LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112619\
Data File : VX013606.D
Acq On : 26 Nov 2019 18:10
Operator : JC/SP
Sample : K5979-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 391120775.1-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\82X112619W.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	1.070	25	30	61	rBV	17277054	42792172	100.00%	38.616%
2	3.027	341	351	369	rBV	8183359	17852221	41.72%	16.110%
3	4.685	607	623	637	rBV	6061328	19584831	45.77%	17.674%
4	5.112	679	693	711	rBV	2001992	5974714	13.96%	5.392%
5	5.484	744	754	765	rBV	375921	1068581	2.50%	0.964%
6	5.648	768	781	794	rBV	652771	1810053	4.23%	1.633%
7	6.051	835	847	855	rBV	428561	1099827	2.57%	0.993%
8	6.325	886	892	902	rVB	164343	453168	1.06%	0.409%
9	6.849	967	978	989	rBV	1044318	2430353	5.68%	2.193%
10	8.709	1276	1283	1290	rBV	2285927	3424347	8.00%	3.090%
11	10.105	1507	1512	1525	rVB	2174322	3095896	7.23%	2.794%
12	10.355	1548	1553	1558	rVB	368730	526662	1.23%	0.475%
13	11.135	1675	1681	1687	rBV	1733448	2325149	5.43%	2.098%
14	12.074	1829	1835	1842	rVB	2315548	3136020	7.33%	2.830%
15	12.812	1949	1956	1961	rBV	438398	629395	1.47%	0.568%
16	12.958	1968	1980	1984	rBV	1860348	2432505	5.68%	2.195%
17	13.525	2068	2073	2077	rBV2	551197	757139	1.77%	0.683%
18	13.641	2087	2092	2102	rBV2	1042673	1420652	3.32%	1.282%

Sum of corrected areas: 110813685

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112619\
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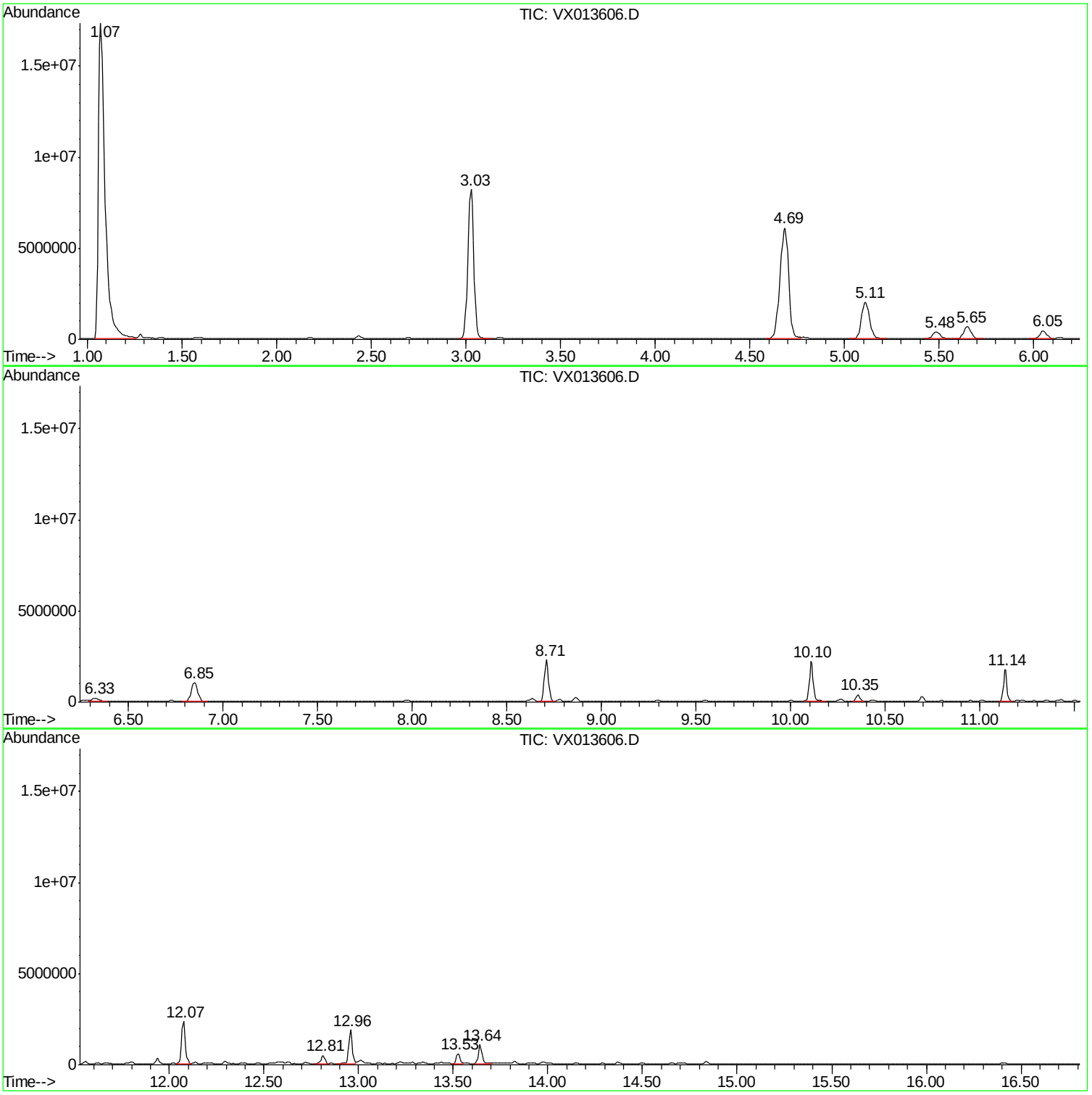
Acq On : 26 Nov 2019 18:10
Operator : JC/SP
Sample : K5979-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
391120775.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.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\VX112619\
Data File : VX013606.D
Acq On : 26 Nov 2019 18:10
Operator : JC/SP
Sample : K5979-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 391120775.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

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

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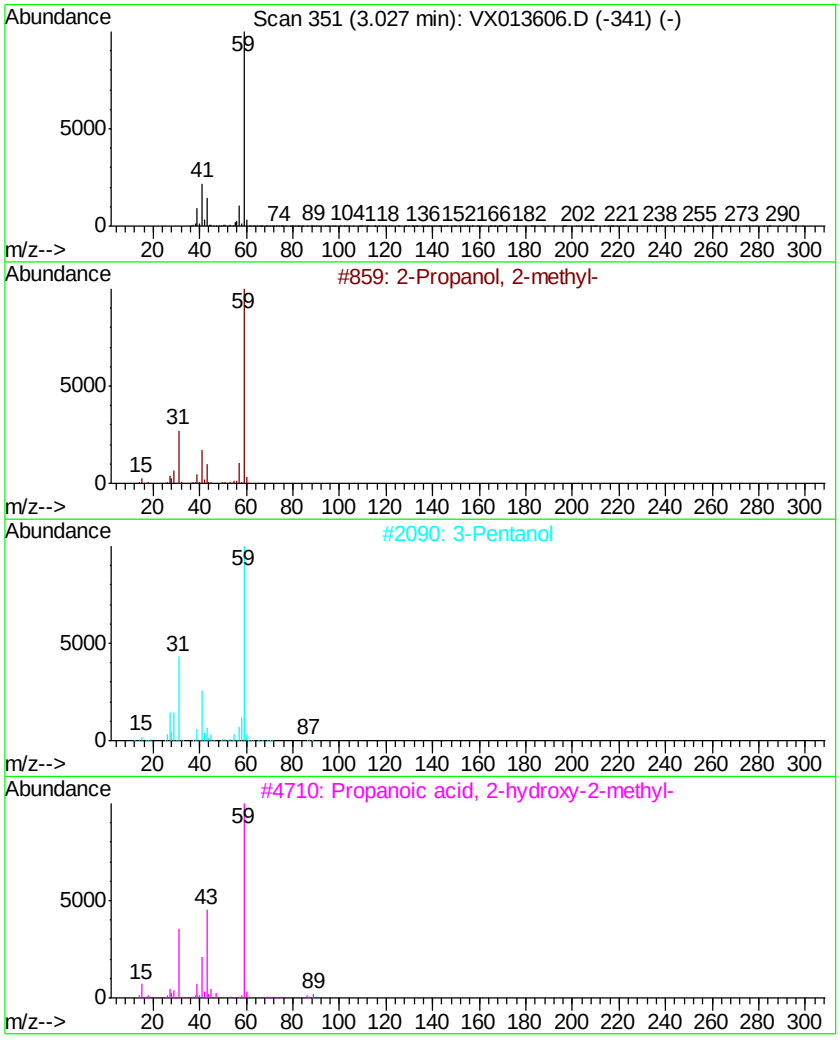
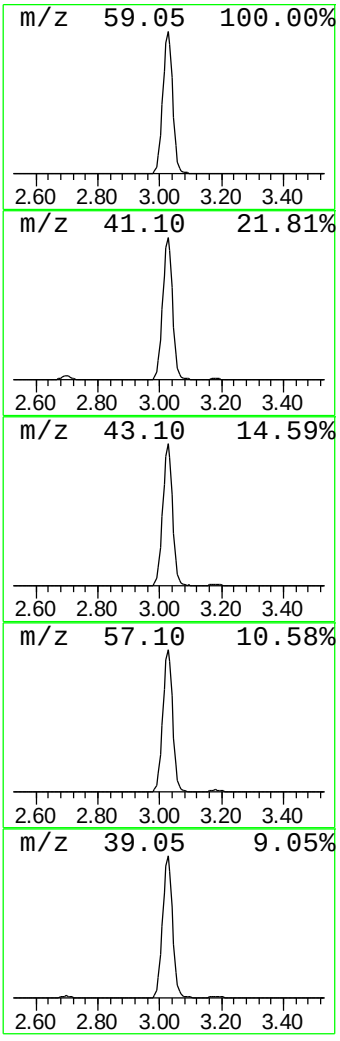
Peak Number 2 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.03	493.14 ug/l	17852200	Pentafluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	74
2	3-Pentanol	88	C5H12O	000584-02-1	9
3	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9
4	Guanidine	59	CH5N3	000113-00-8	4
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112619\
Data File : VX013606.D
Acq On : 26 Nov 2019 18:10
Operator : JC/SP
Sample : K5979-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 391120775.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

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

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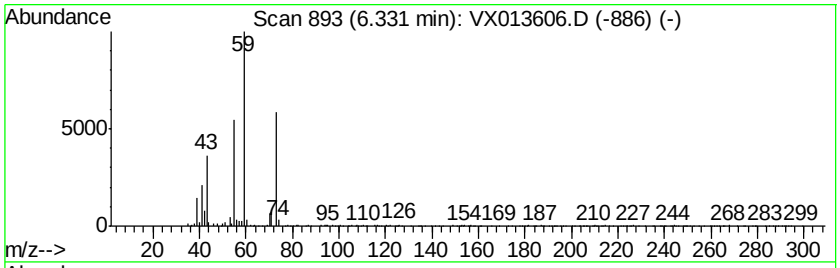
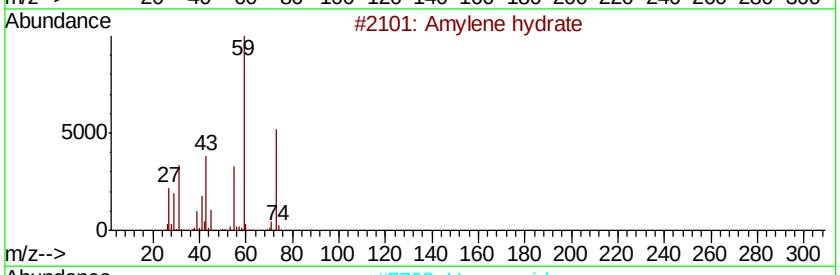
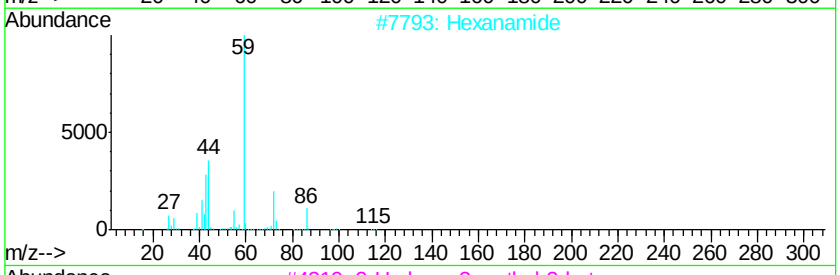
Peak Number 4 Amylene hydrate Concentration Rank 8

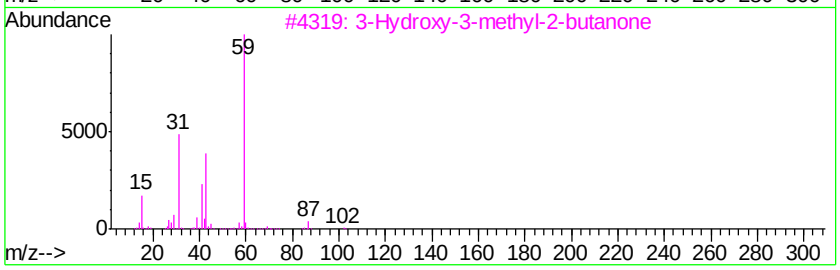
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	9.32 ug/l	453168	1,4-Difluorobenzene	6.85

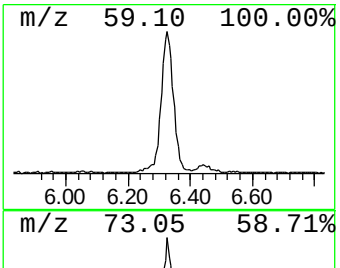
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	64
2	Hexanamide	115	C6H13NO	000628-02-4	45
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	33
4	1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	013588-28-8	9
5	Pentanal, oxime	101	C5H11NO	000628-79-5	9

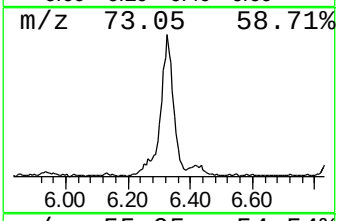


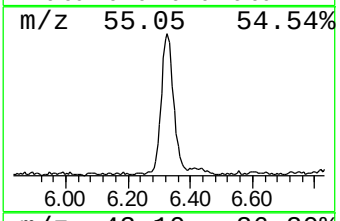


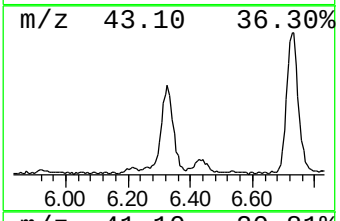


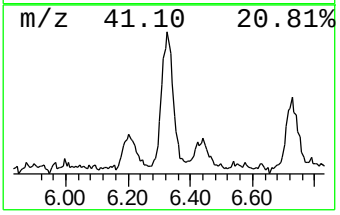












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Data File : VX013606.D
Acq On : 26 Nov 2019 18:10
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 391120775.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

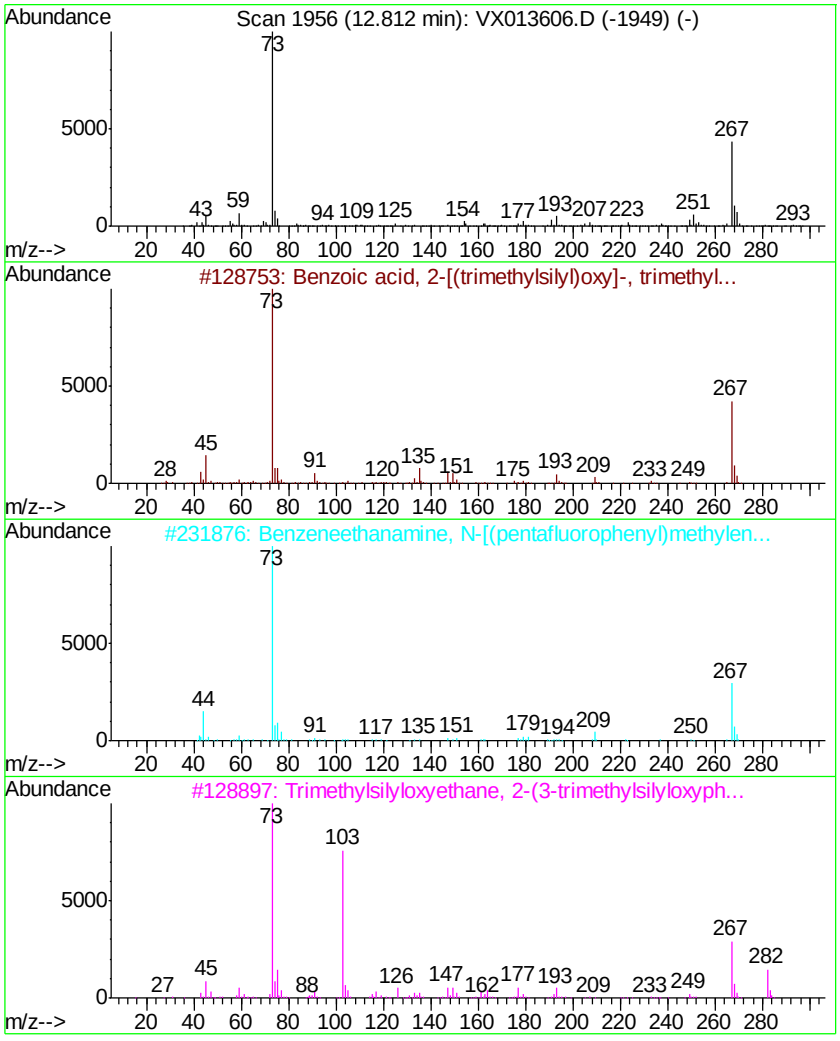
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

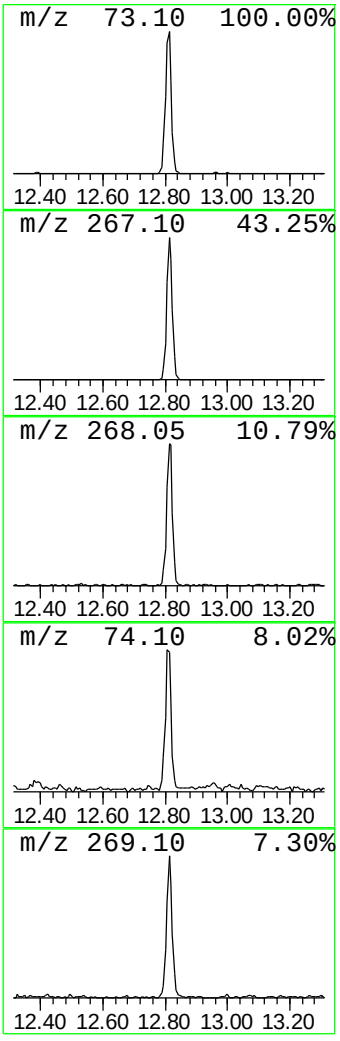
****

Peak Number 5 Benzoic acid, 2-[(trimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	10.03 ug/l	629395	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	50
2	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	45
3	Trimethylsilyloxyethane, 2-(3-tr...	282	C14H26O2Si2	1000365-49-0	39
4	Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	16
5	1-(3-Chlorophenyl)piperazine, 4-...	268	C13H21ClN2Si	1000373-99-3	10





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112619\
Data File : VX013606.D
Acq On : 26 Nov 2019 18:10
Operator : JC/SP
Sample : K5979-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 391120775.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

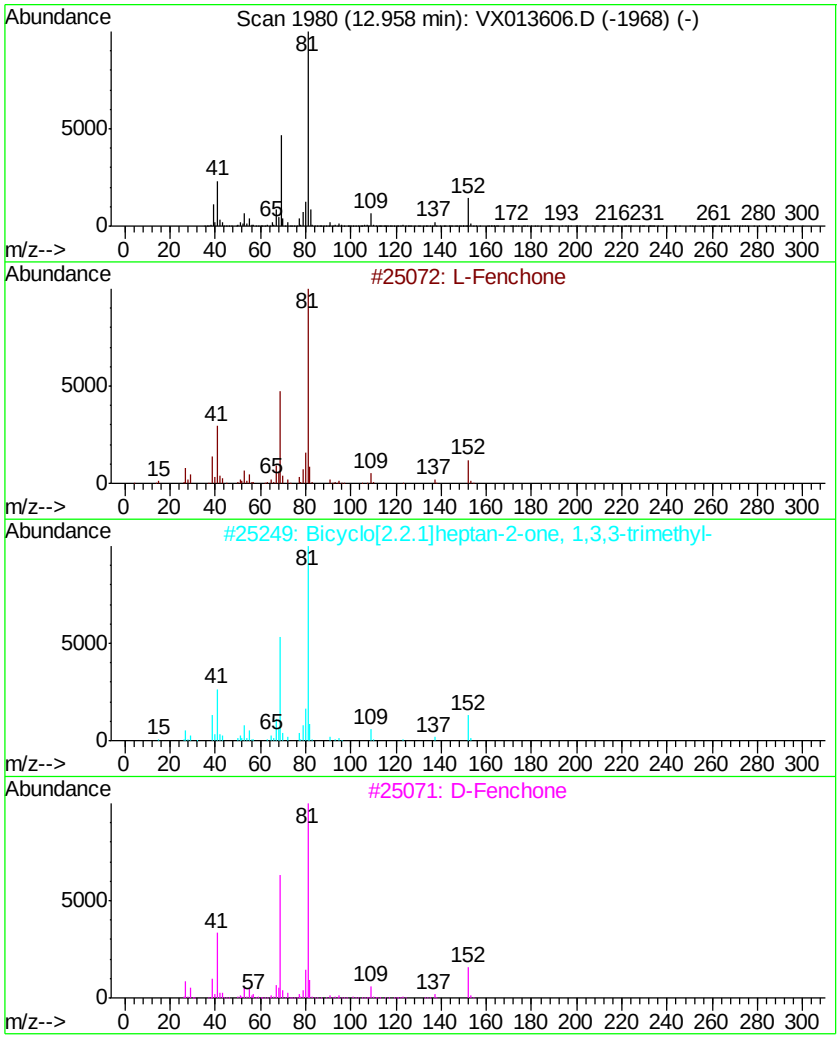
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

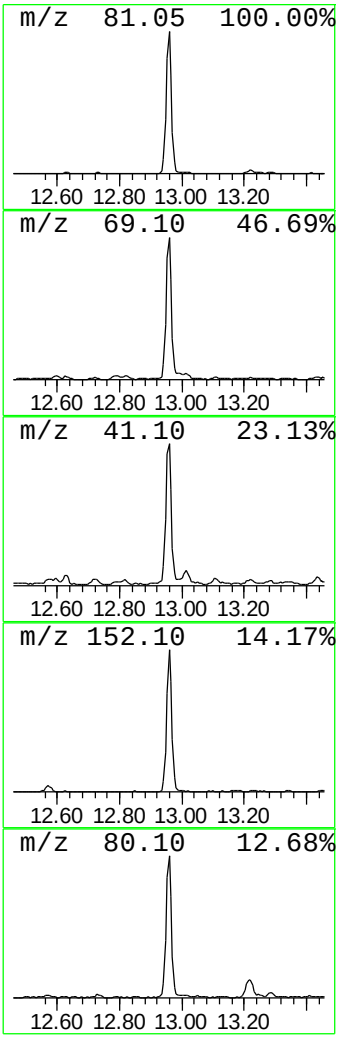
****

Peak Number 6 L-Fenchone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	38.78 ug/l	2432510	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Fenchone	152	C10H16O	007787-20-4	95
2	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42
5	Formic acid, trans-4-methylcyclo...	142	C8H14O2	1000368-24-5	36





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112619\
Data File : VX013606.D
Acq On : 26 Nov 2019 18:10
Operator : JC/SP
Sample : K5979-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 391120775.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

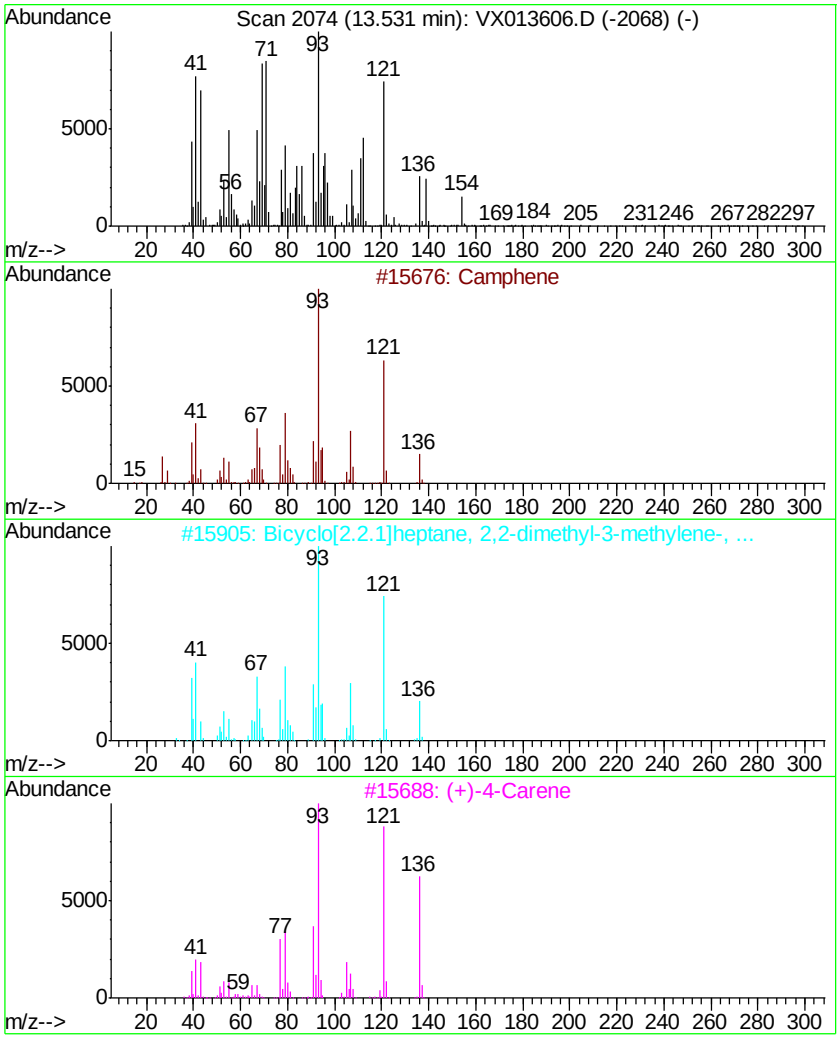
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

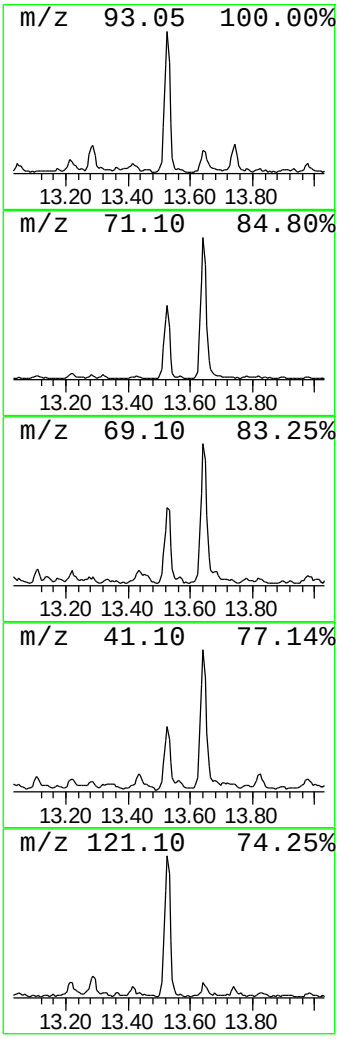
****

Peak Number 7 Camphene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	12.07 ug/l	757139	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphene	136	C10H16	000079-92-5	80
2	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	59
3	(+)-4-Carene	136	C10H16	029050-33-7	30
4	Cyclopentene, 4-ethenyl-1,5,5-tr...	136	C10H16	001727-69-1	30
5	Chlorodimethylethylsilane	122	C4H11ClSi	006917-76-6	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112619\
Data File : VX013606.D
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Sample : K5979-01
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ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 391120775.1-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112619W.M
Quant Title : SW846 8260

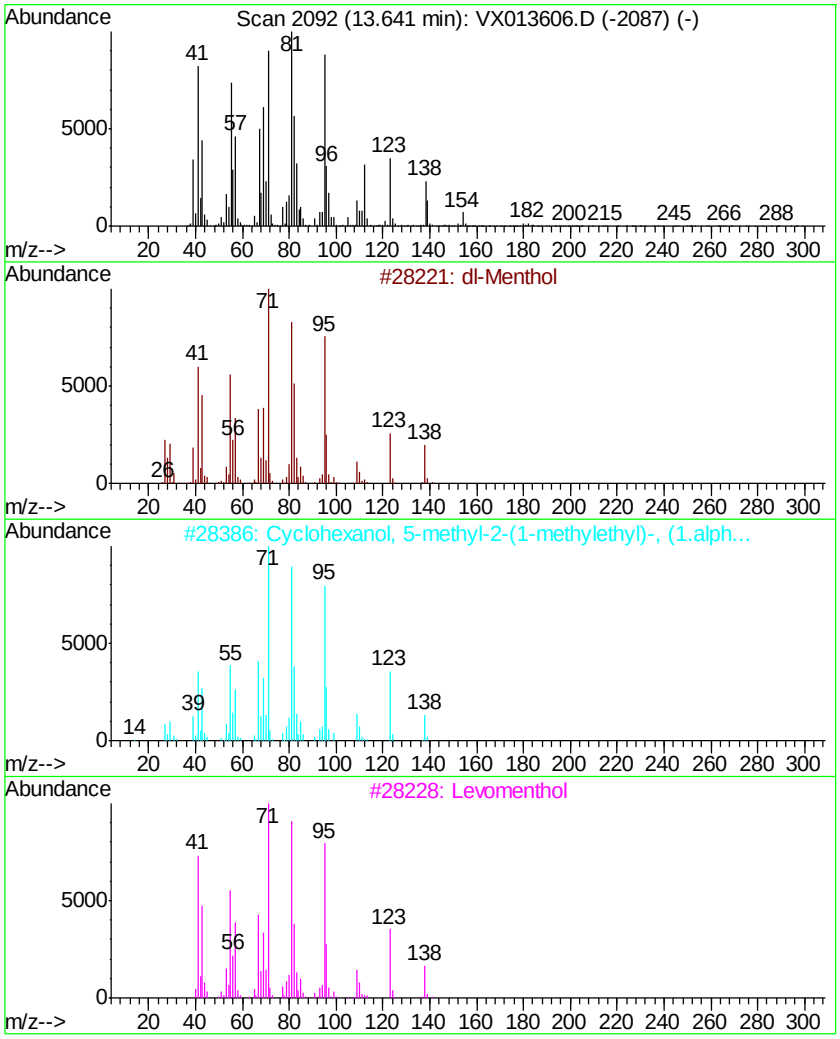
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

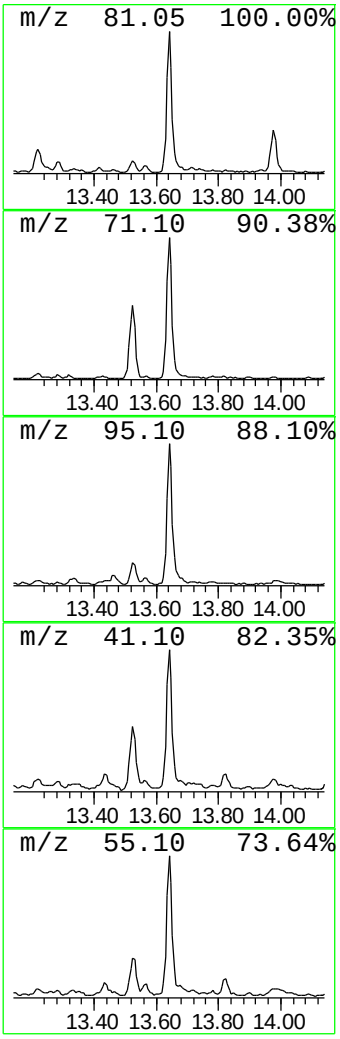
****

Peak Number 8 dl-Menthol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	22.65 ug/l	1420650	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Menthol	156	C10H20O	000089-78-1	87
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	83
3	Levomenthol	156	C10H20O	002216-51-5	83
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	80
5	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	78





Tentatively Identified Compound (LSC) summary

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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
2-Propanol, 2-met...	3.03	493.1	ug/l	17852200	1	5.65	1810050	50.0
Amylene hydrate	6.33	9.3	ug/l	453168	2	6.85	2430350	50.0
Benzoic acid, 2-[...	12.81	10.0	ug/l	629395	4	12.07	3136020	50.0
L-Fenchone	12.96	38.8	ug/l	2432510	4	12.07	3136020	50.0
Camphene	13.53	12.1	ug/l	757139	4	12.07	3136020	50.0
dl-Menthol	13.64	22.6	ug/l	1420650	4	12.07	3136020	50.0