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A COMPUTATIONAL APPROACH OF THE CONCEPT OF SAFE BY DESIGN. APPLICATION FOR CHITIN AND CHITOSAN OLIGOMERS

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ABSTRACT

The concept of safe by design can be addressed using computational studies. The bases of computational approaches concerning the design of safe biomaterials are explained within this study. Furthermore, these approaches are applied for predicting the pharmacokinetics properties and toxicological endpoints of chitin and chitosan oligomers.

Keywords: safe by design, computational approach, chitin oligomers, chitosan oligomers.

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