LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

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\SOMUTR063020WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC: VU039258.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.369	3	9	18	rBV	88950	84079	3.19%	0.519%
2	1.610	74	84	99	rVB2	112352	162407	6.16%	1.002%
3	1.703	103	113	162	rBV	1017847	1634955	61.98%	10.086%
4	1.932	176	184	197	rVB	79244	96160	3.65%	0.593%
5	2.176	253	260	270	rVB3	23970	32913	1.25%	0.203%
6	2.591	372	389	399	rBV2	187363	454147	17.22%	2.802%
7	2.665	399	412	452	rVB	990792	2637991	100.00%	16.274%
8	3.250	573	594	596	rBV2	24367	53621	2.03%	0.331%
9	4.488	957	979	1016	rBV2	183003	497690	18.87%	3.070%
10	4.671	1020	1036	1047	rVV2	114596	303444	11.50%	1.872%
11	4.748	1047	1060	1102	rVB	460210	1263265	47.89%	7.793%
12	5.102	1153	1170	1187	rVB2	139751	308798	11.71%	1.905%
13	5.758	1353	1374	1395	rBV3	266274	693274	26.28%	4.277%
14	6.279	1515	1536	1554	rVB	268095	554111	21.01%	3.418%
15	6.562	1613	1624	1633	rBV9	12701	28965	1.10%	0.179%
16	6.719	1661	1673	1687	rBV	165478	326856	12.39%	2.016%
17	6.800	1687	1698	1719	rVV	164950	320940	12.17%	1.980%
18	6.906	1719	1731	1739	rVV	182403	340782	12.92%	2.102%
19	6.948	1739	1744	1768	rVB	97340	179006	6.79%	1.104%
20	7.591	1931	1944	1961	rVB2	86346	149688	5.67%	0.923%
21	7.922	2032	2047	2063	rBV	308827	538319	20.41%	3.321%
22	8.054	2078	2088	2100	rBV2	27669	51622	1.96%	0.318%
23	8.198	2121	2133	2143	rBV3	64481	116713	4.42%	0.720%
24	8.253	2143	2150	2166	rVB4	16468	31590	1.20%	0.195%
25	8.568	2238	2248	2262	rVB2	77610	123673	4.69%	0.763%
26	8.655	2263	2275	2283	rVV	403737	714327	27.08%	4.407%
27	8.706	2283	2291	2310	rVV	409885	724969	27.48%	4.472%
28	8.806	2310	2322	2347	rVB	244581	424240	16.08%	2.617%
29	9.433	2504	2517	2539	rBV	479797	825481	31.29%	5.092%
30	10.144	2728	2738	2759	rVB	258489	417126	15.81%	2.573%
31	10.250	2760	2771	2783	rBV	227940	371713	14.09%	2.293%
32	10.356	2796	2804	2818	rVB2	43736	71453	2.71%	0.441%
33	10.771	2920	2933	2944	rBV	148534	238033	9.02%	1.468%
34	11.304	3085	3099	3109	rBV5	13942	26805	1.02%	0.165%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

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\SOMUTR063020WMA.M
Title : TRACE VOA SOM01.0

35	11.481	3143	3154	3167	rBV	35928	56664	2.15%	0.350%
36	11.584	3176	3186	3206	rVB	107217	173036	6.56%	1.067%
37	11.822	3248	3260	3276	rVB	401550	642038	24.34%	3.961%
38	12.108	3342	3349	3365	rVB9	16515	36462	1.38%	0.225%
39	12.205	3365	3379	3393	rBV	313163	502662	19.05%	3.101%

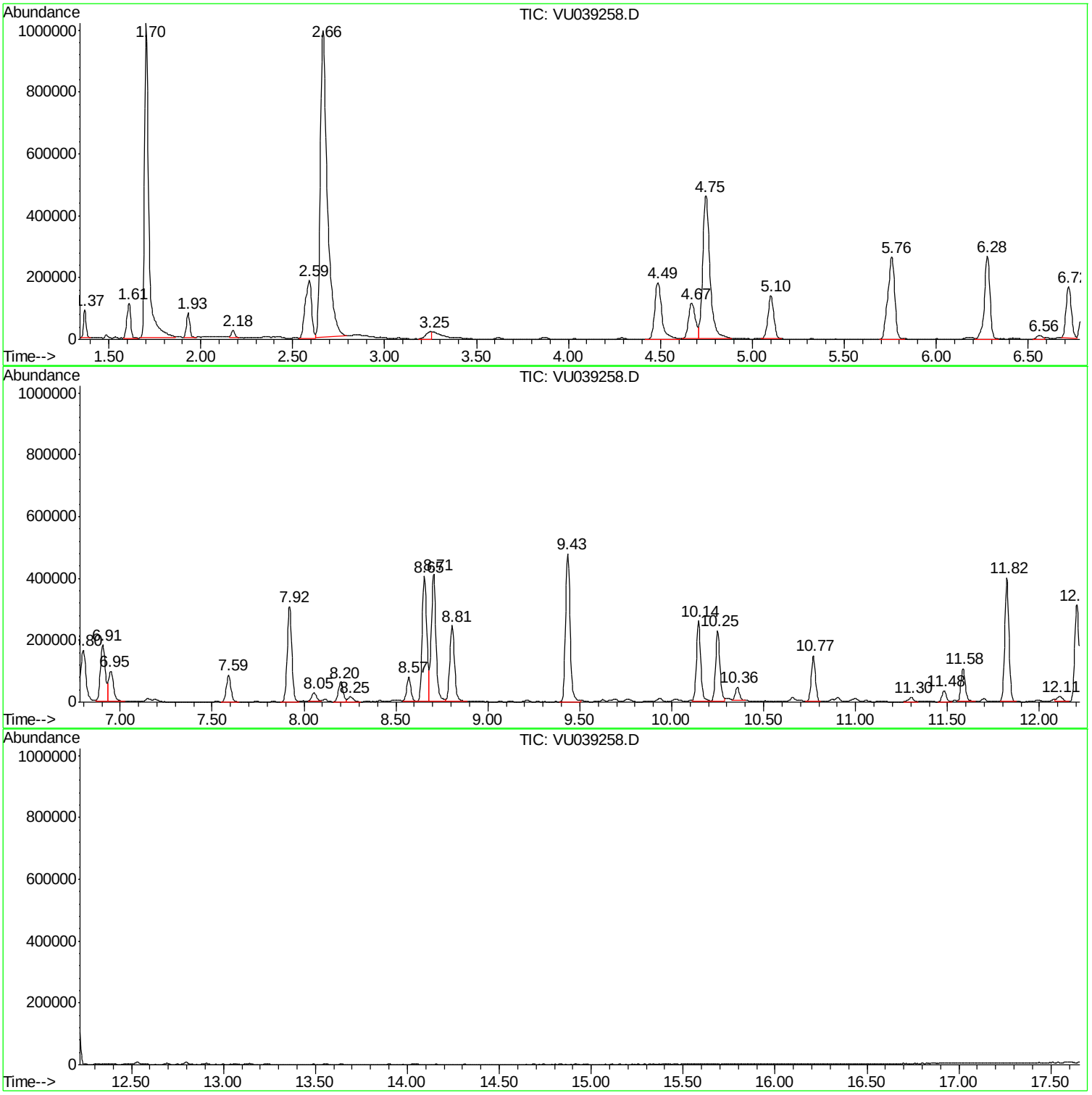
Sum of corrected areas: 16210018

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.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\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

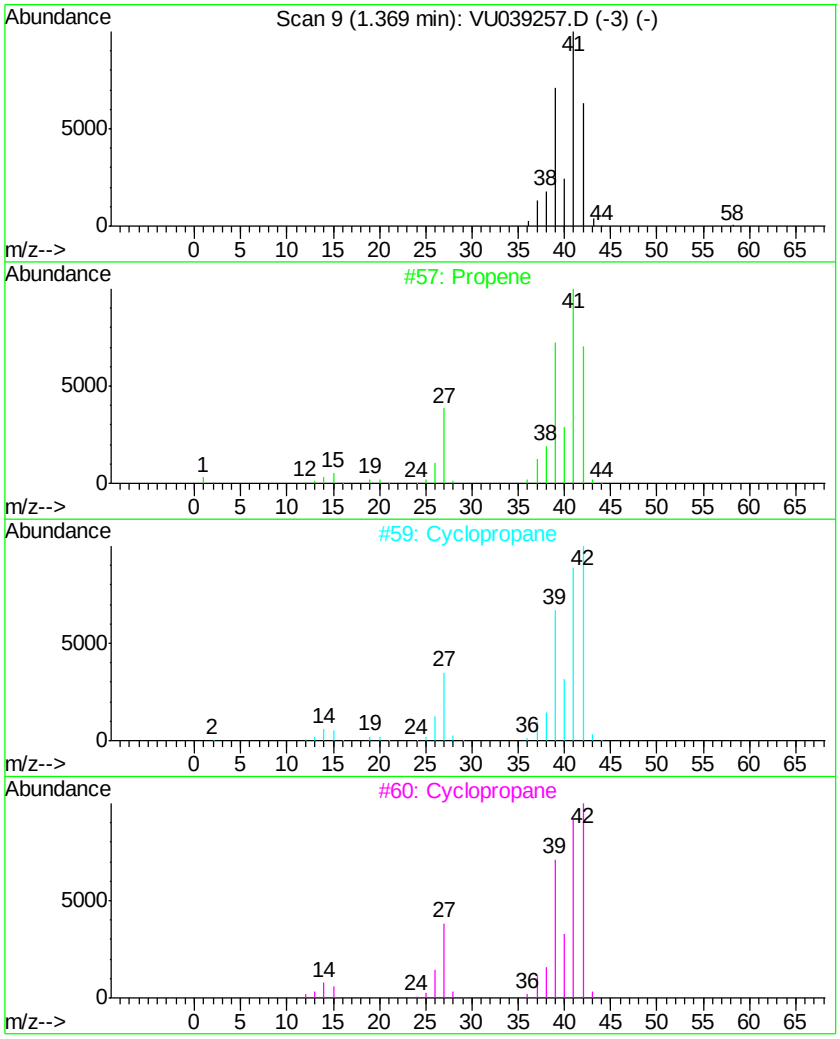
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

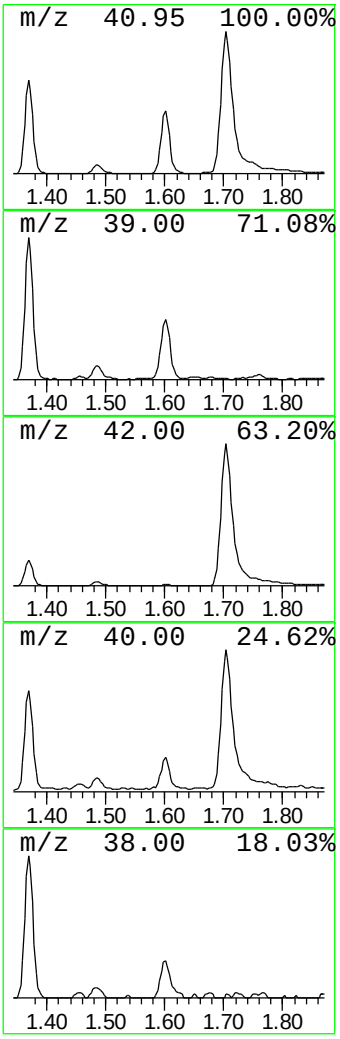
****

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	0.76 ug/L	84079	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Cyclopropane	42	C3H6	000075-19-4	78
3	Cyclopropane	42	C3H6	000075-19-4	78
4	Propene	42	C3H6	000115-07-1	52
5	Cyclopropane	42	C3H6	000075-19-4	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

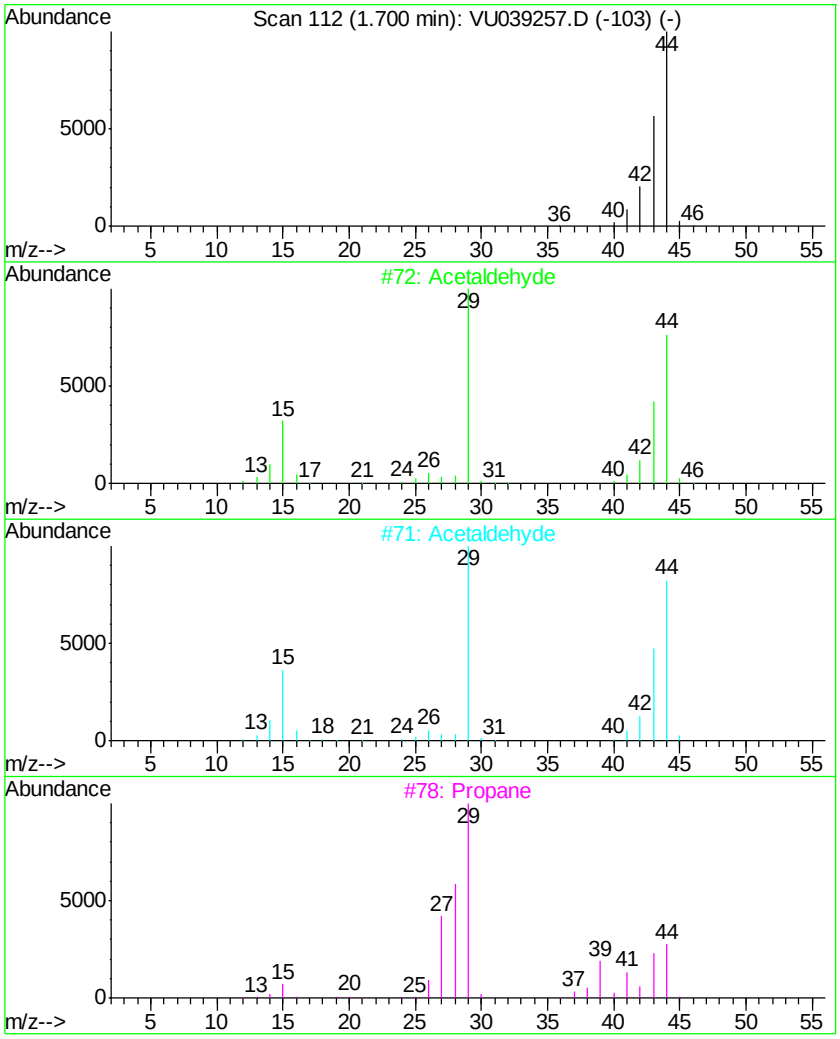
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

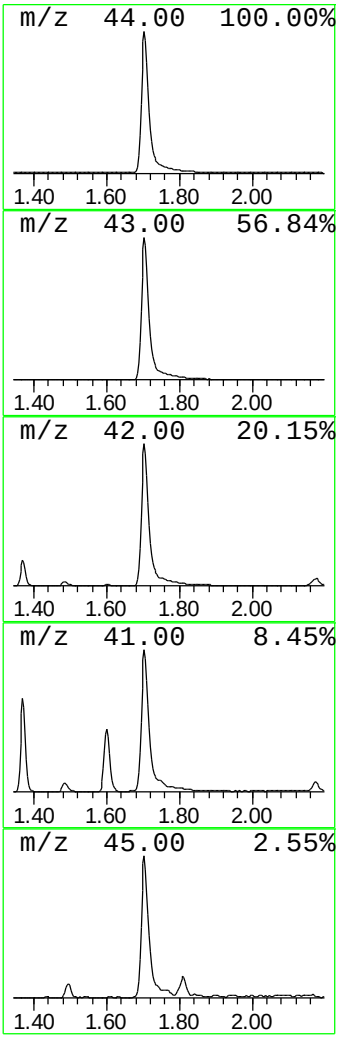
****

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.70	14.75 ug/L	1634960	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	9
2	Acetaldehyde	44	C2H4O	000075-07-0	9
3	Propane	44	C3H8	000074-98-6	5
4	Ethylene oxide	44	C2H4O	000075-21-8	5
5	Ethylene oxide	44	C2H4O	000075-21-8	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

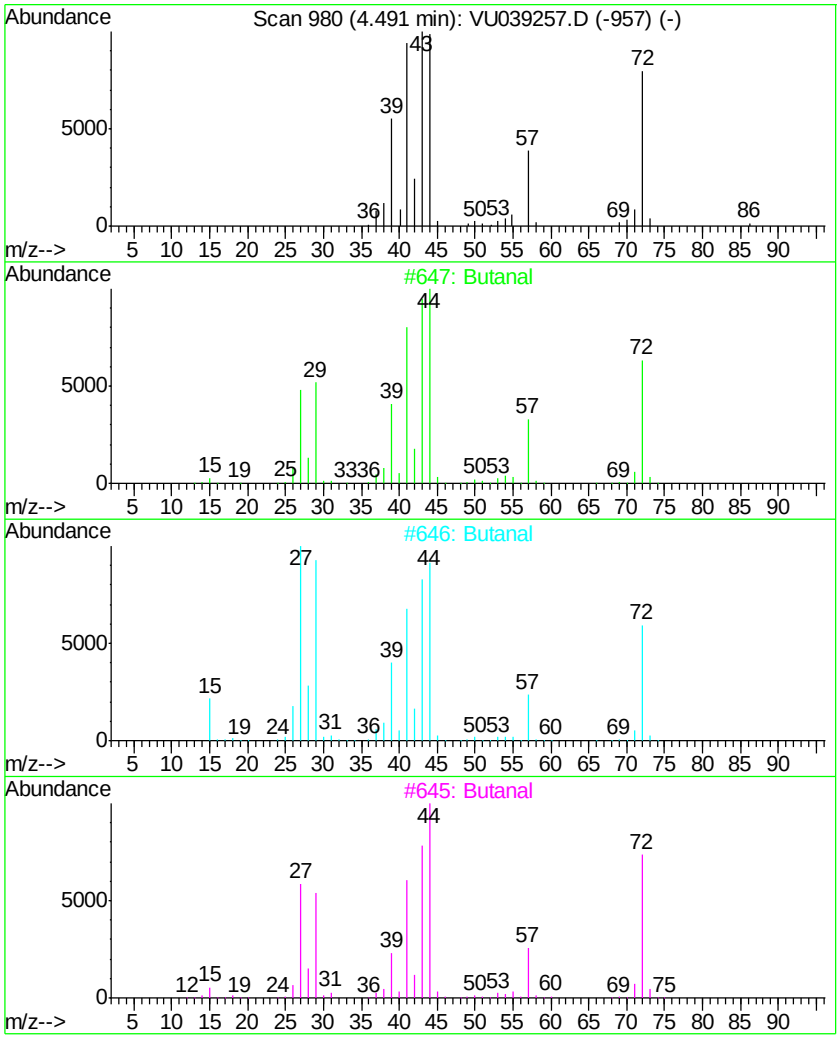
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

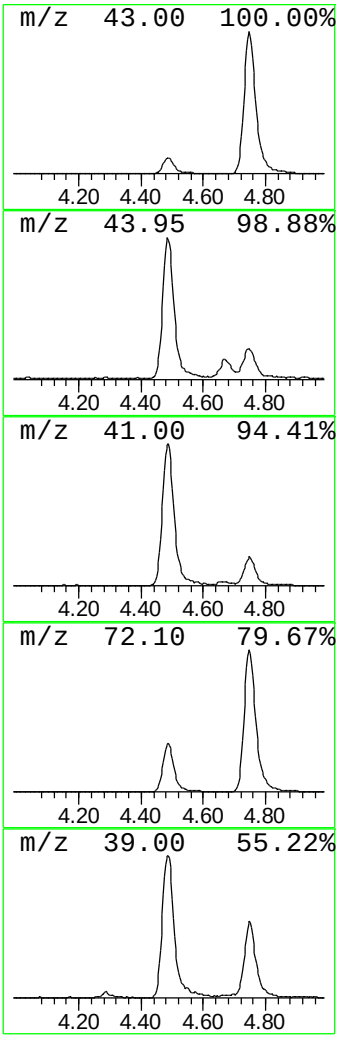
****

Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	4.49 ug/L	497690	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Butanal	72	C4H8O	000123-72-8	91
3	Butanal	72	C4H8O	000123-72-8	59
4	Butanal	72	C4H8O	000123-72-8	59
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

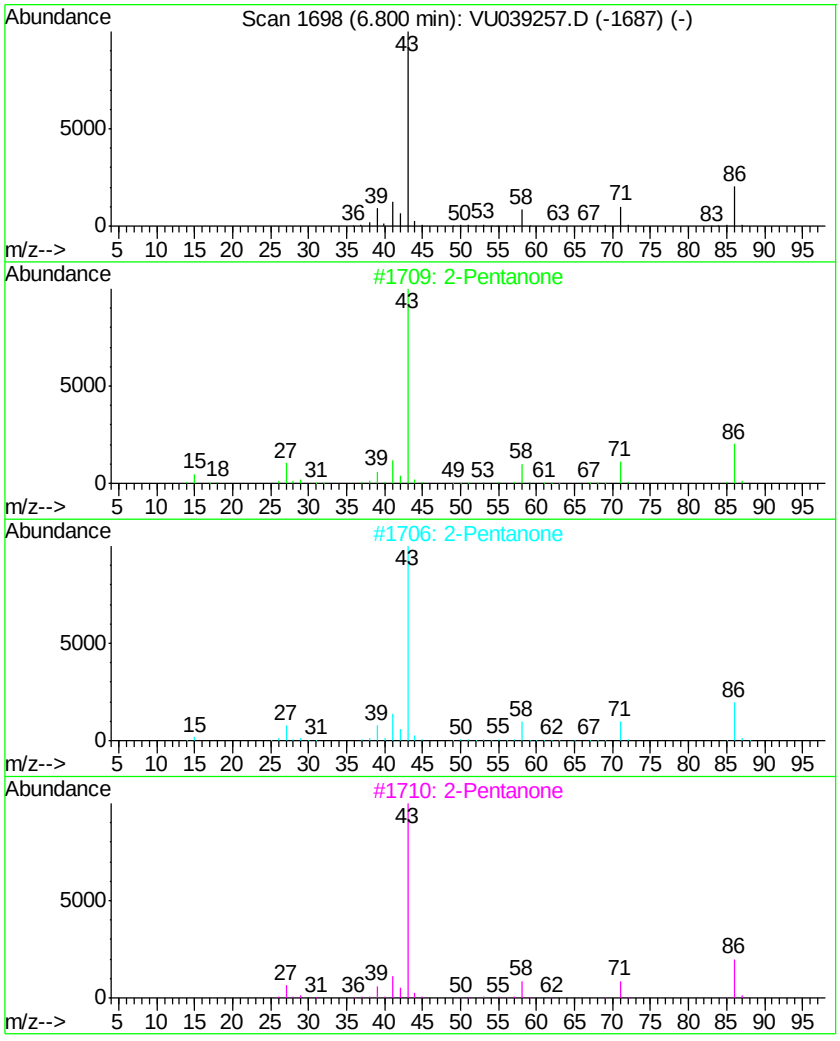
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

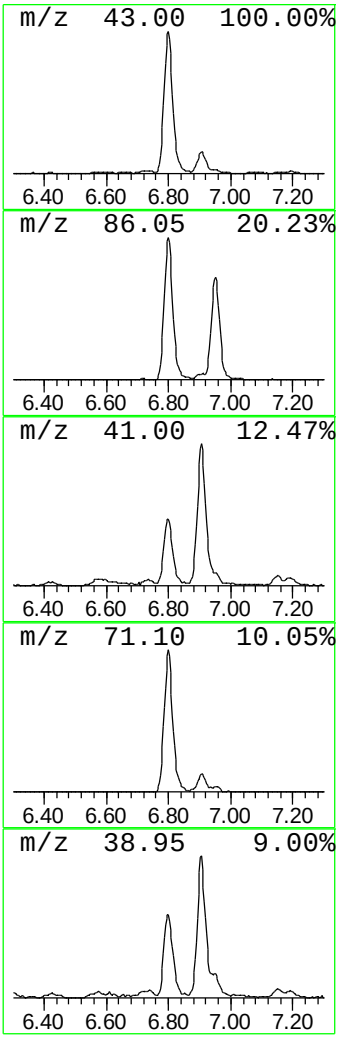
****

Peak Number 4 2-Pentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.80	2.90 ug/L	320940	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	90
2	2-Pentanone	86	C5H10O	000107-87-9	87
3	2-Pentanone	86	C5H10O	000107-87-9	86
4	2,3-Butanedione	86	C4H6O2	000431-03-8	50
5	2,3-Butanedione	86	C4H6O2	000431-03-8	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

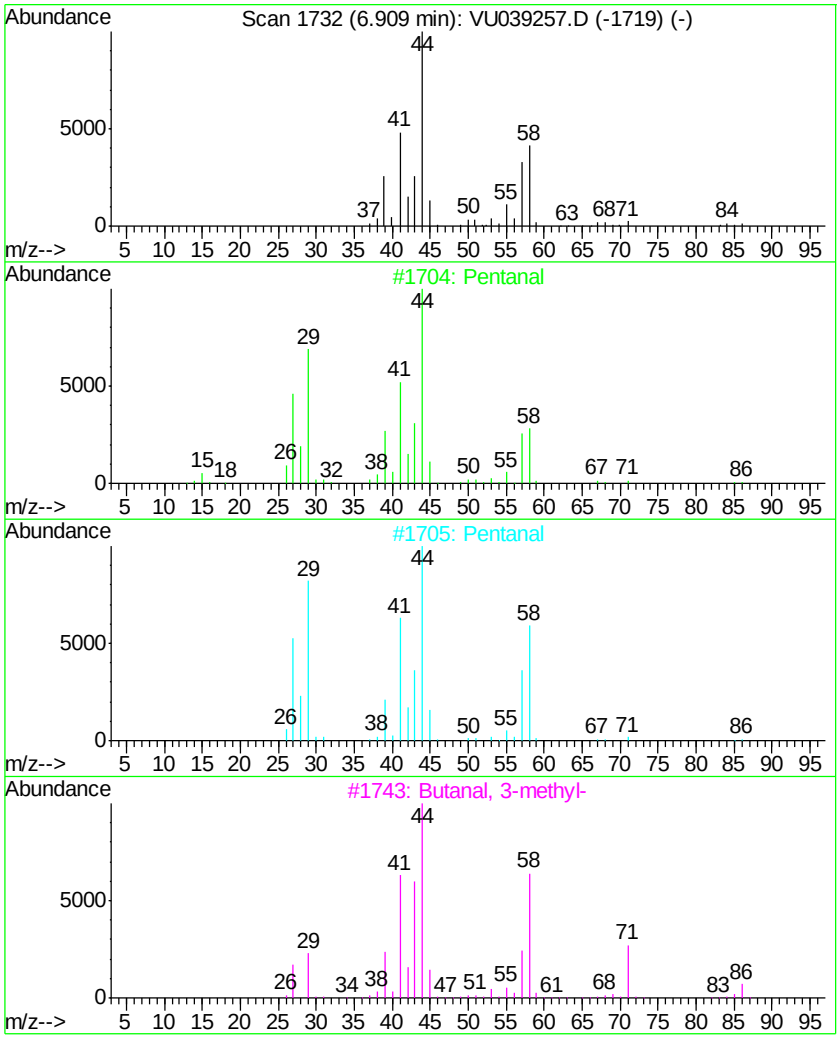
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

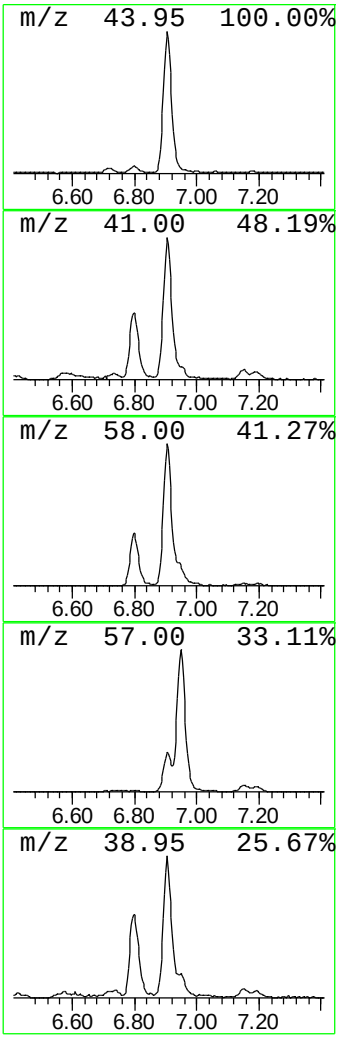
****

Peak Number 5 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.91	3.08 ug/L	340782	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	86
2	Pentanal	86	C5H10O	000110-62-3	86
3	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
4	Pentanal	86	C5H10O	000110-62-3	56
5	Butanal, 3-methyl-	86	C5H10O	000590-86-3	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

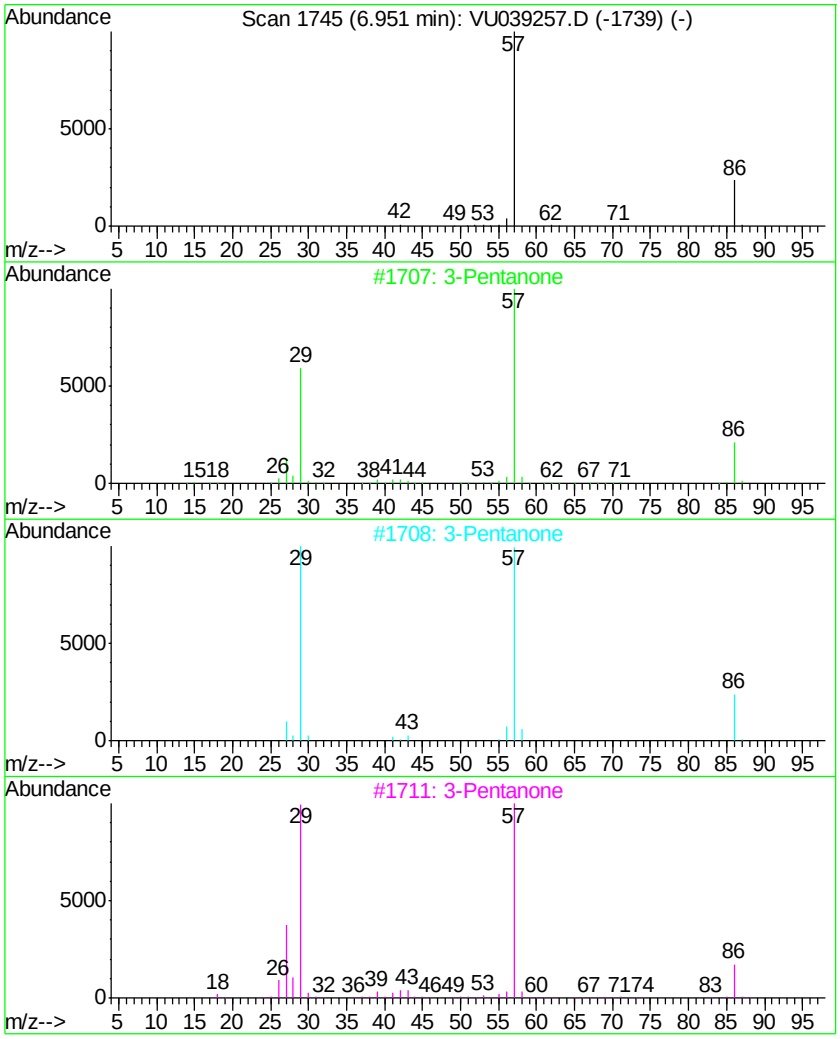
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

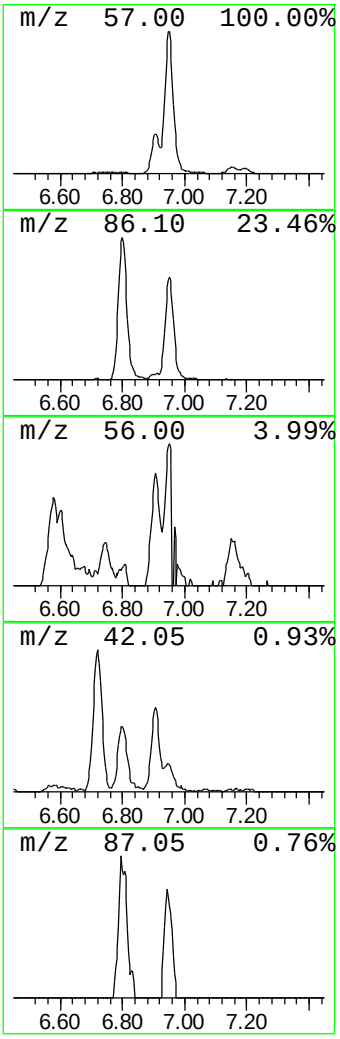
****

Peak Number 6 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	1.62 ug/L	179006	1,4-Difluorobenzene	6.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	50
2	3-Pentanone	86	C5H10O	000096-22-0	7
3	3-Pentanone	86	C5H10O	000096-22-0	7
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	5
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	5





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

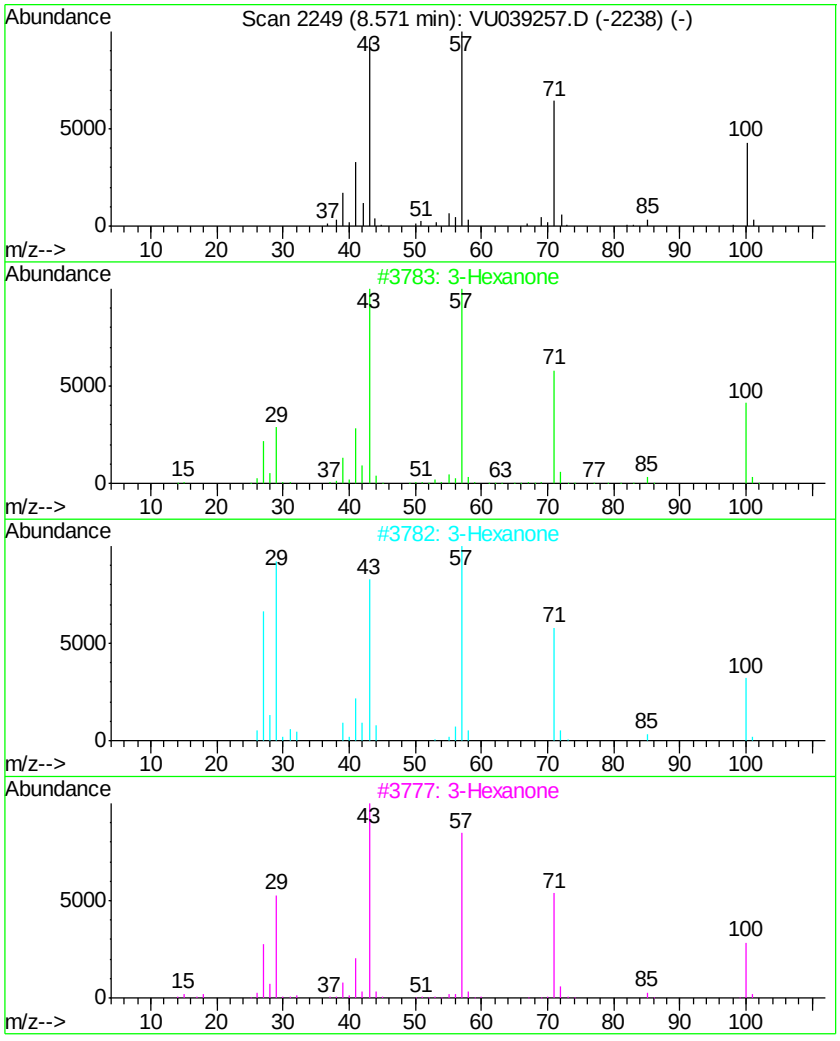
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

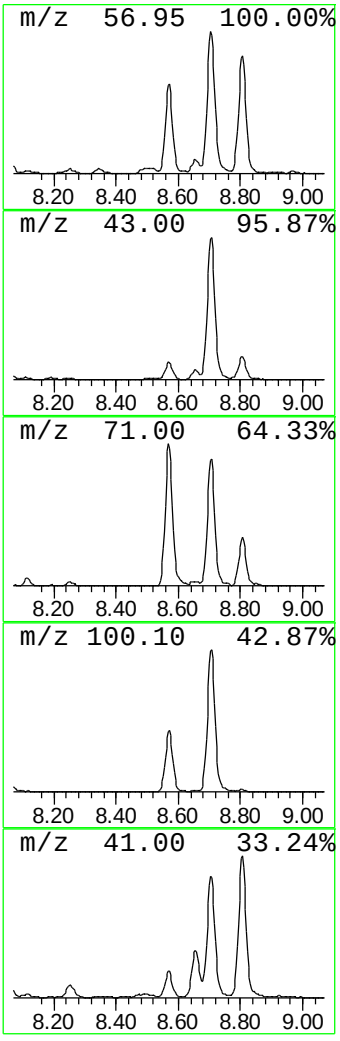
****

Peak Number 8 3-Hexanone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	0.75 ug/L	123673	Chlorobenzene-d5	9.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone	100	C6H12O	000589-38-8	94
2	3-Hexanone	100	C6H12O	000589-38-8	90
3	3-Hexanone	100	C6H12O	000589-38-8	72
4	3-Hexanone	100	C6H12O	000589-38-8	72
5	3-Hexanone	100	C6H12O	000589-38-8	59





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

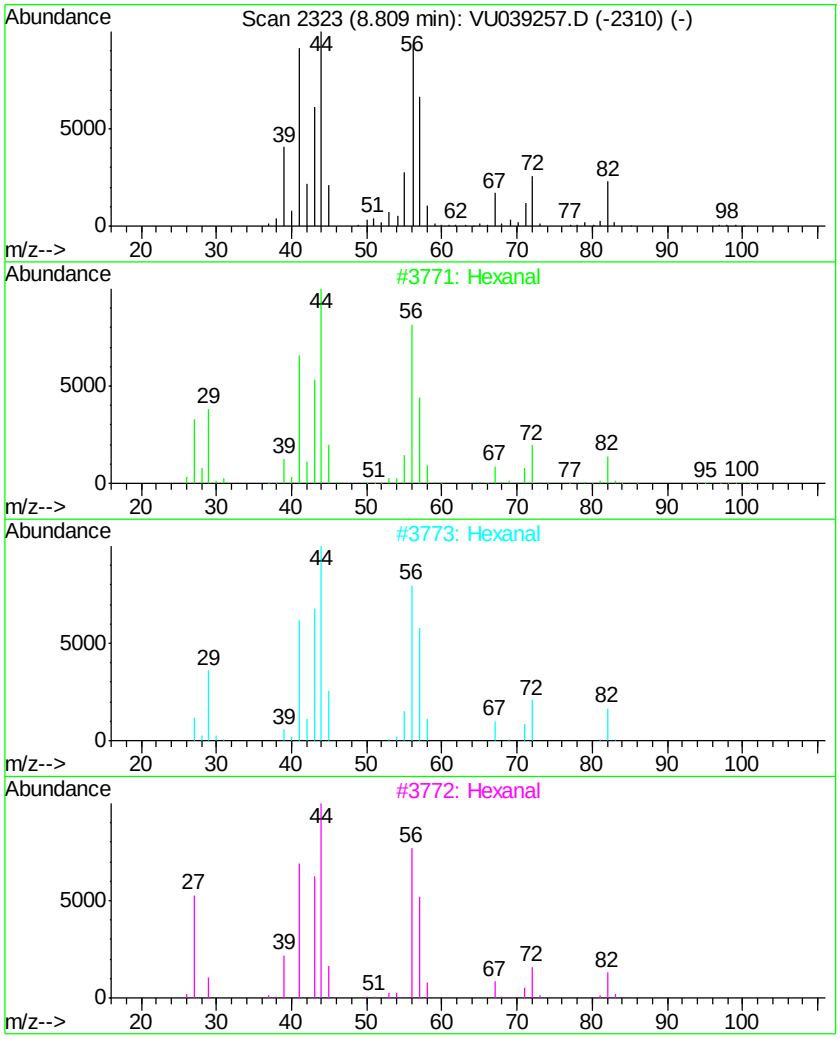
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

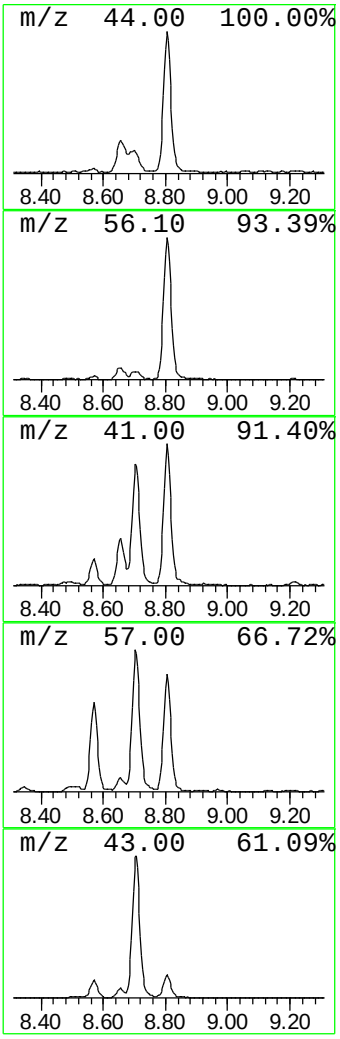
****

Peak Number 9 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.81	2.57 ug/L	424240	Chlorobenzene-d5	9.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	74
2	Hexanal	100	C6H12O	000066-25-1	59
3	Hexanal	100	C6H12O	000066-25-1	53
4	Hexanal	100	C6H12O	000066-25-1	45
5	Butanal, 3-methyl-	86	C5H10O	000590-86-3	32





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

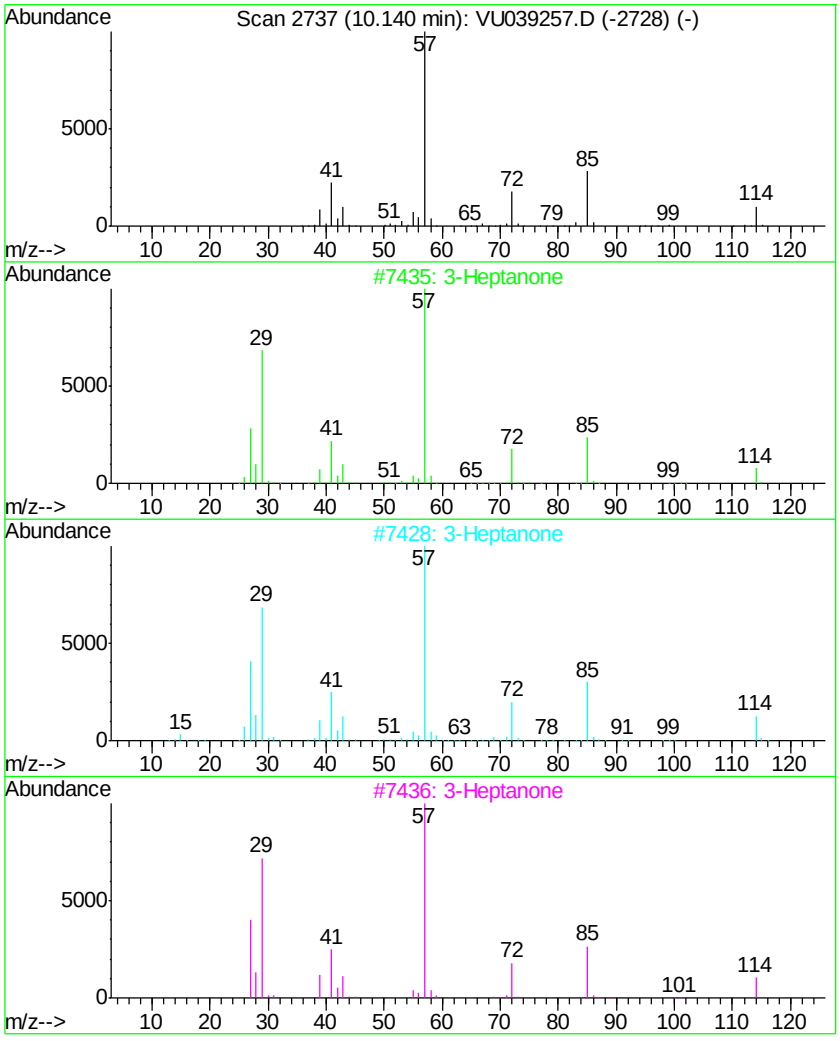
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

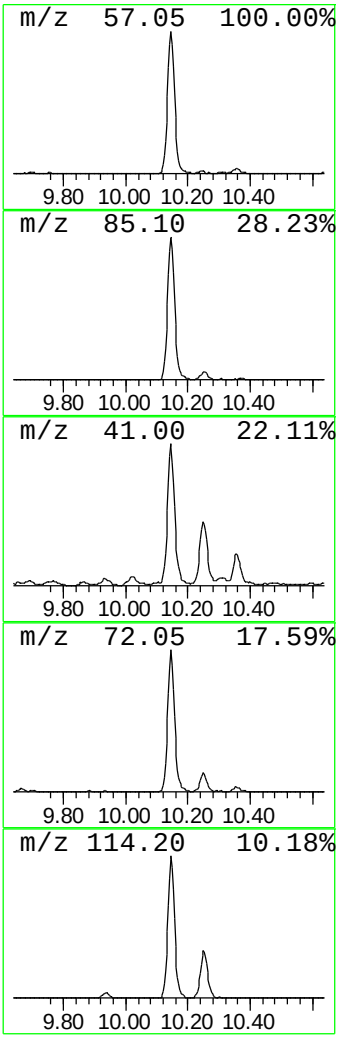
****

Peak Number 10 3-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	2.53 ug/L	417126	Chlorobenzene-d5	9.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone	114	C7H14O	000106-35-4	91
2	3-Heptanone	114	C7H14O	000106-35-4	91
3	3-Heptanone	114	C7H14O	000106-35-4	86
4	3-Heptanone	114	C7H14O	000106-35-4	80
5	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	80





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

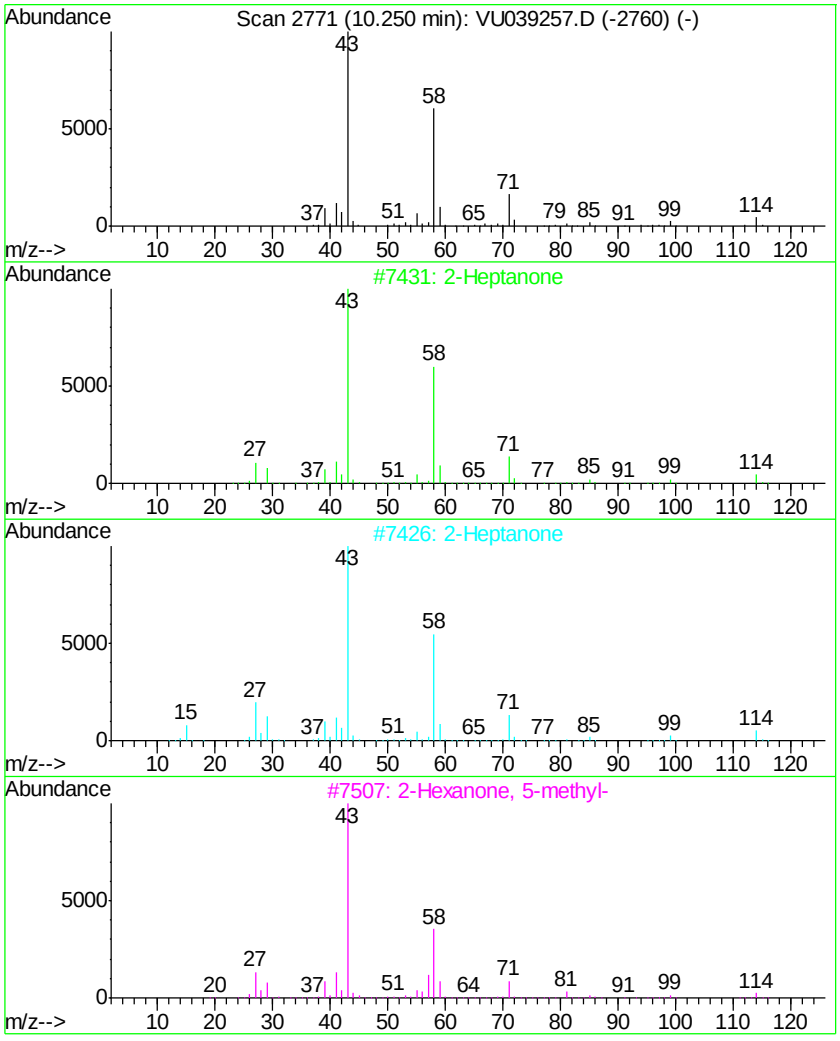
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

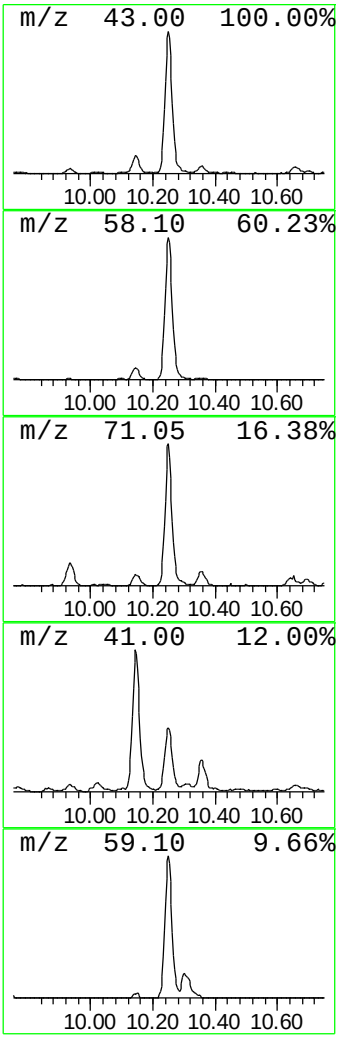
****

Peak Number 11 2-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.25	2.25 ug/L	371713	Chlorobenzene-d5	9.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Heptanone	114	C7H14O	000110-43-0	91
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90
4	2-Heptanone	114	C7H14O	000110-43-0	90
5	2-Heptanone	114	C7H14O	000110-43-0	78





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.M
Quant Title : TRACE VOA SOM01.0

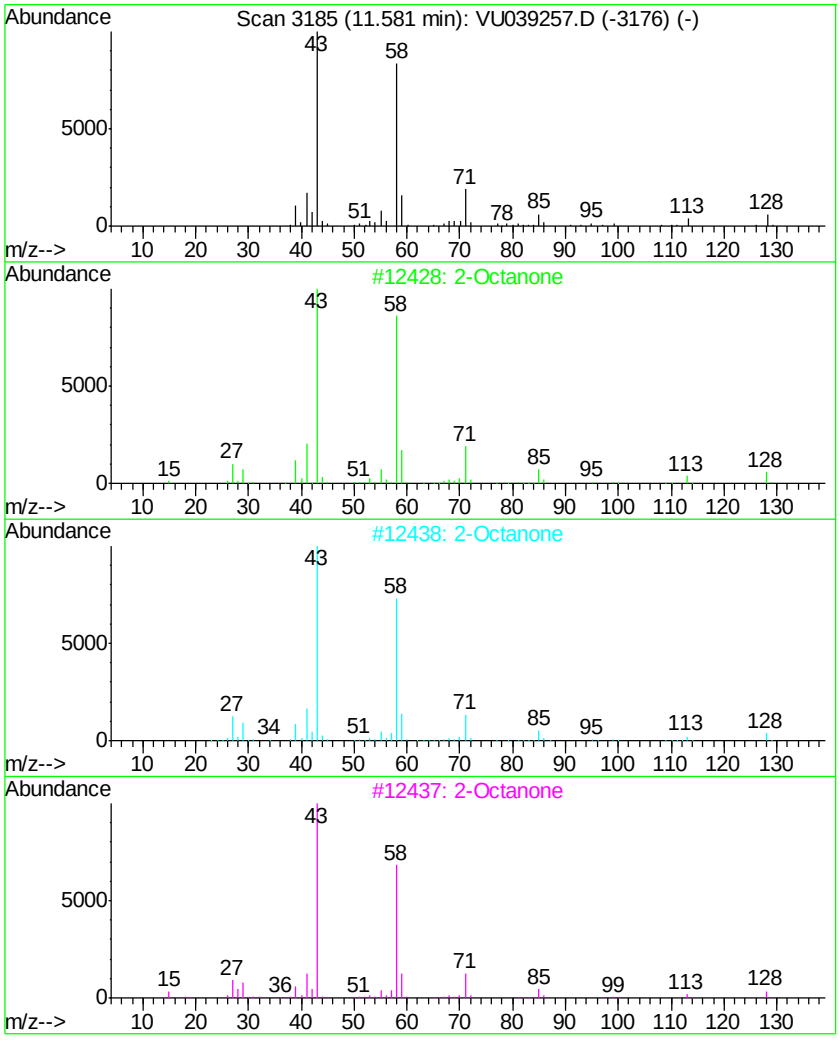
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

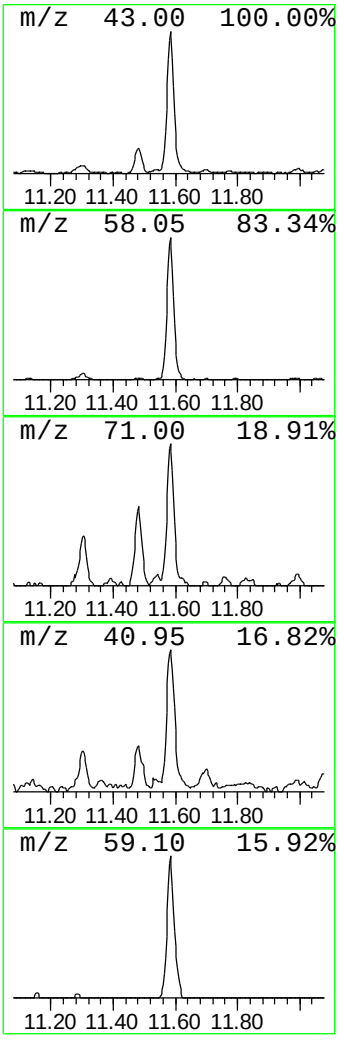
****

Peak Number 12 2-Octanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	1.35 ug/L	173036	1,4-Dichlorobenzene-d4	11.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	94
2	2-Octanone	128	C8H16O	000111-13-7	91
3	2-Octanone	128	C8H16O	000111-13-7	91
4	2-Octanone	128	C8H16O	000111-13-7	91
5	2-Octanone	128	C8H16O	000111-13-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU063020\
Data File : VU039257.D
Acq On : 01 Jul 2020 04:16
Operator : SY/MD
Sample : L3132-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0Y33

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR063020WMA.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
(DEL) Alkane: Str...	1.37	0.8	ug/L	84079	1	6.28	554111	5.0
unknown-01	1.70	14.8	ug/L	1634960	1	6.28	554111	5.0
Butanal	4.49	4.5	ug/L	497690	1	6.28	554111	5.0
2-Pentanone	6.80	2.9	ug/L	320940	1	6.28	554111	5.0
Pentanal	6.91	3.1	ug/L	340782	1	6.28	554111	5.0
3-Pentanone	6.95	1.6	ug/L	179006	1	6.28	554111	5.0
3-Hexanone	8.57	0.8	ug/L	123673	2	9.43	825481	5.0
Hexanal	8.81	2.6	ug/L	424240	2	9.43	825481	5.0
3-Heptanone	10.14	2.5	ug/L	417126	2	9.43	825481	5.0
2-Heptanone	10.25	2.3	ug/L	371713	2	9.43	825481	5.0
2-Octanone	11.58	1.4	ug/L	173036	3	11.82	642038	5.0