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Chapter 1

QM Calculations for Enzyme Activity Screening

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1.1 Introduction

The relevance of describing enzyme catalysis using computational chemistry methods was recently highlighted by awarding the Nobel price 2013 in Chemistry to three pioneering researchers from the field.
In this review, we will highlight recent developments, applications, techniques and methods used to understand and design enzyme catalysts.

Literature:
Fahmi Himo[**(author?)** (2)] (cluster approach), Adrian Mulholland[**(author?)** (1)] (QM/MM applications), Jan Jensen (method development), Baker/Hilvert/Houk[**(author?)** (3)](*de*

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novo design), Stewart[**(author?)** (4)] (semi-empirical methods)

1.2 Applications

1.3 Outlook

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