LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-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\82X081920W.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	40	rVB	206728	258011	1.88%	0.433%
2	2.422	213	219	228	rVB2	237854	433042	3.15%	0.727%
3	3.014	305	316	334	rBV	4679057	10362114	75.46%	17.391%
4	3.172	334	342	352	rVB2	49124	137333	1.00%	0.230%
5	4.666	561	587	600	rBV	4212663	13732778	100.00%	23.048%
6	5.092	646	657	676	rVB	1586316	4700143	34.23%	7.888%
7	5.464	708	718	731	rVV	349625	1012994	7.38%	1.700%
8	5.629	734	745	761	rVB	632714	1786488	13.01%	2.998%
9	6.031	801	811	819	rBV	384761	1010137	7.36%	1.695%
10	6.111	819	824	831	rVB	55063	140032	1.02%	0.235%
11	6.245	837	846	853	rBV2	168655	555458	4.04%	0.932%
12	6.830	930	942	952	rBV	941873	2186807	15.92%	3.670%
13	8.622	1228	1236	1241	rVB2	67741	151563	1.10%	0.254%
14	8.695	1241	1248	1255	rBV	1927106	2973773	21.65%	4.991%
15	8.762	1255	1259	1268	rVB2	106960	187599	1.37%	0.315%
16	8.848	1268	1273	1278	rBV	173275	267918	1.95%	0.450%
17	9.421	1359	1367	1373	rBV	341678	501443	3.65%	0.842%
18	10.098	1468	1478	1489	rBV	2009214	2907181	21.17%	4.879%
19	10.256	1498	1504	1507	rBV	97528	147543	1.07%	0.248%
20	10.341	1513	1518	1524	rVB	368185	519070	3.78%	0.871%
21	10.683	1570	1574	1583	rBV	249935	336156	2.45%	0.564%
22	11.122	1640	1646	1651	rBV	1714068	2175672	15.84%	3.651%
23	11.542	1711	1715	1721	rVB	114795	137626	1.00%	0.231%
24	11.792	1742	1756	1760	rBV	141938	244792	1.78%	0.411%
25	11.927	1770	1778	1785	rVB2	224160	340354	2.48%	0.571%
26	12.061	1794	1800	1808	rVB	2254700	3097649	22.56%	5.199%
27	12.280	1831	1836	1841	rBV	169029	236389	1.72%	0.397%
28	12.561	1878	1882	1888	rBV4	119201	214843	1.56%	0.361%
29	12.615	1888	1891	1895	rVB	166626	196394	1.43%	0.330%
30	12.804	1916	1922	1927	rVB3	228537	335655	2.44%	0.563%
31	12.945	1934	1945	1950	rBV	2155412	2750062	20.03%	4.615%
32	13.000	1950	1954	1959	rVB4	124812	206604	1.50%	0.347%
33	13.329	2002	2008	2012	rBV3	90007	138178	1.01%	0.232%
34	13.518	2034	2039	2041	rBV2	339317	507071	3.69%	0.851%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-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\82X081920W.M
Title : SW846 8260

35	13.548	2041	2044	2050	rVB	2299669	2875919	20.94%	4.827%
36	13.634	2052	2058	2067	rBV	547169	943229	6.87%	1.583%
37	13.810	2083	2087	2092	rVB2	93396	142632	1.04%	0.239%
38	13.963	2107	2112	2120	rBV4	100774	228331	1.66%	0.383%
39	14.133	2136	2140	2146	rBV	249262	343600	2.50%	0.577%
40	14.822	2249	2253	2258	rVB	121518	161656	1.18%	0.271%

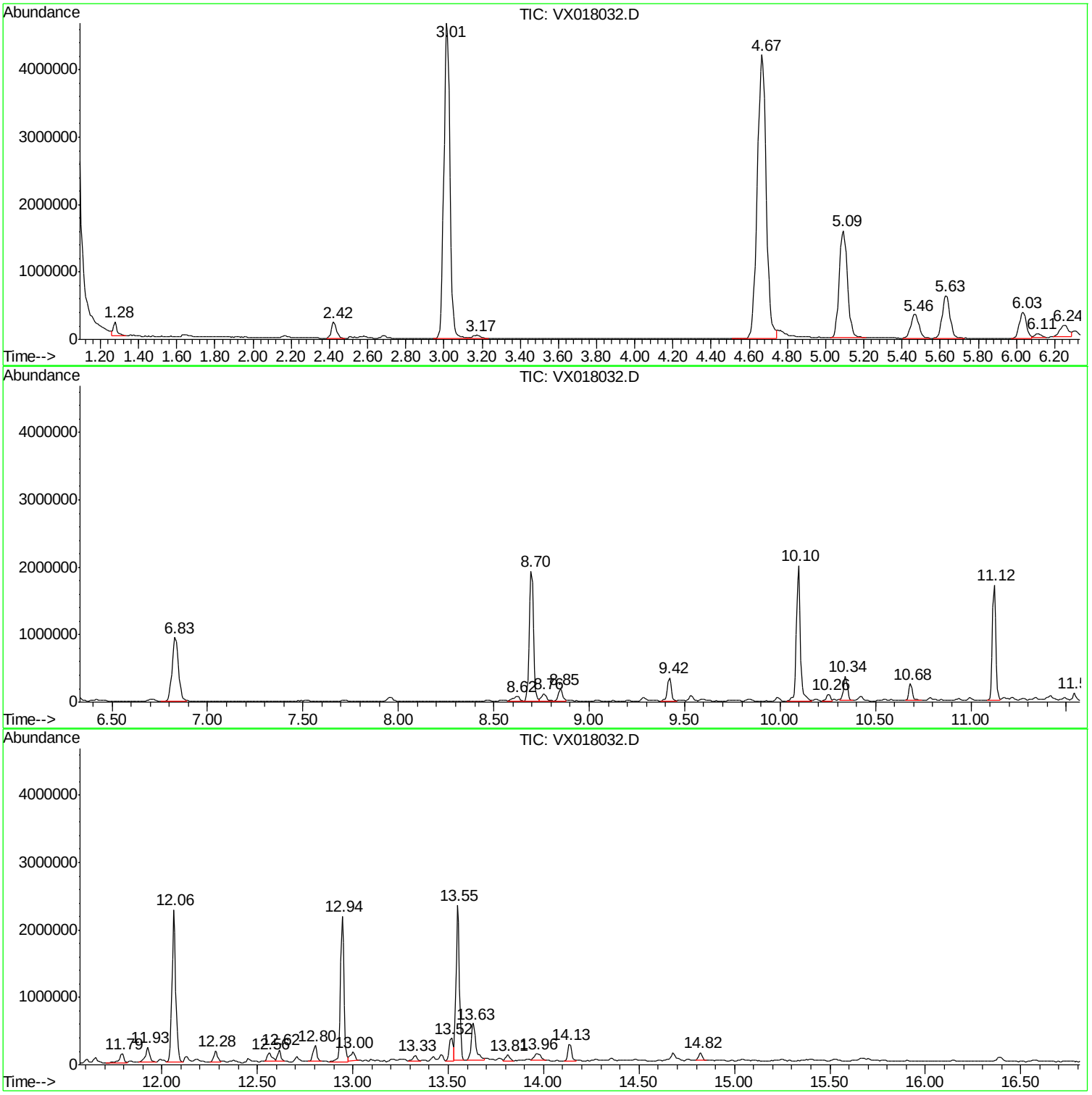
Sum of corrected areas: 59584239

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

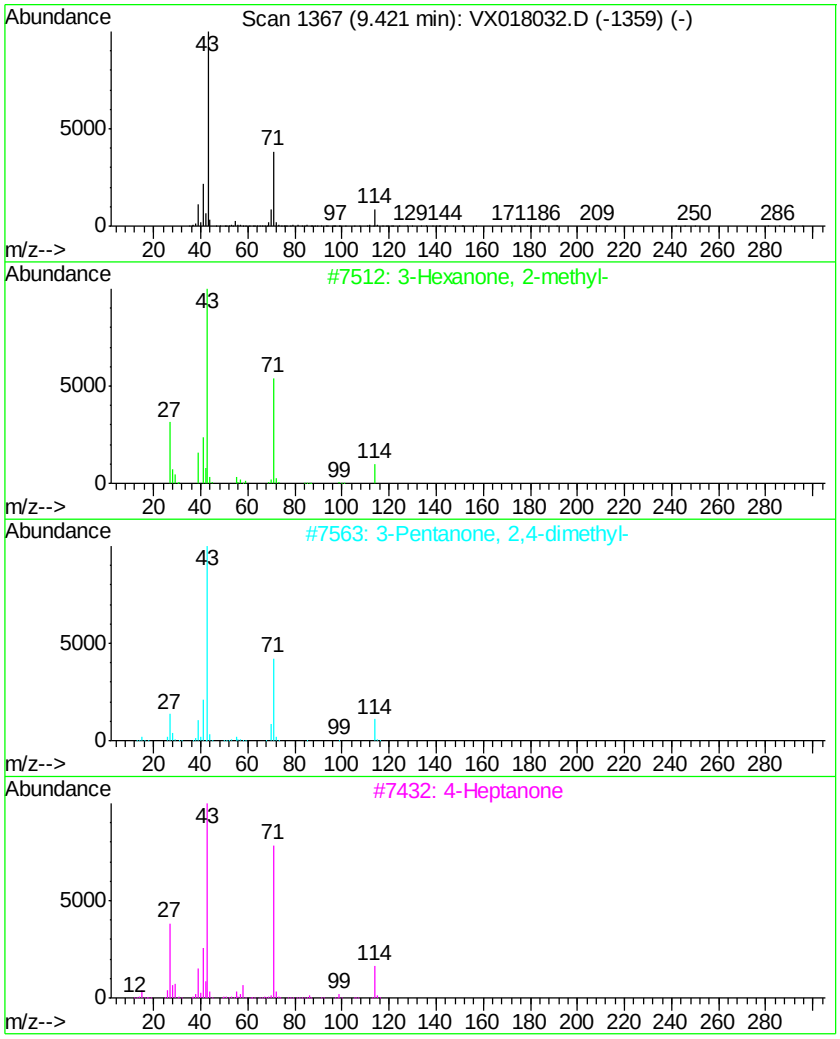
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

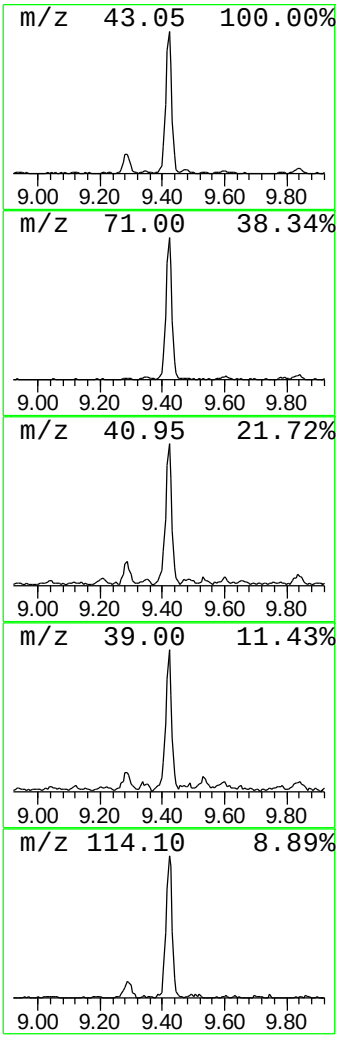
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	8.62 ug/l	501443	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
2	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	72
3	4-Heptanone	114	C7H14O	000123-19-3	53
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	49
5	Pyrrolidine	71	C4H9N	000123-75-1	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

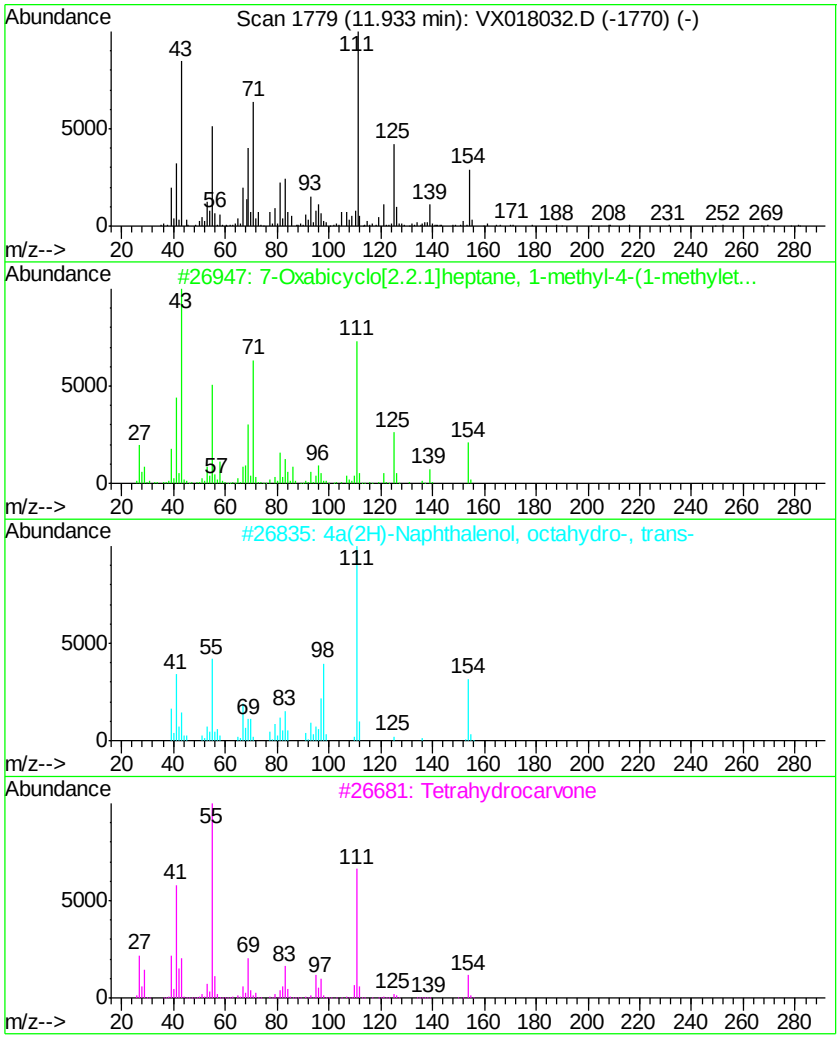
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

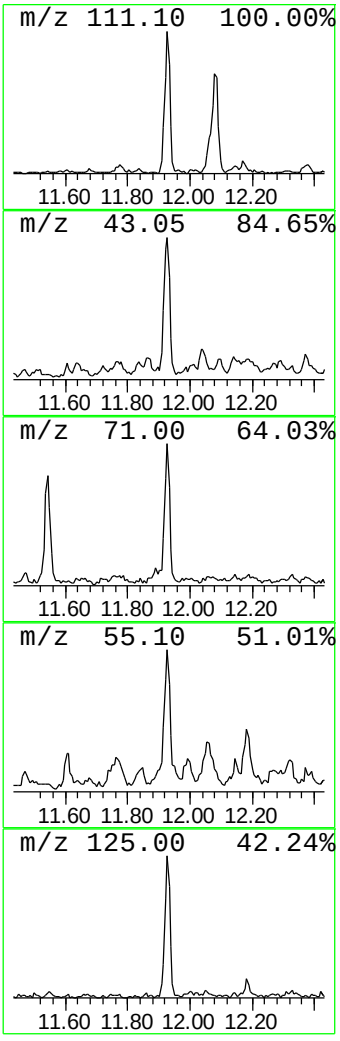
****

Peak Number 4 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	5.49 ug/l	340354	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	90
2	4a(2H)-Naphthalenol, octahydro-,...	154	C10H18O	001654-87-1	45
3	Tetrahydrocarvone	154	C10H18O	000499-70-7	43
4	1-Propanone, 2-methyl-1-[2-(1-me...	154	C10H18O	056259-15-5	43
5	1,2-Propanedione, 1-(2-thienyl)-	154	C7H6O2S	013678-69-8	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

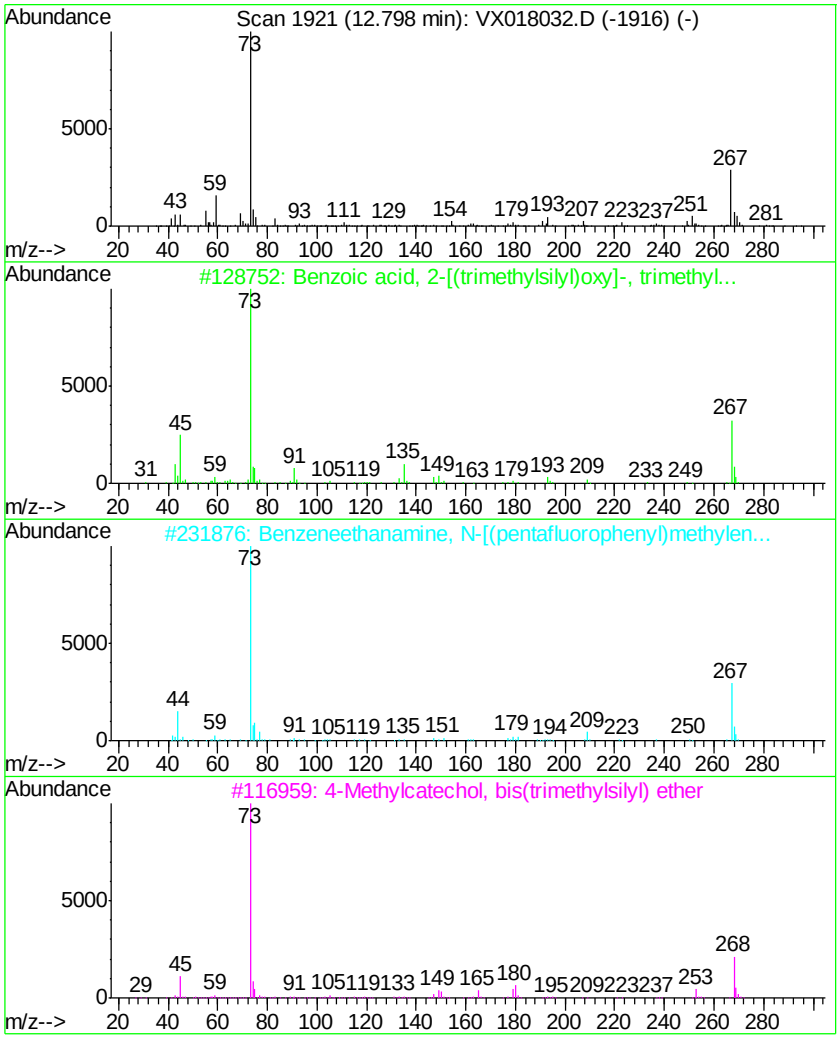
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

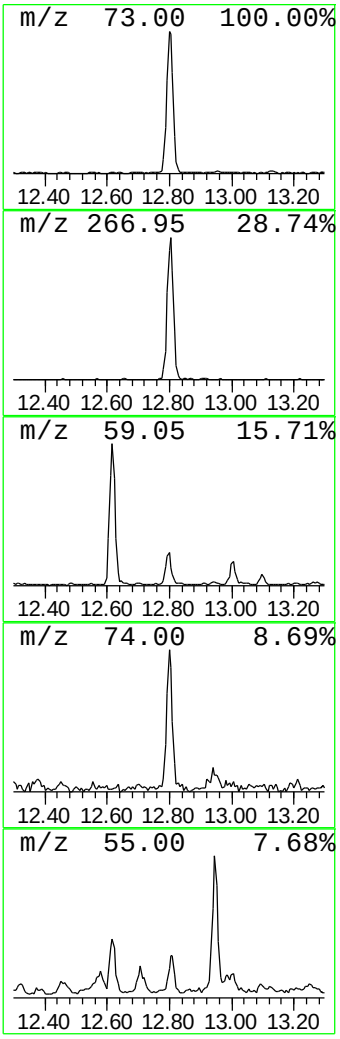
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzoic acid, 2-[(trimethyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	5.42 ug/l	335655	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	59
2	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	38
3	4-Methylcatechol, bis(trimethyls...	268	C13H24O2Si2	1000332-79-9	35
4	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	27
5	1-(3-Chlorophenyl)piperazine, 4-...	268	C13H21ClN2Si	1000373-99-3	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

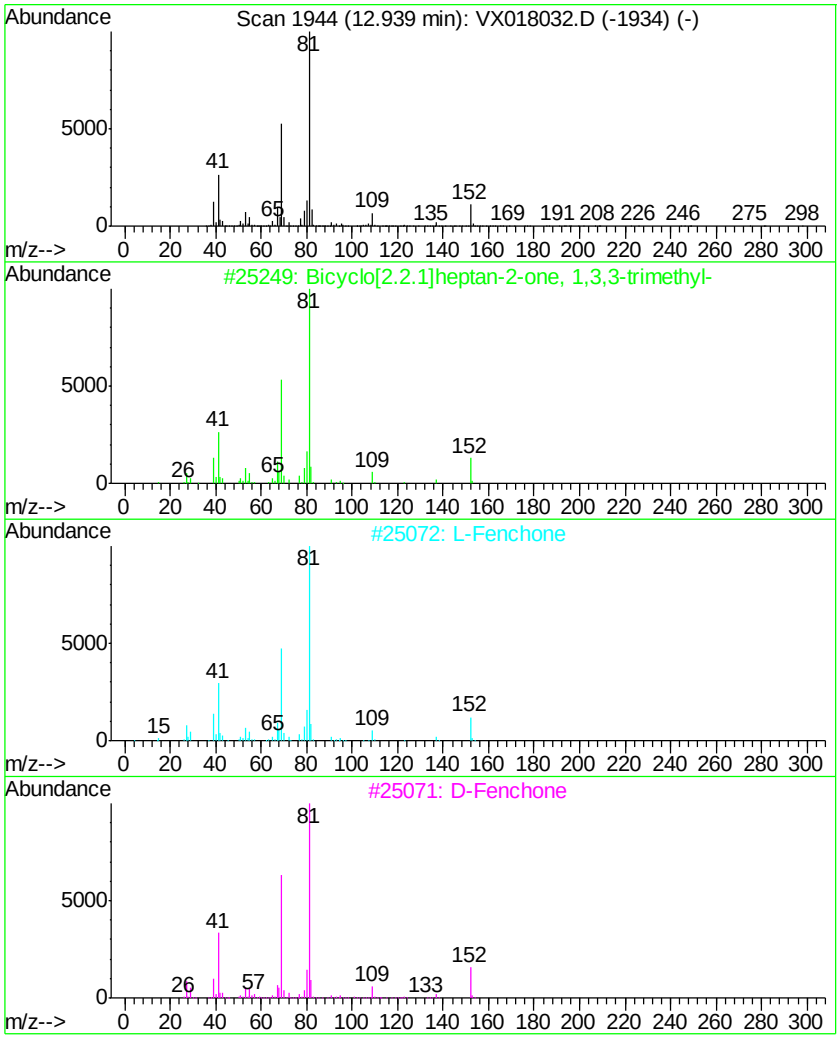
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

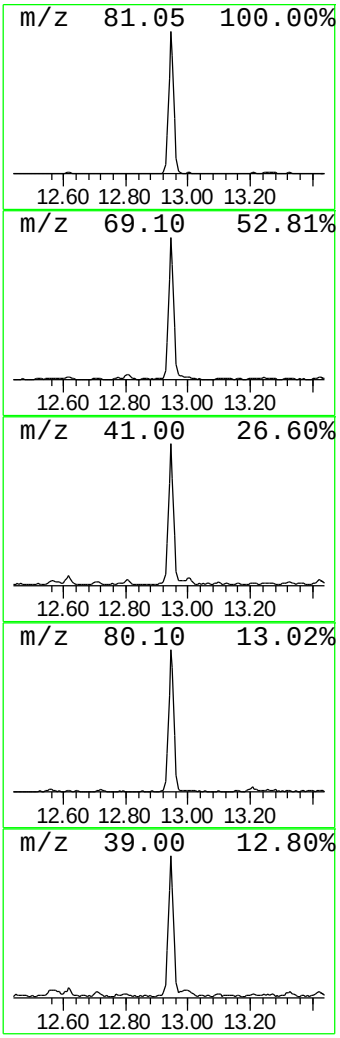
****

Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	44.39 ug/l	2750060	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	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45
5	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

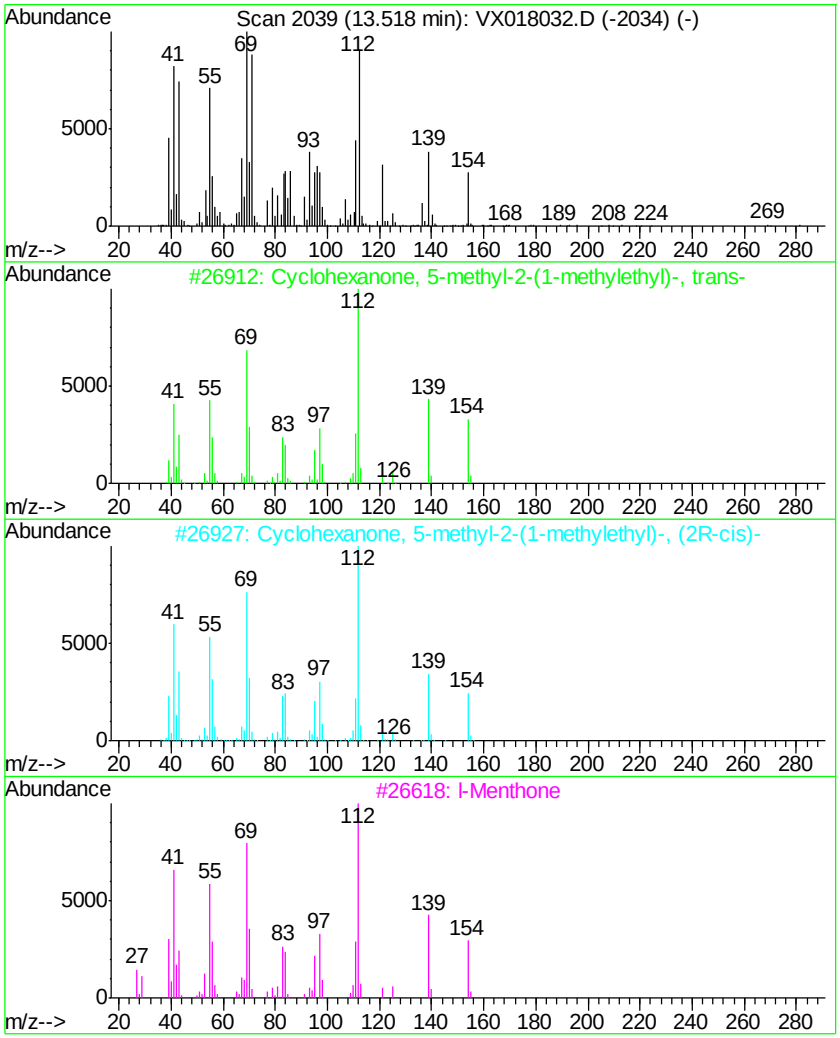
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

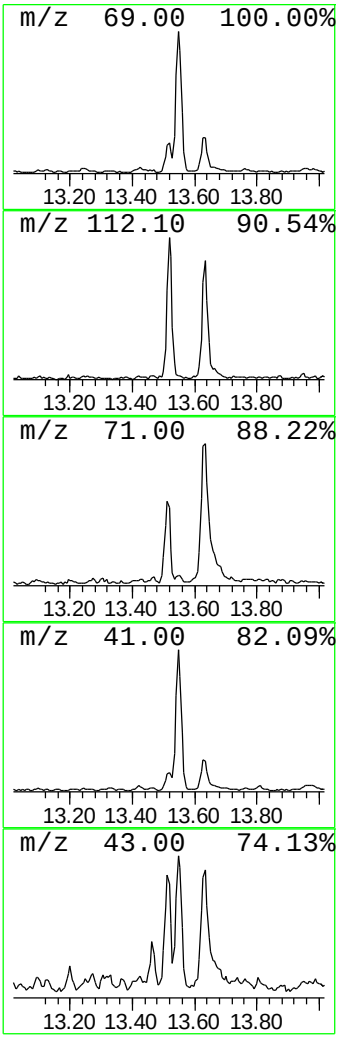
****

Peak Number 7 Cyclohexanone, 5-methyl-2-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	8.18 ug/l	507071	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	83
2	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	78
3	l-Menthone	154	C10H18O	014073-97-3	66
4	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	55
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	53





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

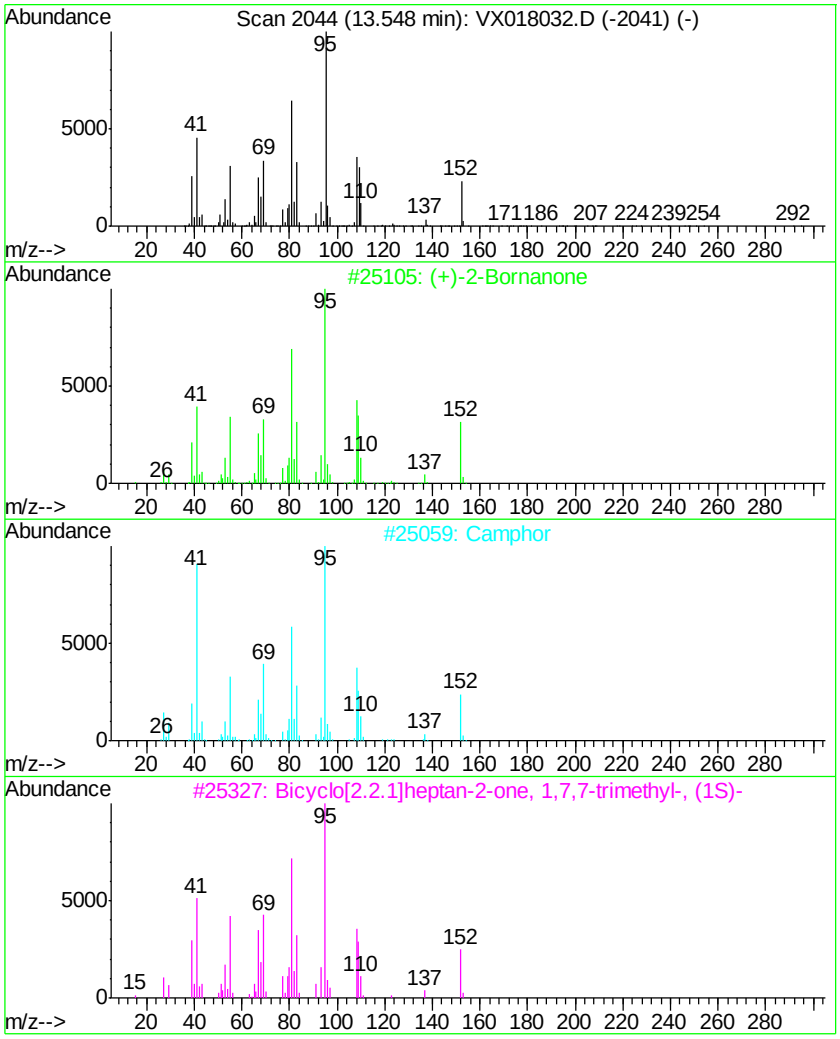
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

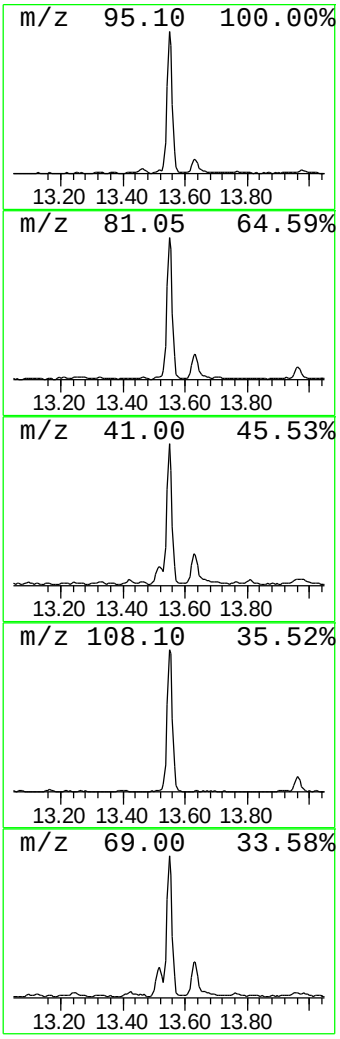
****

Peak Number 8 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	46.42 ug/l	2875920	1,4-Dichlorobenzene-d4	12.06

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-Furancarboxylic acid, 2-propen...	152	C8H8O3	004208-49-5	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

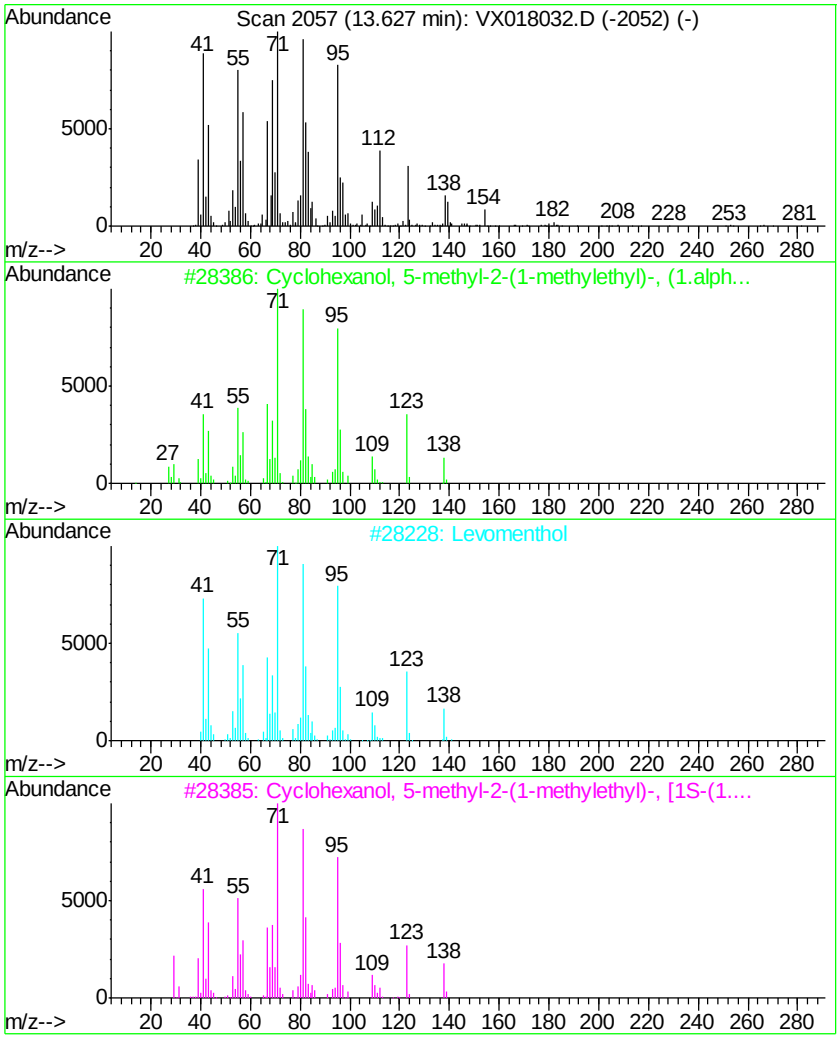
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

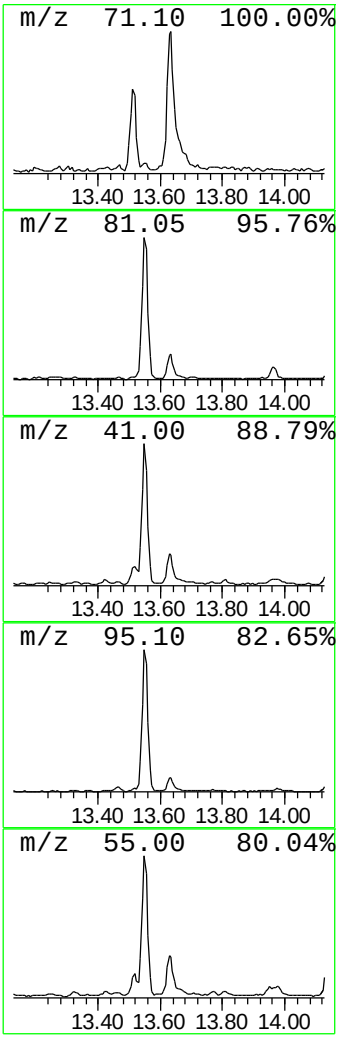
****

Peak Number 9 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	15.22 ug/l	943229	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	87
2	Levomenthol	156	C10H20O	002216-51-5	87
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	80
4	dl-Menthol	156	C10H20O	000089-78-1	72
5	9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

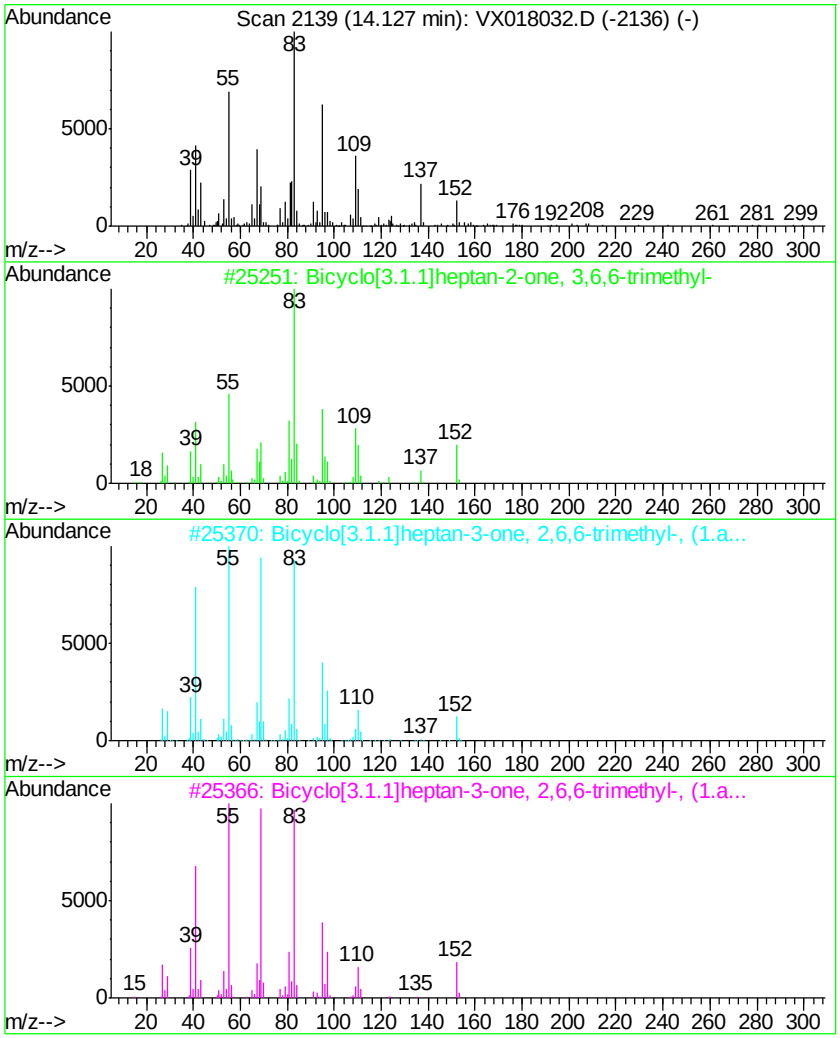
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

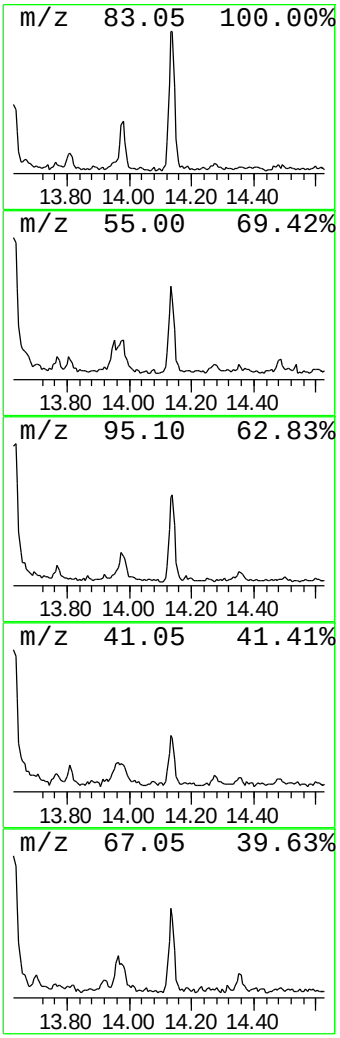
****

Peak Number 10 Bicyclo[3.1.1]heptan-2-one,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	5.55 ug/l	343600	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	70
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	58
3	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	49
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	38
5	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018032.D
Acq On : 20 Aug 2020 14:10
Operator : JC/SP
Sample : L3766-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 200819016-02-VOA

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.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
3-Hexanone, 2-met...	9.42	8.6	ug/l	501443	3	10.10	2907180	50.0
7-Oxabicyclo[2.2....	11.93	5.5	ug/l	340354	4	12.06	3097650	50.0
Benzoic acid, 2-[...	12.80	5.4	ug/l	335655	4	12.06	3097650	50.0
Bicyclo[2.2.1]hep...	12.94	44.4	ug/l	2750060	4	12.06	3097650	50.0
Cyclohexanone, 5-...	13.52	8.2	ug/l	507071	4	12.06	3097650	50.0
(+)-2-Bornanone	13.55	46.4	ug/l	2875920	4	12.06	3097650	50.0
Cyclohexanol, 5-m...	13.63	15.2	ug/l	943229	4	12.06	3097650	50.0
Bicyclo[3.1.1]hep...	14.13	5.5	ug/l	343600	4	12.06	3097650	50.0