

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX042220\
 Data File : VX015850.D
 Acq On : 22 Apr 2020 18:31
 Operator : JC/SP
 Sample : L2379-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SS037MW012-200420

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\82X042220W.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	1.064	24	29	55	rBV2	18446437	60030732	100.00%	44.783%
2	1.777	143	146	158	rVB	400525	608885	1.01%	0.454%
3	2.381	238	245	255	rVB	376822	766056	1.28%	0.571%
4	2.826	308	318	332	rBV	2999492	6589610	10.98%	4.916%
5	4.289	544	558	574	rBV	1830751	5597374	9.32%	4.176%
6	5.472	741	752	763	rBV	492778	1400202	2.33%	1.045%
7	5.636	768	779	784	rVV	898833	2573896	4.29%	1.920%
8	5.703	784	790	804	rVB2	1009263	3031792	5.05%	2.262%
9	6.039	835	845	856	rBV	536321	1441012	2.40%	1.075%
10	6.325	880	892	909	rVB	4865061	14599618	24.32%	10.891%
11	6.837	963	976	986	rBV	1398935	3291958	5.48%	2.456%
12	7.429	1065	1073	1082	rBV	277624	635744	1.06%	0.474%
13	8.038	1163	1173	1185	rBV	3335681	6580585	10.96%	4.909%
14	8.160	1185	1193	1212	rVB	4416039	8969889	14.94%	6.692%
15	8.666	1266	1276	1277	rBV	457057	699752	1.17%	0.522%
16	8.697	1277	1281	1296	rVB	3093381	4767491	7.94%	3.557%
17	10.099	1505	1511	1517	rBV	3179332	4229107	7.04%	3.155%
18	11.123	1673	1679	1684	rBV	2867861	3561322	5.93%	2.657%
19	12.062	1828	1833	1846	rBV	3741892	4673126	7.78%	3.486%

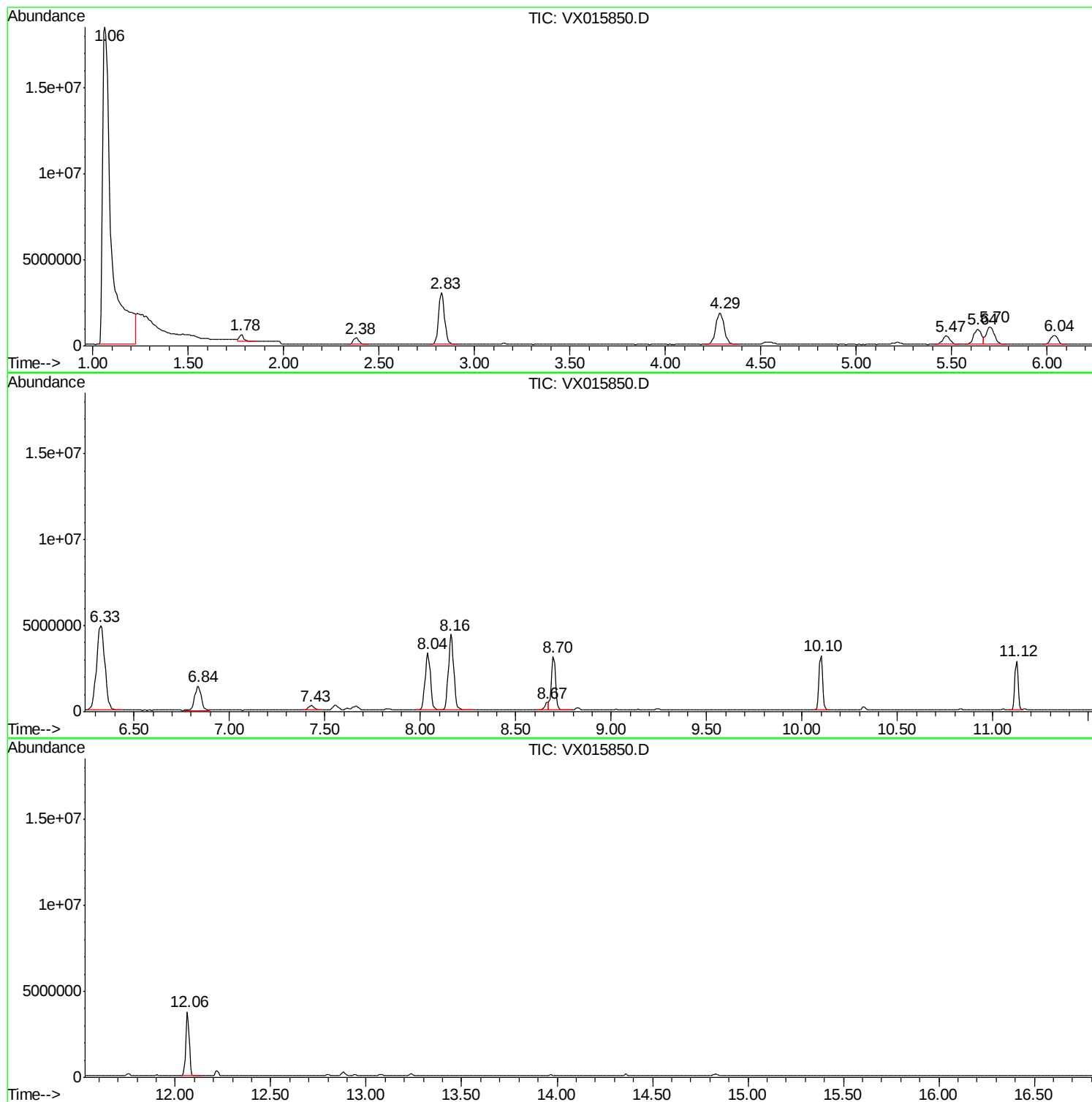
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.M
Quant Title : SW846 8260

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



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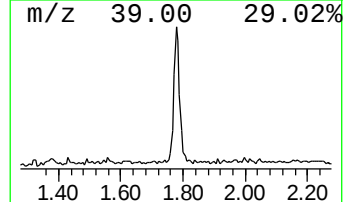
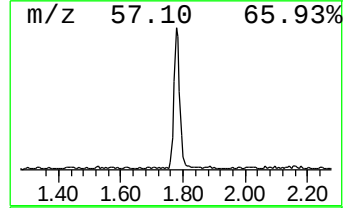
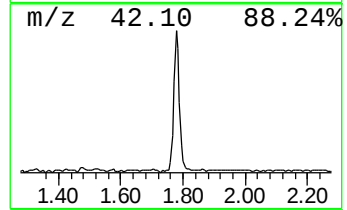
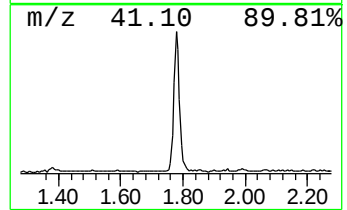
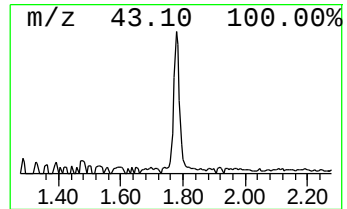
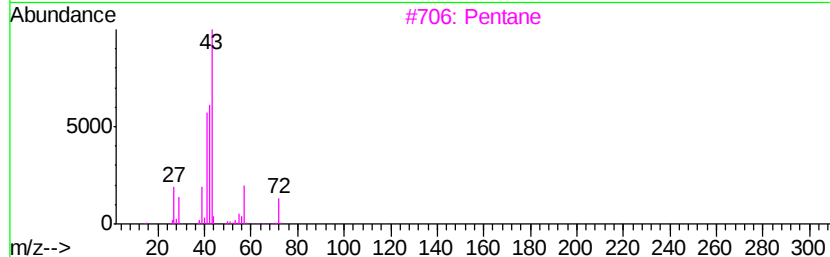
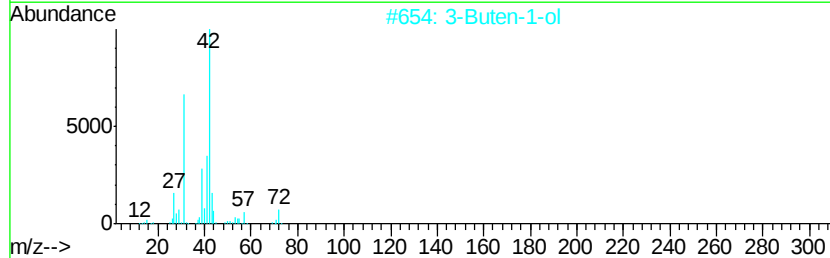
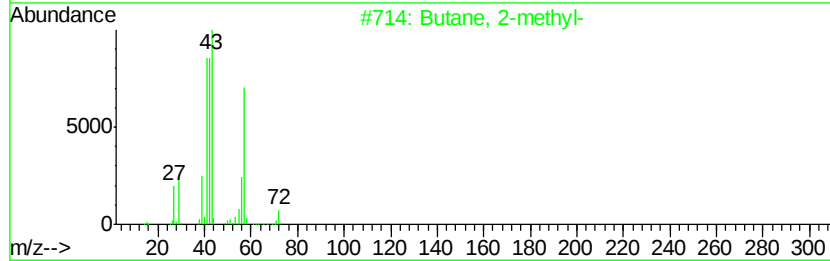
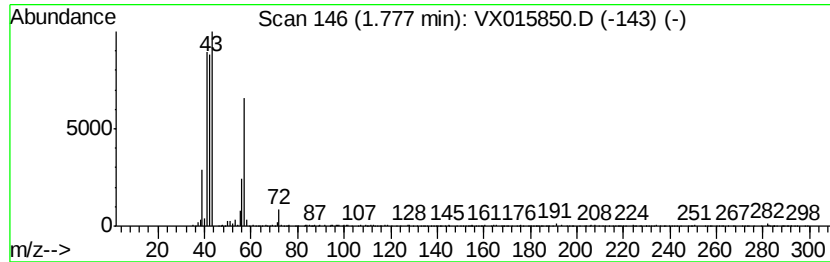
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	11.83 ug/l	608885	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2		3-Buten-1-ol	72	C4H8O	000627-27-0	43
3		Pentane	72	C5H12	000109-66-0	33
4		Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	33
5		2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28



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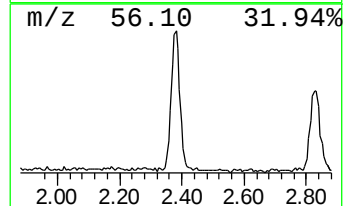
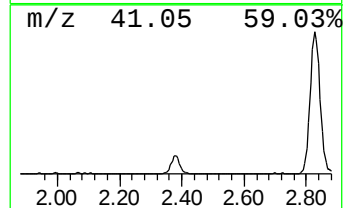
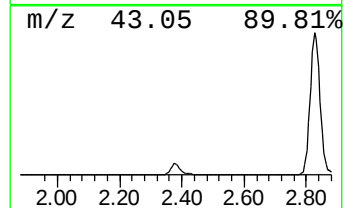
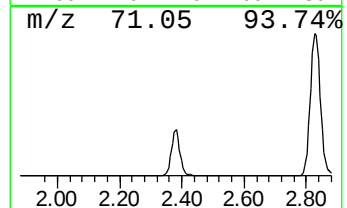
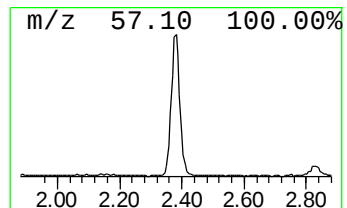
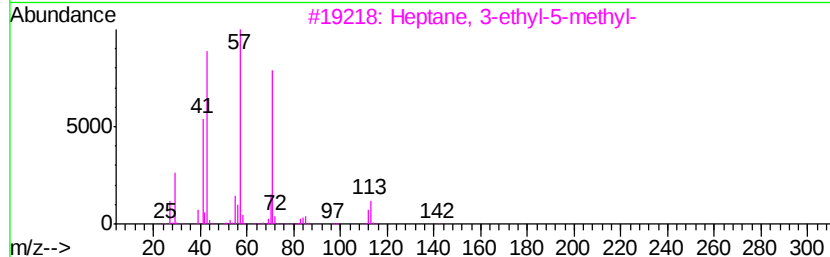
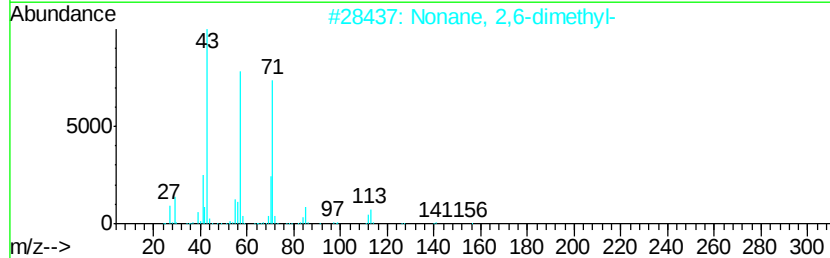
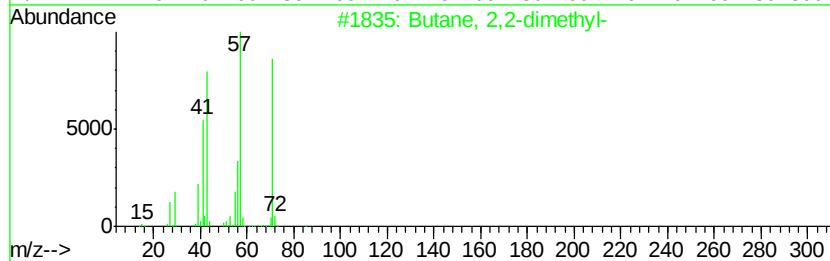
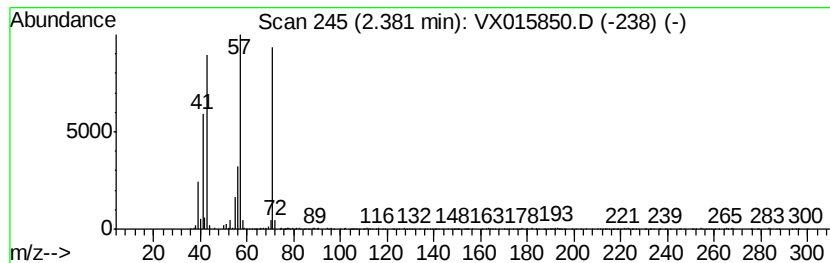
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	14.88 ug/l	766056	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	86
2		Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	72
3		Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	72
4		Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	64
5		Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	50



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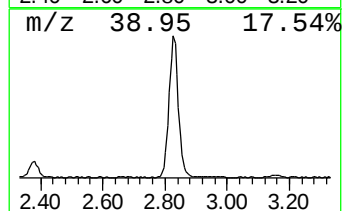
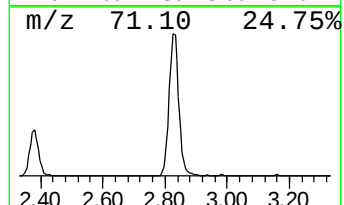
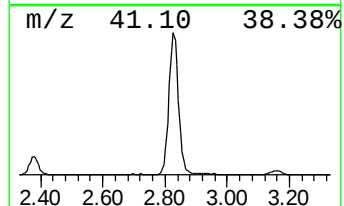
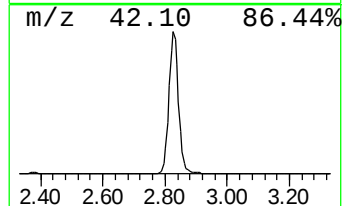
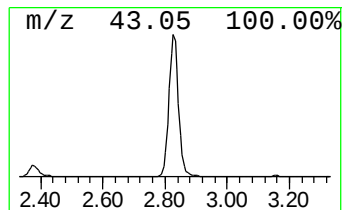
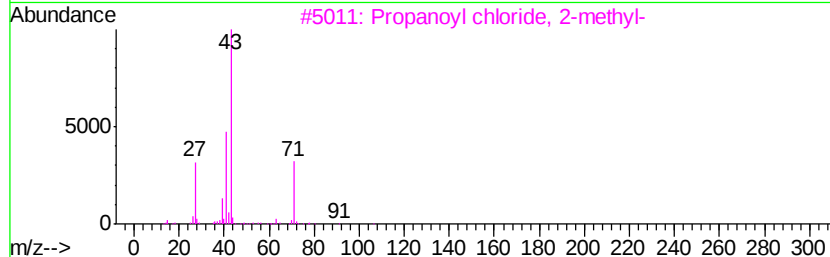
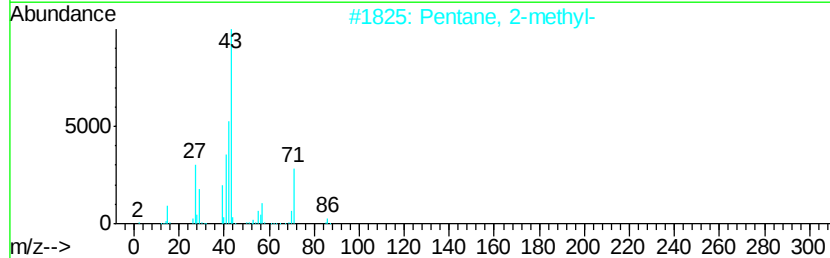
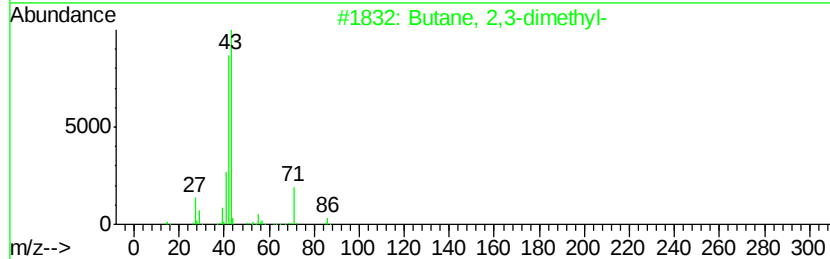
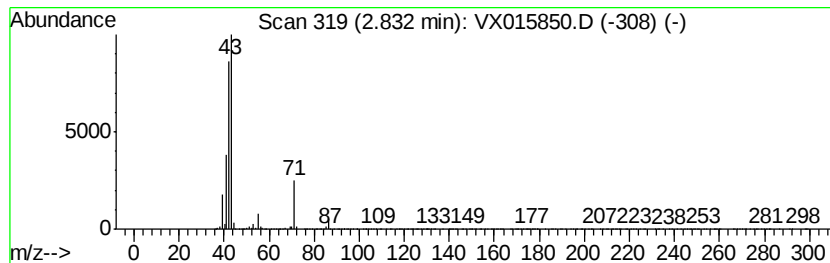
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	128.01 ug/l	6589610	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	16
4		Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	12
5		C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	10



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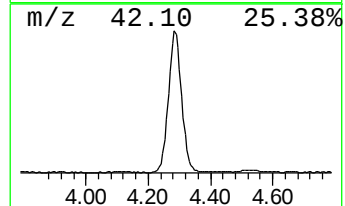
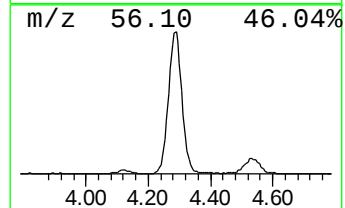
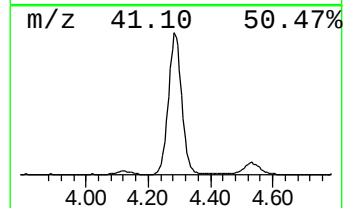
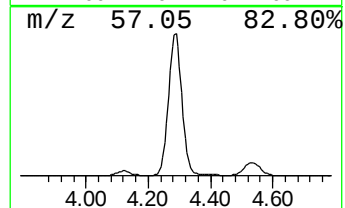
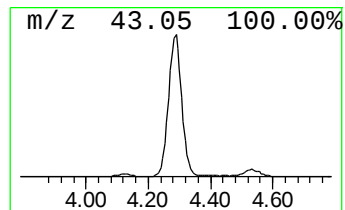
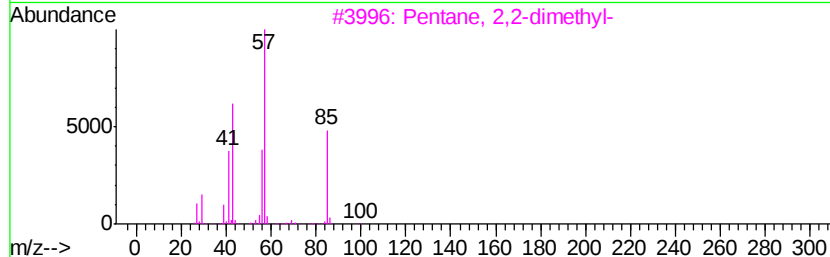
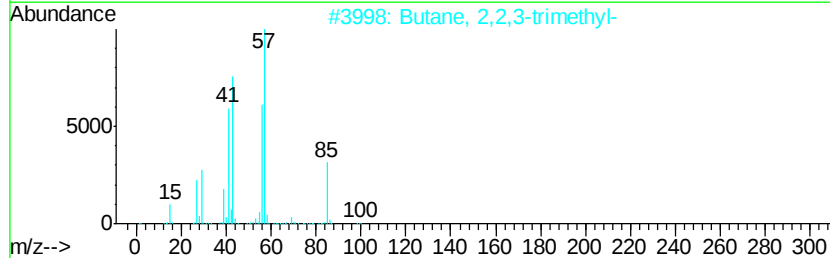
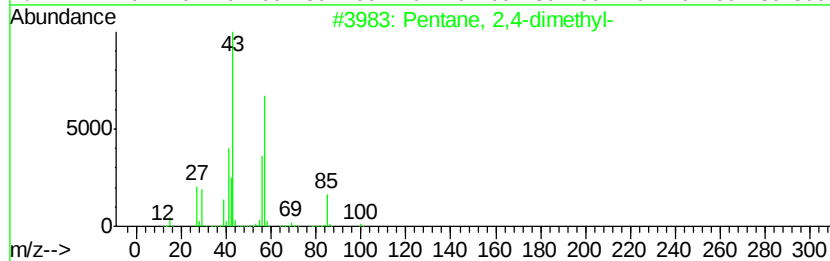
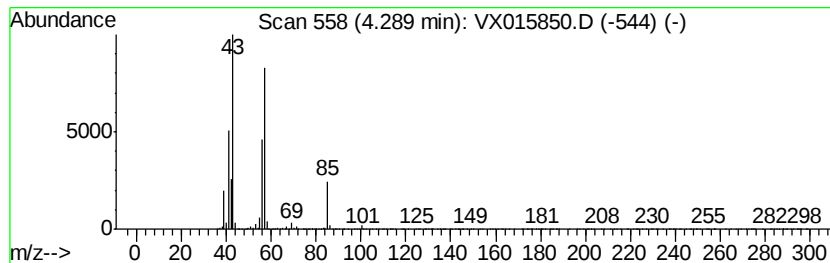
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	108.73 ug/l	5597370	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	90
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	64
4		Oxalic acid, butyl isoheptyl ester	230	C12H22O4	1000309-32-7	50
5		2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	47



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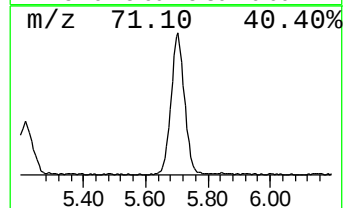
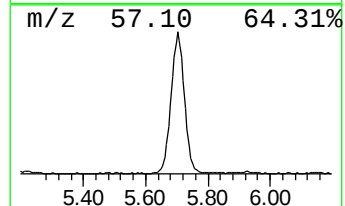
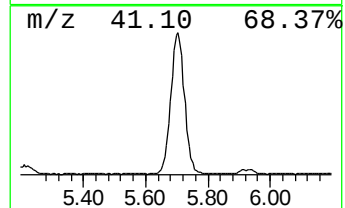
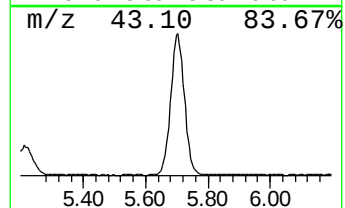
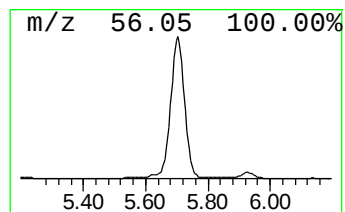
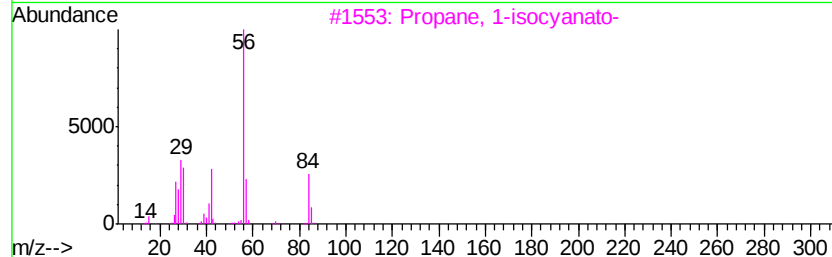
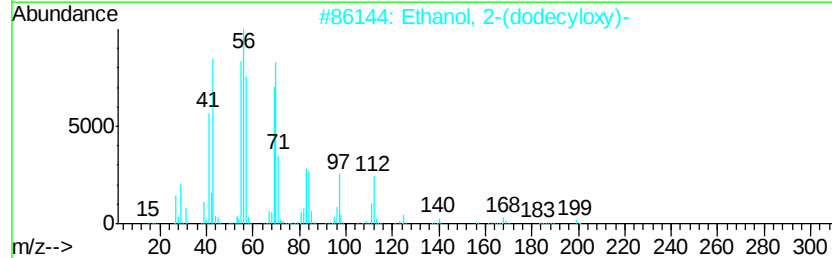
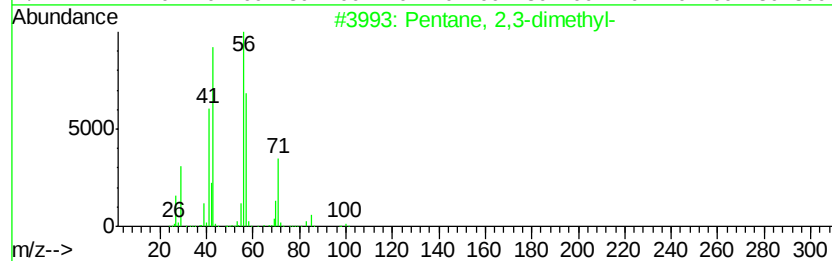
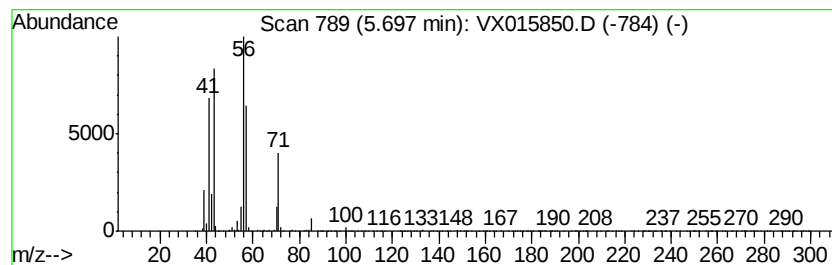
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.M
 Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	58.90 ug/l	3031790	Pentafluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91	
2	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	64	
3	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	47	
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	38	
5	Heptane	100	C7H16	000142-82-5	37	



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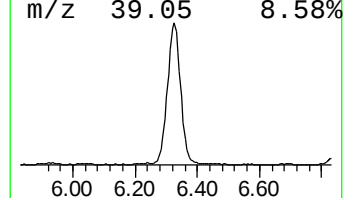
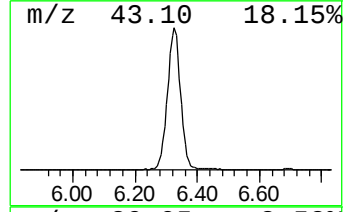
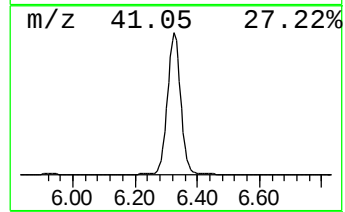
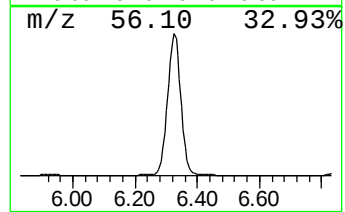
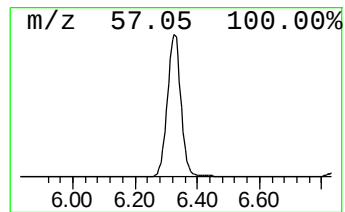
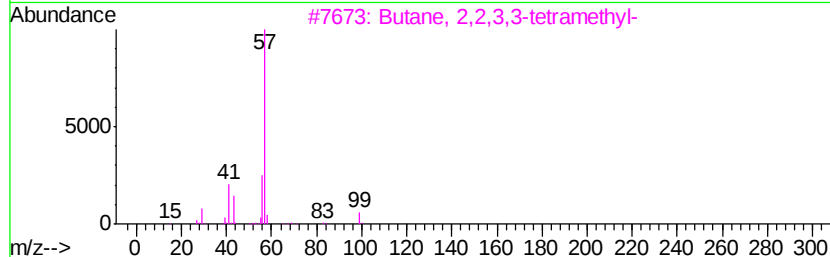
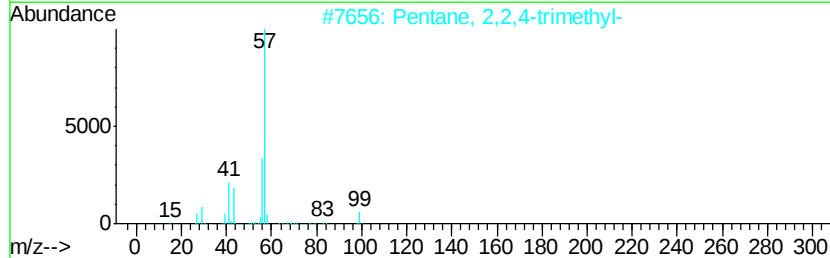
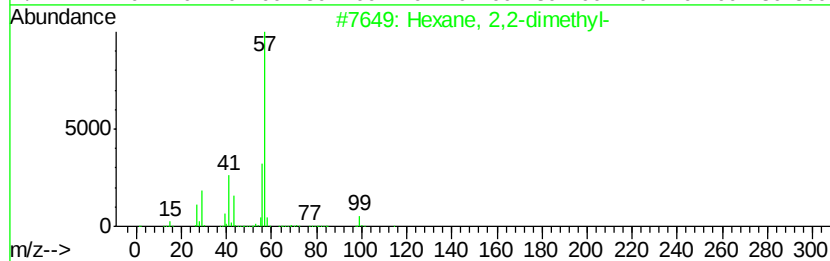
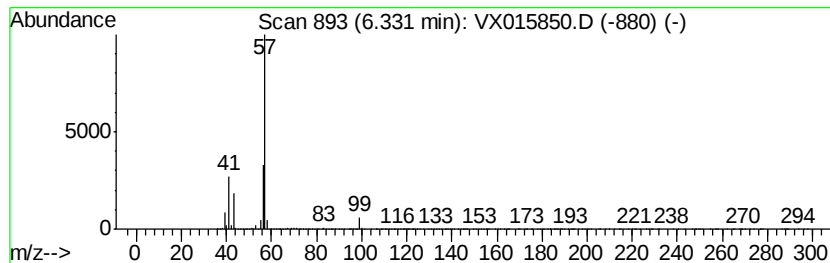
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.M
Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	221.75 ug/l	14599600	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	78
5		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX042220\
Data File : VX015850.D
Acq On : 22 Apr 2020 18:31
Operator : JC/SP
Sample : L2379-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS037MW012-200420

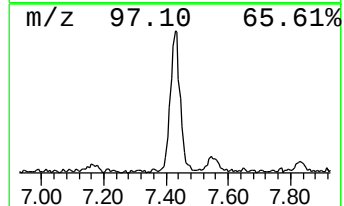
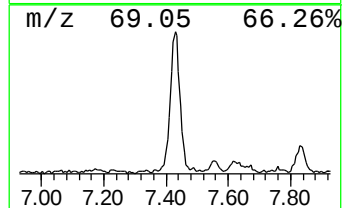
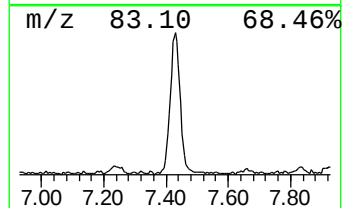
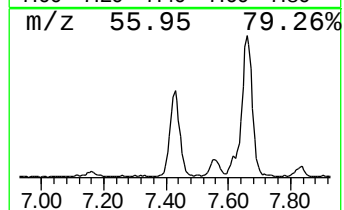
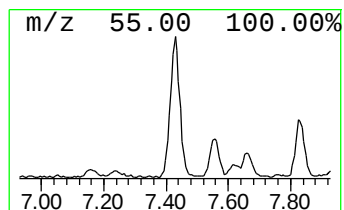
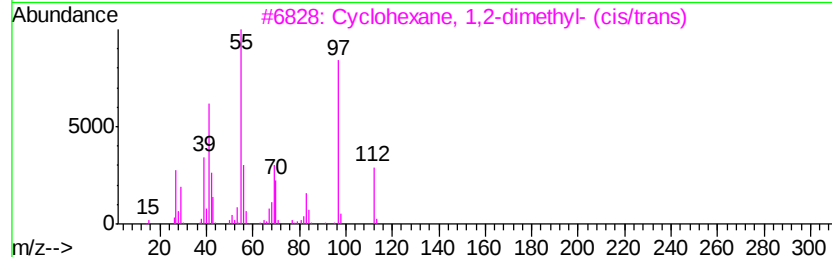
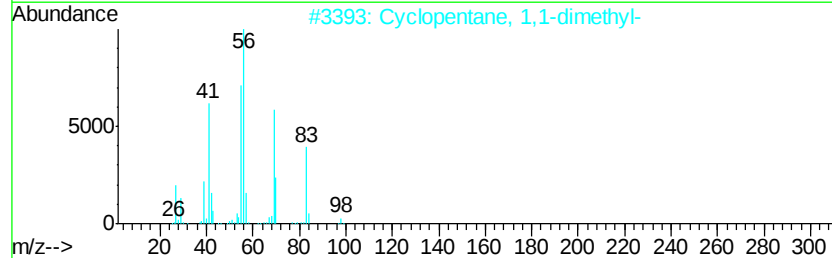
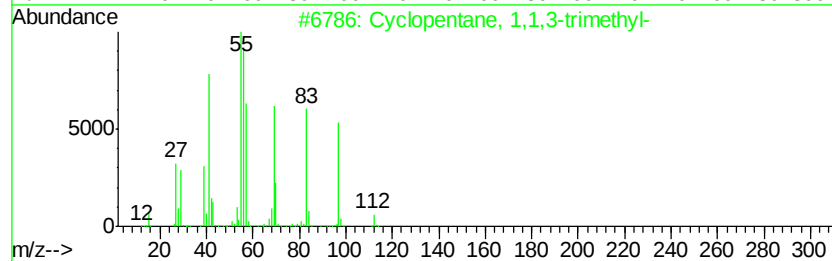
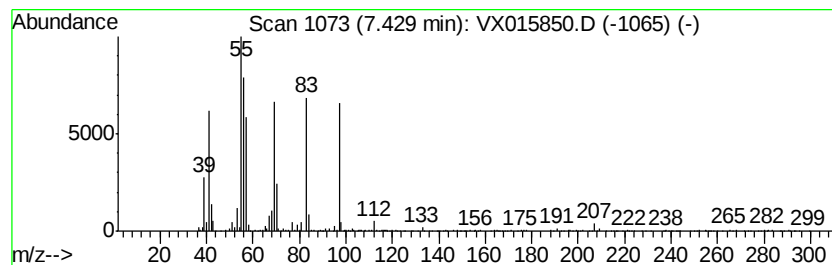
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	9.66 ug/l	635744	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	97
2		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	58
3		Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	46
4		5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	43
5		1-Heptene, 6-methyl-	112	C8H16	005026-76-6	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX042220\
Data File : VX015850.D
Acq On : 22 Apr 2020 18:31
Operator : JC/SP
Sample : L2379-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

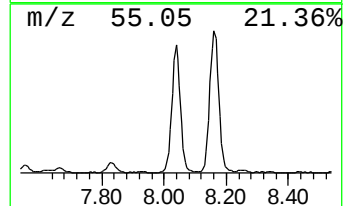
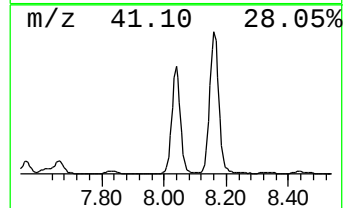
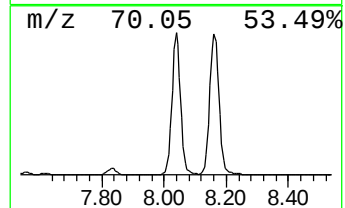
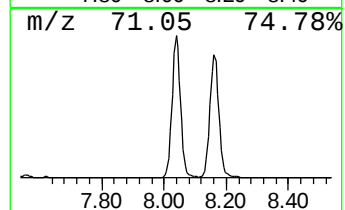
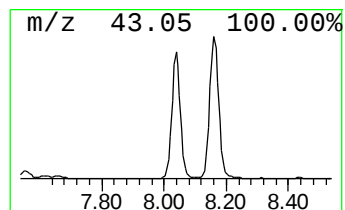
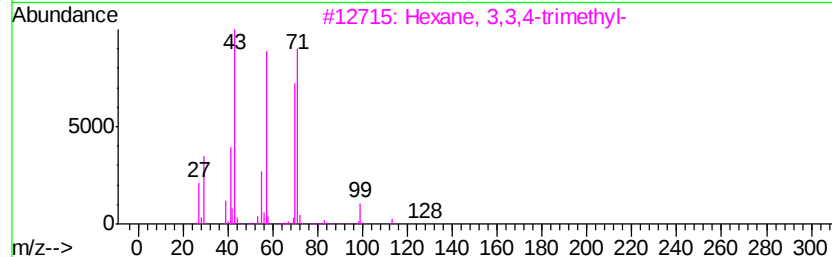
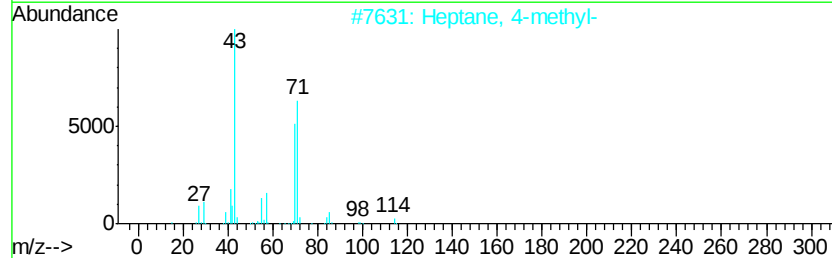
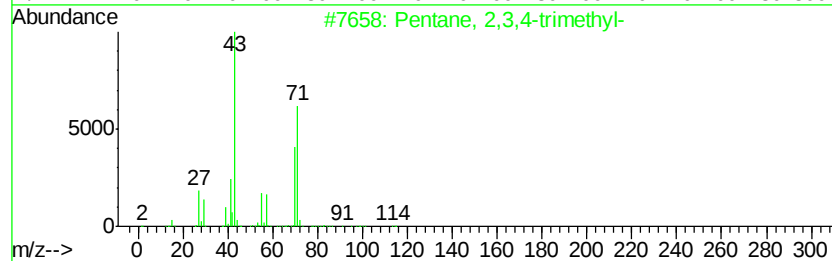
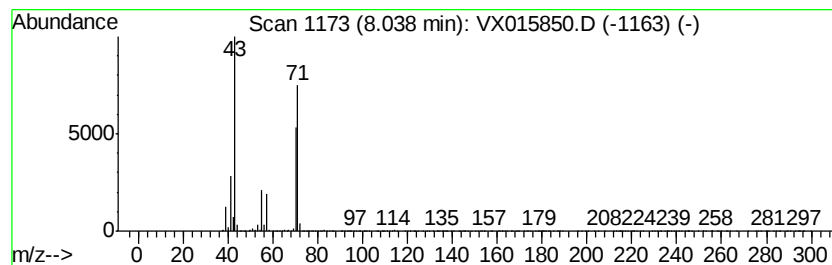
Instrument :
MSVOA_X
ClientSampleId :
SS037MW012-200420

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.M
Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	99.95 ug/l	6580590	1,4-Difluorobenzene	6.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentane, 2,3,4-trimethyl-	114 C8H18	000565-75-3	91
2	Heptane, 4-methyl-	114 C8H18	000589-53-7	83
3	Hexane, 3,3,4-trimethyl-	128 C9H20	016747-31-2	78
4	Heptane, 3,3,4-trimethyl-	142 C10H22	020278-87-9	64
5	Ethanedioic acid, bis(3-methylbu...	230 C12H22O4	002051-00-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX042220\
Data File : VX015850.D
Acq On : 22 Apr 2020 18:31
Operator : JC/SP
Sample : L2379-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS037MW012-200420

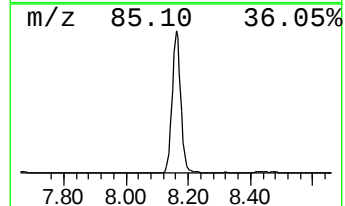
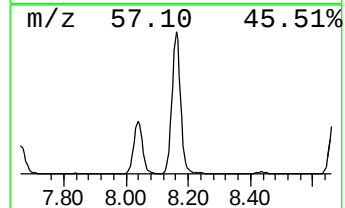
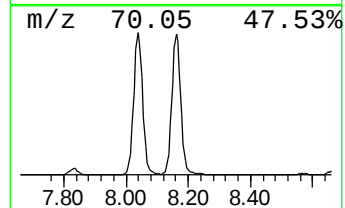
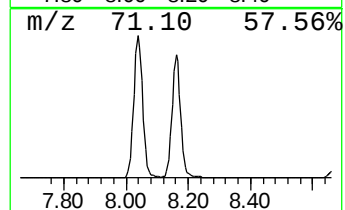
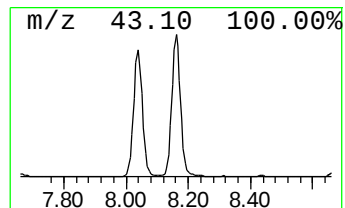
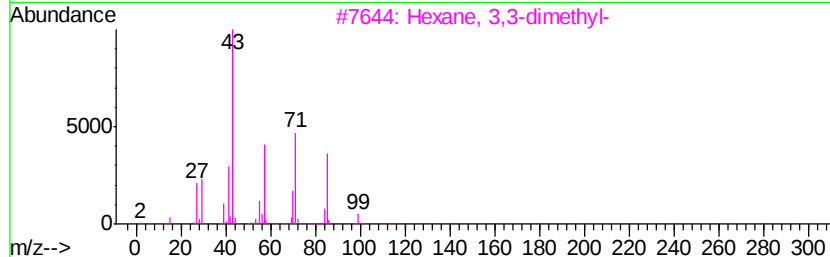
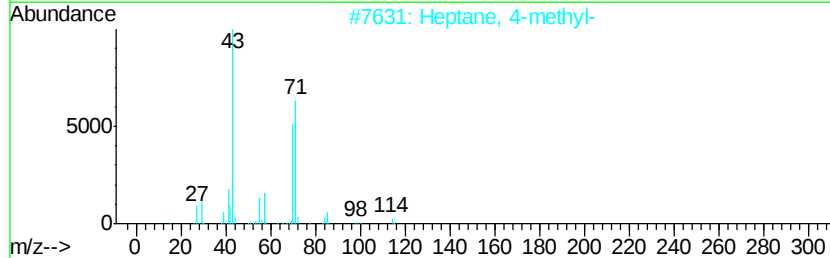
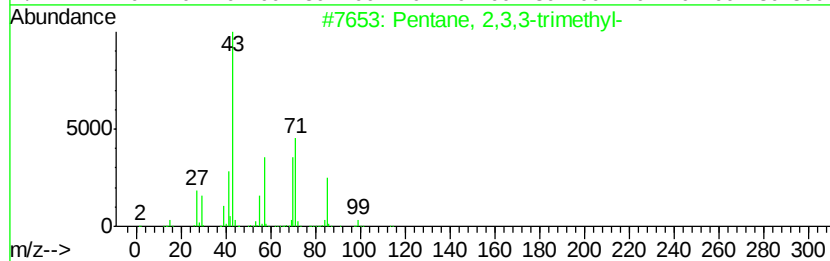
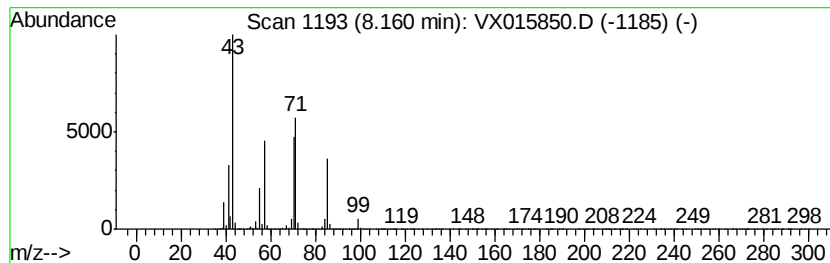
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.M
Quant Title : SW846 8260

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

Peak Number 10 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	136.24 ug/l	8969890	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX042220\
Data File : VX015850.D
Acq On : 22 Apr 2020 18:31
Operator : JC/SP
Sample : L2379-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS037MW012-200420

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X042220W.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	11.8	ug/l	608885	1	5.64	2573900	50.0
Butane, 2,2-dimet...	2.38	14.9	ug/l	766056	1	5.64	2573900	50.0
Butane, 2,3-dimet...	2.83	128.0	ug/l	6589610	1	5.64	2573900	50.0
Pentane, 2,4-dime...	4.29	108.7	ug/l	5597370	1	5.64	2573900	50.0
Pentane, 2,3-dime...	5.70	58.9	ug/l	3031790	1	5.64	2573900	50.0
Hexane, 2,2-dimet...	6.33	221.8	ug/l	14599600	2	6.84	3291960	50.0
Cyclopentane, 1,1...	7.43	9.7	ug/l	635744	2	6.84	3291960	50.0
Pentane, 2,3,4-tr...	8.04	100.0	ug/l	6580590	2	6.84	3291960	50.0
Pentane, 2,3,3-tr...	8.16	136.2	ug/l	8969890	2	6.84	3291960	50.0