

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX041020\
 Data File : VX015624.D
 Acq On : 10 Apr 2020 16:19
 Operator : JC/SP
 Sample : L2210-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 400408742.3-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\82X032720W.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	1.064	23	29	61	rBV	17294998	43309795	100.00%	30.891%
2	2.417	244	251	260	rBV2	253803	485088	1.12%	0.346%
3	3.009	336	348	363	rBV	13906706	30956659	71.48%	22.080%
4	4.655	599	618	631	rBV	7019679	22841366	52.74%	16.292%
5	5.088	678	689	707	rBV	1985217	5948668	13.74%	4.243%
6	5.465	741	751	763	rBV2	614643	1745194	4.03%	1.245%
7	5.630	766	778	792	rBV2	1055228	2921740	6.75%	2.084%
8	6.032	834	844	854	rBV	681399	1782557	4.12%	1.271%
9	6.307	882	889	899	rVB	263468	736151	1.70%	0.525%
10	6.831	966	975	987	rBV	1576148	3814023	8.81%	2.720%
11	8.697	1273	1281	1288	rBV	3477180	5486513	12.67%	3.913%
12	10.099	1499	1511	1518	rBV	3717806	5130584	11.85%	3.659%
13	11.123	1672	1679	1686	rBV	3409782	4273920	9.87%	3.048%
14	12.062	1827	1833	1841	rVB	4558385	5803007	13.40%	4.139%
15	12.800	1946	1954	1959	rBV2	515032	817699	1.89%	0.583%
16	12.982	1981	1984	1992	rVB3	501396	830333	1.92%	0.592%
17	13.513	2066	2071	2074	rBV	773198	1001889	2.31%	0.715%
18	13.549	2074	2077	2085	rVB	704442	949807	2.19%	0.677%
19	13.629	2085	2090	2095	rBV2	399649	587177	1.36%	0.419%
20	13.818	2116	2121	2127	rVB	578634	780081	1.80%	0.556%

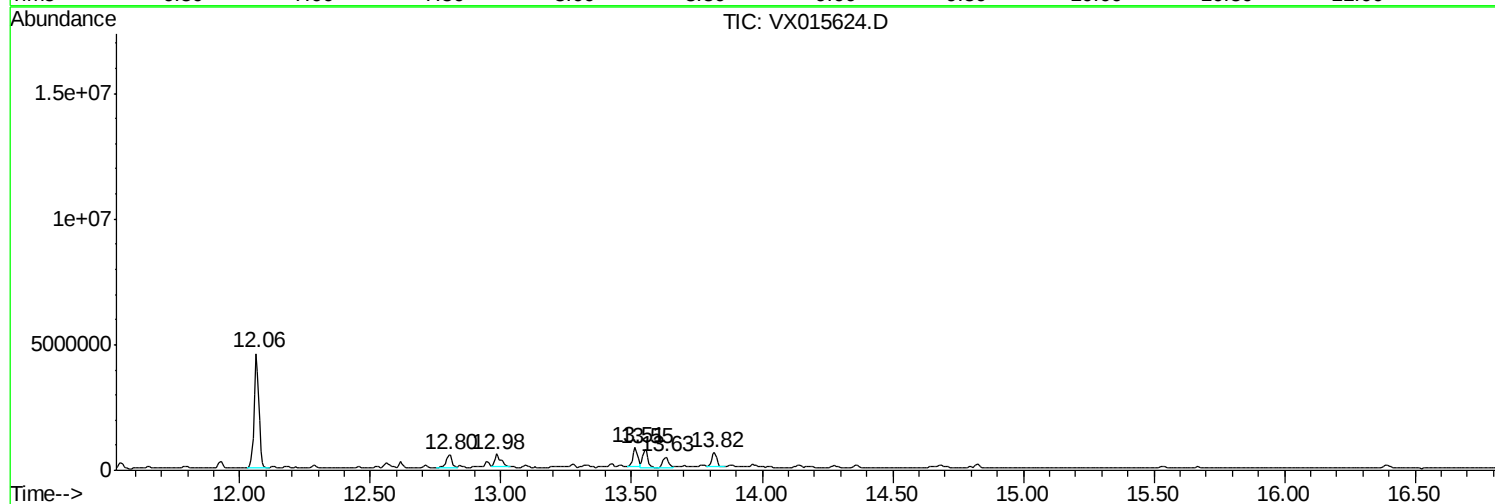
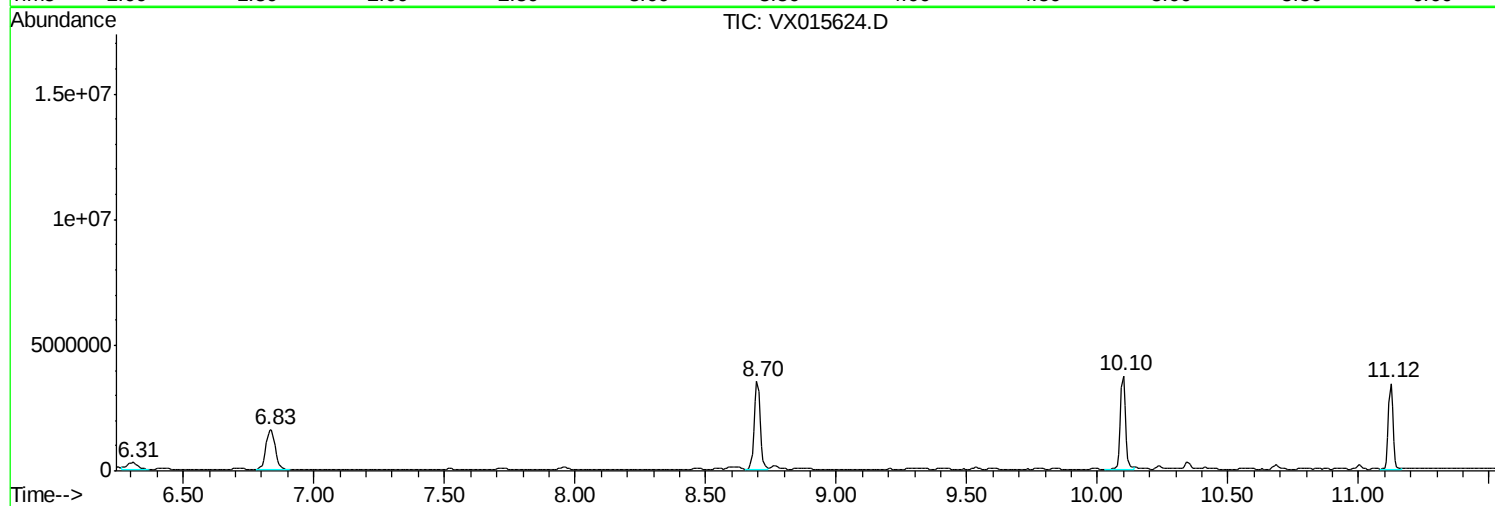
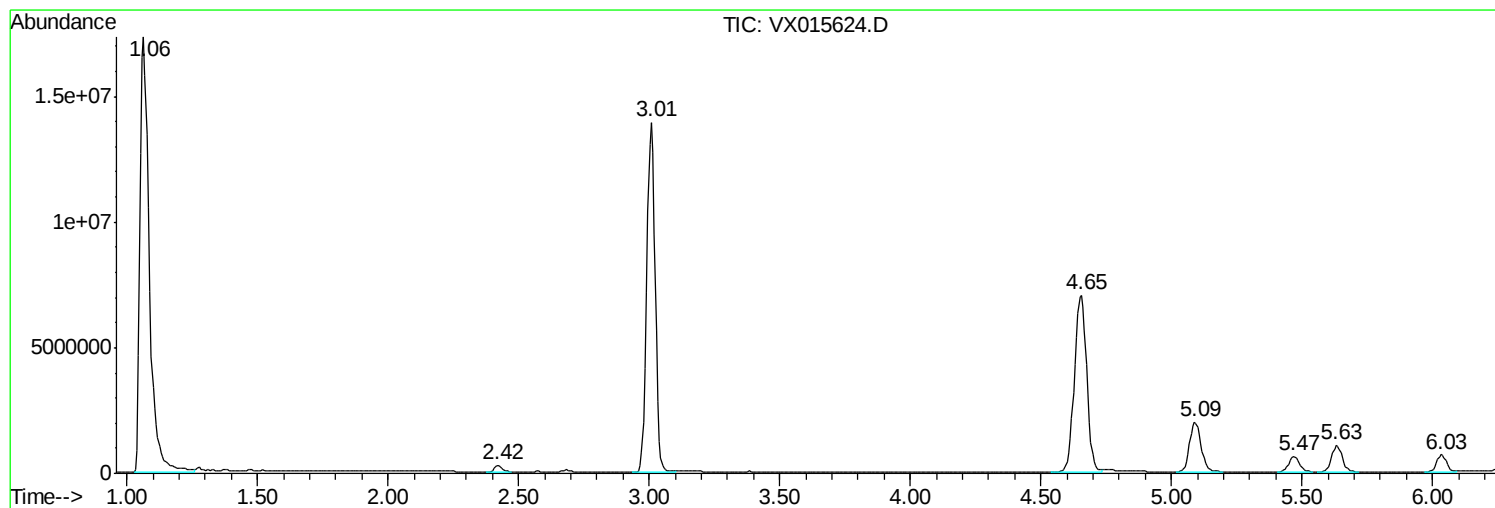
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



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ClientSampleId :
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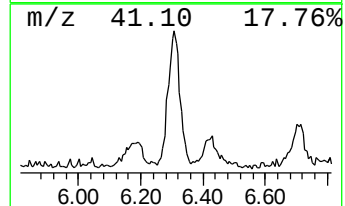
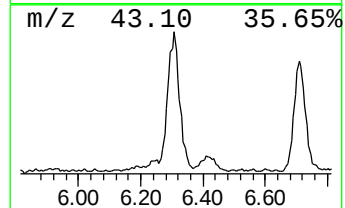
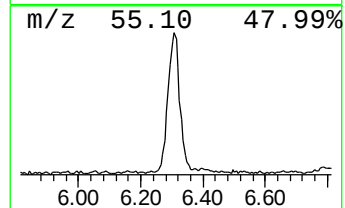
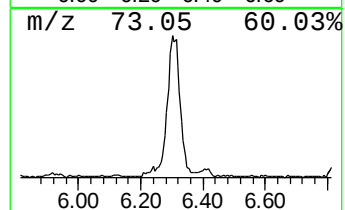
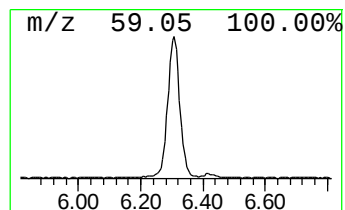
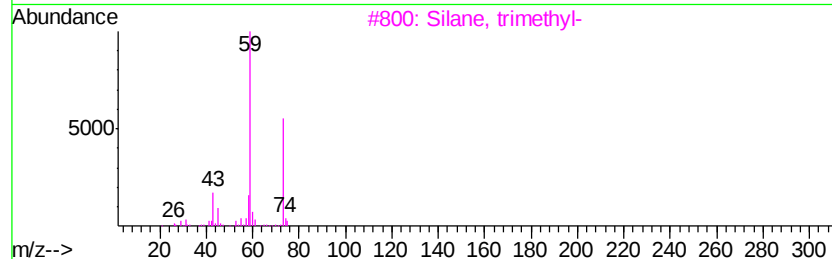
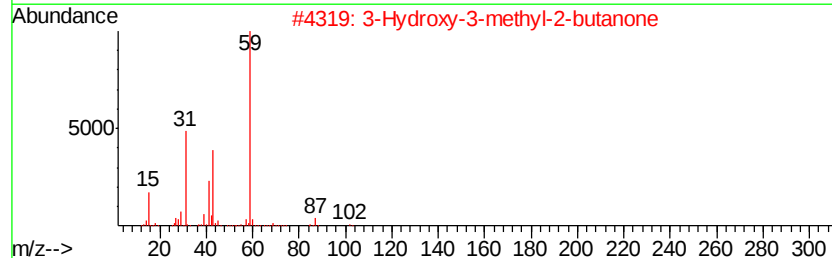
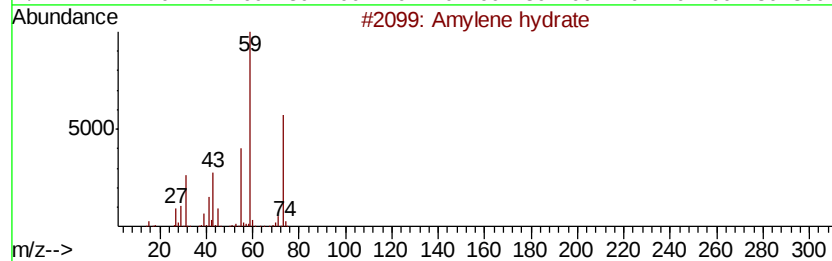
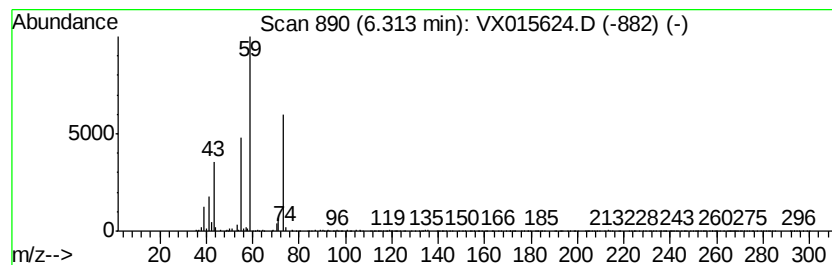
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 2 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	9.65 ug/l	736151	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Amylene hydrate	88	C5H12O	000075-85-4	72
2		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	52
3		Silane, trimethyl-	74	C3H10Si	000993-07-7	39
4		Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	33
5		Silane, trimethylpropyl-	116	C6H16Si	003510-70-1	9



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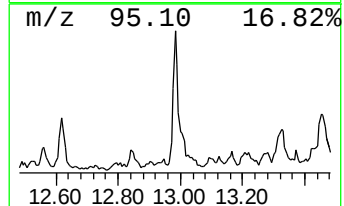
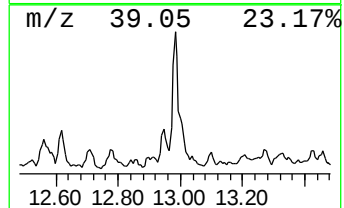
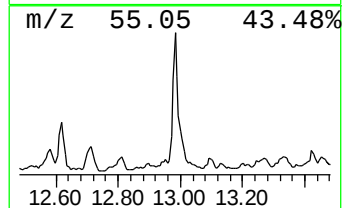
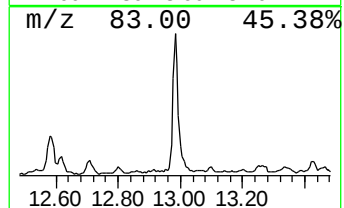
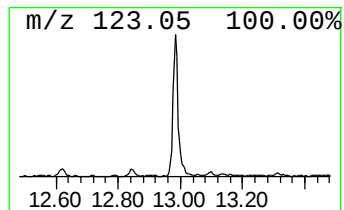
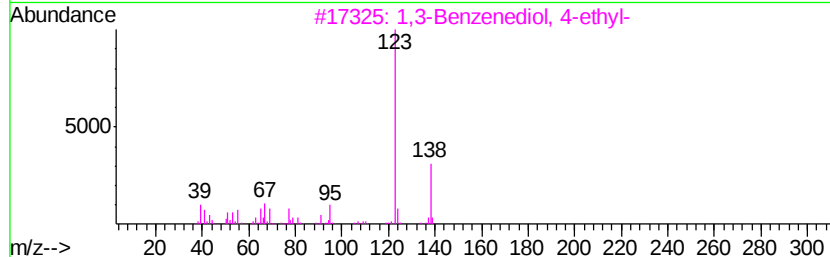
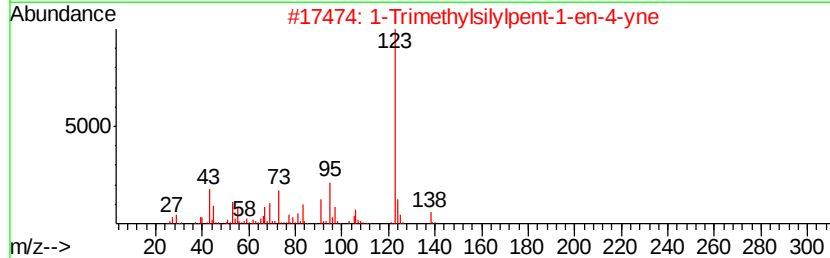
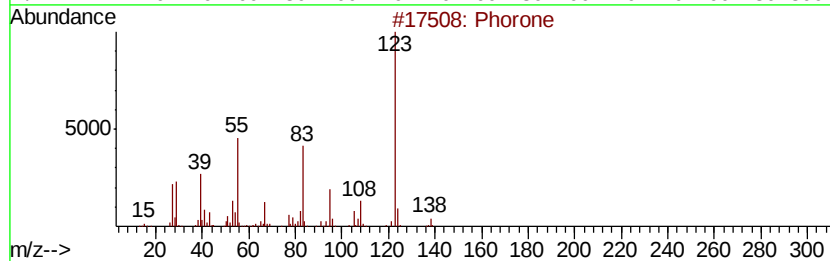
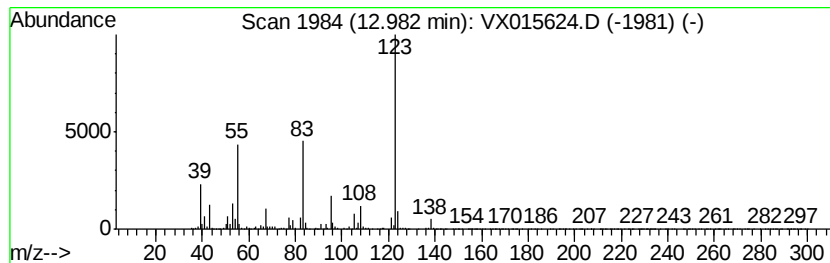
Instrument :
MSVOA_X
ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 4 Phorone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	7.15 ug/l	830333	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phorone		138 C9H14O	000504-20-1 97
2	1-Trimethylsilylpent-1-en-4-yne		138 C8H14Si	079516-25-9 47
3	1,3-Benzenediol, 4-ethyl-		138 C8H10O2	002896-60-8 47
4	3-Pyridinol, 2,6-dimethyl-		123 C7H9NO	001122-43-6 47
5	2-Cyclopenten-1-one, 3,4,5,5-tet...		138 C9H14O	090611-02-2 47



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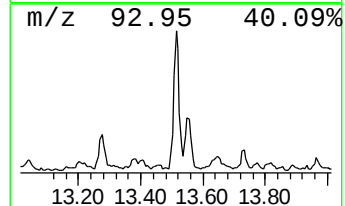
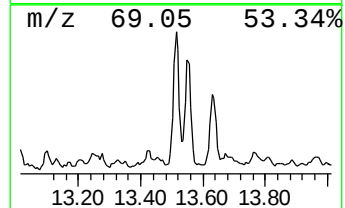
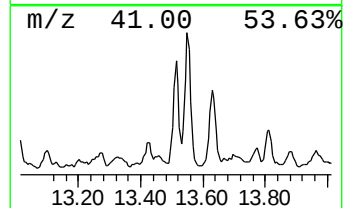
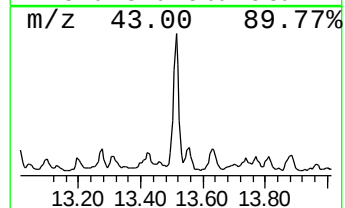
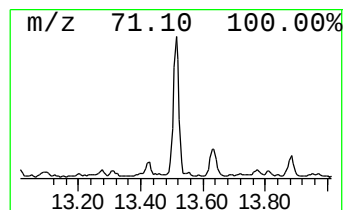
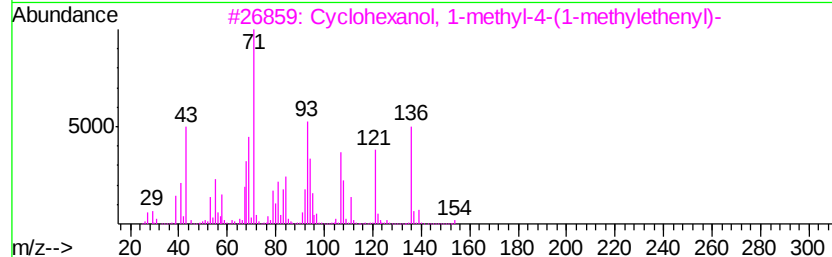
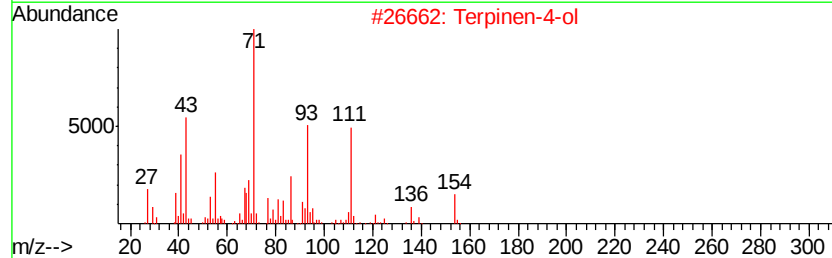
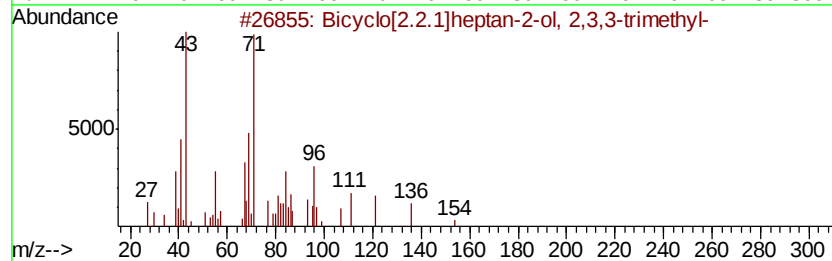
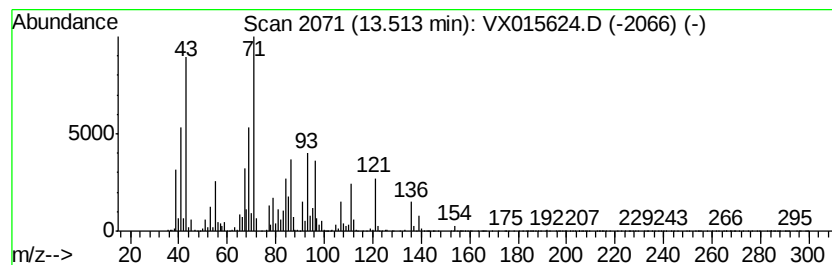
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Bicyclo[2.2.1]heptan-2-ol, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.51	8.63 ug/l	1001890	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	76
2	Terpinen-4-ol	154	C10H18O	000562-74-3	52
3	Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	000138-87-4	50
4	3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	46
5	Phytol	296	C20H40O	000150-86-7	43



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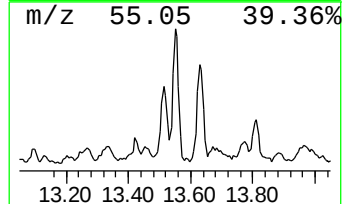
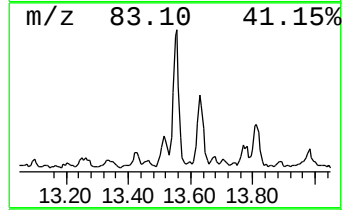
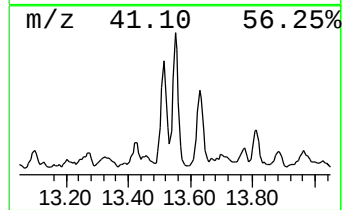
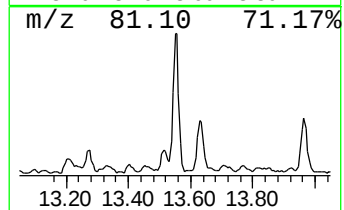
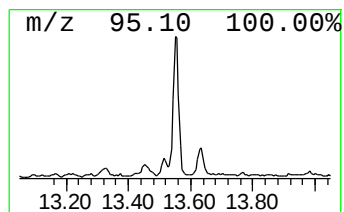
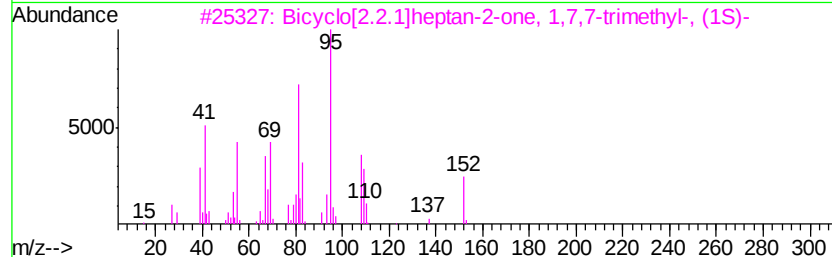
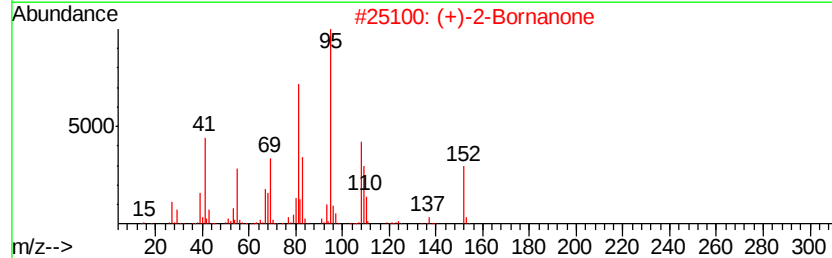
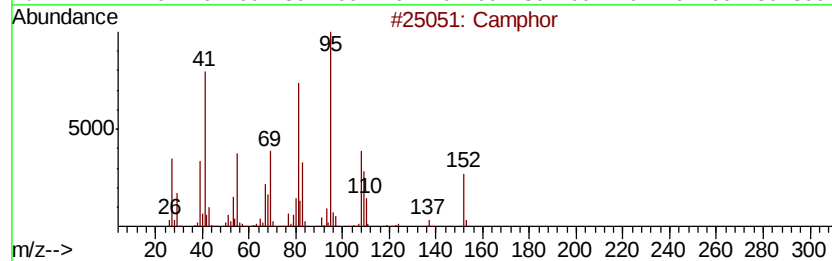
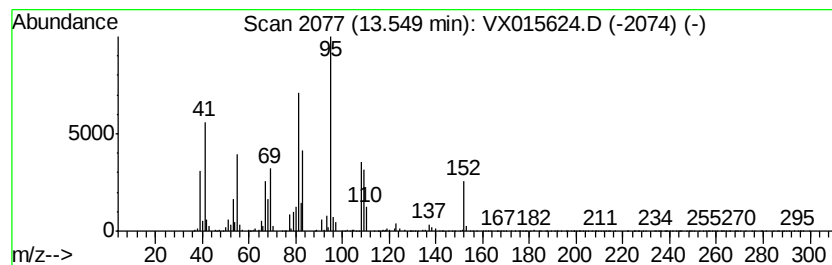
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Camphor Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	8.18 ug/l	949807	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Camphor	152	C10H16O	000076-22-2	98
2		(+)-2-Bornanone	152	C10H16O	000464-49-3	96
3		Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	152	C10H16O	000464-48-2	93
4		5,7-Octadien-4-one, 2,6-dimethyl-, (E)-	152	C10H16O	006752-80-3	49
5		Ketone, 1,5-dimethylbicyclo[2.1.1]hex-2-en-2-ylidene-	138	C9H14O	024081-57-0	43



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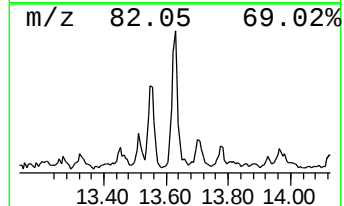
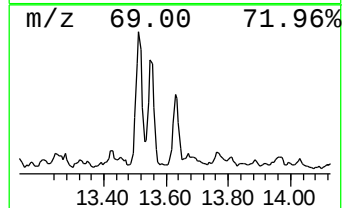
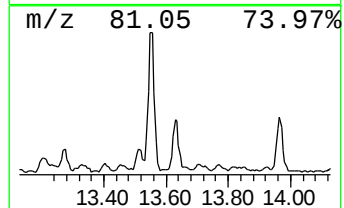
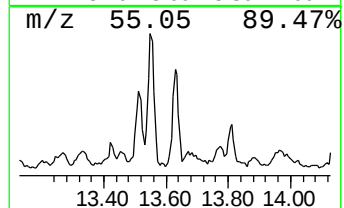
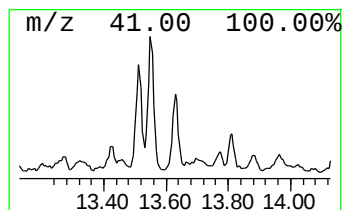
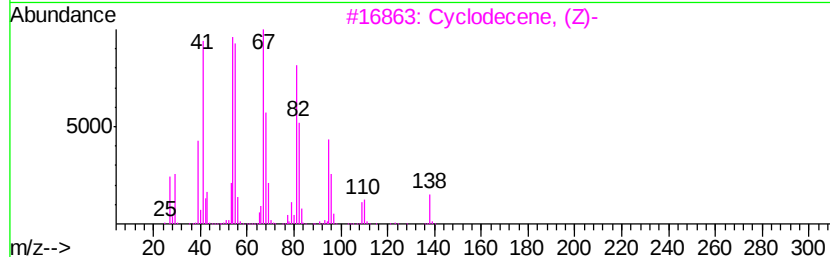
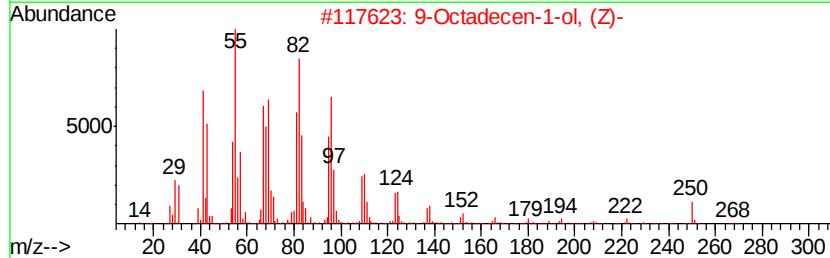
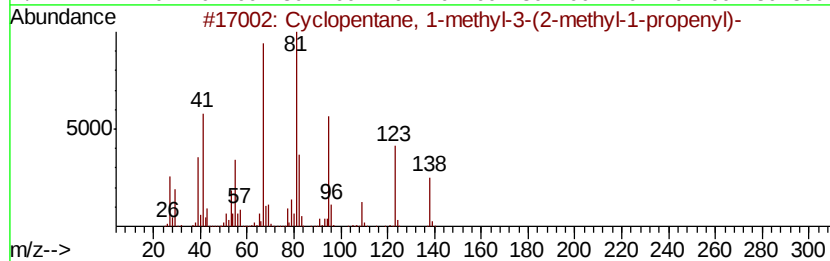
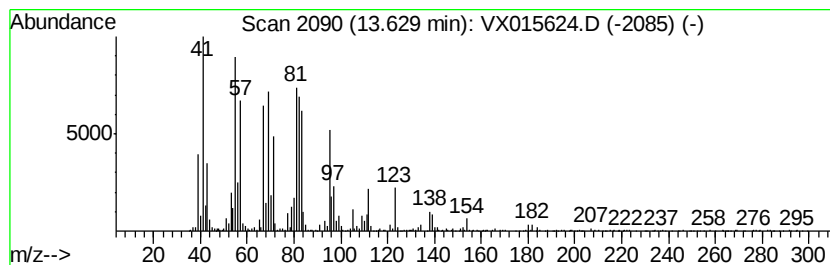
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TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclopentane, 1-methyl-3-(2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.63	5.06 ug/l	587177	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1-methyl-3-(2-meth...	138	C10H18	075873-01-7	60
2	9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	50
3	Cyclodecene, (Z)-	138	C10H18	000935-31-9	46
4	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	45
5	Cyclohexane, (2-methyl-1-propenyl)-	138	C10H18	089656-98-4	41



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	6.31	9.7	ug/l	736151	2	6.84	3814020	50.0
Phorone	12.98	7.2	ug/l	830333	4	12.06	5803010	50.0
Bicyclo[2.2.1]hep...	13.51	8.6	ug/l	1001890	4	12.06	5803010	50.0
Camphor	13.55	8.2	ug/l	949807	4	12.06	5803010	50.0
Cyclopentane, 1-m...	13.63	5.1	ug/l	587177	4	12.06	5803010	50.0