

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
 Data File : VX012587.D
 Acq On : 21 Sep 2019 03:39
 Operator : JC/SP
 Sample : K4978-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 Z2-0161

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

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.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	1.070	26	30	41	rBV	358319	437813	1.43%	1.041%
2	1.783	141	147	161	rVB	1712654	2357196	7.72%	5.604%
3	2.838	308	320	329	rBV	597982	1326997	4.35%	3.155%
4	5.655	774	782	790	rBV	181934	467812	1.53%	1.112%
5	6.142	851	862	877	rVB	11269533	30519879	100.00%	72.552%
6	6.850	969	978	992	rBV	287198	679011	2.22%	1.614%
7	8.709	1275	1283	1289	rBV	593663	925151	3.03%	2.199%
8	8.782	1289	1295	1302	rVB	461153	708529	2.32%	1.684%
9	9.514	1408	1415	1421	rBV	240927	363623	1.19%	0.864%
10	10.062	1499	1505	1509	rBV	229838	327110	1.07%	0.778%
11	10.111	1509	1513	1518	rVB	533857	733174	2.40%	1.743%
12	10.245	1530	1535	1541	rBV	234308	327823	1.07%	0.779%
13	10.355	1547	1553	1560	rVB	736405	963153	3.16%	2.290%
14	11.013	1655	1661	1666	rBV	239383	306792	1.01%	0.729%
15	11.135	1675	1681	1689	rBV	435643	598072	1.96%	1.422%
16	11.806	1786	1791	1795	rVB	298613	375330	1.23%	0.892%
17	12.074	1830	1835	1841	rVB	520098	648519	2.12%	1.542%

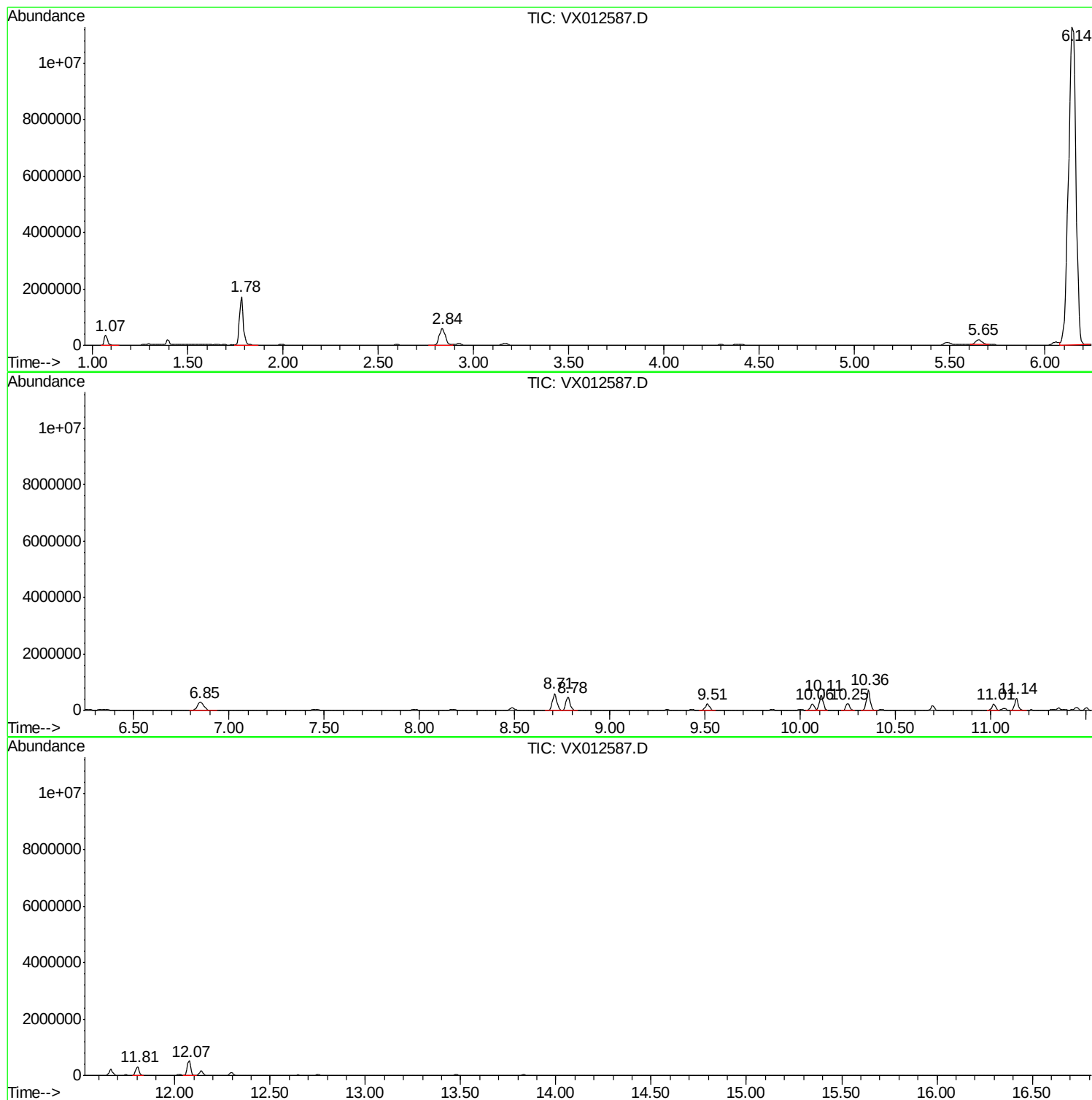
Sum of corrected areas: 42065984

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012587.D
Acq On : 21 Sep 2019 03:39
Operator : JC/SP
Sample : K4978-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0161

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012587.D
Acq On : 21 Sep 2019 03:39
Operator : JC/SP
Sample : K4978-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0161

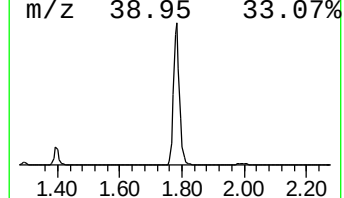
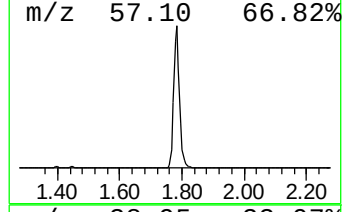
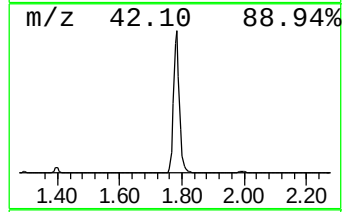
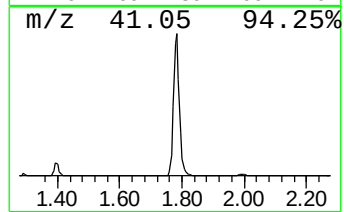
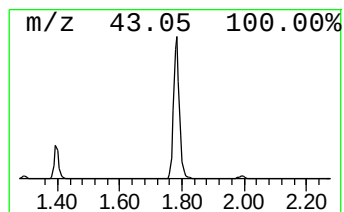
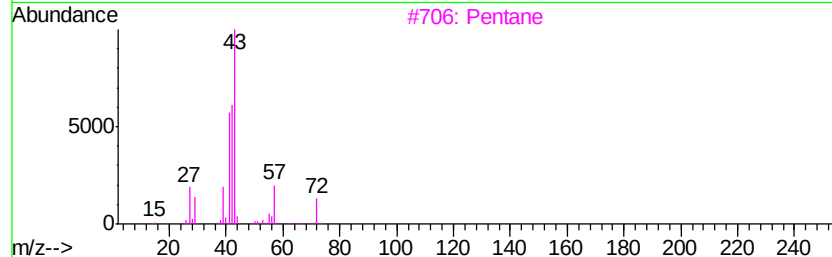
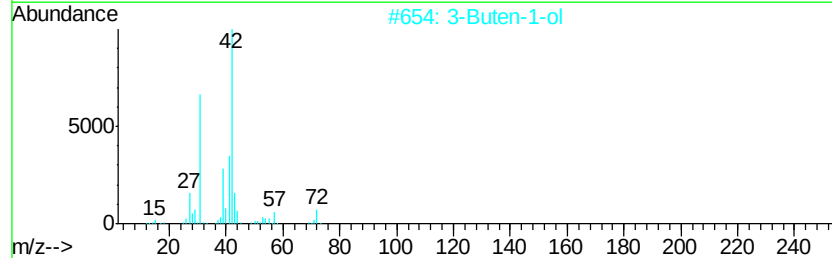
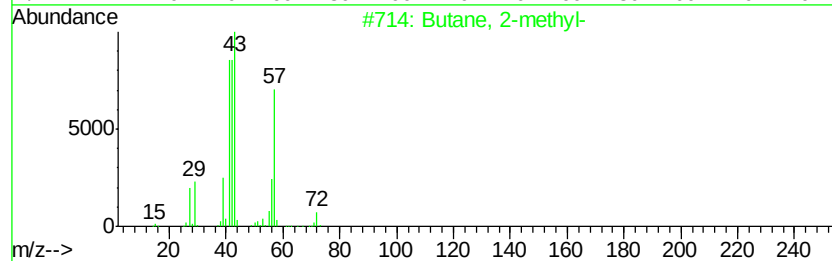
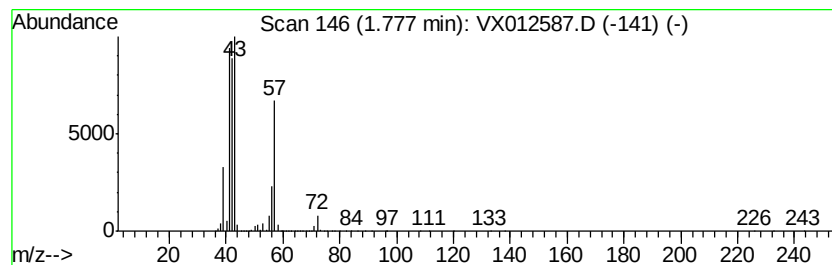
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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.
1.78	251.94 ug/l	2357200	Pentafluorobenzene	5.65

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	40
3		Pentane	72	C5H12	000109-66-0	36
4		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	14



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012587.D
Acq On : 21 Sep 2019 03:39
Operator : JC/SP
Sample : K4978-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0161

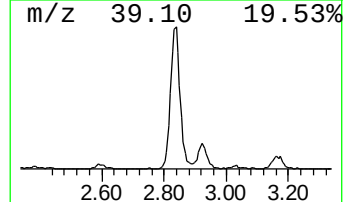
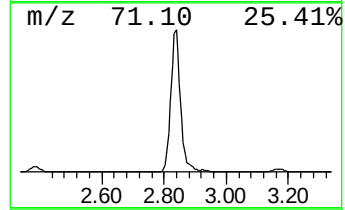
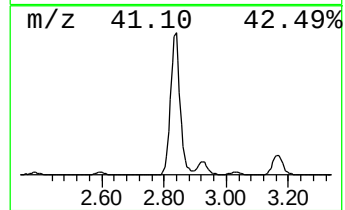
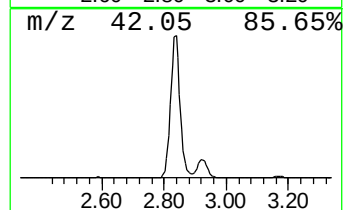
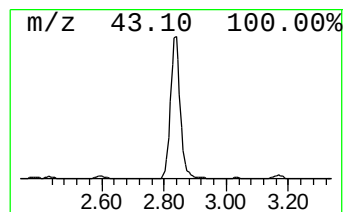
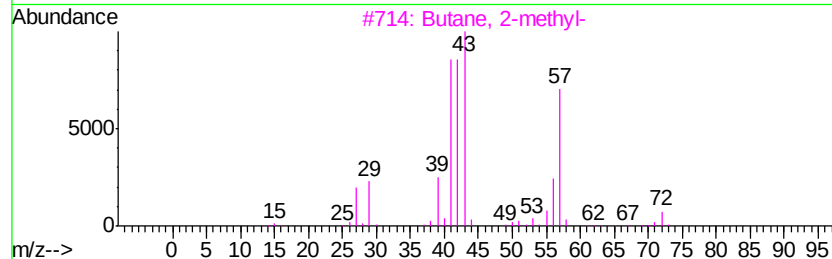
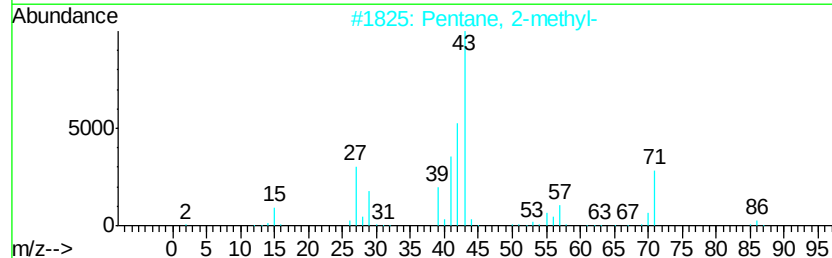
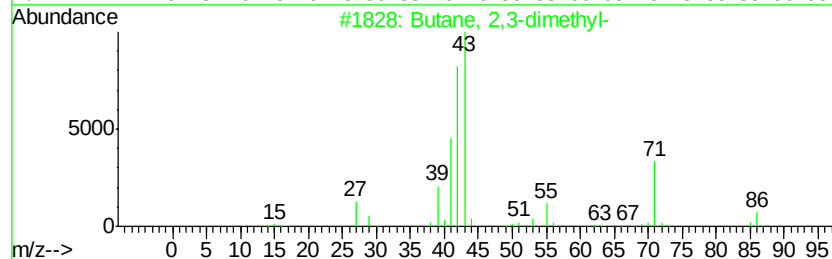
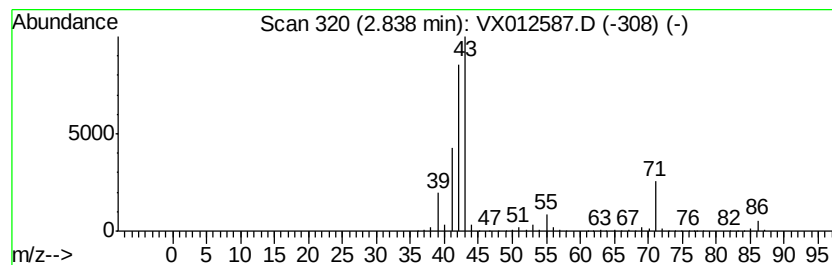
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	141.83 ug/l	1327000	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Butane, 2-methyl-	72	C5H12	000078-78-4	36
4		Cyclobutane, methyl-	70	C5H10	000598-61-8	33
5		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	16



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012587.D
Acq On : 21 Sep 2019 03:39
Operator : JC/SP
Sample : K4978-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
Z2-0161

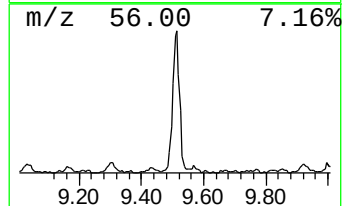
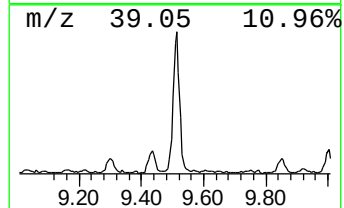
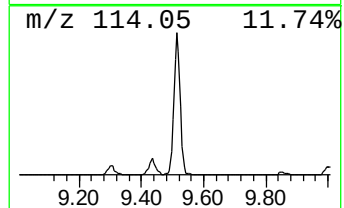
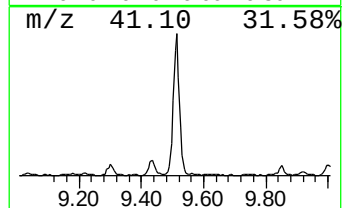
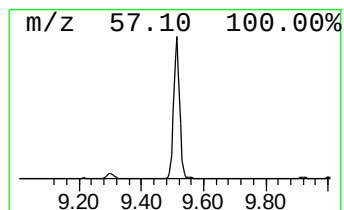
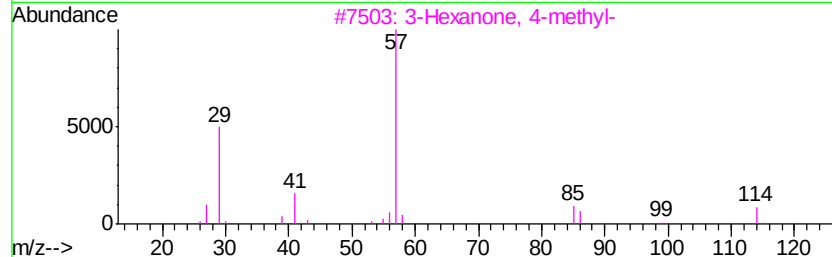
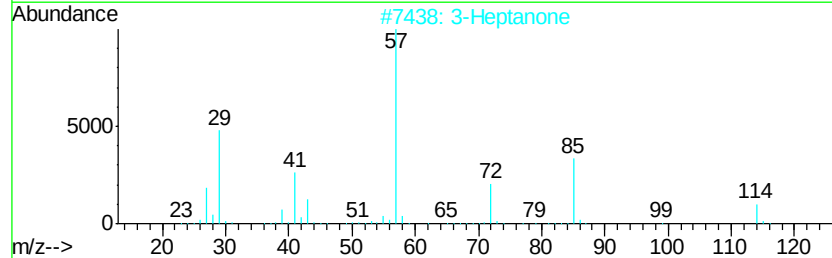
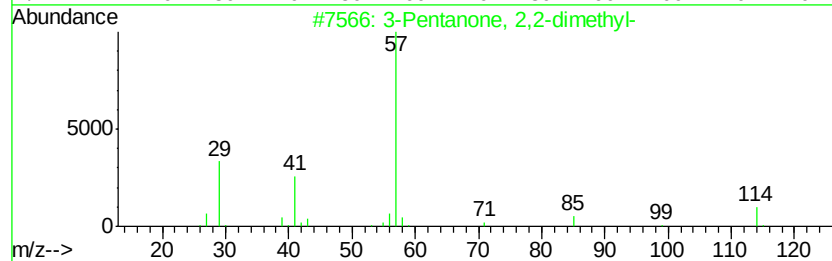
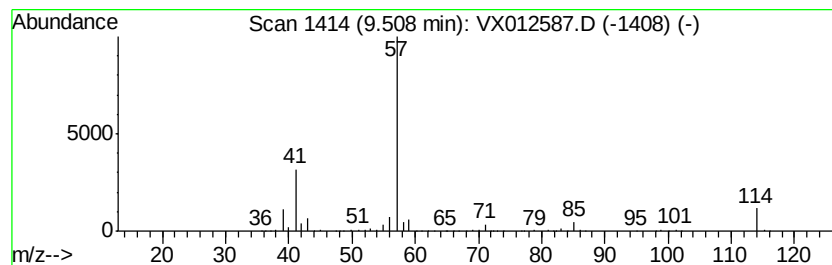
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 4 3-Pentanone, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	24.80 ug/l	363623	Chlorobenzene-d5	10.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	80
2			3-Heptanone	114	C7H14O	000106-35-4	59
3			3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	53
4			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	50
5			2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX092019\
Data File : VX012587.D
Acq On : 21 Sep 2019 03:39
Operator : JC/SP
Sample : K4978-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0161

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.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, 2-methyl-	1.78	251.9	ug/l	2357200	1	5.65	467812	50.0
Butane, 2,3-dimet...	2.84	141.8	ug/l	1327000	1	5.65	467812	50.0
3-Pentanone, 2,2-...	9.51	24.8	ug/l	363623	3	10.11	733174	50.0