

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061319\
 Data File : VX010279.D
 Acq On : 13 Jun 2019 17:46
 Operator : JC/SP
 Sample : K3341-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 14 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 : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.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	1.300	21	24	33	rBV3	50164	89440	5.93%	0.677%
2	1.404	38	41	46	rVV	65966	72082	4.78%	0.545%
3	1.788	99	104	112	rVB	212400	307194	20.36%	2.324%
4	2.001	134	139	148	rVB2	36254	65321	4.33%	0.494%
5	2.263	177	182	192	rVB	30619	54133	3.59%	0.409%
6	2.605	230	238	247	rBV	15385	30252	2.01%	0.229%
7	2.849	270	278	281	rBV2	8299	19012	1.26%	0.144%
8	2.891	281	285	287	rVV2	13096	22371	1.48%	0.169%
9	2.934	287	292	303	rVV2	42297	97323	6.45%	0.736%
10	3.038	305	309	318	rVB2	8371	19177	1.27%	0.145%
11	3.184	323	333	342	rBV3	19104	55572	3.68%	0.420%
12	3.836	430	440	441	rBV2	10935	25076	1.66%	0.190%
13	3.855	441	443	449	rVV2	11319	19752	1.31%	0.149%
14	3.934	449	456	462	rVB6	6730	16306	1.08%	0.123%
15	4.196	490	499	506	rBV4	7964	20854	1.38%	0.158%
16	4.403	522	533	544	rBV2	46073	133765	8.87%	1.012%
17	4.537	547	555	565	rVB6	5255	15889	1.05%	0.120%
18	5.306	671	681	689	rVB2	8127	23955	1.59%	0.181%
19	5.501	700	713	722	rBV2	182788	528644	35.04%	3.999%
20	5.586	722	727	731	rVV3	17647	49075	3.25%	0.371%
21	5.659	731	739	753	rVB	313951	885329	58.68%	6.696%
22	6.062	794	805	812	rBV	169592	449079	29.76%	3.397%
23	6.141	812	818	833	rVB	183920	488591	32.38%	3.696%
24	6.305	837	845	846	rBV3	8262	15862	1.05%	0.120%
25	6.860	924	936	948	rBV	469277	1106601	73.34%	8.370%
26	7.256	993	1001	1009	rVB7	6738	16365	1.08%	0.124%
27	7.470	1023	1036	1047	rBV7	8377	28980	1.92%	0.219%
28	8.214	1152	1158	1164	rBV2	13958	24950	1.65%	0.189%
29	8.567	1211	1216	1225	rVB2	16379	29734	1.97%	0.225%
30	8.713	1233	1240	1247	rBV	967123	1508794	100.00%	11.412%
31	8.787	1247	1252	1261	rVB	89795	146463	9.71%	1.108%
32	10.110	1459	1469	1482	rBV	961011	1299482	86.13%	9.829%
33	10.250	1487	1492	1499	rVV	406022	528505	35.03%	3.998%
34	10.360	1503	1510	1519	rVB	433137	601852	39.89%	4.552%

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35	10.695	1560	1565	1571	rBV	182601	238501	15.81%	1.804%
36	11.018	1612	1618	1622	rBV	44195	58333	3.87%	0.441%
37	11.134	1632	1637	1649	rBV	809146	1028650	68.18%	7.780%
38	11.359	1667	1674	1681	rBV	35156	47354	3.14%	0.358%
39	11.432	1681	1686	1688	rBV	104649	139100	9.22%	1.052%
40	11.506	1694	1698	1705	rVB	76152	93578	6.20%	0.708%
41	11.664	1719	1724	1733	rBV	135760	168257	11.15%	1.273%
42	11.804	1742	1747	1752	rBV	351053	414379	27.46%	3.134%
43	12.073	1786	1791	1797	rBV	936262	1235478	81.89%	9.345%
44	12.140	1797	1802	1807	rVB	142544	171751	11.38%	1.299%
45	12.298	1821	1828	1836	rVB	200694	264427	17.53%	2.000%
46	12.371	1836	1840	1846	rVB2	20956	29278	1.94%	0.221%
47	12.463	1850	1855	1860	rBV6	8979	15787	1.05%	0.119%
48	12.585	1871	1875	1877	rBV	13097	16957	1.12%	0.128%
49	12.670	1885	1889	1891	rBV	22900	30196	2.00%	0.228%
50	12.755	1898	1903	1907	rBV	39608	51440	3.41%	0.389%
51	12.902	1923	1927	1933	rBV3	11412	17497	1.16%	0.132%
52	12.975	1936	1939	1942	rVV	16017	20184	1.34%	0.153%
53	13.018	1942	1946	1950	rVB	21918	28356	1.88%	0.214%
54	13.225	1976	1980	1984	rVB	19639	23388	1.55%	0.177%
55	13.347	1996	2000	2006	rVB2	49431	63317	4.20%	0.479%
56	13.481	2012	2022	2031	rBV9	15065	39804	2.64%	0.301%
57	13.835	2075	2080	2086	rVB	104996	131911	8.74%	0.998%
58	14.365	2162	2167	2174	rBV7	7644	19048	1.26%	0.144%
59	14.694	2218	2221	2225	rVB	14467	17407	1.15%	0.132%
60	15.554	2356	2362	2370	rVB6	19861	40780	2.70%	0.308%
61	16.456	2507	2510	2517	rVB3	11542	19943	1.32%	0.151%

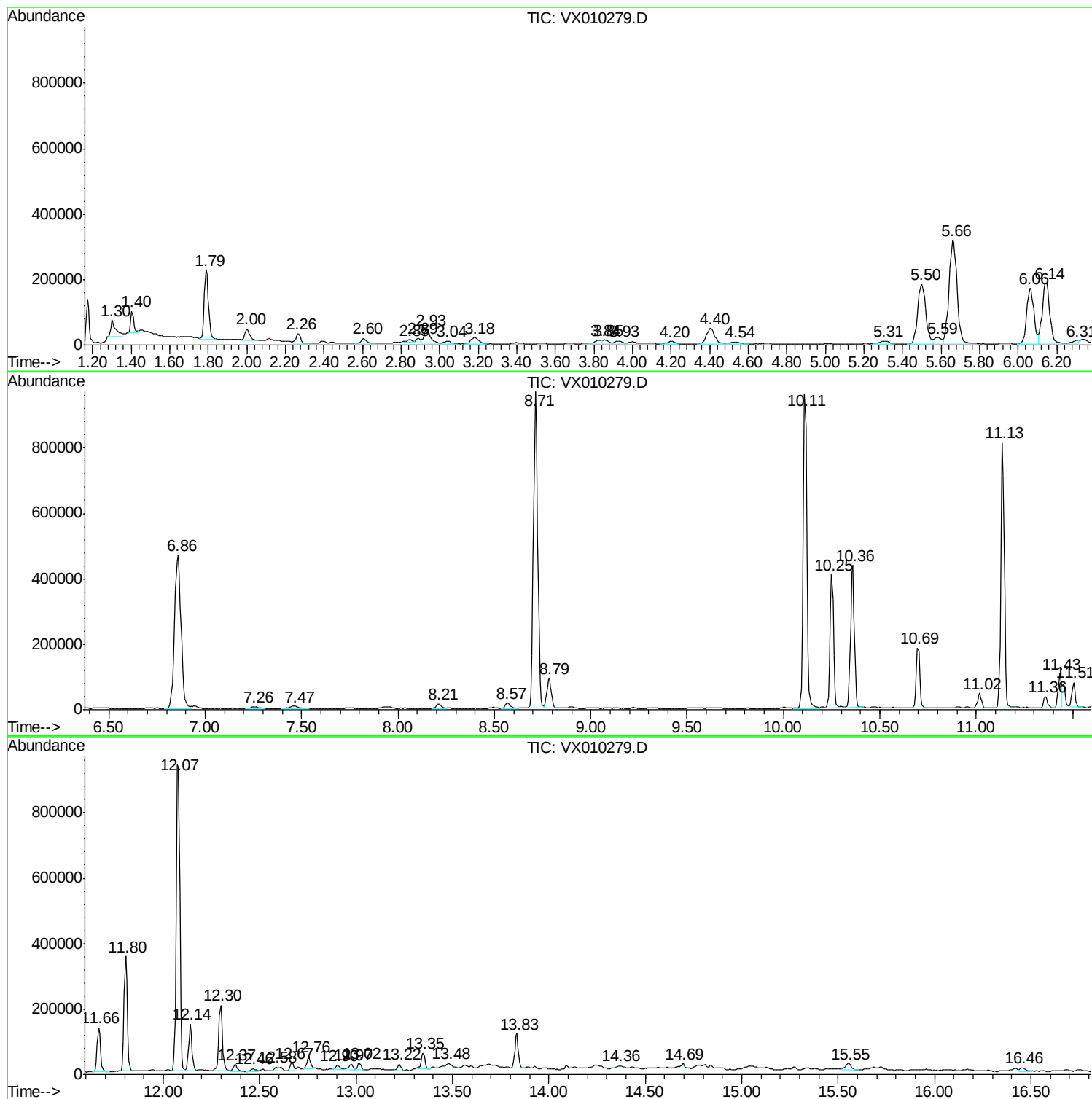
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampled :
MW-4

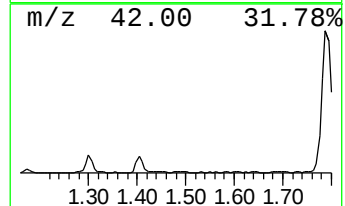
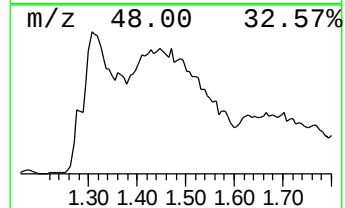
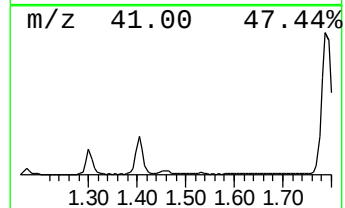
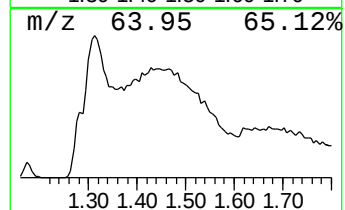
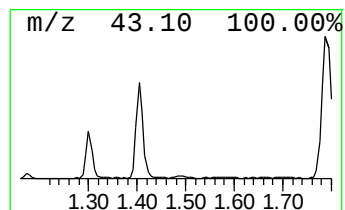
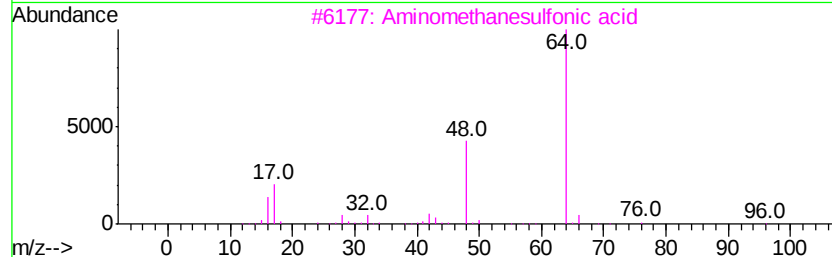
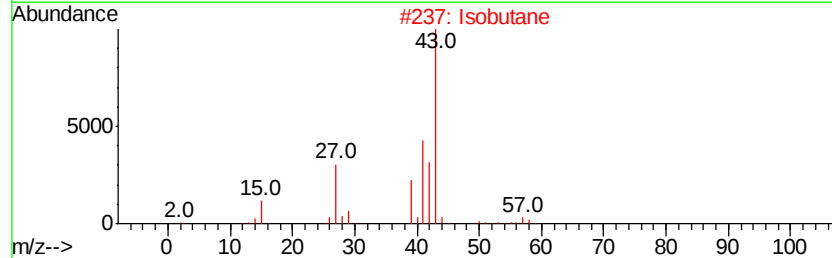
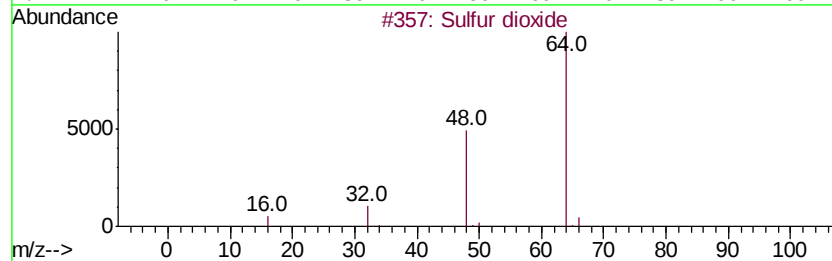
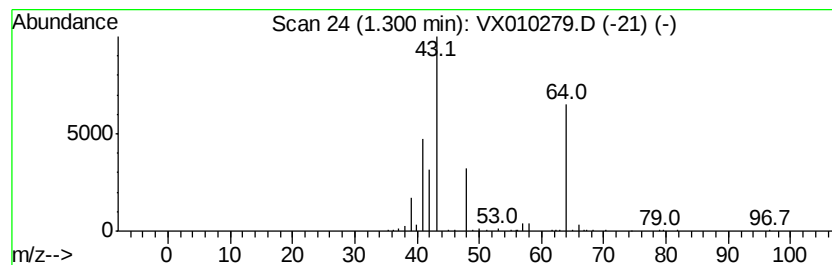
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.30 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	5.05 ug/l	89440	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	45
2			Isobutane	58	C4H10	000075-28-5	10
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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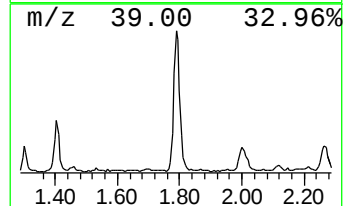
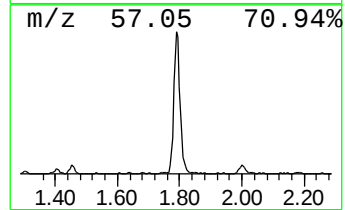
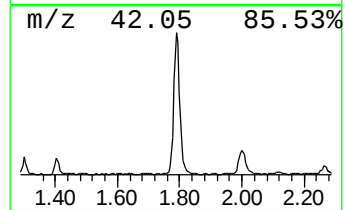
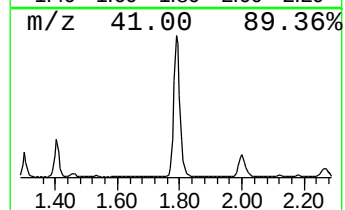
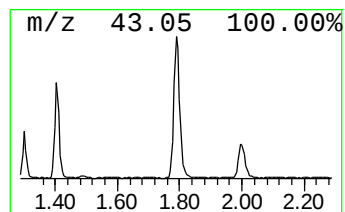
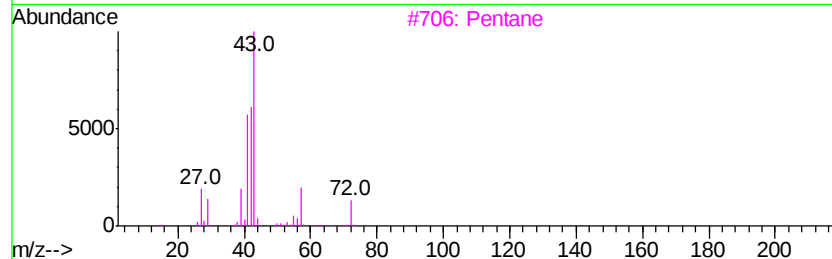
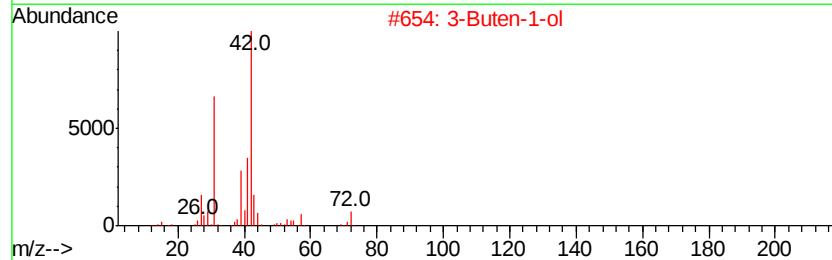
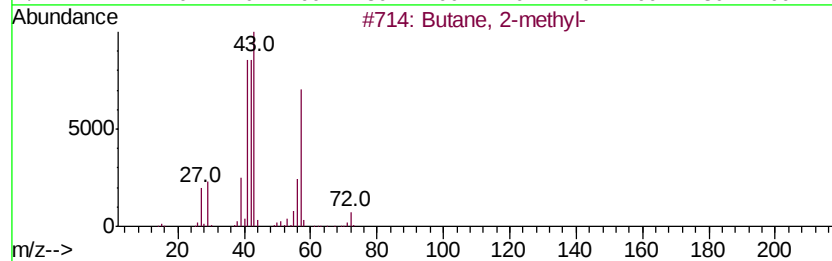
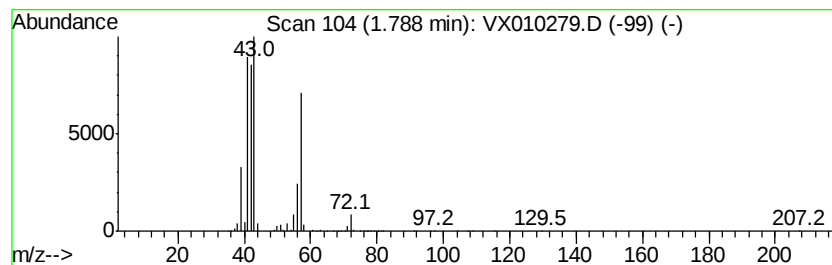
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	17.35 ug/l	307194	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	38
4		2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25
5		1-Butene	56	C4H8	000106-98-9	10



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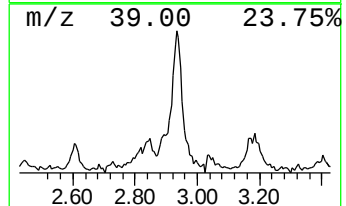
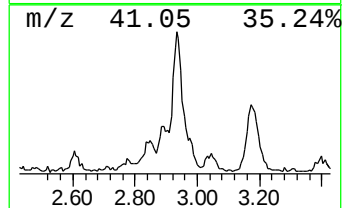
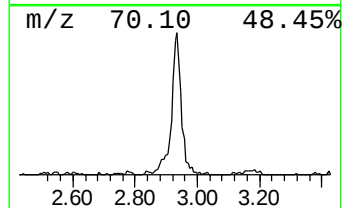
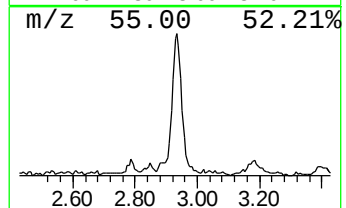
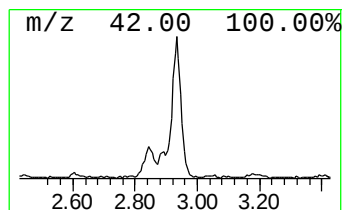
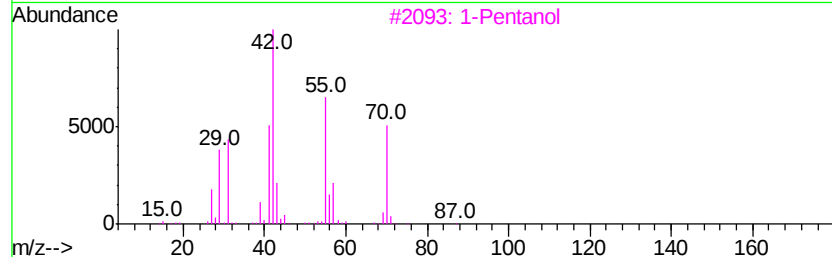
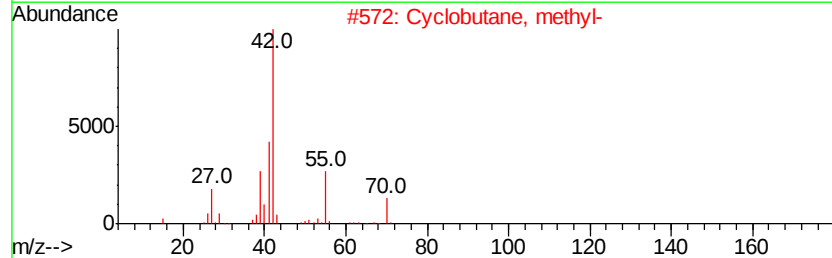
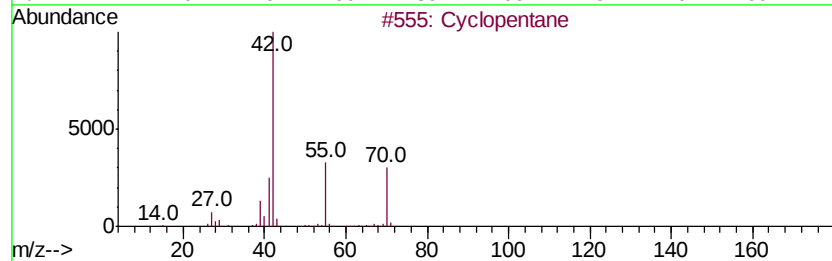
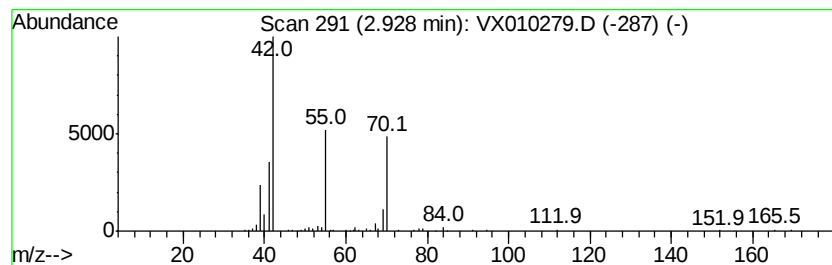
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Peak Number 3 Cyclopentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	5.50 ug/l	97323	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane	70	C5H10	000287-92-3	72
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	64
3		1-Pentanol	88	C5H12O	000071-41-0	56
4		2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	50
5		1-Pentene	70	C5H10	000109-67-1	38



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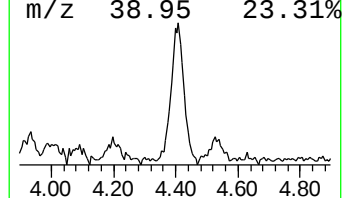
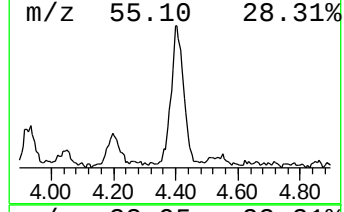
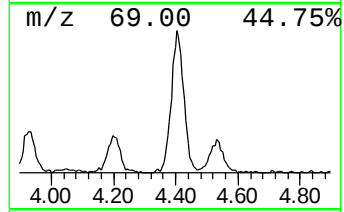
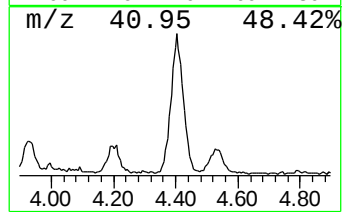
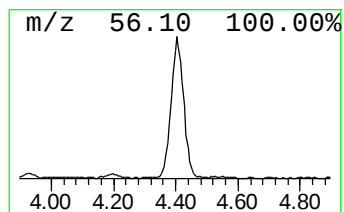
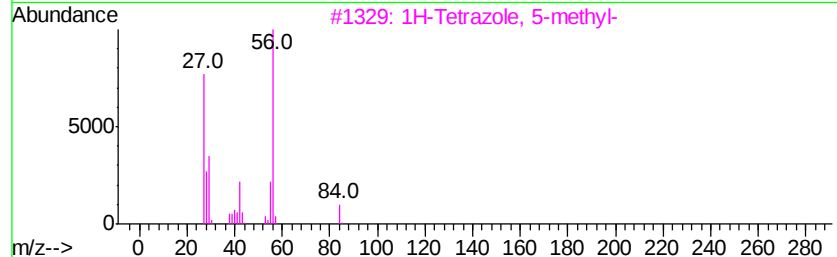
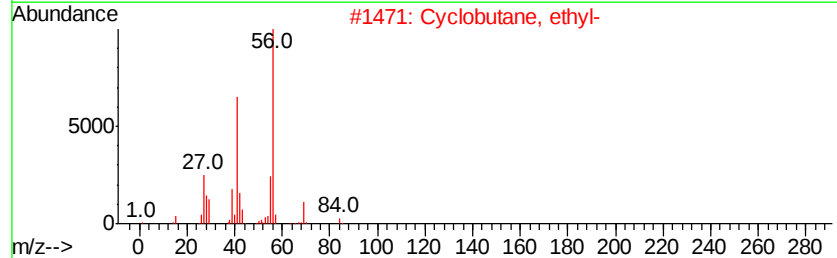
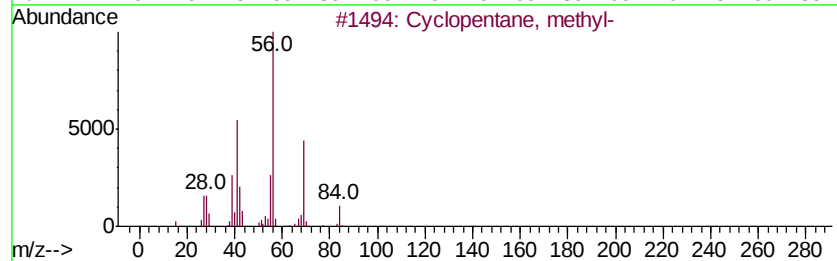
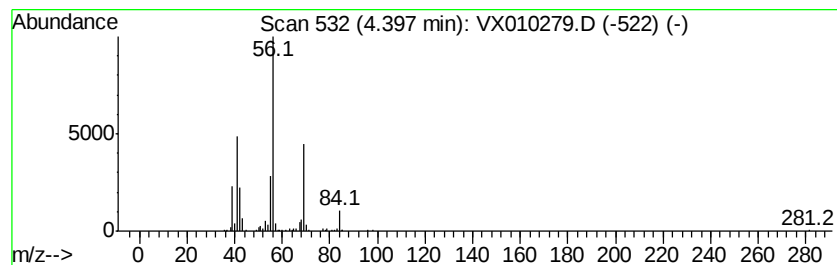
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	7.55 ug/l	133765	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		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	45



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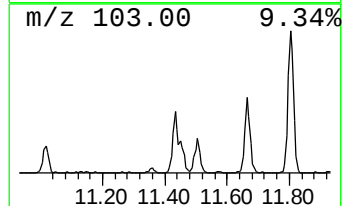
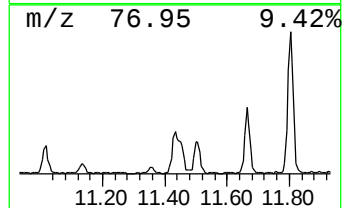
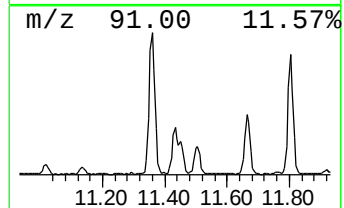
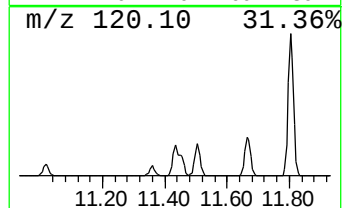
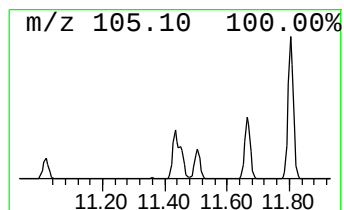
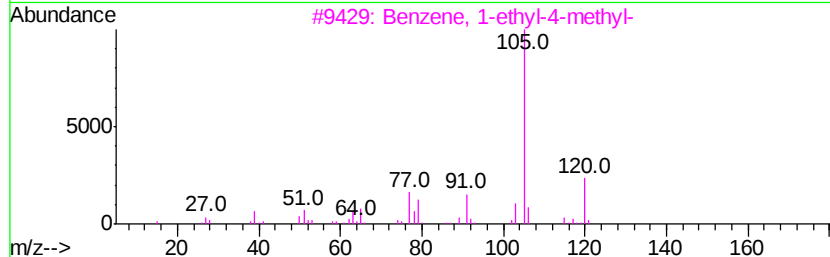
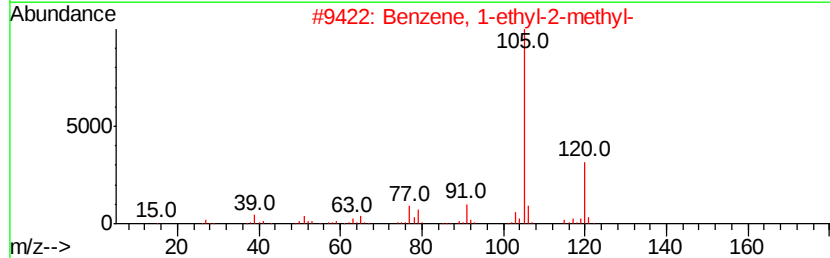
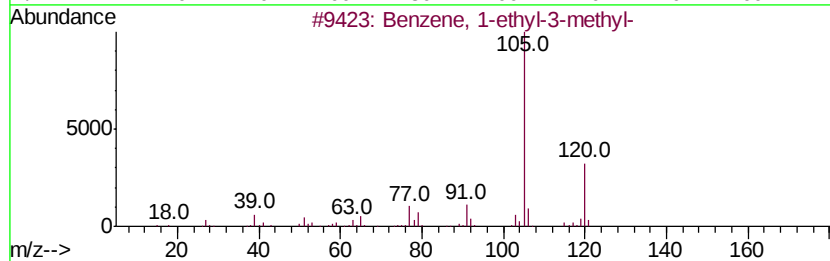
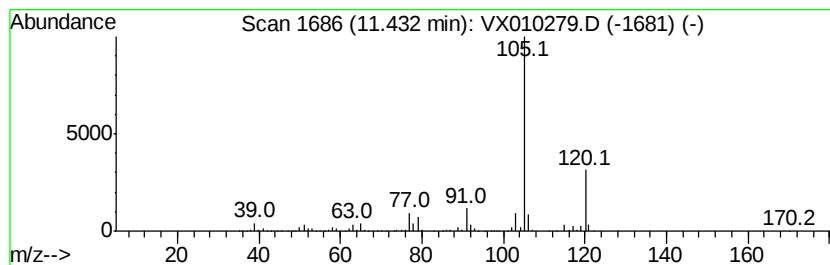
Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	5.63 ug/l	139100	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		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-ethyl-4-methyl-	120 C9H12	000622-96-8 91
4		Mesitylene	120 C9H12	000108-67-8 91
5		Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8 91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061319\
Data File : VX010279.D
Acq On : 13 Jun 2019 17:46
Operator : JC/SP
Sample : K3341-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

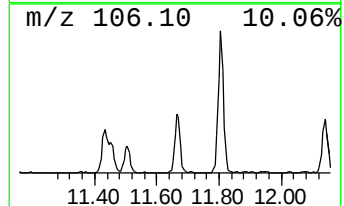
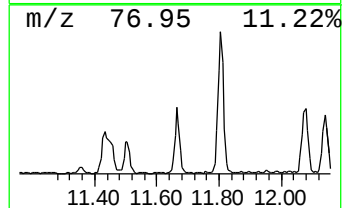
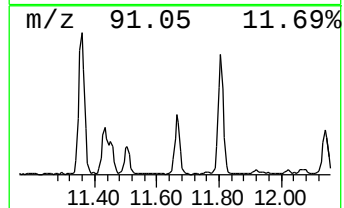
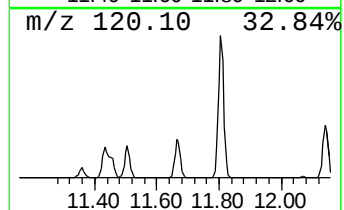
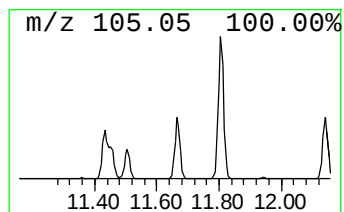
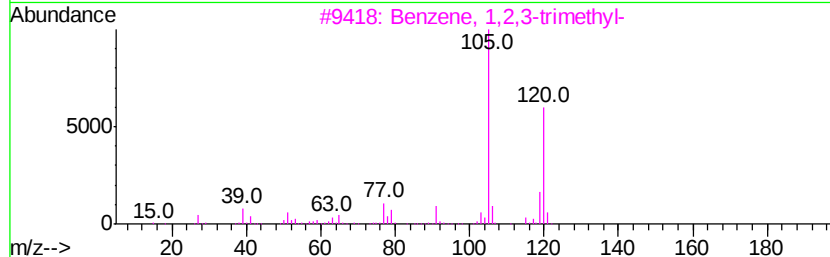
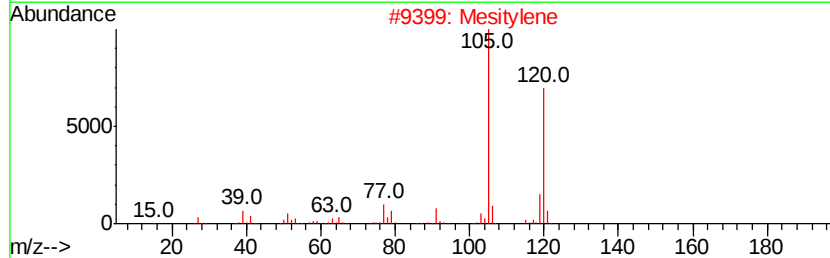
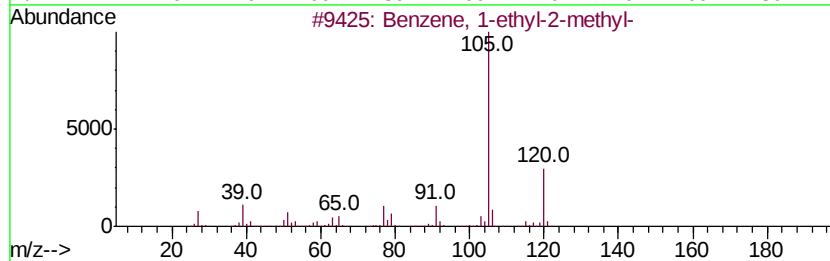
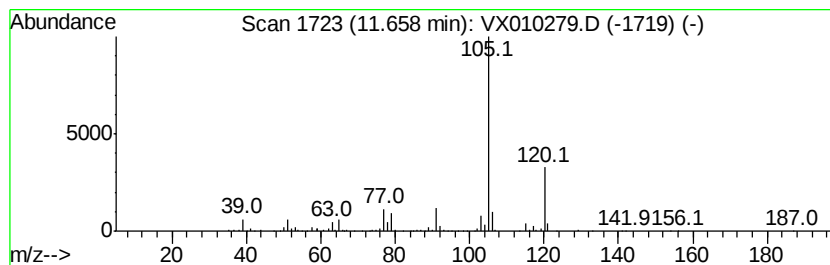
Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.66	6.81 ug/l	168257	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061319\
Data File : VX010279.D
Acq On : 13 Jun 2019 17:46
Operator : JC/SP
Sample : K3341-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
MW-4

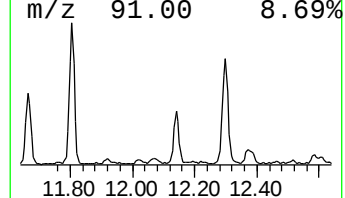
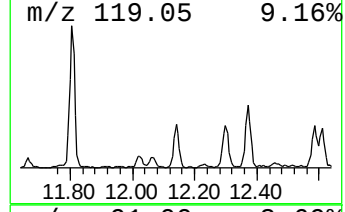
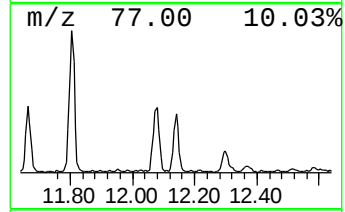
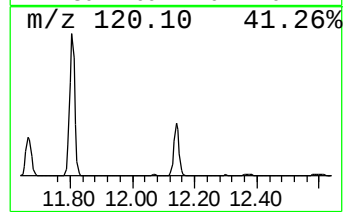
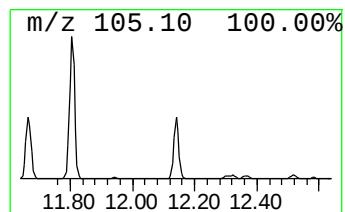
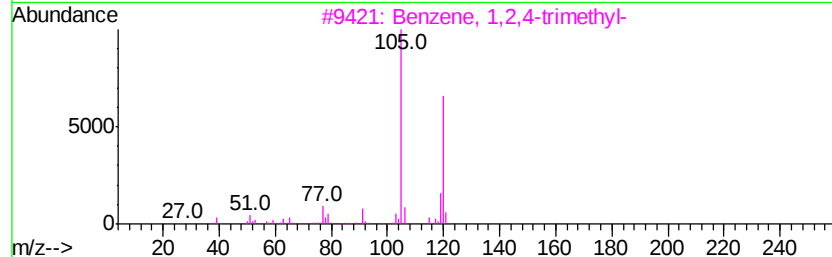
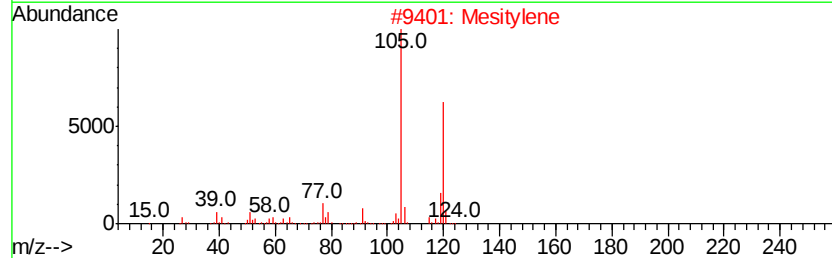
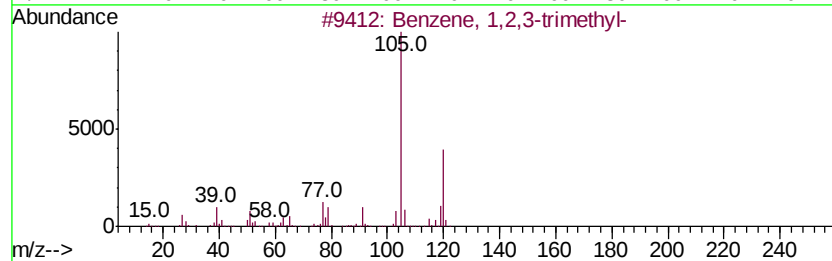
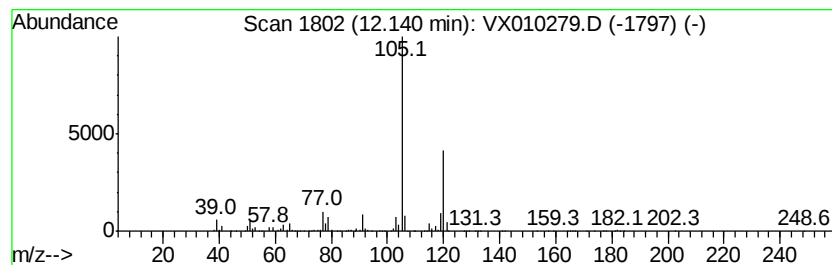
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	6.95 ug/l	171751	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	94
2		Mesitylene	120	C9H12	000108-67-8	93
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061319\
Data File : VX010279.D
Acq On : 13 Jun 2019 17:46
Operator : JC/SP
Sample : K3341-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

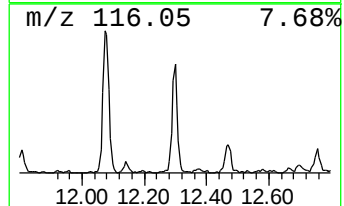
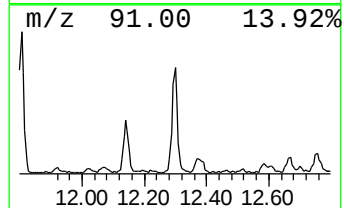
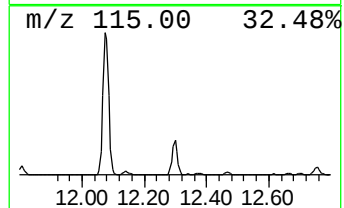
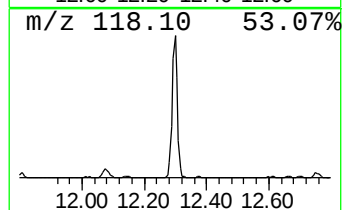
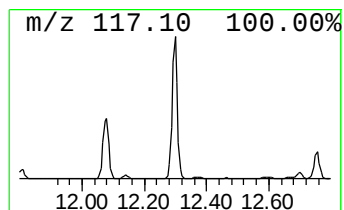
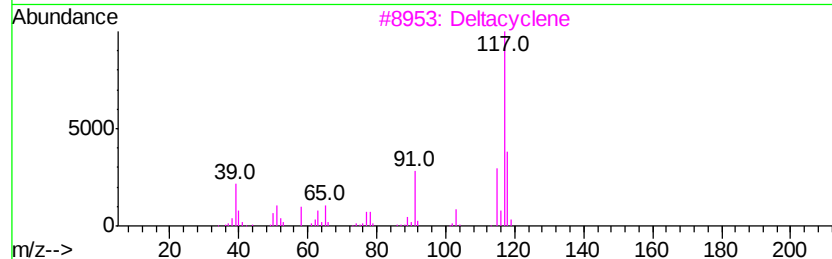
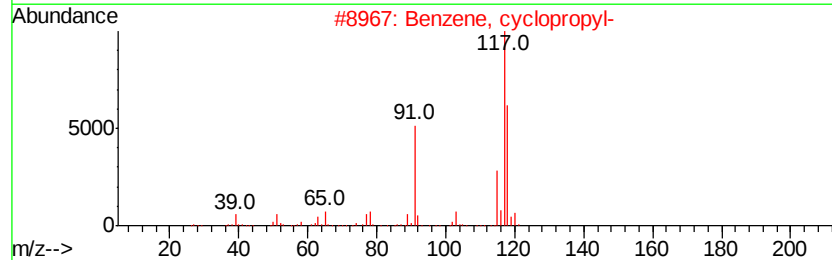
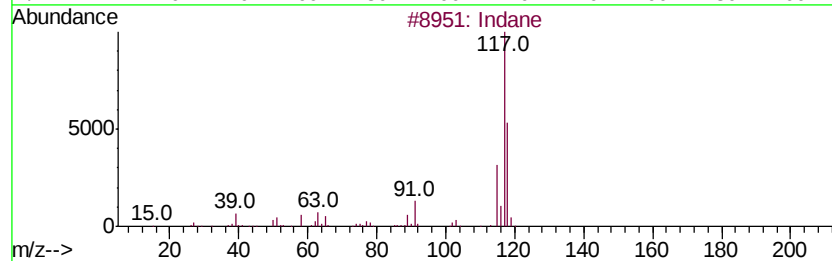
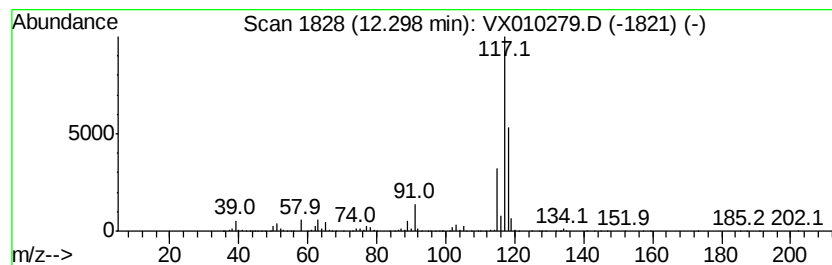
Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	10.70 ug/l	264427	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Indane	118 C9H10	000496-11-7	95
2	Benzene, cyclopropyl-	118 C9H10	000873-49-4	83
3	Deltacyclene	118 C9H10	007785-10-6	72
4	Benzene, 1-ethenyl-4-methyl-	118 C9H10	000622-97-9	64
5	Benzene, 2-propenyl-	118 C9H10	000300-57-2	60



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061319\
Data File : VX010279.D
Acq On : 13 Jun 2019 17:46
Operator : JC/SP
Sample : K3341-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.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
unknown1.30	1.30	5.0	ug/l	89440	1	5.67	885329	50.0
Butane, 2-methyl-	1.79	17.4	ug/l	307194	1	5.67	885329	50.0
Cyclopentane	2.93	5.5	ug/l	97323	1	5.67	885329	50.0
Cyclopentane, met...	4.40	7.5	ug/l	133765	1	5.67	885329	50.0
Benzene, 1-ethyl-...	11.43	5.6	ug/l	139100	4	12.08	1235480	50.0
Benzene, 1-ethyl-...	11.66	6.8	ug/l	168257	4	12.08	1235480	50.0
Benzene, 1,2,3-tr...	12.14	7.0	ug/l	171751	4	12.08	1235480	50.0
Indane	12.30	10.7	ug/l	264427	4	12.08	1235480	50.0