

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082218\
 Data File : VX004209.D
 Acq On : 22 Aug 2018 19:57
 Operator : JC/MD
 Sample : J4579-04
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FL-0544

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\82X082218W.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	75	80	94	rBV	1591386	2102318	4.13%	0.917%
2	1.788	191	197	211	rVB	2571195	3608965	7.09%	1.574%
3	1.995	225	231	246	rVB	1761416	2487444	4.89%	1.085%
4	2.837	361	369	373	rBV	1204329	2594891	5.10%	1.132%
5	2.885	373	377	381	rVV	1036464	2204013	4.33%	0.961%
6	2.922	381	383	400	rVB	673602	1237742	2.43%	0.540%
7	3.166	413	423	437	rBV	972243	2168905	4.26%	0.946%
8	3.513	471	480	496	rBV	648127	1459911	2.87%	0.637%
9	4.300	598	609	615	rBV	252531	754498	1.48%	0.329%
10	4.391	615	624	639	rVB	3062719	8955163	17.60%	3.907%
11	5.574	808	818	828	rVB	3375969	10198173	20.04%	4.449%
12	5.720	836	842	860	rVB	587185	1809495	3.56%	0.789%
13	5.934	864	877	890	rBV6	252966	887804	1.74%	0.387%
14	6.068	890	899	912	rVB	215931	553459	1.09%	0.241%
15	6.257	918	930	935	rBV	189427	549383	1.08%	0.240%
16	6.348	935	945	955	rVV	930059	2845482	5.59%	1.241%
17	6.452	955	962	978	rVB	256541	704572	1.38%	0.307%
18	6.860	1019	1029	1039	rBV	457473	1076556	2.12%	0.470%
19	7.464	1114	1128	1139	rBV	2574495	5751511	11.30%	2.509%
20	8.055	1212	1225	1236	rBV	795225	1579272	3.10%	0.689%
21	8.177	1236	1245	1253	rBV	1397127	2714036	5.33%	1.184%
22	8.671	1318	1326	1329	rBV3	281253	607528	1.19%	0.265%
23	8.714	1329	1333	1342	rVB	1147629	1892932	3.72%	0.826%
24	10.116	1558	1563	1568	rBV	890168	1211152	2.38%	0.528%
25	10.256	1580	1586	1595	rBV	18411822	24199183	47.55%	10.557%
26	10.366	1595	1604	1610	rBV	35747041	50887479	100.00%	22.199%
27	10.701	1653	1659	1671	rVB	13802757	17318919	34.03%	7.555%
28	11.018	1706	1711	1717	rBV	1389325	1726038	3.39%	0.753%
29	11.140	1725	1731	1735	rBV	1007108	1248389	2.45%	0.545%
30	11.360	1762	1767	1774	rBV	1827372	2167922	4.26%	0.946%
31	11.439	1774	1780	1782	rBV	5463072	8184369	16.08%	3.570%
32	11.506	1787	1791	1802	rVB	4447518	5361880	10.54%	2.339%
33	11.670	1812	1818	1827	rBV	4014820	5075782	9.97%	2.214%
34	11.811	1836	1841	1846	rVB	14506382	17350955	34.10%	7.569%

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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	12.079	1880	1885	1890	rVB2	1336013	1751824	3.44%	0.764%
36	12.146	1890	1896	1901	rBV	6797422	7997264	15.72%	3.489%
37	12.298	1914	1921	1929	rBV	3708452	4870889	9.57%	2.125%
38	12.372	1929	1933	1943	rVB3	803798	1206615	2.37%	0.526%
39	12.585	1963	1968	1970	rBV	426869	536556	1.05%	0.234%
40	12.609	1970	1972	1977	rVB	484395	545366	1.07%	0.238%
41	12.670	1977	1982	1985	rBV	677861	789501	1.55%	0.344%
42	12.756	1992	1996	2004	rVB2	554549	884550	1.74%	0.386%
43	12.981	2025	2033	2036	rBV	399448	510842	1.00%	0.223%
44	13.018	2036	2039	2046	rVB	571452	681846	1.34%	0.297%
45	13.225	2065	2073	2078	rBV	659760	826253	1.62%	0.360%
46	13.347	2089	2093	2099	rVB2	1578785	2189847	4.30%	0.955%
47	13.481	2110	2115	2122	rVB	1242188	1452185	2.85%	0.633%
48	13.835	2166	2173	2181	rBV	6583277	7951733	15.63%	3.469%
49	14.700	2307	2315	2326	rBV	1688593	2128659	4.18%	0.929%
50	14.841	2333	2338	2348	rBV	1184751	1433154	2.82%	0.625%

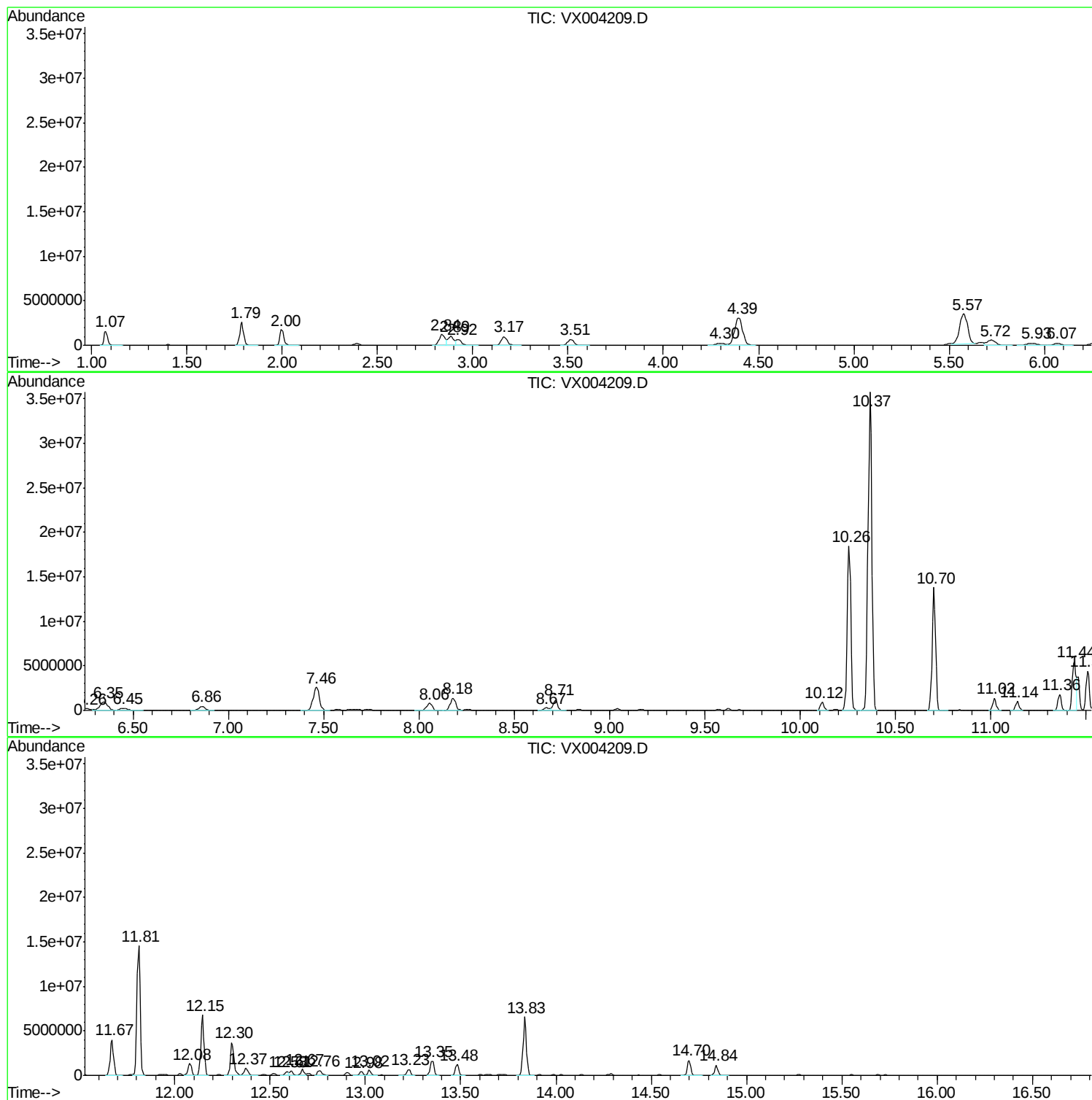
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampled :
FL-0544

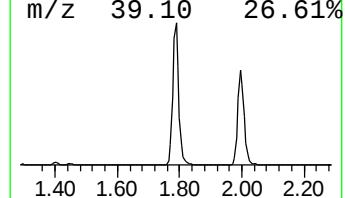
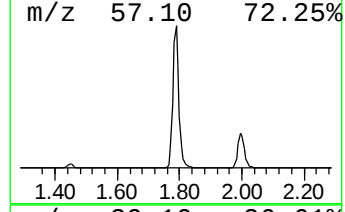
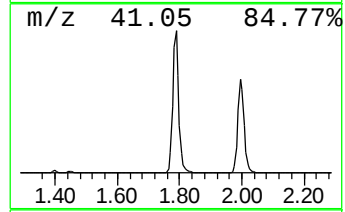
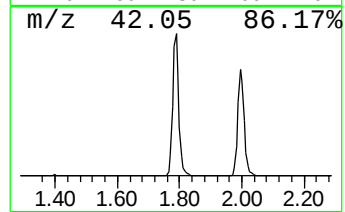
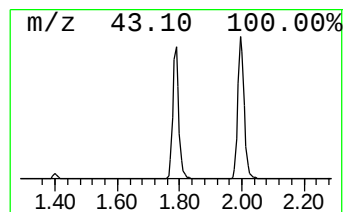
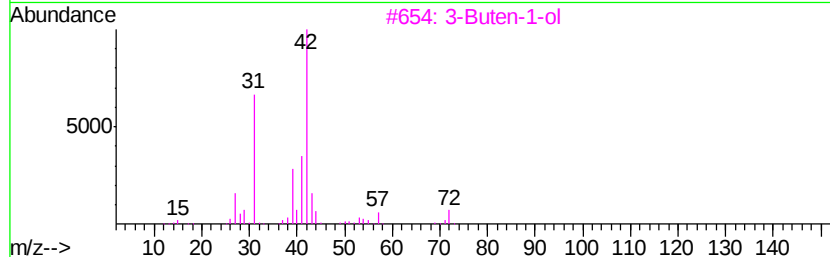
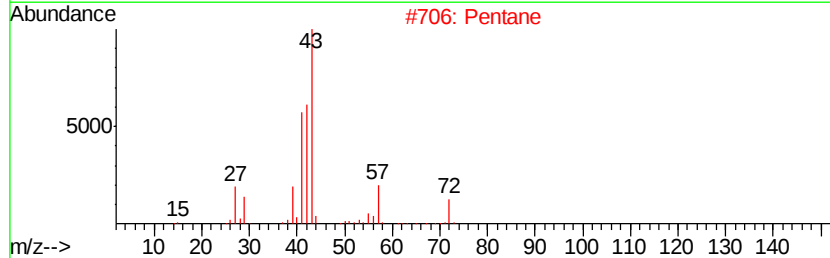
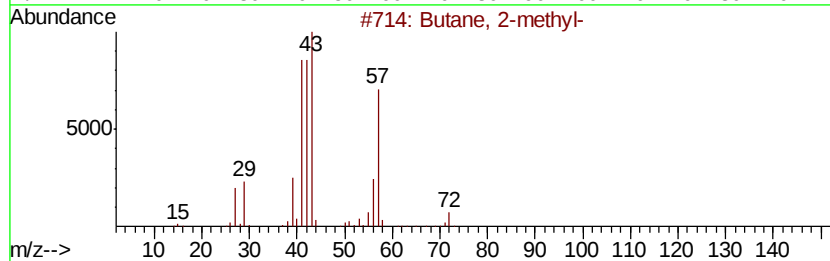
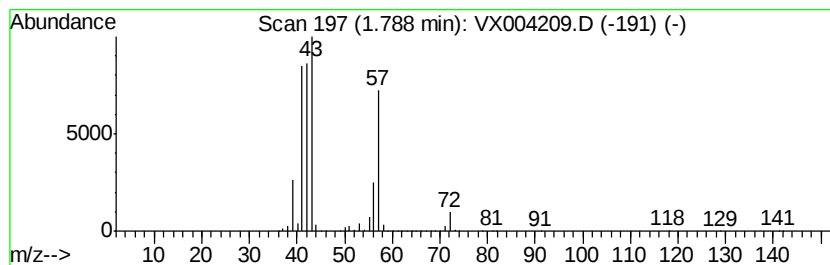
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	99.72 ug/l	3608970	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	43
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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Instrument :
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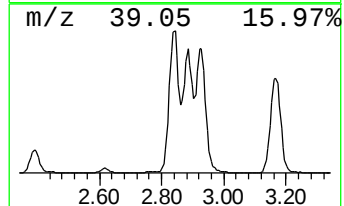
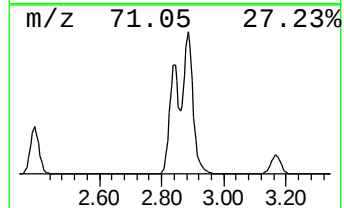
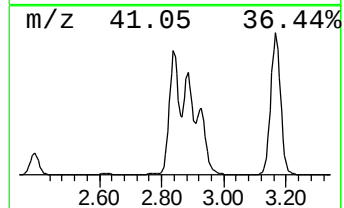
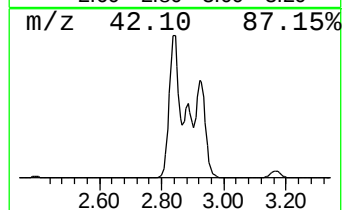
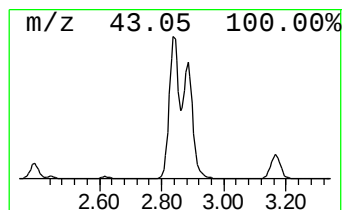
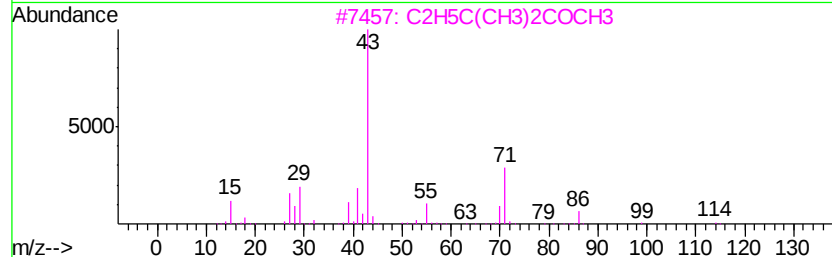
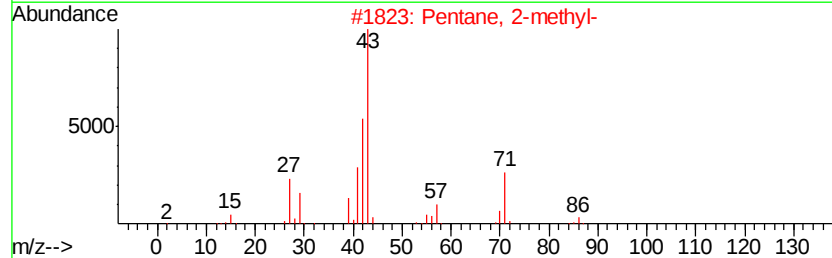
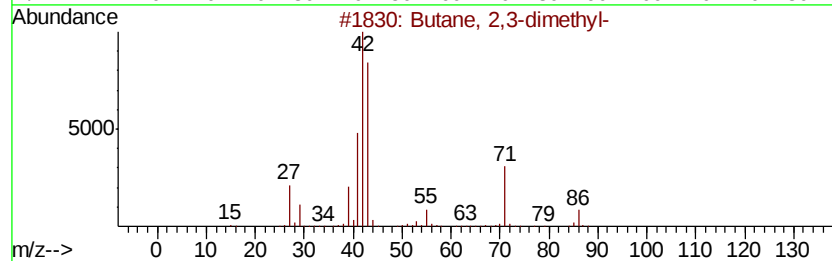
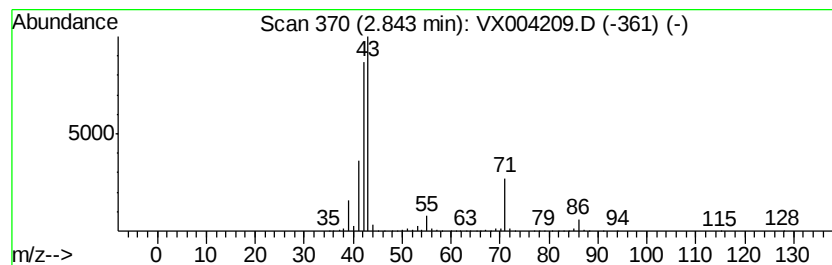
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	71.70 ug/l	2594890	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	12
4		Pyrrolidine	71	C4H9N	000123-75-1	10
5		Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9



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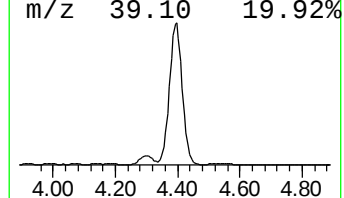
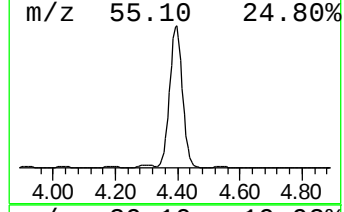
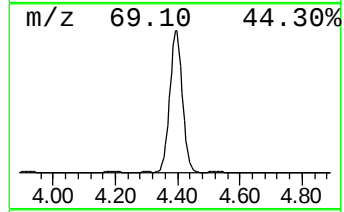
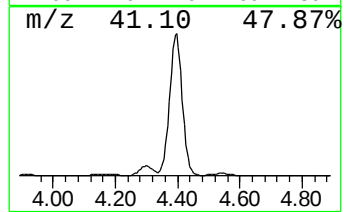
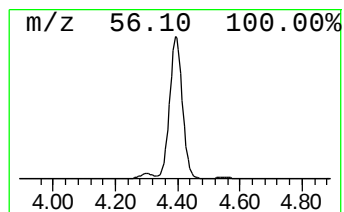
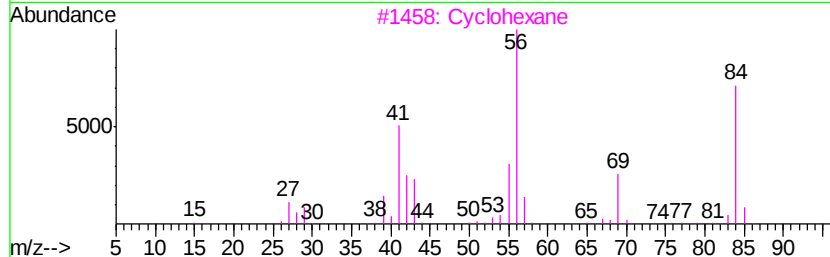
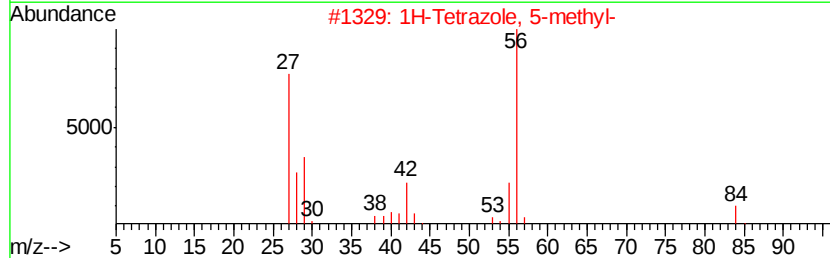
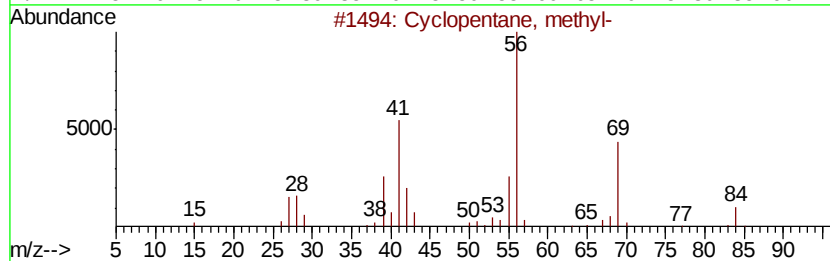
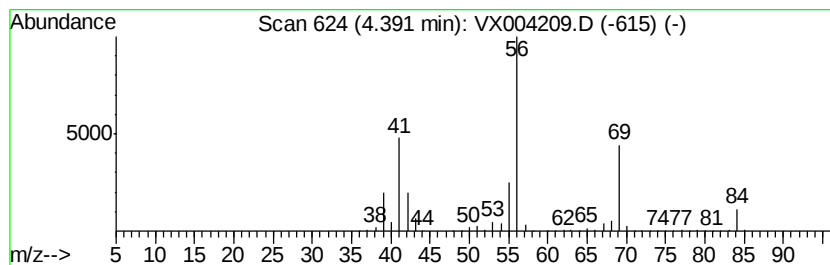
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	247.45 ug/l	8955160	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3		Cyclohexane	84	C6H12	000110-82-7	64
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



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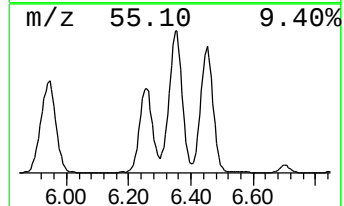
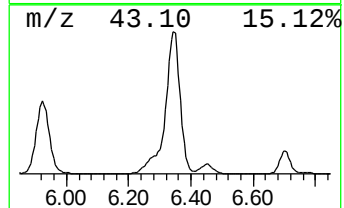
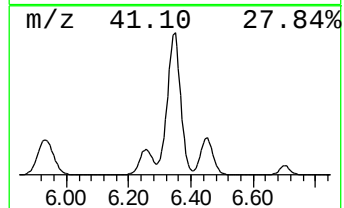
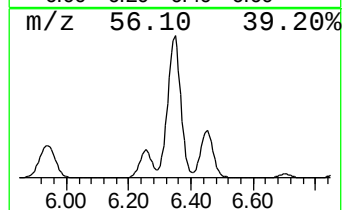
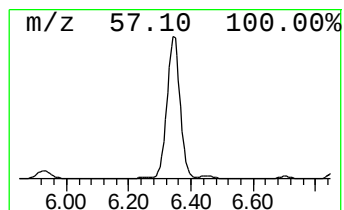
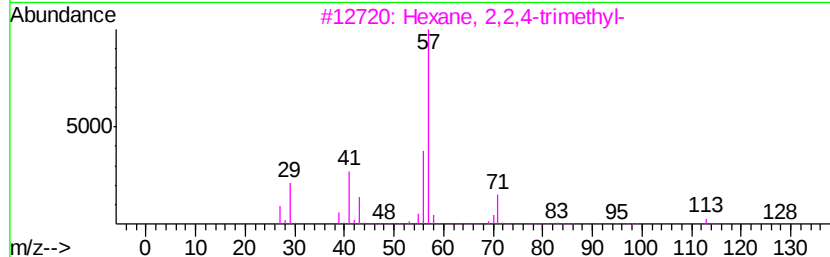
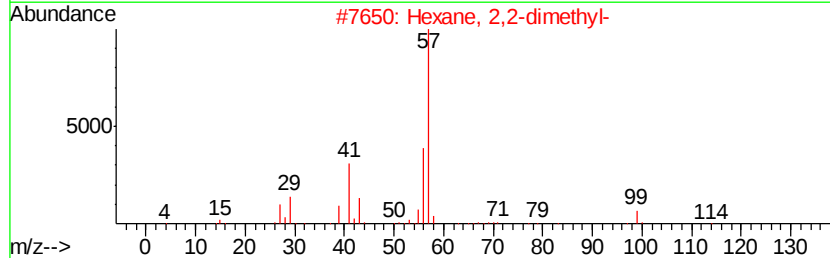
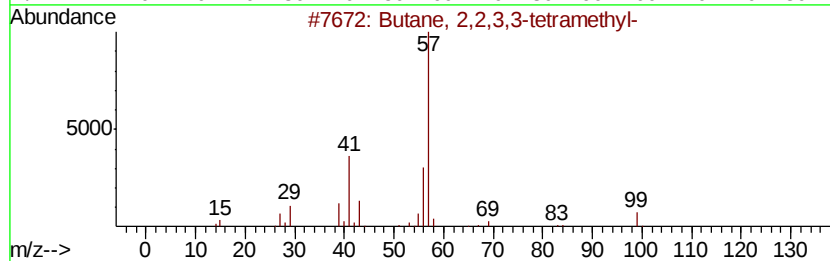
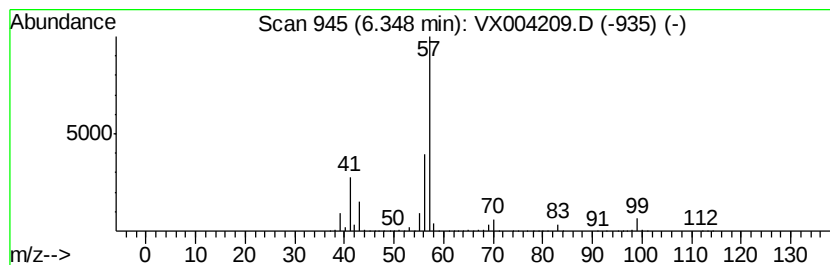
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Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,2,3,3-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	132.16 ug/l	2845480	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
3		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
4		Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	64
5		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64



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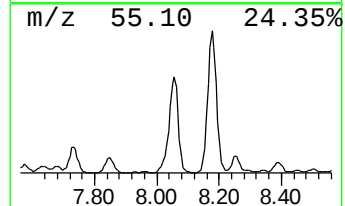
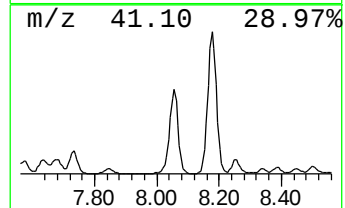
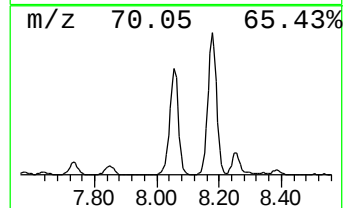
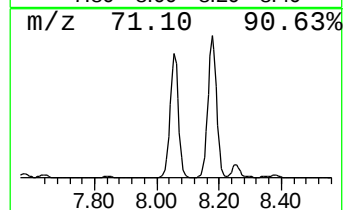
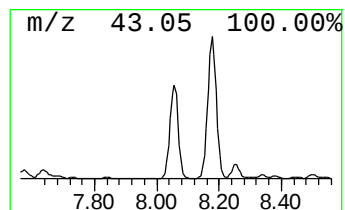
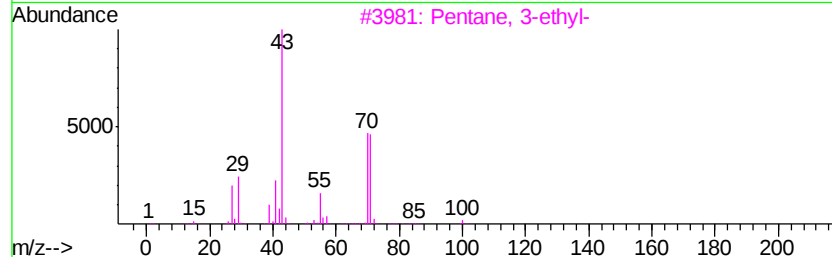
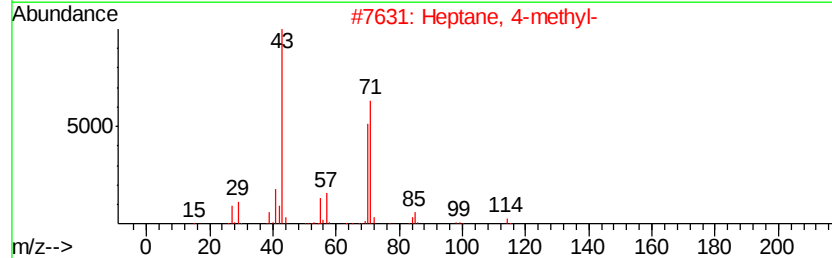
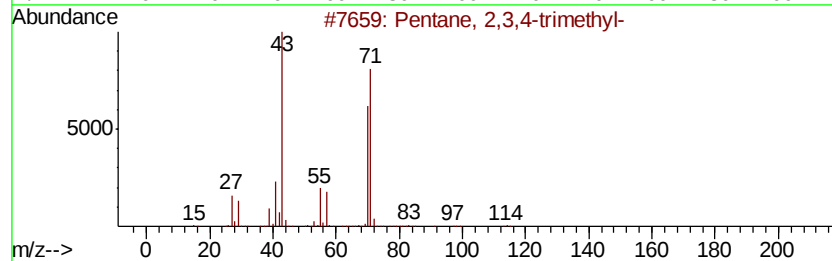
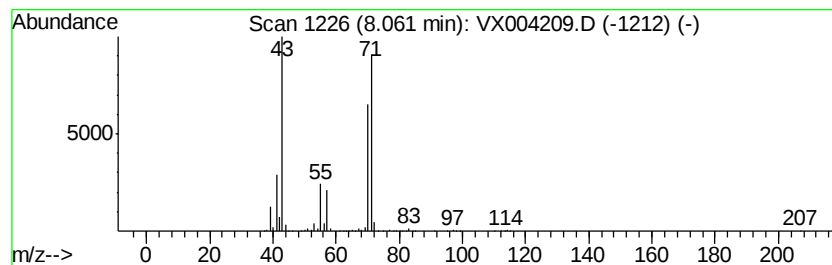
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	73.35 ug/l	1579270	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	78
5		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004209.D
Acq On : 22 Aug 2018 19:57
Operator : JC/MD
Sample : J4579-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0544

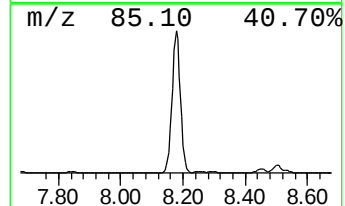
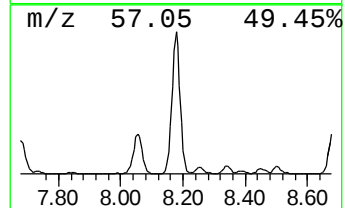
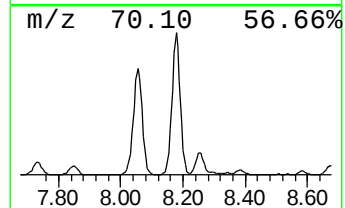
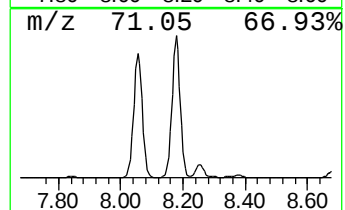
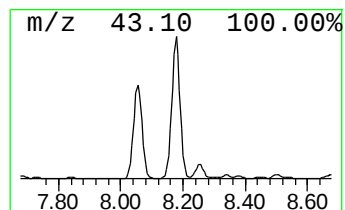
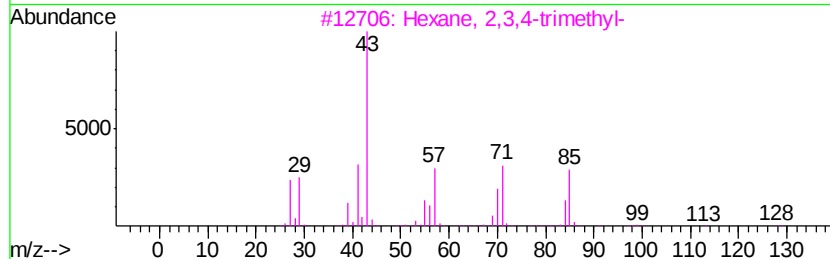
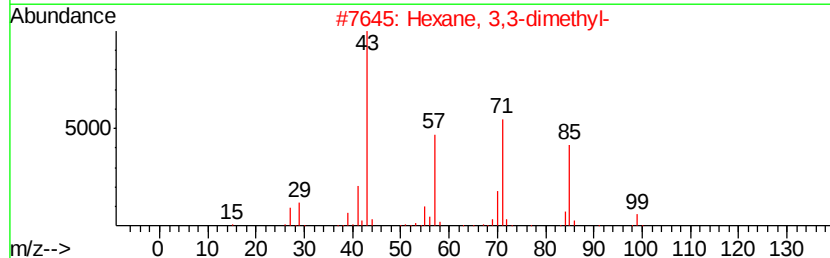
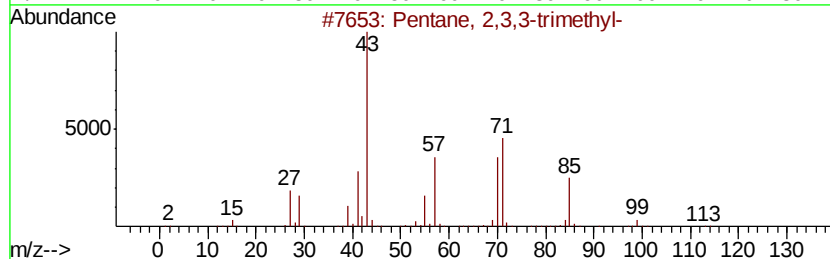
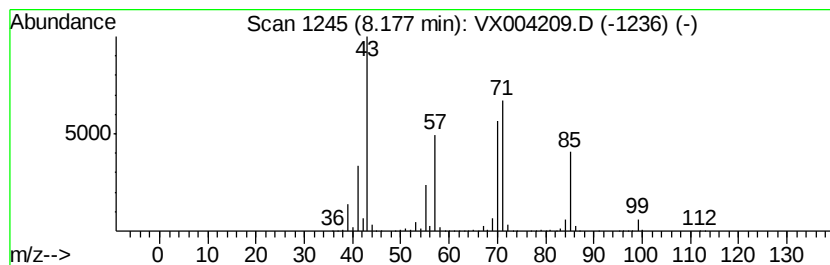
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	126.05 ug/l	2714040	1,4-Difluorobenzene	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90	
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64	
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64	
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	53	
5	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	50	



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004209.D
Acq On : 22 Aug 2018 19:57
Operator : JC/MD
Sample : J4579-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0544

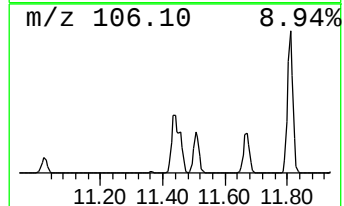
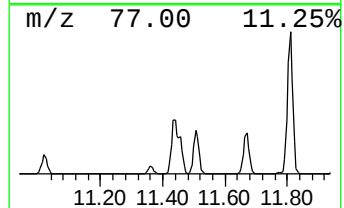
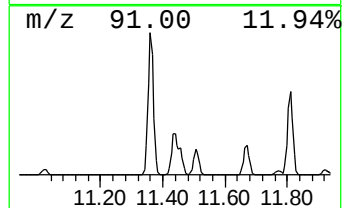
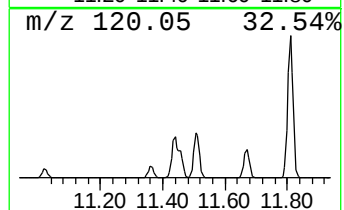
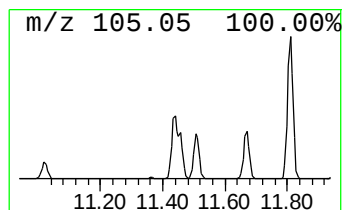
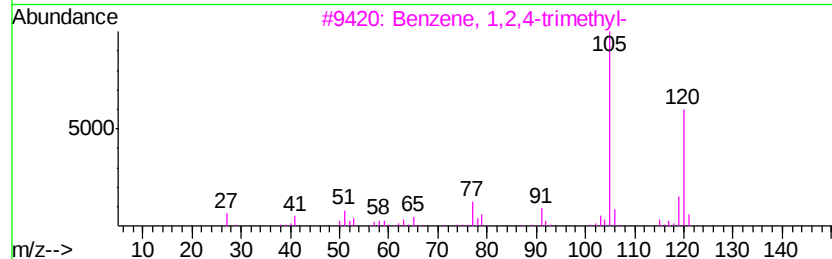
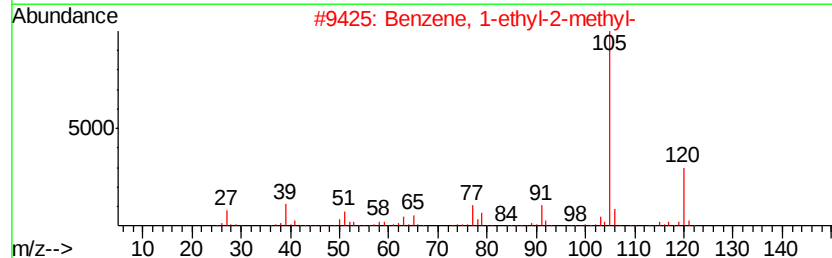
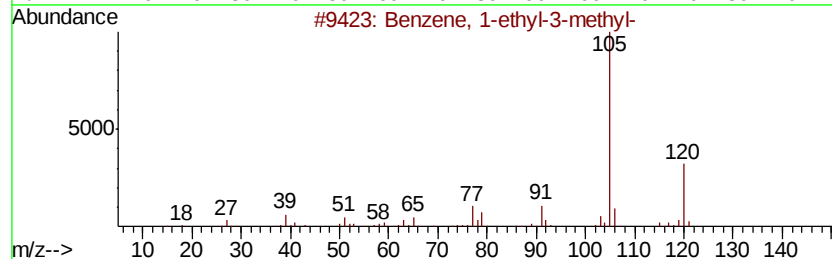
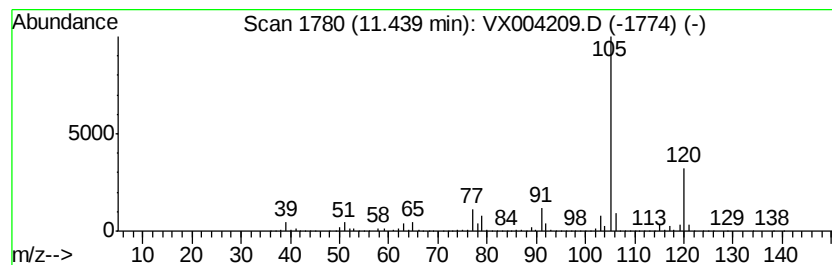
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	233.60 ug/l	8184370	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004209.D
Acq On : 22 Aug 2018 19:57
Operator : JC/MD
Sample : J4579-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0544

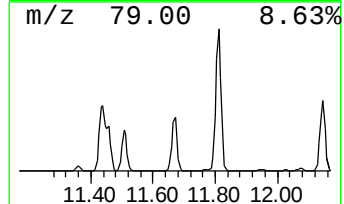
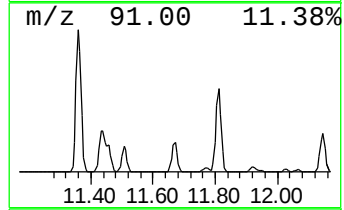
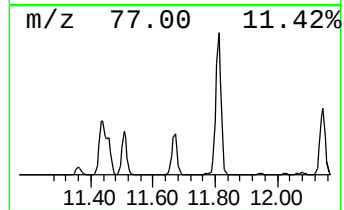
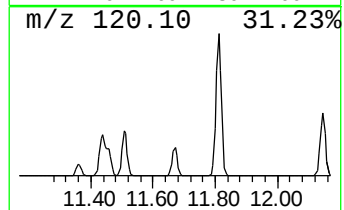
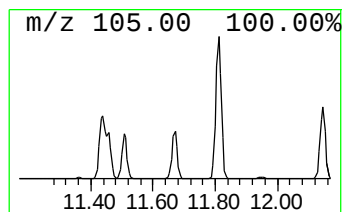
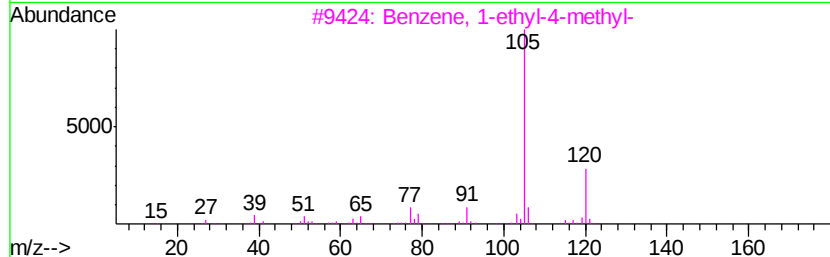
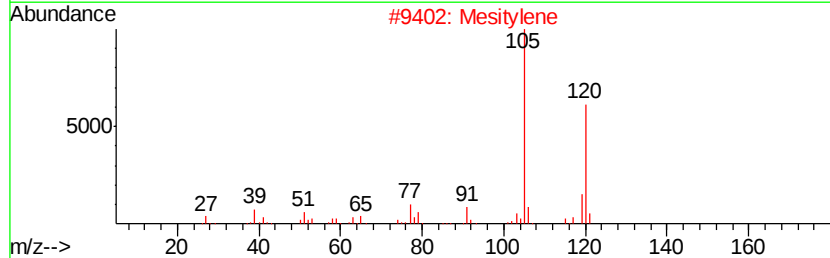
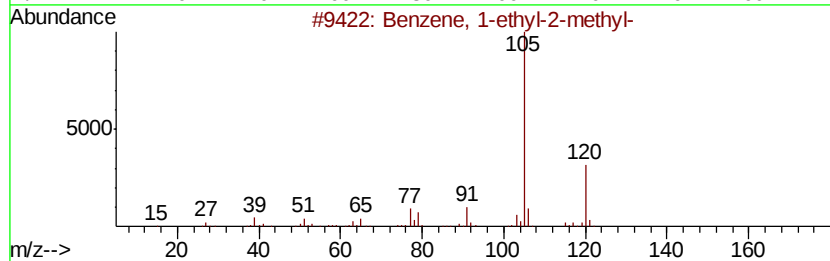
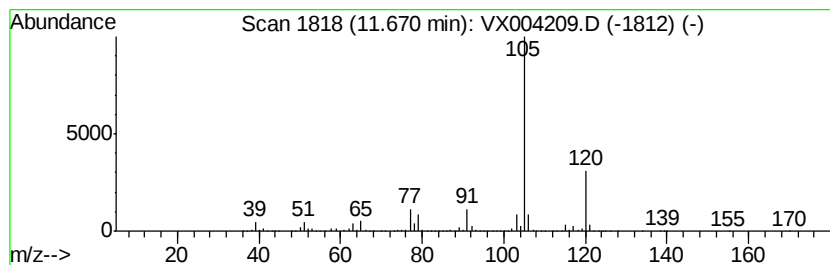
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	144.87 ug/l	5075780	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2		Mesitylene	120	C9H12	000108-67-8	90
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004209.D
Acq On : 22 Aug 2018 19:57
Operator : JC/MD
Sample : J4579-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0544

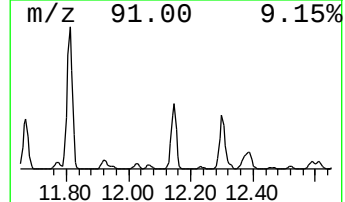
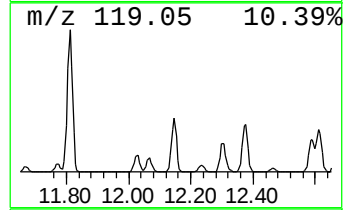
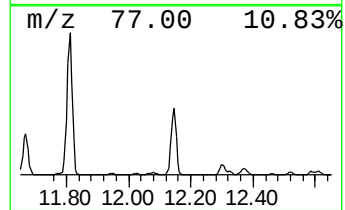
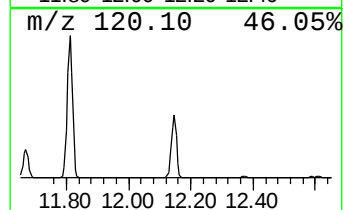
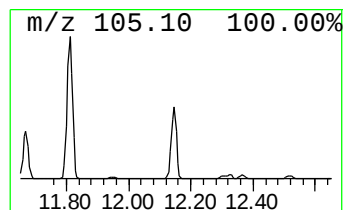
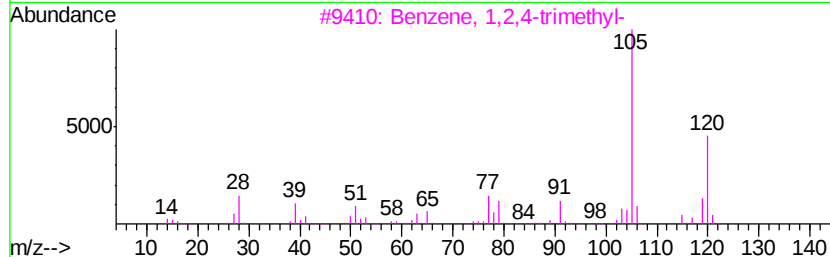
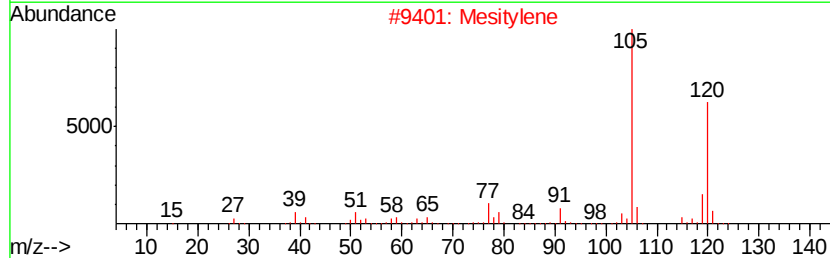
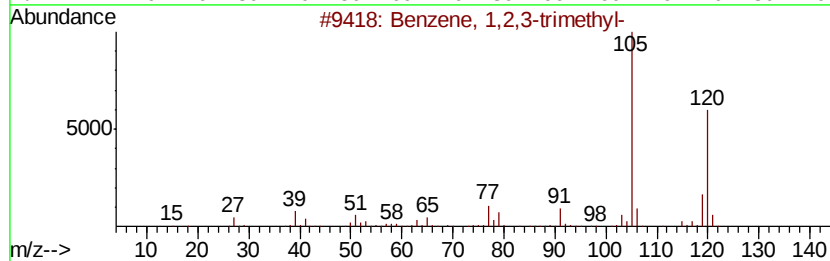
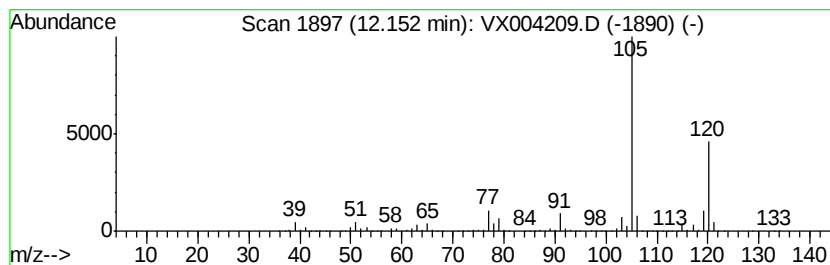
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	228.26 ug/l	7997260	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Mesitylene	120	C9H12	000108-67-8	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX082218\
Data File : VX004209.D
Acq On : 22 Aug 2018 19:57
Operator : JC/MD
Sample : J4579-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FL-0544

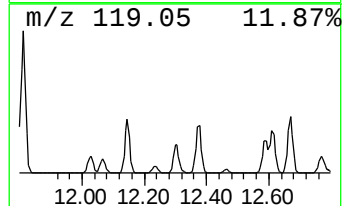
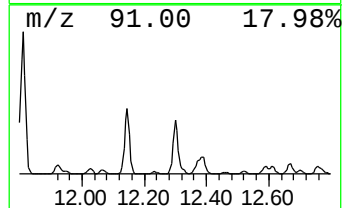
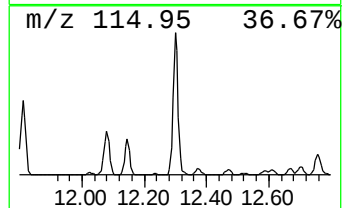
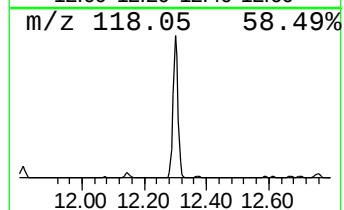
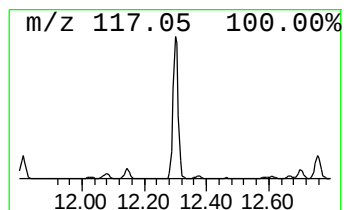
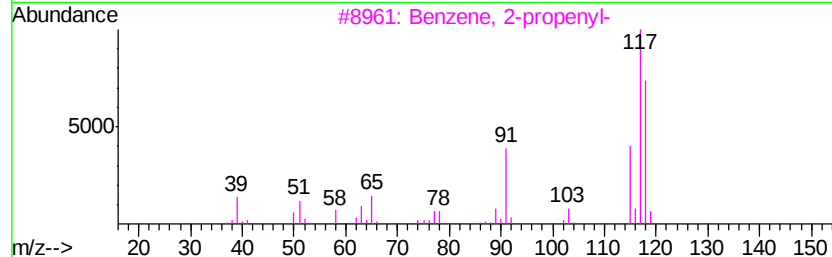
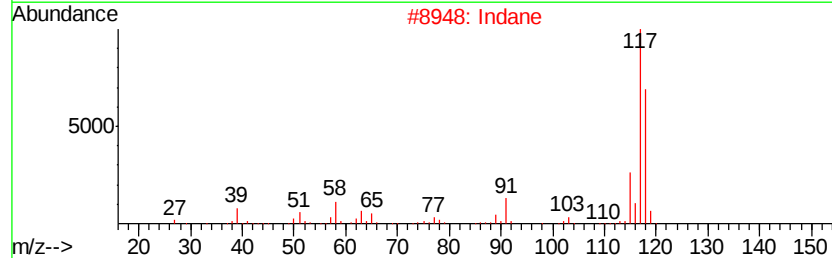
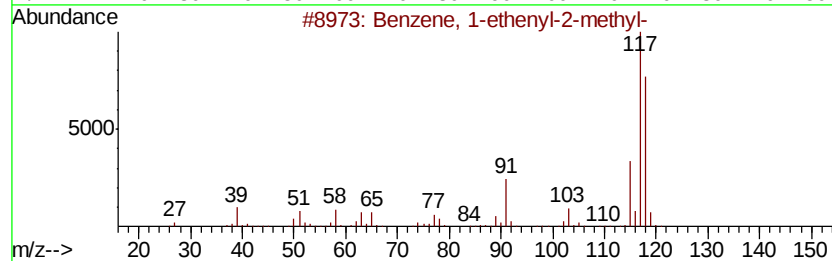
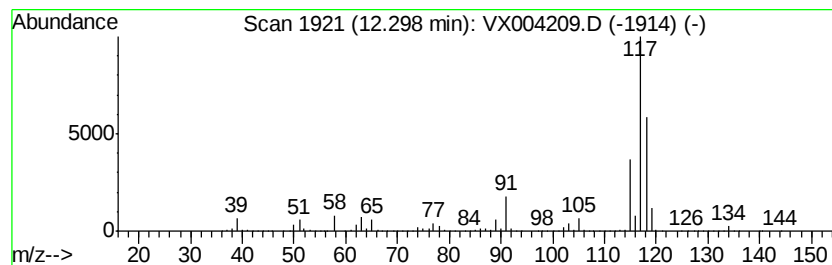
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethenyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	139.02 ug/l	4870890	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
2		Indane	118	C9H10	000496-11-7	81
3		Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4		Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
5		Deltacyclene	118	C9H10	007785-10-6	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082218\
Data File : VX004209.D
Acq On : 22 Aug 2018 19:57
Operator : JC/MD
Sample : J4579-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FL-0544

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.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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Butane, 2,3-dimet...	2.84	71.7	ug/l	2594890	1	5.67	1809500	50.0
Cyclopentane, met...	4.39	247.4	ug/l	8955160	1	5.67	1809500	50.0
Butane, 2,2,3,3-t...	6.35	132.2	ug/l	2845480	2	6.86	1076560	50.0
Pentane, 2,3,4-tr...	8.06	73.3	ug/l	1579270	2	6.86	1076560	50.0
Pentane, 2,3,3-tr...	8.18	126.1	ug/l	2714040	2	6.86	1076560	50.0
Benzene, 1-ethyl-...	11.44	233.6	ug/l	8184370	4	12.08	1751820	50.0
Benzene, 1-ethyl-...	11.67	144.9	ug/l	5075780	4	12.08	1751820	50.0
Benzene, 1,2,3-tr...	12.15	228.3	ug/l	7997260	4	12.08	1751820	50.0
Benzene, 1-etheny...	12.30	139.0	ug/l	4870890	4	12.08	1751820	50.0