

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX051518\
 Data File : VX001726.D
 Acq On : 14 May 2018 23:10
 Operator : JC/MD
 Sample : J2833-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-4

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\82X051518W.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	87	rBV	950863	1156941	83.62%	6.106%
2	1.136	87	90	93	rVV	87894	91251	6.60%	0.482%
3	1.173	93	96	108	rVB	391989	403035	29.13%	2.127%
4	1.301	113	117	120	rBV	90895	79776	5.77%	0.421%
5	1.362	120	127	128	rBV2	33346	73137	5.29%	0.386%
6	1.404	130	134	139	rVB	164854	175555	12.69%	0.927%
7	1.794	193	198	210	rVB	537687	771055	55.73%	4.070%
8	2.002	227	232	244	rVB2	87512	167454	12.10%	0.884%
9	2.118	247	251	257	rBV2	12807	19689	1.42%	0.104%
10	2.270	271	276	285	rVB	92496	145151	10.49%	0.766%
11	2.392	291	296	301	rBV2	11075	20208	1.46%	0.107%
12	2.453	302	306	310	rVV	10113	13934	1.01%	0.074%
13	2.624	330	334	342	rVB	14686	26599	1.92%	0.140%
14	2.892	374	378	379	rBV	11619	17812	1.29%	0.094%
15	2.934	379	385	397	rVB2	111631	268028	19.37%	1.415%
16	3.081	404	409	416	rVB2	8544	18108	1.31%	0.096%
17	3.172	418	424	427	rBV	20629	44419	3.21%	0.234%
18	3.392	453	460	469	rBV5	11315	27587	1.99%	0.146%
19	3.812	522	529	534	rBV	25856	59998	4.34%	0.317%
20	3.879	534	540	543	rBV2	18381	37058	2.68%	0.196%
21	3.995	553	559	568	rVB	11298	26833	1.94%	0.142%
22	4.081	569	573	583	rVB2	7545	18120	1.31%	0.096%
23	4.196	583	592	602	rVB3	20308	56321	4.07%	0.297%
24	4.398	612	625	638	rBV2	81107	239294	17.30%	1.263%
25	4.526	638	646	657	rVB2	16237	48455	3.50%	0.256%
26	5.300	764	773	788	rVB2	28394	88061	6.36%	0.465%
27	5.507	795	807	815	rBV2	175399	504971	36.50%	2.665%
28	5.672	825	834	849	rVB	259172	723688	52.31%	3.820%
29	6.074	889	900	905	rBV	183742	466546	33.72%	2.462%
30	6.147	905	912	927	rVV	503787	1358922	98.22%	7.172%
31	6.306	930	938	945	rVV2	23834	73786	5.33%	0.389%
32	6.397	947	953	961	rVV2	13916	42497	3.07%	0.224%
33	6.464	961	964	976	rVB9	6230	15541	1.12%	0.082%
34	6.867	1020	1030	1041	rBV	367779	885628	64.01%	4.674%

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Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

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 Title : SW846 8260

35	7.257	1087	1094	1105	rVB3	14069	32097	2.32%	0.169%
36	7.464	1118	1128	1135	rBV4	10268	27706	2.00%	0.146%
37	8.214	1245	1251	1257	rBV	24193	41962	3.03%	0.221%
38	8.574	1305	1310	1320	rVB2	25547	52446	3.79%	0.277%
39	8.720	1327	1334	1341	rBV	892090	1383571	100.00%	7.302%
40	8.787	1341	1345	1357	rVB	215524	354888	25.65%	1.873%
41	10.116	1554	1563	1577	rBV	700950	997750	72.11%	5.266%
42	10.256	1581	1586	1597	rVV	922294	1185117	85.66%	6.255%
43	10.366	1598	1604	1617	rVB	950057	1306427	94.42%	6.895%
44	10.701	1651	1659	1671	rVB	351925	478130	34.56%	2.524%
45	11.024	1706	1712	1719	rVB	64221	85996	6.22%	0.454%
46	11.140	1725	1731	1744	rBV	732431	972176	70.27%	5.131%
47	11.366	1763	1768	1774	rBV2	54243	70500	5.10%	0.372%
48	11.439	1775	1780	1788	rVV	170465	315169	22.78%	1.663%
49	11.512	1788	1792	1797	rVB	122098	146913	10.62%	0.775%
50	11.671	1813	1818	1830	rVB	190227	245558	17.75%	1.296%
51	11.811	1836	1841	1850	rVB	497466	616355	44.55%	3.253%
52	12.085	1880	1886	1892	rVV	963244	1196783	86.50%	6.317%
53	12.146	1892	1896	1906	rVB	198882	249830	18.06%	1.319%
54	12.305	1913	1922	1930	rBV	338400	433728	31.35%	2.289%
55	12.378	1930	1934	1942	rVB3	28567	46336	3.35%	0.245%
56	12.475	1944	1950	1954	rBV2	10617	16056	1.16%	0.085%
57	12.591	1964	1969	1971	rBV	14897	19525	1.41%	0.103%
58	12.677	1978	1983	1986	rBV	24918	30955	2.24%	0.163%
59	12.762	1992	1997	2003	rBV	40368	55715	4.03%	0.294%
60	12.981	2028	2033	2036	rVV2	16845	25165	1.82%	0.133%
61	13.024	2036	2040	2045	rVB	24601	29685	2.15%	0.157%
62	13.231	2070	2074	2078	rBV	20262	24465	1.77%	0.129%
63	13.353	2090	2094	2099	rVV2	48937	66306	4.79%	0.350%
64	13.487	2111	2116	2122	rVB3	10897	15640	1.13%	0.083%
65	13.652	2139	2143	2148	rVB6	9342	14122	1.02%	0.075%
66	13.841	2167	2174	2182	rVB	141687	176234	12.74%	0.930%
67	13.932	2182	2189	2194	rBV	10473	16081	1.16%	0.085%
68	14.701	2312	2315	2321	rVB	12269	15325	1.11%	0.081%
69	14.847	2334	2339	2344	rBV3	12166	16599	1.20%	0.088%
70	16.426	2592	2598	2604	rBV2	11668	19981	1.44%	0.105%

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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

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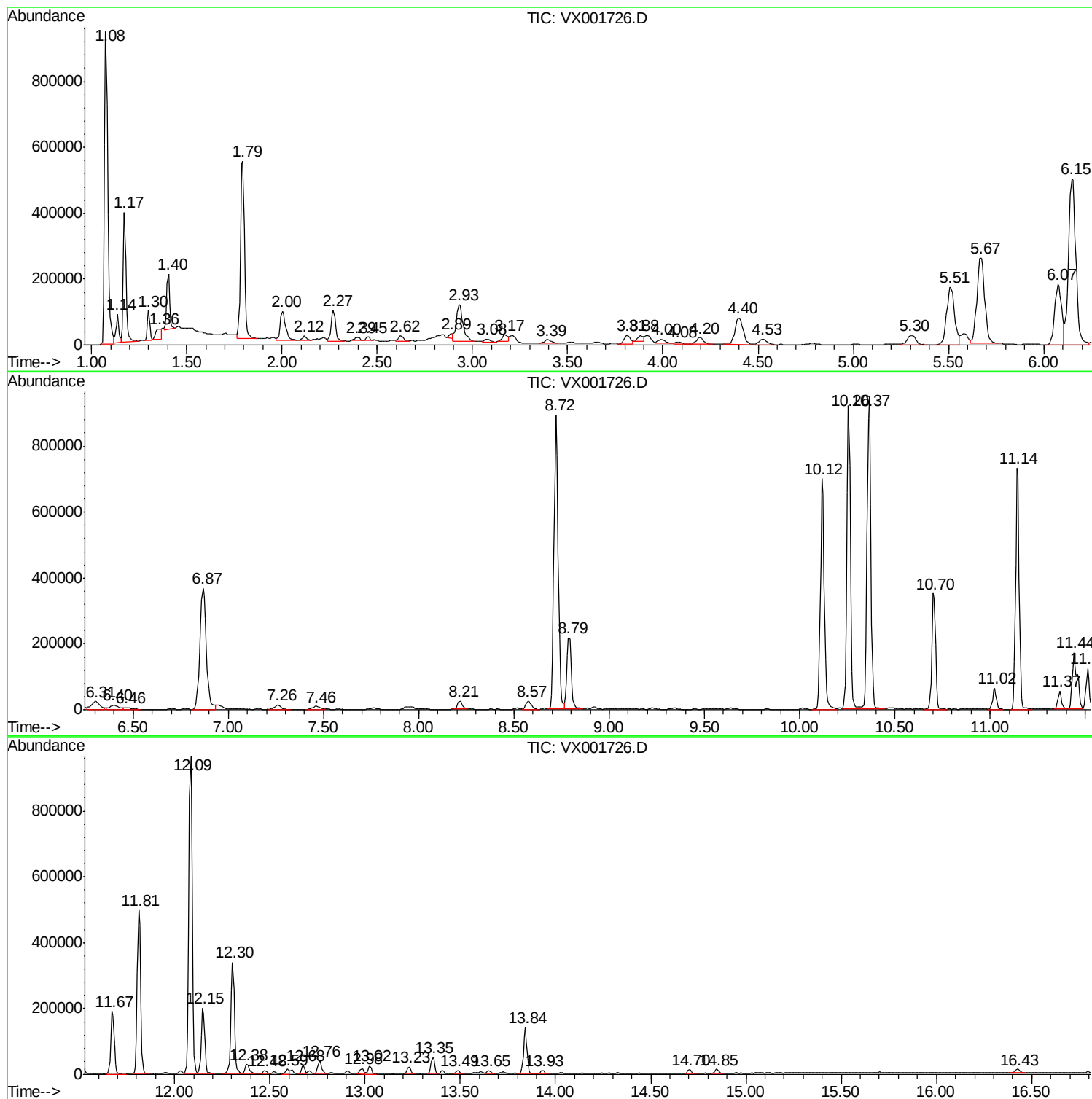
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ClientSampled :
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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X051518W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
ClientSampleId :
MW-4

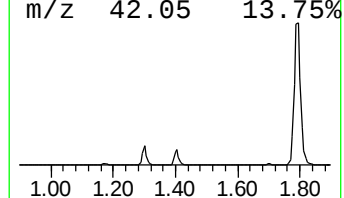
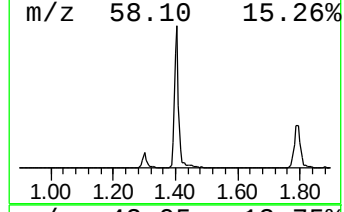
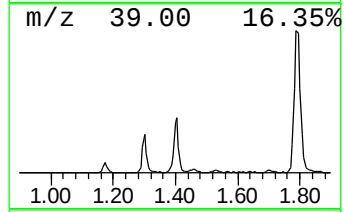
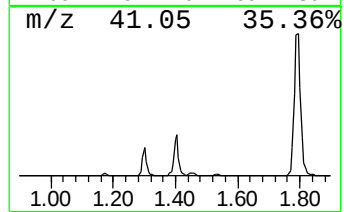
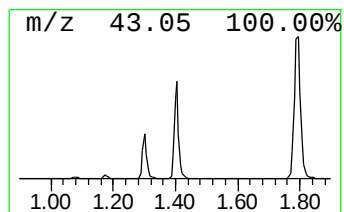
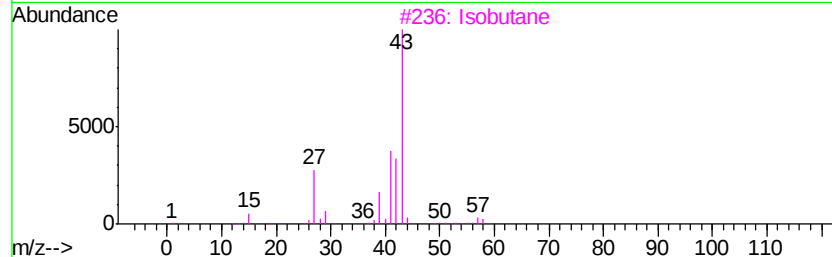
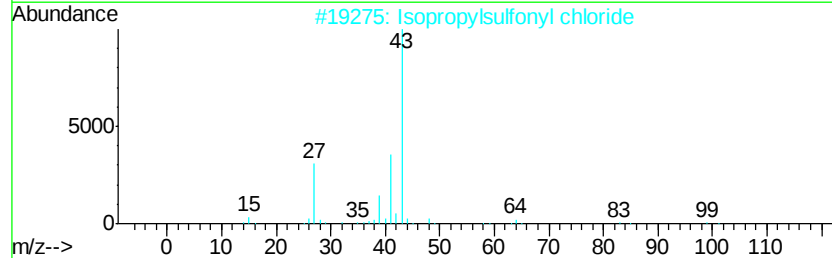
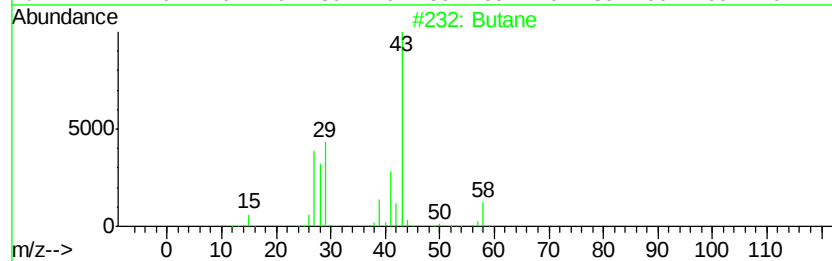
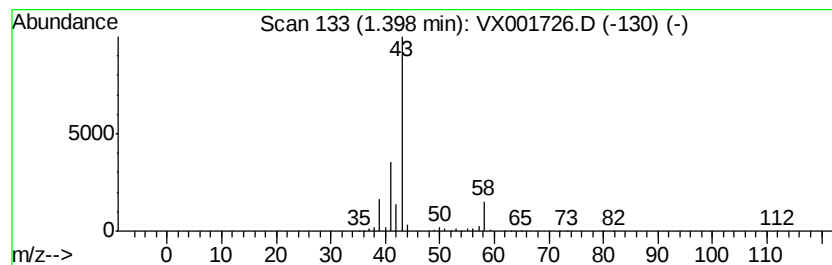
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X051518W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	12.13 ug/l	175555	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane		58	C4H10	000106-97-8	72
2	Isopropylsulfonyl chloride		142	C3H7ClO2S	010147-37-2	9
3	Isobutane		58	C4H10	000075-28-5	9
4	Propane, 1-nitro-		89	C3H7NO2	000108-03-2	9
5	Allyl acetate		100	C5H8O2	000591-87-7	4



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Instrument :
MSVOA_X
ClientSampled :
MW-4

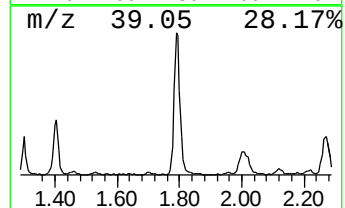
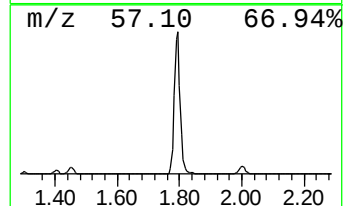
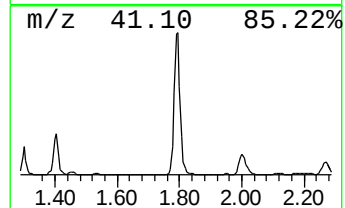
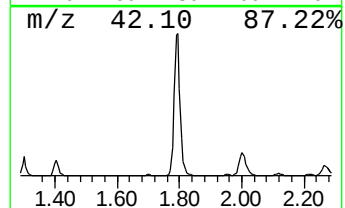
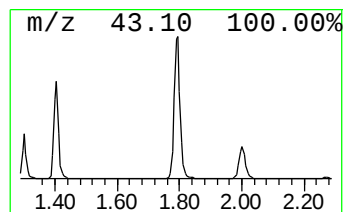
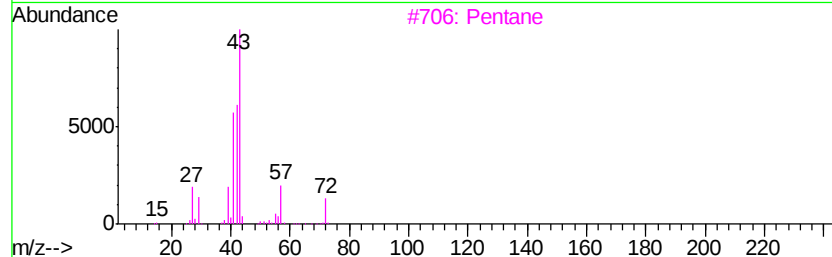
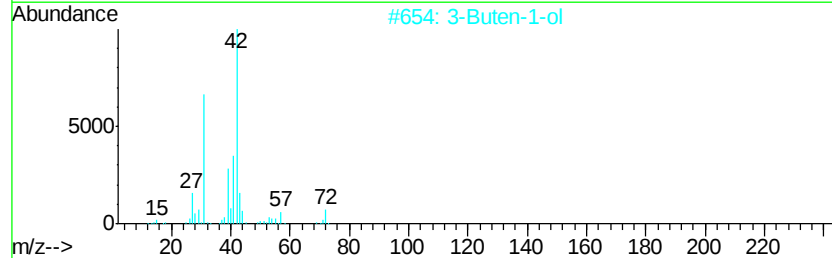
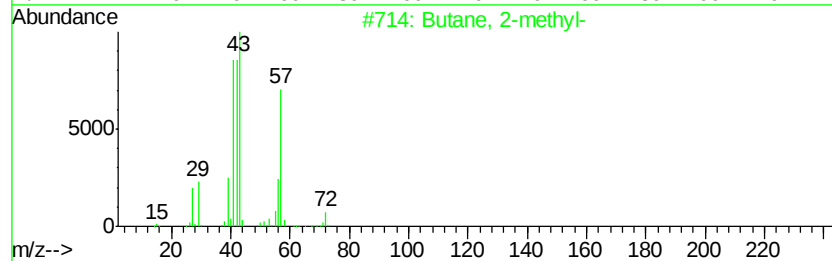
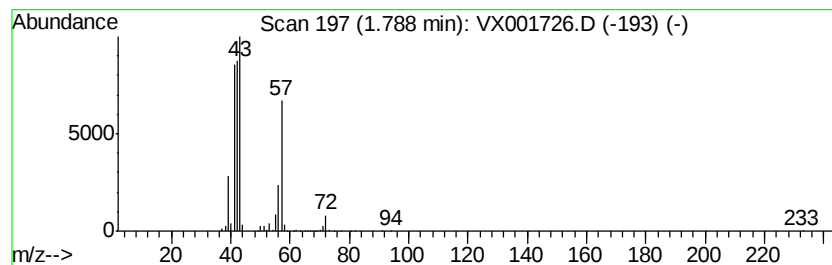
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X051518W.M
Quant Title : SW846 8260

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

Peak Number 4 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	53.27 ug/l	771055	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94	
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47	
3	Pentane	72	C5H12	000109-66-0	36	
4	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	10	
5	Tetrahydrofuran	72	C4H8O	000109-99-9	9	



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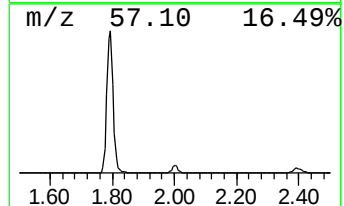
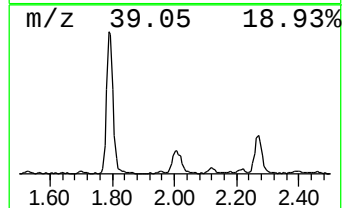
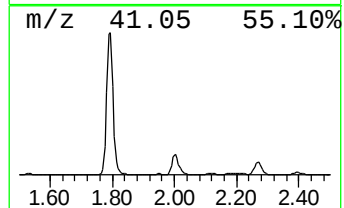
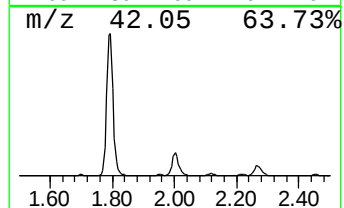
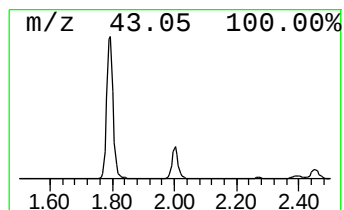
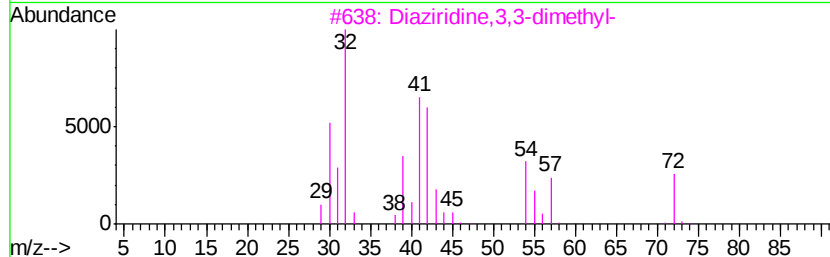
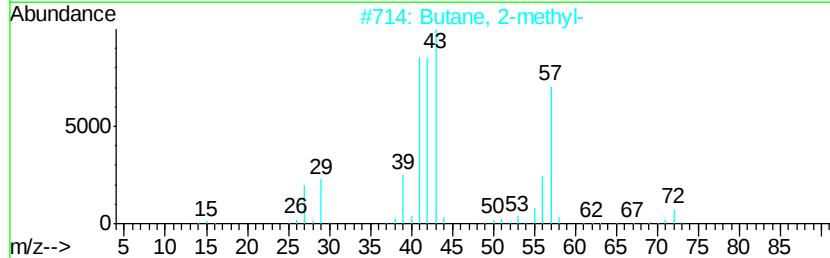
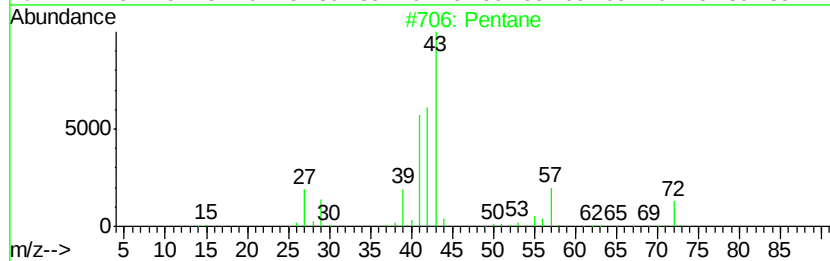
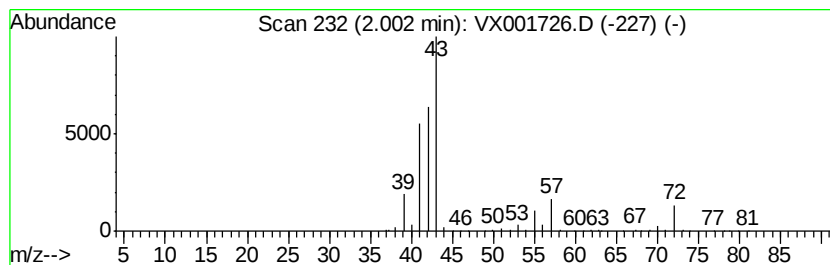
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	11.57 ug/l	167454	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	28
3		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	23
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	12
5		Tetrahydrofuran	72	C4H8O	000109-99-9	9



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ALS Vial : 23 Sample Multiplier: 1

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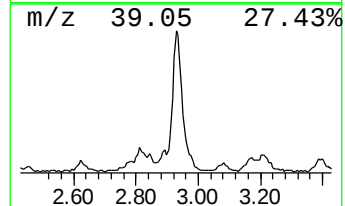
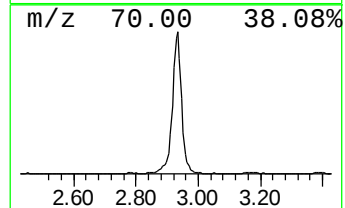
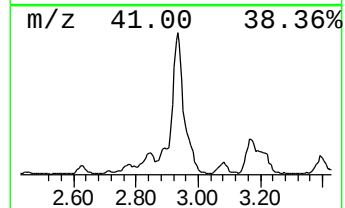
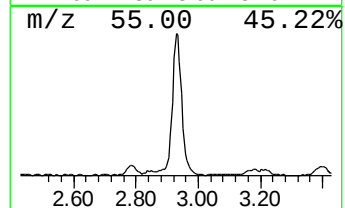
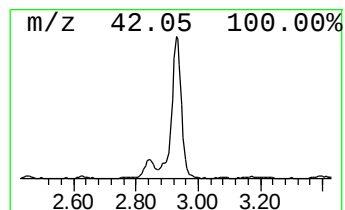
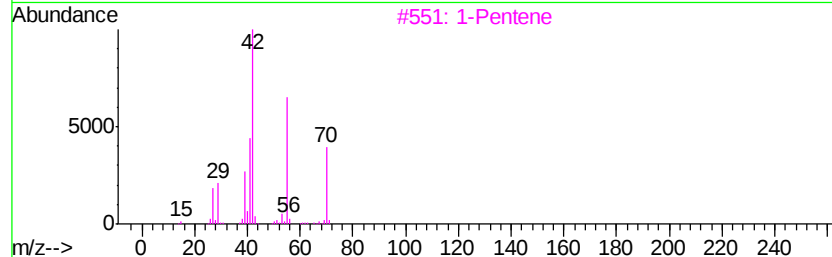
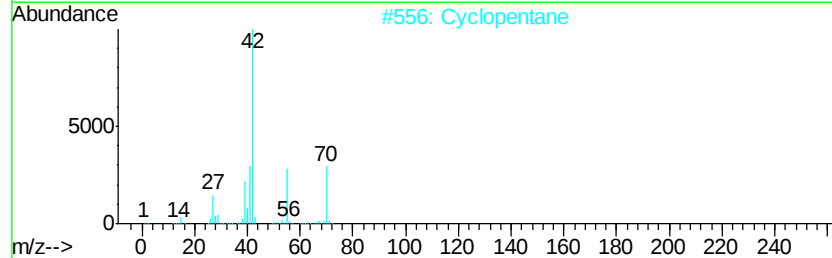
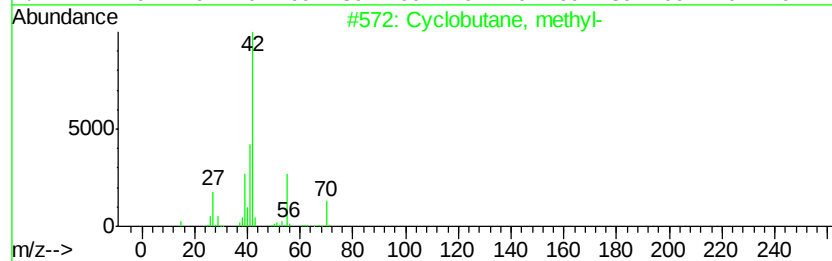
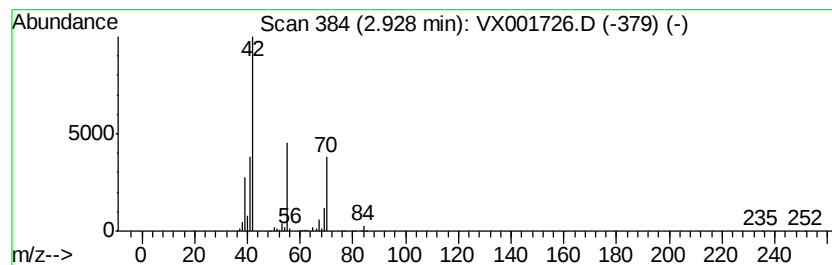
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclobutane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	18.52 ug/l	268028	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2		Cyclopentane	70	C5H10	000287-92-3	72
3		1-Pentene	70	C5H10	000109-67-1	50
4		Cyclopropane, ethyl-	70	C5H10	001191-96-4	45
5		2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	39



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX051518\
Data File : VX001726.D
Acq On : 14 May 2018 23:10
Operator : JC/MD
Sample : J2833-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-4

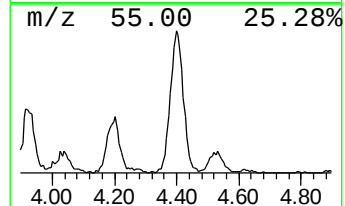
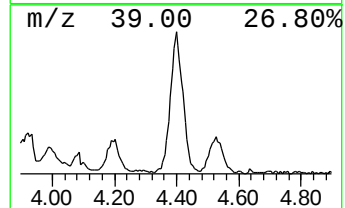
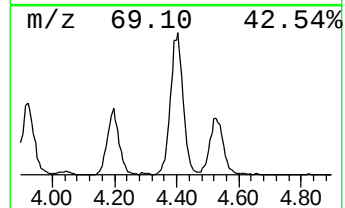
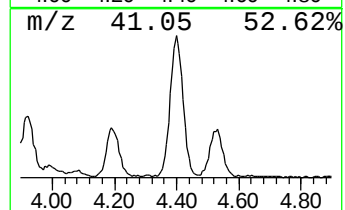
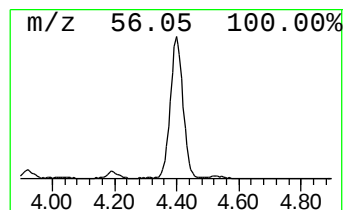
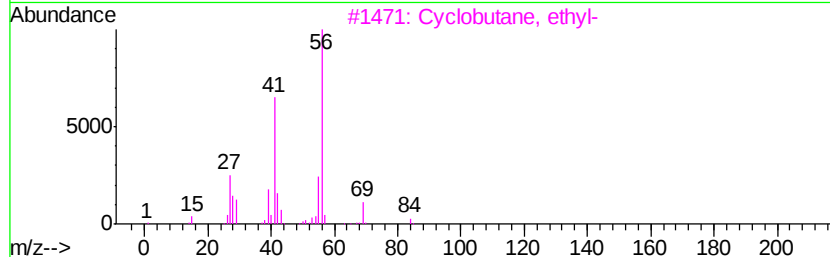
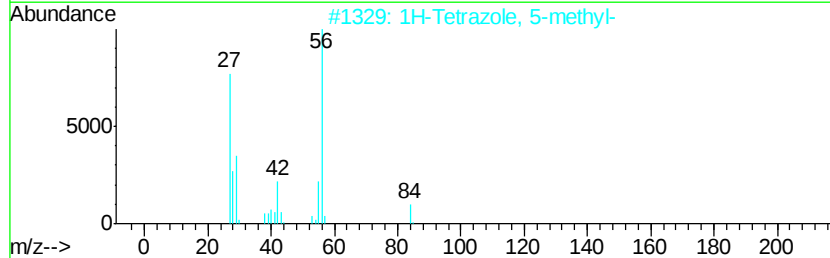
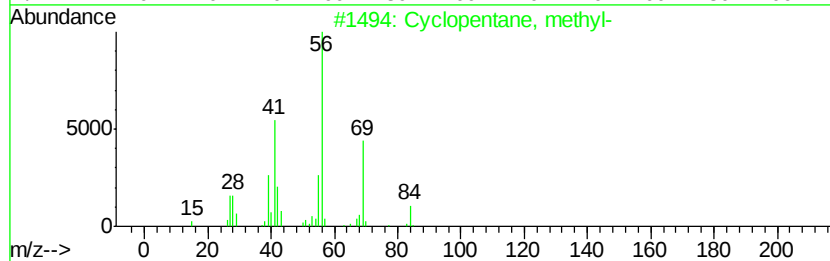
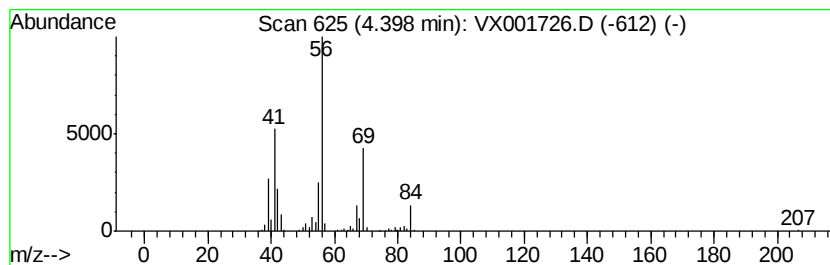
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	16.53 ug/l	239294	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4		Cyclohexane	84	C6H12	000110-82-7	47
5		Cyclobutane	56	C4H8	000287-23-0	47



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX051518\
Data File : VX001726.D
Acq On : 14 May 2018 23:10
Operator : JC/MD
Sample : J2833-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

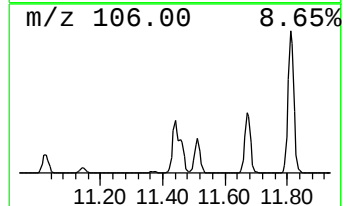
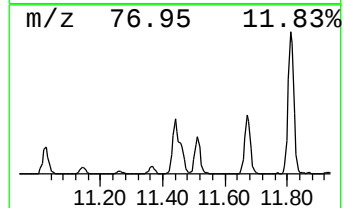
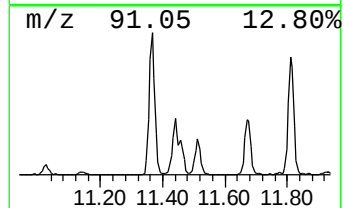
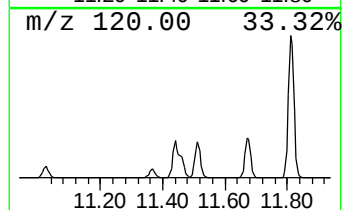
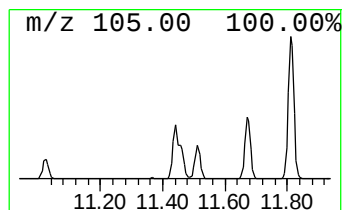
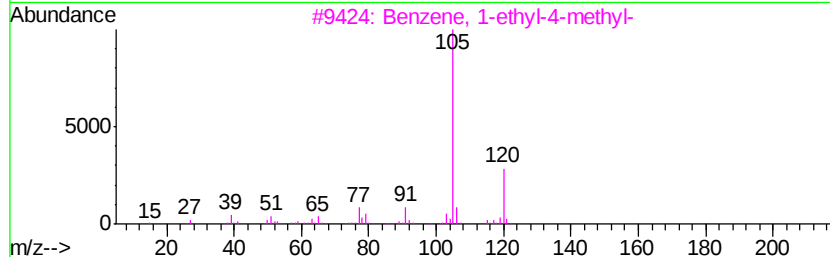
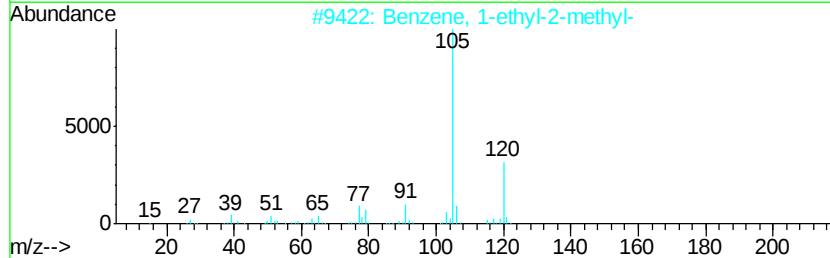
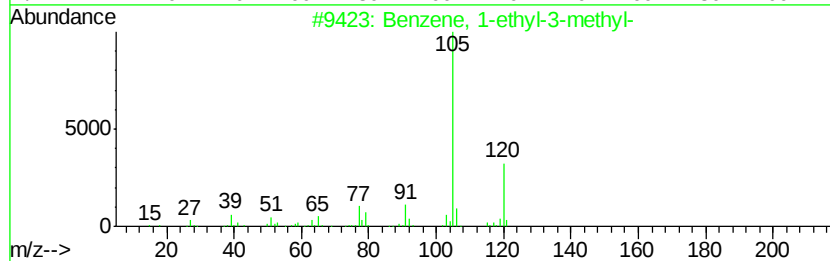
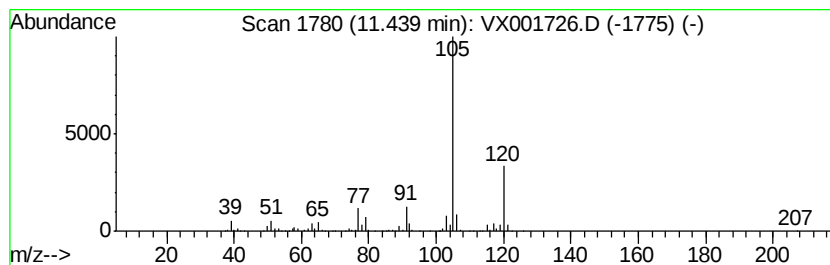
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X051518W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	13.17 ug/l	315169	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX051518\
Data File : VX001726.D
Acq On : 14 May 2018 23:10
Operator : JC/MD
Sample : J2833-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-4

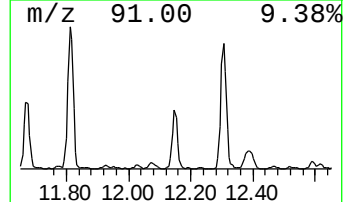
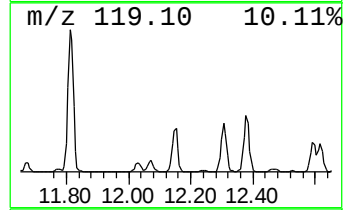
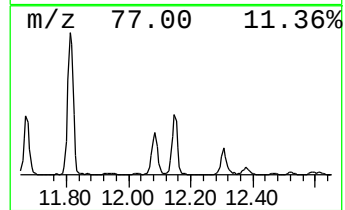
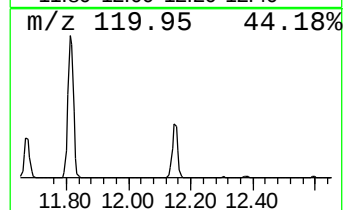
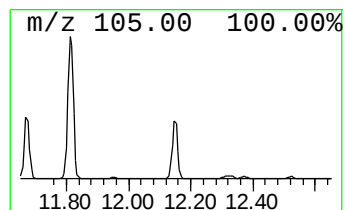
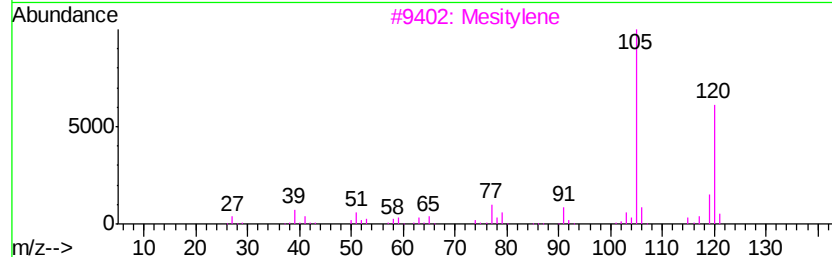
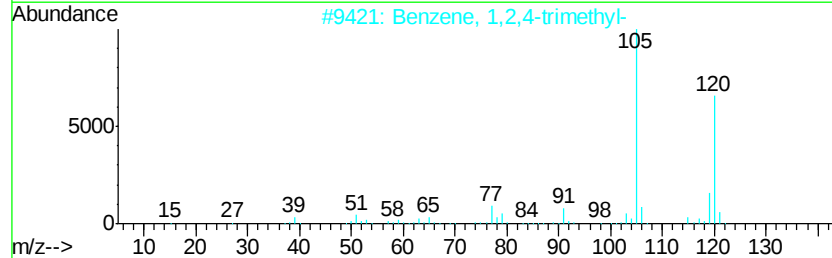
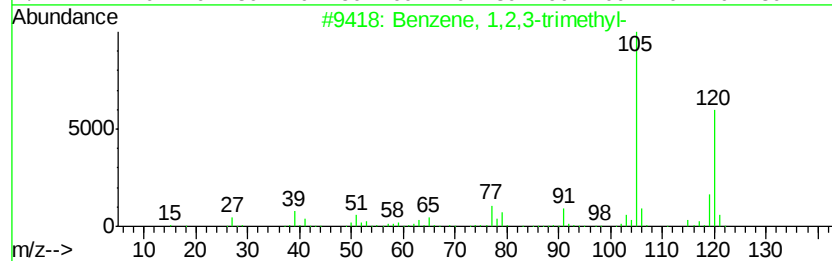
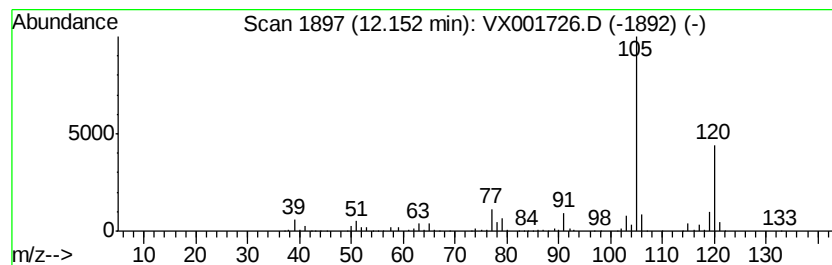
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X051518W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	10.44 ug/l	249830	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3		Mesitylene	120	C9H12	000108-67-8	93
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : W:\HPCHEM1\MSVOA X\DATA\VX051518\
Data File : VX001726.D
Acq On : 14 May 2018 23:10
Operator : JC/MD
Sample : J2833-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

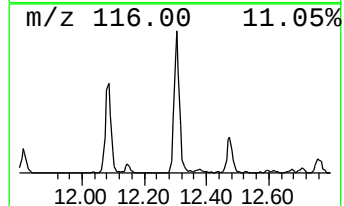
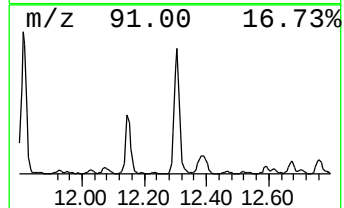
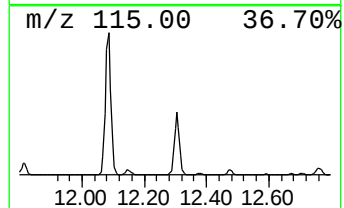
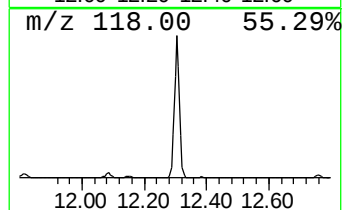
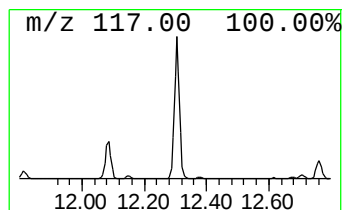
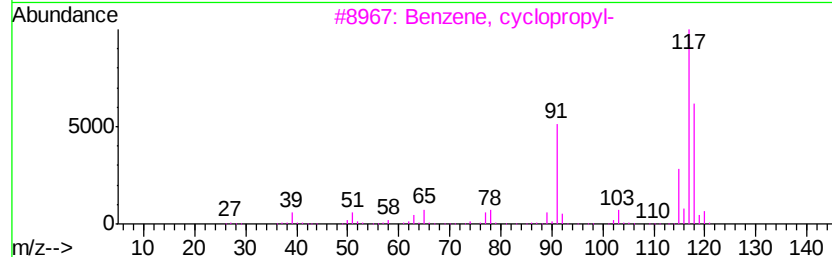
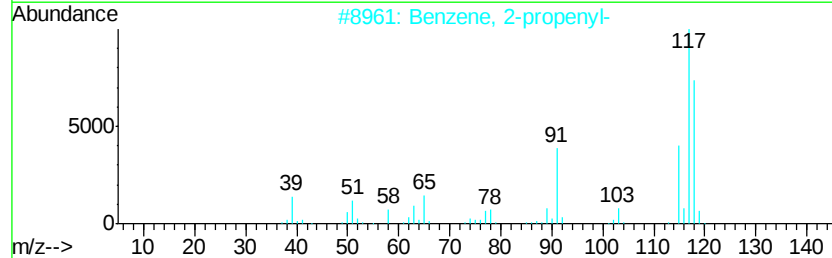
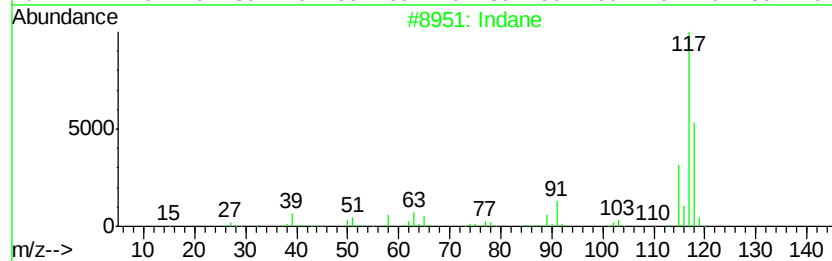
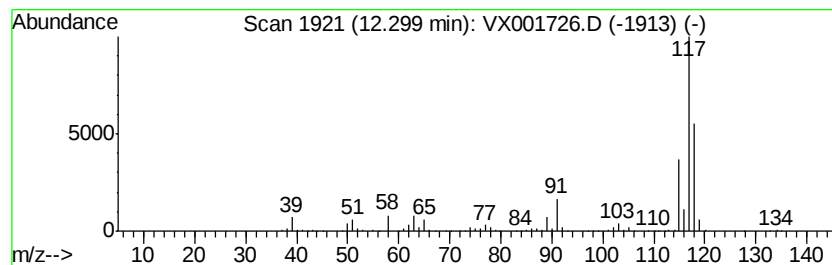
Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X051518W.M
Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	18.12 ug/l	433728	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indane	118	C9H10	000496-11-7	95
2		Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
4		Tetracyclo[3.3.1.0(2,8).0(4,6)]-	118	C9H10	1000191-13-7	80
5		Deltacyclene	118	C9H10	007785-10-6	72



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX051518\
Data File : VX001726.D
Acq On : 14 May 2018 23:10
Operator : JC/MD
Sample : J2833-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X051518W.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	1.40	12.1	ug/l	175555	1	5.67	723688	50.0
Butane, 2-methyl-	1.79	53.3	ug/l	771055	1	5.67	723688	50.0
Pentane	2.00	11.6	ug/l	167454	1	5.67	723688	50.0
Cyclobutane, methyl-	2.93	18.5	ug/l	268028	1	5.67	723688	50.0
Cyclopentane, met...	4.40	16.5	ug/l	239294	1	5.67	723688	50.0
Benzene, 1-ethyl-...	11.44	13.2	ug/l	315169	4	12.09	1196780	50.0
Benzene, 1,2,3-tr...	12.15	10.4	ug/l	249830	4	12.09	1196780	50.0
Indane	12.30	18.1	ug/l	433728	4	12.09	1196780	50.0