LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

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\82N071519W.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	2.294	150	162	247	rBV2	20820557	40989883	100.00%	52.075%
2	3.281	448	469	541	rBV	3255707	8153643	19.89%	10.359%
3	3.696	577	598	617	rBV	176877	460239	1.12%	0.585%
4	3.815	618	635	654	rBV	766938	1972398	4.81%	2.506%
5	4.063	694	712	738	rBV2	171037	487525	1.19%	0.619%
6	6.542	1460	1483	1508	rBV2	839482	2522121	6.15%	3.204%
7	6.834	1553	1574	1589	rBV2	281477	823004	2.01%	1.046%
8	6.928	1589	1603	1635	rVB	587371	1605534	3.92%	2.040%
9	7.590	1790	1809	1820	rBV2	174424	434293	1.06%	0.552%
10	7.664	1821	1832	1853	rVB	288357	678843	1.66%	0.862%
11	8.024	1925	1944	1966	rBV2	194768	483462	1.18%	0.614%
12	8.583	2103	2118	2147	rBV	474310	1000596	2.44%	1.271%
13	8.786	2167	2181	2213	rBV	335337	779442	1.90%	0.990%
14	9.040	2247	2260	2283	rVV	210027	414696	1.01%	0.527%
15	9.982	2540	2553	2572	rBV	470666	871142	2.13%	1.107%
16	10.091	2573	2587	2597	rVV	835111	1671813	4.08%	2.124%
17	10.152	2597	2606	2635	rVB	1404539	2627569	6.41%	3.338%
18	10.853	2810	2824	2851	rBV	2388028	4080946	9.96%	5.185%
19	11.406	2982	2996	3018	rBV	801168	1462166	3.57%	1.858%
20	11.808	3114	3121	3152	rVB	592796	1073829	2.62%	1.364%
21	11.943	3152	3163	3178	rBV	397368	636828	1.55%	0.809%
22	12.400	3293	3305	3329	rVB2	678857	1248153	3.05%	1.586%
23	13.342	3586	3598	3612	rBV	805476	1380627	3.37%	1.754%
24	13.445	3621	3630	3643	rVB	1589434	2393479	5.84%	3.041%
25	14.644	3994	4003	4022	rVB	252849	461225	1.13%	0.586%

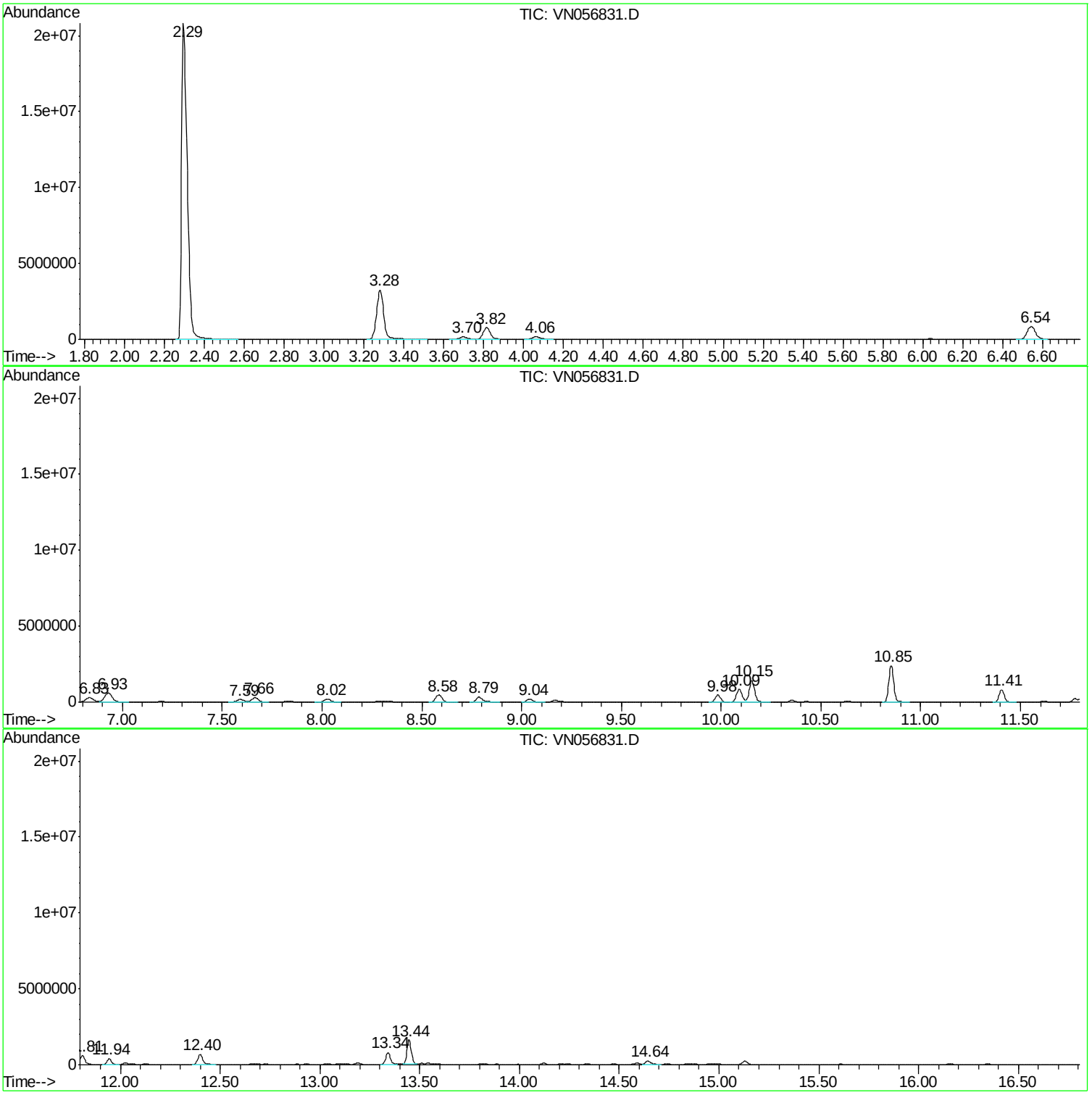
Sum of corrected areas: 78713456

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.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\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.M
Quant Title : SW846 8260

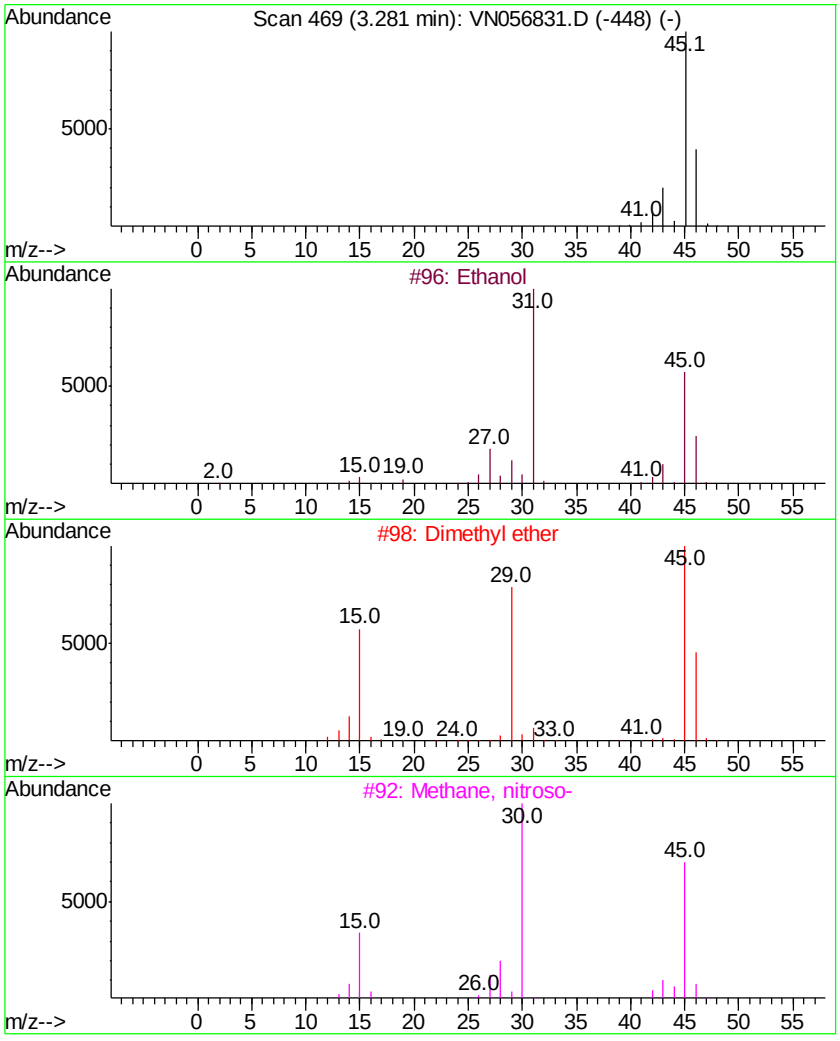
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

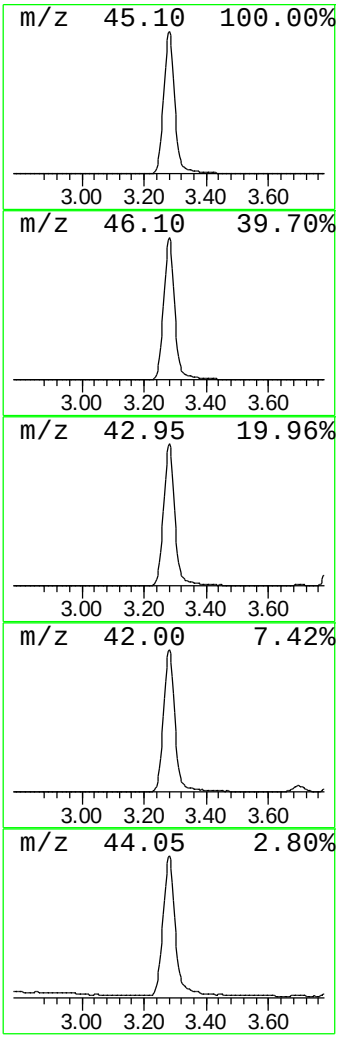
****

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	600.55 ug/l	8153640	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.M
Quant Title : SW846 8260

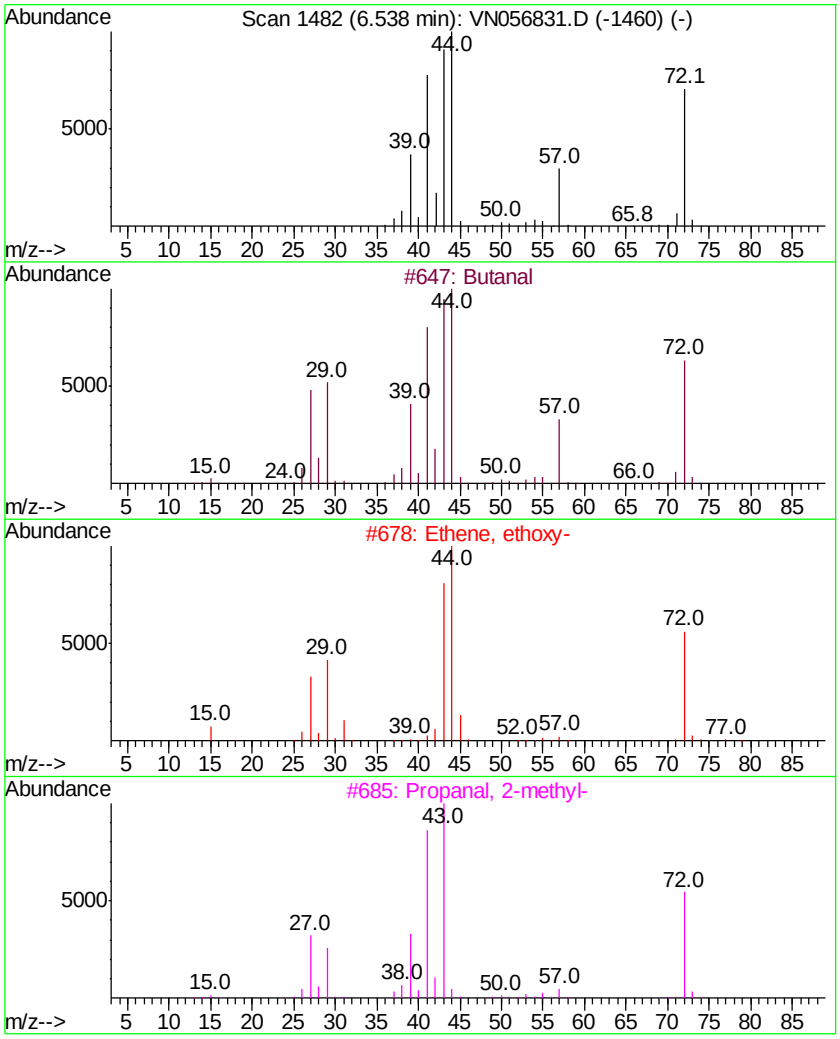
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

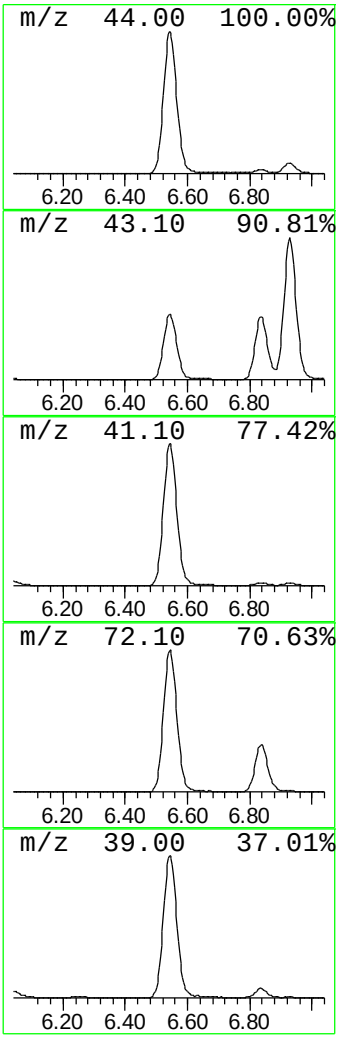
****

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	185.77 ug/l	2522120	Pentafluorobenzene	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	72
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	27
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.M
Quant Title : SW846 8260

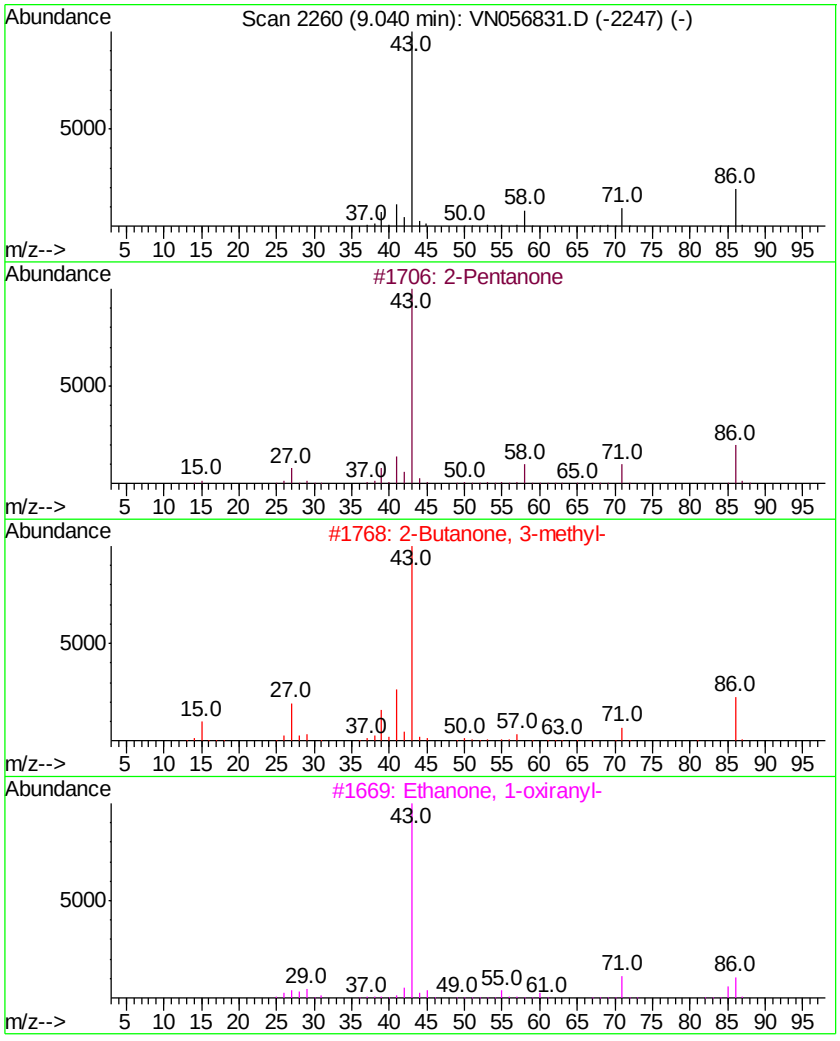
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

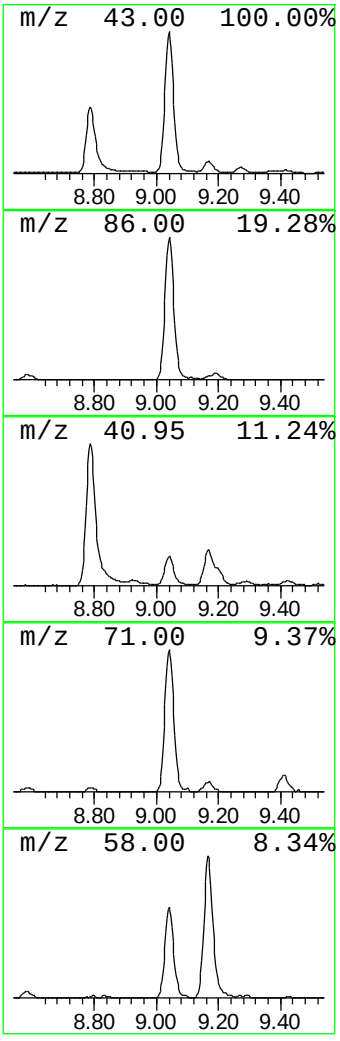
****

Peak Number 4 2-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	20.72 ug/l	414696	1,4-Difluorobenzene	8.59

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	50
3	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	39
4	2,3-Butanedione	86	C4H6O2	000431-03-8	38
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.M
Quant Title : SW846 8260

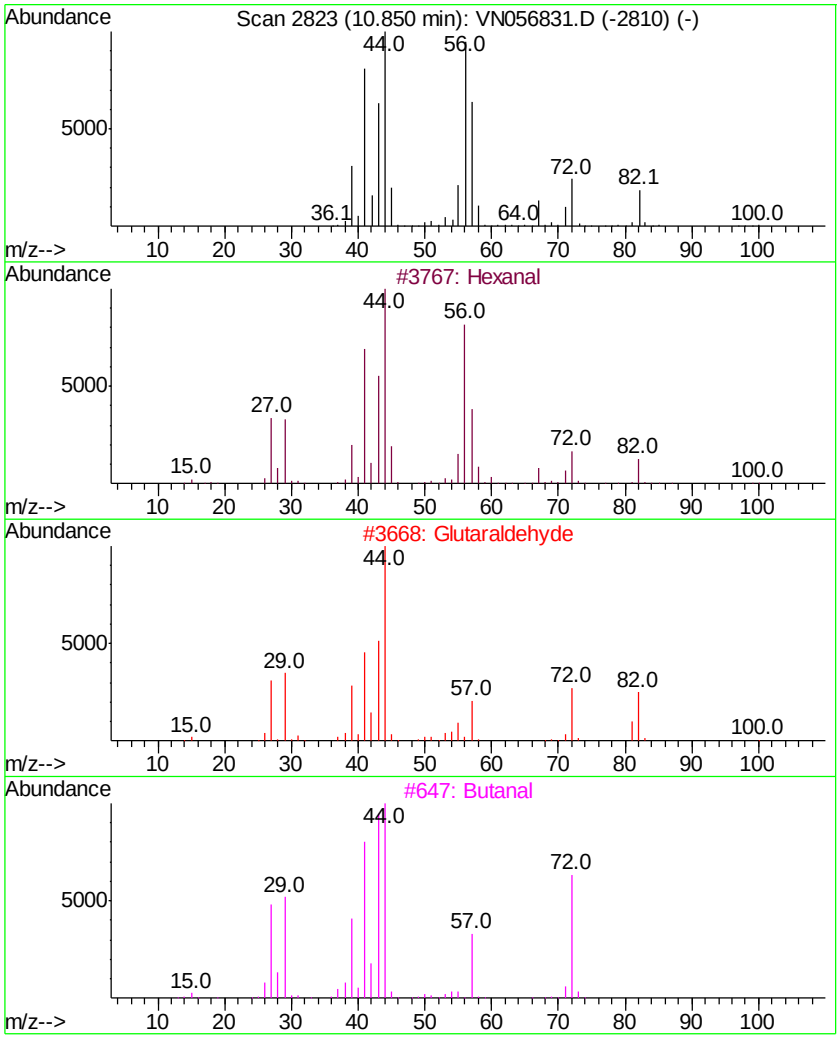
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

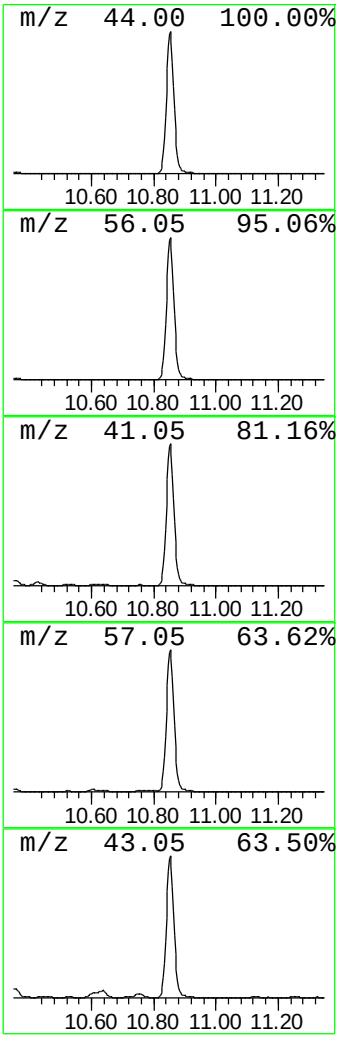
****

Peak Number 5 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	139.55 ug/l	4080950	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	91
2	Glutaraldehyde	100	C5H8O2	000111-30-8	43
3	Butanal	72	C4H8O	000123-72-8	35
4	1,5-Pentanediol	104	C5H12O2	000111-29-5	33
5	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	27





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.M
Quant Title : SW846 8260

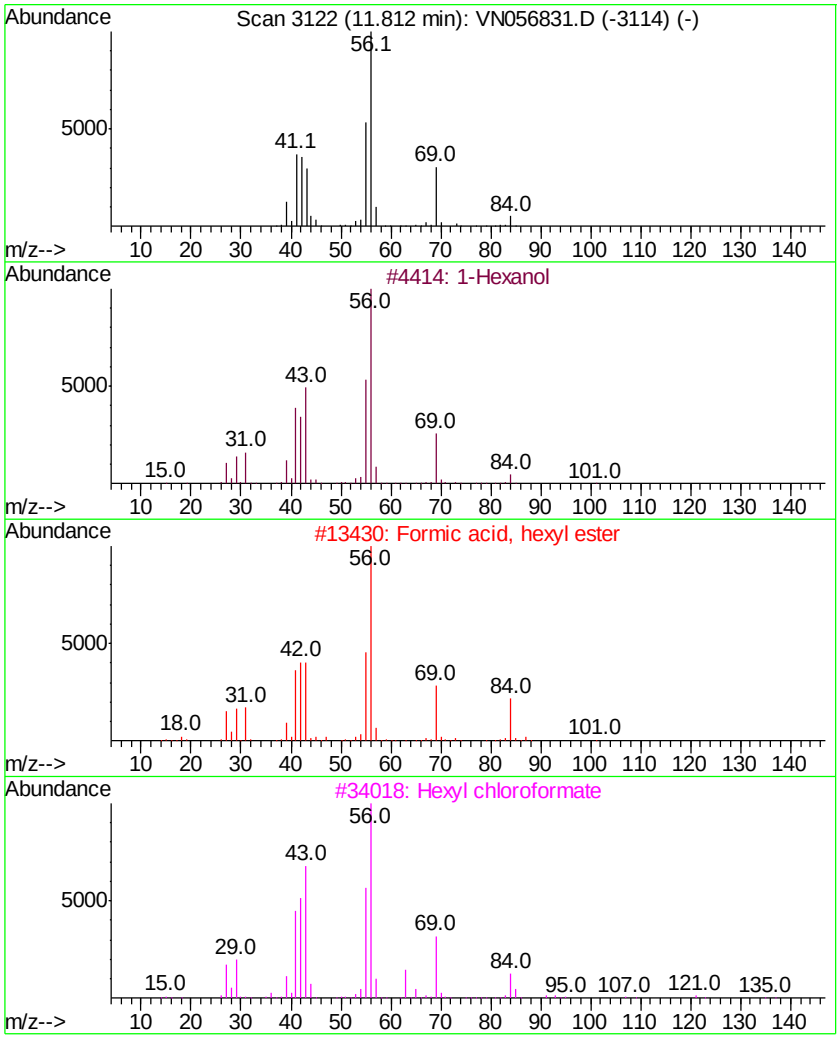
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

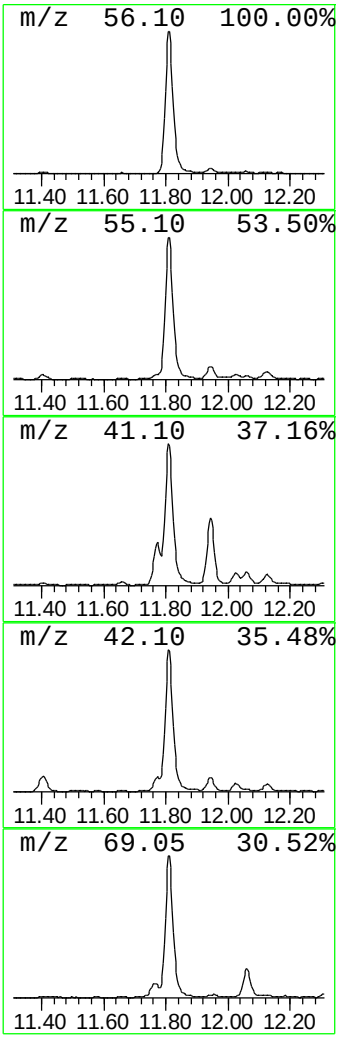
****

Peak Number 6 1-Hexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	36.72 ug/l	1073830	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	78
2	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
3	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
5	2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.M
Quant Title : SW846 8260

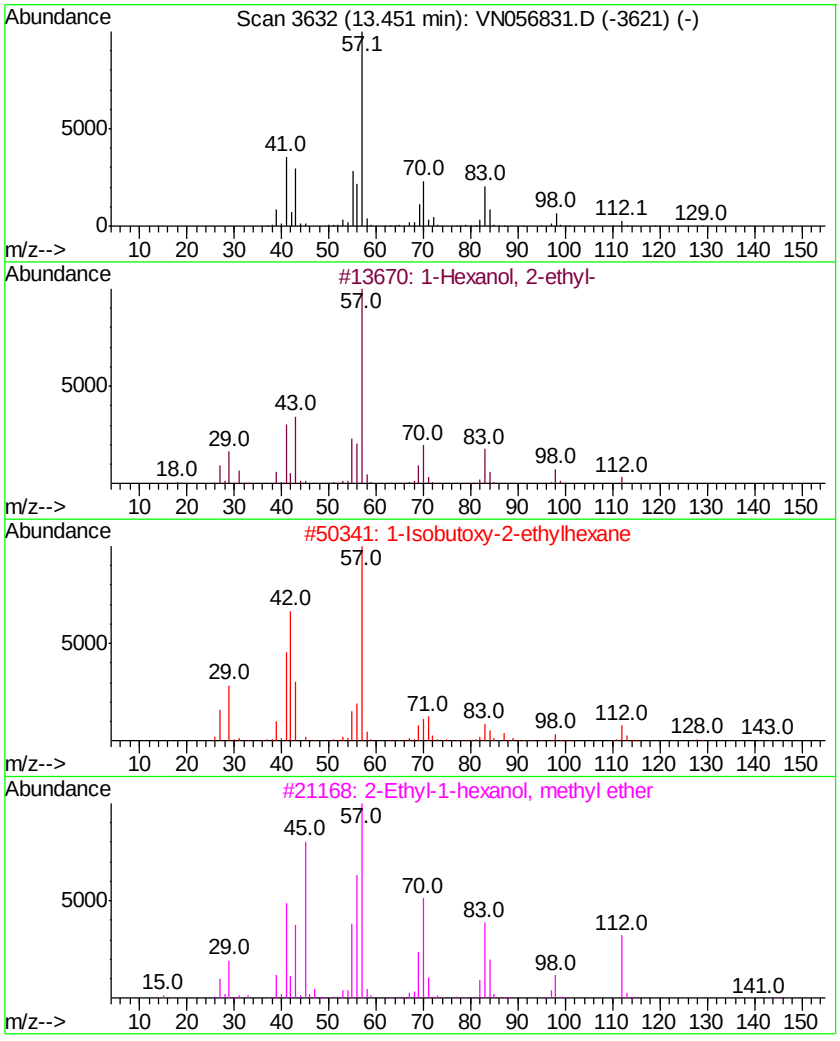
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

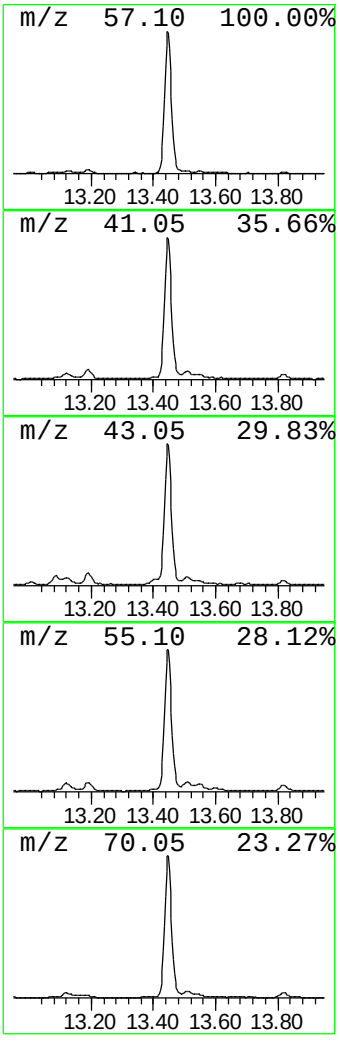
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	86.68 ug/l	2393480	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	78
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.M
Quant Title : SW846 8260

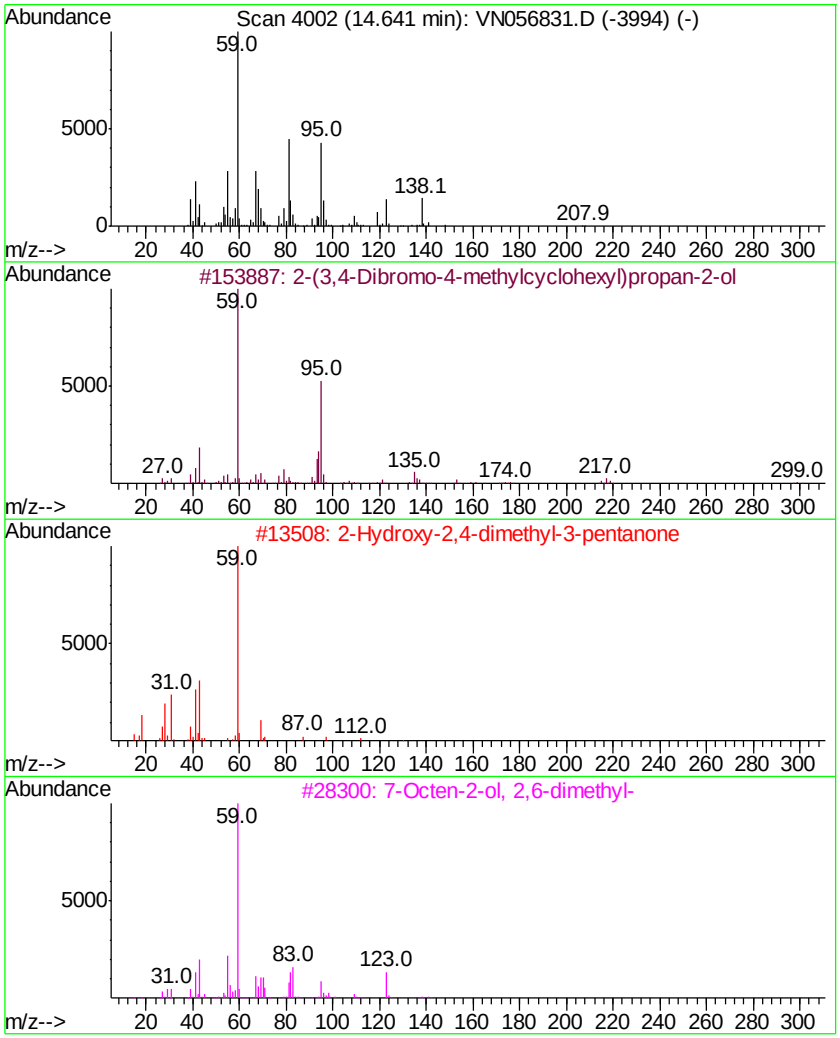
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

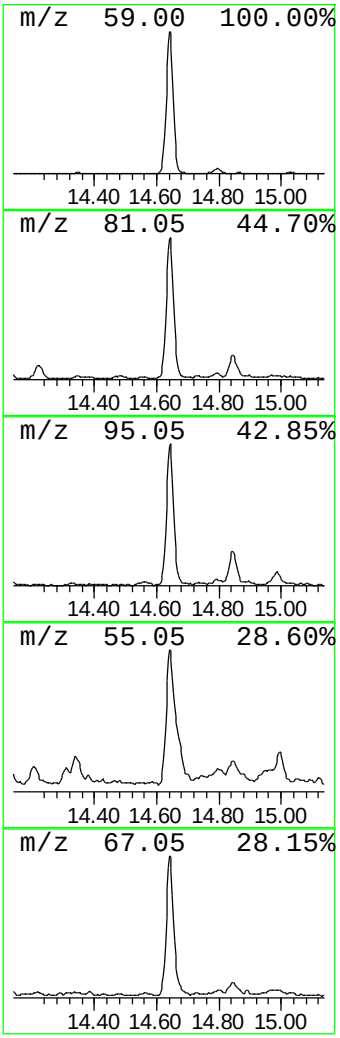
****

Peak Number 8 unknown14.64 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	16.70 ug/l	461225	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3,4-Dibromo-4-methylcyclohexy...	312	C10H18Br2O	110202-13-6	47
2	2-Hydroxy-2,4-dimethyl-3-pentanone	130	C7H14O2	003212-67-7	27
3	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	25
4	Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	25
5	Cyclooctanemethanol, .alpha.,.al...	170	C11H22O	016624-06-9	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN071919\
Data File : VN056831.D
Acq On : 19 Jul 2019 14:54
Operator : JC/SP
Sample : K2646-15
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N071519W.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
Ethanol	3.28	600.5	ug/l	8153640	1	7.66	678843	50.0
Butanal	6.54	185.8	ug/l	2522120	1	7.66	678843	50.0
2-Pentanone	9.04	20.7	ug/l	414696	2	8.59	1000600	50.0
Hexanal	10.85	139.6	ug/l	4080950	3	11.41	1462170	50.0
1-Hexanol	11.81	36.7	ug/l	1073830	3	11.41	1462170	50.0
1-Hexanol, 2-ethyl-	13.45	86.7	ug/l	2393480	4	13.34	1380630	50.0
unknown14.64	14.64	16.7	ug/l	461225	4	13.34	1380630	50.0