

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092718\
 Data File : VX004782.D
 Acq On : 27 Sep 2018 18:50
 Operator : JC/MD
 Sample : J5048-03 10X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-57-SEP18

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\82X092618W.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	2.166	151	166	169	rBV	10454669	25280186	100.00%	23.516%
2	2.452	207	213	226	rVB	378361	726738	2.87%	0.676%
3	2.647	233	245	266	rBV	8864664	18740404	74.13%	17.433%
4	4.080	455	480	502	rBV	2838710	10394070	41.12%	9.669%
5	4.598	555	565	577	rVB2	104463	286456	1.13%	0.266%
6	4.860	599	608	618	rBV	102505	285378	1.13%	0.265%
7	5.501	701	713	728	rVB2	193444	558743	2.21%	0.520%
8	5.665	728	740	754	rBV	209921	612268	2.42%	0.570%
9	6.067	795	806	820	rBV	186445	470145	1.86%	0.437%
10	6.275	828	840	864	rBV	579394	1606848	6.36%	1.495%
11	6.860	926	936	960	rBV	353482	866628	3.43%	0.806%
12	7.214	982	994	1003	rBV	184831	398627	1.58%	0.371%
13	7.366	1003	1019	1046	rBV	5981242	15074666	59.63%	14.023%
14	7.781	1081	1087	1099	rVB	246498	433710	1.72%	0.403%
15	8.713	1234	1240	1249	rBV2	900458	1539966	6.09%	1.433%
16	9.311	1332	1338	1349	rBV	2804724	4551010	18.00%	4.233%
17	9.408	1349	1354	1373	rVV	842652	1534517	6.07%	1.427%
18	9.585	1379	1383	1389	rVV	983693	1452034	5.74%	1.351%
19	9.677	1392	1398	1412	rVB2	222115	579043	2.29%	0.539%
20	10.061	1454	1461	1465	rBV	207869	443292	1.75%	0.412%
21	10.116	1465	1470	1476	rVB	796085	1200287	4.75%	1.117%
22	10.646	1551	1557	1563	rBV	3666434	4987260	19.73%	4.639%
23	10.695	1563	1565	1567	rVV	291327	369631	1.46%	0.344%
24	10.719	1567	1569	1573	rVB	391220	443241	1.75%	0.412%
25	11.140	1630	1638	1654	rVB2	1034780	1641671	6.49%	1.527%
26	11.713	1728	1732	1735	rBV	2013358	2363845	9.35%	2.199%
27	11.768	1735	1741	1752	rVB4	627616	1422446	5.63%	1.323%
28	12.060	1781	1789	1790	rBV	771476	1098491	4.35%	1.022%
29	12.079	1790	1792	1805	rVB	1111129	1300995	5.15%	1.210%
30	12.652	1879	1886	1888	rBV3	599637	1090591	4.31%	1.014%
31	12.676	1888	1890	1899	rVB	560566	700156	2.77%	0.651%
32	12.889	1920	1925	1935	rVB	611508	794440	3.14%	0.739%
33	13.481	2015	2022	2024	rBV2	382675	790597	3.13%	0.735%
34	13.499	2024	2025	2034	rVB	484436	474620	1.88%	0.442%

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Integration Parameters: RTEINT.P

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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35	13.664	2047	2052	2064	rBV	202227	267282	1.06%	0.249%
36	14.225	2139	2144	2145	rBV2	525077	580860	2.30%	0.540%
37	14.243	2145	2147	2155	rVB2	491294	571883	2.26%	0.532%
38	14.932	2254	2260	2276	rBV2	778824	1045646	4.14%	0.973%
39	15.688	2378	2384	2398	rBV	293672	522136	2.07%	0.486%

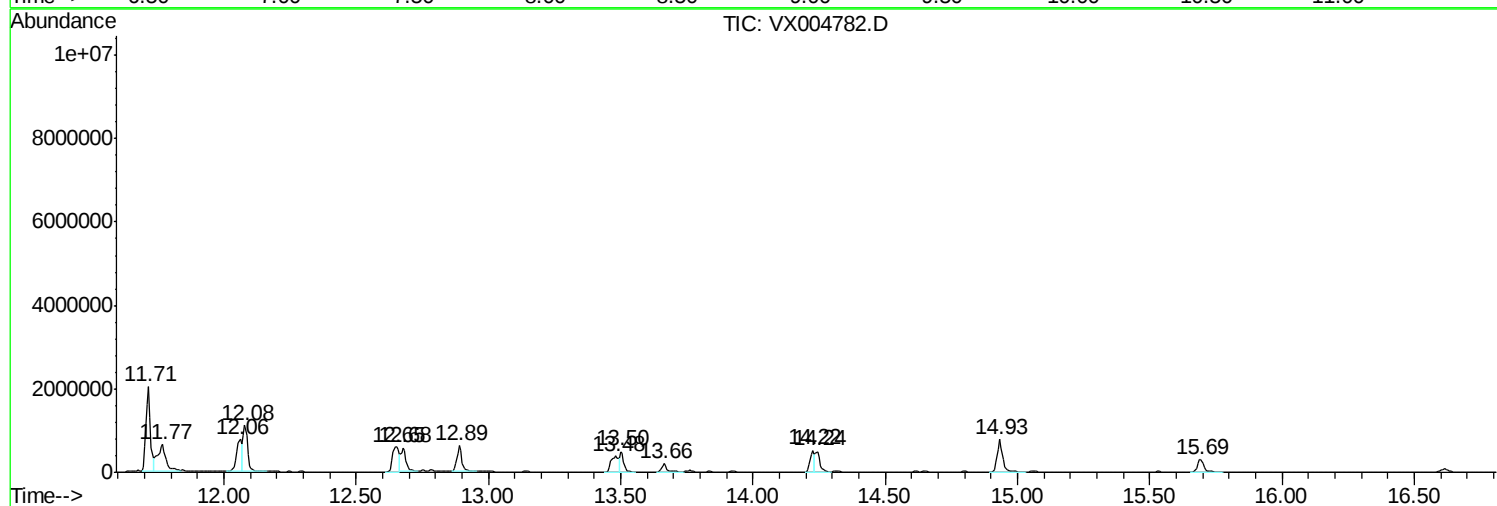
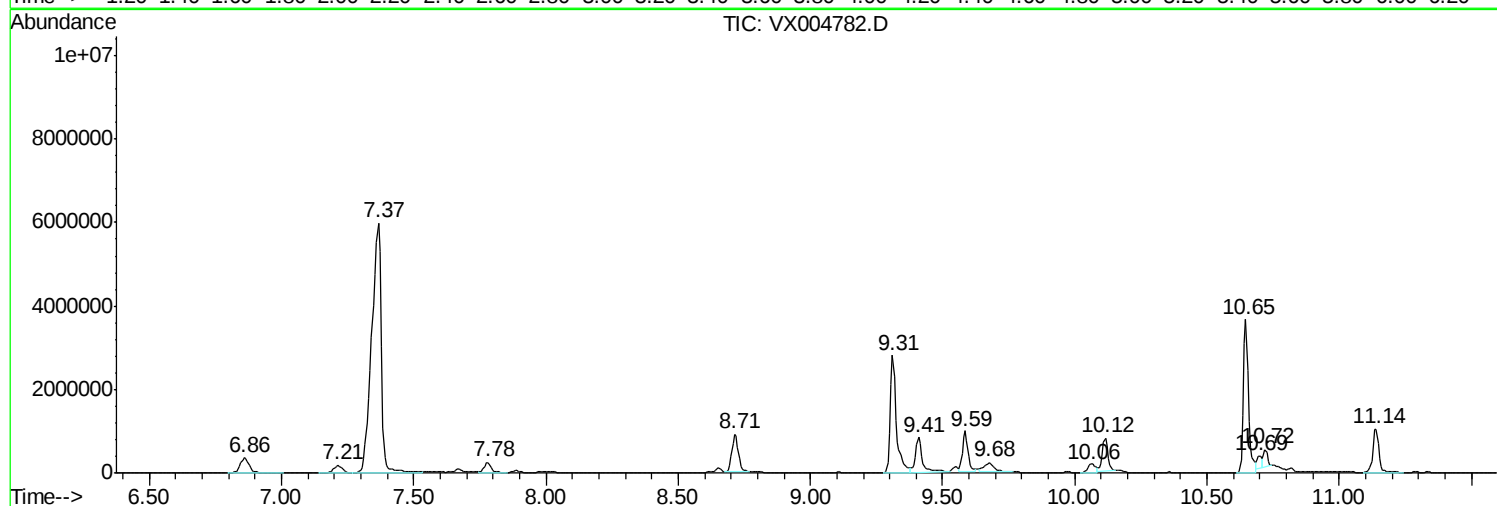
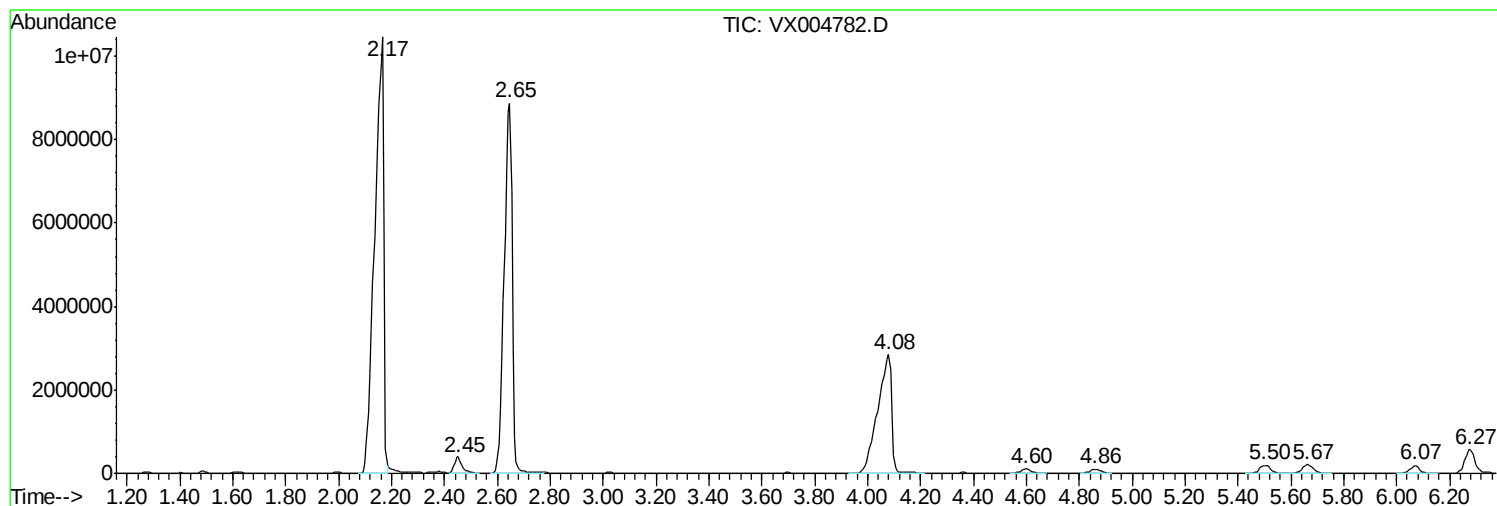
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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



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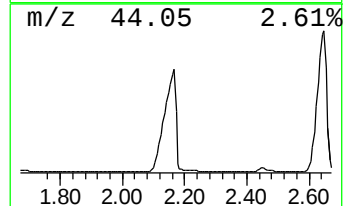
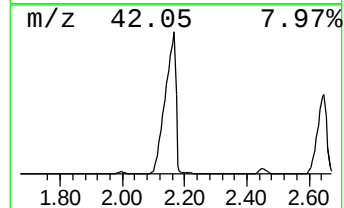
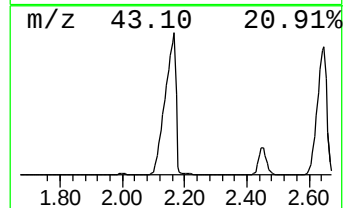
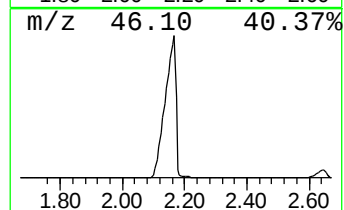
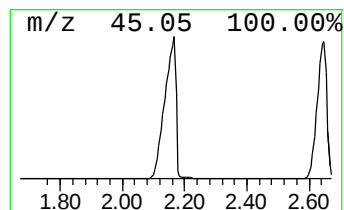
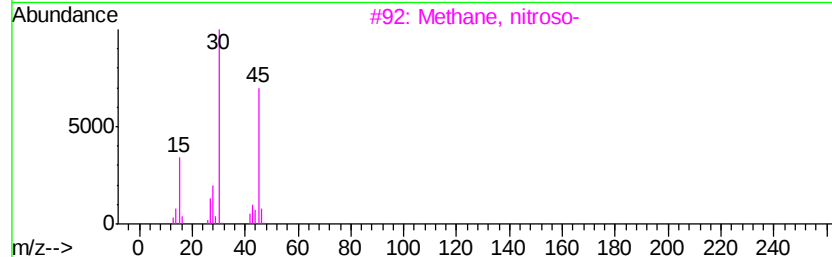
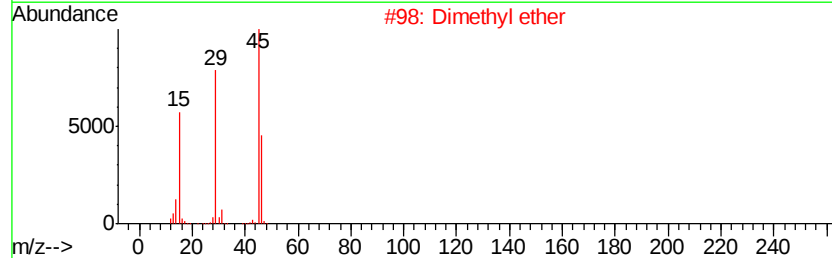
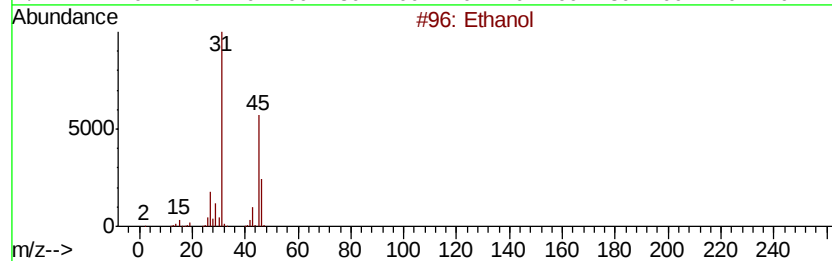
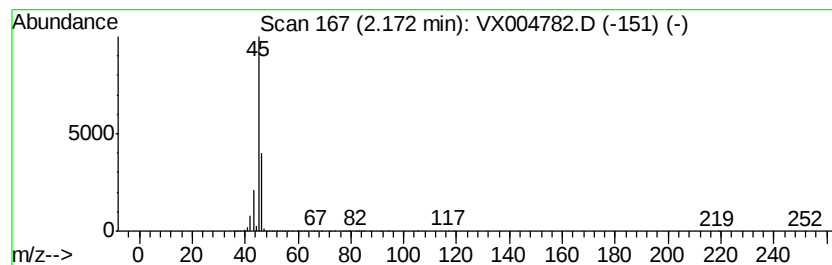
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2064.47 ug/l	25280200	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	83
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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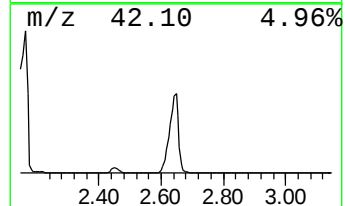
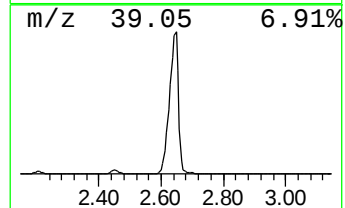
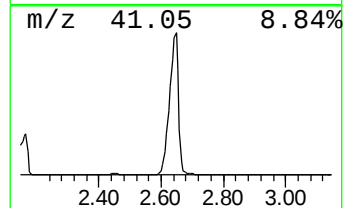
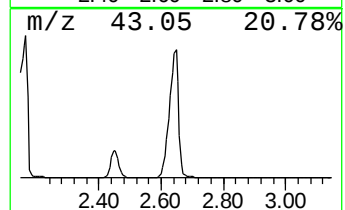
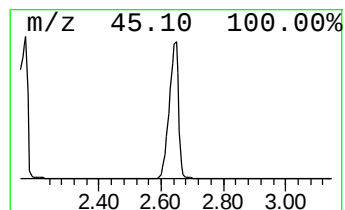
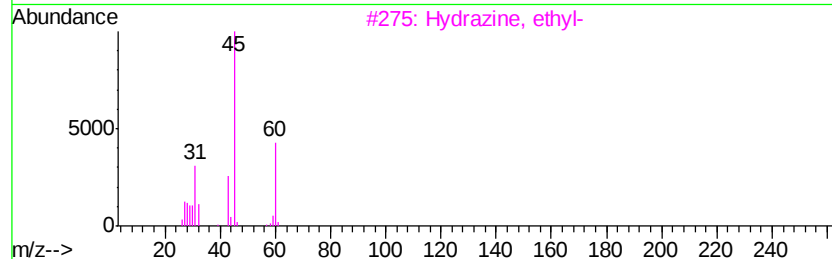
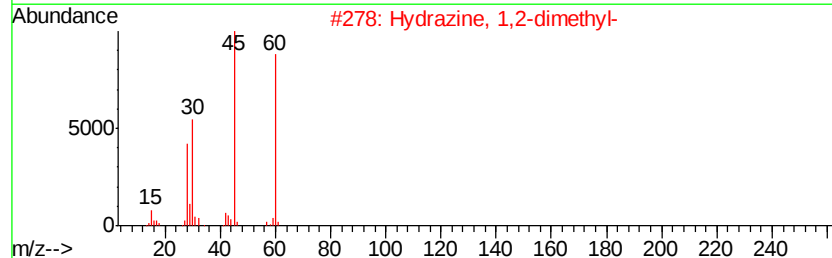
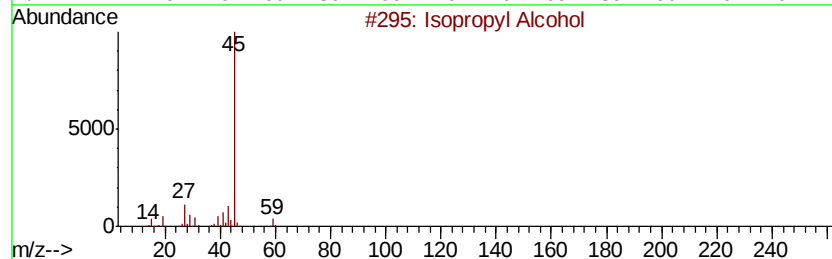
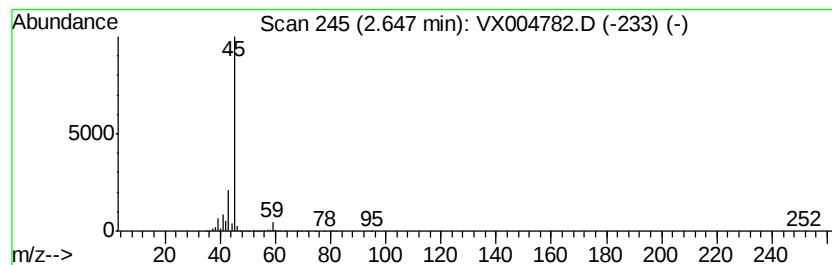
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.65	1530.41 ug/l	18740400	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hvdrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		Hvdrazine, ethyl-	60	C2H8N2	000624-80-6	9
4		Formamide	45	CH3NO	000075-12-7	5
5		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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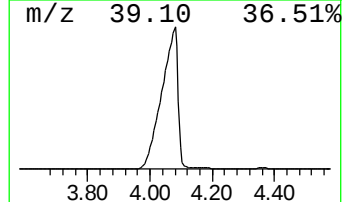
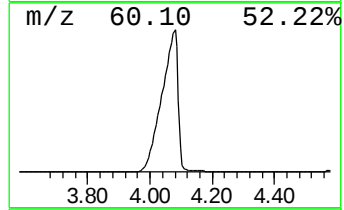
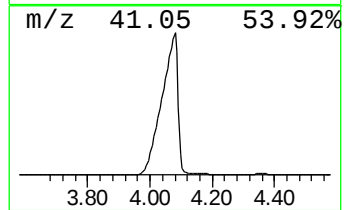
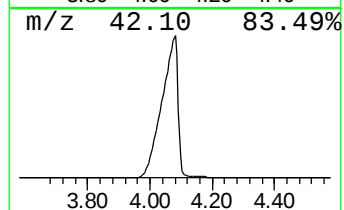
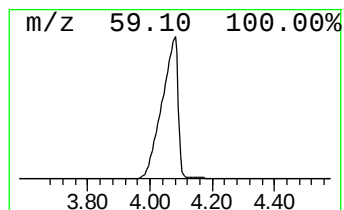
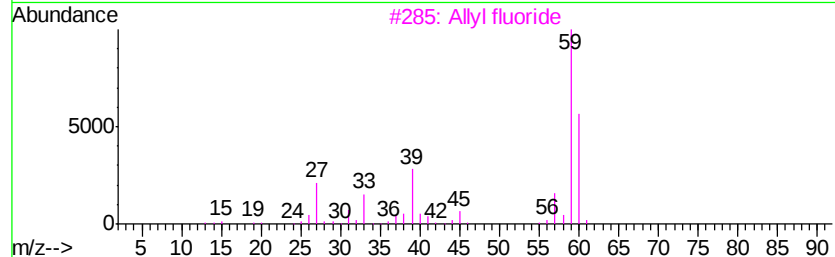
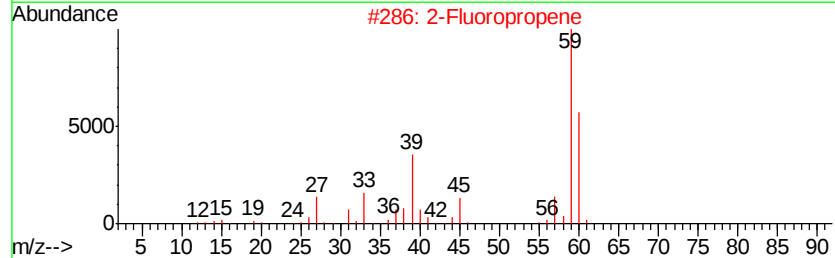
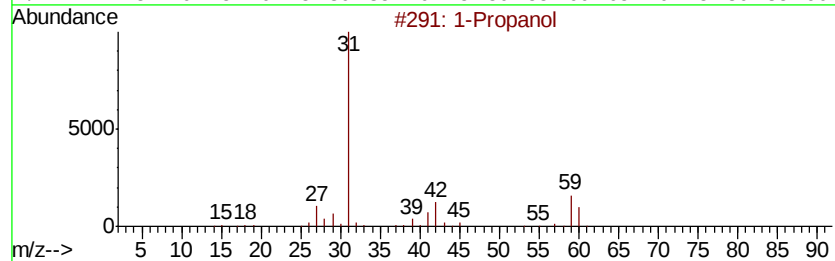
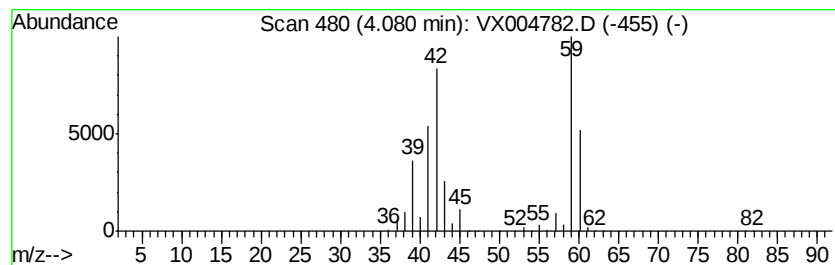
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	848.82 ug/l	10394100	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	49
3		Allyl fluoride	60	C3H5F	000818-92-8	43
4		Cyclopropane	42	C3H6	000075-19-4	9
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



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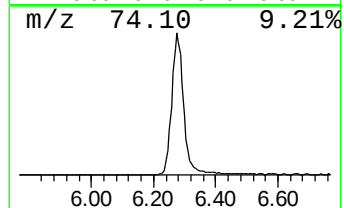
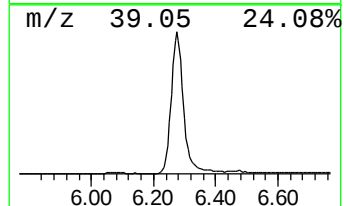
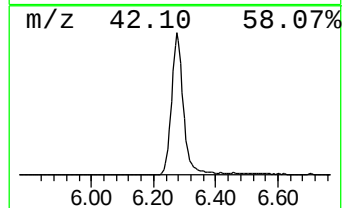
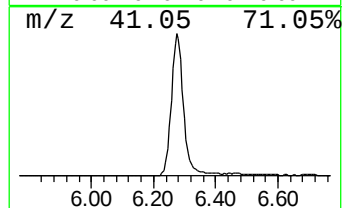
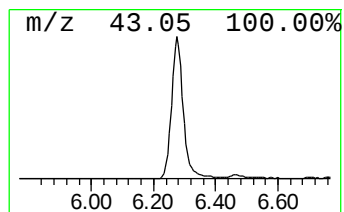
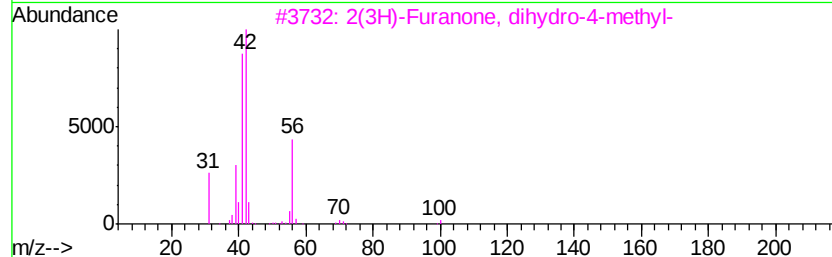
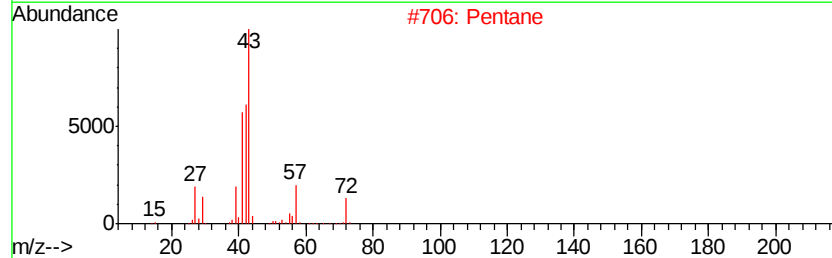
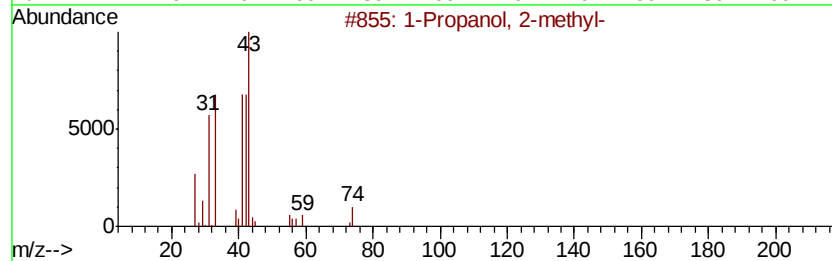
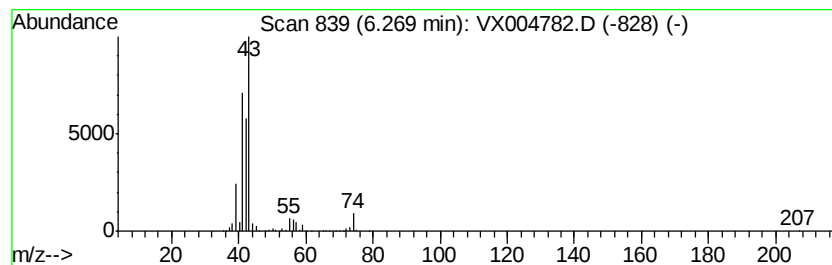
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	92.71 ug/l	1606850	1,4-Difluorobenzene	6.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Propanol, 2-methyl-	74 C4H10O	000078-83-1	86
2	Pentane	72 C5H12	000109-66-0	36
3	2(3H)-Furanone, dihydro-4-methyl-	100 C5H8O2	001679-49-8	25
4	Isobutylene epoxide	72 C4H8O	000558-30-5	25
5	Propanal, 2-methyl-	72 C4H8O	000078-84-2	22



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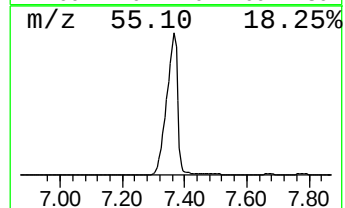
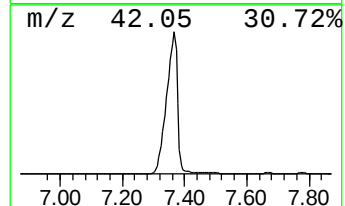
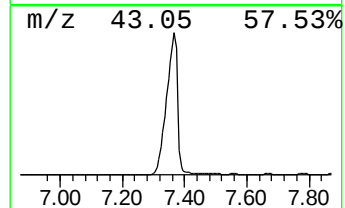
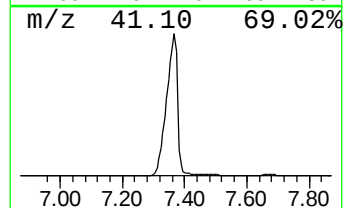
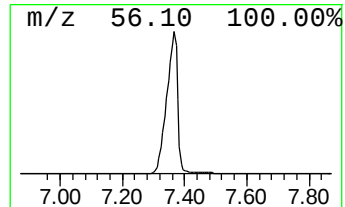
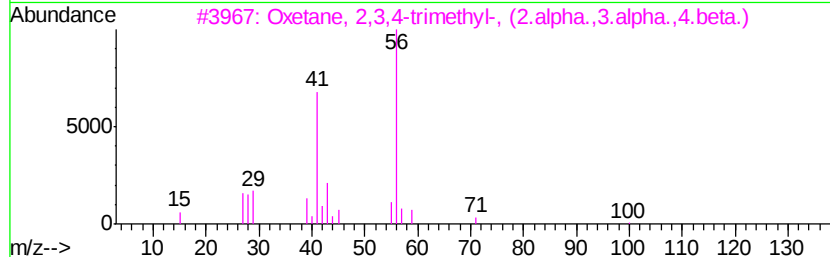
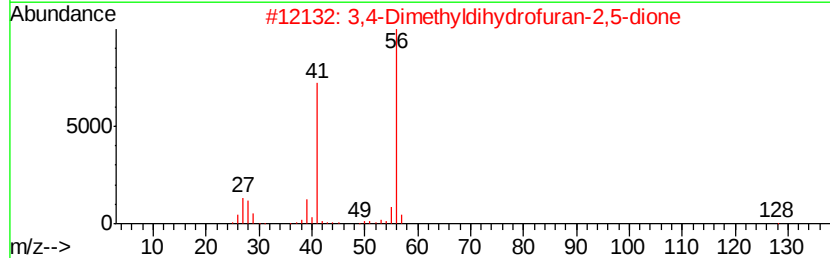
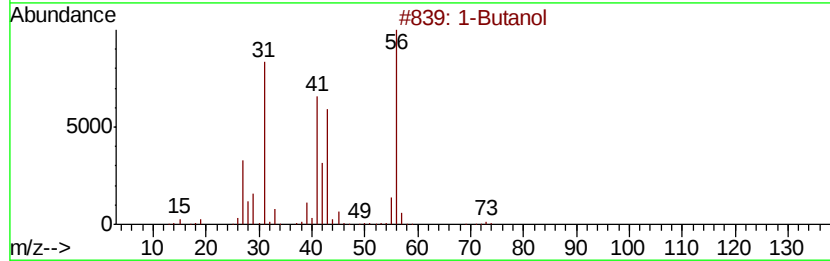
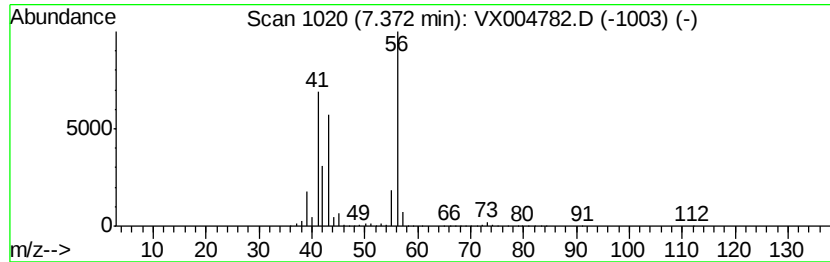
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Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	869.73 ug/l	15074700	1,4-Difluorobenzene	6.86

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
3	Oxetane, 2,3,4-trimethyl-, (2.alpha....	100	C6H12O	032347-12-9	9
4	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092718\
Data File : VX004782.D
Acq On : 27 Sep 2018 18:50
Operator : JC/MD
Sample : J5048-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-57-SEP18

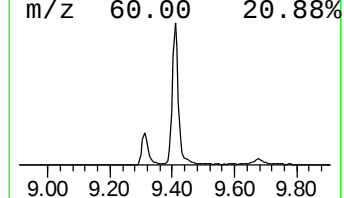
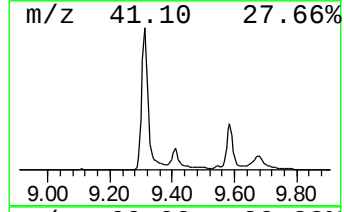
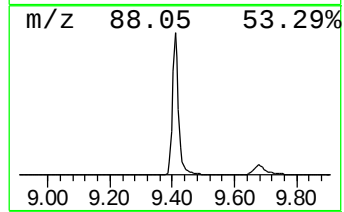
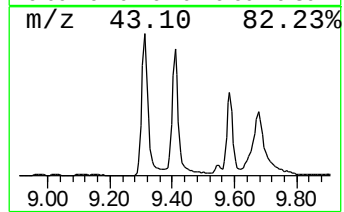
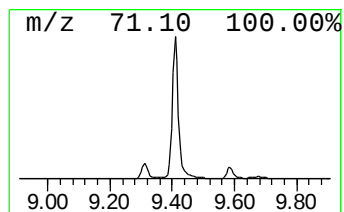
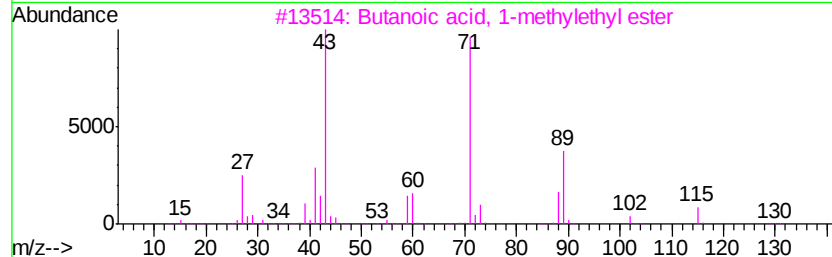
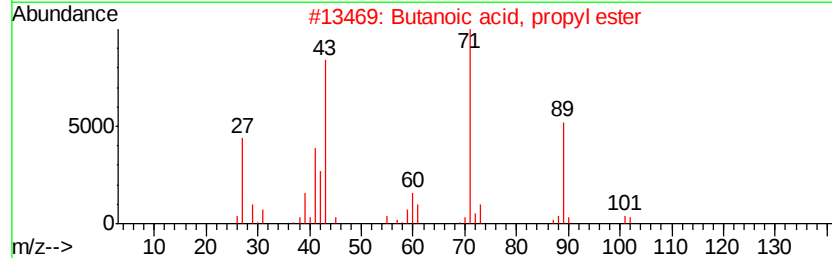
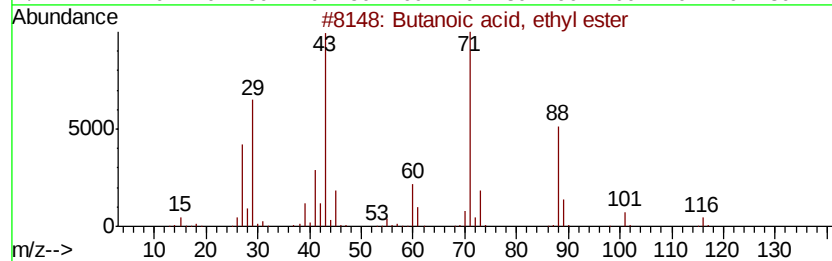
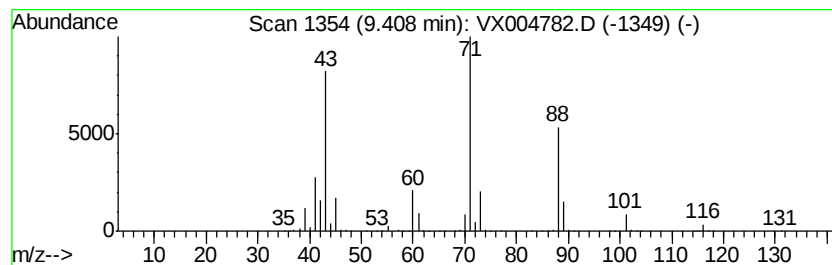
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Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	63.92 ug/l	1534520	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
3		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	43
4		Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
5		Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092718\
Data File : VX004782.D
Acq On : 27 Sep 2018 18:50
Operator : JC/MD
Sample : J5048-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-57-SEP18

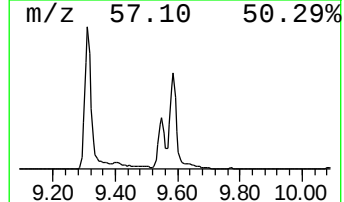
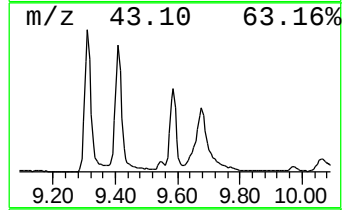
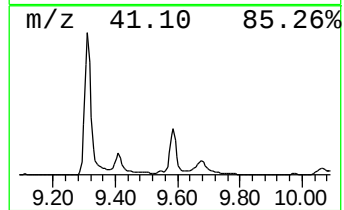
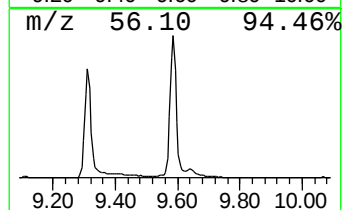
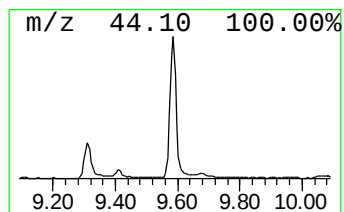
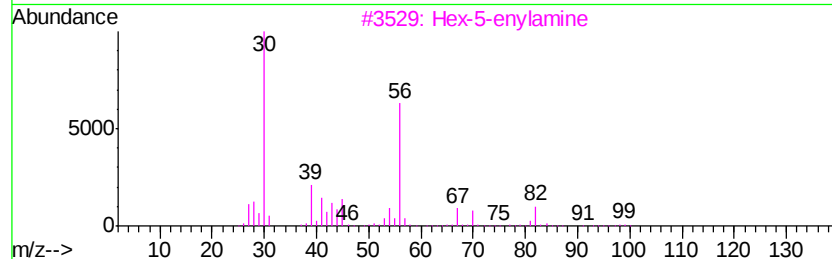
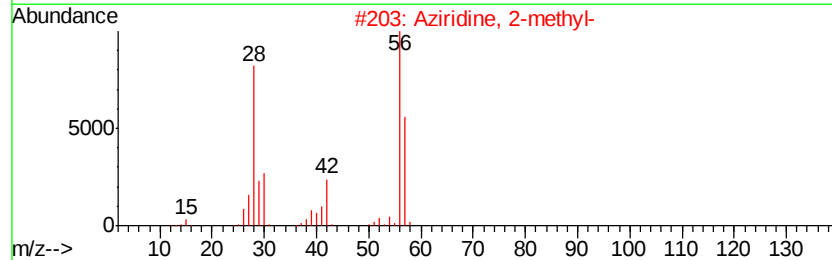
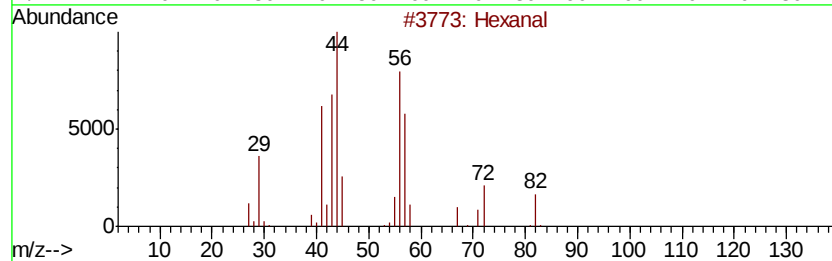
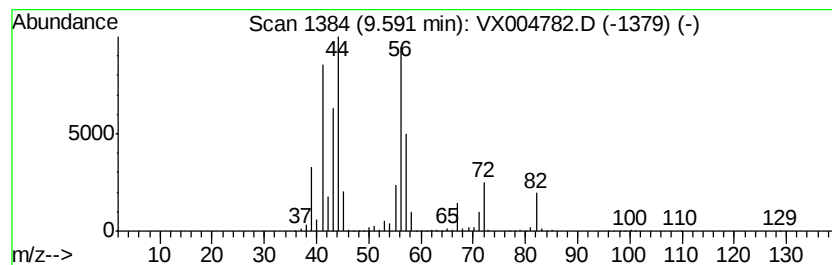
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Quant Title : SW846 8260

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

Peak Number 7 Hexanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	60.49 ug/l	1452030	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	90
2		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	27
3		Hex-5-enylamine	99	C6H13N	034825-70-2	25
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	22
5		Pentanal	86	C5H10O	000110-62-3	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092718\
Data File : VX004782.D
Acq On : 27 Sep 2018 18:50
Operator : JC/MD
Sample : J5048-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-57-SEP18

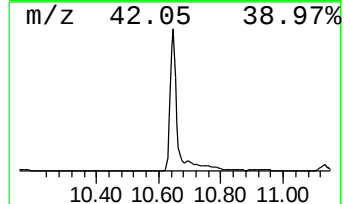
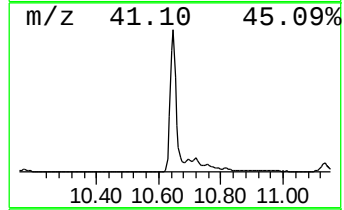
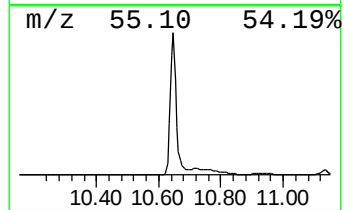
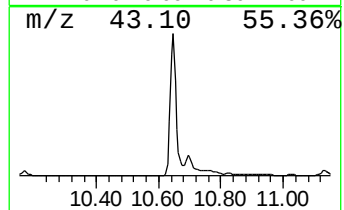
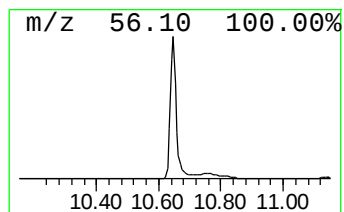
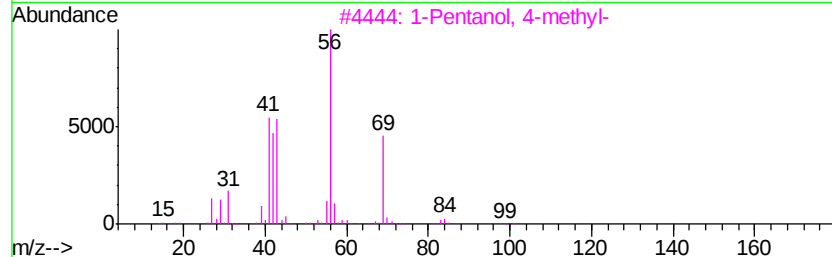
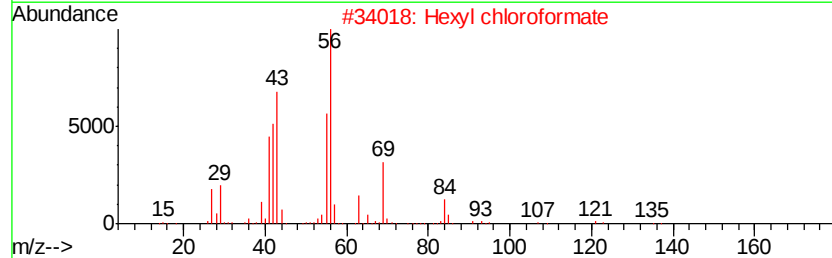
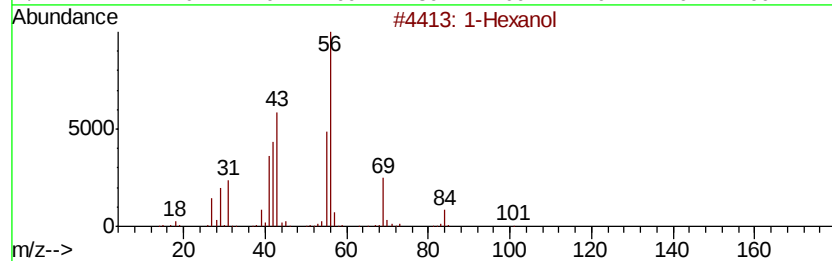
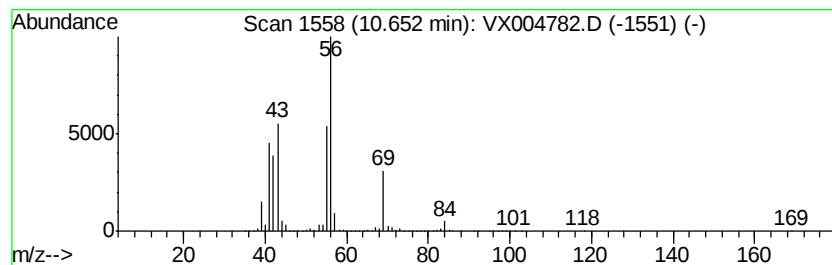
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	207.75 ug/l	4987260	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol	102	C6H14O	000111-27-3	86
2		Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
3		1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
4		Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
5		Cyclopentane, methyl-	84	C6H12	000096-37-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092718\
Data File : VX004782.D
Acq On : 27 Sep 2018 18:50
Operator : JC/MD
Sample : J5048-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

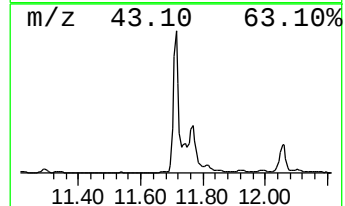
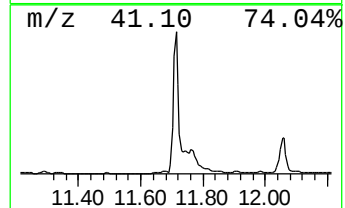
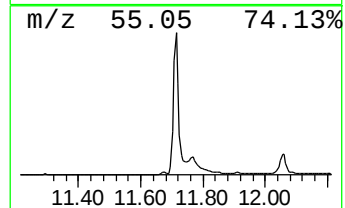
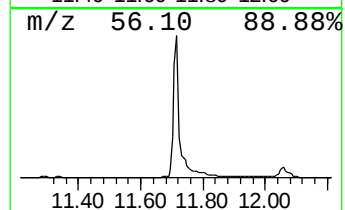
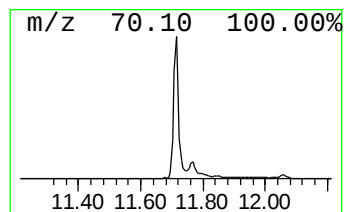
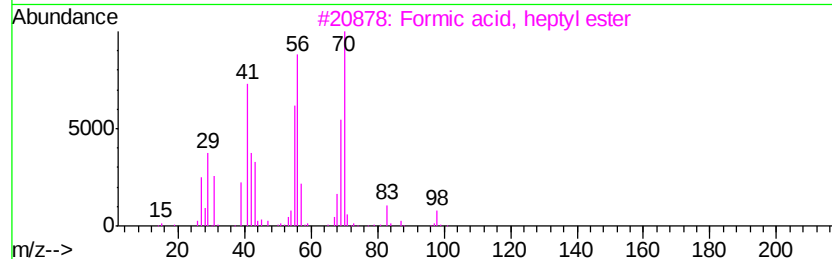
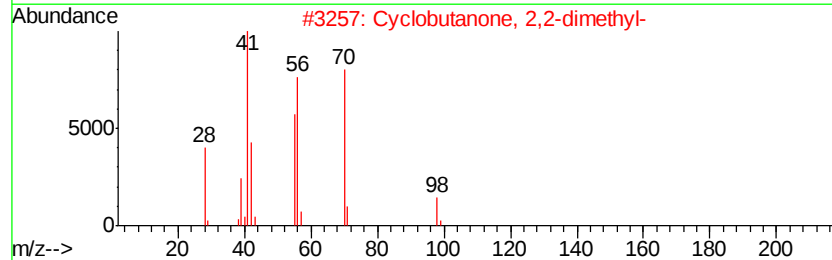
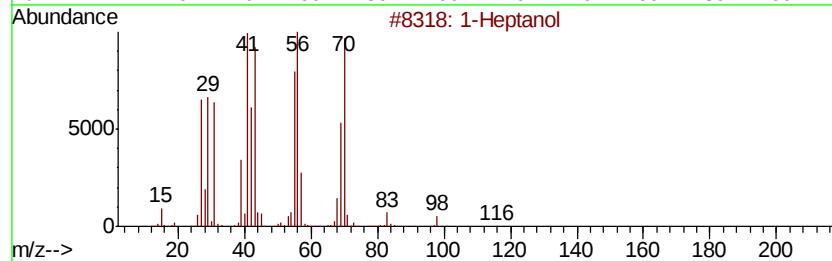
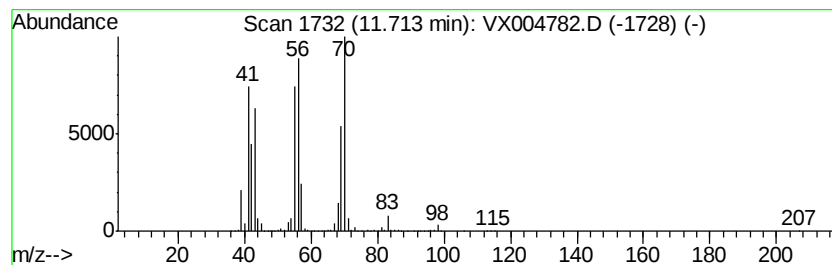
Instrument :
MSVOA_X
ClientSampleId :
MW-57-SEP18

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 9 1-Heptanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	90.85 ug/l	2363850	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptanol	116 C7H16O	000111-70-6	90
2	Cyclobutanone, 2,2-dimethyl-	98 C6H10O	001192-14-9	78
3	Formic acid, heptyl ester	144 C8H16O2	000112-23-2	72
4	Cyclopentane, 1,2-dimethyl-, cis-	98 C7H14	001192-18-3	72
5	Cyclopentane, 1,3-dimethyl-	98 C7H14	002453-00-1	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092718\
Data File : VX004782.D
Acq On : 27 Sep 2018 18:50
Operator : JC/MD
Sample : J5048-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-57-SEP18

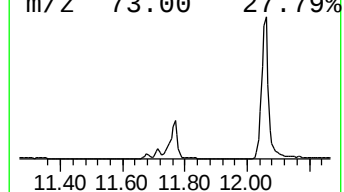
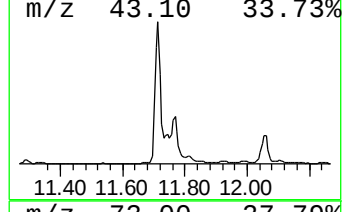
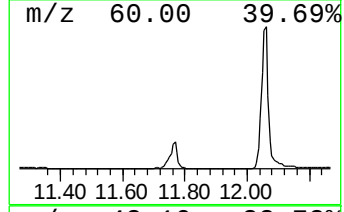
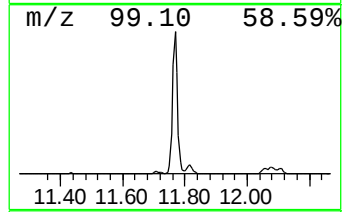
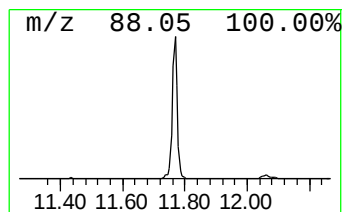
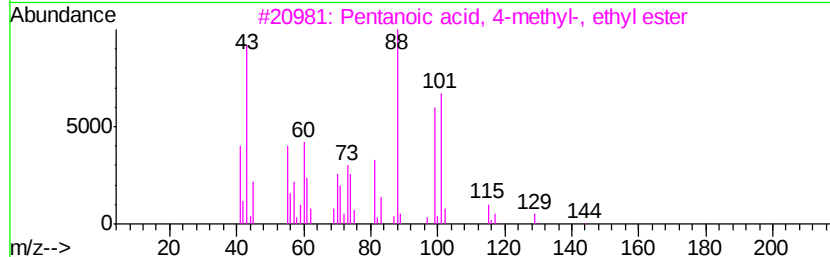
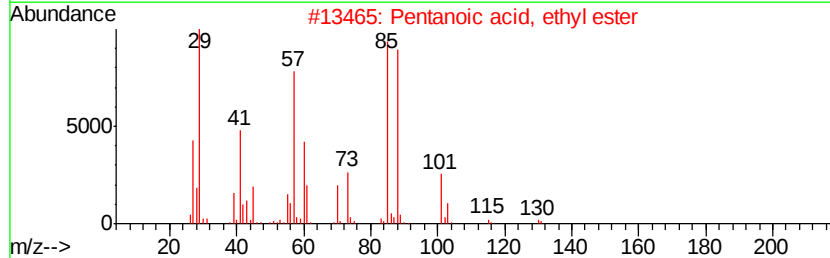
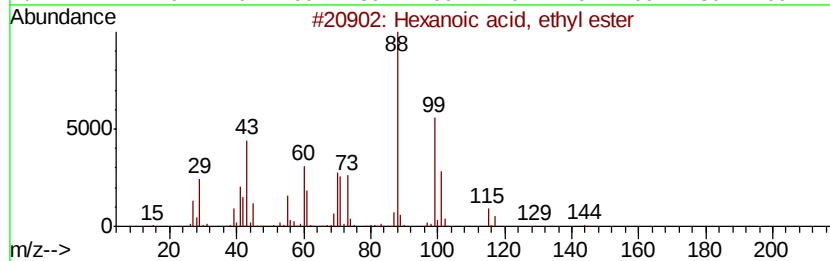
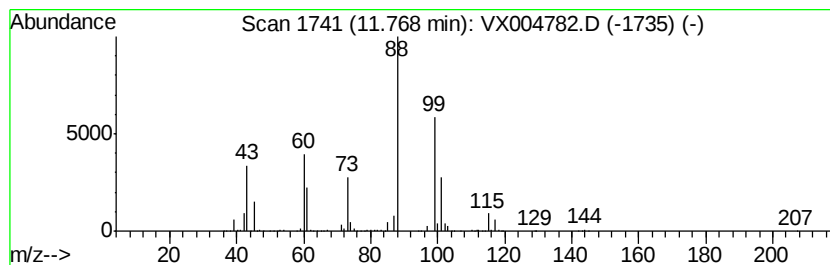
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Quant Title : SW846 8260

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

Peak Number 10 Hexanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	54.67 ug/l	1422450	1,4-Dichlorobenzene-d4	12.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, ethyl ester	144	C8H16O2	000123-66-0	93
2			Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	59
3			Pentanoic acid, 4-methyl-, ethyl...	144	C8H16O2	025415-67-2	56
4			Octanoic acid, ethyl ester	172	C10H20O2	000106-32-1	53
5			Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	45



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092718\
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Operator : JC/MD
Sample : J5048-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-57-SEP18

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.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
Ethanol	2.17	2064.5	ug/l	25280200	1	5.67	612268	50.0
Isopropyl Alcohol	2.65	1530.4	ug/l	18740400	1	5.67	612268	50.0
1-Propanol	4.08	848.8	ug/l	10394100	1	5.67	612268	50.0
1-Propanol, 2-met...	6.27	92.7	ug/l	1606850	2	6.86	866628	50.0
1-Butanol	7.37	869.7	ug/l	15074700	2	6.86	866628	50.0
Butanoic acid, et...	9.41	63.9	ug/l	1534520	3	10.12	1200290	50.0
Hexanal	9.59	60.5	ug/l	1452030	3	10.12	1200290	50.0
1-Hexanol	10.65	207.8	ug/l	4987260	3	10.12	1200290	50.0
1-Heptanol	11.71	90.8	ug/l	2363850	4	12.08	1301000	50.0
Hexanoic acid, et...	11.77	54.7	ug/l	1422450	4	12.08	1301000	50.0