

<b>MetAssimulo</b>	<b>SimulateSpectrum</b>	<b>readParamFile</b>	Read in Parameters when run in 'batch mode'.		
		<b>SetUpPeakShiftInput</b>	Read in peak shift data and convert to NSSD names	<b>Converter</b>	
		<b>PeakShiftInput</b>	Read in peak shift data		
		<b>ReadInConcs</b>	Read in Concentration data		
		<b>MainConverter</b>	Convert synonyms to NSSD names	<b>Converter</b>	
		<b>SimulationOfConcs</b>	Simulate Concentrations	<b>NormalDisCDF</b>	
				<b>InverseNormalDis</b>	
		<b>CorrConcs</b>	Simulate Correlated Concentrations	<b>SimulationOfConcs</b>	Sim uncorrelated metabolites
				<b>SimCorrelated</b>	Sim correlated metabolites
		<b>ReadInExp</b>	Read in Experiment #		
		<b>ReadInProtons</b>	Read in Proton data		
		<b>RemoveWaterAndStandard</b>	Pre-Processing	Set Exclusion Regions to zero	
		<b>BaselineCorrectionWithSplines</b>		Correct baseline using splines	
		<b>RemoveArtifacts</b>		Remove negative artifacts	
		<b>KernelSmootherFinal</b>		Kernel Smoother	
		<b>SimulateSpectrumWithShift</b>	Construct final spectrum with peak shift	<b>PeakDetection</b>	Detect peaks and identify multiplets
				<b>FinalSpectrumShift</b>	Calculate shift
		<b>FinalSpectrumNoShift</b>	Construct final spectrum	<b>KernelSmoothThresh</b>	Smooth spectrum
		<b>Display Results</b>	Display Results		

SynonymConverter

SynonymConverter

Cov_Matrix	Calculate Covariance Matrix
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IndivPeakDetection	Find Peaks	IndivPeakSetBoundaries	Find Peak edges
FindingPeaksToShiftTogether	Find multiplet peaks	FindCorrespondingPeaks	Link multiplet peaks together
GenerateAcidBaseLimits2	Generate AB Limits		
CalculateShift			
KernelSmoothThresh	Smooth spectrum	conv_fft	Convolution using FFT method
conv_fft	Convolution using FFT method		