

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
 Data File : VX030236.D
 Acq On : 27 Jul 2022 17:02
 Operator : JC/MD
 Sample : N3898-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 61422-A

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\82X072522W.M

Title : SW846 8260

Signal : TIC: VX030236.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	55	60	71	rBV	200295	244682	4.78%	1.967%
2	2.385	206	213	222	rBV	40183	69310	1.35%	0.557%
3	2.946	298	305	316	rVB	22945	51683	1.01%	0.416%
4	4.385	530	541	554	rBV	27270	81928	1.60%	0.659%
5	5.391	691	706	723	rBV	127480	372597	7.28%	2.996%
6	5.556	723	733	749	rVB	139888	399164	7.79%	3.209%
7	5.964	789	800	815	rBV	152236	407302	7.95%	3.275%
8	6.769	919	932	940	rBV	226527	546252	10.67%	4.392%
9	6.879	940	950	966	rVB	2223715	5121554	100.00%	41.178%
10	7.214	989	1005	1015	rBV	605190	1321692	25.81%	10.627%
11	8.653	1234	1241	1248	rBV	727747	1116025	21.79%	8.973%
12	8.720	1248	1252	1263	rVB	95799	154518	3.02%	1.242%
13	10.055	1466	1471	1485	rVB	524581	727617	14.21%	5.850%
14	10.317	1505	1514	1524	rBV2	178591	273685	5.34%	2.200%
15	11.085	1634	1640	1647	rBV	565034	702318	13.71%	5.647%
16	12.024	1789	1794	1802	rVB	689573	847177	16.54%	6.811%

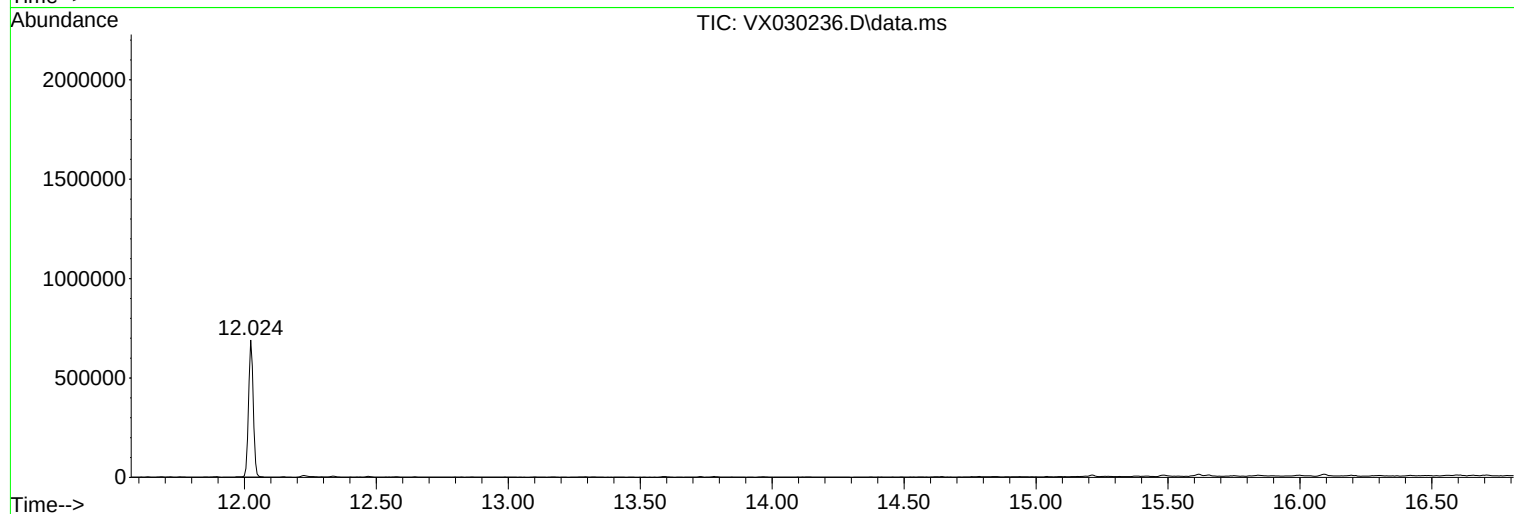
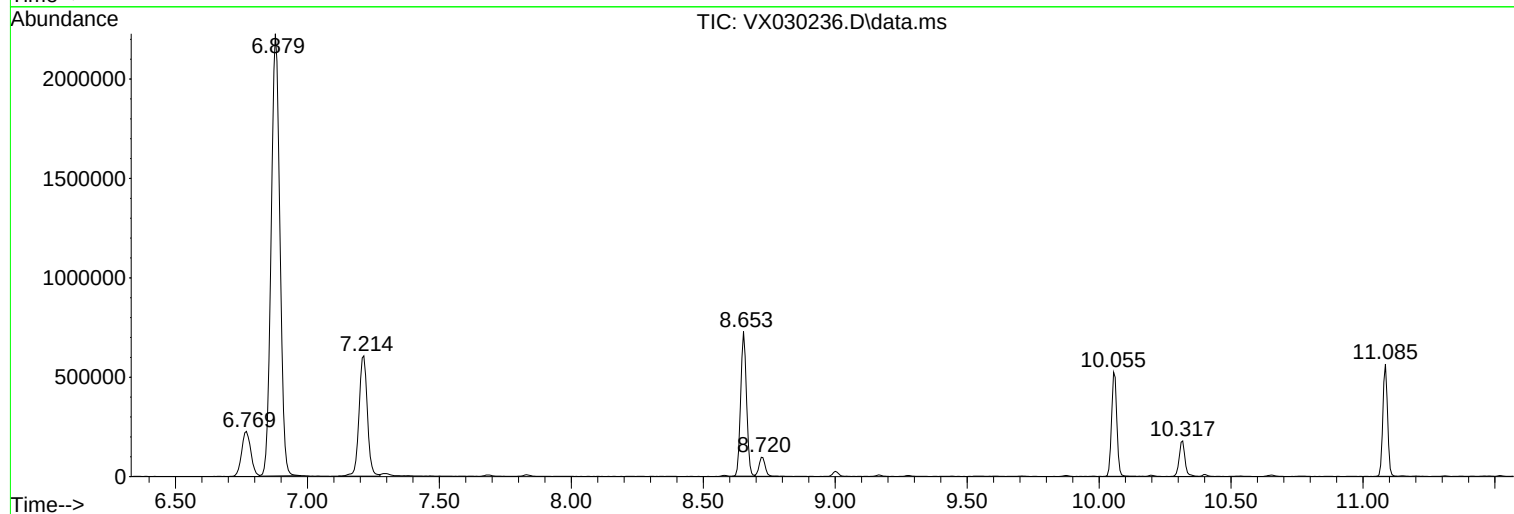
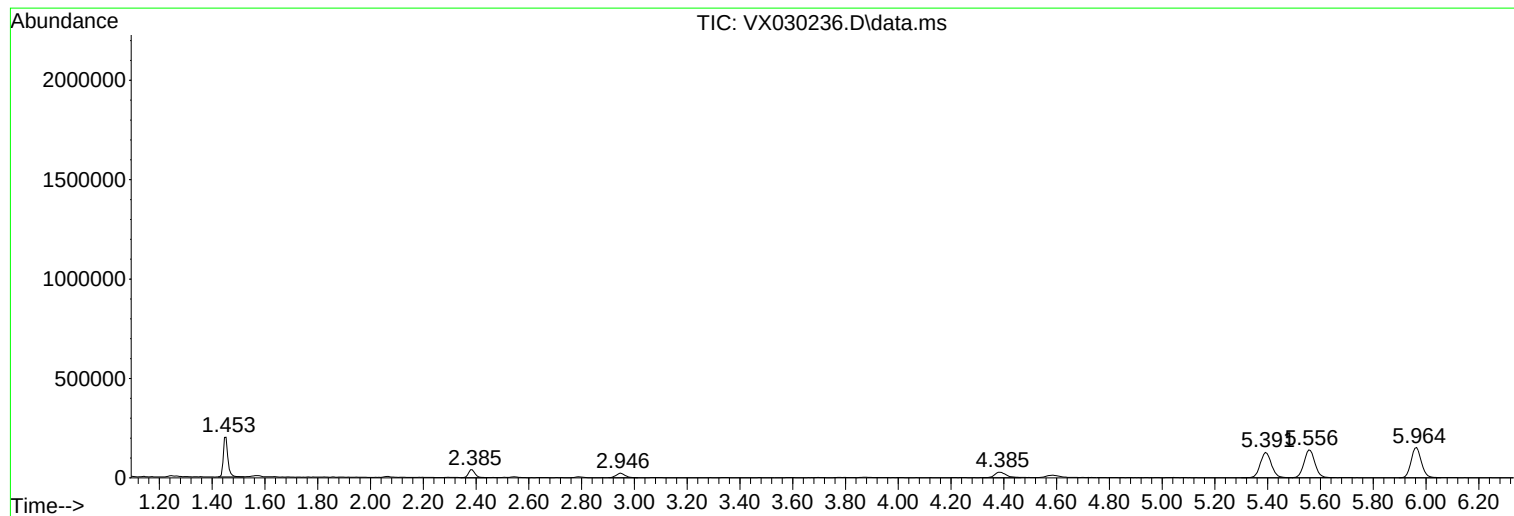
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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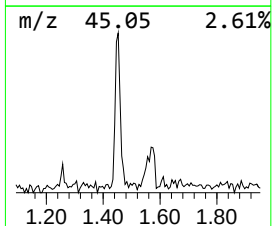
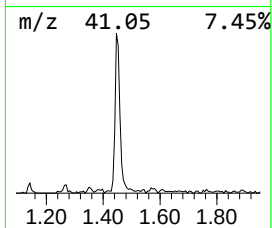
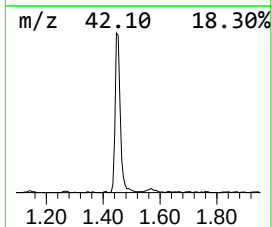
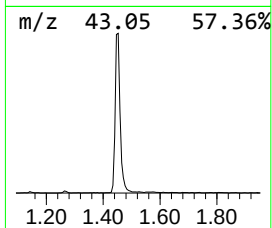
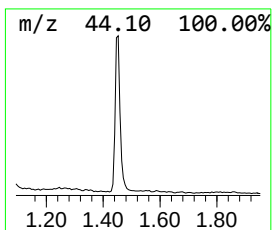
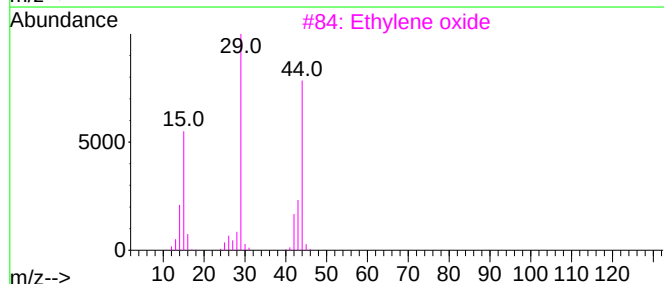
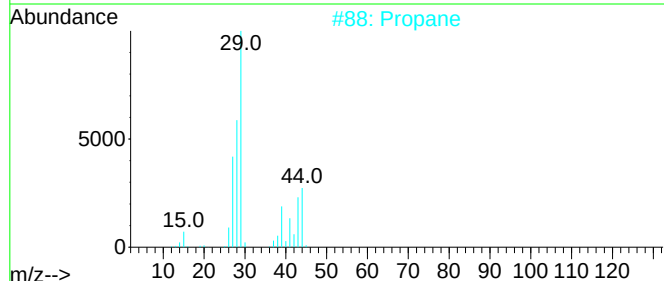
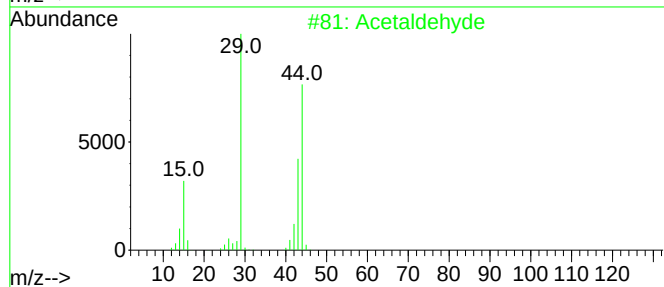
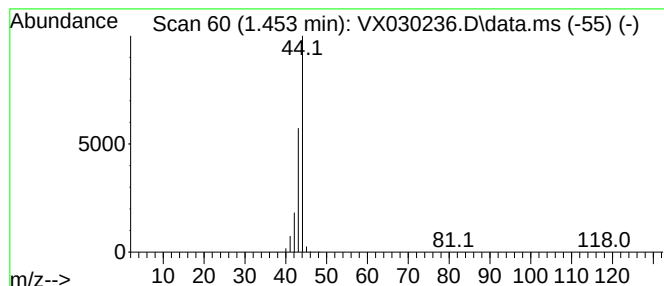
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	30.65 ug/l	244682	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Carbon dioxide	44	CO2	000124-38-9	3



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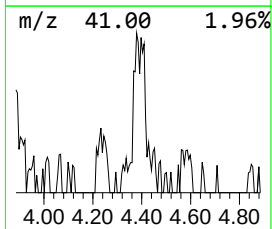
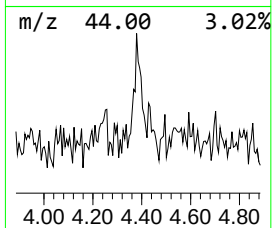
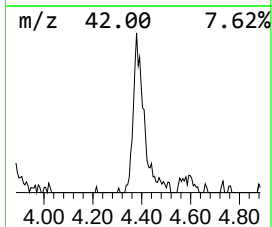
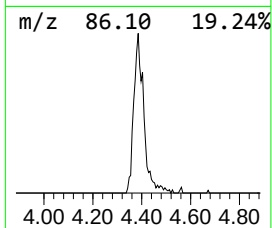
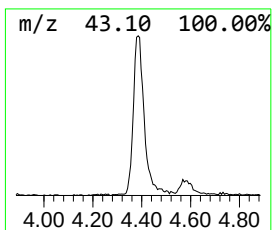
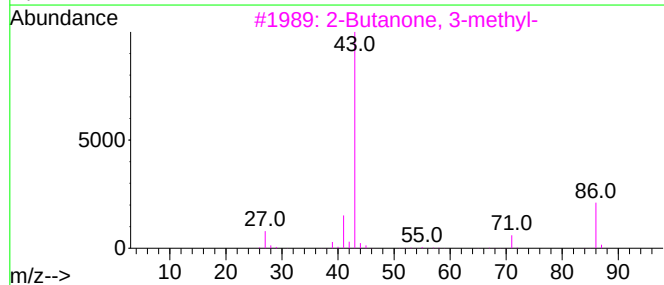
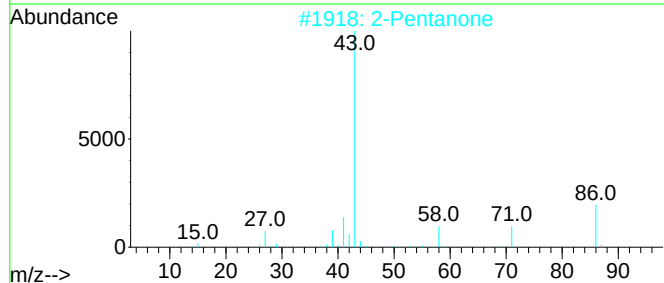
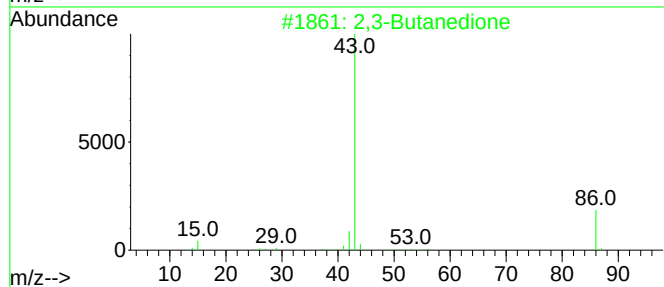
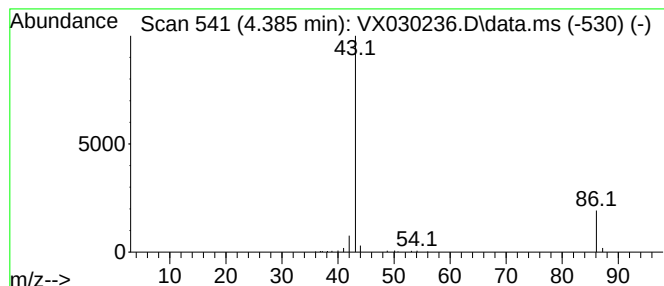
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 3 2,3-Butanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.385	10.26 ug/l	81928	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione			86	C4H6O2	000431-03-8	72
2	2-Pentanone			86	C5H10O	000107-87-9	50
3	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	9
4	Acetic acid ethenyl ester			86	C4H6O2	000108-05-4	7
5	Ethane-1,2-diimine, N,N'-diamino-			86	C2H6N4	1000197-11-5	5



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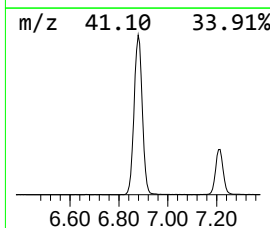
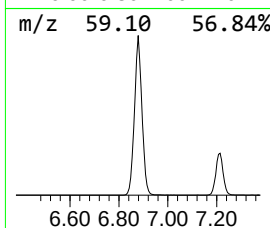
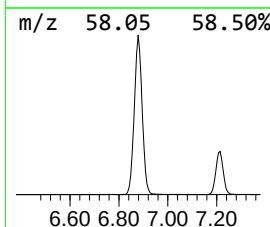
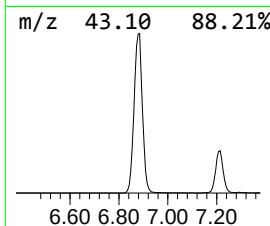
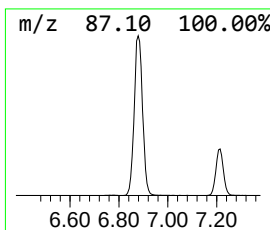
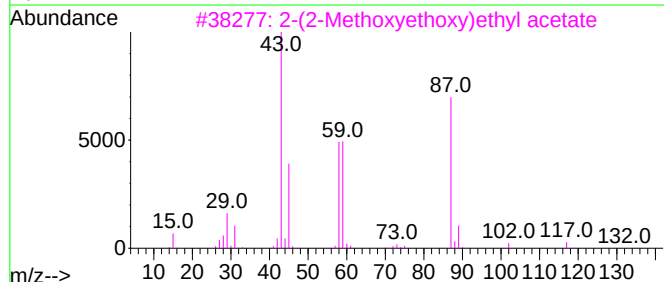
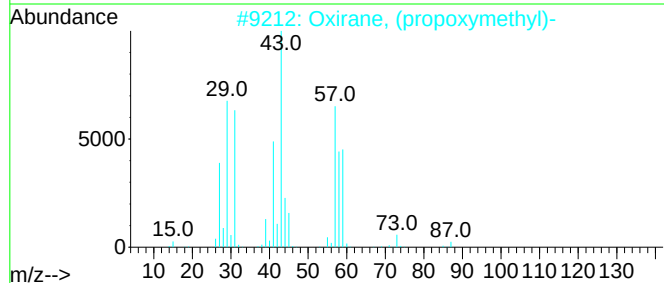
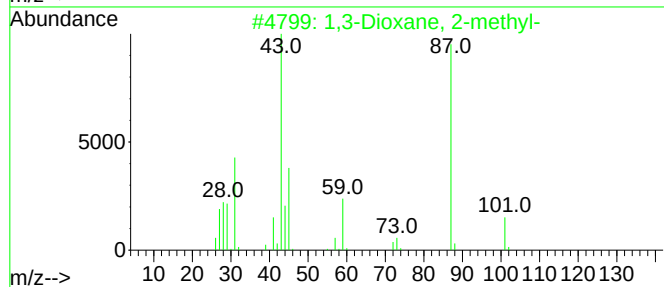
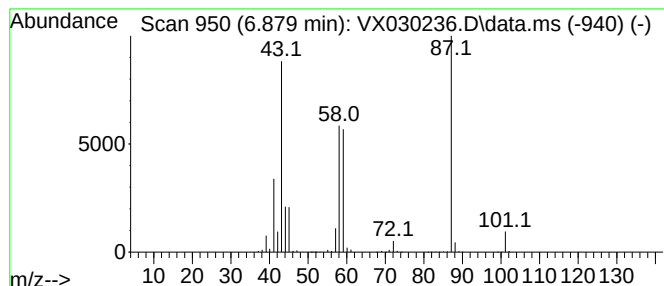
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Peak Number 4 1,3-Dioxane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	468.79 ug/l	5121550	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-			102	C5H10O2	000626-68-6	50
2	Oxirane, (propoxymethyl)-			116	C6H12O2	003126-95-2	43
3	2-(2-Methoxyethoxy)ethyl acetate			162	C7H14O4	1000351-95-4	38
4	Methyl 4-O-methyl-d-arabinopyran...			178	C7H14O5	1000129-79-9	36
5	Oxazolidin-2-one			87	C3H5NO2	000497-25-6	32



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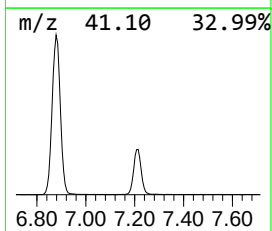
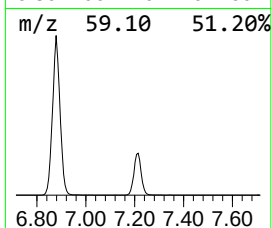
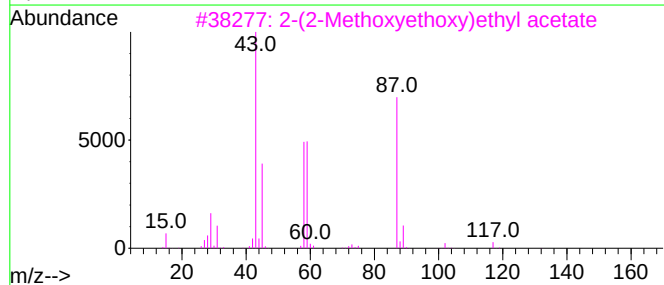
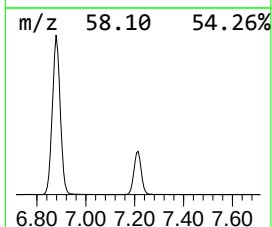
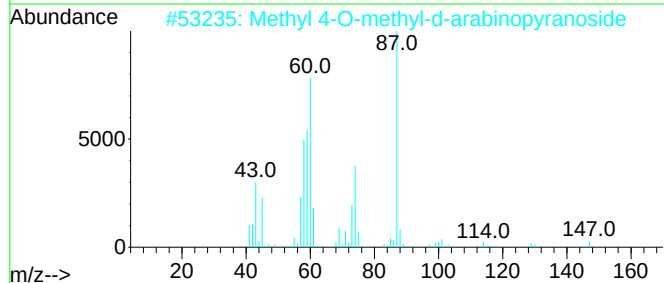
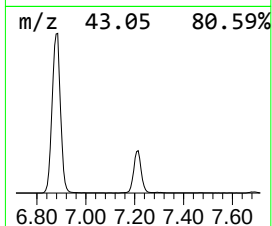
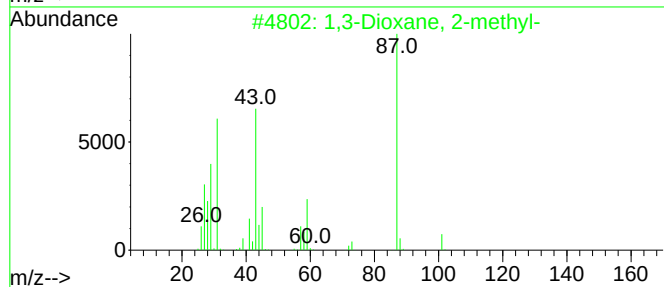
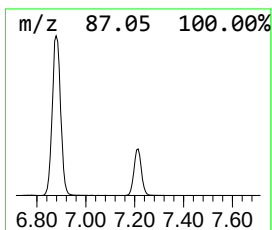
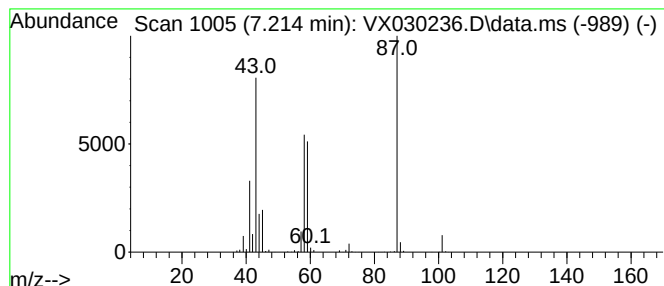
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl 4-O-methyl-d-arabino... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	120.98 ug/l	1321690	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	58
2			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	40
3			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	38
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38
5			Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	30.6	ug/l	244682	1	5.556	399164	50.0
2,3-Butanedione	4.385	10.3	ug/l	81928	1	5.556	399164	50.0
1,3-Dioxane, 2-...	6.879	468.8	ug/l	5121550	2	6.763	546252	50.0
Methyl 4-O-meth...	7.214	121.0	ug/l	1321690	2	6.763	546252	50.0