

Forschung in der Arbeitsgruppe Comba

Koordinationschemie

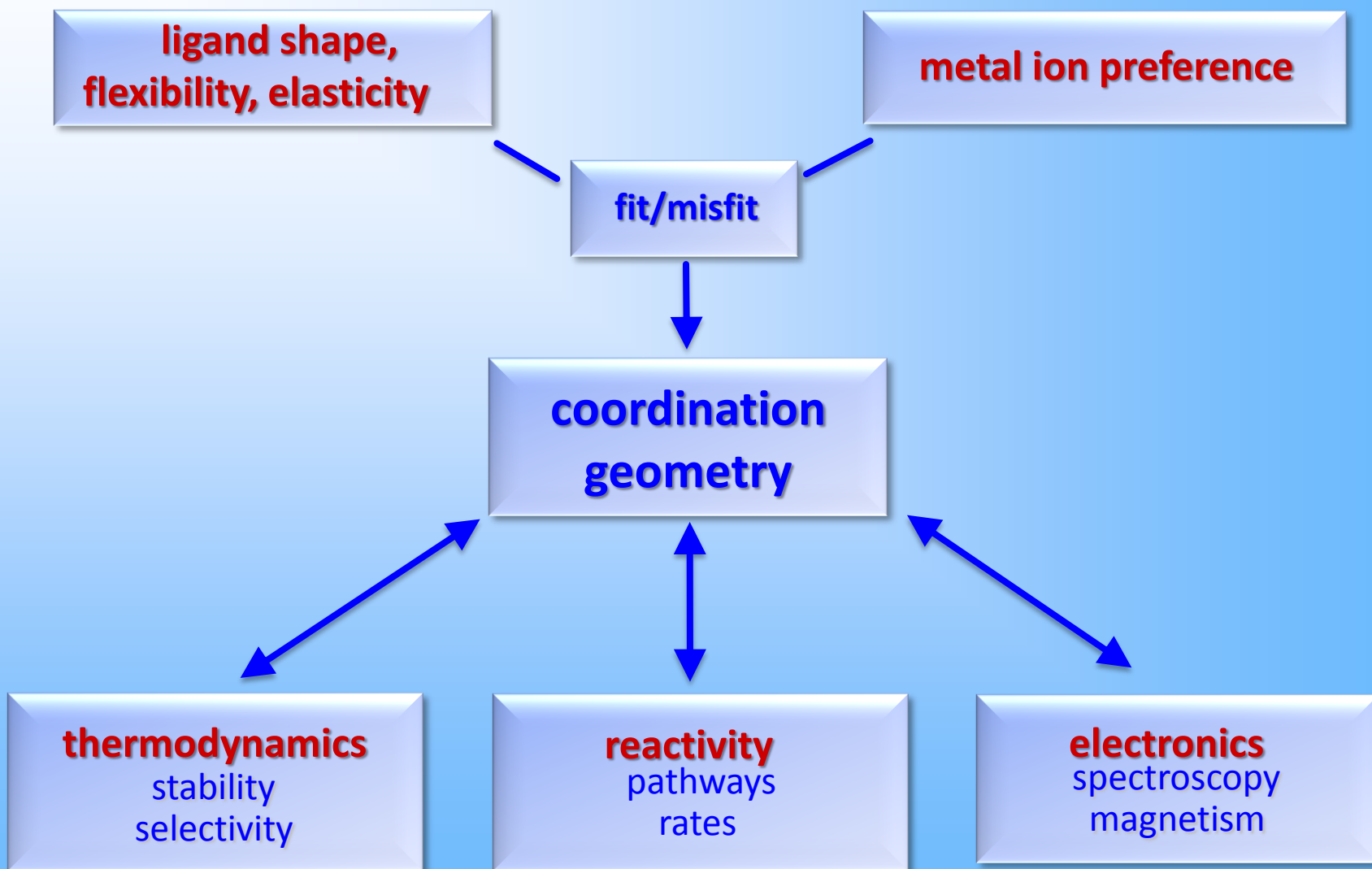
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Struktur und Funktion



Arbeitsmethoden

Ligandensynthese

Bispidine, zyklische Peptide, makrozyklische Liganden, polyfunktionale Liganden

präparative Koordinationschemie

$\text{Fe}^{\text{II/III/IV}}$, $\text{Cu}^{\text{I/II/III}}$, $\text{V}^{\text{III/IV}}$, Ga^{III} , $\text{Co}^{\text{II/III}}$, Ln^{III} , $\text{Ru}^{\text{II/III}}$, Zn^{II} , $\text{Ni}^{\text{II/III}}$ ein- und mehrkernige Komplexe

Strukturanalyse

Kristallographie, Spektroskopie

Spektroskopie, Magnetismus

UV-vis-NIR, ESR, CD, MCD, Mössbauer, NMR, Photophysik, Squid Magnetometrie;
LFT, AOM, QM-basierte Analysen, Spektrensimulationen

Thermodynamik

Stabilitätskonstanten, Redoxpotentiale

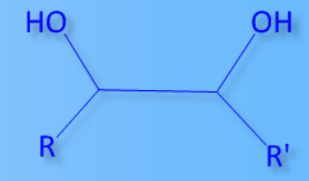
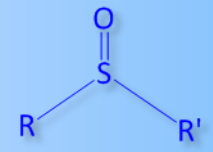
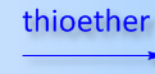
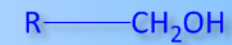
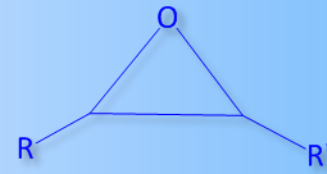
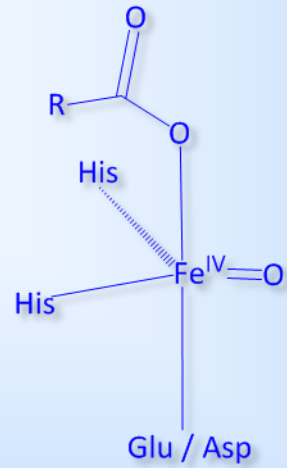
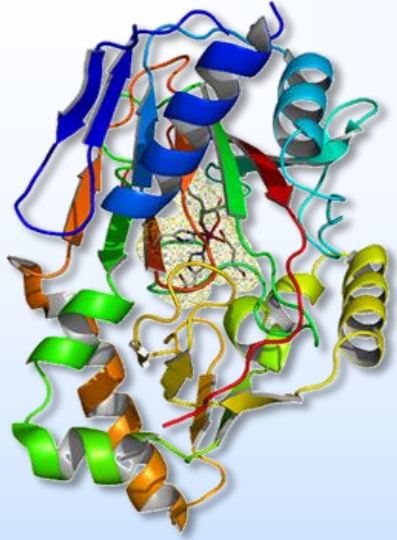
Kinetik und Mechanismus

Elektronentransfer, Oxidationskatalyse, katalytische Hydrolysen; stopped-flow Kinetik,
Tiefemperaturspektroskopie, Produktanalysen, Markierungsexperimente

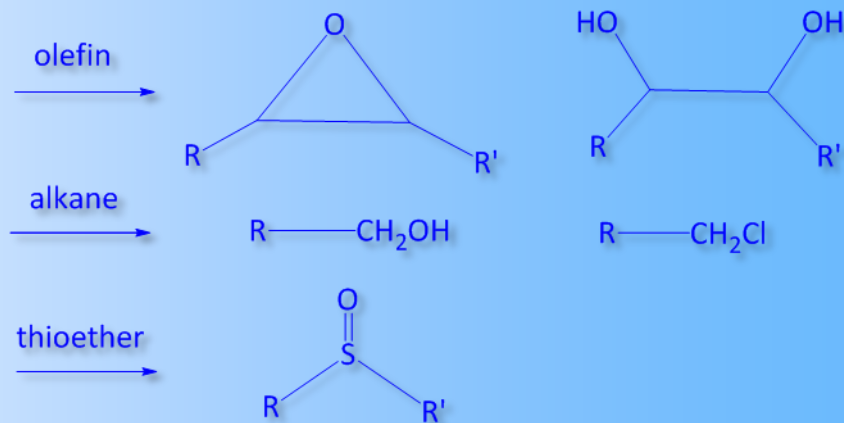
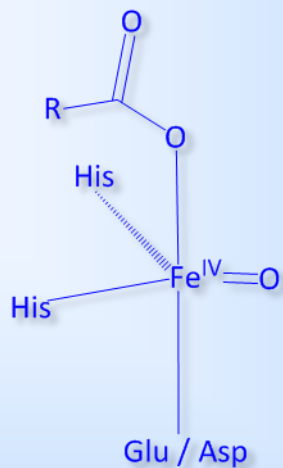
Angewandte Theorie

MM, MD, DFT, ab initio QM, LFT

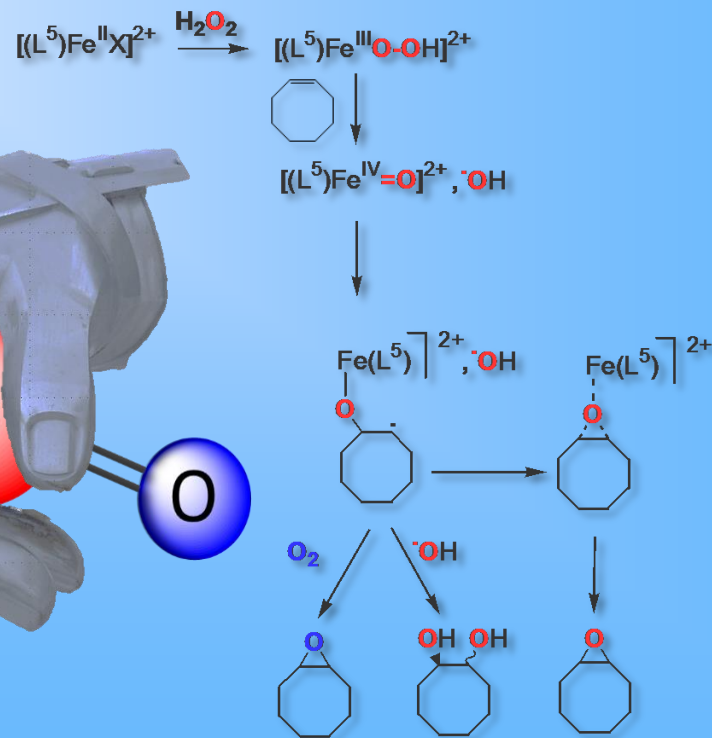
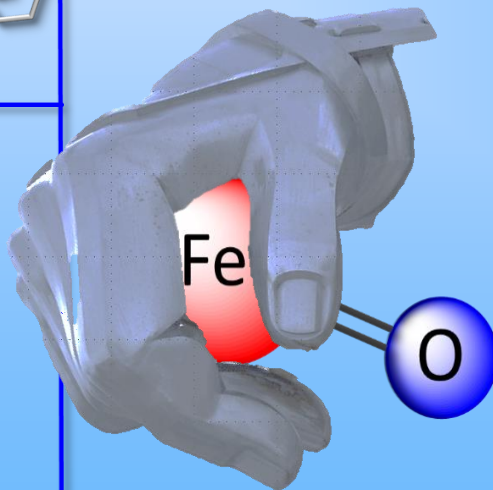
Oxidationskatalyse mit Nichthäm Eisenkomplexen



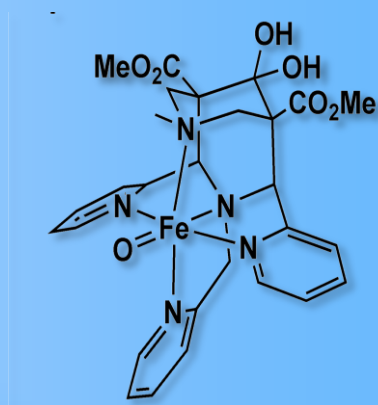
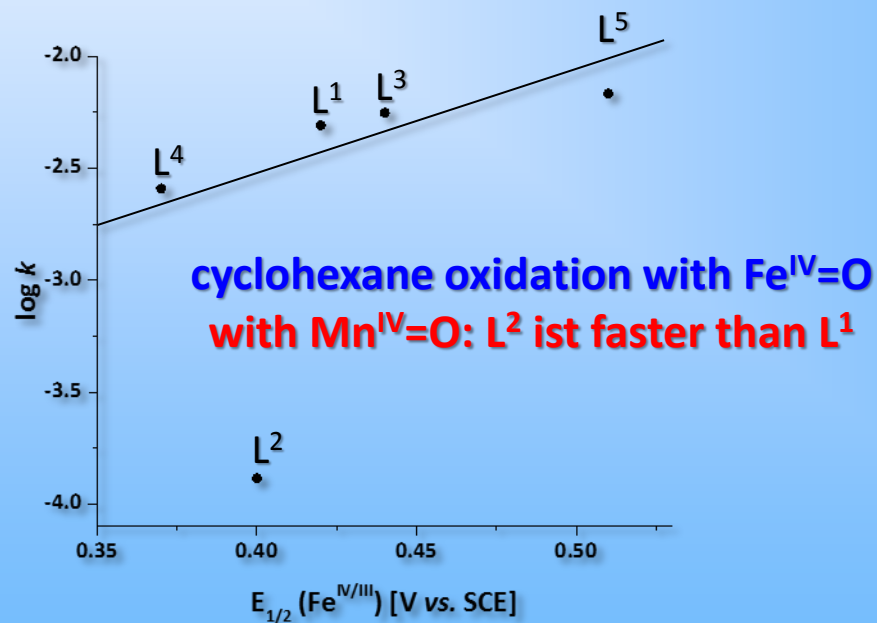
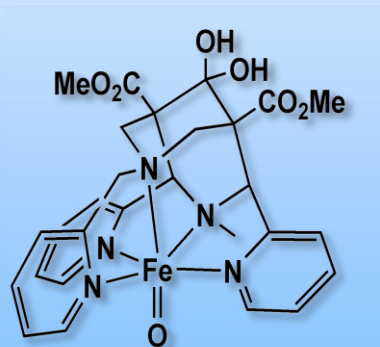
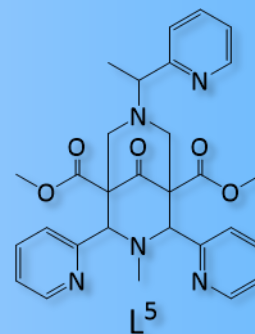
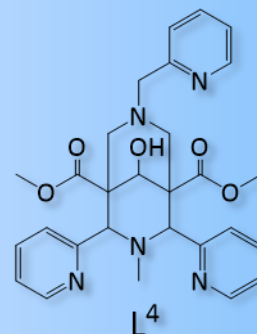
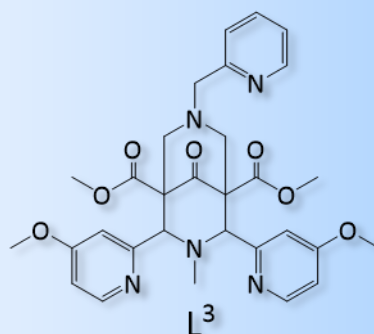
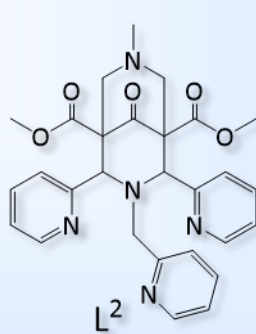
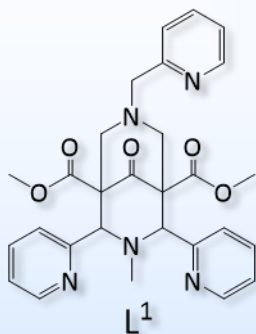
Oxidationskatalyse mit Nichthäm Eisenkomplexen



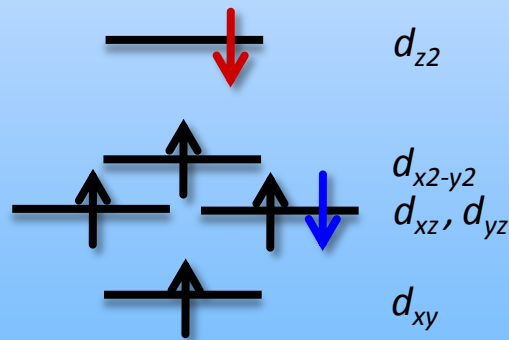
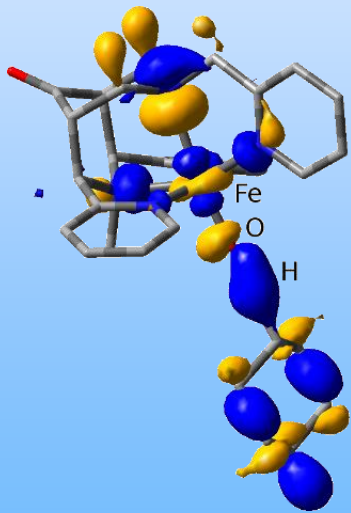
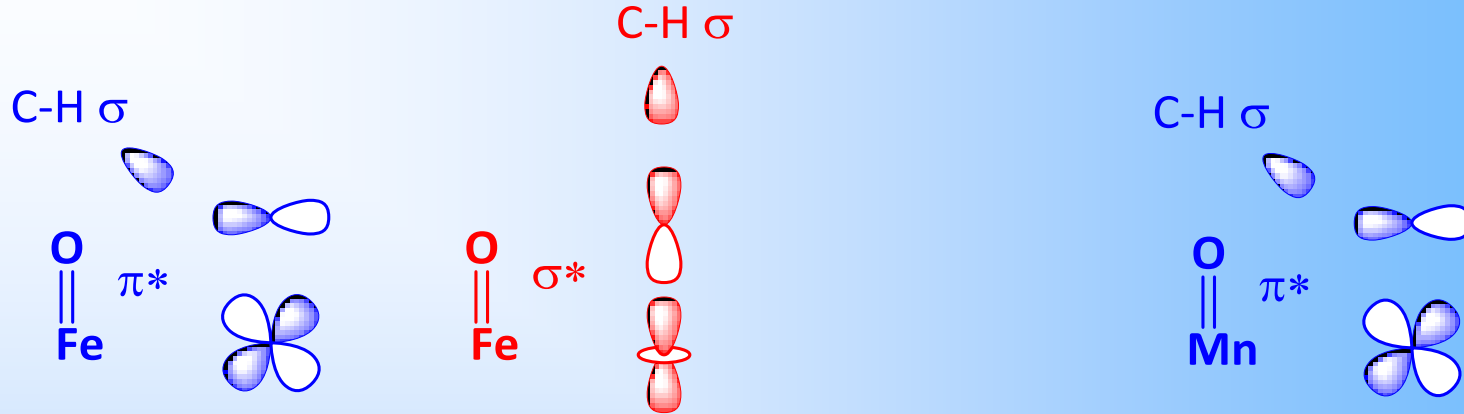
diol;epoxide	0.0; 5.0	1.0; 1.0
epoxide % ¹⁸ O [H ₂ ¹⁸ O ₂ /H ₂ ¹⁸ O/ ¹⁸ O ₂]	15/≈0/85	82/18/-
cis-diol % ¹⁸ O from H ₂ ¹⁸ O ₂ [noO/10/20] H ₂ ¹⁸ O [noO/10/20]	no diol	0/23/77 0/30/0
trans-diol % ¹⁸ O from H ₂ ¹⁸ O ₂ [noO/10/20] H ₂ ¹⁸ O [noO/10/20]		0/56/44 0/50/0



Korrelation von Redoxpotentialen und Reaktivitäten

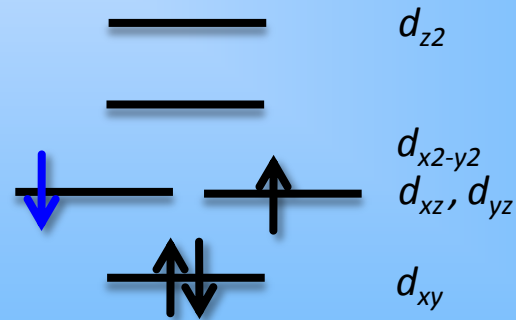


Die σ und π Kanäle der C-H Aktivierung



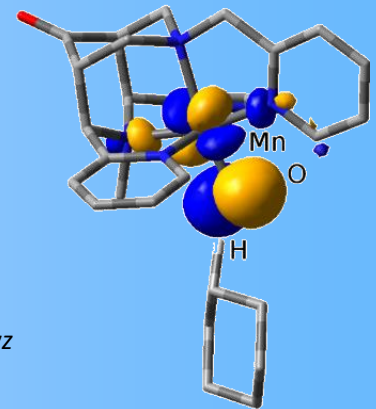
$$S = 2$$

σ or π channel

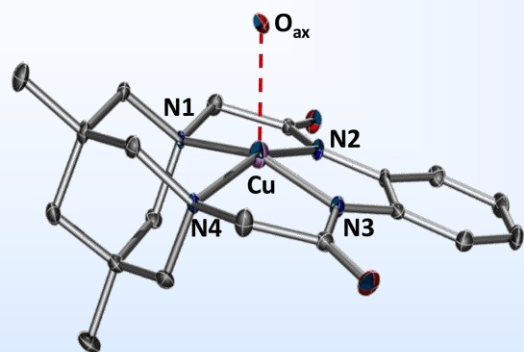


$$S = 1/2$$

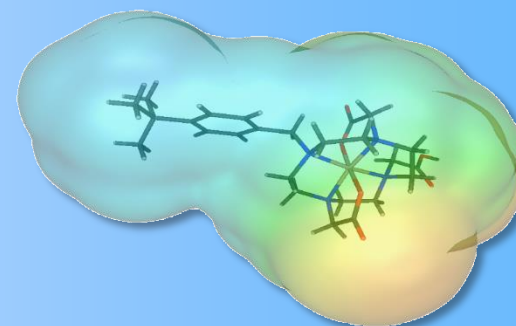
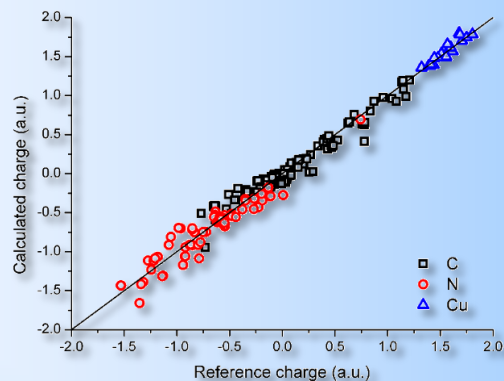
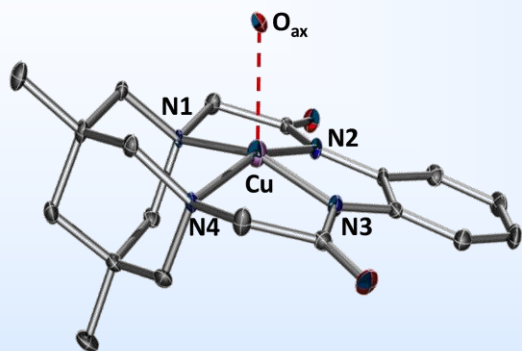
π channel



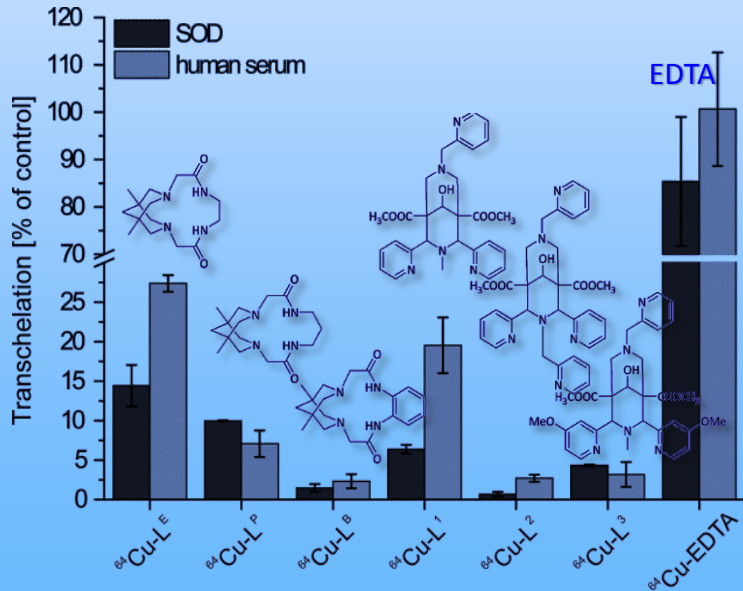
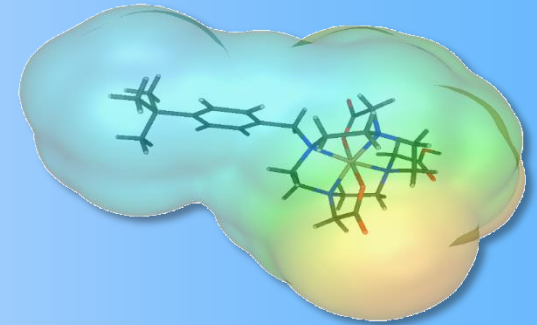
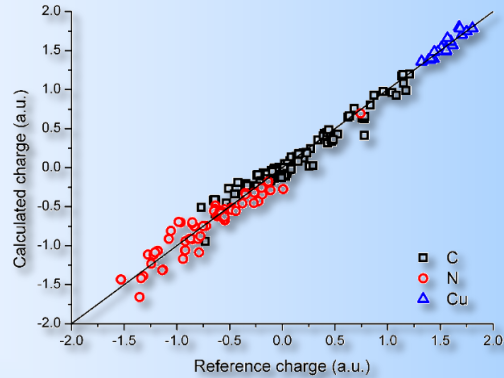
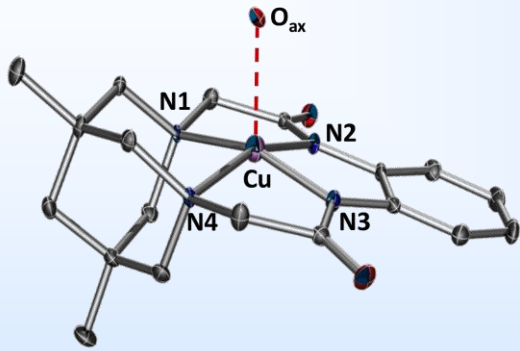
Multimodales Imaging mit ^{64}Cu Verbindungen: PET



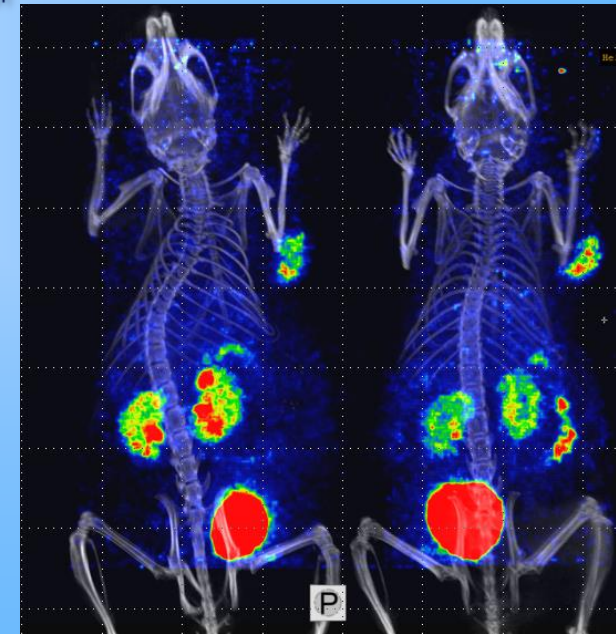
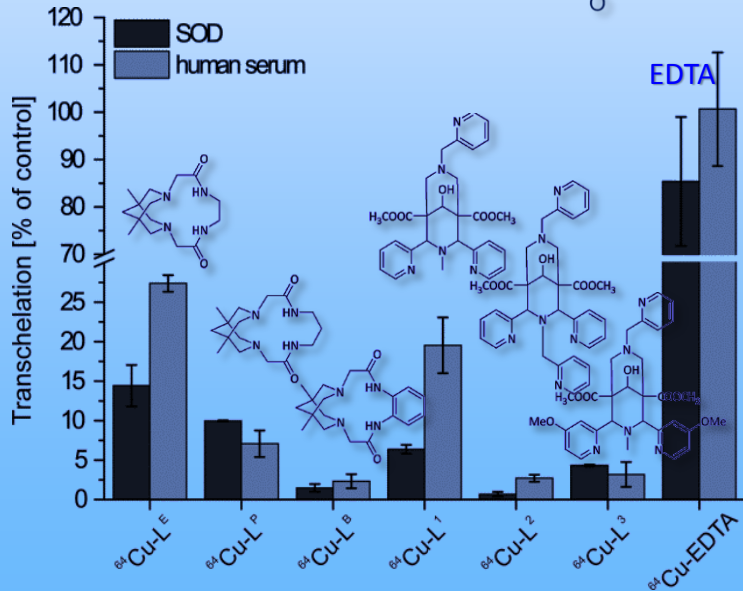
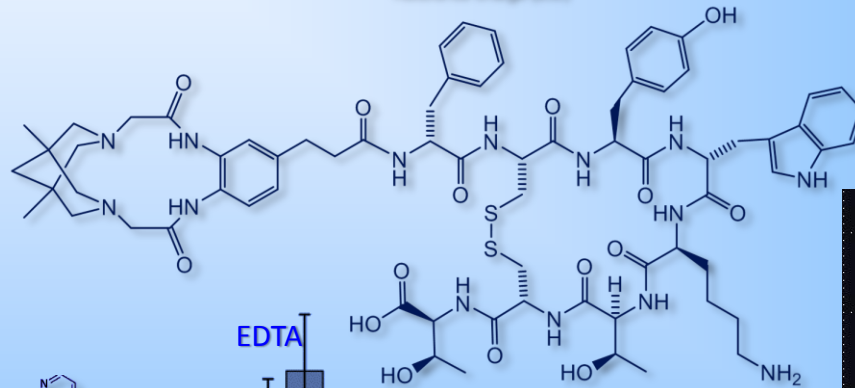
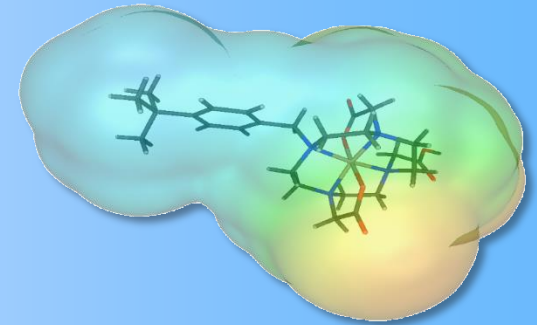
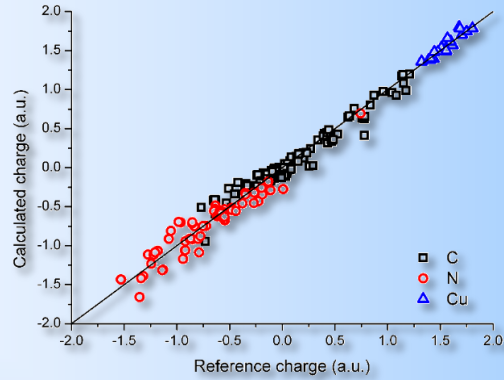
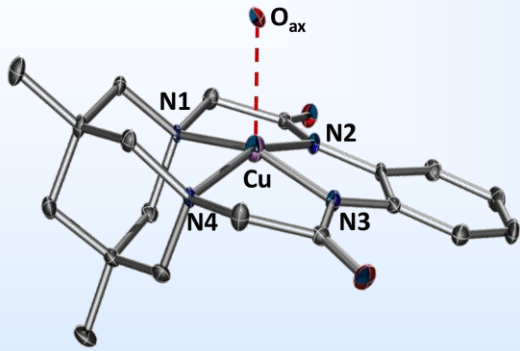
Multimodales Imaging mit ^{64}Cu Verbindungen: PET



Multimodales Imaging mit ^{64}Cu Verbindungen: PET

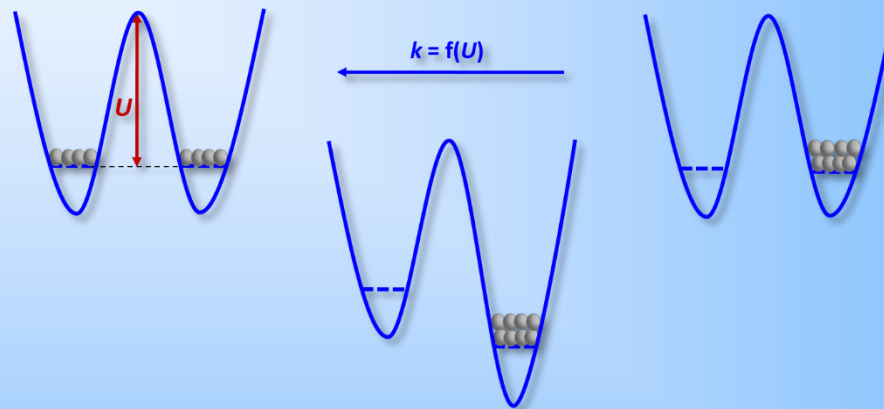


Multimodales Imaging mit ^{64}Cu Verbindungen: PET



Molekularer Magnetismus

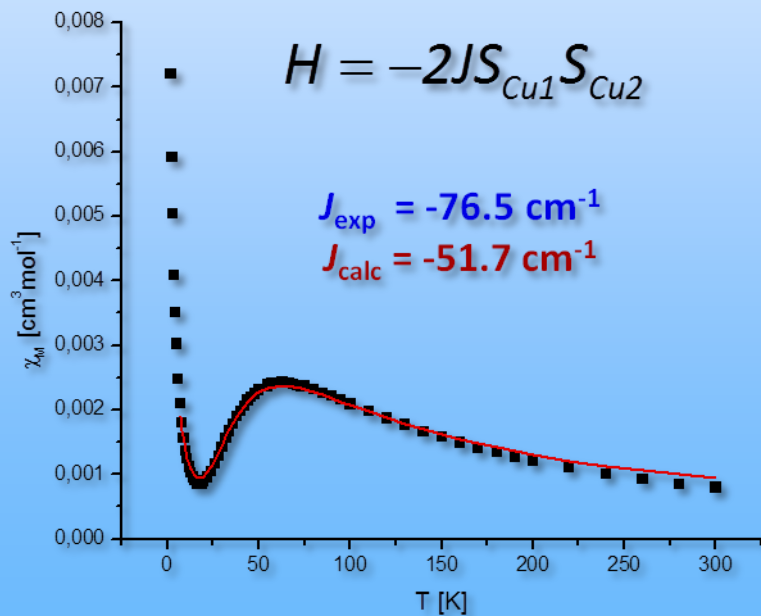
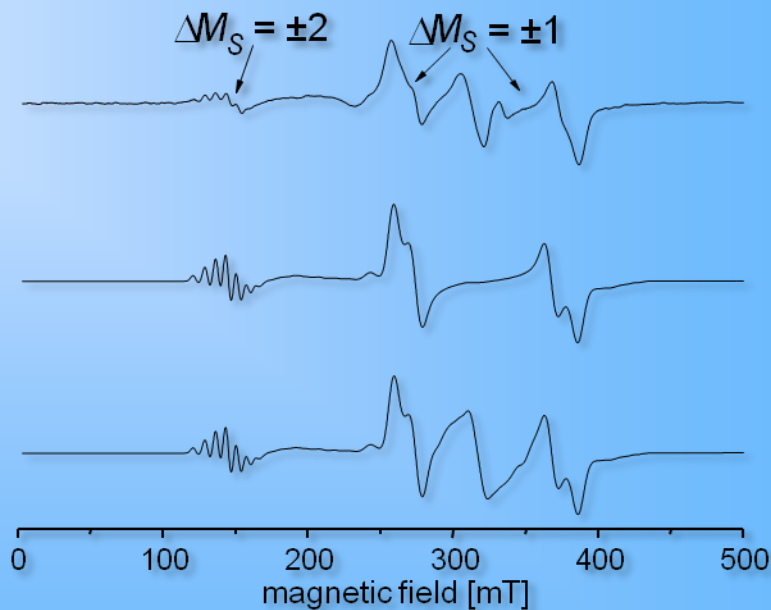
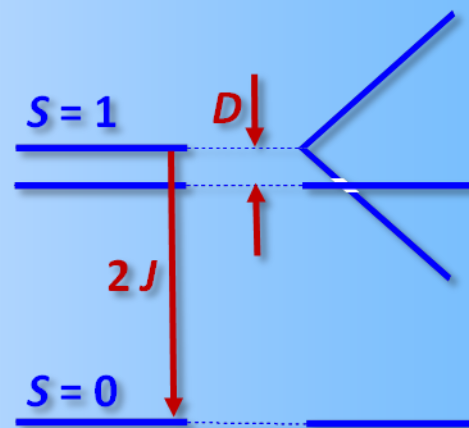
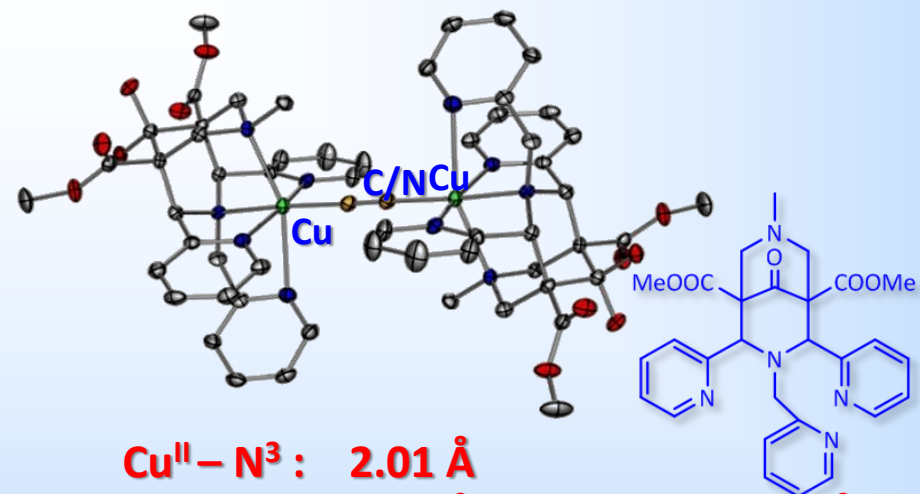
Einzelmolekülmagnetismus



$$U = S^2 |D| \text{ (ganzzahlige Werte von } S \text{)}$$

$$U = (S^2 - \frac{1}{4}) |D| \text{ (halbzahlige Werte von } S \text{)}$$

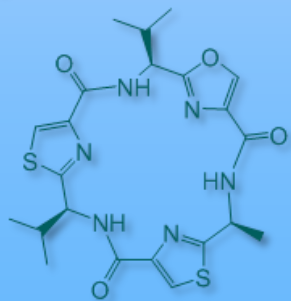
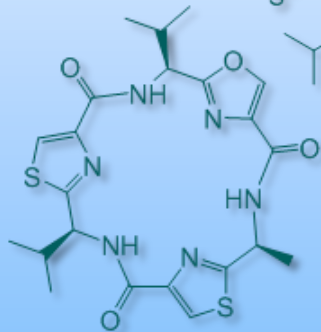
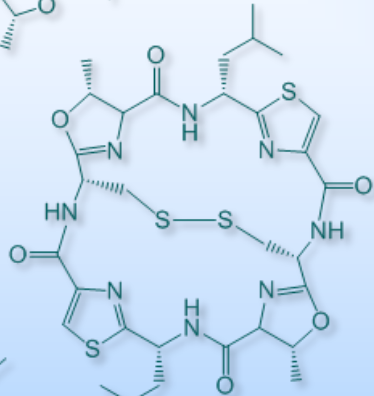
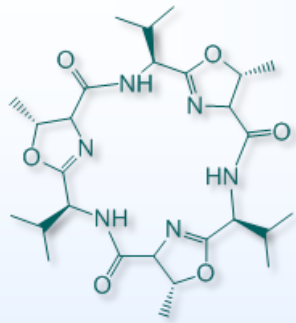
Molekularer Magnetismus



$g_1 = 2.025, g_2 = 2.096, g_3 = 2.240; A_1 = 17, A_2 = 100, A_3 = 149$
 $J = -76.48, D = -0.159 \text{ cm}^{-1}$ with $E/D = 0.08$

J and D are strongly dependent of the structure

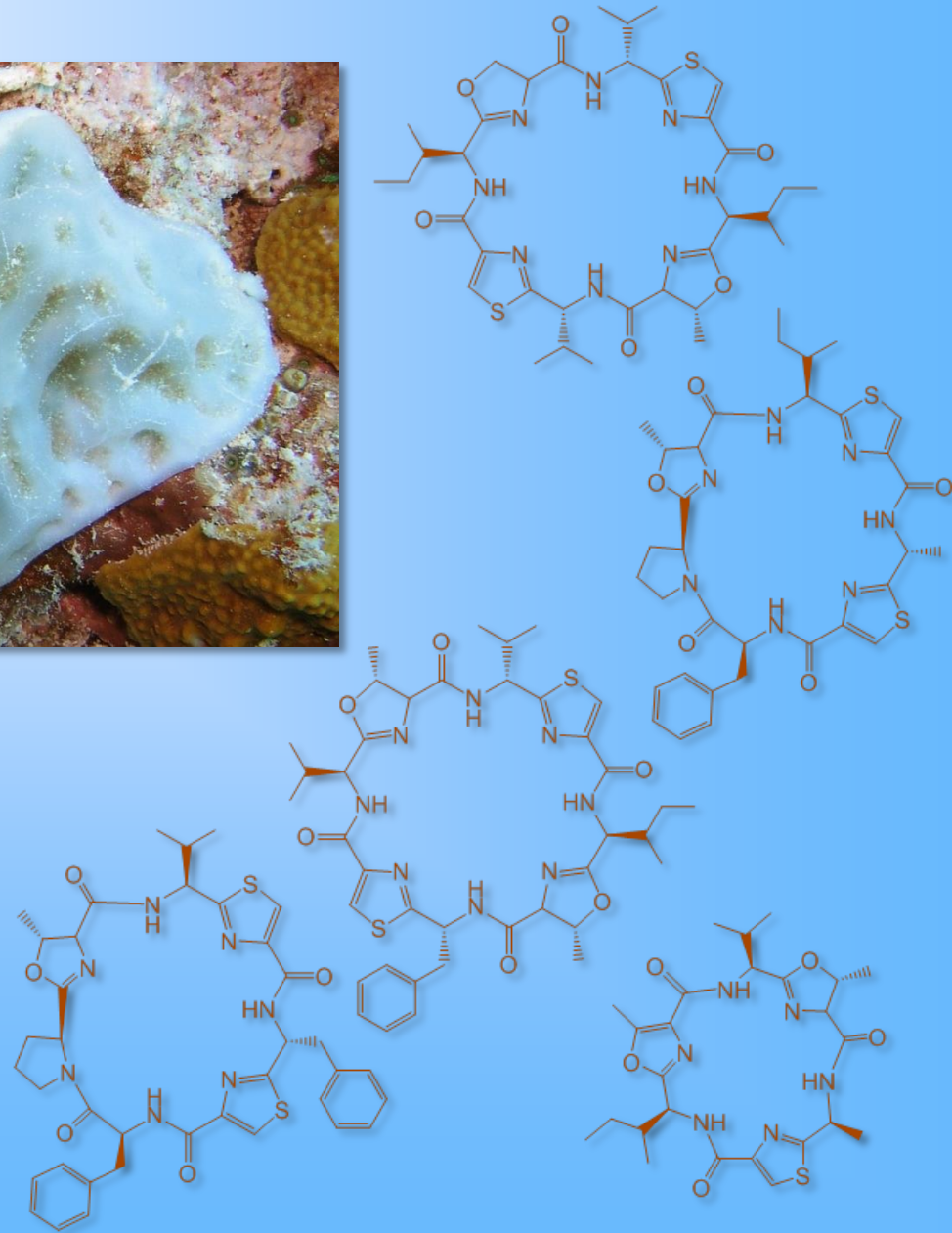
Biomimetische Chemie mit zyklischen Peptiden



Ascidians

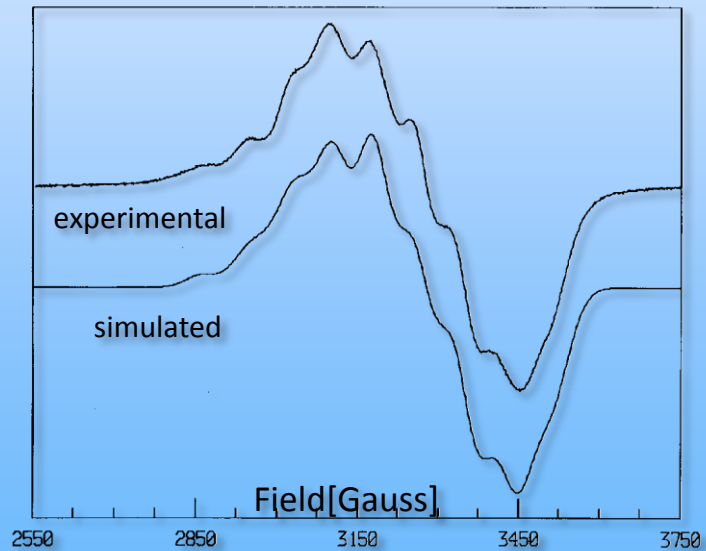
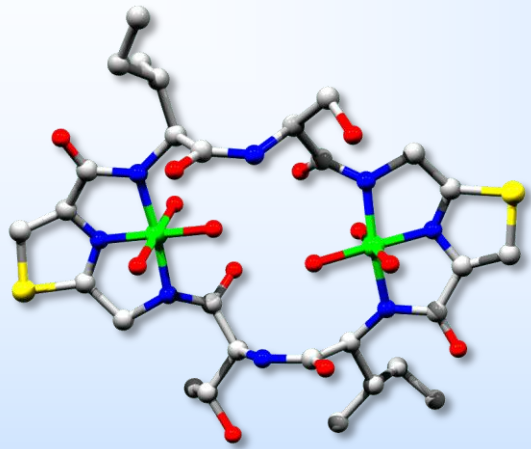
Lissoclinum patella

Lissoclinum bistratum



Biomimetische Chemie mit zyklischen Peptiden

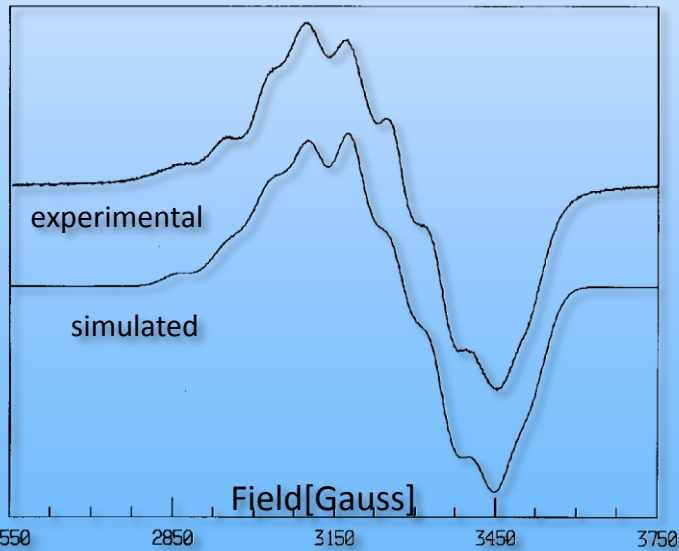
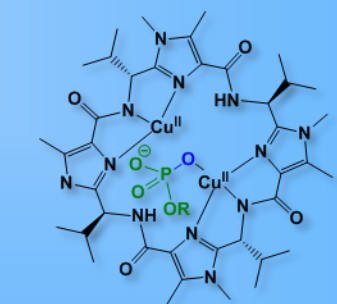
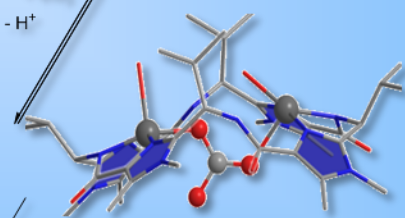
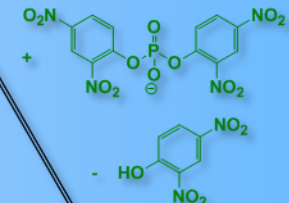
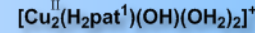
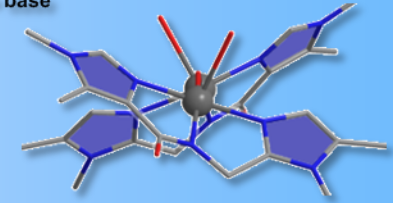
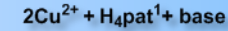
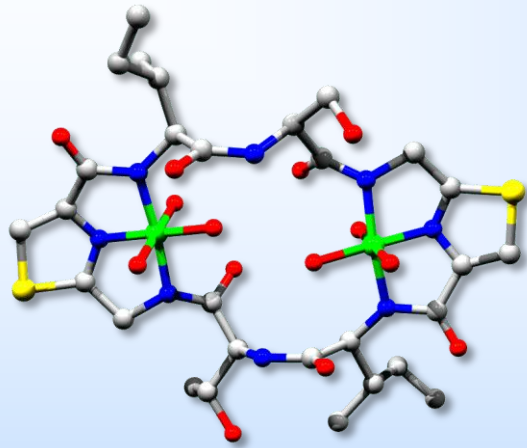
Strukturen in Lösung



Biomimetische Chemie mit zyklischen Peptiden

Strukturen in Lösung

Carboanhydrase & Phosphatase





Kathrin Benzing
Simone Bosch
Annika Eisenschmidt
Biljana Glisic
Michael Grosshauser
Maik Jakob
Marion Kerscher
Bodo Martin
Nina Mehrkens

Dennis Müller
Bianca Pokrandt
Anna-Maria Rensland
Markus Rössler
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Eckhard Bill
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Shunichi Fukuzumi
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Dirk Herten
Frank Keppler
Marcel Maeder

Wonwoo Nam
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Kallol Ray
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Heinfried Schöler
Leone Spiccia
Larry Que
Holger Stephan
Hubert Wadepohl

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