

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
 Data File : VX014427.D
 Acq On : 06 Jan 2020 15:09
 Operator : JC/SP
 Sample : K6484-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30627

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	1.478	93	97	110	rBV	7006052	9332156	1.69%	0.547%
2	2.362	230	242	243	rBV4	47481155	115154247	20.84%	6.754%
3	4.435	491	582	585	rBV	30550223	552653887	100.00%	32.414%
4	6.977	990	999	1022	rVB	2863433	9212268	1.67%	0.540%
5	7.307	1042	1053	1087	rBV3	1124162	6270347	1.13%	0.368%
6	7.660	1099	1111	1135	rBV	2012007	6342503	1.15%	0.372%
7	8.934	1312	1320	1334	rBV	4422692	11563731	2.09%	0.678%
8	9.117	1334	1350	1351	rBV6	120983348	424375438	76.79%	24.890%
9	9.282	1364	1377	1381	rBV6	114473563	340515408	61.61%	19.972%
10	9.312	1381	1382	1390	rVV	6476423	5933043	1.07%	0.348%
11	9.392	1390	1395	1408	rVB	7246058	9716725	1.76%	0.570%
12	9.550	1416	1421	1426	rBV	5774132	7733641	1.40%	0.454%
13	10.135	1508	1517	1524	rVB2	3000300	6658087	1.20%	0.391%
14	10.221	1524	1531	1540	rBV	19632686	26955327	4.88%	1.581%
15	10.769	1612	1621	1636	rVB	5383973	9079035	1.64%	0.532%
16	11.135	1672	1681	1687	rBV3	3466890	5951877	1.08%	0.349%
17	11.214	1687	1694	1699	rVV2	85931789	123439562	22.34%	7.240%
18	11.708	1766	1775	1788	rVB2	10172162	17525413	3.17%	1.028%
19	12.007	1816	1824	1831	rVB	12847783	16590016	3.00%	0.973%

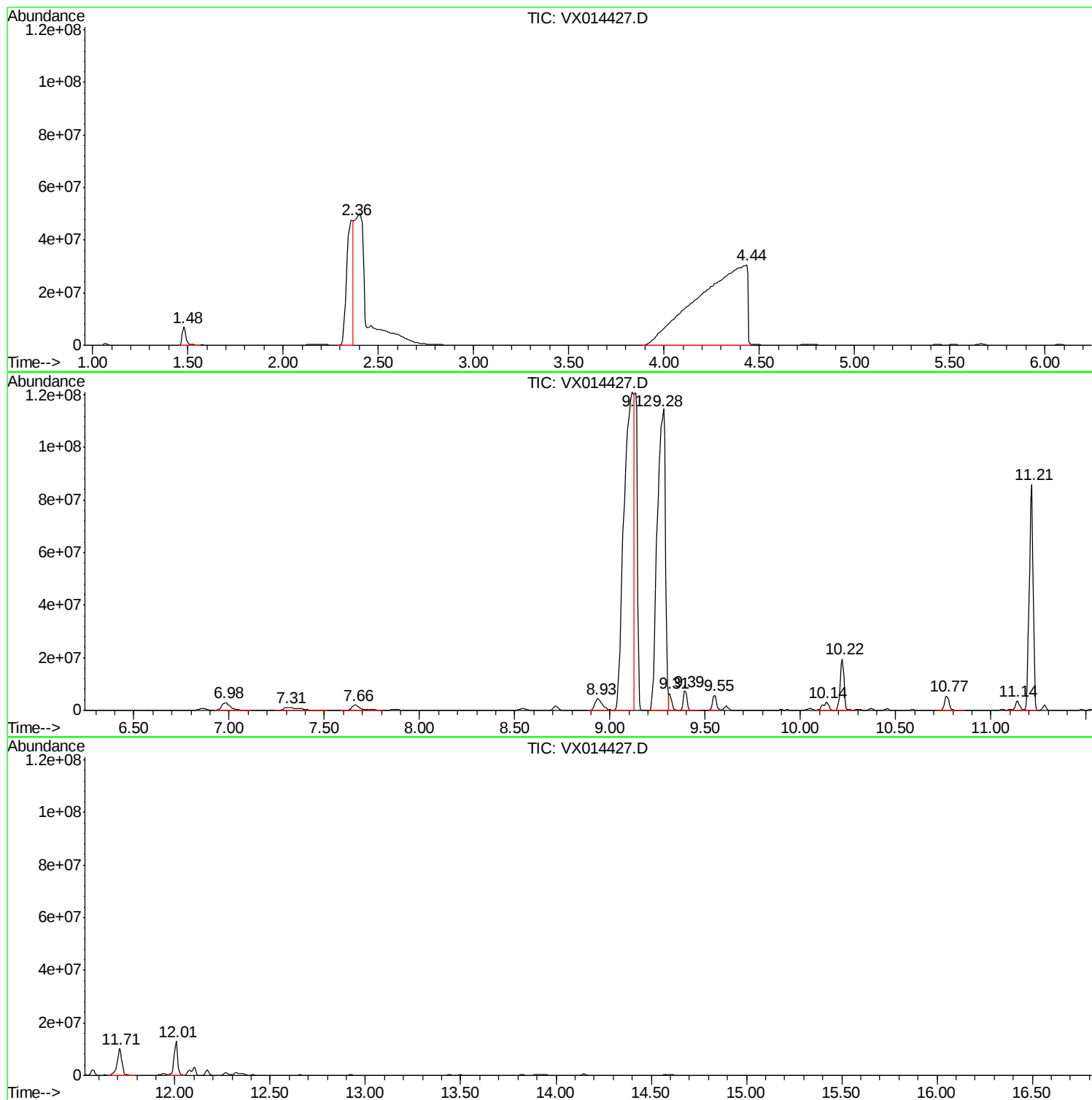
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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



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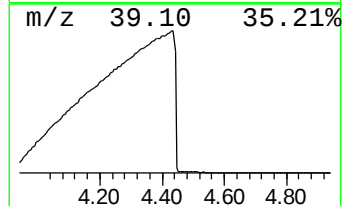
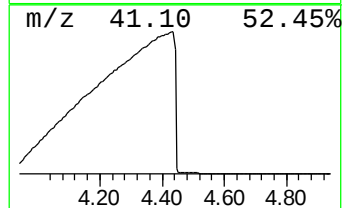
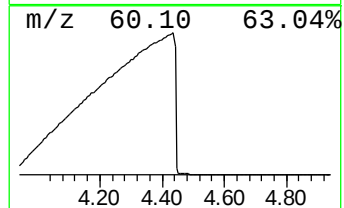
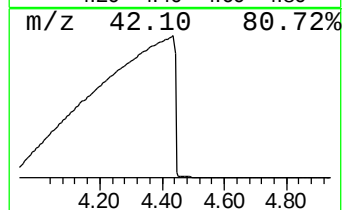
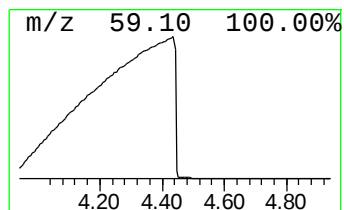
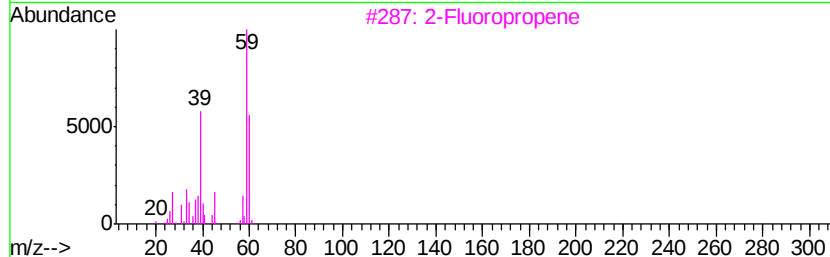
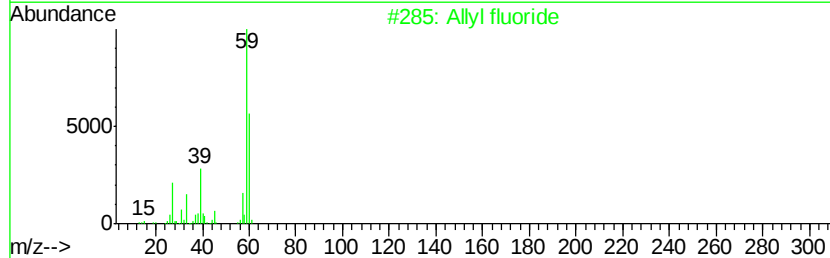
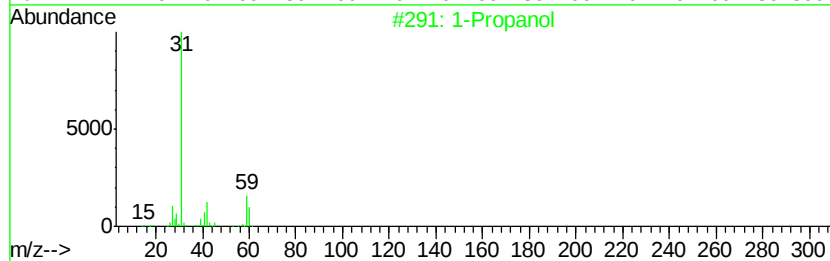
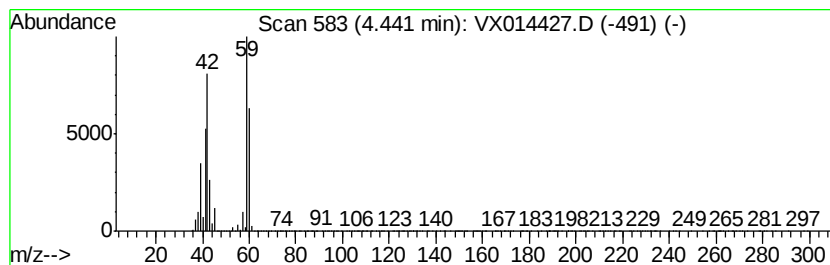
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Propanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	50.00 ug/l	552654000	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	43
3		2-Fluoropropene	60	C3H5F	001184-60-7	43
4		2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	9
5		Cyclopropane	42	C3H6	000075-19-4	9



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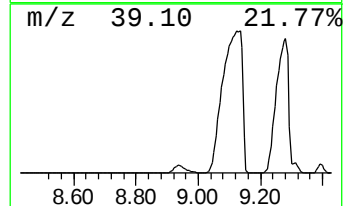
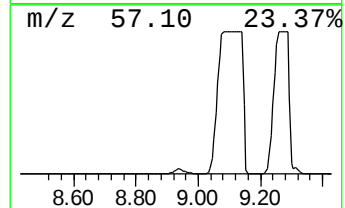
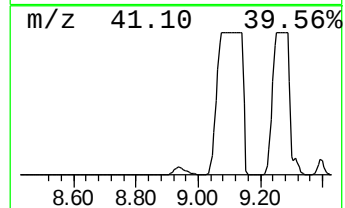
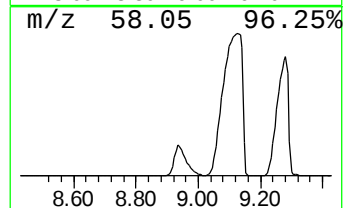
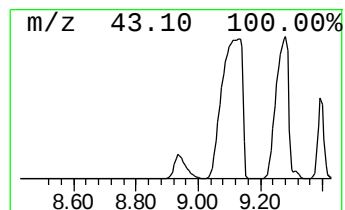
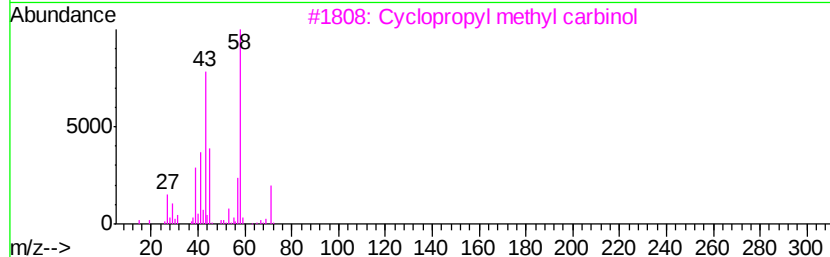
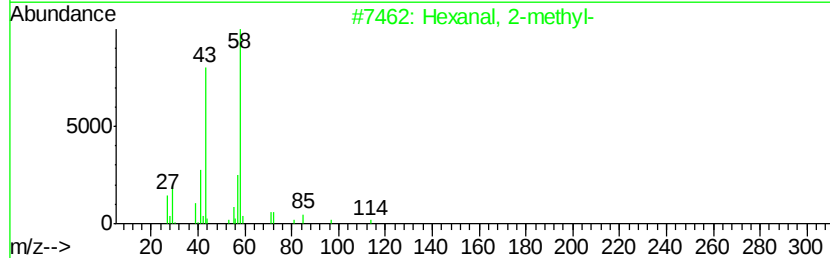
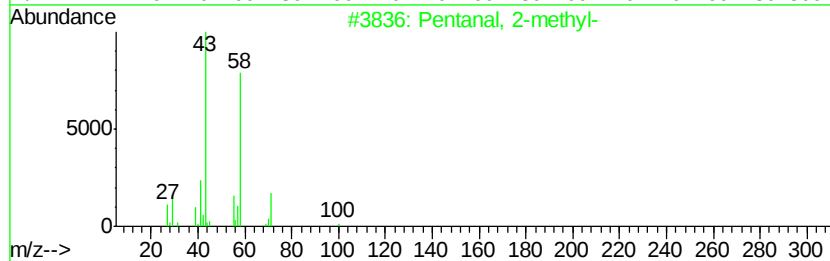
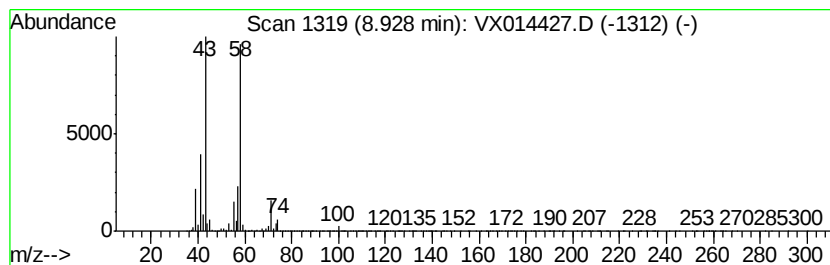
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 Quant Title : SW846 8260

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 TIC Integration Parameters: LSCINT.P

 Peak Number 2 Pentanal, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.93	86.84 ug/l	11563700	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	86
2		Hexanal, 2-methyl-	114	C7H14O	000925-54-2	64
3		Cyclopropyl methyl carbinol	86	C5H10O	000765-42-4	56
4		Butanimidamide	86	C4H10N2	000107-90-4	56
5		2-Propenoic acid, 2-(dimethylami...	143	C7H13NO2	002439-35-2	53



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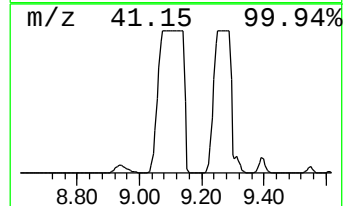
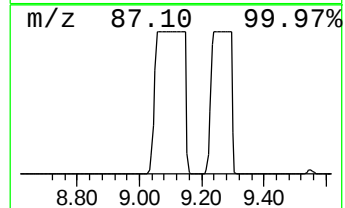
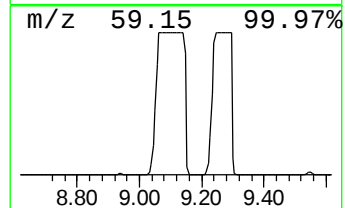
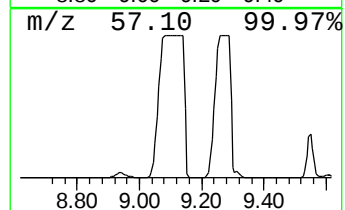
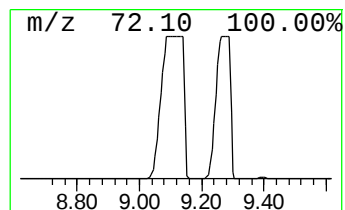
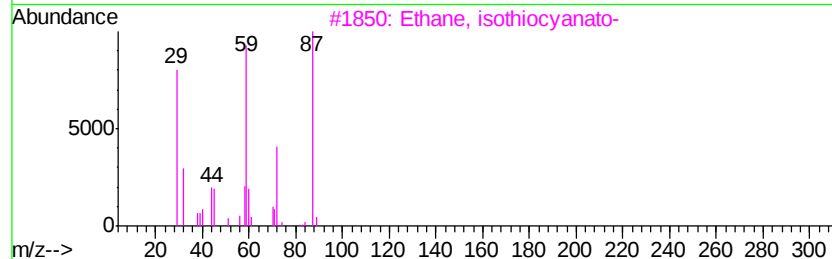
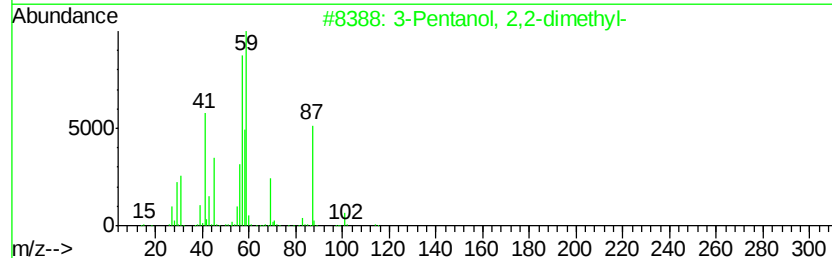
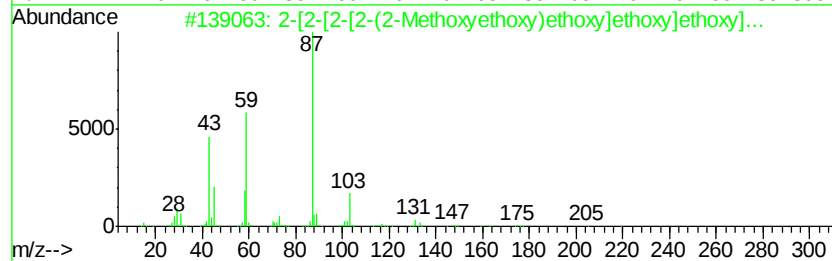
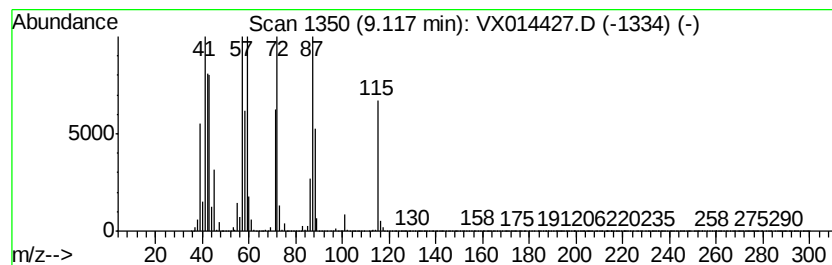
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Peak Number 3 unknown9.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.12	3186.92 ug/l	424375000	Chlorobenzene-d5	10.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	-[2-[2-(2-Methoxyethoxy)etho...	294	C13H26O7	1000351-91-3	30	
2	3	Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	27	
3	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	27		
4	Silane, triethyl-	116	C6H16Si	000617-86-7	25		
5	2-[2-[2-(2-Methoxyethoxy)ethoxy]...	250	C11H22O6	1000351-91-4	22		



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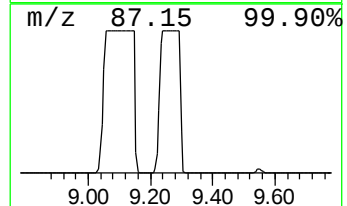
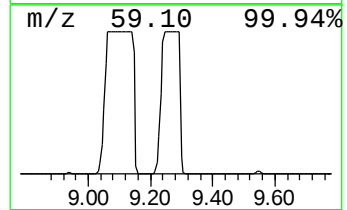
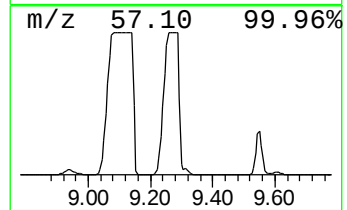
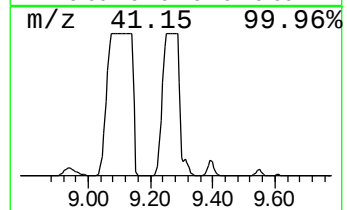
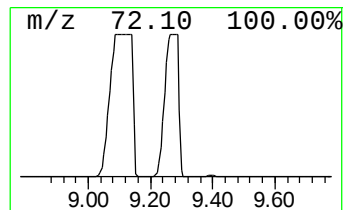
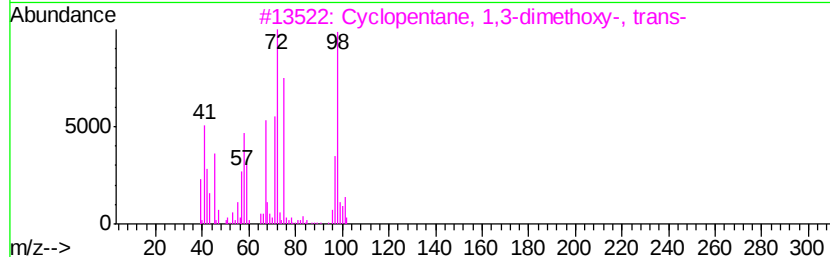
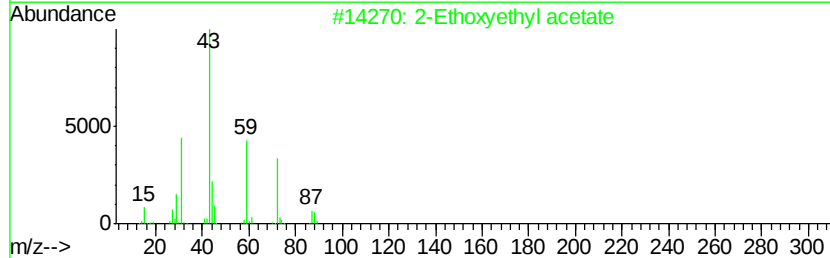
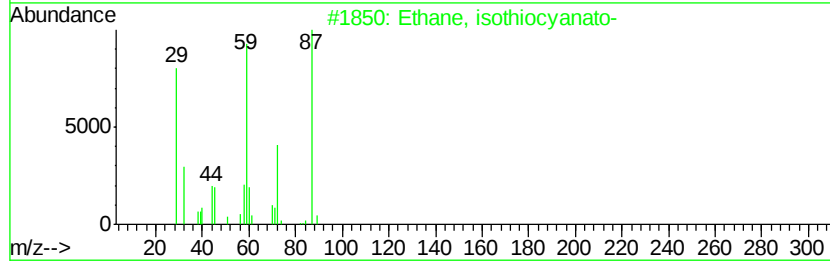
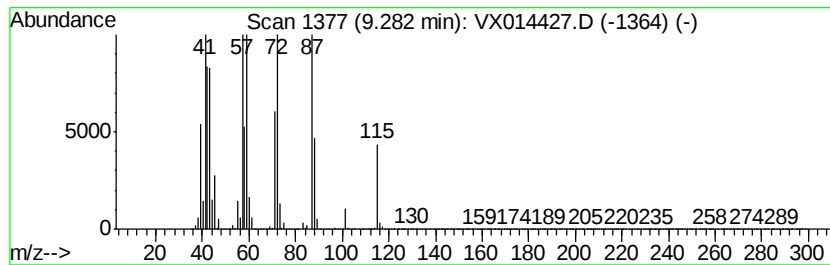
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Peak Number 4 unknown9.28 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.28	2557.16 ug/l	340515000	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	30
2		2-Ethoxyethyl acetate	132	C6H12O3	000111-15-9	27
3		Cyclopentane, 1,3-dimethoxy-, tr...	130	C7H14O2	029887-57-8	27
4		2,2-Diethylacetamide	115	C6H13NO	001114-38-1	25
5		Silane, triethyl-	116	C6H16Si	000617-86-7	22



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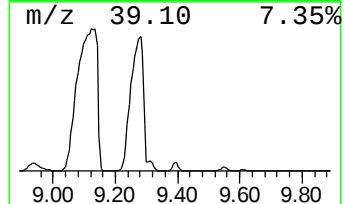
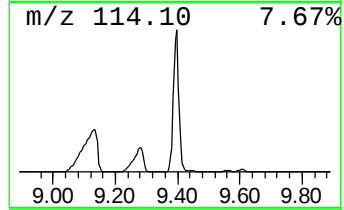
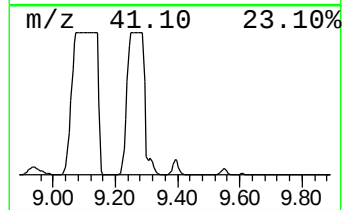
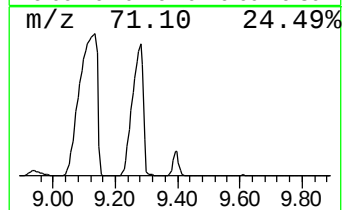
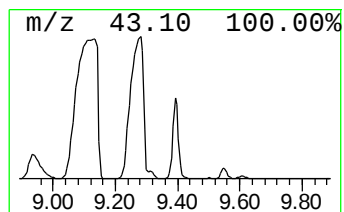
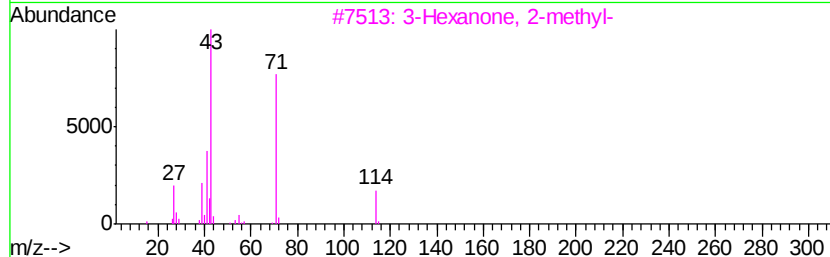
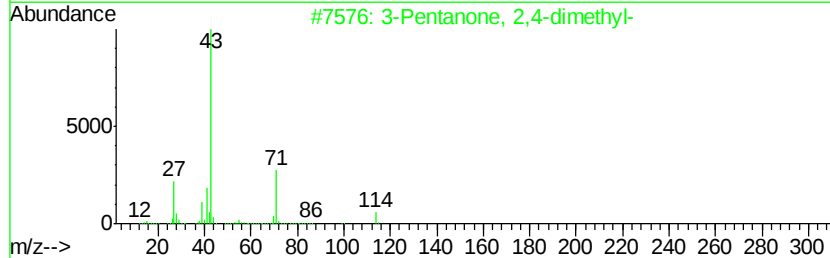
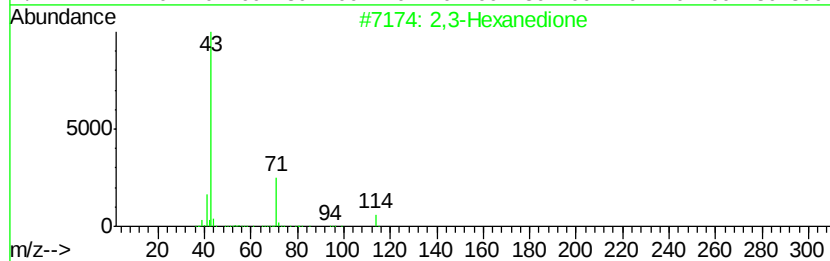
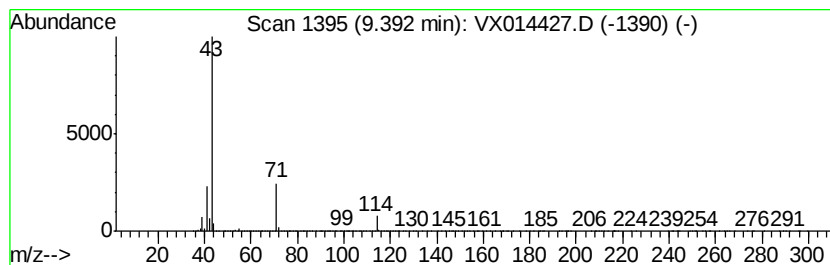
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TIC Integration Parameters: LSCINT.P

Peak Number 5 2,3-Hexanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	72.97 ug/l	9716730	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Hexanedione	114	C6H10O2	003848-24-6	90
2		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	53
3		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	50
4		Butane, 2-(ethenyloxy)-2-methyl-	114	C7H14O	029281-39-8	40
5		2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	9



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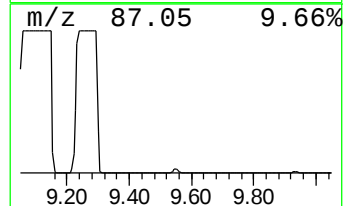
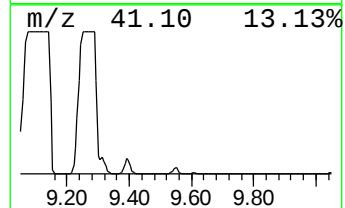
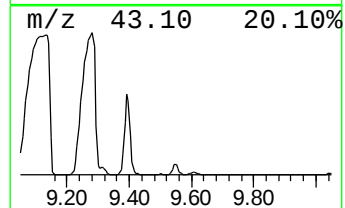
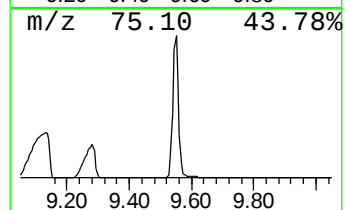
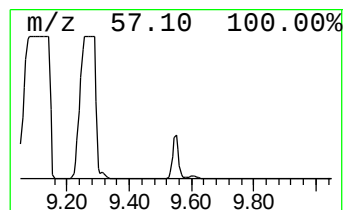
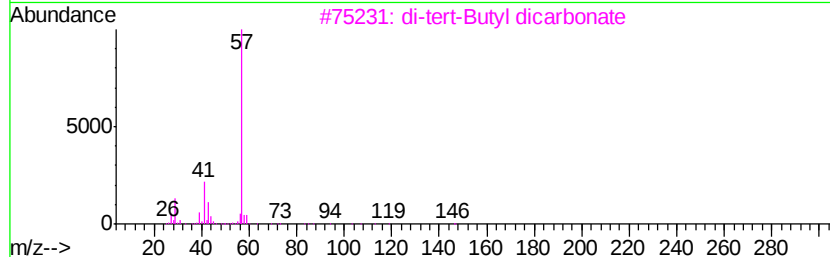
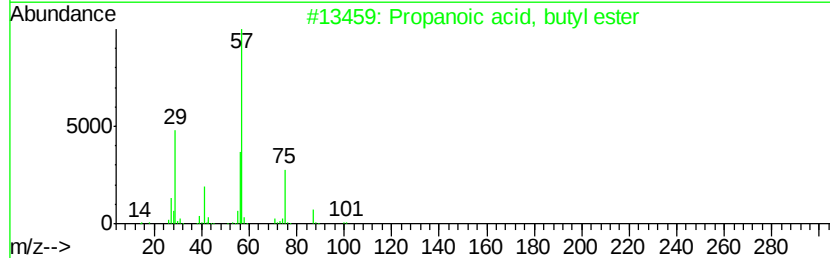
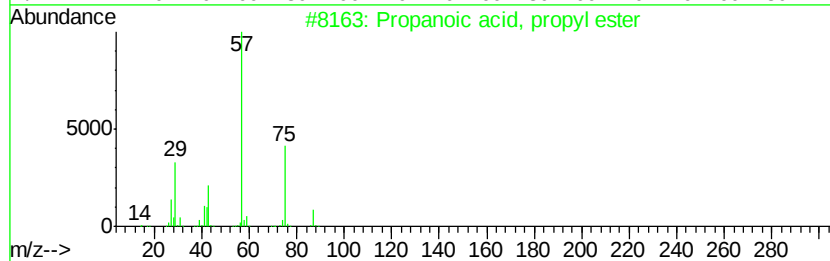
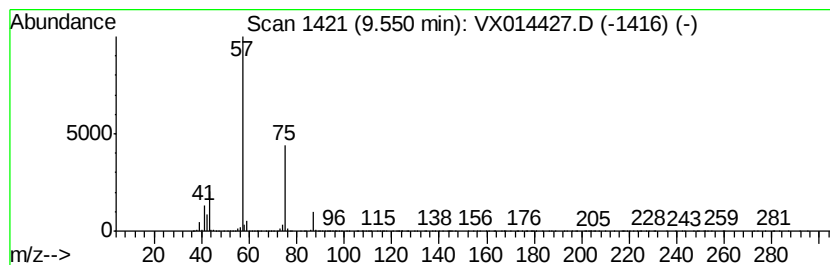
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Quant Title : SW846 8260

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	58.08 ug/l	7733640	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5		1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014427.D
Acq On : 06 Jan 2020 15:09
Operator : JC/SP
Sample : K6484-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30627

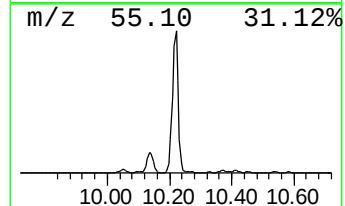
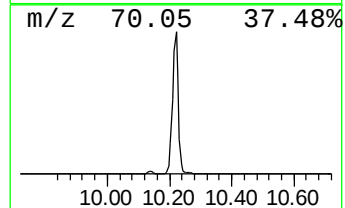
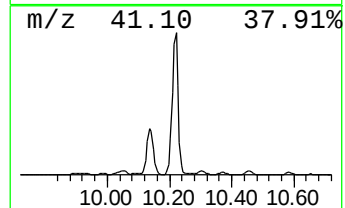
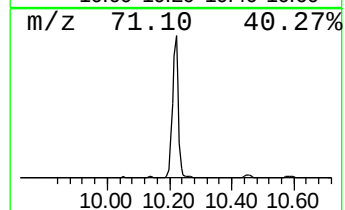
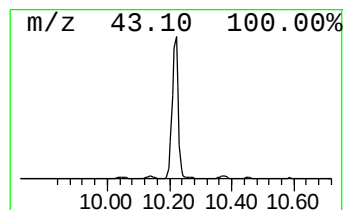
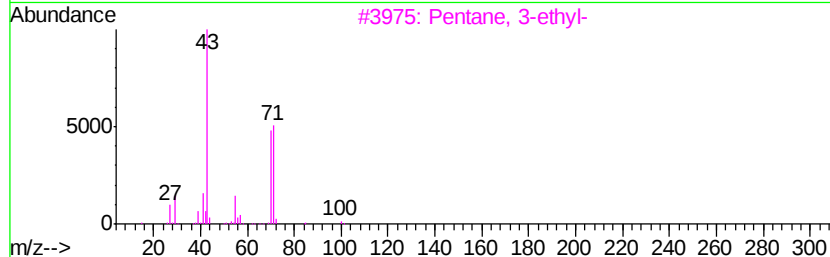
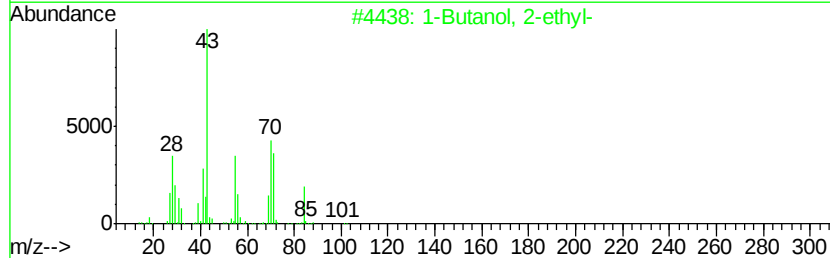
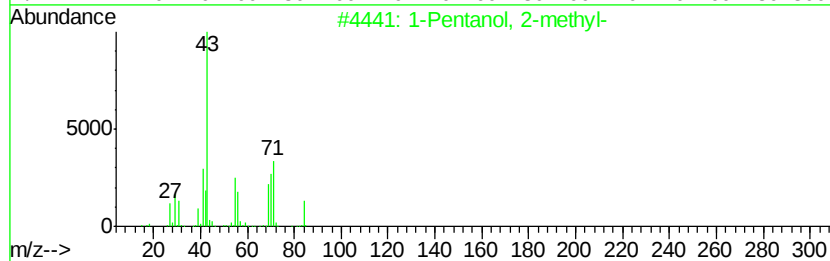
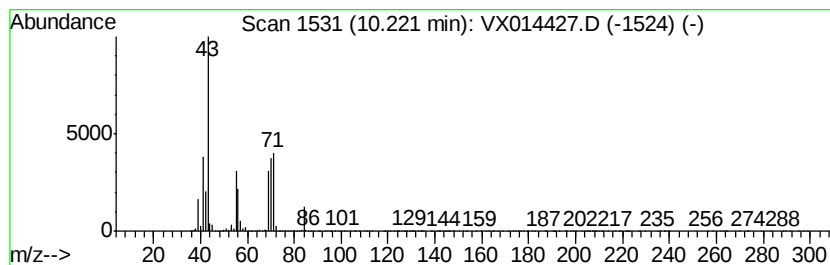
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Quant Title : SW846 8260

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

Peak Number 7 1-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	202.43 ug/l	26955300	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	50
4		Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	42
5		Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014427.D
Acq On : 06 Jan 2020 15:09
Operator : JC/SP
Sample : K6484-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
30627

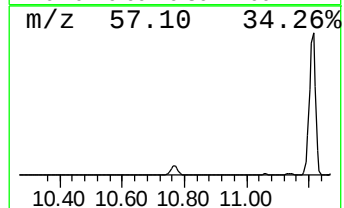
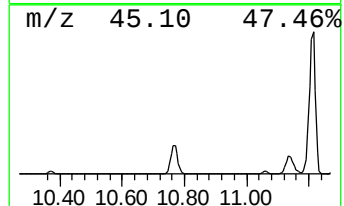
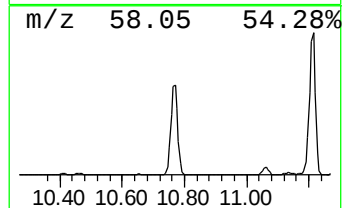
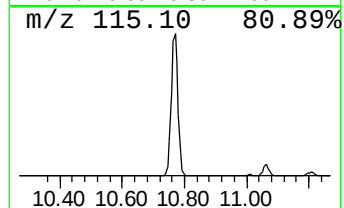
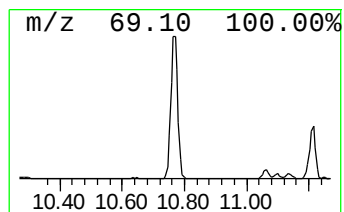
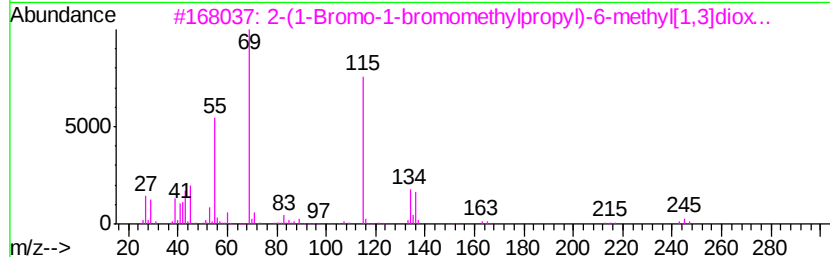
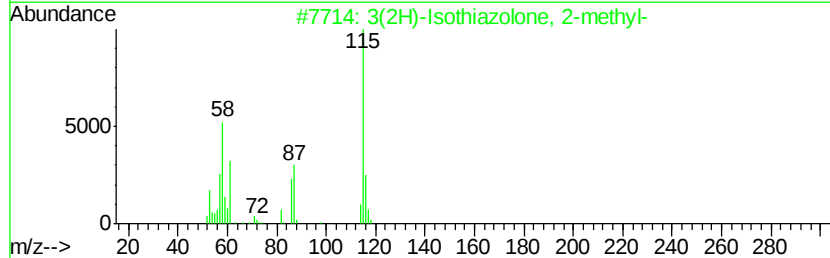
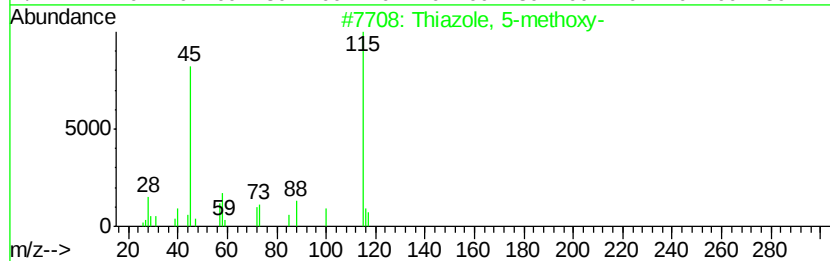
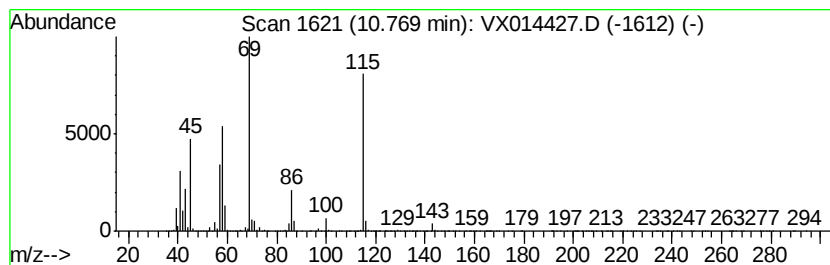
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Quant Title : SW846 8260

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

Peak Number 8 unknown10.77 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	68.18 ug/l	9079040	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiazole, 5-methoxy-	115	C4H5NOS	014542-14-4	38
2		3(2H)-Isothiazolone, 2-methyl-	115	C4H5NOS	002682-20-4	28
3		2-(1-Bromo-1-bromomethylpropyl)-...	328	C9H14Br2O3	1000191-66-9	28
4		4-Octanone, 5-hydroxy-2,7-dimethyl-	172	C10H20O2	006838-51-3	17
5		3-Heptanol, 2,2-dimethyl-	144	C9H20O	019549-70-3	12



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014427.D
Acq On : 06 Jan 2020 15:09
Operator : JC/SP
Sample : K6484-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30627

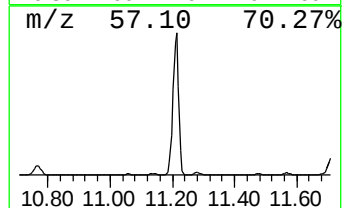
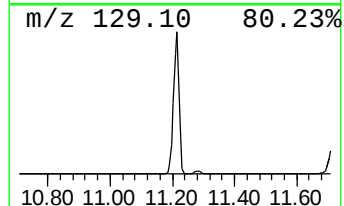
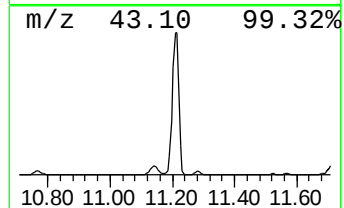
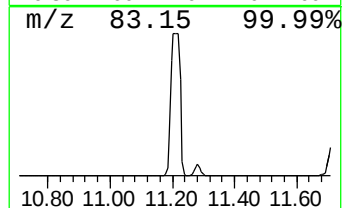
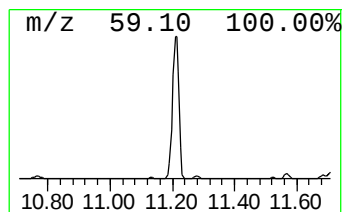
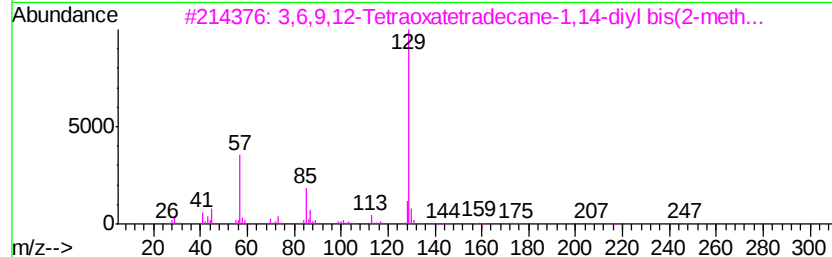
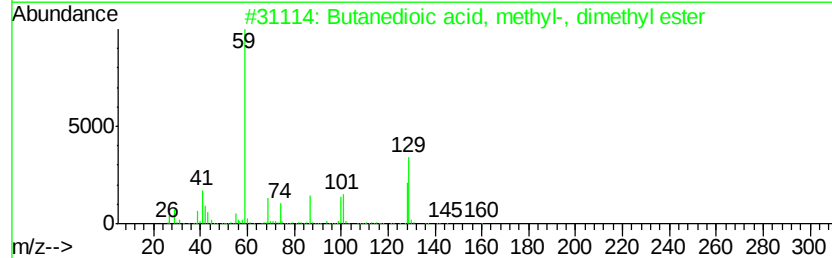
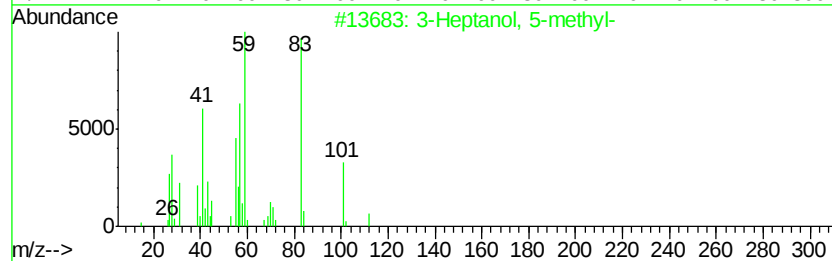
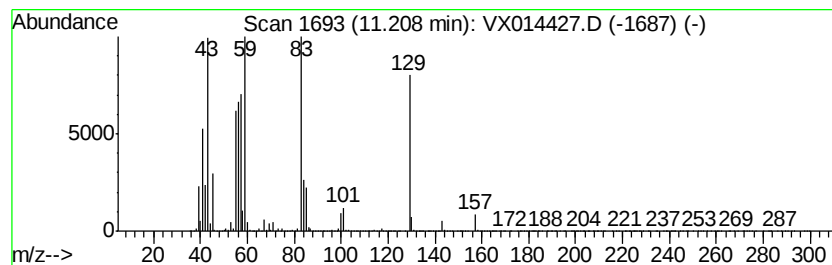
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown11.21 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	372.03 ug/l	123440000	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	43
2		Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	35
3		3,6,9,12-Tetraoxatetradecane-1,1...	406	C20H38O8	1000366-96-9	22
4		Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	18
5		Cyclopropanecarboxylic acid, 1-a...	101	C4H7NO2	022059-21-8	16



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
Data File : VX014427.D
Acq On : 06 Jan 2020 15:09
Operator : JC/SP
Sample : K6484-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
30627

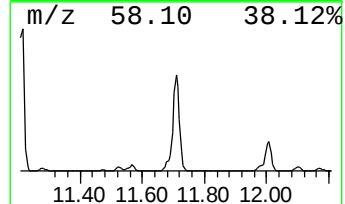
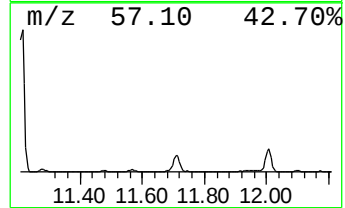
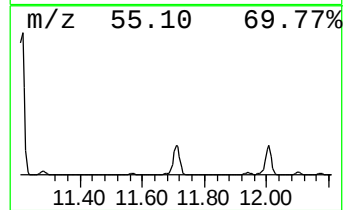
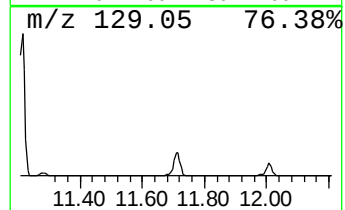
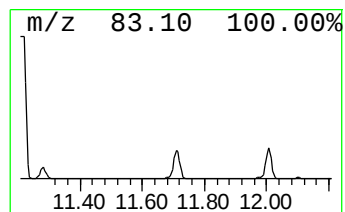
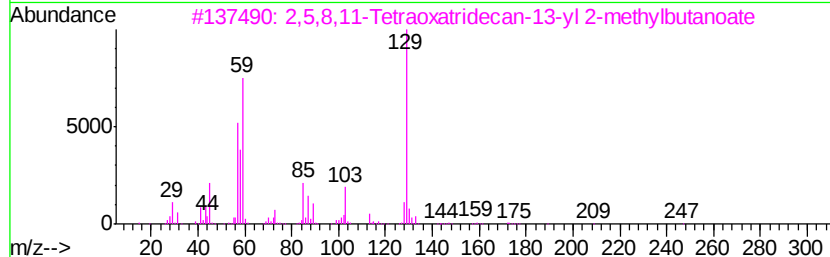
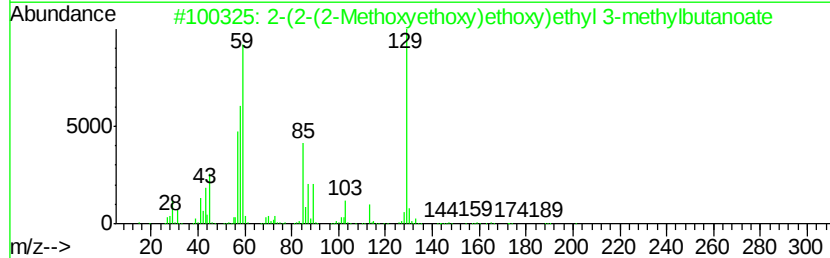
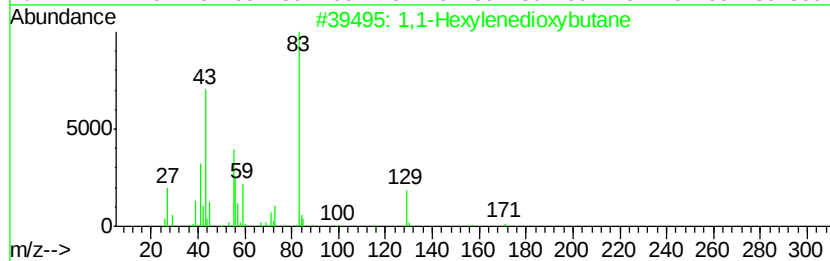
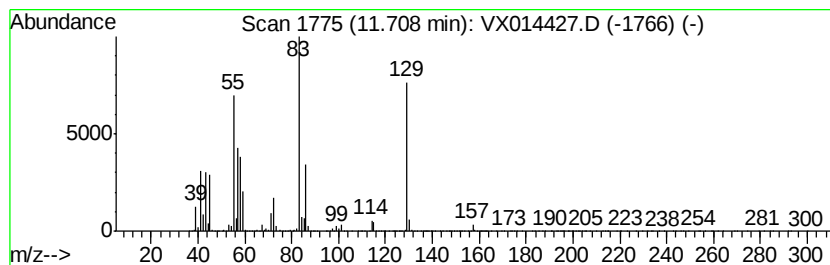
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown11.71 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	52.82 ug/l	17525400	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	37
2		2-(2-(2-Methoxyethoxy)ethoxy)eth...	248	C12H24O5	1000367-05-6	32
3		2,5,8,11-Tetraoxatridecan-13-yl ...	292	C14H28O6	1000366-96-8	25
4		1-Butoxypropan-2-yl 2-methylbut-...	214	C12H22O3	1000367-09-3	16
5		2-Isobutoxy-4-methyl-[1,3,2]diox...	172	C8H17BO3	161616-29-1	16



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX010620\
 Data File : VX014427.D
 Acq On : 06 Jan 2020 15:09
 Operator : JC/SP
 Sample : K6484-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30627

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
1-Propanol	4.44	50.0	ug/l	552654000	1	5.67	552654000	50.0
Pentanal, 2-methyl-	8.93	86.8	ug/l	11563700	3	10.12	6658090	50.0
unknown9.12	9.12	3186.9	ug/l	424375000	3	10.12	6658090	50.0
unknown9.28	9.28	2557.2	ug/l	340515000	3	10.12	6658090	50.0
2,3-Hexanedione	9.39	73.0	ug/l	9716730	3	10.12	6658090	50.0
Propanoic acid, p...	9.55	58.1	ug/l	7733640	3	10.12	6658090	50.0
1-Pentanol, 2-met...	10.22	202.4	ug/l	26955300	3	10.12	6658090	50.0
unknown10.77	10.77	68.2	ug/l	9079040	3	10.12	6658090	50.0
unknown11.21	11.21	372.0	ug/l	123440000	4	12.07	16590000	50.0
unknown11.71	11.71	52.8	ug/l	17525400	4	12.07	16590000	50.0