

Stephanie A. (Mullane) Wankowicz, Ph.D.
Scientific Program Director, Prism
Astera Institute

Education

2023 University of California, San Francisco, San Francisco, CA (PhD, Biophysics; Advisor: James S. Fraser)
2013 University of Massachusetts, Amherst, Amherst, MA (BS, Biochemistry and Molecular Biology)

Academic Appointments

06/2026 - Present Assistant Adjunct Professor, Molecular Physiology and Biophysics, Vanderbilt University
06/2025 - 05/2026 Assistant Professor, Computer Science, Vanderbilt University
12/2024 - 05/2026 Assistant Professor, Biochemistry, Vanderbilt University
08/2024 - 05/2026 Assistant Professor, Molecular Physiology and Biophysics, Vanderbilt University

Employment

05/2026 - Present Scientific Program Director, Prism, Astera Institute, Emeryville, CA
03/2023 - 07/2024 Assistant Professional Researcher, University of California, San Francisco, San Francisco, CA
08/2018 - 02/2023 Graduate Research Assistant, University of California, San Francisco, San Francisco, CA
04/2016 - 07/2018 Computational Biologist, Broad Institute of MIT & Harvard/Dana-Farber Cancer Institute, Boston, MA
06/2013 - 04/2016 Senior Research Data Specialist, Medical Oncology, Dana-Farber Cancer Institute, Boston, MA

Professional Organizations

2024 - 2026 Member, Center for Applied AI in Protein Dynamics, Vanderbilt University
2024 - 2026 Member, Center for Structural Biology, Vanderbilt University
2023 - Present Member, American Crystallographic Association
2023 - Present Member, Biophysical Society
2020 - Present Member, Protein Society

Professional Activities

Intramural: Service, Outreach, Leadership

2025 - 2026 VU School of Medicine Education Strategic Planning Committee
2025 - 2026 VU Computational Resources Faculty Advisory Board
2025 - 2026 Founder and Organizer, VU BioCoDE (Biomedical and Computational Discovery Experience)
2026 VU Center for Structural Biology Retreat Co-Organizer
2025 VU Molecular Physiology & Biophysics Retreat Co-Organizer
2021 - 2023 UCSF Biophysics Peer/Alumni Mentorship Co-Leader
2020 - 2023 UCSF Biophysics Executive Committee

Extramural: Service, Outreach, Leadership

Ad hoc reviewing for the following publications/conferences: *Biochemistry*, *Biophysical Journal*, *Biorxiv*, *Current Opinions in Structural Biology*, *Nature*, *Nature Chemical Biology*, *NeuroIPS*, *PLoS*, *PNAS*, *Protein Science*

2026 Co-organizer, CCP4 Study Weekend
2025 NSF Reviewer
2025 - 2026 Editorial Board Member, Biophysical Journal
2024 - Present Co-organizer, Conformational Ensembles Modeling Conference

Awards/Honors

2026 George M. Sheldrick Award for Contributions to Structural Science, American Union of Crystallography
2024 Rising Stars in Biophysics and Biochemistry, University of Pennsylvania
2023 Clements Award (Best Thesis Award), UCSF
2023 AViDD Mentored Project Award
2023 Intersection Science Fellow
2022 Mentorship Award, UCSF
2021 D.E. Shaw Research Computational Chemistry Fellowship

2020 NSF Graduate Research Fellowship
2020 Discovery Fellowship, UCSF
2016 Winner, MIT Healthcare Hackathon, Primary Care
2013 Commonwealth Honors College Scholar with Greatest Distinction, UMass Amherst
2013 Distinguished Teaching Award, Biochemistry Department, UMass Amherst
2013 George N. Parks Music Leadership Award, UMass Amherst
2012 Distinguished Teaching Award, Biochemistry Department, UMass Amherst

Teaching Activities

Instructor of Record

Molecular Biophysics Training Program Seminar Series, Vanderbilt University - 2025-2026 (contact hours: 20)
Chemical & Physical Biology Discourse & Disquisitions, Vanderbilt University, Course Director - Fall 2024 (contact hours: 38)
Computing for Biophysicists, UCSF, Co-Instructor – Fall 2023 (contact hours: 20)
Biophysics First Year Onboarding, UCSF, Co-organizer – Fall 2020-2022

Other Teaching Instruction

MBTP Journal Club Leader - Winter 2025, 2026
IGP Week in AI Lecture - What do we need to be able to predict protein dynamics accurately? – Winter 2025, 2026
Vanderbilt Data Science Institute Lecture - Predicting how proteins wiggle and jiggle – Winter 2025

Research Supervision

Graduate Students

2024 - 2026 Tonnar Castellano, Chemical & Physical Biology

Graduate Students (Rotations):

Fall 2025, Joseph Crammer, QBC
Summer 2025, Jason Wang, MSTP
Spring 2025, Weizhi (Erika) Cao, QBC
Winter 2025, Tatum Murdock, IGP
Fall 2024, William Harrison, IGP
Fall 2024, Joshua Huang, IGP
Fall 2024, Tonnar Castellano, QBC
QBC=Quantitative & Chemical Biology, IGP=Interdisciplinary Graduate Program; MSTP=Medical Scientist Training Program

Undergraduate Students:

2024 - 2026 Ahmed Alsam, Biochemistry & Computer Science
2024 - 2026 Souella Lou, Biochemistry (*VU Immersion Summer Research Award*)
2025 Carol Xi, Neuroscience & Computer Science (*Nucleate Summer Research Award*)

Research Program

Completed Funding

Co-PI: Wankowicz -2025-2027 Infrastructure to Enable Dynamic Structural Biology. Astera Institute; \$675,000 over 2 years; 25% effort
Co-I: Wankowicz (PI: Fraser) - 2026-2027 Aligning Experiments and Language Models to Improve Protein Function Prediction. DARPA; \$350,000 direct costs per year over 1 year; 25% effort
PI: Wankowicz - 2025 Protein Structural Bioinformatics Tools. Vanderbilt University Provost's Faculty Grant for Immersion Vanderbilt; \$10,000 over 1 year; 0% effort
PI: Wankowicz - 2025 Exploiting differences in the structural dynamics of kinases to achieve selective inhibitor binding. American Cancer Society Pilot Grant; \$60,000 direct costs over 1 year; 0% effort
Co-I: Wankowicz (PI: Krogan) - QCRG Pandemic Response Program 2023-2024 NIAID U19AI171110 62% effort

Other Publications: *corresponding author, #co-first author

1. Srivastava V, Mai H, Collins M, Holton JM, Wall M, Wankowicz SA*. **WaterFlow: Prediction of Ordered Water Molecule Positions on Protein Structures**. *BioRxiv*, 2026.

2. **Wankowicz SA***. (2026) *Recovering Conformational Heterogeneity from the Protein Data Bank at Scale*. The Stacks.
3. Holton J, **Wankowicz SA***. (2026) *Supplying a user-defined bulk solvent map for refinement*. The Stacks.
4. Chrispens K, Collins M, Fraser JS, Mai D, van den Bedem H, **Wankowicz SA***. (2026) *Sampleworks: A modular platform for experimentally guided biomolecular ensemble generation*. The Stacks.
5. Miller CA, **Wankowicz SA***. (2026) *Binding Entropy Can Be Predicted by Crystallographic Ensembles*. eLife.
6. **Wankowicz SA***, Bonomi M. (2026) *From Possibility to Precision in Macromolecular Ensemble Prediction*. Nature Methods.
7. Seo L, Farran I, Aslam A, Li X, Jaishankar P, Ashworth A, Fraser JS, Renslo A, **Wankowicz SA*** (2025) *Crystallographic Ensembles Reveal the Structural Basis of Binding Entropy in SARS-CoV2 Macrodomein*. bioRxiv.
8. **Wankowicz SA***, Fraser JS. (2025) *Advances in uncovering the mechanisms of macromolecular conformational entropy*. Nature Chemical Biology.
9. **Wankowicz SA***. (2025) *10 Rules for a Structural Bioinformatic Analysis*. PLOS Computational Biology.
10. Jin M, Seed RI, Cai G, Shing T, Wang L, Ito S, Cormier A, **Wankowicz SA**, Jespersen JM, Baron JL, Carey ND, Campbell MG, Yu Z, Tang PK, Cossio P, Wen W, Lou J, Marks J, Nishimura SL, Cheng Y. (2024) *Dynamic allostery drives autocrine and paracrine TGF- β signaling*. Cell.
11. **Wankowicz SA***. (2024) *Modeling Bias Toward Binding Sites in PDB Structural Models*. BioRxiv.
12. Flowers J, Echols N, Correy G, Jaishankar P, Togo T, Renslo A, van den Bedem H, Fraser J, **Wankowicz SA***. (2025) *Expanding Automated Multiconformer Ligand Modeling to Macrocycles and Fragments*. eLife.
13. **Wankowicz SA***, Ravikumar A, Sharma S, Riley BT, Raju A, van den Bedem H, Keedy DA, Fraser JS. (2024). *Automated Multiconformer Building in X-ray Crystallography and CryoEM*. eLife.
14. **Wankowicz SA***, Fraser JS. (2024). *Comprehensive encoding of conformational and compositional protein structural ensembles through the mmCIF data structure*. IUCrJ.
15. Du S, **Wankowicz SA**, Yabukarski F, Doukov T, Hershlag, Fraser JS. (2023). *Refinement of Multiconformer Ensemble Models from Multi-temperature X-ray Diffraction Data*. Methods in Enzymology.
16. Lawson CL, Kryshchakovich A, Adams PD, Afonine PV, Baker ML, Barad Ba, Bond P, Burnley T, Cao R, Cheng J, Chojnowski G, Cowtan K, Dill KA, DiMaio F, Farrell DP, Fraser JS, Herzik MA, Wen Hoh S, Hou J, Hung L, Igaev M, Joseph AP, Kihara D, Kumar D, Mittal D, Monastyrskyy B, Olek M, Palmer CM, Patwardhan A, Perez A, Pfab J, Pintilie GD, Richardson JS, Rosenthal PB, Sarkar D, Schäfer LU, Schmid MF, Schröder GF, Shekhar M, Dong Si, Singharoy A, Terashi G, Terwilliger TC, Vaiana A, Wang L, Wang Z, **Wankowicz SA**, Williams CJ, Winn M, Wu T, Yu X, Zhang K, Berman H, Chiu W. (2021). *Cryo-EM model validation recommendations based on outcomes of the 2019 EMDDataResource challenge*. Nature Methods.
17. Riley BT, **Wankowicz SA**, de Oliveira SHP, van Zundert GCP, Hogan DW, Fraser JS, Keedy DA, van den Bedem H. (2021). *qFit 3: Protein and ligand multiconformer modeling for X-ray crystallographic and single particle cryo-EM density maps*. Protein Science.
18. Gitter A, Fraser JS, Gonen T, Patro R, Wayment-Steele HK, Williams A, Haibe-Kains B, Dunbrack RL, Cook C, Kundaje A, Hoffman MM, Carpenter AE, **Wankowicz SA**, Lindorff-Larsen K. (2024). *A renewed call for open artificial intelligence in biomedicine*. OSF Preprints.
19. **Wankowicz SA**, Beltrao P, Cravatt B, Dunbrack R, Gitter A, Lindorff-Larsen K, Ovchinnikov S, Polizzi N, Shoichet B, Fraser JS. (2024) *AlphaFold3 Transparency and Reproducibility*. Zenodo Preprint.
20. Diaz RE, **Wankowicz SA***. (2024) *Ten recommendations for hosting a Diversity, Equity, Inclusion, and Justice (DEIJ) journal club*. PLoS Computational Biology.
21. **Wankowicz SA**, de Oliveira SHP, Hogan DW, van den Bedem H, Fraser JS. (2022). *Ligand binding remodels protein side chain conformational heterogeneity*. eLife.
22. Tewari AK, Cheung ATM, Crowdis J, Conway JR, Camp SY, **Wankowicz SA**, Livitz DG, Park J, Lis RT, Boosma-Moody A, He MX, AlDubayan SH, Zhang Z, McKay RR, Leschiner I, Brown M, Balk S, Getz G, Taplin ME, Van Allen EM. (2021). *Molecular features of exceptional response to neoadjuvant anti-androgen therapy in high-risk localized prostate cancer*. Cell Reports.
23. Crowdis J, Balch S, Sterlin L, Thomas BS, Camp SY, Dunphy M, Anastasio E, Shah S, Damon AL, Ramos R, Sosa DM, Small IK, Tomson B, Nguyen CM, McGillicuddy M, Chastain PS, He MX, Cheung ATM, **Wankowicz SA**, Tewari AK, Kim D, AlDubayan SH, Dowdye A, Zola B, Nowak J, Manarite J, Gunn IH, Olson B, Lander ES,

Painter CA, Wagle N, Van Allen EM. (2021). *A patient-driven clinicogenomic partnership through the Metastatic Prostate Cancer Project*. Cell Genomics.

24. **Wankowicz SA**, Fraser JS. (2020). *Ensemble refinement produces consistent R-free values but smaller ensemble sizes than previously reported*. Computational Crystallography Newsletter.
25. Gordon DE, Jang GM, Bouhaddou M, Xu J, Obernier K, White KM, O'Meara MJ, Rezelj VV, Guo JZ, Swaney DL, Tummino TA, Huettenhain R, Kaake RM, Richards AL, Tutuncuoglu B, Foussard H, Batra J, Haas K, Modak M, Kim M, Haas P, Polacco BJ, Braberg H, Fabius JM, Eckhardt M, Soucheray M, Bennett MJ, Cakir M, McGregor MJ, Li Q, Meyer B, Roesch F, Vallet T, Mac Kain A, Miorin L, Moreno E, Chi Naing ZZ, Zhou Y, Peng S, Shi Y, Zhang Z, Shen W, Kirby IT, Melnyk JE, Chorba JS, Lou K, Dai SA, Barrio-Hernandez I, Memon D, Hernandez-Armenta C, Lyu J, Mathy CJ, Perica T, Pilla KB, Ganesan SJ, Saltzberg DJ, Rakesh R, Liu X, Rosenthal SB, Calviello L, Venkataramanan S, Liboy-Lugo J, Lin Y, Huang X, Liu Y, **Wankowicz SA**, Bohn M, Safari M, Ugur FS, Koh C, Savar NS, Tran QD, Shengjuler D, Fletcher SJ, O'Neal MC, Cai Y, Chang JC, Broadhurst DJ, Klippsten S, Sharp PP, Wenzell NA, Kuzuoglu D, Wang H, Trenker R, Young JM, Caverio DA, Hiatt J, Roth TL, Rathore U, Subramanian A, Noack J, Hubert M, Stroud RM, Frankel AD, Rosenberg OS, Verba KA, Agard DA, Ott M, Emerman M, Jura N, von Zastrow M, Verdin E, Ashworth A, Schwartz O, d'Enfert C, Mukherjee S, Jacobson M, Malik HS, Fujimori DG, Ideker T, Craik CS, Floor SN, Fraser JS, Gross JD, Sali A, Roth BL, Ruggero D, Taunton J, Kortemme T, Beltrao P, Vignuzzi M, García-Sastre A, Shokat KM, Shoichet BK, Krogan NJ. (2020). *A SARS-COV-2 protein interaction map reveals targets for drug repurposing*. Nature.
26. Newberry RW, Arhar T, Costello J, Hartoularos GC, Maxwell AM, Chi Naing ZZ, Pittman M, Reddy NR, Schwarz DM, Wassarman DR, Wu TS, Barrero D, Caggiano C, Catching A, Cavazos TB, Estes L, Faust B, Fink EA, Goldman MA, Gomez YK, Gordon MG, Gunsalus LM, Hoppe N, Jaime-Garza M, Johnson MC, Jones MG, Kung AF, Lopez KE, Lumpe J, Martyn C, McCarthy EE, Miller-Vedam LE, Navarro EJ, Palar A, Pellegrino J, Saylor W, Stephens CA, Strickland J, Torosyan H, **Wankowicz SA**, Wong Dr, Wong G, Redding S, Chow ED, DeGrado WF, Kampmann M. (2020). *Robust Sequence Determinants of alpha-Synuclein Toxicity in Yeast Implicate Membrane Binding*. ACS Chemical Biology.
27. Bellmunt J, Kim J, Reardon B, Perera-Bel J, Orsola A, Rodriguez-Vida A, **Wankowicz SA**, Bowden M, Barletta J, Morote J, de Torres I, Lloreta-Trull J, Mouw K, Taplin ME, Cejas P, Long H, Van Allen E, Getz G, Kwiatkowski D. (2020). *Genomic predictors of good outcome, recurrence, or progression in High grade T1 (HGT1) non-muscle invasive (NMI) bladder cancer*. Cancer Research.
28. Hwang JH, Seo J, Beshiri ML, **Wankowicz SA**, Liu D, Cheung A, Li J, Qiu X, Hong AL, Botta G, Golumb L, Richter C, So J, Sandoval GJ, Giacomelli AO, Ly SH, Han C, Dai C, Pakula H, Sheahan A, Piccioni F, Gjoerup O, Loda M, Sowalsky AG, Ellis L, Long H, Root DE, Kelly K, Van Allen EM, Freedman ML, Choudhury AD, Hahn WC. (2019). *CREB5 promotes resistance to androgen-receptor antagonists and androgen deprivation in prostate cancer*. Cell Reports.
29. Liu D, Abbosh P, Keliher D, Reardon B, Miao D, Mouw K, Weiner-Taylor A, **Wankowicz SA**, Han C, Teo T, Cipolla C, Kim J, Iyer G, Al-Ahmadie H, Dulaimi E, Chen DY, Alpaugh RK, Hoffman-Censits J, Garraway LA, Getz G, Carter SL, Bellmunt J, Plimack E, Rosenberg JE, Van Allen EM. (2019). *Mutational patterns in chemotherapy resistant muscle-invasive bladder cancer*. Nature Communications.
30. **Wankowicz SA**, Armenia J[#], Liu D[#], Gao J, Kundra R, Reznik E, Chatila WK, Chakravarty D, Han GC, Coleman I, Montgomery B, Pritchard C, Morrissey C, Barbieri CE, Beltran H, Sboner A, Zafeiriou Z, Miranda S, Bielski, CM, Penson, AV, Tolonen, C, Huang FW, Robinson, D, Wu YM, Lonigro, R, Garraway LA, Demichelis, F, Kantoff PW, Taplin, M., Abida W, Taylor BS, Scher HI, Nelson PS, de Bono JS, Rubin MA, Sawyers C., Chinnaiyan A, PCF/SU2C International Prostate Cancer Dream Team, Schultz, N., Van Allen, E.M. (2018). *The long tail of oncogenic drivers in prostate cancer*. Nature Genetics.
31. Miao D, Margolis C, Gao W, Voss MH, Li W, Martini D, Norton C, Bossé D, **Wankowicz SA**, Cullen D, Horak C, Wind-Rotolo M, Tracy A, Giannakis M, Hodi FS, Drake CG, Ball MW, Allaf ME, Snyder Charen A, Hellmann M, Ho T, Motzer RJ, Signoretti S, Kaelin Jr WG, Choueiri TK, Van Allen EM. (2018). *Genomic correlates of response to anti-PD-1/PD-L1 therapy in metastatic clear cell renal cell carcinoma*. Science.
32. Viswanathan SR, Ha G, Hoff AM, Wala JA, Carrot-Zhang J, Whelan, CW, Haradhvala NJ, Freeman SS, Reed, SC, Rhoades J, Polak P, Cipicchio M, **Wankowicz SA**, Wong A, Kamath T, Zhang Z, Gydush GJ, Rotem D, PCF/SU2C International Prostate Cancer Dream Team, Love JC, Getz G, Gabriel S, Zhang CZ, Dehm SM, Nelson PS, Van Allen EM, Choudhury AD, Adalsteinsson VA, Beroukhim R, Taplin ME, Meyerson M. (2018). *Structural alterations driving castration-resistant prostate cancer revealed by linked-read genome sequencing*. Cell.

33. Miao D, Margolis CA, Vokes NI, Liu D, Taylor-Weiner A, **Wankowicz SA**, Adeegbe D, Keliher D, Schilling B, Tracy A, Manos M, Chau N, Hanna G, Polak P, Rodig SJ, Signoretti S, Sholl L, Engelman J, Getz G, Janne PA, Haddad RI, Choueiri TK, Barbie DA, Haq R, Awad MM, Schadendorf D, Hodi FS, Bellmunt J, Wong KK, Hammerman P, Van Allen EM. (2018). *Genomic correlates of response to immune checkpoint blockade in microsatellite-stable solid tumors*. Nature Genetics.
34. **Wankowicz SA**, Maile B, Deutsch K, Hayden A, Brown E, Marsilje T, Caldwell B, Simoncell T, Van Allen EM. (2018). *Patient-driven efforts to liberate clinical cancer genomic data*. OSF Preprints.
35. **Wankowicz SA**, Velasco G[#], Madison R, Ali SM, Norton C, Duquette A, Ross JS, Bossé D, Lalani AKA, Miller VA, Stephens PJ, Young L, Hakimi AA, Signoretti SS, Pal SK, Choueiri TK. (2018). *Targeted genomic landscape of metastases compared to primary tumours in clear cell metastatic renal cell carcinoma*. British journal of cancer.
36. **Wankowicz SA**, Gild P[#], Sood A, von Landenberg N, Friedlander DF, Alanee S, Bellmunt J. (2018). *Racial disparities in quality of care and overall survival among muscle-invasive bladder cancer patients treated with radical cystectomy: A national cancer database*. The Journal of Urology.
37. Rodrigues DN, Rescigno P, Liu D, Yuan W, Carreira S, Lambros MB, Seed G, Mateo J, Riisnaes R, **Mullane S**, Margolis C, Miao D, Miranda S, Dolling D, Clarke M, Bertan C, Crespo M, Boysen G, Ferreria A, Sharp A, Figueiredo I, Keliher D, Aldubayan S, Burke K, Sumanasyriya S, Fontes M, Bianchini D, Zafeiriou Z, Mendes L, Mouw K, Schweizer M, Pritchard C, Salipante S, Taplin ME, Beltran H, Rubin M, Cieslik M, Robinson D, Heath E, Schultz N, Armenia J, Abida W, Scher H, Lord C, D'Andrea A, Sawyers C, Chinnaiyan A, Alimonti A, Nelson P, Drake C, Van Allen E, de Bono, JS. (2018). *Immunogenomic analyses associate immunological alterations with mismatch repair defects in prostate cancer*. The Journal of Clinical Investigation.
38. Bellmunt J, Lalani AKA, Jacobus S, **Wankowicz SA**, Polacek L, Takeda DY, Harshman LC, Wagle N, Moreno I, Lundgren K, Bossé D, Van Allen E, Choueiri T, Rosenberg J. (2018). *Everolimus and pazopanib (E/P) benefit genomically selected patients with metastatic urothelial carcinoma*. British journal of cancer.
39. McKay RR, Bossé D, Xie W, **Wankowicz SA**, Flaifel A, Brandao R, Lalani AKA, Martini DJ, Wei XX, Braun DA, Van Allen EM, et al. (2018). *The Clinical Activity of PD-1/PD-L1 Inhibitors in Metastatic Non–Clear Cell Renal Cell Carcinoma*. Cancer immunology research.
40. Sonpavde G, Pond GR, Rosenberg JE, Choueiri TK, Bellmunt J, Regazzi AM, **Mullane SA**, Necchi A, Raggi D, Lee JL, Lee S. (2018). *Nomogram to Assess the Survival Benefit of New Salvage Agents for Metastatic Urothelial Carcinoma in the Era of Immunotherapy*. Clinical genitourinary cancer.
41. Liu D, Abbosh P, Keliher D, Reardon B, Miao D, Mouw K, Taylor-Weiner A, **Mullane SA**, Han C, Teo MY, Cipolla C, Kim J, Iyer G, Al-Ahmadie H, Dulaimi E, Chen DYT, Alpaugh R, Hoffman-Censits J, Garraway L, Getz G, Carter S, Bellmunt J, Plimack E, Rosenberg J, Van Allen EM. (2017). *Mutational Patterns in Chemotherapy-Resistant Muscle-Invasive Bladder Cancer*. Nature Communications.
42. **Wankowicz SA**, Vetterlein, MW[#], Seisen, T, Lander R, Löppenberg B, Chun FK, Menon M, Sun M, Barletta JA, Choueiri TK, Bellmunt J, Trinh QD, Preston, MA (2017). *Neoadjuvant chemotherapy prior to radical cystectomy for muscle-invasive bladder cancer with variant histology*. Cancer.
43. **Wankowicz SA**, Werner L, Orsola A, Novak J, Bowden M, Choueiri TK, de Torres I, Morote J, Freeman GJ, Signoretti S, Bellmunt J. (2017). *Differential Expression Of PD-L1 In High Grade T1 Vs Muscle Invasive Bladder Carcinoma And Its Prognostic Implications*. The Journal of Urology.
44. Han GC, Hwang J, **Wankowicz SA**, Cibulskis C, Zhang Z, McKay RR, PCF-SU2C Dream Team, Carter SL, Hahn WC, Taplin M, Van Allen EM. (2017). *Clinical and genomic resistance to second generation androgen blockade in paired biopsies of metastatic castration-resistant prostate cancer*. JCO Precision Medicine.
45. Huang FW, Mosquera JM, Garofalo A, Oh C, Baco M, Amin-Mansour A, Rabasha B, Bahl S, **Mullane SA**, Robinson BD, Aldubayan S, Khani F, Karir B, Kim E, Chimene-Weiss J, Hofree M, Romanel A, Osborne JR, Kim JW, Azabdaftari G, Woloszynska-Read A, Sfanos K, De Marzo AM, Demichelis F, Gabriel S, Van Allen EM, Mesirov J, Tamayo P, Rubin MA, Powell IJ, Garraway LA. (2017). *Exome Sequencing of African-American Prostate Cancer Reveals Loss-of-Function ERF Mutations*. Cancer Discovery.
46. Teo MY, Bambury RM, Zabor EC, Jordan E, Al-Ahmadie H, Boyd ME, Bouvier N, **Mullane SA**, Cha EK, Roper N, Ostrovnya I, Hyman DM, Bochner BH, Arcila ME, Solit DB, Berger MF, Bajorin DF, Bellmunt J, Iyer G, Rosenberg JE. (2017). *DNA damage response and repair gene alterations are associated with improved survival in patients with platinum-treated advanced urothelial carcinoma*. Clinical Cancer Research.
47. Sevillano E, Werner L, Bossé D, Lalani AA, **Wankowicz SA**, de Velasco G, Farina M, Lundgren K, Choueiri TK, González Del Alba A, Bellmunt J. (2017). *Upper Tract Urothelial Carcinomas: Prognostic Factors and Outcomes in Patients With Non–Lymph Node Distant Metastasis*. Clinical Genitourinary Cancer.

48. Kamran SC, Lennerz JK, Reardon B, **Mullane SA**, Wo JY, Willers H, Corcoran R, Hong TS, Van Allen EM. (2017). *Genomic Evolution and Acquired Resistance to Pre-Operative Chemoradiation Therapy in Locally Advanced Rectal Cancer*. International Journal of Radiation Oncology.
49. Sonpavde G, Pond GR, **Mullane S**, Ramirez AA, Vogelzang NJ, Necchi A, Powles T, Bellmunt J. (2017). *Outcomes in patients with advanced urothelial carcinoma after discontinuation of programmed death (PD)-1 or PD ligand 1 inhibitor therapy*. BJU International.
50. Martini, D., Brandao, R, Hamieh, L, Norton C, **Mullane SA**, Walsh M, Van Allen EM, McKay R, Harshman LC, Choueiri, TK. (2017). *Outcomes in PD-1/PD-L1 responders who discontinued therapy for immune-related adverse events (irAEs): analysis of nine patients with metastatic renal cell carcinoma (mRCC)*. BJU International.
51. **Mullane SA**, Werner L, Rosenberg J, Signoretti S, Callea M, Choueiri TK, Freeman GJ, Bellmunt J. (2016). *Correlation of Apobec mRNA Expression with Overall Survival and PD-L1 Expression in Urothelial Carcinoma*. Scientific Reports.
52. **Mullane SA**, & Van Allen EM. (2016). *Precision medicine for advanced prostate cancer*. Current Opinion in Urology.
53. Cejas P, Li L, O'Neill NK, Duarte M, Rao P, Bowden M, Zhou CW, Mendiola M, Burgos E, Feliu J, Moreno-Rubio J, Guadalajara H, Moreno V, García-Olmo D, Bellmunt J, **Mullane SA**, Hirsch M, Sweeney CJ, Richardson A, Liu XS, Brown M, Shivdasani RA, Long HW. (2016). *Chromatin immunoprecipitation from fixed clinical tissues reveals tumor-specific enhancer profiles*. Nature Medicine.
54. Sonpavde G, Pond GR, Di Lorenzo G, Buonerba C, Rozzi A, Lanzetta G, Necchi A, Giannatempo P, Raggi D, Matsumoto K, Choueiri TK, **Mullane SA**, Niegisch G, Albers P, Lee JL, Kitamura H, Kume H, Bellmunt J. (2016). *Impact of Prior Platinum-Based Therapy on Patients Receiving Salvage Systemic Treatment for Advanced Urothelial Carcinoma*. Clinical Genitourinary Cancer.
55. Bellmunt J, Zhou CW, **Mullane SA**, Werner L, Taplin ME, Fay AP, Choueiri TK, Orsola A, Takeda DY, Hahn WC, Kim J, Sonpavde G, Bowden M. (2016). *Association of tumour microRNA profiling with outcomes in patients with advanced urothelial carcinoma receiving first-line platinum-based chemotherapy*. British Journal of Cancer.
56. **Mullane SA**, & Bellmunt J. (2016). *Cancer immunotherapy: new applications in urologic oncology*. Current Opinion in Urology.
57. Sonpavde G, Pond GR, Choueiri TK, **Mullane SA**, Niegisch G, Albers, P, Necchi A5, Di Lorenzo G, Buonerba C, Rozzi A, Matsumoto K, Lee JL, Kitamura H, Kume H, Bellmunt J. (2016). *Single-agent taxane versus taxane-containing combination chemotherapy as salvage therapy for advanced urothelial carcinoma*. European Urology.
58. Orsola A, **Mullane SA**, Bellmunt J. (2016). Letter to the Editor, Re: van der Heijden AG, Mengual L, Lozano JJ, Ingelmo-Torres M, Ribal MJ, Fernández PL, Oosterwijk E, Schalken JA, Alcaraz A, Witjes JA. *A five-gene expression signature to predict progression in T1G3 bladder cancer*. European Journal of Cancer.
59. **Mullane SA**, Werner L, Guancial EA, Lis RT, Stack EC, Loda, M, Kantoff PW, Choueiri TK, Rosenberg J, Bellmunt, J. (2015). *Expression Levels of DNA Damage Repair Proteins Are Associated With Overall Survival in Platinum-Treated Advanced Urothelial Carcinoma*. Clinical Genitourinary Cancer.
60. Bellmunt J, **Mullane SA**, Werner L, Fay AP, Callea M, Leow J, Choueiri TK, Hodi FS, Freeman GJ, Signoretti S. (2015). *Association of PD-L1 Expression on Tumor Infiltrating Mononuclear Cells and Overall Survival in Patients with Urothelial Carcinoma*. Annals of Oncology.
61. Cole AP, Dalela D, Hanske J, **Mullane SA**, Choueiri TK, Meyer, CP, Nguyen PL, Menon M, Kibel AS, Preston MA, Bellmunt J, Trinh QD. (2015). *Temporal trends in receipt of adequate lymphadenectomy in bladder cancer 1988 to 2010*. Urologic Oncology.
62. Bellmunt J, Werner L, Leow JJ, **Mullane SA**, Fay AP, Riester M, Van Hummelen P, Taplin ME, Choueiri TK, Van Allen E, Rosenberg, J. (2015). *Somatic copy number abnormalities and mutations in PI3K/AKT/mTOR pathway have prognostic significance for overall survival in platinum-treated locally advanced or metastatic urothelial tumors*. PloS one.
63. **Mullane SA**, & Bellmunt J. (2015). Re: John P. Sfakianos, Eugene K. Cha, Gopa Iyer, et al. *Genomic Characterization of Upper Tract Urothelial Carcinoma*. European Urology.
64. Bellmunt J, Werner L, Bamias A, Fay AP, Park RS, Riester M, Selvarajah S, Barletta J, Berman D, de Muga S, Salido M, Gallardo E, Rojo F, Guancial E, Bambury R, **Mullane SA**, Choueiri TK, Loda M, Stack E, Rosenberg, J. (2015). *HER2 as a target in invasive urothelial carcinoma*. Cancer Medicine.
65. Leow J, Fay AP, **Mullane SA**, Bellmunt, J. (2015). *Perioperative Therapy for Invasive Bladder Cancer*. Hematology/Oncology Clinics of North America.

66. Bellmunt J, Selvarajah S, Rodig S, Salido M, de Muga S, Costa I, Bellosillo B, Werner L, **Mullane SA**, Fay AP, O'Brien R, Barretina J, Minoche AE, Signoretti S, Montagut C, Himmelbauer H, Berman D, Kantoff P, Choueiri TK, Rosenberg, J. E. (2014). *Identification of ALK Gene Alterations in Urothelial Carcinoma*. PloS one.
67. Sonpavde G, Pond GR, **Mullane SA**, Qu AQ, Di Lorenzo G, Federico P, Choueiri TK (2014). *Incomplete cross-resistance between taxanes for advanced urothelial carcinoma: implications for clinical practice and trial design*. Clinical Genitourinary Cancer.
68. Orsola A, L. Werner, de Torres I, Martin-Doyle W, Raventos CX, Lozano F, **Mullane SA**, Leow JJ, Barletta JA, Bellmunt J, Morote J. (2014). *Reexamining treatment of high-grade T1 bladder cancer according to depth of lamina propria invasion: a prospective trial of 200 patients*. British Journal of Cancer.

Presentations: *Invited, #Peer Reviewed

External:

- **09/2026**, CAHRA Challenge Workshop, *Building Ensemble Infrastructure for Structural Biology*, Oxford, UK*
- **08/2026**, IUCR Keynote, *Decoding conformational ensembles to leverage entropy for function and design*, Calgary, AB, Canada*
- **08/2026**, SciFoo, *Re-designing structural biology*, Cambridge, UK*
- **07/2026**, Protein Society, *Possibility to Precision in Macromolecular Ensemble Prediction*, Boston, MA*
- **04/2026**, DARPA, *Multimodal Integration of Biophysics and AI for Protein Function Prediction*, Alexandria, VA*
- **03/2026**, CECAM Advances in CryoEM & CryoET, *Modeling Conformational and Compositional Heterogeneity in CryoEM Structures*, Toulouse, France*
- **03/2026**, OpenEye CUP, *Decoding conformational ensembles to leverage entropy for function and design*, Santa Fe, NM*
- **01/2026** CCP4 Study Weekend, *Modeling Conformational and Compositional Heterogeneity for Drug Design*, Nottingham, UK*
- **12/2025** Institute for Protein Design, University of Washington, *Decoding conformational ensembles to leverage entropy for function and design*, Seattle, WA*
- **10/2025** Stanford Cryo-EM Modeling Workshop, *Modeling Conformational and Compositional Heterogeneity in Cryo-EM Structures*, Menlo Park, CA*
- **09/2025** SLAC Users Meeting, *Decoding Conformational Entropy Through Statistical Structural Biology and Conformational Ensembles*, Menlo Park, CA*
- **09/2025** SLAC Users Meeting, *Sampling, Metrics, and New Approaches for Ensemble Modeling in X-ray crystallography*, Menlo Park, CA*
- **09/2025** Microsoft Research, *Using Protein Ensemble Predictions with Experimental Data*, Remote*
- **08/2025** RosettaCon, *Decoding conformational ensembles to leverage entropy for ligand binding affinity*, Cle Elum, WA*
- **07/2025** Protein Dynamics Workshop, Telluride Science & Innovation Center, *How Proteins Optimize Binding: The Role of Pocket Rigidity and Distal Flexibility*, Telluride, CO*
- **07/2025** Flatiron Institute Computational Cryo-EM Workshop, *Modeling Conformational and Compositional Heterogeneity in CryoEM Structures*, New York, NY*
- **06/2025** Genentech, *Decoding conformational ensembles to leverage entropy for ligand binding affinity*, South San Francisco, CA*
- **05/2025** MOISSI Workshop on Software Development for Enzyme Design and Engineering, *Hidden in Plain Sight: Using conformational ensembles better to understand the role of entropy in protein functions*, Atlanta, GA*
- **05/2025** Oak Ridge National Lab, *Decoding Conformational Entropy Through Statistical Structural Biology and Conformational Ensembles*, Oak Ridge, TN*
- **04/2025** American Society for Pharmacology and Experimental Therapeutics, *Hidden in Plain Sight: Heterogeneity underlying Cryo-EM structural models*, Portland, OR*
- **03/2025** Keystone Symposium, Machine Learning Applied to Macromolecular Structure and Function, *Decoding Conformational Entropy Through Statistical Structural Biology and Conformational Ensembles*, Keystone, CO*
- **03/2025** Oak Ridge National Lab-Vanderbilt University Joint Meeting, *Leveraging statistical structural biology for ligand specificity and affinity*, Oak Ridge, TN*
- **11/2024** University of Pennsylvania, *Making sense of the chaos: conformational entropy and ligand binding*, Philadelphia, PA*

- **10/2024** SBGrid, *Automated Multiconformer Model Building for X-ray Crystallography and Cryo-EM*, Remote*
- **09/2024** SLAC National Accelerator Laboratory, Annual Users Meeting, *Hidden in plain sight -- What is underlying structural biology models*, Menlo Park, CA*
- **07/2024** American Crystallographic Association Annual Meeting, Algorithms and computational methods in cryoEM, *Multiconformer protein and ligand models in high-resolution cryoEM*, Denver, CO*
- **06/2024** Macromolecular Conformational Ensembles Workshop, *Automated Multiconformer Model Building for X-ray Crystallography and Cryo-EM*, Redwood City, CA
- **06/2024** Simons Institute for the Theory of Computing, *Automated Multiconformer Model Building for X-ray Crystallography and Cryo-EM*, Berkeley, CA*
- **06/2024** Lawrence Berkeley National Lab, *Automated Multiconformer Model Building for X-ray Crystallography and Cryo-EM*, Berkeley, CA*
- **04/2024** Massachusetts Institute of Technology, *Making sense of the chaos: conformational entropy and ligand binding*, Cambridge, MA*
- **03/2024** University of California, San Diego, *Making sense of the chaos: conformational entropy and ligand binding*, La Jolla, CA*
- **03/2024** Vanderbilt University, *Making sense of the chaos: conformational entropy and ligand binding*, Nashville, TN*
- **02/2024** University of California, Irvine, *Making sense of the chaos: conformational entropy and ligand binding*, Irvine, CA*
- **01/2024** CASP Special Interest Group on Modeling Ensembles and Alternative Conformations of Proteins, *Comprehensive encoding of conformational and compositional protein structural ensembles through mmCIF data structure*, Virtual*
- **12/2023** EMBL Computational Structural Biology, *Water Molecule Likelihood Map for Protein and Ligand Structural Models*, Heidelberg, Germany#
- **11/2023** Machine Learning for Structural Biology Seminar, *Improving Structural Ensembles in X-ray Crystallography and CryoEM Data*, Remote*
- **10/2023** St. Jude Structural Biology Symposium, *Making sense of the chaos: conformational entropy and ligand binding*, Memphis, TN*
- **10/2023** University of California, San Francisco, Clements Lecture, *Making sense of the chaos: conformational entropy and ligand binding*, San Francisco, CA*
- **10/2023** Intersection Science Fellows Symposium, *Making sense of the chaos: conformational entropy and ligand binding*, Remote#
- **03/2023** Keystone Symposia, Computational Design and Modeling of Biomolecules, *Water Molecule Likelihood Map for Protein and Ligand Structural Models*, Banff, AB, Canada#
- **10/2022** University of Massachusetts Medical School, *How does ligand binding impact protein conformational heterogeneity?* Worcester, MA*
- **10/2022** Dana-Farber Cancer Institute, *How does ligand binding impact protein conformational heterogeneity?* Boston, MA*
- **10/2022** Pittsburg Diffraction Conference, *Leveraging machine learning to detect heterogeneous features from diffraction data*, Argonne National Lab, Lemont, IL*
- **04/2022** Phenix Developers Meeting, *Identifying and improving the modeling of water molecules in multiconformer models*, Lawrence Berkeley National Lab, Berkeley, CA
- **06/2021** Hamburg-Harvard Series of Crystallographic Curiosities, *Assessing how side chain conformational heterogeneity changes upon ligand binding*, Remote*
- **05/2021** D.E. Shaw Research, *Assessing how side chain conformational heterogeneity changes upon ligand binding*, Remote#

Internal:

- **03/2026** Center for Structural Biology/Center for AI in Protein Dynamics Symposium, *Decoding conformational ensembles to leverage entropy for ligand binding*, Nashville, TN*
- **2/2026** Molecular Biophysics Training Program, *Making sense of chaos: conformational entropy and ligand binding*, Nashville, TN*

- **10/2025** Vanderbilt University School of Medicine Scientific Advisory Board, *Modeling Conformational and Compositional Heterogeneity in Structural Biology Data*, Nashville, TN*
- **08/2025** Molecular Physiology and Biophysics Department Meeting, *Decoding conformational ensembles to leverage entropy for ligand binding*, Nashville, TN*
- **04/2025** Molecular Physiology and Biophysics Retreat, *Decoding Binding Entropy Through Statistical Structural Biology and Conformational Ensembles*, Antioch, TN*
- **03/2025** Vanderbilt University AI Days, *What is Underlying AlphaFold Models*, Nashville, TN*
- **12/2024** Vanderbilt University Scientific Advisory Board, *Hidden in Plain Sight: The Role of Entropy in Ligand Binding*, Nashville, TN*
- **11/2024** Center for Structural Biology, *Hidden in Plain Sight: Heterogeneity underlying Cryo-EM and X-ray structural models*, Nashville, TN*
- **10/2024** Biochemistry Department Retreat, *Making sense of the chaos: conformational entropy and ligand binding*, Nashville, TN*
- **09/2024** Molecular Physiology and Biophysics Department Meeting, *Decoding conformational ensembles to leverage entropy for ligand binding*, Nashville, TN*
- **11/2022** UCSF Quantitative Biology Retreat, *How does ligand binding impact protein conformational heterogeneity?*, Santa Cruz, CA[#]
- **11/2017** Center for Cancer Precision Medicine, Dana Farber Cancer Institute, *Expanding the molecular landscape of advanced prostate cancer*, Boston, MA
- **09/2017** Cancer Program, Broad Institute of MIT & Harvard, *Expanding the molecular landscape of advanced prostate cancer*, Cambridge, MA