



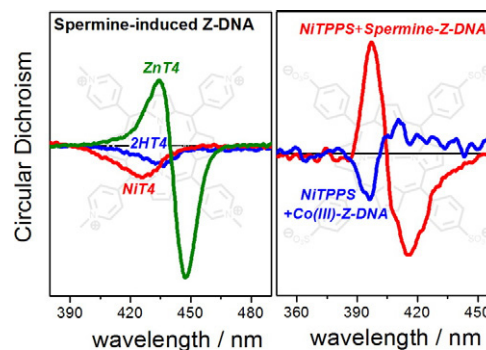
Contents

Jung Kyu Choi, Alessandro D'Urso, Milan Balaz

Journal of Inorganic Biochemistry 127 (2013) 1–6

Chiroptical properties of anionic and cationic porphyrins and metalloporphyrins in complex with left-handed Z-DNA and right-handed B-DNA

Chiroptical properties of charged metalloporphyrins and their metal-free counterparts in complex with Z-DNAs induced by cobalt(III) or spermine are described.

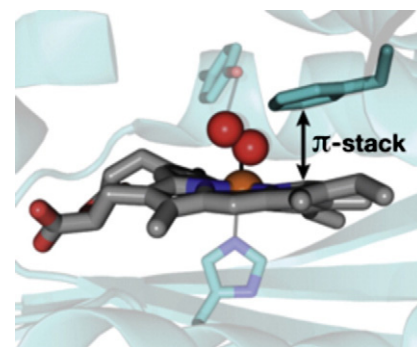


Emily E. Weinert, Christine M. Phillips-Piro, Michael A. Marletta

Journal of Inorganic Biochemistry 127 (2013) 7–12

Porphyrin π -stacking in a heme protein scaffold tunes gas ligand affinity

A phenylalanine-porphyrin off-set π -stack was found to exert significant effects on ligand binding properties of *Tt* H-NOX, without changing the protein structure. Removal of the π -stack resulted in a modest change (~ 40 mV) in midpoint potential and an order of magnitude change in O_2 affinity.

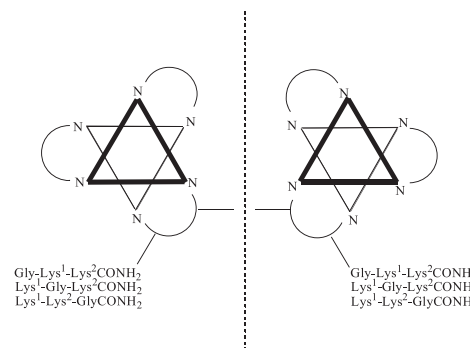


Konstantina Karidi, Konstantinos Ypsilantis, Athanasios Papakyriakou, Achilleas Garoufis

Journal of Inorganic Biochemistry 127 (2013) 13–23

Synthesis and characterization of ruthenium(II)-oligopyridine-peptide conjugates. Interactions of the diastereomers Δ - and Λ -[Ru(bpy)₂(4-COY-4'-Mebpy)]Cl₂ (Y = Gly-Lys¹-Lys²CONH₂, Lys¹-Gly-Lys²CONH₂, Lys¹-Lys²-GlyCONH₂) with the oligonucleotide d(5'-CGCGAATTCGCG-3')₂

Diastereomeric complexes of the general formulae Λ - and Δ -[Ru(bpy)₂(4-COY-4'-Mebpy)]Cl₂ where Y = Gly-Lys¹-Lys²CONH₂, Lys¹-Gly-Lys²CONH₂, Lys¹-Lys²-GlyCONH₂, were synthesized and characterized. The ability of these compounds to bind to the oligonucleotide duplex d(5'-CGCGAATTCGCG-3')₂ was studied with NMR techniques.

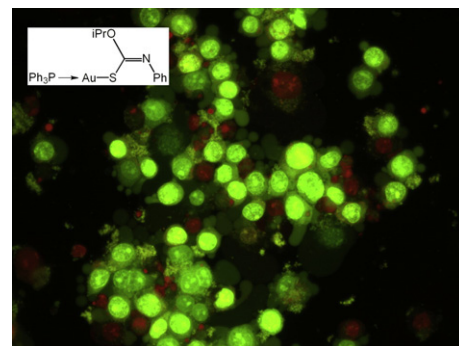


**Chien Ing Yeo, Kah Kooi Ooi,
Abdah Md Akim, Kok Pian Ang,
Zainal Abidin Fairuz,
Siti Nadiyah Binti Abdul Halim, Seik Weng Ng,
Hoi-Ling Seng, Edward R.T. Tiekink**

Journal of Inorganic Biochemistry 127 (2013)
24–38

The influence of R substituents in triphenylphosphinegold(I) carbonimidothioates, $\text{Ph}_3\text{PAu}[\text{SC}(\text{OR}) = \text{NPh}]$ (R = Me, Et and iPr), upon in vitro cytotoxicity against the HT-29 colon cancer cell line and upon apoptotic pathways

The $\text{Ph}_3\text{PAu}[\text{SC}(\text{OR}) = \text{NPh}]$ compounds are cytotoxic to the HT-29 cancer cell line and induce apoptosis by both extrinsic and intrinsic pathways.

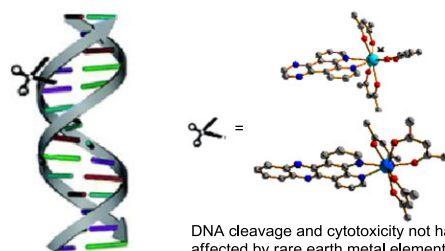


**Gong-Jun Chen, Zhi-Gang Wang, Xin Qiao,
Jing-Yuan Xu, Jin-Lei Tian, Shi-Ping Yan**

Journal of Inorganic Biochemistry 127 (2013)
39–45

Synthesis, DNA binding, photo-induced DNA cleavage, cytotoxicity studies of a family of heavy rare earth complexes

A family of heavy rare earth complexes, $[\text{RE}(\text{acac})_3(\text{dpq})]$ and $[\text{RE}(\text{acac})_3(\text{dppz})]$ CH_3OH have been synthesized, their DNA binding and photo-induced DNA cleavage activity are investigated. DNA binding, DNA cleavage and cytotoxicity not have affected by rare earth metal elements.

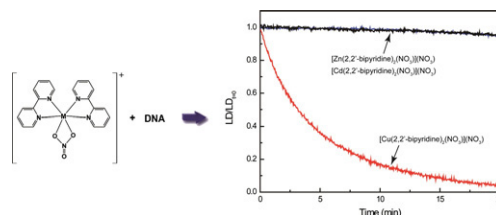


**Hee-Jin Park, Ji Hye Kwon, Tae-Sub Cho,
Jong Moon Kim, In Hong Hwang,
Cheal Kim, Soojin Kim, Jinheung Kim,
Seog K. Kim**

Journal of Inorganic Biochemistry 127 (2013)
46–52

Real-time detection of DNA cleavage induced by $[\text{M}(2,2'\text{-bipyridine})_2(\text{NO}_3)](\text{NO}_3)$ (M = Cu(II), Zn(II) and Cd(II)) complexes using linear dichroism technique

Decrease of linear dichroism according to the cleavage of DNA by $[\text{M}(2,2'\text{-bipyridine})_2(\text{NO}_3)](\text{NO}_3)$ complexes.

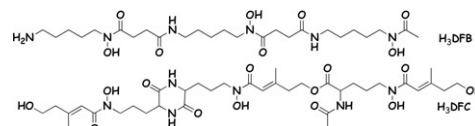


**Gyula Tircsó, Zoltán Garda,
Ferenc K. Kálmán, Zsolt Baranyai,
István Pócsi, György Balla, Imre Tóth**

Journal of Inorganic Biochemistry 127 (2013)
53–61

Lanthanide(III) complexes of some natural siderophores: A thermodynamic, kinetic and relaxometric study

The given manuscript reports on the complexation properties of desferrioxamine B and desferricoprogen towards lanthanide(III) ions in solution studied by means of pH-potentiometry, UV-vis spectrophotometry, ^1H - and ^{17}O -relaxometry. The natural hydroxamates studied form mostly mononuclear complexes with Ln(III) ions of relatively low stability, which are kinetically labile.

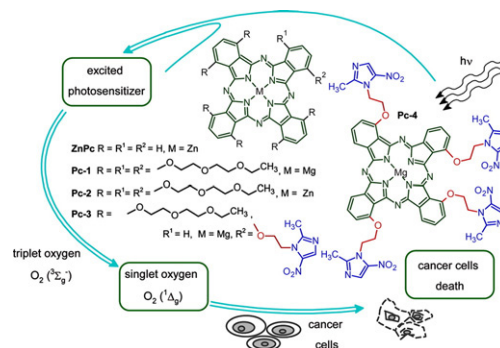


Marcin Wierzchowski, Lukasz Sobotta, Paulina Skupin-Mrugalska, Justyna Kruk, Weronika Jusiak, Michael Yee, Krystyna Konopka, Nejat Düzgüneş, Ewa Tykarska, Maria Gdaniec, Jadwiga Mielcarek, Tomasz Goslinski

Journal of Inorganic Biochemistry 127 (2013) 62–72

Phthalocyanines functionalized with 2-methyl-5-nitro-1*H*-imidazolelethoxy and 1,4,7-trioxanonyl moieties and the effect of metronidazole substitution on photocytotoxicity

Four novel zinc(II) and magnesium(II) phthalocyanines bearing non-peripheral polyether substituents (**Pc-1**, **Pc-2** and **Pc-3**) and (2-methyl-5-nitro-1*H*-imidazol-1-yl) ethoxy substituents (**Pc-3** and **Pc-4**) were synthesized. All photosensitizers revealed interesting photophysical properties and high values of singlet oxygen generation. The photocytotoxicity of the novel macrocycles was also evaluated.

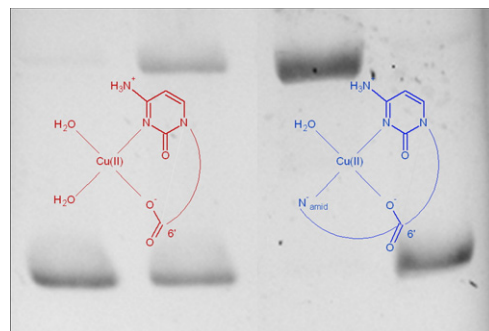


Kamila Stokowa-Sołtys, Małgorzata Jeżowska-Bojczuk

Journal of Inorganic Biochemistry 127 (2013) 73–78

A rice fungicide blasticidin S efficiently binds Cu(II) ions and prevents DNA from metal-induced damage

Copper(II) complex of blasticidin S was studied regarding its coordination pattern as well as the impact on the plasmid DNA. Surprisingly, DNA damage is not observed. This result indicates that BS can be considered as a ligand that effectively lowers the oxidative activity of Cu(II) ion.

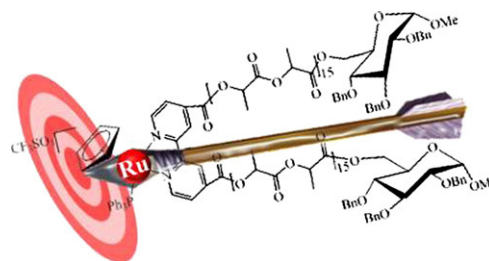


Andreia Valente, Maria Helena Garcia, Fernanda Marques, Yong Miao, Cyril Rousseau, Philippe Zinck

Journal of Inorganic Biochemistry 127 (2013) 79–81

First polymer “ruthenium-cyclopentadienyl” complex as potential anticancer agent

First polymer “ruthenium-cyclopentadienyl” complex active against several human cancer cells.

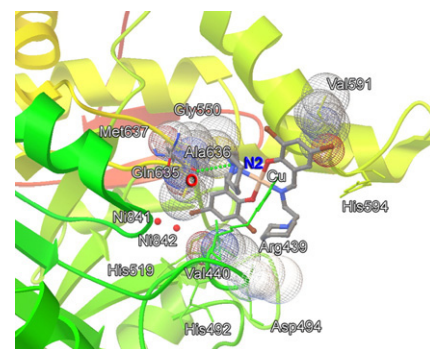


Xiongwei Dong, Taolian Guo, Yuguang Li, Yongming Cui, Qiang Wang

Journal of Inorganic Biochemistry 127 (2013) 82–89

Synthesis, structure and urease inhibition studies of Schiff base copper(II) complexes with planar four-coordinate copper(II) centers

Seven new copper(II) complexes of Schiff bases were synthesized and structurally characterized. Inhibition of jack bean urease by all the obtained copper(II) complexes with planar four-coordinate copper(II) centers was evaluated. A docking analysis via a DOCK program supports their potent inhibitory activities.

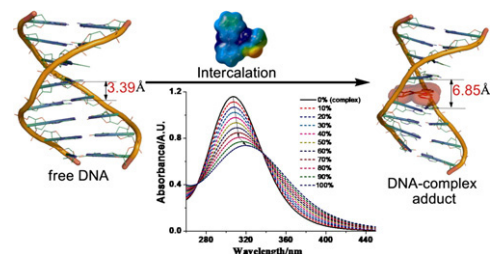


**Wei Hu, Suwen Deng, Jianyin Huang,
Yanmei Lu, Xueyi Le, Wenxu Zheng**

Journal of Inorganic Biochemistry 127 (2013)
90–98

Intercalative interaction of asymmetric copper(II) complex with DNA: Experimental, molecular docking, molecular dynamics and TDDFT studies

A combined experimental/theoretical investigation of intercalative interaction between metallointercalator copper(II) complex and DNA is reported. An analytical method was proposed to simulate the dynamically changing absorption spectra of complex/DNA intercalation. A rational explanation for the red shift of the absorption spectra has been proposed.

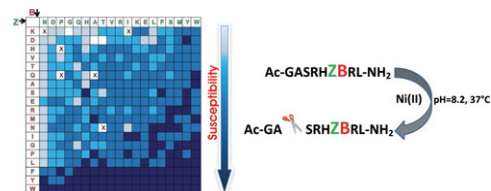


**Anna Maria Protas,
Hanieh Hossein Nejad Ariani,
Arkadiusz Bonna,
Agnieszka Polkowska-Nowakowska,
Jarosław Poznański, Wojciech Bal**

Journal of Inorganic Biochemistry 127 (2013)
99–106

Sequence-specific Ni(II)-dependent peptide bond hydrolysis for protein engineering: Active sequence optimization

Aromatic residues downstream of the Ni(II) binding site enhance nickel dependent peptide bond hydrolysis.

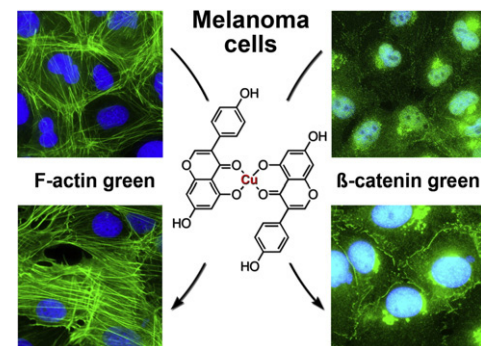


**Cornelia Spoerlein, Katharina Mahal,
Holger Schmidt, Rainer Schobert,**

Journal of Inorganic Biochemistry 127 (2013)
107–115

Effects of chrysin, apigenin, genistein and their homoleptic copper(II) complexes on the growth and metastatic potential of cancer cells

Complexation of chrysin, apigenin, and genistein to Cu(II) trebles their cytotoxicity against cancer cells. While the apigenin complex destabilizes their F-actin cytoskeleton and stimulates the expression of matrix metalloproteinases, the genistein complex supports cell–cell adhesion by actin remodeling, cadherin–catenin complex formation, and a reduced expression and secretion of MMPs.

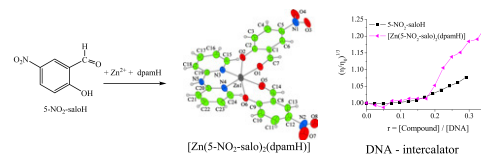


**Ariadni Zianna, George Psomas,
Antonis Hatzidimitriou,
Evdoxia Coutouli-Argyropoulou,
Maria Lalia-Kantouri,**

Journal of Inorganic Biochemistry 127 (2013)
116–126

Zinc complexes of salicylaldehydes: Synthesis, characterization and DNA-binding properties

Zinc complexes of the formulae $[Zn(X-salo)_2(CH_3OH)_2]$ and $[Zn(X-salo)_2(\alpha\text{-diimine})]$ with 5-substituted salicylaldehydes (X-saloH) and N,N'-donor ligands (α -diimine) have been synthesized and characterized. The complexes can bind tightly to CT DNA probably by intercalation and compete to ethidium bromide for the intercalation site of DNA.



Special Issue from the 11th European Biological Inorganic Chemistry Conference (EUROBIC11)

**Alicia Domínguez-Martín,
Juan Niclós-Gutiérrez**

Journal of Inorganic Biochemistry 127 (2013)
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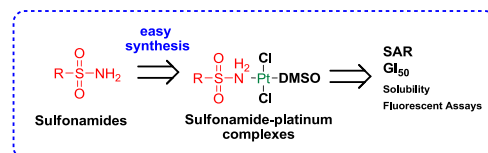
Preface

Metals in Medicine

**Virginia del Solar,
Adolfo Quiñones-Lombrana,
Silvia Cabrera, José M. Padrón,
Carla Ríos-Luci, Amparo Alvarez-Valdés,
Carmen Navarro-Ranninger, José Alemán**

Journal of Inorganic Biochemistry 127 (2013)
128–140

Expanding the synthesis of new *trans*-sulfonamide platinum complexes: Cytotoxicity, SAR, fluorescent cell assays and stability studies

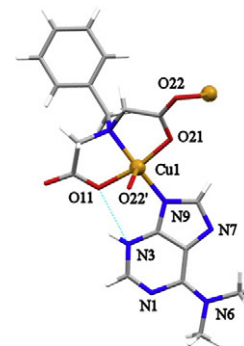


**Alicia Domínguez-Martín,
Ángel García-Raso, Catalina Cabot,
Duane Choquesillo-Lazarte,
Inmaculada Pérez-Toro,
Antonio Matilla-Hernández,
Alfonso Castiñeiras, Juan Niclós-Gutiérrez**

Journal of Inorganic Biochemistry 127 (2013)
141–149

Structural insights on the molecular recognition patterns between N^6 -substituted adenines and *N*-(aryl-methyl)iminodiacetate copper(II) chelates

N^6 -monosubstituted-adenines recognize Cu^{II} -IDA chelates by cooperation of the $\text{Cu}-\text{N}3$ (purine) bond and one intra-molecular interligand $\text{N}9-\text{H} \cdots \text{O}$ (carboxy) interaction. In contrast, N^6, N^6 -dimethyladenine shows the rare tautomer $\text{H}(\text{N}3)\text{dimAP}$, unprecedented for this ligand, and the molecular recognition pattern $\text{Cu}-\text{N}9 + \text{N}3-\text{H} \cdots \text{O}$ (carboxy) interaction. Only the free cycloalkyladenine ligands showed cytokinin activity.

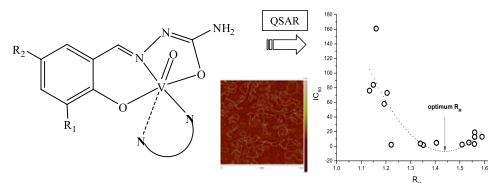


**Mariana Fernández, Lorena Becco,
Isabel Correia, Julio Benítez, Oscar E. Piro,
Gustavo A. Echeverría, Andrea Medeiros,
Marcelo Comini, María Laura Lavaggi,
Mercedes González, Hugo Cerecetto,
Virtudes Moreno, Joao Costa Pessoa,
Beatriz Garat, Dinorah Gambino**

Journal of Inorganic Biochemistry 127 (2013)
150–160

Oxidovanadium(IV) and dioxidovanadium(V) complexes of tridentate salicylaldehyde semicarbazones: Searching for prospective antitrypanosomal agents

New $[\text{V}^{\text{VO}}_2(\text{L}-2\text{H})]$ and $[\text{V}^{\text{VO}}(\text{L}-2\text{H})(\text{NN})]$ complexes with salicylaldehyde semicarbazones (L) and polypyridyl ligands (NN) were synthesized and evaluated on trypanosomatid parasites. A QSAR study was performed.

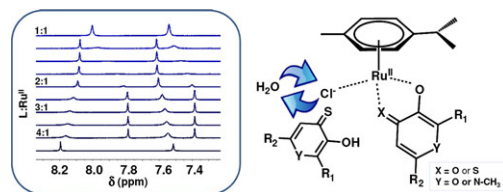


Éva A. Enyedy, Éva Sija, Tamás Jakusch, Christian G. Hartinger, Wolfgang Kandioller, Bernhard K. Keppler, Tamás Kiss

Journal of Inorganic Biochemistry 127 (2013) 161–168

Solution equilibria of anticancer ruthenium(II)-(η^6 -*p*-cymene)-hydroxy(thio)pyr(id)one complexes: Impact of sulfur vs. oxygen donor systems on the speciation and bioactivity

A comparative study on the antitumor ruthenium(II)- η^6 -*p*-cymene complexes of bidentate (O,O) hydroxypyrrone and (O, S) hydroxythiopyr(id)one type ligands revealed that the hydroxythiopyr(id)one ligands form complexes of significantly higher stability compared with the hydroxypyrrones; their complexes are biologically more active. The simultaneous bi- and monodentate coordination of the ligands in the bis complexes (ML_2 and ML_2H) was also demonstrated.

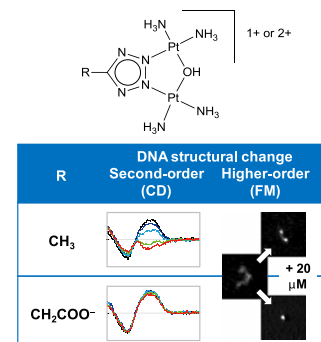


Masako Uemura, Yuko Yoshikawa, Kenichi Yoshikawa, Takaji Sato, Yoshiki Mino, Masahiko Chikuma, Seiji Komeda

Journal of Inorganic Biochemistry 127 (2013) 169–174

Second- and higher-order structural changes of DNA induced by antitumor-active tetrazolato-bridged dinuclear platinum(II) complexes with different types of 5-substituent

The second- and higher-order DNA structural changes were monitored upon addition of antitumor tetrazolato-bridged dinuclear platinum(II) complexes with different types of 5-substituent, using circular dichroism and fluorescence microscopy. The types of 5-substituent exert unique or different magnitudes of influence on the second-order structure, which is not necessarily linked to higher-order ones.

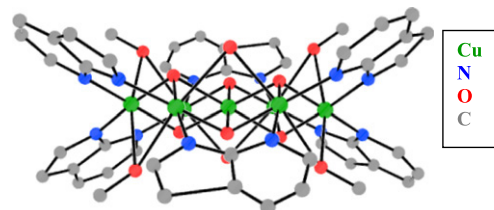


Jacob A. Przyowski, Nicole N. Myers, Hadi D. Arman, Andrey Prosvirin, Kim R. Dunbar, Mohan Natarajan, Manickam Krishnan, Sumathy Mohan, Judith A. Walmsley

Journal of Inorganic Biochemistry 127 (2013) 175–181

Dinuclear and heptanuclear complexes of copper(II) with 7-azaindole ligand: Synthesis, characterization, magnetic properties, and biological activity

A dinuclear complex and a heptanuclear complex of Cu(II) with 7-azaindole have been synthesized and characterized.

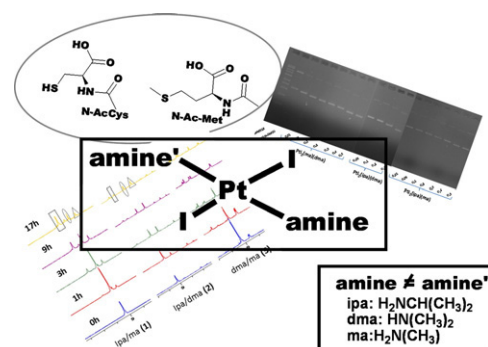


Thalia Parro, María Angeles Medrano, Leticia Cubo, Sandra Muñoz-Galván, Amancio Carnero, Carmen Navarro-Ranninger, Adoración G. Quiroga

Journal of Inorganic Biochemistry 127 (2013) 182–187

The second generation of iodido complexes: *trans*-[Pt₂(amine)(amine')] bearing different aliphatic amines

The antitumoral potential for platinum iodido complexes bearing different aliphatic amines was studied. One of the complexes is especially active towards cell lines where cisplatin has no effect. These complexes' interaction with biological models such as pBR322, 5'-GMP, 9EtG, N-AcMet and N-AcCys has been studied and compared to cisplatin's.

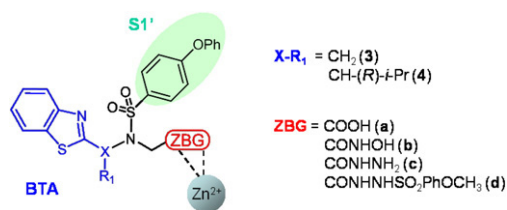


Sérgio M. Marques, Claudia C. Abate, Sílvia Chaves, Fernanda Marques, Isabel Santos, Elisa Nuti, Armando Rossello, M. Amélia Santos

Journal of Inorganic Biochemistry 127 (2013) 188–202

New bifunctional metalloproteinase inhibitors: an integrated approach towards biological improvements and cancer therapy

A new set of bifunctional MMP inhibitors bearing a benzothiazole moiety reveals high inhibitory activity (sub-nanomolar to high micromolar) against MMP2 and also high anti-proliferative activity of A2780 ovarian cancer cell line. These properties combined with the high resistance to hydrolysis suggest that these compounds may be considered for a new generation of anti-cancer MMPi.

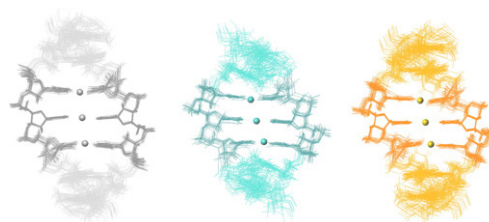


Sadhana Kumbhar, Silke Johannsen, Roland K.O. Sigel, Mark P. Waller, Jens Müller,

Journal of Inorganic Biochemistry 127 (2013) 203–210

A QM/MM refinement of an experimental DNA structure with metal-mediated base pairs

QM/MM geometry optimizations of an NMR structure of a DNA duplex with silver(I)-mediated base pairs led to additional distance constraints that were successfully applied in re-refining the original NMR structure, leading to a higher resolution experimental structure.

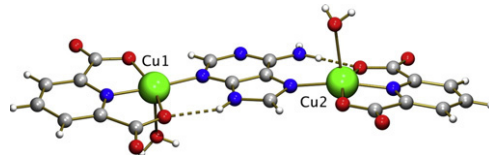


María del Pilar Brandi-Blanco, Duane Choquesillo-Lazarte, Alicia Domínguez-Martín, Antonio Matilla-Hernández, Josefa María González-Pérez, Alfonso Castiñeiras, Juan Niclós-Gutiérrez

Journal of Inorganic Biochemistry 127 (2013) 211–219

Molecular recognition modes between adenine or adeninium(1+) ion and binary M^{II}(pdc) chelates (M=Co–Zn; pdc = pyridine-2,6-dicarboxylate(2-) ion)

M^{II}(pdc) chelates (Co–Zn) recognize H(N9)adenine via the M–N7 bond and the N6–H···O interligand interaction irrespective of the coordination geometry, the different hydrates of the ternary complexes and the neutral or cationic adenine coligand. μ₂-Hade mode (figure) involves Cu–N3 and Cu–N7 bonds and the N9–H···O and N6–H···O interactions, respectively.



Leonardo Toso, Guido Crisponi, Valeria M. Nurchi, Miriam Crespo-Alonso, Joanna I. Lachowicz, M. Amelia Santos, Sergio M. Marques, Juan Niclós-Gutiérrez, Josefa M. González-Pérez, Alicia Domínguez-Martín, Duane Choquesillo-Lazarte, Zbigniew Szewczuk

Journal of Inorganic Biochemistry 127 (2013) 220–231

A family of hydroxypyrrone ligands designed and synthesized as iron chelators

A series of iron chelators composed by two kojic units joined by different linkers was synthesized. These molecules are easy and cheap to produce. Their structural characterization, the protonation and the iron^{III} complex formation equilibria studied by potentiometry, UV–Vis spectrophotometry, ESI-MS and ¹H NMR spectroscopy are presented.



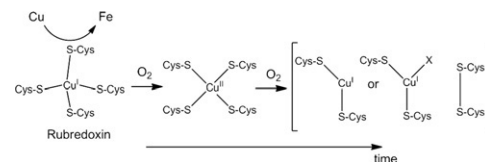
Metals in Proteins

Anders Thapper, Alberto C. Rizzi, Carlos D. Brondino, Anthony G. Wedd, Ricardo J. Pais, Biplab K. Maiti, Isabel Moura, Sofia R. Pauleta, José J.G. Moura

Journal of Inorganic Biochemistry 127 (2013) 232–237

Copper-substituted forms of the wild type and C42A variant of rubredoxin

The interplay between Cu(I) and Cu(II) in sulfur-rich protein environments is studied in the copper-substituted forms of the wild-type rubredoxin from *Desulfovibrio vulgaris* Hildenborough and of its variant C42A-rubredoxin. The results emphasize the redox instability of $\text{Cu}^{\text{II}}\text{-(S-Cys)}_n$ centers.

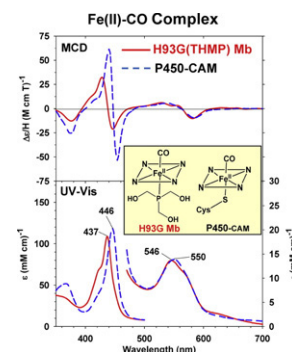


Shengfang Sun, Masanori Sono, John H. Dawson

Journal of Inorganic Biochemistry 127 (2013) 238–245

Mono- and bis-phosphine-ligated H93G myoglobin: Spectral models for ferrous-phosphine and ferrous-CO cytochrome P450

Ferric/ferrous tris(hydroxymethyl)phosphine (THMP)-H93G myoglobin (Mb) complexes having THMP/X (X = none, THMP, imidazole, CO and O_2) heme axial ligand(s) have been prepared and examined here with UV-visible and magnetic circular dichroism (MCD) spectroscopy. Interestingly, THMP/CO- (shown here, a hyperporphyrin) and bis-THMP-bound ferrous H93G Mb exhibited P450-type UV-Vis and MCD spectra.

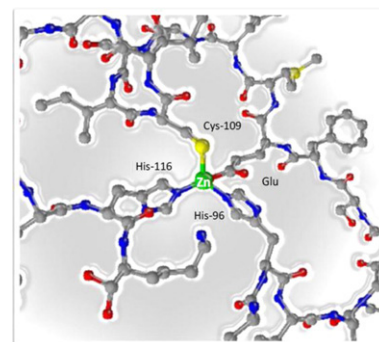


Slawomir Potocki, Daniela Valensin, Francesca Camponeschi, Henryk Kozłowski

Journal of Inorganic Biochemistry 127 (2013) 246–252

The extracellular loop of IRT1 ZIP protein – the chosen one for zinc?

Zinc complexes with the extracellular loop of IRT1, a ZIP family protein from *Arabidopsis thaliana*, has been studied. The complexes with the Ac-(95) MHVLPDSFEMLSICLEENPWHK(117)- NH_2 peptide revealed surprisingly high thermodynamic stability. The relative IRT1 stability has been shown using several Zn^{2+} complexes with multi-cysteine sequences.

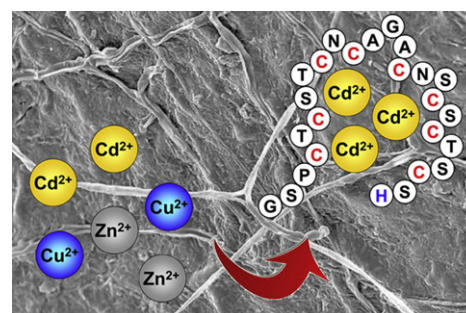


Jens Loebus, Barbara Leitenmaier, Diana Meissner, Bianca Braha, Gerd-Joachim Krauss, Dirk Dobritzsch, Eva Freisinger

Journal of Inorganic Biochemistry 127 (2013) 253–260

The major function of a metallothionein from the aquatic fungus *Heliscus lugdunensis* is cadmium detoxification

The aquatic fungus *Heliscus lugdunensis*, occurring in a spring highly contaminated with heavy metal ions, expresses a metallothionein that is exclusively induced by Cd^{2+} ions, which is unprecedented so far. Spectroscopic analyses reveal different coordination modes for Zn^{2+} and Cd^{2+} at a physiologically relevant concentration range.



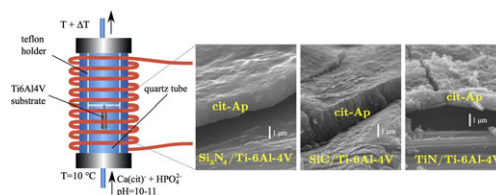
Metals in Biomineralization

**José Manuel Delgado-López,
Michele Iafisco, Isaac Rodríguez-Ruiz,
Jaime Gómez-Morales**

Journal of Inorganic Biochemistry 127 (2013)
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Bio-inspired citrate-functionalized apatite thin films crystallized on Ti–6Al–4V implants pre-coated with corrosion resistant layers

Crystallization of citrate-apatite (cit-Ap) on Ti–6Al–4V implants pre-coated with corrosion resistant layers of Ni_3Si_4 , SiC and TiN by induction heating method using Ca-citrate/phosphate metastable flowing solutions.



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