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A Novel Approach for Computing Cross-Sections in Ion-Mobility Measurements LUCA LARINI, OSCAR MARIN, Rutgers University - Camden — Mass spectrometry allows the identification of molecules based on their mass to charge ratio. One of the advantages of this technique is that it is able to distinguish molecules that differ for a small value of the mass. In addition, once the molecule of interest has been selected by the mass spectrometer, it can be further analyzed in an ion mobility tube that can characterize the conformations adopted by the molecule. This is extremely useful when dealing with unstructured proteins that populate multiple conformations. However, ion mobility distinguishes structures based on their cross-section. In order to associate a well-defined tridimensional structure to a specific cross-section, molecular dynamics simulations must be performed first, and then the theoretical cross-section compared to the experimental one. Computing a cross-section starting from molecular dynamics data is extremely computationally expensive. For this reason, we have developed a software that takes advantage on the multicore and multimode architecture of modern computer clusters.

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