

## Testfile\_rdata

properties	values
Number of m/z features	10111
Range of m/z values	1000.02 – 1199.99
Number of pixels	20
Range of x coordinates	1 – 20
Range of y coordinates	1 – 1
Range of intensities	0 – 0
Number of NA intensities	0
Number of Inf intensities	0
Number of duplicated coordinates	0
Median of intensities	0
Intensities > 0	0 %
Number of empty spectra	20
Median TIC $\pm$ sd	0 $\pm$ 0
Median # peaks per spectrum $\pm$ sd	0 $\pm$ 0
maximum m/z window size	0.02
Centroided	TRUE
input m/z (#valid/#input) in inputcalibrantfile2.txt	1 / 3