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## Modelling copper-containing proteins

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# **MODELLING COPPER- CONTAINING PROTEINS**

Proefschrift

ter verkrijging  
van de graad van Doctor  
aan de Universiteit Leiden,  
op gezag van de Rector Magnificus  
dr. D.D. Breimer, hoogleraar in de  
faculteit der Wiskunde en Natuurwetenschappen  
en die der Geneeskunde, volgens besluit  
van het College voor Promoties te  
verdedigen op 18 januari 2006  
klokke 16.15 uur.

door

Marieke van den Bosch  
geboren te Helmond in 1975

## **Promotiecommissie:**

|                |                                                                                       |
|----------------|---------------------------------------------------------------------------------------|
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|                | Prof. dr. M. C. van Hemert                                                            |

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Voor mijn ouders

### **Omslag voorzijde**

Leÿda, Batavorum Lugdunum, volgo Leÿden, concinna edificiorum et incolarum freque[n]tia pulcherrimum nitidissimumq[ue] opp[idum] ab Hispanis obsidione cinctum, ab Auriacis autem com[m]eatus invectione liberatum anno parte salutis MDLXXIIII.

vrij vertaald:

Leÿda, Lugdunum van Batavia, ook bekend als Leÿden, versierd door gebouwen en gevuld met bewoners, mooie en blinkende stad, bezet door de Spanjaarden en bevrijd door de Prins van Oranje in het jaar 1574.

[Braun en Hogenberg, 1576]

### **Omslag achterzijde, van boven naar beneden**

Kaart van Leiden en omgeving, kopie uit de 19-de eeuw  
[Sluyter, 1550]

Leiden  
[Blaeu, 1649]

Beschrijving der Stad Leyden  
[Orlers, 1780]

Stafkaart Leiden en omgeving  
[Topografische dienst, 2005]

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## ABBREVIATIONS

|           |                                 |
|-----------|---------------------------------|
| 2,3QD     | 2,3 quercetin dioxygenase       |
| DFT       | Density Functional Theory       |
| EPR       | Electron Paramagnetic Resonance |
| IR        | Infra-Red                       |
| KMP       | kaempferol                      |
| MD        | Molecular Dynamics              |
| MM        | Molecular Mechanics             |
| NMR       | Nuclear Magnetic Resonance      |
| PC        | Plastocyanin                    |
| QM        | Quantum Mechanics               |
| RR        | resonance Raman                 |
| RMS       | root mean square                |
| <i>wt</i> | wild type                       |
| UV-vis    | ultraviolet and visible light   |
| UFF       | Universal Force Field           |
| XRD       | X-ray Diffraction               |