LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 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\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	1.613	75	85	100	rVB	177034	210017	7.87%	1.138%
2	1.748	120	127	138	rVB	48997	61540	2.31%	0.333%
3	1.932	176	184	202	rVB	143324	187054	7.01%	1.013%
4	2.398	320	329	343	rVB	22133	36421	1.37%	0.197%
5	2.594	375	390	402	rBV	269184	446859	16.75%	2.421%
6	2.668	403	413	437	rVB	47911	126504	4.74%	0.685%
7	2.835	448	465	466	rBV2	23032	40066	1.50%	0.217%
8	3.263	570	598	665	rBV2	385775	2667694	100.00%	14.453%
9	3.620	696	709	724	rVB2	13043	29976	1.12%	0.162%
10	3.906	786	798	813	rVB2	18045	42936	1.61%	0.233%
11	4.031	818	837	862	rBV	356378	924075	34.64%	5.006%
12	4.671	1018	1036	1080	rVB2	271959	845069	31.68%	4.578%
13	5.099	1153	1169	1190	rBV	233999	516426	19.36%	2.798%
14	5.758	1350	1374	1406	rBV2	485100	1275344	47.81%	6.910%
15	6.279	1511	1536	1557	rVB	357384	784677	29.41%	4.251%
16	6.719	1659	1673	1693	rBV	305206	594662	22.29%	3.222%
17	6.941	1724	1742	1758	rBV	83130	165561	6.21%	0.897%
18	7.195	1804	1821	1837	rVB3	24031	49803	1.87%	0.270%
19	7.536	1916	1927	1934	rBV2	37697	63500	2.38%	0.344%
20	7.591	1934	1944	1960	rVB	156274	275915	10.34%	1.495%
21	7.739	1974	1990	2007	rBV	302736	567619	21.28%	3.075%
22	7.919	2033	2046	2061	rBV	566749	976622	36.61%	5.291%
23	8.198	2120	2133	2152	rBV	106092	183429	6.88%	0.994%
24	8.655	2256	2275	2314	rBV	954801	1697935	63.65%	9.199%
25	9.433	2504	2517	2538	rBV2	507118	961459	36.04%	5.209%
26	10.275	2765	2779	2801	rBV	496736	920466	34.50%	4.987%
27	10.372	2801	2809	2824	rVB6	14026	30876	1.16%	0.167%
28	10.562	2860	2868	2887	rVB3	26530	48061	1.80%	0.260%
29	10.771	2916	2933	2948	rBV	253585	417446	15.65%	2.262%
30	11.044	3000	3018	3042	rBV	680009	1153787	43.25%	6.251%
31	11.822	3248	3260	3283	rVB2	506940	904523	33.91%	4.901%
32	12.205	3361	3379	3402	rBV2	588373	1251196	46.90%	6.779%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 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\SOMUTR062320WMA.M
Title : TRACE VOA SOM01.0

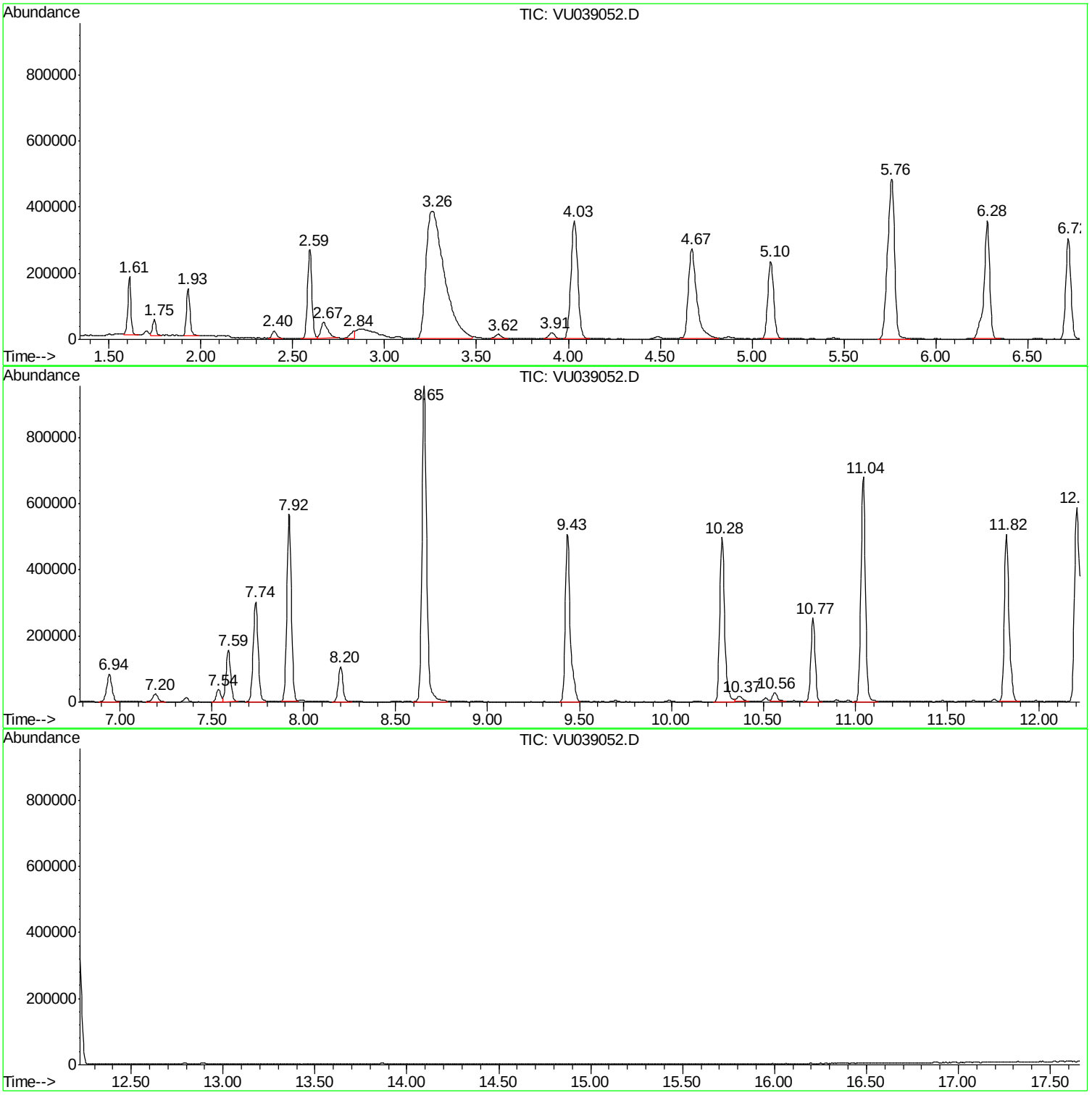
Sum of corrected areas: 18457518

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

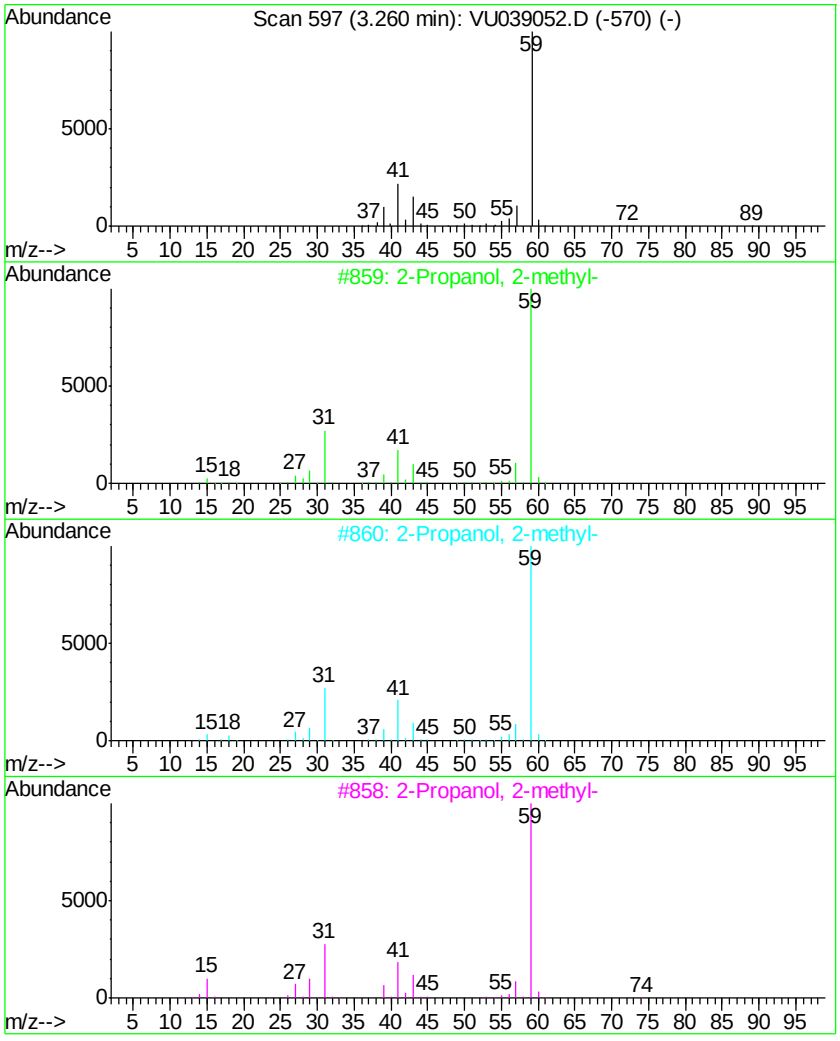
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

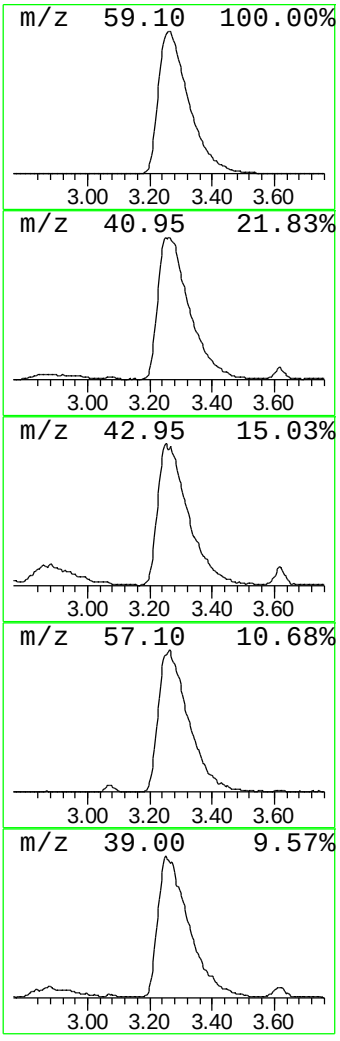
****

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	17.00 ug/L	2667690	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	78
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4	3-Pentanol	88	C5H12O	000584-02-1	64
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

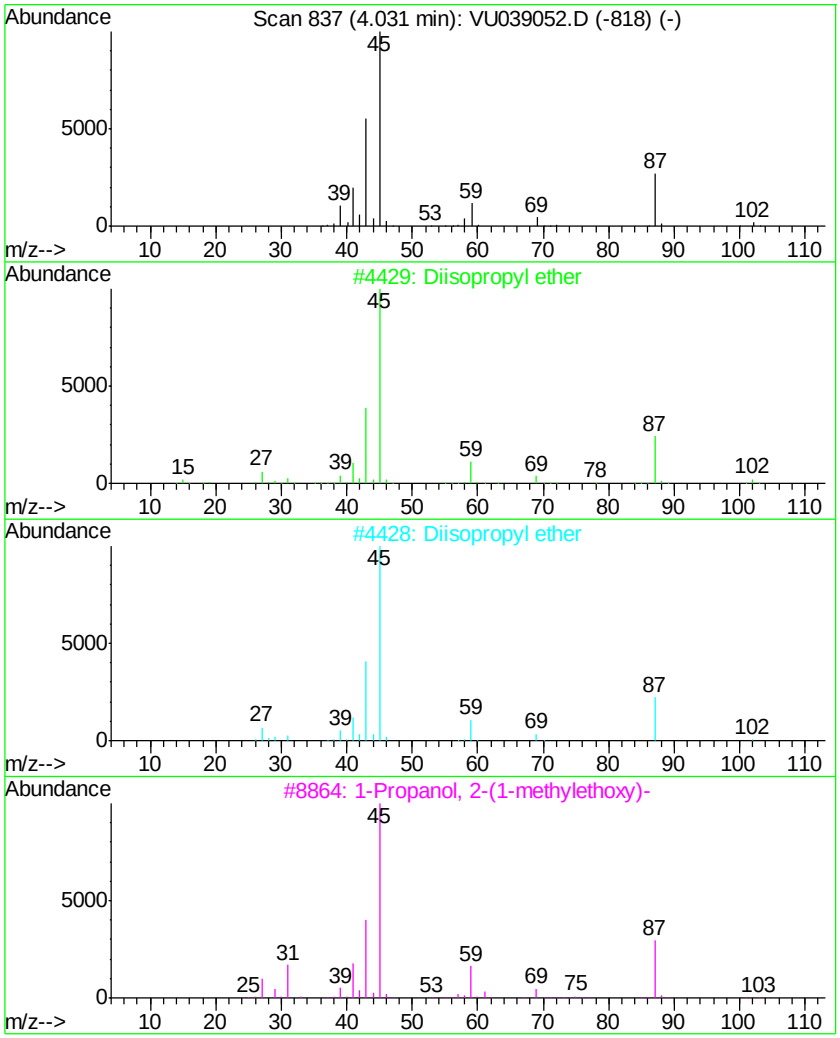
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

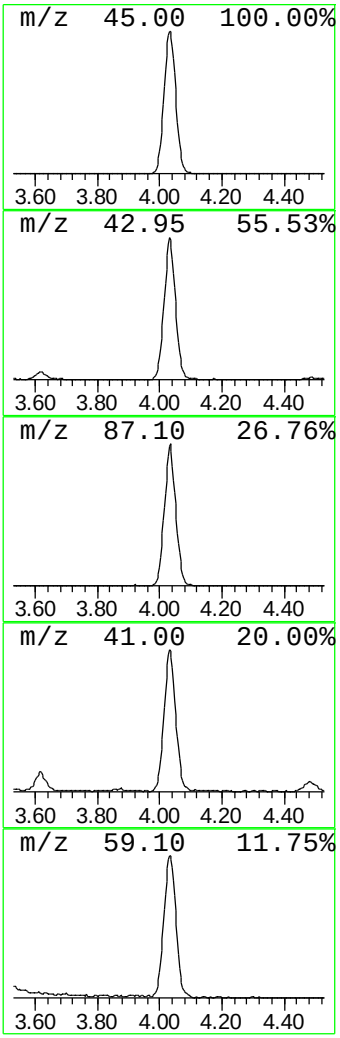
****

Peak Number 2 Diisopropyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	5.89 ug/L	924075	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	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64
4	Diisopropyl ether	102	C6H14O	000108-20-3	64
5	2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

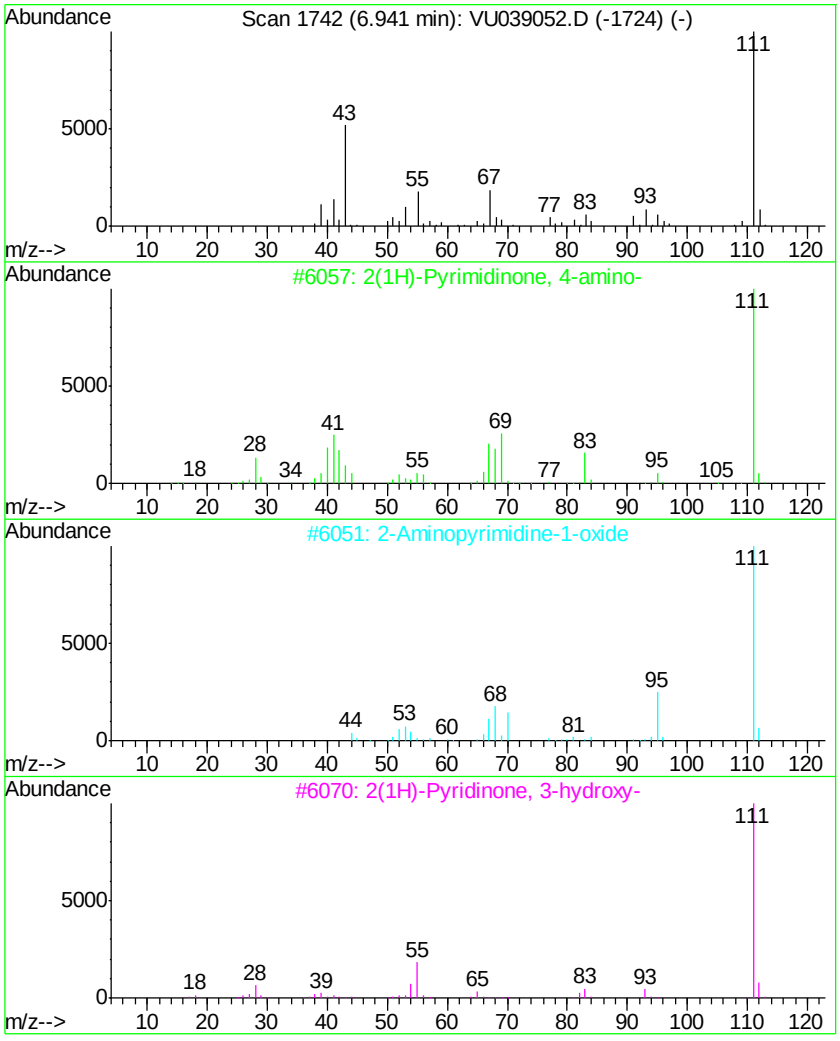
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

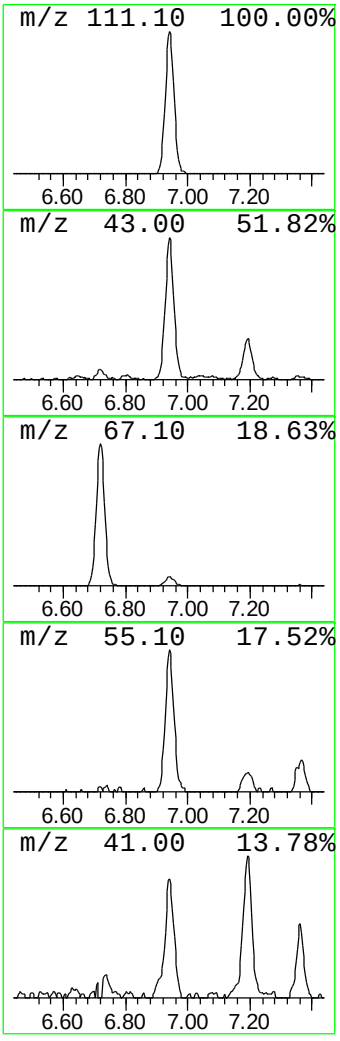
****

Peak Number 3 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	1.05 ug/L	165561	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-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	56
3	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	53
4	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	45
5	Bruceantin	548	C28H36O11	041451-75-6	45





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

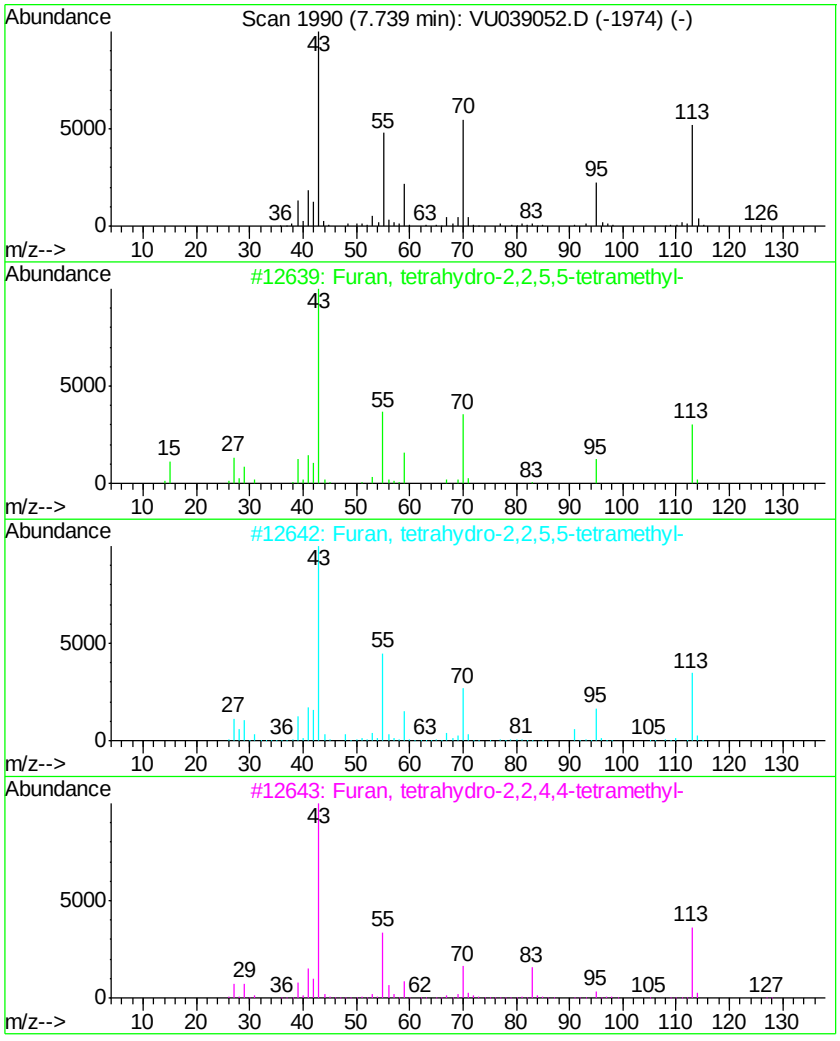
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

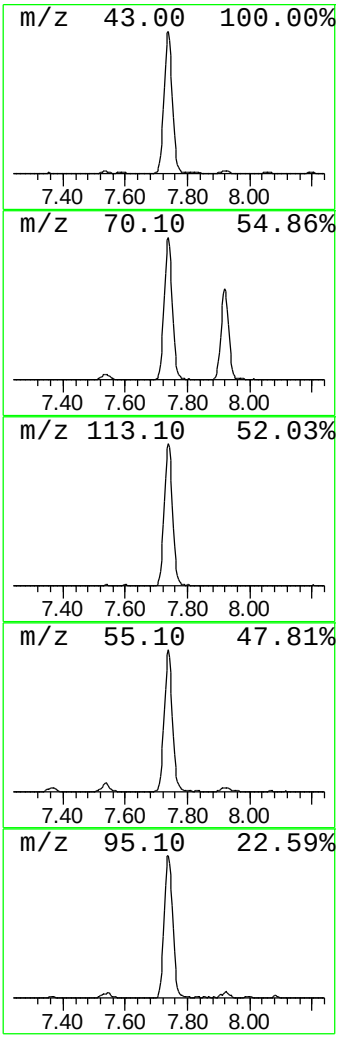
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	3.62 ug/L	567619	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	64
2	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	56
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	Ethosuximide	141	C7H11NO2	000077-67-8	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

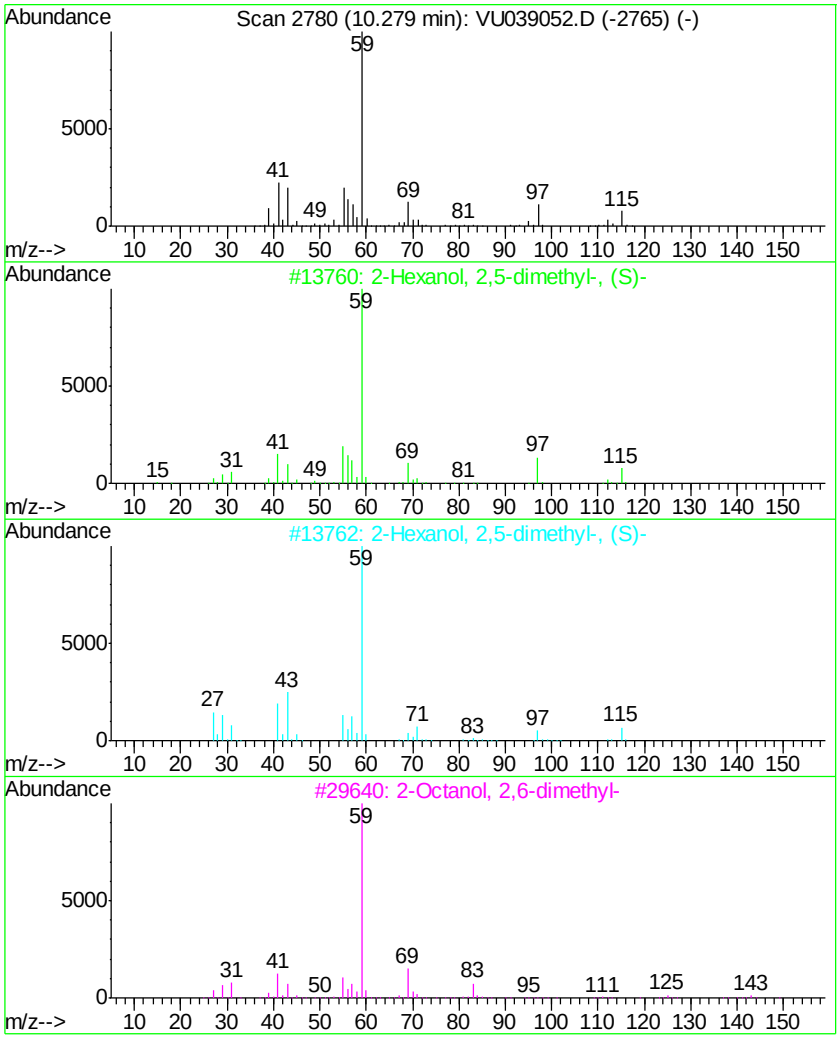
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

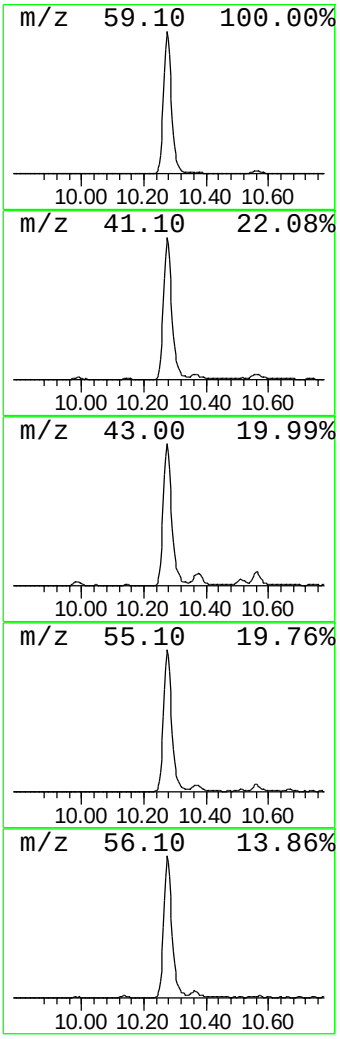
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	4.79 ug/L	920466	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	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	56
3	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45
5	2-Hydroxy-2,4-dimethyl-3-pentanone	130	C7H14O2	003212-67-7	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062320\
Data File : VU039052.D
Acq On : 23 Jun 2020 20:02
Operator : SY/MD
Sample : L3061-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFXJ2

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

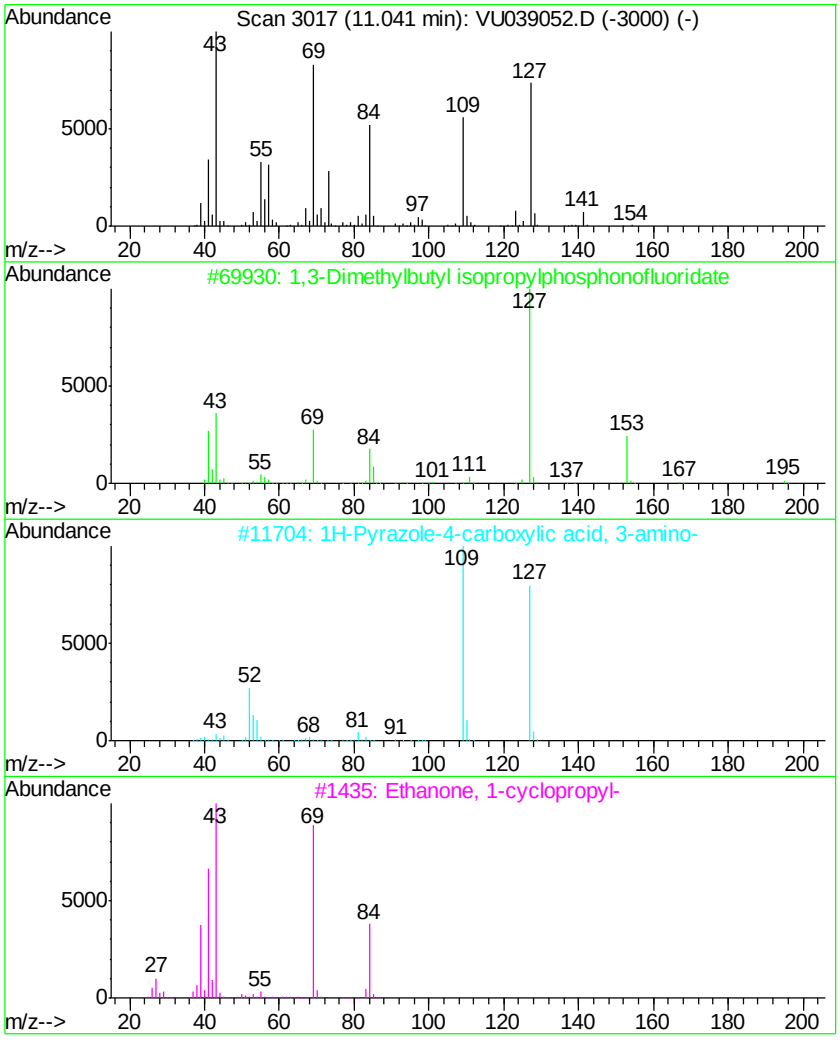
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

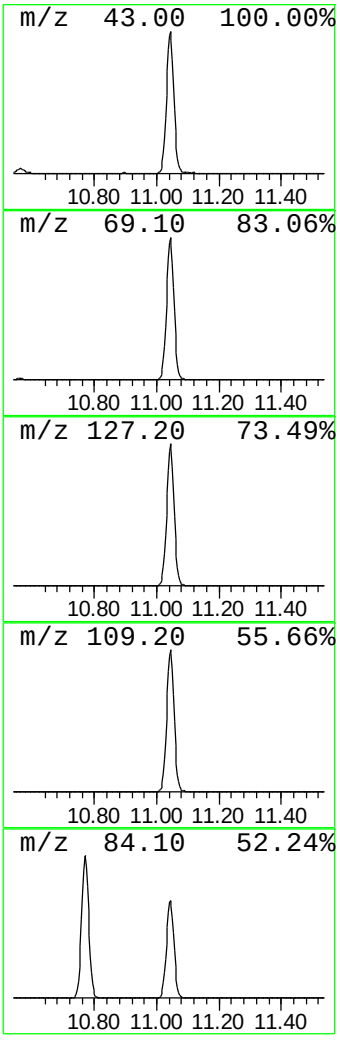
****

Peak Number 7 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	6.38 ug/L	1153790	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethylbutyl isopropylphosp...	210	C9H20FO2P	1000298-25-6	42
2	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
4	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
5	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062320\
Data File : VU039052.D
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Operator : SY/MD
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ClientSampleId : BFXJ2

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Propanol, 2-met...	3.26	17.0	ug/L	2667690	1	6.28	784677	5.0
Diisopropyl ether	4.03	5.9	ug/L	924075	1	6.28	784677	5.0
2(1H)-Pyrimidinon...	6.94	1.1	ug/L	165561	1	6.28	784677	5.0
Furan, tetrahydro...	7.74	3.6	ug/L	567619	1	6.28	784677	5.0
2-Hexanol, 2,5-di...	10.28	4.8	ug/L	920466	2	9.43	961459	5.0
unknown-01	11.04	6.4	ug/L	1153790	3	11.82	904523	5.0