

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042523\
 Data File : VX035286.D
 Acq On : 25 Apr 2023 16:13
 Operator : JC/MD
 Sample : 02431-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AUD-1979

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035286.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	56	60	72	rVB	56335	73928	5.64%	0.822%
2	2.392	206	214	223	rVB	11490	24000	1.83%	0.267%
3	3.007	302	315	326	rBV3	6301	26063	1.99%	0.290%
4	3.958	455	471	472	rBV4	8709	29643	2.26%	0.330%
5	4.391	534	542	558	rBV2	10858	39863	3.04%	0.443%
6	5.385	693	705	720	rBV2	143130	412276	31.47%	4.584%
7	5.550	720	732	749	rVB	257572	733777	56.02%	8.159%
8	5.952	788	798	813	rBV	161144	424771	32.43%	4.723%
9	6.147	818	830	852	rBV3	74597	334973	25.57%	3.725%
10	6.763	920	931	941	rBV	397300	959137	73.22%	10.665%
11	6.873	941	949	968	rVB	380320	922383	70.41%	10.256%
12	7.208	996	1004	1014	rBV	232288	495229	37.81%	5.507%
13	8.647	1232	1240	1249	rBV	848379	1309925	100.00%	14.566%
14	8.781	1257	1262	1273	rBV	12584	26418	2.02%	0.294%
15	10.055	1465	1471	1482	rBV	845244	1141347	87.13%	12.691%
16	10.311	1505	1513	1518	rBV4	13393	21434	1.64%	0.238%
17	11.079	1634	1639	1654	rBV	697840	896301	68.42%	9.966%
18	12.024	1788	1794	1801	rBV	858357	1103044	84.21%	12.265%
19	12.219	1822	1826	1832	rBV3	9895	18764	1.43%	0.209%

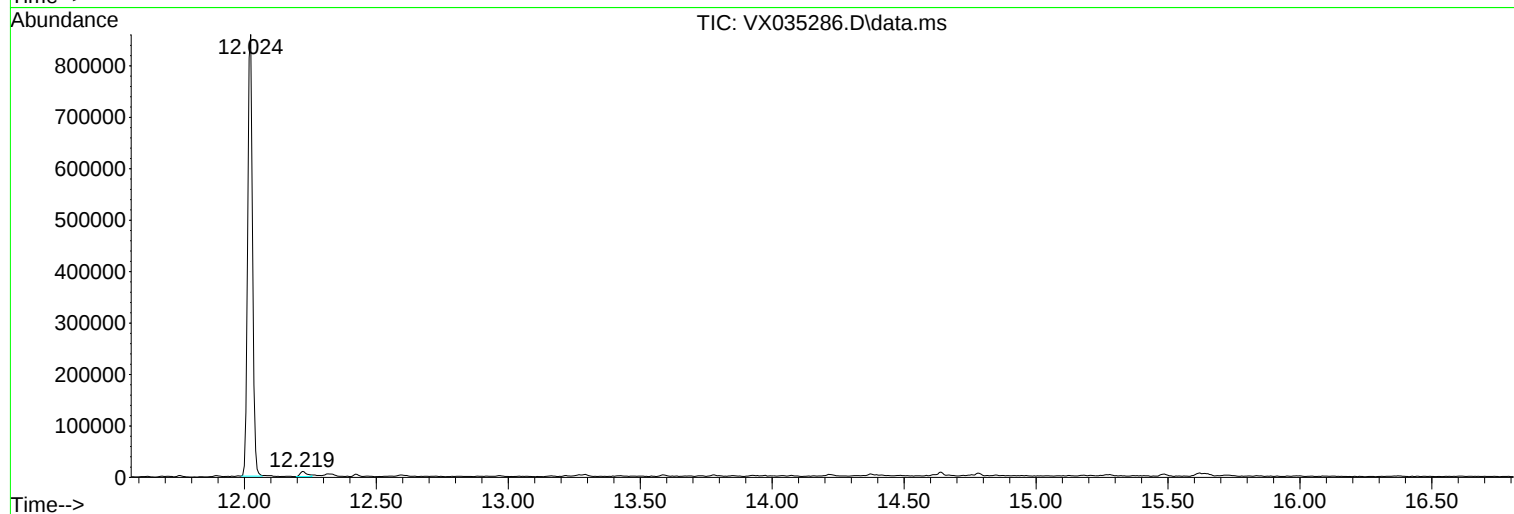
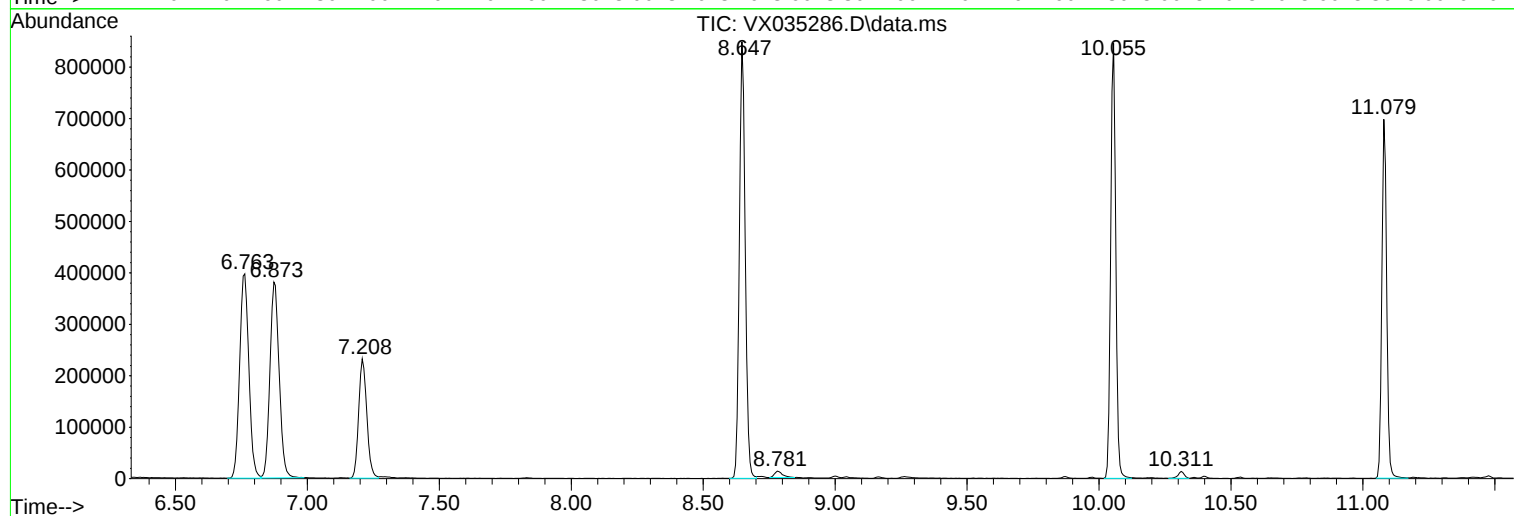
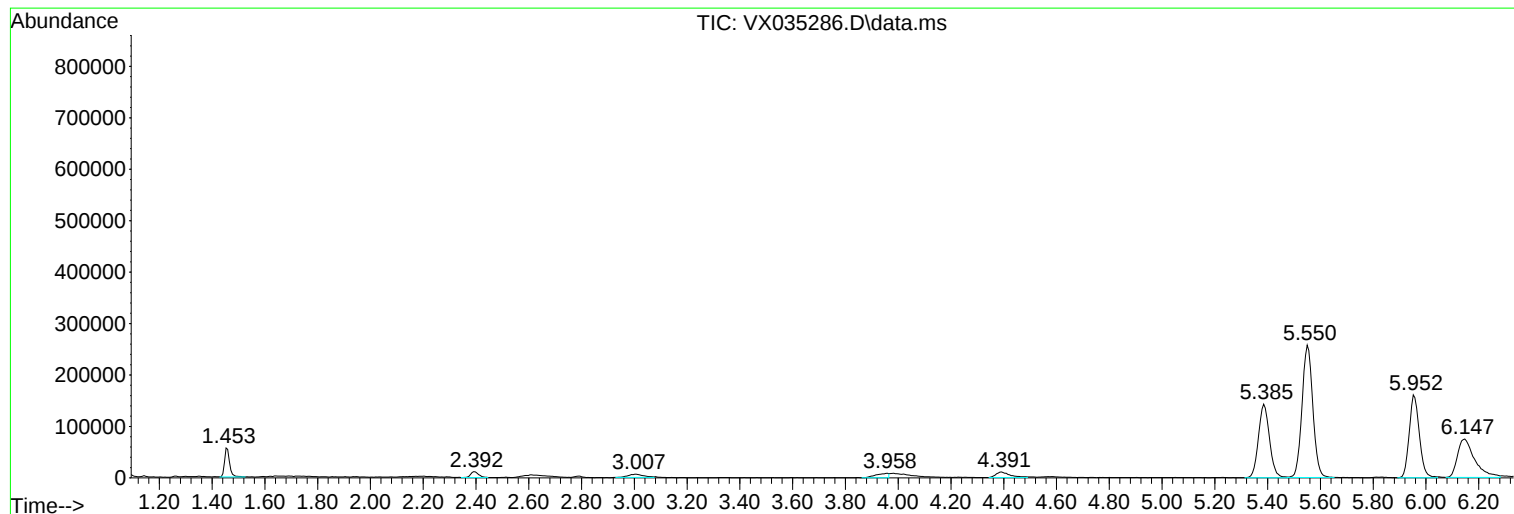
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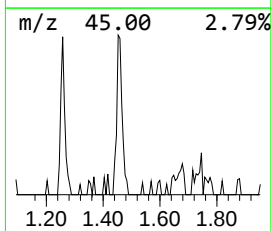
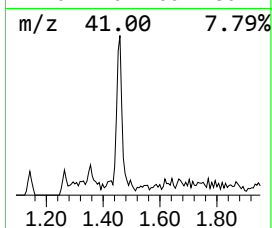
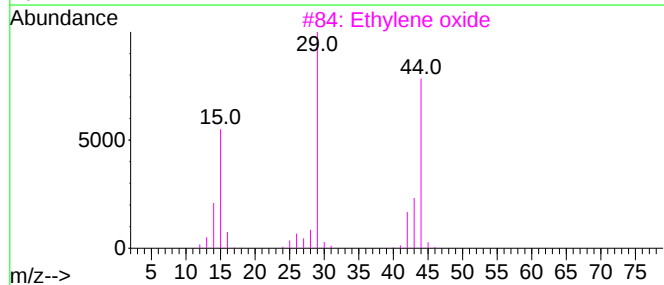
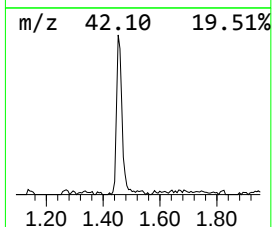
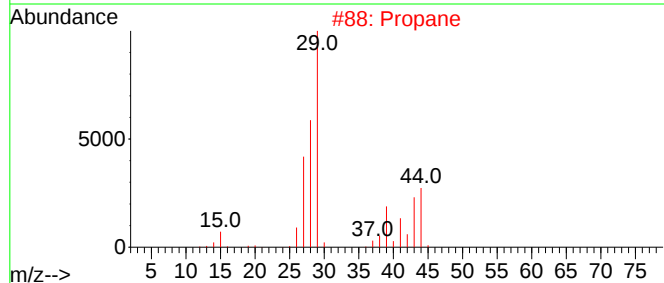
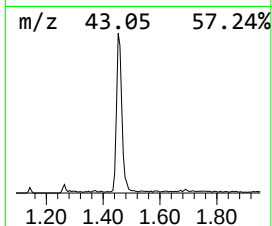
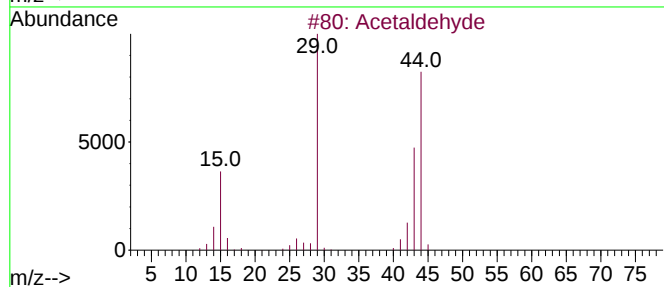
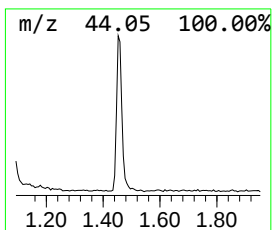
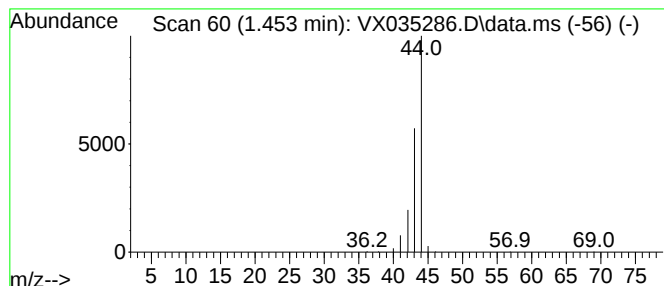
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	5.04 ug/l	73928	Pentafluorobenzene	5.550

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			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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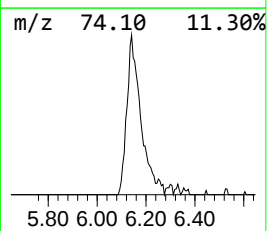
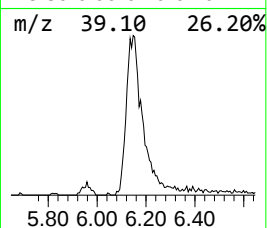
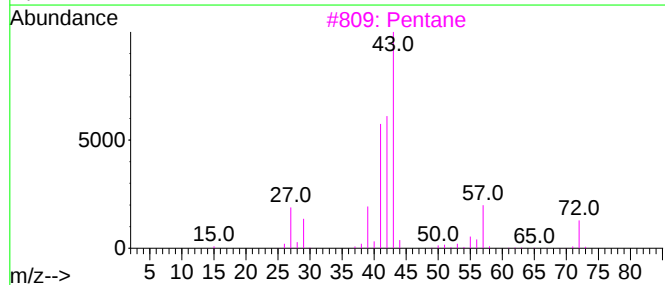
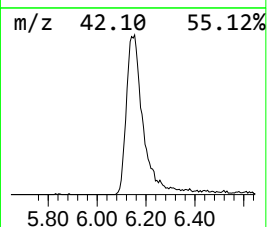
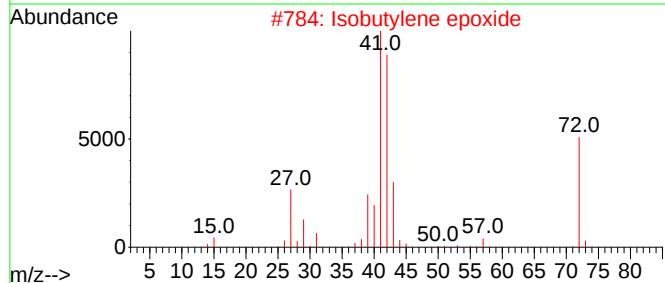
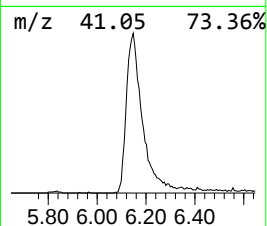
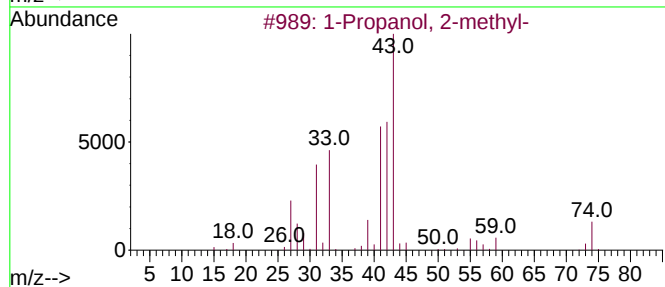
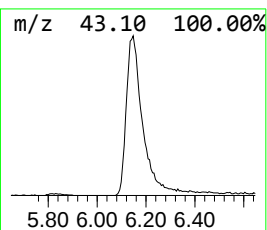
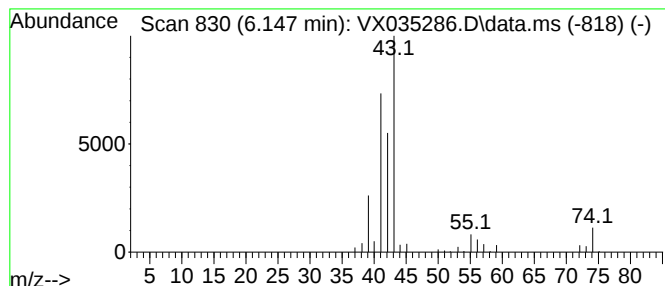
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.147	22.83 ug/l	334973	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	90
2		Isobutylene epoxide	72	C4H8O	000558-30-5	40
3		Pentane	72	C5H12	000109-66-0	39
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	35
5		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	28



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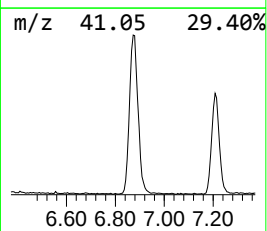
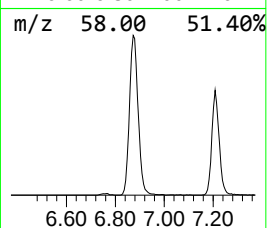
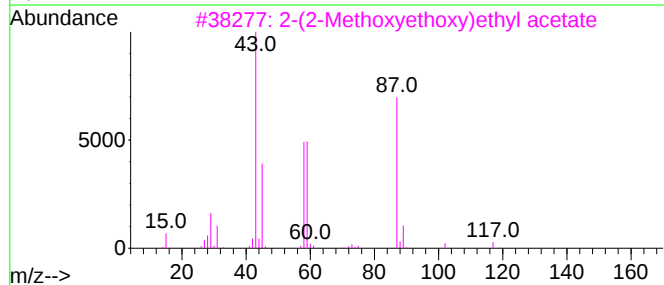
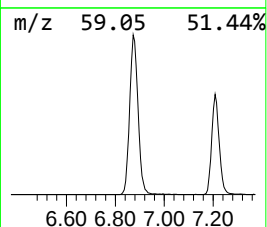
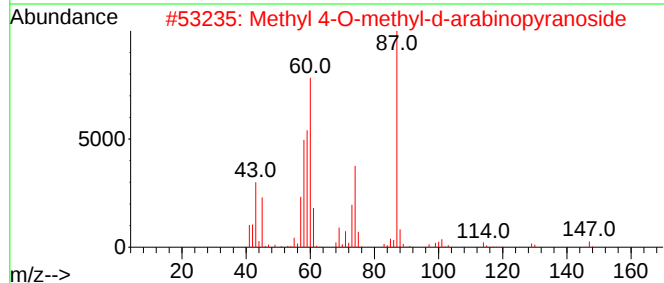
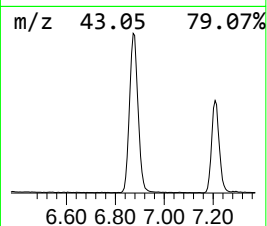
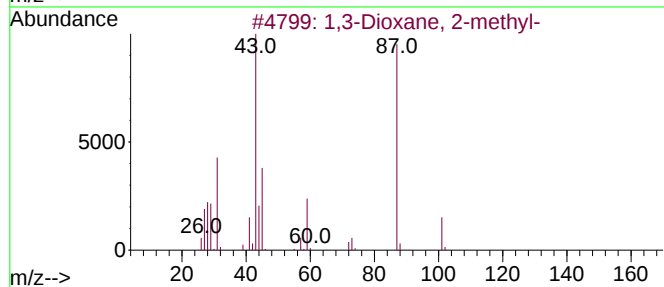
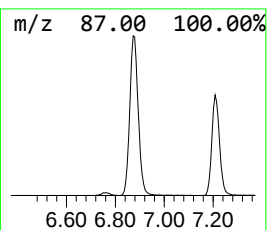
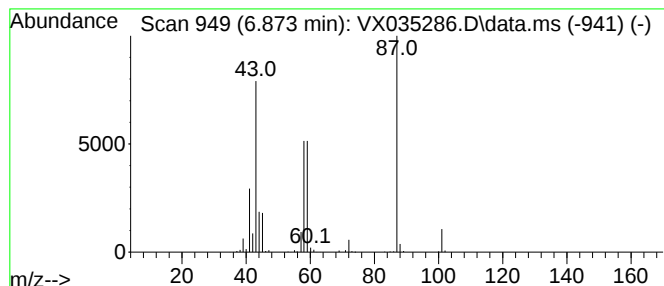
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Peak Number 3 1,3-Dioxane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	48.08 ug/l	922383	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			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
3			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	33
4			Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	32
5			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	28



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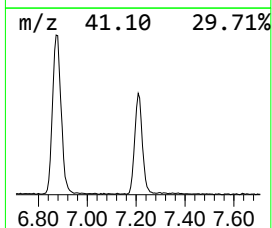
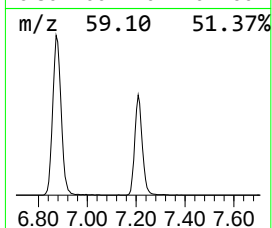
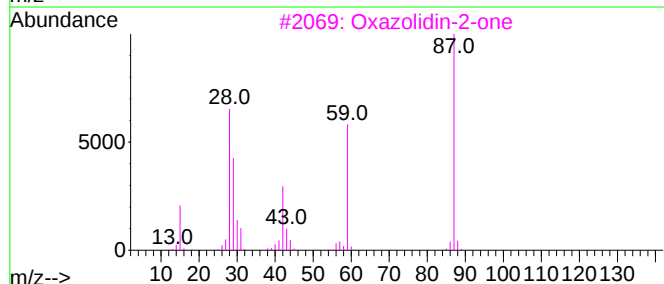
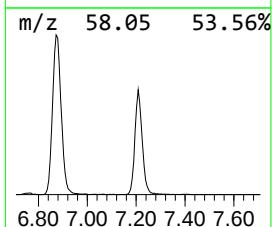
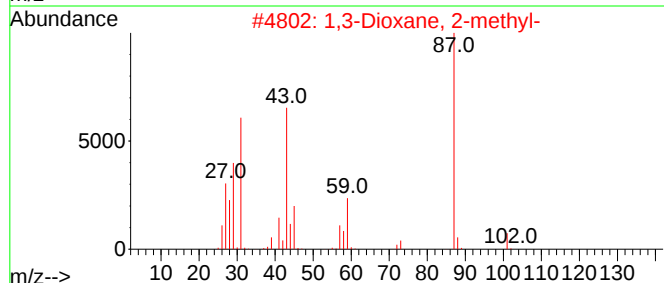
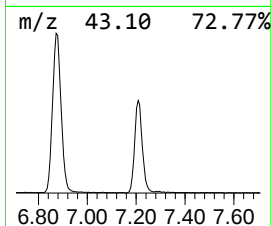
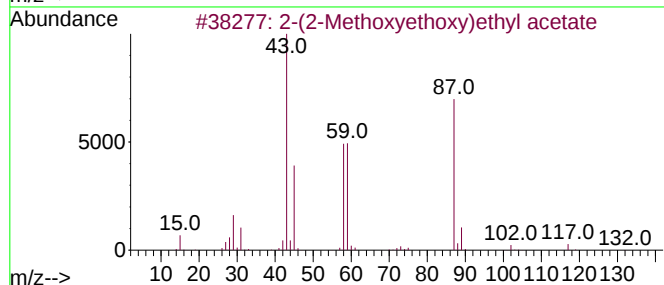
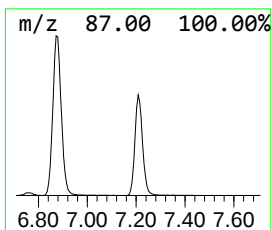
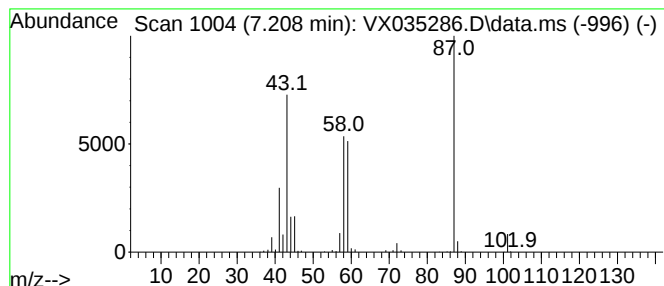
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Peak Number 4 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	25.82 ug/l	495229	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	56	
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	47	
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40	
4	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	40	
5	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	36	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	5.0	ug/l	73928	1	5.550	733777	50.0
1-Propanol, 2-m...	6.147	22.8	ug/l	334973	1	5.550	733777	50.0
1,3-Dioxane, 2-...	6.873	48.1	ug/l	922383	2	6.763	959137	50.0
2-(2-Methoxyeth...	7.208	25.8	ug/l	495229	2	6.763	959137	50.0