Steven K. Albanese

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EDUCATION

PH.D., Biomedical Sciences: Cancer Biology, Gerstner Sloan Kettering 2014-present

Committee: John D. Chodera (thesis advisor, MSKCC), Sarat Chandarlapaty(MSKCC), Daniel A. Heller(MSKCC)

Robert Abel (Schrödinger, Inc)

B.A., Biological Sciences, Chemistry, Cornell University, cum laude 2010-14

RESEARCH EXPERIENCE

Gerstner Sloan Kettering, Ph.D. research with John D. Chodera 2015-present

Selective kinase inhibitor design, computational modeling of hyperactivating mutations in mTOR, laboratory

automation, kinase inhibitor resistance, allosteric regulation of Aurora Kinase A

Schrödinger, Inc, Summer Internship in the Desmond Dev Group

Worked with Lingle Wang to use FEP+ to predict kinase inhibitor selectivity

Cornell University, Undergraduate research with Holger Sondermann 2011-14

Developing high-throughput screen for atlastin-1 drug design, identification and characterization of atlastin-1 binding partners.

ACADEMIC LEADERSHIP EXPERIENCE

Gerstner Sloan Kettering Student Council, Co-Chair	2015-2017
Experimental Therapeutics Symposium at Gerstner Sloan Kettering, Organizer	2016
Biology Scholars Program, Cornell University, Study Group Leader	2011-2014

AWARDS AND HONORS

B.A. awarded *cum laude* for original research from Cornell University 2014

SCIENCE COMMUNICATION AND OUTREACH

Judge for Three Minute Thesis Competition at Weill Cornell and Gerstner Sloan Kettering	2017
Organizer for Experimental Therapeutics Symposium at Gerstner Sloan Kettering	2016
Recruiter for Gerstner Sloan Kettering at SACNAS	2016
Volunteer with Rockefeller University Outreach: Lab Experiences, program to introduce NYC public school	2015-present
students to scientific research	
Recruiter for Gerstner Sloan Kettering at Annual Biomedical Research Conference for Minority Students	2015

PROFESSIONAL MEMBERSHIP

New York Academy of Sciences	2014-present
Biophysical Society	2015-2016

Summer 2017

TALKS AND POSTERS

Rational approach to selective inhibitor design using multitarget constraints Poster, Workshop on Free Energy Methods in Drug Design: Targeting Cancer - Boston, MA Albanese SK, Grinaway P, Hanson S, Rodriguez L, Tan Z, Chodera JD	2016
Simulating mTOR hyperactivating mutations to understand functionally significant structural rearrangements Poster, 60th Annual Biophysical Society Meeting - Los Angeles, CA Albanese SK, Xu J, Hsieh J, Chodera JD	2016
Simulating mTOR hyperactivating mutations to understand functionally significant structural rearrangements Poster, Protein Kinases in Drug Discovery Conference - San Diego, CA Albanese SK, Xu J, Hanson S, Fass J, Hsieh J, Chodera JD	2017
Using physical modeling to direct biophysical experiments and predict the functional impact of clinical cancer mutations in kinases on drug susceptibility	2017

Talk, EMBO Workshop: Integrating genomics and biophysics to comprehend functional genetic variation - Turin, Italy Albanese SK, Parton D, Hauser K, Negron C, Hanson S, Rodriguez-Laureano L, Isik M, Wang L, Abel R, Chodera JD

Using physical modeling to direct biophysical experiments and predict the functional impact of clinical cancer mutations in kinases on drug susceptibility

Talk, Med Into grad Symposium: Precision Medicine - Columbia University, New York, NY **Albanese SK**, Parton D, Hauser K, Negron C, Hanson S, Rodriguez-Laureano L, Isik M, Wang L, Abel R, Chodera JD

PUBLICATIONS

 st asterisks or † daggers denote that marked authors contributed equally

Xu J, Pham CG, Albanese SK, Dong Y, Oyama T, Lee CH, Rodrik-Outmezguine V, Yao Z, Han S, Chen D, Parton DL, Chodera JD, Rosen N, Cheng EH, and Hsieh JJ.

Mechanistically distinct cancer-associated mTOR activation clusters predict sensitivity to rapamycin. Journal of Clinical Investigation 126:3529, 2016 \cdot DOI

We use massively parallel distributed molecular simulations on Folding@home to probe the mechanism activating mutations of the mTOR kinase identified in clinical populations.

Ruff EF, Muretta JM, Thompson A, Lake E, Cyphers S, **Albanese SK**, Hanson SM, Behr JM, David DD, Chodera JD, Levinson NM

A dynamic mechanism for allosteric activation of Aurora kinase A by activation loop phosphorylation. *eLife* 7:e32766, 2018 · DOI

MD modeling of AURKA to investigate impact of TPX2 and phosphorylation on structure using massively parallel simulations on Folding@Home. We also modeled DEER experiments by simulation spin probe-labeled AURKA in different conformations and conditions

Intelkofer A, Shih A, Wang B, Nazir A, Rustenburg A, **Albanese SK**, Patel M, Famulare C, Arcila M, Taylor J, Tallman M, Roshal M, Petsko G, Chodera JD, Thompson C, Levine R, Stein E

Acquired clinical resistance to IDH inhibition through in trans IDH2 mutations. In Press, Nature Medicine \cdot Structural modeling of the clinical mutants

Hauser K, Negron C, Albanese SK, Ray S, Wang L, Lupyan D, Steinbrecher T, Abel R, and Chodera JD Accurately predicting targeted kinase inhibitor resistance to clinical Abl mutations using alchemical free-energy calculations. In Press, Nature Communications Biology ·

We show how alchemical free energy calculations can be used to predict whether clinical point mutations in human kinase domains confer resistance or susceptibility to targeted kinase inhibitors

Albanese SK*, Parton DL*, Rodriguez-Laureano L † , Isik M † , Hanson SM, Behr J, Gradia S, Jeans C, Seeliger M, Levinson N, Chodera JD

An open library of human kinase domain constructs for automated bacterial expression. Preprint at bioR χ v, In press ACS Biochemistry

Designed, automated, and executed thermophoretic melt experiments and biophysical binding measurements to demonstrate the proteins were folded, identified and test expressed clinically observed mutants, wrote the manuscript











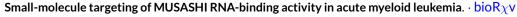
Preprints, Submitted and Under Review

 * asterisks or † daggers denote that marked authors contributed equally

Wojnarowicz P, Desai B, Chin Y, Lima e Silva R, Ohnaka M, Lee SB, Cao MG, Ouerfelli O, Xu S, Goldgur Y, Miller M, Chaudhary J, Garland W, Stoller G, Albanese SK, Soni R, Philip J, Healey J, Vinagolu R, Norton L, Rosen N, Hendrickson R, Iavarone A, Dannenberg A, Chodera JD, Pavletich N, Lasorella A, Campochiaro P, Benezra R. A small-molecule pan Id antagonist, AGX51, shows strong anti-tumor and anti-neovascular activity In revision

We identify the binding site of a new small-molecule pan-Id antagonist prior to its confirmation by mass spectrometry crosslinking data

Minuesa G, **Albanese SK**, Chow A, Schurer A, Park S, Rotsides CZ, Taggart J, Rizzi A, Naden L, Chou T, Gourkanti S, Cappel D, Passarelli M, Fairchild L, Adura C, Glickman FJ, Schulman J, Famulare C, Patel M, Eibl JK, Ross GM, Tan DS, Leslie CS, Beuming T, Goldgur T, Chodera JD, Kharas MG



Physical modeling and free energy calculations for an RNA-competitive small molecule inhibitor of Musashi

