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De-Novo Structural Elucidation from Mass/NMR Spectra

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Abstract : The structure elucidation based on Mass Spectra (MS) data of unknown substances is an unresolved problem that affects many different fields of application. The recent overview of software available for structure elucidation of small molecules has shown the demand for efficient computational tool that will be able to perform structure elucidation of unknown small molecules and peptides. We developed an algorithm for De-Novo fragment analysis based on MS data that proposes a set of scored and ranked structures that are compatible with the MS and MSMS spectra. Several different algorithms were developed depending on the initial set of fragments and the structure building processes. Also, in all cases, several scores for the final molecule ranking were computed. They were validated with small and middle databases (DB) with the eleven test set compounds. Similar results were obtained from any of the databases that contained the fragments of the expected compound. We presented an algorithm. Or De-Novo fragment analysis based on only mass spectrometry (MS) data only that proposed a set of scored/ranked structures that was validated on different types of databases and showed good results as proof of concept. Moreover, the solutions proposed by Mass Spectrometry were submitted to the prediction of NMR spectra in order to elucidate which of the proposed structures was compatible with the NMR spectra collected.

Keywords : De Novo, structure elucidation, mass spectrometry, NMR
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