Simulation data set has 25 groups of data. Each group consists of 100 spectra. Real data has 8 groups of data, Each group consists of 25 spectra. Please refer to http://bioinformatics.ust.hk/MSPeakComparison.html for more information.

Part one: parameters

Program Name	Parameters Names In Package
CWT	peakScaleRange,snr and amp.Th
PROcess	snr,area and ratio
LIMPIC	factor, mz_block, iupac_thres and peak_width
LMS	neighbor_size and scale_thres
Cromwell	waveletThreshold

Part two: parameter values

*MassSpecWavelet parameters:
peakScaleRange=[2, 4, 6];
snr=[1, 3, 5];
amp.Th=[0.0001, 0.01, 0.1]

*PROcess parameters:
snr=[1, 3, 5];
area=[0.3, 0.003, 0.0003];
ratio=[0.001, 0.01, 0.1, 0.5]

*LIMPIC parameters:
factor=[10, 20, 30, 40];
mz_block=[50, 100, 150, 200];

iupac_thres=[3, 5, 7];
peak_width=[0.5, 1, 2];

*Local maximum search:
When data resolution is low (e.g. When most intervals between two adjacent points are around 1Da to 3Da), the neighborhood is set as around 15Da. the neighbor_size in the unit of points is determined as 15/1 = 15 points, scale_thres is set as 5.
In experiment:
neighbor_size = [1, 4, 8, 12, 16, 20, 26, 30];
scale_thres = [1, 3, 5, 7, 9]

When data resolution is high (e.g. When most intervals between two adjacent points are around 0.02Da), the same neighbor_size of 15Da will result in different number of points: 15/0.02=750 points
In experiment:
neighbor_size=[70, 100, 150, 300, 450, 600, 850, 1240]
scale_thres=[8, 12, 16, 10, 24]

*Cromwell
Similar argument as in *Local maximum search
When data resolution is low, wavelet threshold is set as around 15,
In experiment:
waveletThreshold=4:2:30

When data resolution is high, wavelet threshold is set as around 750,
In experiment:
waveletThreshold=[60, 100, 300, 400, 600, 700, 900, 1000, 1200, 1400, 1800];

Part three: parameters for obtaining the best F1 measure

In our paper, we use a method similar to ROC curve to measure the overall performance for each algorithm. And we use F1 measure to obtain a best compromise between false

discovery rate and sensitivity. We also test peak detection precision for each algorithm with its best parameter combination.

	Using Simulation Data			U
Program Name	Parameter Values	The number of times to generate maximal F1 (Total number is 2500)	Median m/z error	Paramete
CWT	[peakScaleRange,snr,amp.Th]= [2,1,0.01]	1068	0.32 %	[peakScaleRange,sn 0.1]
PROcess	[snr,area,ratio]=[1,0.003,0.01]	632	0.35 %	[snr,area,ratio]=[1,0
LIMPIC	[factor,mz_block,iupac_thres,peak_width]= [40,50,3,0.5]	306	0.40 %	[factor,mz_block,iupa h]= [10,50,7,0.5]
LMS	[neighbor_size,scale_thres] = [8,5]	1471	0.52 %	[neighbor_size,scale_
Cromwell	waveletThreshold=30	2050	0.40 %	waveletThreshold=1