

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071620\
 Data File : VX017392.D
 Acq On : 16 Jul 2020 15:43
 Operator : JC/SP
 Sample : L3321-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 200715084-02-VOA

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	42	rVB	266950	287114	2.72%	0.697%
2	1.605	83	85	109	rVB2	84207	161272	1.53%	0.391%
3	2.416	212	218	235	rVB	561525	1026190	9.74%	2.491%
4	2.575	235	244	257	rBV	227770	419402	3.98%	1.018%
5	3.014	305	316	333	rBV	2823593	6255530	59.35%	15.183%
6	4.660	564	586	599	rBV2	2924890	10539275	100.00%	25.579%
7	5.086	644	656	675	rBV2	1227249	3714674	35.25%	9.016%
8	5.471	708	719	731	rVB	182556	519825	4.93%	1.262%
9	5.629	733	745	759	rVB	295029	826172	7.84%	2.005%
10	6.031	800	811	819	rBV	188992	494385	4.69%	1.200%
11	6.306	851	856	866	rVB	51510	136716	1.30%	0.332%
12	6.830	931	942	955	rBV	462191	1108957	10.52%	2.691%
13	7.269	1007	1014	1025	rBV	127693	288982	2.74%	0.701%
14	8.696	1241	1248	1254	rBV	1019478	1584624	15.04%	3.846%
15	8.763	1254	1259	1266	rVV2	110857	188045	1.78%	0.456%
16	8.848	1268	1273	1278	rVB	75358	112190	1.06%	0.272%
17	9.275	1338	1343	1350	rBV2	99756	179034	1.70%	0.435%
18	9.421	1358	1367	1373	rVB	235052	358353	3.40%	0.870%
19	10.098	1467	1478	1489	rBV	1144538	1685714	15.99%	4.091%
20	10.238	1496	1501	1511	rBV2	157371	254146	2.41%	0.617%
21	10.342	1512	1518	1524	rVV	220024	305966	2.90%	0.743%
22	10.616	1559	1563	1570	rBV	213422	301148	2.86%	0.731%
23	10.683	1570	1574	1586	rVB	142834	212229	2.01%	0.515%
24	11.122	1640	1646	1651	rBV	1039622	1305161	12.38%	3.168%
25	11.927	1771	1778	1785	rVB2	95644	135416	1.28%	0.329%
26	12.061	1794	1800	1808	rBV	1491926	1934997	18.36%	4.696%
27	12.140	1808	1813	1817	rBV3	140788	212359	2.01%	0.515%
28	12.616	1888	1891	1895	rVB	112553	129932	1.23%	0.315%
29	12.805	1913	1922	1926	rBV2	103589	169528	1.61%	0.411%
30	12.945	1938	1945	1950	rBV	1139340	1405554	13.34%	3.411%
31	13.000	1950	1954	1959	rVB3	97468	146593	1.39%	0.356%
32	13.372	2011	2015	2021	rBV	138761	199661	1.89%	0.485%
33	13.512	2034	2038	2040	rBV2	188268	251941	2.39%	0.611%
34	13.548	2040	2044	2052	rVB	1710306	2222018	21.08%	5.393%

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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 >
Peak separation: 5

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Title : SW846 8260

35	13.628	2052	2057	2066	rBV2	567505	791937	7.51%	1.922%
36	13.768	2076	2080	2084	rBV2	133235	167104	1.59%	0.406%
37	13.817	2084	2088	2094	rVB	588994	704523	6.68%	1.710%
38	13.975	2107	2114	2119	rBV5	50225	119097	1.13%	0.289%
39	14.134	2134	2140	2152	rBV	241682	346456	3.29%	0.841%

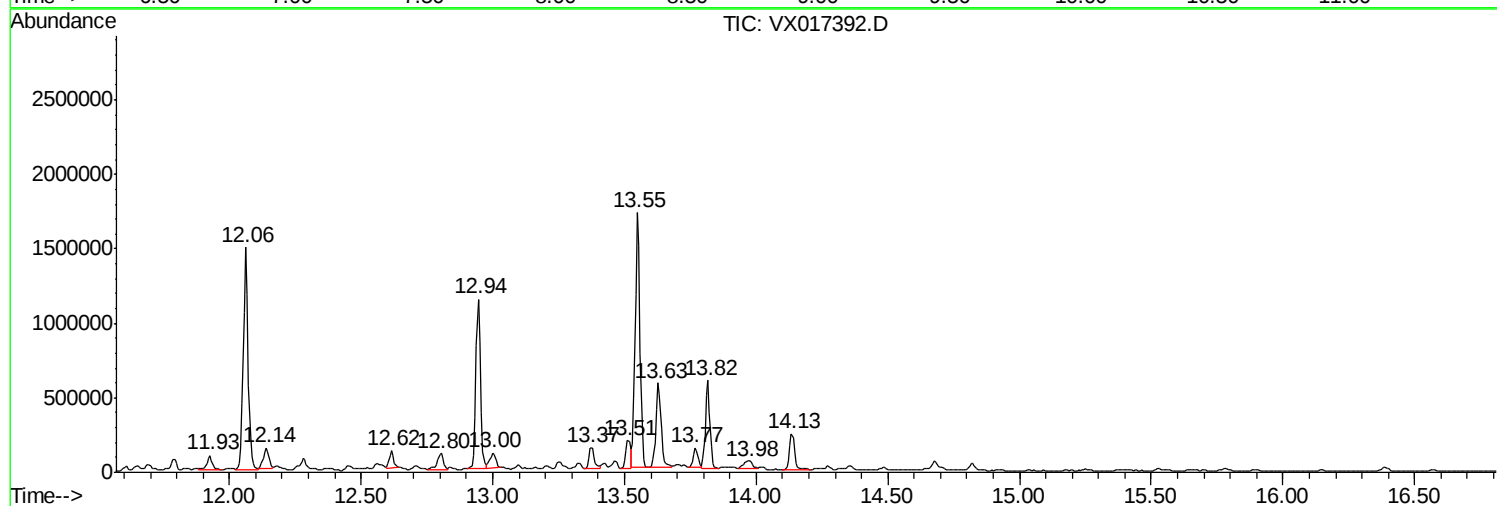
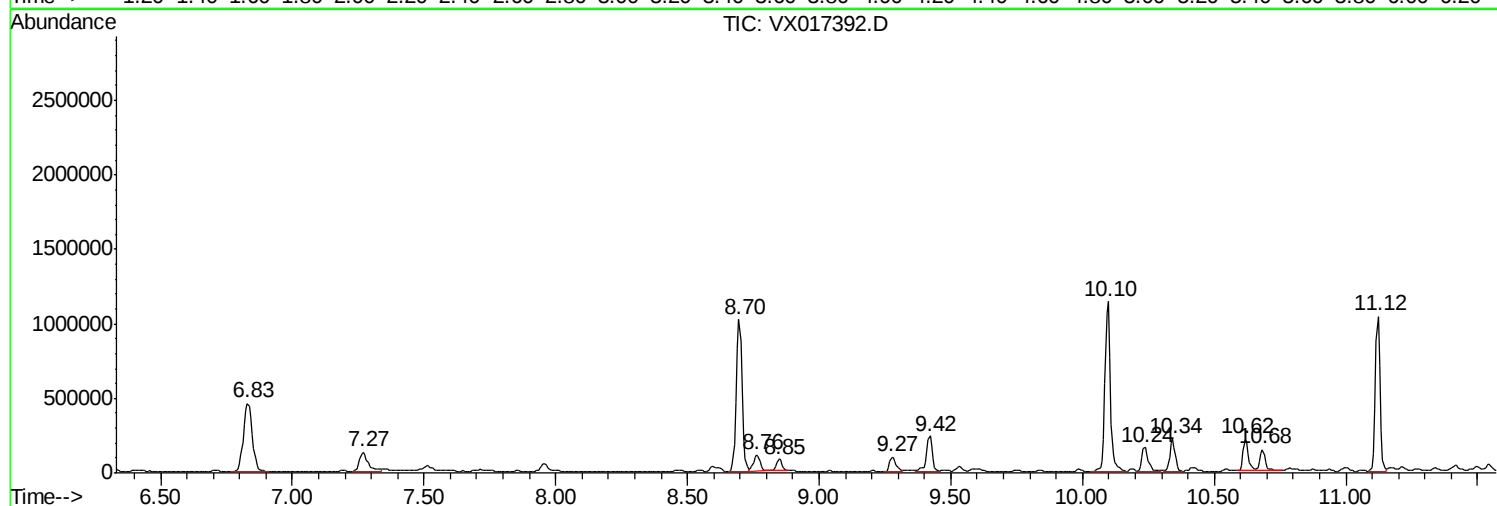
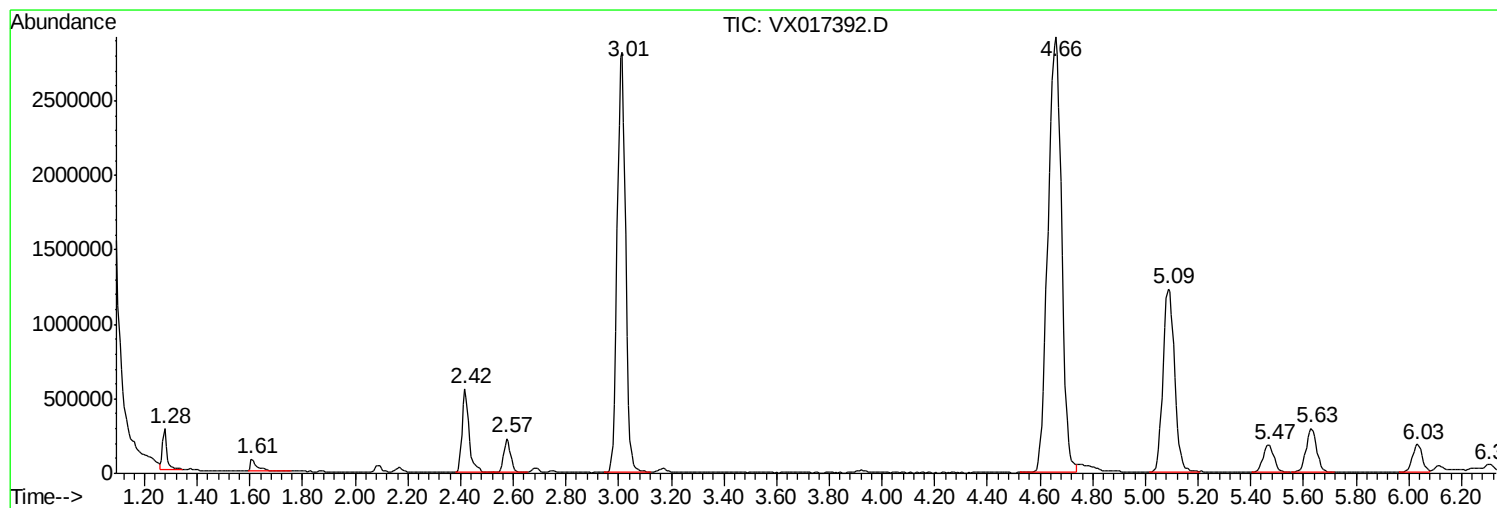
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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



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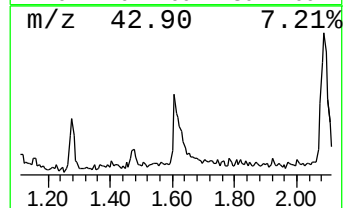
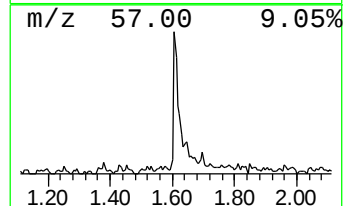
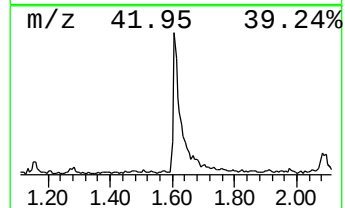
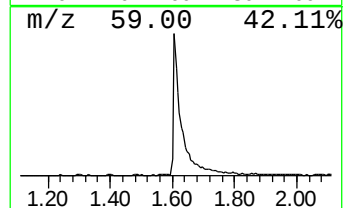
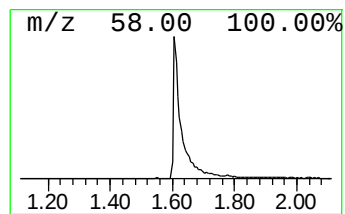
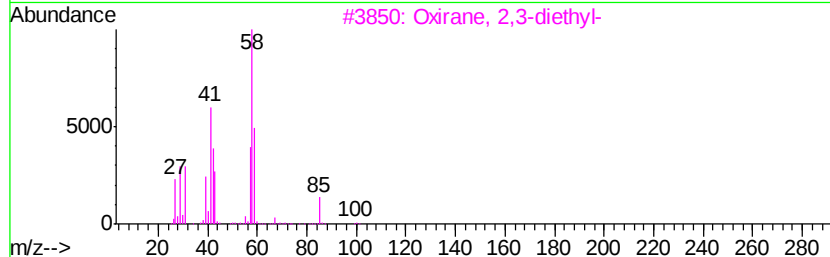
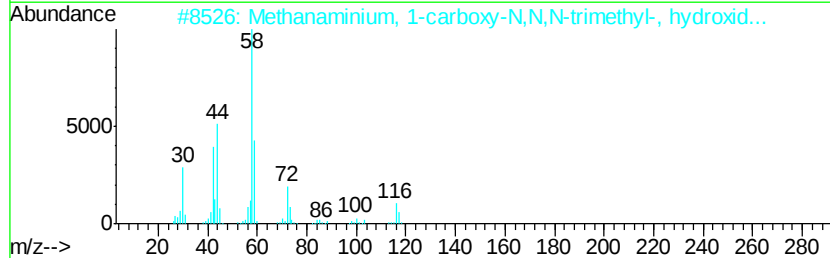
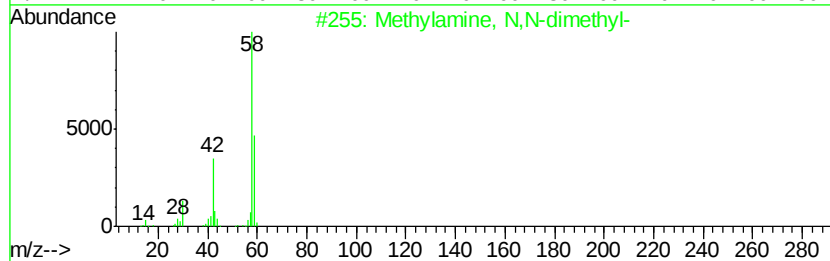
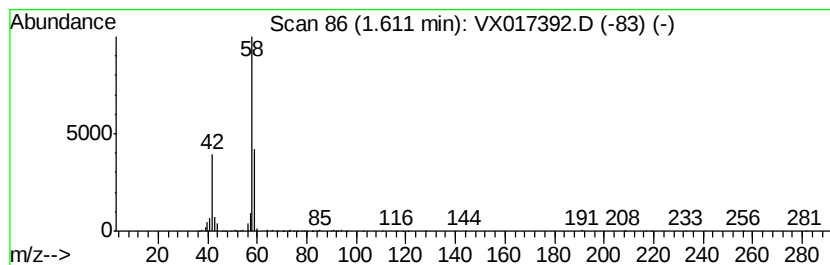
Instrument :
MSVOA_X
ClientSampleId :
200715084-02-VOA

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 2 Methylamine, N,N-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.61	9.76 ug/l	161272	Pentafluorobenzene	5.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	90
2		Methanaminium, 1-carboxy-N,N,N-t...	117	C5H11N02	000107-43-7	40
3		Oxirane, 2,3-diethyl-	100	C6H12O	004468-66-0	9
4		2-Propanone, 1-(dimethylamino)-	101	C5H11NO	015364-56-4	9
5		2-Methyl-1,2-propanediamine	88	C4H12N2	000811-93-8	9



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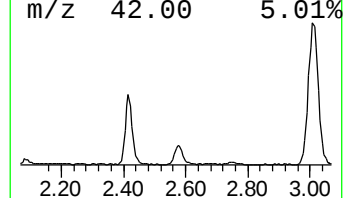
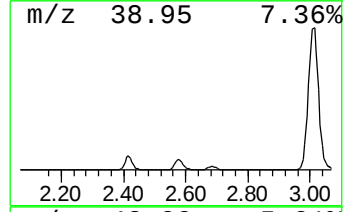
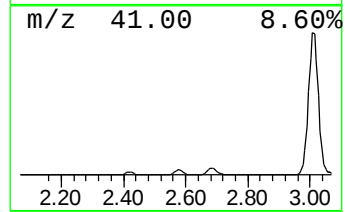
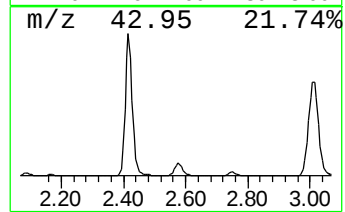
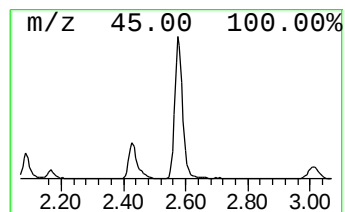
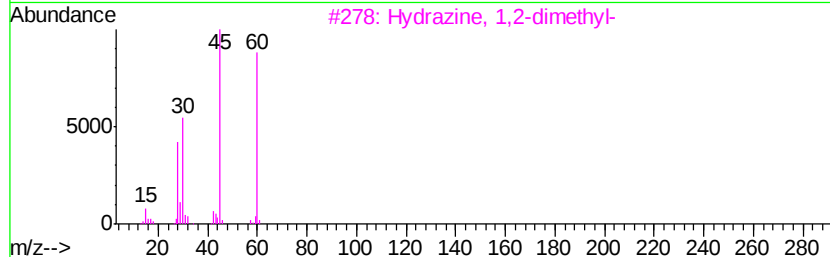
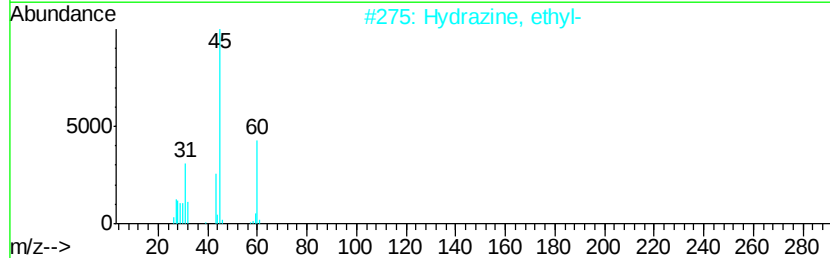
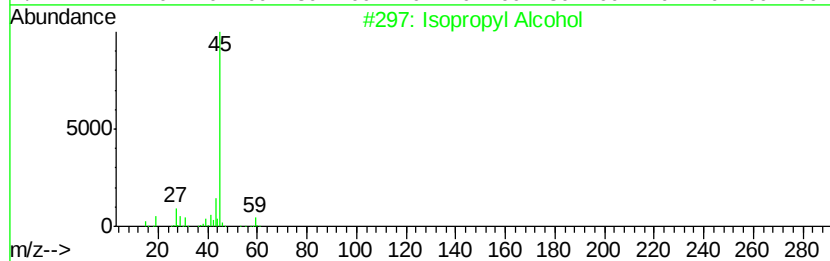
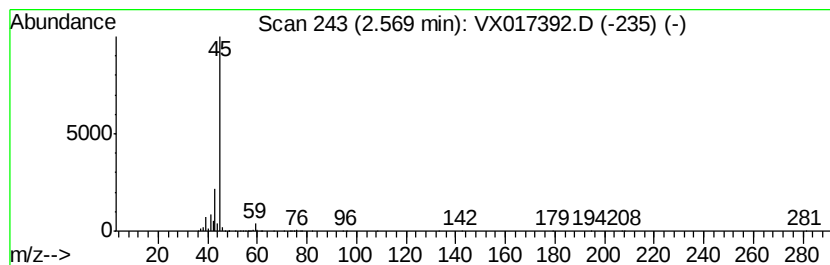
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X071320W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.57	25.38 ug/l	419402	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2		Hvdrazine, ethyl-	60	C2H8N2	000624-80-6	9
3		Hvdrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4		Formamide	45	CH3NO	000075-12-7	5
5		2-Butanol	74	C4H10O	000078-92-2	4



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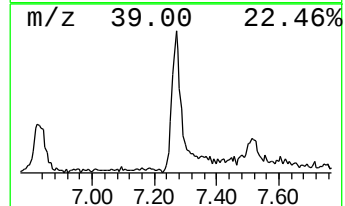
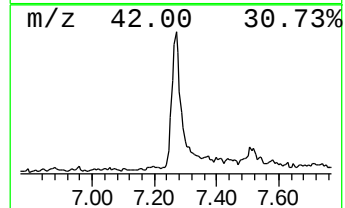
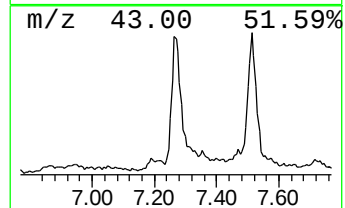
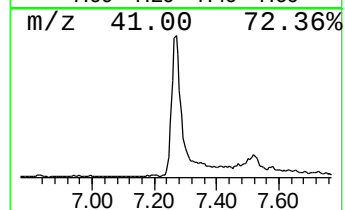
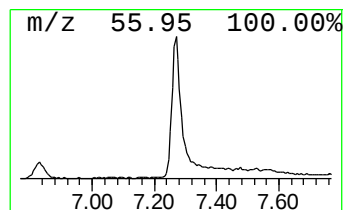
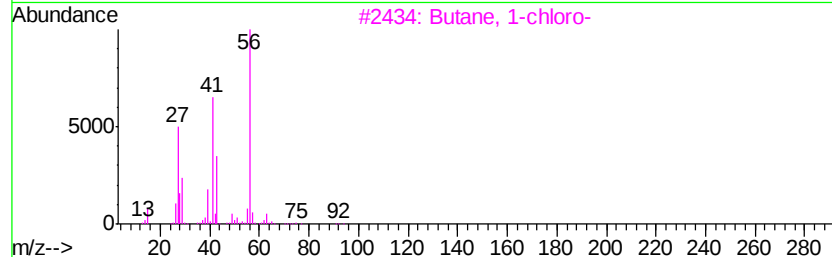
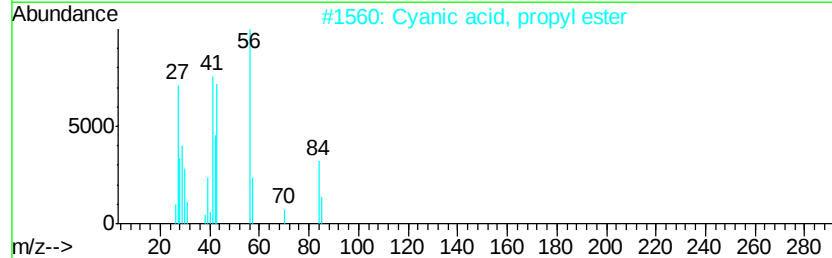
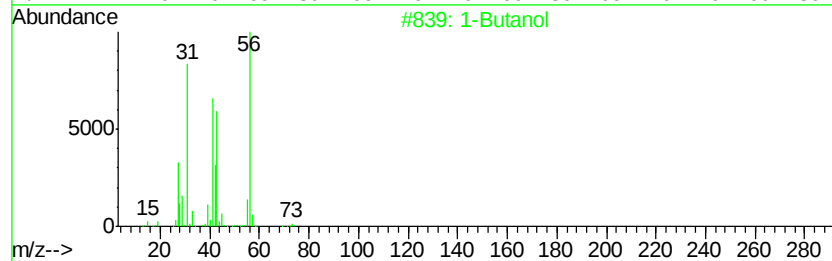
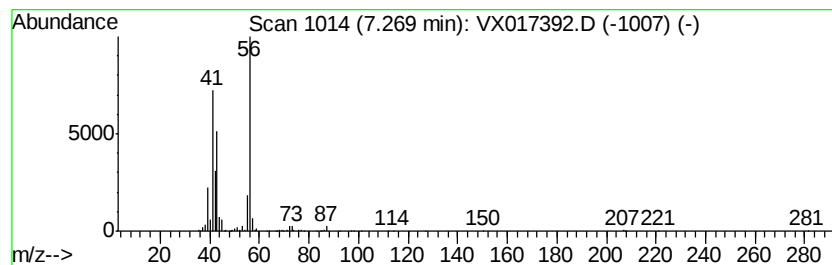
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	13.03 ug/l	288982	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	80
2		Cyanoic acid, propyl ester	85	C4H7NO	001768-36-1	50
3		Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
4		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	42
5		Hexyl chloroformate	164	C7H13ClO2	006092-54-2	40



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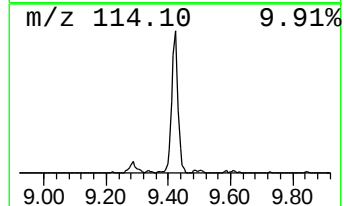
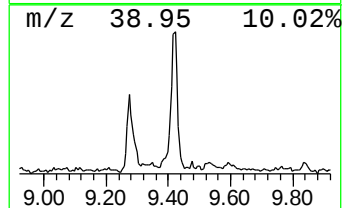
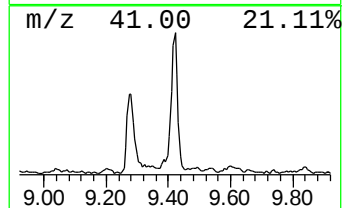
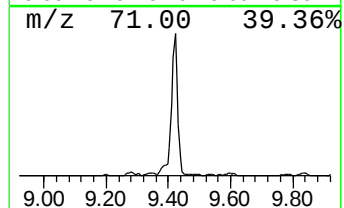
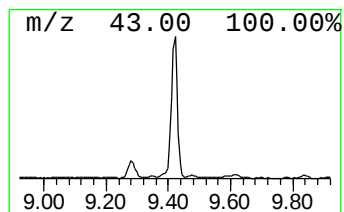
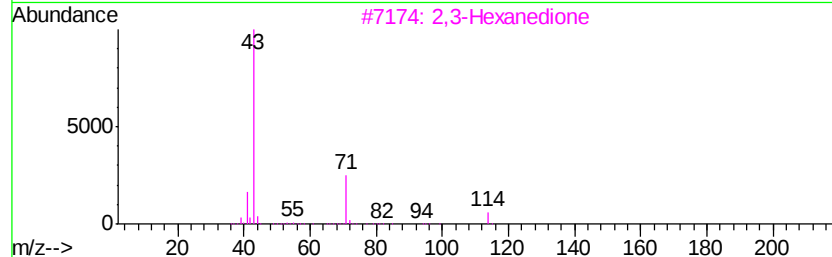
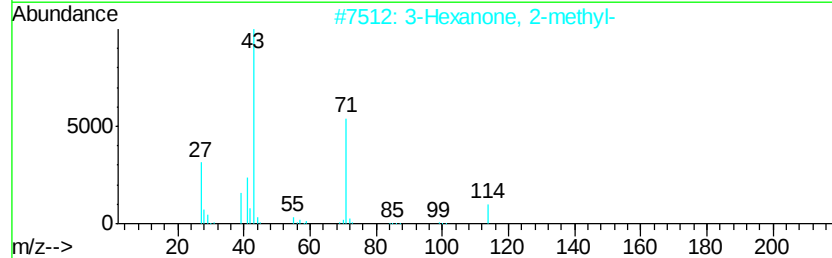
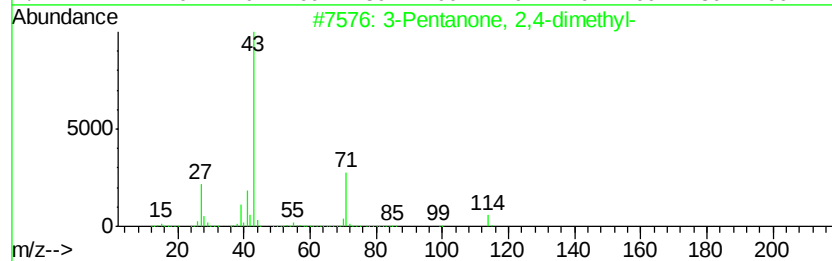
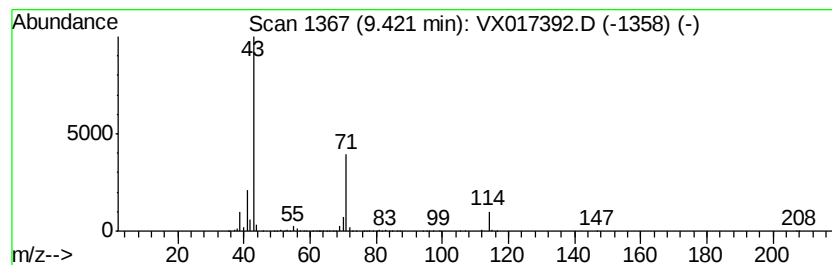
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	10.63 ug/l	358353	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	80
3		2,3-Hexanedione	114	C6H10O2	003848-24-6	64
4		4-Heptanone	114	C7H14O	000123-19-3	53
5		Pyrrolidine	71	C4H9N	000123-75-1	42



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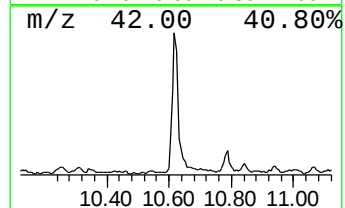
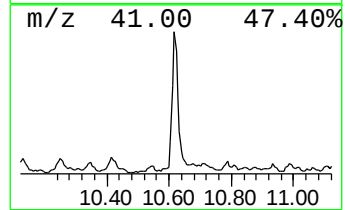
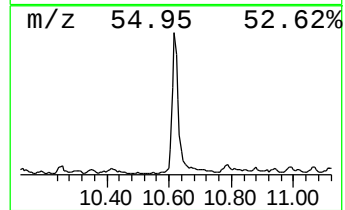
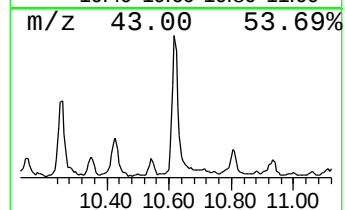
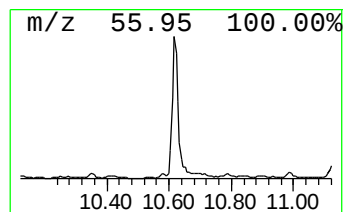
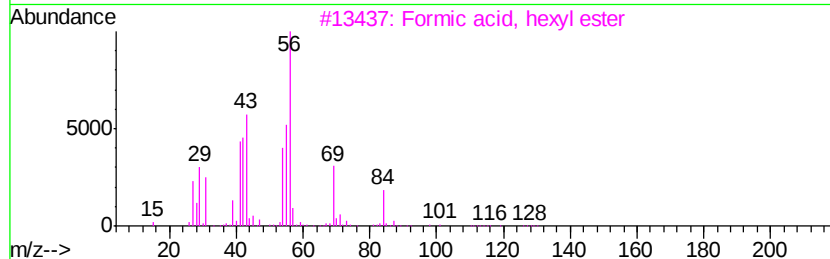
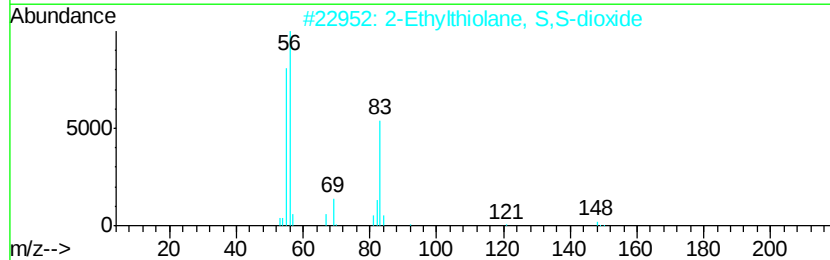
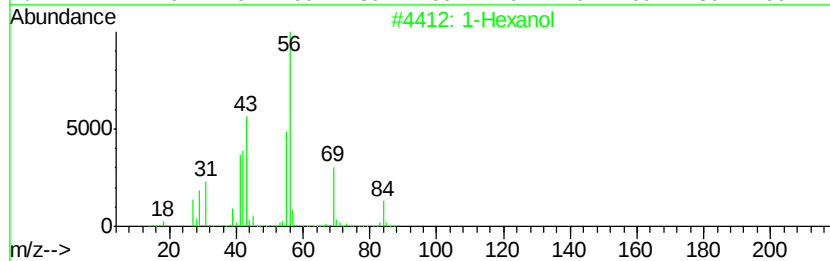
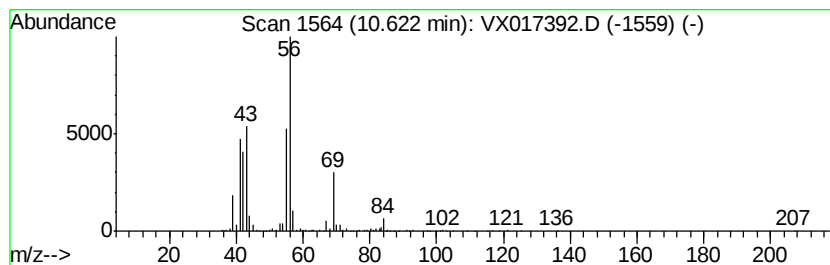
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	8.93 ug/l	301148	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol	102	C6H14O	000111-27-3	86
2		2-Ethylthiolane, S,S-dioxide	148	C6H12O2S	010178-59-3	83
3		Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
4		Hexyl chloroformate	164	C7H13ClO2	006092-54-2	64
5		1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX017392.D
Acq On : 16 Jul 2020 15:43
Operator : JC/SP
Sample : L3321-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
200715084-02-VOA

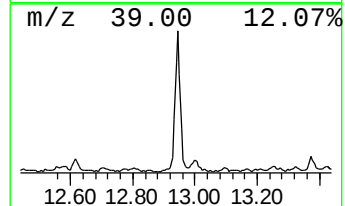
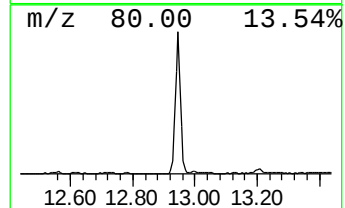
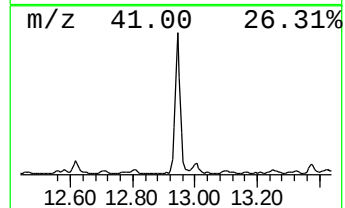
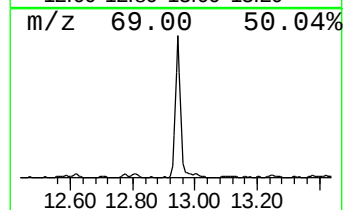
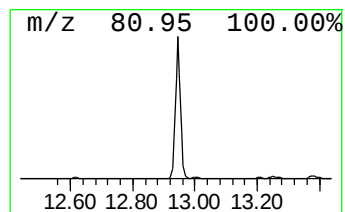
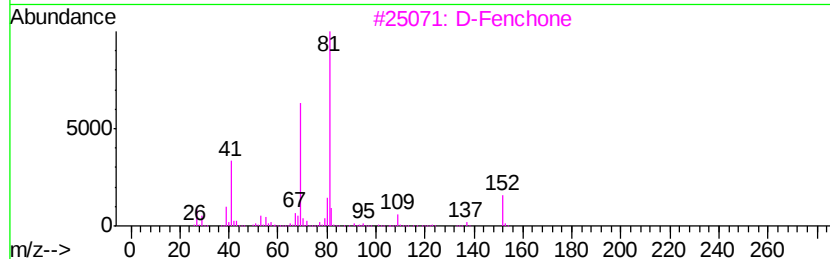
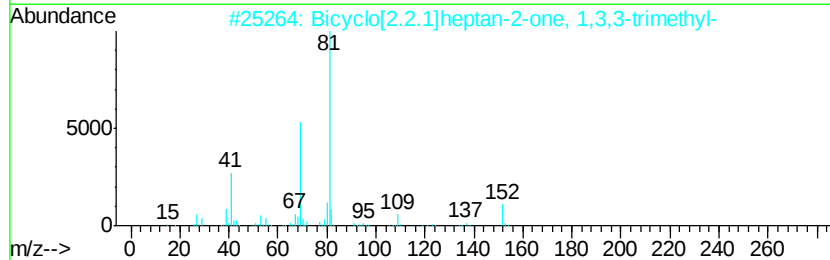
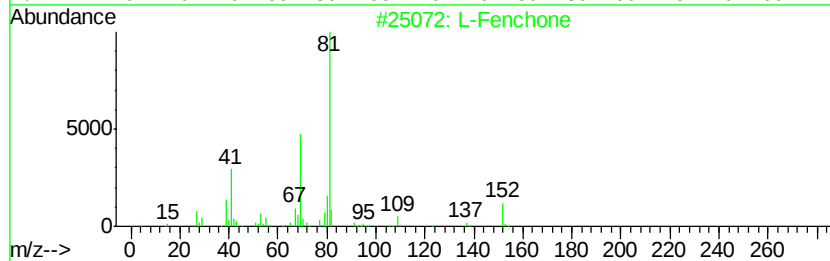
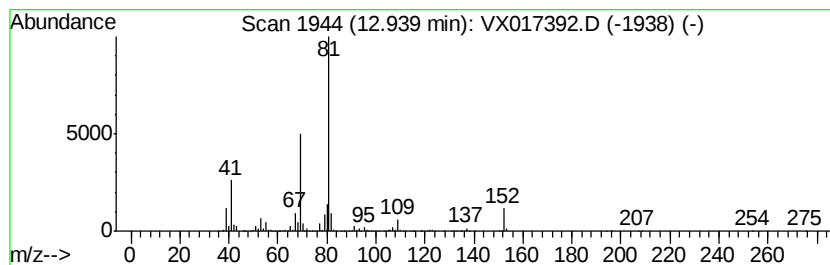
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Quant Title : SW846 8260

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

Peak Number 7 L-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	36.32 ug/l	1405550	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Ethanone, 1-(2-methyl-2-cyclopent...	124	C8H12O	001767-84-6	42
5		1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3N02	1000301-43-3	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX017392.D
Acq On : 16 Jul 2020 15:43
Operator : JC/SP
Sample : L3321-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

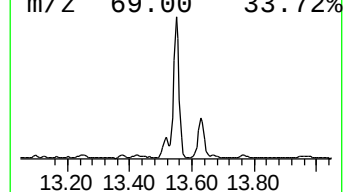
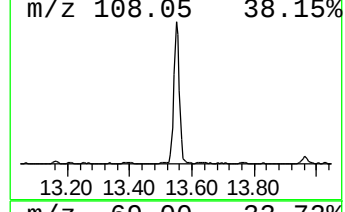
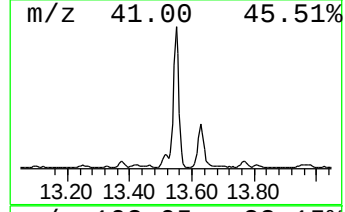
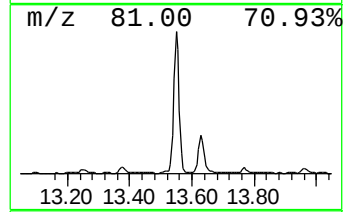
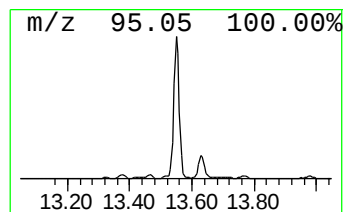
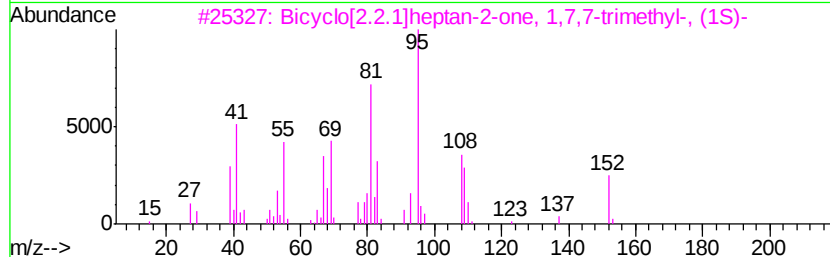
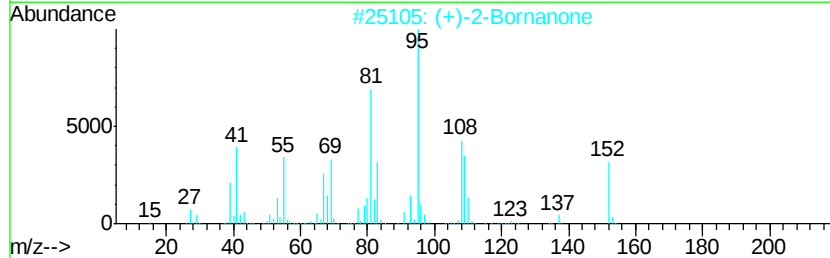
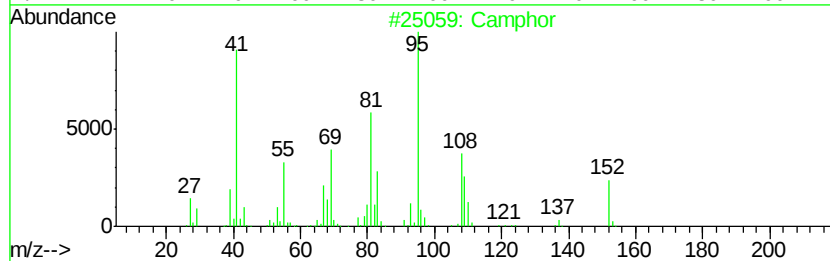
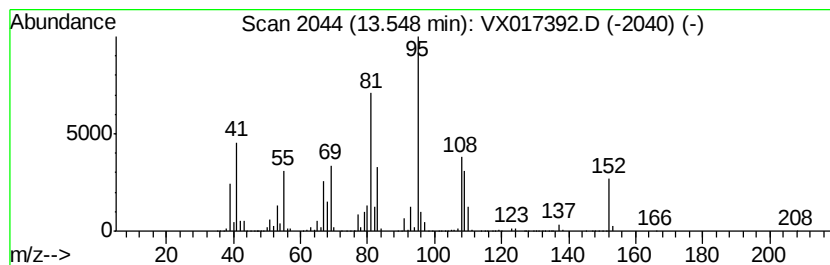
Instrument :
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ClientSampleId :
200715084-02-VOA

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 Camphor Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	57.42 ug/l	2222020	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Camphor		152 C10H16O	000076-22-2 98
2	(+)-2-Bornanone		152 C10H16O	000464-49-3 98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...		152 C10H16O	000464-48-2 98
4	2-Butanone, 4-(5-methyl-2-furanyl)-		152 C9H12O2	013679-56-6 47
5	1,4-Pentadiene, 2,3,3-trimethyl-		110 C8H14	000756-02-5 38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX071392.D
Acq On : 16 Jul 2020 15:43
Operator : JC/SP
Sample : L3321-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

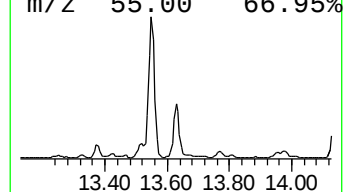
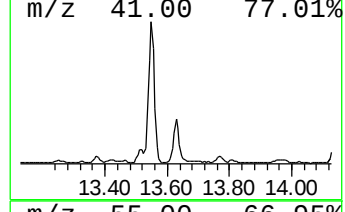
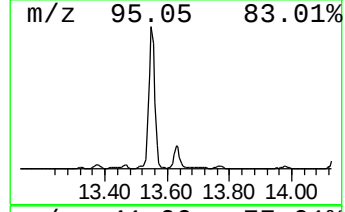
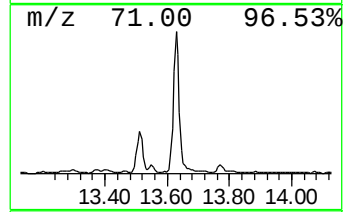
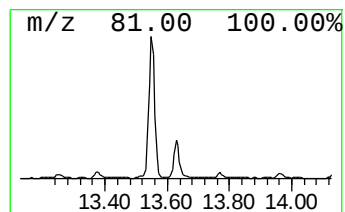
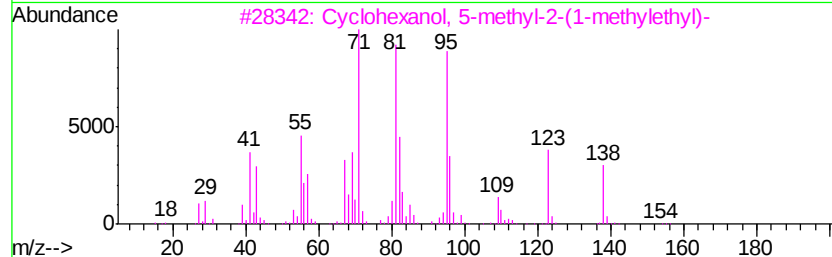
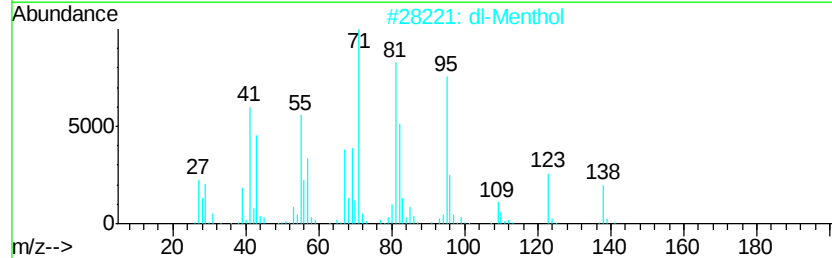
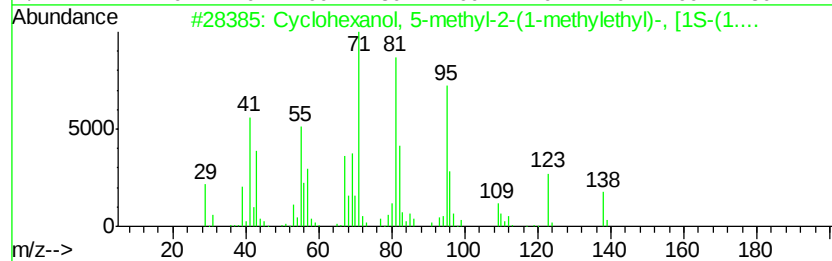
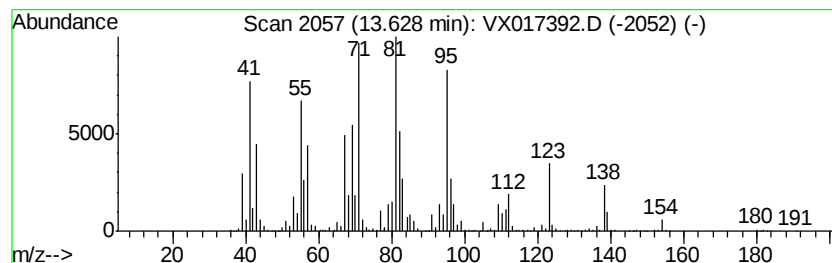
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ClientSampleId :
200715084-02-VOA

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 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	20.46 ug/l	791937	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexanol, 5-methyl-2-(1-meth...	156 C10H20O	002216-52-6 91
2		dl-Menthol	156 C10H20O	000089-78-1 91
3		Cyclohexanol, 5-methyl-2-(1-meth...	156 C10H20O	001490-04-6 86
4		Cyclohexanol, 5-methyl-2-(1-meth...	156 C10H20O	015356-70-4 83
5		Levomenthol	156 C10H20O	002216-51-5 83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX071620\
Data File : VX017392.D
Acq On : 16 Jul 2020 15:43
Operator : JC/SP
Sample : L3321-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
200715084-02-VOA

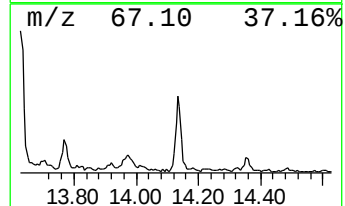
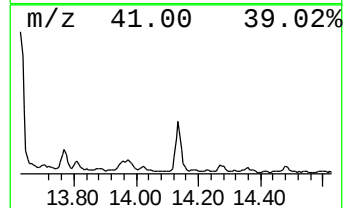
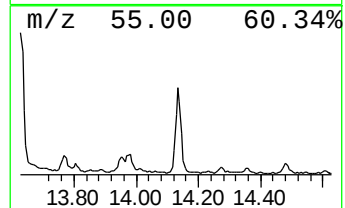
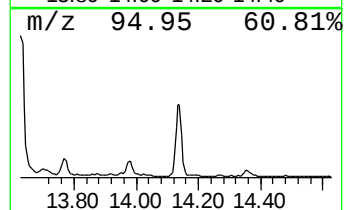
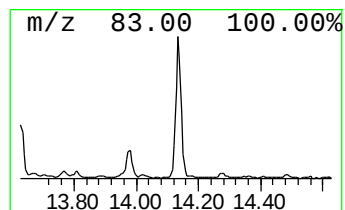
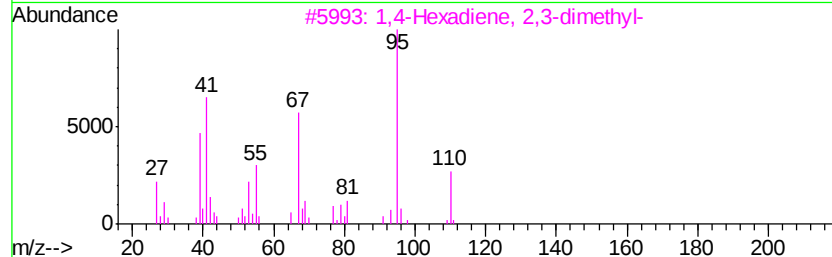
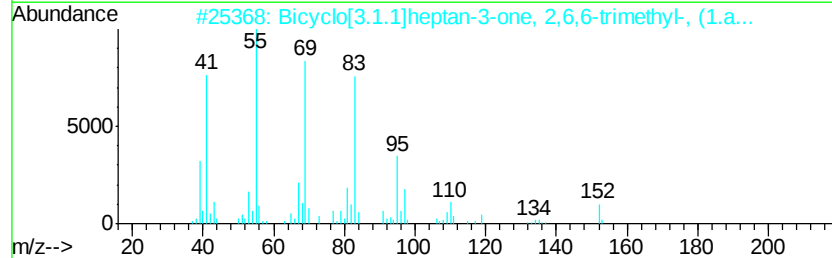
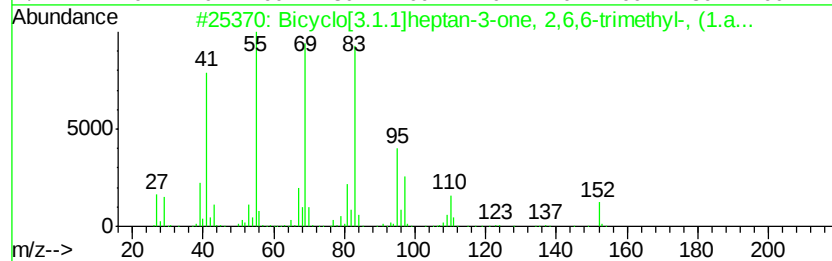
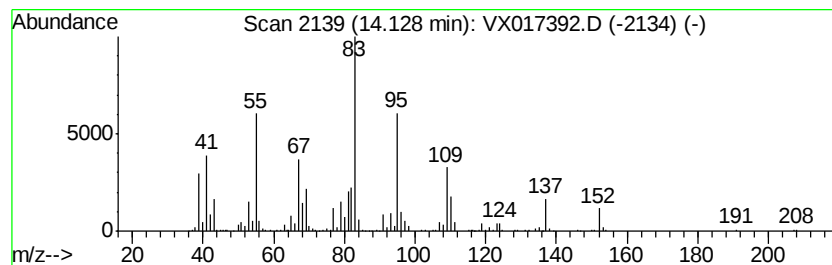
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Quant Title : SW846 8260

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

Peak Number 10 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	8.95 ug/l	346456	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	58
3		1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38
4		2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	38
5		5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	35



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071620\
Data File : VX017392.D
Acq On : 16 Jul 2020 15:43
Operator : JC/SP
Sample : L3321-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
200715084-02-VOA

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	9.8	ug/l	161272	1	5.63	826172	50.0
Isopropyl Alcohol	2.57	25.4	ug/l	419402	1	5.63	826172	50.0
1-Butanol	7.27	13.0	ug/l	288982	2	6.83	1108960	50.0
3-Pentanone, 2,4-...	9.42	10.6	ug/l	358353	3	10.10	1685710	50.0
1-Hexanol	10.62	8.9	ug/l	301148	3	10.10	1685710	50.0
L-Fenchone	12.94	36.3	ug/l	1405550	4	12.06	1935000	50.0
Camphor	13.55	57.4	ug/l	2222020	4	12.06	1935000	50.0
Cyclohexanol, 5-m...	13.63	20.5	ug/l	791937	4	12.06	1935000	50.0
Bicyclo[3.1.1]hep...	14.13	8.9	ug/l	346456	4	12.06	1935000	50.0