

3MT TRAINEE ACHIEVEMENTS 2008-2009

PUBLICATIONS

1. Song, K., Campbell, A. J.,* Bergonzo, C.,* de los Santos, C., Grollman, A.P., & Simmerling, C. (2009). An Improved Reaction Coordinate for Nucleic Acid Base Flipping Studies. *Journal of Chemical Theory and Computation*, submitted April 2009.
2. Scharer, O. D., & Campbell, A. J.* (2009). Wedging out DNA damage. *Nature Structural and Molecular Biology* 16, 102-104.
3. Cohn, C.A., Pedigo, C.E. Hylton, S.N.,* Simon, S.R. & Schoonen, M.A.A. (2009). Evaluating the use of 3' -(p-Aminophenyl) fluorescein for determining particulate-induced formation of highly reactive oxygen species. *Geochemical Transactions*, in review April 2009.
4. Emmetsberger, J.,* Mirrione, M.,* Zhou, C., Fernandez-Monreal, M., & Tsirka, S. (2009) Tissue Plasminogen Activator promotes neuronal survival against zinc toxicity by interacting with the zinc transporter ZIP4. *Journal of Cell Biology*, submitted April 2009.
5. Barros, C. S., Nguyen, T.,* Spencer, K. S. R., Nishiyama, A., Colognato, H. & Müller, U. (2009) Beta1 integrins are essential for CNS myelination and promote Akt-dependent myelin outgrowth. *Development*, acceptance pending revision submitted April 2009.
6. Benotti, M. J., Fisher, S.,* Furlong, E. T., & Brownawell, B. J.... (2009). Occurrence and transport of pharmaceuticals in shallow groundwater on Long Island. *Ground Water*, in review April 2009.

CONFERENCES AND WORKSHOPS

Bergonzo, C.,* & Simmerling, C. (2008, August). Hamiltonian replica exchange molecular dynamics and its application to biologically relevant protein motions. Poster session presented at The 236th ACS National Meeting, Philadelphia, PA.

Bergonzo, C,* & Simmerling, C. (2008, October). Collective protein motions studied through a combination of coarse-grain and atomistic models. Poster session presented at The 2nd Annual ICB&DD Symposium, "Frontiers in Chemical Biology and Drug Discovery," Stony Brook, NY.

Bergonzo, C.,* Song, K. & Campbell, A.J.,* de los Santos, C., Grollman, A.P., & Simmerling, C. (2009, February). Base Flipping Mechanism of DNA Repair Enzyme Fpg Examined via Nudged Elastic Band Simulations. Poster session presented at the 49th Annual Sanibel Symposium, St. Simons Island, GA.

Bergonzo, C.,* & Simmerling, C. (2009, March). Modification of the Nudged Elastic Band Code in Amber11. Poster session presented at The AMBER (Assisted Model Building with Energy Refinement) Developers Meeting, Sanibel Island, FL.

Bobiak, M.,* & Bogenhagen, D. (2009, February). ABH7 is a Mitochondrial Protein that Catalyzes the Direct Reversal of 1,N⁶-Ethenoadenine. Poster session presented at The 3rd US/EU Conference of Endogenous Genome Damage, Galveston TX.

Campbell, A. J.,* Song, K., Guainazzi, A., Scharer, O. & Simmerling, C. (2008, October) Modeling DNA Interstrand Crosslinks to Validate Experimental Analogs. Poster session presented at The 2nd Annual ICB&DD Symposium, "Frontiers in Chemical Biology and Drug Discovery," Stony Brook, NY.

Guainazzi, A., Angelov, Campbell, A. J.,* Scharer, O. & Simmerling, C. (2008, October). Exploring structure and biochemistry of nitrogen mustard interstrand crosslinks through synthetic analogs. Poster session presented at The 2nd Annual ICB&DD Symposium, "Frontiers in Chemical Biology and Drug Discovery," Stony Brook, NY.

Campbell, A. J.,* Song, K., Guainazzi, A., Scharer, O. & Simmerling, C. (2008, May). Modeling Damaged DNA using Molecular Dynamics Simulations. Poster session presented at The ACS 40th Mid-Atlantic Regional Meeting, Queens, NY.

Guainazzi, A., Campbell, A. J.* Angelov, T., Simmerling, C. & Scharer, O. (2008, May). Exploring structure and biochemistry of nitrogen mustard interstrand crosslinks through synthetic analogs. Poster session presented at The ACS 40th Mid-Atlantic Regional Meeting, Queens, NY.

Guainazzi, A., Campbell, A. J.,* Angelov, T., Simmerling, C. & Scharer, O. (2009, February). Synthesis and Molecular Modeling of Nitrogen Mustard Interstrand Crosslinks. Poster session presented at Gordon Research Conferences: Mammalian DNA Repair, Ventura, CA.

Dutton, J.* & Nick Fisher (2008, May). Intraspecific differences in metal bioaccumulation in the Atlantic silverside (*Menidia menidia*) inferences regarding the effects of key biological processes. Poster session presented at the 2008 IGERT Project Meeting, Arlington, VA.

Dutton, J.* & Nick Fisher (2008, November). Assessing the bioaccumulation of metals in killifish (*Fundulus heteroclitus*), a bioindicator organism. Poster session presented at The SETAC North America 29th Annual Meeting, Tampa, FL.

Emmetsberger, J.,* Heppner, F.L., & Tsirka, S.E. (2008, November). The spatio-temporal distribution of microglia determines microglial neuroprotective and neurotoxic behaviors following spinal cord injury. Poster session presented at 38th Annual Meeting of the Society for Neuroscience, Washington, DC.

Emmetsberger, J.* (2008, July) Attended and participated in workshops at the Glia in Health & Disease Conference, Cold Spring Harbor Laboratory, Cold Spring Harbor, NY.

Emmetsberger, J.,* Mirrione, M. M.,* Zhou, C., Fernandez-Monreal, M., & Tsirka, S.E. (2009, March-April). Tissue Plasminogen Activator Promotes Neuronal Survival Against Zinc Toxicity by Interacting with the Zinc Transporter ZIP4. Oral presentation at The Molecular and Cellular Plasminogen Activation Conference, Cold Spring Harbor, NY.

Fisher, S.,* Hylton, S.,* Brownawell, B., and Schoonen, M.A.A. (2008, November). Hydroxyl radical-specific oxidation of phenylalanine by pyrite in model biological and marine environments. Poster session presented at The SETAC North America 29th Annual Meeting, Tampa, FL.

Fisher, S.* (2008, November). Attended and participated in the Mass Spectrometry Short Course at The SETAC North America 29th Annual Meeting, Tampa, FL.

Hylton, S.* (2008, October). Served as a biological sciences poster judge at the HBCU-UP National Research Conference, Atlanta, GA.

Morgan, K,* Cabana, J., Sideris, P., Kim, J., Nielsen, U. G. & Grey, C. P..(2008, August). Sorption and structural studies of manganese oxides via ²³Na MAS NMR. Poster session presented at The 236th ACS National Meeting, Philadelphia, PA.

Morgan, K,* Cabana, J., Sideris, P., Kim, J., Nielsen, U. G. & Grey, C. P. (2008, December). Investigation of Sodium Manganese Oxide Model Compounds and Local Environments of Sodium in Synthetic Analogues of Naturally Occurring Manganese Oxides by ²³Na Solid State NMR. Poster session presented at the Synchrotron Environmental Science IV Meeting, San Francisco, CA.

Nguyen, T.,* & H. Colognato, (2008, July). Beta 1 integrin regulates oligodendrocyte development and CNS myelination. Platform presentation at the Glia in Health & Disease Conference, Cold Spring Harbor Laboratory, Cold Spring Harbor, NY.

Nguyen, T.* (2008, October) Attended workshops and recruited at the SACNAS (Society for Advancement of Chicanos and Native Americans) National Conference: "International Polar Year: Global Change in Our Communities," Salt Lake City, UT.

AWARDS

Emmetsberger, J. (2008, September). Van der Kloot Award for Excellence in Teaching. Presented at the Annual Fall Symposium of the Graduate Program in Molecular and Cellular Pharmacology, Old Field, NY.