

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX050818\
 Data File : VX001520.D
 Acq On : 08 May 2018 18:00
 Operator : JC/MD
 Sample : J2644-15
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SS037MW012-180426

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.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	1.075	76	80	93	rBV	1375355	1713190	56.52%	10.241%
2	1.788	193	197	202	rVB	25355	33226	1.10%	0.199%
3	2.392	289	296	303	rBV	62316	122664	4.05%	0.733%
4	2.630	329	335	343	rVB	21221	39985	1.32%	0.239%
5	2.843	361	370	380	rBV	161856	354939	11.71%	2.122%
6	4.306	594	610	626	rBV	91519	286606	9.45%	1.713%
7	4.556	639	651	667	rBV3	27130	100078	3.30%	0.598%
8	5.239	751	763	776	rBV3	17666	60356	1.99%	0.361%
9	5.513	793	808	823	rBV	190241	537560	17.73%	3.213%
10	5.672	823	834	859	rVV	219586	772881	25.50%	4.620%
11	6.074	889	900	919	rBV	212491	545951	18.01%	3.263%
12	6.348	925	945	972	rBV	1000272	3031349	100.00%	18.120%
13	6.867	1018	1030	1046	rBV	315521	745326	24.59%	4.455%
14	7.452	1118	1126	1137	rVB3	20143	48317	1.59%	0.289%
15	7.684	1152	1164	1174	rVB	24507	67324	2.22%	0.402%
16	8.061	1216	1226	1237	rBV	772580	1485268	49.00%	8.878%
17	8.183	1237	1246	1271	rVB	1192828	2345298	77.37%	14.019%
18	8.683	1319	1328	1329	rBV	68150	89839	2.96%	0.537%
19	8.720	1329	1334	1351	rVV	929967	1539823	50.80%	9.204%
20	9.317	1428	1432	1440	rVB2	15950	31856	1.05%	0.190%
21	10.116	1557	1563	1575	rBV	579634	835987	27.58%	4.997%
22	11.079	1712	1721	1726	rBV	29188	47250	1.56%	0.282%
23	11.146	1726	1732	1737	rBV	751005	996937	32.89%	5.959%
24	12.085	1880	1886	1897	rVB	743956	897047	29.59%	5.362%

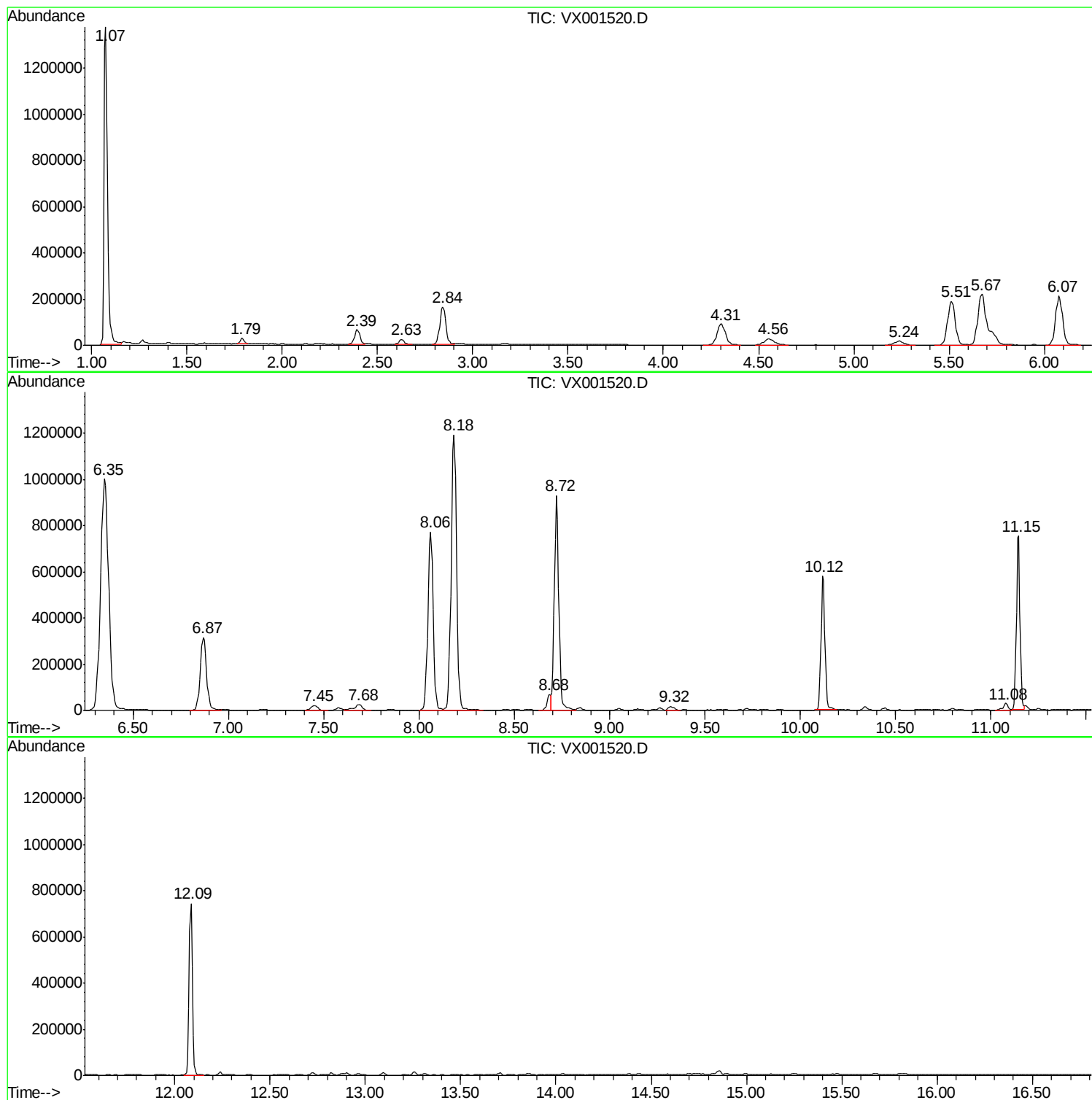
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Quant Title : SW846 8260

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



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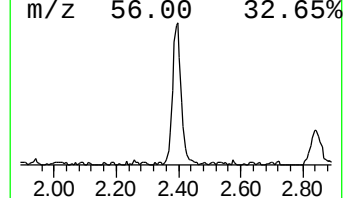
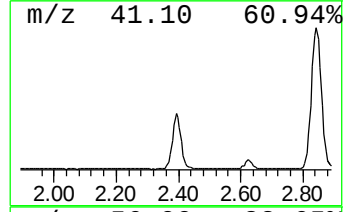
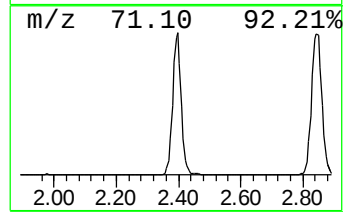
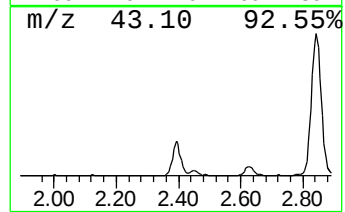
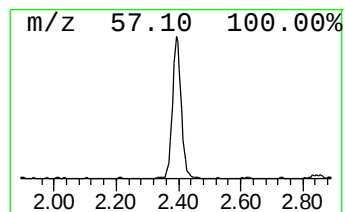
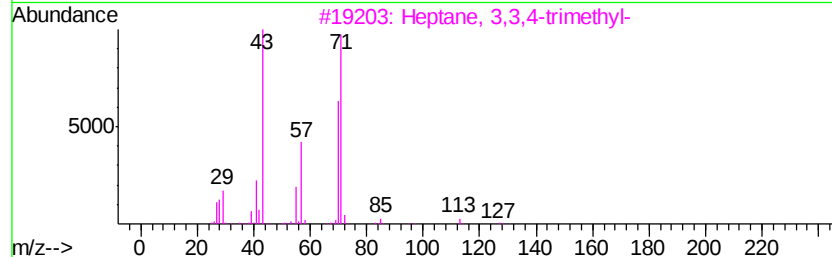
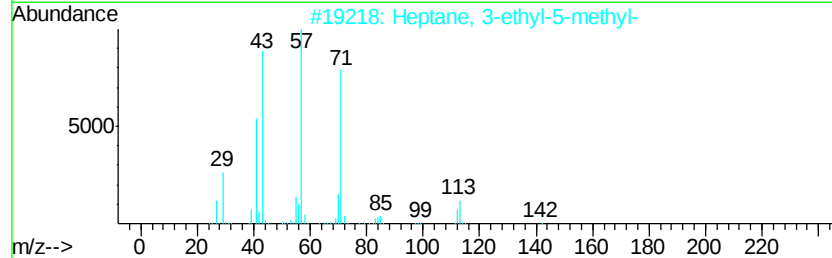
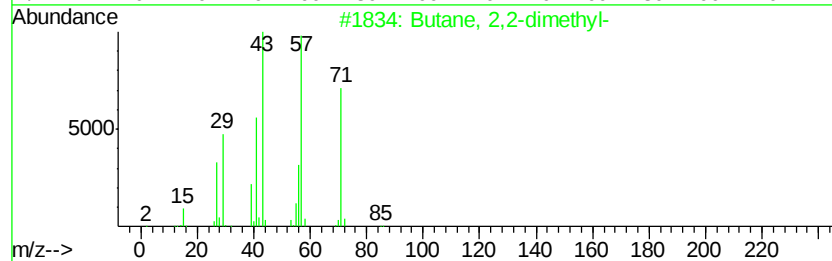
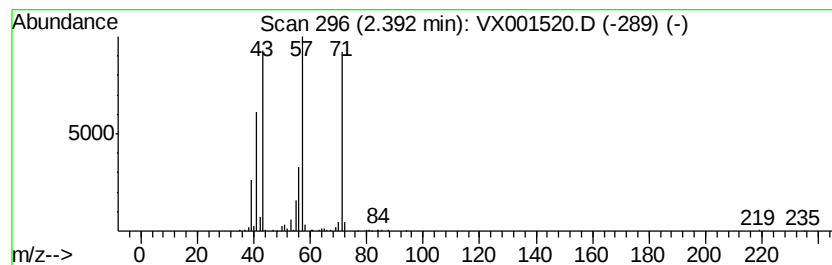
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.39	7.94 ug/l	122664	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	78
2		Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	56
3		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53
4		Butanoic acid, anhydride	158	C8H14O3	000106-31-0	47
5		Butyric acid, 2,2-dimethyl-, vin...	142	C8H14O2	013170-00-8	45



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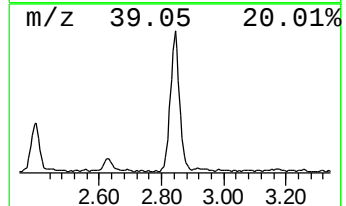
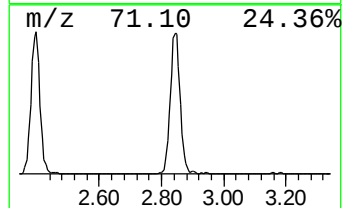
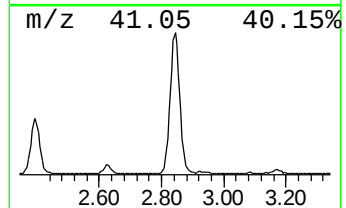
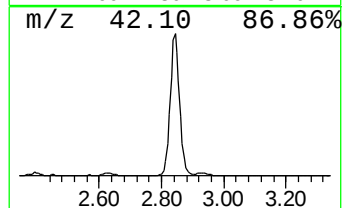
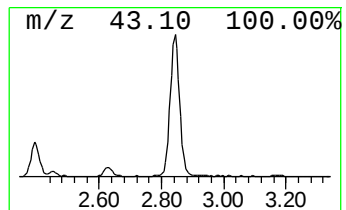
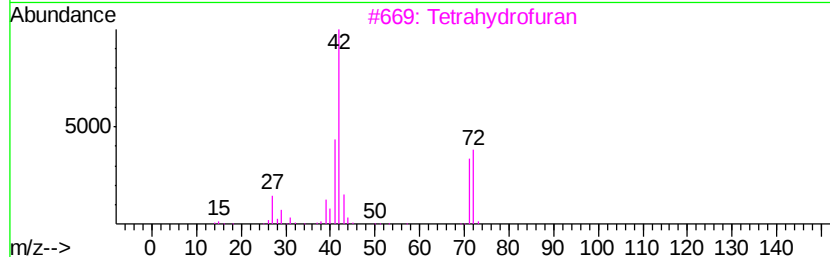
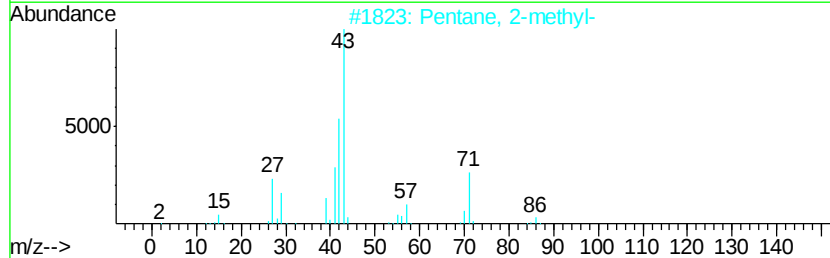
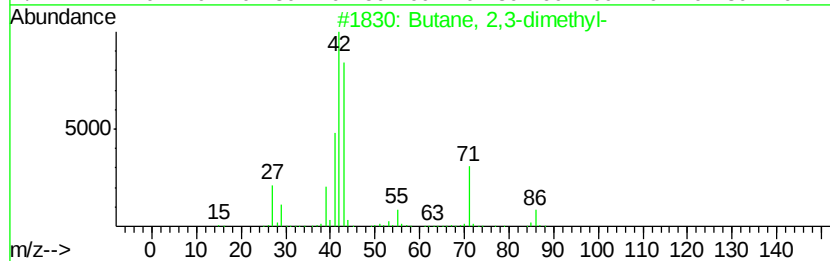
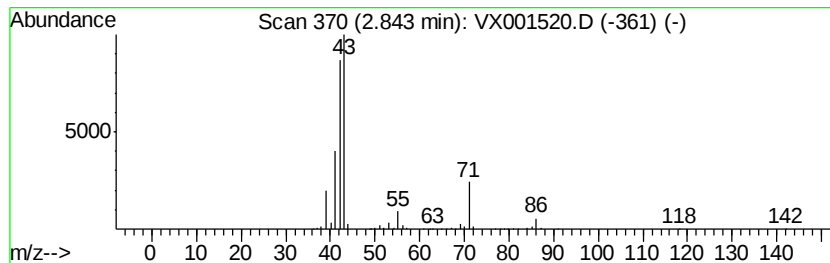
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Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	22.96 ug/l	354939	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	38
3		Tetrahydrofuran	72	C4H8O	000109-99-9	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	36
5		Cyclobutane, methyl-	70	C5H10	000598-61-8	33



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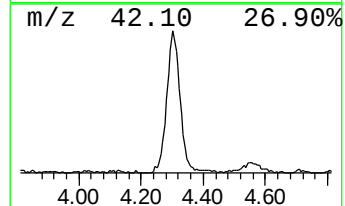
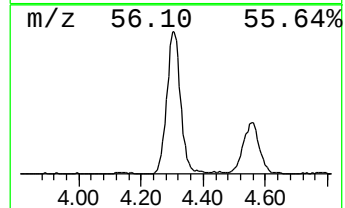
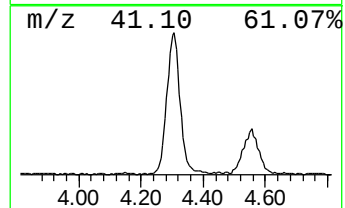
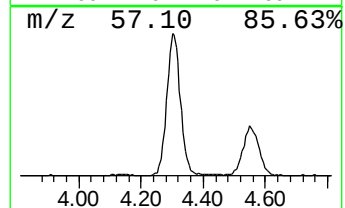
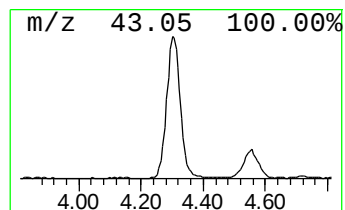
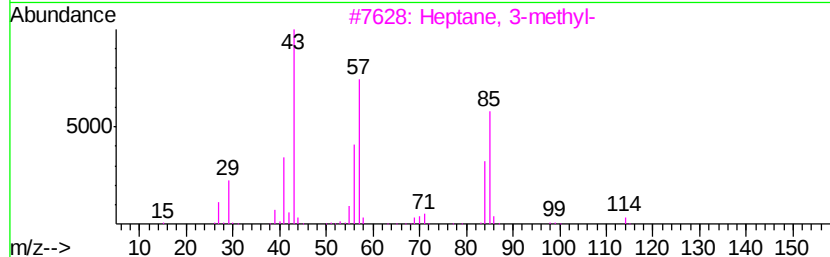
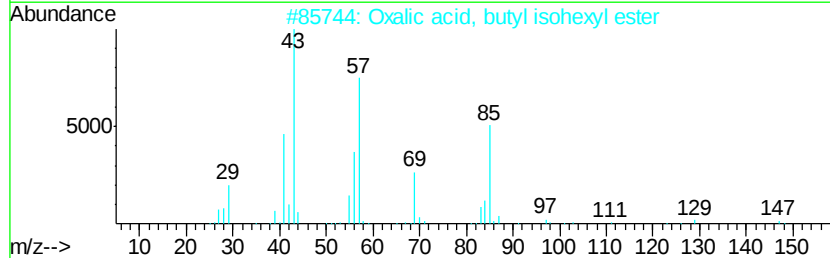
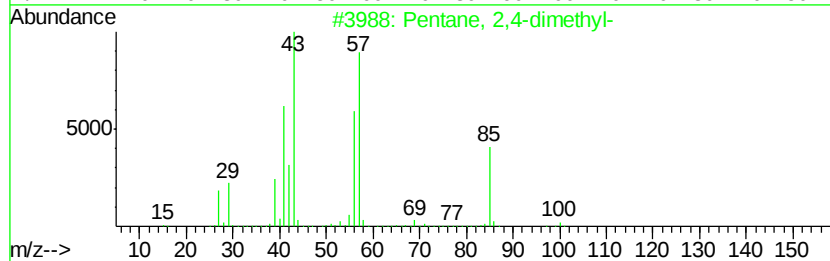
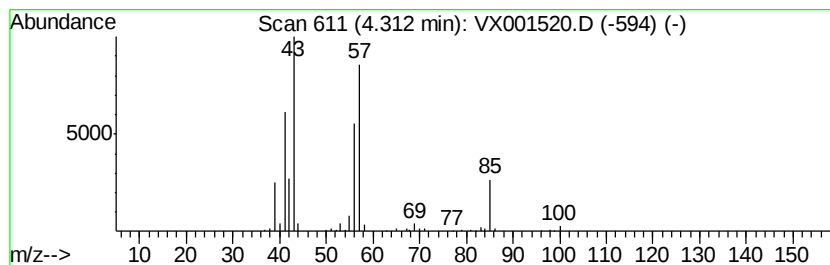
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Peak Number 4 Pentane, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.31	18.54 ug/l	286606	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	94
2		Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3		Heptane, 3-methyl-	114	C8H18	000589-81-1	56
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53



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ALS Vial : 14 Sample Multiplier: 1

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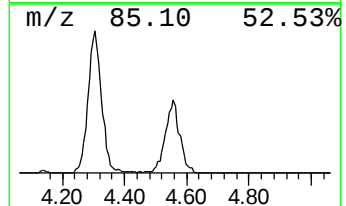
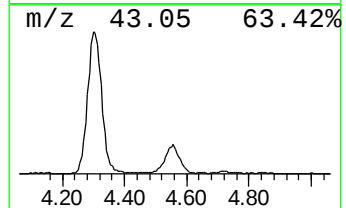
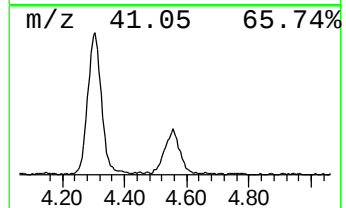
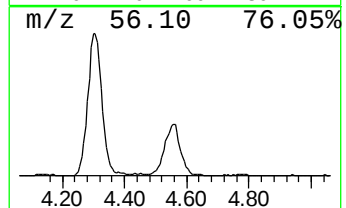
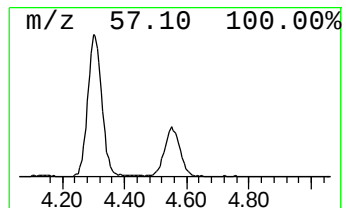
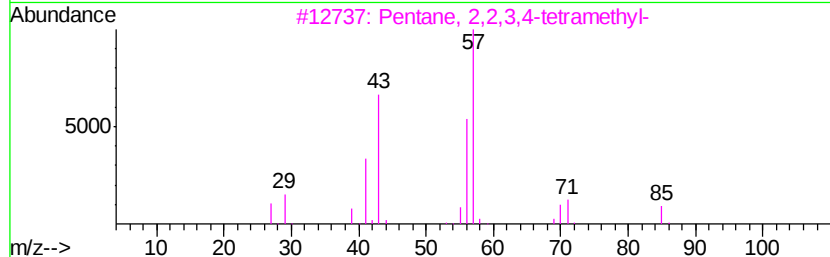
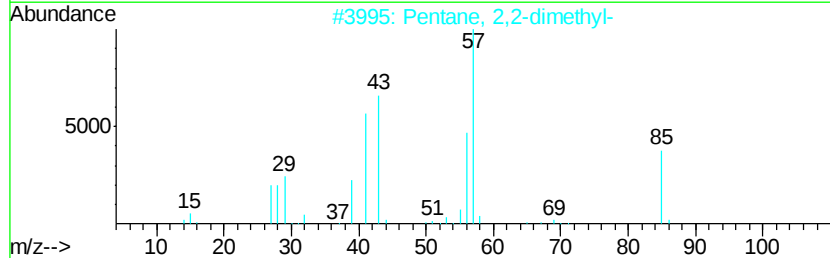
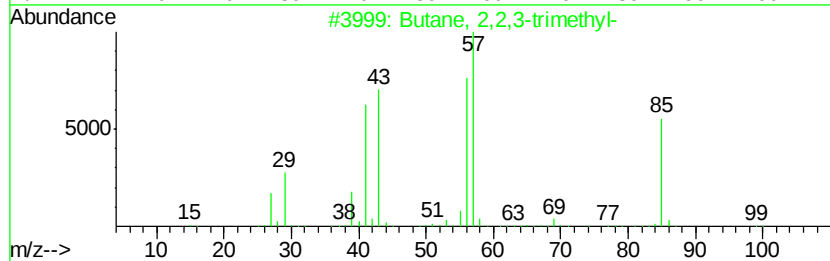
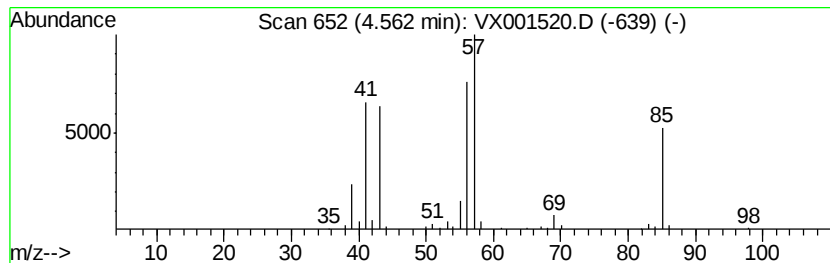
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butane, 2,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	6.47 ug/l	100078	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
2		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	72
3		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53
4		Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	50
5		Cyclobutanone, oxime	85	C4H7NO	002972-05-6	43



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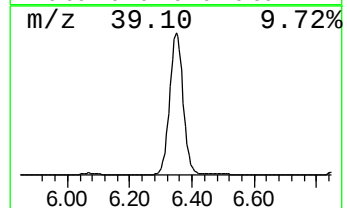
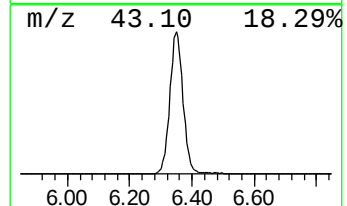
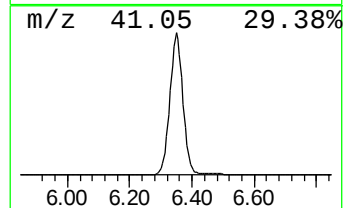
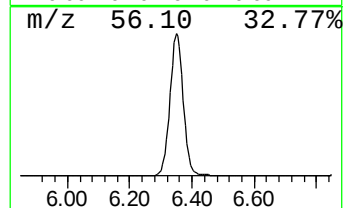
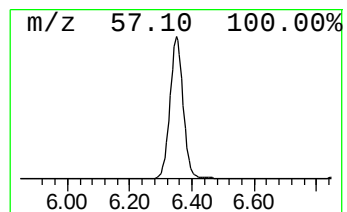
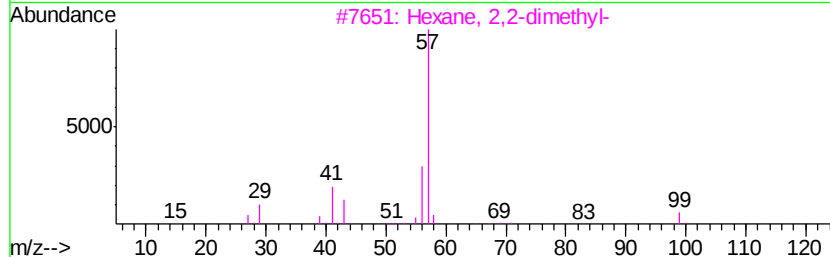
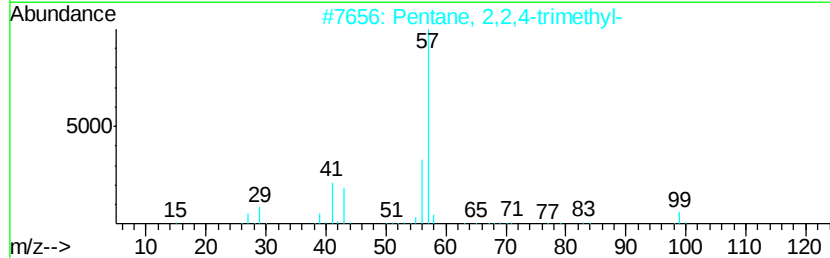
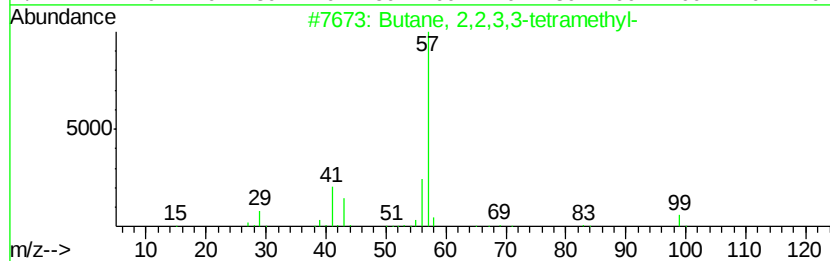
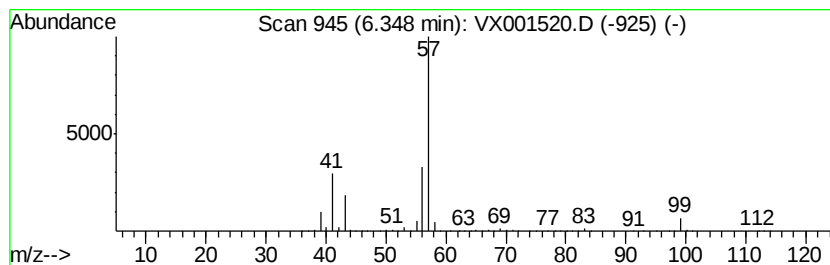
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	203.36 ug/l	3031350	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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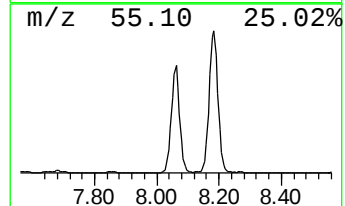
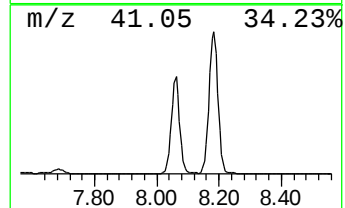
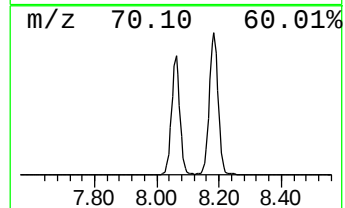
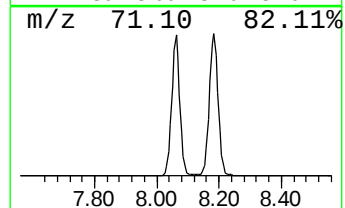
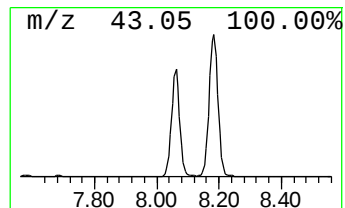
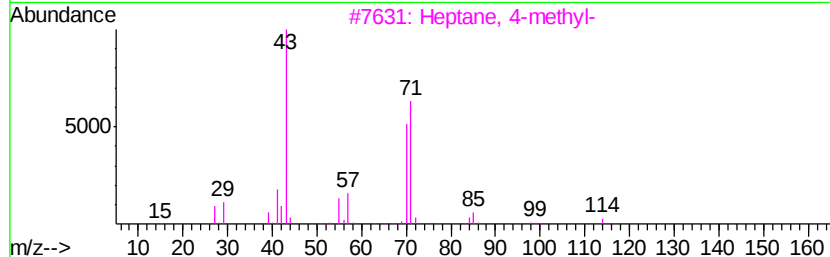
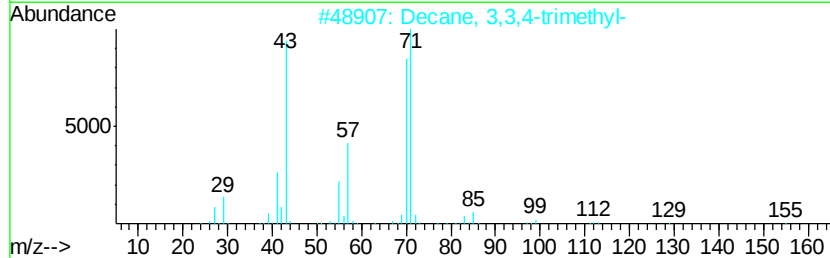
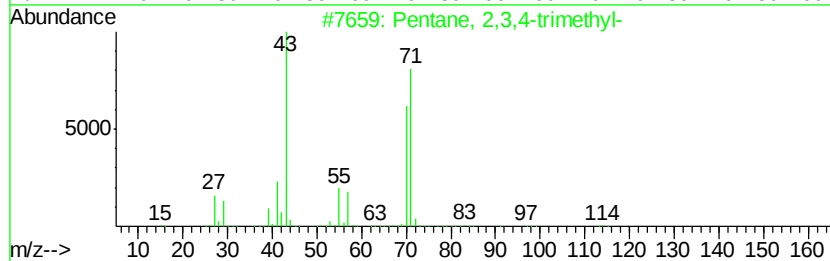
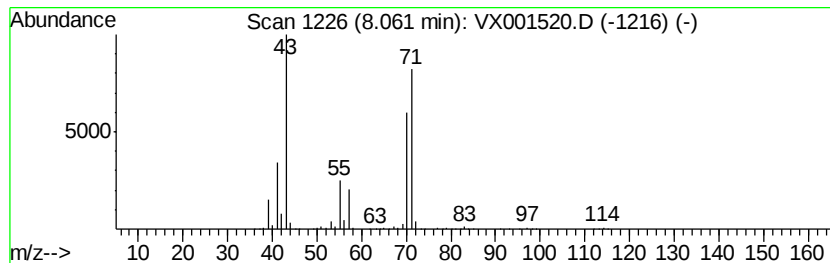
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	99.64 ug/l	1485270	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	83
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	78



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX050818\
Data File : VX001520.D
Acq On : 08 May 2018 18:00
Operator : JC/MD
Sample : J2644-15
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS037MW012-180426

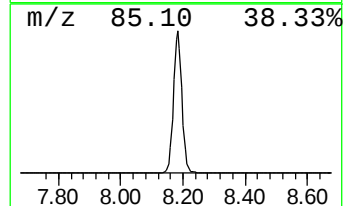
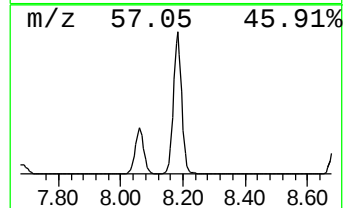
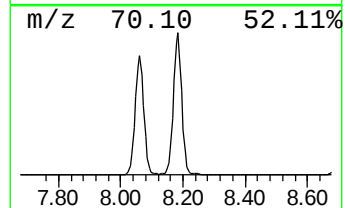
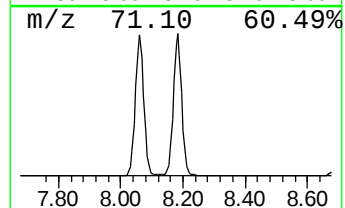
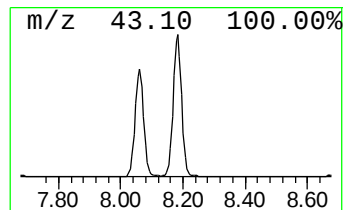
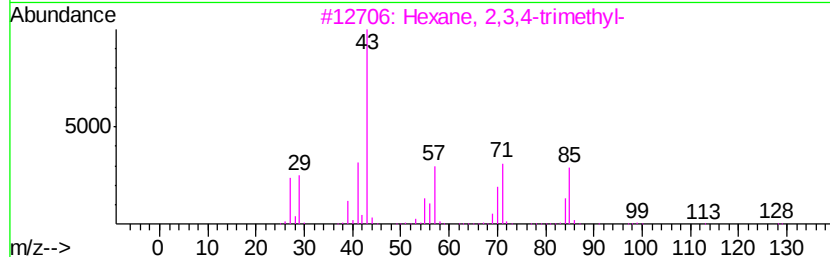
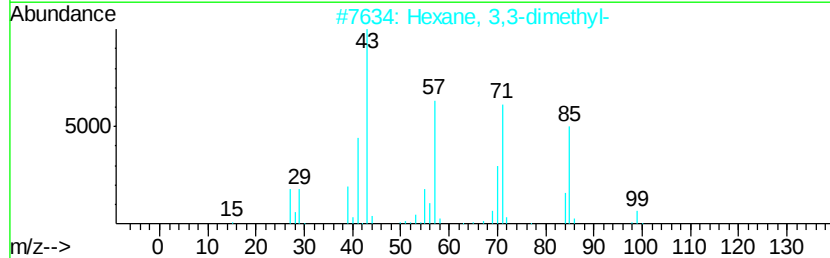
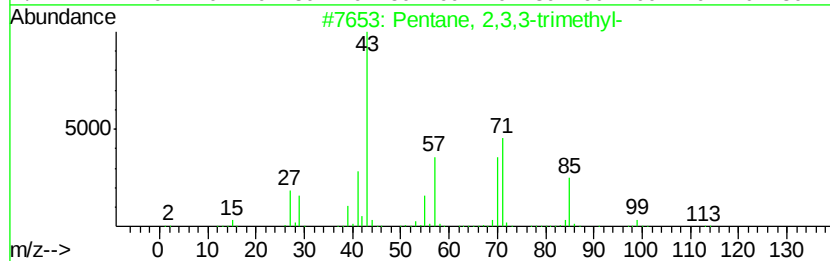
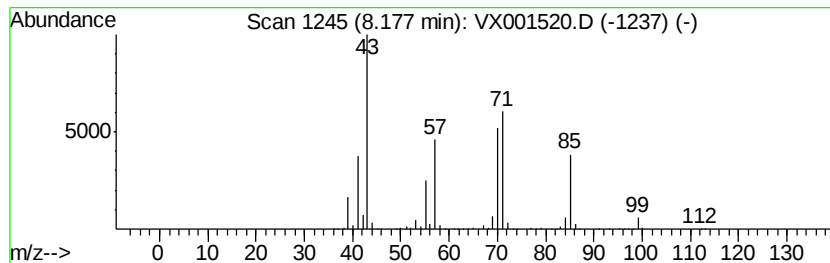
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.M
Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	157.33 ug/l	2345300	1,4-Difluorobenzene	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	72
3		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4		Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	50
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX050818\
Data File : VX001520.D
Acq On : 08 May 2018 18:00
Operator : JC/MD
Sample : J2644-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS037MW012-180426

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X050518W.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
Butane, 2,2-dimet...	2.39	7.9	ug/l	122664	1	5.67	772881	50.0
Butane, 2,3-dimet...	2.84	23.0	ug/l	354939	1	5.67	772881	50.0
Pentane, 2,4-dime...	4.31	18.5	ug/l	286606	1	5.67	772881	50.0
Butane, 2,2,3-tri...	4.56	6.5	ug/l	100078	1	5.67	772881	50.0
Butane, 2,2,3,3-t...	6.35	203.4	ug/l	3031350	2	6.87	745326	50.0
Pentane, 2,3,4-tr...	8.06	99.6	ug/l	1485270	2	6.87	745326	50.0
Pentane, 2,3,3-tr...	8.18	157.3	ug/l	2345300	2	6.87	745326	50.0