

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081919\
 Data File : VX011632.D
 Acq On : 19 Aug 2019 15:19
 Operator : JC/SP
 Sample : K4351-09
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PH2-0138

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\82X081519W.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	1.398	36	40	46	rBV	1632168	1530427	3.63%	1.200%
2	1.782	98	103	114	rVB	766962	1032217	2.45%	0.810%
3	1.995	133	138	148	rVB	735020	1050143	2.49%	0.824%
4	2.928	286	291	302	rVB	331930	691206	1.64%	0.542%
5	4.397	519	532	546	rVB	933359	2662223	6.32%	2.088%
6	5.495	702	712	716	rBV2	211663	590662	1.40%	0.463%
7	5.574	716	725	734	rVV	2191602	6667768	15.83%	5.230%
8	5.653	734	738	746	rVB	366865	893771	2.12%	0.701%
9	5.940	775	785	796	rBV3	156144	499136	1.19%	0.392%
10	6.056	796	804	813	rBV	208334	528130	1.25%	0.414%
11	6.257	826	837	846	rBV2	201981	629263	1.49%	0.494%
12	6.354	846	853	861	rVV2	216561	588514	1.40%	0.462%
13	6.452	861	869	882	rVB	277824	745313	1.77%	0.585%
14	6.854	925	935	946	rBV	575823	1341809	3.19%	1.053%
15	7.458	1021	1034	1048	rBV	2795173	6378298	15.14%	5.003%
16	8.714	1234	1240	1247	rVB	1047954	1721776	4.09%	1.351%
17	10.110	1463	1469	1475	rBV	1133540	1515593	3.60%	1.189%
18	10.250	1486	1492	1500	rVB	842559	1081542	2.57%	0.848%
19	10.360	1500	1510	1521	rBV	28728337	42115082	100.00%	33.035%
20	10.701	1560	1566	1578	rVB	22655692	30006584	71.25%	23.537%
21	11.134	1632	1637	1643	rBV	998988	1249247	2.97%	0.980%
22	11.433	1680	1686	1693	rBV	2602004	4536897	10.77%	3.559%
23	11.506	1693	1698	1705	rVB	2838835	3546884	8.42%	2.782%
24	11.664	1719	1724	1729	rBV	4058075	4933896	11.72%	3.870%
25	11.804	1742	1747	1753	rVB	4443682	5192757	12.33%	4.073%
26	12.073	1786	1791	1797	rVB	1283090	1673114	3.97%	1.312%
27	12.140	1797	1802	1807	rVB	1256851	1467573	3.48%	1.151%
28	12.298	1821	1828	1835	rBV	437970	634788	1.51%	0.498%
29	12.756	1898	1903	1910	rVB2	337681	546574	1.30%	0.429%
30	13.341	1995	1999	2004	rVB2	425694	556228	1.32%	0.436%
31	13.829	2072	2079	2088	rVB	647362	877840	2.08%	0.689%

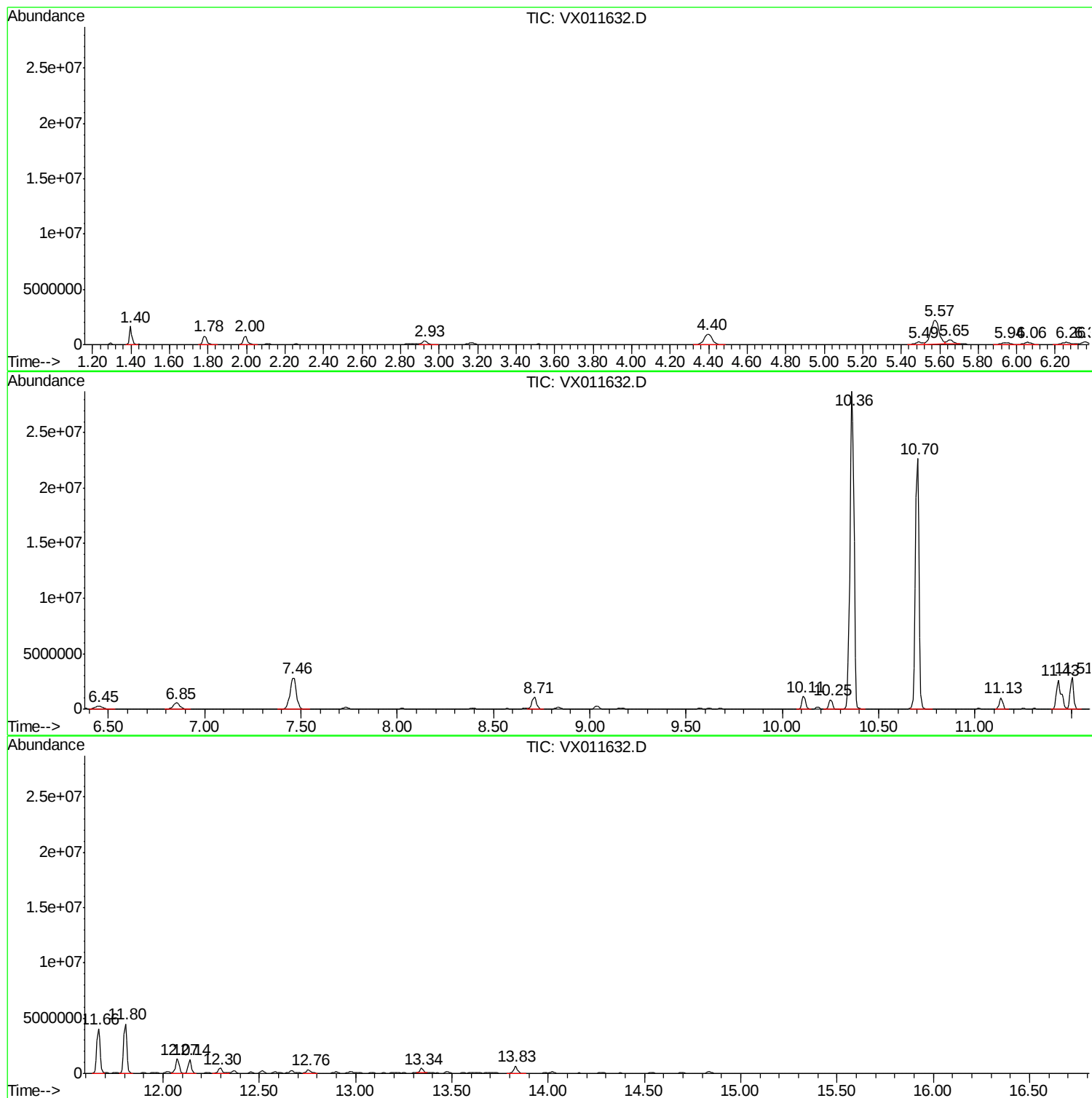
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Instrument :
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ClientSampleId :
PH2-0138

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

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



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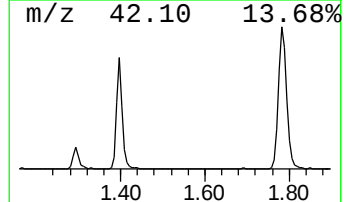
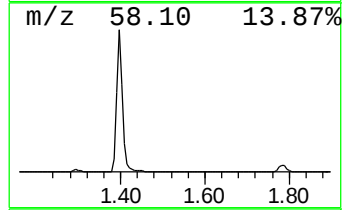
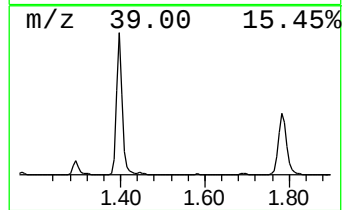
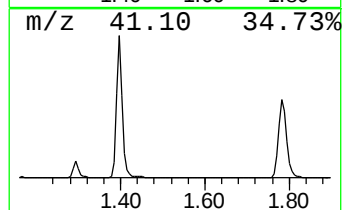
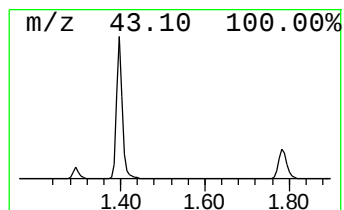
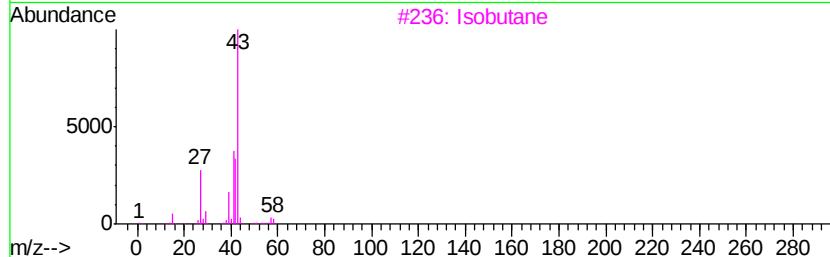
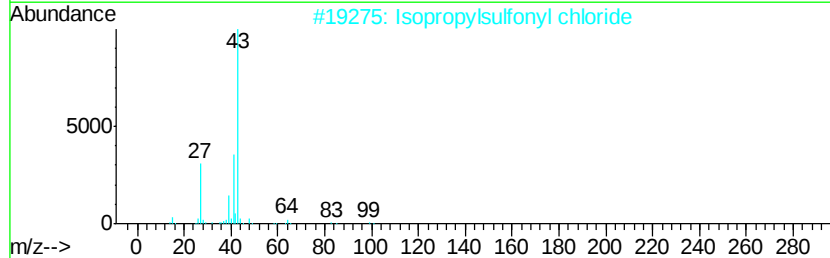
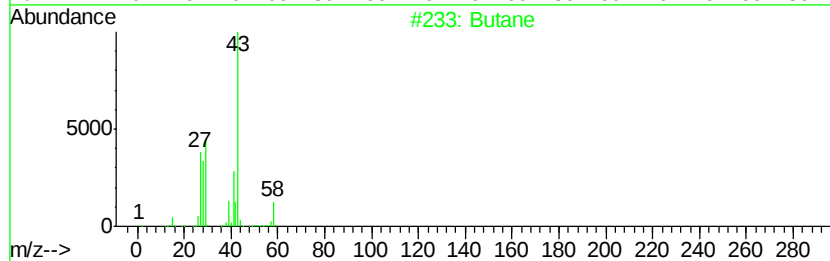
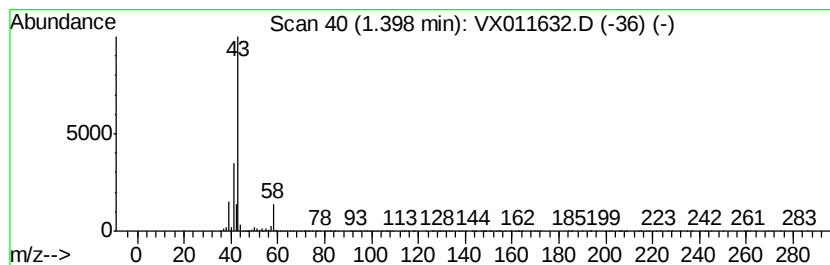
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	85.62 ug/l	1530430	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane		58	C4H10	000106-97-8	80
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	Diazene, dimethyl-		58	C2H6N2	000503-28-6	5



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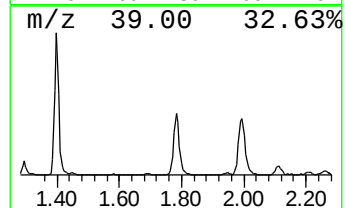
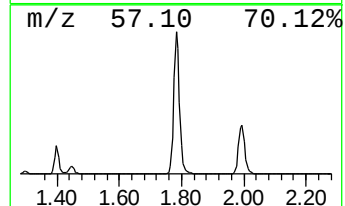
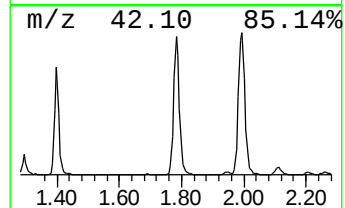
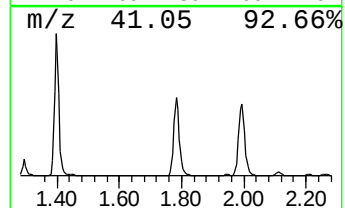
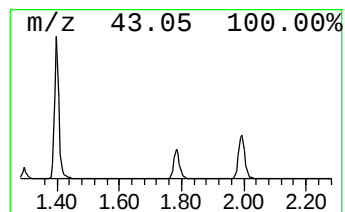
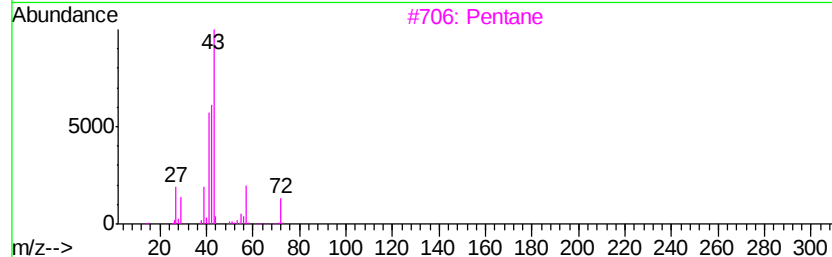
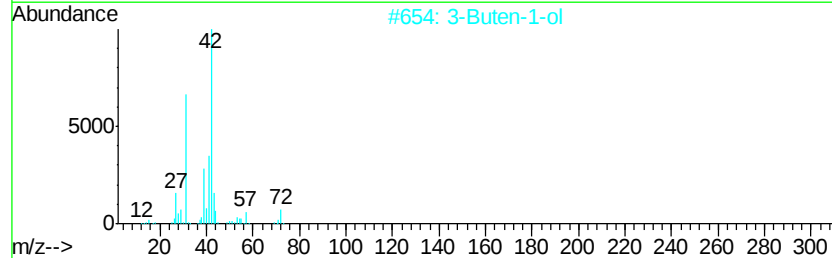
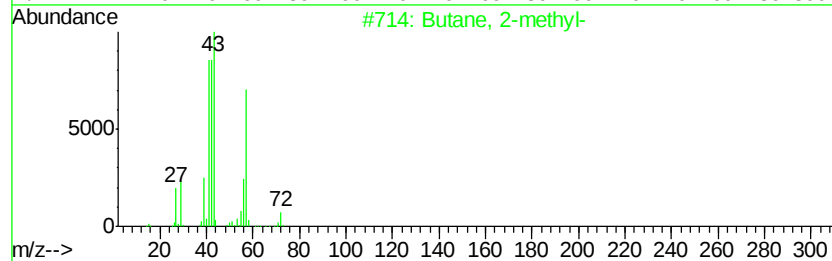
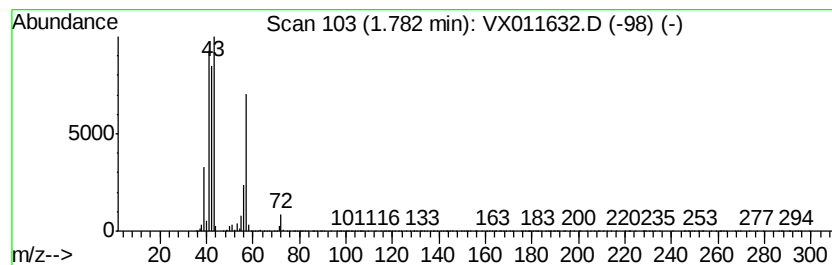
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Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	57.75 ug/l	1032220	Pentafluorobenzene	5.66

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	36
4		Azetidine	57	C3H7N	000503-29-7	9
5		3-Buten-2-ol	72	C4H8O	000598-32-3	9



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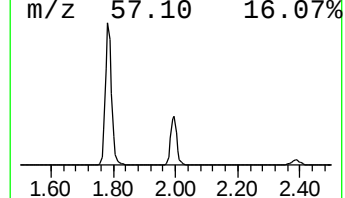
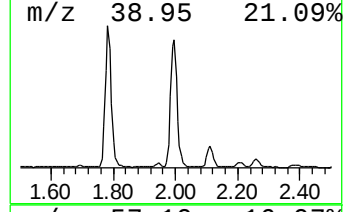
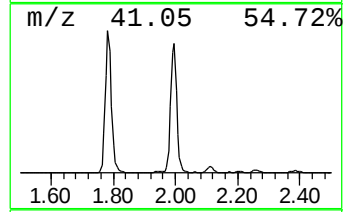
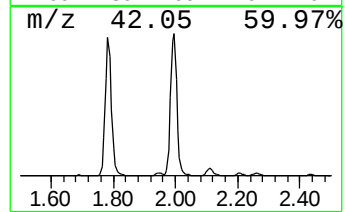
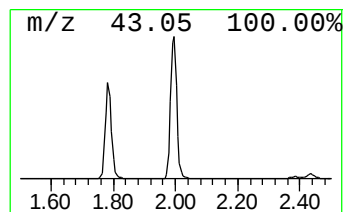
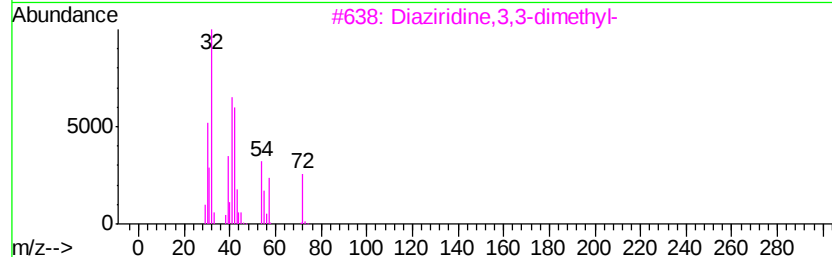
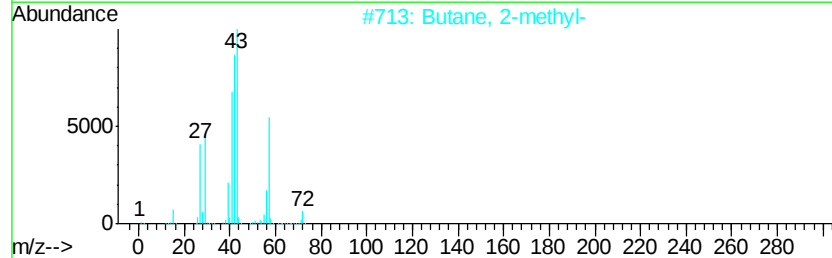
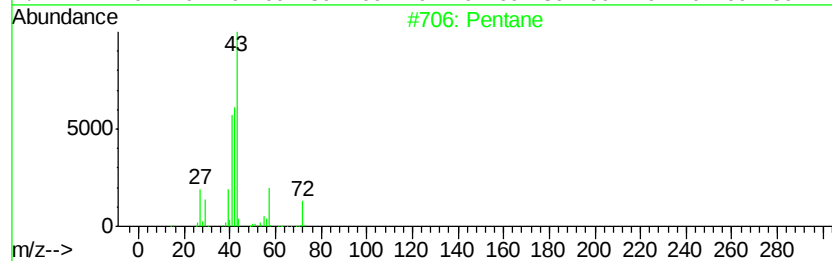
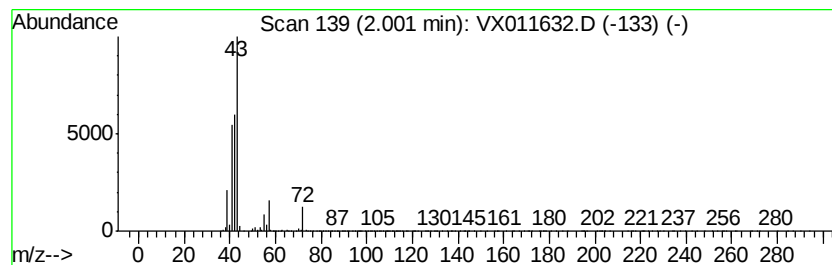
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	58.75 ug/l	1050140	Pentafluorobenzene	5.66

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	45
3	Diaziridine,3,3-dimethyl-		72	C3H8N2	004901-76-2	35
4	Tetrahydrofuran		72	C4H8O	000109-99-9	9
5	Isobutyl nitrite		103	C4H9NO2	000542-56-3	9



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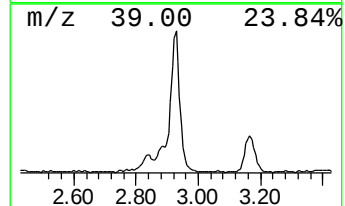
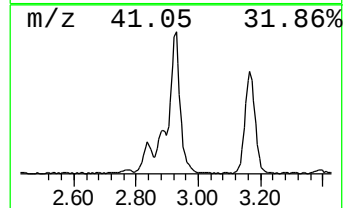
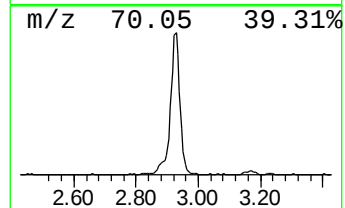
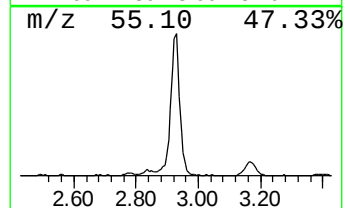
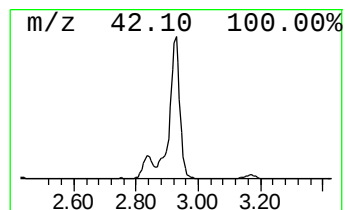
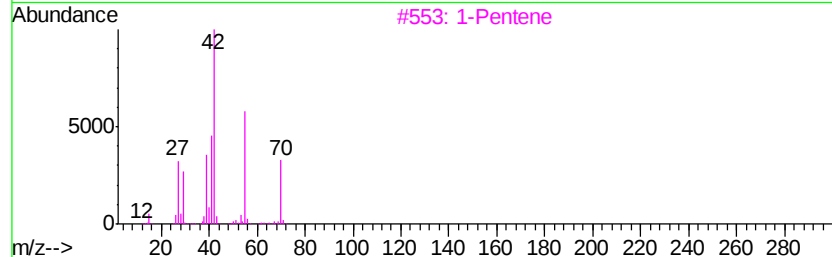
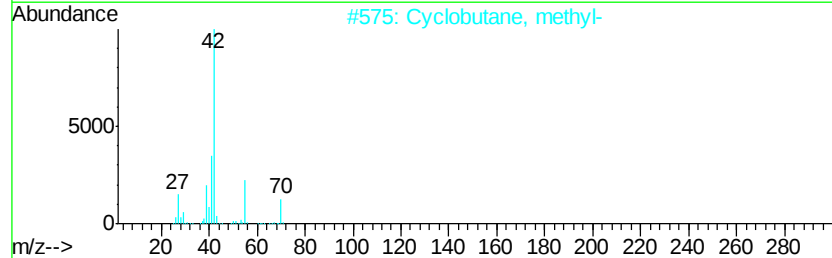
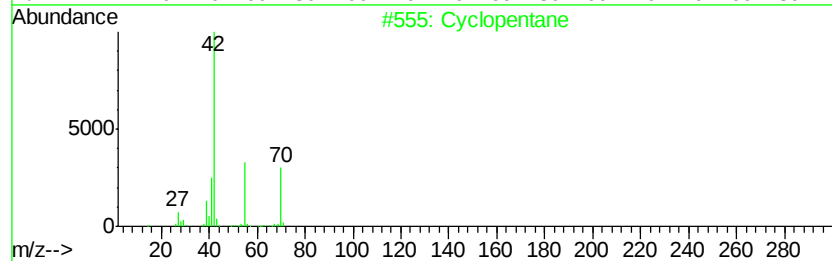
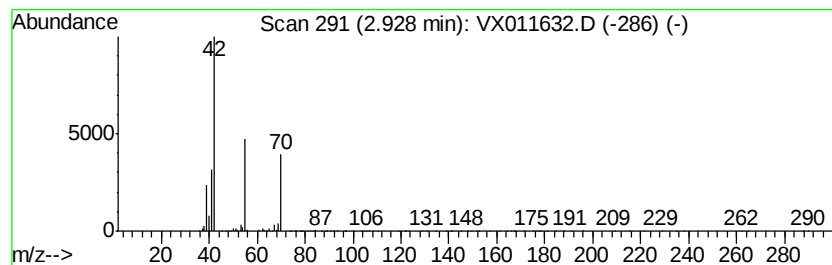
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Peak Number 4 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	38.67 ug/l	691206	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane	70	C5H10	000287-92-3	78
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	56
3		1-Pentene	70	C5H10	000109-67-1	9
4		Cyclopropane, ethyl-	70	C5H10	001191-96-4	7
5		Methyl propargyl ether	70	C4H6O	000627-41-8	7



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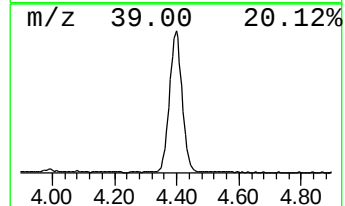
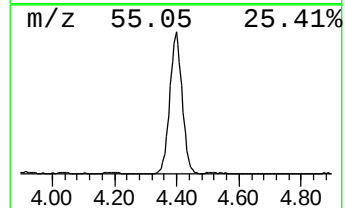
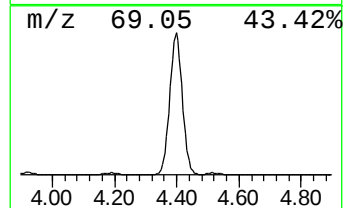
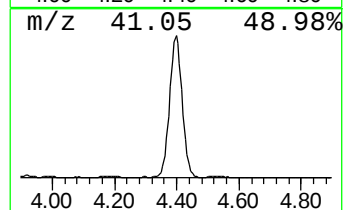
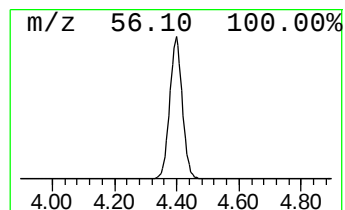
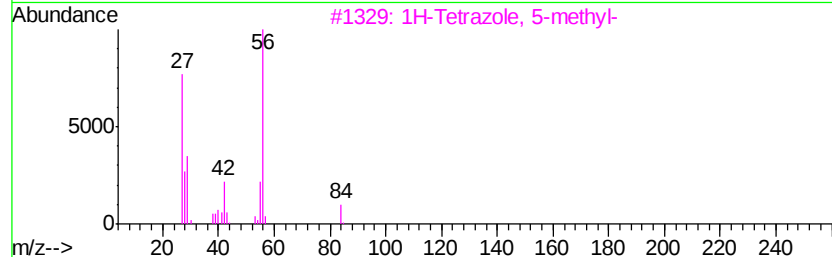
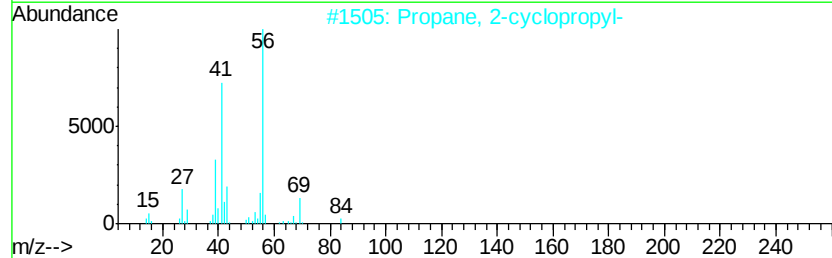
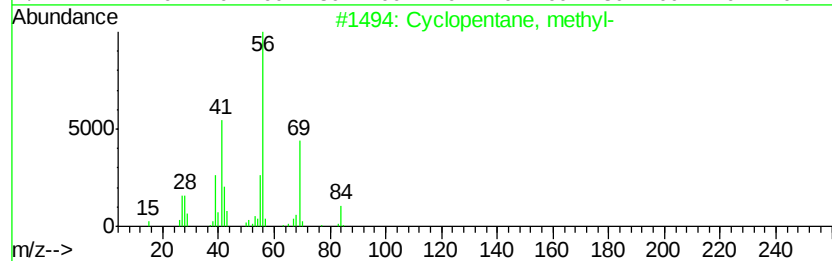
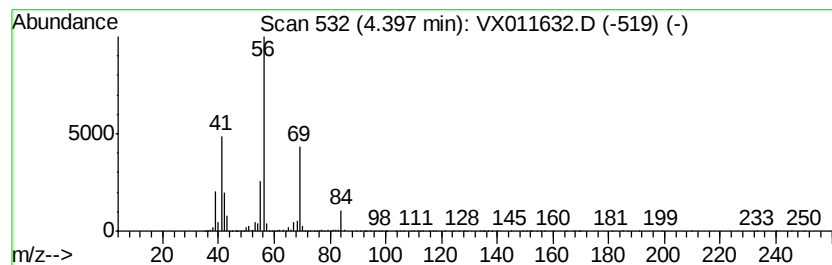
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	148.93 ug/l	2662220	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64



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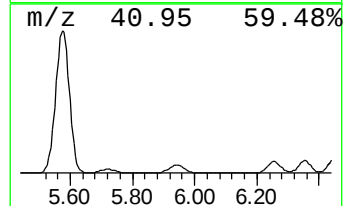
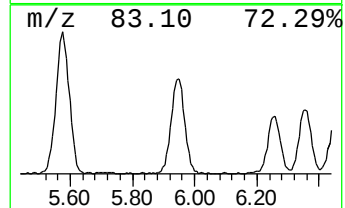
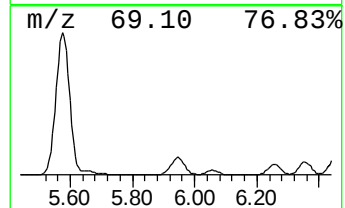
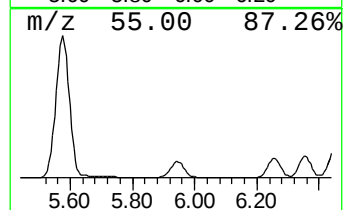
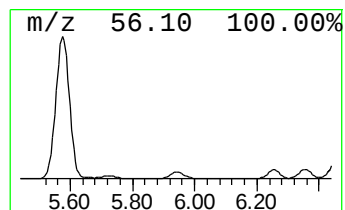
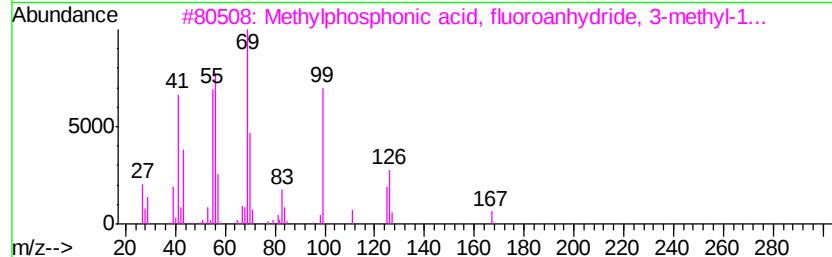
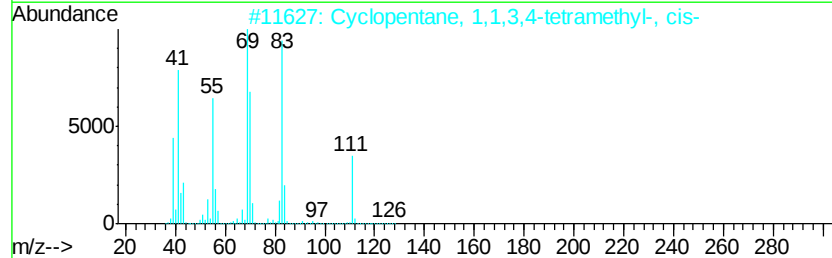
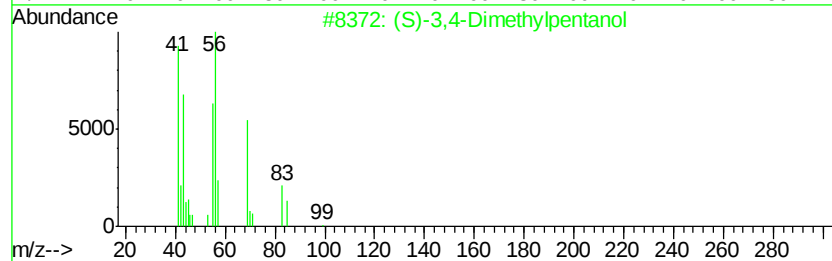
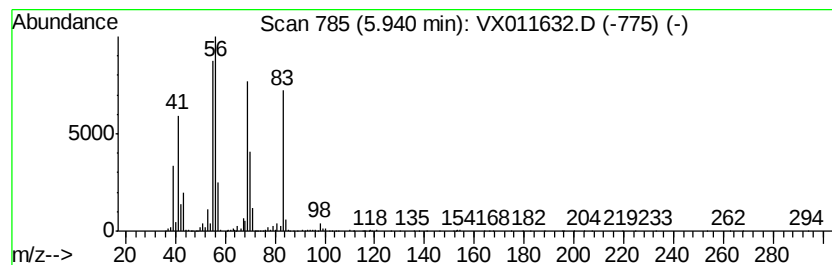
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Quant Title : SW846 8260

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

Peak Number 6 (S)-3,4-Dimethylpentanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.94	27.92 ug/l	499136	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-3,4-Dimethylpentanol	116	C7H16O	1000143-83-9	72	
2	Cyclopentane, 1,1,3,4-tetramethyl-	126	C9H18	053907-60-1	62	
3	Methylphosphonic acid, fluoroanhydride	224	C10H22F02P	193090-16-3	59	
4	3-Heptene, (E)-	98	C7H14	014686-14-7	53	
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	46	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX081919\
Data File : VX011632.D
Acq On : 19 Aug 2019 15:19
Operator : JC/SP
Sample : K4351-09
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
PH2-0138

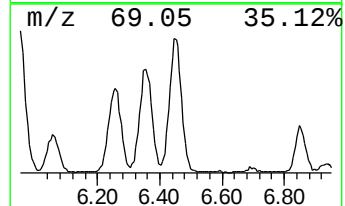
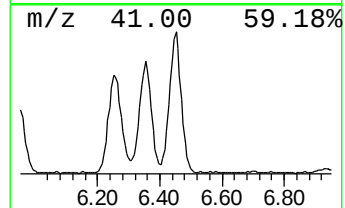
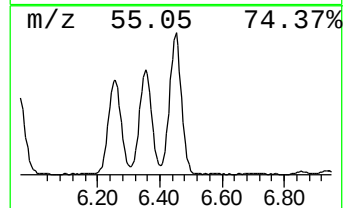
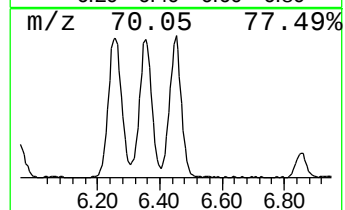
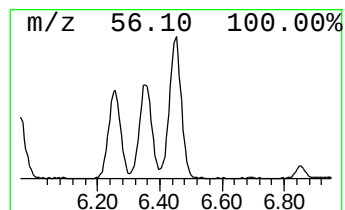
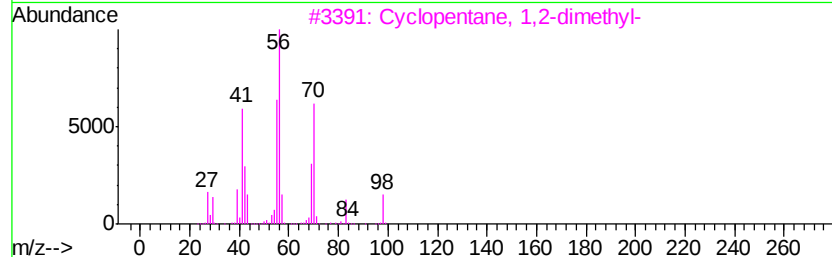
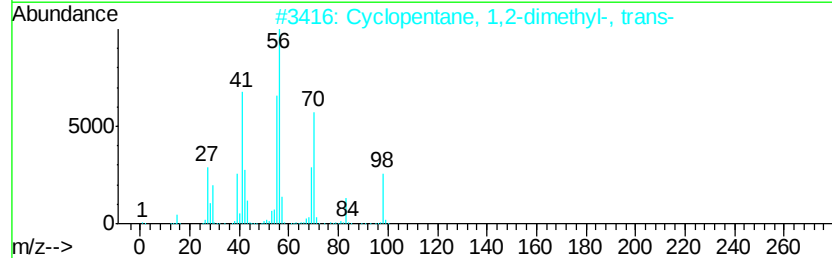
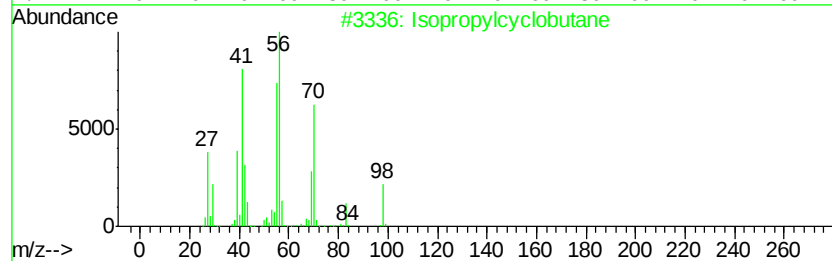
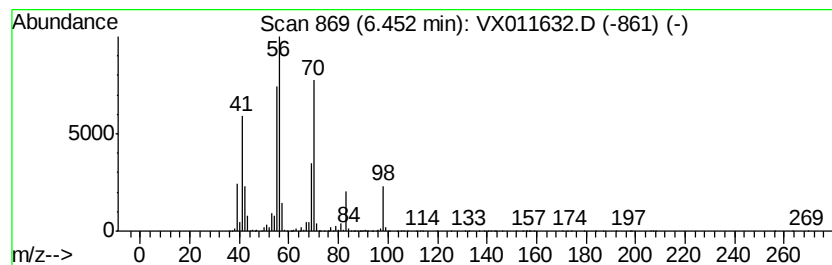
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

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

Peak Number 7 Isopropylcyclobutane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	27.77 ug/l	745313	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropylcyclobutane	98	C7H14	000872-56-0	94
2		Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
3		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	87
4		Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	86
5		Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	86



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX081919\
Data File : VX011632.D
Acq On : 19 Aug 2019 15:19
Operator : JC/SP
Sample : K4351-09
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
PH2-0138

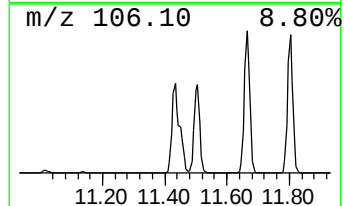
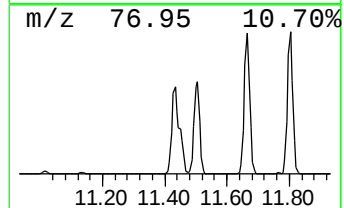
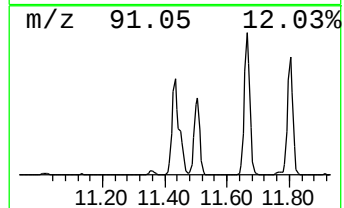
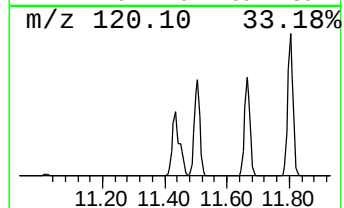
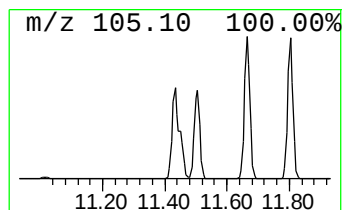
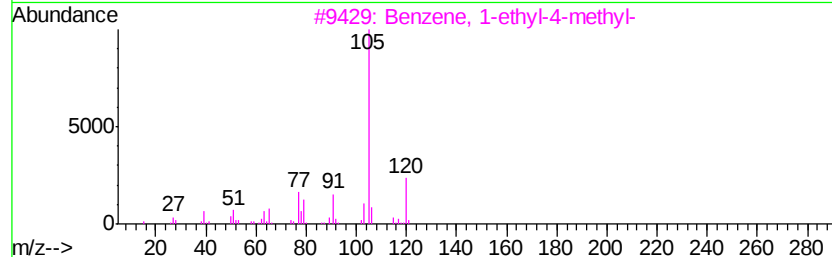
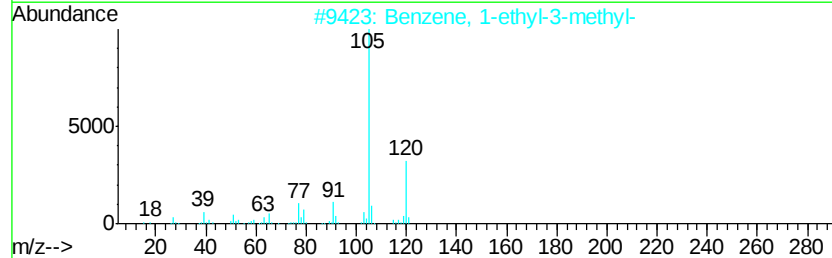
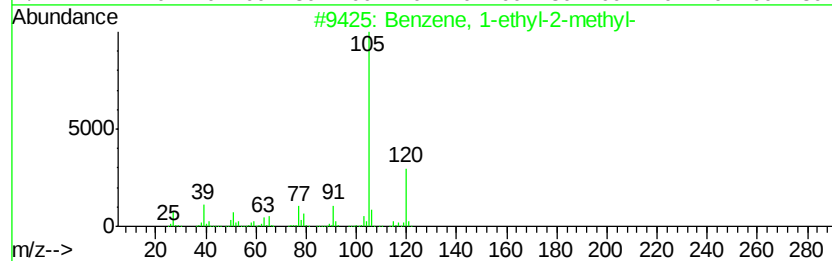
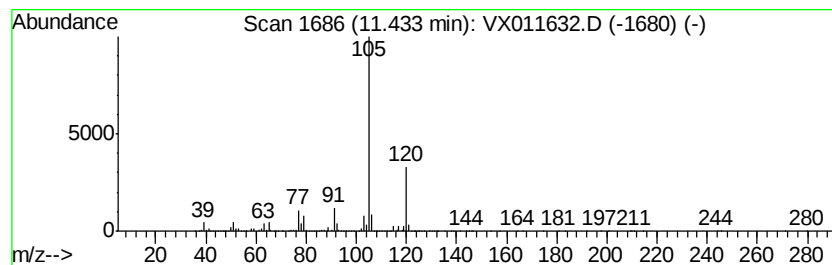
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	135.58 ug/l	4536900	1,4-Dichlorobenzene-d4	12.07

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081919\
Data File : VX011632.D
Acq On : 19 Aug 2019 15:19
Operator : JC/SP
Sample : K4351-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PH2-0138

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.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	85.6	ug/l	1530430	1	5.66	893771	50.0
Butane, 2-methyl-	1.78	57.8	ug/l	1032220	1	5.66	893771	50.0
Pentane	2.00	58.8	ug/l	1050140	1	5.66	893771	50.0
Cyclopentane	2.93	38.7	ug/l	691206	1	5.66	893771	50.0
Cyclopentane, met...	4.40	148.9	ug/l	2662220	1	5.66	893771	50.0
(S)-3,4-Dimethylp...	5.94	27.9	ug/l	499136	1	5.66	893771	50.0
Isopropylcyclobutane	6.45	27.8	ug/l	745313	2	6.85	1341810	50.0
Benzene, 1-ethyl-...	11.43	135.6	ug/l	4536900	4	12.07	1673110	50.0