

VORTRAG IM RAHMEN DES SONDERFORSCHUNGSBEREICHS 623
DER UNIVERSITÄT HEIDELBERG
MOLEKULARE KATALYSATOREN: STRUKTUR UND FUNKTIONSDESIGN

Donnerstag, 28. Juni 2007, 16 Uhr

OCI Seminarraum Nr. 129, Gebäude 270

Prof. Dr. M. Iwaoka

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Japan**

**„Modeling of Anti-oxidant Catalysis of
Glutathione Peroxidase.
Experimental and Theoretical
Approaches“**

Summary: Glutathione peroxidase is an anti-oxidant enzyme involving selenocysteine at the active site. We have designed three sorts of small organic selenium compounds as the enzyme models based on the active-site structure:

aromatic diselenides with a weak nonbonded interaction from a nearby heteroatom (N,O,F,etc.), water-soluble alkyl selenides, and selenocysteine derivatives.

These model compounds were synthesized, and their chemical properties were characterized by spectroscopy and quantum chemical calculation. The structures were also simulated by using the single amino acid potential (SAAP) force field developed recently in our group.

Gäste sind herzlich willkommen.

DER SPRECHER
gez. Prof. Dr. P. Hofmann