LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

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\82N011320W.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	2.291	147	161	179	rBV	471495	746504	2.54%	0.768%
2	3.233	440	454	500	rBV	241322	574525	1.96%	0.591%
3	3.664	570	588	645	rBV	10131178	29363899	100.00%	30.215%
4	6.050	1287	1330	1371	rBV	5268306	20430340	69.58%	21.022%
5	7.567	1784	1802	1813	rBV2	135118	333523	1.14%	0.343%
6	7.645	1813	1826	1855	rVB	256725	615231	2.10%	0.633%
7	8.005	1920	1938	1963	rVB	148790	356674	1.21%	0.367%
8	8.567	2096	2113	2132	rBV	369031	761896	2.59%	0.784%
9	8.764	2160	2174	2205	rBV	175715	369809	1.26%	0.381%
10	10.079	2563	2583	2600	rBV	575430	1065975	3.63%	1.097%
11	11.326	2954	2971	2982	rBV	353008	586569	2.00%	0.604%
12	11.400	2982	2994	3017	rVB	534525	938451	3.20%	0.966%
13	12.397	3291	3304	3323	rVB	433049	717630	2.44%	0.738%
14	13.339	3586	3597	3606	rBV	537119	875038	2.98%	0.900%
15	13.403	3606	3617	3624	rVV	2667472	4430646	15.09%	4.559%
16	13.445	3624	3630	3651	rVB	2175689	3250093	11.07%	3.344%
17	14.123	3826	3841	3852	rBV	223161	358451	1.22%	0.369%
18	14.204	3854	3866	3887	rBV	2134618	3221073	10.97%	3.314%
19	14.310	3887	3899	3902	rBV	2568481	3608219	12.29%	3.713%
20	14.339	3902	3908	3931	rVB	5785144	9044350	30.80%	9.306%
21	14.667	3998	4010	4048	rBV	8798964	13079987	44.54%	13.459%
22	14.844	4055	4065	4076	rBV	594529	983674	3.35%	1.012%
23	14.995	4101	4112	4123	rBV	550427	897795	3.06%	0.924%
24	15.789	4348	4359	4373	rVB	322810	573138	1.95%	0.590%

Sum of corrected areas: 97183490

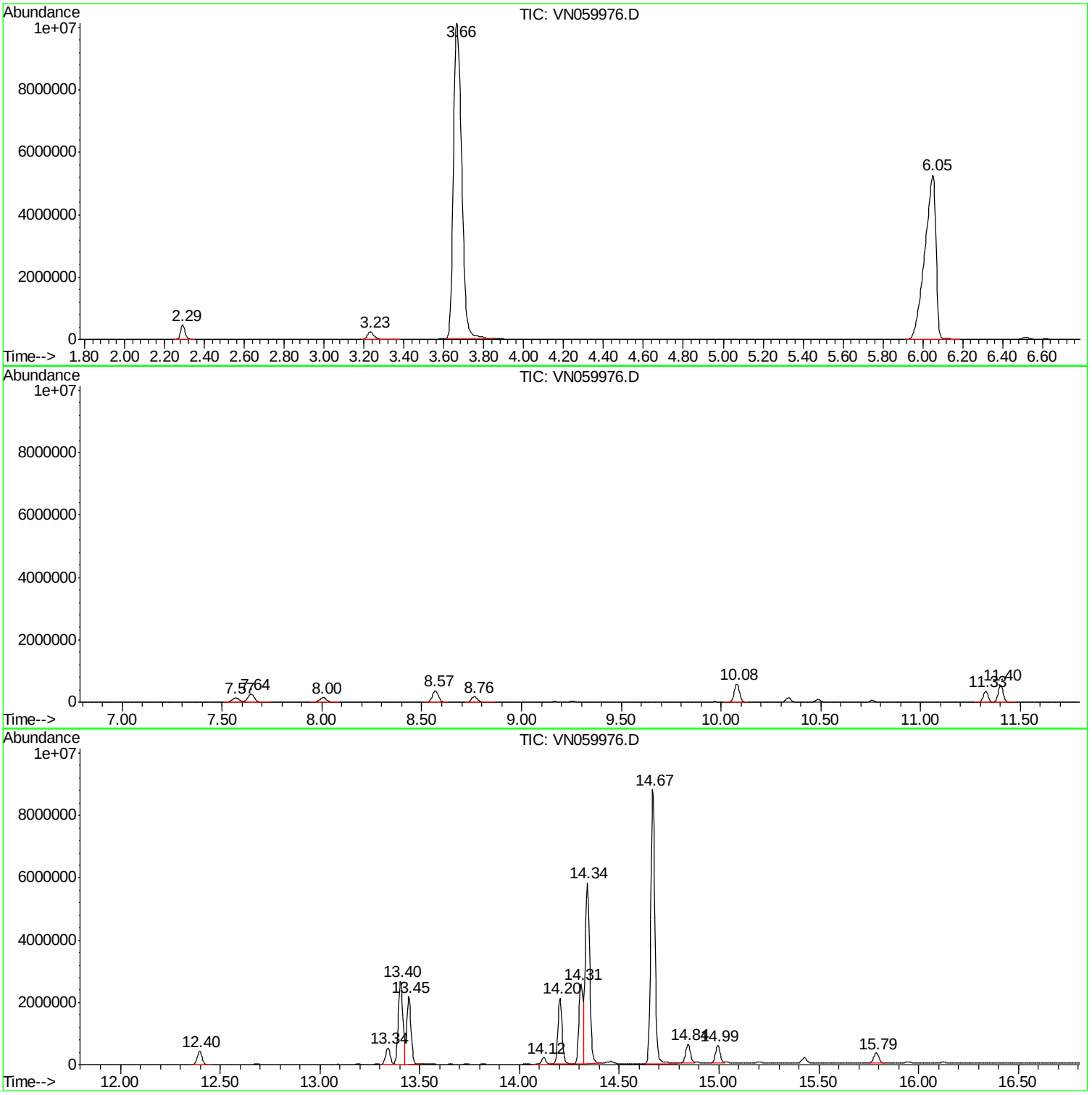
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.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\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

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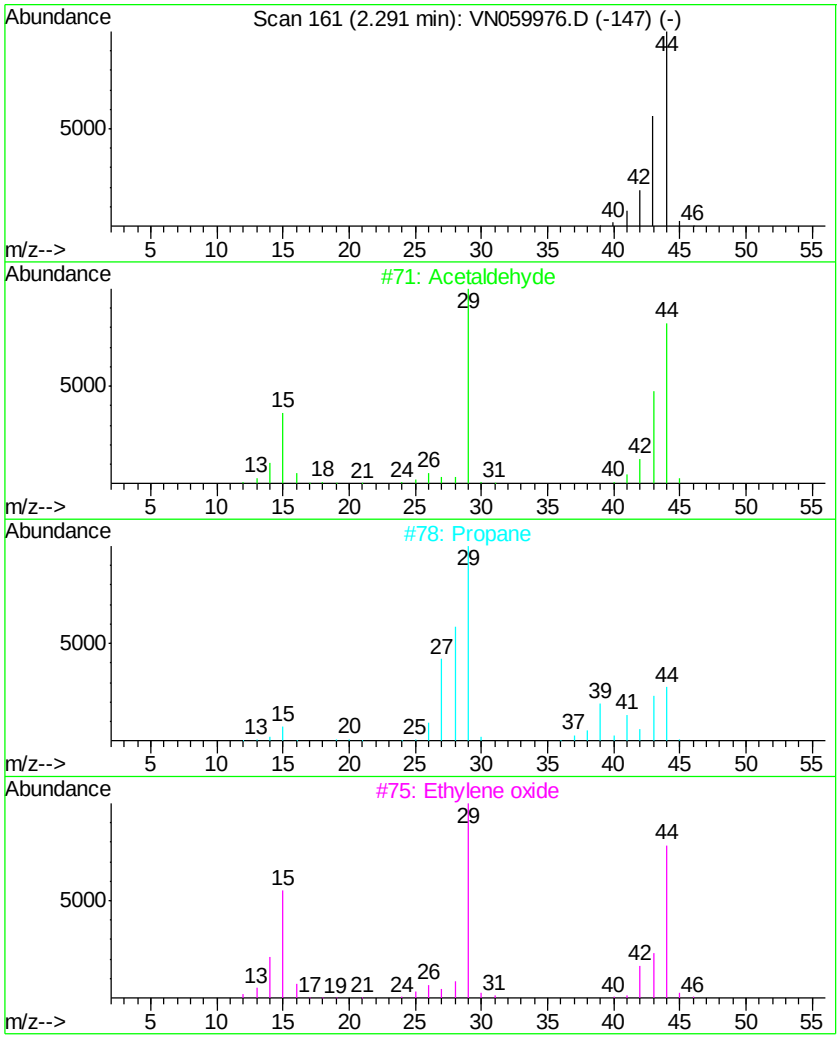
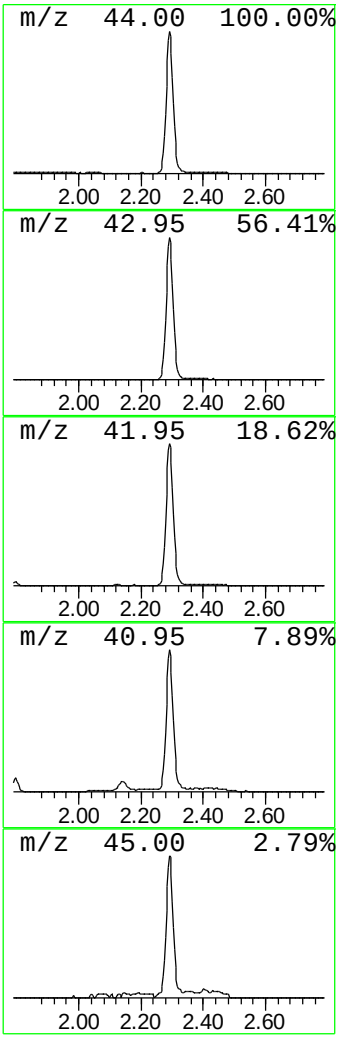
Peak Number 1 Acetaldehyde Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	60.67 ug/l	746504	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5	Alanine	89	C3H7NO2	000056-41-7	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

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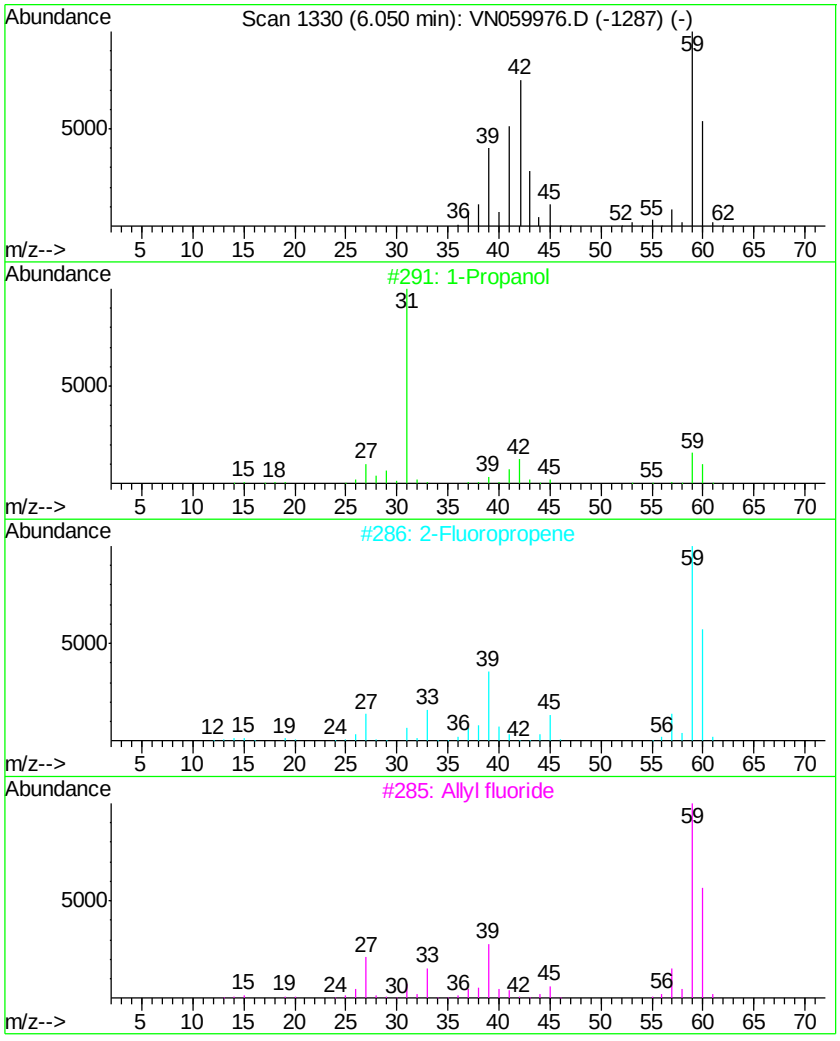
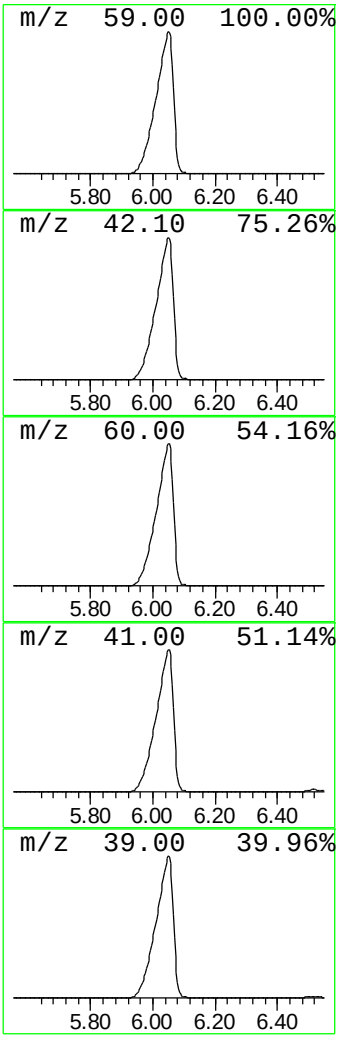
Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.05	1660.38 ug/l	20430300	Pentafluorobenzene	7.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	59
2	2-Fluoropropene	60	C3H5F	001184-60-7	50
3	Allyl fluoride	60	C3H5F	000818-92-8	32
4	Cyclopropane	42	C3H6	000075-19-4	25
5	Propene	42	C3H6	000115-07-1	17





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

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

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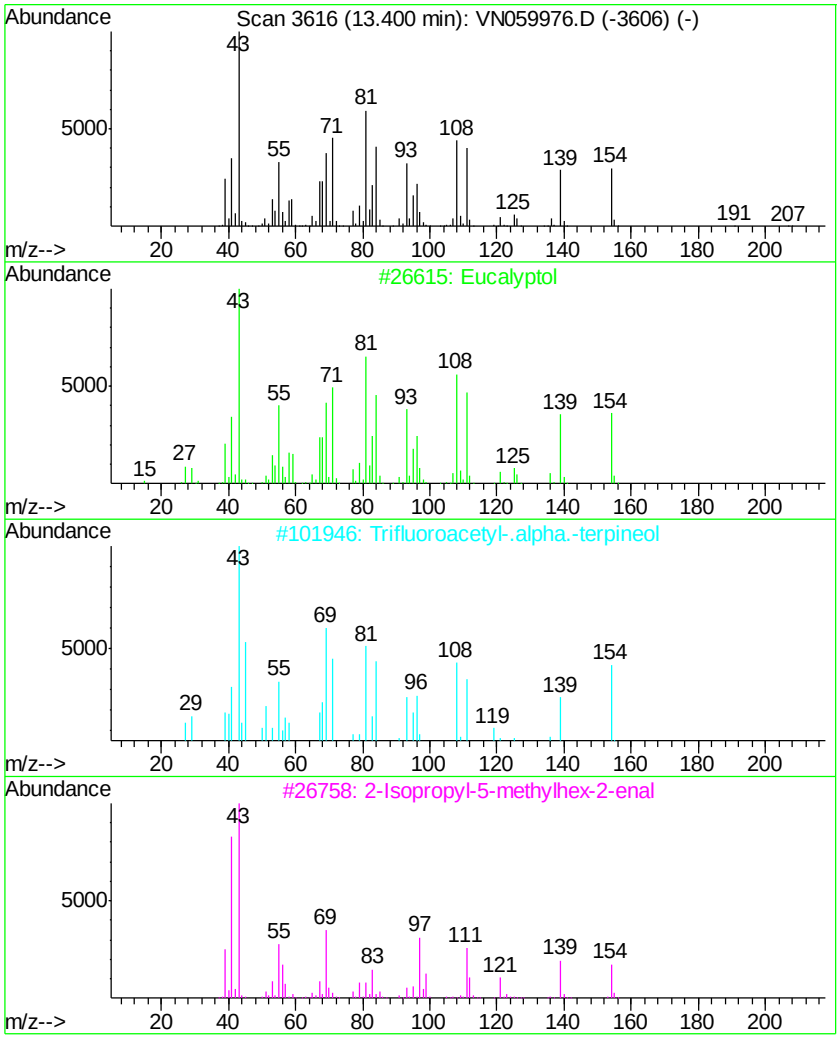
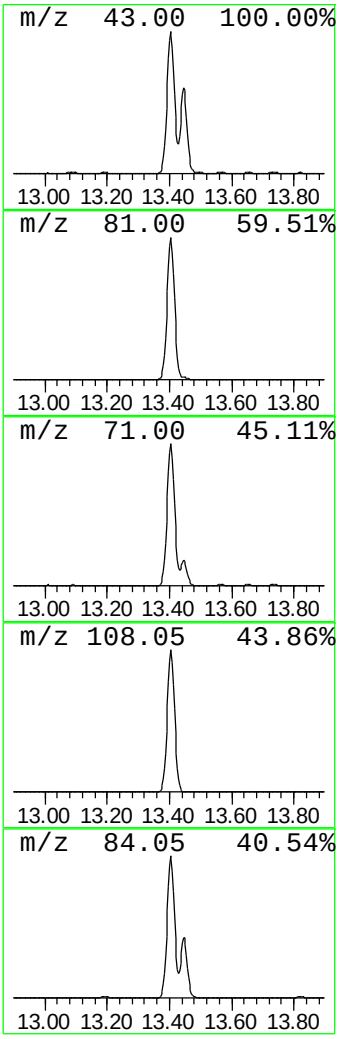
Peak Number 4 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	253.17 ug/l	4430650	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	43
3	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27
4	1-Hepten-6-one, 2-methyl-	126	C8H14O	010408-15-8	27
5	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

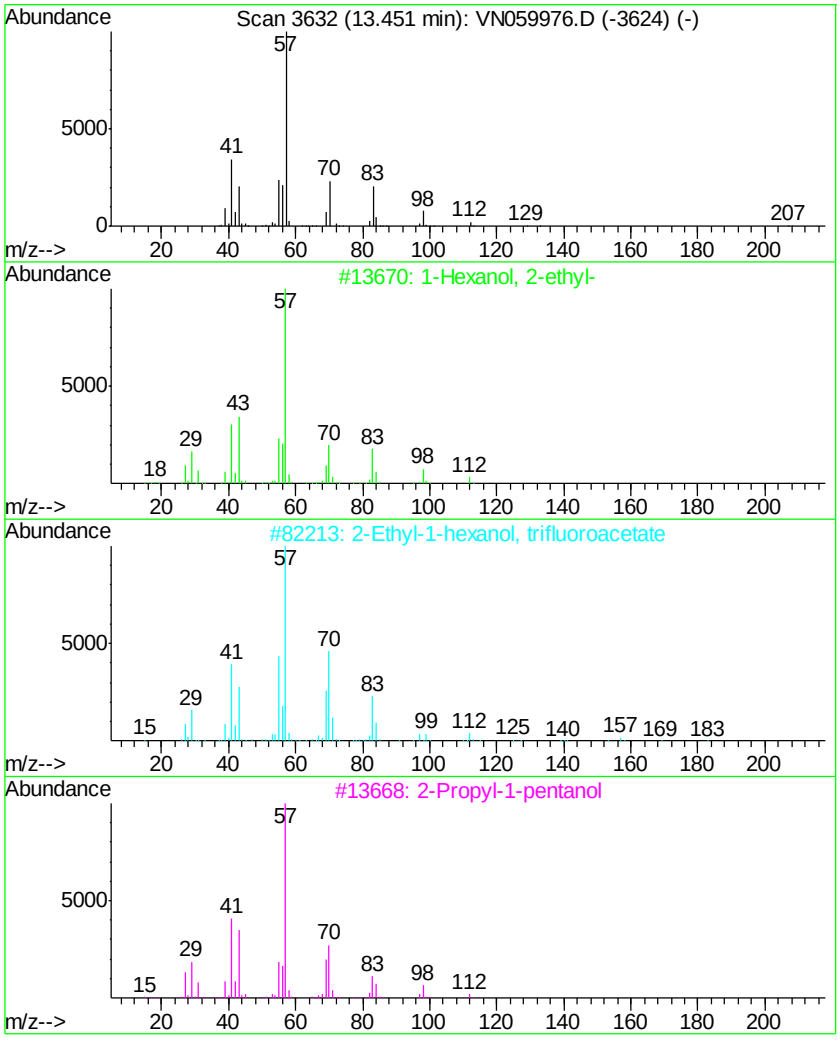
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

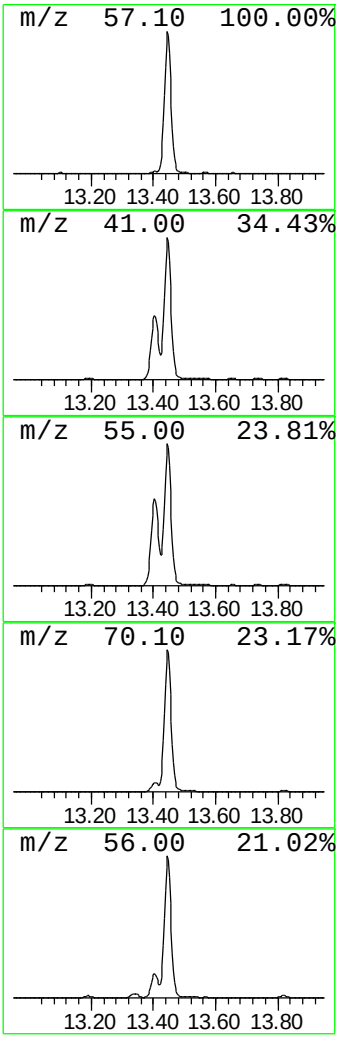
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	185.71 ug/l	3250090	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	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	43
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	43
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	38
5	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	37





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

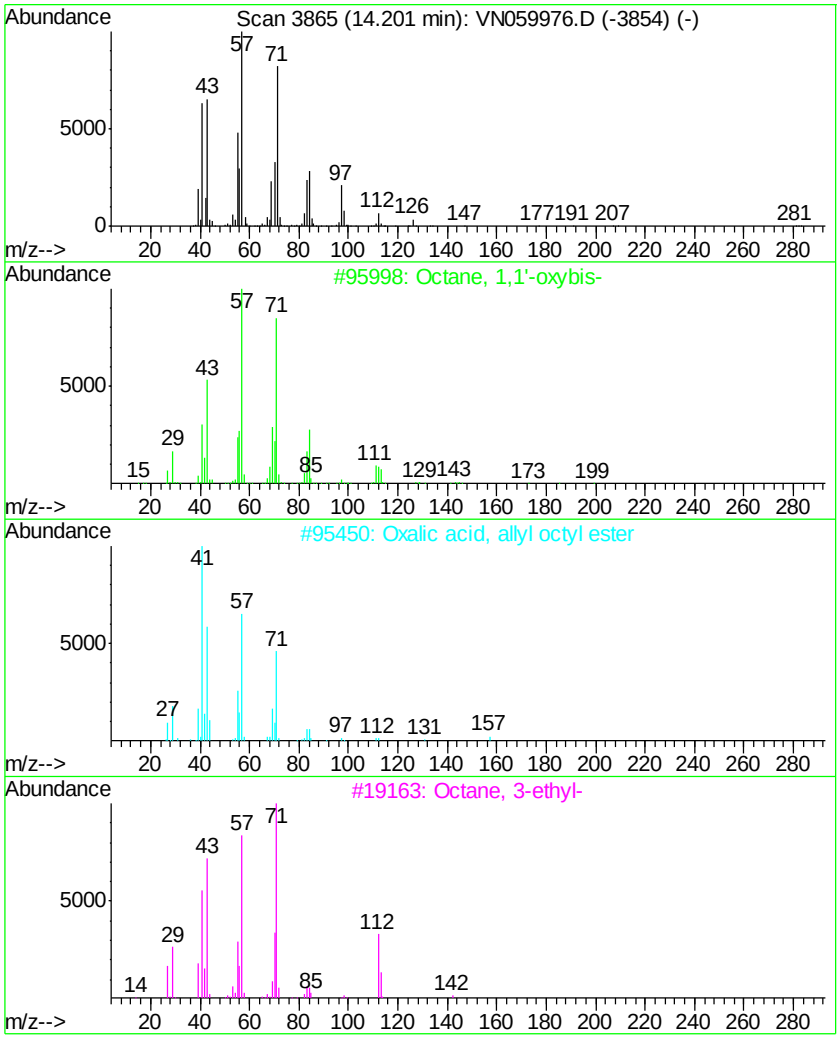
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

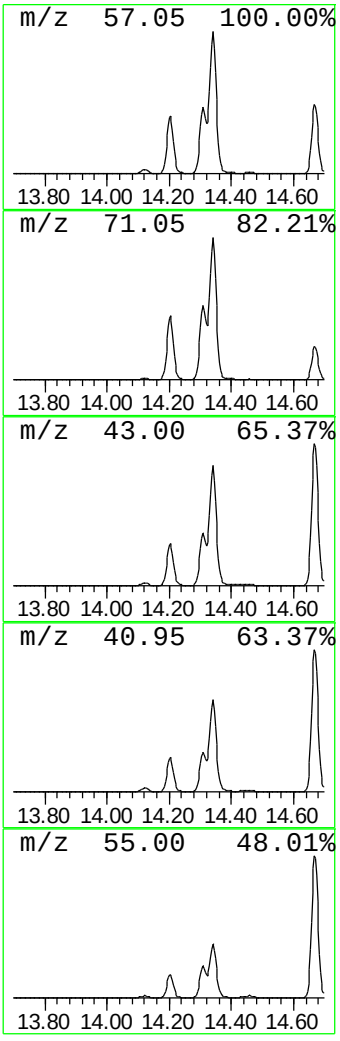
****

Peak Number 6 Octane, 1,1'-oxybis- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	184.05 ug/l	3221070	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
2	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	53
3	Octane, 3-ethyl-	142	C10H22	005881-17-4	50
4	1-Decene, 4-methyl-	154	C11H22	013151-29-6	47
5	Isobutyl octyl carbonate	230	C13H26O3	1000372-74-6	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

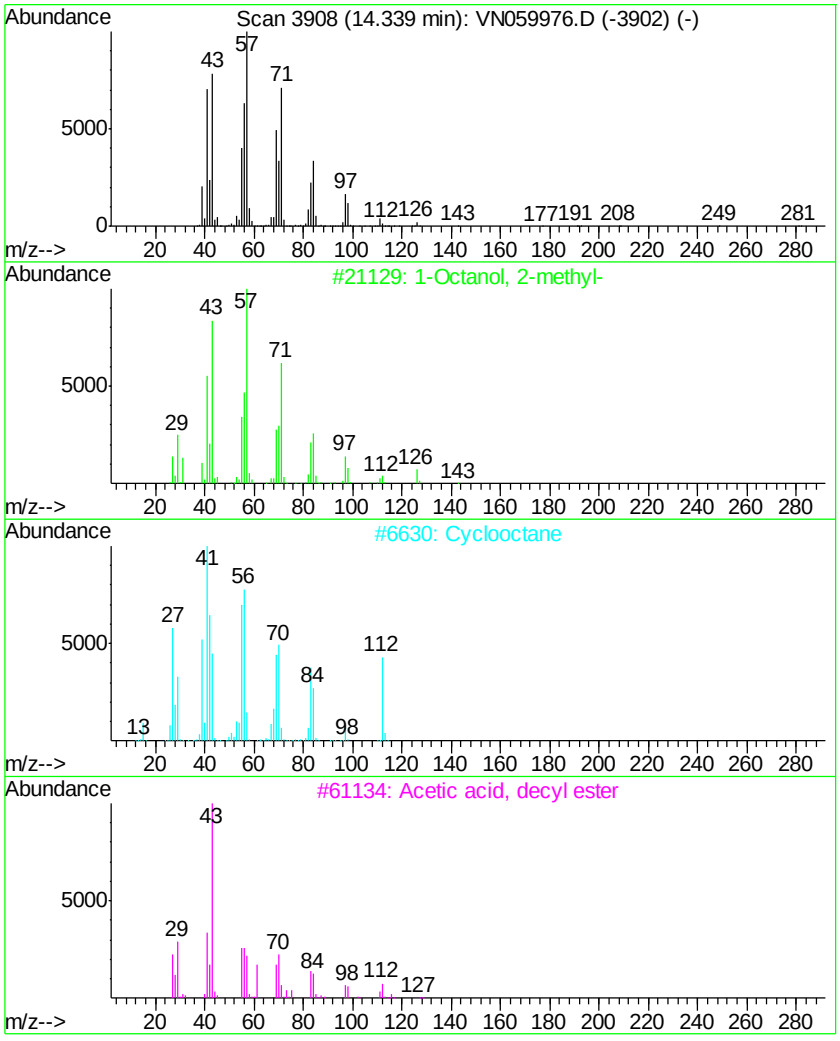
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

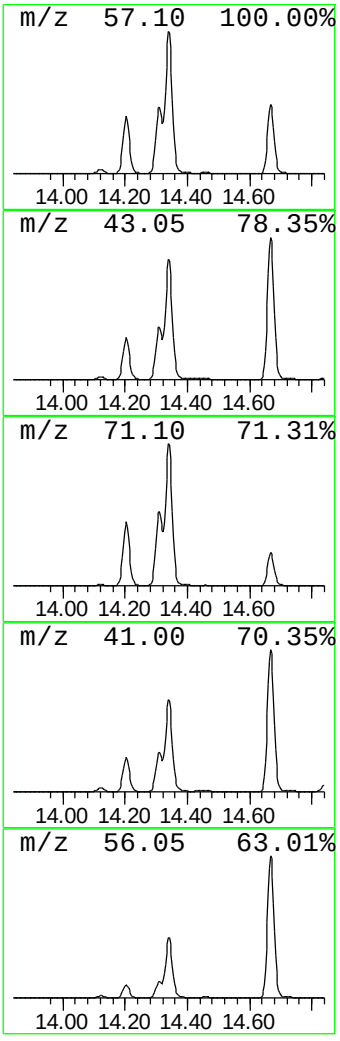
****

Peak Number 8 1-Octanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	516.80 ug/l	9044350	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	90
2	Cyclooctane	112	C8H16	000292-64-8	43
3	Acetic acid, decyl ester	200	C12H24O2	000112-17-4	43
4	Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	38
5	1-Heptene	98	C7H14	000592-76-7	38





Library Search Compound Report

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Sample : L1329-17
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

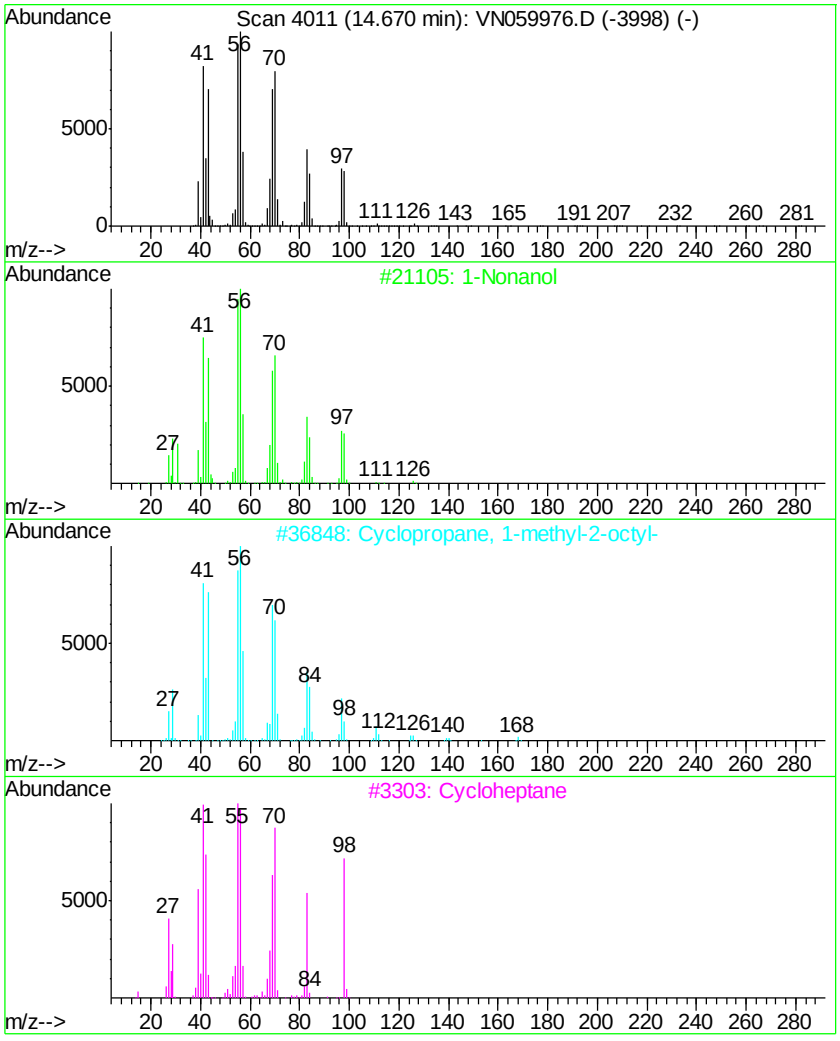
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

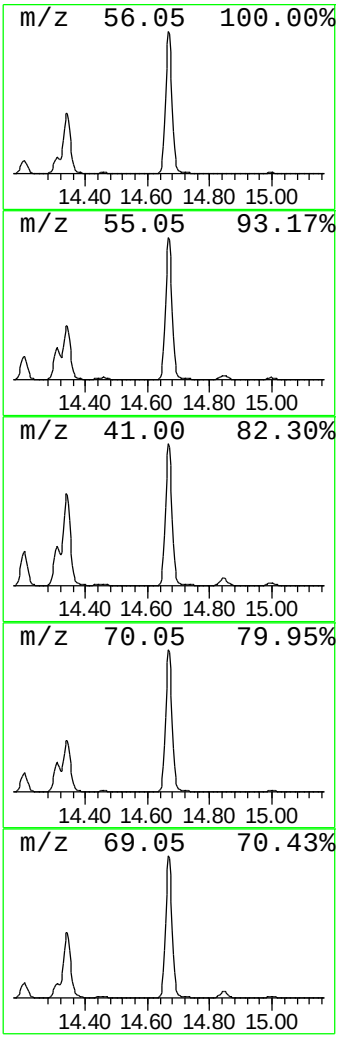
****

Peak Number 9 1-Nonanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	747.40 ug/l	13080000	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
3	Cycloheptane	98	C7H14	000291-64-5	72
4	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	70
5	Isopropylcyclobutane	98	C7H14	000872-56-0	62





Library Search Compound Report

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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.M
Quant Title : SW846 8260

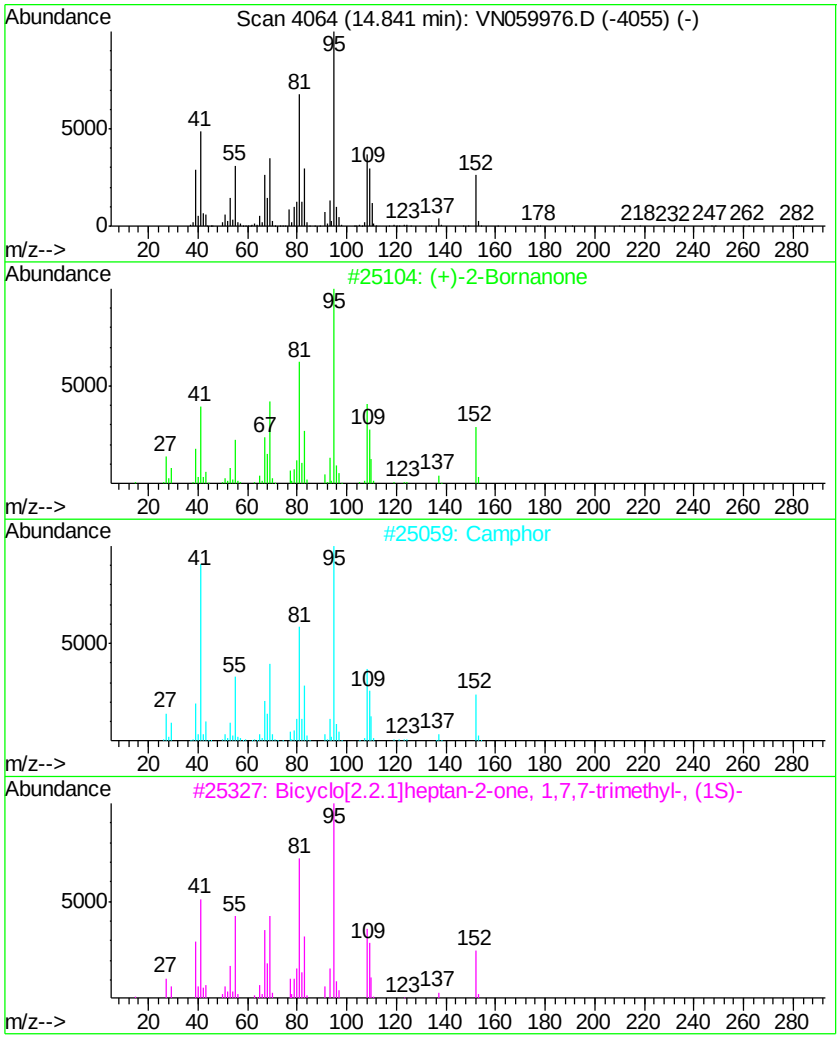
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

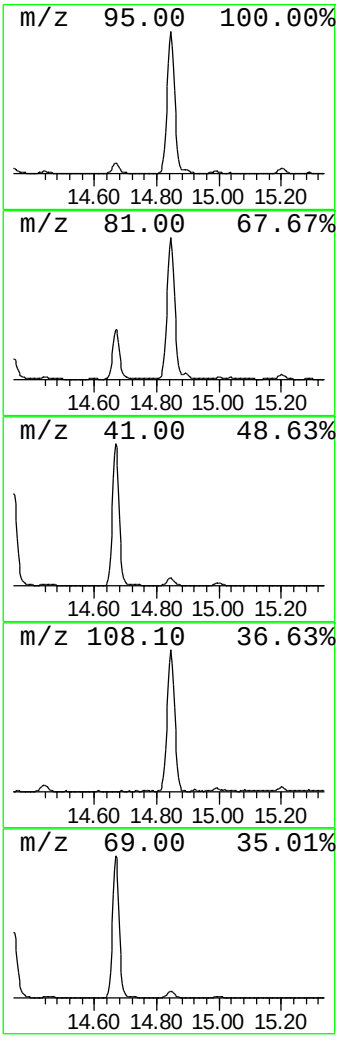
****

Peak Number 10 (+)-2-Bornanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	56.21 ug/l	983674	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020320\
Data File : VN059976.D
Acq On : 3 Feb 2020 15:48
Operator : JC/MD
Sample : L1329-17
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 40098

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N011320W.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
Acetaldehyde	2.29	60.7	ug/l	746504	1	7.64	615231	50.0
1-Propanol	6.05	1660.4	ug/l	20430300	1	7.64	615231	50.0
Eucalyptol	13.40	253.2	ug/l	4430650	4	13.34	875038	50.0
1-Hexanol, 2-ethyl-	13.45	185.7	ug/l	3250090	4	13.34	875038	50.0
Octane, 1,1'-oxybis-	14.20	184.1	ug/l	3221070	4	13.34	875038	50.0
1-Octanol, 2-methyl-	14.34	516.8	ug/l	9044350	4	13.34	875038	50.0
1-Nonanol	14.67	747.4	ug/l	13080000	4	13.34	875038	50.0
(+)-2-Bornanone	14.84	56.2	ug/l	983674	4	13.34	875038	50.0