

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX053119\
 Data File : VX009981.D
 Acq On : 31 May 2019 13:11
 Operator : JC/SP
 Sample : K2964-04
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 51030

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\82X052819W.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	1.489	51	55	66	rVB	2391455	2890252	7.96%	3.890%
2	2.123	153	159	170	rBV	293789	443221	1.22%	0.596%
3	2.446	205	212	228	rBV	508725	857844	2.36%	1.154%
4	4.489	536	547	568	rBV	712078	2098834	5.78%	2.825%
5	5.665	727	740	757	rVB	178089	517775	1.43%	0.697%
6	6.860	926	936	945	rBV	272979	692435	1.91%	0.932%
7	6.994	945	958	991	rVB	14449361	36303875	100.00%	48.858%
8	7.311	991	1010	1017	rBV	9948941	20902999	57.58%	28.131%
9	7.378	1017	1021	1031	rVB	426315	787182	2.17%	1.059%
10	7.750	1074	1082	1099	rBV	282589	515150	1.42%	0.693%
11	8.713	1233	1240	1247	rBV	618547	946350	2.61%	1.274%
12	9.055	1288	1296	1310	rBV	685342	1018445	2.81%	1.371%
13	9.219	1317	1323	1332	rBV	469856	651127	1.79%	0.876%
14	10.110	1460	1469	1481	rVB	580394	871931	2.40%	1.173%
15	10.366	1499	1511	1521	rBV2	1820393	2644423	7.28%	3.559%
16	11.134	1632	1637	1643	rBV	447375	575591	1.59%	0.775%
17	12.024	1774	1783	1788	rBV	749046	949866	2.62%	1.278%
18	12.073	1788	1791	1799	rVB	489422	637421	1.76%	0.858%

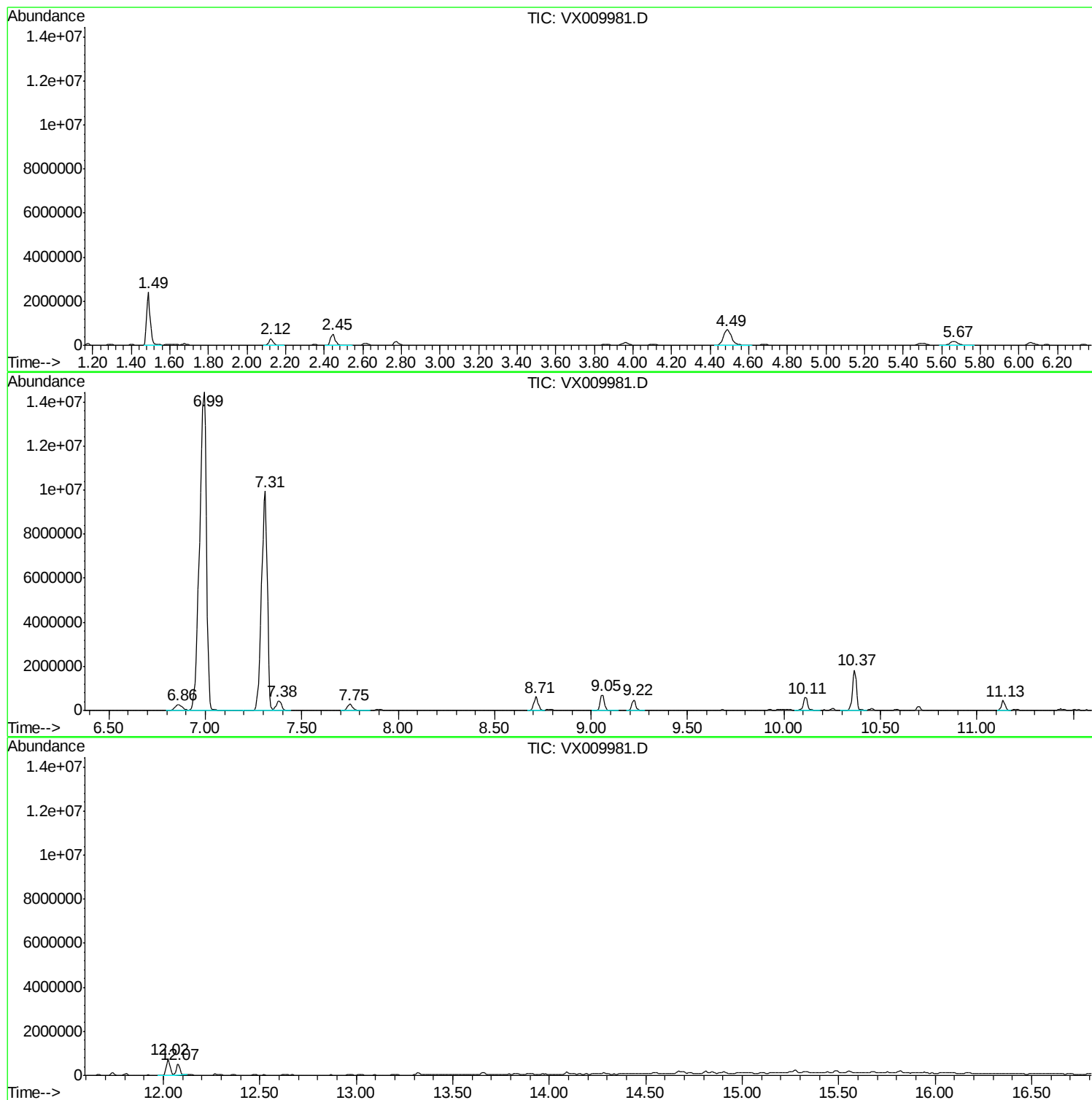
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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



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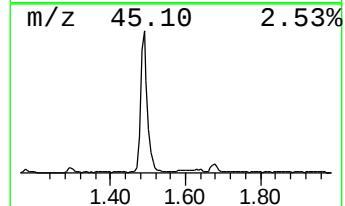
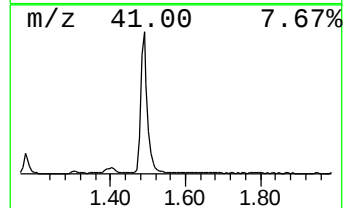
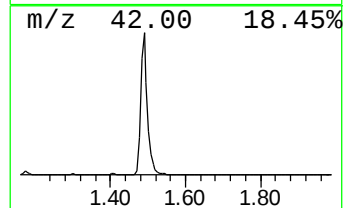
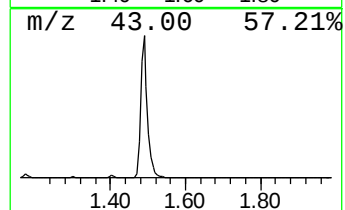
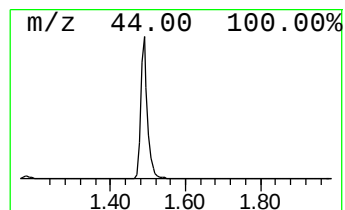
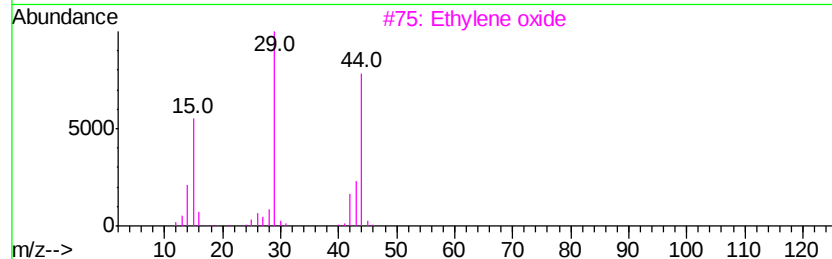
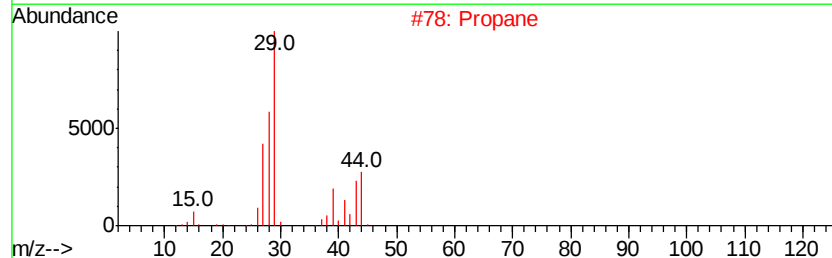
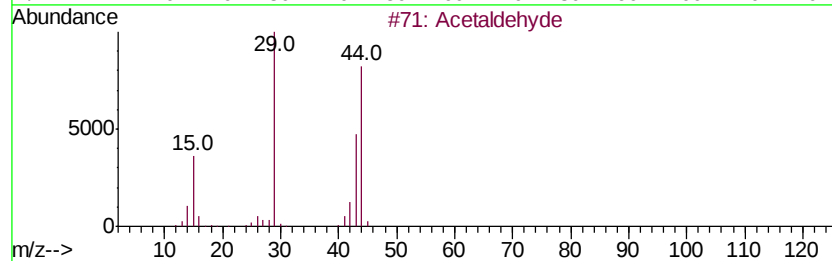
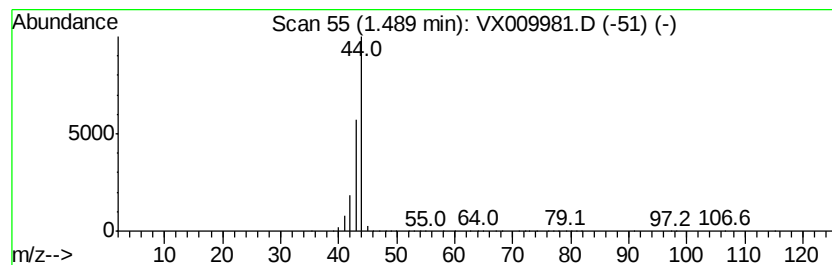
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	279.10 ug/l	2890250	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehyd	44	C2H4O	000075-07-0	9
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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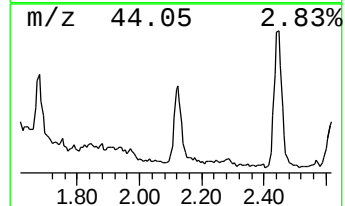
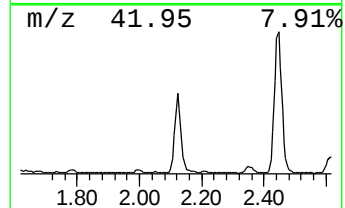
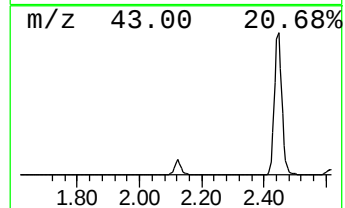
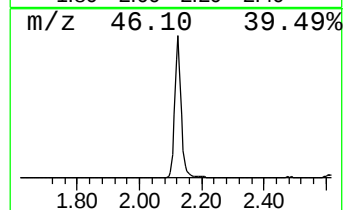
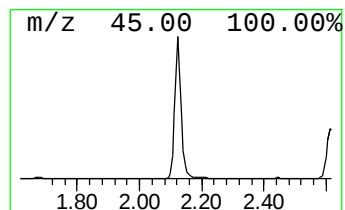
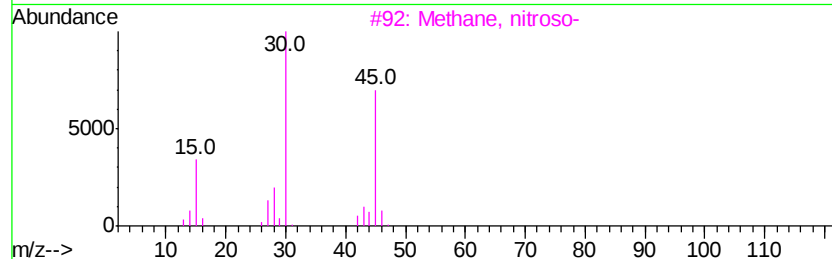
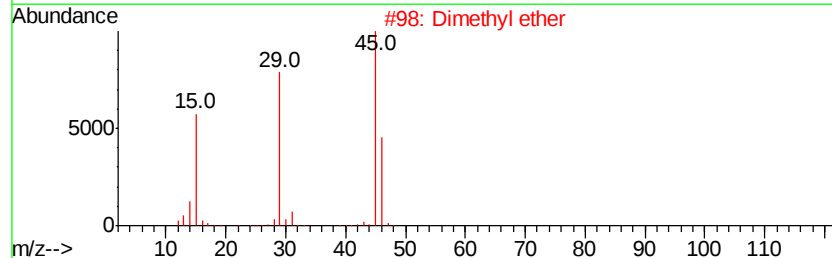
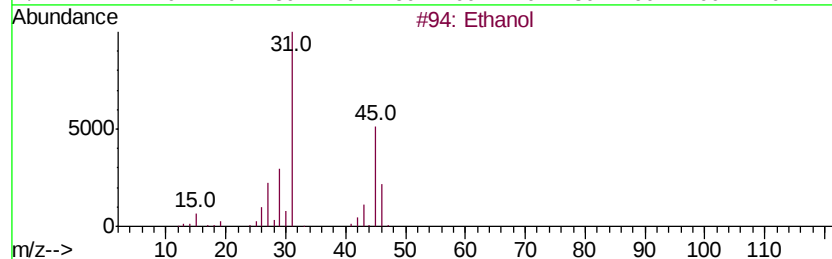
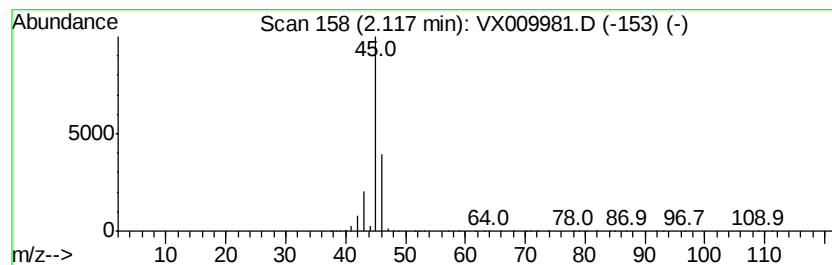
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	42.80 ug/l	443221	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	64
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	Oxalic acid		90	C2H2O4	000144-62-7	4



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

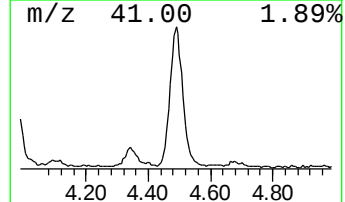
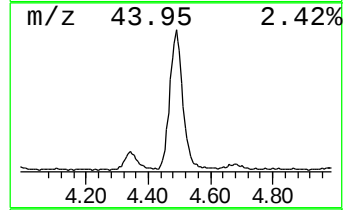
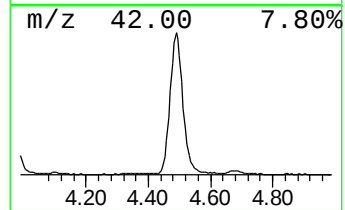
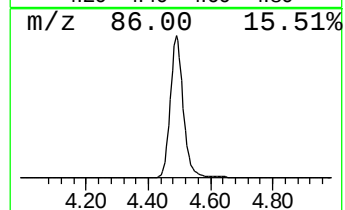
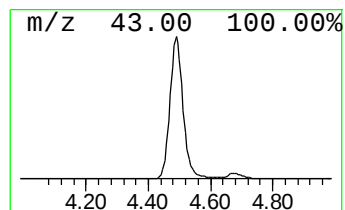
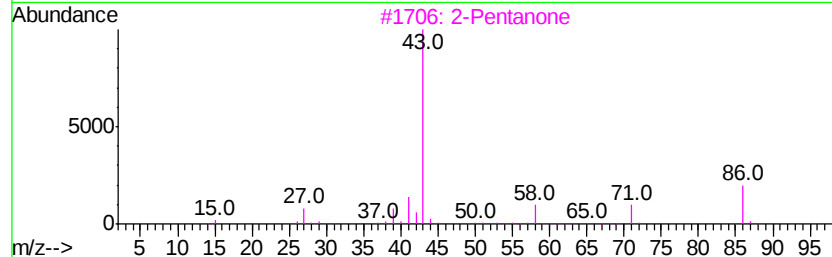
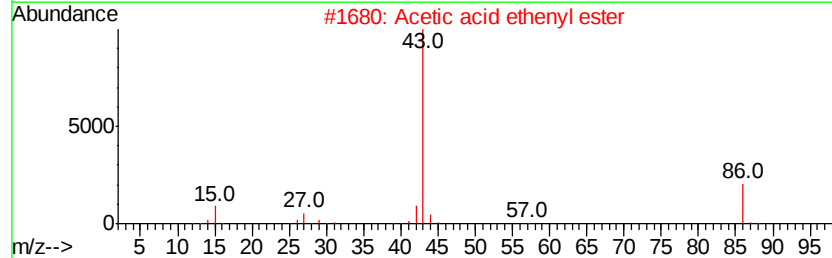
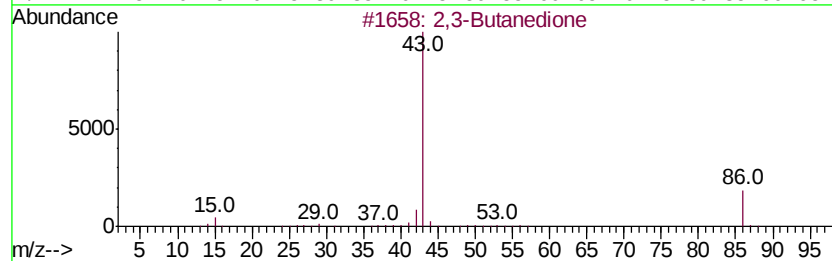
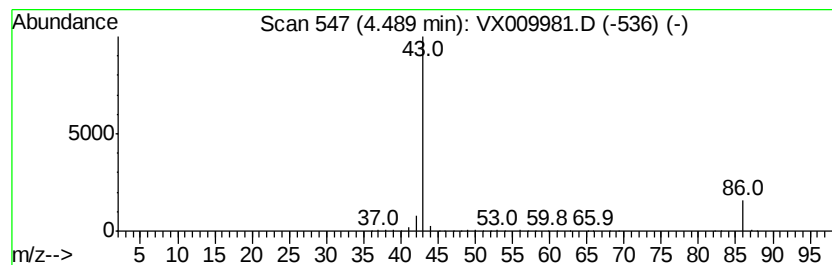
Instrument :
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ClientSampleId :
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Peak Number 3 2,3-Butanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
4.49	202.68 ug/l	2098830	Pentafluorobenzene	5.66		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione		86	C4H6O2	000431-03-8	80
2	Acetic acid ethenyl ester		86	C4H6O2	000108-05-4	9
3	2-Pentanone		86	C5H10O	000107-87-9	5
4	2-Butanone, 3-methyl-		86	C5H10O	000563-80-4	5
5	Propane, 2-(ethenyloxy)-		86	C5H10O	000926-65-8	5



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Instrument :
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ClientSampleId :
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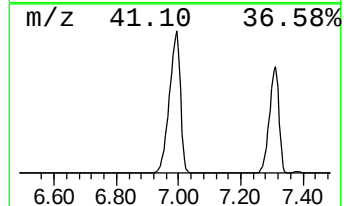
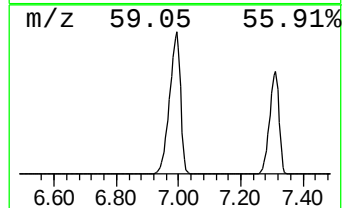
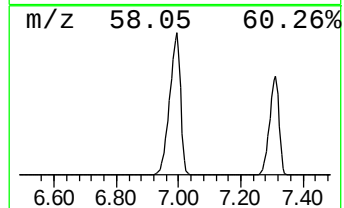
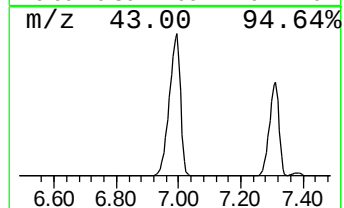
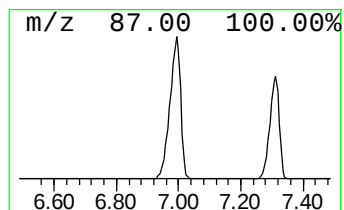
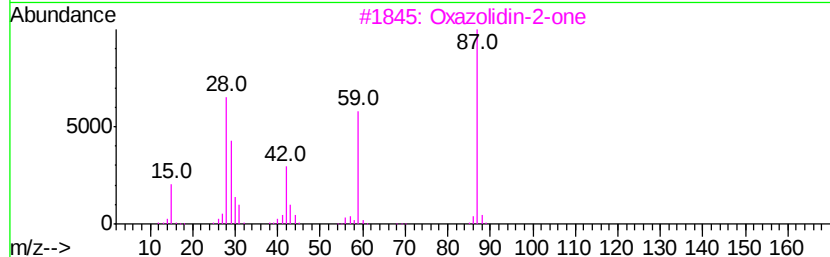
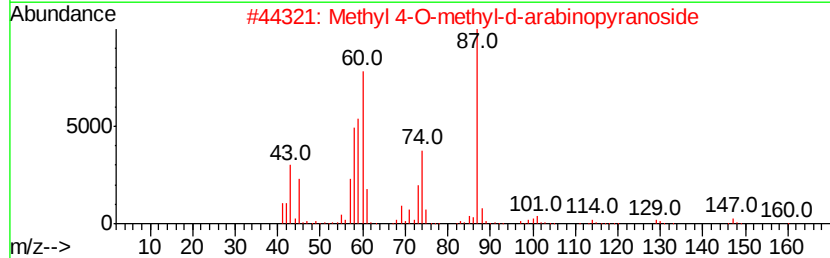
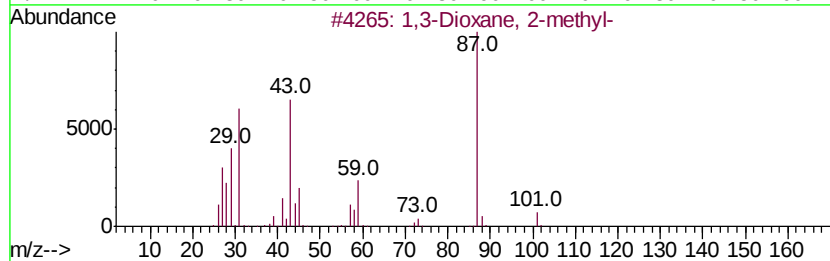
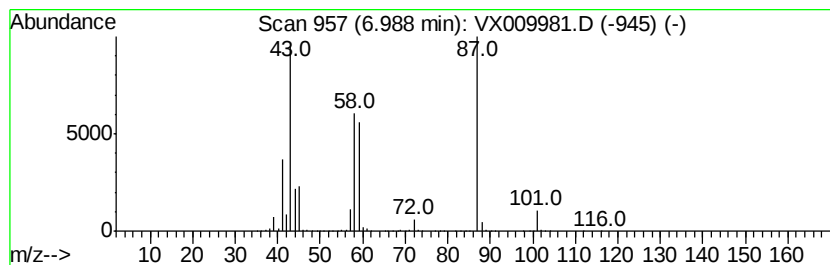
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Quant Title : SW846 8260

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

Peak Number 4 1,3-Dioxane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	2621.46 ug/l	36303900	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	59
2		Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	36
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	32
4		1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	28
5		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	28



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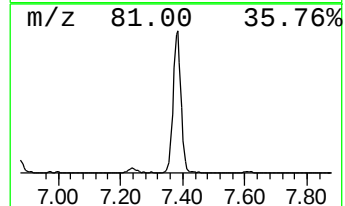
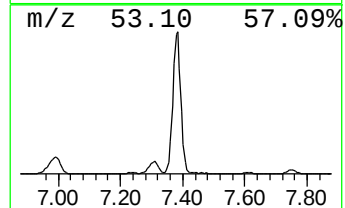
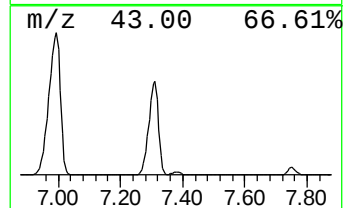
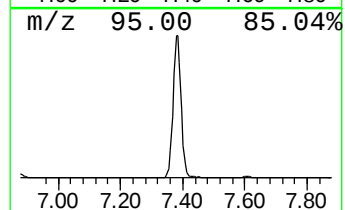
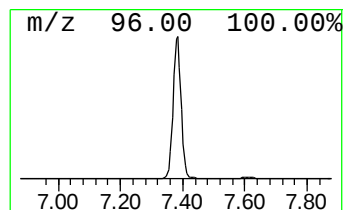
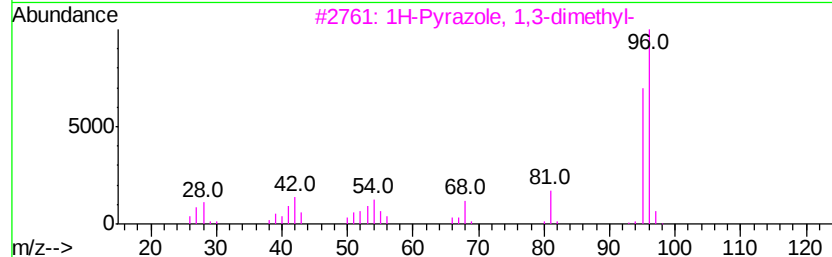
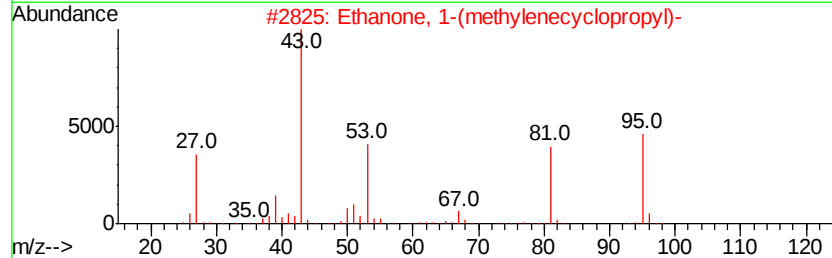
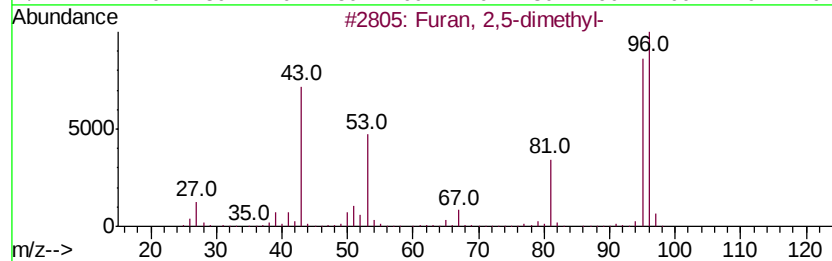
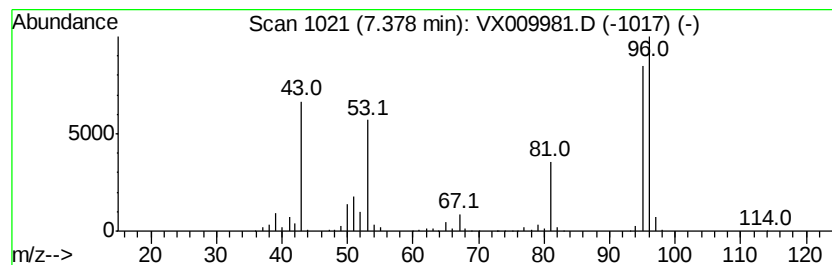
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Furan, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	56.84 ug/l	787182	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	94
2		Ethanone, 1-(methylenecyclopropyl)-	96	C6H8O	062266-35-7	59
3		1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	000694-48-4	38
4		1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	000694-31-5	38
5		3,5-Dimethylpyrazole-1-methanol	126	C6H10N2O	085264-33-1	35



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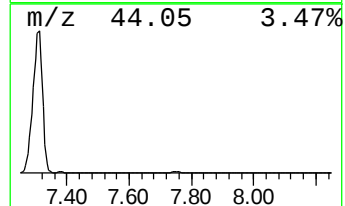
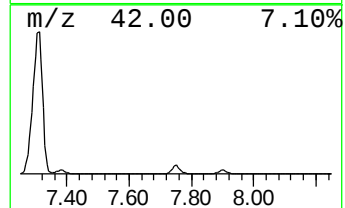
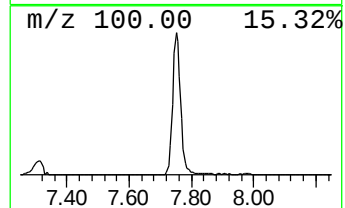
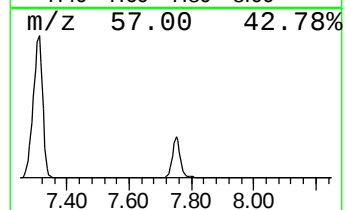
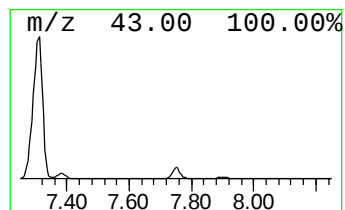
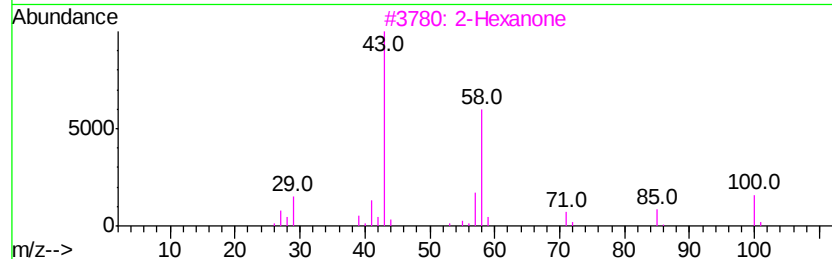
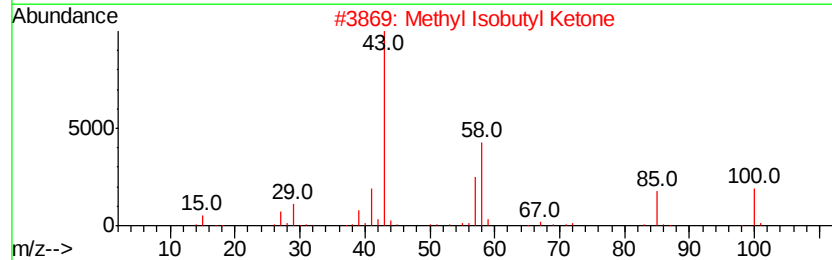
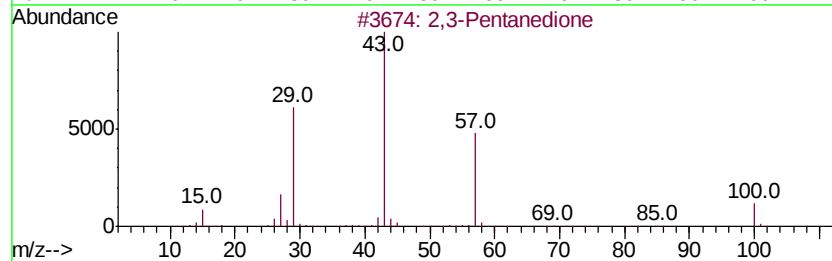
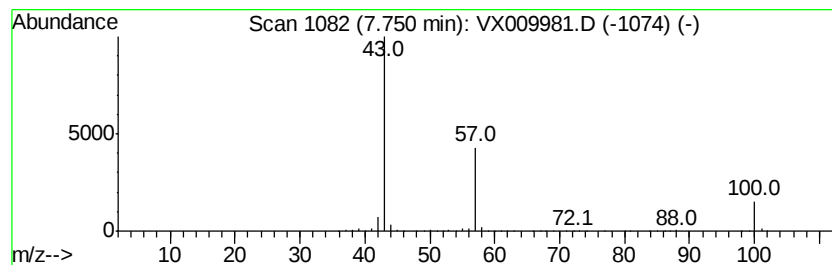
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 7 2,3-Pentanedione Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	37.20 ug/l	515150	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Pentanedione	100	C5H8O2	000600-14-6	78
2		Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	45
3		2-Hexanone	100	C6H12O	000591-78-6	39
4		3-Penten-2-one, 4-(acetyloxy)-, ...	142	C7H10O3	038365-58-1	33
5		Acetylacetone	100	C5H8O2	000123-54-6	28



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009981.D
Acq On : 31 May 2019 13:11
Operator : JC/SP
Sample : K2964-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
51030

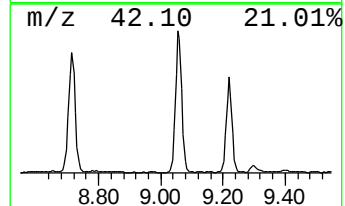
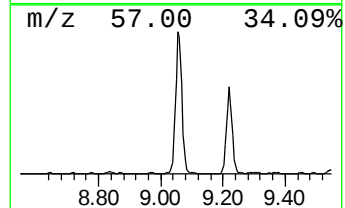
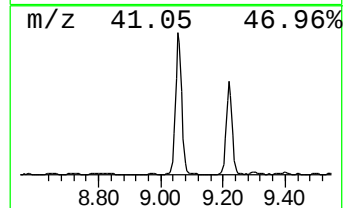
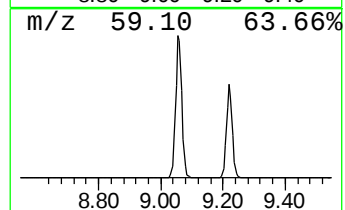
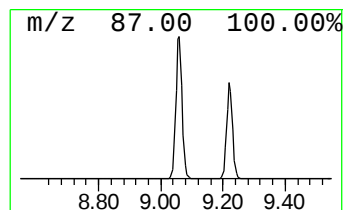
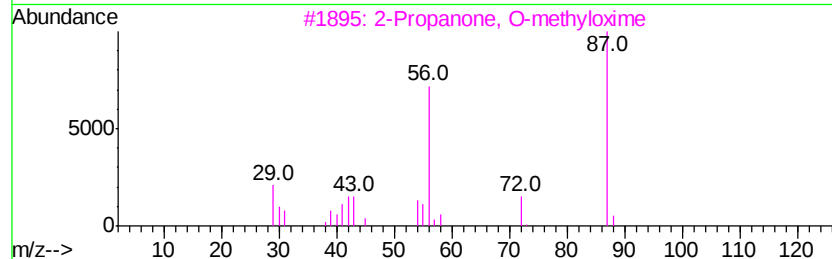
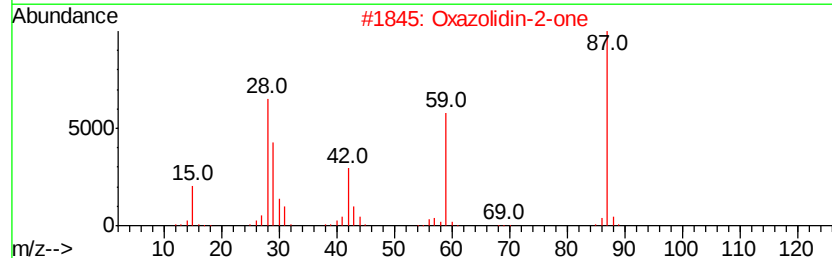
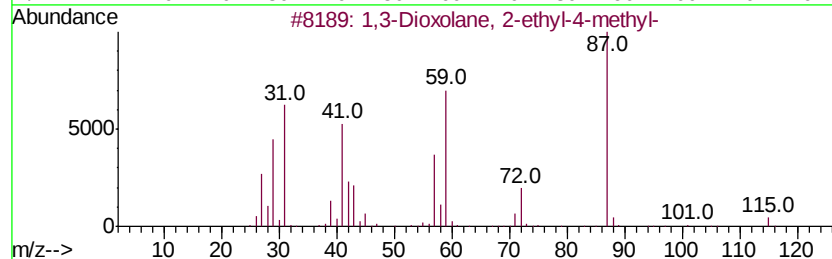
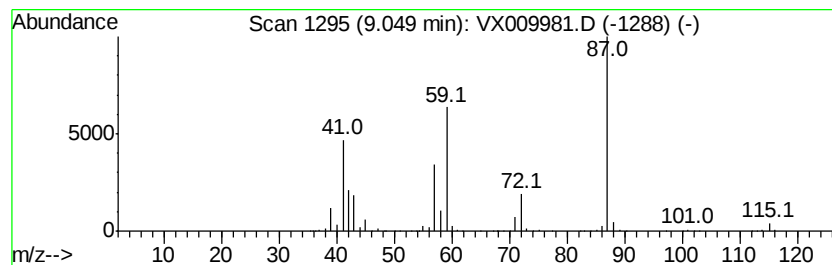
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Quant Title : SW846 8260

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

Peak Number 8 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.05	58.40 ug/l	1018450	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	95
2		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	59
3		2-Propanone, O-methyl-oxime	87	C4H9NO	003376-35-0	58
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
5		Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009981.D
Acq On : 31 May 2019 13:11
Operator : JC/SP
Sample : K2964-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 10 Sample Multiplier: 1

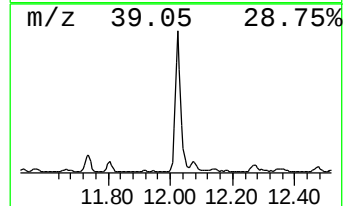
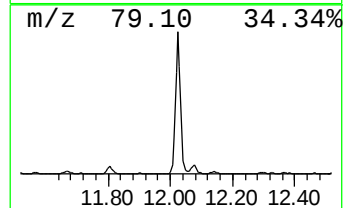
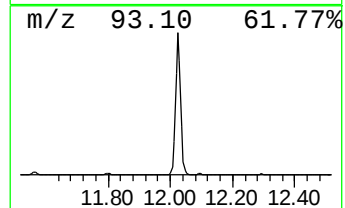
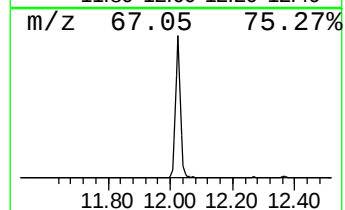
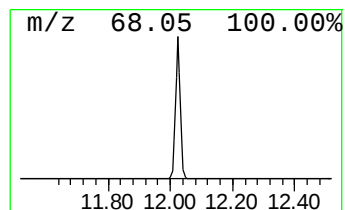
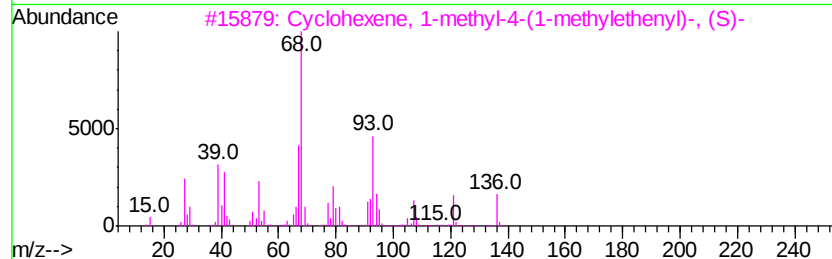
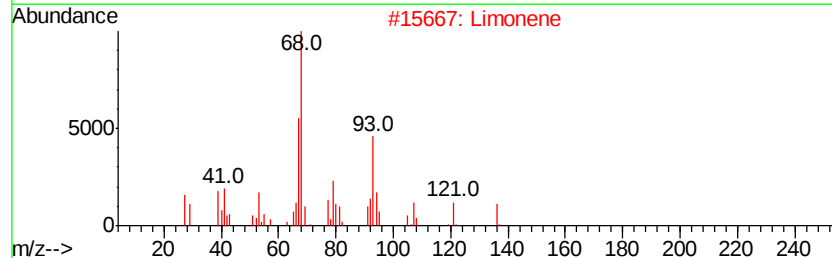
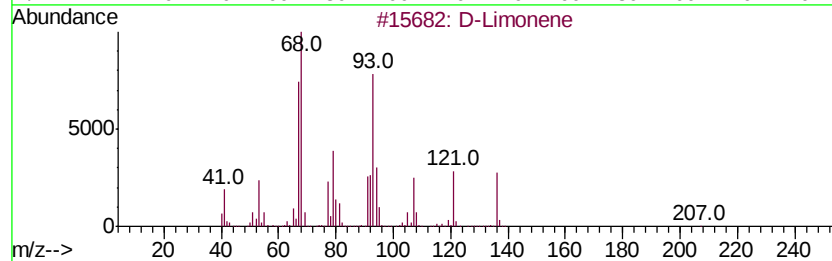
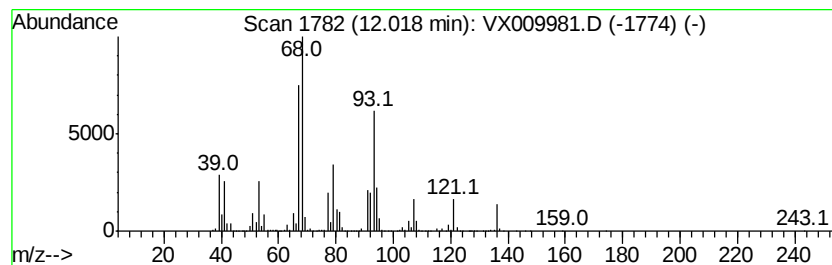
Instrument :
MSVOA_X
ClientSampleId :
51030

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 10 D-Limonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.02	74.51 ug/l	949866	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	97
2	Limonene	136	C10H16	000138-86-3	94
3	Cyclohexene, 1-methyl-4-(1-methyl-4-ethenyl)-, (S)-	136	C10H16	005989-54-8	87
4	1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	70
5	Cyclohexene, 4-ethenyl-1,4-dimethyl-	136	C10H16	001743-61-9	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX053119\
Data File : VX009981.D
Acq On : 31 May 2019 13:11
Operator : JC/SP
Sample : K2964-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
51030

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.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	1.49	279.1	ug/l	2890250	1	5.66	517775	50.0
Ethanol	2.12	42.8	ug/l	443221	1	5.66	517775	50.0
2,3-Butanedione	4.49	202.7	ug/l	2098830	1	5.66	517775	50.0
1,3-Dioxane, 2-me...	6.99	2621.5	ug/l	36303900	2	6.86	692435	50.0
Furan, 2,5-dimethyl-	7.38	56.8	ug/l	787182	2	6.86	692435	50.0
2,3-Pentanedione	7.75	37.2	ug/l	515150	2	6.86	692435	50.0
1,3-Dioxolane, 2-...	9.05	58.4	ug/l	1018450	3	10.11	871931	50.0
D-Limonene	12.02	74.5	ug/l	949866	4	12.08	637421	50.0