LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

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_X\METHOD\82X120420W.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	1.276	28	31	44	rVB	241466	280642	3.03%	0.752%
2	2.435	213	221	237	rBV2	100799	276034	2.98%	0.739%
3	3.008	304	315	333	rBV	3403800	7460679	80.59%	19.982%
4	4.660	562	586	598	rBV	2894007	9257641	100.00%	24.795%
5	5.080	644	655	683	rVB	1294468	3857798	41.67%	10.333%
6	5.458	706	717	730	rBV	177679	501499	5.42%	1.343%
7	5.623	733	744	759	rVB	319760	894782	9.67%	2.397%
8	6.025	800	810	819	rBV	201304	530387	5.73%	1.421%
9	6.251	839	847	850	rBV2	48560	130815	1.41%	0.350%
10	6.824	932	941	954	rVV	488591	1157048	12.50%	3.099%
11	7.952	1119	1126	1132	rBV	56317	103024	1.11%	0.276%
12	8.696	1241	1248	1254	rBV	1030301	1599959	17.28%	4.285%
13	8.763	1254	1259	1267	rVB2	124081	213967	2.31%	0.573%
14	8.848	1267	1273	1278	rBV	133536	210386	2.27%	0.563%
15	9.415	1358	1366	1372	rBV	344219	532362	5.75%	1.426%
16	10.092	1466	1477	1489	rBV	1032546	1597195	17.25%	4.278%
17	10.250	1497	1503	1507	rBV2	52205	95648	1.03%	0.256%
18	10.342	1513	1518	1523	rVB	204025	291404	3.15%	0.780%
19	10.683	1569	1574	1578	rBV	151736	203333	2.20%	0.545%
20	11.122	1640	1646	1651	rBV	844098	1092125	11.80%	2.925%
21	11.927	1769	1778	1786	rVB3	126832	190404	2.06%	0.510%
22	12.061	1793	1800	1807	rVB	1092209	1430078	15.45%	3.830%
23	12.140	1807	1813	1817	rBV2	263098	392394	4.24%	1.051%
24	12.280	1828	1836	1841	rBV2	66708	130878	1.41%	0.351%
25	12.561	1878	1882	1887	rBV3	58248	116220	1.26%	0.311%
26	12.616	1887	1891	1902	rVB	194571	261432	2.82%	0.700%
27	12.799	1914	1921	1926	rBV2	356292	512007	5.53%	1.371%
28	12.945	1933	1945	1950	rBV	1741771	2238632	24.18%	5.996%
29	13.000	1950	1954	1959	rVB3	115005	168798	1.82%	0.452%
30	13.518	2033	2039	2043	rBV3	232146	384711	4.16%	1.030%
31	13.628	2051	2057	2067	rBV	817084	1224032	13.22%	3.278%

Sum of corrected areas: 37336314

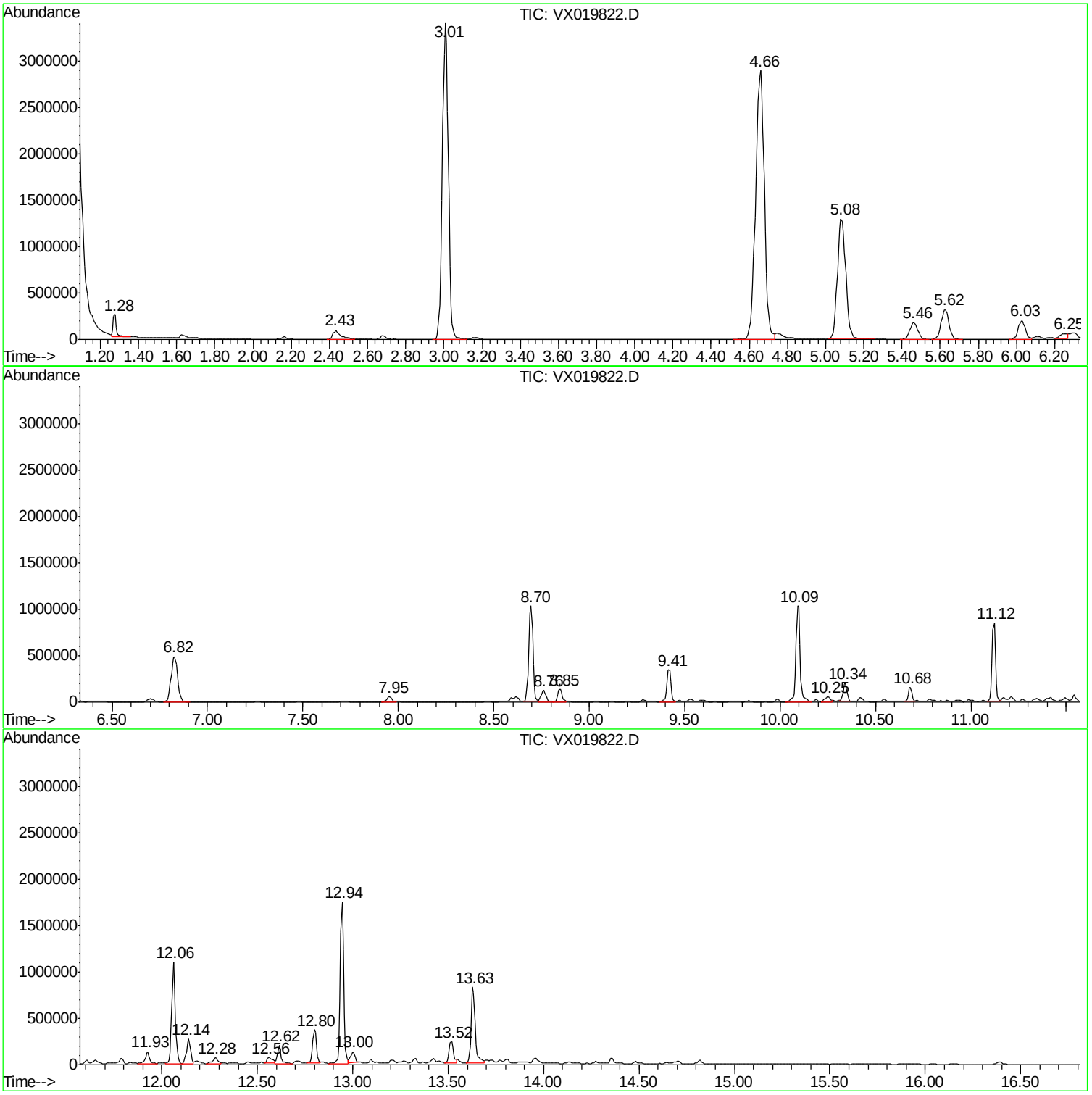
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.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 X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

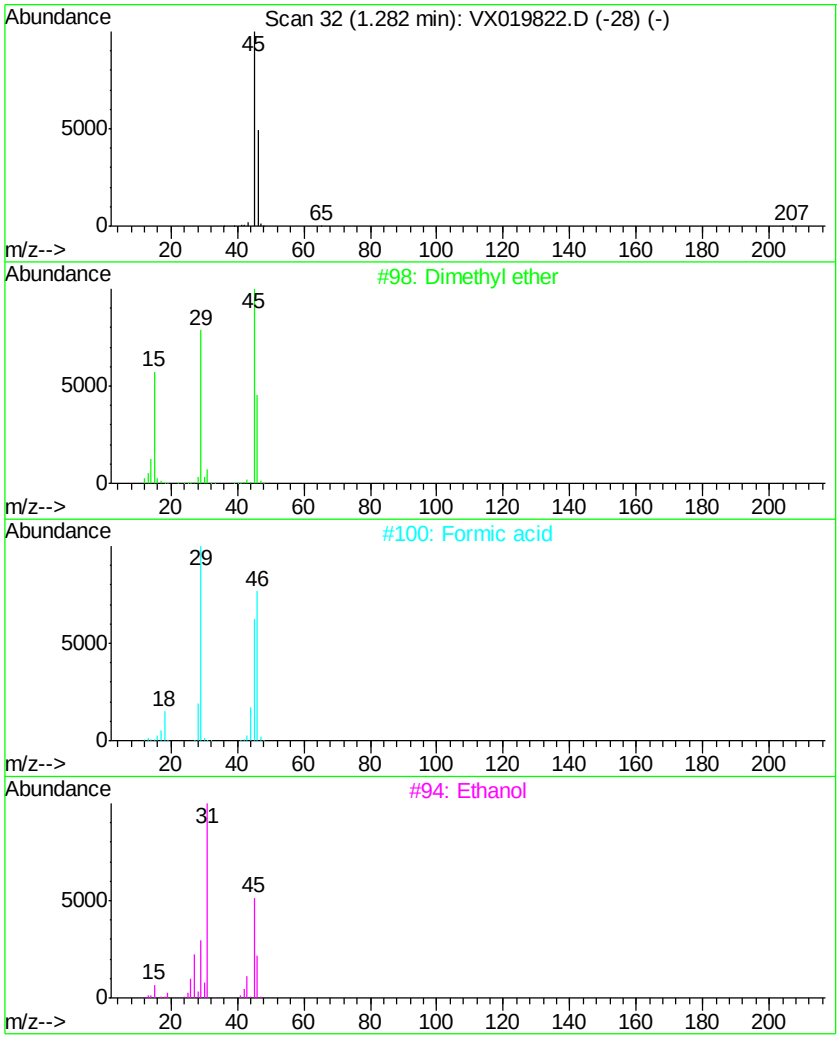
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

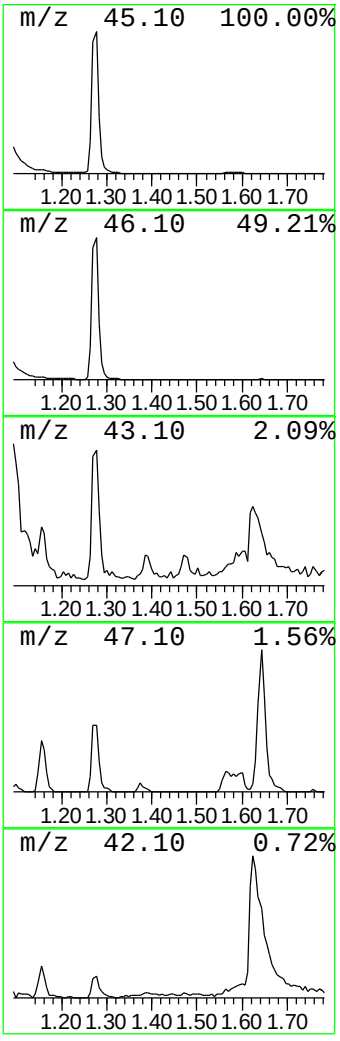
****

Peak Number 1 Dimethyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	15.68 ug/l	280642	Pentafluorobenzene	5.62

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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

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

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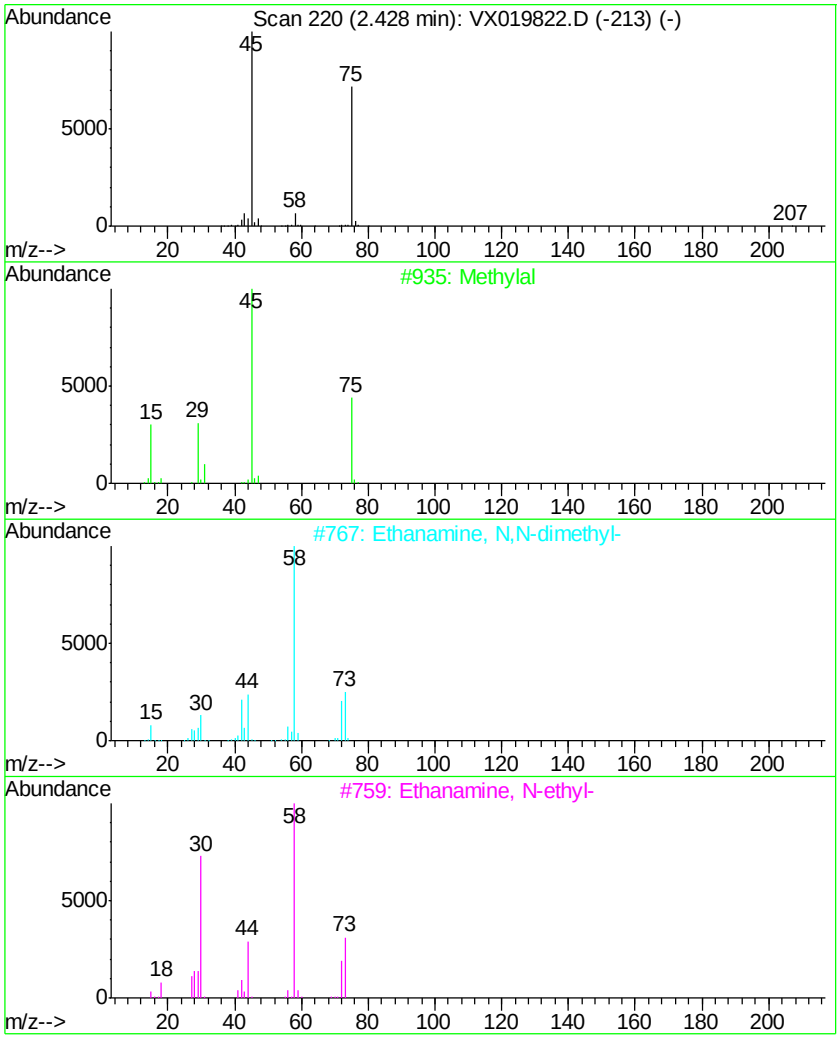
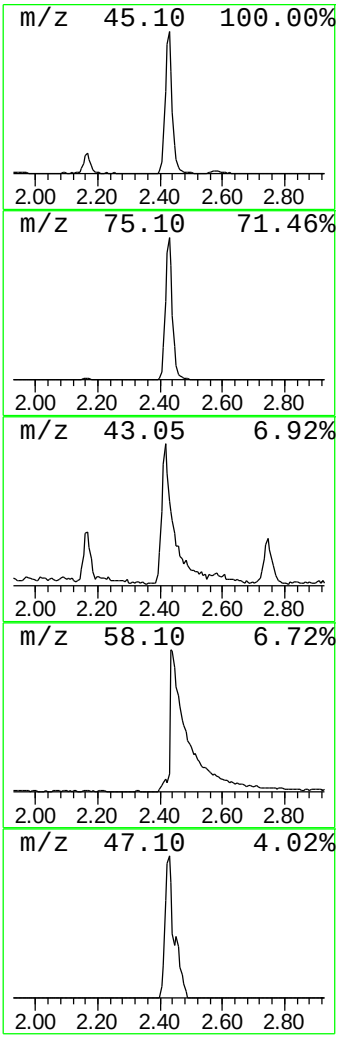
Peak Number 2 unknown2.43 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	15.42 ug/l	276034	Pentafluorobenzene	5.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylal	76	C3H8O2	000109-87-5	25
2	Ethanamine, N,N-dimethyl-	73	C4H11N	000598-56-1	18
3	Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	18
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	16
5	2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	12





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

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

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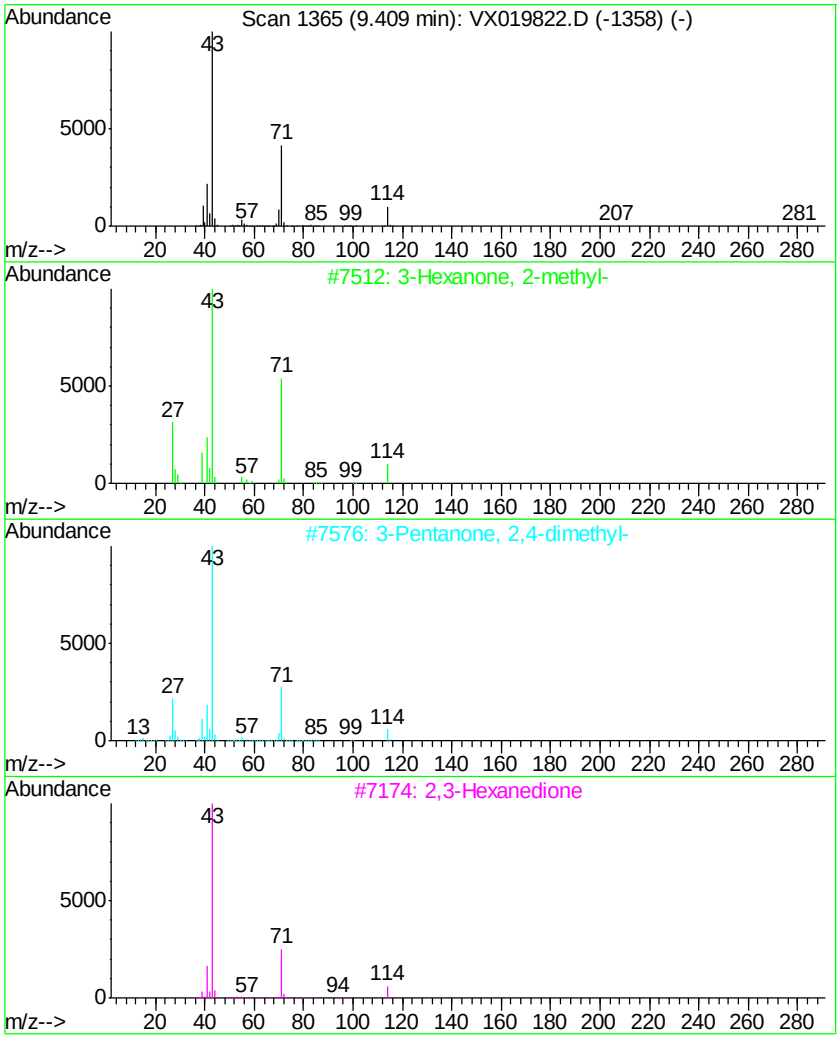
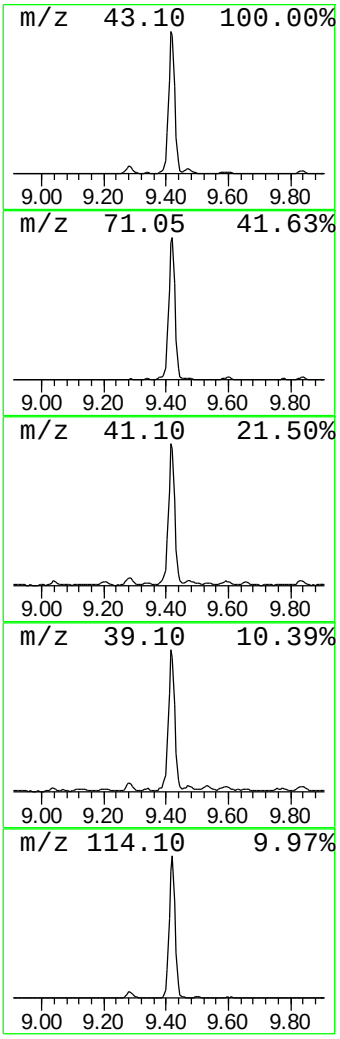
Peak Number 4 3-Hexanone, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	16.67 ug/l	532362	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
2	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	80
4	4-Heptanone	114	C7H14O	000123-19-3	59
5	Pyrrolidine	71	C4H9N	000123-75-1	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

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

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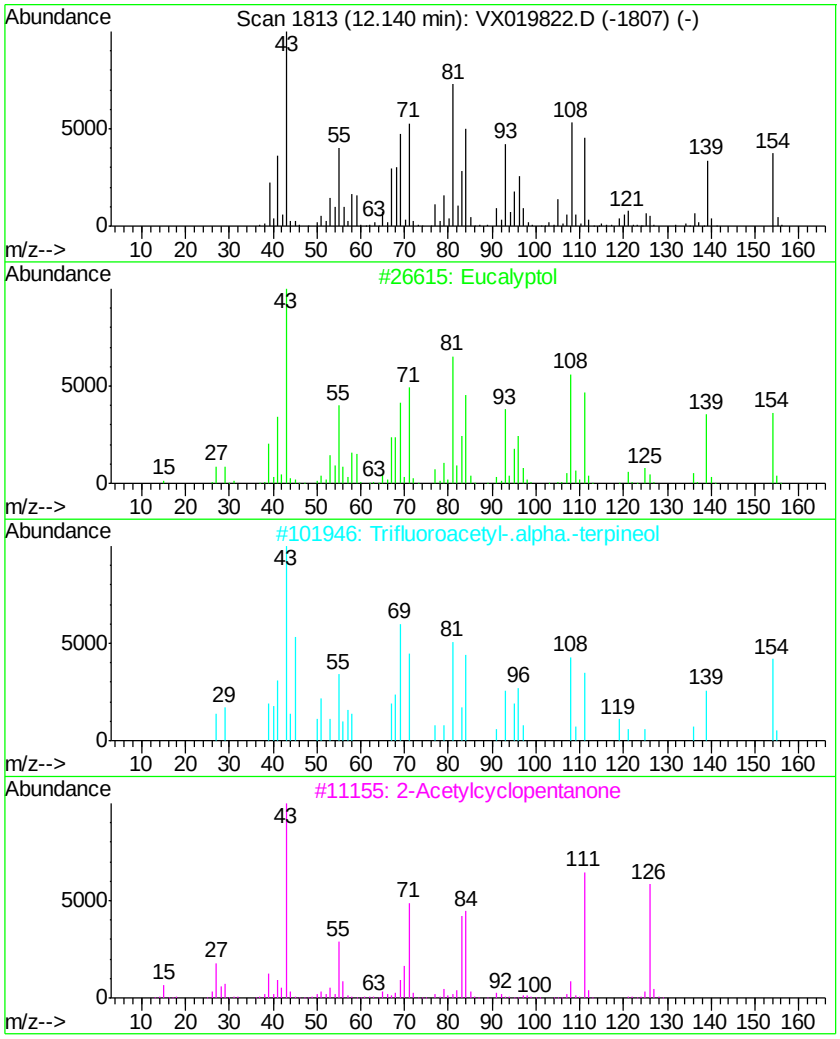
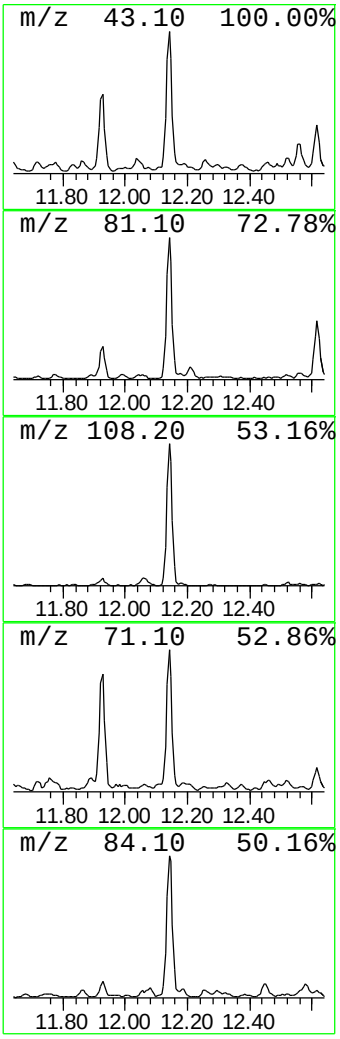
Peak Number 5 Eucalyptol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	13.72 ug/l	392394	1,4-Dichlorobenzene-d4	12.06

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	90
3	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
4	4-Chlorobenzoic acid, 2-tetrahyd...	240	C12H13ClO3	004650-87-7	32
5	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

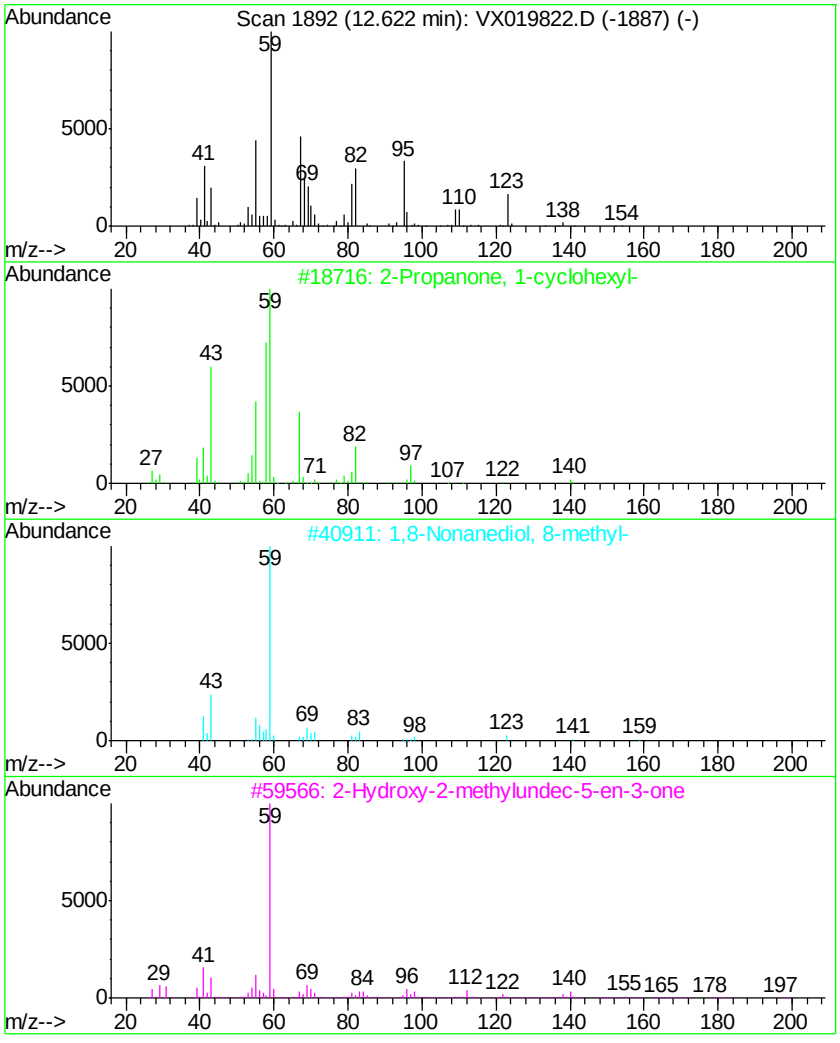
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

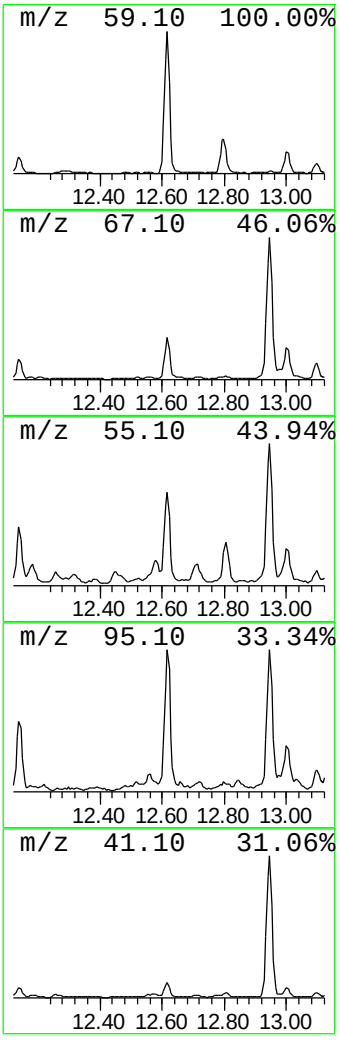
****

Peak Number 6 unknown12.62 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	9.14 ug/l	261432	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	40
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	27
3	2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	25
4	3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-97-5	16
5	5-Hexyn-3-ol	98	C6H10O	019780-84-8	12





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

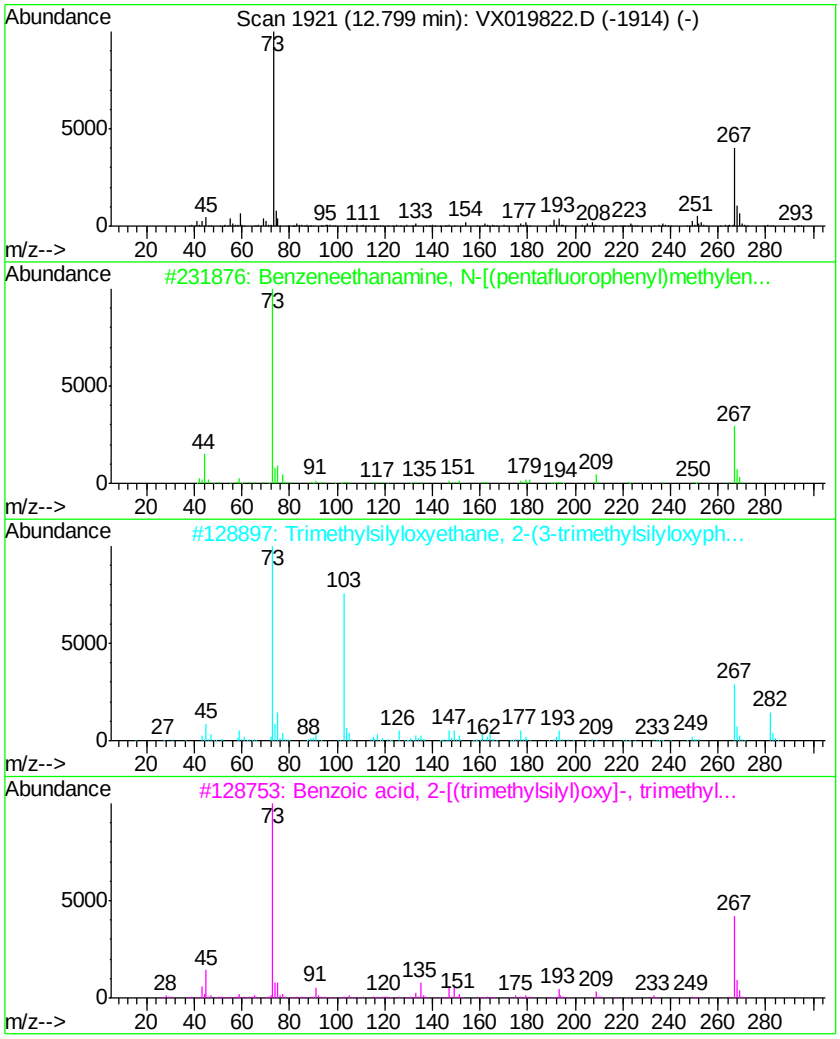
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

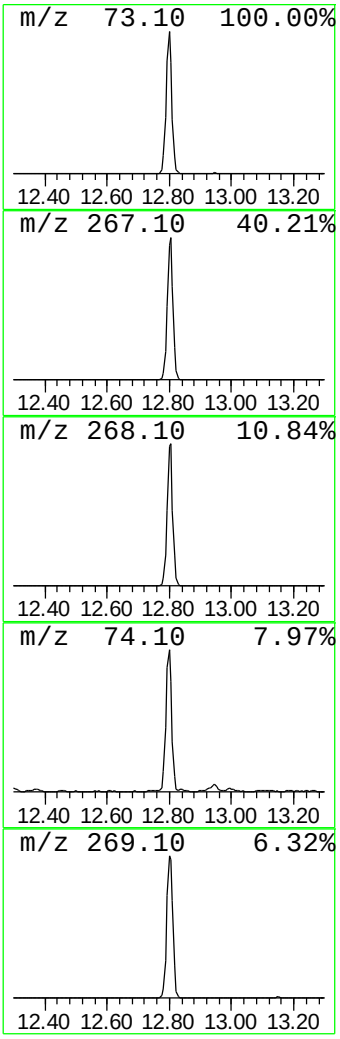
****

Peak Number 7 unknown12.80 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	17.90 ug/l	512007	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	45
2	Trimethylsilyloxyethane, 2-(3-tr...	282	C14H26O2Si2	1000365-49-0	39
3	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	39
4	1-(3-Chlorophenyl)piperazine, 4-...	268	C13H21ClN2Si	1000373-99-3	14
5	Propanal, 2-methyl-, (2,4-dinitr...	252	C10H12N4O4	002057-82-1	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

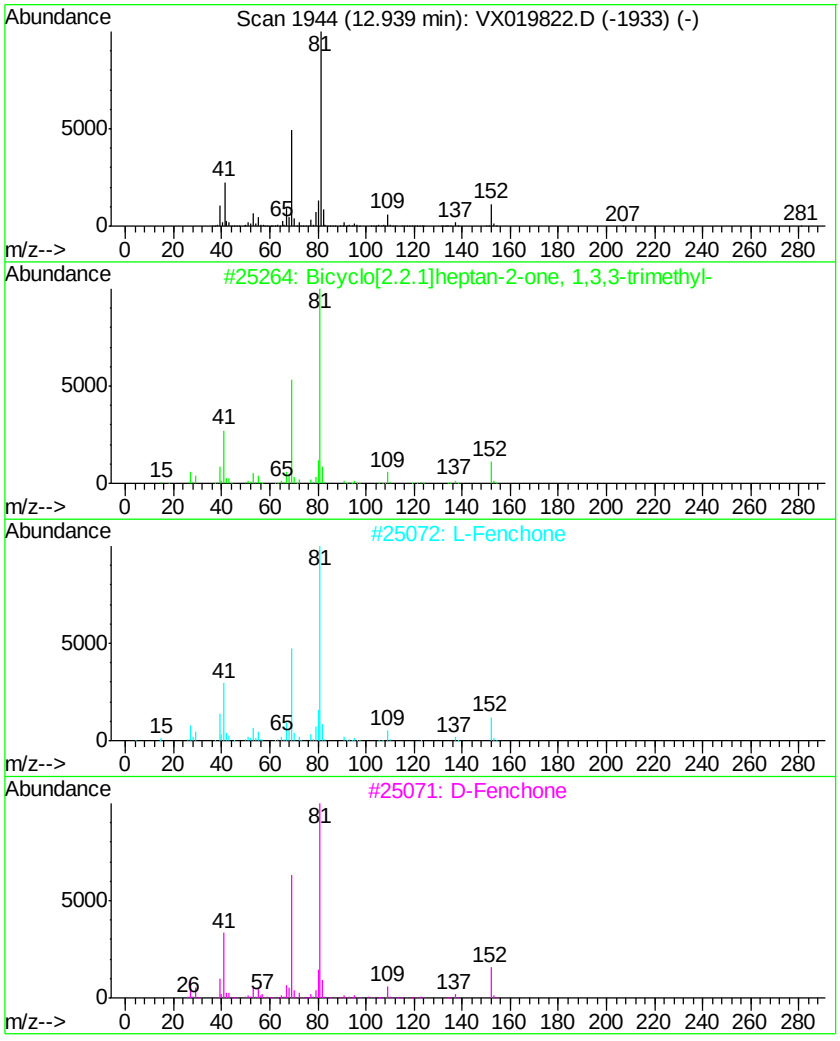
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

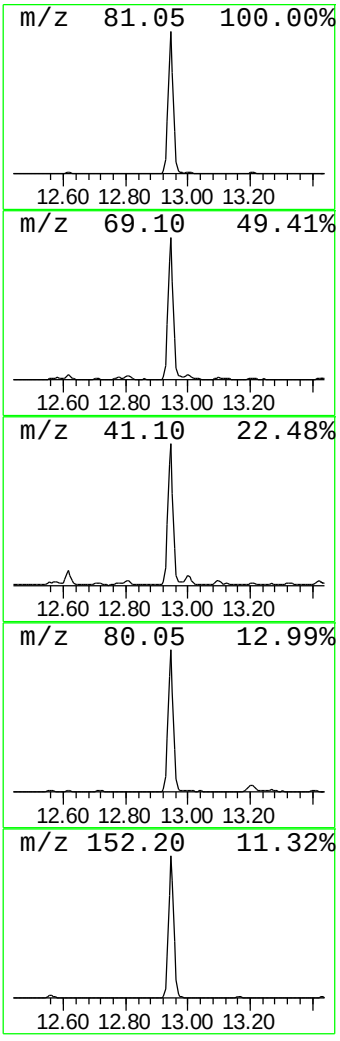
****

Peak Number 8 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	78.27 ug/l	2238630	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	95
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42
5	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

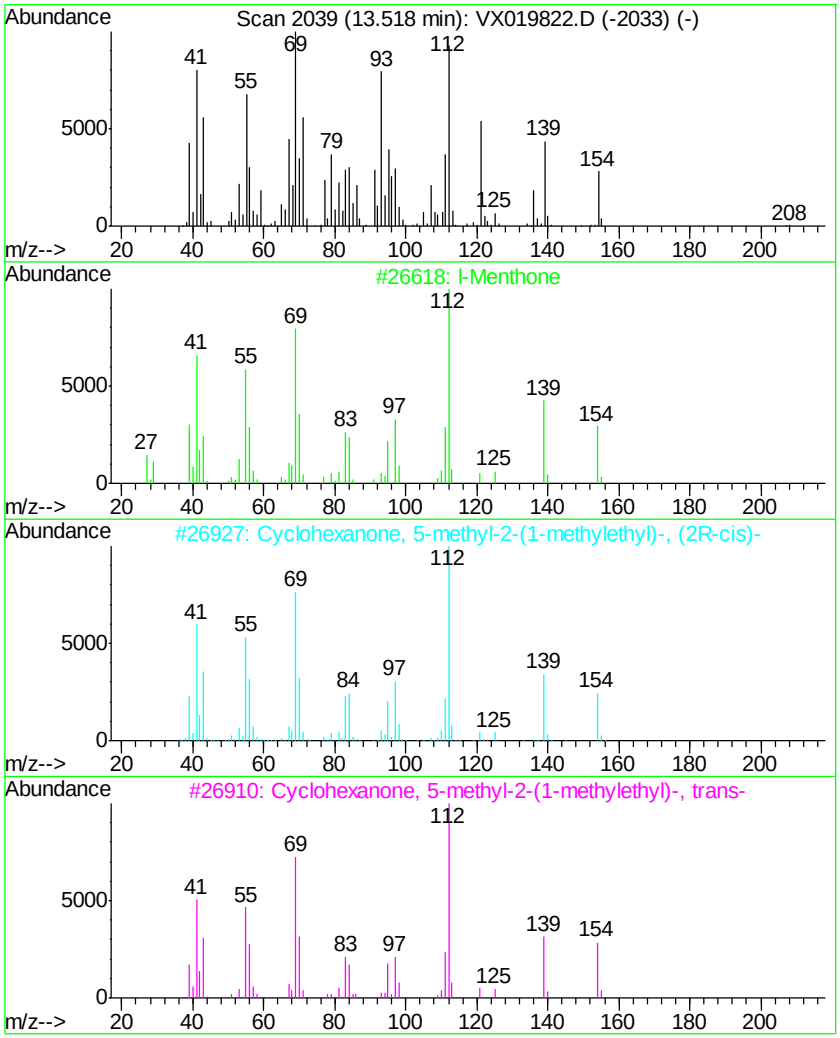
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

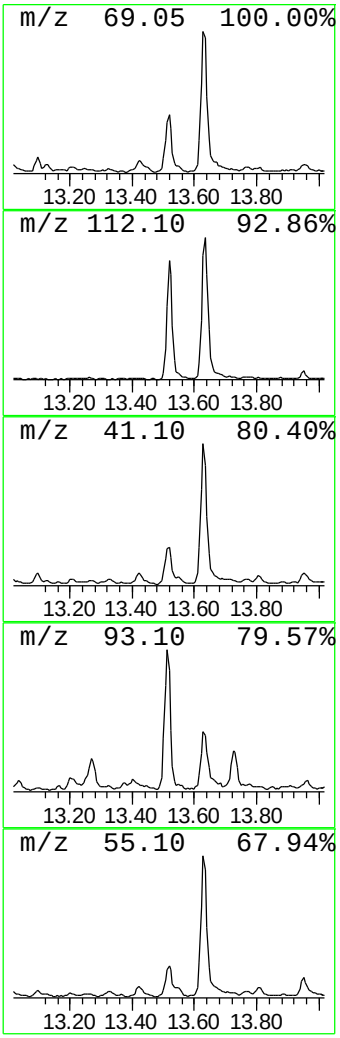
****

Peak Number 9 l-Menthone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	13.45 ug/l	384711	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	l-Menthone	154	C10H18O	014073-97-3	98
2	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	96
3	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	86
4	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	86
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	52





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.M
Quant Title : SW846 8260

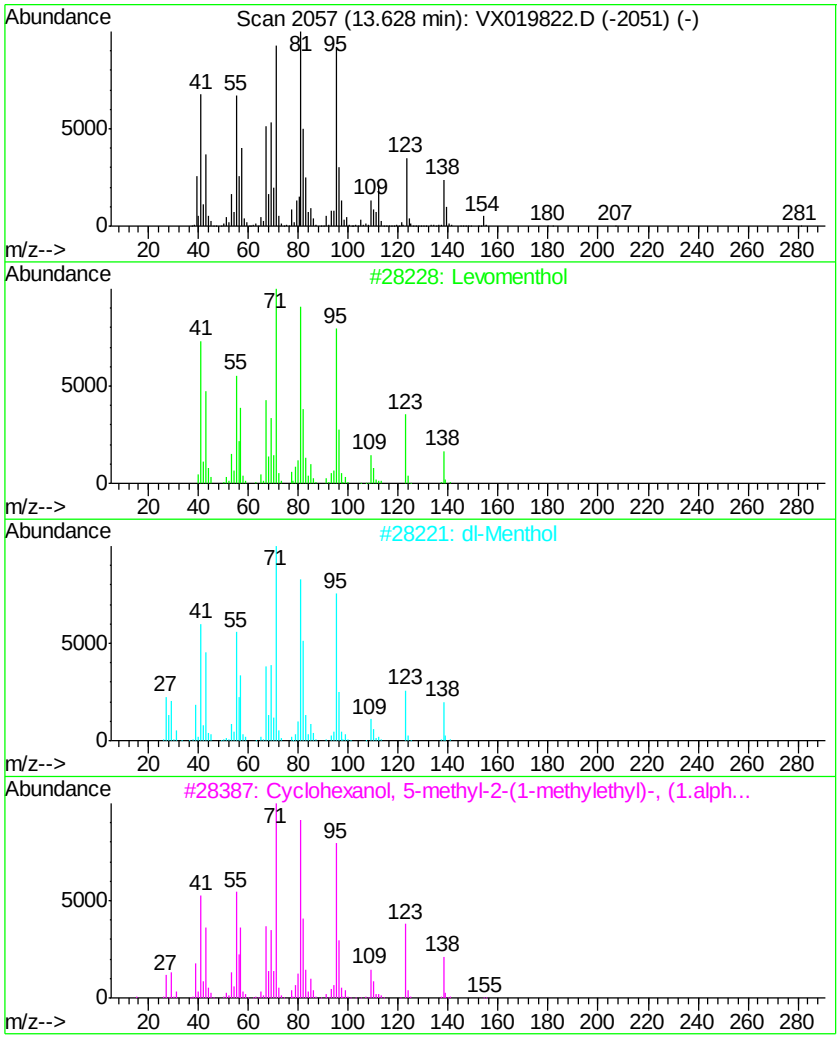
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

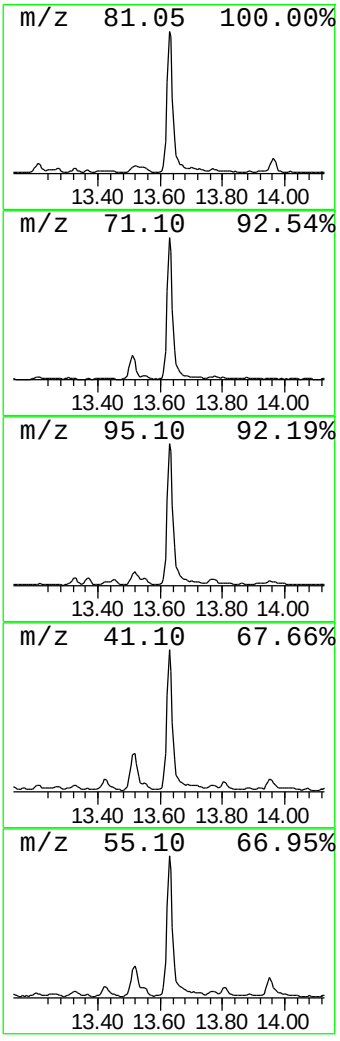
****

Peak Number 10 Levomenthol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	42.80 ug/l	1224030	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Levomenthol	156	C10H20O	002216-51-5	90
2	dl-Menthol	156	C10H20O	000089-78-1	87
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	87
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	87
5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121020\
Data File : VX019822.D
Acq On : 10 Dec 2020 13:57
Operator : JC/MD
Sample : L5020-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 201209058-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X120420W.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
Dimethyl ether	1.28	15.7	ug/l	280642	1	5.62	894782	50.0
unknown2.43	2.43	15.4	ug/l	276034	1	5.62	894782	50.0
3-Hexanone, 2-met...	9.41	16.7	ug/l	532362	3	10.10	1597200	50.0
Eucalyptol	12.14	13.7	ug/l	392394	4	12.06	1430080	50.0
unknown12.62	12.62	9.1	ug/l	261432	4	12.06	1430080	50.0
unknown12.80	12.80	17.9	ug/l	512007	4	12.06	1430080	50.0
Bicyclo[2.2.1]hep...	12.94	78.3	ug/l	2238630	4	12.06	1430080	50.0
l-Menthone	13.52	13.4	ug/l	384711	4	12.06	1430080	50.0
Levomenthol	13.63	42.8	ug/l	1224030	4	12.06	1430080	50.0