

MatLab ROI-MCR-ALS Cheat Sheet

Parameter Tests:

```
[TestPeak,TestTime] = LoadTestData  
  
[MSroi_test,mzroi_test,Times] = TestROI(TestPeak,TestTime)  
  
MSroiBaseCorr=TestBaseCorrect (MSroi_test,Times)  
  
MSroiSmooth=TestGolaySmooth (MSroiBaseCorr,Times)
```

ROI:

```
[MSroi_end,mzroi_end,time_end,nRows,Parameters] = ROIprocess
```

When running into out of memory error:

```
[MSroi_end,mzroi_end,time_end,nRows,Parameters] = seqROIprocess
```

MCR-ALS:

Run mcr_main.m

Output Table:

```
ReportTable = MCRout (copt,sopt,mzroi_end,time_end,nRows,Parameters)
```

Check Correlation between each Average Concentration Profile and main mz EIC for all Components:

```
[EICs,ReportTable]=CheckConcProfiles (ReportTable,Parameters)
```

Plot Correlation of Component and EIC for selected Components:

```
PlotProfileCheck (EICs,ReportTable)
```

Evaluate Database MS1 Search:

Databank Results must be comma separated List

```
ReportTable=evalDatabaseQuery (ReportTable)
```

Find MS2 Spectra:

```
ReportTable = extractMSMS (ReportTable,Parameters)
```

Compare to Suspect List:

```
ReportTable = compare2suspects (ReportTable,Parameters)
```