

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071620\
 Data File : VX017394.D
 Acq On : 16 Jul 2020 16:28
 Operator : JC/SP
 Sample : L3325-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 200715091-01

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.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	38	rVB	258369	254260	2.50%	0.627%
2	1.605	83	85	91	rBV	84002	118025	1.16%	0.291%
3	2.416	212	218	232	rVB	489586	913315	8.99%	2.253%
4	2.575	237	244	256	rBV	251039	451495	4.45%	1.114%
5	3.008	304	315	334	rBV	2839446	6241343	61.46%	15.394%
6	4.660	563	586	599	rBV2	2823504	10155398	100.00%	25.048%
7	5.087	644	656	680	rBV2	1247001	3780154	37.22%	9.324%
8	5.464	708	718	731	rBV2	173983	495491	4.88%	1.222%
9	5.629	733	745	761	rVB	284499	791591	7.79%	1.952%
10	6.031	799	811	819	rBV2	181985	477650	4.70%	1.178%
11	6.306	850	856	866	rVB	50259	139395	1.37%	0.344%
12	6.830	931	942	956	rBV	445682	1064670	10.48%	2.626%
13	7.269	1006	1014	1024	rBV	167529	365873	3.60%	0.902%
14	8.696	1241	1248	1255	rBV	978106	1530381	15.07%	3.775%
15	8.763	1255	1259	1265	rVV2	108001	175209	1.73%	0.432%
16	8.848	1269	1273	1278	rVV	73615	105304	1.04%	0.260%
17	9.281	1338	1344	1350	rBV2	96433	174624	1.72%	0.431%
18	9.421	1358	1367	1373	rVB	243275	368102	3.62%	0.908%
19	10.098	1466	1478	1489	rBV	1103206	1637913	16.13%	4.040%
20	10.232	1496	1500	1511	rBV2	146875	245098	2.41%	0.605%
21	10.342	1511	1518	1524	rVV	218241	312039	3.07%	0.770%
22	10.616	1559	1563	1570	rBV	198977	292365	2.88%	0.721%
23	10.683	1570	1574	1585	rVB	141780	211420	2.08%	0.521%
24	11.122	1640	1646	1651	rBV	1014388	1264390	12.45%	3.119%
25	11.927	1770	1778	1785	rVB2	93308	135950	1.34%	0.335%
26	12.061	1794	1800	1807	rBV	1432171	1879641	18.51%	4.636%
27	12.140	1807	1813	1817	rBV3	138741	209587	2.06%	0.517%
28	12.280	1828	1836	1841	rBV2	78782	146976	1.45%	0.363%
29	12.616	1888	1891	1895	rVB	112299	130165	1.28%	0.321%
30	12.805	1913	1922	1926	rBV3	107445	172358	1.70%	0.425%
31	12.945	1933	1945	1950	rBV	1151910	1433272	14.11%	3.535%
32	13.000	1950	1954	1959	rVB2	97561	148752	1.46%	0.367%
33	13.372	2011	2015	2019	rBV	140924	181272	1.78%	0.447%
34	13.518	2034	2039	2040	rBV2	193853	253658	2.50%	0.626%

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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 >
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35	13.548	2040	2044	2052	rVB	1704196	2187773	21.54%	5.396%
36	13.628	2052	2057	2067	rBV3	568838	782968	7.71%	1.931%
37	13.768	2076	2080	2084	rBV2	124731	159010	1.57%	0.392%
38	13.817	2084	2088	2094	rVB	577087	707841	6.97%	1.746%
39	13.975	2107	2114	2119	rBV7	49046	110619	1.09%	0.273%
40	14.134	2134	2140	2152	rBV	238902	338055	3.33%	0.834%

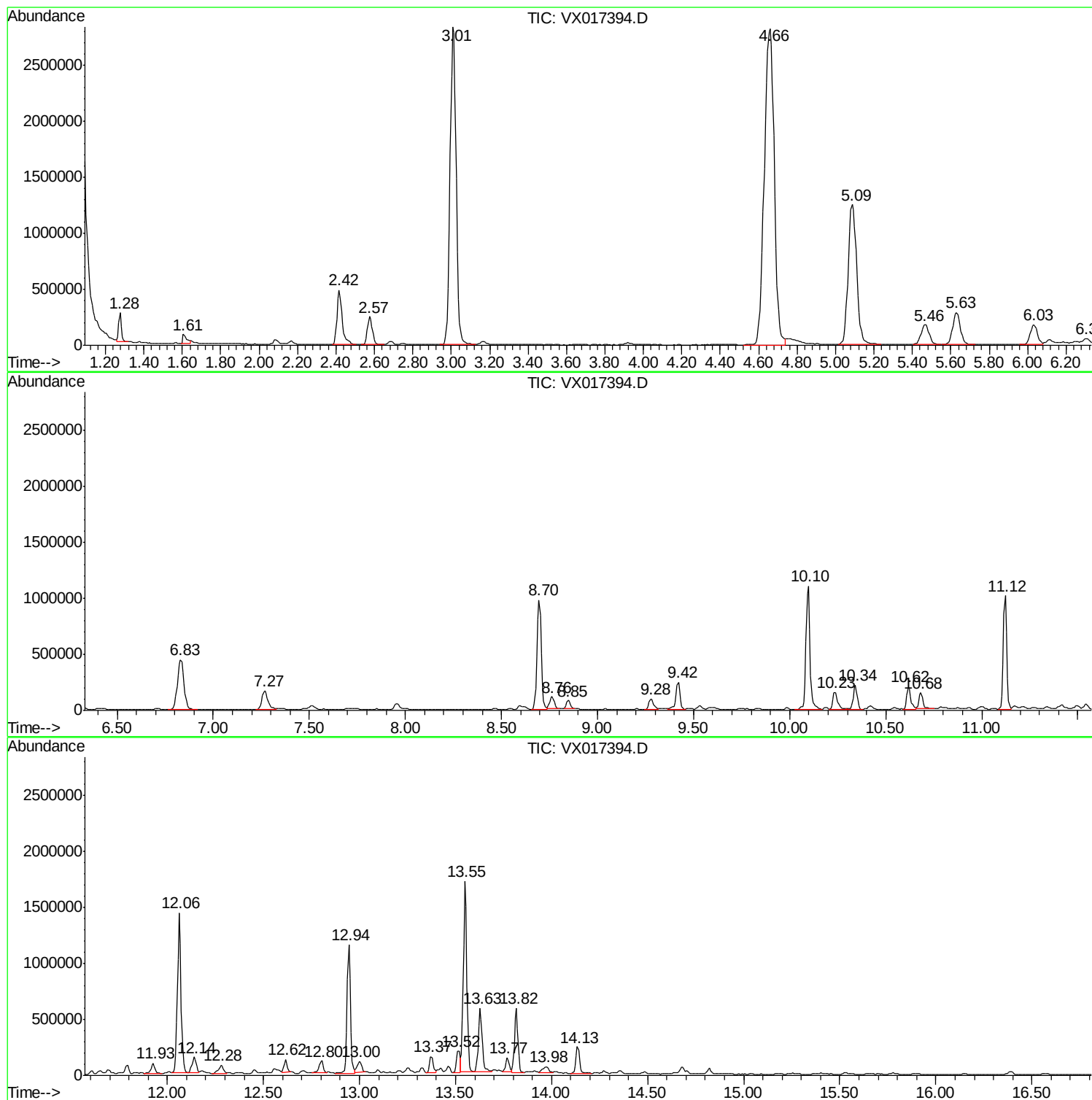
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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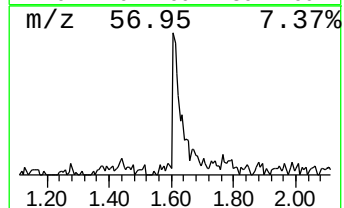
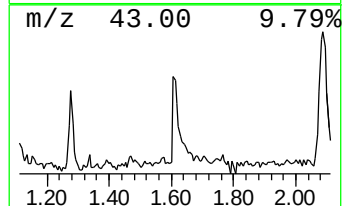
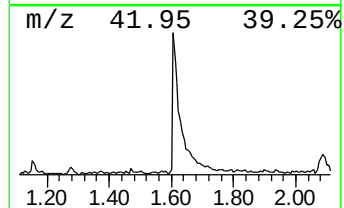
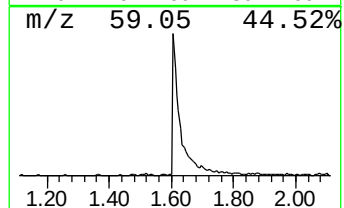
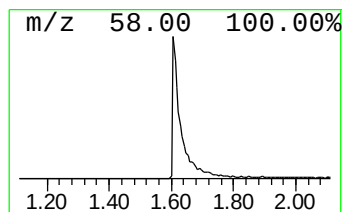
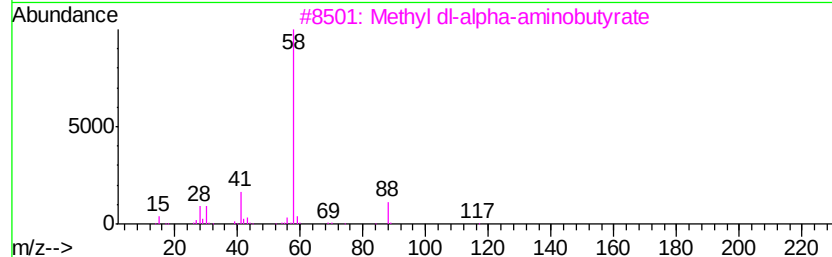
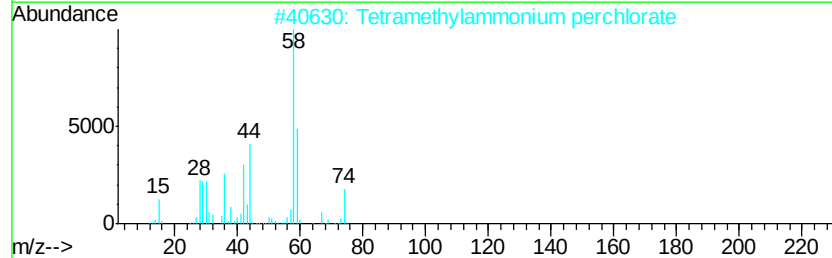
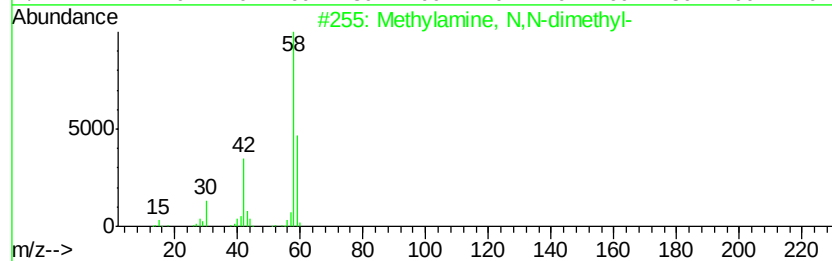
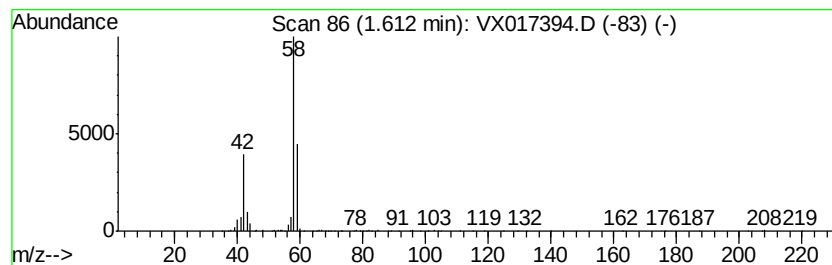
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Peak Number 2 Methylamine, N,N-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.61	7.45 ug/l	118025	Pentafluorobenzene	5.63
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Methylamine, N,N-dimethyl-	59 C3H9N	000075-50-3 91
2		Tetramethylammonium perchlorate	173 C4H12ClN04	002537-36-2 43
3		Methyl dl-alpha-aminobutvrate	117 C5H11N02	002483-62-7 9
4		Propylamine	59 C3H9N	000107-10-8 9
5		Butanoic acid, 4-(dimethylamino)...	147 C6H13N03	003688-46-8 9



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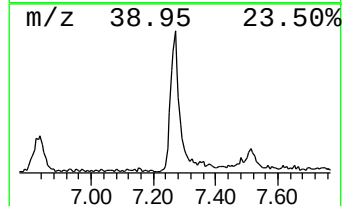
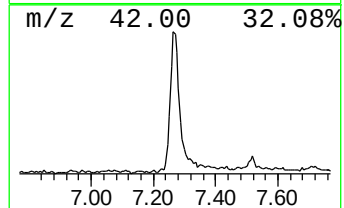
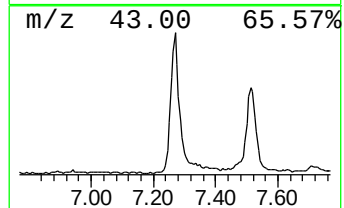
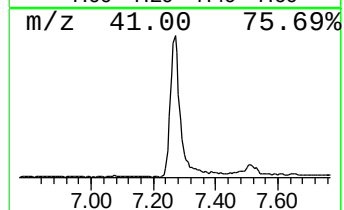
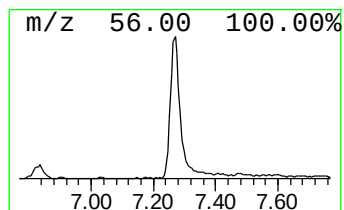
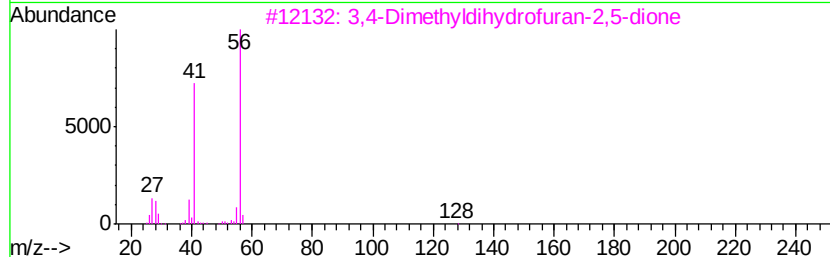
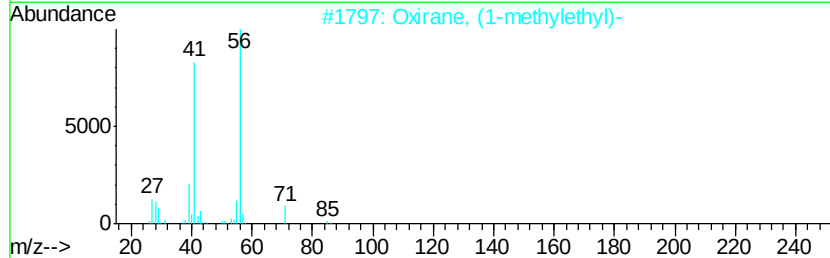
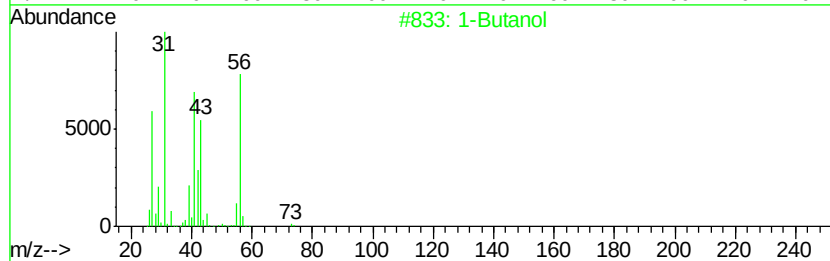
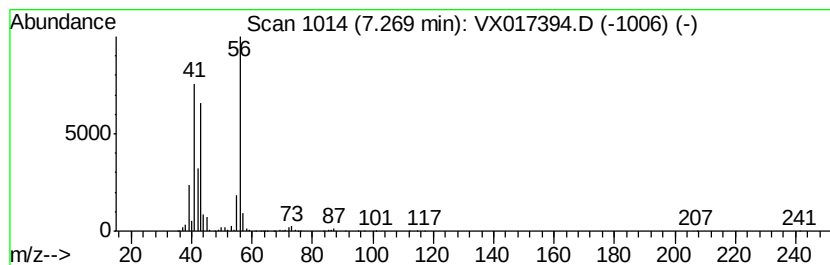
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	17.18 ug/l	365873	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	86
2		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	64
3		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	59
4		Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	50
5		Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	50



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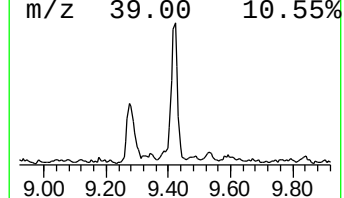
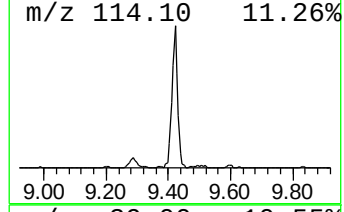
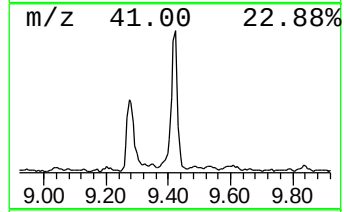
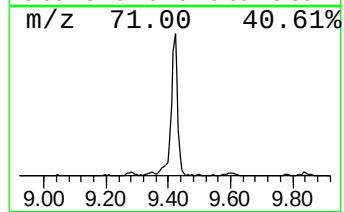
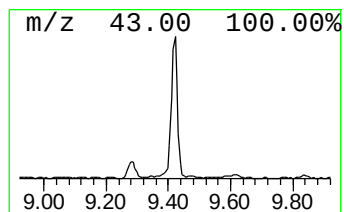
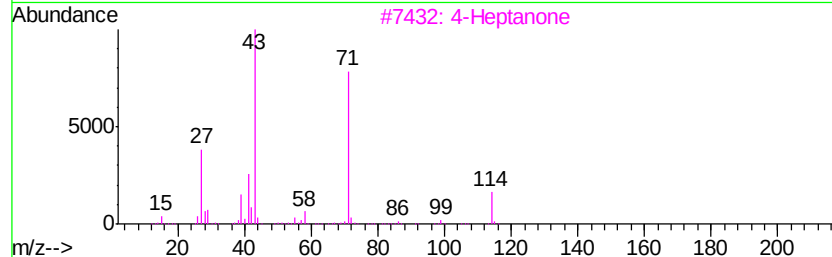
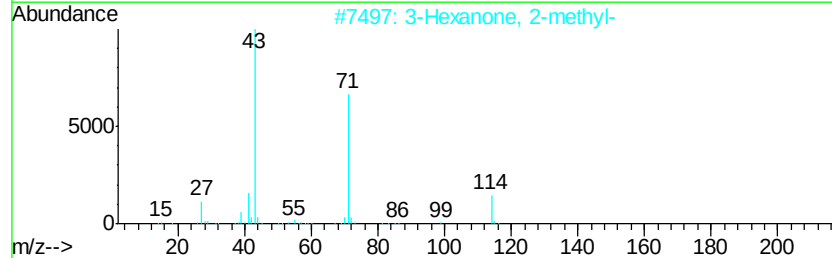
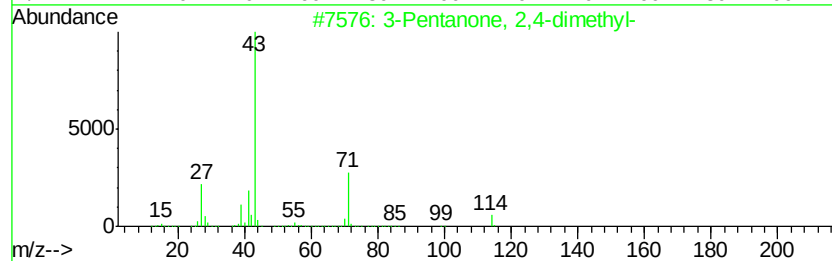
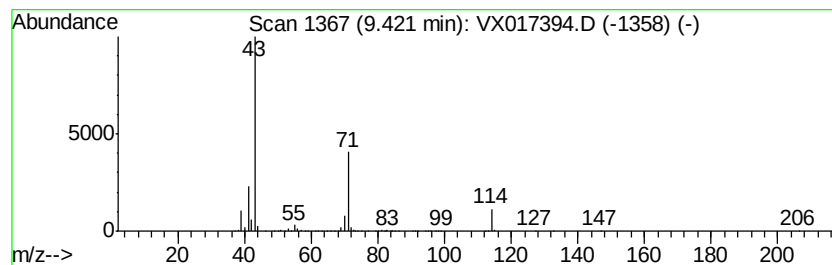
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	11.24 ug/l	368102	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	59
3		4-Heptanone	114	C7H14O	000123-19-3	53
4		2,3-Hexanedione	114	C6H10O2	003848-24-6	47
5		Pyrrolidine	71	C4H9N	000123-75-1	42



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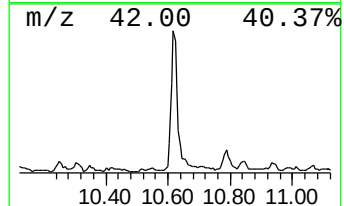
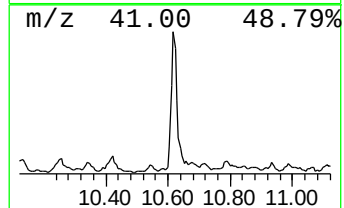
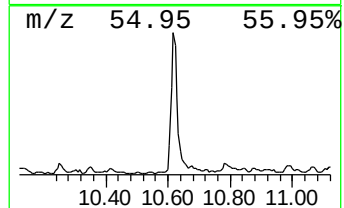
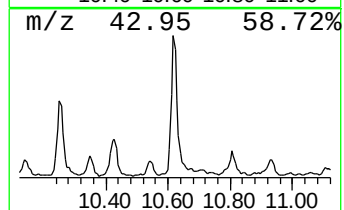
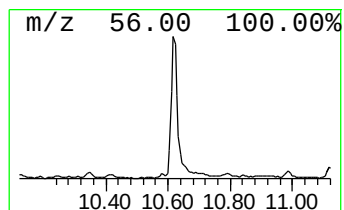
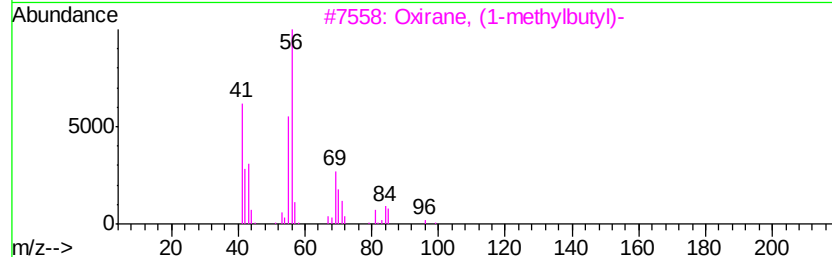
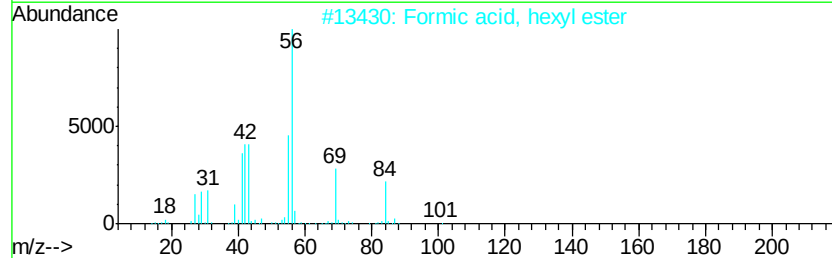
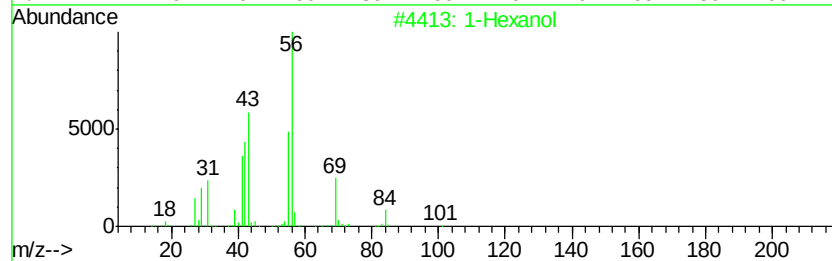
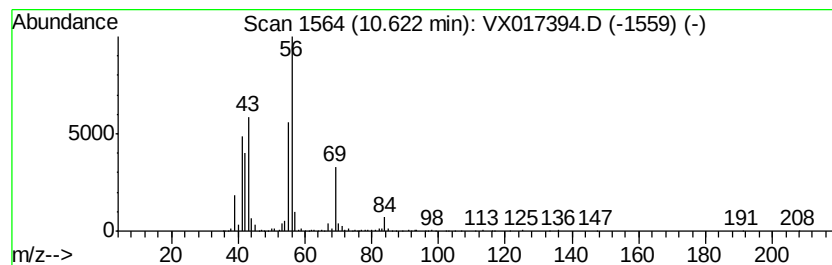
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Hexanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	8.92 ug/l	292365	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol	102	C6H14O	000111-27-3	83
2		Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
3		Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	74
4		1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
5		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	64



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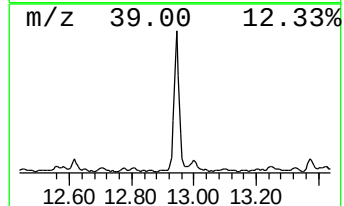
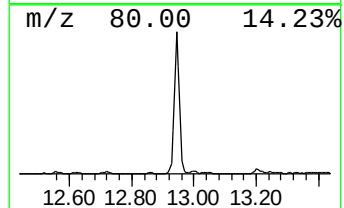
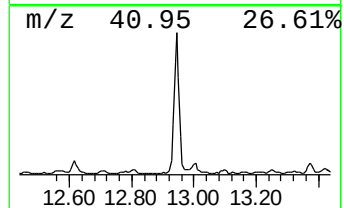
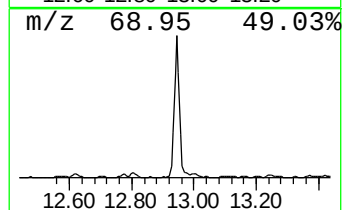
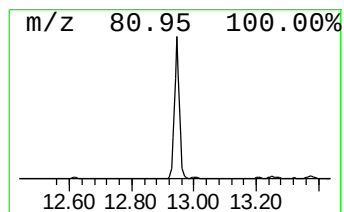
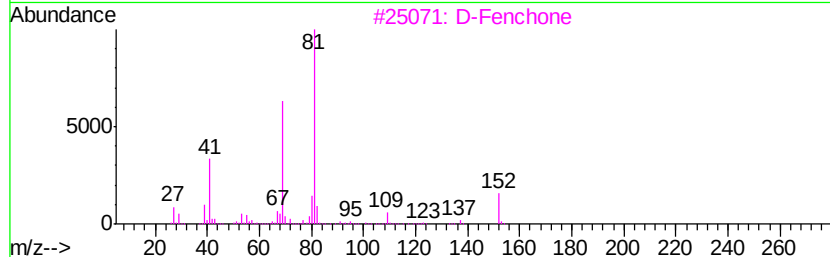
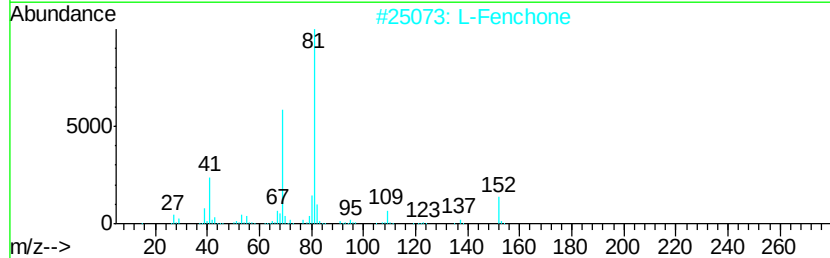
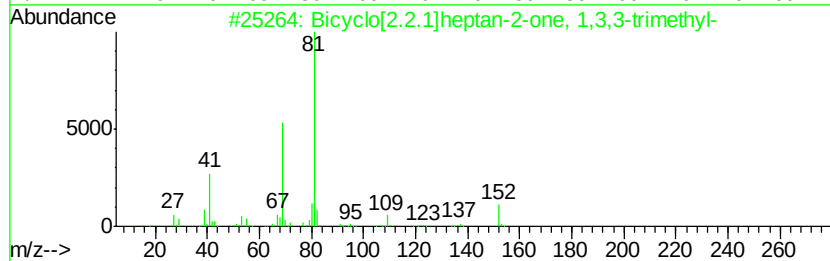
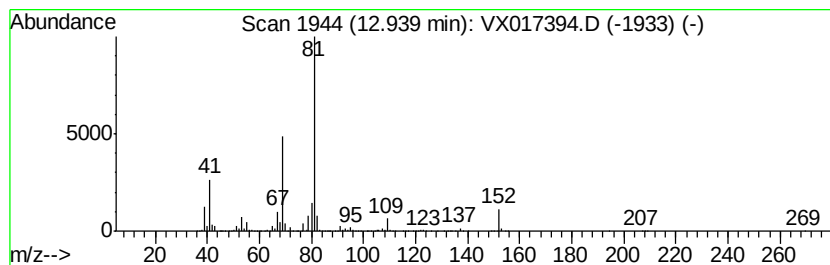
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Peak Number 6 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.94	38.13 ug/l	1433270	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	94
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3N02	1000301-43-3	50
5	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX017394.D
Acq On : 16 Jul 2020 16:28
Operator : JC/SP
Sample : L3325-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

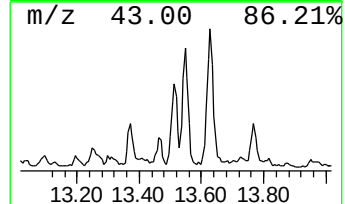
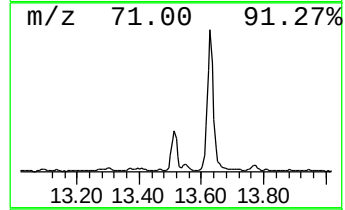
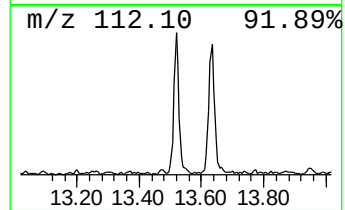
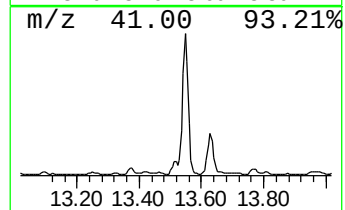
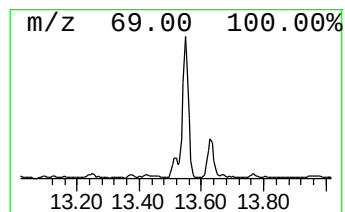
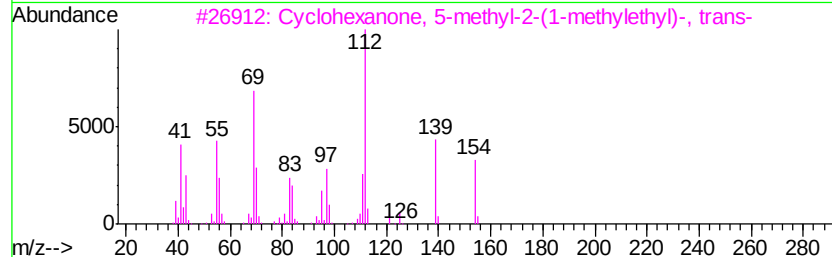
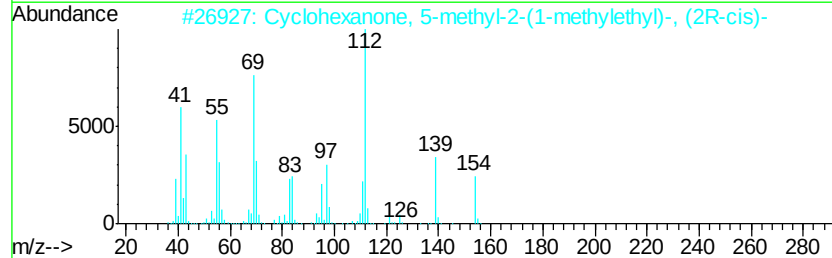
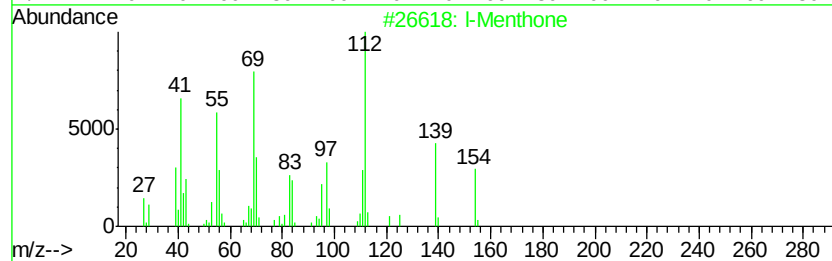
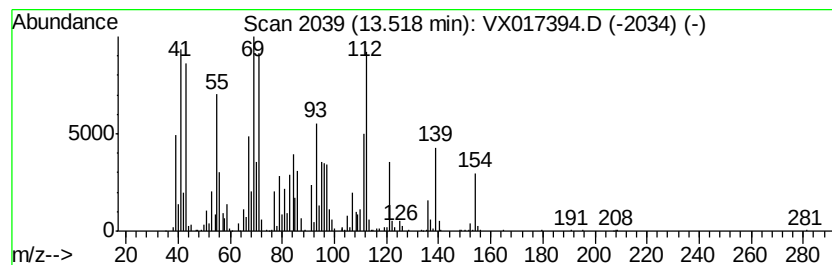
Instrument :
MSVOA_X
ClientSampleId :
200715091-01

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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

Peak Number 7 l-Menthone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	6.75 ug/l	253658	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		l-Menthone	154 C10H18O	014073-97-3 86
2		Cyclohexanone, 5-methyl-2-(1-met...	154 C10H18O	001196-31-2 78
3		Cyclohexanone, 5-methyl-2-(1-met...	154 C10H18O	000089-80-5 55
4		Cyclohexanone, 5-methyl-2-(1-met...	154 C10H18O	000491-07-6 49
5		Cyclohexanone, 5-methyl-2-(1-met...	154 C10H18O	010458-14-7 42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX017394.D
Acq On : 16 Jul 2020 16:28
Operator : JC/SP
Sample : L3325-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

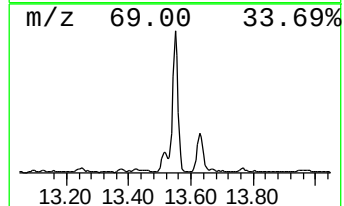
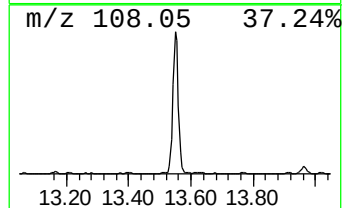
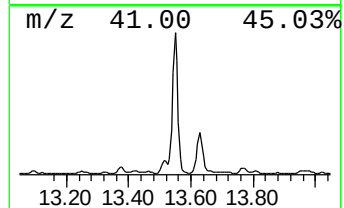
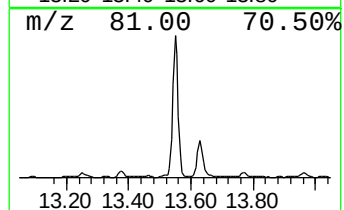
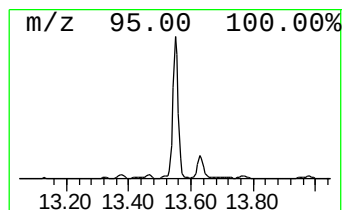
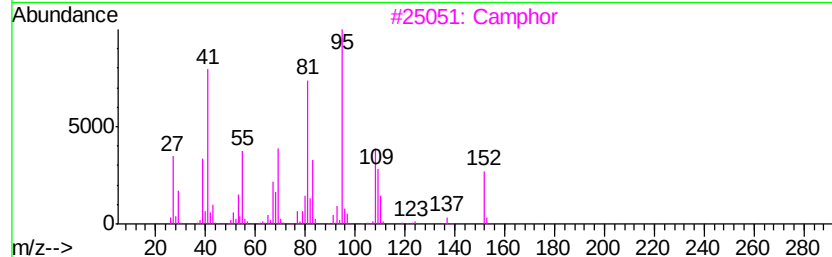
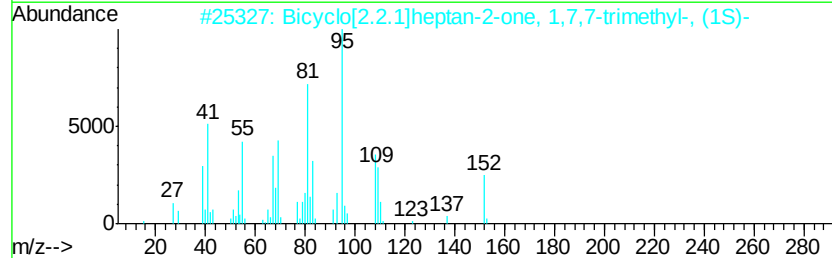
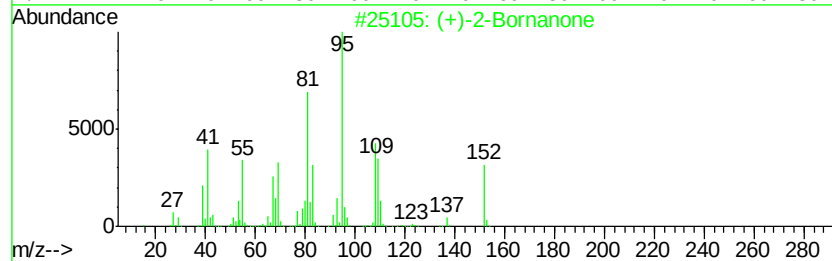
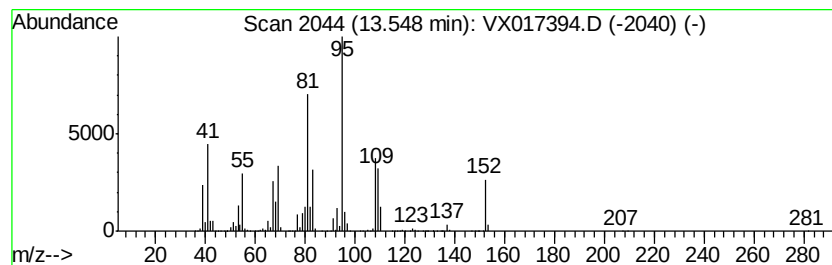
Instrument :
MSVOA_X
ClientSampleId :
200715091-01

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.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	58.20 ug/l	2187770	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	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
3	Camphor	152	C10H16O	000076-22-2	96
4	2-Furancarboxylic acid, 2-propen...	152	C8H8O3	004208-49-5	43
5	7-Octene-1,2-diol	144	C8H16O2	085866-02-0	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX017394.D
Acq On : 16 Jul 2020 16:28
Operator : JC/SP
Sample : L3325-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

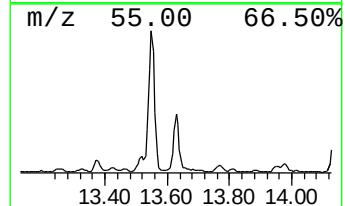
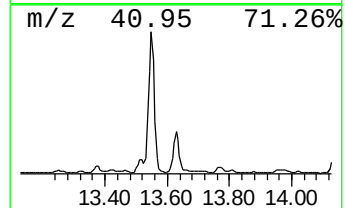
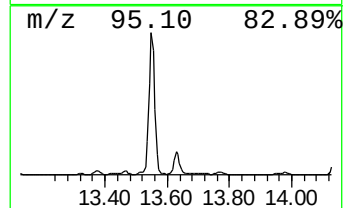
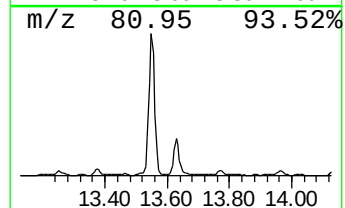
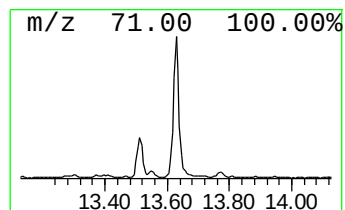
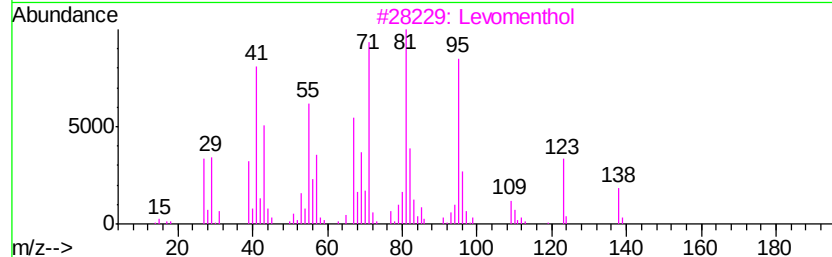
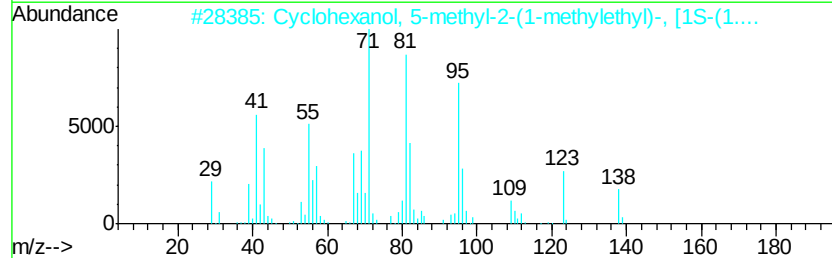
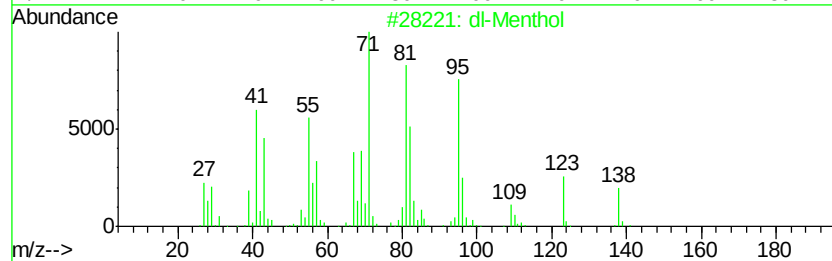
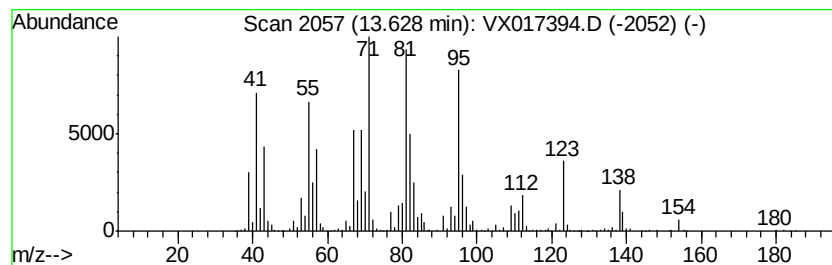
Instrument :
MSVOA_X
ClientSampleId :
200715091-01

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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

Peak Number 9 dl-Menthol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	20.83 ug/l	782968	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	dl-Menthol	156 C10H20O	000089-78-1	91
2	Cyclohexanol, 5-methyl-2-(1-meth...	156 C10H20O	002216-52-6	91
3	Levomenthol	156 C10H20O	002216-51-5	87
4	Cyclohexanol, 5-methyl-2-(1-meth...	156 C10H20O	015356-70-4	87
5	d-Menthol	156 C10H20O	015356-60-2	80



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX017394.D
Acq On : 16 Jul 2020 16:28
Operator : JC/SP
Sample : L3325-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
200715091-01

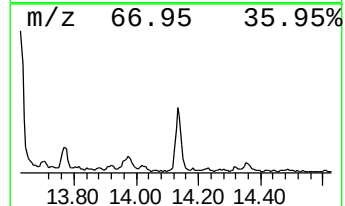
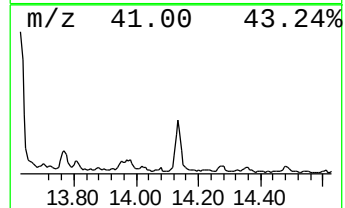
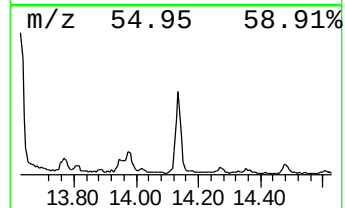
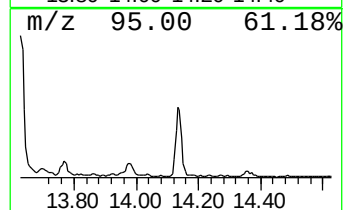
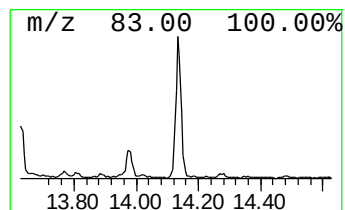
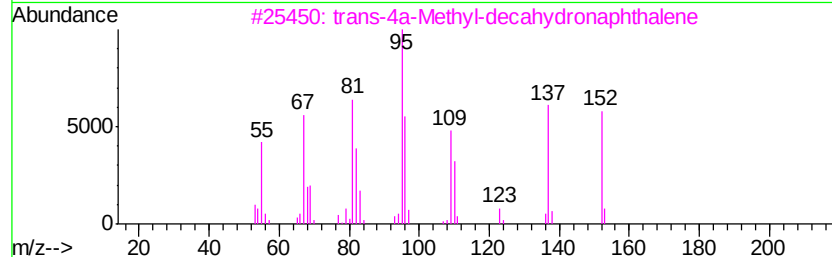
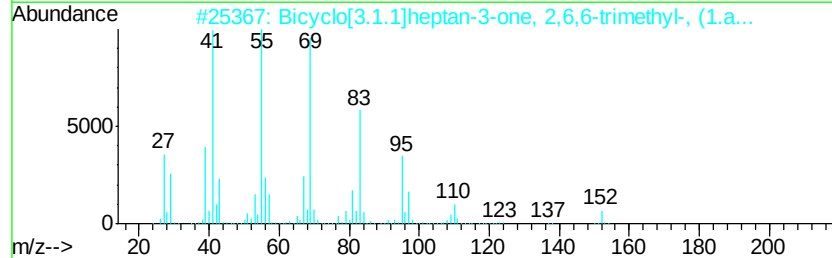
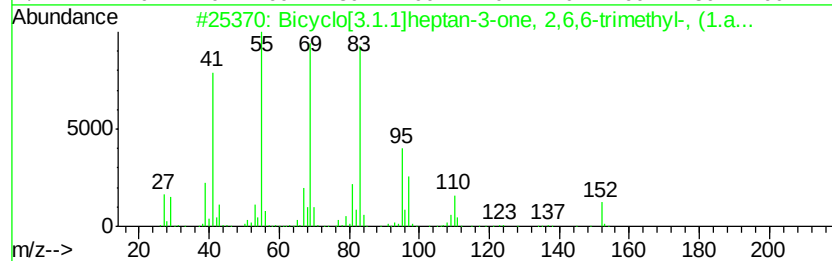
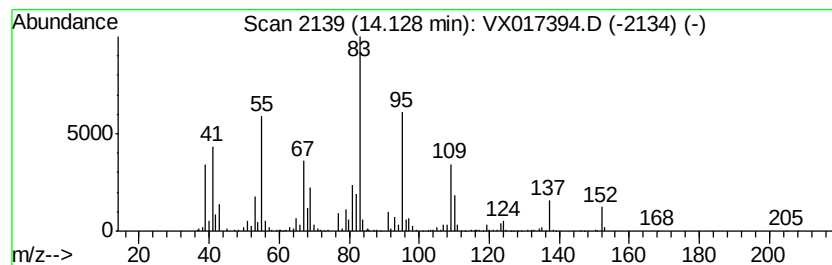
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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

Peak Number 10 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	8.99 ug/l	338055	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	76
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	64
3		trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	46
4		2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	30
5		Bicyclo[2.2.1]heptane, 2-ethyl-	124	C9H16	002146-41-0	25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071620\
Data File : VX017394.D
Acq On : 16 Jul 2020 16:28
Operator : JC/SP
Sample : L3325-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
200715091-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methylamine, N,N-...	1.61	7.5	ug/l	118025	1	5.63	791591	50.0
1-Butanol	7.27	17.2	ug/l	365873	2	6.83	1064670	50.0
3-Pentanone, 2,4-...	9.42	11.2	ug/l	368102	3	10.10	1637910	50.0
1-Hexanol	10.62	8.9	ug/l	292365	3	10.10	1637910	50.0
Bicyclo[2.2.1]hep...	12.94	38.1	ug/l	1433270	4	12.06	1879640	50.0
l-Menthone	13.52	6.8	ug/l	253658	4	12.06	1879640	50.0
(+)-2-Bornanone	13.55	58.2	ug/l	2187770	4	12.06	1879640	50.0
dl-Menthol	13.63	20.8	ug/l	782968	4	12.06	1879640	50.0
Bicyclo[3.1.1]hep...	14.13	9.0	ug/l	338055	4	12.06	1879640	50.0