

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050724\
Data File : VX041403.D
Acq On : 07 May 2024 13:54
Operator : JC/MD
Sample : P2389-03 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1402

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\82X043024W.M

Title : SW846 8260

Signal : TIC: VX041403.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.300	186	199	204	rBV	10125182	18795074	100.00%	52.735%
2	2.361	204	209	268	rVB2	2771375	11659022	62.03%	32.713%
3	3.892	450	460	480	rBV	138975	414713	2.21%	1.164%
4	5.385	694	705	721	rVB2	91166	270233	1.44%	0.758%
5	5.550	721	732	751	rVB	174252	494011	2.63%	1.386%
6	5.952	788	798	822	rBV	94354	255385	1.36%	0.717%
7	6.757	921	930	955	rBV	217787	560066	2.98%	1.571%
8	8.647	1234	1240	1256	rBV	434857	698474	3.72%	1.960%
9	8.994	1292	1297	1313	rVB	204615	316710	1.69%	0.889%
10	9.159	1318	1324	1340	rVB	139351	201207	1.07%	0.565%
11	10.055	1465	1471	1486	rBV	455999	785933	4.18%	2.205%
12	11.079	1634	1639	1646	rBV	397382	501739	2.67%	1.408%
13	12.024	1788	1794	1804	rBV	534671	688044	3.66%	1.931%

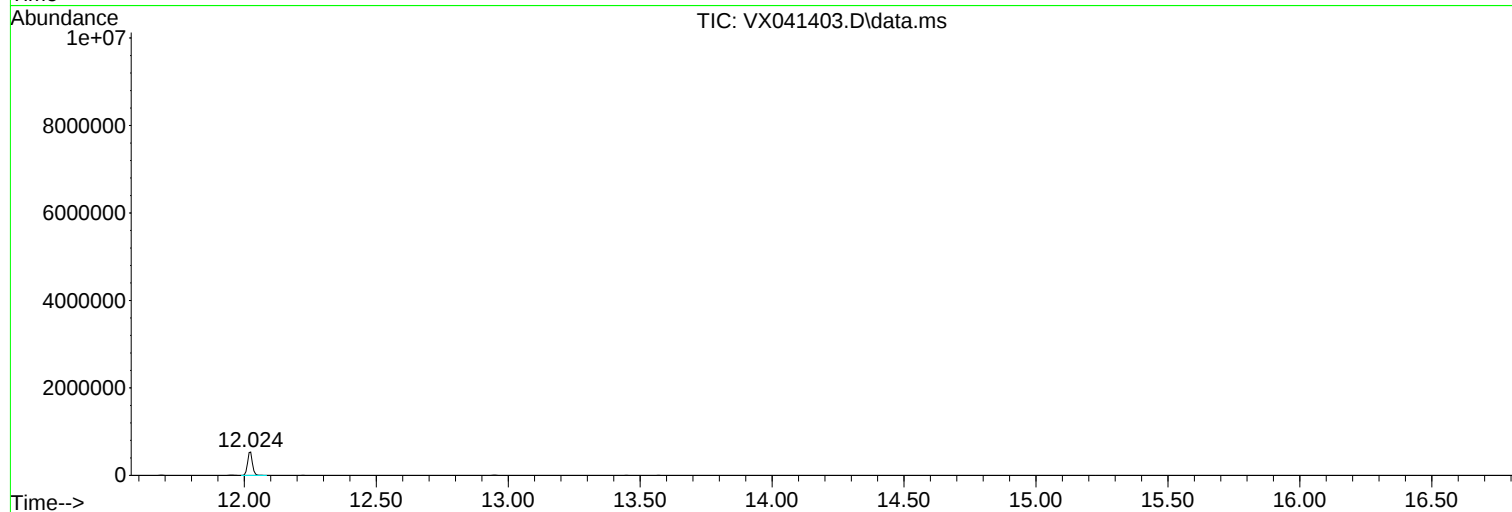
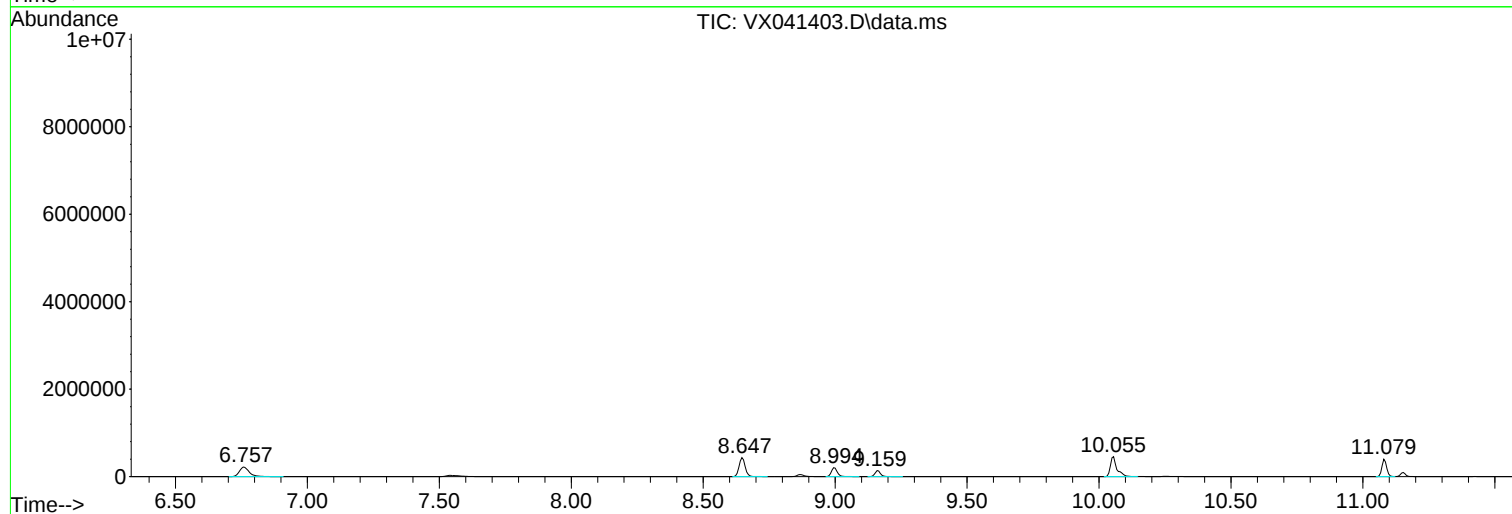
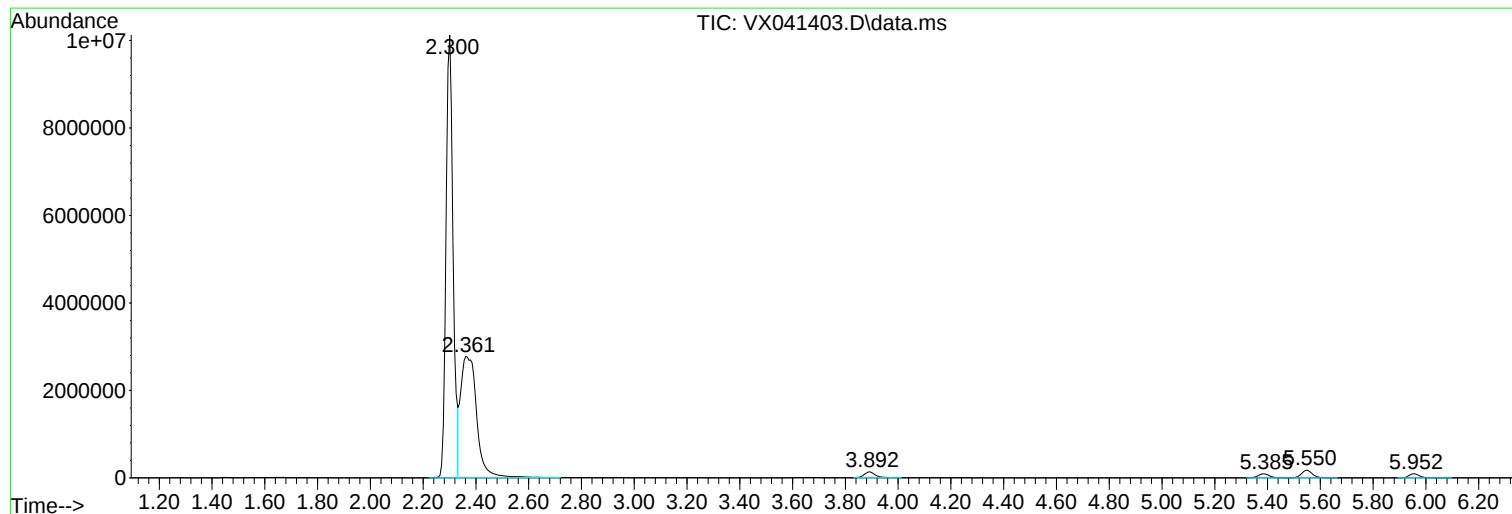
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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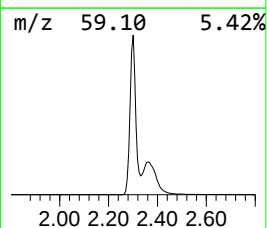
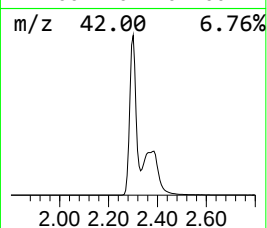
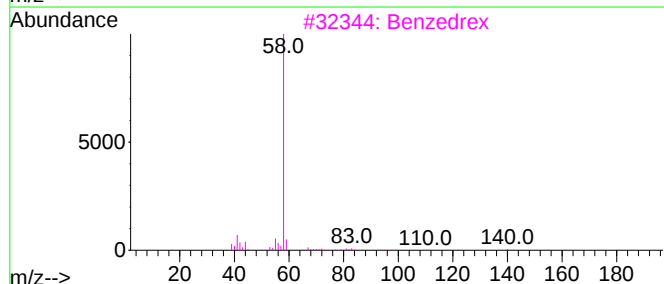
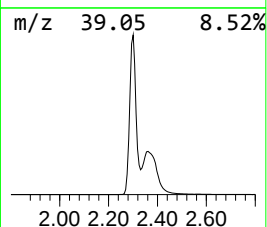
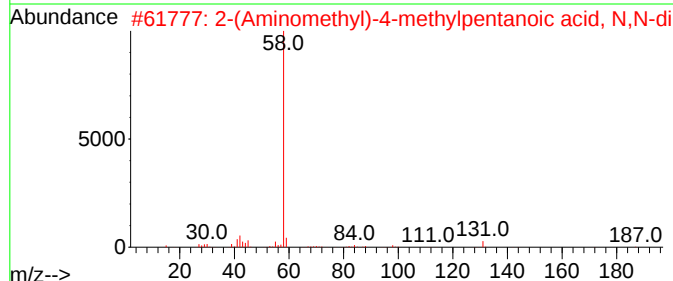
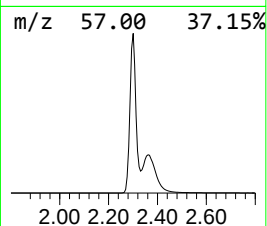
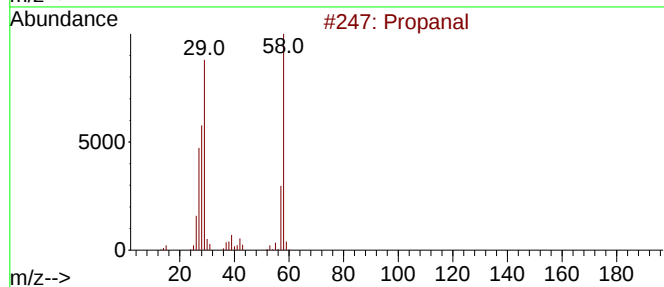
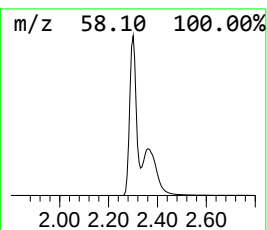
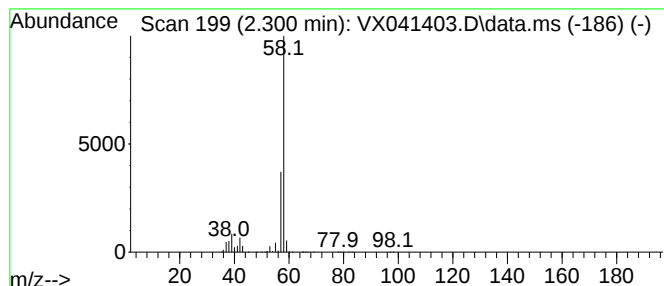
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.300	1902.29 ug/l	18795100	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	86
2			2-(Aminomethyl)-4-methylpentanoic...	187	C10H21NO2	1891211-54-3	9
3			Benzedrex	155	C10H21N	000101-40-6	9
4			Propylene oxide	58	C3H6O	000075-56-9	7
5			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7



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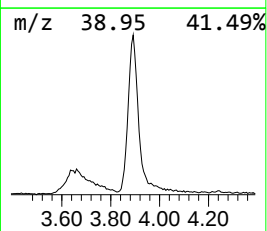
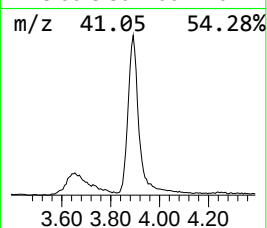
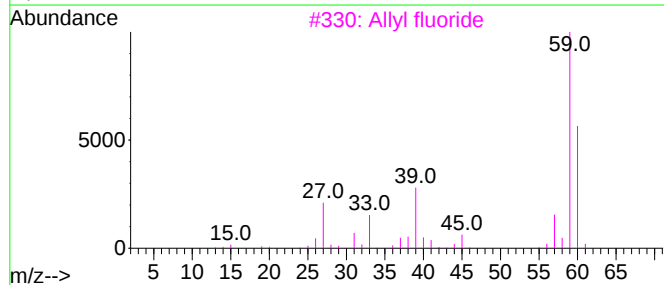
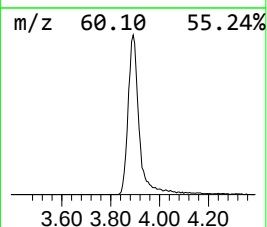
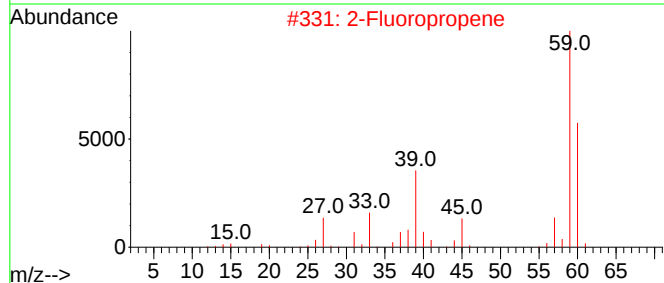
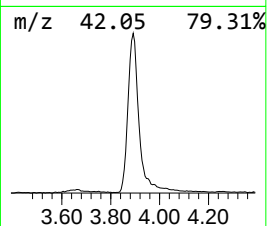
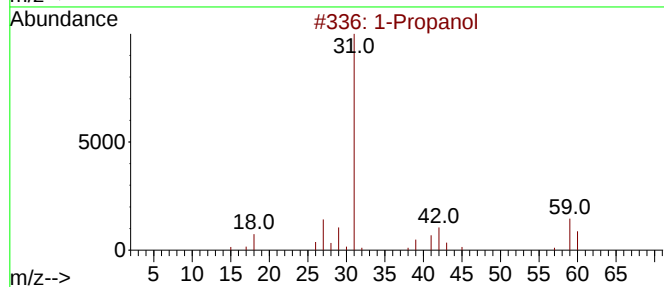
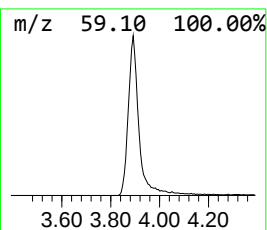
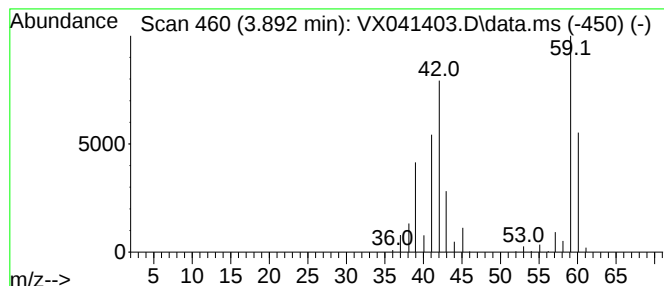
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.892	41.97 ug/l	414713	Pentafluorobenzene	5.550

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	52
3	Allyl fluoride			60	C3H5F	000818-92-8	38
4	Cyclopropane			42	C3H6	000075-19-4	25
5	Propene			42	C3H6	000115-07-1	17



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1402

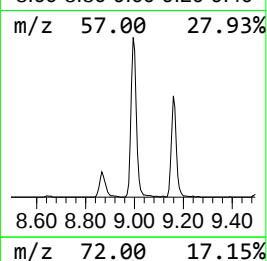
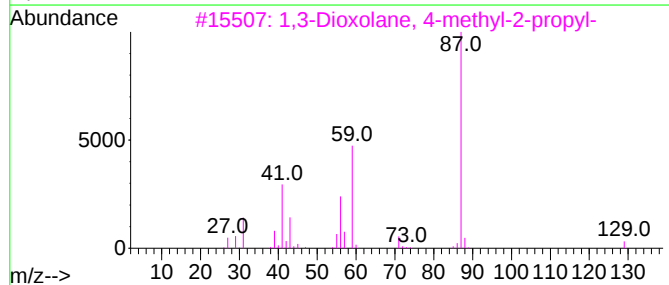
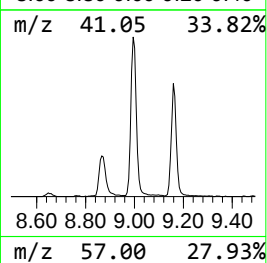
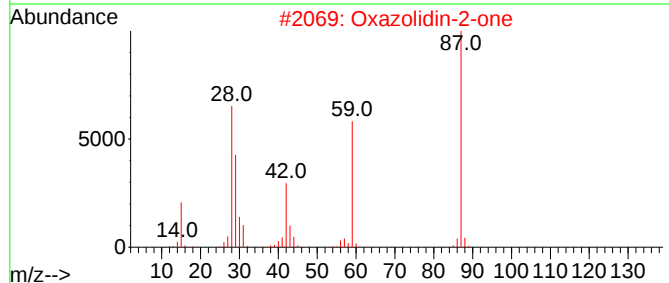
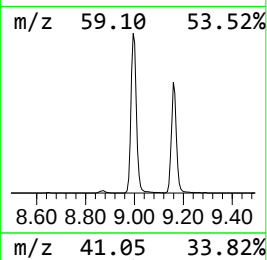
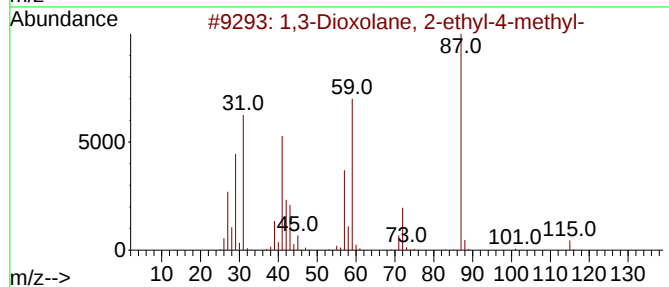
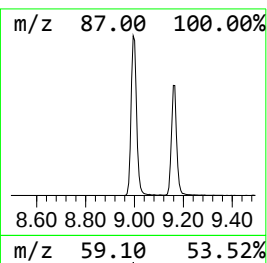
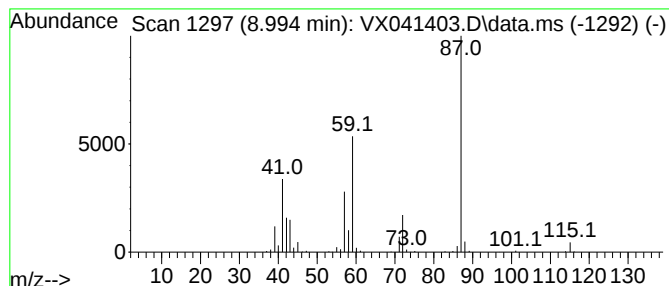
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Peak Number 3 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.994	20.15 ug/l	316710	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	90		
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64		
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59		
4	2-[2-[2-(2-Methoxyethoxy)ethoxy]...	250	C11H22O6	1000351-91-4	59		
5	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	56		



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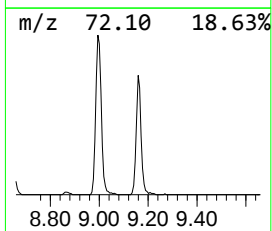
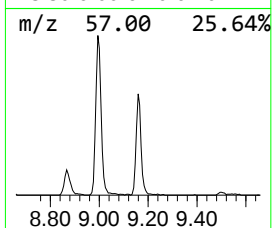
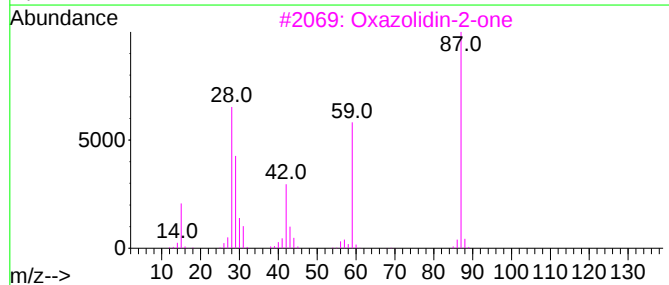
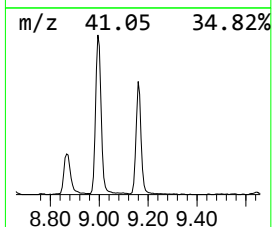
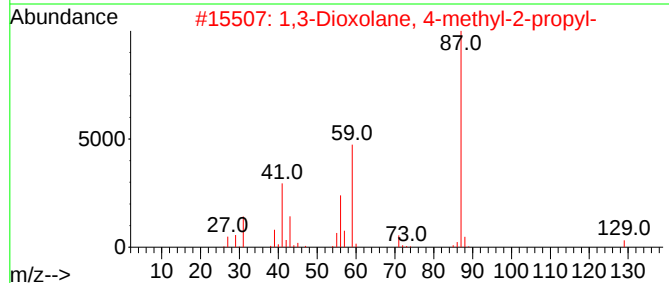
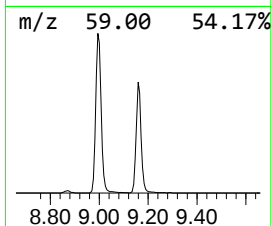
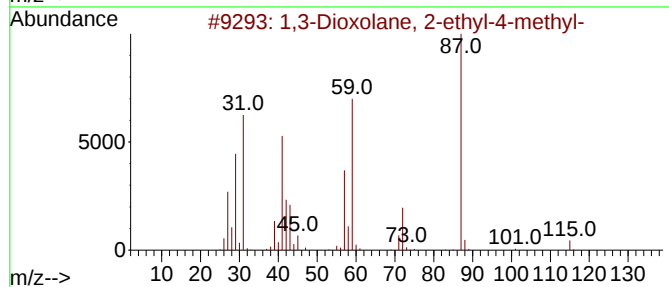
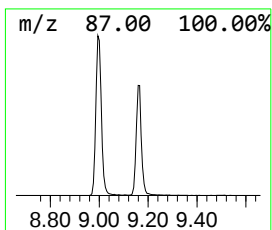
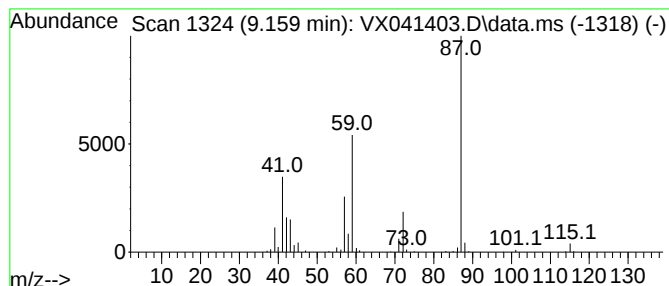
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Quant Title : SW846 8260

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Peak Number 4 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.159	12.80 ug/l	201207	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91		
2	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64		
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	56		
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53		
5	2-Propanone, O-methylloxime	87	C4H9NO	003376-35-0	52		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	2.300	1902.3	ug/l	18795100	1	5.550	494011	50.0
1-Propanol	3.892	42.0	ug/l	414713	1	5.550	494011	50.0
1,3-Dioxolane, ...	8.994	20.1	ug/l	316710	3	10.055	785933	50.0
1,3-Dioxolane, ...	9.159	12.8	ug/l	201207	3	10.055	785933	50.0