LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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	1.494	41	48	62	rBV	154451	313920	20.39%	1.994%
2	1.610	78	84	91	rVB	193836	211737	13.76%	1.345%
3	1.929	176	183	200	rVB	141251	191687	12.45%	1.218%
4	2.395	324	328	343	rVB	23523	36633	2.38%	0.233%
5	2.588	376	388	401	rBV	290062	477314	31.01%	3.032%
6	2.658	402	410	422	rVB2	14135	25747	1.67%	0.164%
7	2.800	440	454	482	rBV	147171	321212	20.87%	2.041%
8	3.221	568	585	609	rBV	135373	317720	20.64%	2.018%
9	3.620	692	709	721	rBV3	8467	20415	1.33%	0.130%
10	3.906	779	798	817	rVB3	20119	47683	3.10%	0.303%
11	4.035	817	838	866	rBV3	351355	917372	59.60%	5.828%
12	4.665	1019	1034	1077	rBV2	279808	740289	48.09%	4.703%
13	4.848	1081	1091	1109	rVB4	7146	19342	1.26%	0.123%
14	5.099	1153	1169	1191	rVB	236235	518151	33.66%	3.292%
15	5.758	1353	1374	1402	rBV2	493021	1272921	82.70%	8.086%
16	6.279	1516	1536	1560	rVB	358384	683944	44.43%	4.345%
17	6.719	1658	1673	1694	rBV	307300	593625	38.57%	3.771%
18	6.944	1723	1743	1756	rBV2	91585	183020	11.89%	1.163%
19	7.192	1808	1820	1833	rVB5	7329	15515	1.01%	0.099%
20	7.362	1861	1873	1888	rBV	48931	86156	5.60%	0.547%
21	7.539	1910	1928	1935	rBV	95565	173180	11.25%	1.100%
22	7.591	1935	1944	1958	rVB	126307	225537	14.65%	1.433%
23	7.739	1976	1990	2010	rBV2	293935	555510	36.09%	3.529%
24	7.922	2032	2047	2063	rBV	575928	996530	64.74%	6.331%
25	8.202	2121	2134	2150	rBV	84300	144203	9.37%	0.916%
26	8.655	2257	2275	2316	rBV	835422	1539258	100.00%	9.778%
27	9.436	2503	2518	2545	rBV2	531981	1009735	65.60%	6.415%
28	10.275	2765	2779	2798	rBV	274423	587956	38.20%	3.735%
29	10.366	2800	2807	2820	rVB6	11451	22997	1.49%	0.146%
30	10.562	2860	2868	2882	rVB4	16726	30454	1.98%	0.193%
31	10.771	2918	2933	2955	rBV	246750	400317	26.01%	2.543%
32	11.044	3005	3018	3036	rBV	460600	804563	52.27%	5.111%
33	11.822	3248	3260	3280	rBV2	534988	947459	61.55%	6.019%
34	12.205	3365	3379	3401	rBV3	616865	1309251	85.06%	8.317%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

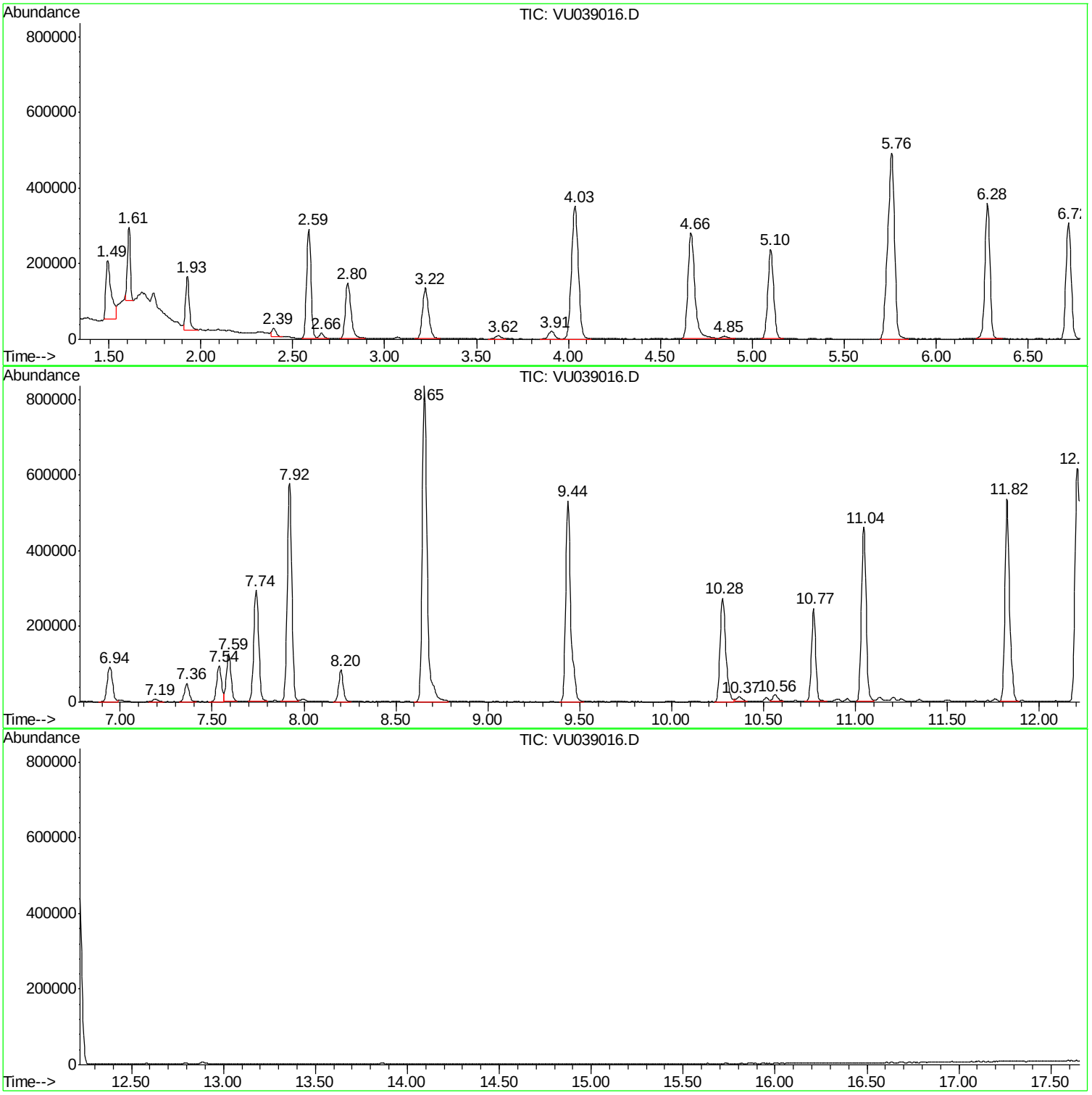
Sum of corrected areas: 15741353

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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 : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

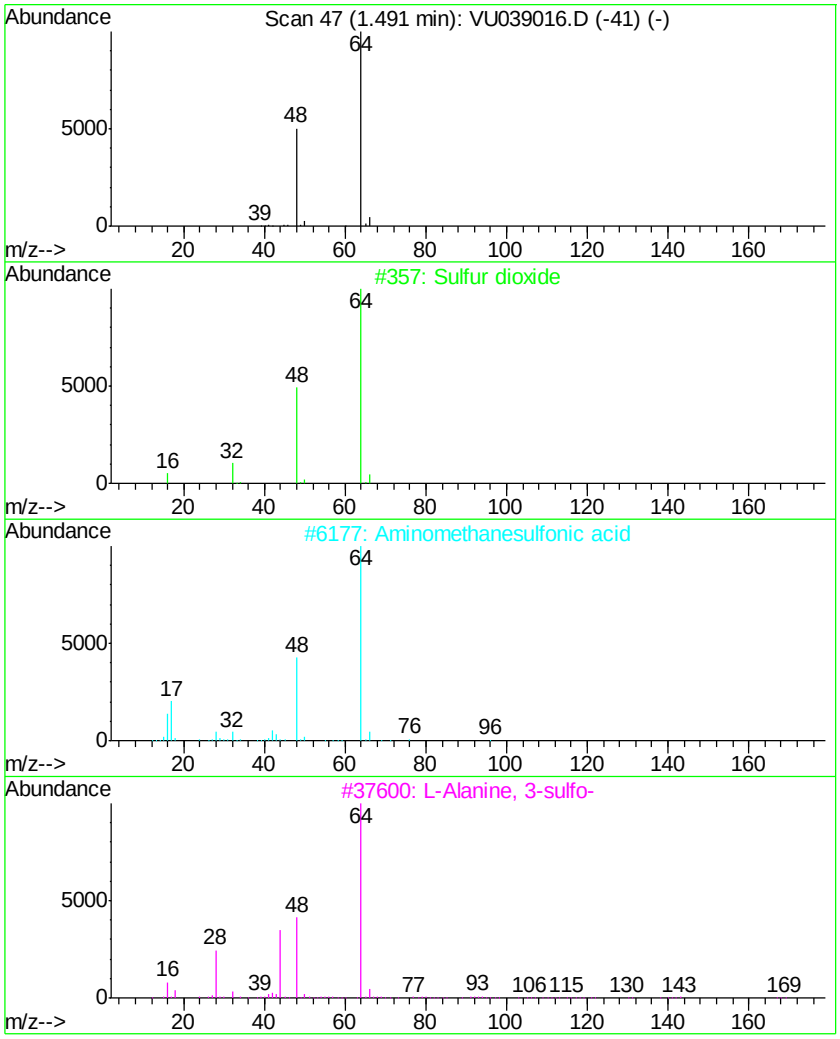
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

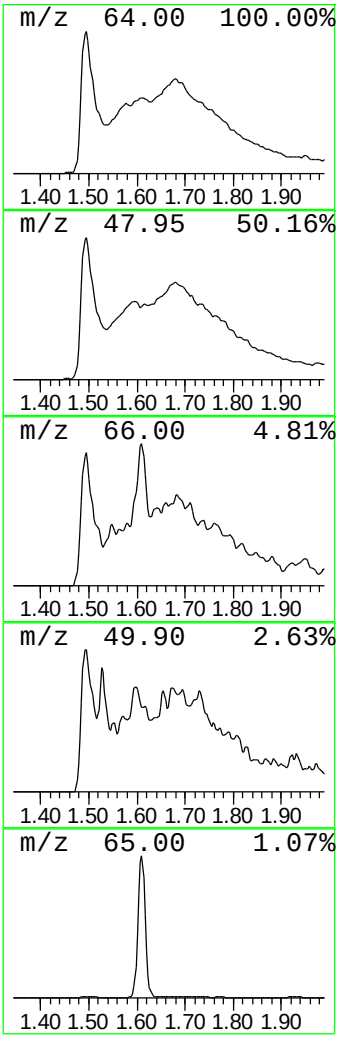
****

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	2.29 ug/L	313920	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	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

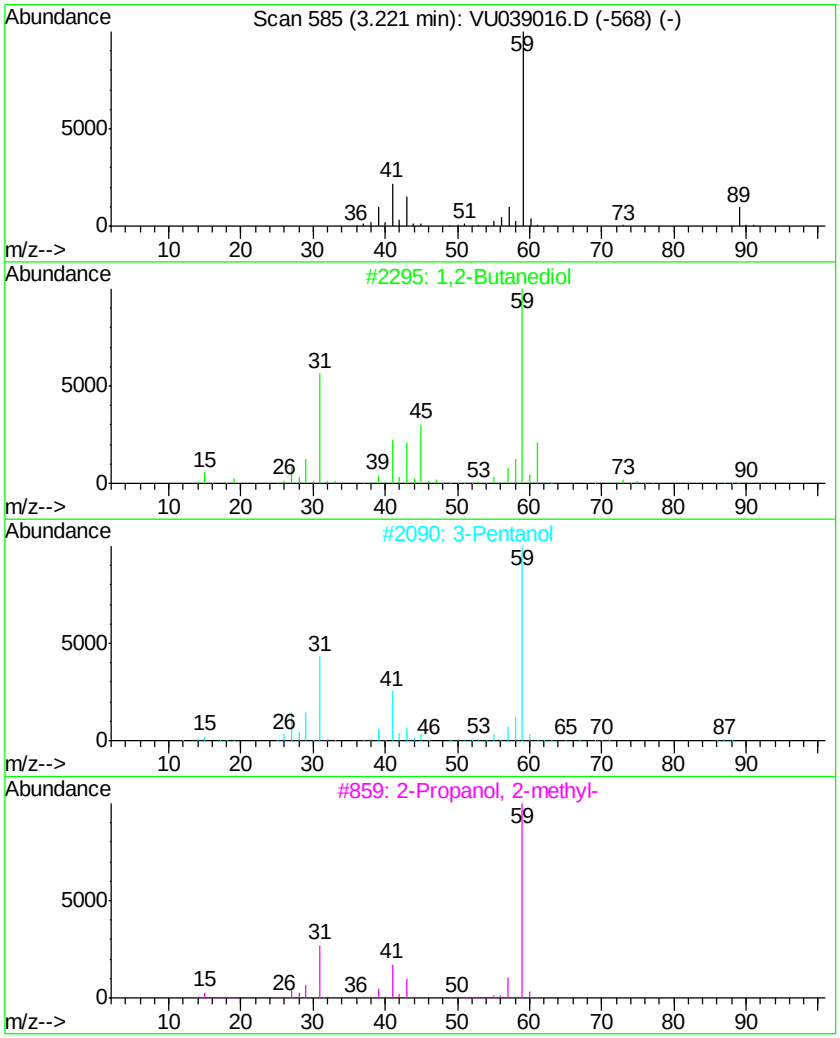
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

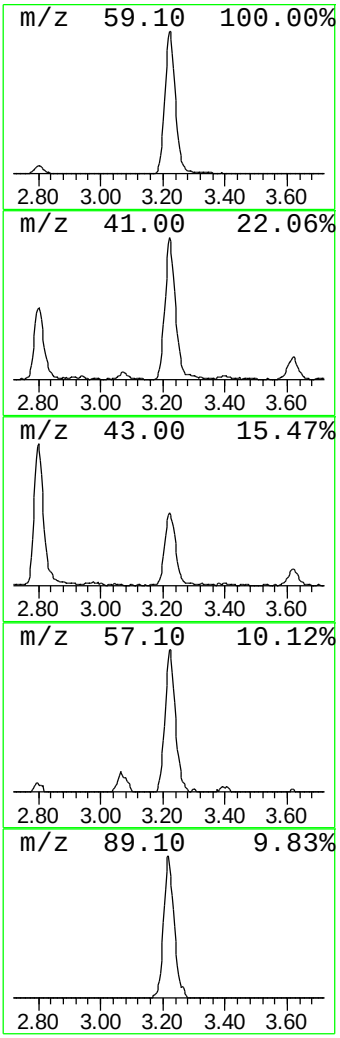
****

Peak Number 2 1,2-Butanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	2.32 ug/L	317720	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Butanediol	90	C4H10O2	000584-03-2	64
2	3-Pentanol	88	C5H12O	000584-02-1	50
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

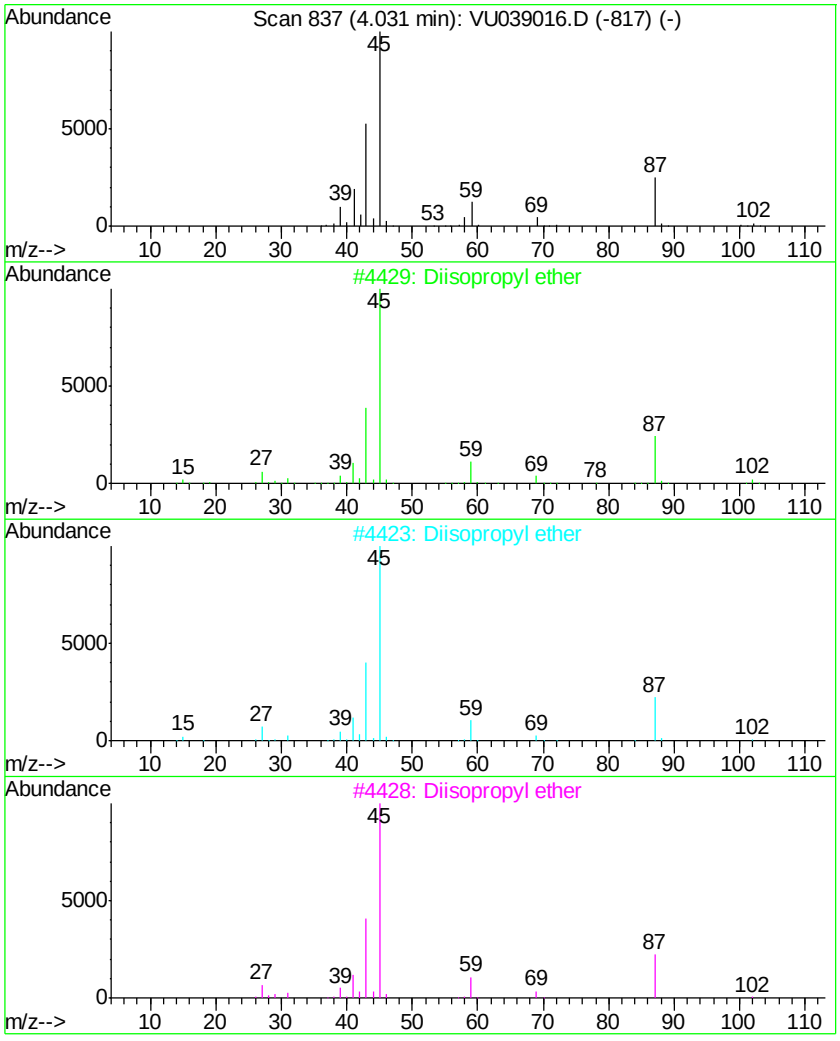
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

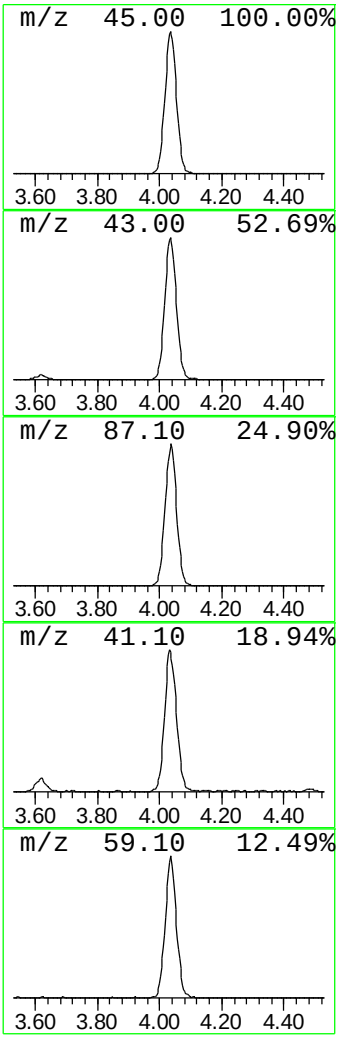
****

Peak Number 3 Diisopropyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	6.71 ug/L	917372	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl ether	102	C6H14O	000108-20-3	86
2	Diisopropyl ether	102	C6H14O	000108-20-3	78
3	Diisopropyl ether	102	C6H14O	000108-20-3	78
4	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64
5	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

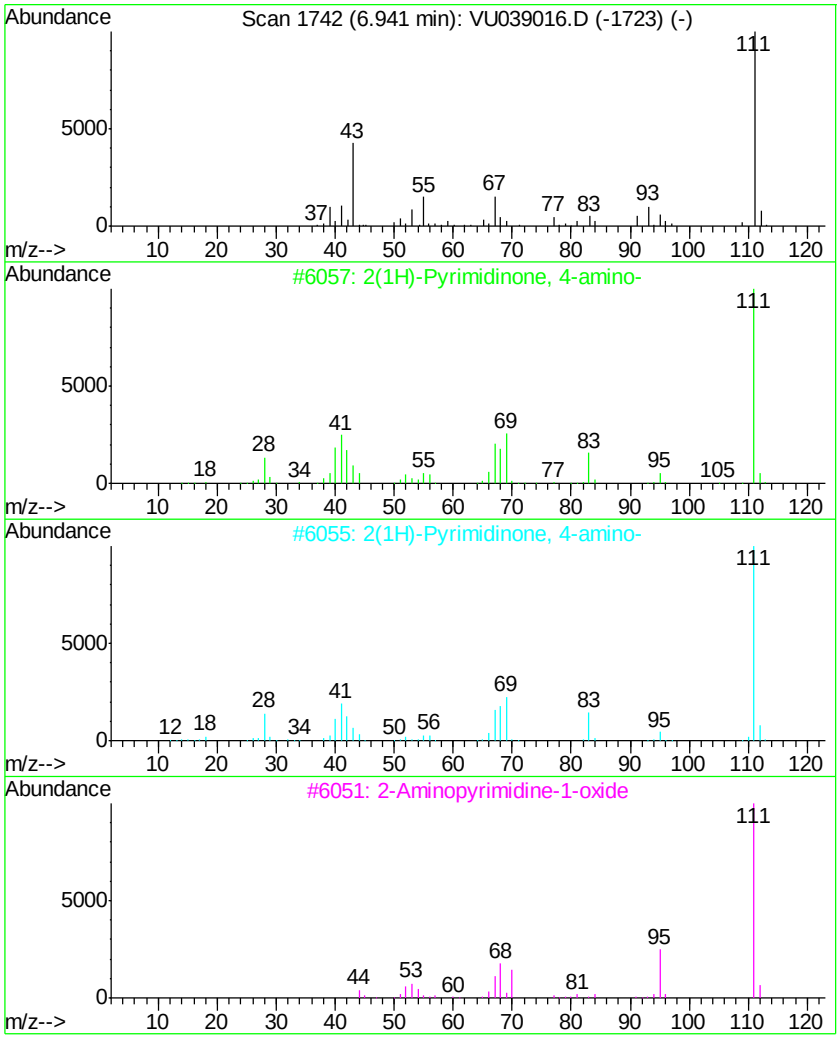
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

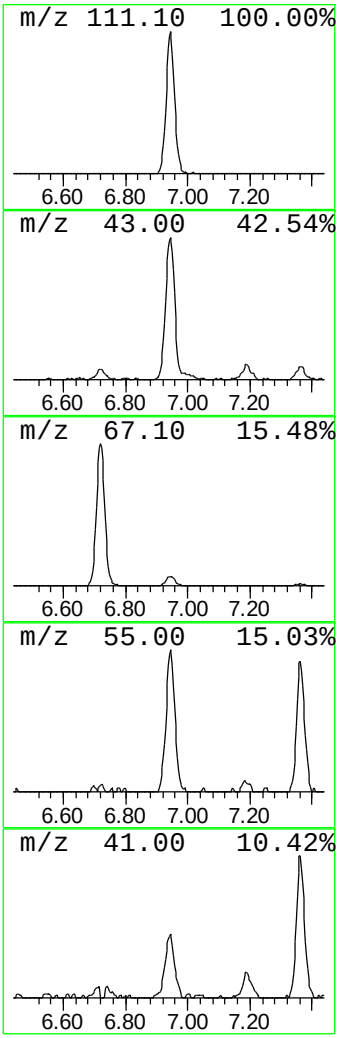
****

Peak Number 4 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	1.34 ug/L	183020	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(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
3	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	53
4	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	53
5	Pyrazol-4-amine, 1,5-dimethyl-	111	C5H9N3	121983-36-6	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

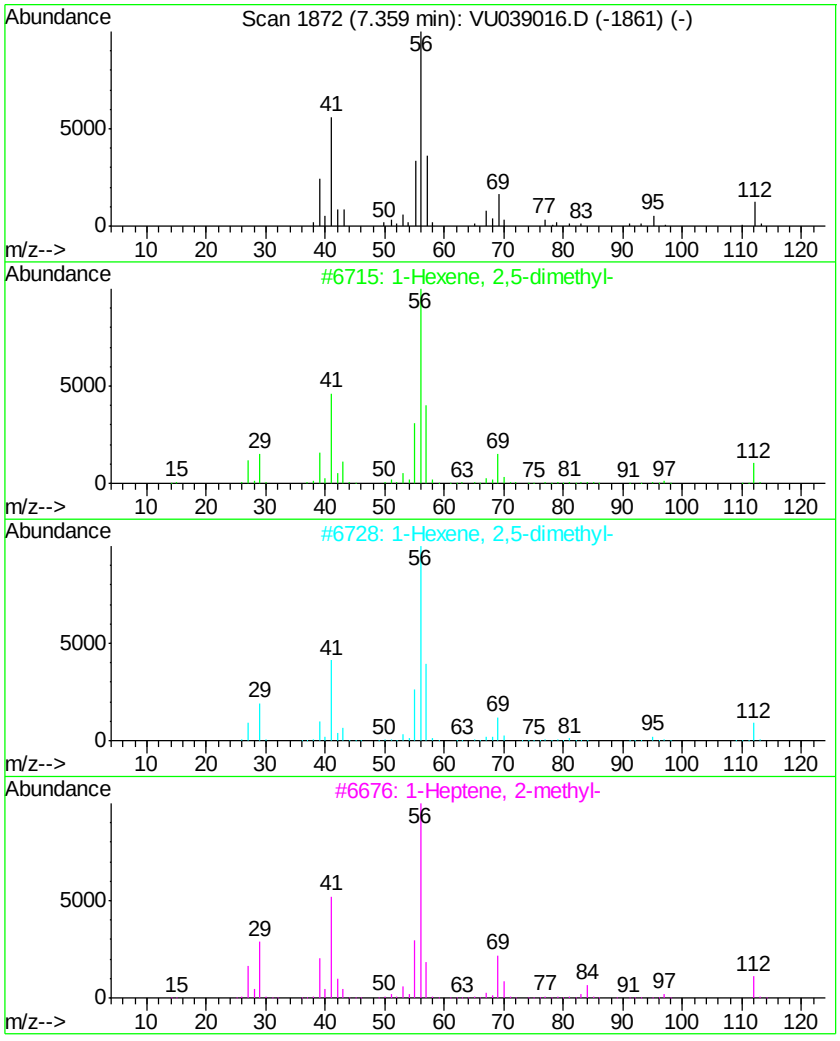
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

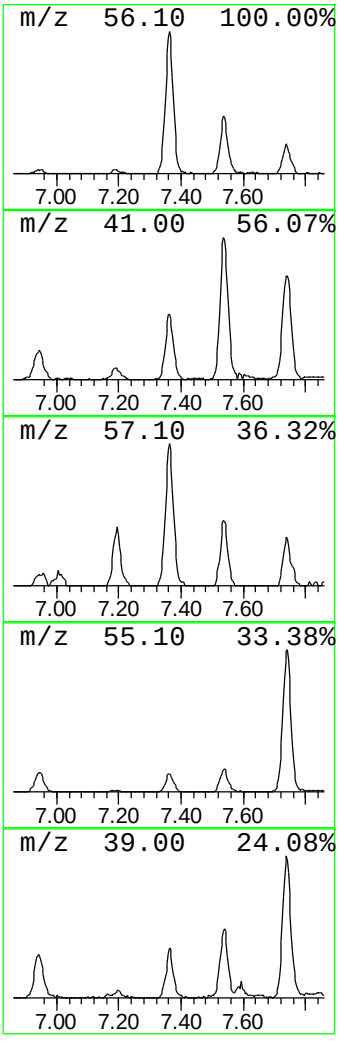
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	0.63 ug/L	86156	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	87
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	86
3	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	64
4	2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	64
5	4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

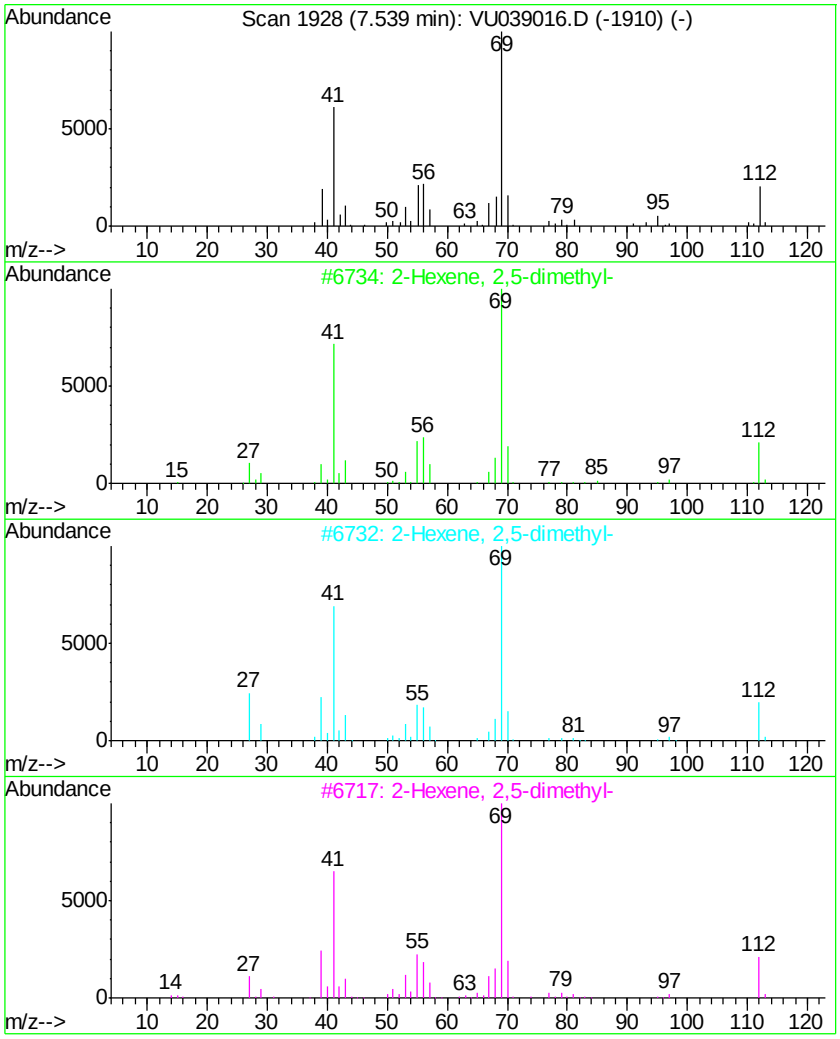
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

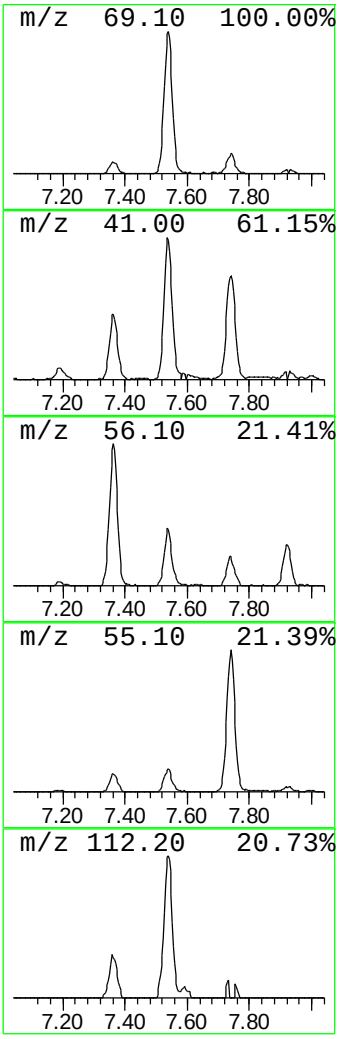
****

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	1.27 ug/L	173180	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	87
2	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	87
3	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	86
4	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	86
5	3-Hexene, 2,5-dimethyl-, (E)-	112	C8H16	000692-70-6	83





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

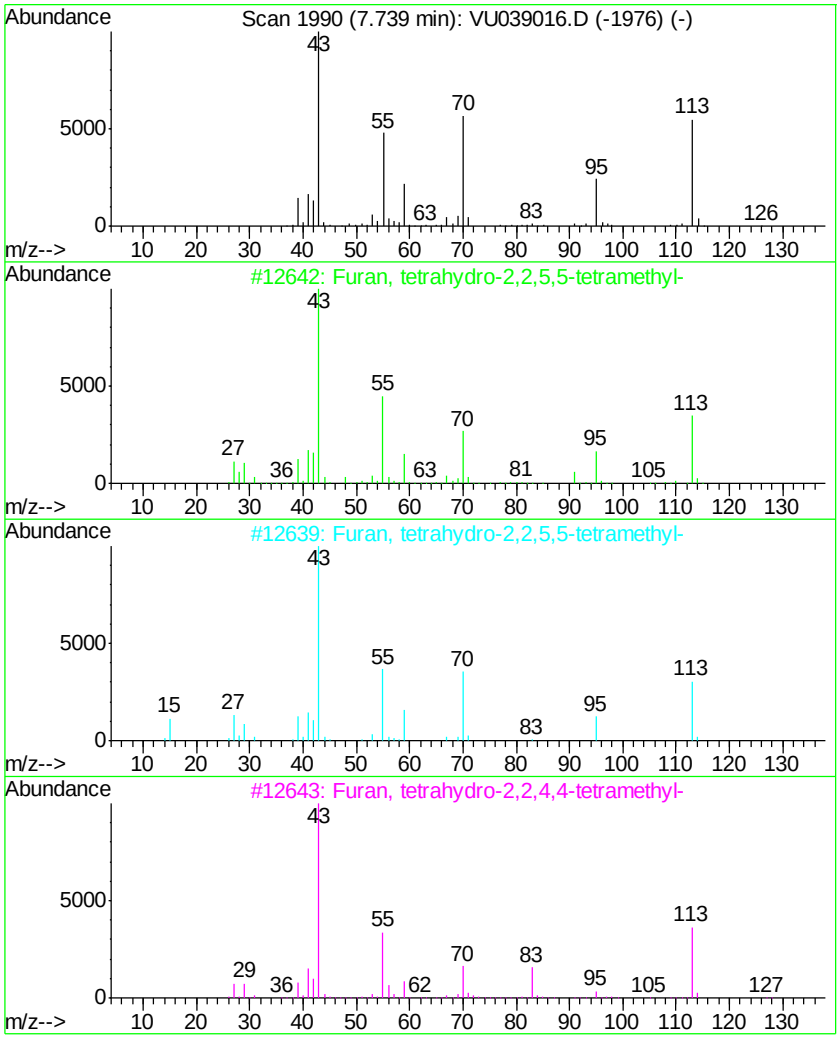
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

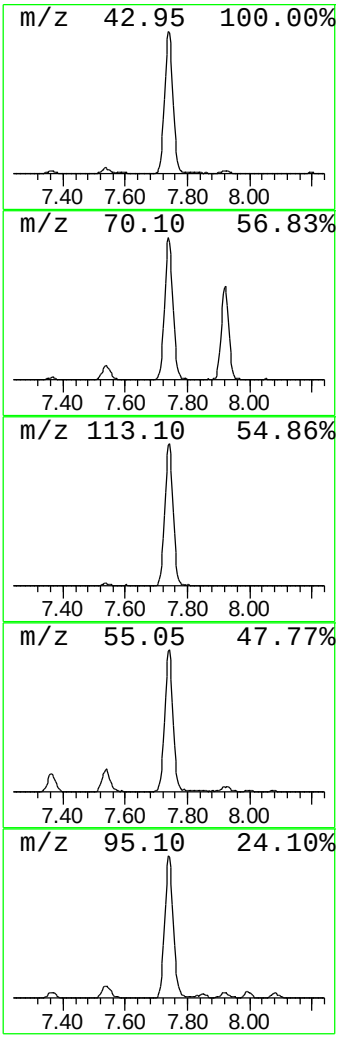
****

Peak Number 8 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	4.06 ug/L	555510	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	64
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	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

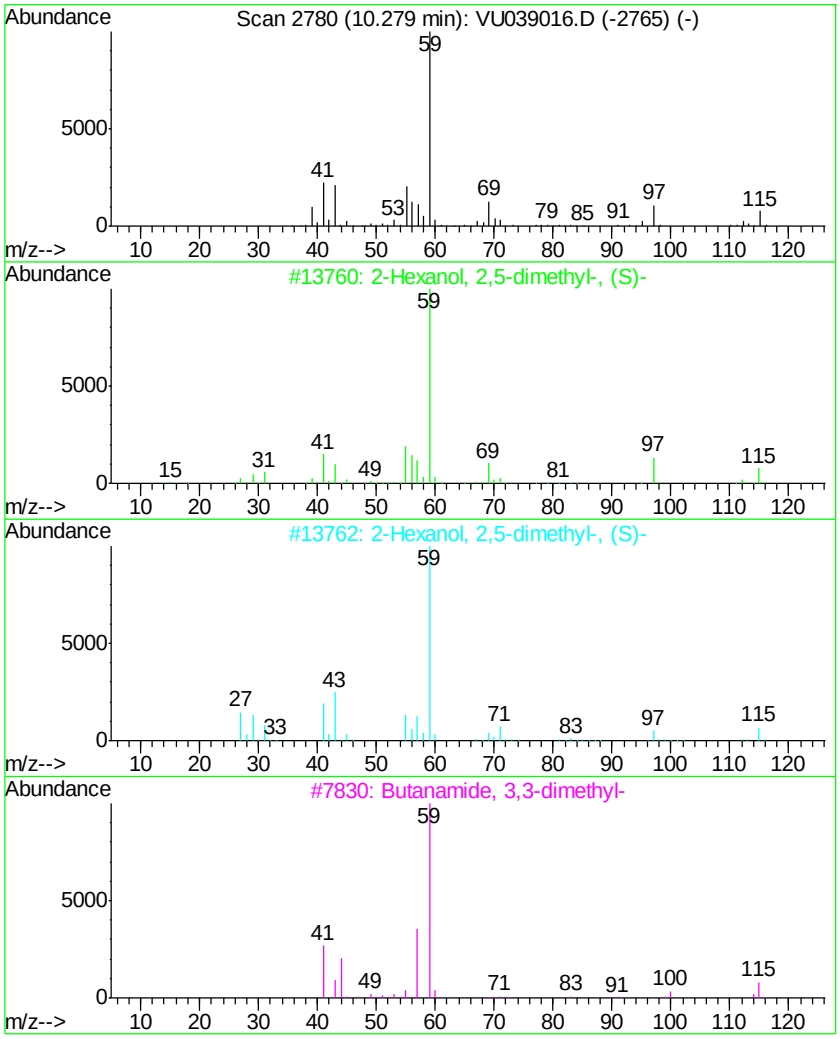
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

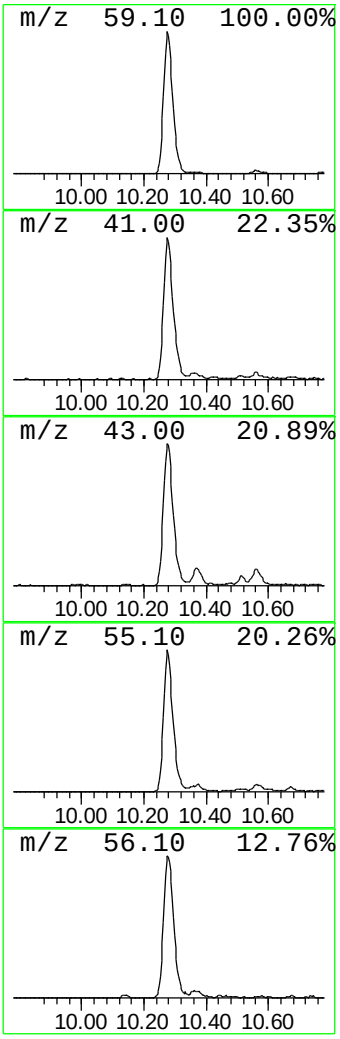
****

Peak Number 9 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.91 ug/L	587956	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	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	52
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

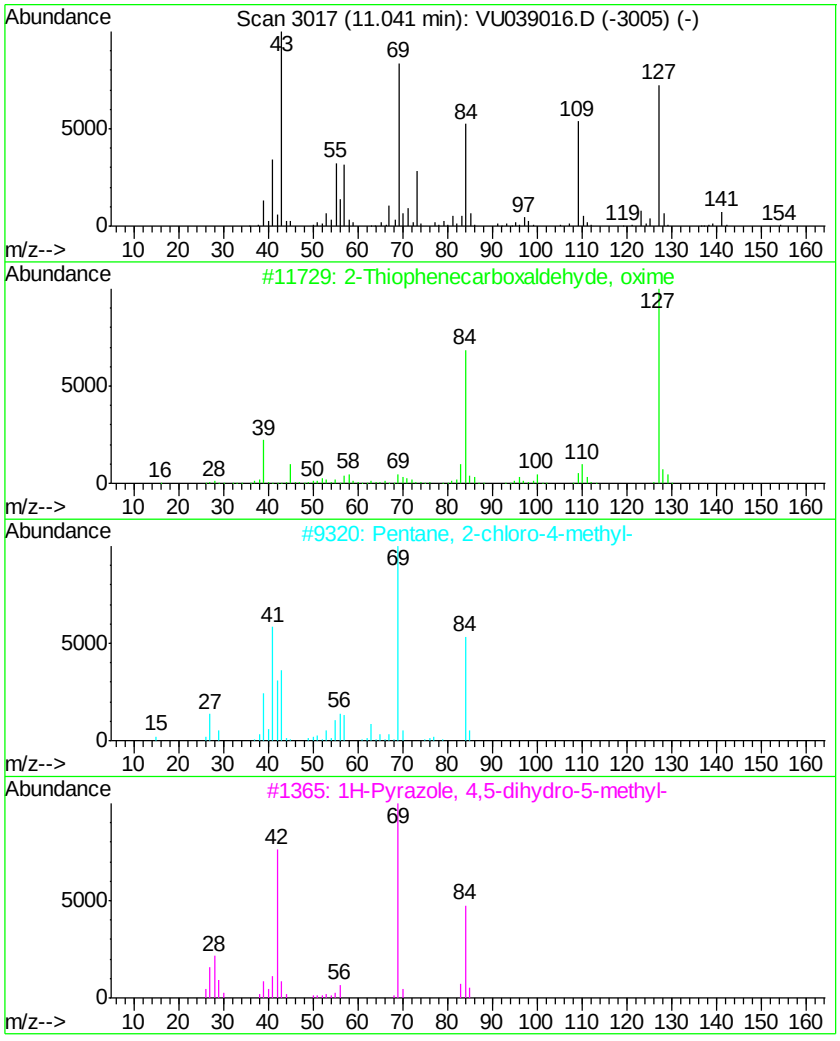
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

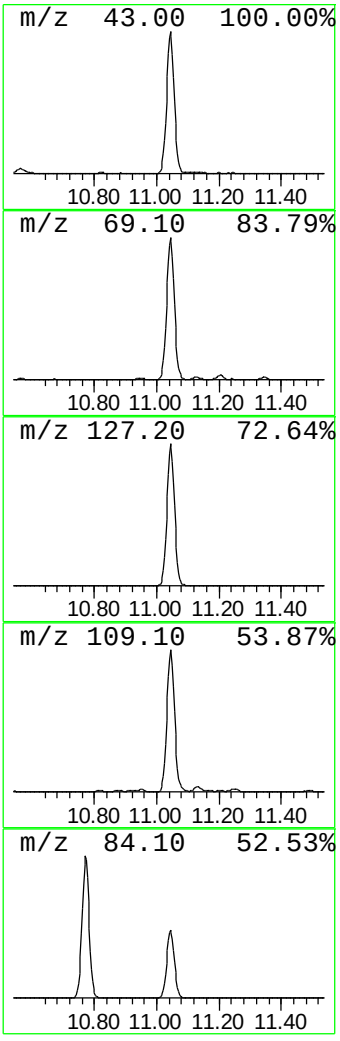
****

Peak Number 10 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	4.25 ug/L	804563	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
2	Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
3	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
4	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27
5	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
Data File : VU039016.D
Acq On : 22 Jun 2020 20:01
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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	2.3	ug/L	313920	1	6.28	683944	5.0
1,2-Butanediol	3.22	2.3	ug/L	317720	1	6.28	683944	5.0
Diisopropyl ether	4.03	6.7	ug/L	917372	1	6.28	683944	5.0
2(1H)-Pyrimidinon...	6.94	1.3	ug/L	183020	1	6.28	683944	5.0
(DEL) Alkane: Str...	7.36	0.6	ug/L	86156	1	6.28	683944	5.0
(DEL) Alkane: Str...	7.54	1.3	ug/L	173180	1	6.28	683944	5.0
Furan, tetrahydro...	7.74	4.1	ug/L	555510	1	6.28	683944	5.0
2-Hexanol, 2,5-di...	10.28	2.9	ug/L	587956	2	9.44	1009740	5.0
unknown-01	11.04	4.3	ug/L	804563	3	11.83	947459	5.0