

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092818\
 Data File : VX004829.D
 Acq On : 28 Sep 2018 18:45
 Operator : JC/MD
 Sample : J5130-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FA18-JMW-3284

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	162855	161366	3.76%	0.632%
2	1.788	98	104	125	rVB	3050180	4294137	100.00%	16.815%
3	2.001	134	139	150	rVB2	163707	266577	6.21%	1.044%
4	2.617	233	240	251	rVB	79331	142331	3.31%	0.557%
5	2.843	267	277	282	rBV	701088	1558032	36.28%	6.101%
6	3.166	321	330	343	rBV	164291	374505	8.72%	1.466%
7	4.306	505	517	525	rBV	183110	571702	13.31%	2.239%
8	4.397	525	532	544	rVV	74440	227807	5.31%	0.892%
9	4.550	546	557	575	rVB6	25354	120091	2.80%	0.470%
10	5.507	701	714	720	rBV	175954	512004	11.92%	2.005%
11	5.574	721	725	732	rVV2	57366	161422	3.76%	0.632%
12	5.665	732	740	745	rVV	214298	646350	15.05%	2.531%
13	5.720	746	749	763	rVB	194518	510441	11.89%	1.999%
14	5.934	774	784	796	rVB4	31293	114337	2.66%	0.448%
15	6.068	796	806	813	rBV	191401	489951	11.41%	1.919%
16	6.141	813	818	828	rVB	60725	156987	3.66%	0.615%
17	6.263	828	838	841	rBV	32992	89622	2.09%	0.351%
18	6.348	841	852	864	rVV	1321529	4066855	94.71%	15.925%
19	6.452	865	869	891	rVB3	48155	151785	3.53%	0.594%
20	6.860	926	936	956	rBV	356970	903740	21.05%	3.539%
21	7.458	1022	1034	1044	rBV4	61483	167204	3.89%	0.655%
22	7.573	1046	1053	1058	rVV	96341	203632	4.74%	0.797%
23	7.641	1058	1064	1068	rVV	127768	304409	7.09%	1.192%
24	7.677	1068	1070	1076	rVV	88084	159910	3.72%	0.626%
25	7.732	1076	1079	1090	rVV2	19707	44898	1.05%	0.176%
26	8.055	1118	1132	1144	rBV	713835	1461999	34.05%	5.725%
27	8.177	1144	1152	1160	rVV	926383	1855526	43.21%	7.266%
28	8.250	1160	1164	1170	rVB	37676	67153	1.56%	0.263%
29	8.451	1192	1197	1203	rVB	28235	51524	1.20%	0.202%
30	8.677	1226	1234	1236	rBV3	175783	304722	7.10%	1.193%
31	8.713	1236	1240	1256	rVV	854244	1536069	35.77%	6.015%
32	8.842	1256	1261	1266	rVB	33374	58205	1.36%	0.228%
33	9.043	1288	1294	1303	rVB	58822	98439	2.29%	0.385%
34	9.165	1306	1314	1320	rBV3	25260	50859	1.18%	0.199%

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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 >
Peak separation: 5

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Title : SW846 8260

35	9.677	1393	1398	1403	rVV	34691	51506	1.20%	0.202%
36	10.116	1464	1470	1479	rBV	785934	1113558	25.93%	4.360%
37	10.250	1487	1492	1502	rVB	30816	51506	1.20%	0.202%
38	10.360	1502	1510	1516	rVB5	17760	47420	1.10%	0.186%
39	11.140	1632	1638	1644	rBV	814618	1035245	24.11%	4.054%
40	12.079	1786	1792	1799	rBV	1054362	1260558	29.36%	4.936%
41	12.304	1821	1829	1835	rBV3	27908	49100	1.14%	0.192%
42	12.755	1899	1903	1911	rVB3	23681	44593	1.04%	0.175%

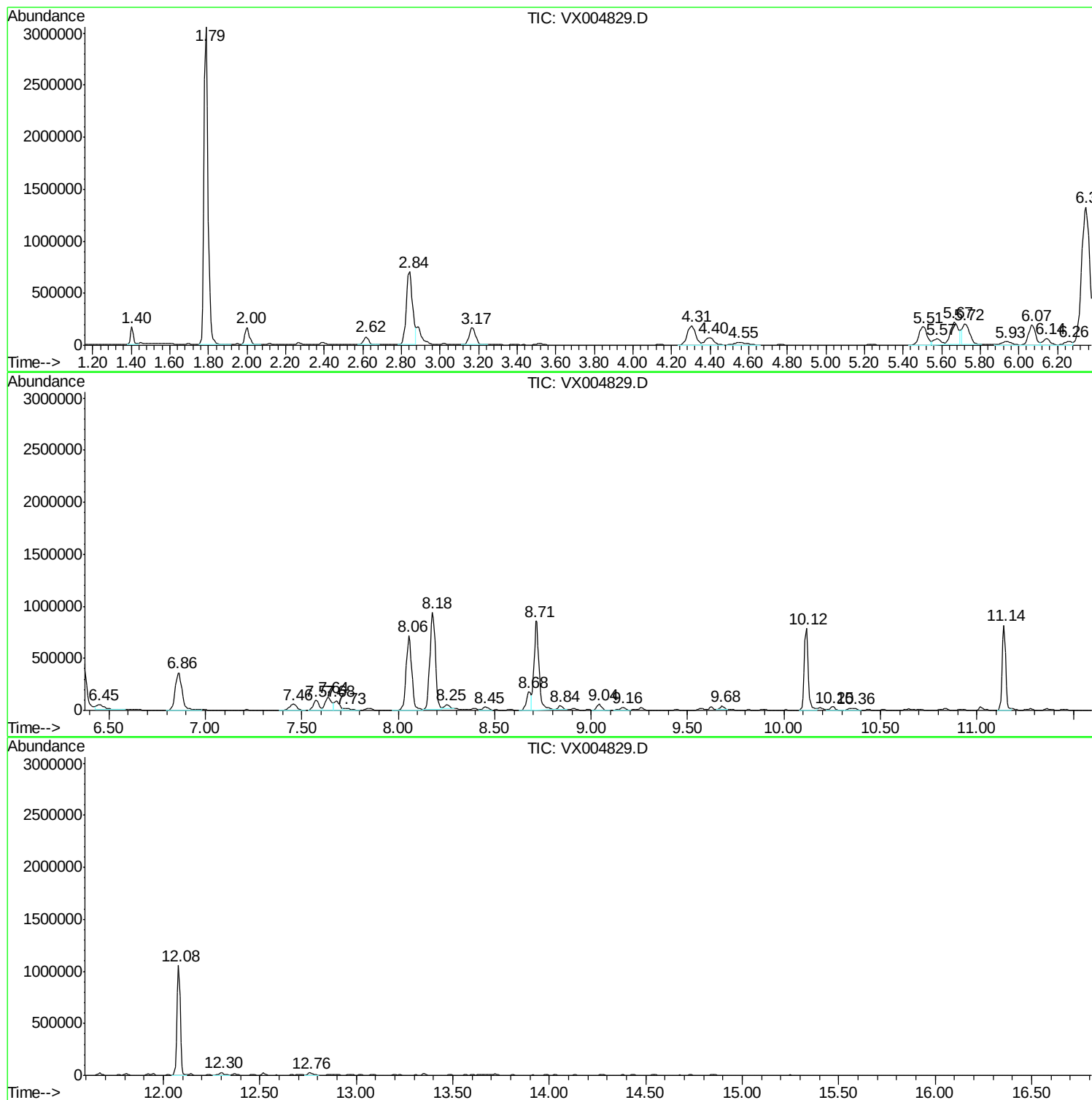
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Quant Title : SW846 8260

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



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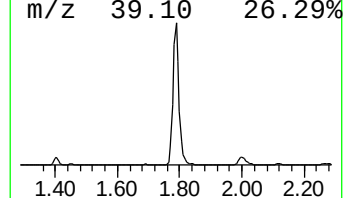
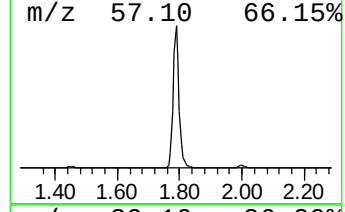
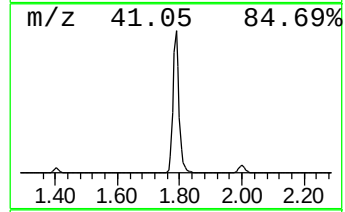
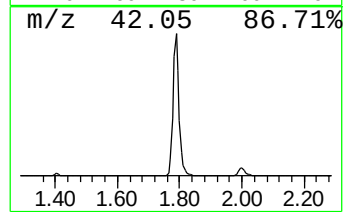
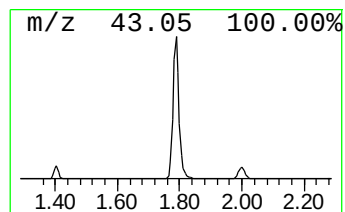
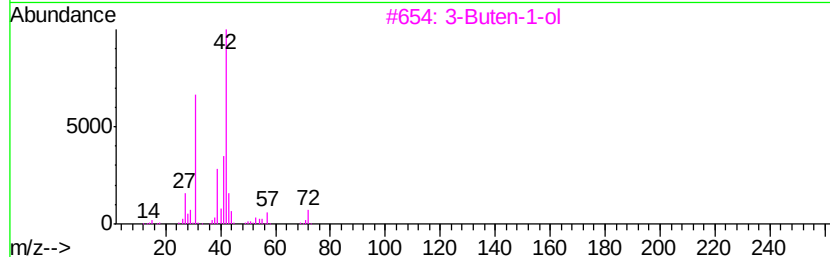
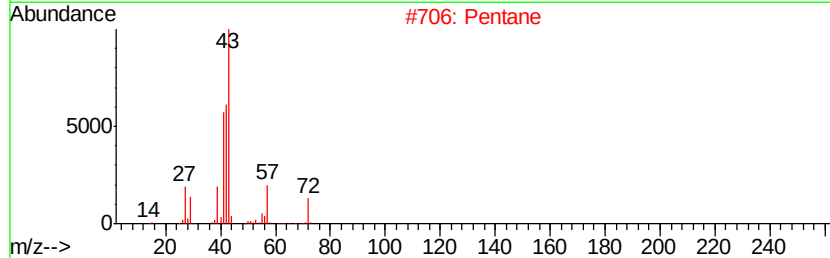
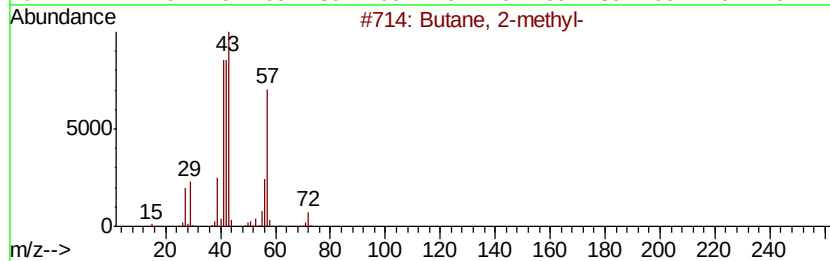
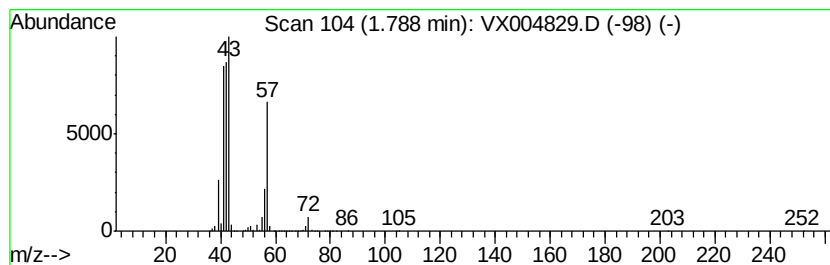
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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	332.18 ug/l	4294140	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	64
3		3-Buten-1-ol	72	C4H8O	000627-27-0	28
4		1-Butene	56	C4H8	000106-98-9	10
5		Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FA18-JMW-3284

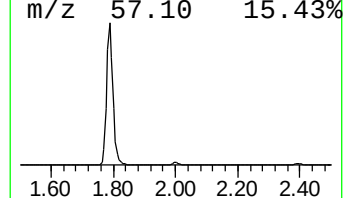
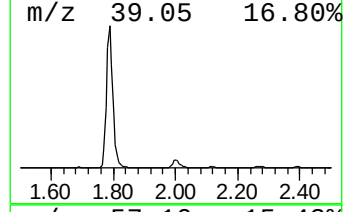
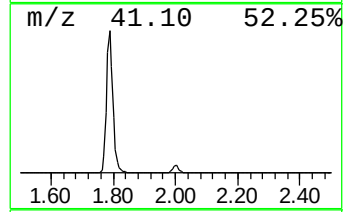
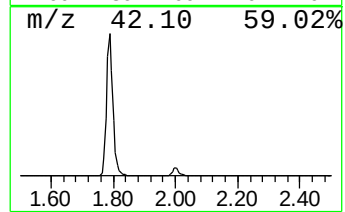
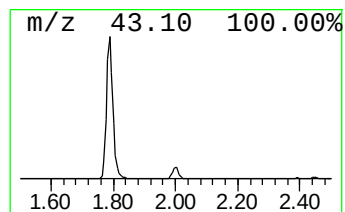
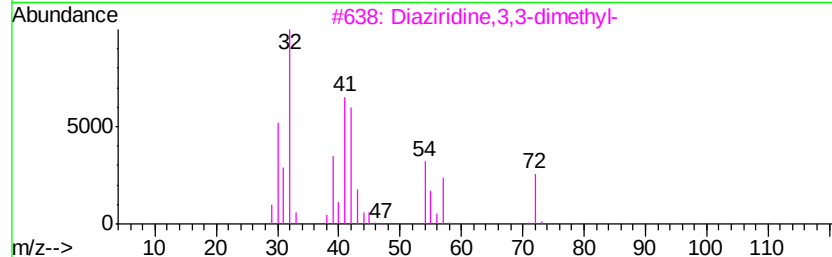
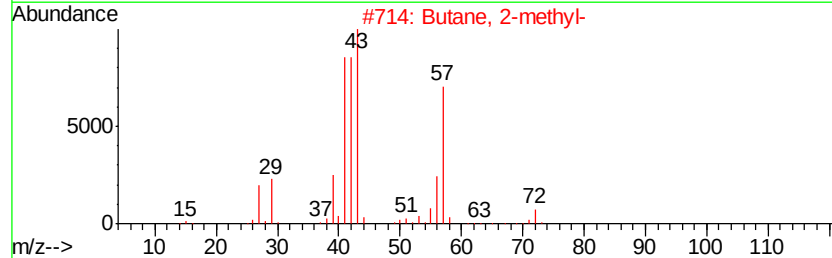
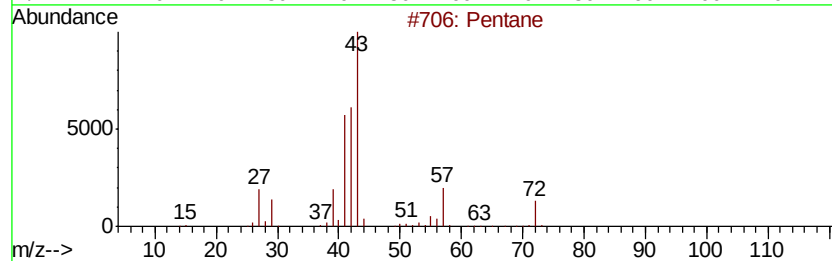
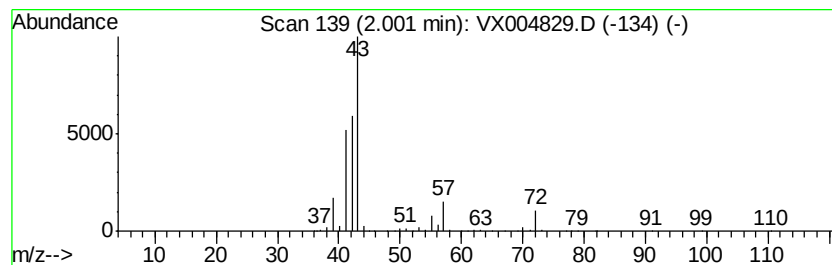
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	20.62 ug/l	266577	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane		72	C5H12	000109-66-0	91
2	Butane, 2-methyl-		72	C5H12	000078-78-4	42
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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FA18-JMW-3284

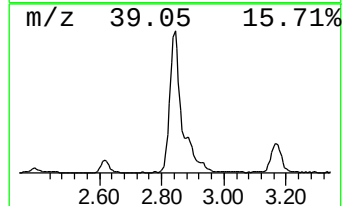
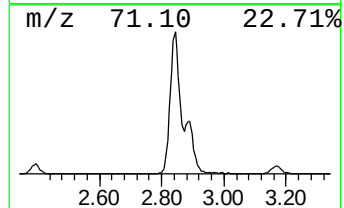
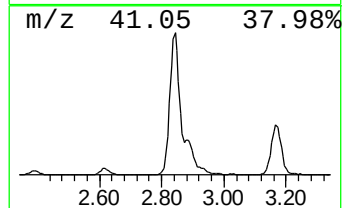
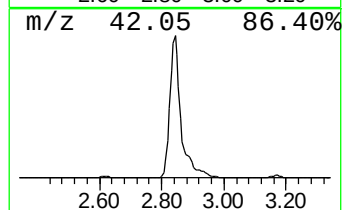
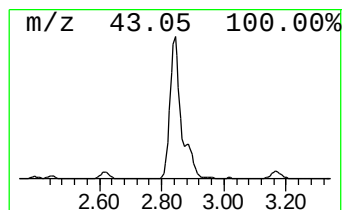
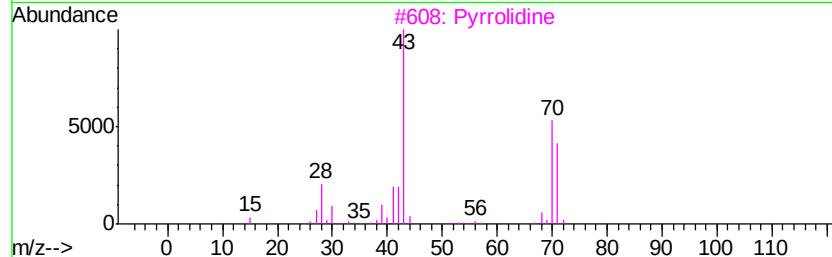
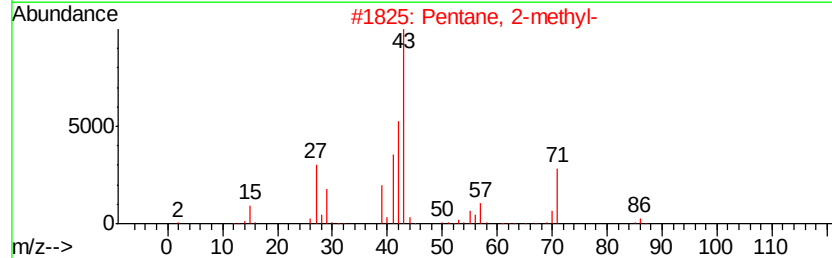
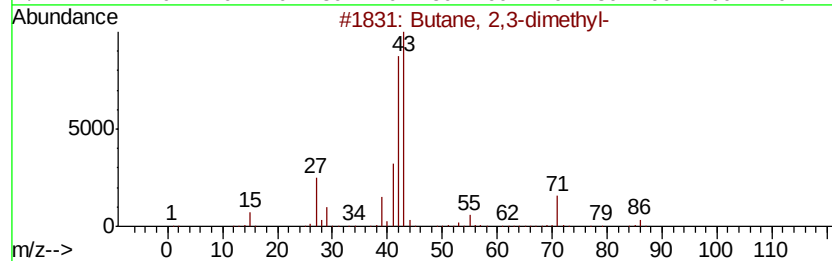
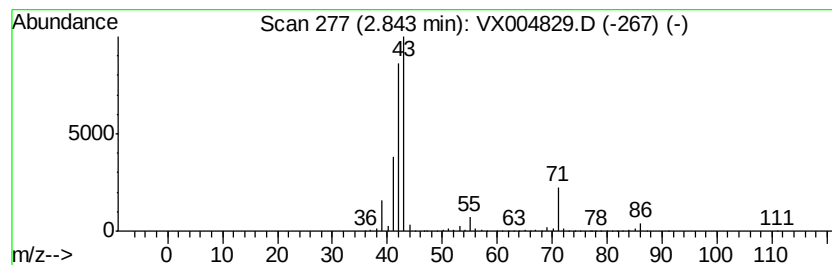
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	120.53 ug/l	1558030	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3		Pyrrolidine	71	C4H9N	000123-75-1	9
4		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	9
5		Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	9



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JMW-3284

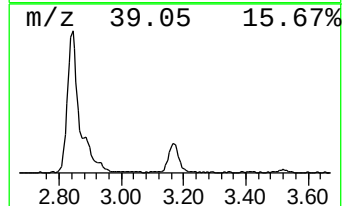
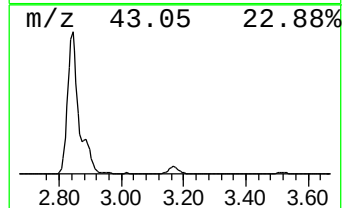
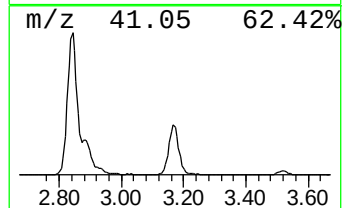
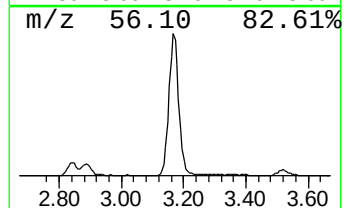
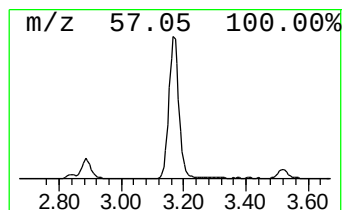
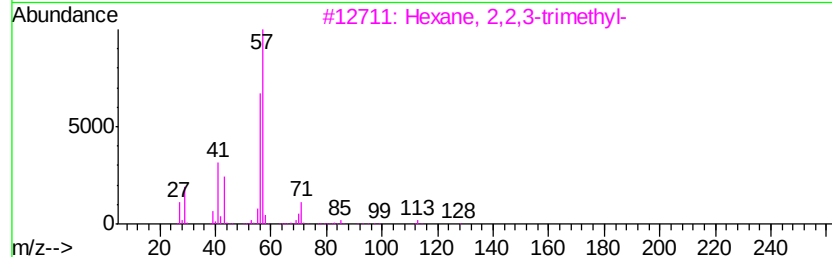
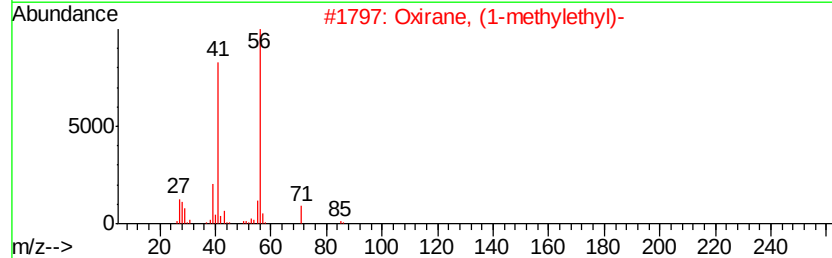
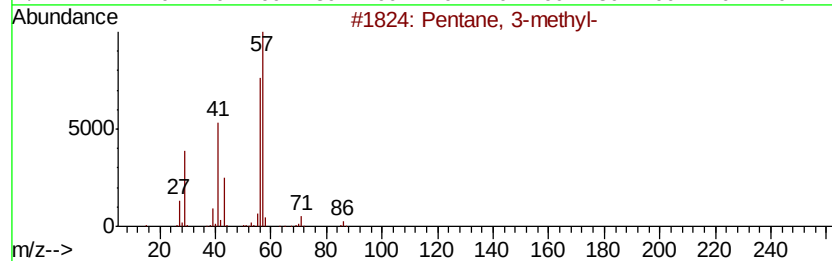
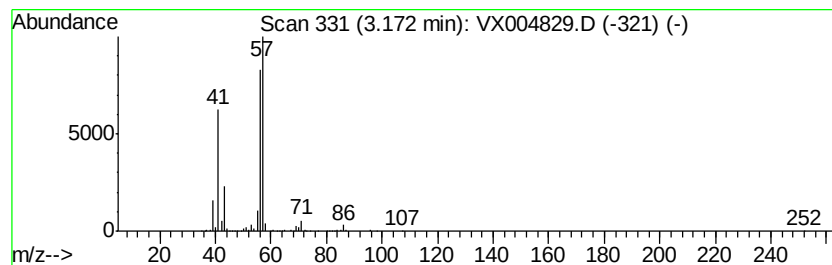
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	28.97 ug/l	374505	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59
3		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45
5		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43



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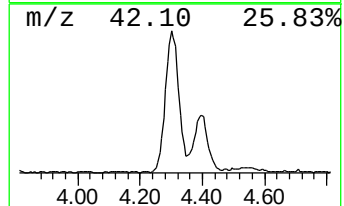
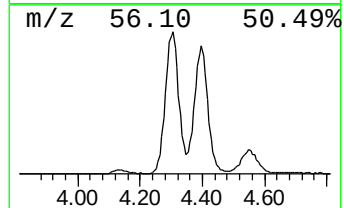
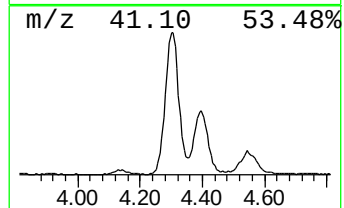
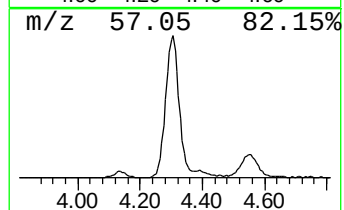
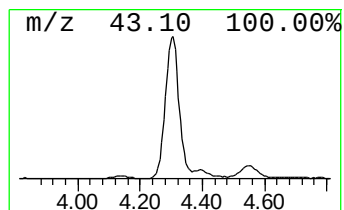
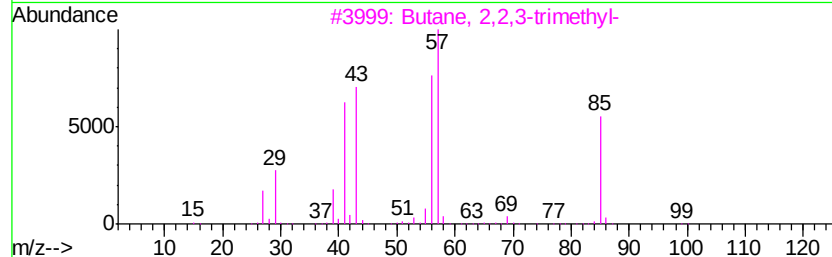
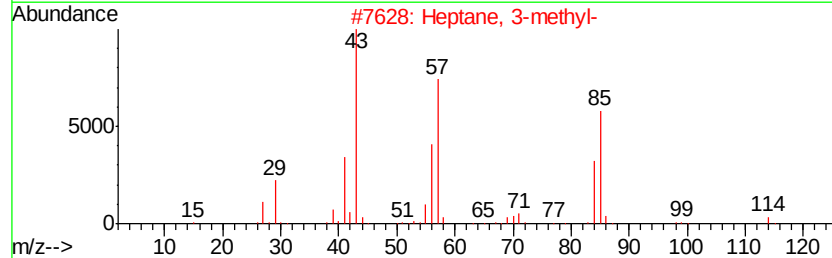
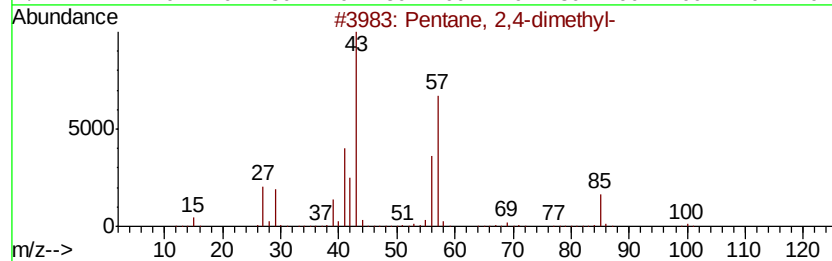
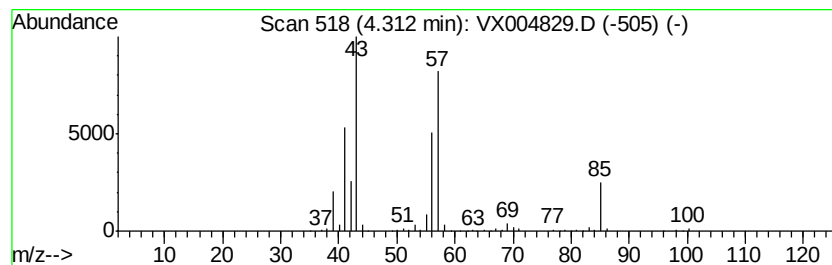
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.31	44.23 ug/l	571702	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2		Heptane, 3-methyl-	114	C8H18	000589-81-1	72
3		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004829.D
Acq On : 28 Sep 2018 18:45
Operator : JC/MD
Sample : J5130-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FA18-JMW-3284

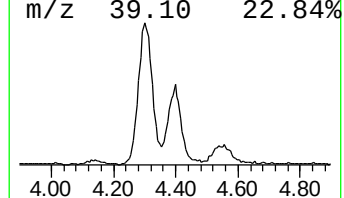
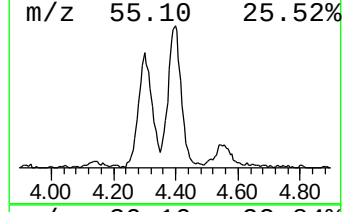
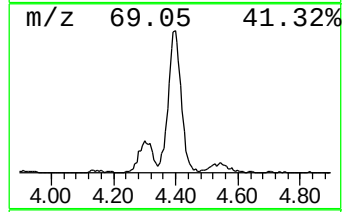
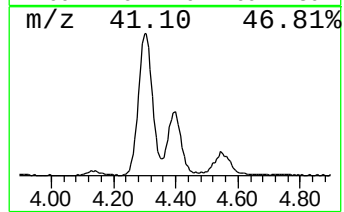
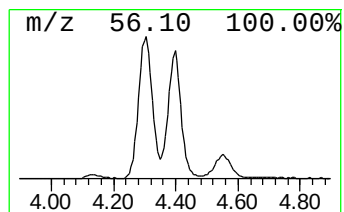
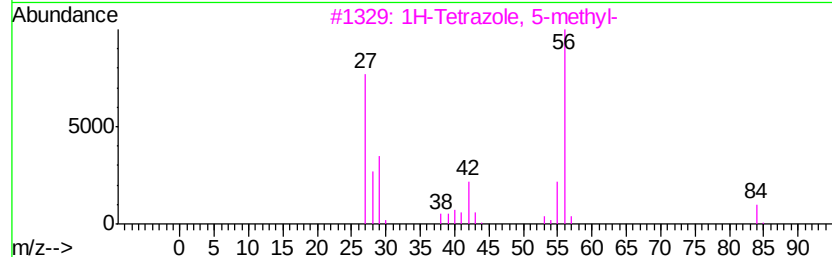
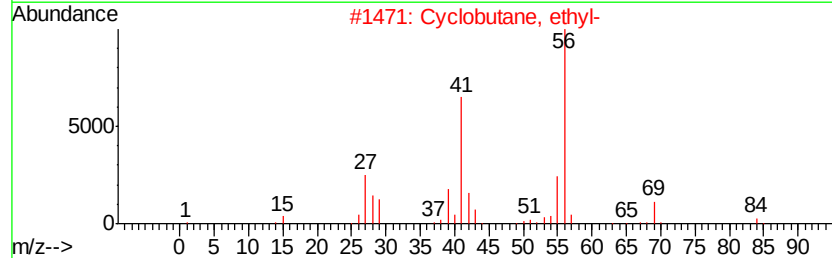
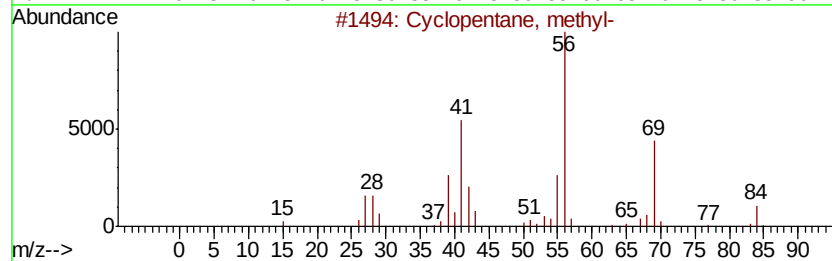
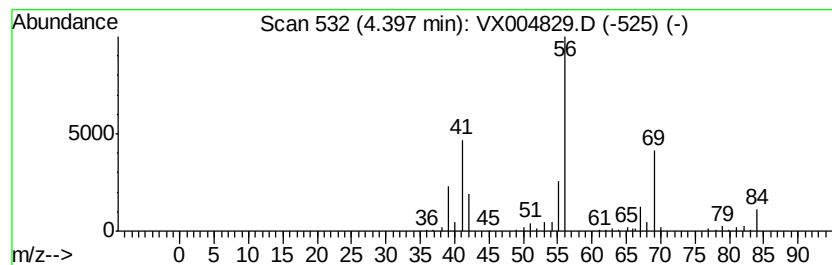
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	17.62 ug/l	227807	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
4		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	40
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004829.D
Acq On : 28 Sep 2018 18:45
Operator : JC/MD
Sample : J5130-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FA18-JMW-3284

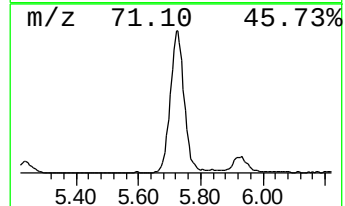
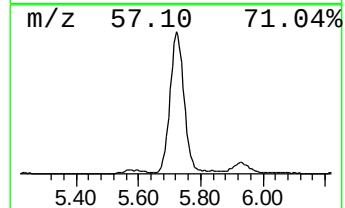
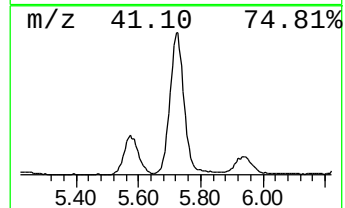
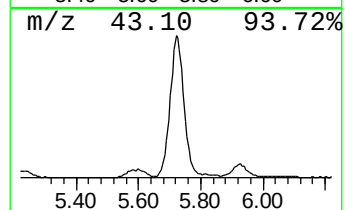
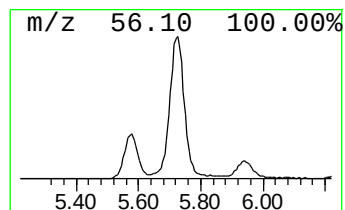
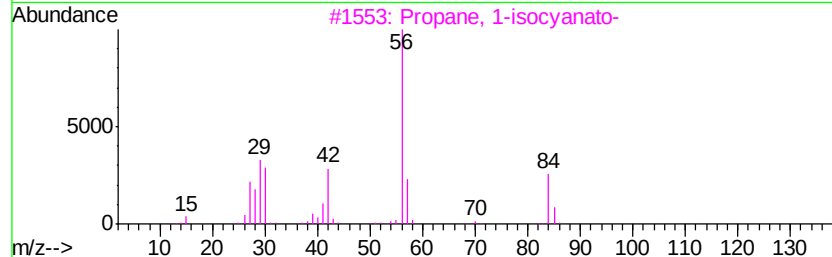
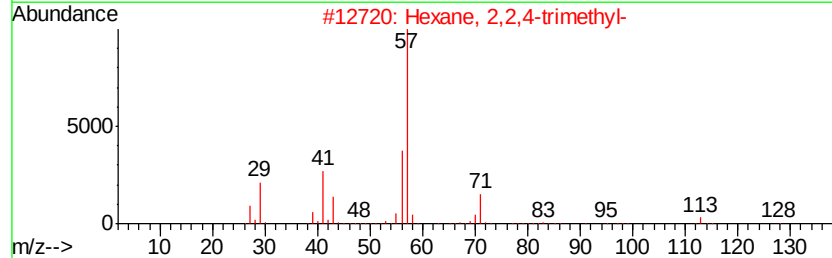
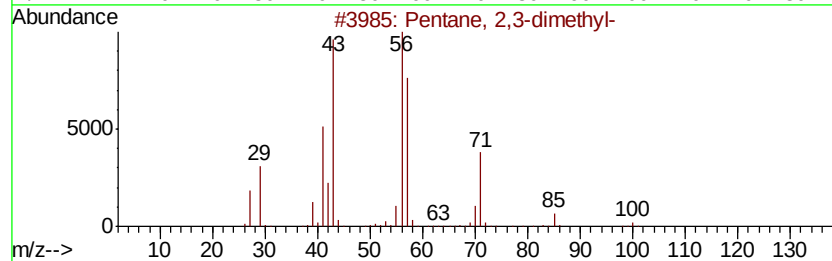
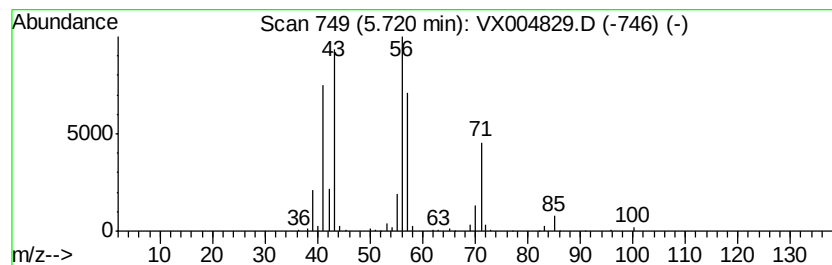
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	39.49 ug/l	510441	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
3		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	43
4		Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	40
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	37



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004829.D
Acq On : 28 Sep 2018 18:45
Operator : JC/MD
Sample : J5130-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JMW-3284

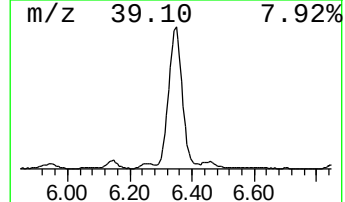
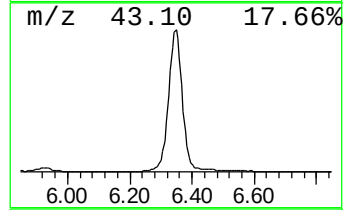
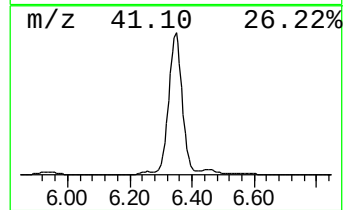
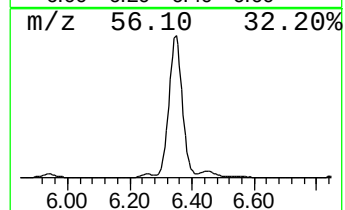
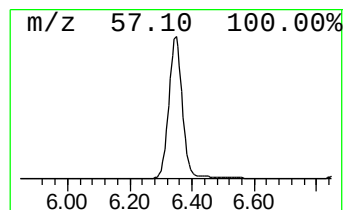
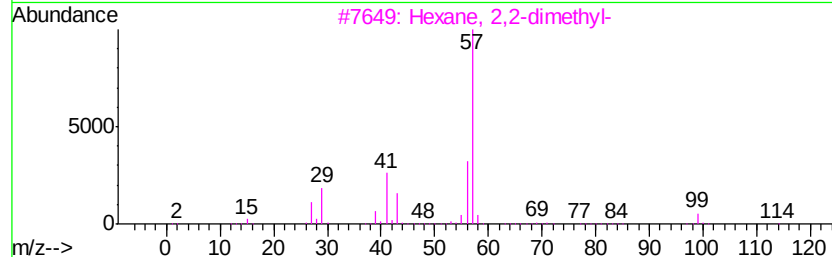
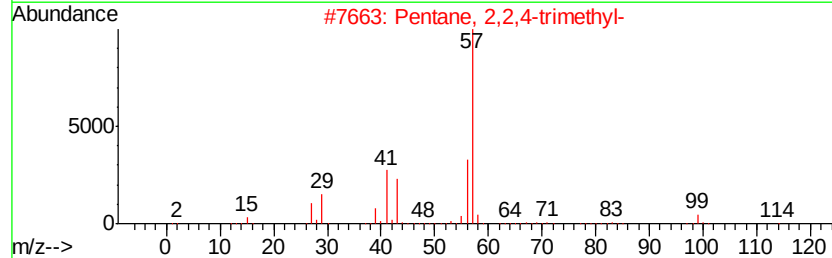
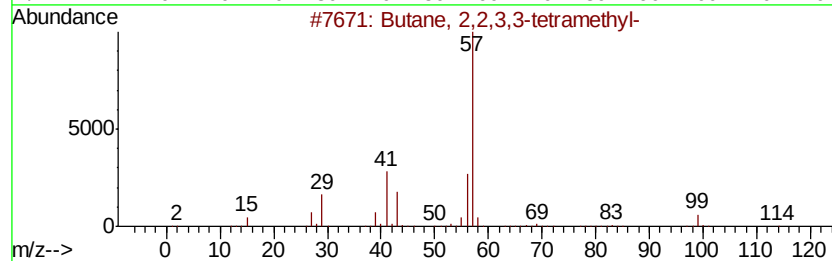
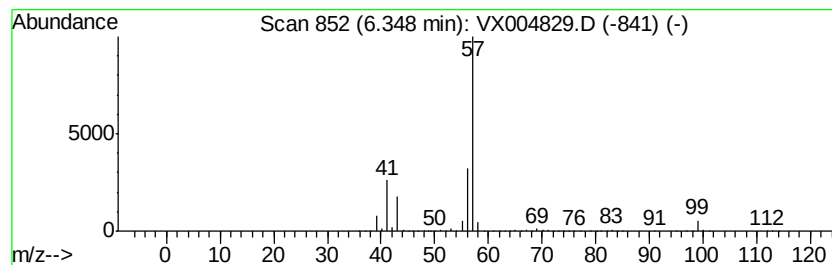
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Quant Title : SW846 8260

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

Peak Number 8 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	225.00 ug/l	4066860	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	83
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	78
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004829.D
Acq On : 28 Sep 2018 18:45
Operator : JC/MD
Sample : J5130-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JMW-3284

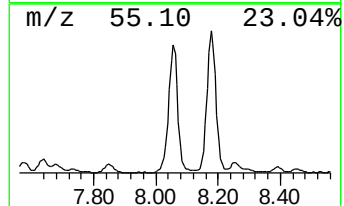
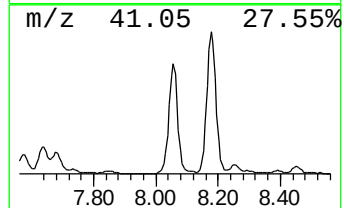
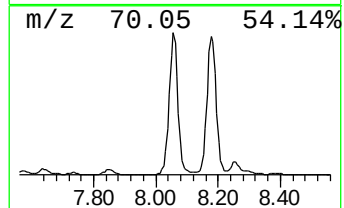
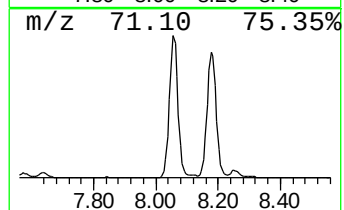
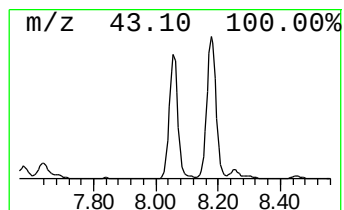
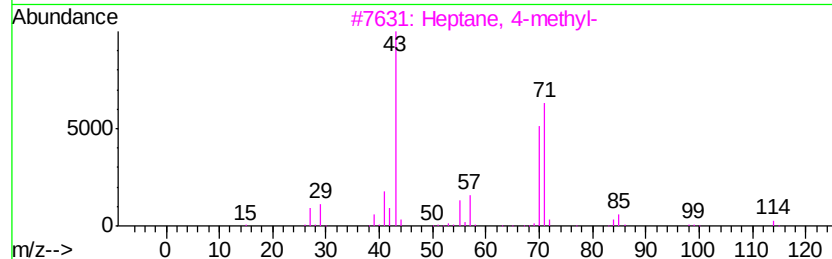
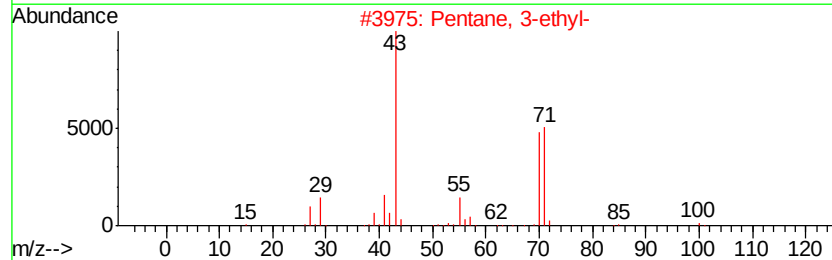
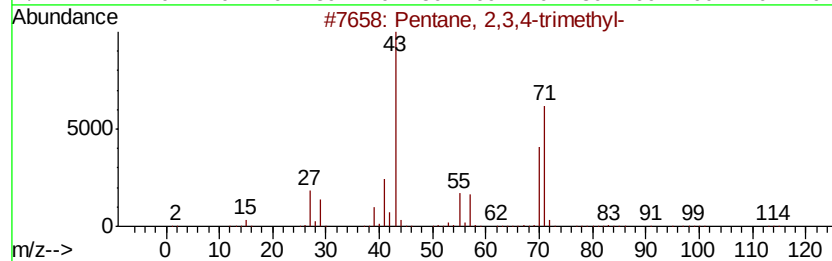
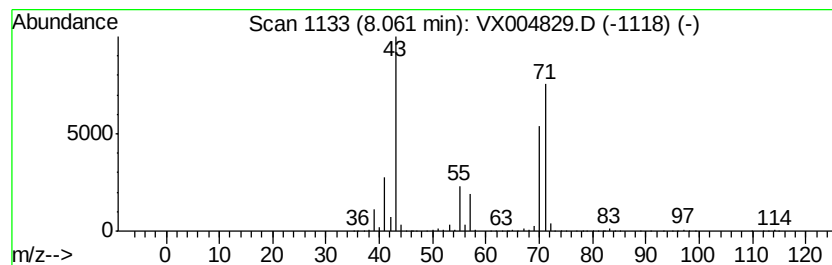
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	80.89 ug/l	1462000	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		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004829.D
Acq On : 28 Sep 2018 18:45
Operator : JC/MD
Sample : J5130-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JMW-3284

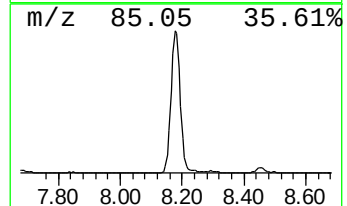
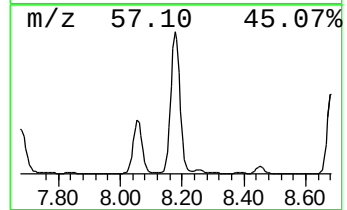
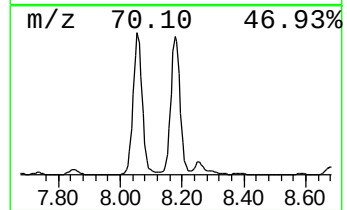
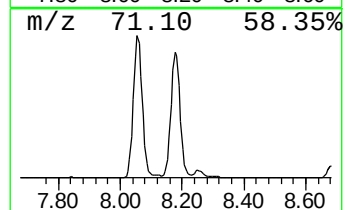
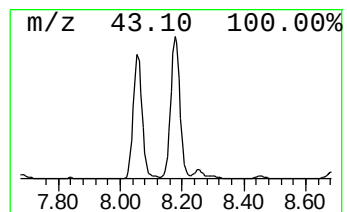
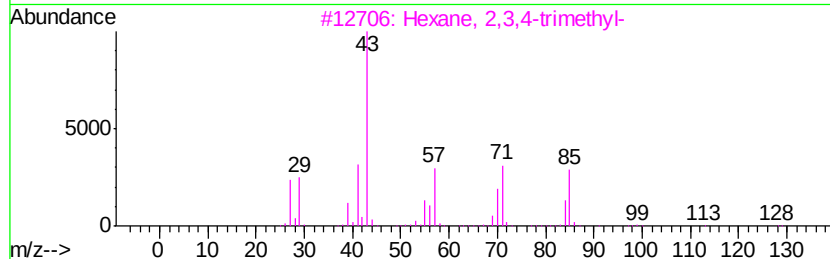
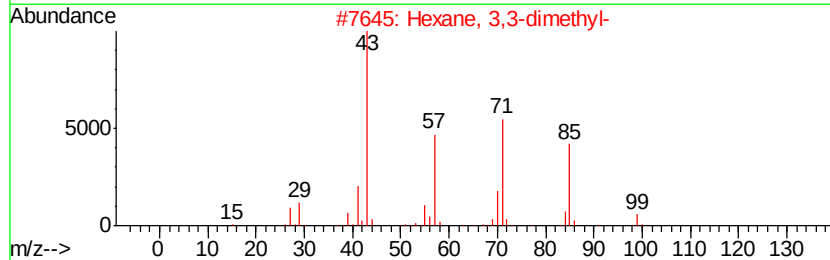
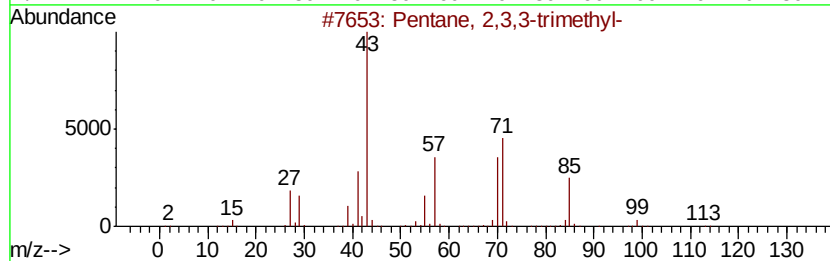
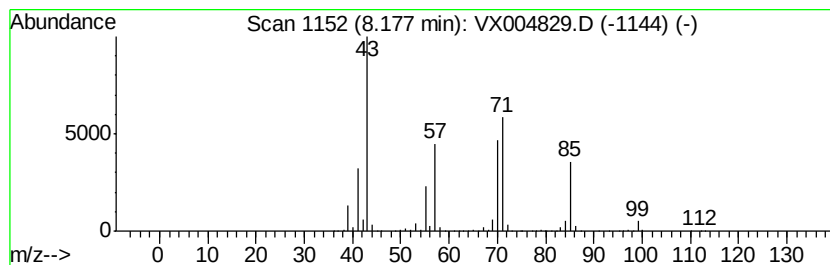
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 10 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	102.66 ug/l	1855530	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	59
3		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004829.D
Acq On : 28 Sep 2018 18:45
Operator : JC/MD
Sample : J5130-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA18-JMW-3284

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
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Pentane	2.00	20.6	ug/l	266577	1	5.67	646350	50.0
Butane, 2,3-dimet...	2.84	120.5	ug/l	1558030	1	5.67	646350	50.0
Pentane, 3-methyl-	3.17	29.0	ug/l	374505	1	5.67	646350	50.0
Pentane, 2,4-dime...	4.31	44.2	ug/l	571702	1	5.67	646350	50.0
Cyclopentane, met...	4.40	17.6	ug/l	227807	1	5.67	646350	50.0
Pentane, 2,3-dime...	5.72	39.5	ug/l	510441	1	5.67	646350	50.0
Butane, 2,2,3,3-t...	6.35	225.0	ug/l	4066860	2	6.87	903740	50.0
Pentane, 2,3,4-tr...	8.06	80.9	ug/l	1462000	2	6.87	903740	50.0
Pentane, 2,3,3-tr...	8.18	102.7	ug/l	1855530	2	6.87	903740	50.0