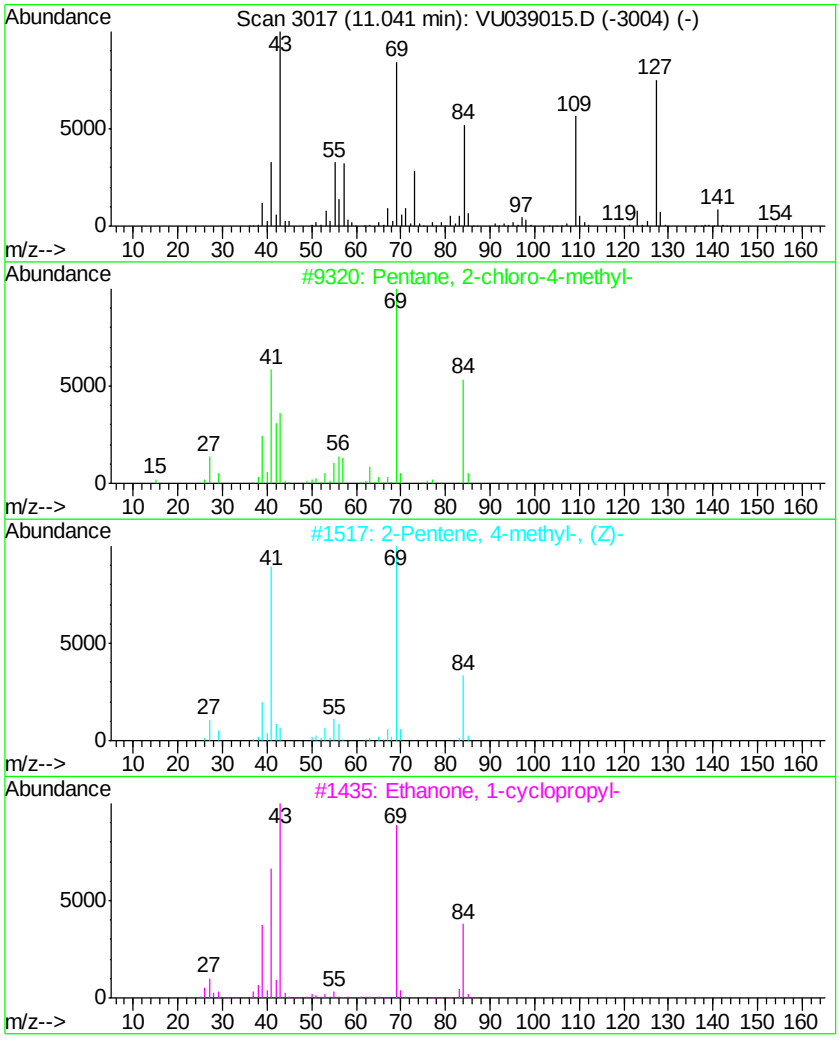
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

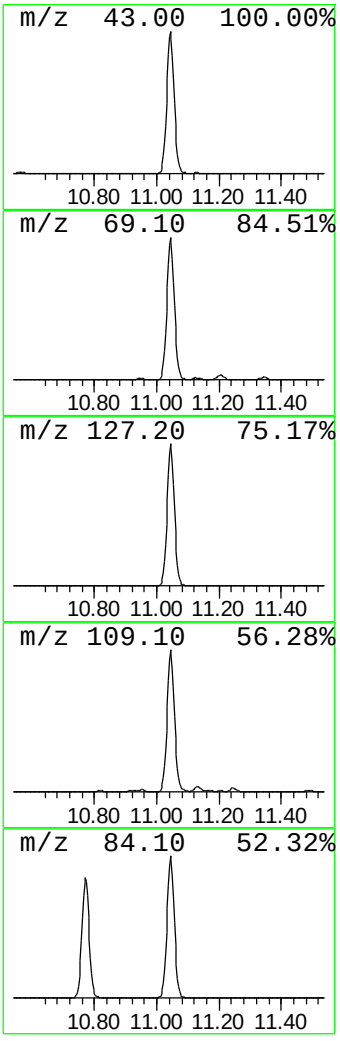
****

Peak Number 9 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	11.20 ug/L	1874620	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
2	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
4	Pentane, 3-methylene-	84	C6H12	000760-21-4	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 : VU039015.D
Acq On : 22 Jun 2020 19:37
Operator : SY/MD
Sample : L3061-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ1

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
3-Pentanol	3.23	6.5	ug/L	837045	1	6.28	643188	5.0
Diisopropyl ether	4.03	1.1	ug/L	147797	1	6.28	643188	5.0
2(1H)-Pyrimidinon...	6.94	9.8	ug/L	1259050	1	6.28	643188	5.0
(DEL) Alkane: Str...	7.36	0.7	ug/L	88298	1	6.28	643188	5.0
(DEL) Alkane: Str...	7.54	1.9	ug/L	243676	1	6.28	643188	5.0
Furan, tetrahydro...	7.74	3.1	ug/L	395266	1	6.28	643188	5.0
2-Hexanol, 2,5-di...	10.28	2.7	ug/L	484634	2	9.44	885849	5.0
unknown-01	11.04	11.2	ug/L	1874620	3	11.82	836620	5.0