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Séminaire :

**«Computer-aided rational
design of new biological catalysts.»**

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Two main strategies have raised in recent years in order to improve the catalytic power of catalytic antibodies (CA), the rational design approach that consists in direct mutation of residues on selected specific positions on the active site of the protein, and directed in vitro evolution consisting of search of sequence space and iterative cycling of variation and selection, strategies that can be combined as proposed by some authors.

Here we show a computer aided rational design protocol to improve the efficiency of CAs. The information derived from Theoretical and Computational Chemistry techniques has allowed proposing mutations at the active site of several CAs, some of them never done up to now, that enhance the rate constant of the chemical step.