

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041723\
 Data File : VX035106.D
 Acq On : 17 Apr 2023 14:06
 Operator : JC/MD
 Sample : 02353-05 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BUR-1263

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\82X032923W.M
 Title : SW846 8260

Signal : TIC: VX035106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	207	214	225	rBV	14661	32151	1.63%	0.258%
2	2.617	237	251	275	rBV	24435	173201	8.76%	1.388%
3	3.008	302	315	347	rVB	29849	155927	7.89%	1.249%
4	5.385	693	705	719	rBV	178095	526177	26.61%	4.215%
5	5.550	719	732	747	rVB	316136	909926	46.02%	7.290%
6	5.952	788	798	818	rBV	202814	550257	27.83%	4.408%
7	6.147	818	830	856	rVV2	63713	296202	14.98%	2.373%
8	6.757	920	930	940	rBV	499043	1204103	60.90%	9.646%
9	6.873	940	949	962	rVB	828008	1977219	100.00%	15.840%
10	7.208	994	1004	1016	rBV	322611	703824	35.60%	5.638%
11	8.647	1233	1240	1249	rBV	1042280	1643101	83.10%	13.163%
12	8.781	1256	1262	1274	rVB2	23020	48084	2.43%	0.385%
13	9.256	1333	1340	1348	rBV3	11890	29276	1.48%	0.235%
14	9.872	1435	1441	1450	rVB2	19291	27691	1.40%	0.222%
15	10.055	1465	1471	1483	rBV	1008649	1418926	71.76%	11.367%
16	10.396	1523	1527	1534	rVB	14688	20416	1.03%	0.164%
17	11.079	1634	1639	1647	rBV	871440	1109726	56.13%	8.890%
18	11.890	1766	1772	1781	rBV2	21223	37653	1.90%	0.302%
19	12.024	1788	1794	1803	rVB	1054877	1357634	68.66%	10.876%
20	12.219	1822	1826	1831	rBV	22076	34798	1.76%	0.279%
21	12.274	1831	1835	1839	rVV3	12047	28331	1.43%	0.227%
22	12.335	1843	1845	1858	rVB	16612	26272	1.33%	0.210%
23	13.780	2078	2082	2088	rVB	13861	20682	1.05%	0.166%
24	14.603	2213	2217	2220	rBV2	23860	31504	1.59%	0.252%
25	14.640	2220	2223	2227	rVB	23394	28819	1.46%	0.231%
26	14.780	2240	2246	2250	rBV2	20886	29556	1.49%	0.237%
27	15.481	2356	2361	2367	rBV2	15412	26799	1.36%	0.215%
28	15.615	2378	2383	2387	rBV2	20921	34339	1.74%	0.275%

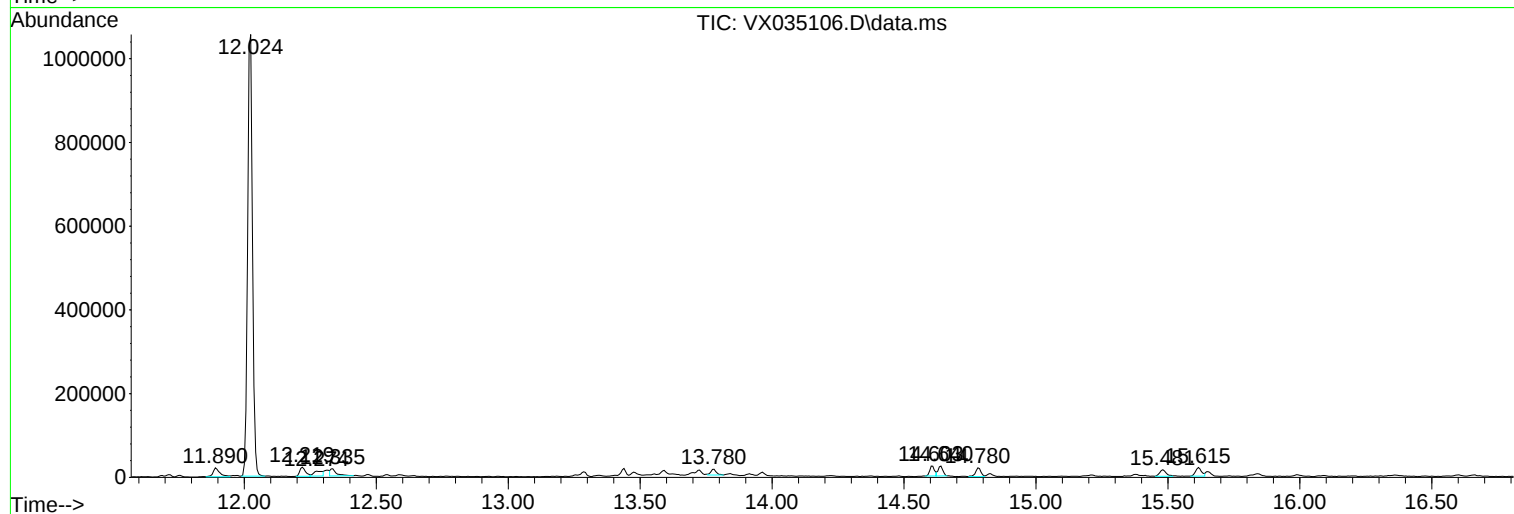
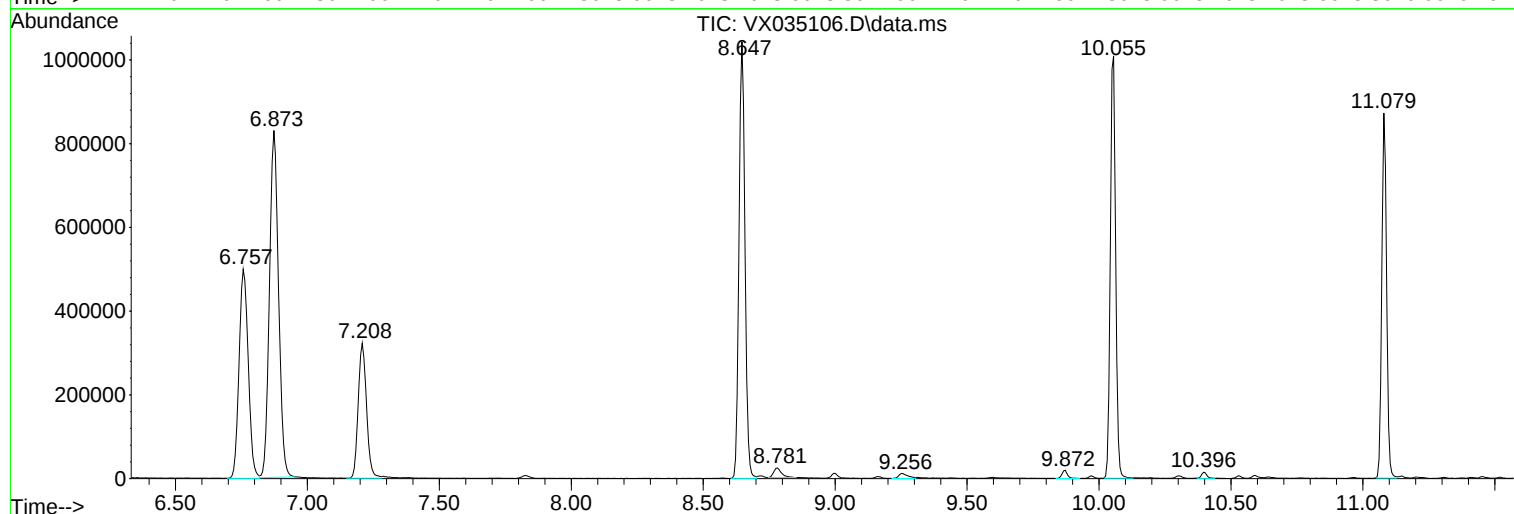
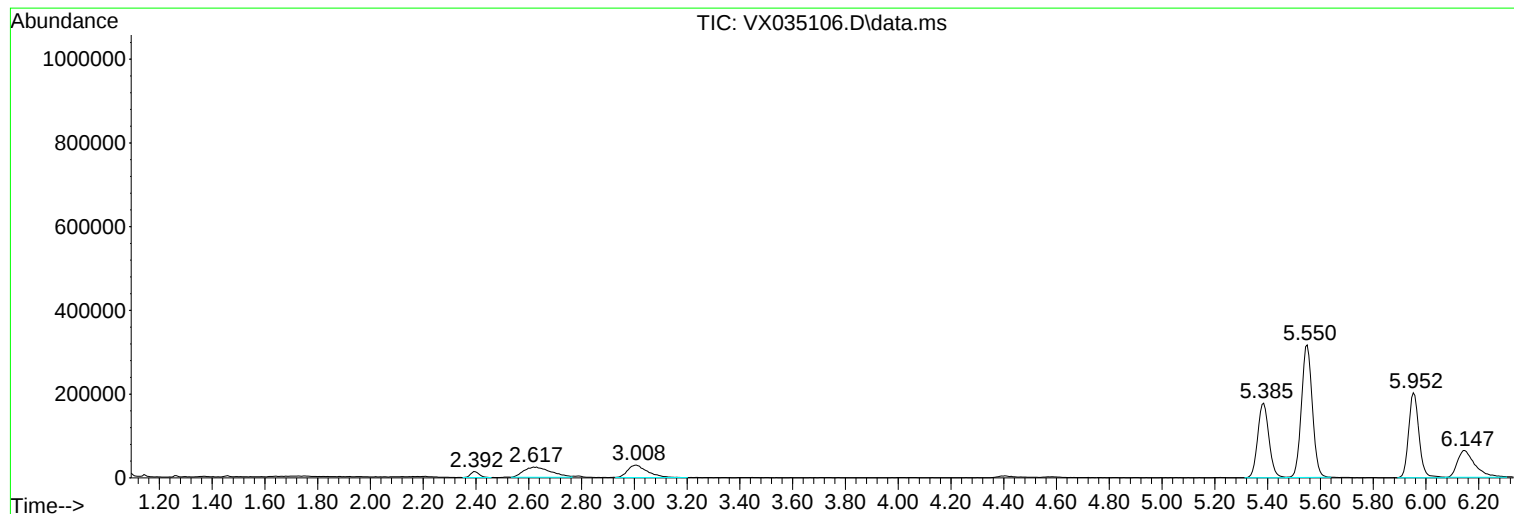
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



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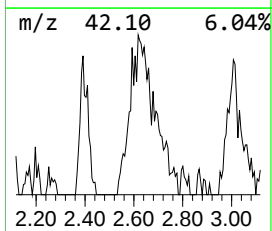
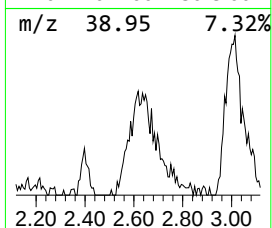
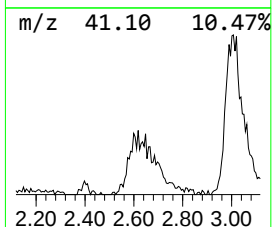
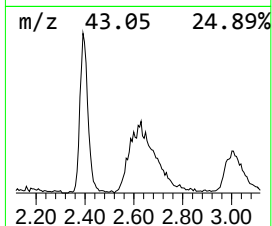
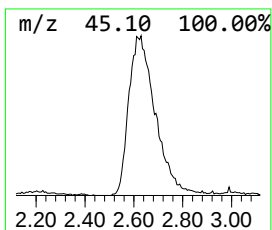
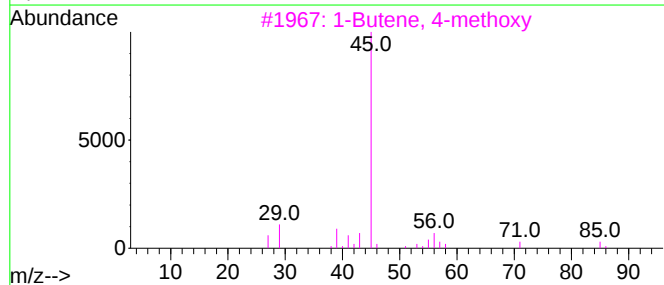
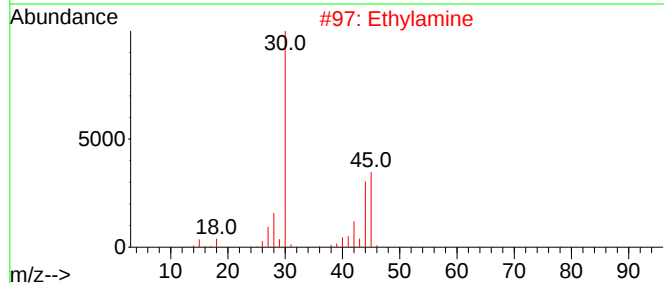
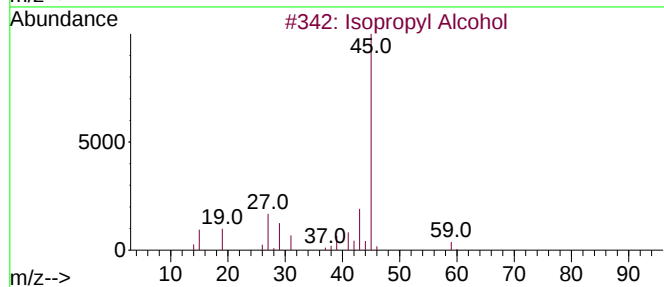
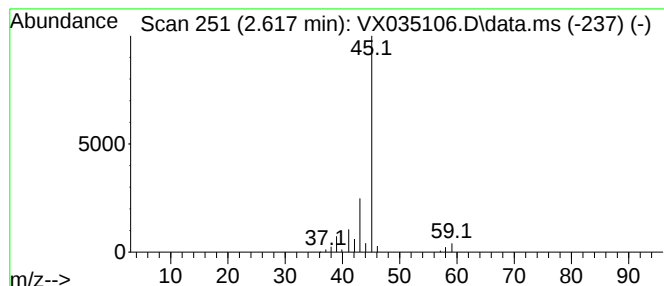
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.617	9.52 ug/l	173201	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2			Ethylamine	45	C2H7N	000075-04-7	7
3			1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4
4			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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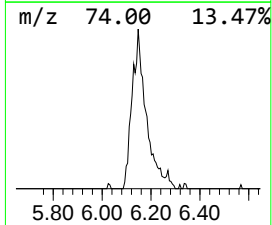
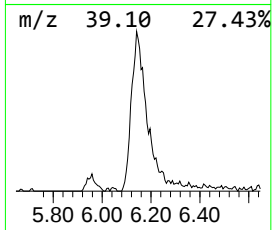
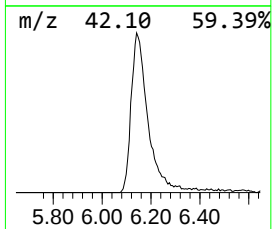
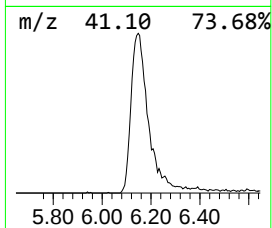
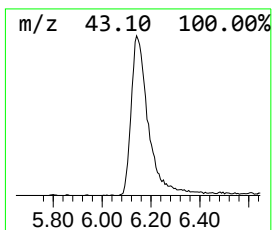
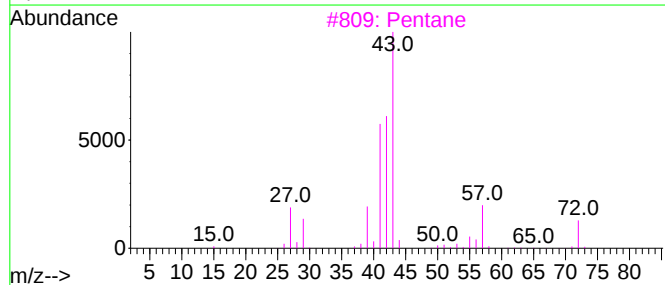
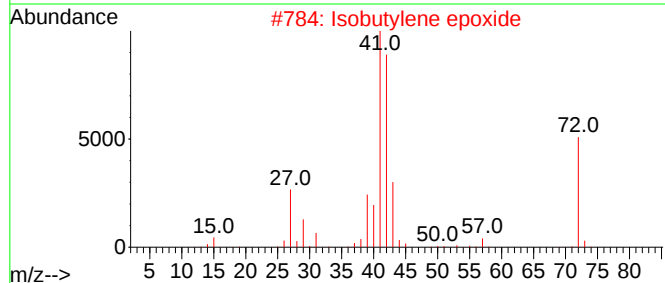
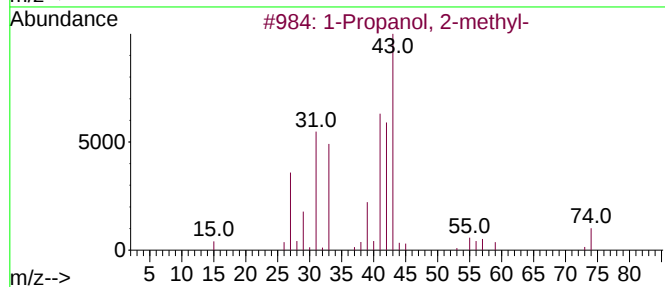
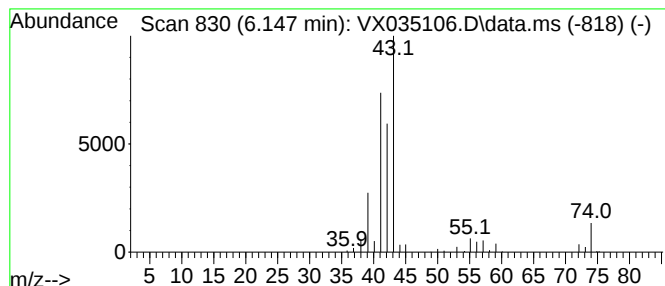
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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	16.28 ug/l	296202	Pentafluorobenzene	5.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	91
2		Isobutylene epoxide	72	C4H8O	000558-30-5	38
3		Pentane	72	C5H12	000109-66-0	38
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	35
5		Butane, 2-methyl-	72	C5H12	000078-78-4	33



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Instrument :
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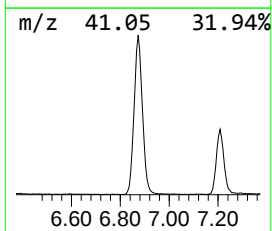
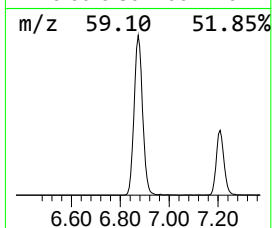
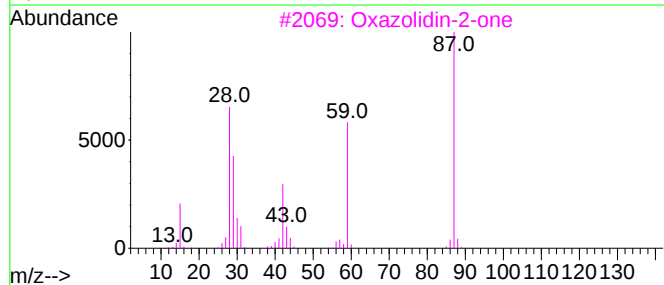
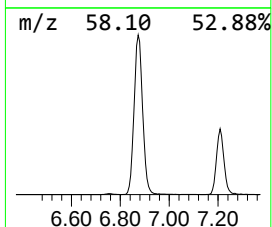
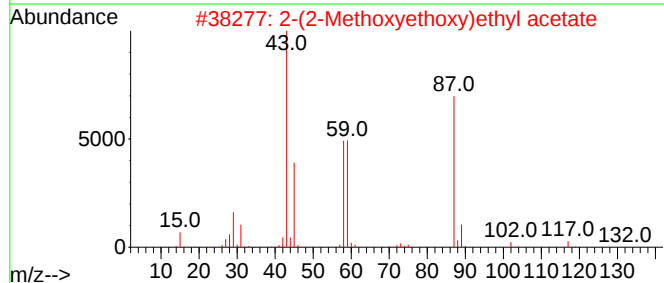
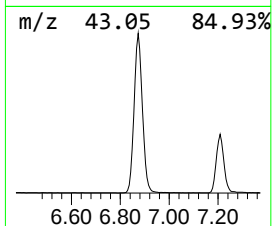
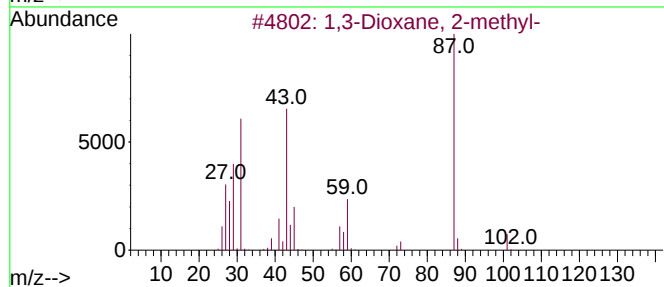
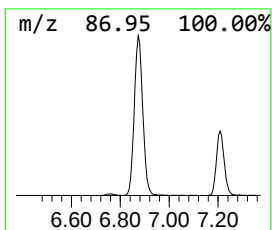
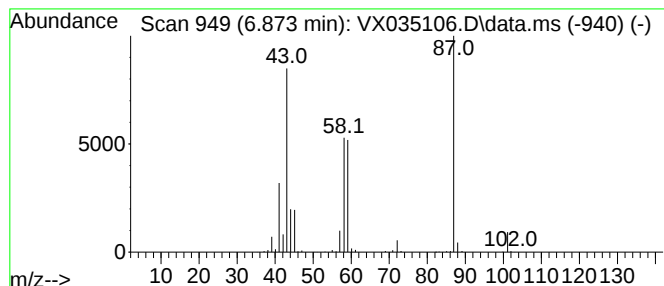
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Peak Number 3 unknown6.873 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	82.10 ug/l	1977220	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	42
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	38
3			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	32
4			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	28
5			Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	27



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Instrument :
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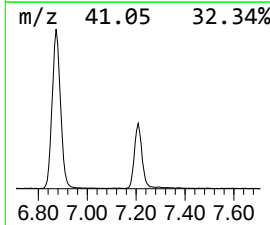
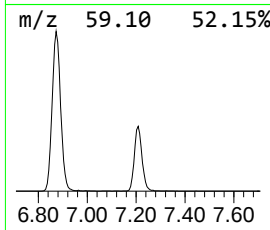
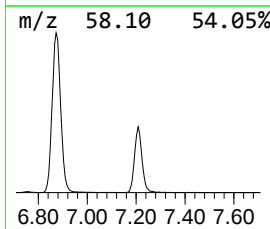
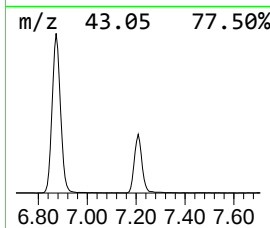
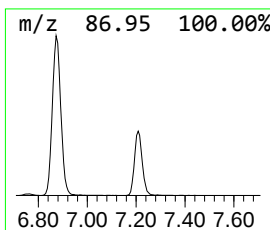
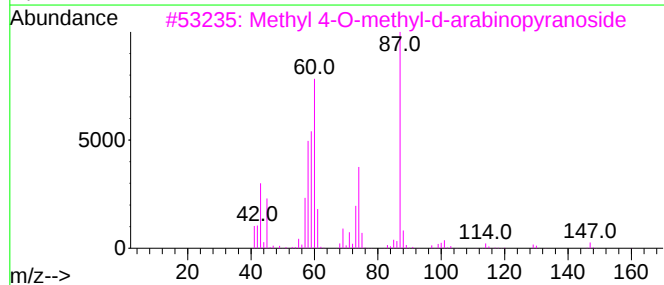
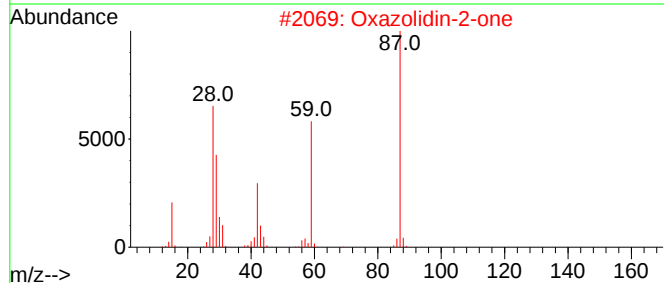
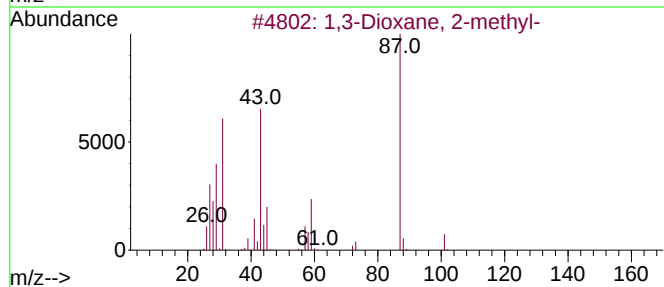
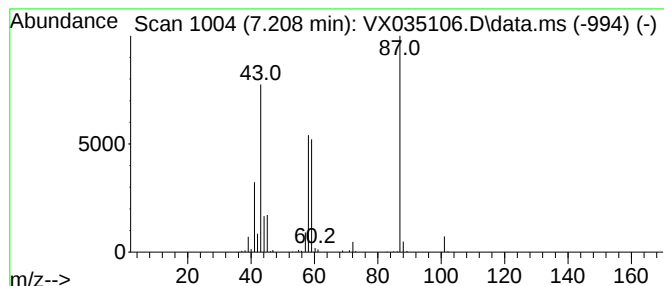
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	29.23 ug/l	703824	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	59
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
3			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	36
4			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	33
5			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.617	9.5	ug/l	173201	1	5.550	909926	50.0
1-Propanol, 2-m...	6.147	16.3	ug/l	296202	1	5.550	909926	50.0
unknown6.873	6.873	82.1	ug/l	1977220	2	6.757	1204100	50.0
1,3-Dioxane, 2-...	7.208	29.2	ug/l	703824	2	6.757	1204100	50.0