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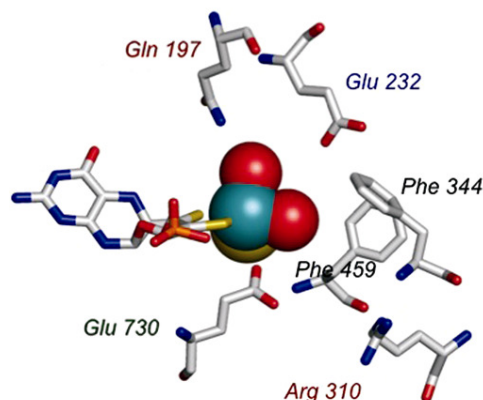
NUMBER 3-4

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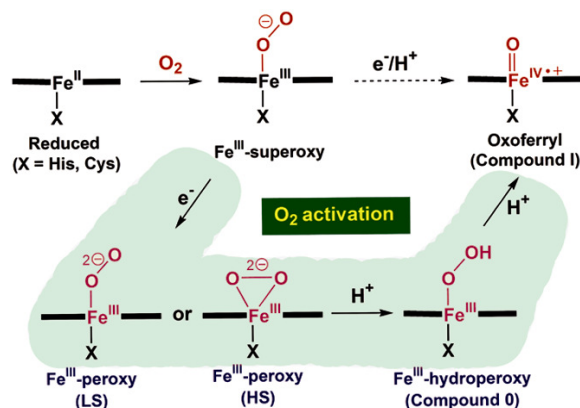
Advances in Contemporary Research

- 355 **Substrate orientation and the origin of catalytic power in xanthine oxidoreductase** Recent efforts towards understanding the role of active site amino acid residues in accelerating reaction rate have been reviewed.



Hongnan Cao, James Pauff & Russ Hille*

- 363 **Probing dioxygen activation mechanisms in heme-containing enzymes by heme models** Recent synthetic model studies on the mechanism of dioxygen reduction reaction involved in cytochrome *c* oxidase as well as on the dioxygen binding and activation associated with general heme-containing enzymes have been summarized.



Jin-Gang Liu & Yoshinori Naruta*

374 Bacterial model systems for cytochrome *c* oxidase biogenesis

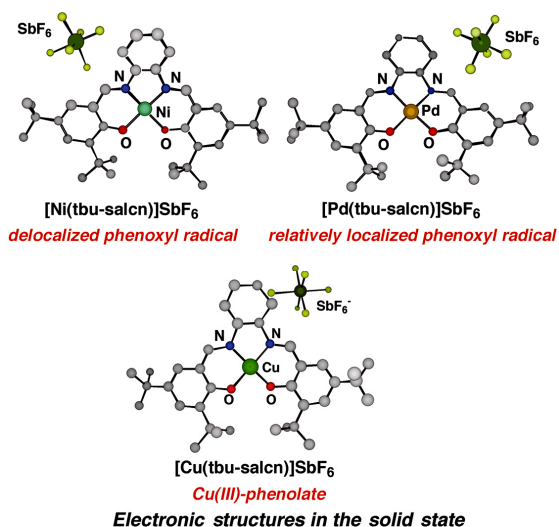
Biogenesis of the enzyme is a complex process involving up to 30 accessory proteins in higher eukaryotes. The chaperones required during early biogenesis steps have been reviewed, with special emphasis on the bacterial counterparts.



A Hannappel, F A Bundschuh, P Greiner,
M Alles, C Werner, O M Richter & B Ludwig*

383 Recent advances in metal-phenoxyl radical chemistry

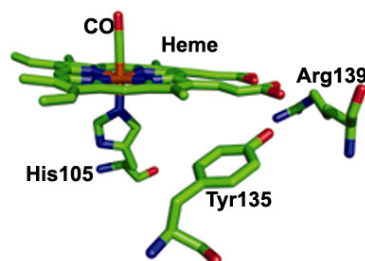
The phenolate ligand is well-known as one of the non-innocent ligands in inorganic and coordination chemistry. This review focuses on metal-phenolate complexes and their one-electron oxidized species and compares the properties of the metal-phenoxyl and high-valent metal-phenolate complexes.



Yuichi Shimazaki* & Osamu Yamauchi*

- 395 **Differences between two active forms of CO-bound soluble guanylate cyclase in the presence of activators and substrate and their populations revealed by resonance Raman spectroscopy**

Effects of exogenous compounds, YC-1 and BAY 41-2272, on CO-bound soluble guanylate cyclase are discussed. Structural changes of heme, including the vinyl and propionate side chains, upon binding of YC-1/BAY 41-2272 play an important role in the activation of this enzyme.

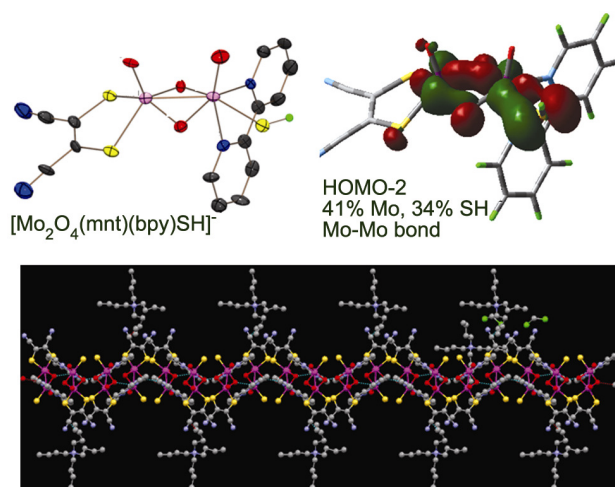


Biswajit Pal & Teizo Kitagawa*

Papers

- 401 **Hydrosulfido molybdenum(V) complexes in relevance to xanthine oxidase**

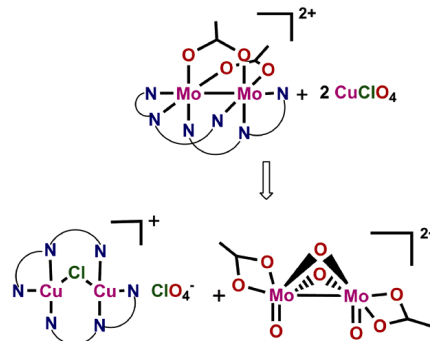
Rare hydrosulfido coordinated Mo(V) complexes are synthesized in relevance to xanthine oxidase. The dimeric form, and not the monomeric form, could be stabilized due to high reactivity. DFT calculations show involvement of Mo and S (from SH) orbitals in HOMO.



Joyee Mitra & Sabyasachi Sarkar*

- 409** Perchlorate reduction to chloride by the dimolybdenum(II) core: Making a case for molybdenum cofactor (MoCo) in the perchlorate reductase enzyme

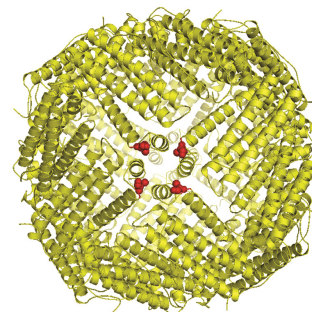
Ligand-transfer reaction from quadruply bonded $[\text{Mo}^{\text{II}}\equiv\text{Mo}^{\text{II}}]$ core to $[\text{Cu}^{\text{I}}\dots\text{Cu}^{\text{I}}]$ unit proceeds with concomitant reduction of $\text{ClO}_4^- \rightarrow \text{Cl}^-$.



Moumita Majumdar & Jitendra K Bera*

- 414** Moving iron in ferritin: Leucine 154, a residue near Fe(III) during mineral buildup minimizes mineral dissolution

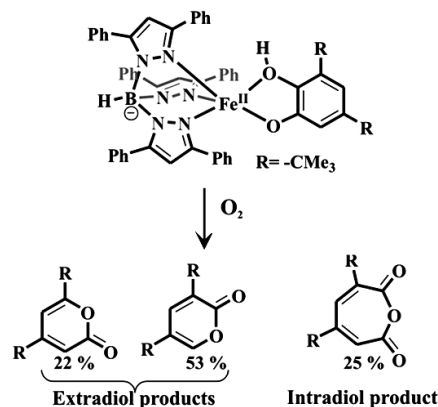
Mineral dissolution from eukaryotic ferritin protein nanocages is influenced by conserved residue leucine 154. The residue (illustrated in red) is identified by proximity to ferric oxo mineral nuclei by NMR; view from the inside of the ferritin protein cage (yellow polypeptide helices). Each L154 residue is at the entry to the mineralization cavity, $\sim 60\%$ of the protein cage volume, from each of the 24-subunit nucleation channels, and, because of cage geometry, in a group of four L154 residues around the four-fold axes of the cage



Suranjana Haldar, Takehiko Tosha & Elizabeth C Theil*

- 420** Iron(II)-catecholate complexes of a monoanionic facial N_3 ligand: Structural and functional models of the extradiol cleaving catechol dioxygenases

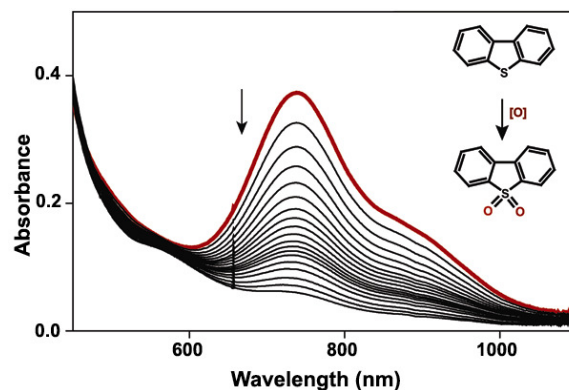
The iron(II)-3,5-di-*tert*-butylcatecholate complex of hydrotris(3,5-diphenylpyrazole-1-yl)borate ligand reacts with dioxygen to selectively give extradiol cleavage products of catechol.



Sayantan Paria, Partha Halder, Biswarup Chakraborty & Tapan Kanti Paine*

- 427 **Oxidation of dibenzothiophene by mononuclear non-heme iron complexes: A biomimetic approach for oxidative desulphurization**

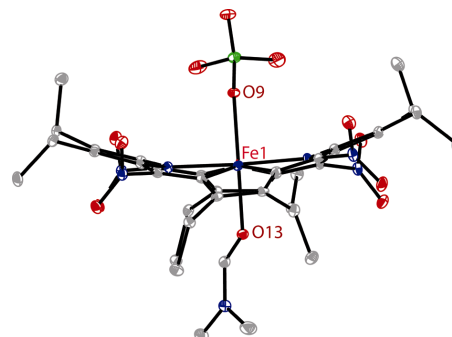
Anil Kumar Vardhaman, Subhajit Sikdar & Chivukula V Sastri*



- 432 **Synthesis, structure and properties of a high-spin Fe(III) porphyrin with non-equivalent axial ligands: Implications for the hemoproteins**

Arvind Chaudhary, Ranjan Patra & Sankar Prasad Rath*

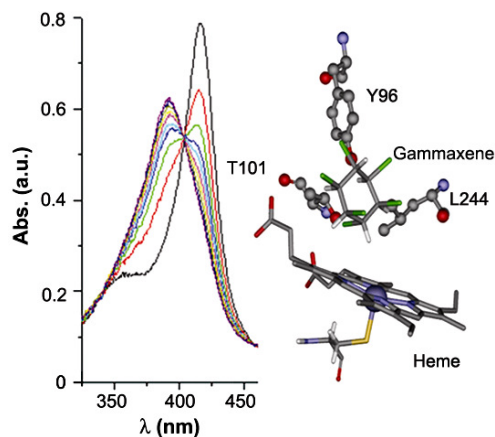
Synthesis and X-ray structure of a six-coordinate (porphinato)iron(III) derivative, having mixed-axial ligation of perchlorate and dimethylformamide with no displacement of metal in a nonplanar porphyrinic environment, is reported for the first time.



- 438 **Interaction of gammaxene with site specific mutants of cytochrome P450_{cam}**

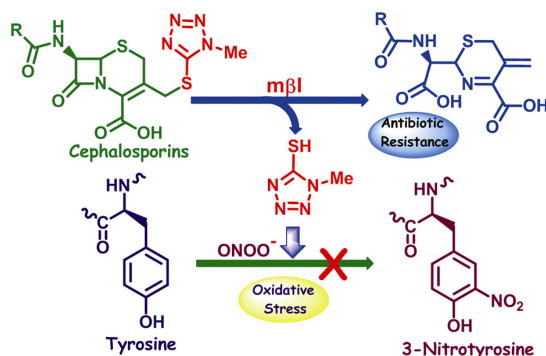
Saptaswa Sen, Soumen Kanti Manna & Shyamalava Mazumdar*

Site-specific mutation studies of cytochrome P450_{cam} show that Y96F, Y96F/L244A and Y96F/T101V mutants of the enzyme bind and metabolize the halogenated pesticide, gammaxene, making them potential green biocatalysts for environmental applications.



- 447 Effect of β -lactamase-catalyzed hydrolysis of cephalosporins on peroxynitrite-mediated nitration of serum albumin and cytochrome c

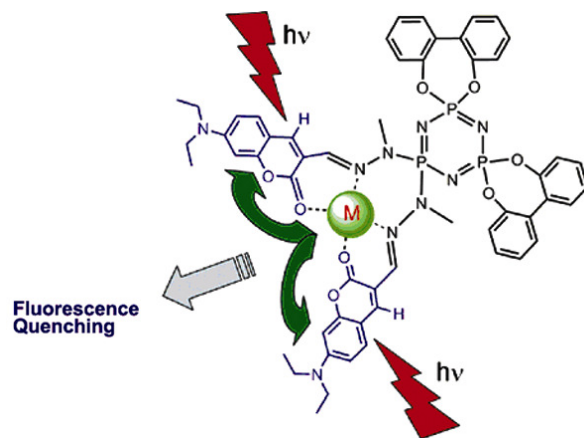
Some cephalosporin-based antibiotics effectively inhibit peroxynitrite-mediated protein tyrosine nitration upon hydrolysis by β -lactamase. The inhibition is mainly due to the elimination of heterocyclic thiol/thione moieties from cephalosporins by the β -lactamase-mediated hydrolysis.



Surendar Reddy Jakka & Govindasamy Mugesh*

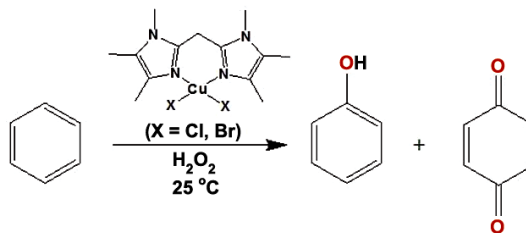
- 453 A phosphorus-supported coumarin-containing ligand as a fluorescence probe for detection of Cu(II) and Ag(I) ions

A phosphorus-supported fluorescent probe, $N_3P_3(O_2C_{12}H_8)_2[N(Me)N=CHR]_2$, ($RCHO = 7$ -diethylamino-coumarin-3-aldehyde) has been synthesized by the condensation of *gem*- $N_3P_3(O_2C_{12}H_8)_2[N(Me)NH_2]_2$ with 7-diethylamino-coumarin-3-aldehyde. It is shown to be an excellent fluorescence-based chemosensor of Cu^{2+} and Ag^+ ions in aqueous solutions.



Vadapalli Chandrasekhar*, Mrituanjay D Pandey, Biswanath Das, Bani Mahanti & Tapas Senapati

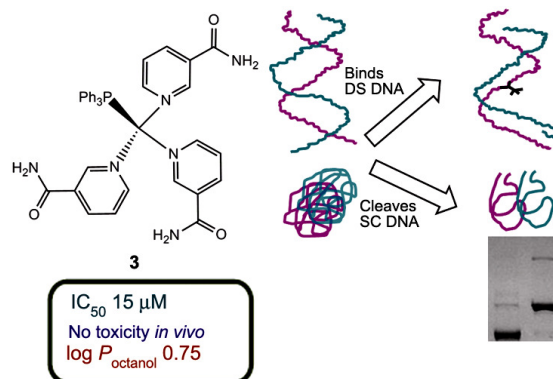
- 459 Catalytic oxidation of benzene by mononuclear copper(II) complexes with a bis(imidazolyl)methane ligand



Mana Goto, Yuji Kajita & Hideki Masuda*

- 465 **Copper(I) complexes of modified nucleobases and vitamin B3 as potential chemotherapeutic agents: *In vitro* and *in vivo* studies**

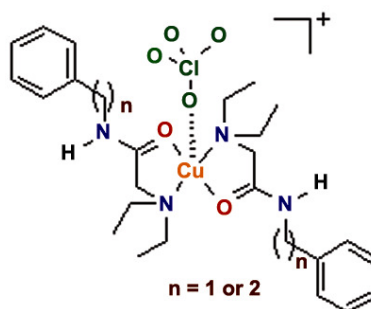
Thionucleobase and nicotinamide containing copper(I) phosphine complexes with potent anticancer activities are reported.



N J M Sanghamitra, M K Adwankar, A S Juvekar, V Khurajjam, C Wycliff, A G Samuelson*

- 474 **Synthesis, structure and anticancer activity of copper(II) complexes of *N*-benzyl-2-(diethylamino)acetamide and 2-(diethylamino)-*N*-phenylethylacetamide**

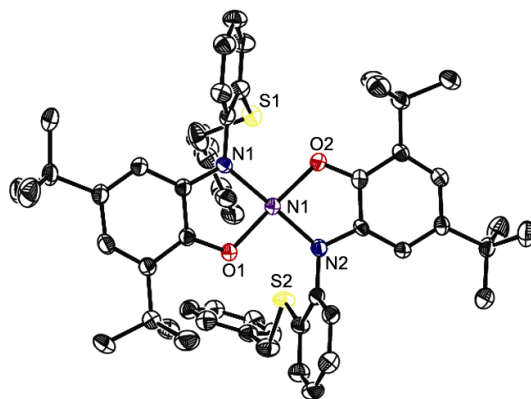
Two copper(II) complexes have been synthesized with two new bidentate amide-based ligands. Anti-proliferative studies against the U87 and HeLa cancerous cells indicate promising cytotoxicity. Despite potent *in vitro* activity, both complexes exhibit diminished cytotoxicity against the normal human HEK cells.



Amit P Singh, Nagendra K Kaushik, Akhilesh K Verma & Rajeev Gupta*

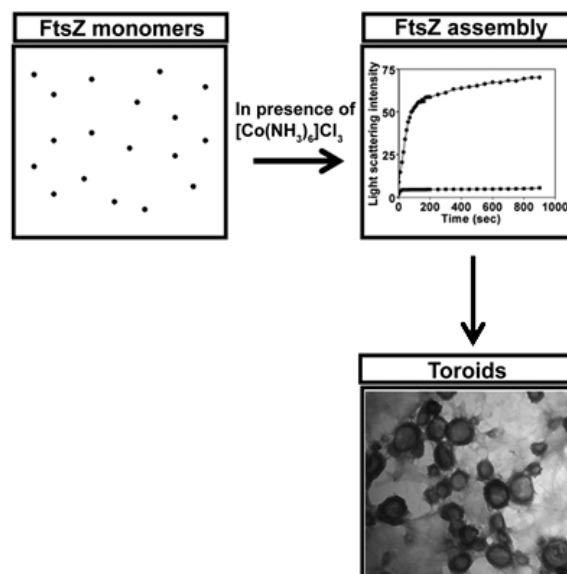
- 484 **Bidentate coordination of a potentially tridentate ligand. A mononuclear four-coordinate Ni(II) complex supported by two *o*-iminobenzosemiquinonato units**

A potentially tridentate ligand with *N,O,S* donor sites coordinates to a Ni^{II} ion as a bidentate ligand, utilizing only *N* and *O* donor sites in its *o*-iminobenzosemiquinonato(1-) π -radical form.



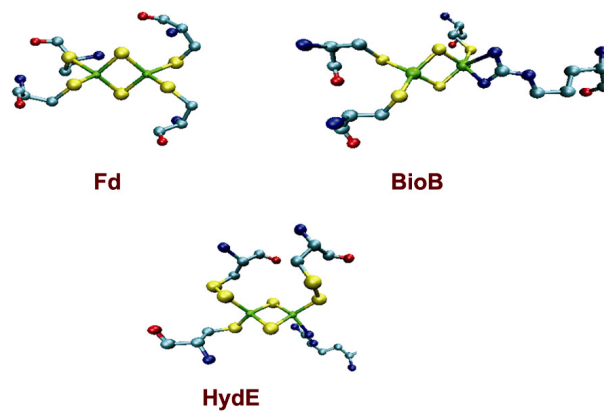
Atasi Mukherjee & Rabindranath Mukherjee*

- 491 Cobalt hexamine trichloride induced toroidal condensation of FtsZ



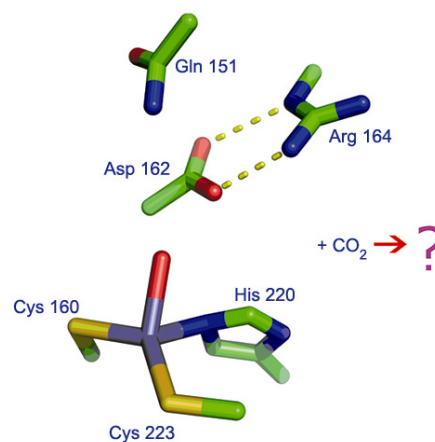
Anuradha Kuchibhatla, Jayesh Bellare & Dulal Panda*

- 498 Density functional theory calculations on Fe_2S_2 clusters: Effect of ligand environment on geometric/electronic structure and reduction potential



Abhishek Dey

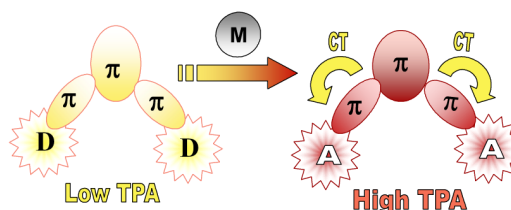
- 503 Density functional theory investigations of the catalytic mechanism of β -carbonic anhydrase



V Hakkim, V Rajapandian & V Subramanian*

- 511 **A comparative study of third-order optical nonlinearity of symmetrical dipolar chromogenic probes and their enhancement by different metal ions**

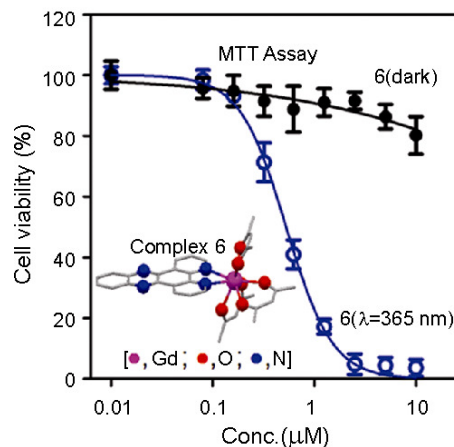
Three dipolar NLO-phores consisting of different conjugation lengths as well as binding sites have been synthesized to obtain symmetrical D- π -D systems. In presence of metal ions, these dipolar moieties transform into A- π -A systems showing very large two-photon absorption cross-section values.



Atanu Jana, Jong Min Lim, Sun Woo Park,
Dongho Kim* & Parimal K Bharadwaj*

- 519 **Photocytotoxicity and DNA photocleavage activity of La(III) and Gd(III) complexes of phenanthroline bases**

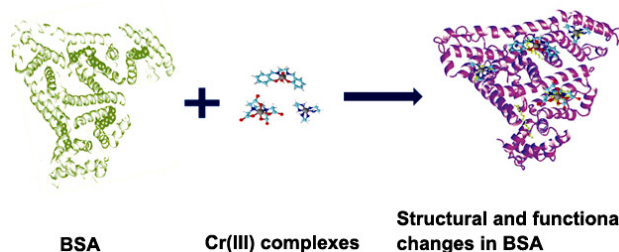
The lanthanum(III) and gadolinium(III) complexes of dipyrrophenazine base show significant photo-induced plasmid DNA cleavage activity and photocytotoxicity in HeLa cancer cells in UV-A light of 365 nm. The dark toxicity of the dppz base is significantly reduced upon binding to the lanthanide(III) ions, while retaining its photocytotoxicity.



Akhtar Hussain, Sounik Saha, Ritankar Majumdar,
Rajan R Dighe & Akhil R Chakravarty*

- 531 **Chromium(III) mediated conformational changes associated with alterations in the enzymatic activity of BSA: Influence of the coordinated ligand**

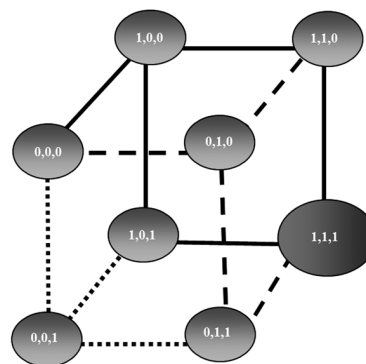
The structural and functional changes brought about in BSA due to interaction with Cr(III) complexes is largely dependent on the ligand environment of the complex.



Natesasn Sella Raja, H Yamini Shrivastava &
Balachandran Unni Nair*

539 Structural basis for preferential Ca^{2+} -displacement by a paramagnetic ion (Ce^{3+}) in non-myristoylated neuronal calcium sensor-1

The relative specificity of the individual Ca^{2+} -binding sites present in a 190 amino acid long neuronal calcium sensor protein ($M^r = 23$ kDa) has been studied at the microscopic level by NMR by looking at the Ca^{2+} -displacement by a paramagnetic metal ion (Ce^{3+}).



Kousik Chandra, A L Susmitha, Y Sharma & K V R Chary*

Authors for correspondence are indicated by (*)