
BIOGRAPHICAL SKETCH

Provide the following information for the key personnel and other significant contributors.
Follow this format for each person. **DO NOT EXCEED FOUR PAGES.**

NAME Kristen A. Marino	POSITION TITLE Postdoctoral Fellow		
eRA COMMONS USER NAME N/A			
EDUCATION/TRAINING (<i>Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.</i>)			
INSTITUTION AND LOCATION	DEGREE (if applicable)	YEAR(s)	FIELD OF STUDY
Lehigh University, Bethlehem, PA	B.S.E	2004	Chemical Engineering
Princeton University, Princeton, NJ	Ph.D.	2009	Chemical Engineering
University of Amsterdam, the Netherlands	Post-doc	2009-2011	Comp. Chem. & Biology
École Normale Supérieure, Paris, France	Post-doc	2012-2013	Comp. Chemistry
UCL, London, UK	Post-doc	2013-2015	Comp. Chem. & Biology
Icahn School of Medicine at Mount Sinai	Post-doc	2015-	Comp. Struct. Biology

A. Personal Statement

My research interests lie in applying enhanced sampling techniques to understand the molecular level mechanisms of pharmaceutically relevant proteins, which occur on timescales unattainable by traditional molecular dynamics (MD). I recently joined the group of Marta Filizola in the Department of Chemical and Structural Biology at the Icahn School of Medicine at Mount Sinai to further my training by studying a key pharmaceutical target, GRCRs. After completing my Ph.D. in the group of Emily A. Carter in the Department of Chemical Engineering at Princeton University studying the kinetics and thermodynamics of diffusion in NiAl, I moved to the group of Peter G. Bolhuis at the University of Amsterdam. In Amsterdam, I used enhanced sampling techniques, replica-exchange and transition interface sampling, to examine the effect of confinement on protein folding. I then moved to the group of Damien Laage at École Normale Supérieure to use QM/MM simulations to study the role of water molecules in catalysis in organic solvents. Prior to joining the Filizola group, I was a Marie Curie Fellow with Francesco L. Gervasio at UCL in London where I used parallel-tempering metadynamics to understand the effect of a key oncogenic mutation on the conformational changes of the B-Raf kinase. The information gleaned from this work could provide a valuable pathway for the development of novel kinase inhibitors to treat melanoma.

B. Positions and Honors

Positions

2004-2009	Graduate student, Department of Chemical Engineering, Princeton University
2009-2011	Postdoctoral Research Associate, Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, the Netherlands
2012-2013	Postdoctoral Research Associate, Department of Chemistry, École Normale Supérieure, Paris, France
2013-2015	Marie Curie Research Fellow, Department of Chemistry, University College London, London, UK
2015-	Postdoctoral Research Associate, Department of Chemical and Structural Biology, Icahn School of Medicine at Mount Sinai, New York, NY

Honors

2011	Marie Curie Intra-European Fellowship for Career Development
2014	Outstanding Poster Award, Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery Meeting, September 2014, Istanbul, Turkey

C. Selected peer-reviewed publications

1. K. A. Marino and E. A. Carter, "First-Principles characterization of Ni diffusion kinetics in β -NiAl" *Phys. Rev. B*, **78** (2008) 184104.
2. K. A. Marino and E. A. Carter, "The effect of platinum on diffusion kinetics in β -NiAl: Implications for thermal barrier coatings lifetime" *ChemPhys Chem*, **10** (2009) 226.
3. K. A. Marino and E. A. Carter, "The effect of platinum on Al diffusion kinetics in β -NiAl: Implications for thermal barrier coating lifetime" *Acta Materialia* **58** (2010) 2726.
4. K. A. Marino, B. Hinnemann, and E. A. Carter, "Atomic-scale insight and design principles for turbine engine thermal barrier coatings from theory" *Proceedings of the National Academy of Sciences of the U.S.A.*, **108** (2011) 5480.
5. W. Du, K. A. Marino, and P. G. Bolhuis, "Multiple state transition path sampling of alanine dipeptide in explicit solvent" *Journal of Chemical Physics*, **135** (2011) 145102.
6. K. A. Marino and P. G. Bolhuis, "Confinement-induced states in the folding landscape of the Trp-cage miniprotein" *Journal of Physical Chemistry B*, **116** (2012) 11872.
7. H. Meuzelaar, K. A. Marino, A. Huerta-Viga, M. R. Panman, L. E. J. Smeenk, A. J. Kettelarij, J. H. van Maarseveen, P. Timmerman, P. G. Bolhuis, and S. Woutersen, "Folding dynamics of the Trp-cage miniprotein: Evidence for a native-like intermediate from combined time-resolved vibrational spectroscopy and molecular dynamics simulations" *Journal of Physical Chemistry B*, **117** (2013) 11490.

D. Research Support

COMPLETED (last three years)

Marie Curie Actions, FP7/2007-2013, Grant Number 299136; Improving the selectivity of kinase inhibitors: Characterizing binding mechanisms of inhibitors targeting inactive states and allosteric site; 02/01/2013-02/28/2015