LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_N\METHODS\82N022720W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.780	606	624	651	rBV	254449	666259	16.89%	3.692%
2	4.014	679	697	718	rBV2	23791	70425	1.79%	0.390%
3	4.288	765	782	808	rBV	60111	172160	4.36%	0.954%
4	4.523	832	855	882	rBV	169958	516329	13.09%	2.861%
5	6.510	1451	1473	1499	rBV2	64059	196569	4.98%	1.089%
6	6.799	1539	1563	1588	rBV	56248	176863	4.48%	0.980%
7	7.567	1783	1802	1813	rBV	135017	334805	8.49%	1.855%
8	7.645	1813	1826	1853	rVB	257456	609248	15.45%	3.376%
9	8.005	1916	1938	1964	rBV	164982	418698	10.62%	2.320%
10	8.567	2097	2113	2130	rBV	396919	821899	20.84%	4.554%
11	8.763	2162	2174	2185	rBV	61695	131357	3.33%	0.728%
12	9.021	2243	2254	2270	rVB	40376	78648	1.99%	0.436%
13	9.969	2537	2549	2562	rBV	75354	136699	3.47%	0.757%
14	10.079	2569	2583	2592	rBV	626580	1153051	29.23%	6.389%
15	10.143	2592	2603	2629	rVB	2166290	3944396	100.00%	21.856%
16	10.268	2631	2642	2657	rVB	65193	113049	2.87%	0.626%
17	10.516	2710	2719	2735	rVB3	19585	39547	1.00%	0.219%
18	10.844	2809	2821	2836	rBV	283089	465725	11.81%	2.581%
19	11.400	2981	2994	3010	rBV	614156	1090942	27.66%	6.045%
20	11.503	3016	3026	3042	rVB	105676	183304	4.65%	1.016%
21	11.612	3045	3060	3081	rBV	490048	967599	24.53%	5.362%
22	11.940	3152	3162	3172	rBV	292448	521301	13.22%	2.889%
23	11.988	3173	3177	3185	rVB	61821	81693	2.07%	0.453%
24	12.397	3293	3304	3317	rBV	497214	823913	20.89%	4.565%
25	12.824	3426	3437	3450	rVB	906667	1448755	36.73%	8.028%
26	12.908	3455	3463	3477	rVB	126703	191250	4.85%	1.060%
27	13.069	3505	3513	3516	rBV2	111223	149227	3.78%	0.827%
28	13.101	3517	3523	3533	rVB	257313	383449	9.72%	2.125%
29	13.201	3549	3554	3567	rVB3	29210	43786	1.11%	0.243%
30	13.339	3586	3597	3610	rBV	598391	996706	25.27%	5.523%
31	13.445	3621	3630	3645	rVB	608708	933719	23.67%	5.174%
32	14.477	3946	3951	3963	rVB4	32496	52295	1.33%	0.290%
33	14.811	4048	4055	4073	rVB5	52131	133317	3.38%	0.739%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_N\METHODS\82N022720W.M
Title : SW846 8260

Sum of corrected areas: 18046983

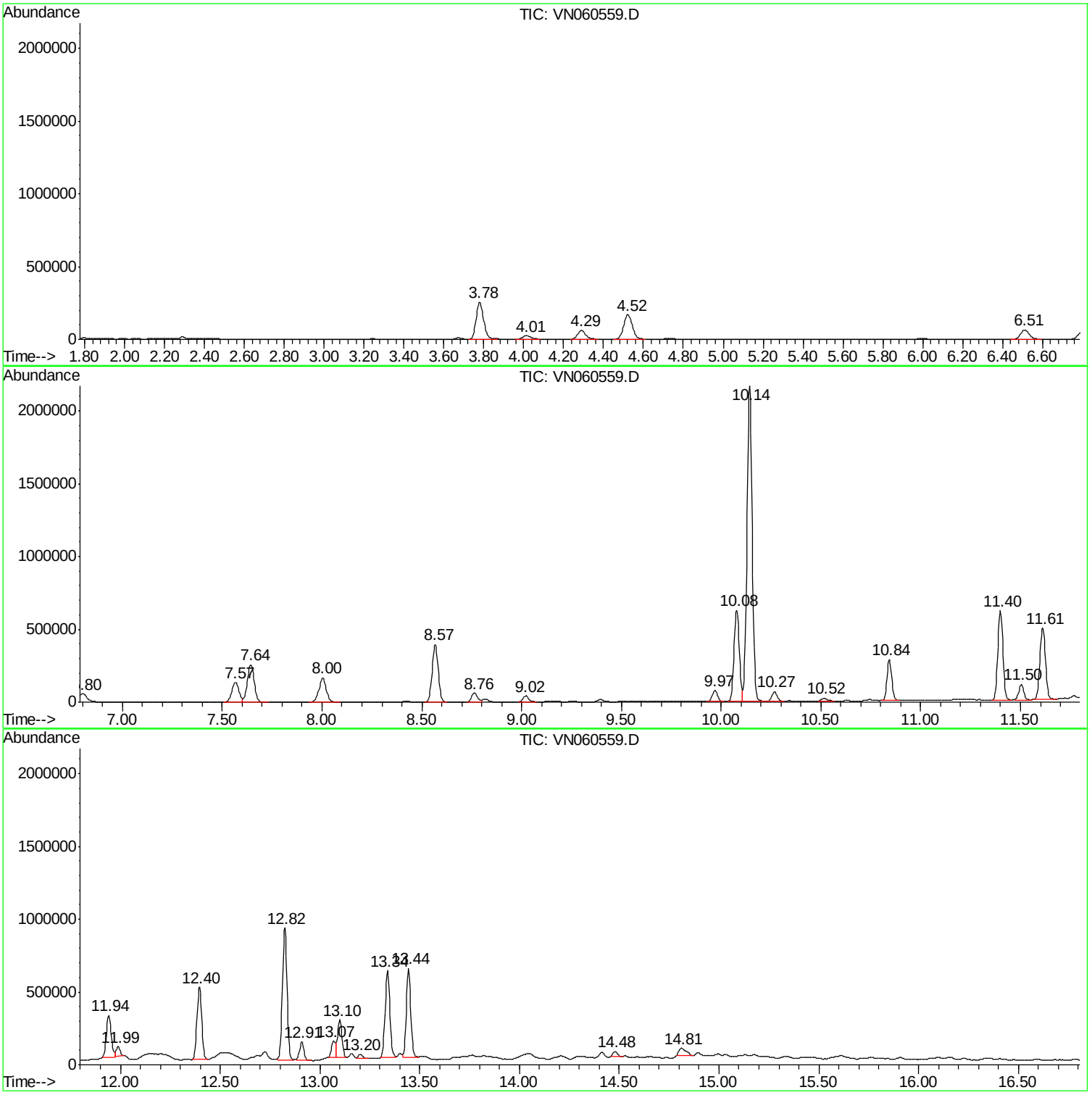
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

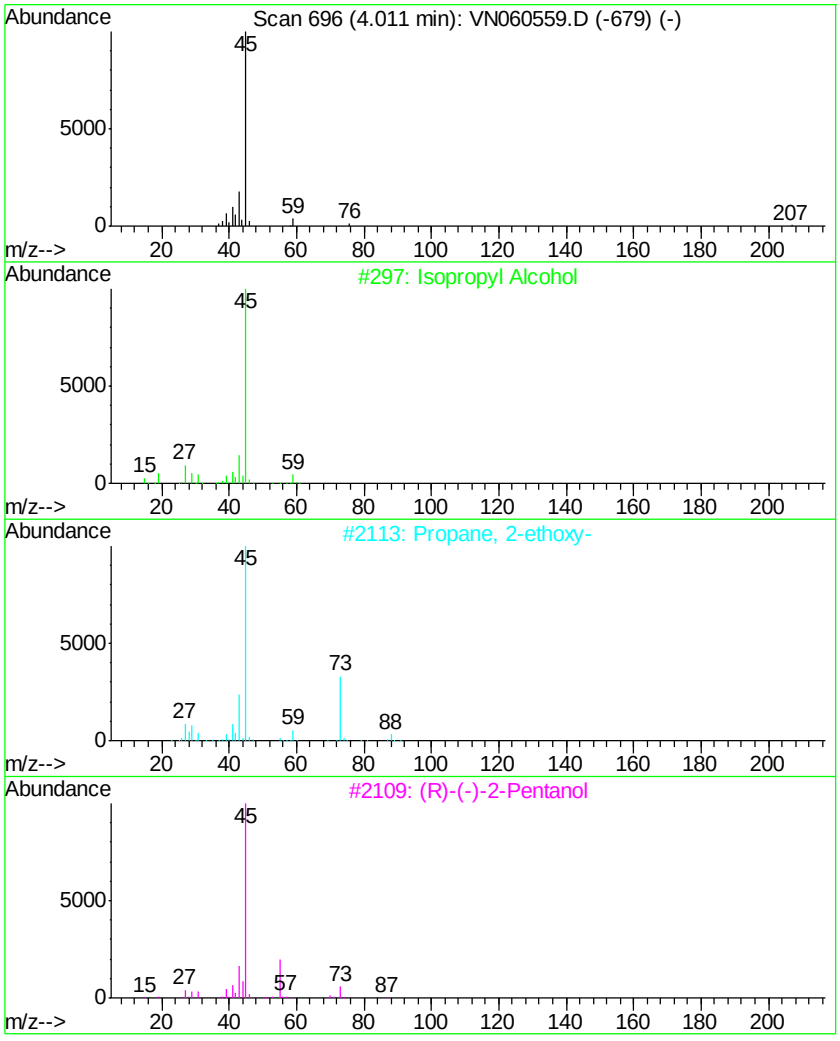
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

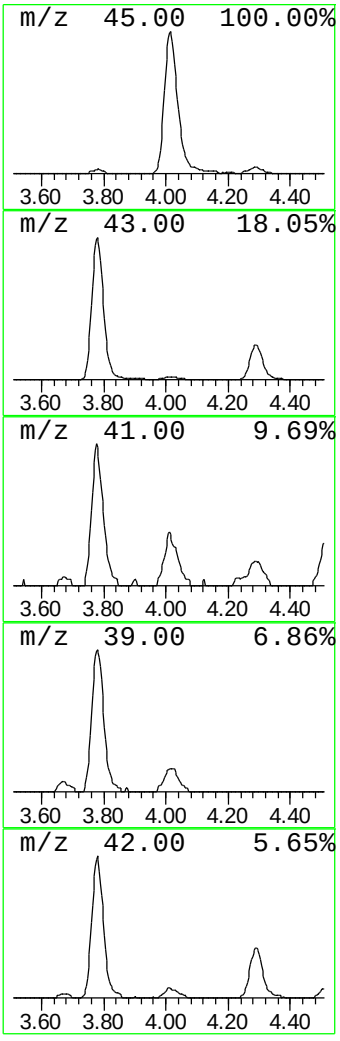
****

Peak Number 1 Isopropyl Alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	5.78 ug/l	70425	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
3	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
4	2-Pentanol	88	C5H12O	006032-29-7	9
5	4-Penten-2-ol	86	C5H10O	000625-31-0	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

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

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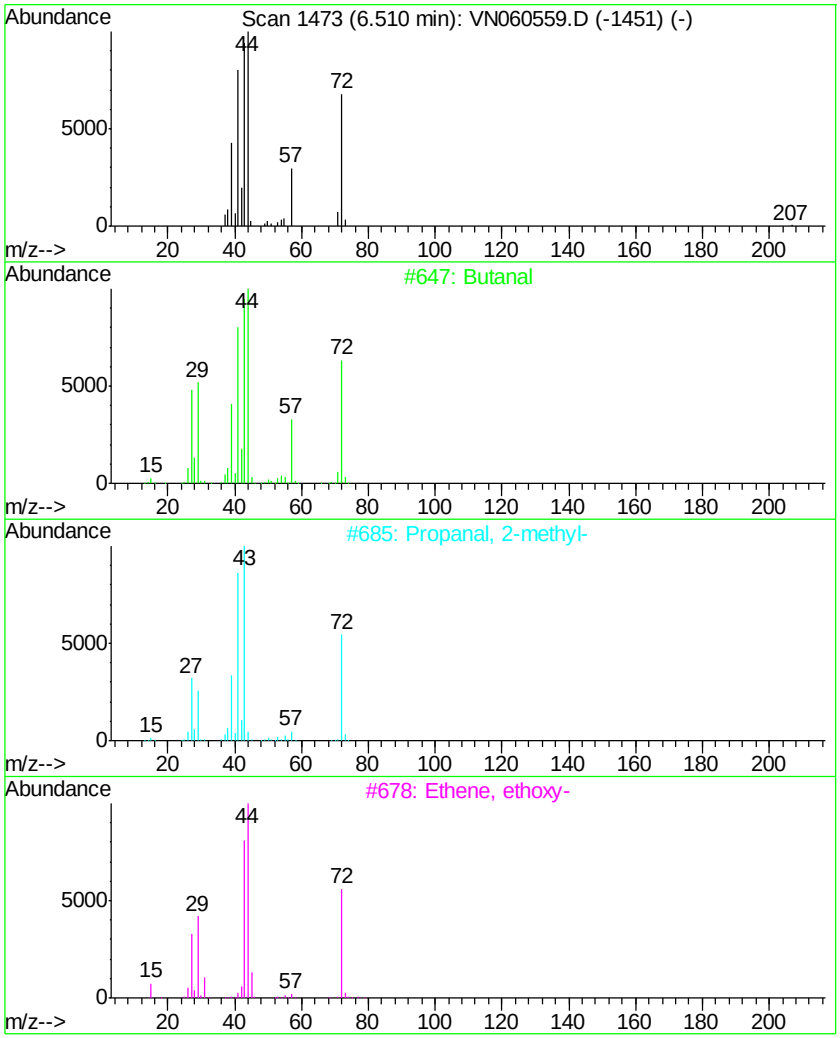
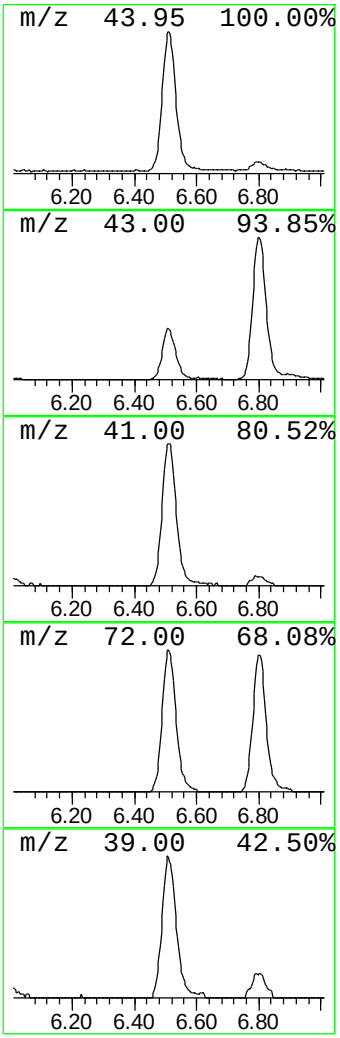
Peak Number 2 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	16.13 ug/l	196569	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
4	Adenine-9-propanoic acid, .alpha...	322	C13H18N6O4	055387-36-5	38
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

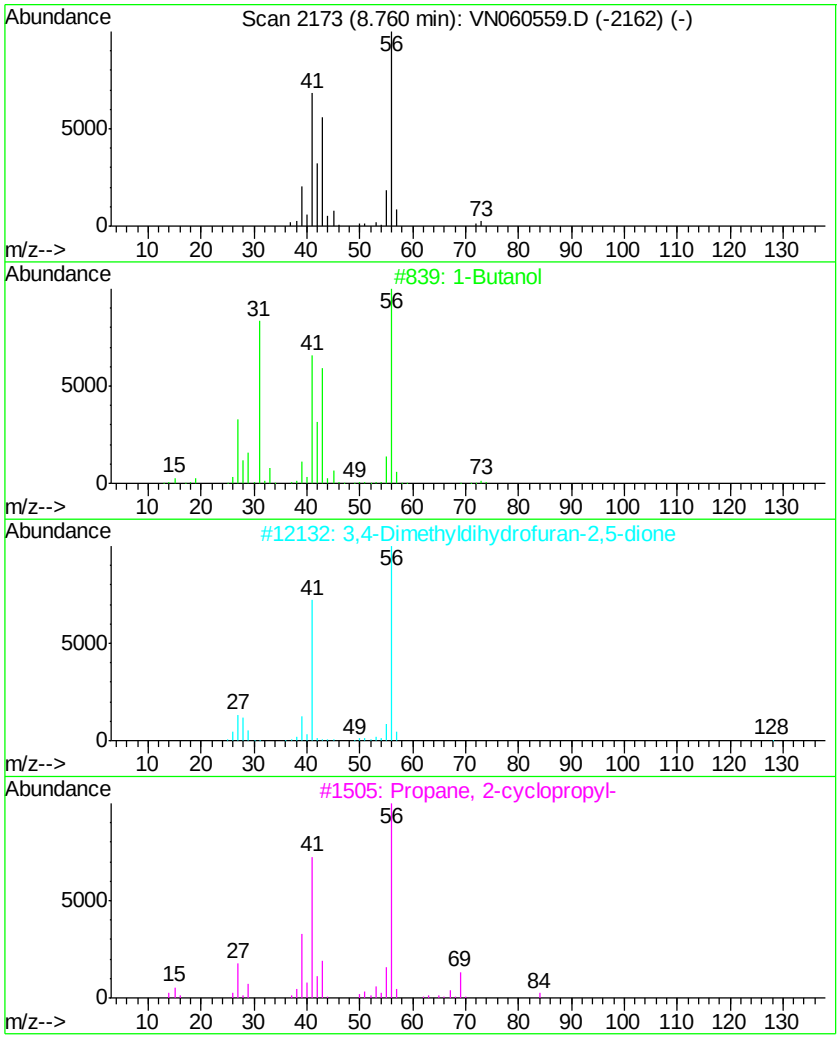
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

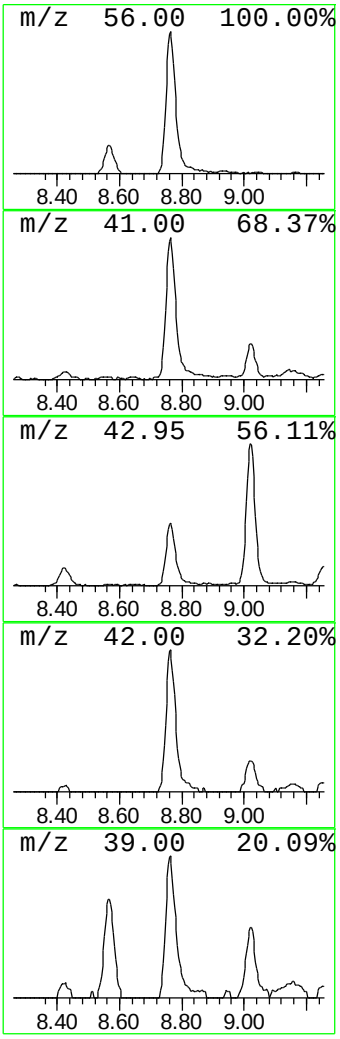
****

Peak Number 3 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	7.99 ug/l	131357	1,4-Difluorobenzene	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
4	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

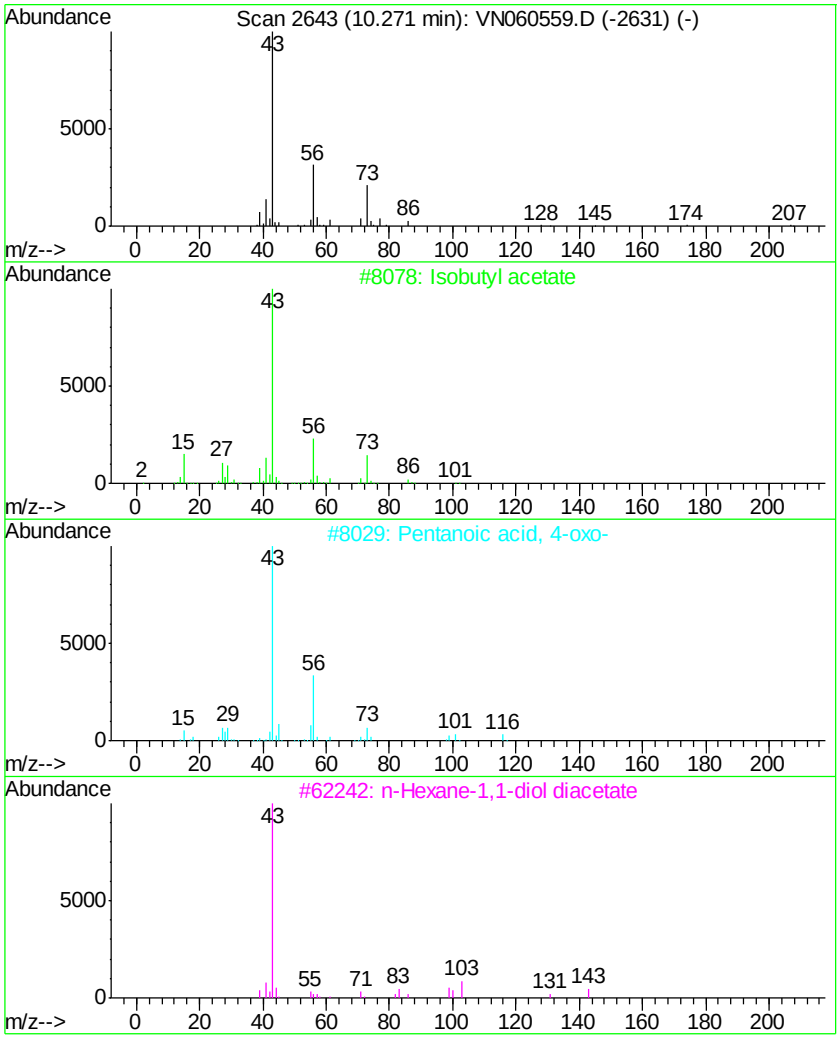
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

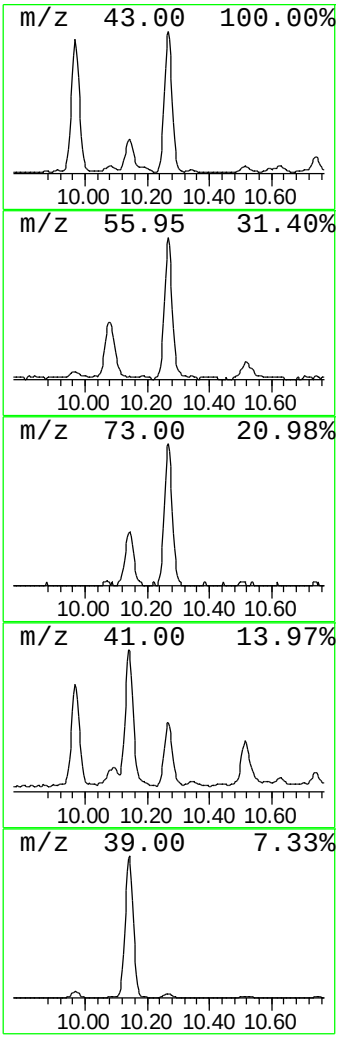
****

Peak Number 4 Isobutyl acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	5.18 ug/l	113049	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	36
3	n-Hexane-1,1-diol diacetate	202	C10H18O4	064847-81-0	23
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

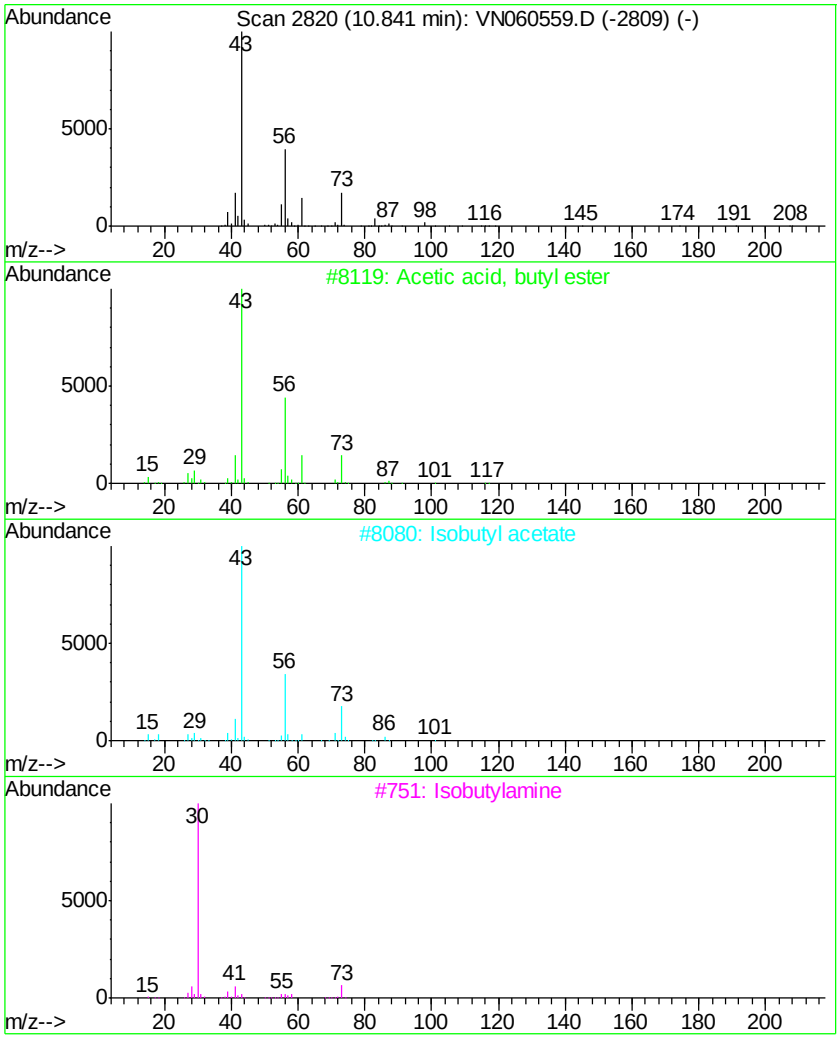
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

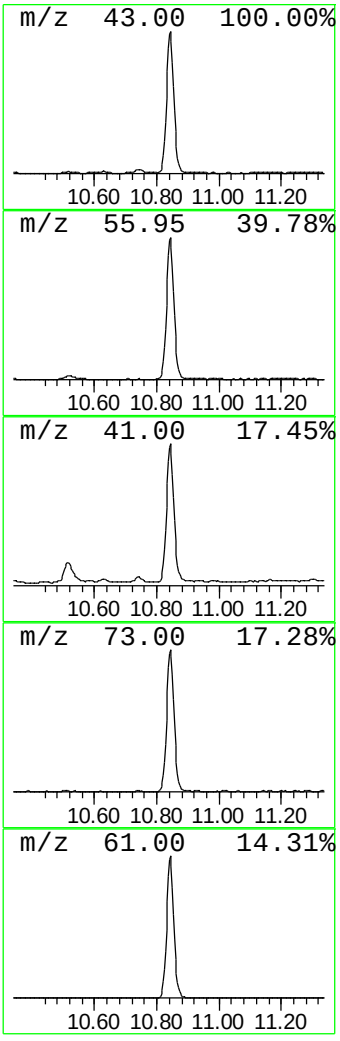
****

Peak Number 5 Acetic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	21.35 ug/l	465725	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2	Isobutyl acetate	116	C6H12O2	000110-19-0	39
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Ethane, diazo-	56	C2H4N2	001117-96-0	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

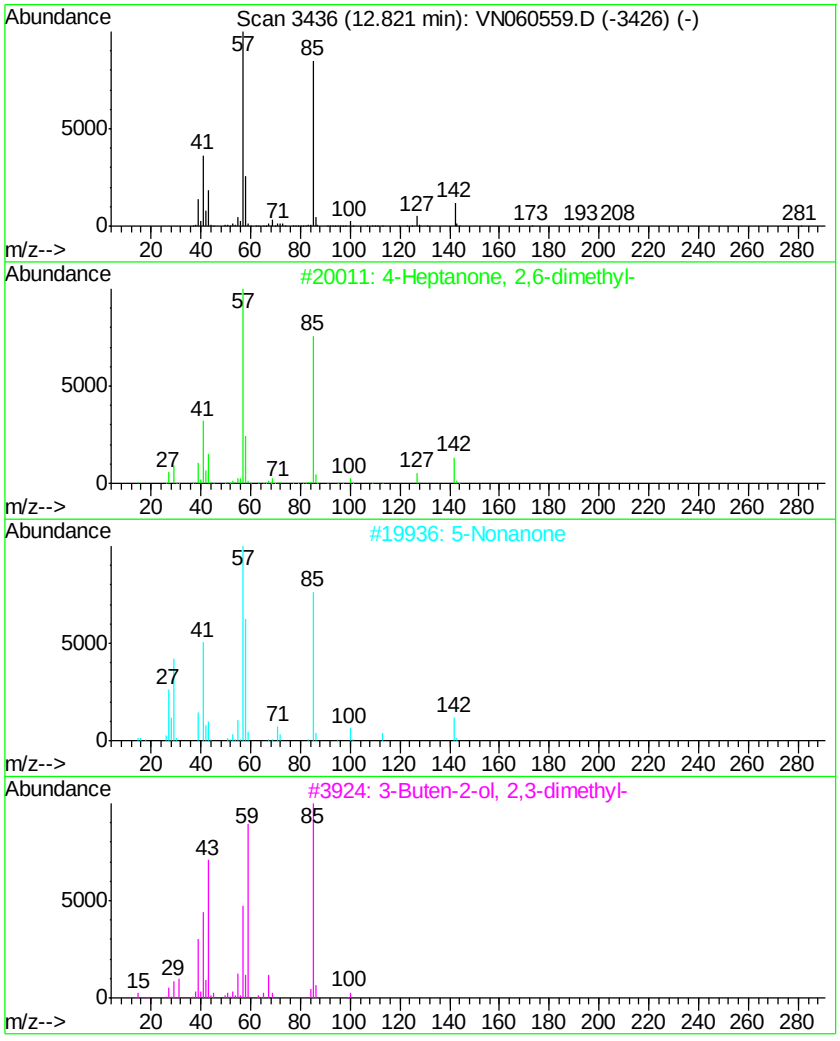
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

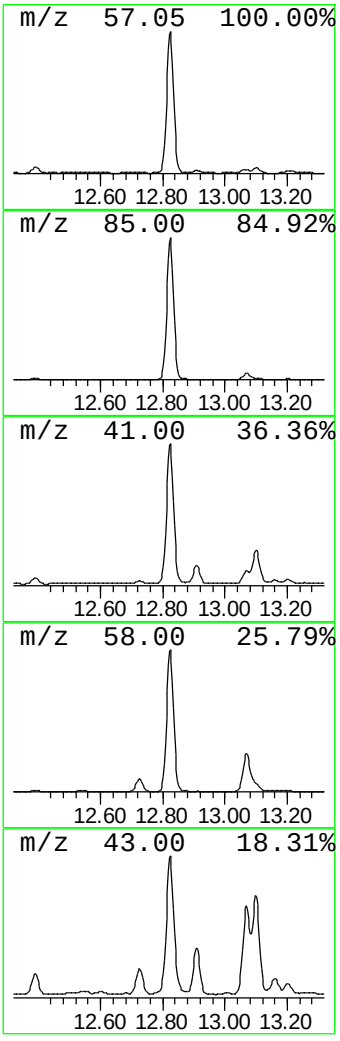
****

Peak Number 6 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	72.68 ug/l	1448760	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	5-Nonanone	142	C9H18O	000502-56-7	59
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50
4	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	49
5	Pentanethioic acid, S-propyl ester	160	C8H16OS	002432-76-0	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

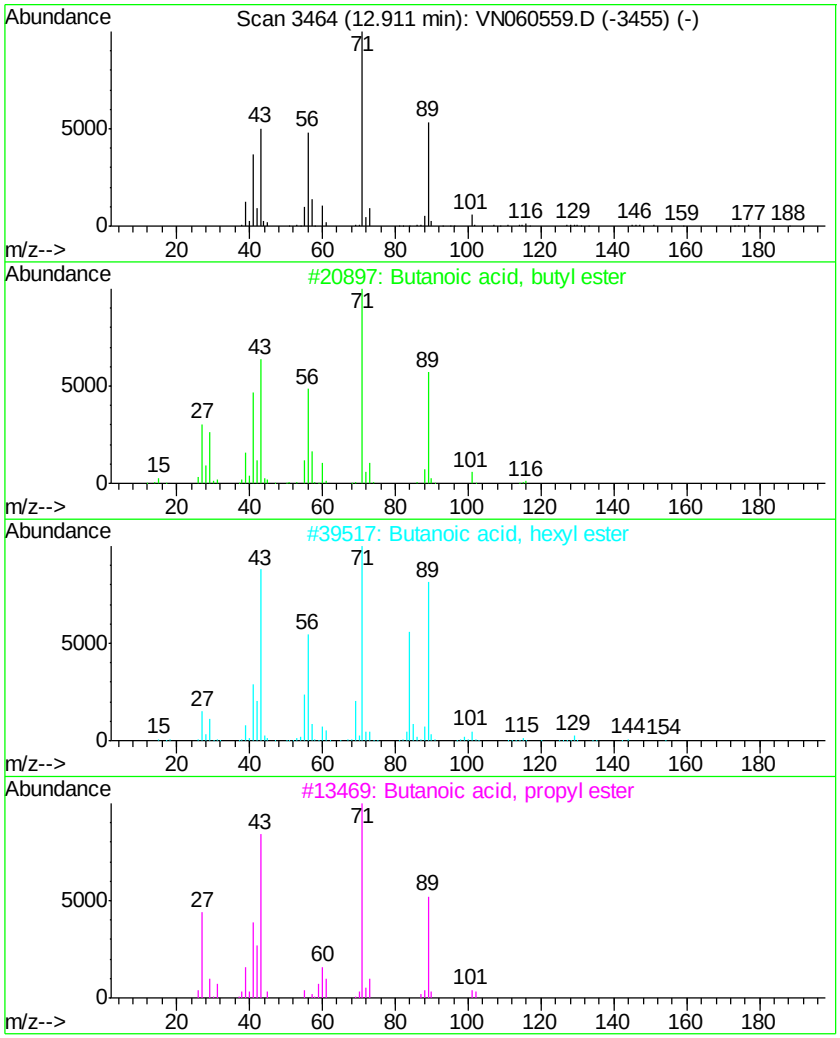
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

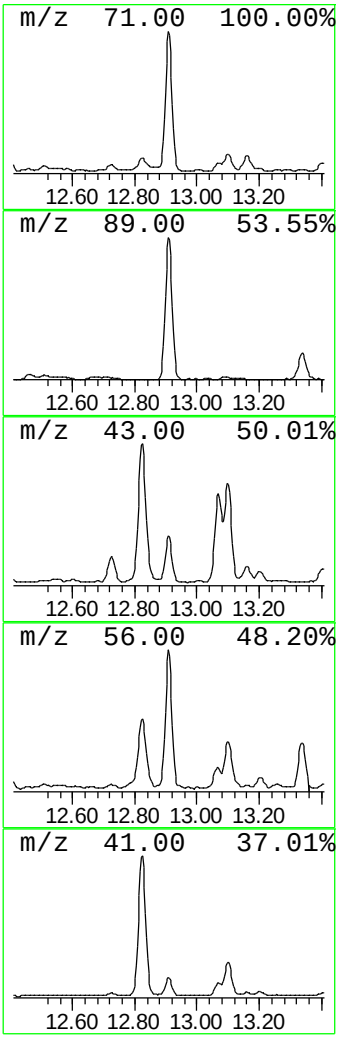
****

Peak Number 7 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	9.59 ug/l	191250	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
5	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

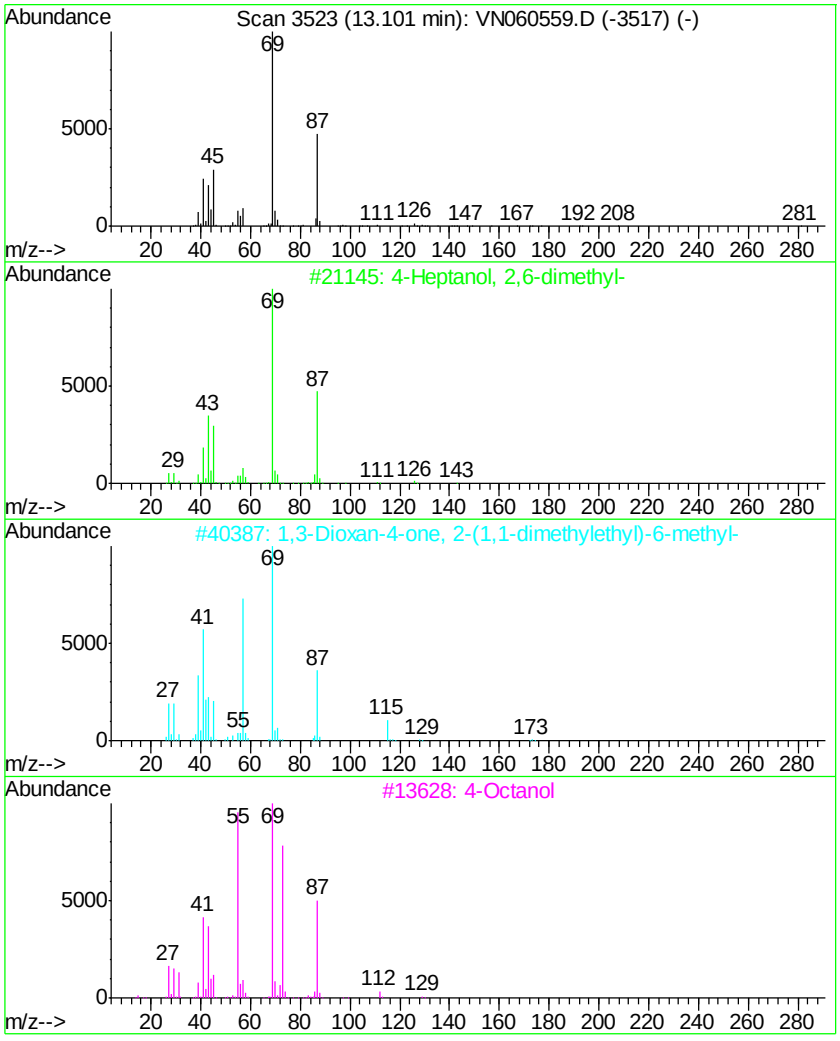
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

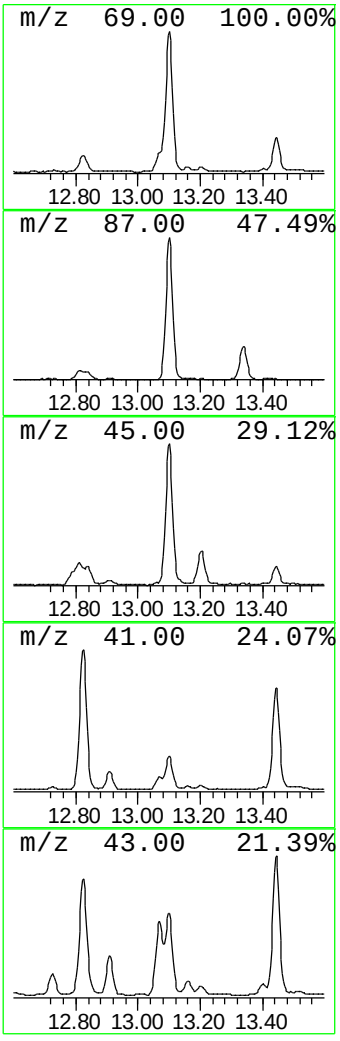
****

Peak Number 8 4-Heptanol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	19.24 ug/l	383449	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2	1,3-Dioxan-4-one, 2-(1,1-dimethy...	172	C9H16O3	113505-75-2	78
3	4-Octanol	130	C8H18O	000589-62-8	72
4	1-Octen-4-ol	128	C8H16O	040575-42-6	64
5	1,2-Hexanediol	118	C6H14O2	006920-22-5	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

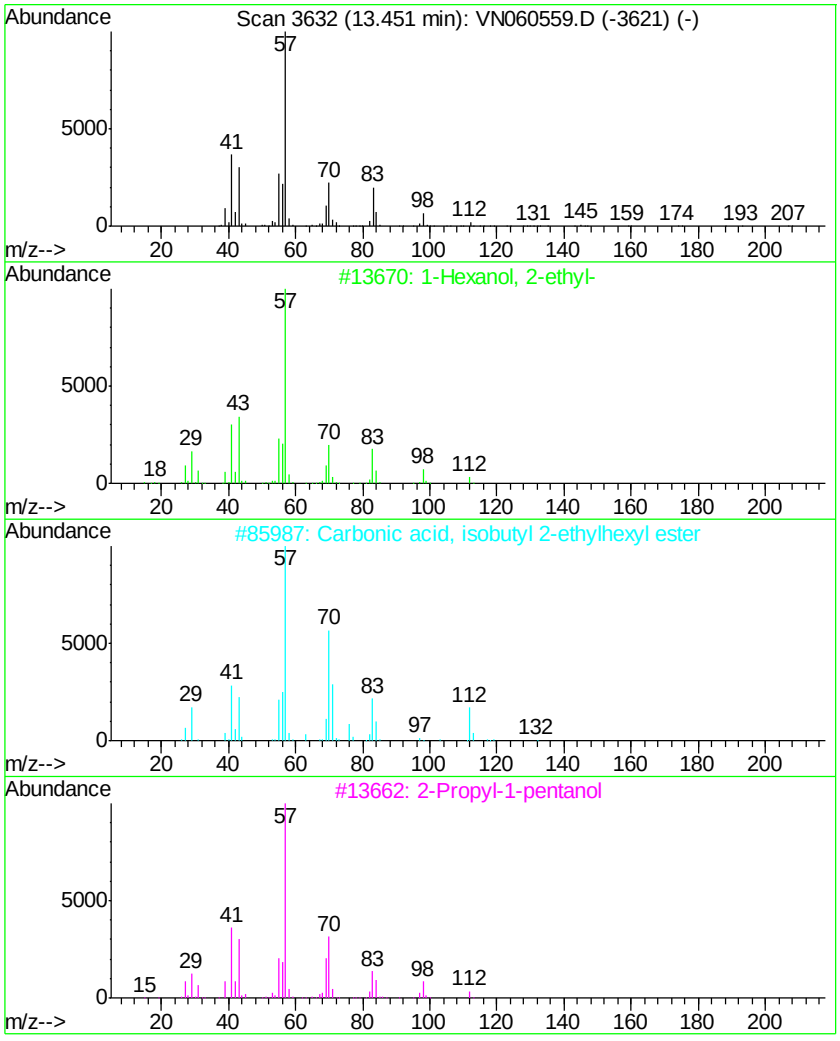
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

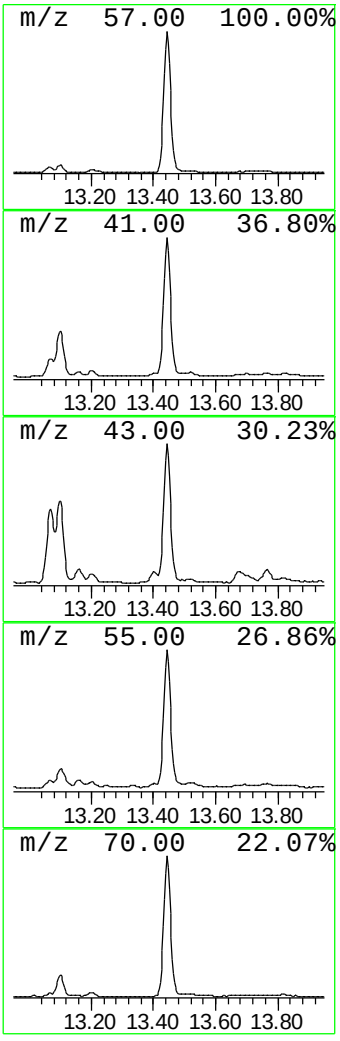
****

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	46.84 ug/l	933719	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

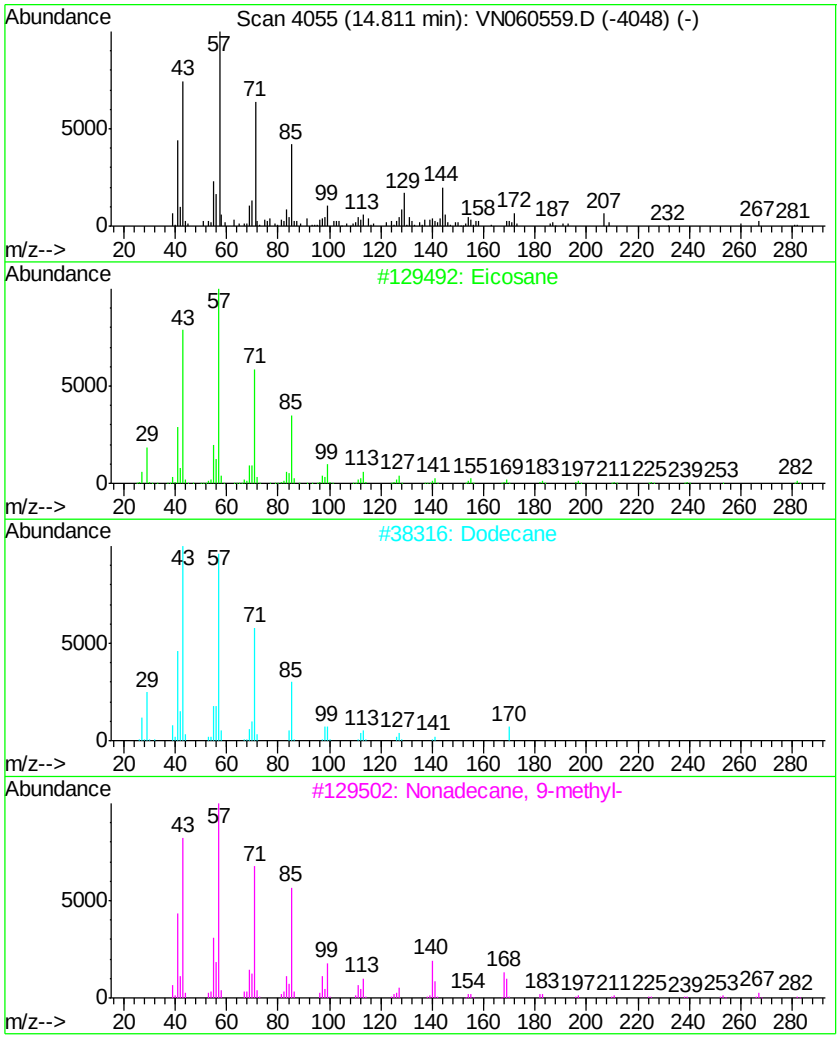
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

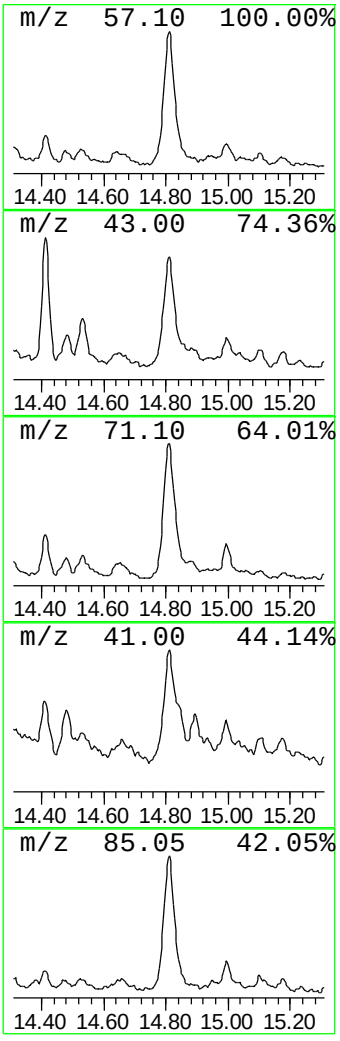
****

Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	6.69 ug/l	133317	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Dodecane	170	C12H26	000112-40-3	70
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	64
4	Octacosane	394	C28H58	000630-02-4	62
5	Heptadecane	240	C17H36	000629-78-7	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031720\
Data File : VN060559.D
Acq On : 17 Mar 2020 16:11
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N022720W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl Alcohol	4.01	5.8	ug/l	70425	1	7.64	609248	50.0
Butanal	6.51	16.1	ug/l	196569	1	7.64	609248	50.0
1-Butanol	8.76	8.0	ug/l	131357	2	8.57	821899	50.0
Isobutyl acetate	10.27	5.2	ug/l	113049	3	11.40	1090940	50.0
Acetic acid, buty...	10.84	21.4	ug/l	465725	3	11.40	1090940	50.0
4-Heptanone, 2,6-...	12.82	72.7	ug/l	1448760	4	13.34	996706	50.0
Butanoic acid, bu...	12.91	9.6	ug/l	191250	4	13.34	996706	50.0
4-Heptanol, 2,6-d...	13.10	19.2	ug/l	383449	4	13.34	996706	50.0
1-Hexanol, 2-ethyl-	13.45	46.8	ug/l	933719	4	13.34	996706	50.0
Eicosane	14.81	6.7	ug/l	133317	4	13.34	996706	50.0