

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
 Data File : VX021256.D
 Acq On : 16 Mar 2021 19:54
 Operator : JC/MD
 Sample : M1665-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30821

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\82X031621W.M

Title : SW846 8260

Signal : TIC: VX021256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.470	62	65	96	rVB	5876867	6434939	12.91%	8.451%
2	6.188	858	867	896	rVB	390723	1032658	2.07%	1.356%
3	10.347	1564	1574	1583	rBV2	462208	687630	1.38%	0.903%
4	11.630	1783	1792	1796	rBV	29596090	49852166	100.00%	65.473%
5	11.871	1827	1833	1838	rBV	5816908	7198442	14.44%	9.454%
6	11.930	1838	1843	1849	rVB	3153306	4019507	8.06%	5.279%
7	12.141	1871	1879	1888	rBV	2214331	2883516	5.78%	3.787%
8	13.253	2064	2068	2073	rVB	432920	505058	1.01%	0.663%
9	13.771	2149	2156	2160	rBV	2010858	2368724	4.75%	3.111%
10	13.818	2160	2164	2170	rVB	887042	1158610	2.32%	1.522%

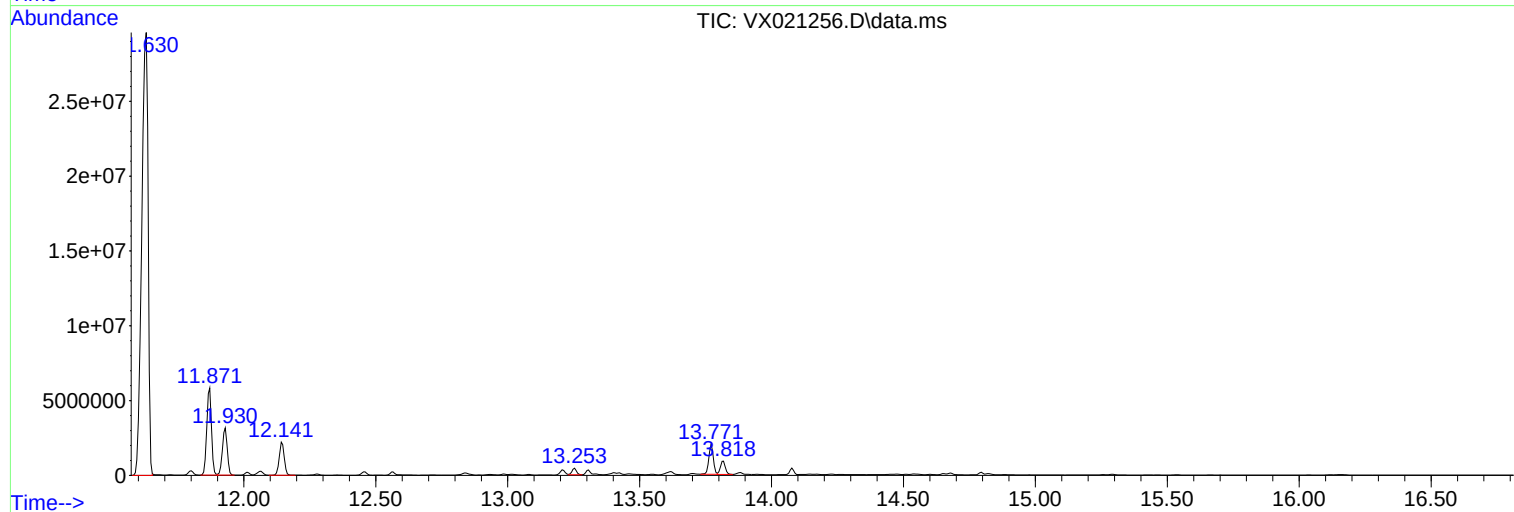
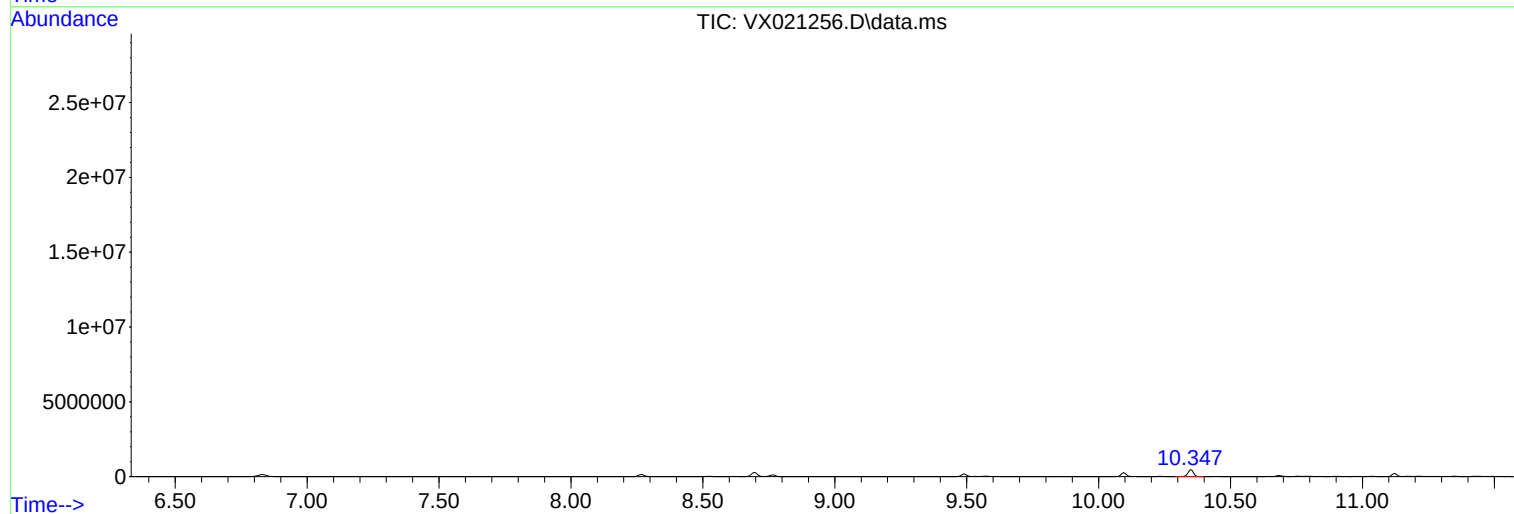
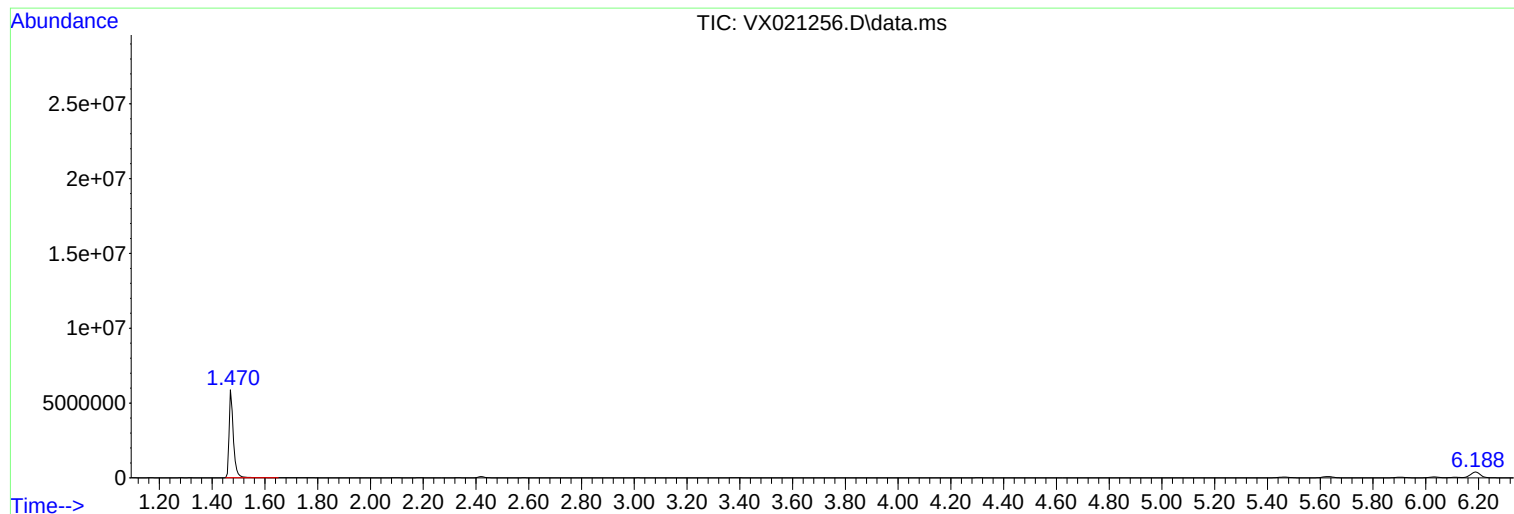
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

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



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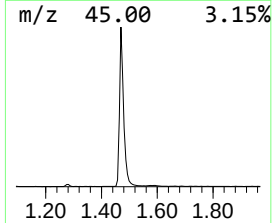
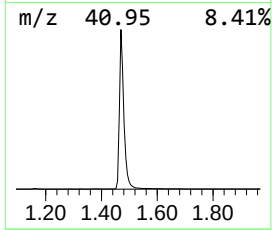
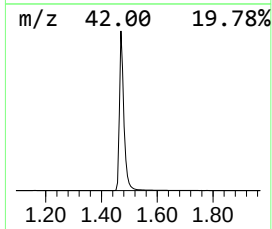
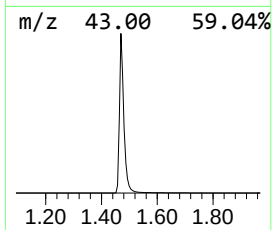
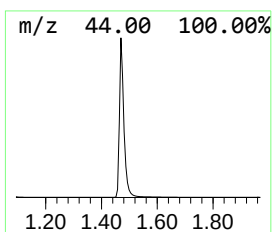
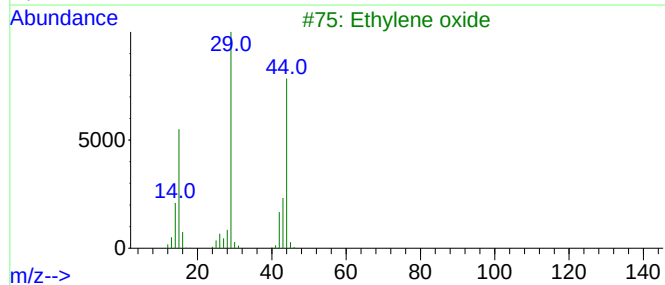
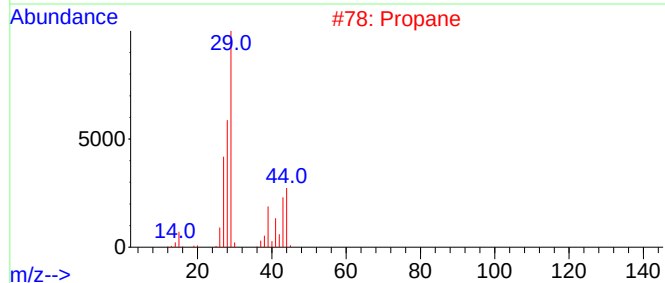
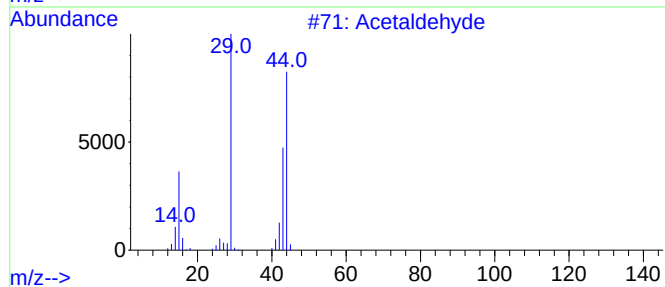
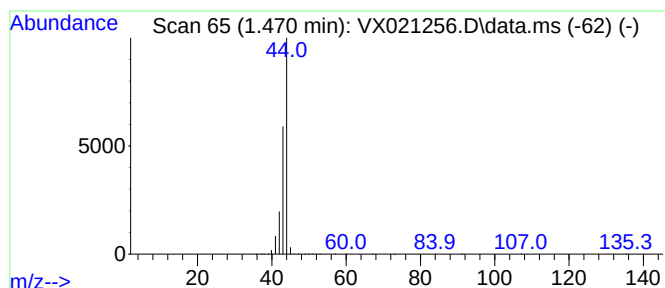
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.470	311.57 ug/l	6434940	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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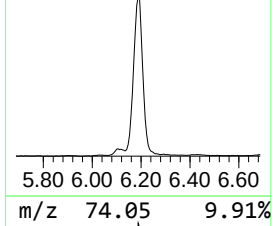
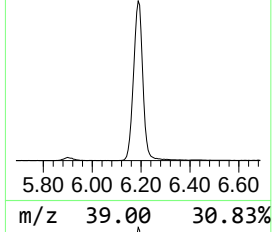
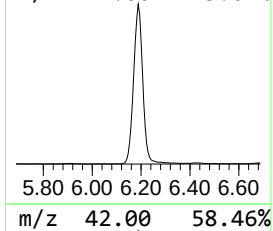
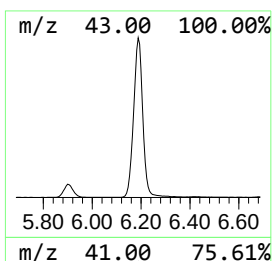
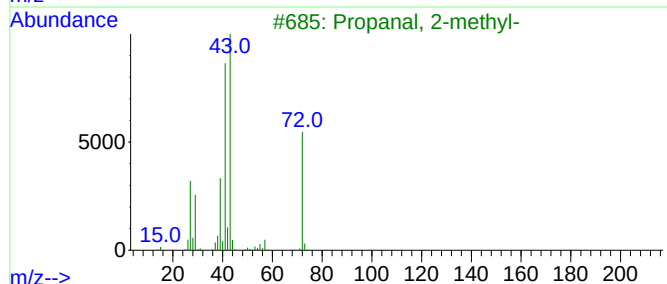
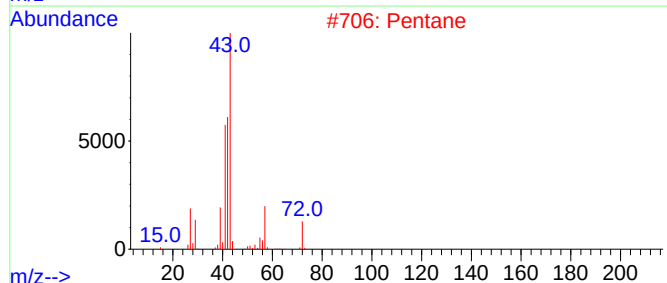
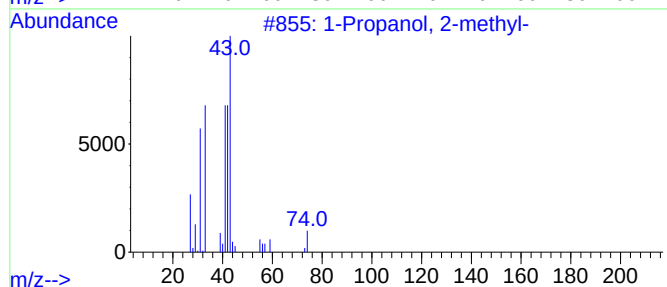
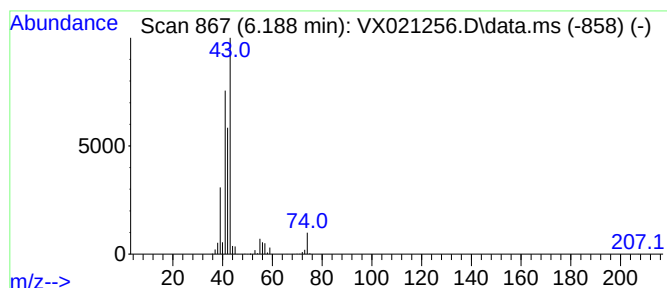
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.188	50.00 ug/l	1032660	Pentafluorobenzene	5.629

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	90	
2	Pentane	72	C5H12	000109-66-0	45	
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	35	
4	Isobutylene epoxide	72	C4H8O	000558-30-5	33	
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	28	



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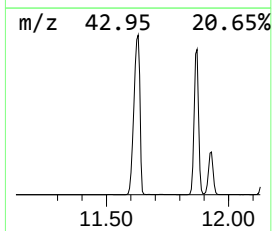
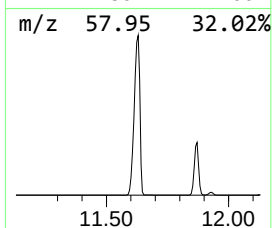
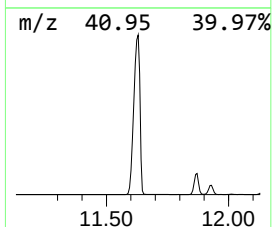
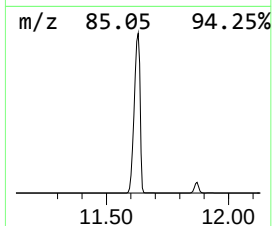
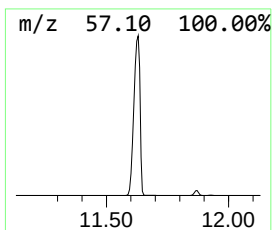
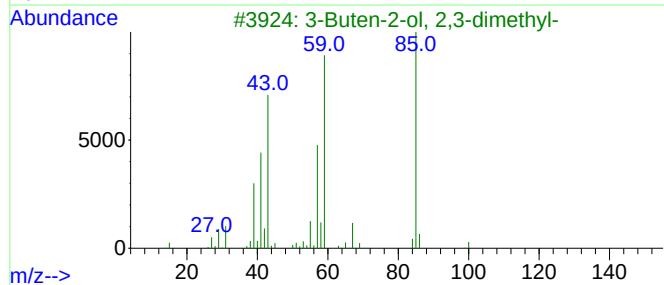
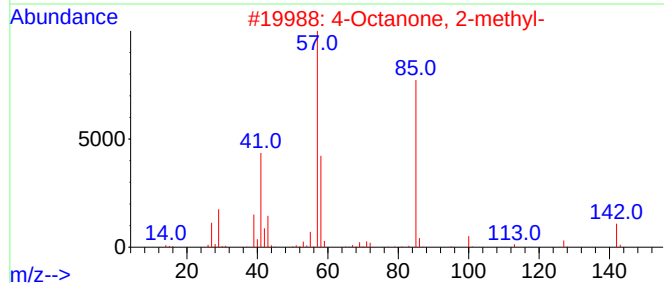
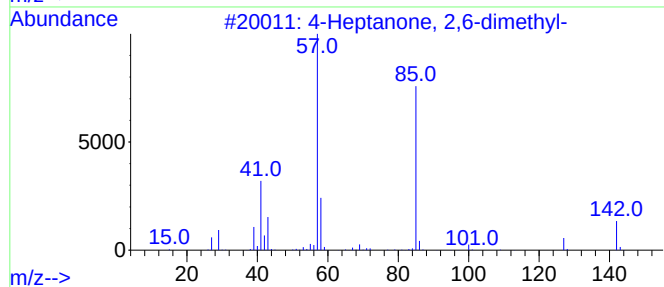
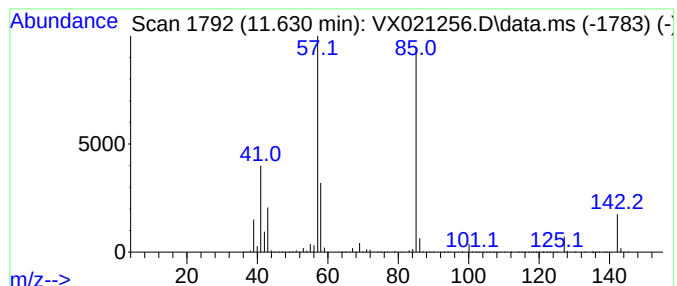
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

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

Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.630	864.43 ug/l	49852200	1,4-Dichlorobenzene-d4	12.065	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	74
3	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	59
4	1-Propoxypropan-2-yl 2-methylbut...	202	C11H22O3	1000367-10-7	56
5	5-Nonanone	142	C9H18O	000502-56-7	53



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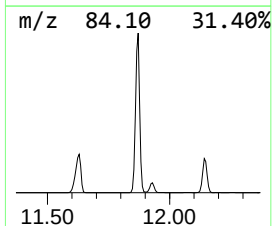
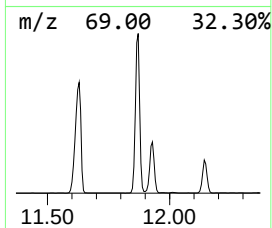
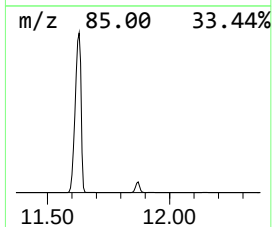
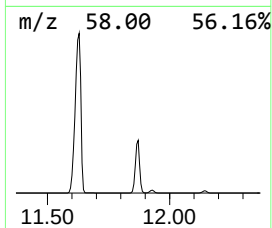
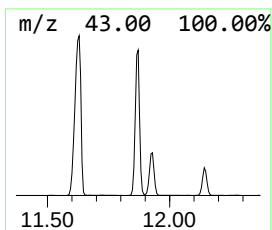
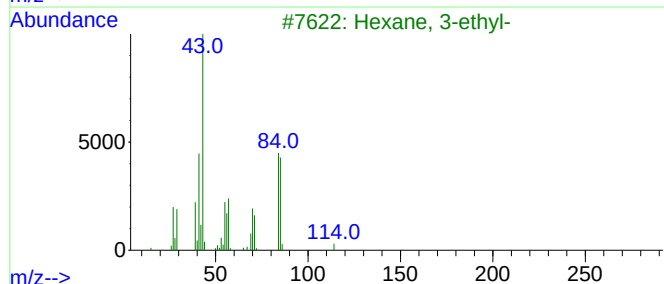
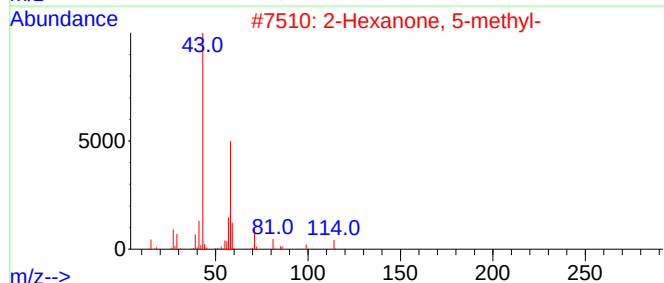
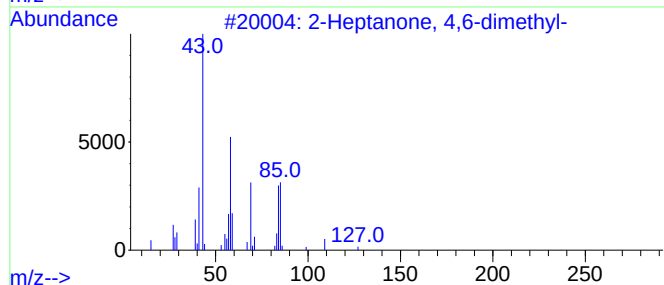
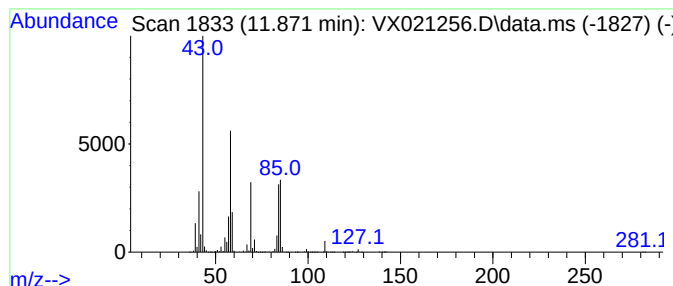
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.871	124.82 ug/l	7198440	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
3			Hexane, 3-ethyl-	114	C8H18	000619-99-8	43
4			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43
5			Butanoic acid, 3-oxo-, 2-propeny...	142	C7H10O3	001118-84-9	43



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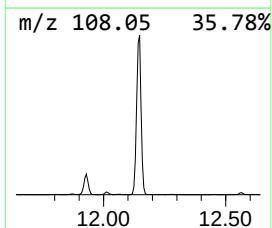
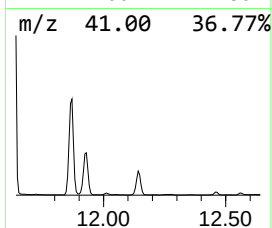
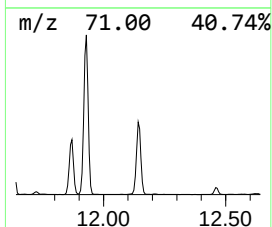
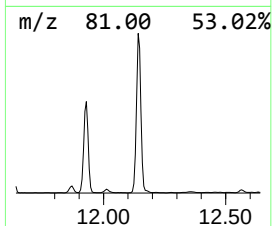
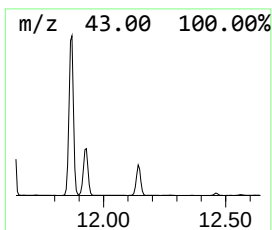
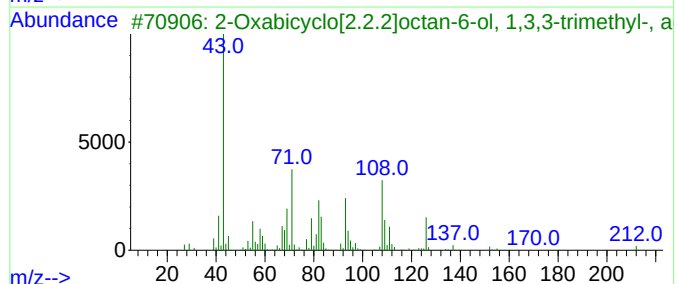
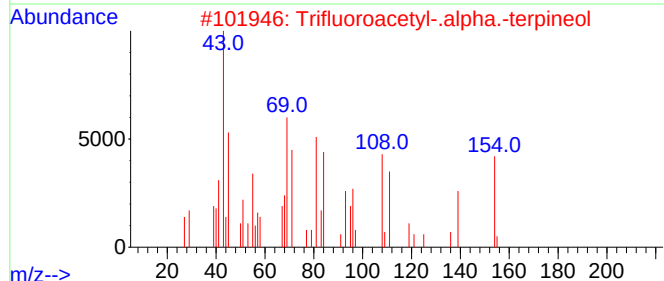
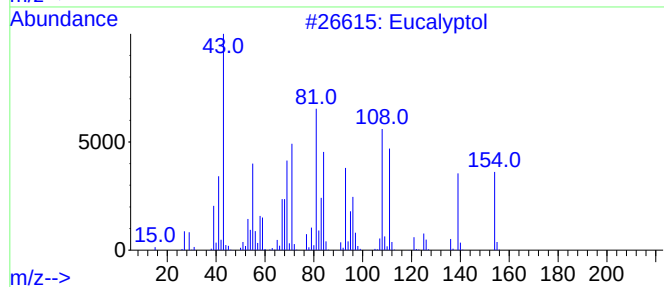
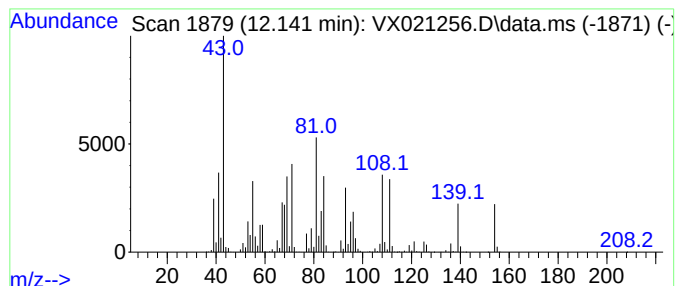
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Quant Title : SW846 8260

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

Peak Number 5 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.142	50.00 ug/l	2883520	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	97
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	78
3			2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	43
4			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	27
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	12



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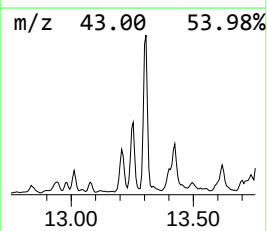
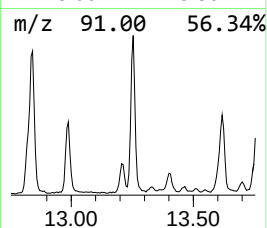
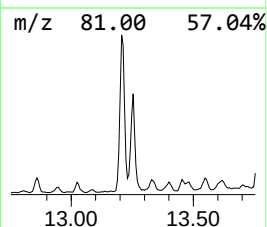
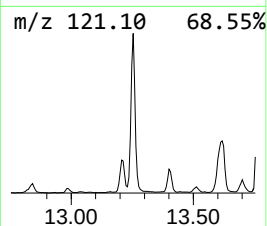
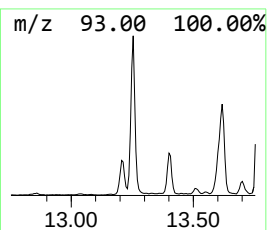
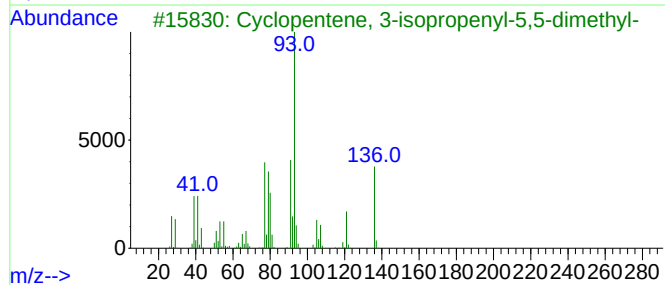
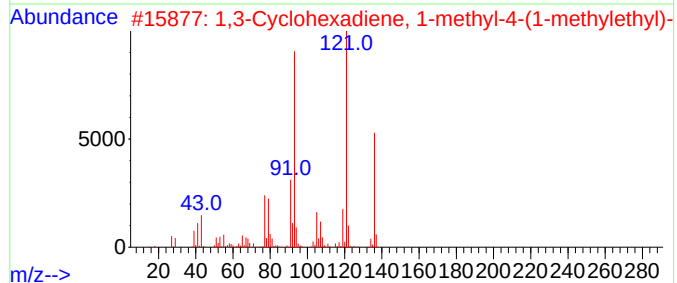
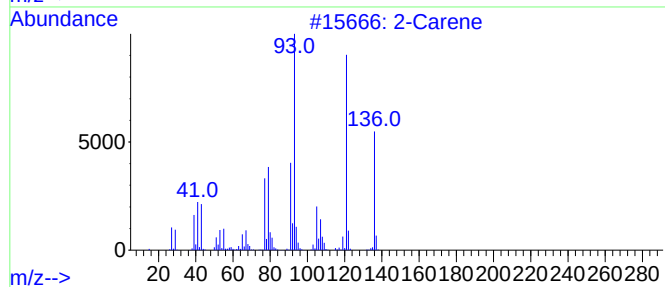
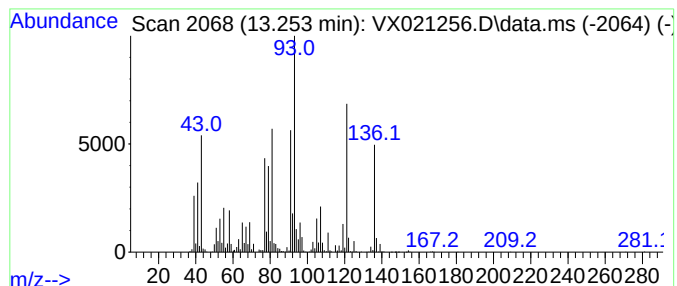
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

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

Peak Number 6 2-Carene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.253	8.76 ug/l	505058	1,4-Dichlorobenzene-d4	12.065

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Carene	136	C10H16	000554-61-0	94
2			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	93
3			Cyclopentene, 3-isopropenyl-5,5-...	136	C10H16	1000162-25-4	91
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	91
5			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031621\
Data File : VX021256.D
Acq On : 16 Mar 2021 19:54
Operator : JC/MD
Sample : M1665-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30821

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.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
Acetaldehyde	1.470	311.6	ug/l	6434940	1	5.629	1032660	50.0
1-Propanol, 2-m...	6.188	50.0	ug/l	1032660	1	5.629	1032660	50.0
4-Heptanone, 2,...	11.630	864.4	ug/l	49852200	4	12.065	2883520	50.0
2-Heptanone, 4,...	11.871	124.8	ug/l	7198440	4	12.065	2883520	50.0
Eucalyptol	12.142	50.0	ug/l	2883520	4	12.065	2883520	50.0
2-Carene	13.253	8.8	ug/l	505058	4	12.065	2883520	50.0