

## The Pilot Study

Our purpose in the pilot study is to create an ontology or ontologies and a term database for enzyme chemistry, based on available recommendations, in particular from the Gold Book and ODBMB.<sup>1,3</sup> For a start, we have chosen to work in two narrow subfields: enzyme inhibition and protein structure. By using principles of terminology we intend to avoid creating inconsistencies when expanding the ontologies. We are using the concept modelling tool i-Model from i-Term;<sup>4</sup> the system i-Term is a terminology and knowledge management system that combines facilities of a traditional term base with a concept modelling tool.

## How to Define Terms

Instead of focusing on each definition, we work according to the terminological method with the concepts in a *concept system* (an *ontology*). Therefore, we need to formalize the relations between the concepts and to introduce characteristics delimiting related concepts (*feature specifications*, consisting of *attribute-value pairs*). On the basis of these feature specifications, *subdivision criteria* are introduced, which group concepts and thereby give a good overview. These methods are described in conference proceedings referenced below.<sup>5,6</sup>

In our work, we use an iterative process: analyzing the concepts as well as placing them in draft concept systems in the form of hierarchies or networks on the basis of their characteristics, then drafting definitions, and, finally, refining concept systems as well as definitions. In this way, we arrive at consistent definitions referring to the superordinate concept (i.e., *genus proximum* or nearest kind) and followed by the delimiting characteristic.

In the example shown to the right in Figure 1, the *genus proximum* is inhibition, one subdivision criterion or attribute is MECHANISM, and one of the attribute values is “*a product of the reaction is the inhibitor.*”

The superordinate concept and the attribute of the feature specification must be the same in definitions of *subordinate* concepts falling under one subdivision criterion.

## Inhibition as Kinetics and Mechanism

Figure 1 clarifies the differences between various subtypes of *inhibition*. Seven of these concepts fall within two groups according to the two subdivision criteria: KINETICS and MECHANISM.

The three concepts *allosteric inhibition*, *substrate inhibition*, and *product inhibition* differ with respect to

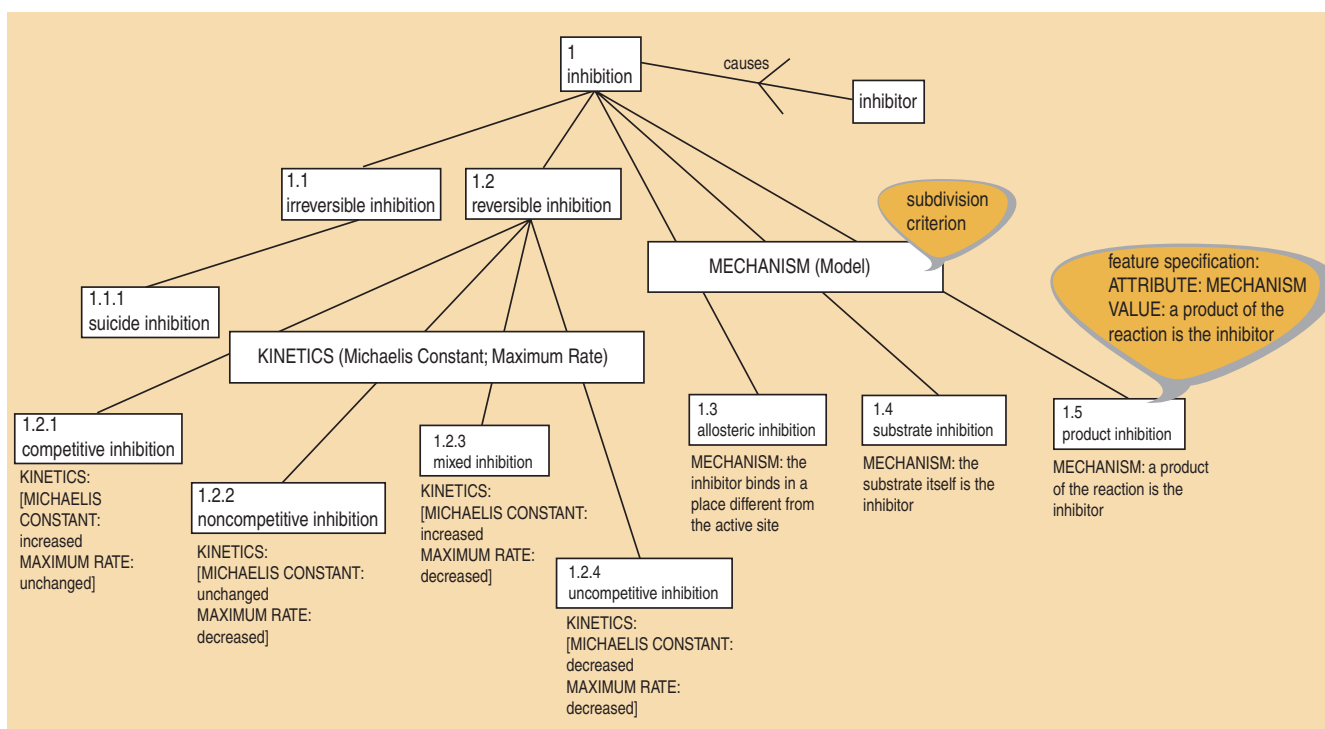


Figure 1. Extract of the inhibition diagram.