

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
 Data File : VX030241.D
 Acq On : 27 Jul 2022 18:59
 Operator : JC/MD
 Sample : N3916-03 100X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 998

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: VX030241.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	70	rBV	393907	461666	40.32%	7.263%
2	2.294	193	198	203	rBV2	8673	14262	1.25%	0.224%
3	2.386	206	213	218	rBV	11227	18131	1.58%	0.285%
4	2.953	297	306	316	rBV	18542	43185	3.77%	0.679%
5	3.861	446	455	469	rBV5	9435	25332	2.21%	0.399%
6	4.379	530	540	555	rBV2	58682	168423	14.71%	2.650%
7	4.580	565	573	583	rBV2	12689	38536	3.37%	0.606%
8	5.391	695	706	720	rBV	130763	372543	32.54%	5.861%
9	5.556	723	733	744	rBV	136414	383322	33.48%	6.030%
10	5.958	790	799	815	rBV2	158153	420262	36.71%	6.612%
11	6.769	919	932	942	rBV2	213441	520000	45.42%	8.181%
12	6.879	942	950	960	rVB	179025	424009	37.03%	6.670%
13	7.214	997	1005	1014	rBV2	28598	63674	5.56%	1.002%
14	8.653	1233	1241	1251	rBV	736633	1144949	100.00%	18.012%
15	9.000	1292	1298	1304	rBV	21515	30680	2.68%	0.483%
16	10.055	1465	1471	1483	rBV	509449	690418	60.30%	10.862%
17	11.085	1634	1640	1646	rBV	552167	706700	61.72%	11.118%
18	12.024	1789	1794	1804	rVB	651843	789656	68.97%	12.423%
19	12.225	1820	1827	1836	rBV	19605	40771	3.56%	0.641%

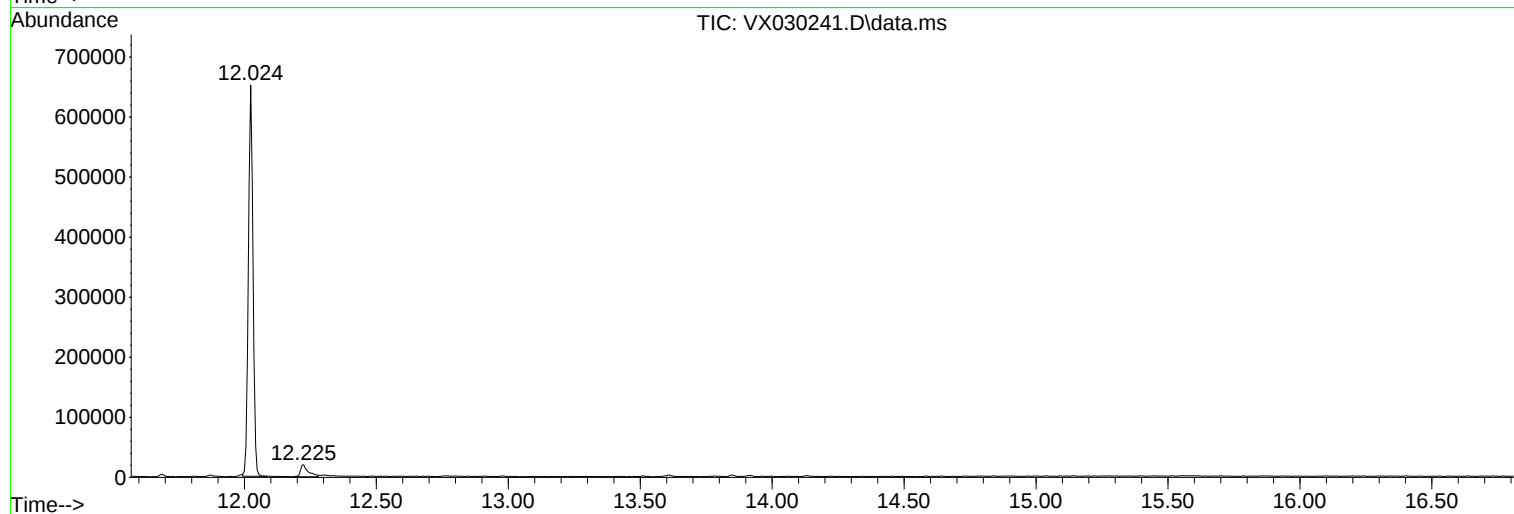
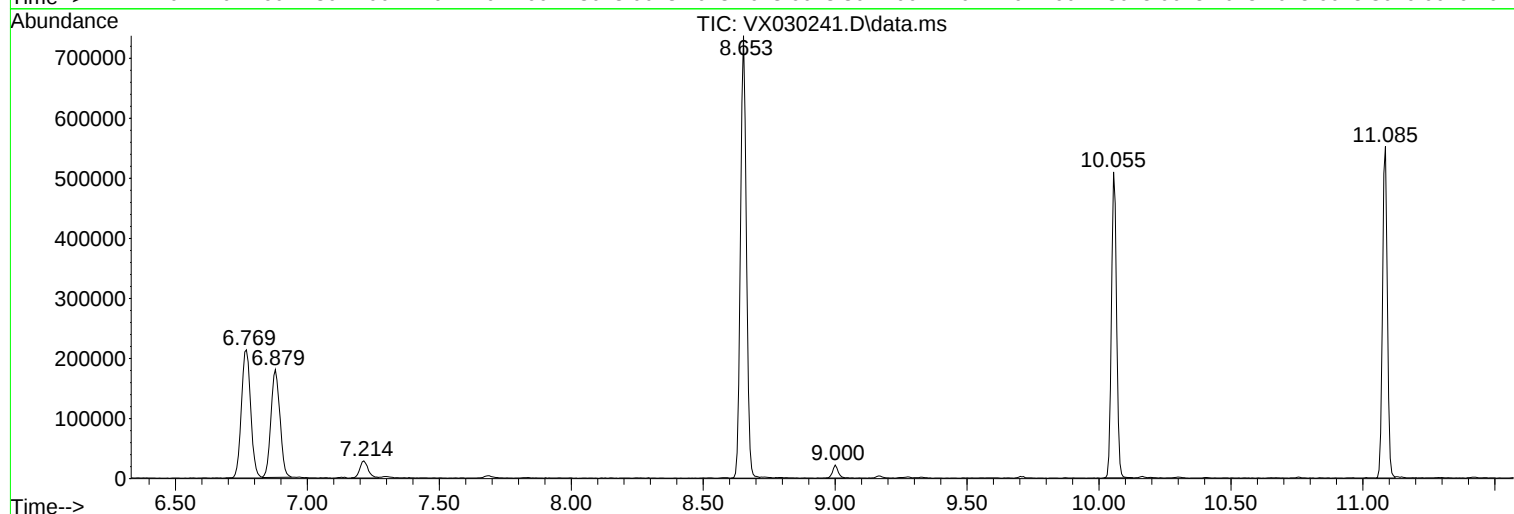
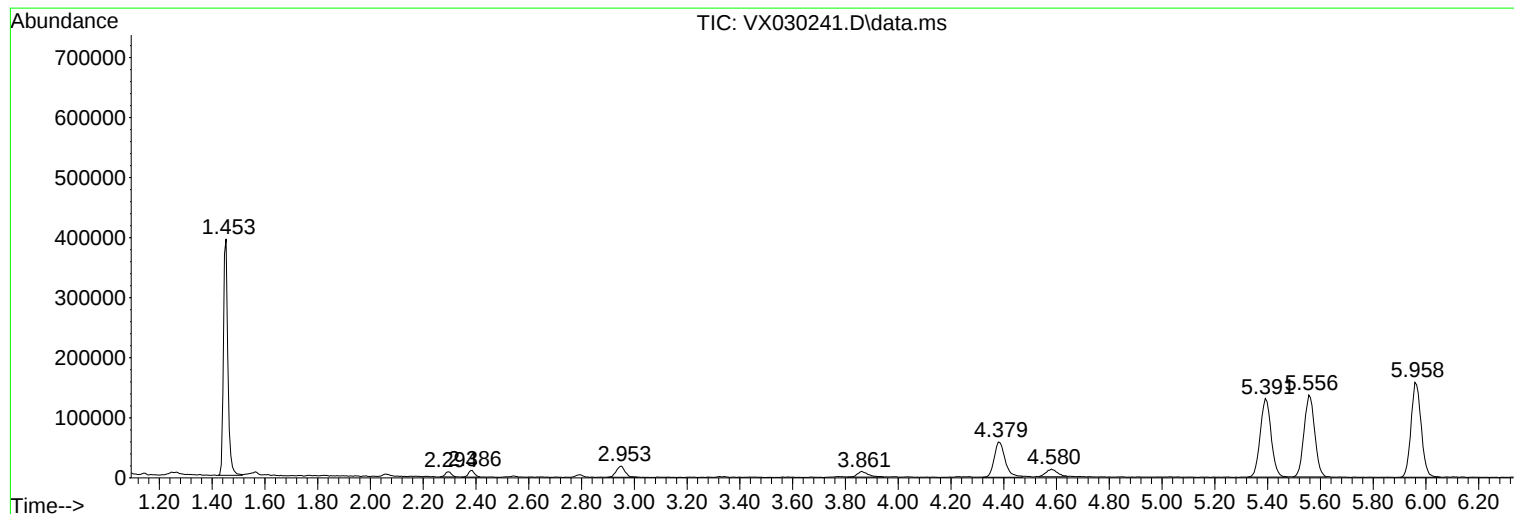
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TIC Integration Parameters: LSCINT.P



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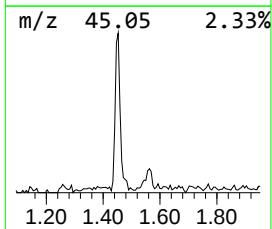
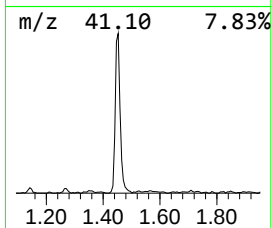
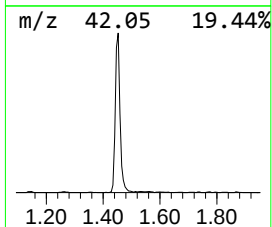
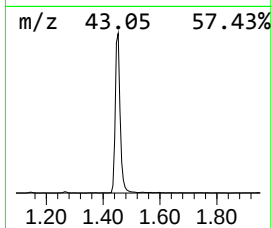
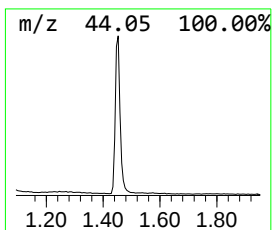
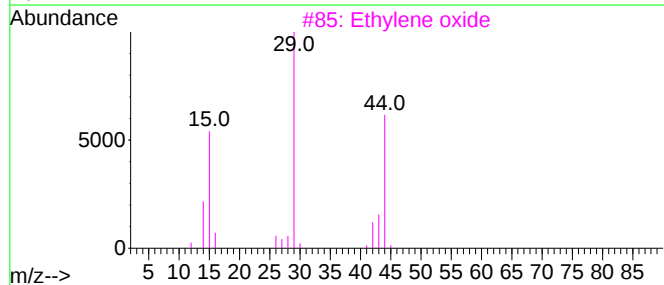
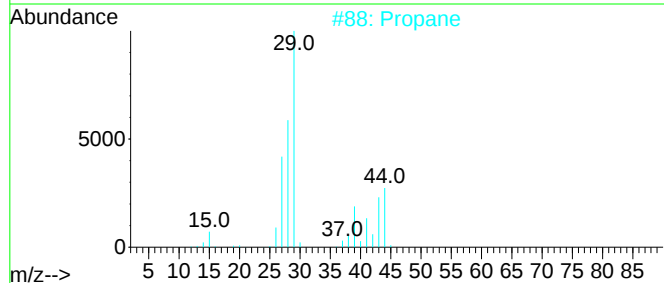
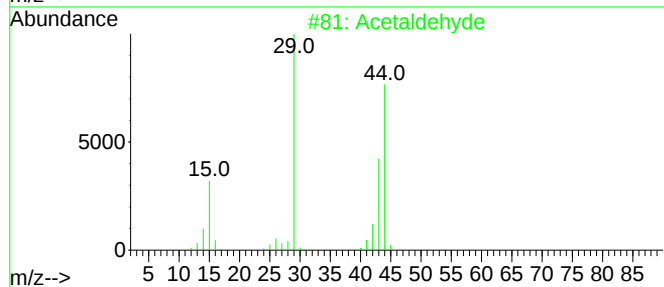
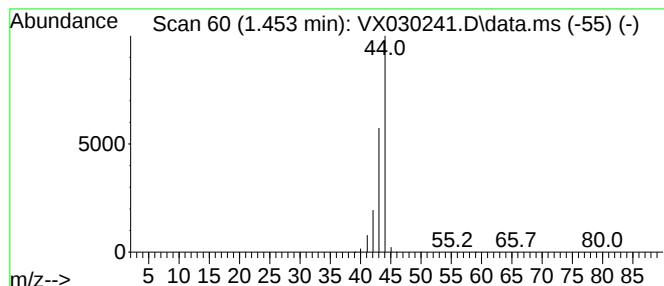
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	60.22 ug/l	461666	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
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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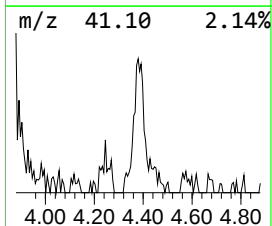
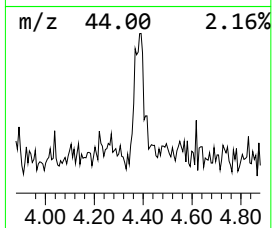
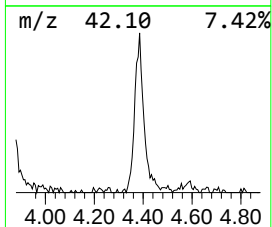
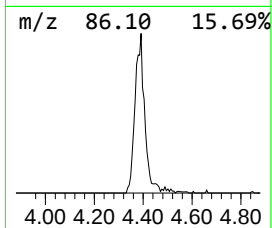
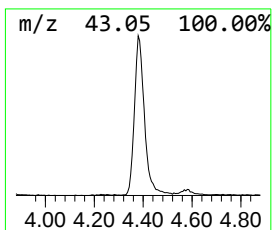
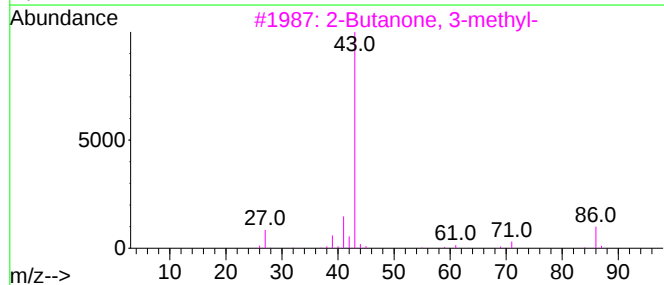
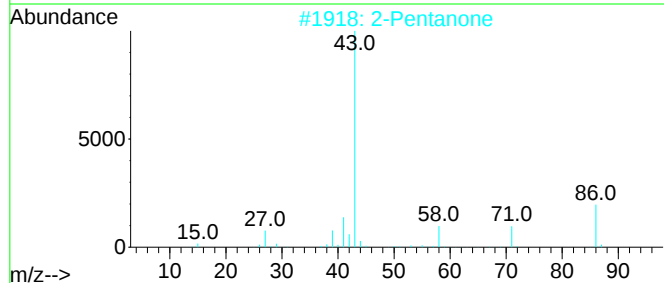
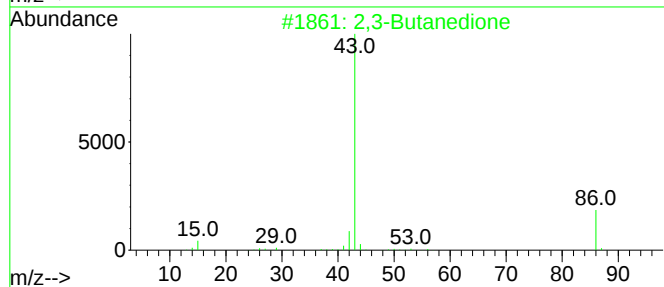
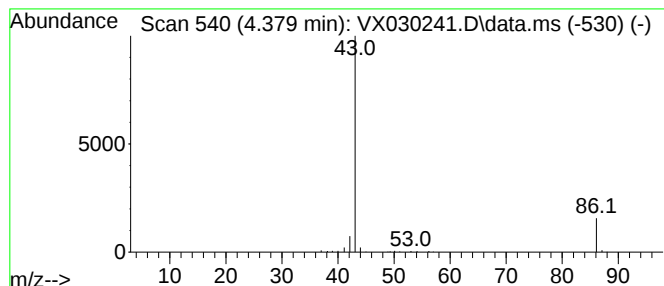
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 3 2,3-Butanedione Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.379	21.97 ug/l	168423	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione			86	C4H6O2	000431-03-8	86
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	9
5	Ethanone, 1-oxiranyl-			86	C4H6O2	004401-11-0	9



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Instrument :
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ClientSampleId :
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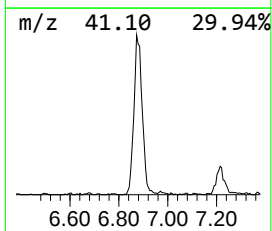
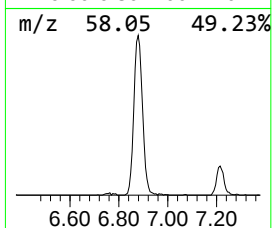
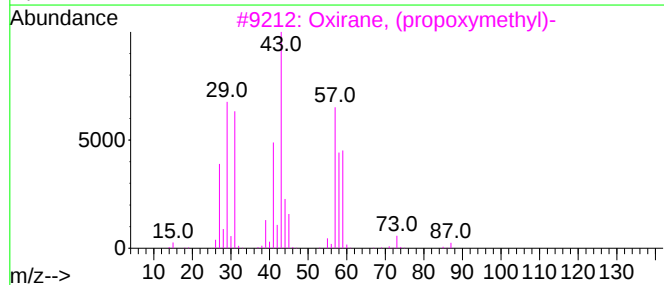
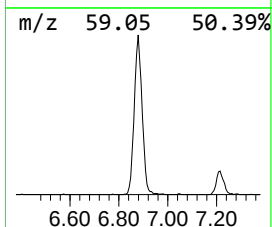
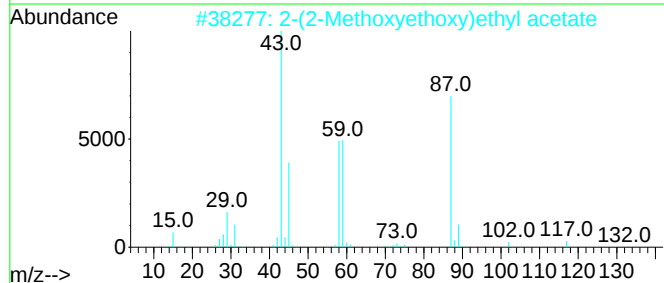
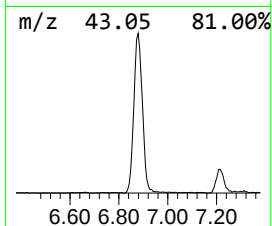
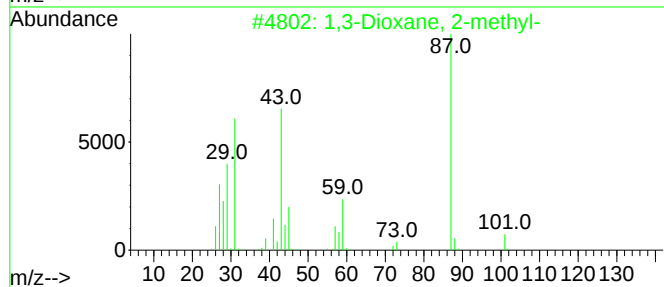
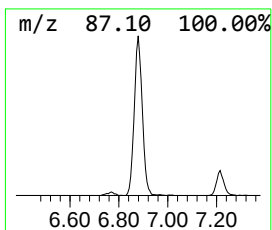
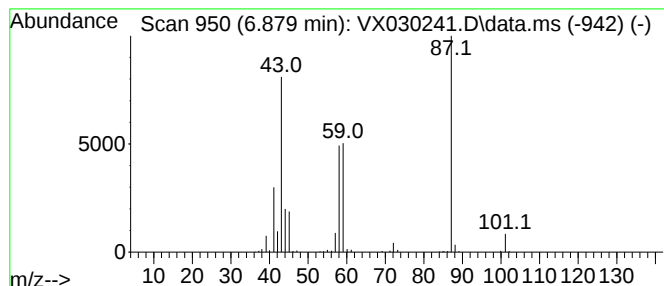
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Peak Number 4 unknown6.879 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	40.77 ug/l	424009	1,4-Difluorobenzene	6.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	40
2		2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
3		Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	38
4		1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	28
5		Monomethyl malonate	118	C4H6O4	016695-14-0	28



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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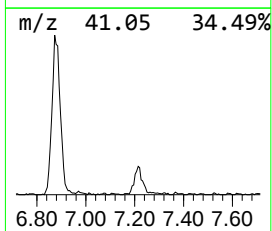
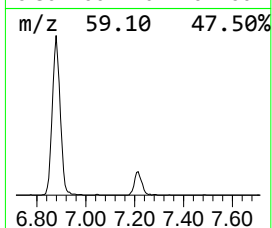
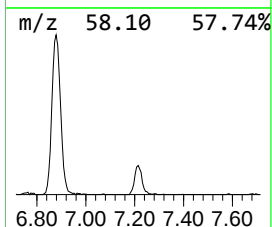
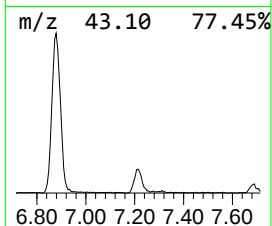
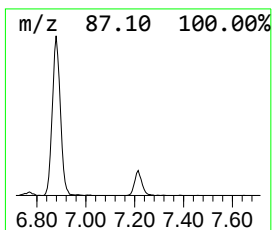
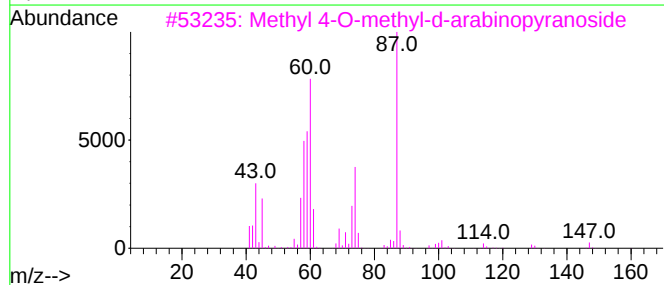
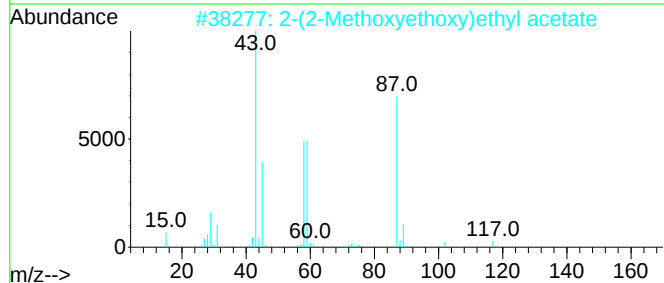
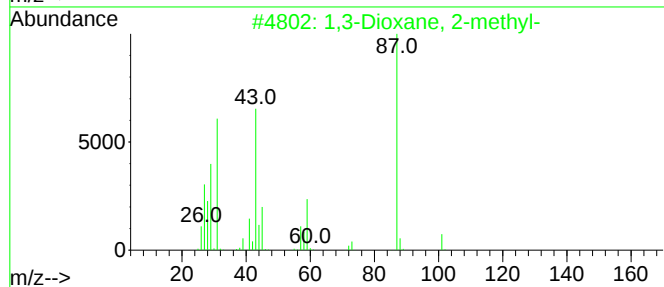
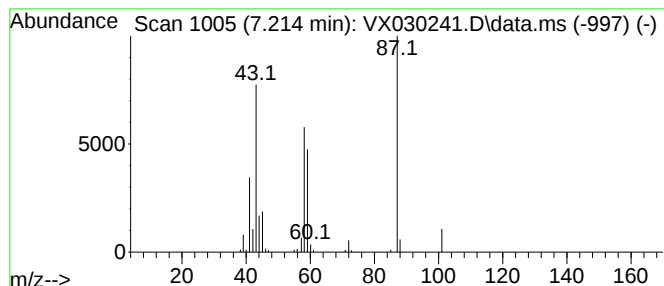
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	6.12 ug/l	63674	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	53
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	33
5			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	28



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.453	60.2	ug/l	461666	1	5.562	383322	50.0
2,3-Butanedione	4.379	22.0	ug/l	168423	1	5.562	383322	50.0
unknown6.879	6.879	40.8	ug/l	424009	2	6.769	520000	50.0
1,3-Dioxane, 2-...	7.214	6.1	ug/l	63674	2	6.769	520000	50.0