

3rd BioXAS Study WE

<i>POSTER number</i>	<i>TITLE</i>	<i>Authors</i>
PO-01	Inorganic Physiology : Distribution and speciation of metal Ions in cells	<p style="text-align: center;">Carol Fierke¹, Matthew Kidd¹, Thomas V. O'Halloran³, James E. Penner-Hahn^{1,2}, Janet Wolford³, and Nathan Zahler¹</p> <p style="text-align: center;"><i>¹Department of Chemistry and ²Biophysics Research Division, The University of Michigan, Ann Arbor, MI 48109-1055 USA. ³Department of Chemistry, Northwestern University,</i></p>
PO-02	K β -detected high resolution XANES in models of catechol oxygenase	<p style="text-align: center;">Ana Mijovilovich^a, Hisashi Hayashi^b, Naomi Kawamura^c, Hitoshi Osawa^c, Pieter C.A.Bruijninx^d, Robert J.K. Klein Gebbink^d, Frank M.F. de Groot^a and Bert M. Weckhuysen^a</p> <p style="text-align: center;"><i>^aInorganic Chemistry and Catalysis, Faculty of Science, Utrecht University, , Utrecht, The Netherlands ^bJapan Women's University, 2-8-1, Mejirodai, Bunkyo-ku, Tokyo, 112-8681, Japan. ^cJAERI-SPring8, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5198, Japan ^dOrganic Chemistry and Catalysis, Faculty of Science, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands</i></p>
PO-03	X-Ray Absorption Spectroscopic Analysis of Plastocyanin and its Complexes with Cytochrome f and Photosystem I: the Methionine-Copper Coordination and its Relevance to Electron Transfer.	<p style="text-align: center;">Díaz-Moreno, I.^a, Díaz-Moreno, S.^b, Subías, G.^c, De la Rosa, M.A. 1 & <u>Díaz-Quintana, A.</u>^a</p> <p style="text-align: center;"><i>^aInstituto de Bioquímica Vegetal y Fotosíntesis. Universidad de Sevilla-CSIC. ^bDiamond Light Source Ltd. Rutherford Appleton Laboratory. Oxford, U.K. ^c Instituto de Ciencia de Materiales de Aragón. Universidad de Zaragoza-CSIC.</i></p>

PO-04	Determination of structural parameters of cobalt cysteine complexes combining EXAFS experiments and molecular dynamics Simulations	<p>Carole Bresson^a, Riccardo Spezia^b, <u>Pier Lorenzo Solari</u>^c and Christophe Den Auwer^d</p> <p>^a CEA Saclay, DEN/DPC/SECR/LSRM, 91191 Gif sur Yvette, France</p> <p>^b LAMBE, UMR CNRS 8587, Université d'Evry-Val-d'Essonne, 91025 Evry Cedex, France</p> <p>^c SOLEIL, BP48 Saint Aubin, 91192, Gif sur Yvette, France</p> <p>^d CEA Marcoule, DEN/DRCP/SCPS, 30207 Bagnols sur Cèze Cedex, France</p>
PO-05	Study of Cu,Zn superoxide dismutase in extreme pressure conditions: interest in combining X-ray diffraction and BioXAS	<p>I. Ascone¹, A. Cognigni², E. Girard¹, A.-C. Dhaussy³ R. Kahn⁴ & R. Fourme¹</p> <p>¹ Synchrotron-Soleil, Saint Aubin, France</p> <p>² Synchrotron Elettra, Italy</p> <p>³ CRISMAT/ENSI Caen</p> <p>⁴ IBS, Grenoble, France</p>
PO-06	EXAFS study of native and oxidized states of proteus mirabilis catalase combination with Mössbauer spectroscopy and DFT calculations	<p><u>Pier Lorenzo Solari</u>^a and H�el�ene Marie Jouve^b</p> <p>^a SOLEIL, BP48 Saint Aubin, 91192, Gif sur Yvette, France</p> <p>^b Institut de Biologie Structurale Jean-Pierre Ebel, CEA/CNRS/UJF, 41 rue Jules Horowitz, 38027 Grenoble Cedex 1, France</p>
PO-07	MARS: The Radioactive Matter Beamline for Diffraction and Absorption at the SOLEIL Synchrotron	<p><u>Pier Lorenzo Solari</u>^a, Herv�e Hermange^a and Bruno Sitaud^a</p> <p>^a SOLEIL, BP48 Saint Aubin, 91192, Gif sur Yvette, France</p>
PO-08	The Monte-Carlo Method in XAS: from Classical usage to Model Selection Tools	<p>Emmanuel CURIS^a, Ioannis NICOLIS^a, Patrick DESCHAMPS^a, Simone BENAZETH^a</p> <p>^a Laboratoire de biomath�ematiques, Facult�e de pharmacie, universit�e Paris Descartes, 4, avenue de l'Observatoire, F-75006 Paris, France,</p>

PO-09	Towards automatic BioXAS refinement - ABRA	<p style="text-align: center;"><u>Gerd Wellenreuther^a</u>, Wolfram Meyer-Klaucke^a</p> <p>^a <i>European Molecular Biology Laboratory, Hamburg outstation, Notkestr. 85, 22603 Hamburg, Germany</i></p>
PO-10	Element-Selective Valence Electron Configuration by X-Ray Emission Spectroscopy	<p style="text-align: center;">GLATZEL Pieter</p> <p style="text-align: center;">ESRF</p>
PO-11	Structural analysis of cyanomet-MB and carbon monoxy-Mb active site through first-principles xanes ca	<p style="text-align: center;">M. Arfaoui ^a, D. Cabaret ^a, S. Della Longa ^b and F. Mauri ^a</p> <p><i>a IMPMC, UMR 7590, CNRS, Université Pierre et Marie Curie (Paris 6), Université Denis Diderot (Paris 7), IPGP, 140 rue de Lourmel 75015 Paris, France</i></p> <p><i>b Dipartimento di Medicina Sperimentale, Università dell'Aquila, I-67100 L'Aquila, Italy</i></p>
PO-12	Structural characterization of binuclear and mononuclear copper centres of metalloproteins and models	<p style="text-align: center;">Elena Borghi</p> <p><i>Università di Roma "La Sapienza", Dipartimento di Chimica, p.le A. Moro, 5, I-00185 Roma, Italy</i></p>