

# Steven K. Albanese



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## EDUCATION

- 2014-present **Ph.D., Biomedical Sciences: Cancer Biology, Gerstner Sloan Kettering**  
Committee: [John D. Chodera](#) (Thesis Advisor, MSKCC), [Sarat Chandarlapaty](#) (MSKCC),  
[Daniel A. Heller](#) (MSKCC), [Robert Abel](#) (Schrödinger, Inc)  
2010-14 **B.A., Biological Sciences, Chemistry, Cornell University, cum laude**

## RESEARCH EXPERIENCE

- 2015-present **Gerstner Sloan Kettering**, Ph.D. research with [John D. Chodera](#)  
Applications of free energy calculations, molecular dynamics, and automated biophysical measurements to understand the selectivity of small molecule kinase inhibitors, the functional impact of clinical kinase mutations, and kinase conformational dynamics. Performed physical modeling on a number of academic drug discovery projects resulting in novel tool compounds.
- Summer 2017 **Schrödinger, Inc**, Summer Internship in the Desmond Dev Group  
Worked with Lingle Wang to use FEP+ to predict kinase inhibitor selectivity
- 2011-14 **Cornell University**, Undergraduate research with [Holger Sondermann](#)  
Developing high-throughput screen for atlastin-1 drug design, identification and characterization of atlastin-1 binding partners.

## ACADEMIC LEADERSHIP AND TEACHING

- 2018 Gerstner Sloan Kettering Core Course, **Teaching Fellow**  
2015-2017 Gerstner Sloan Kettering Student Council, **Co-Chair**  
2016 Experimental Therapeutics Symposium at Gerstner Sloan Kettering, **Organizer**  
2011-2014 Biology Scholars Program, Cornell University, **Study Group Leader**

## Mentorship

- 6/18-present **Erin Grundy, Technician**  
*High-throughput cloning and protein purification, measurements of small molecule kinase inhibitor affinities, cell free protein expression*
- Summer 2018 **Jessica Tom, Summer Undergraduate Researcher**  
*Large-scale protein purification of human Abl kinase mutants, measurements of small molecule kinase inhibitor affinities to mutant kinases*  
Current position: Undergraduate Student, **Stonybrook University**  
Lucelenie Rodríguez-Laureano, **Technician**
- 12/17-7/18 *Measurements of small molecule kinase inhibitor affinities, fluorescence-based thermostability assays*  
Current position: Medical Student, **NYU School of Medicine**

## AWARDS AND HONORS

- 2014      B.A. awarded *cum laude* for original research from Cornell University  
2013      Summer Institute of Life Sciences ([SILS](#)) Research grant, Cornell University

## SCIENCE COMMUNICATION AND OUTREACH

- 2017      Three Minute Thesis Competition at Weill Cornell and Gerstner Sloan Kettering, **Judge**  
2015, 2017    [Annual Biomedical Research Conference for Minority Students](#), **Recruitment for GSK**  
2016      Experimental Therapeutics Symposium at Gerstner Sloan Kettering, **Organizer**  
2016      [SACNAS](#) Conference, **Recruitment for GSK**  
2015-present    [LAB Experience Program](#), **Volunteer**  
*Program at Rockefeller University that introduces NYC public school students to scientific research through a molecular biology laboratory exercise and case studies*  
2013      Undergraduate Research Discussion, [Prefreshman Summer Program](#) at Cornell University, **Panelist**

## PROFESSIONAL MEMBERSHIP

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

## TALKS AND POSTERS

- 2016      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
- 2017      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  
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
- 2017      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
- 2018      Using physical modeling to direct biophysical experiments and predict the functional impact of clinical cancer mutations in kinases on drug susceptibility  
Invited Chalk Talk, Gerstner Sloan Kettering 5th Biennial Retreat- Gerstner Sloan Kettering, New Paltz, NY  
**Albanese SK**, Parton D, Hauser K, Negron C, Hanson S, Rodriguez-Laureano L, Isik M, Wang L, Abel R, Chodera JD

## PUBLICATIONS

\* asterisks or † daggers denote that marked authors contributed equally

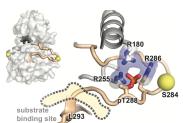


Xu J, Pham CG, **Albanese SK**, Dong Y, Oyama T, Lee CH, Rodrik-Outmezguine V, Yao Z, Han S, Chen D, Parton DL, Chodera JD, Rosen N, Cheng EH, and Hsieh JJ

### Mechanistically distinct cancer-associated mTOR activation clusters predict sensitivity to rapamycin

*Journal of Clinical Investigation* 126:3529, 2016 · [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.

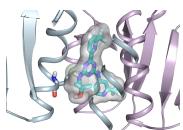


Ruff EF, Muretta JM, Thompson A, Lake E, Cyphers S, **Albanese SK**, Hanson SM, Behr JM, David DD, Chodera JD, Levinson NM

### 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

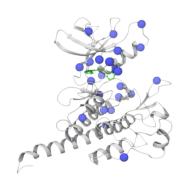


Intelkofer A, Shih A, Wang B, Nazir A, Rustenburg A, **Albanese SK**, Patel M, Famulare C, Arcila M, Taylor J, Tallman M, Roshal M, Petsko G, Chodera JD, Thompson C, Levine R, Stein E

### Acquired clinical resistance to IDH inhibition through *in trans* IDH2 mutations.

*Nature*, 559(7712):125-129, 2018 · [DOI](#)

Structural modeling of the clinical mutants that cause resistance to an IDH inhibitor

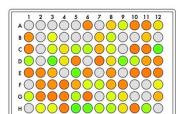


Hauser K, Negron C, **Albanese SK**, Ray S, Wang L, Lupyan D, Steinbrecher T, Abel R, and Chodera JD

### Accurately predicting targeted kinase inhibitor resistance to clinical Abl mutations using alchemical free-energy calculations.

*Communications Biology* 1, Article number: 70, 2018 · [DOI](#)

The emergence of resistance mutations are a significant problem in precision cancer therapy. As it becomes routine to collect sequencing data for cancer patients, it is increasingly apparent that the vast majority of missense mutations in kinases – for which more than 36 small molecule inhibitors are available – are rare enough that no information will be available as to whether these mutations might have therapeutic implications by inducing resistance to certain inhibitors. Here, we take the first steps toward using physical modeling to predict individualized therapeutic response, assessing how accurately the impact of clinical Abl mutations on inhibitor binding affinity can be predicted. Our results suggest free energy calculations are a promising tool for aiding therapeutic decision making.



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

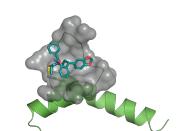
### An open library of human kinase domain constructs for automated bacterial expression.

*Biochemistry* 7:57(31):4675-4689, 2018 · [DOI](#)

We engineer a library of human kinase domains with useful bacterial expression using a novel phosphatase coexpression technique. We used automated thermophoretic melt experiments and biophysical binding measurements to demonstrate the proteins were folded with well formed ATP-binding sites. We also identified and test expressed clinically observed mutants to demonstrate the constructs utility for studying resistance and the development of next-generation inhibitors.

## 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, Stolberg 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

### Small-molecule targeting of MUSASHI RNA-binding activity in acute myeloid leukemia

bioRxiv

We use free energy calculations and docking to identify a putative binding site and likely interactions for an RNA-competitive small molecule inhibitor of Musashi