

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072823\
 Data File : VN078689.D
 Acq On : 28 Jul 2023 16:53
 Operator : JC\MD
 Sample : 03806-01 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 ORA-1694

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_N\methods\82N071023W.M

Title : SW846 8260

Signal : TIC: VN078689.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.671	115	122	131	rBV	453720	800687	2.08%	0.949%
2	4.300	387	399	419	rBV	13345305	38538830	100.00%	45.680%
3	6.741	802	814	836	rBV	889245	2728007	7.08%	3.233%
4	8.176	1048	1058	1062	rBV	605768	1362201	3.53%	1.615%
5	8.235	1062	1068	1081	rVB	951138	2140943	5.56%	2.538%
6	8.588	1116	1128	1141	rBV	545366	1240439	3.22%	1.470%
7	9.112	1208	1217	1234	rVB	1539844	3195560	8.29%	3.788%
8	10.576	1456	1466	1479	rBV	2046776	3864069	10.03%	4.580%
9	10.812	1497	1506	1522	rBV	7911918	13963667	36.23%	16.551%
10	10.953	1522	1530	1546	rVB	4722674	8061006	20.92%	9.555%
11	11.870	1675	1686	1699	rBV	1851844	3408482	8.84%	4.040%
12	12.853	1847	1853	1863	rVB	1427147	2531856	6.57%	3.001%
13	13.800	2006	2014	2023	rBV	1483344	2531534	6.57%	3.001%

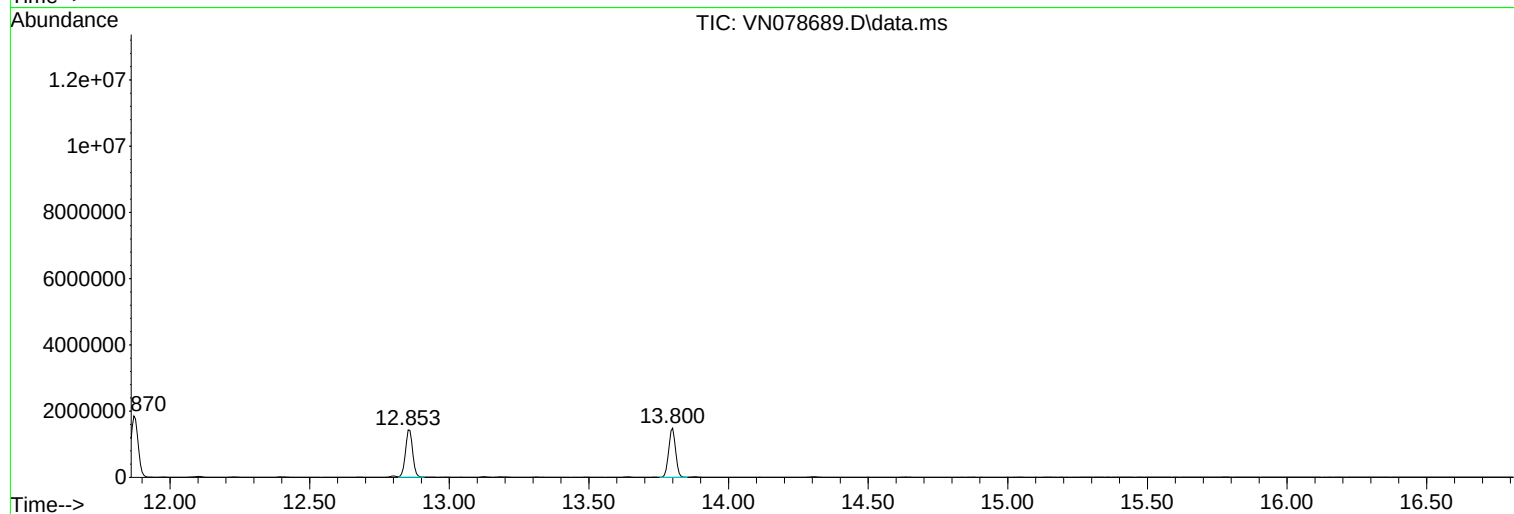
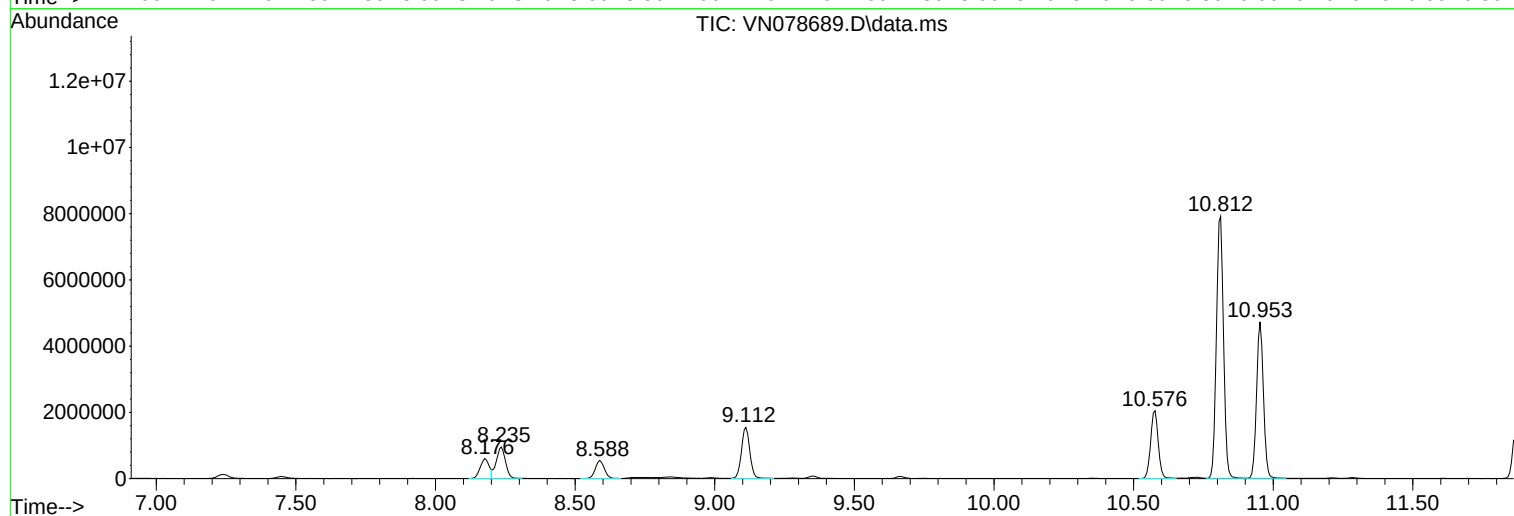
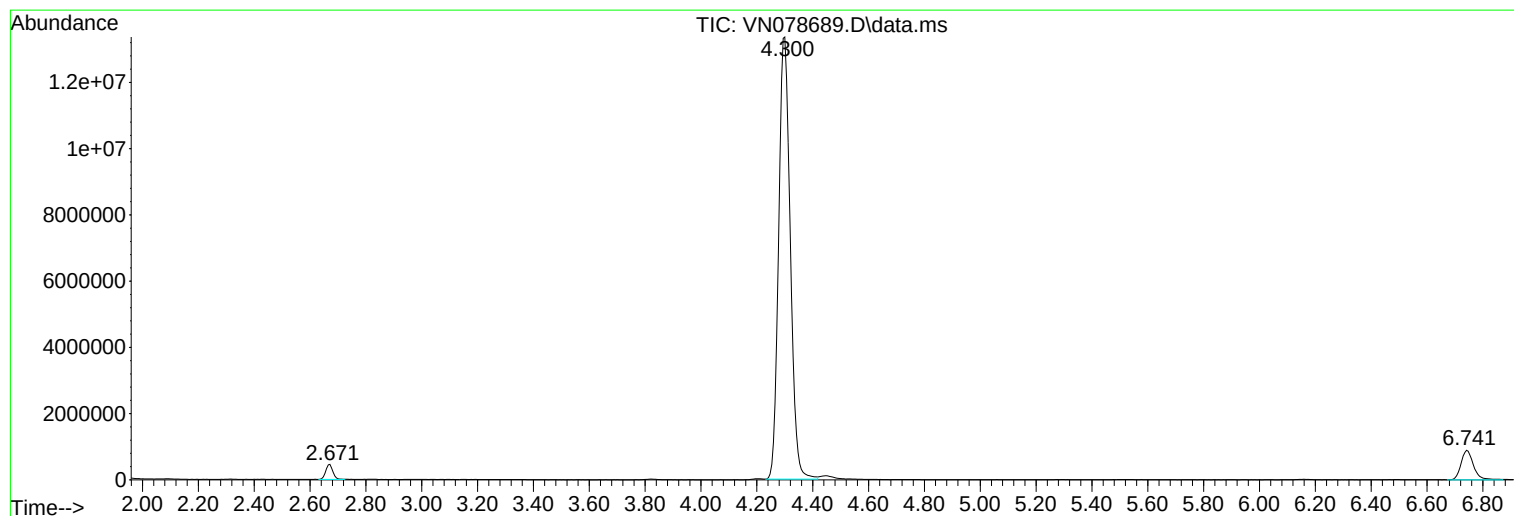
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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



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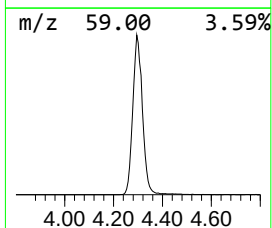
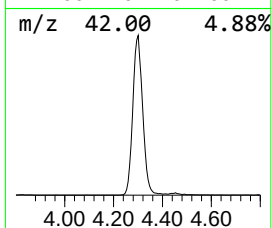
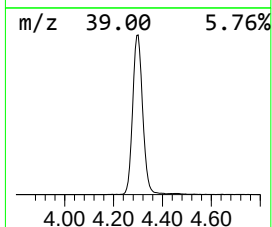
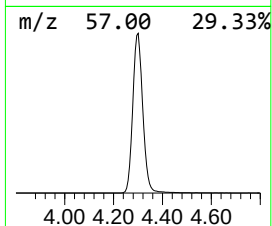
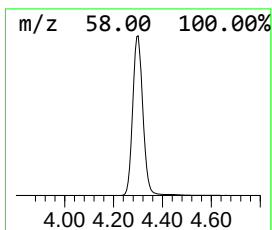
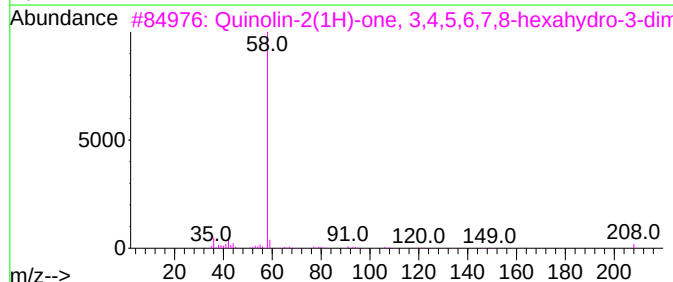
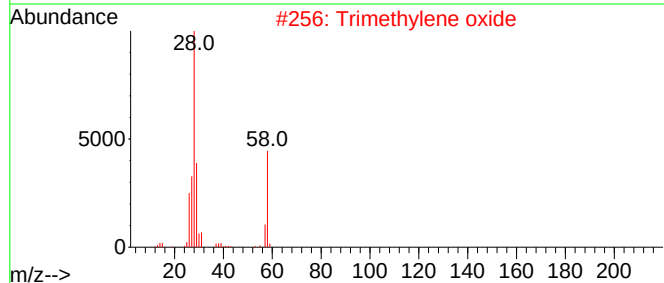
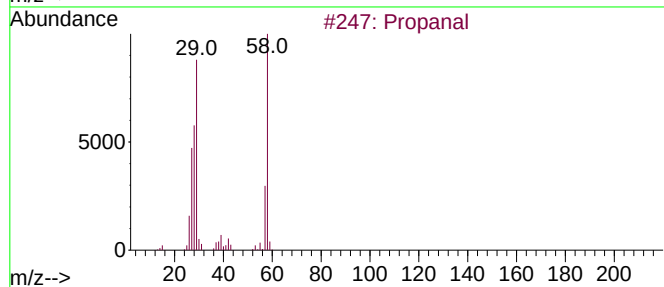
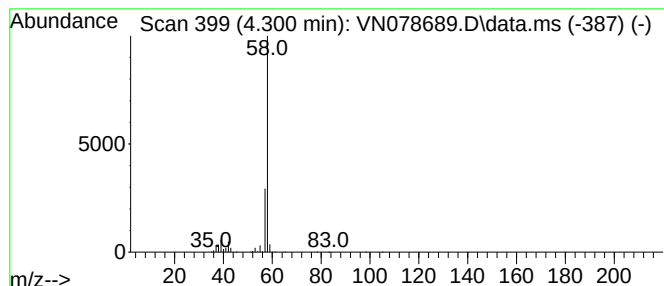
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071023W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	900.04 ug/l	38538800	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	64
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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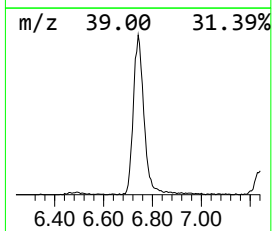
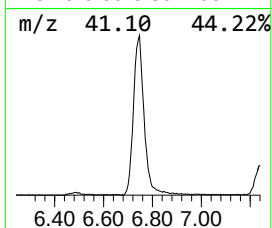
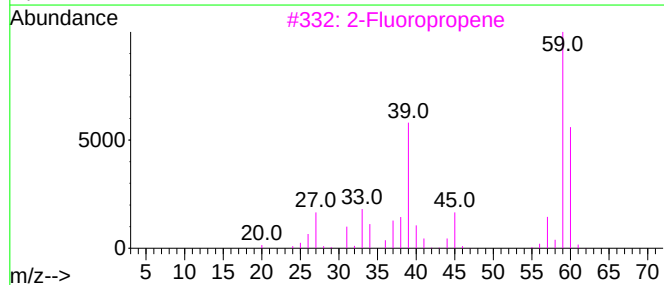
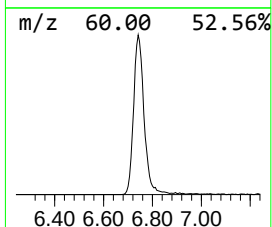
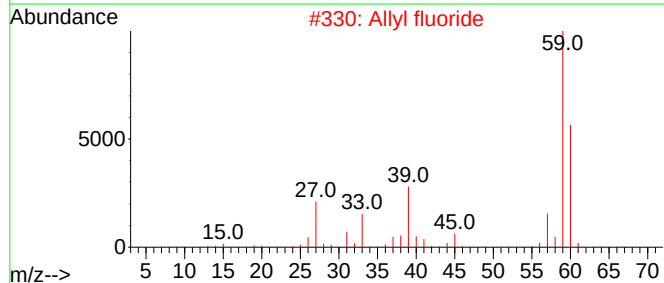
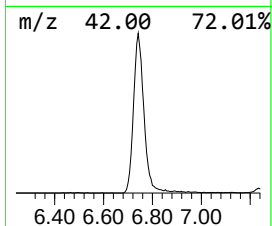
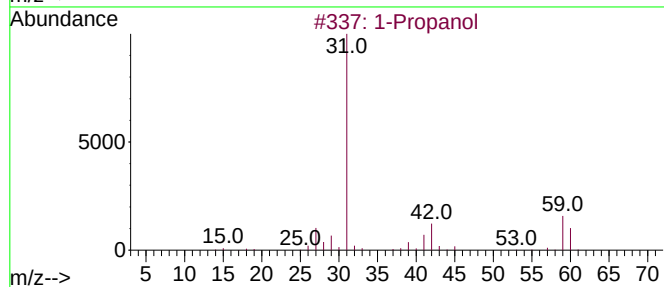
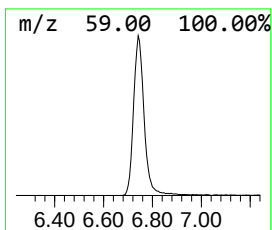
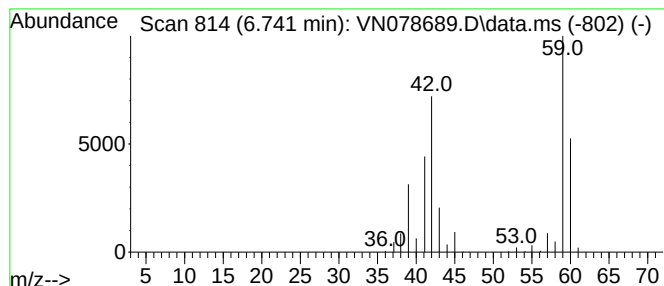
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Quant Title : SW846 8260

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Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.741	63.71 ug/l	2728010	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	78
2	Allyl fluoride			60	C3H5F	000818-92-8	53
3	2-Fluoropropene			60	C3H5F	001184-60-7	40
4	Acetaldoxime			59	C2H5NO	000107-29-9	7
5	Formic acid hydrazide			60	CH4N2O	000624-84-0	5



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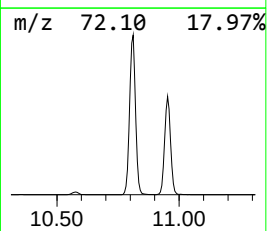
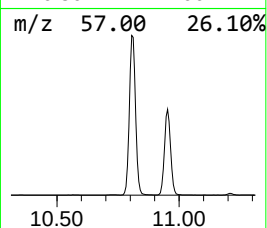
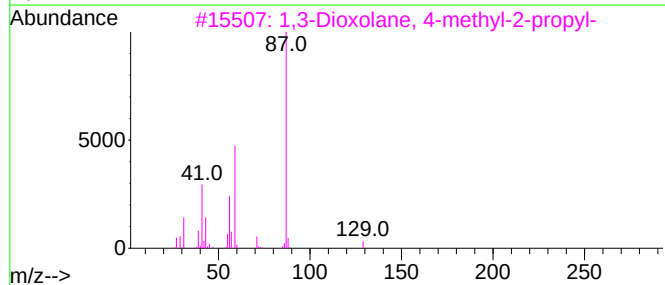
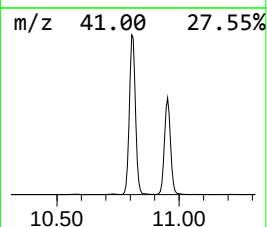
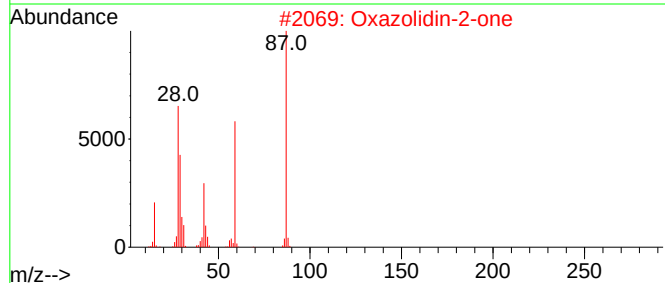
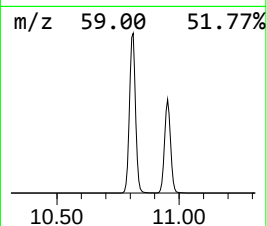
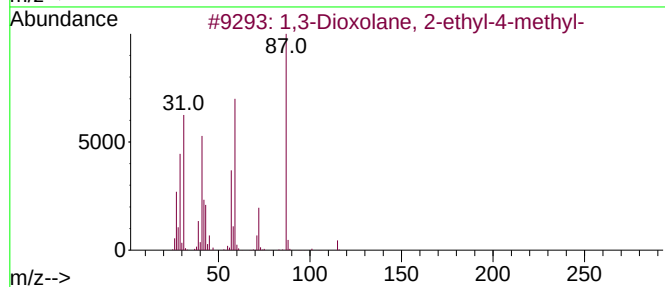
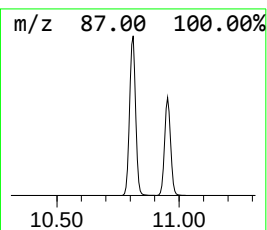
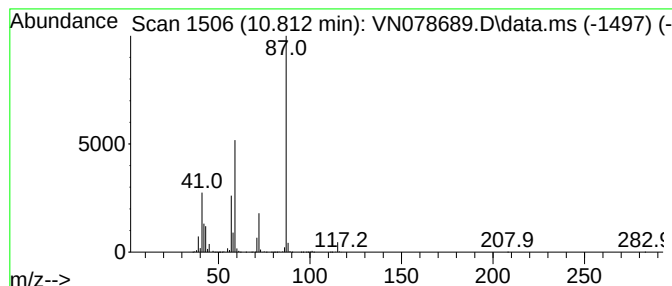
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Peak Number 4 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.812	204.84 ug/l	13963700	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
4			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	56
5			2-Propanone, 0-methyloxime	87	C4H9NO	003376-35-0	52



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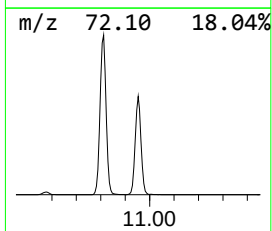
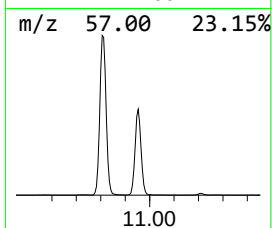
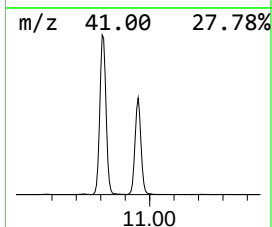
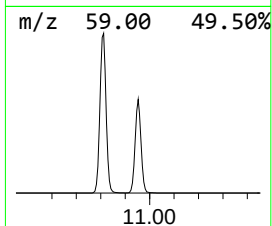
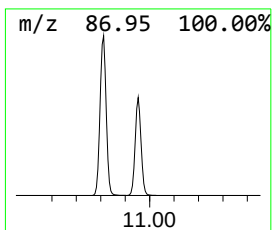
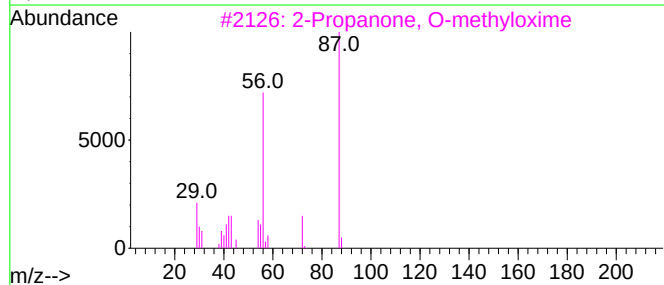
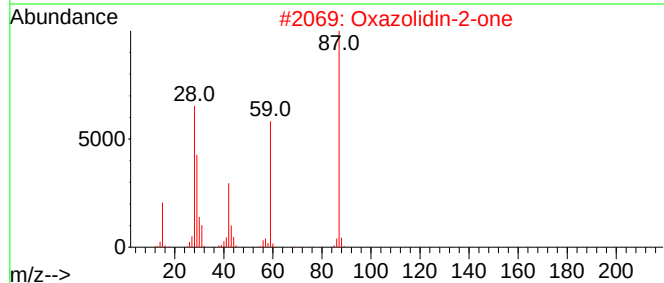
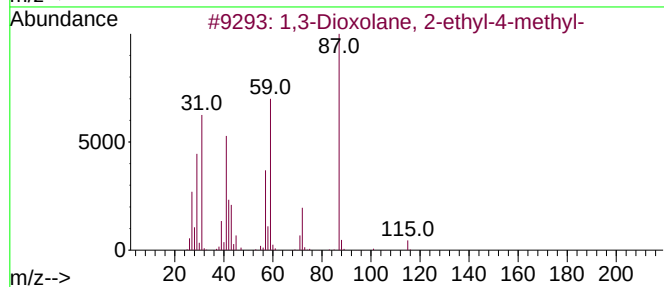
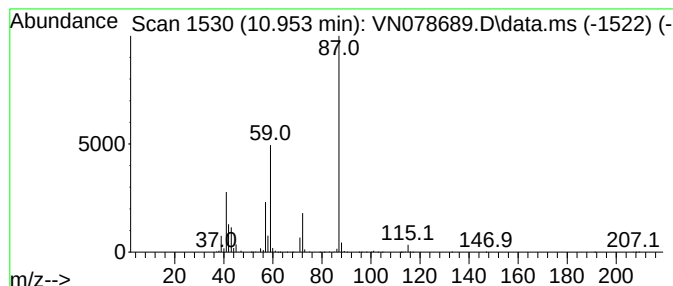
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Peak Number 5 Oxazolidin-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.953	118.25 ug/l	8061010	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	80
3			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50
5			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	4.300	900.0	ug/l	38538800	1	8.235	2140940	50.0
1-Propanol	6.741	63.7	ug/l	2728010	1	8.235	2140940	50.0
1,3-Dioxolane, ...	10.812	204.8	ug/l	13963700	3	11.870	3408480	50.0
Oxazolidin-2-one	10.953	118.3	ug/l	8061010	3	11.870	3408480	50.0