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Chapter 1

Working title: Calculations

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1.1 Motivation

Let us imagine two companies A and B. Both companies use very similar technical equipment to carry out a biotechnological process where a chemical reaction is catalyzed by an enzyme. Company A uses an enzyme with a rate constant $k_{\mathrm{A}} = 1000s^{-1}$ while company B uses an enzyme with $k_{\mathrm{B}} = 2000s^{-1}$. Letting all other things be equal, the process of company B will therefore only require half the time to produce one Mole of product compared to the time required for company A. Company B therefore can save energy required to heat up the reaction volume, the commercial implications of this are immediate.
The need for efficient catalysts arises from such an outline.[1] Increasing the performance of enzymes however is still far from

[1] We use the terms *enzme* and *bio-/catalyst* interchangeably.

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trivial and forms a growing body of research. What is clear though is that the development of such catalysts is costly, in terms of manpower, material and energy – if it is carried out in the laboratory. A number of companies have in fact formed around this quest: Novozymes (DK), Genzyme (US) or DSM (NL) to name but a few[1].
The laboratory costs can however be saved almost entirely if the development is carried out *in silico*.

1.2 Applications

1.3 Outlook

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