

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092818\
 Data File : VX004831.D
 Acq On : 28 Sep 2018 19:39
 Operator : JC/MD
 Sample : J5130-04
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FA18-JBW-7333-9001

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	1.404	37	41	46	rBV	879878	863947	3.04%	0.914%
2	1.788	98	104	126	rVB	19475978	28397156	100.00%	30.039%
3	2.001	134	139	152	rVB2	1595743	2576917	9.07%	2.726%
4	2.842	267	277	282	rBV	3189116	7304732	25.72%	7.727%
5	2.885	282	284	301	rVB	1389308	2665695	9.39%	2.820%
6	3.166	321	330	347	rVB	907287	2083792	7.34%	2.204%
7	3.519	378	388	402	rBV	369229	862675	3.04%	0.913%
8	4.306	504	517	524	rBV	634450	1936141	6.82%	2.048%
9	4.397	524	532	546	rVB	666622	1949762	6.87%	2.062%
10	5.500	700	713	718	rBV2	174332	510199	1.80%	0.540%
11	5.580	718	726	735	rVV2	631887	2197576	7.74%	2.325%
12	5.665	735	740	742	rVV	247305	539869	1.90%	0.571%
13	5.726	743	750	772	rVV	667676	2188009	7.71%	2.314%
14	5.933	772	784	797	rVV5	268061	951006	3.35%	1.006%
15	6.067	797	806	812	rVV	192489	509385	1.79%	0.539%
16	6.147	812	819	828	rVV	244464	648555	2.28%	0.686%
17	6.256	828	837	842	rVV	190131	554024	1.95%	0.586%
18	6.348	842	852	863	rVV	2659169	8137749	28.66%	8.608%
19	6.452	863	869	902	rVB	269750	844861	2.98%	0.894%
20	6.860	926	936	957	rBV	367801	923374	3.25%	0.977%
21	7.464	1022	1035	1045	rBV	921949	2202147	7.75%	2.329%
22	7.573	1046	1053	1058	rVV	257894	546685	1.93%	0.578%
23	7.634	1058	1063	1068	rVV	343030	770839	2.71%	0.815%
24	7.677	1068	1070	1075	rVV	184883	334004	1.18%	0.353%
25	7.732	1075	1079	1091	rVB	156074	310851	1.09%	0.329%
26	8.055	1121	1132	1144	rBV	1509216	3075109	10.83%	3.253%
27	8.177	1144	1152	1160	rVV	2005714	4029887	14.19%	4.263%
28	8.256	1160	1165	1176	rVB	292802	585873	2.06%	0.620%
29	8.677	1225	1234	1237	rBV2	410930	924194	3.25%	0.978%
30	8.713	1237	1240	1248	rVB	867020	1437840	5.06%	1.521%
31	9.043	1288	1294	1305	rVB	219924	364990	1.29%	0.386%
32	9.622	1385	1389	1394	rBV	210567	300708	1.06%	0.318%
33	10.116	1464	1470	1478	rBV	786621	1113907	3.92%	1.178%
34	10.256	1487	1493	1502	rVB	623089	896413	3.16%	0.948%

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Instrument :
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ClientSampleId :
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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 >
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35	10.359	1502	1510	1522	rBV	1406537	1991017	7.01%	2.106%
36	11.018	1613	1618	1632	rVB	288924	395446	1.39%	0.418%
37	11.140	1632	1638	1643	rBV	838522	1080269	3.80%	1.143%
38	11.359	1665	1674	1681	rBV	338213	427217	1.50%	0.452%
39	11.438	1681	1687	1688	rVV	400424	533566	1.88%	0.564%
40	11.457	1688	1690	1694	rVV	404149	437688	1.54%	0.463%
41	11.506	1694	1698	1706	rVB	484029	596179	2.10%	0.631%
42	11.670	1719	1725	1734	rBV	441684	569047	2.00%	0.602%
43	11.810	1743	1748	1758	rVB	1166031	1437917	5.06%	1.521%
44	12.079	1787	1792	1798	rVV2	1123620	1462987	5.15%	1.548%
45	12.146	1798	1803	1808	rVB	307358	392019	1.38%	0.415%
46	12.322	1830	1832	1836	rVV	244636	284221	1.00%	0.301%
47	12.371	1836	1840	1850	rVB3	293442	460310	1.62%	0.487%
48	12.761	1899	1904	1911	rBV4	158456	335290	1.18%	0.355%
49	14.694	2209	2221	2226	rBV	199630	304126	1.07%	0.322%
50	14.840	2240	2245	2259	rVB	203768	289666	1.02%	0.306%

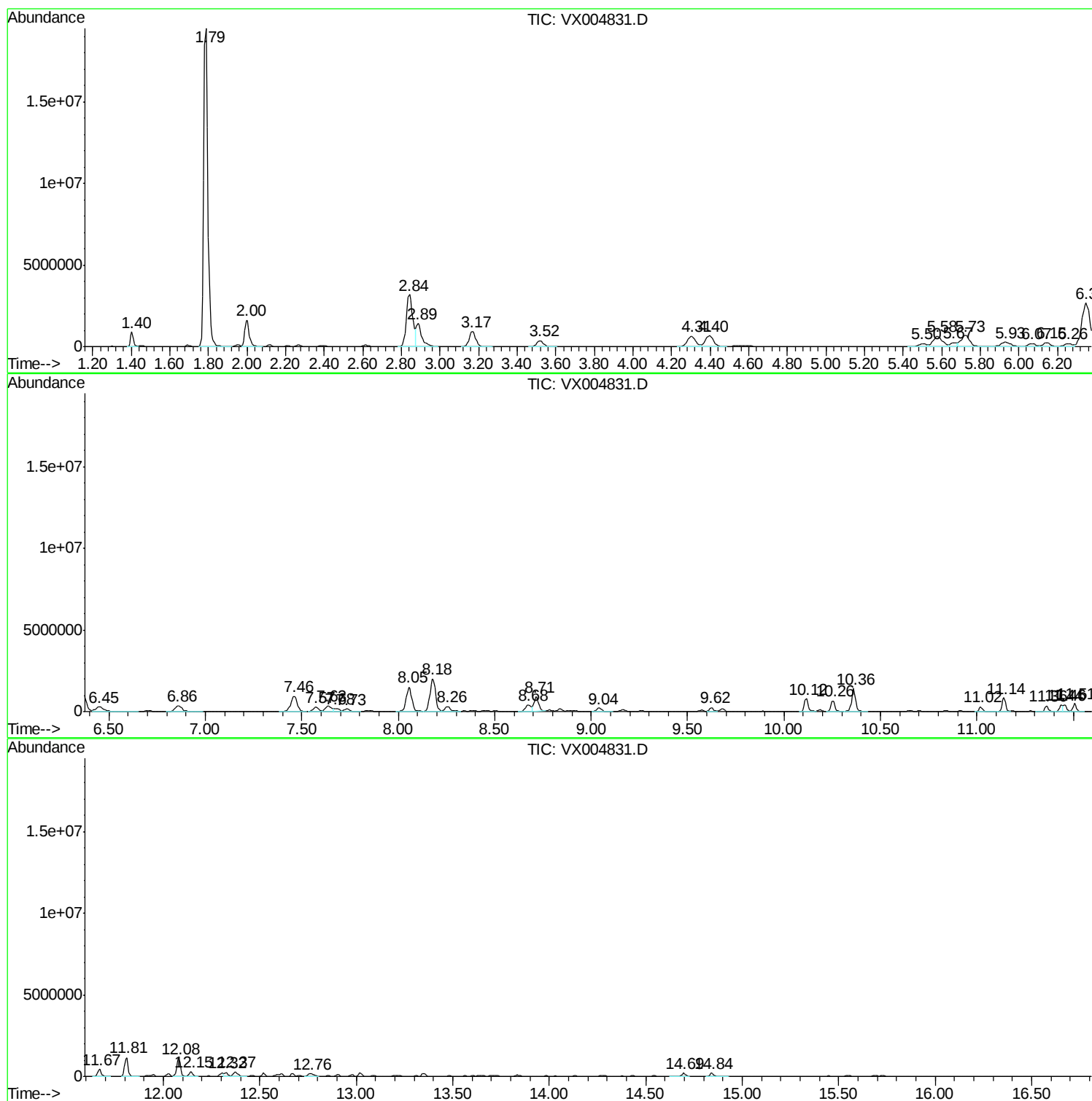
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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



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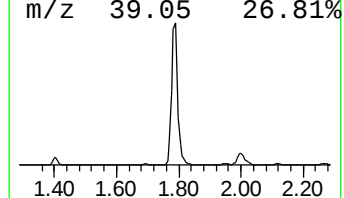
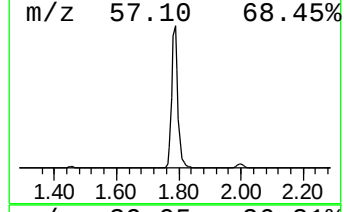
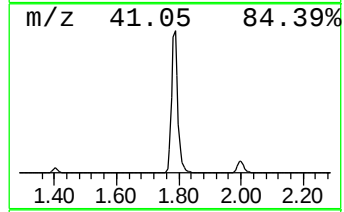
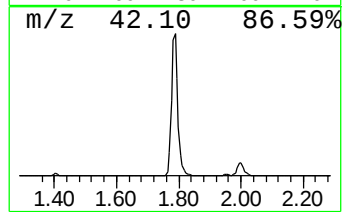
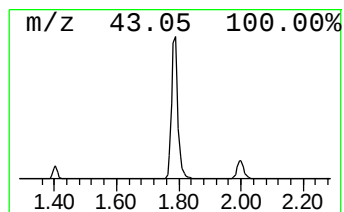
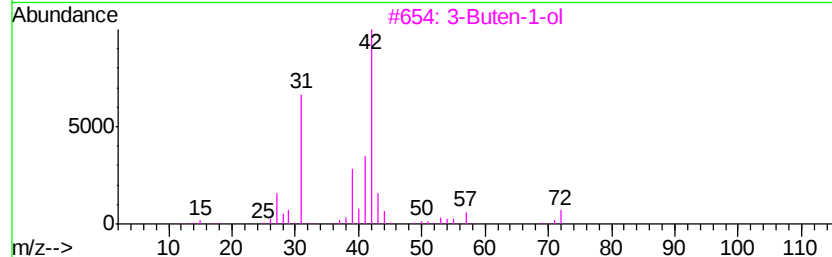
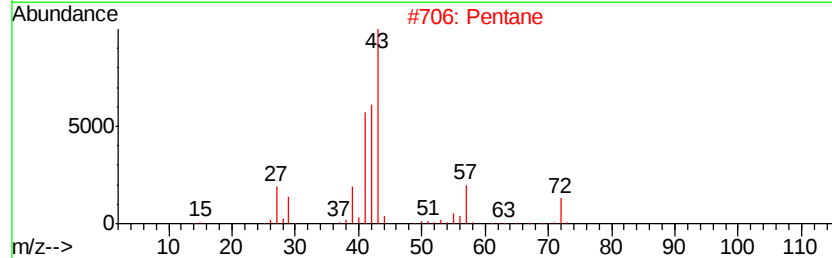
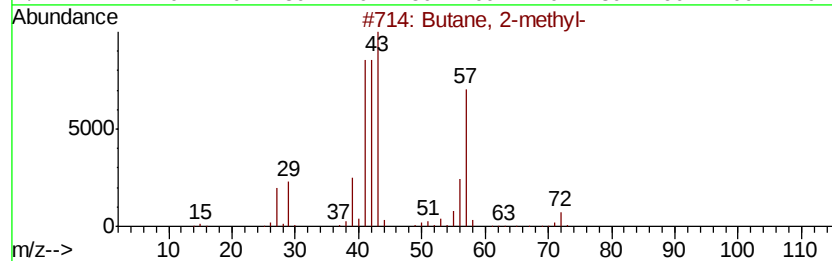
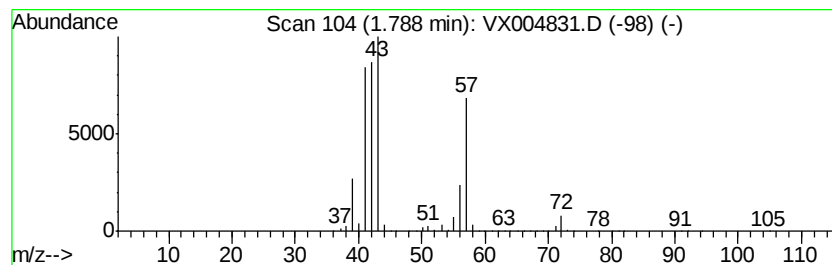
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	2630.00 ug/l	28397200	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		Pentane	72	C5H12	000109-66-0	33
3		3-Buten-1-ol	72	C4H8O	000627-27-0	28
4		1-Butene	56	C4H8	000106-98-9	10
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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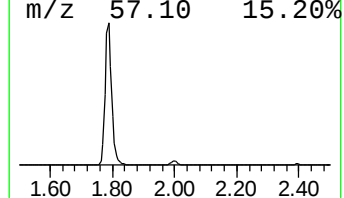
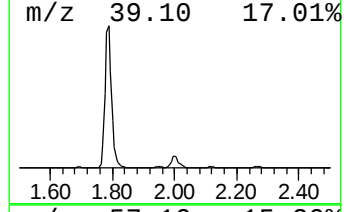
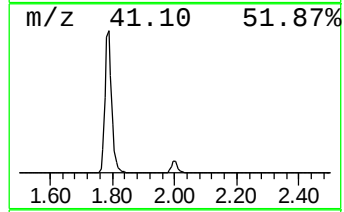
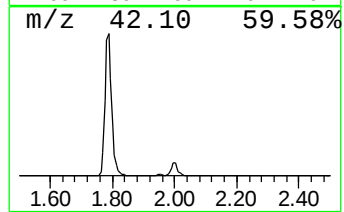
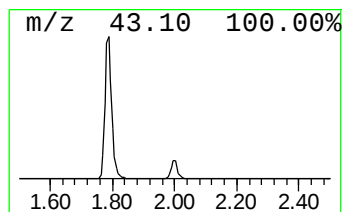
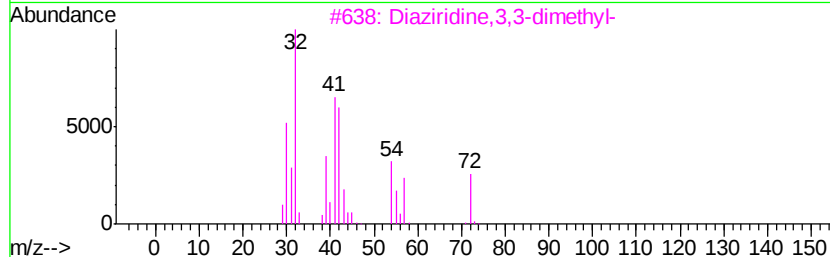
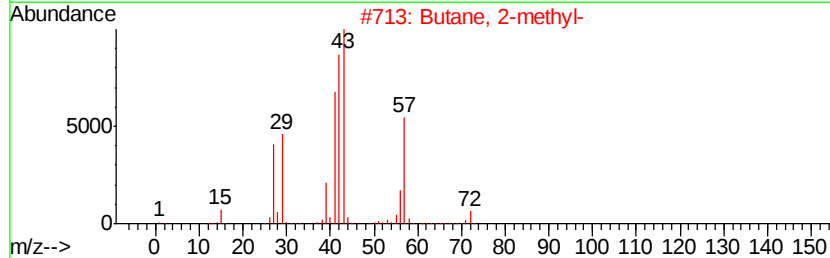
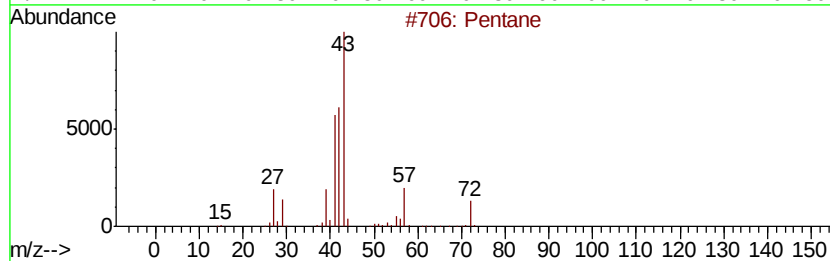
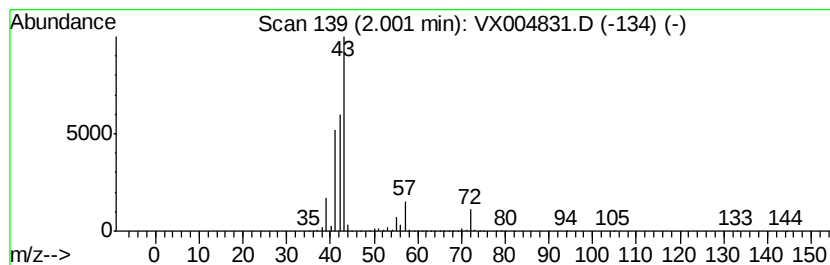
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	238.66 ug/l	2576920	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	45
3		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4		Oxirane, ethyl-	72	C4H8O	000106-88-7	9
5		1-Pentanol	88	C5H12O	000071-41-0	9



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ALS Vial : 21 Sample Multiplier: 1

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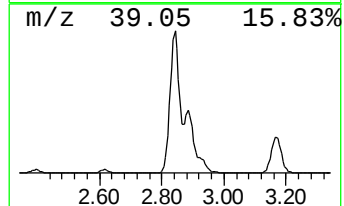
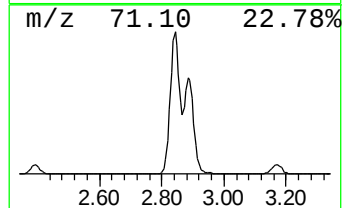
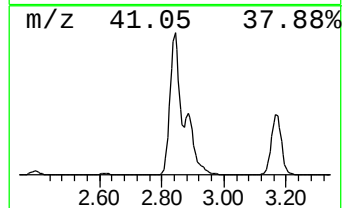
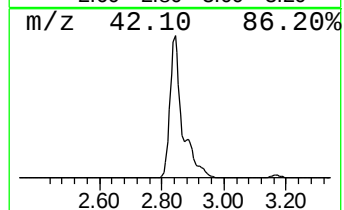
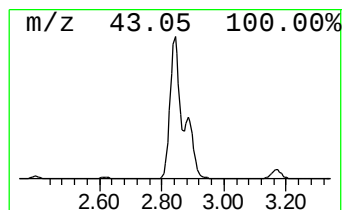
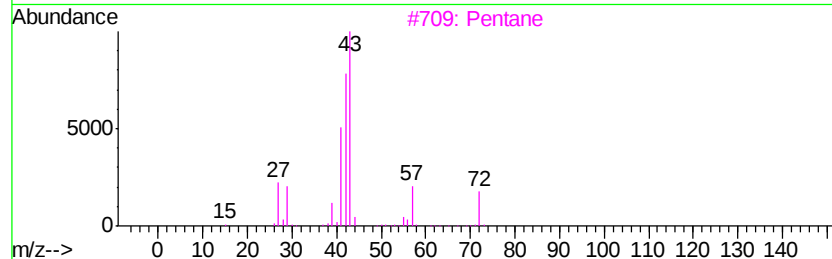
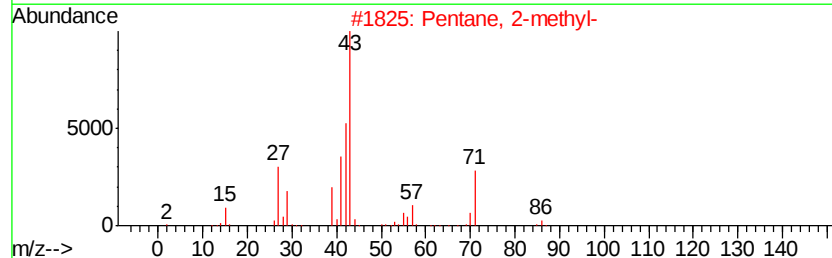
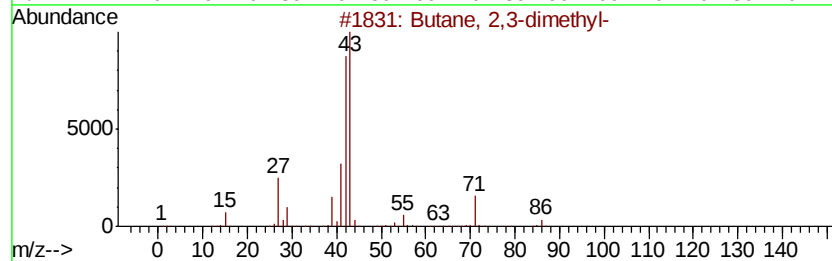
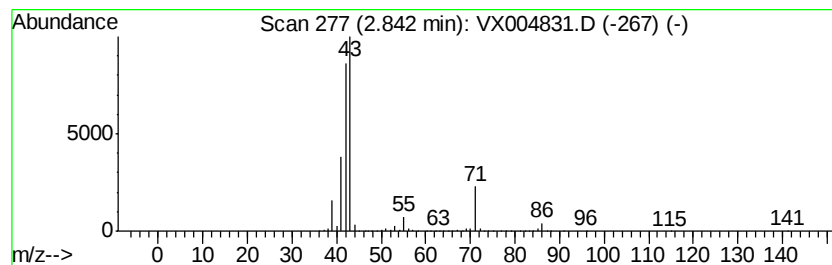
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	676.53 ug/l	7304730	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3			Pentane	72	C5H12	000109-66-0	36
4			Pyrrolidine	71	C4H9N	000123-75-1	10
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9



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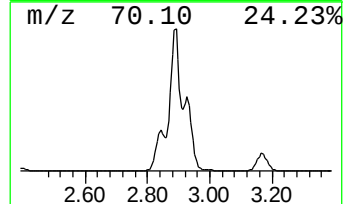
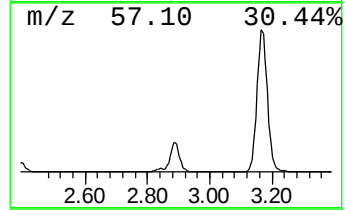
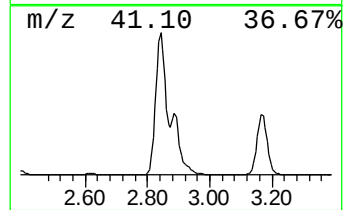
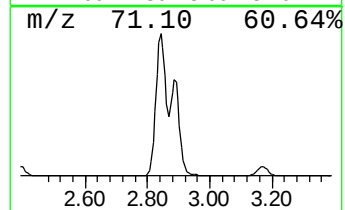
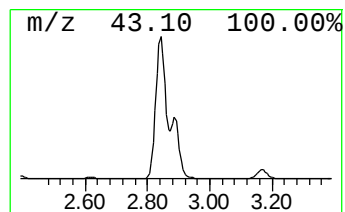
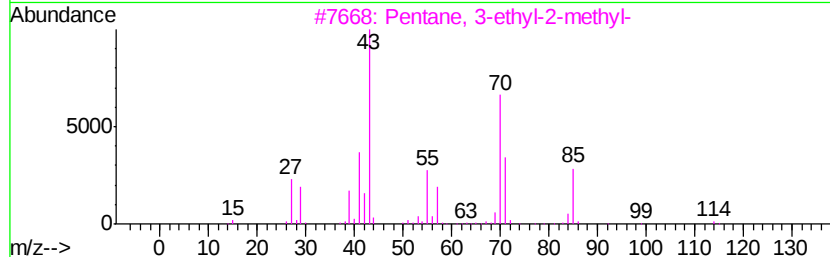
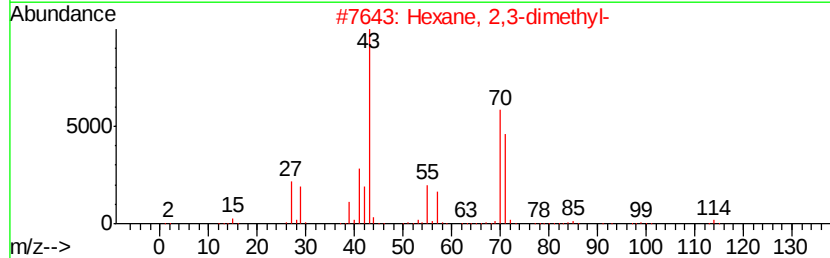
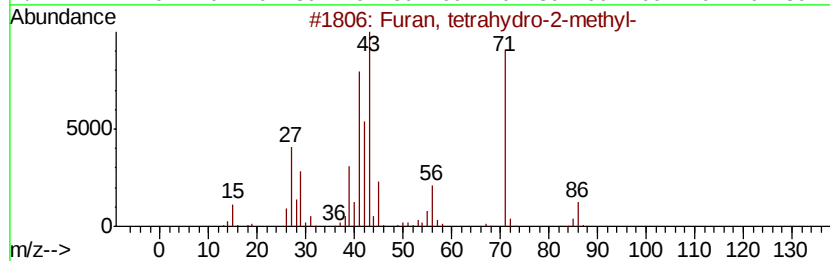
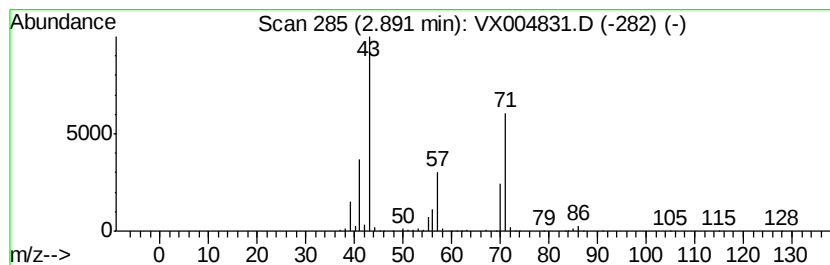
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown2.89 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	246.88 ug/l	2665700	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	38
2		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
3		Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	33
4		Octane, 4-methyl-	128	C9H20	002216-34-4	28
5		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	25



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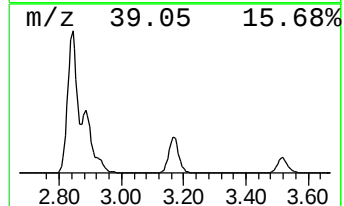
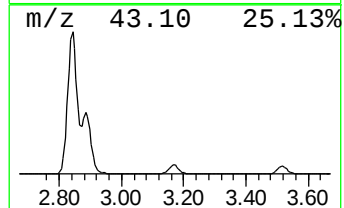
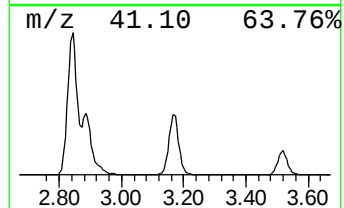
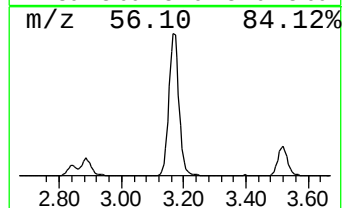
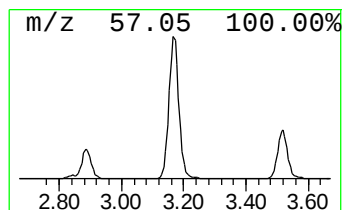
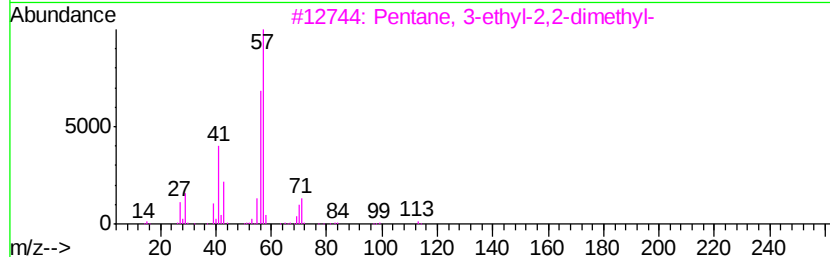
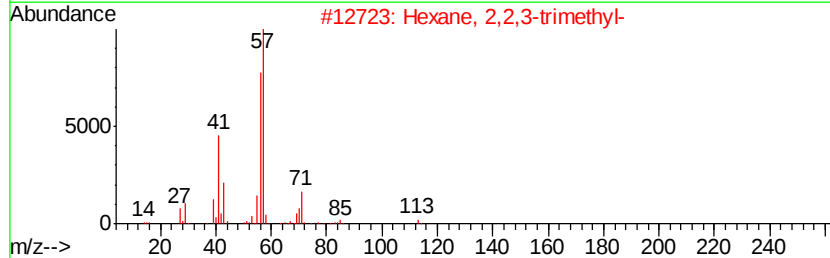
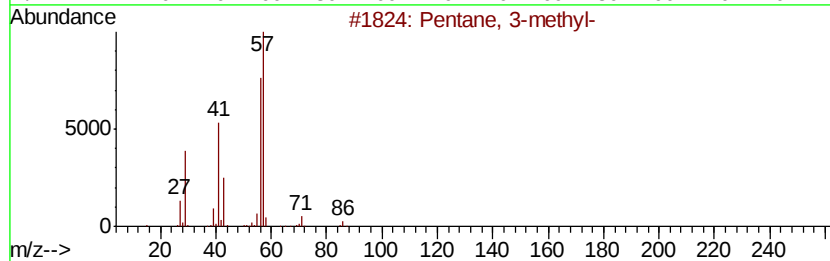
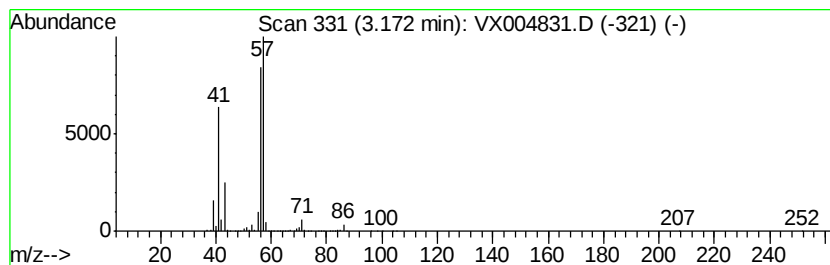
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	192.99 ug/l	2083790	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50
5		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004831.D
Acq On : 28 Sep 2018 19:39
Operator : JC/MD
Sample : J5130-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JBW-7333-9001

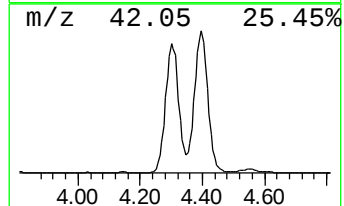
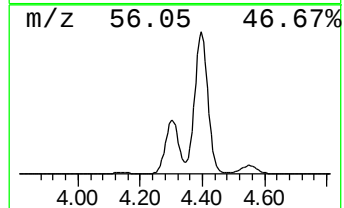
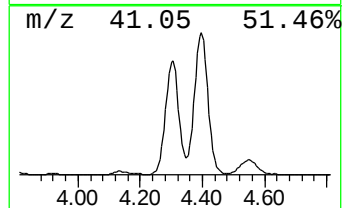
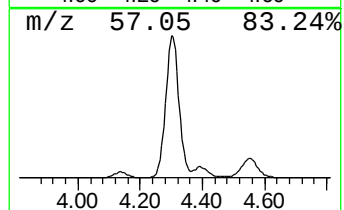
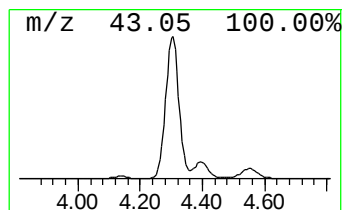
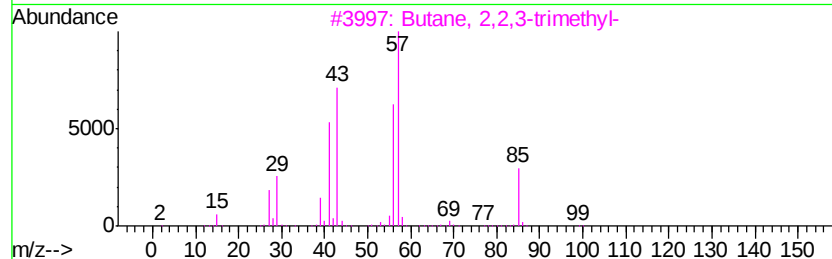
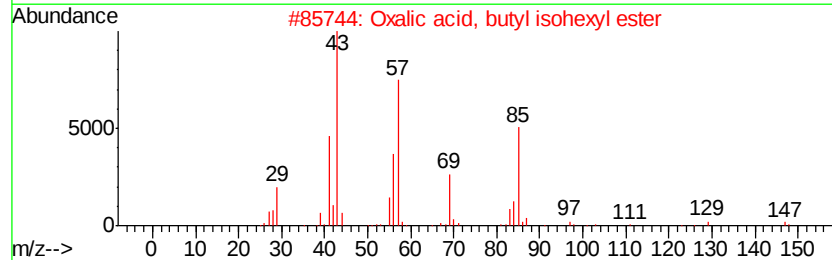
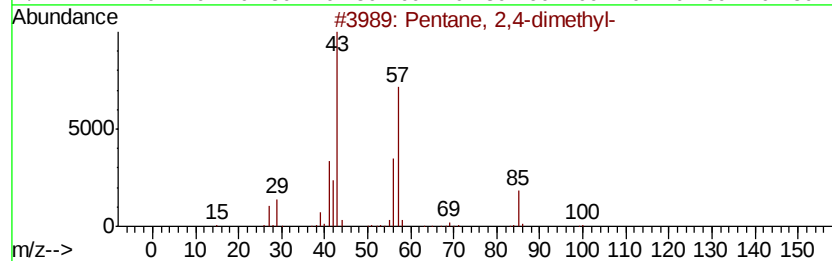
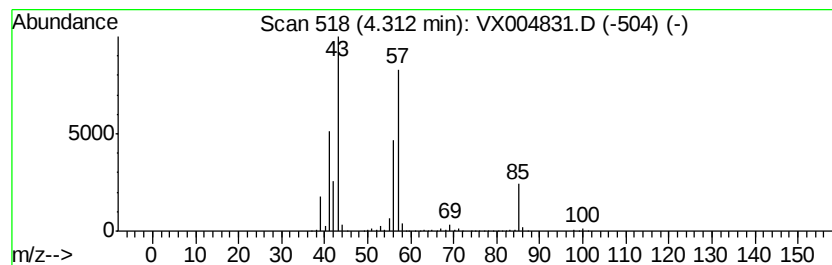
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.31	179.32 ug/l	1936140	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2		Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	72
3		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
4		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
5		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004831.D
Acq On : 28 Sep 2018 19:39
Operator : JC/MD
Sample : J5130-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JBW-7333-9001

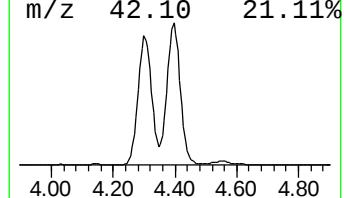
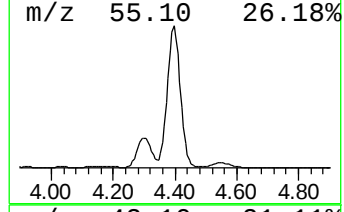
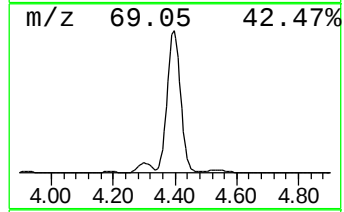
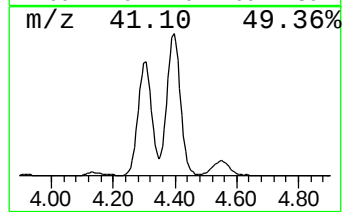
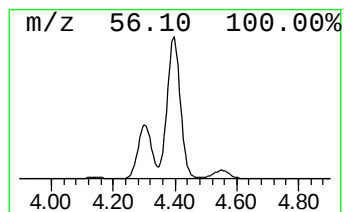
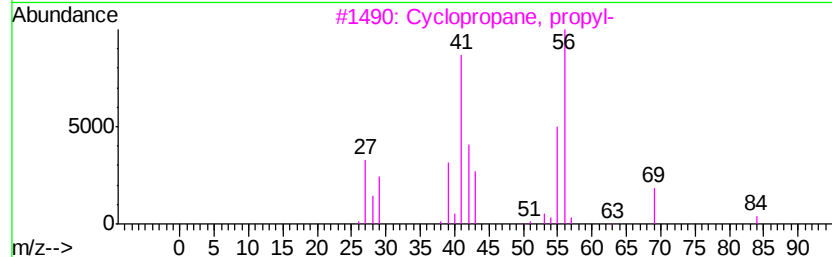
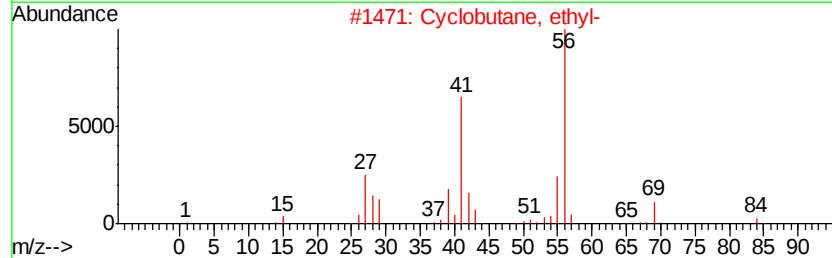
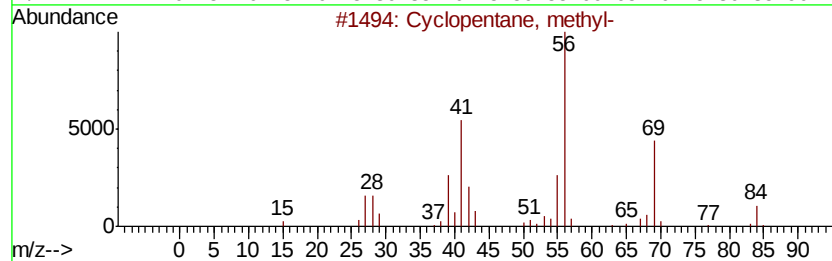
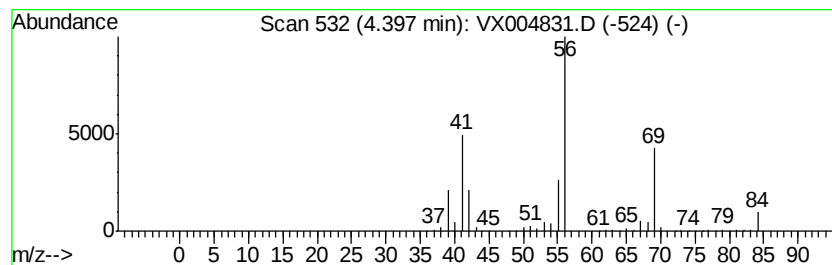
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	180.58 ug/l	1949760	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3		Cyclopropane, propyl-	84	C6H12	002415-72-7	72
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004831.D
Acq On : 28 Sep 2018 19:39
Operator : JC/MD
Sample : J5130-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JBW-7333-9001

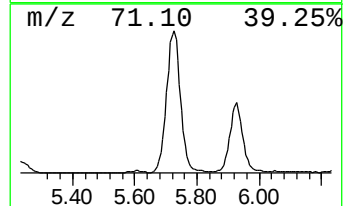
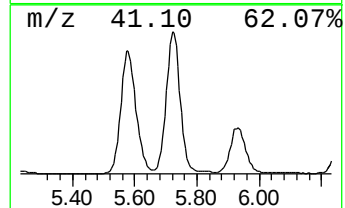
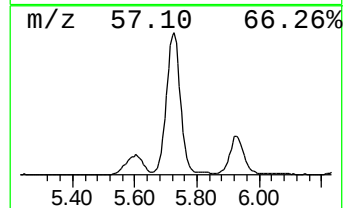
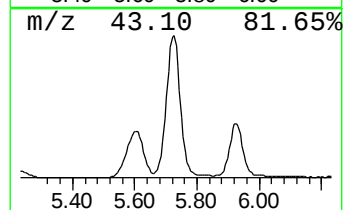
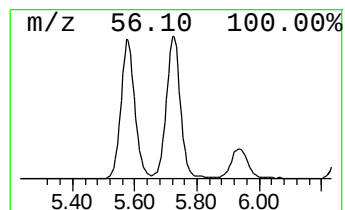
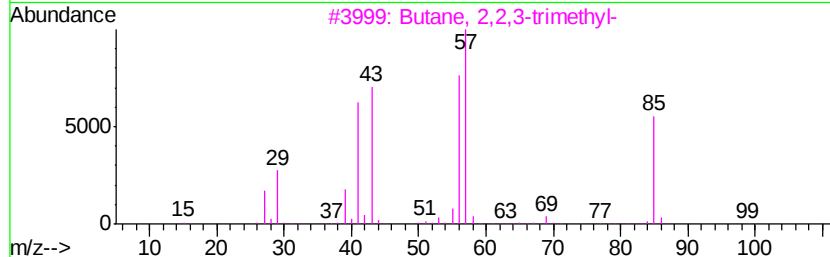
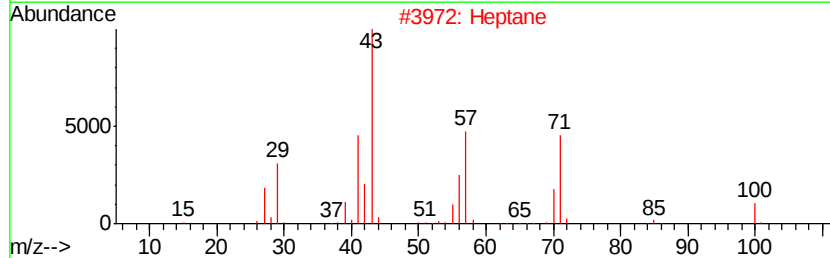
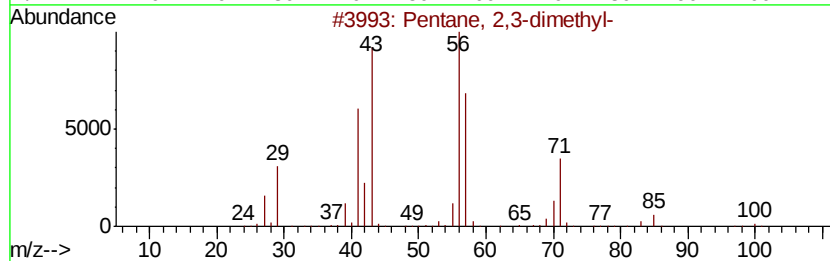
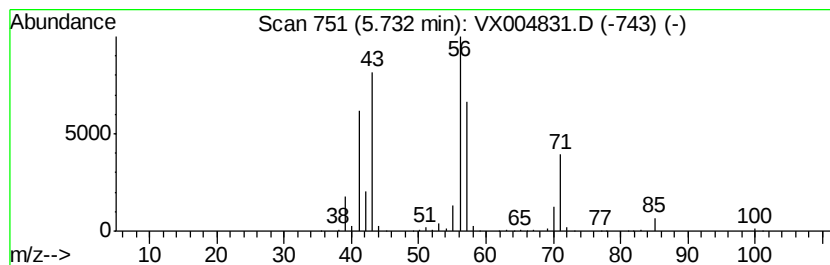
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	202.64 ug/l	2188010	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Heptane	100	C7H16	000142-82-5	37
3		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	37
4		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	37
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	36



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004831.D
Acq On : 28 Sep 2018 19:39
Operator : JC/MD
Sample : J5130-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

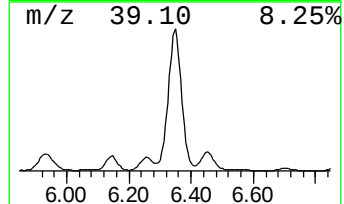
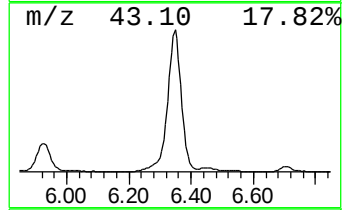
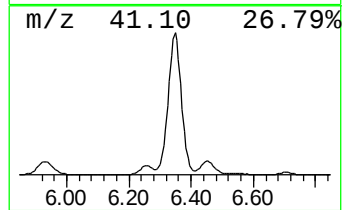
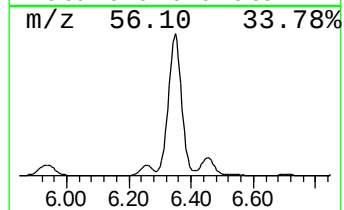
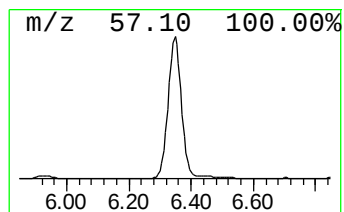
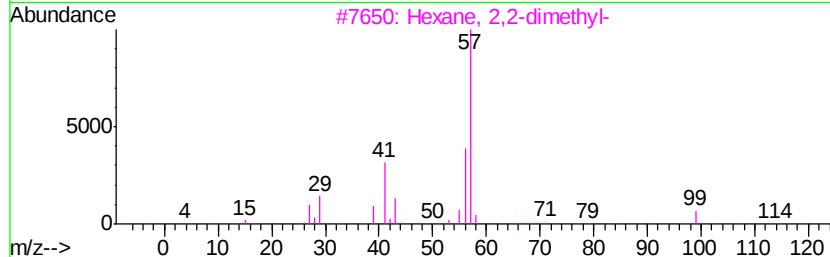
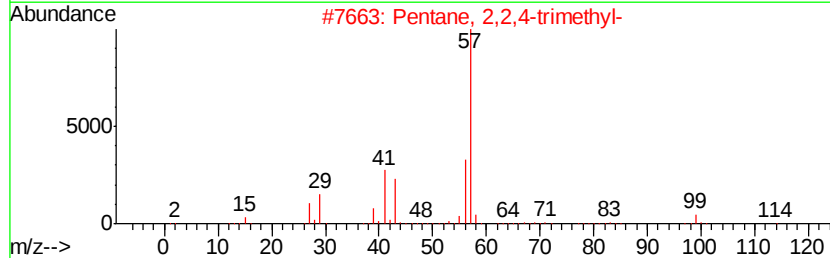
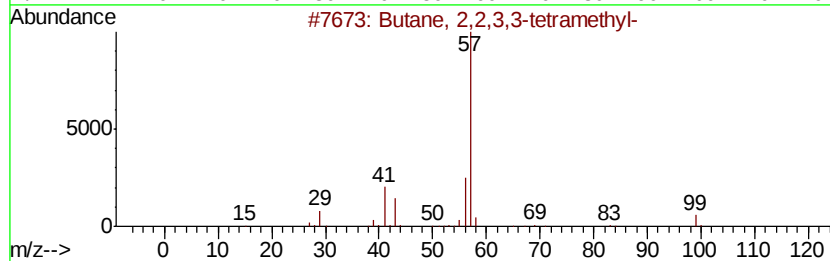
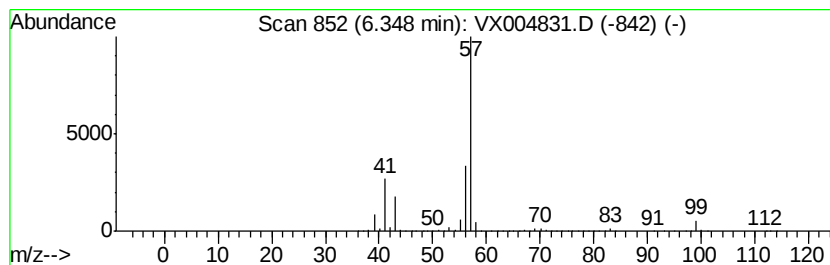
Instrument :
MSVOA_X
ClientSampleId :
FA18-JBW-7333-9001

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 Butane, 2,2,3,3-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.35	440.65 ug/l	8137750	1,4-Difluorobenzene	6.86	
Hit# of	5	Tentative ID	MW MolForm	CAS#	Qual
1		Butane, 2,2,3,3-tetramethyl-	114 C8H18	000594-82-1	72
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	59
5		Pentane, 2,2,4,4-tetramethyl-	128 C9H20	001070-87-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004831.D
Acq On : 28 Sep 2018 19:39
Operator : JC/MD
Sample : J5130-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JBW-7333-9001

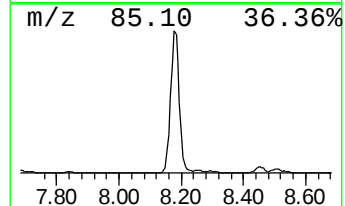
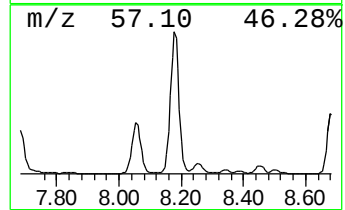
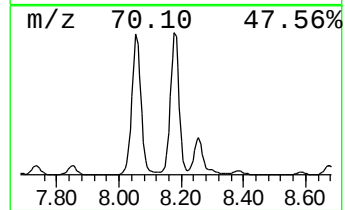
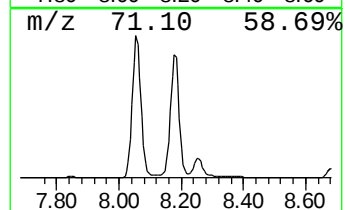
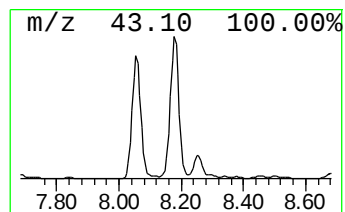
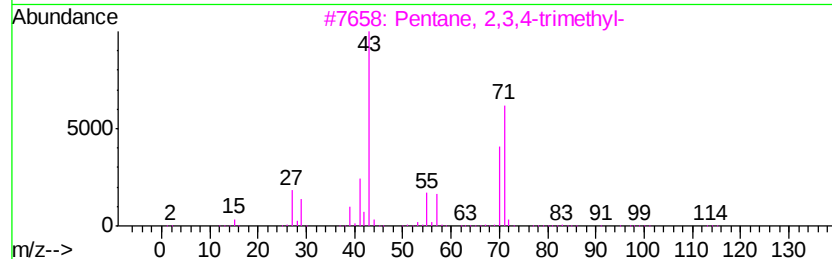
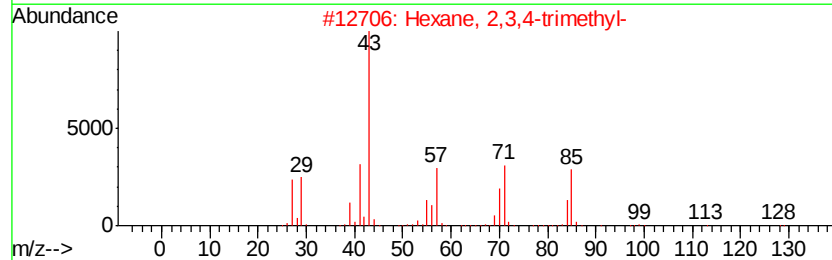
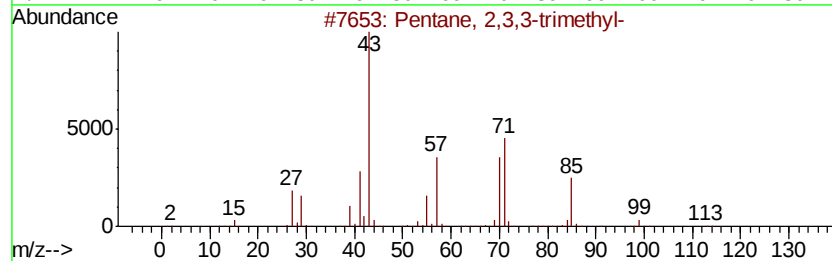
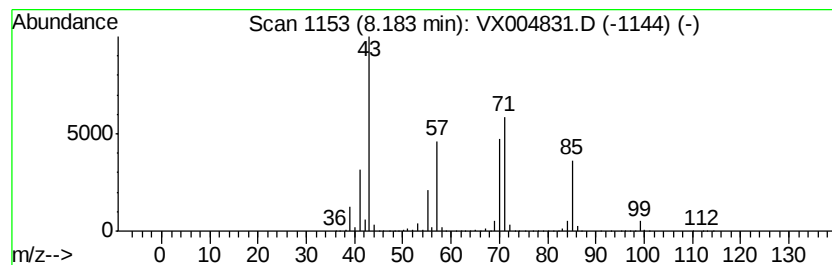
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 10 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	218.22 ug/l	4029890	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004831.D
Acq On : 28 Sep 2018 19:39
Operator : JC/MD
Sample : J5130-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JBW-7333-9001

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
Butane, 2-methyl-	1.79	2630.0	ug/l	28397200	1	5.67	539869	50.0
Pentane	2.00	238.7	ug/l	2576920	1	5.67	539869	50.0
Butane, 2,3-dimet...	2.84	676.5	ug/l	7304730	1	5.67	539869	50.0
unknown2.89	2.89	246.9	ug/l	2665700	1	5.67	539869	50.0
Pentane, 3-methyl-	3.17	193.0	ug/l	2083790	1	5.67	539869	50.0
Pentane, 2,4-dime...	4.31	179.3	ug/l	1936140	1	5.67	539869	50.0
Cyclopentane, met...	4.40	180.6	ug/l	1949760	1	5.67	539869	50.0
Pentane, 2,3-dime...	5.73	202.6	ug/l	2188010	1	5.67	539869	50.0
Butane, 2,2,3,3-t...	6.35	440.6	ug/l	8137750	2	6.86	923374	50.0
Pentane, 2,3,3-tr...	8.18	218.2	ug/l	4029890	2	6.86	923374	50.0