

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091620\
 Data File : VX018435.D
 Acq On : 16 Sep 2020 12:45
 Operator : JC/SP
 Sample : L4008-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 13703

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\82X082120W.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	1.471	59	63	72	rBV	2084357	2517413	1.14%	0.879%
2	2.099	159	166	188	rBV	1222942	3605976	1.64%	1.259%
3	2.331	198	204	212	rBV	4396557	6990622	3.17%	2.440%
4	2.422	212	219	236	rVV	2712786	4952176	2.25%	1.729%
5	4.239	452	517	521	rBV	18723502	220378184	100.00%	76.924%
6	6.946	952	961	972	rVB	1245164	2823507	1.28%	0.986%
7	8.622	1229	1236	1242	rBV	1581887	2415158	1.10%	0.843%
8	8.696	1242	1248	1254	rVV	1589947	2442495	1.11%	0.853%
9	8.769	1254	1260	1266	rVV	4570761	6931950	3.15%	2.420%
10	9.043	1299	1305	1320	rVB	6580667	9233068	4.19%	3.223%
11	9.208	1324	1332	1341	rBV	4459139	6407922	2.91%	2.237%
12	9.616	1394	1399	1404	rVV2	1322422	3190308	1.45%	1.114%
13	9.671	1404	1408	1427	rVB	1914324	2982910	1.35%	1.041%
14	10.098	1470	1478	1489	rBV	1651260	2241450	1.02%	0.782%
15	10.342	1507	1518	1525	rBV	3264059	4239823	1.92%	1.480%
16	12.061	1795	1800	1807	rVB	1899451	2341233	1.06%	0.817%
17	12.256	1827	1832	1839	rBV	2284233	2795528	1.27%	0.976%

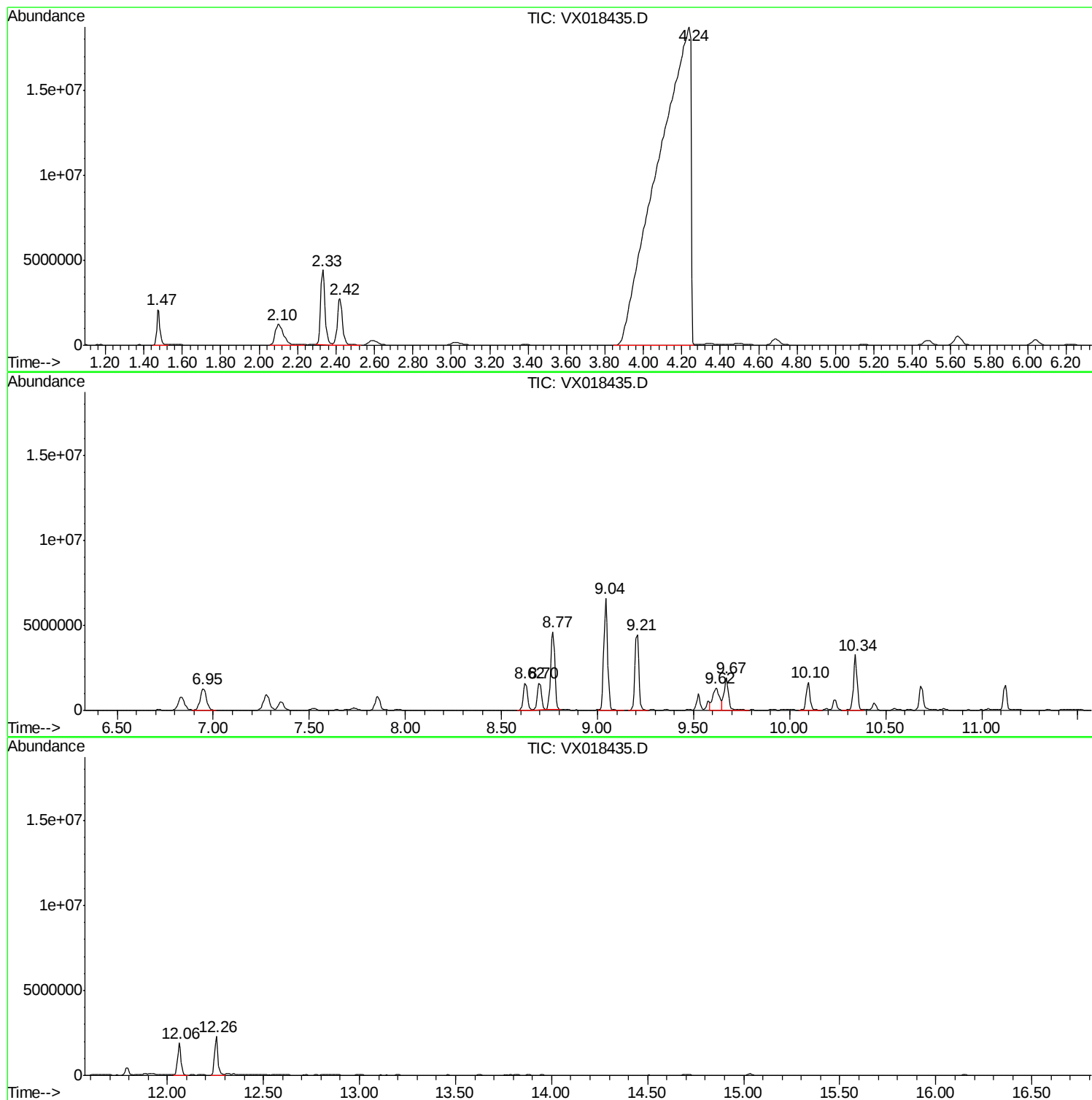
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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



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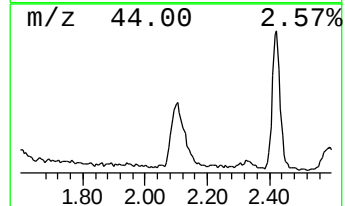
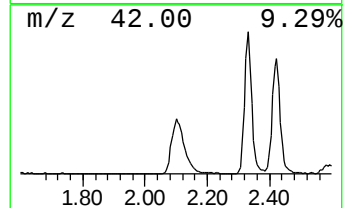
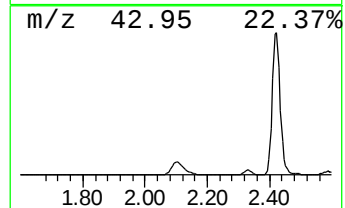
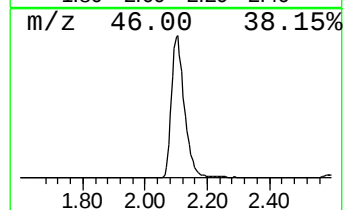
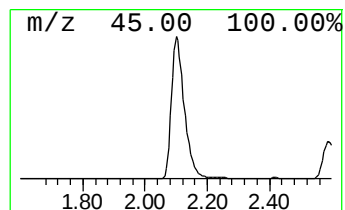
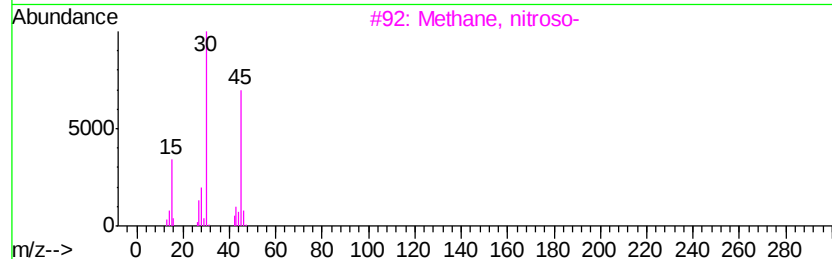
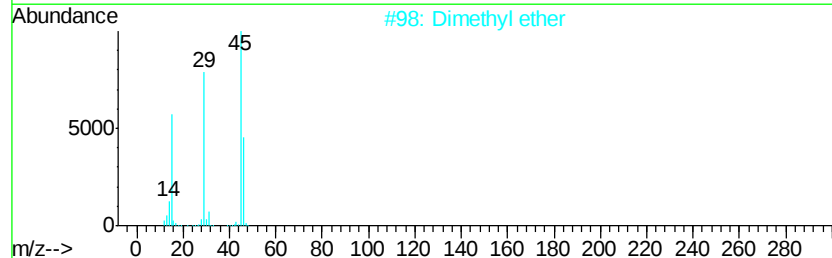
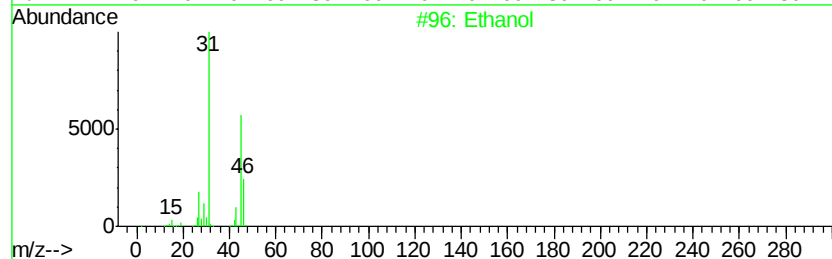
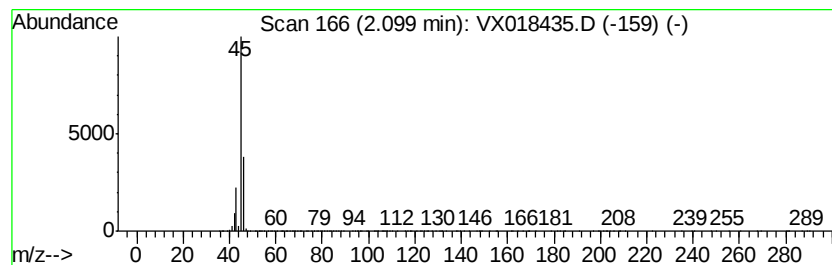
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
 Quant Title : SW846 8260

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

 Peak Number 2 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.10	63.86 ug/l	3605980	Pentafluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	64
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	L-Lactic acid		90	C3H6O3	000079-33-4	2



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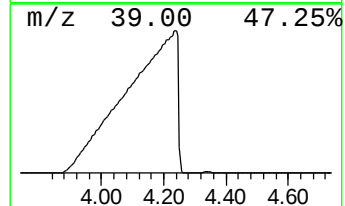
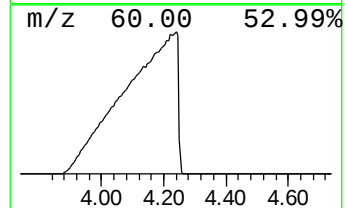
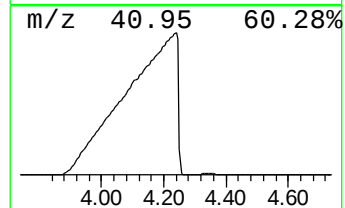
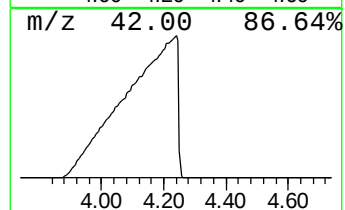
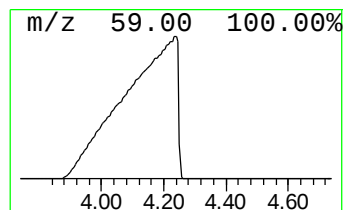
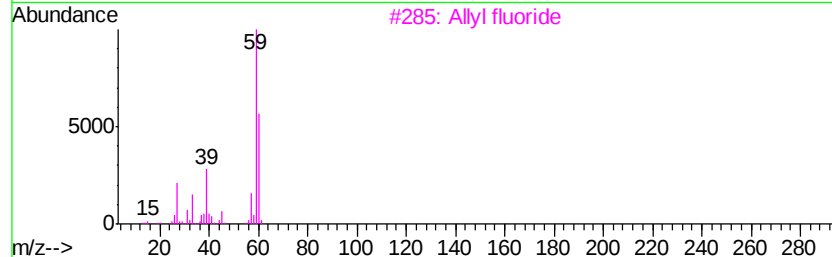
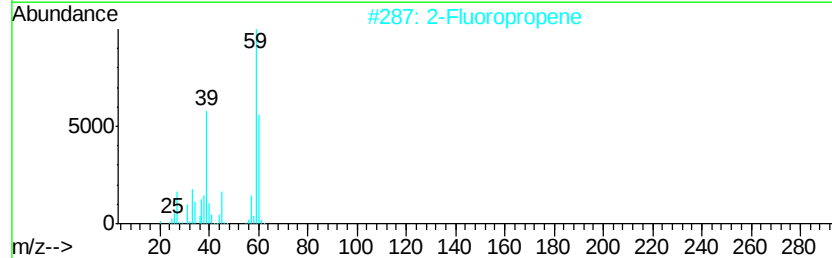
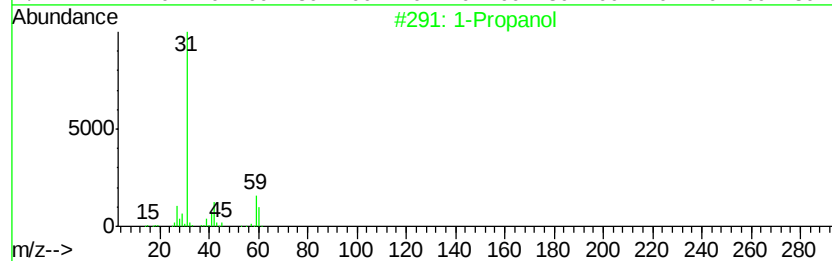
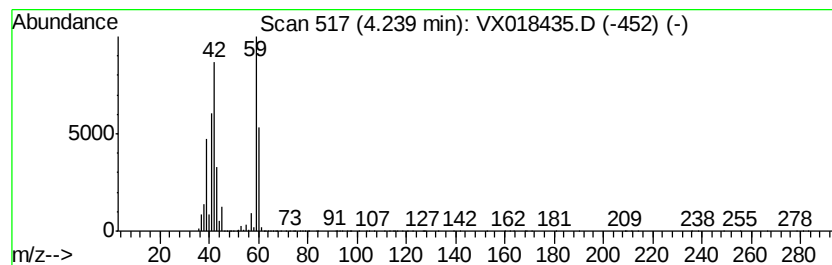
Instrument :
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ClientSampleId :
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Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
4.24	3902.56 ug/l	220378000	Pentafluorobenzene	5.64		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol		60	C3H8O	000071-23-8	59
2	2-Fluoropropene		60	C3H5F	001184-60-7	50
3	Allyl fluoride		60	C3H5F	000818-92-8	38
4	Cyclopropane		42	C3H6	000075-19-4	25
5	Propene		42	C3H6	000115-07-1	25



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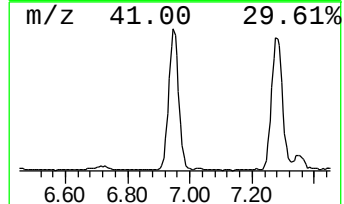
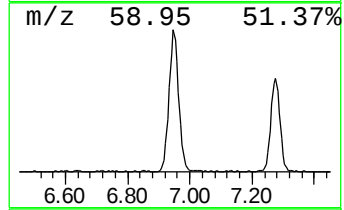
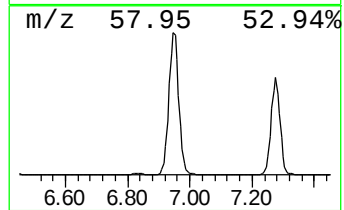
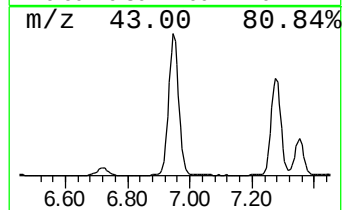
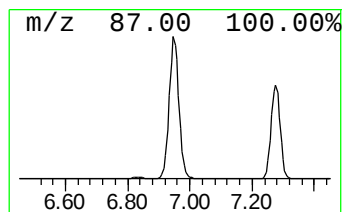
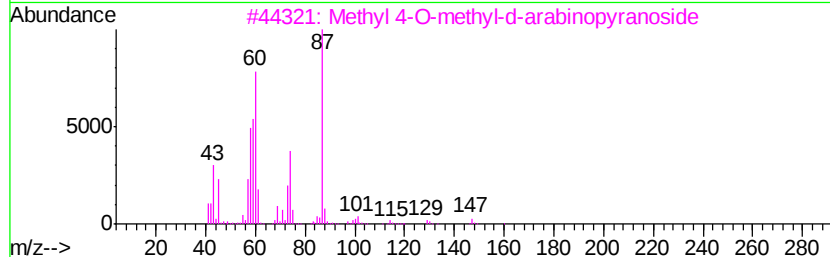
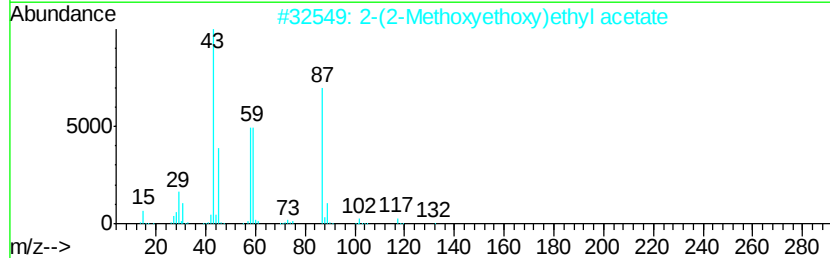
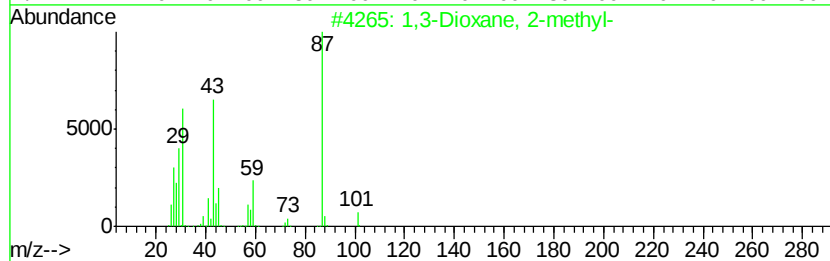
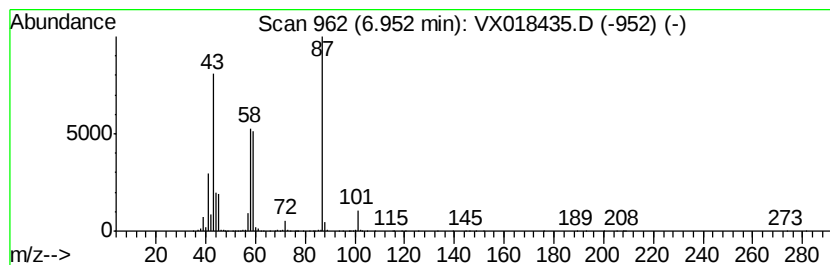
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Peak Number 4 unknown6.95 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	50.00 ug/l	2823510	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	40
2		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
3		Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4		Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
5		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37



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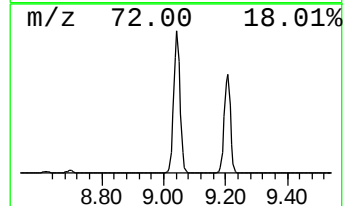
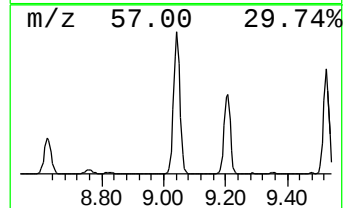
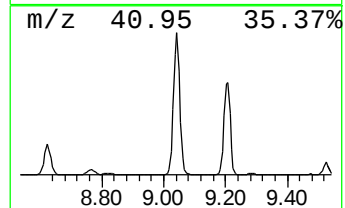
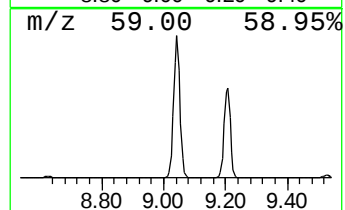
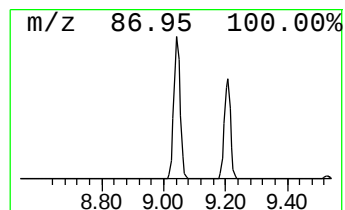
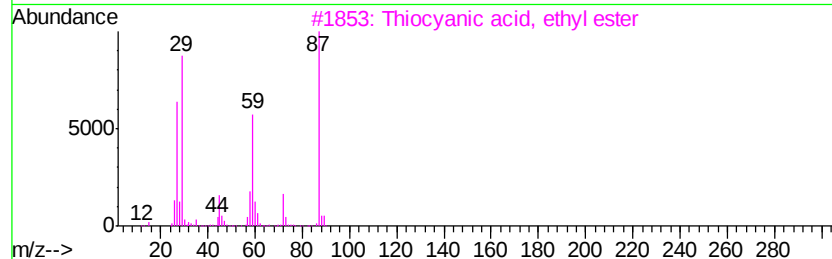
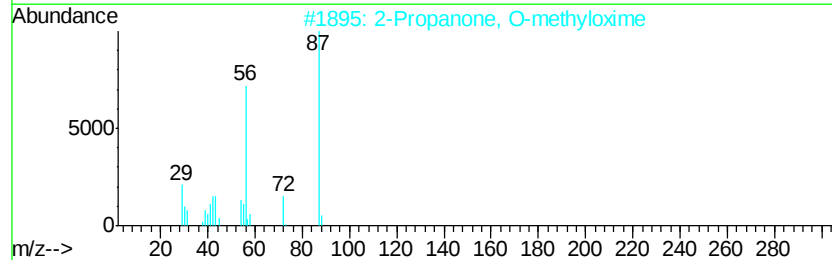
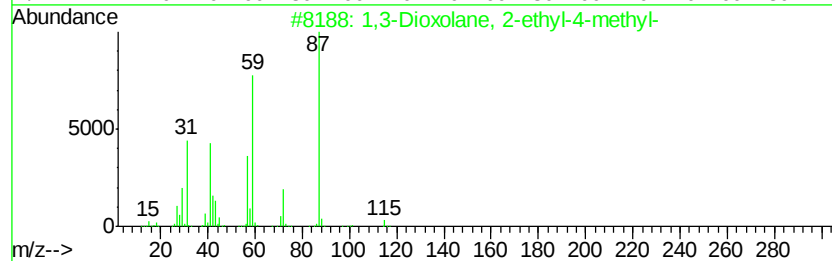
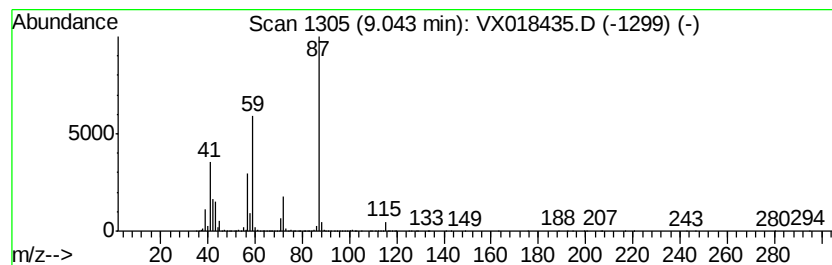
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	205.96 ug/l	9233070	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2		2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
3		Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	47
5		2-[2-[2-(2-Methoxyethoxy)etho...	294	C13H26O7	1000351-91-3	45



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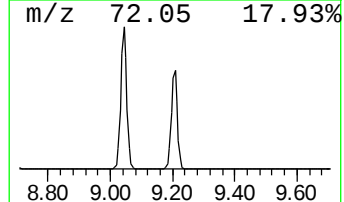
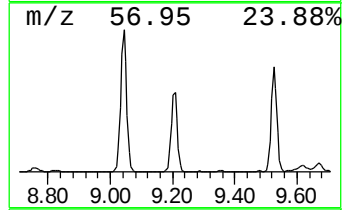
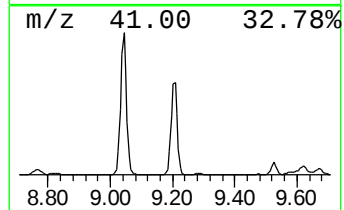
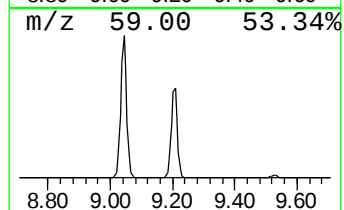
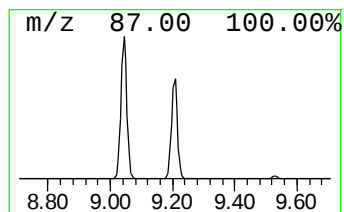
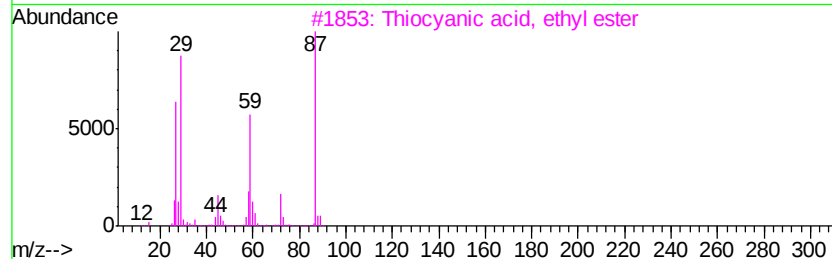
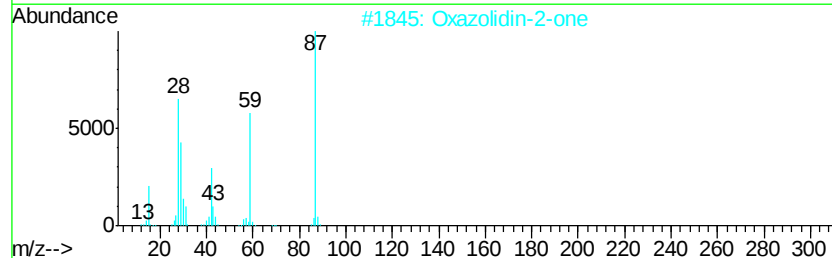
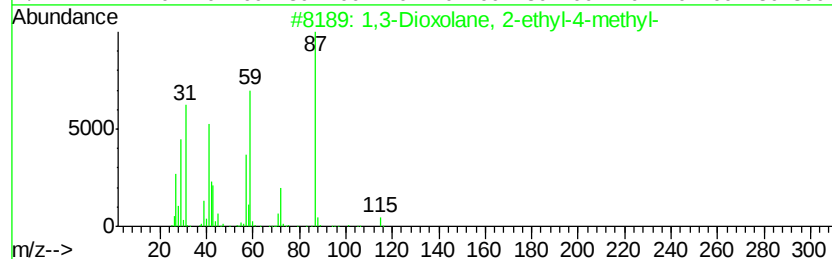
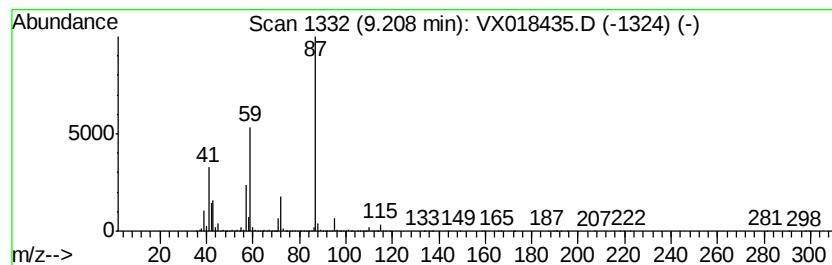
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Peak Number 6 Oxazolidin-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.21	142.94 ug/l	6407920	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90
2		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	50
3		Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	50
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50
5		2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	47



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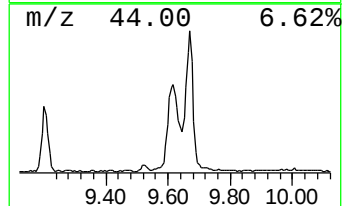
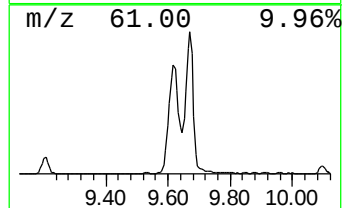
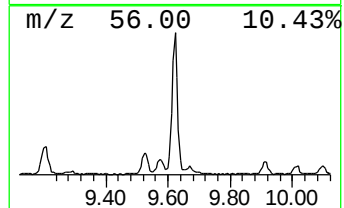
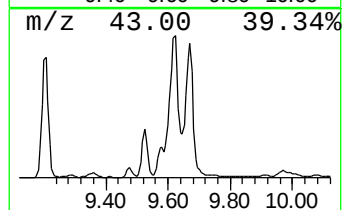
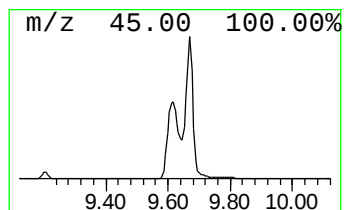
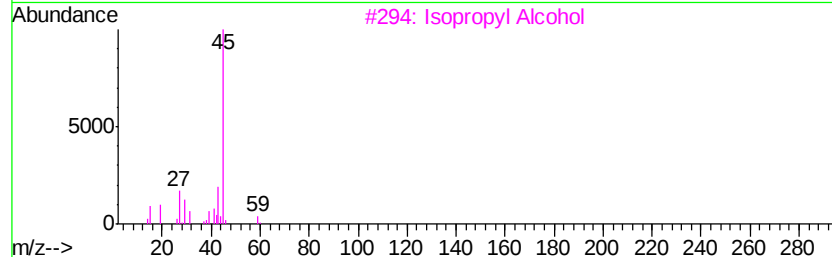
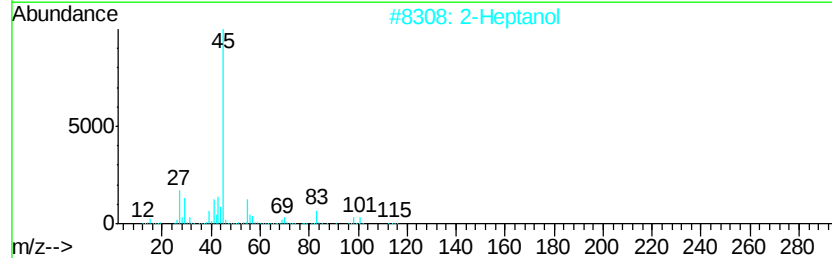
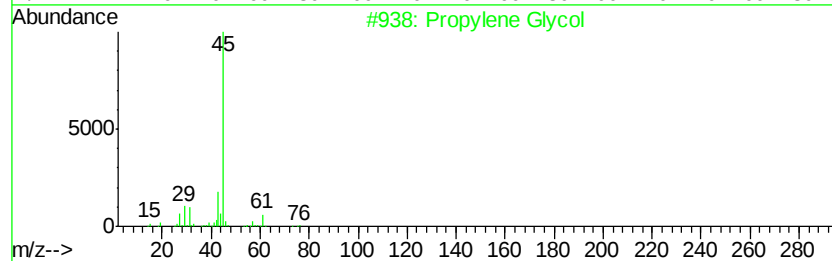
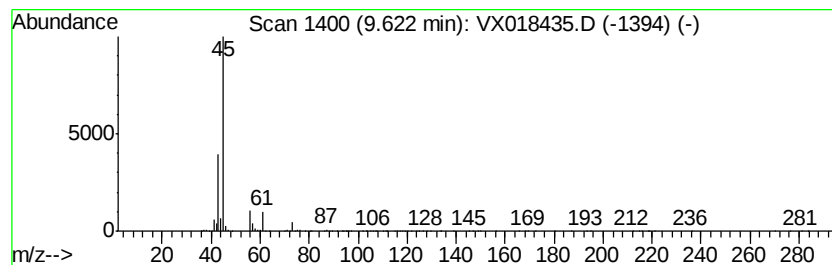
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	71.17 ug/l	3190310	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	86
2		2-Heptanol	116	C7H16O	000543-49-7	40
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5		2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091620\
Data File : VX018435.D
Acq On : 16 Sep 2020 12:45
Operator : JC/SP
Sample : L4008-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
13703

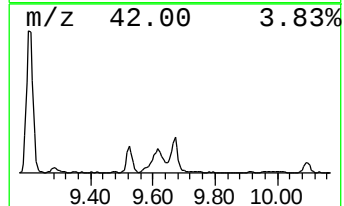
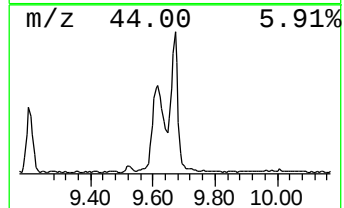
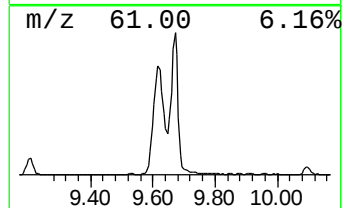
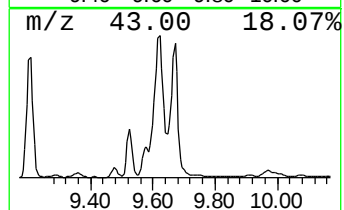
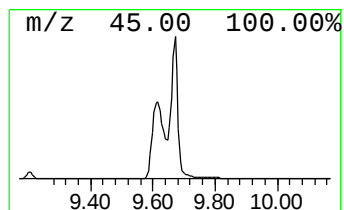
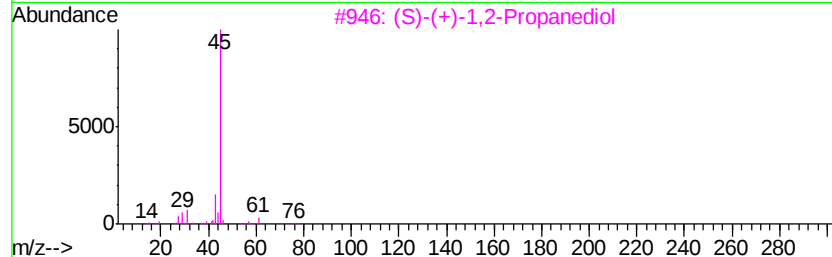
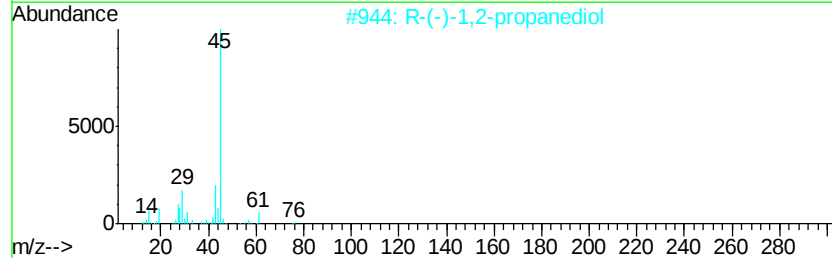
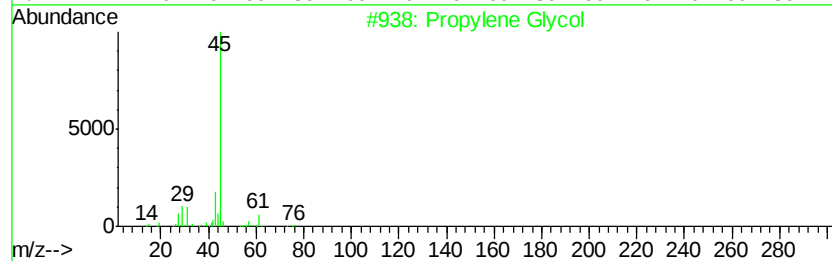
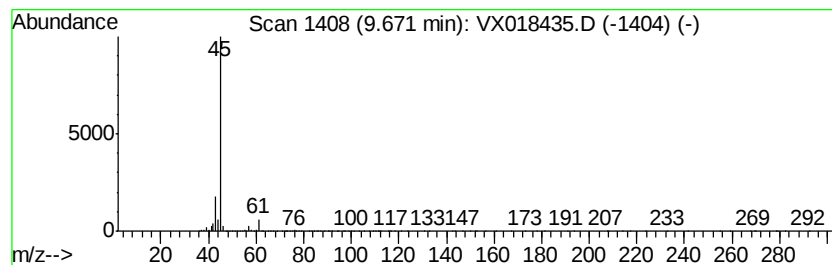
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Quant Title : SW846 8260

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

Peak Number 8 R-(-)-1,2-propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.67	66.54 ug/l	2982910	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	90
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5		2-Pentanol	88	C5H12O	006032-29-7	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091620\
Data File : VX018435.D
Acq On : 16 Sep 2020 12:45
Operator : JC/SP
Sample : L4008-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

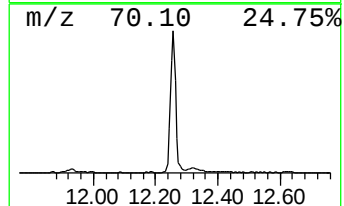
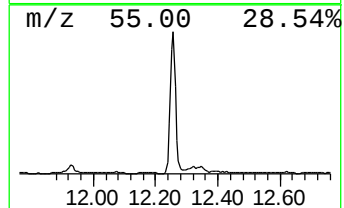
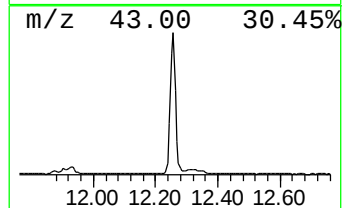
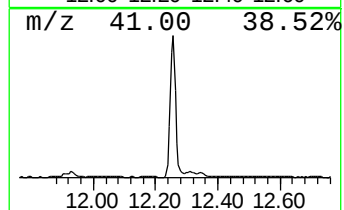
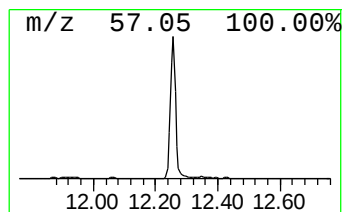
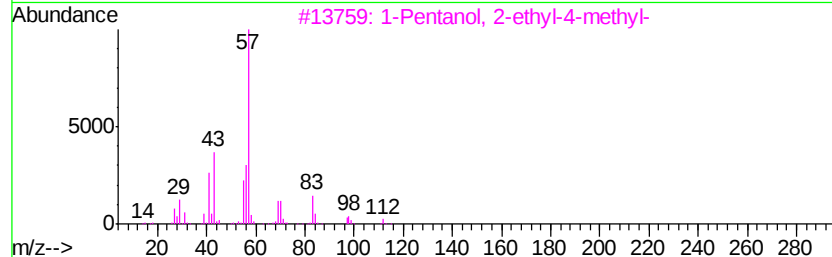
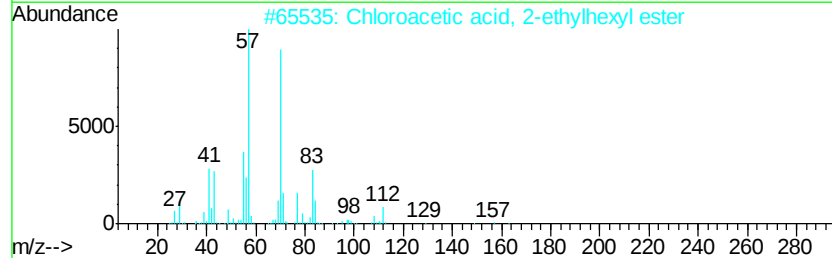
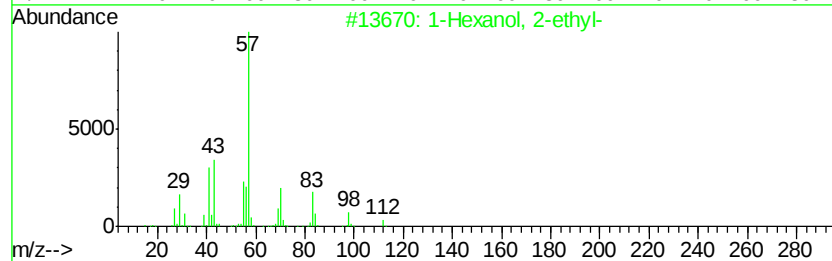
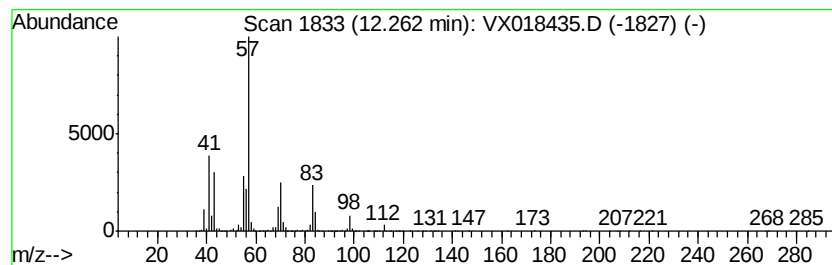
Instrument :
MSVOA_X
ClientSampleId :
13703

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	59.70 ug/l	2795530	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	83
2	Chloroacetic acid, 2-ethylhexyl ...	206 C10H19ClO2	005345-58-4	59
3	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	56
4	Heptane, 1,1'-oxybis-	214 C14H30O	000629-64-1	53
5	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091620\
Data File : VX018435.D
Acq On : 16 Sep 2020 12:45
Operator : JC/SP
Sample : L4008-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
13703

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.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
Ethanol	2.10	63.9	ug/l	3605980	1	5.64	2823510	50.0
1-Propanol	4.24	3902.6	ug/l	220378000	1	5.64	2823510	50.0
unknown6.95	6.95	50.0	ug/l	2823510	2	6.84	2823510	50.0
1,3-Dioxolane, 2-...	9.04	206.0	ug/l	9233070	3	10.10	2241450	50.0
Oxazolidin-2-one	9.21	142.9	ug/l	6407920	3	10.10	2241450	50.0
Propylene Glycol	9.62	71.2	ug/l	3190310	3	10.10	2241450	50.0
R-(-)-1,2-propane...	9.67	66.5	ug/l	2982910	3	10.10	2241450	50.0
1-Hexanol, 2-ethyl-	12.26	59.7	ug/l	2795530	4	12.06	2341230	50.0