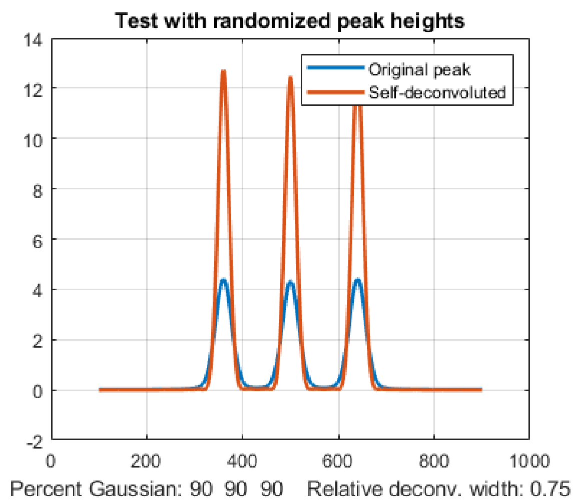
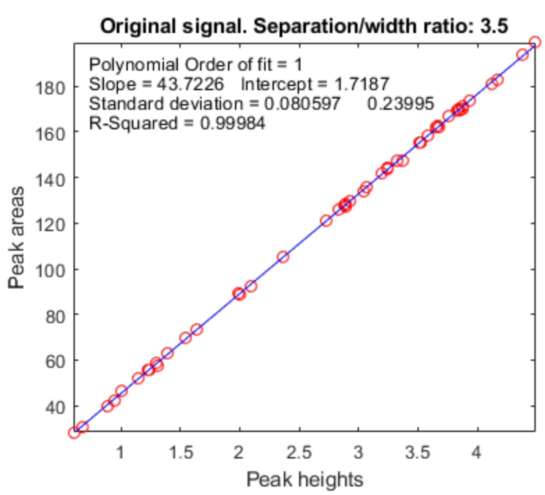
Area measurements with randomized peak heights with equal widths

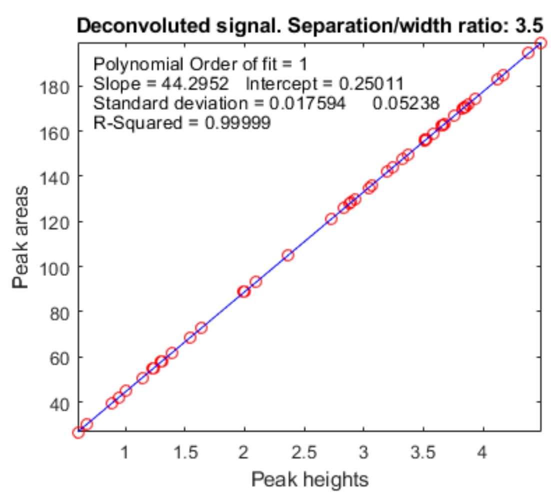
In the following simulations, the areas of a group of three partially overlapping peaks is measured, by the perpendicular drop method, before and after peak sharpening by Fourier self-deconvolution. The measurements are repeated with random peak heights from 0.5 to 4.5, to test how the peak overlap interferes with precise area measurement. Sixteen trials with randomized peak heights, the true peak area are plotted against the measured areas, and the R2 for each case are compared before and after deconvolution. Link to Matlab script: GLSDPerpDropDemo16.m. Conclusion: in every case, from the “easiest” to the most challenging, deconvolution yields the best results.

Test 1: Well-separated Gaussian peaks work well with or without deconvolution

90% Gaussian peaks; positions =360 500 640; SeparationWidthRatio =**3.5**
MeanPercentErrorOfMeasuredAreas = 0.9419 1.3087 0.6015
PRSDPercentErrorOfMeasuredAreas -2.5021 -6.0390 -5.4700
MeanErrorsOfDeconvolutedAreas = 0.1377 0.1391 0.1098
PRSDPercentErrorsOfDeconvolutedAreas =- 1.3568 -1.0600 2.9387
AccuracyImprovementFactor = 7.2412

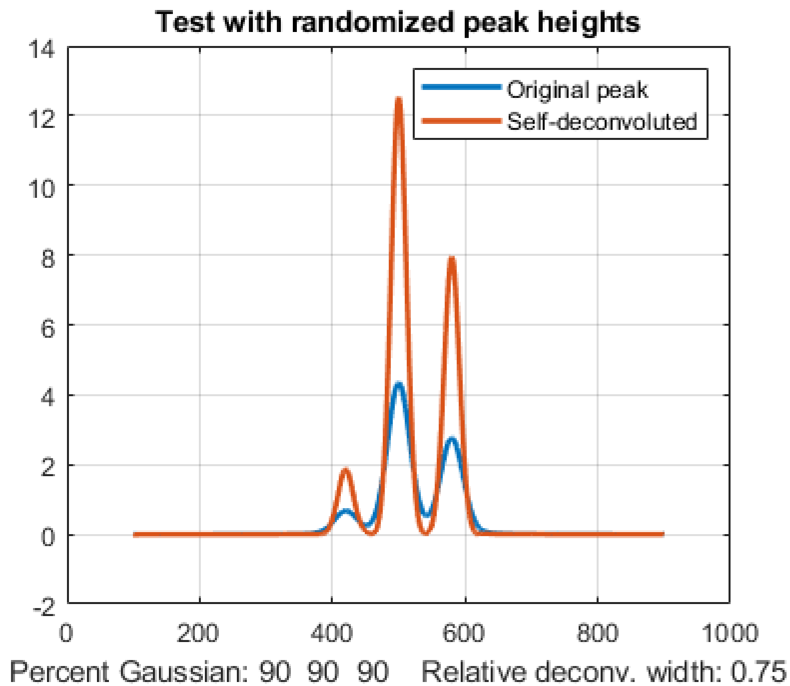


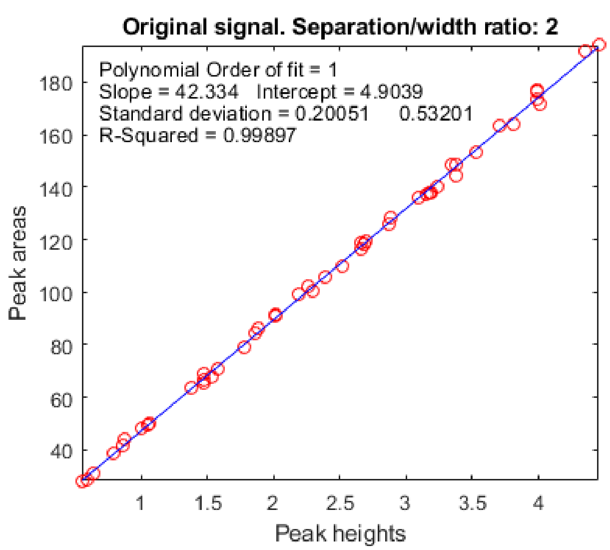


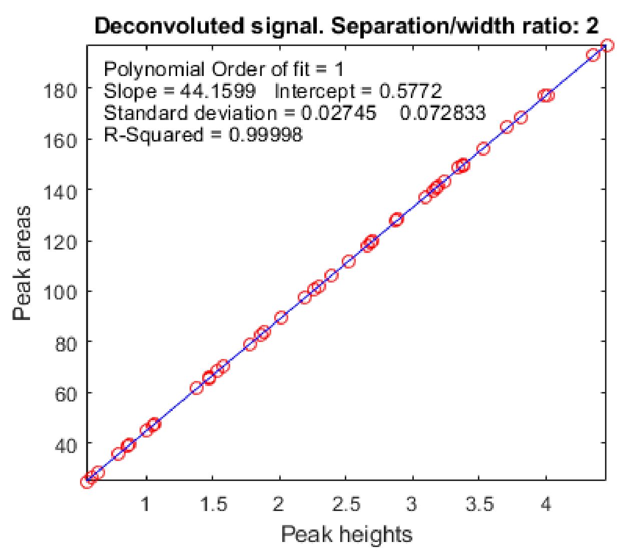


Test 2: For slightly-overlapped peaks, deconvolution yields baseline resolution, better results.

positions =420   500   580
SeparationWidthRatio =**2**
MeanPercentErrorOfMeasuredAreas =4.1019   3.1636   2.8436
PRSDPercentErrorOfMeasuredAreas =-1.3072   4.4501   -1.9798
MeanErrorsOfDeconvolutedAreas =0.5096   0.4006   0.3542
PRSDPercentErrorsOfDeconvolutedAreas =-1.2460   3.7374   -1.7393
AccuracyImprovementFactor =7.9922







Test 3: More-overlapped peaks work better with deconvolution

positions =430   500   570

SeparationWidthRatio =**1.75**

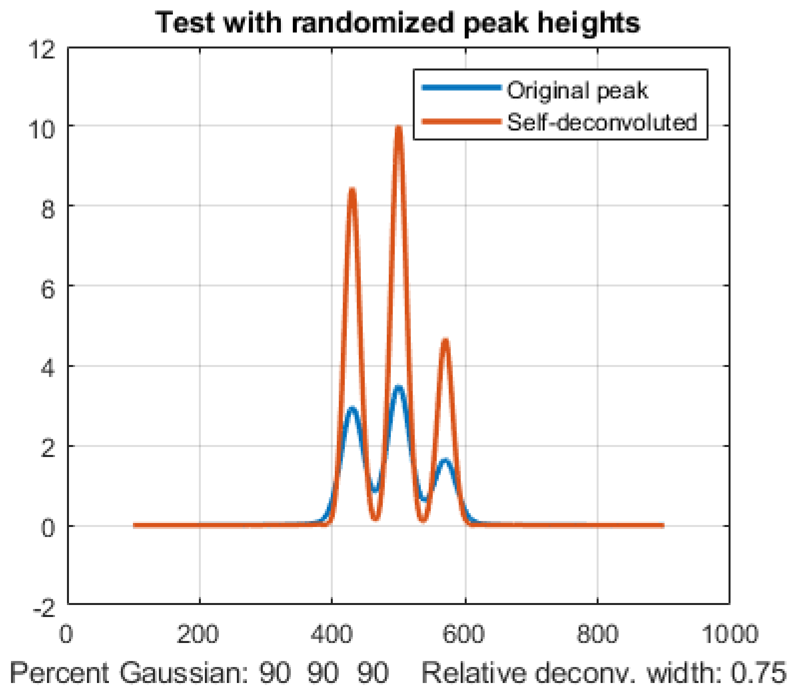
MeanPercentErrorOfMeasuredAreas =1.9730   3.1958   3.4725

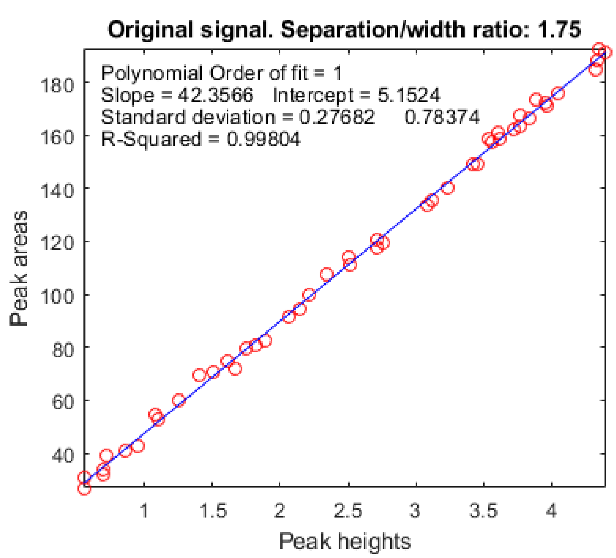
PRSDPercentErrorOfMeasuredAreas =-5.6076 -12.8715   -1.8906

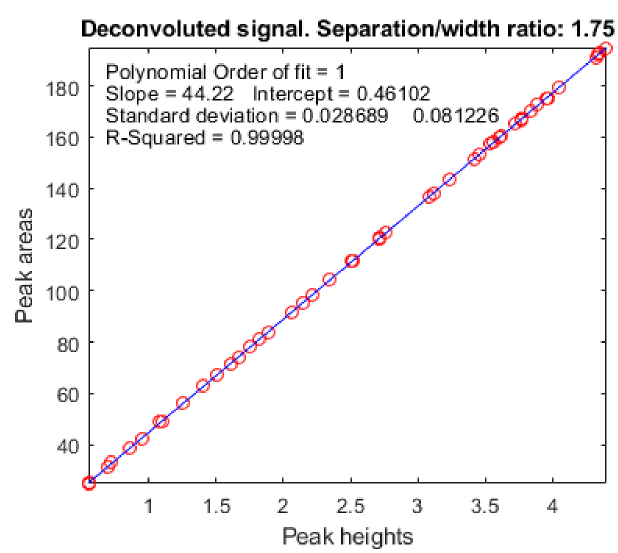
MeanErrorsOfDeconvolutedAreas =0.1963   0.3229   0.3720

PRSDPercentErrorsOfDeconvolutedAreas =-3.1952   7.5383   -1.6257

AccuracyImprovementFactor =9.7603

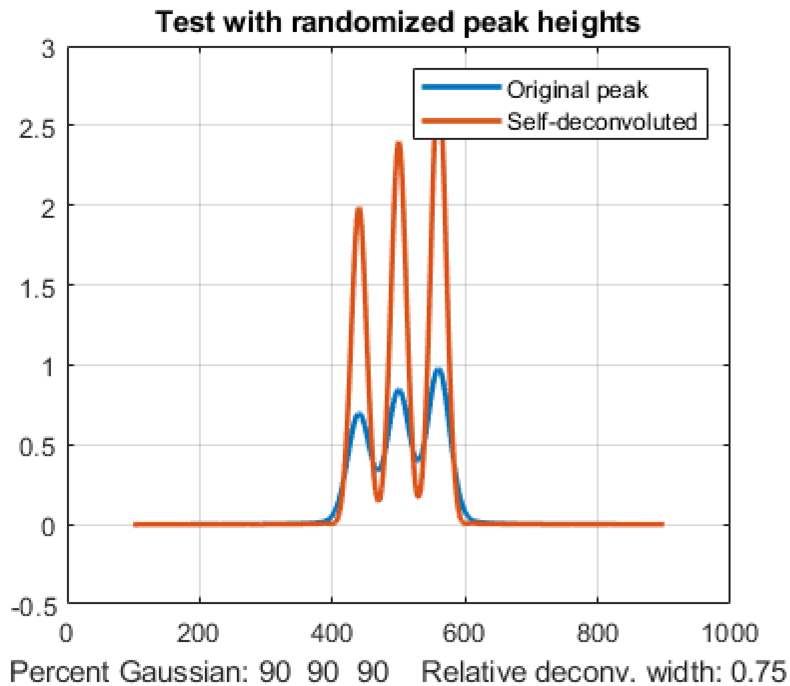


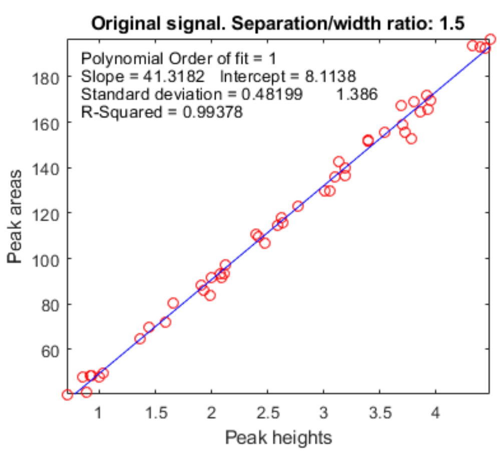


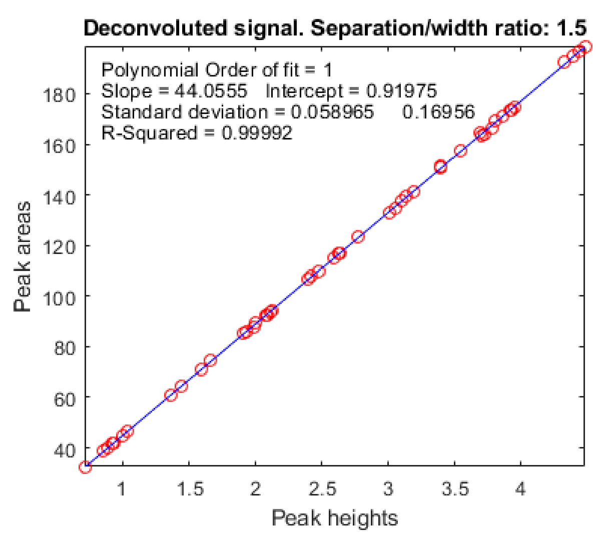


Test 4: Heavily-overlapped peaks work significantly better with deconvolution

positions =440 500 560
SeparationWidthRatio =**1.5**
MeanPercentErrorOfMeasuredAreas =4.0260 9.2013 3.6862
PRSDPercentErrorOfMeasuredAreas =-2.9061 -2.2265 -7.6087
MeanErrorsOfDeconvolutedAreas =0.4809 1.0074 0.4135
PRSDPercentErrorsOfDeconvolutedAreas =-2.2622 -2.6433 -5.3338
AccuracyImprovementFactor =8.8068







Test 5: Severely-merged peaks work far better with deconvolution

positions = 460   500   540

SeparationWidthRatio =**1.0**

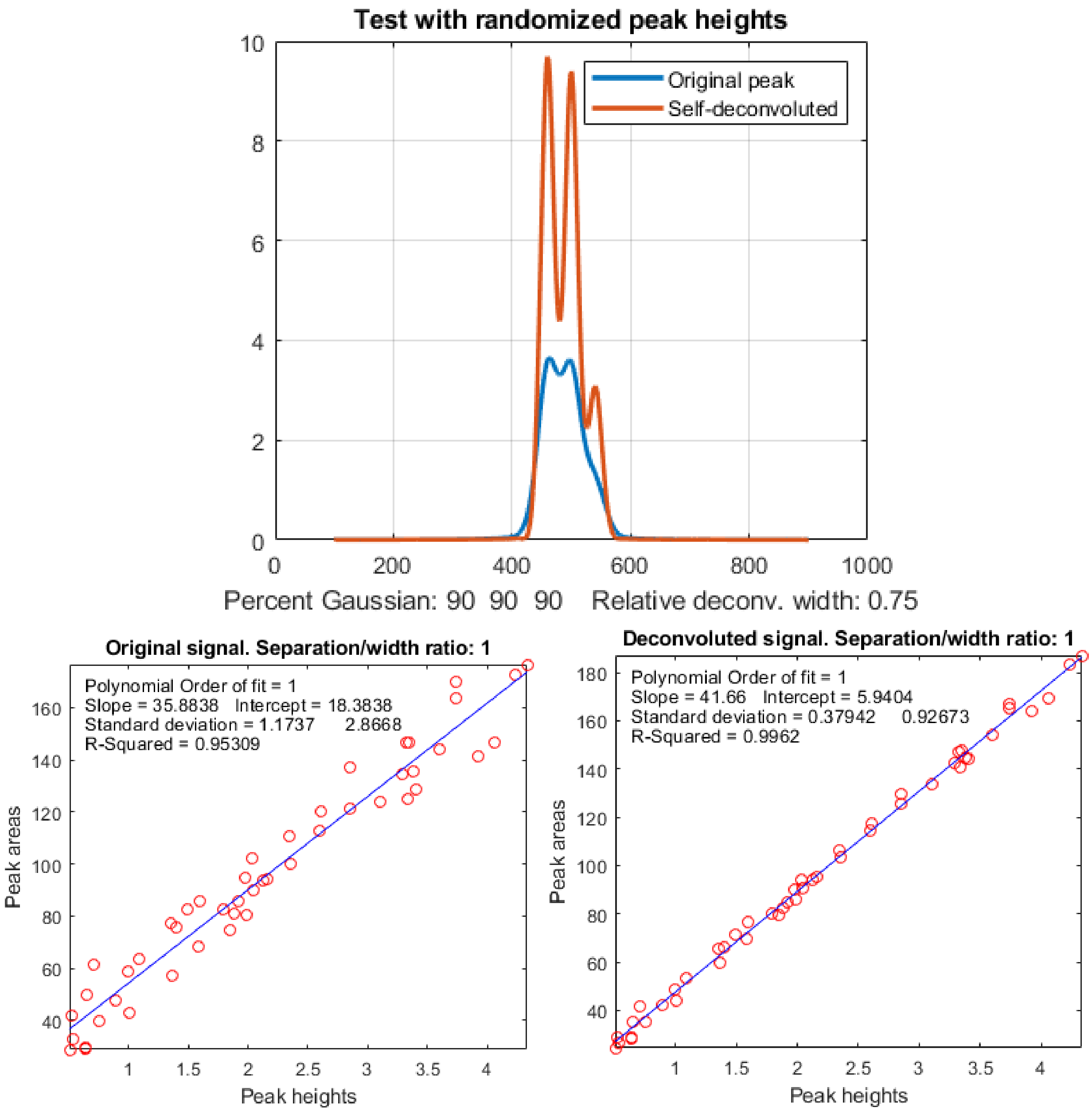
MeanPercentErrorOfMeasuredAreas =12.1553   17.4832   13.9822

PRSDPercentErrorOfMeasuredAreas =-1.7285   -4.9517   -2.5153

MeanErrorsOfDeconvolutedAreas =4.0401   5.9301   4.7017

PRSDPercentErrorsOfDeconvolutedAreas =-1.6747   -3.9970   -2.4296

AccuracyImprovementFactor =2.9769



Test 6: Well-separated Lorentzian peaks still interact slightly, but even then deconvolution is better.

90% Lorentzian (10% Gaussian) peaks

positions =360   500   640

SeparationWidthRatio =**3.5**

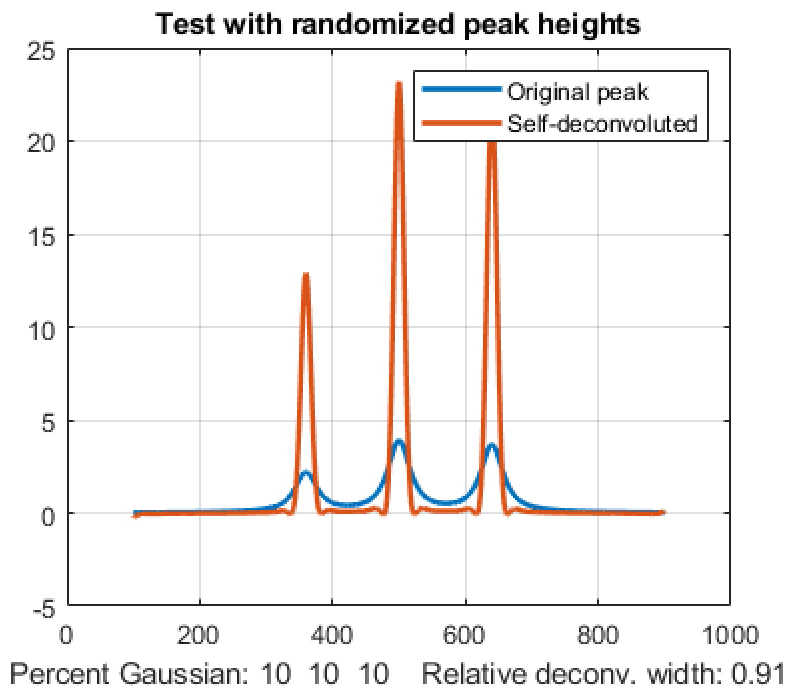
MeanPercentErrorOfMeasuredAreas =4.5783   6.6357   9.9925

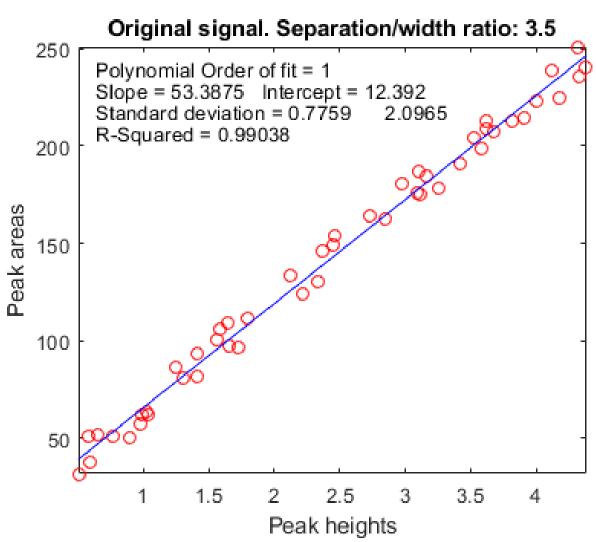
PRSDPercentErrorOfMeasuredAreas =-2.1666   2.7683   -1.7190

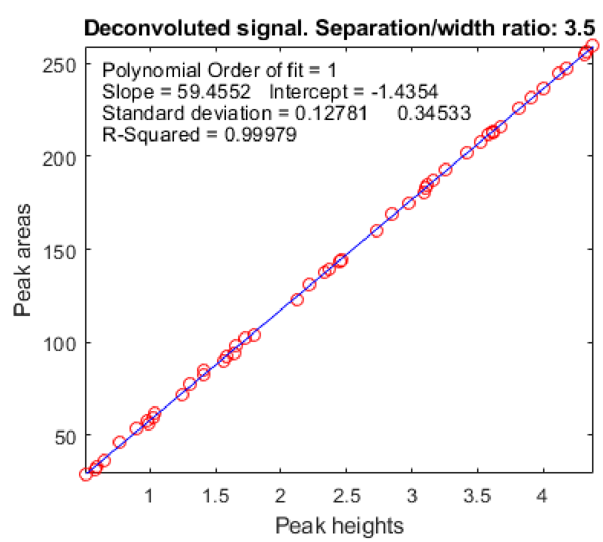
MeanErrorsOfDeconvolutedAreas =0.9209   0.6279   1.7969

PRSDPercentErrorsOfDeconvolutedAreas =3.1201   -0.9316   1.6664

AccuracyImprovementFactor =7.0335







Test 7 With more overlap, the deconvolution method is far better.

90% Lorentzian (10% Gaussian) peaks

positions =420   500   580

SeparationWidthRatio =**2.0**

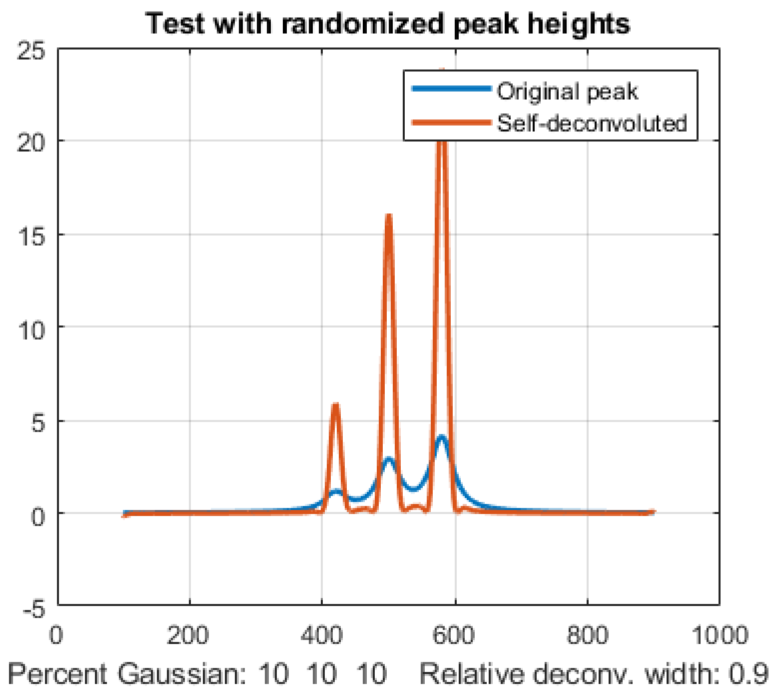
MeanPercentErrorOfMeasuredAreas =13.7536   19.6947   6.7218

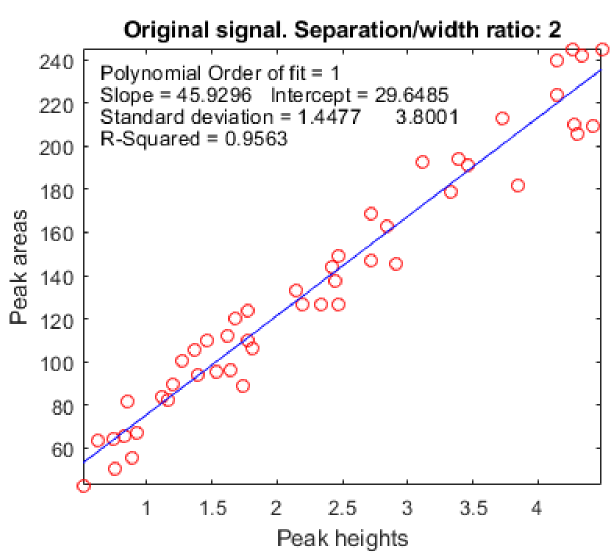
PRSDPercentErrorOfMeasuredAreas =-1.7772   -3.2485 -16.2214

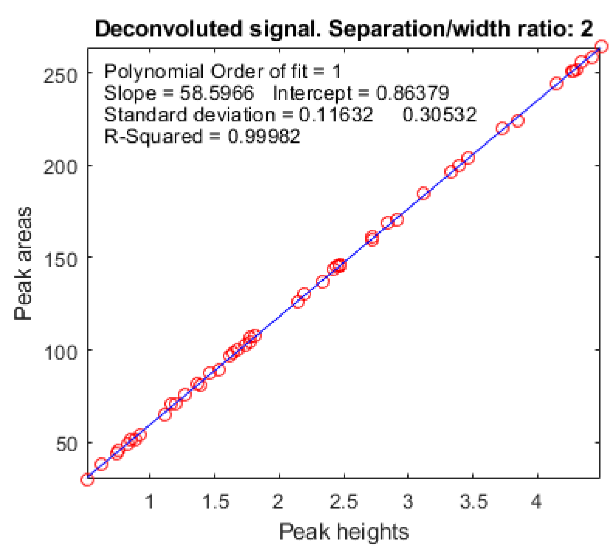
MeanErrorsOfDeconvolutedAreas = 0.6554   2.4280   0.5624

PRSDPercentErrorsOfDeconvolutedAreas =3.7026   -1.5151   3.8531

AccuracyImprovementFactor =13.6825







Test 8: Even closer spacing, deconvolution method achieves flat baseline between peaks.

90% Lorentzian (10% Gaussian) peaks

positions =440   500   560

SeparationWidthRatio =**1.5**

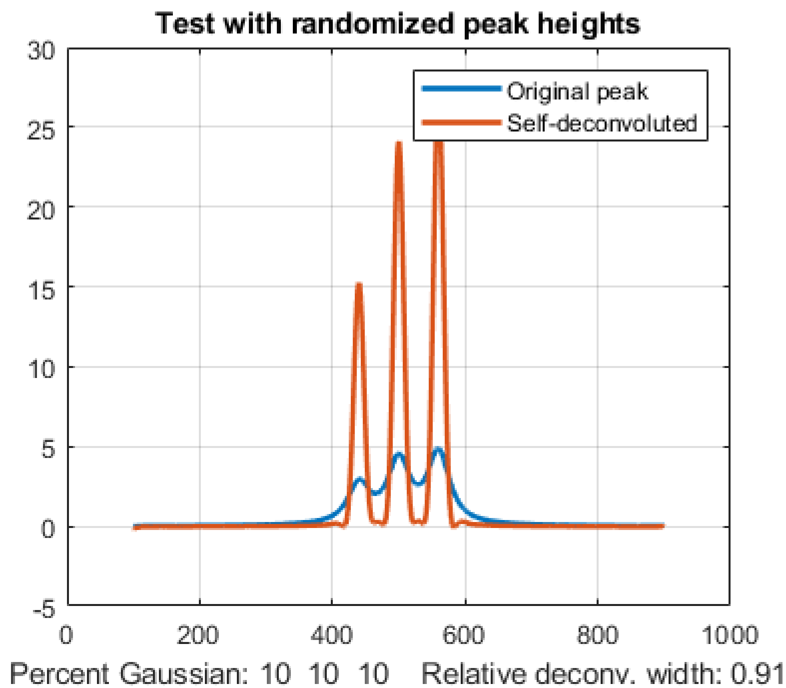
MeanPercentErrorOfMeasuredAreas =14.4434   19.3372   8.5846

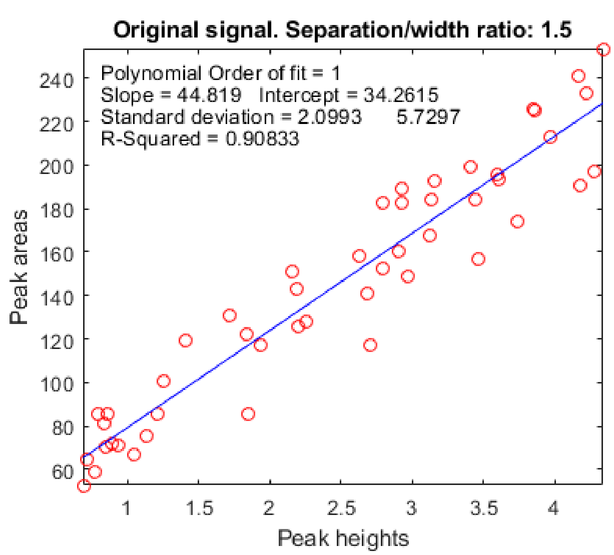
PRSDPercentErrorOfMeasuredAreas = -1.7901   -5.2272   -5.9883

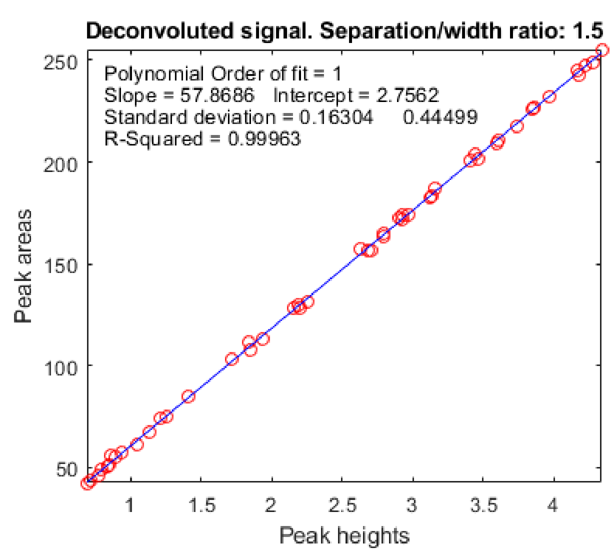
MeanErrorsOfDeconvolutedAreas =0.6605   2.2794   0.4722

PRSDPercentErrorsOfDeconvolutedAreas = 9.3058   -1.8957   2.6210

AccuracyImprovementFactor = 16.1773







Test 9: Even closer spacing; deconvolution method still achieves baseline resolution

90% Lorentzian (10% Gaussian) peaks

positions =450 500 550

SeparationWidthRatio =**1.25**

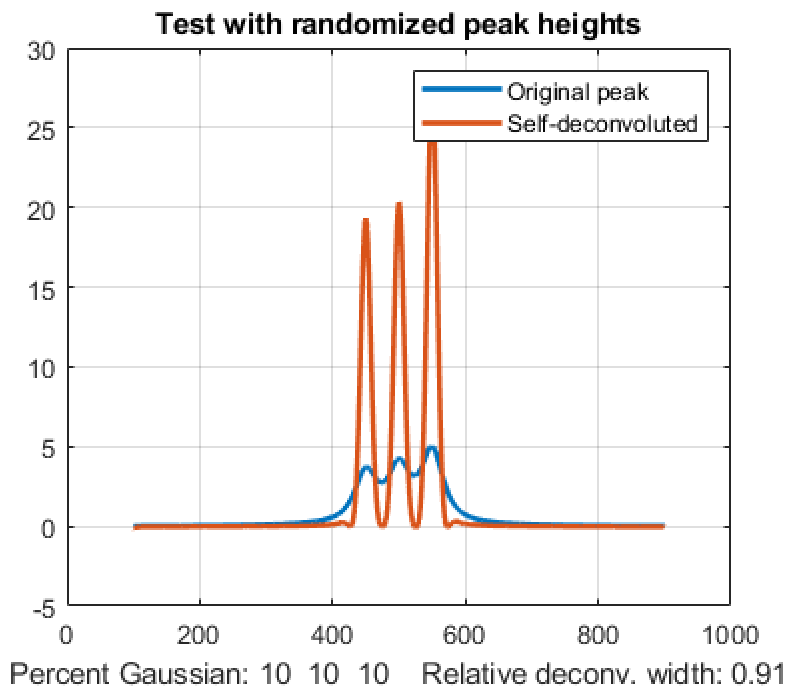
MeanPercentErrorOfMeasuredAreas = 24.0318 16.2420 32.2423

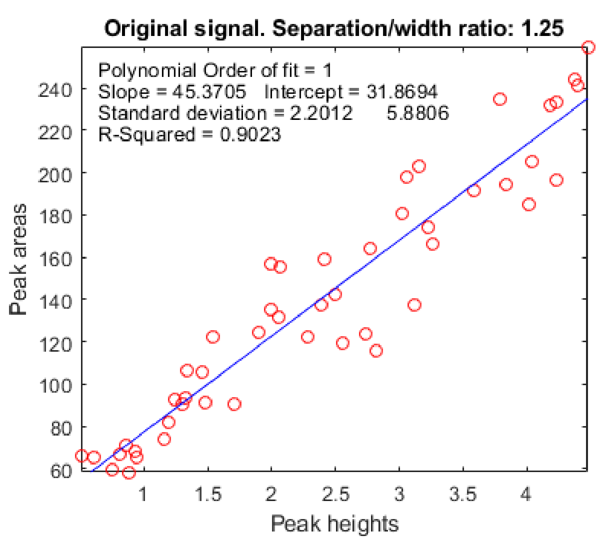
PRSDPercentErrorOfMeasuredAreas = -1.4414 0.7382 -1.5508

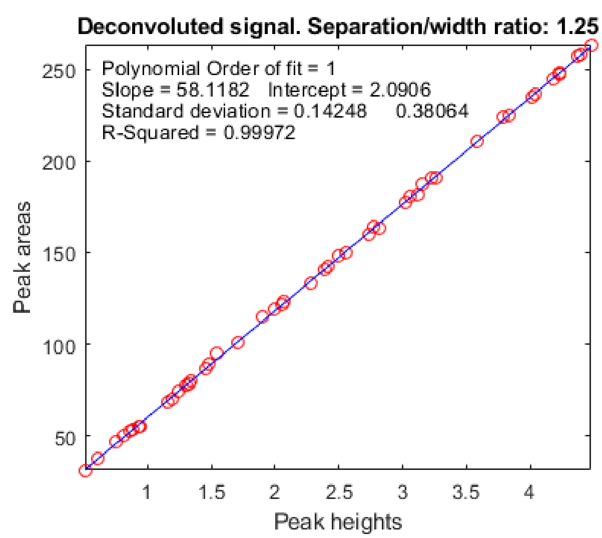
MeanErrorsOfDeconvolutedAreas =1.0915 0.8485 1.5102

PRSDPercentErrorsOfDeconvolutedAreas = -1.8925 2.6568 -1.6747

AccuracyImprovementFactor = 20.8365







Test 10: With extreme overlap, deconvolution method nearly achieves baseline resolution

positions =460   500   540

SeparationWidthRatio = **1.0**

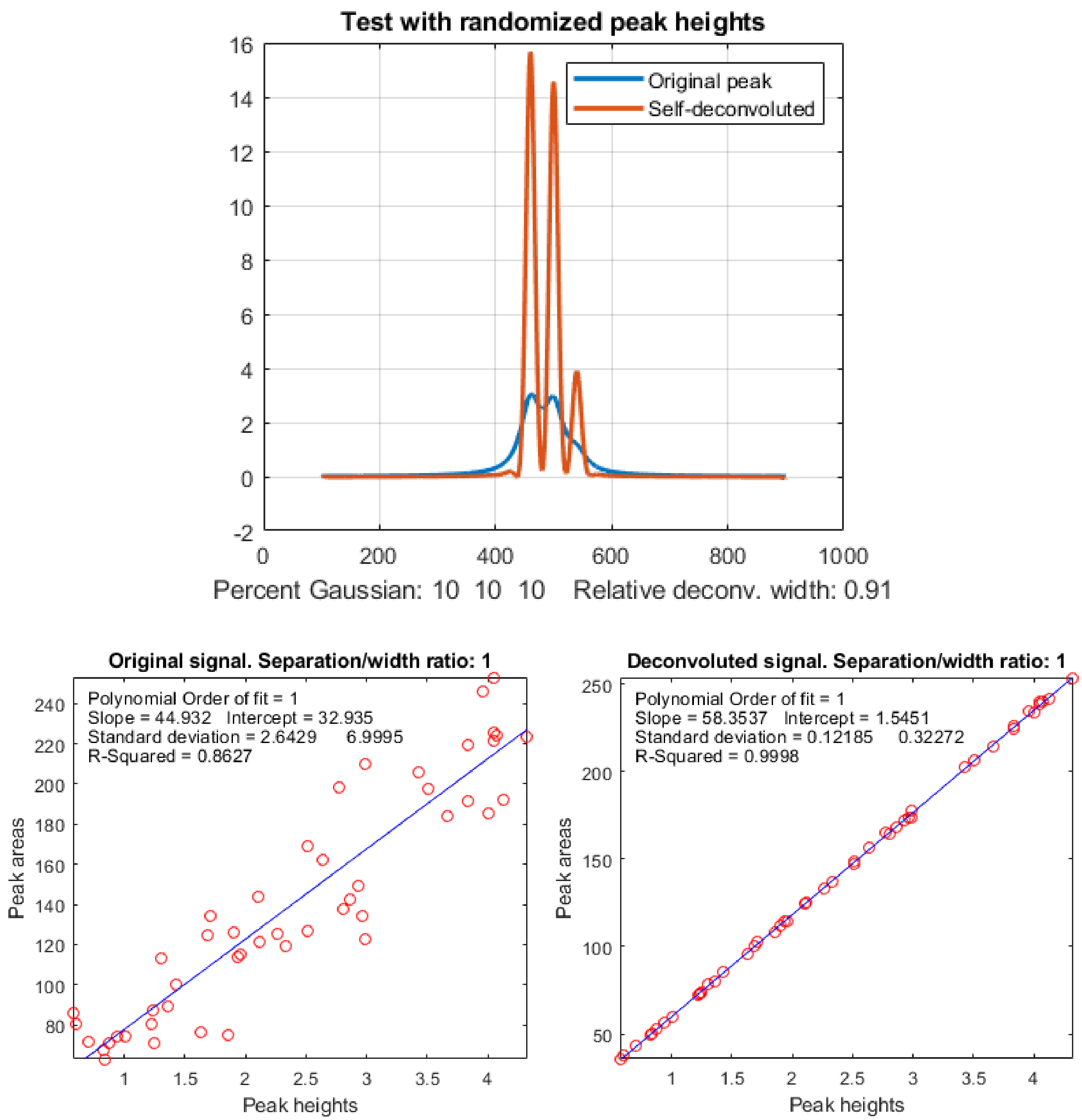
MeanPercentErrorOfMeasuredAreas = 22.0323   26.4398   24.1916

PRSDPercentErrorOfMeasuredAreas = -2.6072 -13.0751   -1.6612

MeanErrorsOfDeconvolutedAreas = 1.0100   1.6524   0.8971

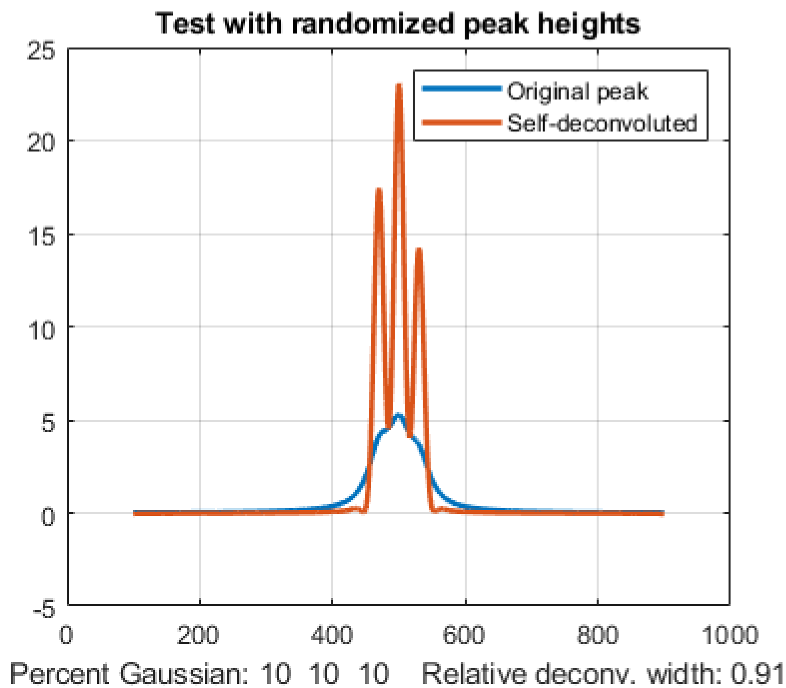
PRSDPercentErrorsOfDeconvolutedAreas = -2.9719   -3.3261   -2.0592

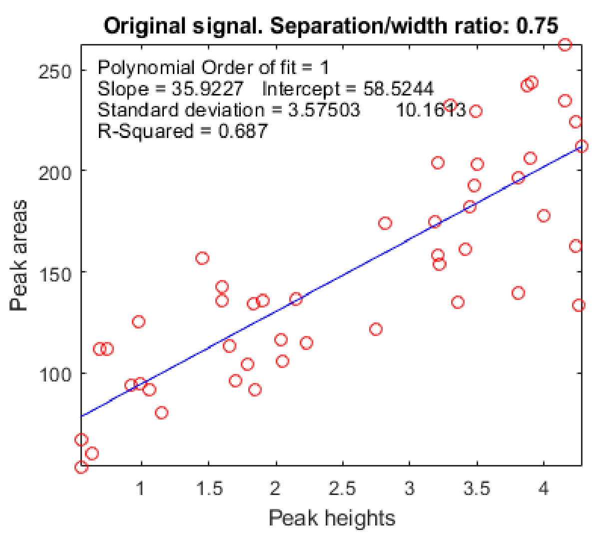
AccuracyImprovementFactor =21.5936

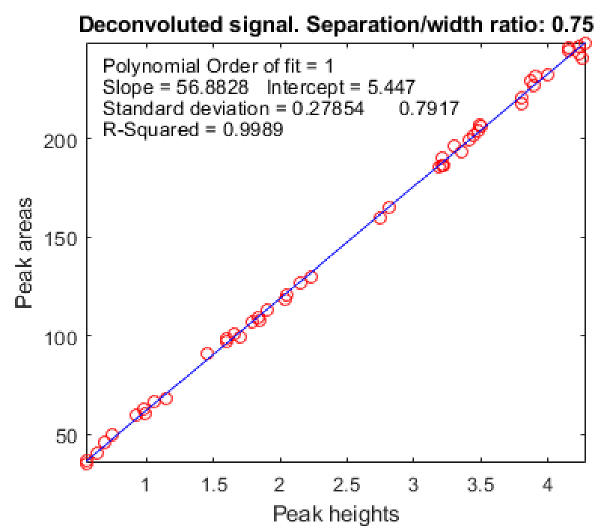


Test 11: When peaks merge into a blob with bumps: deconvolution method still works well.

positions =470   500   530
SeparationWidthRatio =**0.75**
MeanPercentErrorOfMeasuredAreas =17.0494   37.3584   31.3426
PRSDPercentErrorOfMeasuredAreas =-2.3349 110.2535   -1.6326
MeanErrorsOfDeconvolutedAreas = 1.3488   3.8740   2.4266
PRSDPercentErrorsOfDeconvolutedAreas =-3.2312   -5.1943   -1.8989
AccuracyImprovementFactor = 11.7332







Test 12: If peaks fuse into one peak, even the deconvolution method performs poorly.

positions =480 500 520
SeparationWidthRatio =**0.5**
MeanPercentErrorOfMeasuredAreas =47.2747 44.7142 29.4886
PRSDPercentErrorOfMeasuredAreas =-1.4058 8.3318 -1.8355
MeanErrorsOfDeconvolutedAreas = 9.1199 15.4335 5.7621
PRSDPercentErrorsOfDeconvolutedAreas =-1.9862 -3.4480 -3.7076
AccuracyImprovementFactor =4.3995