Supplementary material

Optimization of Resolving Power, fragmentation and mass calibration in an Orbitrap Spectrometer for analysis of 24 pesticide metabolites in urine

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Table SI.1. Scheme of the Resolving power optimization study

Ionization mode	ESI NEG			ESI POS		
Resolving power (FWHM)	**10,000**	**25,000**	**50,000**	**10,000**	**25,000**	**50,000**
Nº aliquotes (spiked urine) injected[a]	6	6	6	6	6	6
Nº acquisitions non-applying fragmentation[a] (diagnostic ions)	6	6	6	6	6	6
Nº acquisitions applying fragmentation (HCD 20 eV)[a] (fragment ions)	6	6	6	6	6	6

[a]Each injection allowed both "applying fragmentation" and "non-applying fragmentation" acquisitions quasi-simultaneously

Total ions

□ [100-80]%   ■ < 80%

Diagnostic ions

□ [100-80]%   ■ < 80%

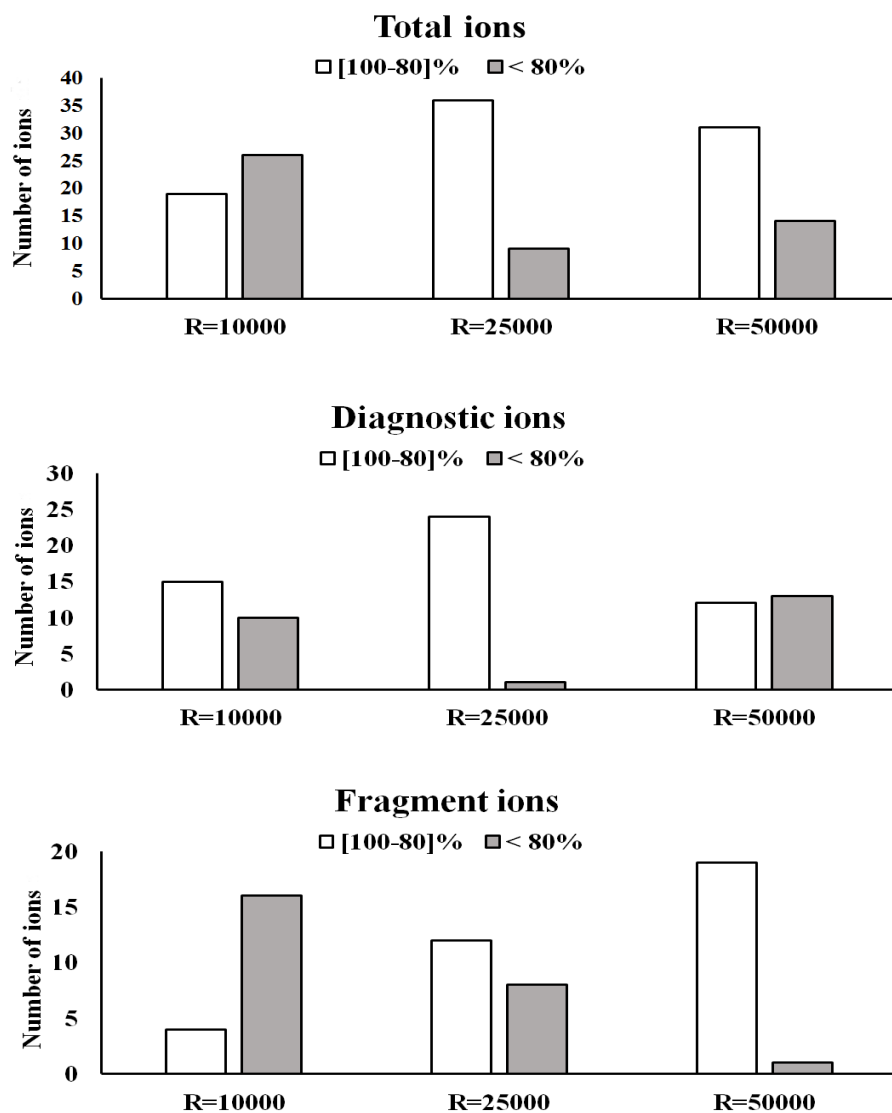## Fragment ions

□ [100-80]%   ■ < 80%

Figure SI.1. Number of ions with high ([100-80]%) and low (<80%) peak areas at R=10,000, R=25,000 and R=50,000 (FWHM), for total, diagnostic and fragment ions. The percentage (%) is calculated dividing the area of an ion by the highest area obtained for that ion and multiplying by 100.