

Curriculum Vitae (09.2025)

Aleksandra Karolak, PhD

Assistant Member

Machine Learning, Moffitt Cancer Center
12902 Magnolia Drive, Tampa, FL 33612
Phone: (813)-745-7872
Email: aleks.karolak@moffitt.org

Education

2010 – 2015 PhD in Biophysical and Computational Chemistry, University of South Florida (USF), Tampa, United States. Title: *Application and development of computational methods in conformational studies of biomolecules: proteins and DNA*

1995 – 2000 MSc in Metal-Organic Chemistry, Maxima Cum Laude, Individual Curriculum, Adam Mickiewicz University, Posen, Poland. Title: *Reactions of hydroxysilanes with Ni(0) and Ni(II) complexes*

Postgraduate Training and Fellowship Appointments

10/2019 – 9/2021 Assistant Research Professor, Beckman Research Institute of City of Hope, Department of Population Sciences and Division of Mathematical Oncology, Department of Computational and Quantitative Medicine, Duarte, CA

7/2018 – 9/2019 H2020 Marie Skłodowska-Curie Actions and Barcelona Institute of Science and Technology COFUND postdoctoral fellowship, Genome Data Science, Institute for Research in Biomedicine, Barcelona, Spain

6/2015 – 6/2018 Postdoctoral Researcher, Moffitt Cancer Center, Integrated Mathematical Oncology, Tampa, FL

Appointments

2021 – present Assistant Member at Moffitt Cancer Center, Department of Machine Learning, Division of Quantitative Science, Tampa, FL

2021 – present Assistant Professor at the Morsani College of Medicine, University of South Florida, Department of Oncologic Sciences, Tampa, FL

2021 – present (Secondary Appointment) Assistant Member at Moffitt Cancer Center, Department of Gastrointestinal Oncology, Tampa, FL

2021 – present (Secondary Appointment) Assistant Member at Moffitt Cancer Center, Molecular Medicine, Drug Discovery, Tampa, FL

2022 – present (Affiliation) Assistant Professor at USF, Department of Chemical, Biological, and Materials, Tampa, FL

Teaching Experience

2024 – present **ECH4914 Instructor**, 3 credits, Advanced Research Methods for Undergrads, Chemical, Biological, and Materials Engineering Department, USF

2024 – present **AS.020.503 Instructor**, 1 credit, Research Methods, Undergraduate, John Hopkins University

2024 – present **DS4940 Instructor**, 1 credit, Research Methods, Undergraduate, University of Florida

2023 – present Moffitt Cancer Center, Faculty in the **PhD Chemical Cancer Biology Program**

2023 – present **CIS4940 Instructor**, 1 credit, Practical Work, University of Florida

Spring 2021 City of Hope, Co-instructor in Quantitative Models for Biomedicine (graduate course)

Spring 2015 USF, Teaching Assistant (TA) in Organic Chemistry II Lab, Solomon Weldegirma, PhD

Spring 2014 USF, TA in Organic Chemistry II Lab, Solomon Weldegirma, PhD

Fall 2013 USF, Head TA in Chemistry for Today Discussion, Daniel Cruz, Ushiri Kulatunga, PhDs

Spring 2013 USF, TA in Historical Perspectives in Chemistry, Patricia Muisener, PhD

Spring 2013 USF, TA in Use of Literature in Chemistry, Patricia Muisener, PhD

Spring 2013 USF, TA in Organic Chemistry II Lab, Solomon Weldegirma, PhD

Spring 2010 USF, TA in General Chemistry I Lab, Vasiliki Lykourinou, PhD

Honors and Awards

1. **Biophysical Society Annual Meeting Travel Awards** (for two group members) – 69th Biophysical Conference, Los Angeles, USA (2025)
2. Postdoctoral Fellowship H2020 Marie Skłodowska-Curie Actions and BIST, IRB Barcelona, Spain (2018-2019)
3. **The NCI Travel Award** – PS-ON Annual Investigators Meeting, Boston, USA (2017)

4. The **NCI Travel Award** – Cancer Systems Biology Consortium and Physical Sciences in Oncology Network Junior Investigators Meeting, Bethesda, USA (2017)
5. The **Landahl Travel Awards** – Society for Mathematical Biology Annual Meetings:
 - Salt Lake City, USA (2017)
 - Nottingham, United Kingdom (2016)
6. The Centre International de Rencontres Mathématiques (CIRM) **Travel Award**: “Present Challenges of Mathematics in Oncology and Biology of Cancer” Marseille, France (2015)
7. **1st Place** for Graduate Student Talk, 12th USF Castle Conference, Tampa, USA (2014)
8. **1st Place** for Graduate Student Talk, 10th USF Castle Conference, Tampa, USA (2012)
9. The **Martin Travel Endowment Award** at the USF, Tampa, USA (2012)
10. **3rd Place** for Graduate Student Poster Presentation, 9th USF Castle Conference, Tampa, USA (2011)
11. **Maxima Cum Laude** in Master of Science in Chemistry, UAM, Posen, Poland (2000)

Committees:

2024 – present	Member, Team Science Scientific Review Committee
2023 – present	Member, SRC Laurel Study Section at Moffitt (mtg once a month, 2h/wk commitment)
2023 – present	Member, Women in Oncology Professional Development Subcommittee
2023 – present	Review Committee and Member of the Faculty for PhD Program at Moffitt
2023 – present	Review Committee and Member of the Postdoctoral Program at Moffitt
2022 – present	Chair of the ML Research in Progress Seminars (EMERGE) , Moffitt
2022 – present	Organizer of the Machine Learning Departmental Journal Club , Moffitt
2021 – 2022	Member of the Faculty Search Committee (Machine Learning), Moffitt
2021 – present	Co-Leader and Moffitt Liaison for the Biomedical AI Moffitt – USFStudy Sections
2024 – present	Scientific Reviewer : Cancer Prevention and Research Institute of Texas (CPRIT)
2024 – present	Ad Hoc Reviewer : Cancer Prevention and Research Institute of Texas (CPRIT)
2023 – present	Scientific Reviewer: DoD Ovarian Study Section – Ovarian Cancer Research Program (OCR) for the Department of Defense (DOD) Congressionally Directed Medical Research Programs (CDMRP)

Professional Association Memberships

2015 - present	Member , American Association for Cancer Research
2010 - present	Member , Biophysical Society

Publications

1. K.Mizgalska, K.Urbaniak, DJ.Imbody, EB.Haura, WC.Guida, S.Branciamore, **A.Karolak** *Integrating computational chemistry and machine learning to predict KRAS mutation-induced resistance* – submitted to Biophysical Journal
2. EW.Davis, MA.Park, ..., **A.Karolak**, ..., JB.Fleming, MP.Malafa, D.Jeong, JB.Permuth, Florida Pancreas Collaborative. *The Impact of Edema on Skeletal Muscle Changes among Patients with Pancreatic Ductal Adenocarcinoma*. Cancer Epidemiol. Biomarkers Prev. 34, 9 (2025)
3. RE.Noor, S.Islam, T.Smalley, K.Mizgalska, M.Eschenfelder, D.Keramisanou, A.Joshua Astalos, JW.Leahy, WC.Guida, **A.Karolak**, I.Gelis, M.Acevedo-Duncan. *Biophysical Insights into the Binding Interactions of Inhibitors (ICA-IS/IT) Targeting Protein Kinase C-1*, Biophysica 5, 3 (2025)
4. T.Nguyen, **A.Karolak**. *Transformer Graph Variational Autoencoder for Generative Molecular Design*, Biophysical Journal 124, 1–9 (2025) PMID: 39885689
5. A.Wojtulewski, A.Sikora, S.Dineen, M.Raof, **A.Karolak**. *Using artificial intelligence and statistics for managing peritoneal metastases from gastrointestinal cancers*, Briefings in Functional Genomics, elae049 (2025)
6. MA.Park, K.Gumpper-Fedus, SG.Krishna, MC.Genilo-Delgado, S.Brantley, PA.Hart, ME.Dillhoff, MF.Gomez, TL.Basinski, SR.Mok, AK.Luthra, JB.Fleming, A.Mohammadi, BA.Centeno, K.Jiang, **A.Karolak**, D.Jeong, DT.Chen, P.Stewart, JK.Teer, Z.Cruz-Monserrate, JB.Permuth. *Molecular Pathway and Immune Profile Analysis of IPMN-Derived Versus PanIN-Derived Pancreatic Ductal Adenocarcinomas*. International Journal of Molecular Sciences. 25(23):13164 (2024)
7. E.Mohan, G.Shen, S.Ren, HH.Fan, KT.Ying Moua, **A.Karolak**, RC.Rockne, R.Nakamura, DA.Horne, CG.Kanakry, DE.Mager, J.McCune. *Challenges with sirolimus experimental data to inform QSP model of post-transplantation cyclophosphamide regimens*. Clin. Transl. Sci. DOI: 10.1111/cts.70014 (2024)
8. M.Gubanov, A.Pyayt, **A.Karolak**. *CancerKG.ORG - a Web-scale, Interactive, Verifiable Knowledge Graph-LLM Hybrid for Assisting with Optimal Cancer Treatment and Care* ACM CIKM (2024)
9. A.Mukund⁺, MA.Afridi⁺, **A.Karolak**, JB.Permuth, MA.Park, G.Rasool *Pancreatic Ductal Adenocarcinoma: A Review of Recent Advancements Enabled by Artificial Intelligence*. Cancers (2024) <https://doi.org/10.3390/cancers16122240>
10. **A.Karolak**, K.Urbaniak, A.Monastyrskyi, D.Duckett, S.Branciamore⁺, P. Stewart⁺ *Structure-independent machine learning predictions of the CDK12 interactome*. Biophys.J. (2024):<https://doi.org/10.1016/j.bpj.2024.05.017>

11. A.Sikora, K.Sullivan, S.Dineen, M.Raouf*, **A.Karolak***. *Emerging therapeutic approaches for peritoneal metastases from gastrointestinal cancers*. Molecular Therapy Oncolytics Volume 32, Issue 1 (2024) <https://doi.org/10.1016/j.omton.2024.200767>
*co-senior authors
12. TI.Shaw, B.Zhao, Y.Li, H.Wang, L.Wang, B.Manley, PA.Stewart, **A.Karolak**. *Multi-omics approach to identifying isoform variants as therapeutic targets in cancer patients*. Front. Oncology (2022) PMID: **36505834** PMCID: [PMC9730332](https://pubmed.ncbi.nlm.nih.gov/PMC9730332/)
13. JS.McCune, R.Nakamura, D.O'Meally, TW.Randolph, BM.Sandmaier, **A.Karolak**, D.Hockenbery, SL.Navarro. *Pharmacometabonomic Association of Cyclophosphamide 4-hydroxylation in Hematopoietic Cell Transplant Recipients*. Clin Transl Sci. (2022) PMID: 35106927 PMCID: [PMC9099130](https://pubmed.ncbi.nlm.nih.gov/PMC9099130/)
14. **A.Karolak**, J. Levatic, F. Supek. *A framework for mutational signature analysis based on DNA shape parameters*. PLoS ONE 17(1): e0262495 (2022) PMID: 35015788 PMCID: [PMC8752002](https://pubmed.ncbi.nlm.nih.gov/PMC8752002/)
15. **A.Karolak**, S.Poonja, DA.Markov, LJ.McCawley, KA.Rejniak *Morphophenotypic classification of tumor organoids as an indicator of drug exposure and penetration potential* Plos.Comp.Biol. 15(7): e1007214 (2019) PMID: 31310602 PMCID: [PMC6660094](https://pubmed.ncbi.nlm.nih.gov/PMC6660094/)
16. A.Khabibullin, **A.Karolak**, M.Budzevich, M.Mclaughlin, D.Morse, L.Woods *Structure and properties of DOTA-chelated radiopharmaceuticals within the ²²⁵Ac decay pathway*, Med.Chem.Comm.,6;9(7), p155 (2018) PMID: 30109003 PMCID: [PMC6072494](https://pubmed.ncbi.nlm.nih.gov/PMC6072494/)
17. **A.Karolak**, DA.Markov, LJ.McCawley, KA.Rejniak, *Toward personalized computational oncology: from spatial models of tumor spheroids to organoids to tissues*, J.R.Soc Interface, 15:20170703 (2018) PMID: 29367239 PMCID: PMC5805971
18. **A.Karolak**, KA.Rejniak *Micropharmacology: an in silico approach for assessing drug efficacy within a tumor tissue*, Bull. Math. Biol. P1 (2018) PMID: 29423880 PMCID: [PMC6082744](https://pubmed.ncbi.nlm.nih.gov/PMC6082744/)
19. **A.Karolak**, V.Estrella, T.Chen, AS.Huynh, DL.Morse, KA.Rejniak *Targeting imaging agents efficacy linked to tumor tissue topological heterogeneity via single-cell micro-pharmacological modelling*, Scientific Reports, 8 (1), p3638 (2018)
20. **A.Karolak**, Estrella VC, Huynh AS, Chen T, Vagner J, Morse DL, Rejniak KA. *Targeting Ligand Specificity Linked to Tumor Tissue Topological Heterogeneity via Single-Cell Micro-Pharmacological Modeling*. Sci Rep. 2018 Feb 26;8(1):3638. doi: 10.1038/s41598-018-21883-z. PMID: 29483578; PMCID: [PMC5827036](https://pubmed.ncbi.nlm.nih.gov/PMC5827036/).
21. S.Mukherjee, **A.Karolak**, Y.Renaudineau, M.Debant, P.Buscaglia, O.Mignen, WC.Guida, WH.Brooks *Molecular dynamics simulations of membrane bound STIM1 to investigate conformational changes during STIM1 activation upon calcium release*, J. Chem. Inf. Model. 57 (2), p335 (2017) PMID: 28151650 DOI: [10.1021/acs.jcim.6b00475](https://doi.org/10.1021/acs.jcim.6b00475)
22. TA.Word, **A.Karolak**, C.Cioce, A.van der Vaart, RW.Larsen, *Using photoacoustic calorimetry to study the cis to trans photo isomerization of the [Ru(II)(2,2'-bipyridine)₂(H₂O)₂]²⁺ complex in aqueous solution*, Comment. Inorg. Chem. 36, p343 (2016) DOI: [10.1080/02603594.2016.1183488](https://doi.org/10.1080/02603594.2016.1183488)
23. **A.Karolak**, A.van der Vaart *Molecular dynamics simulations of 5-hydroxycytosine damaged DNA* J. Phys. Chem. B, 120, p42 (2016) PMID: 26654566 DOI: [10.1021/acs.jpcc.5b09250](https://doi.org/10.1021/acs.jpcc.5b09250)
24. J. Pérez-Velázquez, JL. Gevertz, **A.Karolak**, KA. Rejniak. *Microenvironmental Niches and Sanctuaries: A Route to Acquired Resistance*. Adv Exp Med Biol. 2016;936:149-164. doi: 10.1007/978-3-319-42023-3_8. PMID: 27739047; PMCID: PMC5113820.
25. **A.Karolak**, A.van der Vaart *BII stability and base step flexibility of N6-adenine methylated GATC motifs* Biophys. Chem. 203, p22 (2015) PMID: 26004863 DOI: [10.1016/j.bpc.2015.05.001](https://doi.org/10.1016/j.bpc.2015.05.001)
26. TA.Word, CL.Whittington, **A.Karolak**, MT.Kemp, HL.Woodcock, A.van der Vaart, RW. Larsen *Photoacoustic calorimetry study of ligand photorelease from the Ru(II)bis(2,2'-bipyridine)(6,6'-dimethyl-2,2'-bipyridine) complex in aqueous solution* Chem. Phys. Lett. 619, p214 (2015) <https://doi.org/10.1016/j.cplett.2014.11.012>
27. **A.Karolak**, A.van der Vaart *Enhanced sampling simulations of DNA step parameters* J. Comp. Chem. 35, 2297-2304 (2014) PMID: 25303338 DOI: [10.1002/jcc.23751](https://doi.org/10.1002/jcc.23751)
28. **A.Karolak**, A.van der Vaart *Importance of local interactions for the ETS1 stability of inhibitory helix 1* Biophys. Chem. 165, p74 (2012) PMID: 22494801 DOI: [10.1016/j.bpc.2012.03.007](https://doi.org/10.1016/j.bpc.2012.03.007)
29. H.Maciejewski, B.Marciniak, J.Gulinski, **A.Karolak**, NK.Skvortsov *From isothiocyanato- to silyl-nickel complexes* Inorg. Chem. Comm. 5, p464 (2002)

Invited Peer-Reviewed Publications

30. M.Stitou, J.Koomen, D.Imbody, Y.Liao, A.Monastryskiy, U.Rix, D.Duckett, E.Haura, **A.Karolak**. *Does AI need companionship to assist drug discovery? The KRAS study*. BJR AI, Volume 1, Issue 1 (2024) <https://doi.org/10.1093/bjrai/ubae001>
31. **A.Karolak**, V.Schoning, A.Khurana. *Spotlight on AI in Experimental Pharmacology and Drug Discovery*. Front. Pharmacology, (2023) PMID: 37711179 PMCID: PMC10498275
32. I.El Naqa, **A.Karolak**, Y.Luo, L.Folio, A.Tarhini, D.Rollison, K.Parodi. *Translation of AI into clinical practice*. Oncogene (2023) DOI: 10.1038/s41388-023-02826-z PMID: 37684407
33. **A.Karolak**, S.Branciamore, JS.McCune, PP.Lee, AS.Rodin, RC.Rockne. *Concepts and applications of information theory to immuno-oncology* Trends in Cancer, Special Issue: Quantitative Cancer Biology 7(4) (2021) PMID: 33618998 PMCID: [PMC8156485](https://pubmed.ncbi.nlm.nih.gov/PMC8156485/)

Non-Peer Reviewed Publications

1. T.Nguyen, **A.Karolak**. *Expanding Molecular Design with Graph Variational Autoencoders: A Comparative Study of Pair-Encoding and Character Tokenization*. ChemRxiv doi: 10.26434/chemrxiv-2025-j1p93 (2025)
2. MA.Park, K.Gumpper-Fedus, SG.Krishna, MC.Genilo-Delgado, S.Brantley, PA.Hart, ME.Dillhoff, MF.Gomez, TL.Basinski, SR.Mok, AK.Luthra, JB.Fleming, A.Mohammadi, BA.Centeno, K.Jiang, **A.Karolak**, D.Jeong, DT.Chen, P.Stewart, JK.Teer, Z.Cruz-Monserrate, JB.Permuth. *Molecular Pathway and Immune Profile Analysis of IPMN- vs. PanIN-Derived Pancreatic Ductal Adenocarcinomas*. Preprints <https://doi.org/10.20944/preprints202409.2045.v1> (2024)
3. T.Nguyen, **A.Karolak**. *Transformer Graph Variational Autoencoder for Generative Molecular Design*, bioRxiv <https://doi.org/10.1101/2024.07.22.604603> (2024)
4. N.Nguyen, MA.Park, JK.Teer, P.McDonald, JB.Fleming, JB.Permuth, KC.Chen, **A.Karolak**. *Text-based Integration of Mutational Profiles for Risk Predictions and Biomarker Identification of Intraductal Papillary Mucinous Neoplasms of the Pancreas*, medRxiv (2023)
5. **A.Karolak**, J. Levatic, F. Supek *A framework for mutational signature analysis based on DNA shape parameters*, BioRxiv doi: <https://doi.org/10.1101/2020.09.28.316794> (2020)
6. M.Damaghi, S.Byrne, L.Xu, N.Tafreshi, B.Fang, JM. Koomen, **A.Karolak**, T.Chen, J.Johnson, ND. Gallant, A.Marusyk, RJ.Gillies *Collagen production and niche engineering: a novel strategy for cancer cells to survive acidosis and evolve*. BioRxiv 711978; doi: <https://doi.org/10.1101/711978> (2019)
7. S.Nizzero, JC. Alfonso, A.Alvarez-Arenas, I.Mirzaev, I. Zervantonakis, T.Lewin, A.Rishi, E.Piretto, T. Joshi, DN. Santiago, **A.Karolak**, R.Howard, H.Enderling, FA.Karreh, J.Torres-Roca *Overcoming non-small cell lung cancer radiation resistance by modulating the tumor-immune ecosystem* BioRxiv <https://doi.org/10.1101/458372> (2018)
8. **A.Karolak**, B.Huffstutler, Z.Khan, KA.Rejniak *Assessment of patient-specific efficacy of chemo- and targeted-therapies: a micro pharmacology approach* NIH/NCI Handbook of Mathematical Methods in Cancer Biology, BioRxiv, doi.org/10.1101/236653 (2017)
9. R.Walker, PE.Navas, SH.Friedman, S.Galliani, **A.Karolak**, F.Macfarlane, R.Noble, J.Poleszczuk, S.Russell, KA.Rejniak, A.Shahmoradi, Fireball, J.Brayer, D.Abate-Daga, H.Enderling *Enhancing synergy of CAR T cell therapy and oncolytic virus therapy for pancreatic cancer* BioRxiv doi: 10.1101/055988 (2016)

Book Chapters

1. **A.Karolak**, S.Agrawal, S.Lee, KA.Rejniak *Dissecting tumor heterogeneity with single-cell-based in silico models*, Chapter in “*Encyclopedia of Biomedical Engineering: Single Cell Mathematical Models*”, Wiley (2019)
2. **A.Karolak**, KA.Rejniak *Mathematical modeling of tumor organoids: toward personalized medicine*, Chapter in “*Tumor Organoids: Cancer Drug Delivery and Development*”, Springer (2017)
3. J.Pérez-Velázquez, JL.Gevertz, **A.Karolak**, KA.Rejniak *Microenvironmental niches and sanctuaries: A route to acquired resistance*, Chapter in “*Advances in Experimental Medicine and Biology*”, Springer (2016)

Conference proceedings (Published abstracts):

1. K.Mizgalska, DJ.Imbody, EB.Haura, WC.Guida, **A.Karolak** *A computational chemistry and AI-driven framework for structure-based drug design informed by underlying factors of mutation-induced drug resistance: A study of KRAS*. Clinical Cancer Research 31 (13_Supplement), A016 (2025)
2. **A.Karolak**, EW.Davis, M.Isukapalli, R.Veligeti, MA.Park, JK.Teer, DK.Jeong, K.Jiang, DT.Chen, JB.Permuth, G.Rasool *Mutational profiling and machine learning for risk stratification and biomarker identification in intraductal papillary mucinous neoplasms progressing to pancreatic cancer*. Clinical Cancer Research 31 (13_Supplement), A043 (2025)
3. EW.Davis, [.] **A.Karolak** [.] JB.Permuth *Say it ain't psoas: addressing edema in pancreatic cancer body composition analyses*, Cancer Research 85 (8_Supplement_1), 4904-4904 (2025)
4. K.Mizgalska, WC.Guida, **A.Karolak** *Mutations in drug binding sites: integrating computational chemistry and machine learning to understand mutation-induced resistance – 69th Biophysical Conference, Los Angeles, CA*. Biophysical Journal 124 (3), 522a (2025)
5. T.Nguyen, **A.Karolak** *Molecular Design with Generative AI: A Transformer Graph Variational Autoencoder Approach – 69th Biophysical Conference, Los Angeles, CA*. Biophysical Journal 124 (3), 321a (2025)
6. N.Nguyen, JK.Teer, MA.Park, P.McDonald, JB.Fleming, JB.Permuth, KC.Chen, **A.Karolak** *Reinforcing risk prediction for intraductal papillary mucinous neoplasms of the pancreas with AI-optimized nucleotide-to-amino acid analyses*, Cancer Res. 84 (2 Suppl.), B109 (2024)
7. A.Matache, **A.Karolak**, S.Branciamore, A.Rodin, PP.Lee, RC.Rockne, *A communication theory framework for modeling cytokine-mediated signaling in healthy and breast cancer derived peripheral blood immune cells*, Cancer Res. 82 (12 Suppl.), 2741 (2022)
8. R.Singh, R. Falahat, E.Williams, JO.Johnson, N.Alcantar, **A.Karolak**, KA.Rejniak, M. Wiranowska, *Cross-disciplinary optimization of nano-drug delivery to ovarian carcinoma and glioma cells*, Cancer Res. 77 (13 Supplement), 2185-2185 (2017)
9. **A.Karolak**, A.Khabibullin, MM.Budzevich, M.Martinez, M.Doliganski, M.McLaughlin, L.Woods, DL.Morse, *The stability of DOTA-chelated radiopharmaceuticals within 225Ac decay pathway studied with density functional theory*, Bull. Amer. Phys. Soc. 62 (2017)

10. **A.Karolak**, B.Huffstutler, DA.Markov, LJ.McCawley, KA.Rejniak, *Elucidating the role of tumor micro environmental heterogeneity with computational model of 3D breast spheroids*, Biophys.J.112(3),45a (2017)
11. **A.Karolak**, V.Estrella, T.Chen, AS.Huynh, DL.Morse, KA.Rejniak, *Imaged-based computational predictions of imaging agent efficacy in pancreatic tumors expressing TLR2*, Cancer Res. 77 (2 Supplement), A28-A28 (2017)
12. AR.Khabibullin, **A.Karolak**, MM.Budzevich, LM.Woods, MV.Martinez, ML.McLaughlin, DL.Morse, *DFT calculations of the stability of DOTA-based-radiopharmaceuticals* AAPM 58th American Association of Physicists in Medicine Conference, Washington DC, (2016)
13. **A.Karolak**, V.Estrella, T.Chen, AS.Huynh, DL.Morse, KA.Rejniak, *Using computational modeling to quantify targeted agent binding and internalization in pancreatic cancer*, Cancer Res. 76 (3 Supplement), B21-B21 (2016)
14. **A.Karolak**, A.van der Vaart, *Enhanced Sampling of DNA Step Parameters: Impact of methylation on DNA shape and flexibility* Biophys. J. 108 (2), 396a (2015)
15. RW.Larsen, **A.Karolak**, TA.Word, MT.Kemp, CL.Whittington, HL.Woodcock, A.van der Vaart, *Ru(II)Bis(2,2')Bipyridine)L complexes as photo release agents for bioactive molecules: photo thermal studies of ligand release*, Biophys.J. 106(2) 477a-478a (2015)
16. **A.Karolak**, A.van der Vaart, *Novel coarse-grained model for molecular dynamics simulations of DNA* Biophys. J. 106 (2), 804a (2014)
17. **A.Karolak**, A.van der Vaart, *Importance of local interactions for the stability of ETS1 inhibitory helix 1*, Biophys. J. 102 (3), 447a (2012)

Selected presentations

2025:

- Poster D.Bhattacharjee*, B.Fang, V.Izumi, Y.Liao, E.Welsh, J.Koomen, D.Duckett, **A.Karolak**, E.Haura, A.Monastyrskiy, U.Rix, *Comprehensive Profiling of Unique Targets in Lung Cancer via High-Throughput Chemical Proteomics*, ChemBio, ICBS Conference, Paris (10/2025)
- Poster K.Mizgalska*, WC.Guida, **A.Karolak** *Mutations in drug binding sites: integrating computational chemistry and machine learning to understand mutation-induced resistance* – Moffitt Scientific Symposium, Tampa, FL (5/2025)
- Poster KC.Craig*, S.Xiang, G.Mahankai, X.Lou, DL.Welch, DR.Reed, W.Guida, **A.Karolak**, HR.Lawrence, NJ.Lawrence, MG.Alexandrow *Synthesis of Novel CMG Helicase Inhibitors (CMGi) for Treatment of K-Ras-Driven Tumors* – Basic Science Retreat, Moffitt CC (3/2025)
- Talk **K.Mizgalska***, WC.Guida, **A.Karolak** – *Mutations in drug binding sites: integrating computational chemistry and machine learning to understand mutation-induced resistance* – 69th Biophysical Conference, Los Angeles, CA (2/2025)

2024:

- Talk **A.Karolak** *AI in de novo Drug Design* – Drug Discovery Chemistry Conference, Barcelona, Spain (12/2024)
- Talk **A.Karolak** *AI Innovations in Molecular Design* – Dr. Gillies Machine Learning Workshop, Moffitt (11/2024)
- Poster M.Isukapalli*, R.Veligeti*, M.Park, J.Tier, G.Rasool, J.Permuth, **A.Karolak** *AI-Enhanced Origin Prediction of Pancreatic Adenocarcinoma: IPMN-derived vs. non-IPMN-derived Tumors*
 - Dr. Gillies Machine Learning Workshop (11/2024)
 - ORIEN 5th Scientific Summit (10/2024)
- Poster K.Mizgalska, EI.Lawrence, TL.Siev, WC.Guida, **A.Karolak**. *Mutations in drug binding sites: integrating computational chemistry and machine learning to understand mutation-induced resistance*
 - Dr. Gillies Machine Learning Workshop (11/2024)
 - ORIEN 5th Scientific Summit (10/2024)
- Poster T.Nguyen, D.Imbody, E.Haura, **A.Karolak** *Transformer Graph Variational Autoencoder for De Novo Drug Design*
 - 3rd Annual Oktoberfest Moffitt Cancer Center, Tampa, FL (10/2024)
 - ORIEN 5th Summit (10/2024)
 - Moffitt Scientific Symposium (5/2024)
- Poster M.Manjith, **A.Karolak** *Investigating Role of Mucins, Biofilm-Related Biomarkers, to Predict Response to Therapy in Colorectal Cancer* Moffitt Scientific Symposium (5/2024)
- Poster M.Stitou, T.Nguyen, **A.Karolak** *Integrating Artificial Intelligence and Chemistry for Cancer Research: From Mutational Signatures to De Novo Drug Design*
 – 2nd Annual Bioengineering at Moffitt Meeting (2/2024)
- Talk M.Stitou, **A.Karolak** *KRAS acquired resistance* – ODSi Meeting (2/2024)

2023:

- Poster A.Wojtulewski, Y.Balagurunathan, D.Anaya, **A.Karolak** *Heterogeneity in survival among patients with metastatic colorectal cancer.* – 2nd Annual QS Oktoberfest, Moffitt (10/2023)
- Poster T.Nguyen, M.Stitou, D.Imbody, E.Haura, **A.Karolak** *AI-enabled Pharmacophore-Guided Drug Design: A Novel Approach*

for Targeting Double KRAS G12C/Y96C Mutation. – 2nd Annual QS Oktoberfest, Moffitt (10/2023)

- Poster M.Froid, A.Karolak, G.Marcucci, R.Rockne, D.Basanta – 2nd Annual QS Oktoberfest, Moffitt (10/2023)
- Poster MM.Froid, R.Rockne, B.Zhang, G.Marcucci, **A.Karolak**, D.Basanta *A hybrid modeling approach illuminates physical and genetic factors contributing to resistance in the AML bone marrow niche*
- Moffitt Scientific Symposium, Moffitt, Tampa, FL (5/2023)
- Talk+Poster N.Nguyen, J.Fleming, P.McDonald, KC.Chen, **A.Karolak** *Intelligent Personalized Risk Prediction for Intraductal Papillary Mucinous Neoplasms of Pancreas*
- GRC Cancer Genetics and Epigenetics, Barga, Italy (5/2023)
- 67th Biophysical Society Annual Meeting, San Diego, CA (2/2023)
- Bioengineering at Moffitt Inaugural Symposium, Moffitt, Tampa, FL (2/2023)
- 2022:**
- The Gillies Machine Learning in Image Analytics Workshop, Clearwater, FL (11/2022)
 - International Society for Computational Biology RSGDREAM Meeting, Las Vegas, NV (11/2022)
 - American Pancreas Association Annual Meeting, Orlando, FL (11/2022)
 - Oktoberfest Scientific Celebration, Moffitt Cancer Center (10/2022)
- Poster N.Nguyen, **A.Karolak**, KC.Chen *Advancing Modeling and Biomedicine using Quantum Machine Intelligence*
- International Society for Computational Biology RSGDREAM Meeting, Las Vegas, NV (11/2022)
- Oktoberfest Scientific Celebration, Moffitt Cancer Center (10/2022)
- Poster **A.Karolak** *A Framework for Mutational Signature Analysis Based on DNA Shape Parameters*
- GRC Conference on Multiscale Modeling of Complex Systems, Castelldefels, Spain (7/2022)
- Talk **A.Karolak** *Machine Learning and Computational Oncology for Cancer Research* (invited talks)
- Pancreas Working Group Seminar Series, GI Department, Moffitt Cancer Center (6/2022)
- Bio2 Weekly Seminar, Moffitt Cancer Center (5/2022)
- Poster A.Matache, **A.Karolak**, S.Branciamore, A.Rodin, PP.Lee, RC.Rockne *A Communication Theory Framework for Modeling Cytokine-Mediated Signaling in Healthy and Breast Cancer Derived Peripheral Blood Immune Cells*
- AACR, New Orleans, USA (4/2022)

2021 and earlier:

- Poster **A.Karolak**, J.Levatic, F.Supek *A Framework for Mutational Signature Analysis based on DNA Shape Parameters*
- NCI Symposium on Mutational Signatures in Cancer, NIH/NCI, USA (12/2021)
- Gordon Research Conference in Computational Chemistry, Spain (7/2022)
- Poster **A.Karolak**, RC.Rockne, DE.Mager, CG.Kanakry, E.Mohanan, R.Nakamura, M.Shiferaw, CM.Quinones, J.S.McCune *A Quantitative Systems Pharmacology Model to Improve Graft Versus Host Disease Outcomes*
- CSBC Annual Meeting, NIH/NCI, USA (9/2021)
- NCI CSBC/PS-ON/BD-STEP JI Meeting, USA (8/2021)
- Poster **A.Karolak**, RC.Rockne, DE.Mager, CG.Kanakry, E.Mohanan, R.Nakamura, M.Shiferaw, CM.Quinones, J.S.McCune *A Quantitative Systems Pharmacology Model to Improve Graft Versus Host Disease Outcomes*
- SMB Minisymposium, USA (6/2021)
- City of Hope RSO (Research Staff Organization) Retreat, USA (4/2021)
- Talk **A.Karolak**, RC.Rockne, DE.Mager, CG.Kanakry, R.Nakamura, M.Shiferaw, CM.Quinones, J.S.McCune *Improving Graft Versus Host Disease Outcomes with Quantitative Systems Pharmacology*
- VPH2020 (Virtual Physiological Human) Paris, France (8/2020) - virtual
- QSPC2020 (Quantitative Systems Pharmacology), Leiden, Netherlands (4/2020) - cancelled
- Talk **A.Karolak**, RC.Rockne, DE.Mager, CG.Kanakry, R.Nakamura, M.Shiferaw, K.Littlejohn, J.S.McCune *Optimization of Graft Versus Host Disease with Quantitative Systems Pharmacology*
- SIAM-LS (Society for Industrial and Applied Mathematics-Life Sciences) Garden Grove, USA (6/2020)
- City of Hope RSO (Research Staff Organization) Retreat, Lake Arrowhead, CA (3/2020)
- City of Hope Young PIs retreat, Oxnard, USA (12/2019)
- Talk **A.Karolak**, L.Palenzuela, TH. Stracker, F.Supek *Interacting with interactome: improved protein-protein interactions prediction by integrating biotin identification mass-spectrometry experiments with ML*
- Cancer Research Seminars, IRB Barcelona, Spain (3/2019)
- IRB Scientific Symposium, Barcelona, Spain (10/2018)
- Talk **A.Karolak**, S.Poonja, DA.Markov, LJ.McCawley, KA.Rejniak *Computational predictions of morpho-phenotypic features of tumor organoids under various microenvironments and treatments*
- Evolution Therapy Moffitt Scientific Retreat, St. Petersburg, USA (2018)
- Moffitt Scientific Symposium, Tampa, USA (2018)
- Cancer Genomics and Mathematical Analysis Symposium, Columbia University, NY, USA (2018)
- Poster **A.Karolak**, B.Huffstutler, Z.Khan, DA.Markov, LJ.McCawley, KA.Rejniak *Organoid3D: the role of micro- environmental heterogeneity on the development of breast tumor spheroids elucidated with computational modeling*

- CBSC/PS-ON Junior Investigators (JI) Meeting at NIH, Bethesda, USA (2017)
- Society for Mathematical Biology (SMB) Annual Meeting, Salt Lake City, USA (2017)
- Poster **A.Karolak**, V.C.Estrella, T.Chen, A.S.Huynh, B.Huffstutler, Z. Khan, D.L. Morse, D.A. Markov, L.J. McCawley, K.A. Rejniak, *From Single Cells to Organoids: Studying the Interplay between Therapeutic Agents and Tumor Microenvironment* Cancer Biology and Evolution Symposium, Tampa, USA (2017)
- Poster **A.Karolak**, B.Huffstutler, Z.Khan, D.A.Markov, L.J.McCawley, K.A.Rejniak *Linking mutations, drug mechanisms and microenvironmental heterogeneity to predict treatment efficacy in the 3D in silico model of tumor organoids*
 - Gordon Research Conference, Galveston, USA (2017)
 - Moffitt Scientific Symposium, Tampa, USA (2017)
- Talk **A.Karolak**, V.Estrella, T.Chen, A.S.Huynh, D.L.Morse, K.A.Rejniak *Quantitative intravital image-based modeling of targeted nanoparticle delivery and cellular uptake*
 - American Institute of Mathematical Sciences 11th Conference on Dynamical Systems, Differential Equations and Applications, Orlando, USA (2016)
 - SMB and ECMTB (European Conference for Mathematical and Theoretical Biology) Meeting, Nottingham, UK (2016)
- Poster **A.Karolak**, V.Estrella, T.Chen, A.S.Huynh, D.L.Morse, K.A.Rejniak *Imaged-based computational predictions of imaging agent efficacy in pancreatic tumors expressing TLR2* American Association of Cancer Research, Boston, USA (2016)
- Poster **A.Karolak**, V.Estrella, T.Chen, A.S.Huynh, D.L.Morse, K.A.Rejniak *Targeting solid tumors - a microscopic perspective in treatment optimization* Systems Approaches to Cancer Biology, Woods Hole, USA (2016)
- Poster **A.Karolak**, V.Estrella, T.Chen, A.S.Huynh, D.L.Morse, K.A.Rejniak *Using computational modelling to quantify targeted agent binding and internalization in pancreatic cancers* Centre International de Rencontres Mathématiques (CIRM), Marseille, France (2015)
- Talk **A.Karolak**, V.Estrella, T.Chen, A.S.Huynh, D.L.Morse, K.A.Rejniak *An integrated approach to modelling targeted agent penetration into pancreatic tumors using intravital fluorescence microscopy* World Molecular Imaging Society Conference, Honolulu, USA (2015)
- Talk **A.Karolak**, A.van der Vaart *Impact of N6-methyladenine on the shape and flexibility of DNA* American Chemical Society 66th South-East Regional Meeting (SERMACS), Nashville, USA (2014)
- Talk **A.Karolak**, A.van der Vaart *Enhanced sampling of DNA step parameters* ACS 90th Florida Annual Meeting and Exposition, Palm Harbor, USA (2014)
- Poster **A.Karolak**, A.van der Vaart *Development of a novel coarse-grained model for protein – DNA binding* ACS 89th Florida Annual Meeting and Exposition (FAME), Palm Harbor, USA (2013)
- Poster **A. Karolak**, A.van der Vaart *Importance of local interactions for the stability of inhibitory helix 1 of the ETS-1 in the apo state* ACS 88th FAME Palm Harbor, USA (2012)
- Poster **A. Karolak**, A.van der Vaart *Replica exchange simulations of the inhibitory helix 1 of ETS-1* ACS 87th FAME, Palm Harbor, USA (2011)
- Talk **A.Karolak**, J.Gulinski, H.Maciejewski *Synthesis of polycarbosilanes* World Polymer Congress, Warsaw, Poland (2000)
- Poster **A.Karolak**, H.Maciejewski *Nickel-silyl complexes* International School of Coordination Chemistry, Polanica Zdroj, Poland (1999)

Invited Talks/Seminars

- A.Karolak** – *Integrating AI and Computational Strategies to Overcome Resistance in Cancer*
 - Conference: Discovery on Target by Cambridge Healthtech, Boston (9/2025)
- A.Karolak** – *AI Meets Biophysics: Intelligent Molecular Design*
 - Conference: The Future of Cancer Research: Unleashing the Power of Machine Learning, Syracuse, Italy (5/2025)
 - Invited talk: City of Hope Cancer Center, Monrovia, CA (2/2025)
- A.Karolak** – *Using AI to Enhance Collaboration, Productivity, and Innovation in Cancer Drug Resistance Research*
 - Invited talk to the Tampa VA Research Week, Tampa, FL (5/2025)
- A.Karolak** – *Next-gen drug design: AI, chemistry, and biophysics against resistance*
 - Invitation for ACS Innovative Program Session, American Chemical Society Spring 2025 Meeting, San Diego, CA (3/2025)
- A.Karolak** – *Utilizing AI in Drug Discovery: Instances from Cancer Center*
 - Invited talk: Networking Tea, Moffitt (2/2025)
 - Invited talk: USF Career Expo (2/2025)
- A.Karolak** *AI Innovations in Molecular Design* – Cancer Biology Seminar, USF, Tampa, FL (1/2025)
- A.Karolak** *In Control of Your Career Trajectory* – Virtual Postdoc Event at Moffitt (11/2024)
- T.Nguyen, **A.Karolak** *Transformer Graph Variational Autoencoder for De Novo Drug Design*
 - Invited talk at the SPRINTD meeting, Moffitt, Tampa, Florida (12/2024) – A.Karolak
 - Invited Talk at the 2nd AI-X Conference at USF, Tampa, Florida (10/2024) – T.Nguyen
 - Invited Talk at the 1st Prescriptomics and Personalized Medicine Conference at Lisbon, Portugal (5/2024) – A.Karolak
- A.Karolak** *Utilizing AI in Drug Discovery: Instances from Cancer Center*–Stevens Institute of Technology, NJ (10/2024)

T.Nguyen, **A.Karolak** *Machine Learning for De Novo Drug Design* (invited talk) Bio2 Seminar Series, Moffitt Cancer Center (4/2024)

A.Karolak *Machine Learning and Molecular AI at Moffitt* – Invited Panelist at the Breakout Session on AI in Healthcare, 3rd Global and National Security Institute (GNSI) Tampa Summit, USF (3/2024)

A.Karolak *In Control of Your Career Trajectory* – Virtual Postdoc Event at Moffitt (2/2024)

A.Karolak *AI applications to Fragment Based Drug Discovery – part 2* (8/2023)

- Screening and Proteomics Initiative for Novel Targets and Drugs Platform (SPRINTD), Molecular Medicine Program, Moffitt, Tampa, FL

A.Karolak *Concepts and Applications of AI and Computational Modeling to Peritoneal Disease*

- GI Peritoneal Disease Site Retreat, Gastrointestinal Oncology, Moffitt (8/2023)

A.Karolak *AI-enabled Development of Protein Specific Fragment Libraries – part 1* (8/2023)

- Screening and Proteomics Initiative for Novel Targets and Drugs Platform (SPRINTD), Molecular Medicine Program, Moffitt, Tampa, FL

A.Karolak *AI applications to Fragment Based Drug Discovery*

- Screening and Proteomics Initiative for Novel Targets and Drugs Platform (SPRINTD), Molecular Medicine Program, Moffitt, Tampa, FL (6/2023)

A.Karolak *Molecular AI at Moffitt*

- Molecular Medicine Program at Moffitt (8/2023)
- Department of Chemical, Biological, and Materials Engineering, College of Engineering, USF (4/2023)
- St. Leo University (4/2023)