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ACCEPTED MANUSCRIPT

Negative mode MS/MS to read digital information encoded in sequence-defined oligo(urethane)s: a mechanistic study

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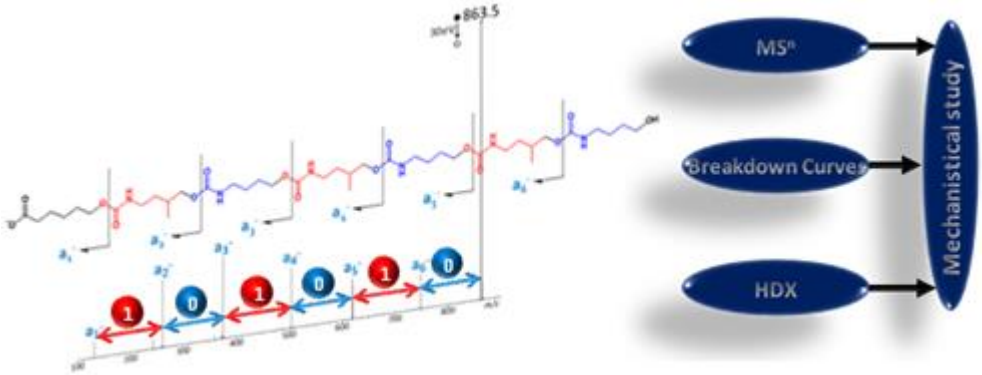
Running title: MS/MS of deprotonated sequence-controlled polyurethanes

Graphical Abstract



Highlights

- ► Small polyurethanes (PUs) were studied to anticipate MS/MS behavior of long chains
- ► Three mechanisms were evidenced for O–(CO)NH bond cleavage in deprotonated PUs
- ► Main issue with long chains was not related to CID but to negative mode ESI yield
- ► A new design of PU end-groups allowed this sensitivity issue to be addressed

Abstract

MS/MS sequencing is an unrivaled technique to decipher binary information chemically encoded in the backbone of sequence-controlled synthetic polymers constructed with two co-monomers of different mass, arbitrarily designated as the 0- and 1-bit of the ASCII alphabet. Efficiency of this "reading" step relies however on the simplicity of MS/MS patterns, which

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