LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 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\82N031820W.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	2.288	151	160	174	rBV	16912	26572	1.03%	0.168%
2	3.780	607	624	659	rVV	268971	704992	27.23%	4.447%
3	4.014	681	697	723	rBV2	26821	77435	2.99%	0.488%
4	4.291	765	783	810	rBV2	53639	151498	5.85%	0.956%
5	4.522	833	855	880	rBV	143185	439230	16.96%	2.770%
6	6.509	1454	1473	1500	rBV2	63635	193869	7.49%	1.223%
7	6.799	1540	1563	1586	rBV2	61118	187126	7.23%	1.180%
8	7.567	1784	1802	1813	rBV	135115	330589	12.77%	2.085%
9	7.644	1813	1826	1854	rVB	257354	604873	23.36%	3.815%
10	8.005	1915	1938	1957	rBV	162600	417582	16.13%	2.634%
11	8.567	2097	2113	2130	rBV	387515	812689	31.39%	5.126%
12	8.763	2160	2174	2186	rBV	69341	146046	5.64%	0.921%
13	9.021	2241	2254	2276	rBV	43454	88049	3.40%	0.555%
14	9.394	2360	2370	2386	rBV3	14305	28050	1.08%	0.177%
15	9.969	2537	2549	2567	rVB	71387	129237	4.99%	0.815%
16	10.078	2567	2583	2592	rBV	631842	1146065	44.26%	7.229%
17	10.143	2592	2603	2630	rVB	1418084	2589200	100.00%	16.331%
18	10.268	2630	2642	2656	rBV	52236	96875	3.74%	0.611%
19	10.516	2709	2719	2735	rBV3	20607	41162	1.59%	0.260%
20	10.844	2809	2821	2837	rBV	223912	375454	14.50%	2.368%
21	11.400	2979	2994	3013	rBV	618673	1094236	42.26%	6.902%
22	11.503	3016	3026	3040	rVB	62486	111770	4.32%	0.705%
23	11.609	3045	3059	3079	rVV2	294721	592506	22.88%	3.737%
24	11.766	3102	3108	3117	rBV2	17408	26365	1.02%	0.166%
25	11.940	3152	3162	3171	rBV	206527	370541	14.31%	2.337%
26	11.988	3172	3177	3202	rVB2	86876	190228	7.35%	1.200%
27	12.397	3292	3304	3317	rBV	484127	815797	31.51%	5.145%
28	12.824	3425	3437	3454	rVV	749382	1225248	47.32%	7.728%
29	12.908	3455	3463	3477	rVB	92448	141638	5.47%	0.893%
30	13.069	3505	3513	3516	rBV2	94190	130598	5.04%	0.824%
31	13.101	3517	3523	3534	rVV	243447	365357	14.11%	2.304%
32	13.159	3536	3541	3548	rVV	29670	40967	1.58%	0.258%
33	13.204	3549	3555	3571	rVB4	25371	45480	1.76%	0.287%
34	13.339	3585	3597	3610	rBV	590644	995783	38.46%	6.281%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 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\82N031820W.M
Title : SW846 8260

35	13.445	3621	3630	3645	rVB	597378	905139	34.96%	5.709%
36	14.413	3924	3931	3941	rVB3	31931	53261	2.06%	0.336%
37	14.480	3944	3952	3961	rVV5	35116	62523	2.41%	0.394%
38	14.811	4046	4055	4062	rBV4	45176	100666	3.89%	0.635%

Sum of corrected areas: 15854696

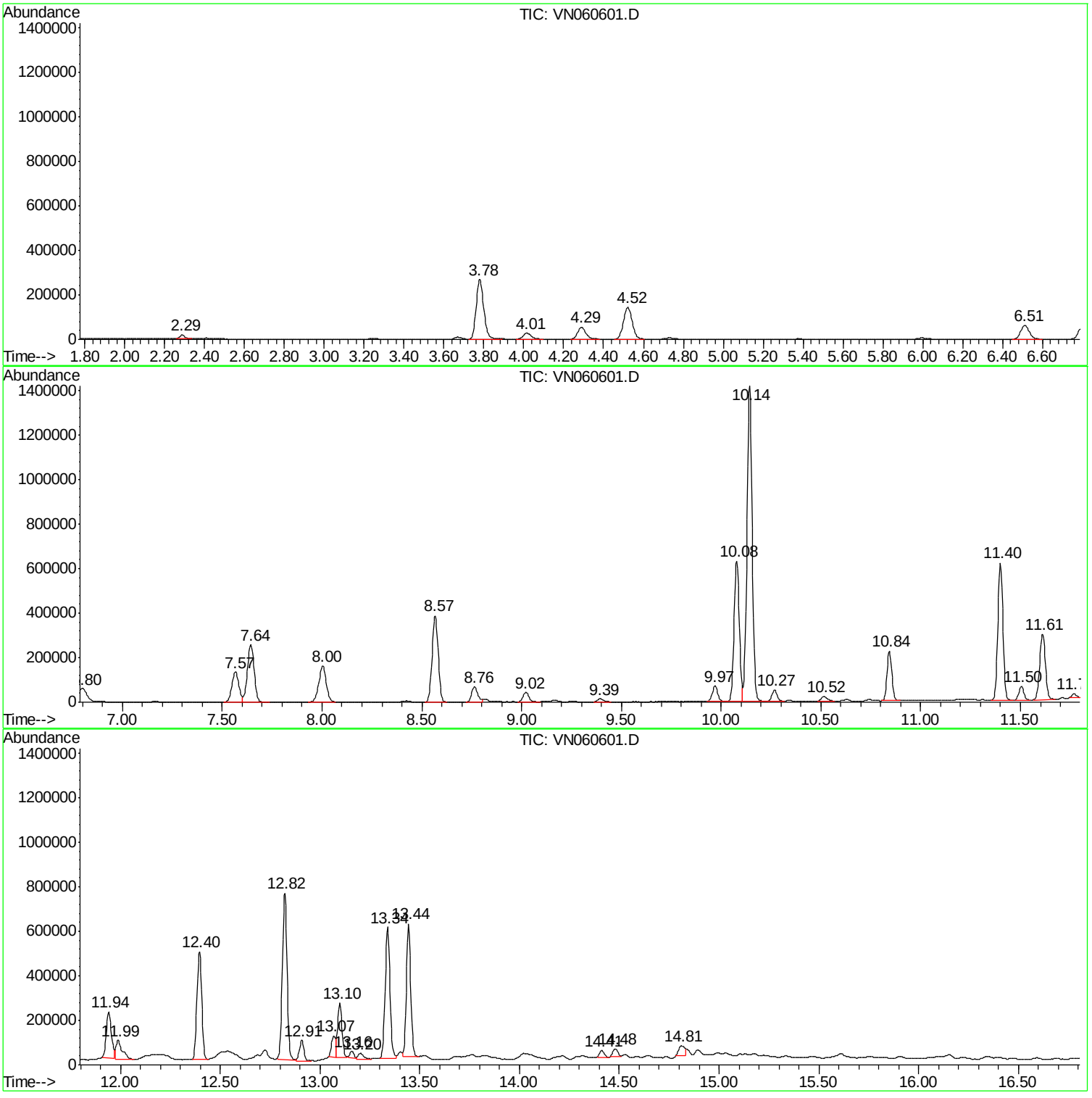
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.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\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

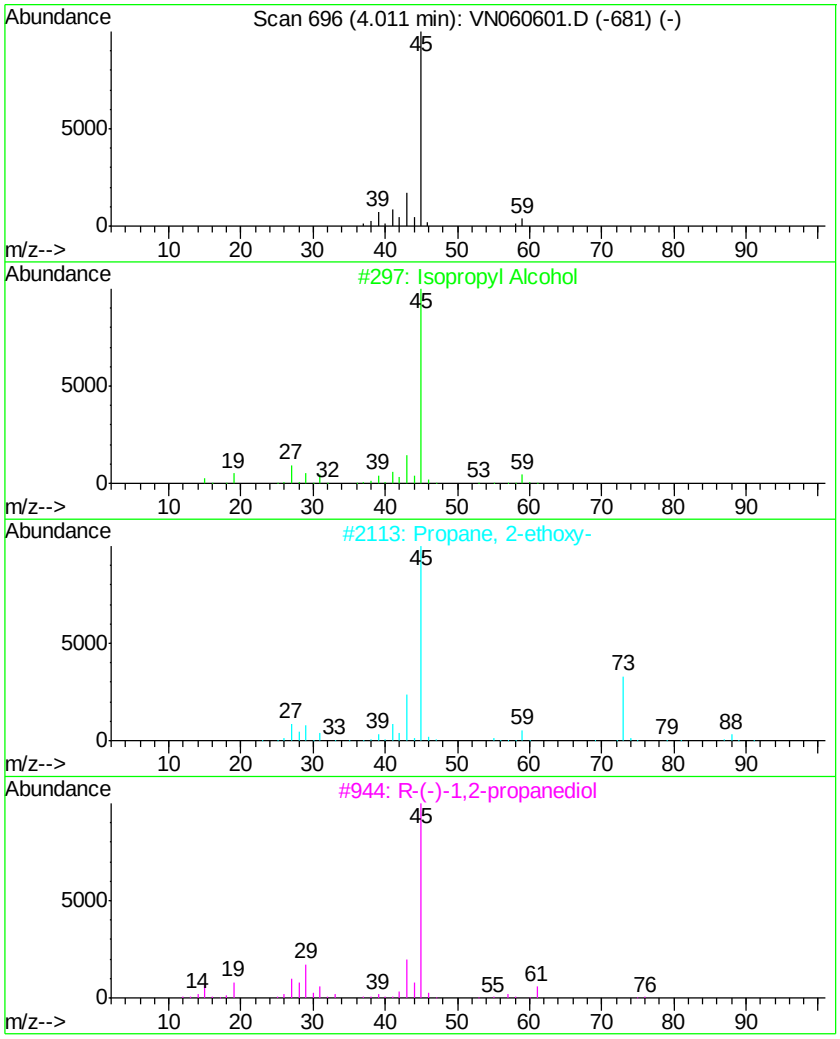
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

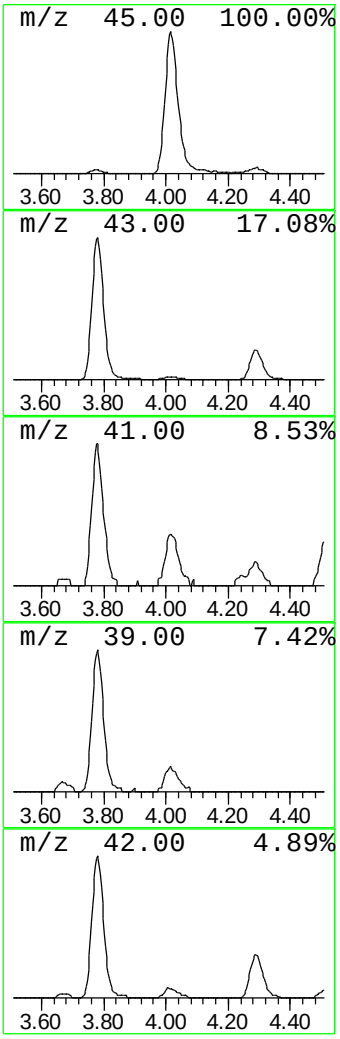
****

Peak Number 1 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	6.40 ug/l	77435	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
5	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

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

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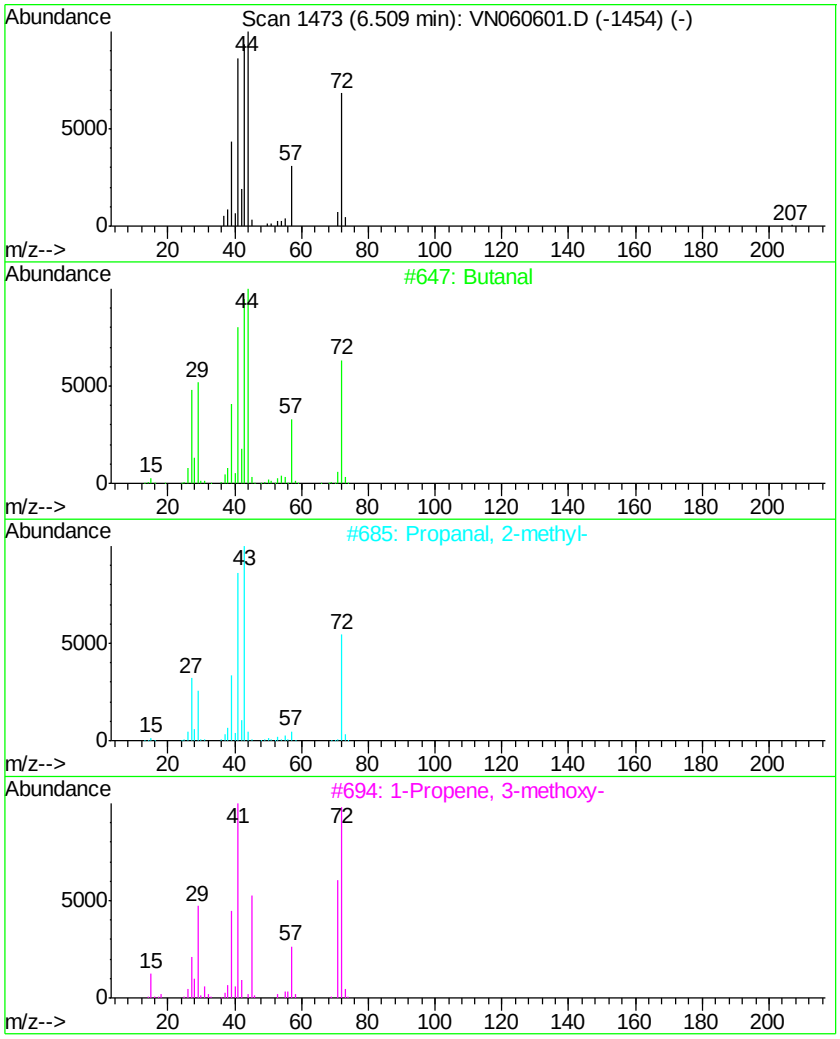
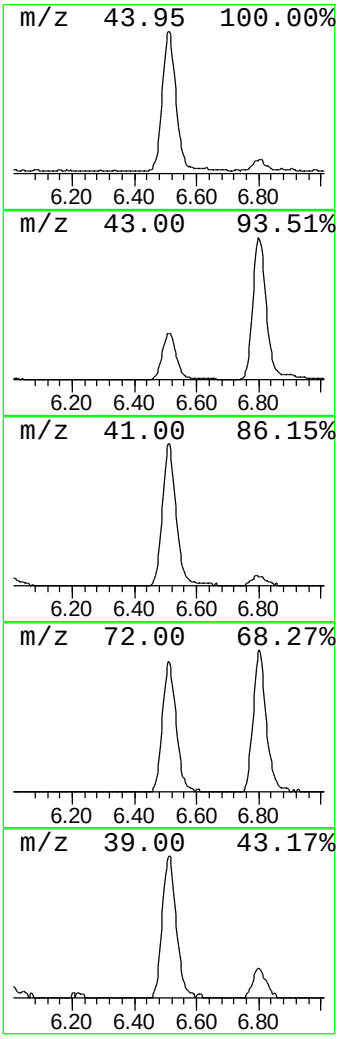
Peak Number 2 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	16.03 ug/l	193869	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	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
5	3-Bromopropyl isothiocyanate	179	C4H6BrNS	002799-73-7	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

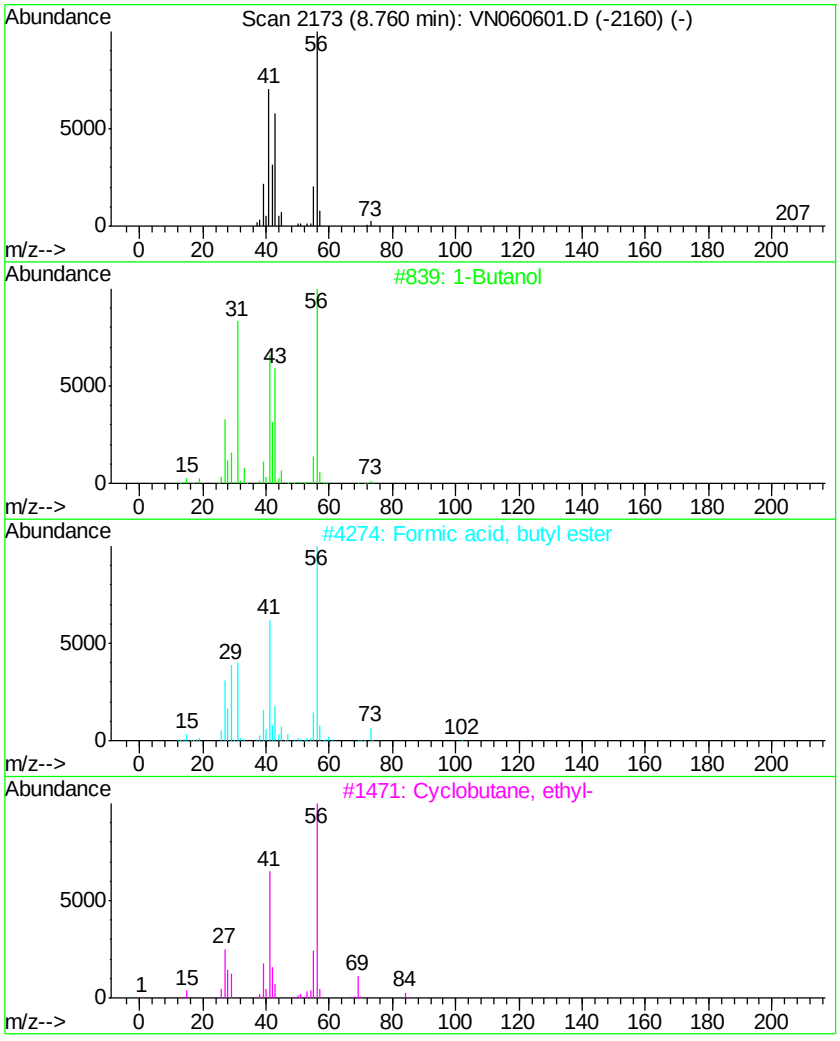
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

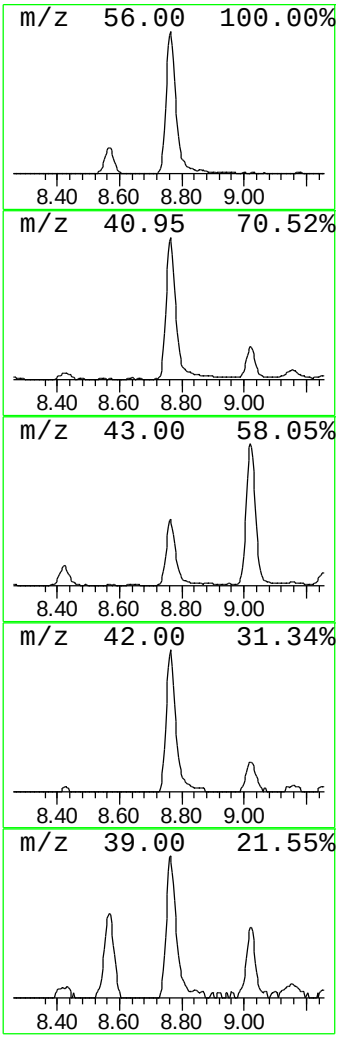
****

Peak Number 3 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	8.99 ug/l	146046	1,4-Difluorobenzene	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

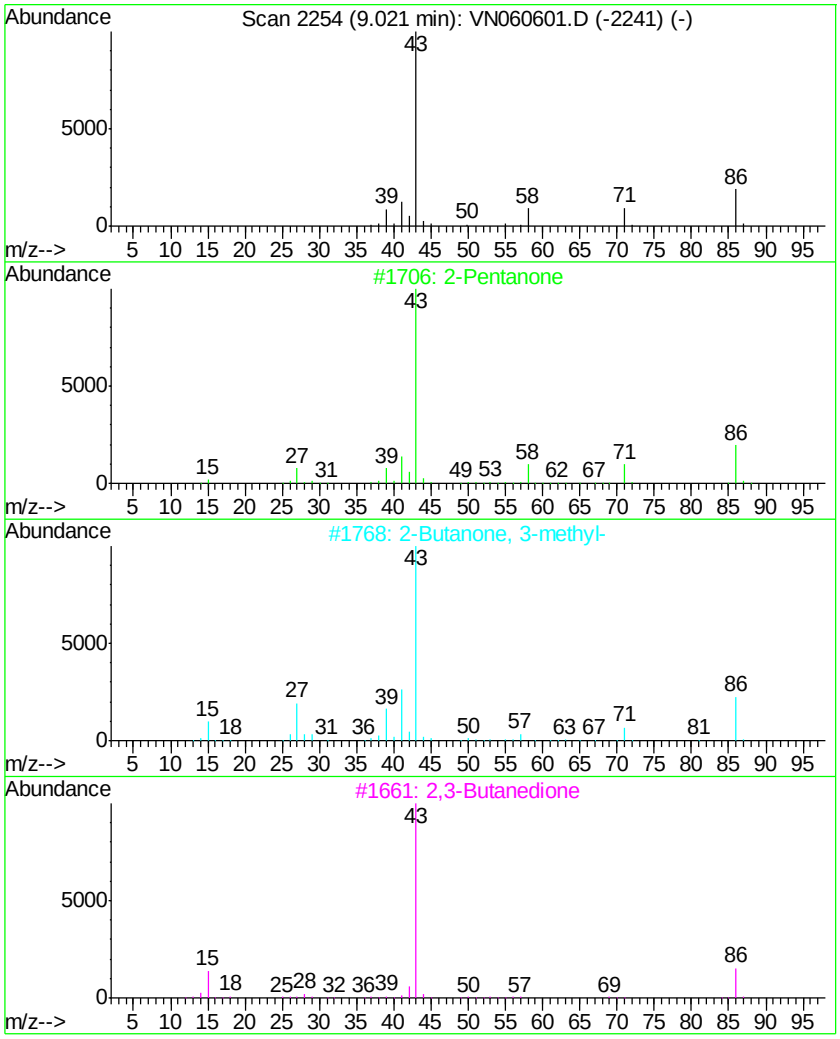
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

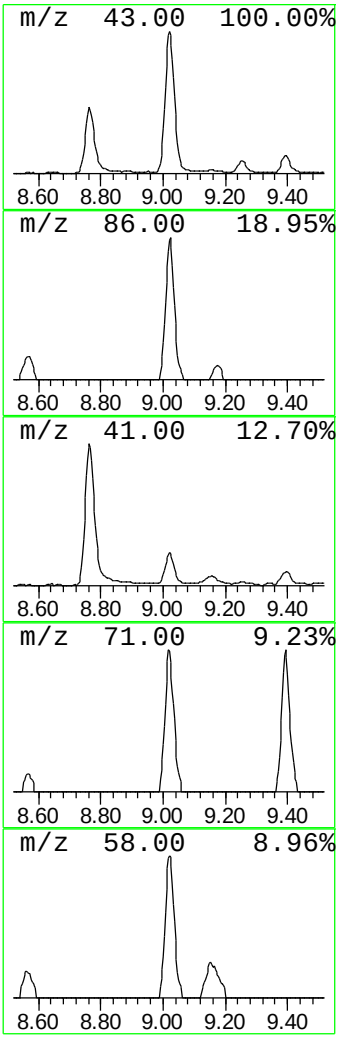
****

Peak Number 4 2-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	5.42 ug/l	88049	1,4-Difluorobenzene	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	87
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	2,3-Butanedione	86	C4H6O2	000431-03-8	47
4	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	38
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

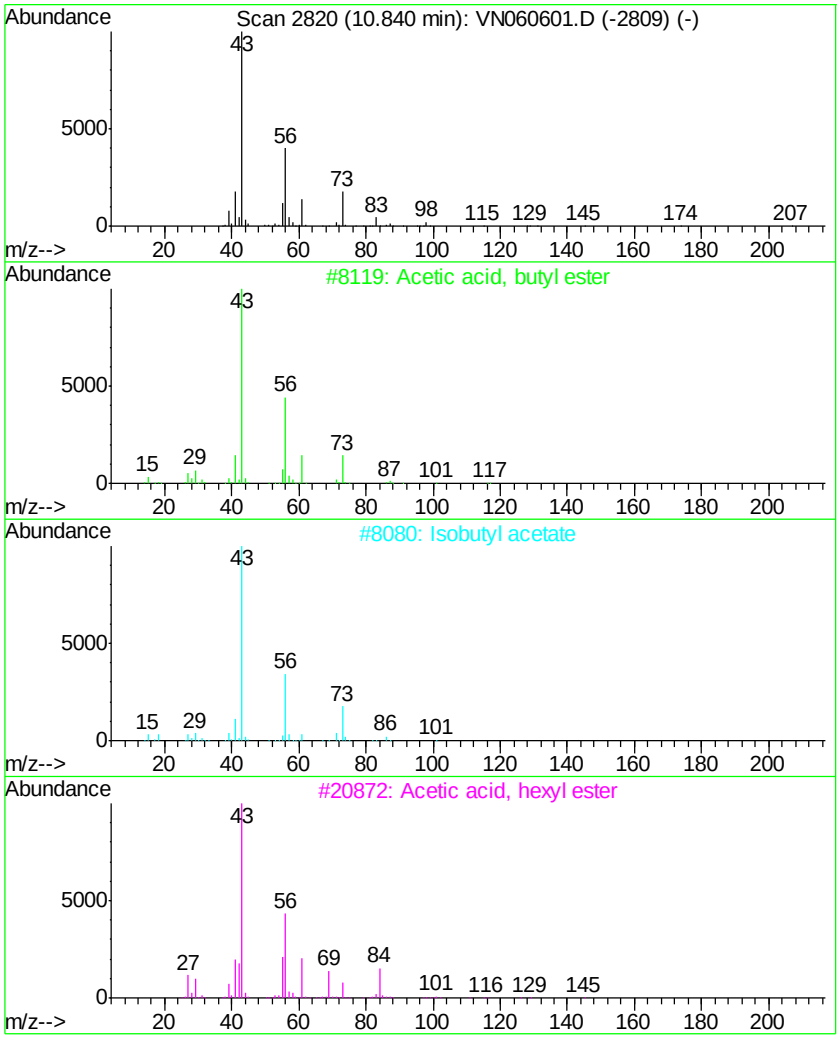
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

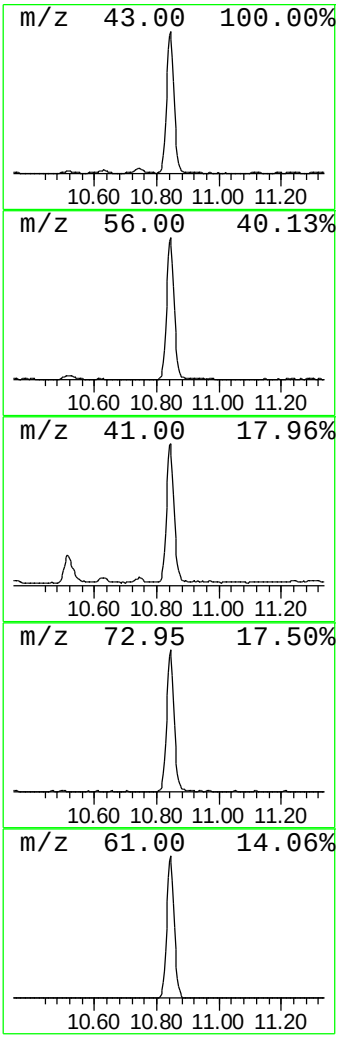
****

Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	17.16 ug/l	375454	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	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	38
4	1-Butanol, 2-methylene-, acetate	128	C7H12O2	055670-09-2	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

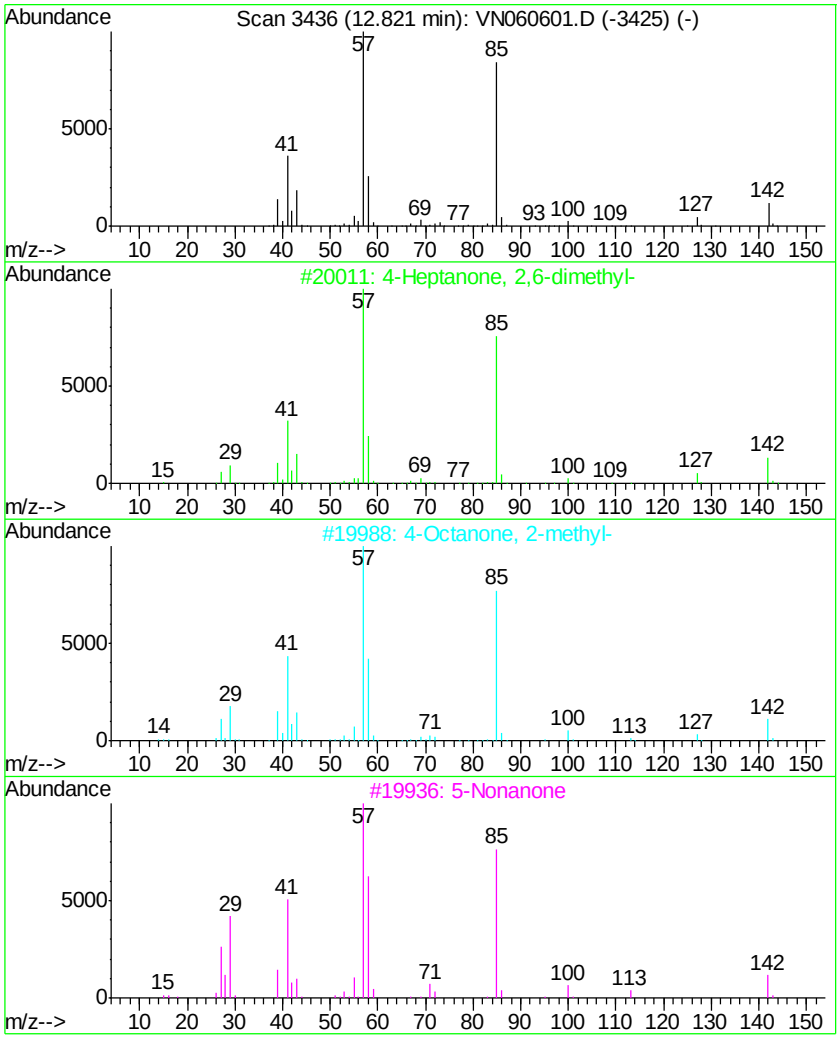
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

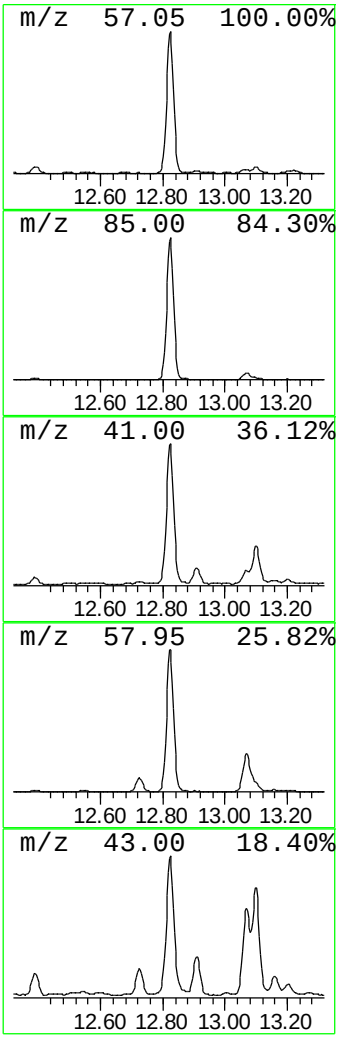
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	61.52 ug/l	1225250	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	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
3	5-Nonanone	142	C9H18O	000502-56-7	59
4	2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	53
5	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

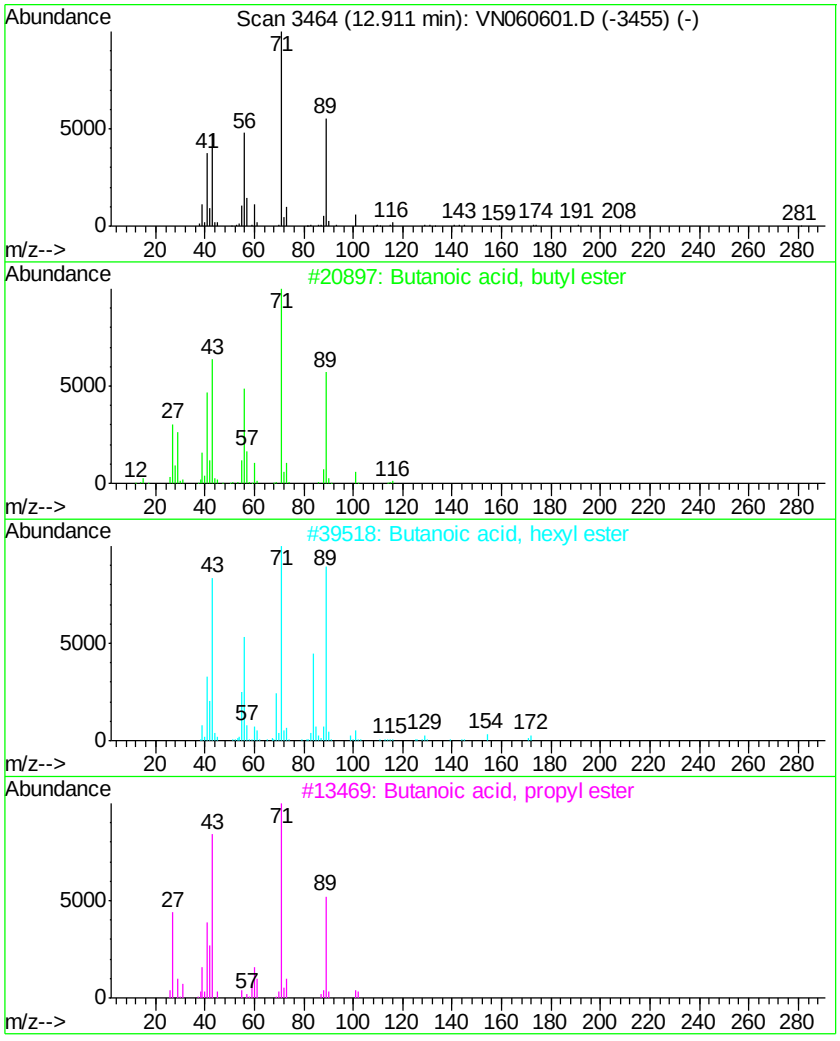
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

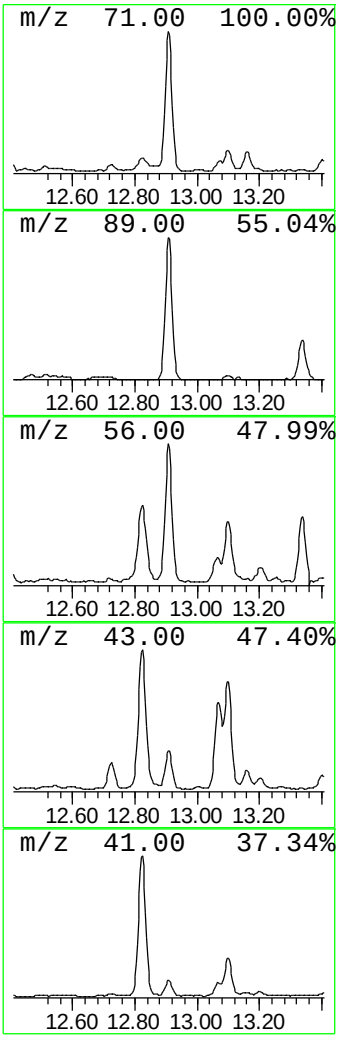
****

Peak Number 7 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	7.11 ug/l	141638	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

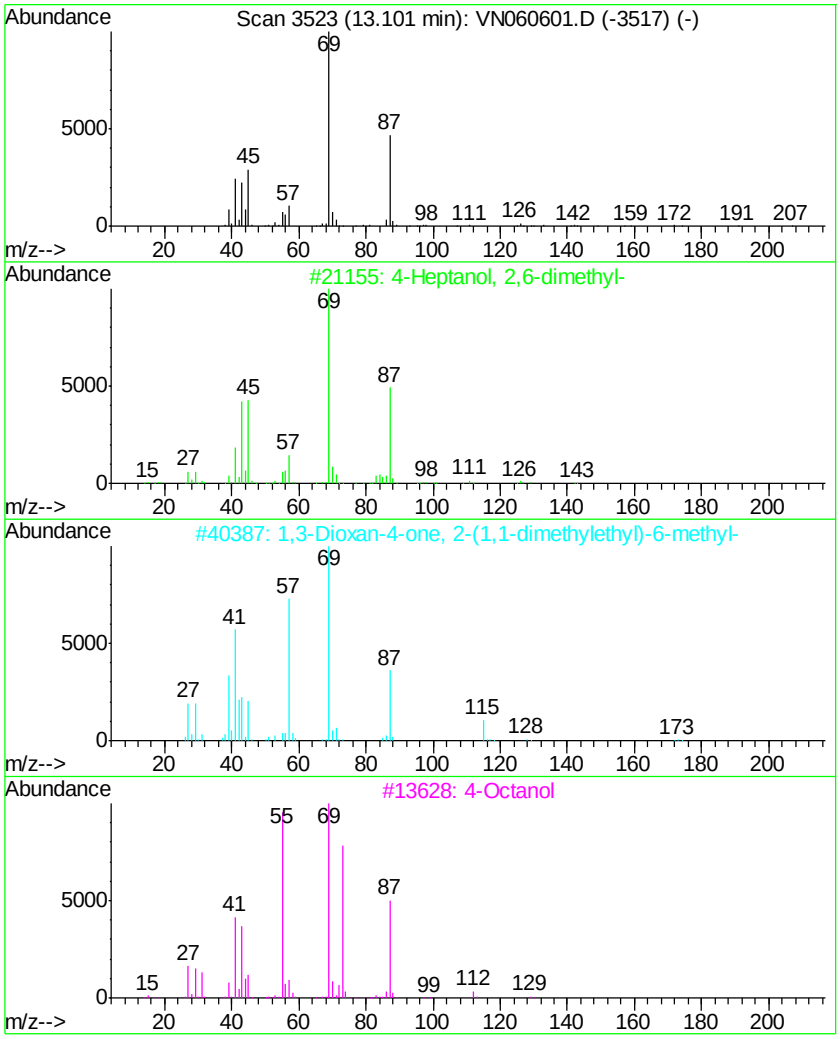
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

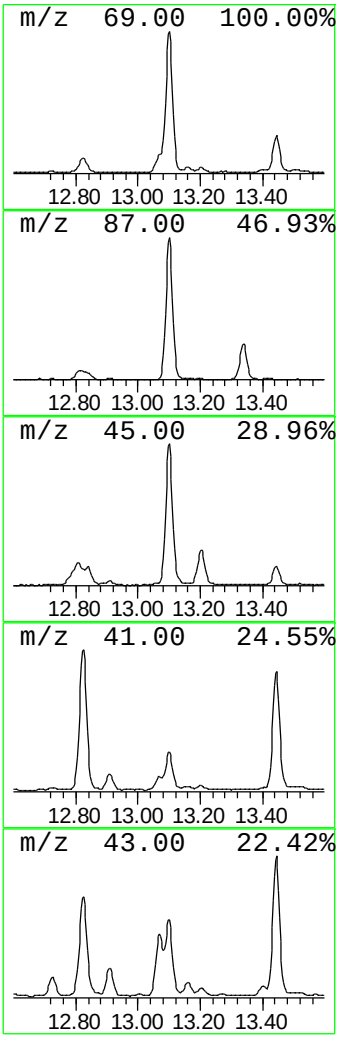
****

Peak Number 8 4-Heptanol, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	18.35 ug/l	365357	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	5-Nonanol	144	C9H20O	000623-93-8	72
5	1,2-Hexanediol	118	C6H14O2	006920-22-5	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

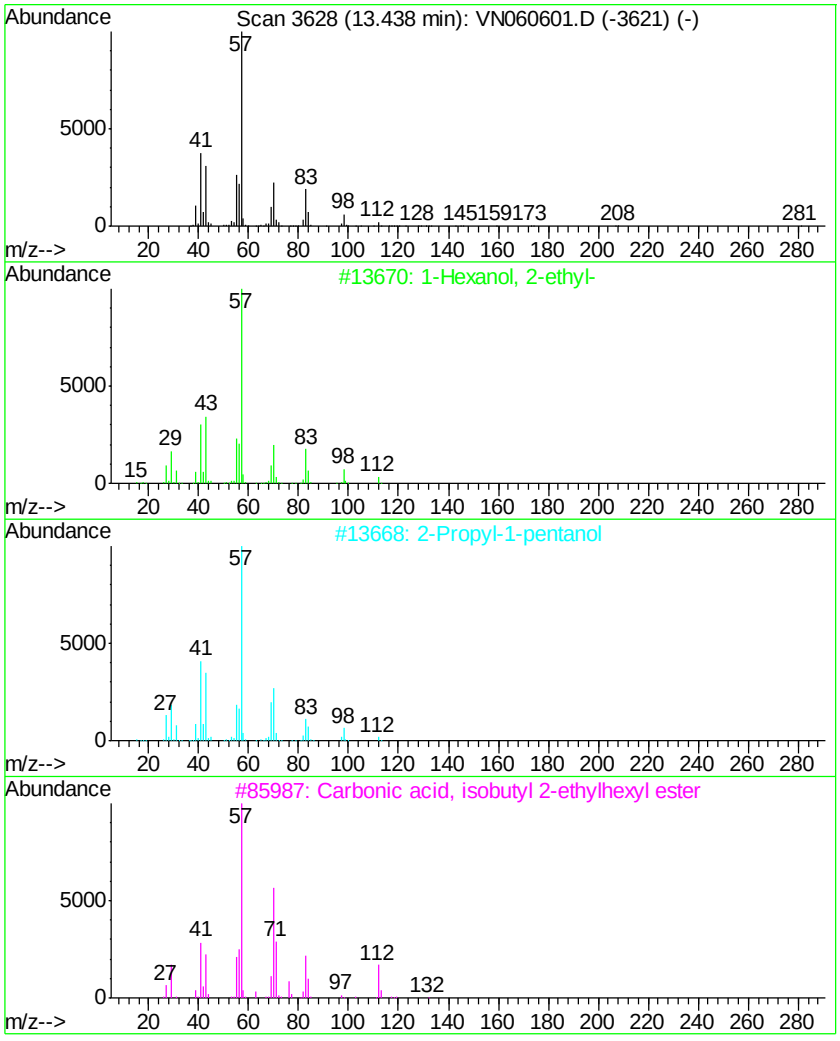
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

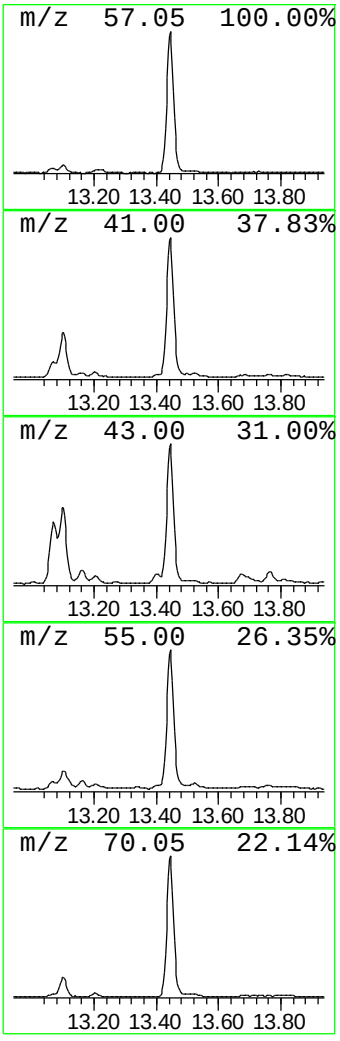
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	45.45 ug/l	905139	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	74
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	59
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.M
Quant Title : SW846 8260

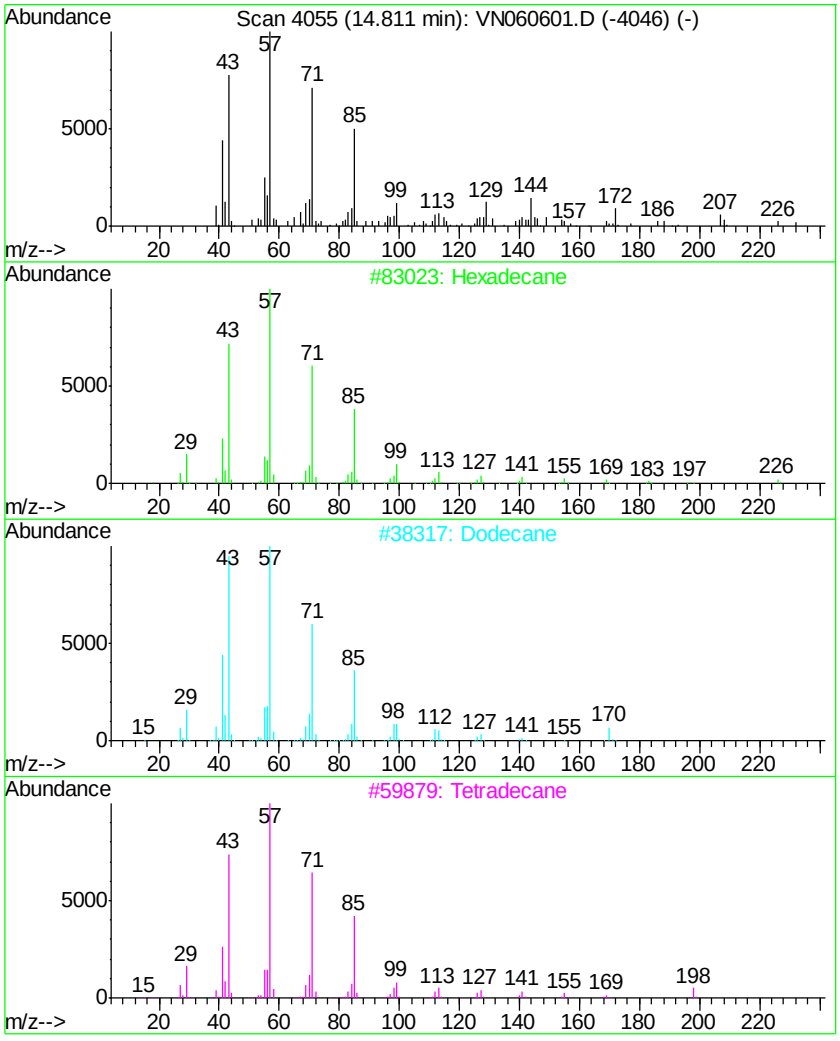
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

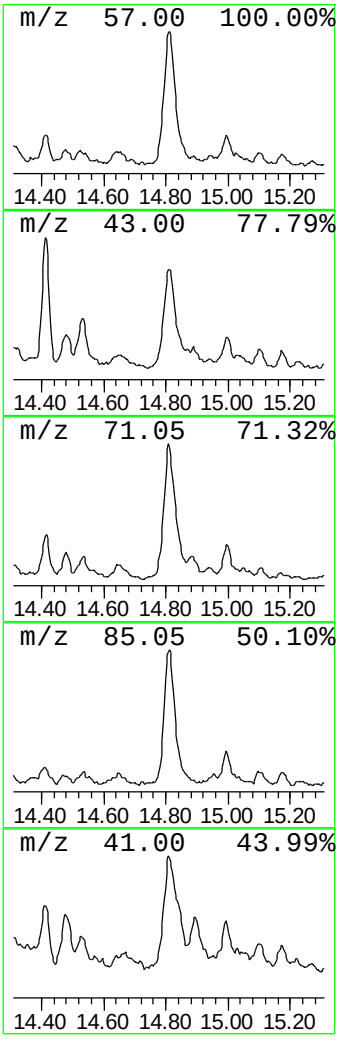
****

Peak Number 10 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	5.05 ug/l	100666	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Dodecane	170	C12H26	000112-40-3	89
3	Tetradecane	198	C14H30	000629-59-4	68
4	Nonadecane	268	C19H40	000629-92-5	68
5	Heptadecane	240	C17H36	000629-78-7	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN031820\
Data File : VN060601.D
Acq On : 18 Mar 2020 18:42
Operator : JC/MD
Sample : L1946-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N031820W.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	6.4	ug/l	77435	1	7.64	604873	50.0
Butanal	6.51	16.0	ug/l	193869	1	7.64	604873	50.0
1-Butanol	8.76	9.0	ug/l	146046	2	8.57	812689	50.0
2-Pentanone	9.02	5.4	ug/l	88049	2	8.57	812689	50.0
Acetic acid, buty...	10.84	17.2	ug/l	375454	3	11.40	1094240	50.0
4-Heptanone, 2,6-...	12.82	61.5	ug/l	1225250	4	13.34	995783	50.0
Butanoic acid, bu...	12.91	7.1	ug/l	141638	4	13.34	995783	50.0
4-Heptanol, 2,6-d...	13.10	18.4	ug/l	365357	4	13.34	995783	50.0
1-Hexanol, 2-ethyl-	13.44	45.5	ug/l	905139	4	13.34	995783	50.0
Hexadecane	14.81	5.0	ug/l	100666	4	13.34	995783	50.0