

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121919\
 Data File : VX014130.D
 Acq On : 19 Dec 2019 18:57
 Operator : JC/SP
 Sample : K6347-02 10X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-2

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\82X121319W.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	39	rBV	803746	948289	27.81%	4.088%
2	1.295	63	67	75	rBV	245467	263455	7.73%	1.136%
3	1.399	80	84	93	rVB	557387	526462	15.44%	2.269%
4	1.606	108	118	123	rVB	35754	92662	2.72%	0.399%
5	1.783	142	147	158	rVB	396508	568768	16.68%	2.452%
6	1.990	177	181	190	rVB	189046	263371	7.72%	1.135%
7	2.259	221	225	233	rVB	59751	102517	3.01%	0.442%
8	2.850	314	322	323	rBV5	19864	36945	1.08%	0.159%
9	2.881	323	327	330	rVV	35186	69670	2.04%	0.300%
10	2.923	330	334	342	rVB	79067	167974	4.93%	0.724%
11	3.027	345	351	360	rVB	40204	93364	2.74%	0.402%
12	3.167	366	374	382	rBV	28557	67041	1.97%	0.289%
13	4.392	566	575	588	rVB	64239	187342	5.49%	0.808%
14	5.490	745	755	763	rBV	281240	807278	23.68%	3.480%
15	5.569	763	768	773	rVV3	63765	173048	5.08%	0.746%
16	5.654	773	782	794	rVB	514096	1447709	42.46%	6.240%
17	6.051	838	847	853	rBV	321660	822864	24.13%	3.547%
18	6.136	853	861	878	rVB	1288911	3409762	100.00%	14.698%
19	6.325	884	892	905	rVB	416496	1128592	33.10%	4.865%
20	6.849	967	978	989	rBV	814691	1874239	54.97%	8.079%
21	7.453	1069	1077	1084	rBV3	31554	69069	2.03%	0.298%
22	8.489	1241	1247	1254	rBV	61853	107006	3.14%	0.461%
23	8.562	1254	1259	1266	rVV	234041	366418	10.75%	1.579%
24	8.709	1276	1283	1291	rBV	1667211	2581858	75.72%	11.129%
25	8.898	1308	1314	1320	rBV	238214	368397	10.80%	1.588%
26	9.501	1409	1413	1418	rBV	36182	53560	1.57%	0.231%
27	10.074	1502	1507	1508	rBV	74354	90241	2.65%	0.389%
28	10.105	1508	1512	1518	rVB	1571495	2173208	63.73%	9.367%
29	10.196	1523	1527	1533	rVB	87876	118093	3.46%	0.509%
30	10.696	1603	1609	1617	rBV	377413	495902	14.54%	2.138%
31	11.129	1675	1680	1690	rBV	1256544	1660090	48.69%	7.156%
32	11.666	1763	1768	1772	rBV	39696	53461	1.57%	0.230%
33	12.074	1830	1835	1842	rBV	1642772	1966503	57.67%	8.476%
34	12.141	1842	1846	1851	rVB	30549	44390	1.30%	0.191%

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

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\82X121319W.M
Title : SW846 8260

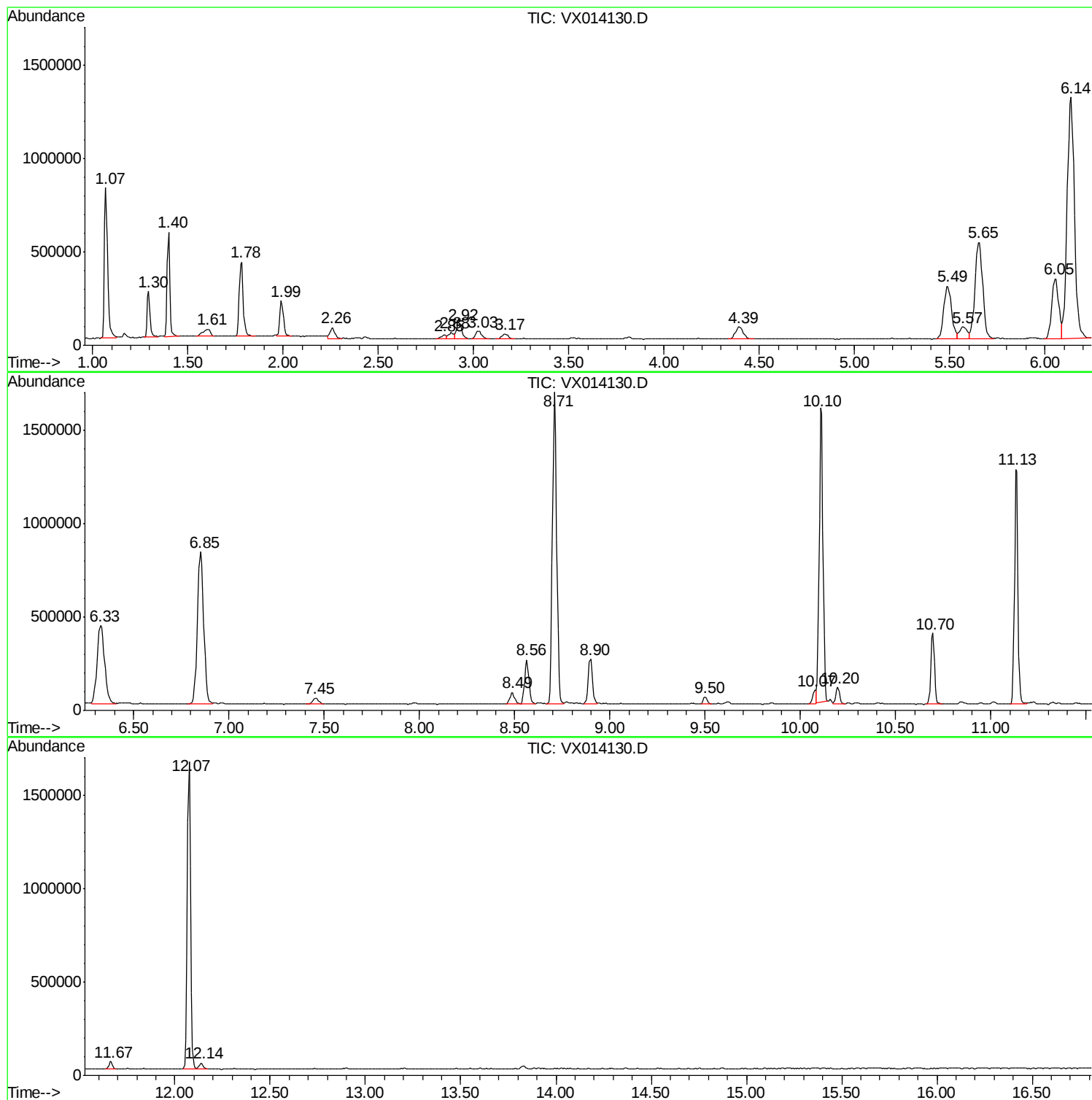
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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



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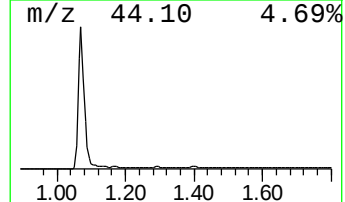
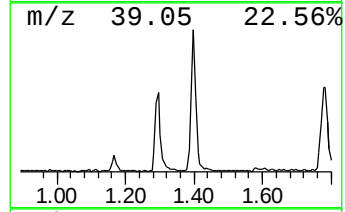
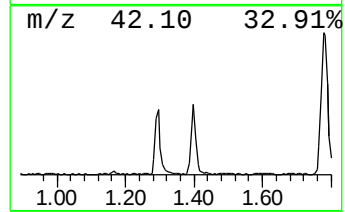
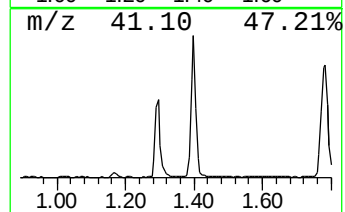
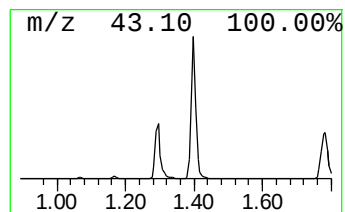
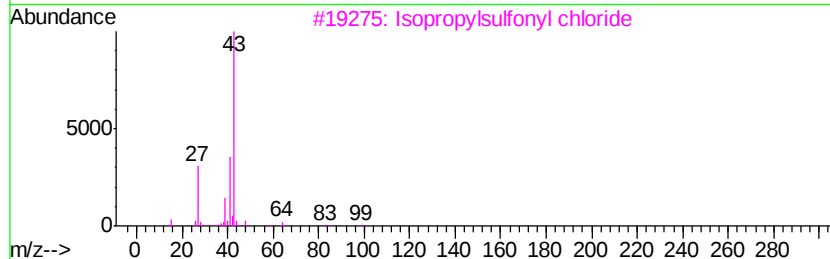
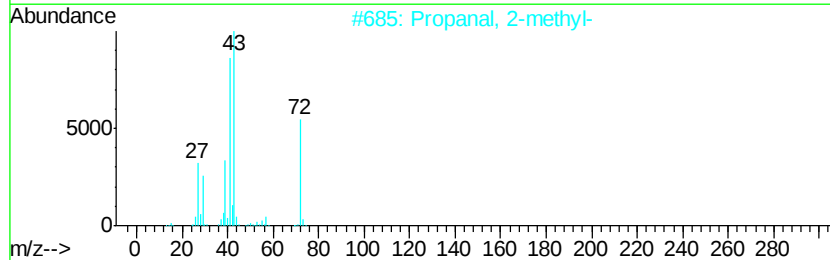
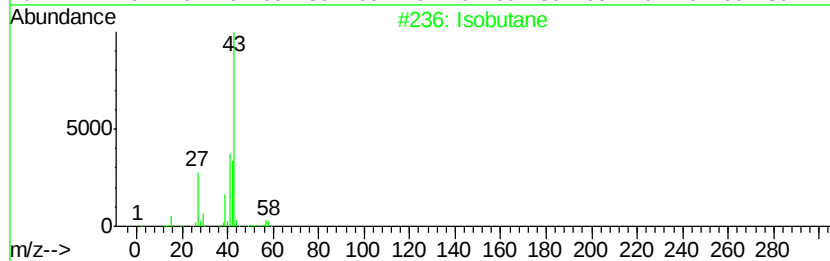
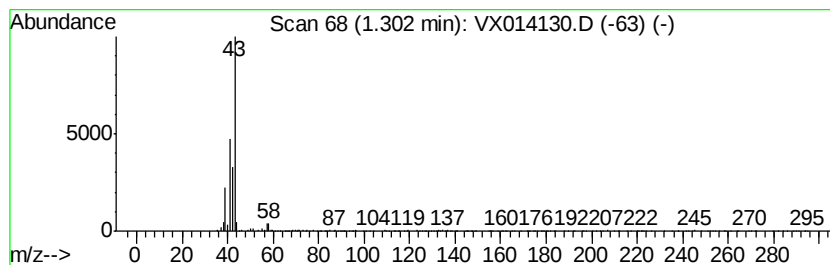
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 2 Isobutane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	9.10 ug/l	263455	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutane	58	C4H10	000075-28-5	80
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	25
3		Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4		2-Propanone, 1-hydroxy-, oxime	89	C3H7NO2	068113-52-0	5
5		1,3-Dioxolan-2-one, 4,4,5,5-tetr...	144	C7H12O3	019424-29-4	4



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ClientSampleId :
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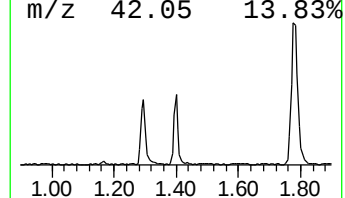
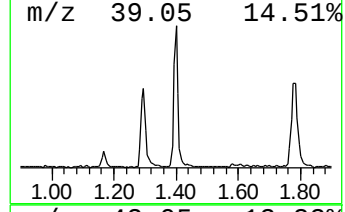
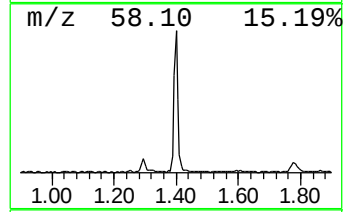
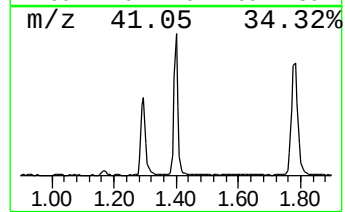
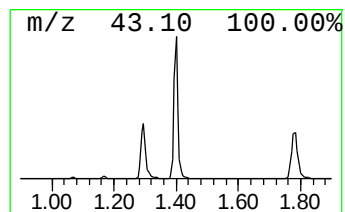
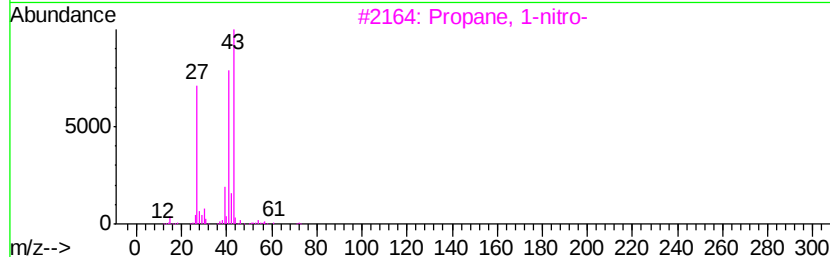
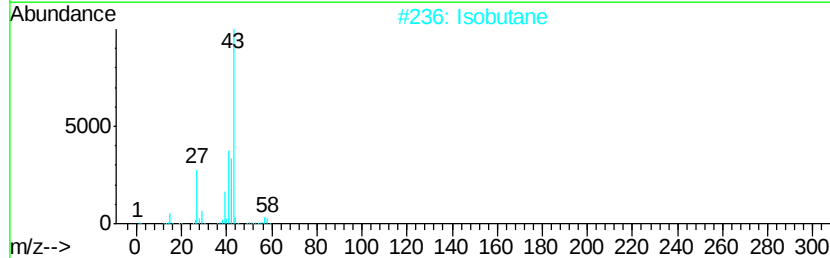
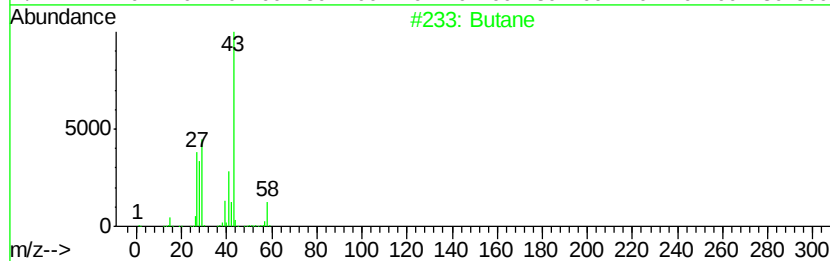
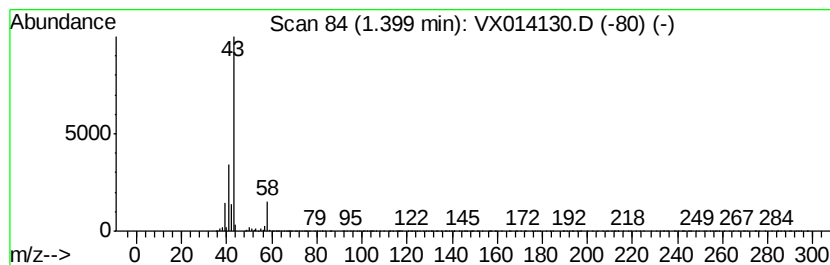
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	18.18 ug/l	526462	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane		58	C4H10	000106-97-8	72
2	Isobutane		58	C4H10	000075-28-5	9
3	Propane, 1-nitro-		89	C3H7NO2	000108-03-2	9
4	Isopropylsulfonyl chloride		142	C3H7ClO2S	010147-37-2	9
5	Diazene, dimethyl-		58	C2H6N2	000503-28-6	5



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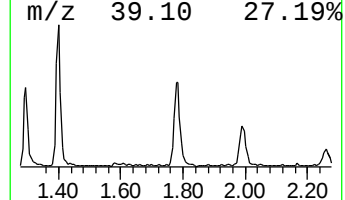
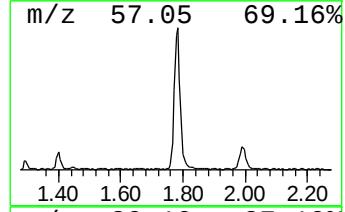
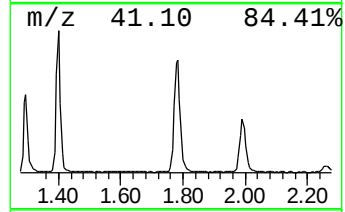
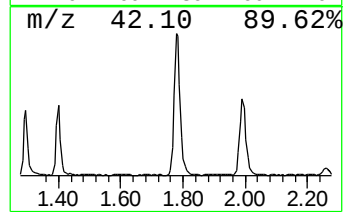
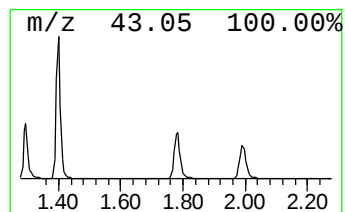
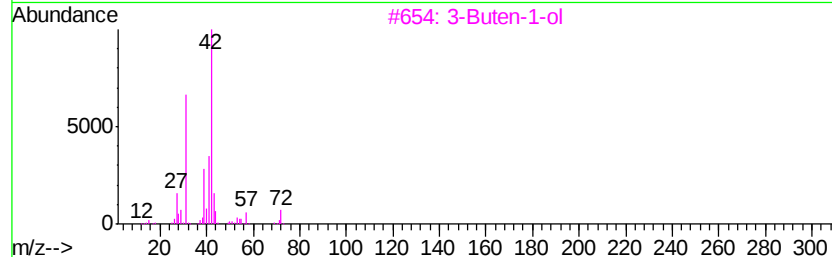
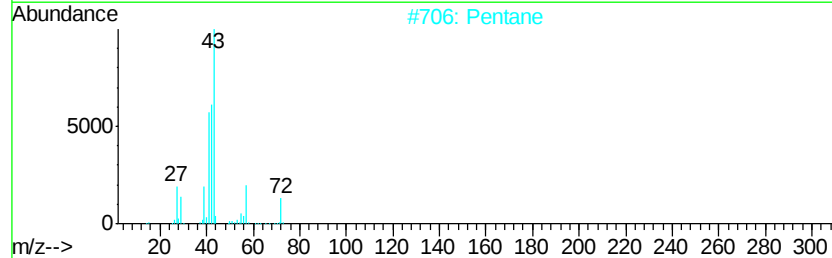
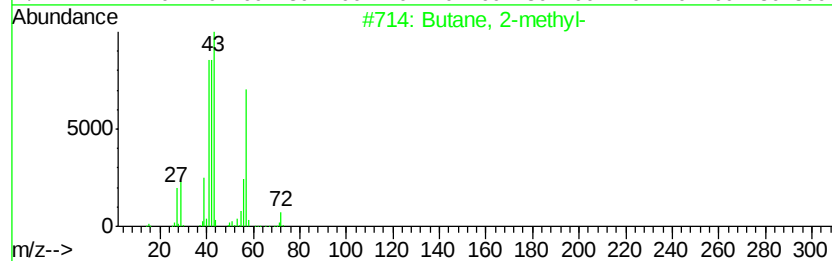
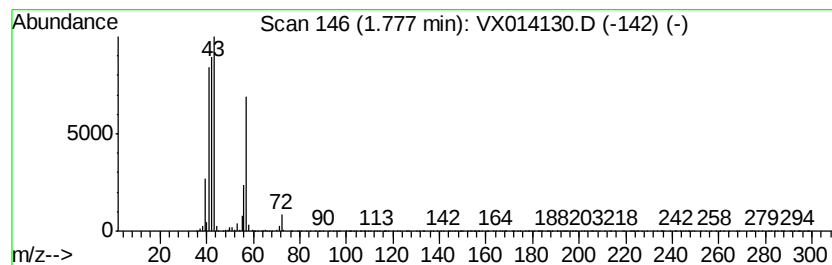
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	19.64 ug/l	568768	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		Pentane	72	C5H12	000109-66-0	50
3		3-Buten-1-ol	72	C4H8O	000627-27-0	47
4		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5		Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

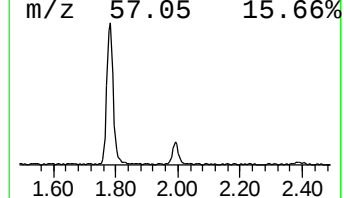
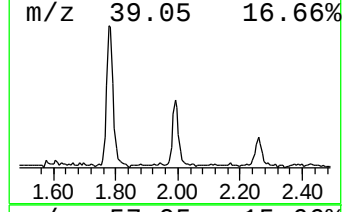
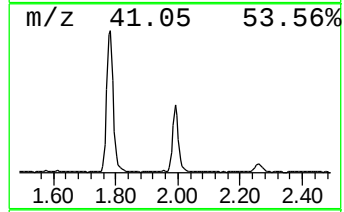
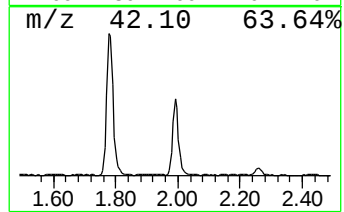
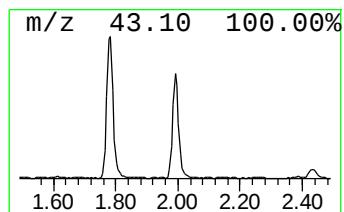
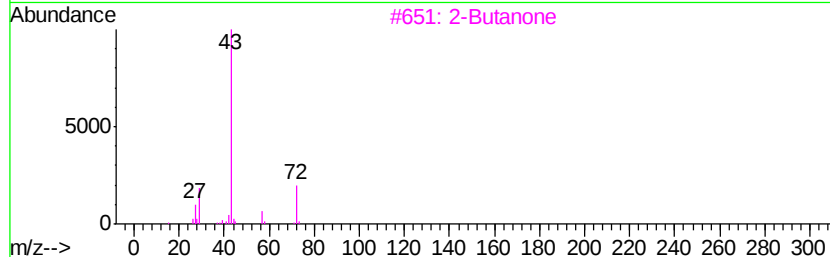
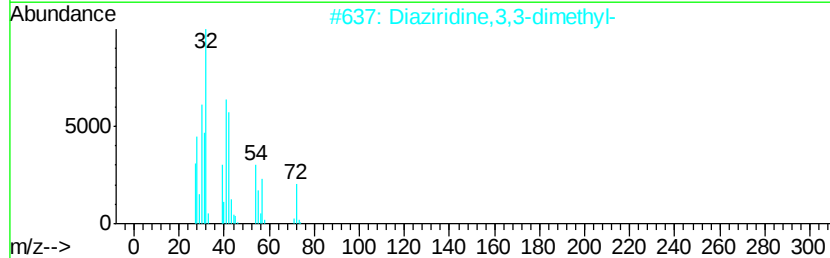
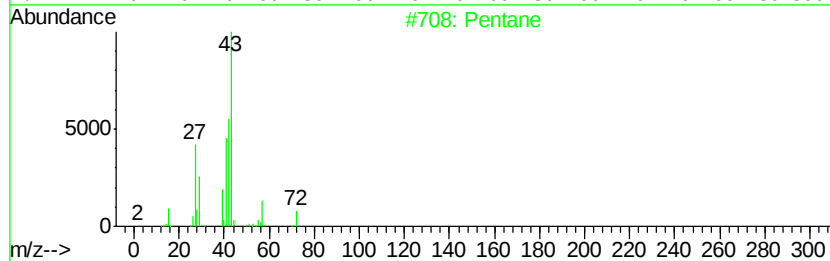
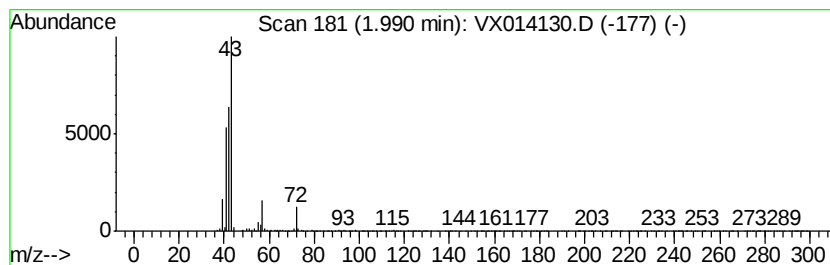
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Quant Title : SW846 8260

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

Peak Number 5 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.99	9.10 ug/l	263371	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	80
2		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	17
3		2-Butanone	72	C4H8O	000078-93-3	9
4		2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	9
5		2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	9



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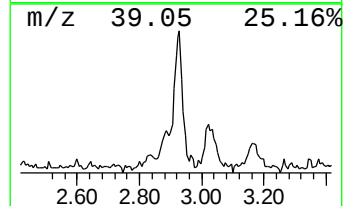
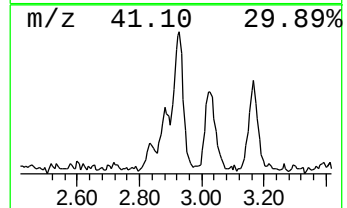
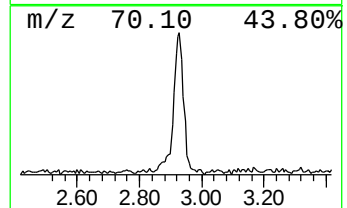
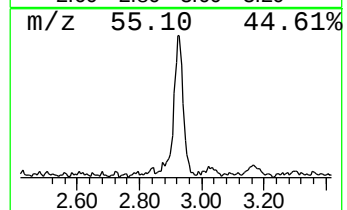
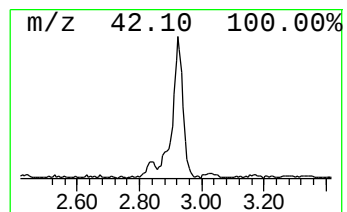
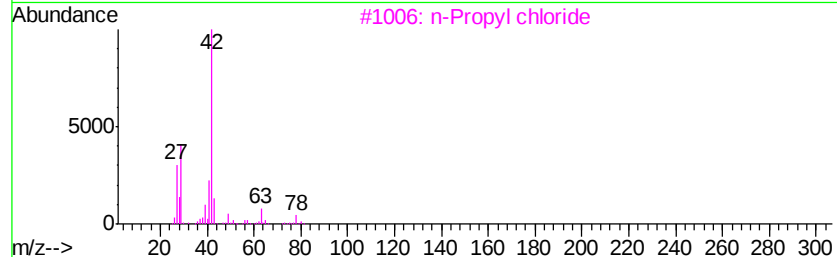
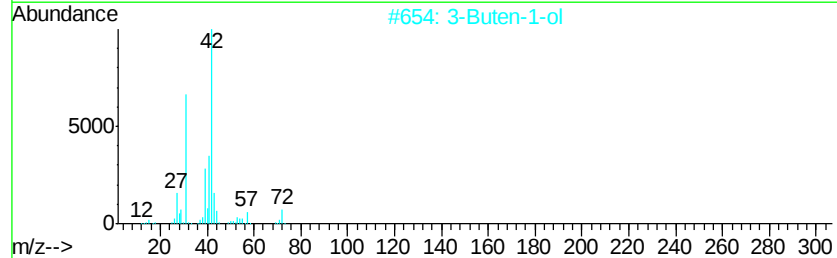
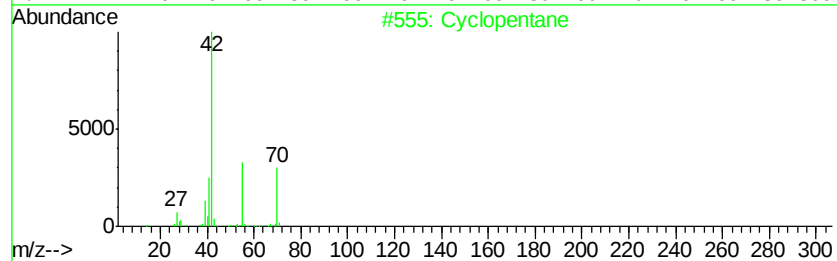
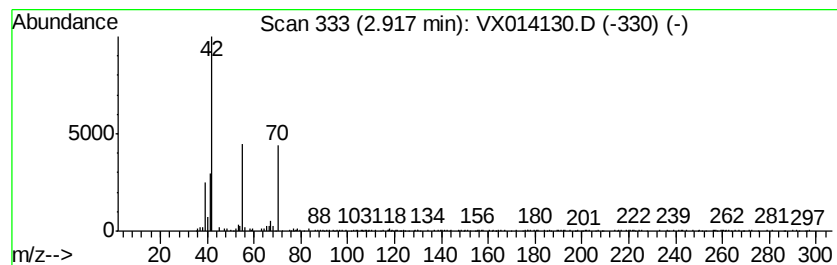
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.92	5.80 ug/l	167974	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane	70	C5H10	000287-92-3	72
2		3-Buten-1-ol	72	C4H8O	000627-27-0	37
3		n-Propyl chloride	78	C3H7Cl	000540-54-5	25
4		Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	9
5		3,4-Epoxytetrahydrothiophene-1,1...	134	C4H6O3S	004509-11-9	9



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ClientSampleId :
MW-2

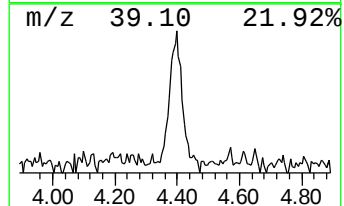
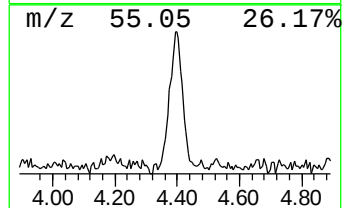
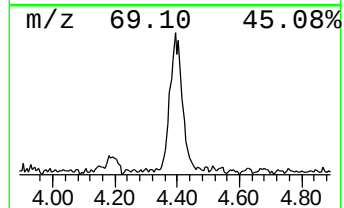
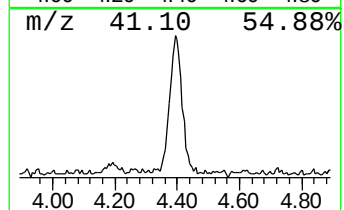
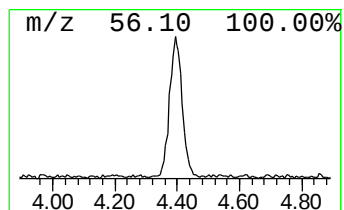
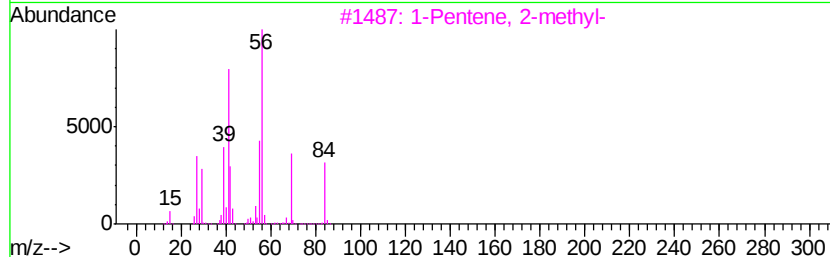
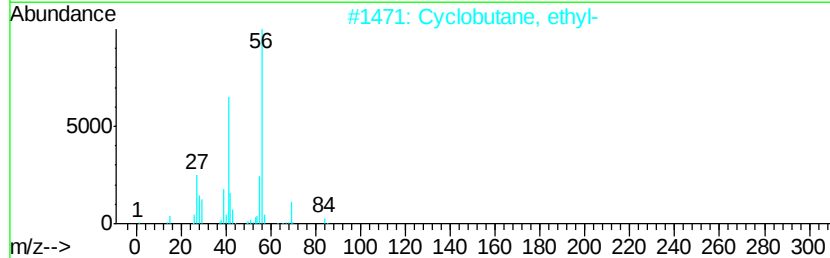
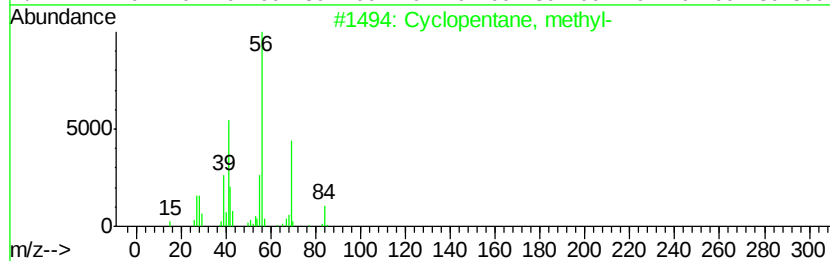
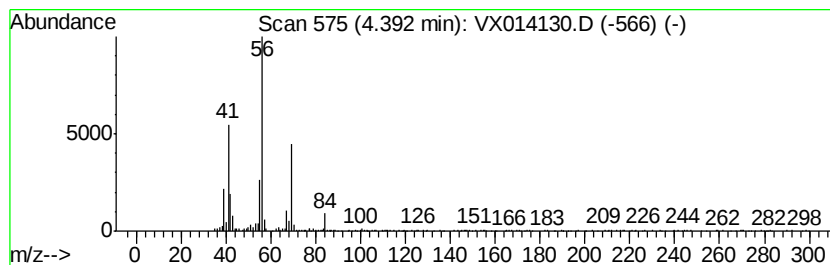
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 7 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	6.47 ug/l	187342	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014130.D
Acq On : 19 Dec 2019 18:57
Operator : JC/SP
Sample : K6347-02 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

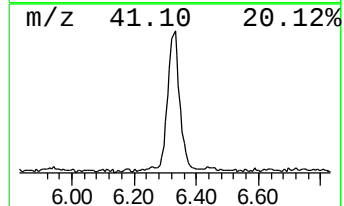
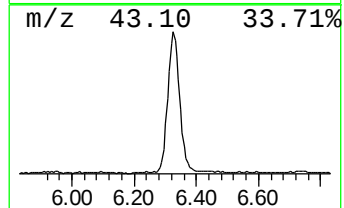
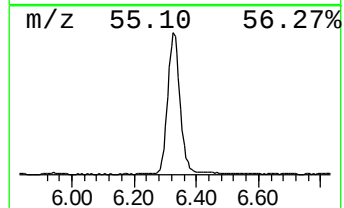
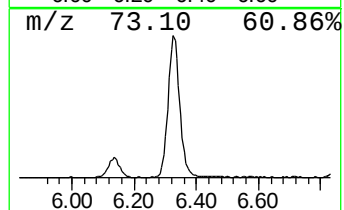
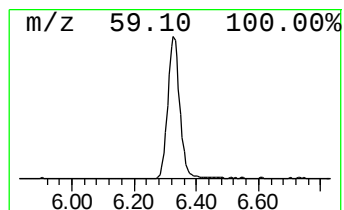
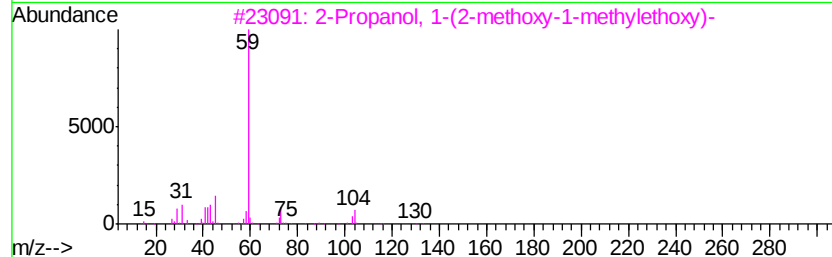
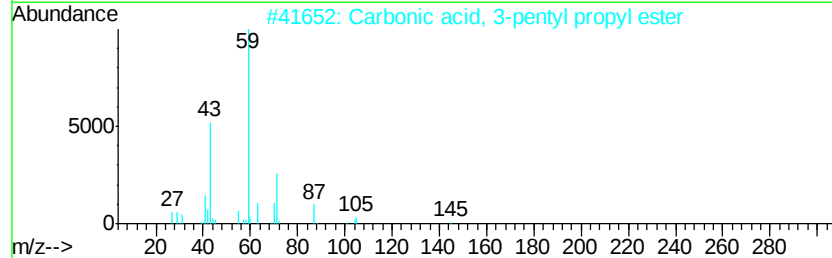
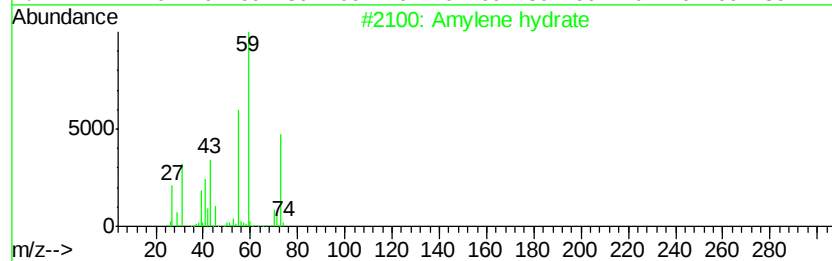
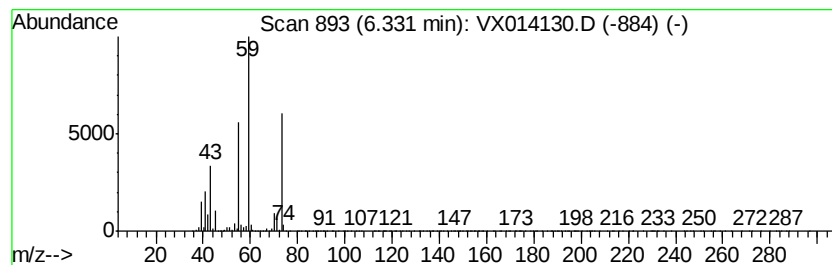
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Quant Title : SW846 8260

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

Peak Number 8 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	30.11 ug/l	1128590	1,4-Difluorobenzene	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Amylene hydrate	88	C5H12O	000075-85-4	83
2		Carbonic acid, 3-pentyl propyl e...	174	C9H18O3	1000325-64-0	42
3		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	42
4		3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	39
5		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014130.D
Acq On : 19 Dec 2019 18:57
Operator : JC/SP
Sample : K6347-02 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

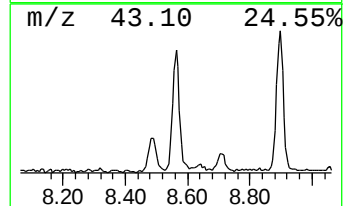
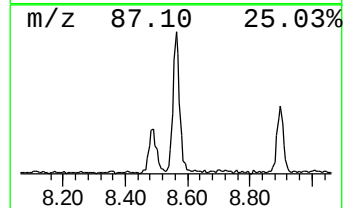
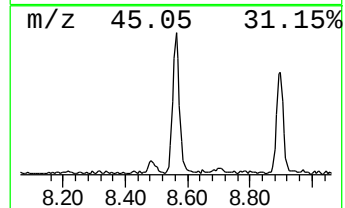
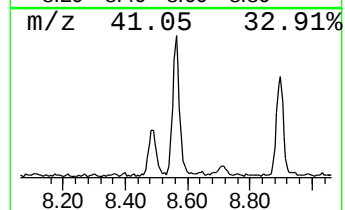
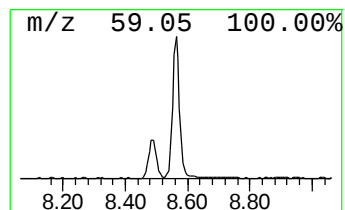
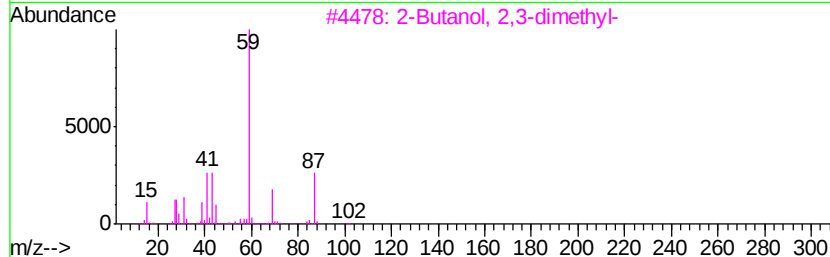
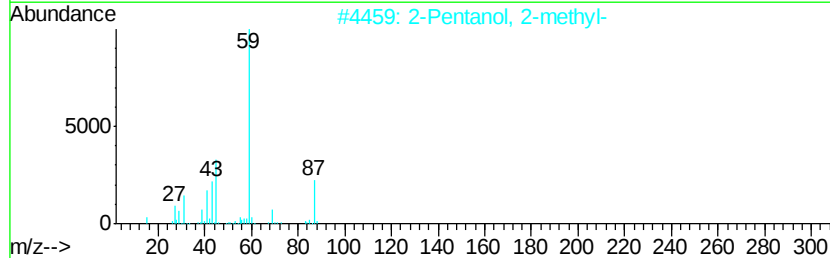
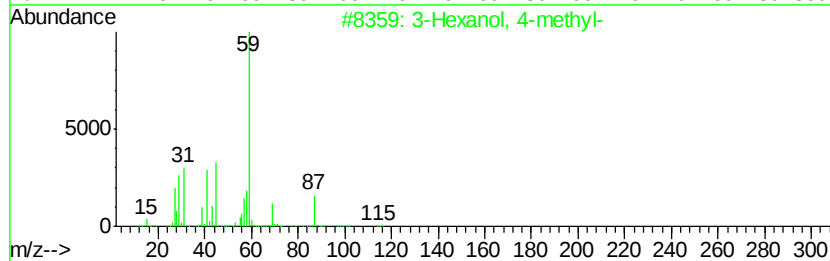
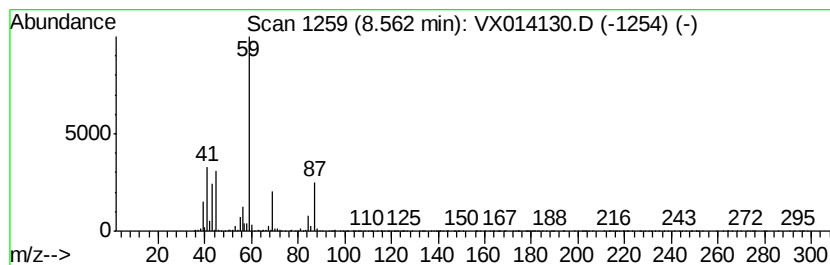
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Quant Title : SW846 8260

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

Peak Number 9 3-Hexanol, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	8.43 ug/l	366418	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	78
2		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
3		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
4		3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	56
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121919\
Data File : VX014130.D
Acq On : 19 Dec 2019 18:57
Operator : JC/SP
Sample : K6347-02 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

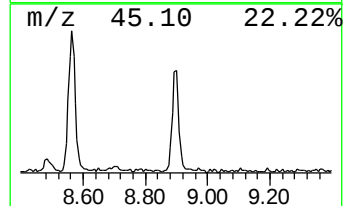
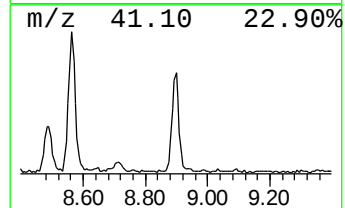
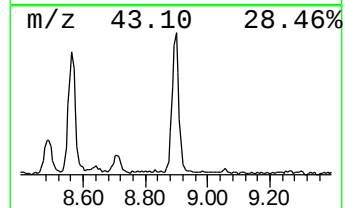
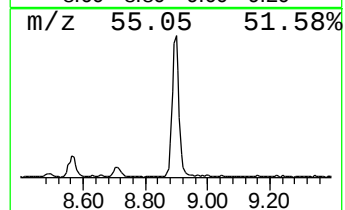
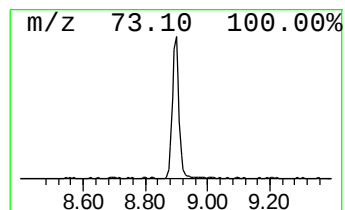
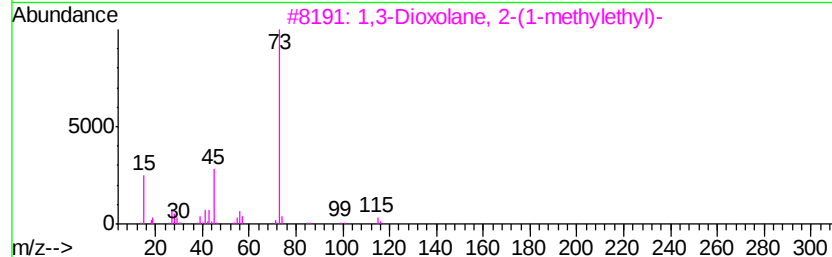
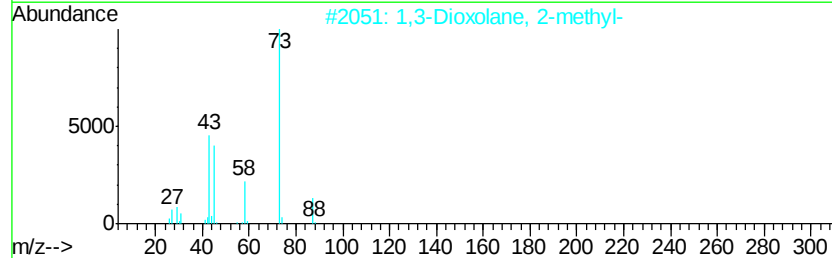
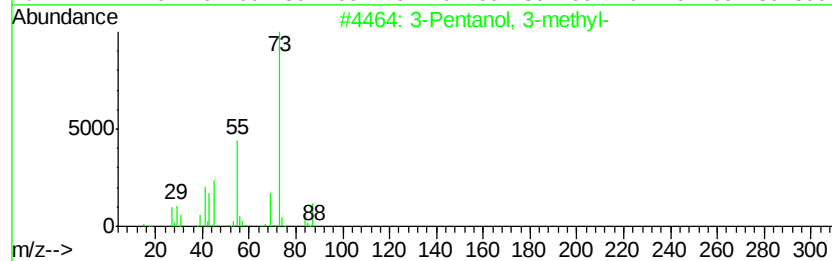
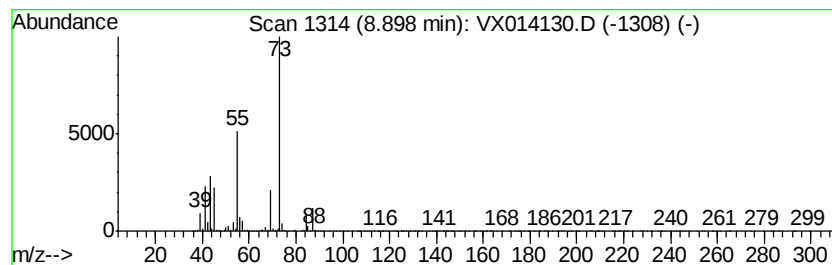
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 10 3-Pentanol, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	8.48 ug/l	368397	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	86
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	37
4		4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	36
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121919\
Data File : VX014130.D
Acq On : 19 Dec 2019 18:57
Operator : JC/SP
Sample : K6347-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.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
Isobutane	1.30	9.1	ug/l	263455	1	5.65	1447710	50.0
Butane	1.40	18.2	ug/l	526462	1	5.65	1447710	50.0
Butane, 2-methyl-	1.78	19.6	ug/l	568768	1	5.65	1447710	50.0
Pentane	1.99	9.1	ug/l	263371	1	5.65	1447710	50.0
Cyclopentane	2.92	5.8	ug/l	167974	1	5.65	1447710	50.0
Cyclopentane, met...	4.39	6.5	ug/l	187342	1	5.65	1447710	50.0
Amylene hydrate	6.33	30.1	ug/l	1128590	2	6.85	1874240	50.0
3-Hexanol, 4-methyl-	8.56	8.4	ug/l	366418	3	10.11	2173210	50.0
3-Pentanol, 3-met...	8.90	8.5	ug/l	368397	3	10.11	2173210	50.0