

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX040620\
 Data File : VX015514.D
 Acq On : 06 Apr 2020 15:49
 Operator : JC/SP
 Sample : L2152-05
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40734

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\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	1.466	91	95	112	rVB	21469588	41601328	8.79%	3.151%
2	2.350	227	240	244	rBV6	62984870	272642422	57.58%	20.650%
3	2.576	276	277	289	rVB	15427418	13247697	2.80%	1.003%
4	4.252	493	552	555	rBV2	40198096	473512036	100.00%	35.863%
5	6.862	970	980	991	rVB	2115415	5120884	1.08%	0.388%
6	7.599	1094	1101	1106	rBV	2746777	6104993	1.29%	0.462%
7	7.654	1106	1110	1115	rVV	2160645	5110933	1.08%	0.387%
8	7.715	1116	1120	1142	rVB2	1578107	7024459	1.48%	0.532%
9	8.709	1276	1283	1292	rBV	4436917	8336463	1.76%	0.631%
10	8.922	1312	1318	1332	rVV	39397629	68066802	14.37%	5.155%
11	9.056	1332	1340	1353	rVB2	55911848	92845847	19.61%	7.032%
12	9.215	1360	1366	1375	rVB	17364767	25011723	5.28%	1.894%
13	10.142	1504	1518	1525	rBV4	107460680	230230122	48.62%	17.437%
14	10.196	1525	1527	1535	rVV	9159151	11230735	2.37%	0.851%
15	10.288	1536	1542	1559	rVB	7315687	16290119	3.44%	1.234%
16	11.123	1673	1679	1684	rBV	4495066	5794394	1.22%	0.439%
17	11.190	1684	1690	1699	rVB	11307492	18082821	3.82%	1.370%
18	11.702	1765	1774	1779	rVB	3503225	5275624	1.11%	0.400%
19	12.062	1828	1833	1841	rBV	5878870	7614306	1.61%	0.577%
20	12.147	1841	1847	1857	rVB	5277727	7189504	1.52%	0.545%

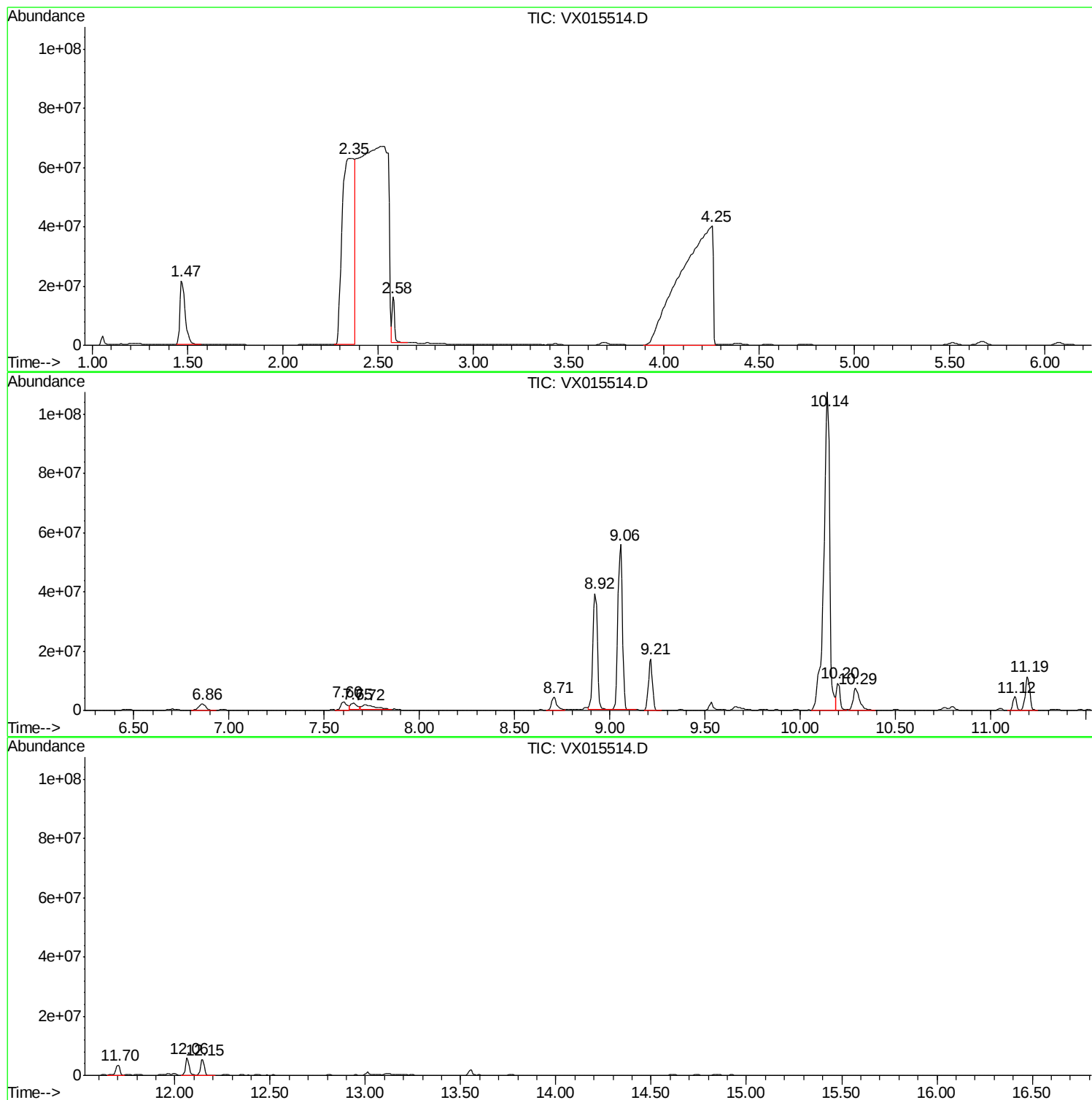
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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



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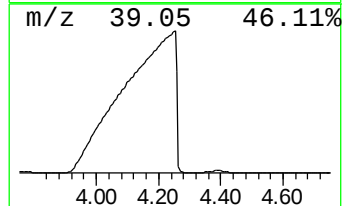
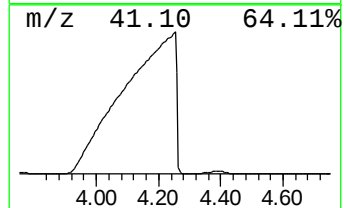
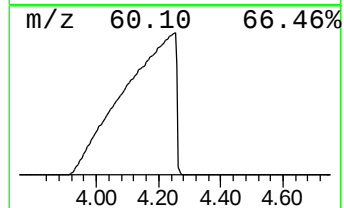
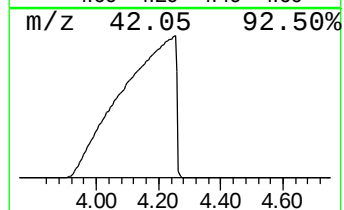
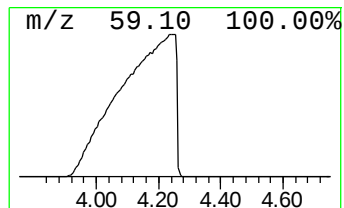
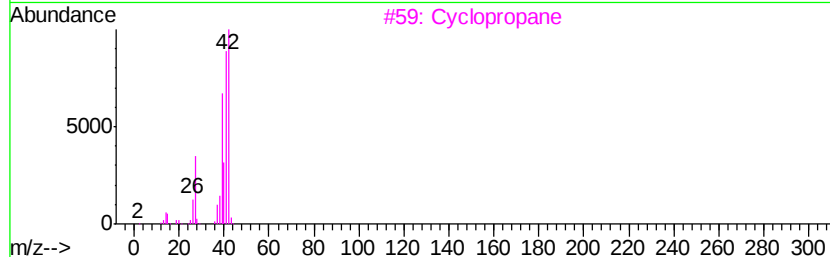
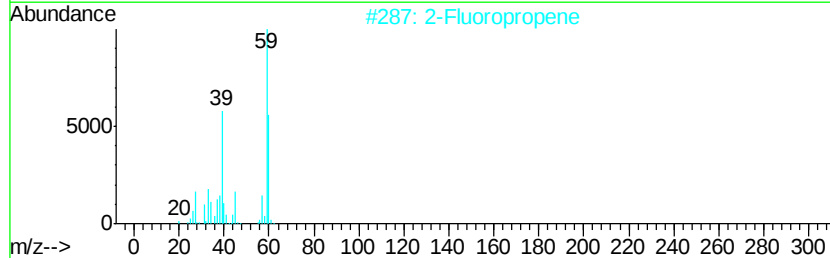
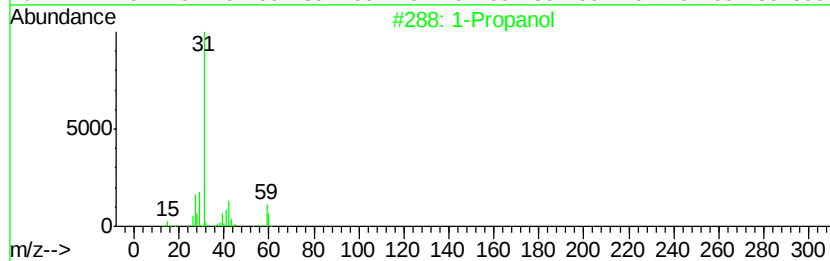
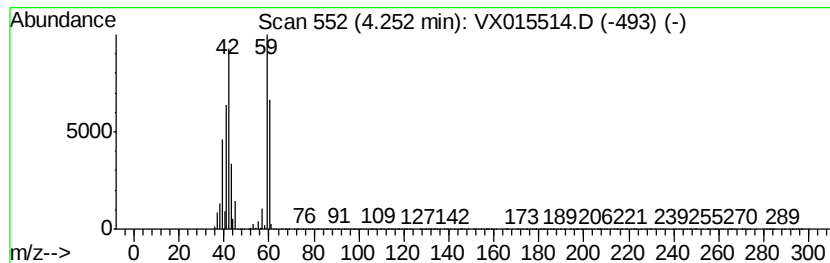
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	4623.34 ug/l	473512000	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	64
2		2-Fluoropropene	60	C3H5F	001184-60-7	52
3		Cyclopropane	42	C3H6	000075-19-4	25
4		Allyl fluoride	60	C3H5F	000818-92-8	9
5		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9



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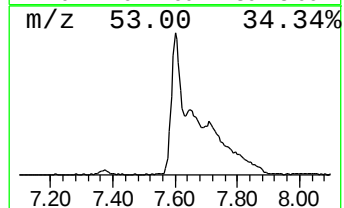
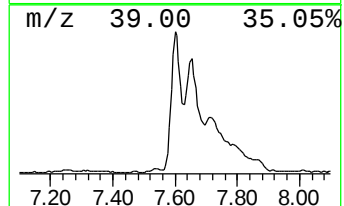
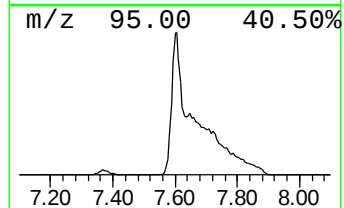
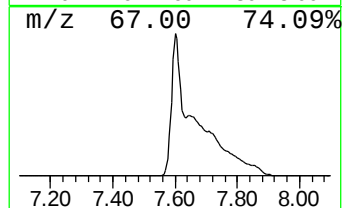
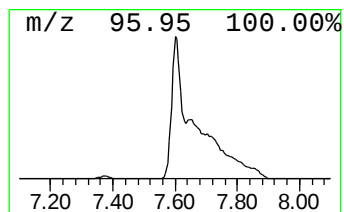
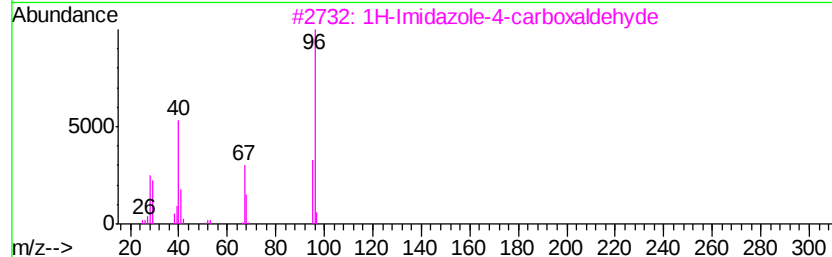
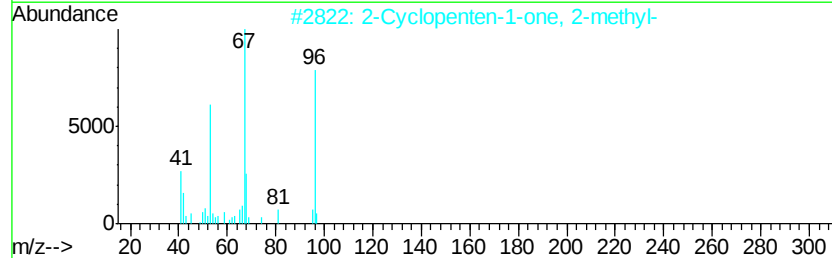
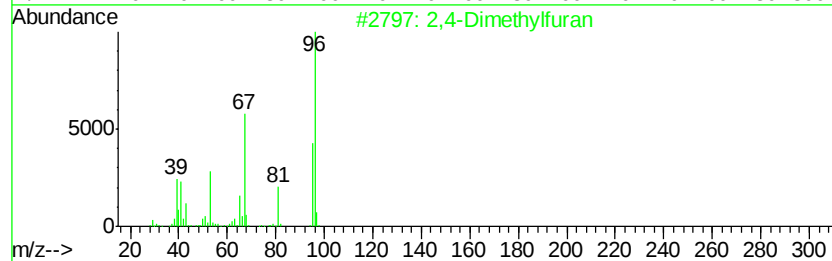
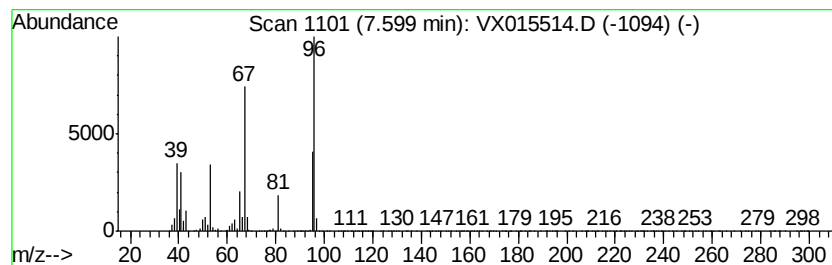
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Quant Title : SW846 8260

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

Peak Number 4 2,4-Dimethylfuran Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	59.61 ug/l	6104990	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Dimethylfuran	96	C6H8O	003710-43-8	95
2		2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	001120-73-6	59
3		1H-Imidazole-4-carboxaldehyde	96	C4H4N2O	003034-50-2	43
4		2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	38
5		3-Heptyne	96	C7H12	002586-89-2	38



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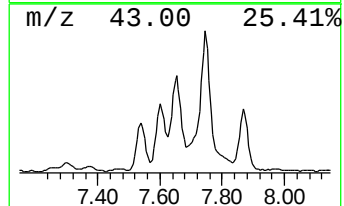
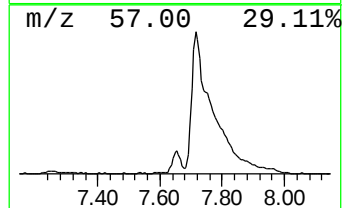
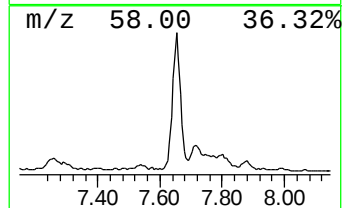
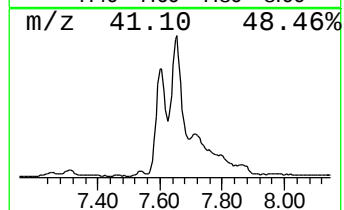
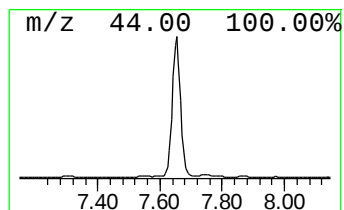
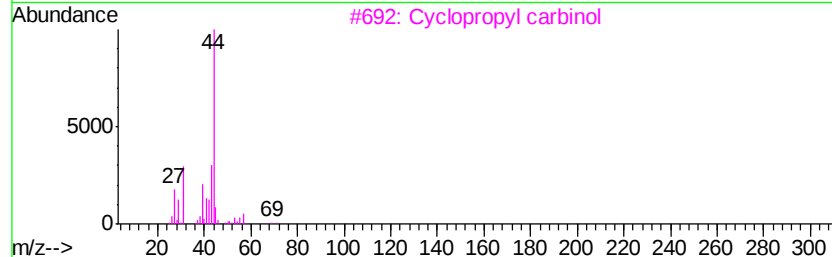
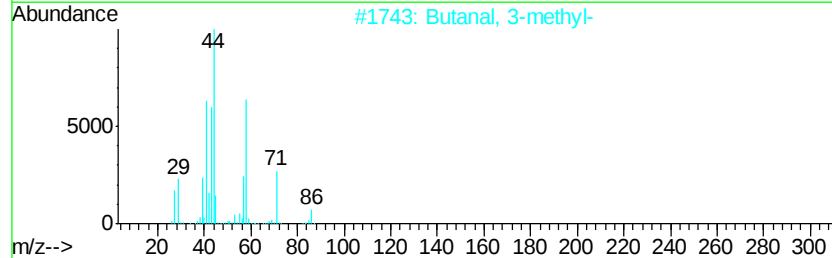
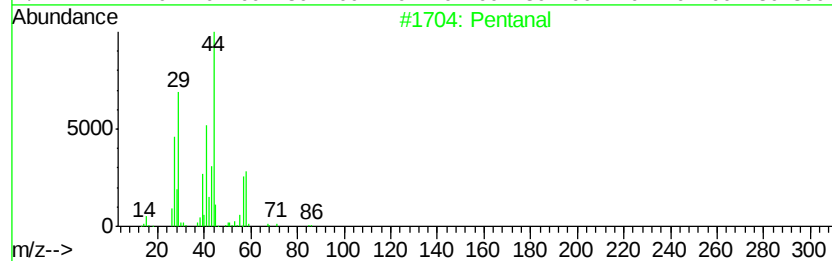
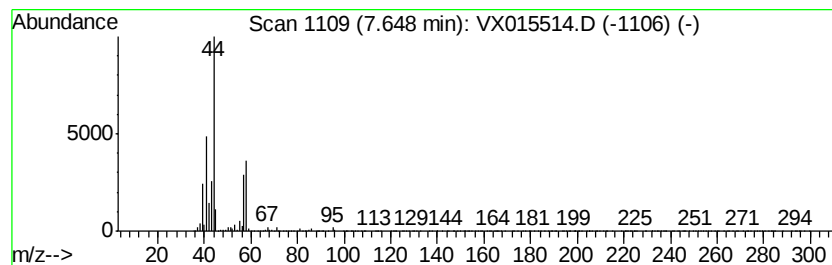
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	49.90 ug/l	5110930	1,4-Difluorobenzene	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal		86	C5H10O	000110-62-3	80
2	Butanal, 3-methyl-		86	C5H10O	000590-86-3	74
3	Cyclopropyl carbinol		72	C4H8O	002516-33-8	40
4	Glycidol		74	C3H6O2	000556-52-5	33
5	Succindialdehyde		86	C4H6O2	000638-37-9	9



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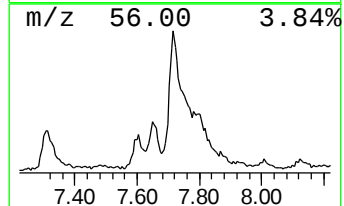
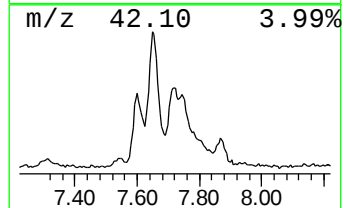
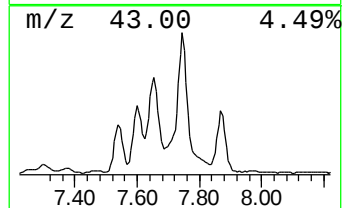
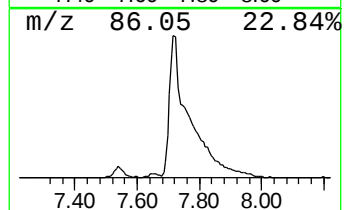
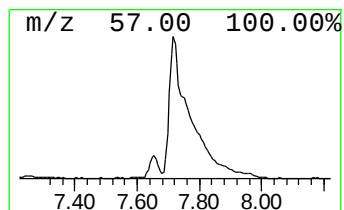
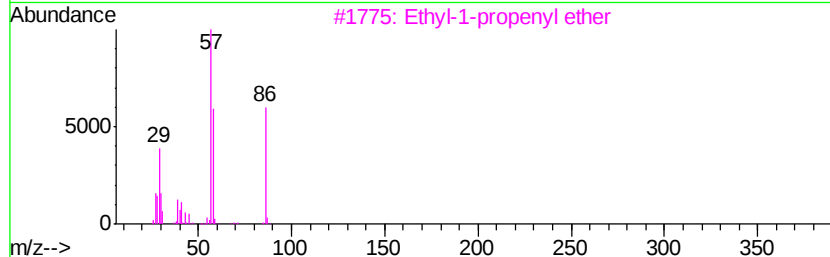
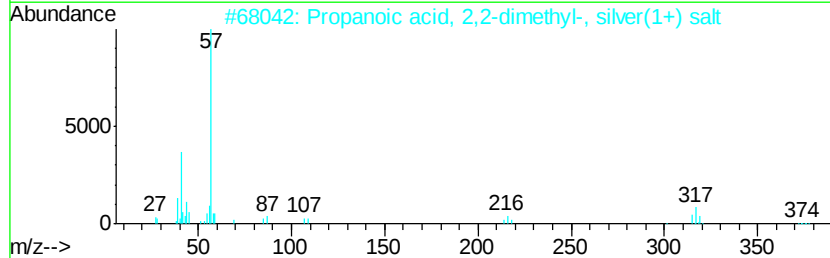
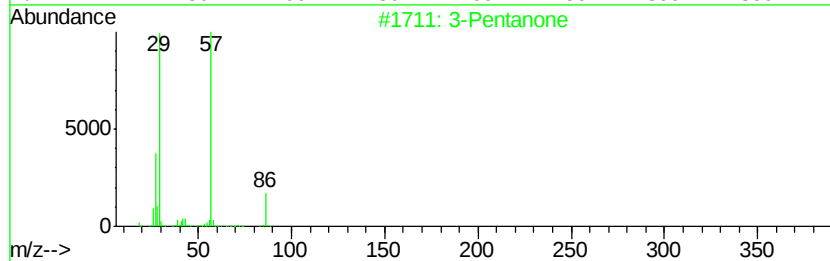
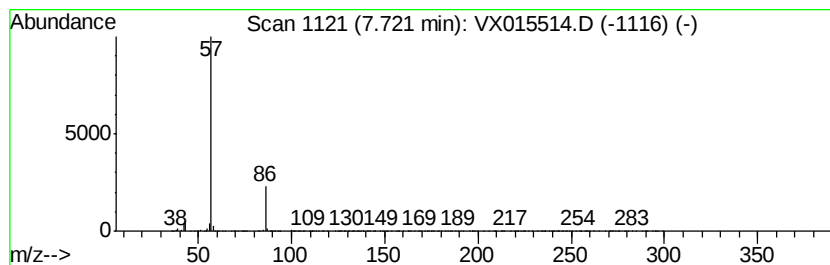
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	68.59 ug/l	7024460	1,4-Difluorobenzene	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone		86	C5H10O	000096-22-0	72
2	Propanoic acid, 2,2-dimethyl-, s...		208	C5H9AqO2	007324-58-5	9
3	Ethyl-1-propenyl ether		86	C5H10O	000928-55-2	5
4	2-Imidazolidinone		86	C3H6N2O	000120-93-4	5
5	Propanal, 2,2-dimethyl-		86	C5H10O	000630-19-3	5



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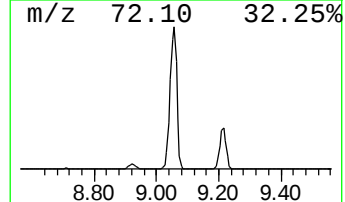
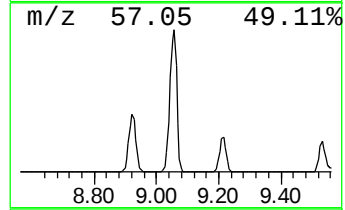
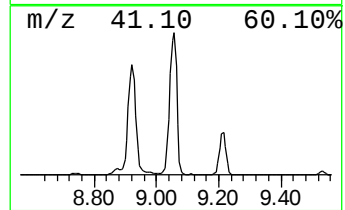
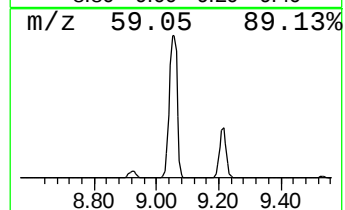
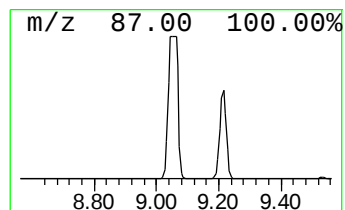
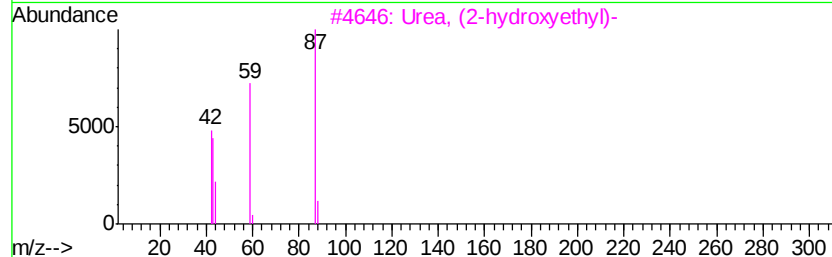
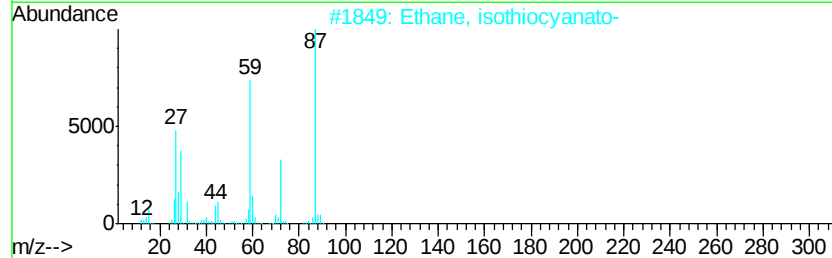
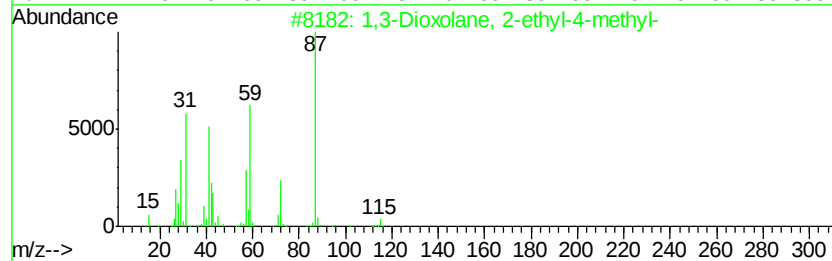
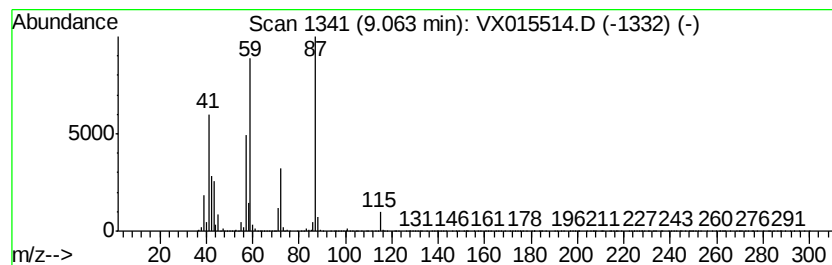
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	20.16 ug/l	92845800	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	62
2		Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	53
3		Urea, (2-hydroxyethyl)-	104	C3H8N2O2	002078-71-9	53
4		Ethanol, 2-[2-(2-methoxyethoxy)ethyl]-	206	C9H18O5	003610-27-3	38
5		Ethoxycitronellal	198	C12H22O2	1000132-02-6	38



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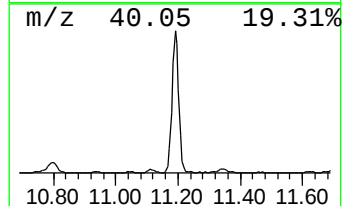
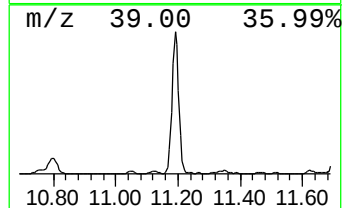
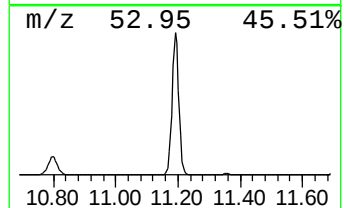
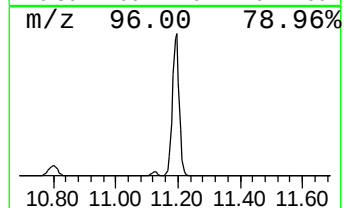
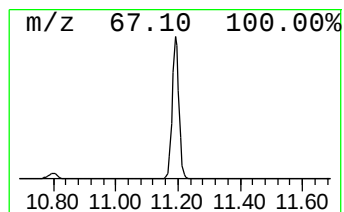
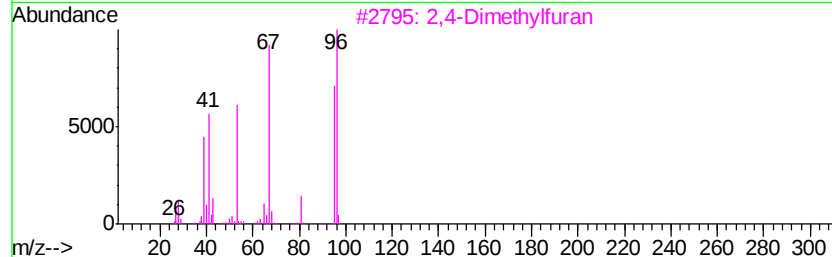
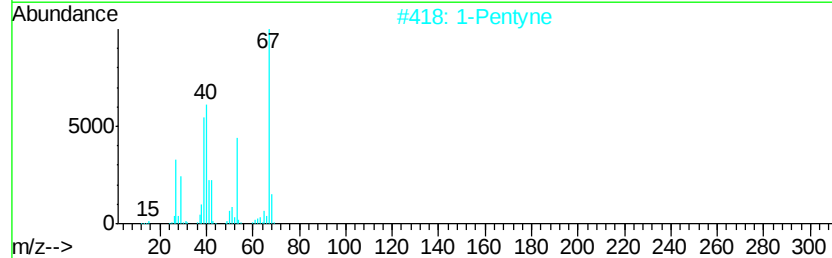
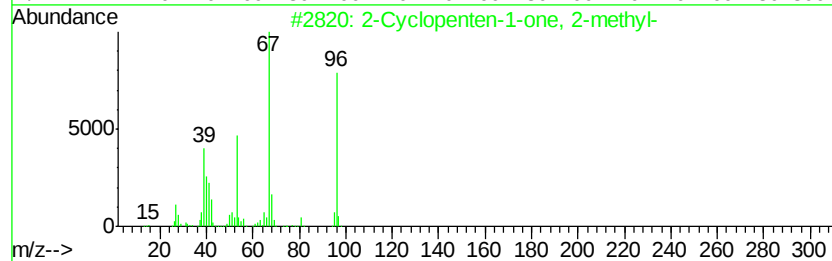
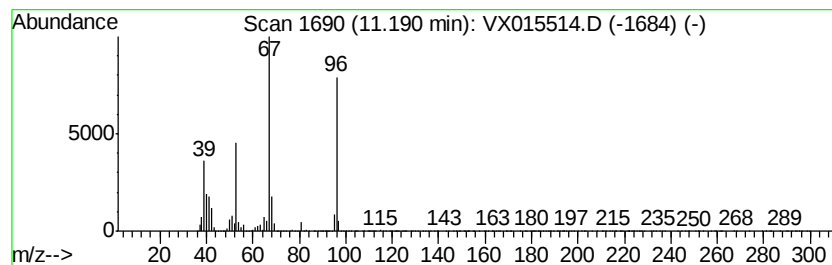
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Quant Title : SW846 8260

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

Peak Number 8 2-Cyclopenten-1-one, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	118.74 ug/l	18082800	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	001120-73-6	97
2		1-Pentyne	68	C5H8	000627-19-0	76
3		2,4-Dimethylfuran	96	C6H8O	003710-43-8	64
4		1-Butyne, 3-methyl-	68	C5H8	000598-23-2	58
5		1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	55



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX040620\
Data File : VX015514.D
Acq On : 06 Apr 2020 15:49
Operator : JC/SP
Sample : L2152-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40734

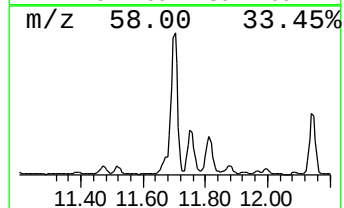
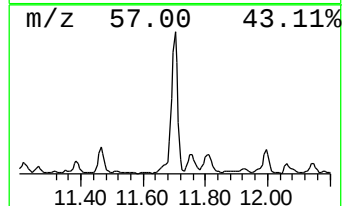
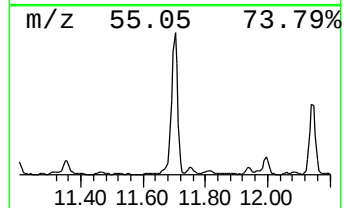
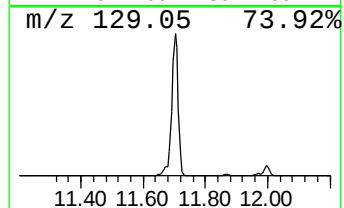
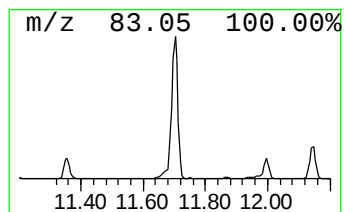
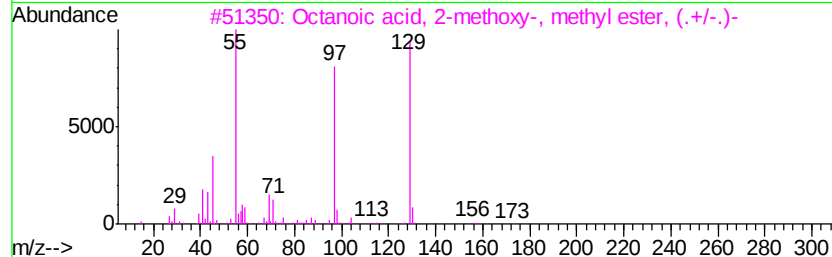
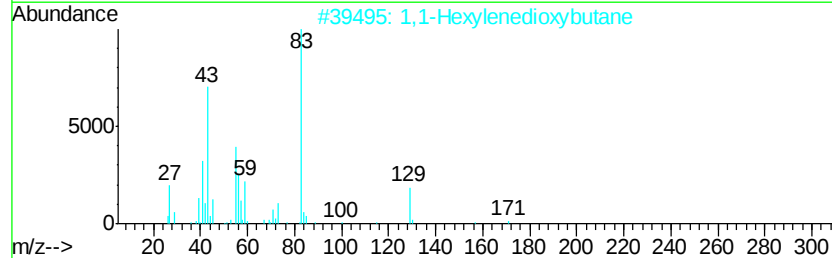
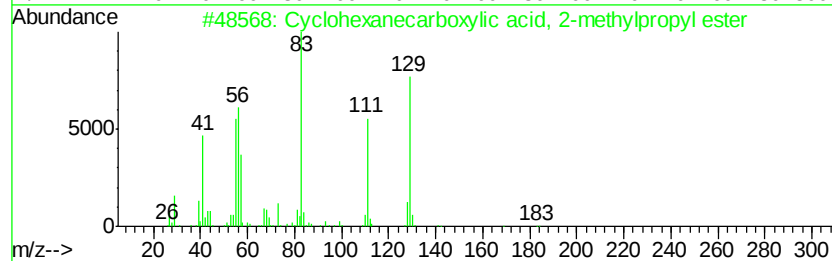
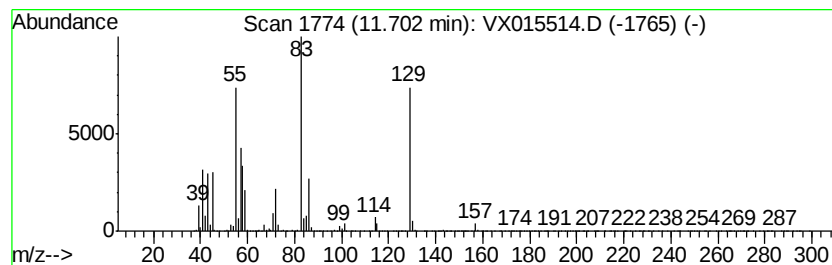
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Quant Title : SW846 8260

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

Peak Number 9 unknown11.70 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	34.64 ug/l	5275620	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanecarboxylic acid, 2-me...	184	C11H20O2	037139-85-8	38
2		1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	37
3		Octanoic acid, 2-methoxy-, methv...	188	C10H20O3	1000332-74-2	35
4		1-Butoxypropan-2-yl 2-methylbut-...	214	C12H22O3	1000367-09-3	27
5		Flucytosine	129	C4H4FN3O	002022-85-7	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX040620\
Data File : VX015514.D
Acq On : 06 Apr 2020 15:49
Operator : JC/SP
Sample : L2152-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40734

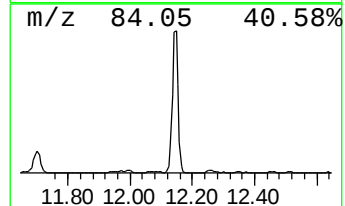
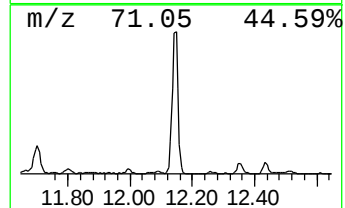
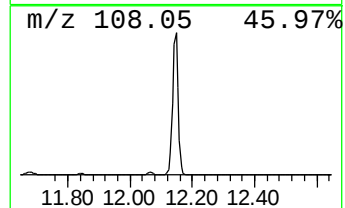
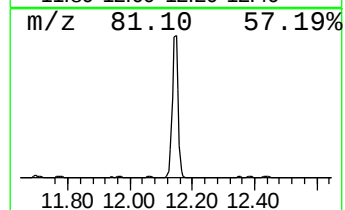
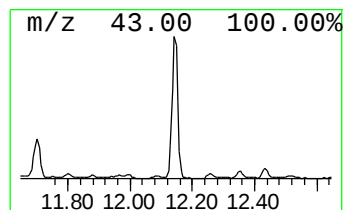
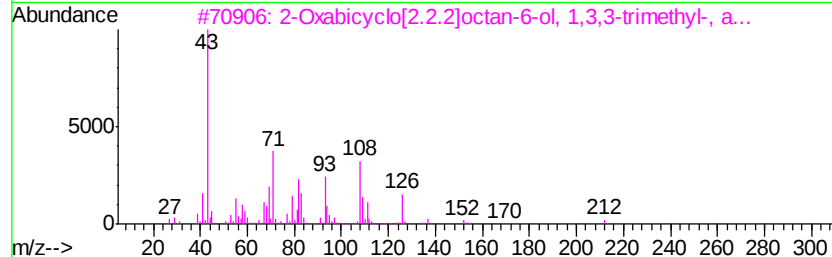
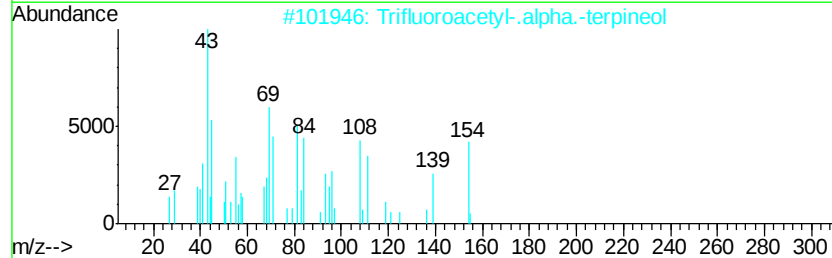
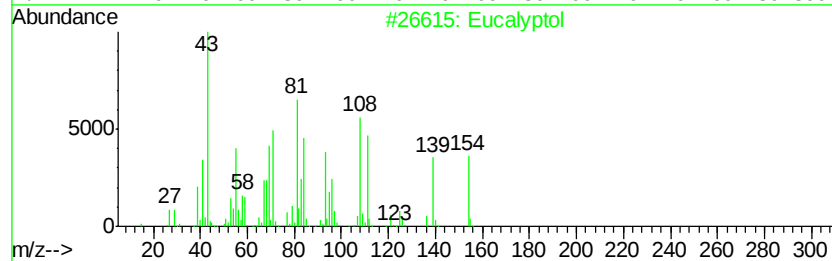
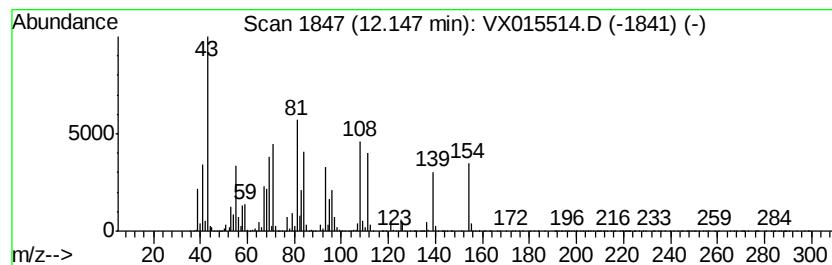
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.M
Quant Title : SW846 8260

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

Peak Number 10 Eucalyptol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	47.21 ug/l	7189500	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eucalyptol	154	C10H18O	000470-82-6	99
2		Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	49
3		2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	32
4		2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27
5		1-Hepten-6-one, 2-methyl-	126	C8H14O	010408-15-8	27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX040620\
 Data File : VX015514.D
 Acq On : 06 Apr 2020 15:49
 Operator : JC/SP
 Sample : L2152-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40734

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032720W.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
1-Propanol	4.25	4623.3	ug/l	473512000	1	5.67	5120880	50.0
2,4-Dimethylfuran	7.60	59.6	ug/l	6104990	2	6.86	5120880	50.0
Pentanal	7.65	49.9	ug/l	5110930	2	6.86	5120880	50.0
3-Pentanone	7.72	68.6	ug/l	7024460	2	6.86	5120880	50.0
1,3-Dioxolane, 2-...	9.06	20.2	ug/l	92845800	3	10.11	230230000	50.0
2-Cyclopenten-1-o...	11.19	118.7	ug/l	18082800	4	12.06	7614310	50.0
unknown11.70	11.70	34.6	ug/l	5275620	4	12.06	7614310	50.0
Eucalyptol	12.15	47.2	ug/l	7189500	4	12.06	7614310	50.0