DIANE JOSEPH-MCCARTHY

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Senior life science executive and educator with extensive experience driving the translation of science into medical breakthroughs, and leading innovative teams in a fast-paced, entrepreneurial setting. Significant expertise in chemical biology applied across a broad range of therapeutic areas and modalities in both the pharmaceutical and biotechnology sectors as well as in an academic setting. Ability to interact with high-level functional leaders across disciplines to foster a culture of urgency, excellence, and collaboration.

PROFESSIONAL EXPERIENCE

Executive Director, Bioengineering Technology & Entrepreneurship Center, Boston University 2019-date
Professor of the Practice, Department of Biomedical Engineering, Boston University 2020-date
Hariri Institute for Computing and Computational Science & Engineering, Research Fellow 2022-date

- Established a new facility and built industrial partnerships with top-tier companies
- Co-taught biomedical engineering senior design course
- Research on elucidating fundamental protein-ligand interactions and enhancing drug design & delivery

Senior Vice President, Discovery & Early Development, EnBiotix 2019
Vice President, Translational Science, EnBiotix 2012-2018

- Built company based on academic innovations as part of an initial team of three
  - Secured partners, grants, and investors including closing Series A and B financings; the company is now traded as SPEX.SW
- Member of executive leadership team developing the R&D strategy and leading the science
  - Anti-persister, linear peptide antibiotics, engineered bacteriophage, and in-licensed products
- Translated early-stage assets into pre-clinical development for respiratory infections and rare diseases
- Initiated and led EnBiotix's Artificial Intelligence MINE platform collaborations
  - Target identification and pathway analysis, Gates Grand Challenges Explorations award
- Outward-facing interactions with external stakeholders and collaborators
  - Leveraged a strong professional relationship network to identify business opportunities
  - Regular presenter to investors, partners, SAB, board members, and at scientific conferences
- Due diligence on a variety of late-stage assets to identify products to strengthen the pipeline
- Company liaison to the FDA
  - Successful pre-IND submission, Qualified Infectious Disease Product and Orphan Drug designations, and shortly after departure an approved IND application

Associate Director, Chemistry, Infection Innovative Medicines Unit, AstraZeneca 2008-2012

- Head of a group of 11 PhD-level scientists
  - Provided modeling, bioinformatics, and cheminformatics support to Infection
  - Discovery and selection of candidates based on potency, PK, and tox including one FIM
- Infection Target Evaluation Team, 2008-2011
  - Assessed druggability, optimal screening approaches, target product profile
  - Multiple project starts resulting in verified leads
- Leader/member of task forces aimed at creating innovation in the early portfolio
  - Lead Generation Task Force, (2011), Irreversible Inhibitors Task Force Chair (2010), Early Portfolio Task Force Chair (2009)
- Leader, Global Structure-Based Design Team, 2010-2012
  - Across 3 international sites accountable for 3 postdocs and 6 external collaborations
- Chair, Scientific Computing Governance Committee, 2010-2011
- Predictive Chemistry Program Steering Committee, 2011-2012
  - Strategy and fund allocation ($Ms) for Predictive Science
- Chair, Infection Seminar Committee, 2011-2012; member, 2009-2010

Cambridge Site Head for Computational Chemistry, Wyeth Research 2006-2008
Principal Research Scientist, Wyeth Research 2001-2006
Staff Scientist II, Wyeth Research 1998-2001

- Led a group of 3 PhD-level scientists and several interns
- Computational chemistry liaison for all Inflammation projects
  - Assessed the druggability of targets and areas for impact for early stage projects
- HTS data analysis and lead optimization for drug discovery in Inflammation, Cardiovascular and Metabolic Disease, Infectious Disease, and Neuroscience
  - Expert on kinases, matrix metalloproteases, phosphatases, GPCRs, PPIs, other novel classes
  - Actively involved in discovery of compounds that reached Phase 2 trials in osteoarthritis
- Lead developer of virtual screening platform and aided in desktop modeling toolkit design

Associate, Harvard University 1998-2003
Research Fellow, Harvard Medical School 1992-1998
Science Scholar, Radcliffe Bunting Institute 1994-1995

EDUCATION

Harvard Medical School, Boston, MA 1992-1998
Postdoctoral Fellow, Biological Chemistry & Molecular Pharmacology
Research with Professor James M. Hogle and Nobelist Martin Karplus

Massachusetts Institute of Technology, Cambridge, MA 1986-1992
Ph.D., Physical Chemistry
Thesis with Professor Gregory A. Petsko and Nobelist Martin Karplus

Boston University, Boston, MA 1982-1986
B.A., Chemistry with a Minor in Computer Science
Summa cum laude with Distinction in Chemistry, Phi Beta Kappa, Trustee Scholar

HONORS AND AWARDS

Fellow, American Institute for Medical and Biological Engineering	2023
Boston University Chemistry Convocation Distinguished Alumni Speaker	2016
"Wyeth Women as Leaders in Discovery" Two-Year Program	2006-2007
Wyeth Above and Beyond Award	2005
Wyeth CSS Publication Award, Wyeth Research Team of the Year Award	2004
Giovanni Armenise-Harvard Foundation Fellowship	1997-1998
Charles A. King/Medical Foundation Fellowship	1995-1997
Radcliffe Bunting Institute Science Scholarship	1994-1995
A.A.U.W. Dissertation Fellowship	1990-1991

PROFESSIONAL ACTIVITIES

- MIT Venture Mentor Service 2019- date
- New England Women in Science Executives (NEWISE), Co-Chair Board of Directors 2019- date
- Advisor, Fractal Therapeutics 2019- date
- HBA Executive Exchange Program 2018-2019
- Editorial Advisory Boards (JCIM, JCAMD) 2010- date
- Boston University Kindle Program Mentor 2012-2016
- Boston University Ignition Awards Review Committee 2013
- MIT Start Smart Boot Camp, HBA Mentoring Program 2012
- National Academies of Sciences Polio Antiviral Workshop Committee 2005-2006

PUBLICATIONS, PATENTS, PRESENTATIONS

81 publications and patents/patent applications and 98 professional presentations

Publications

1. Lehrer, S.S. and **Joseph, D.** (1987) Differences in local conformation around cysteine residues in αα, αβ, and ββ rabbit skeletal tropomyosin. *Arch. Biochem. Biophys.* **256**, 1-9.
2. **Joseph, D**., Petsko, G.A., Karplus, M. (1990) Anatomy of a protein conformational change: Hinged 'lid' motion of the triosephosphate isomerase loop. *Science* **249**, 1425-1428.
3. Karplus, M., Evanseck, J.D., **Joseph, D.**, Bash, P.A., Field, M.J. (1992) Simulation analysis of triosephosphate isomerase: Conformation transition and catalysis. *Faraday Discuss.* **93**, 239-248.
4. Schmidt, J.M., Bruschweiler, R., Ernst, R.R., Dunbrack, R.L., **Joseph, D.**, Karplus, M. (1993) Molecular-dynamics simulation of the proline conformational equilibrium and dynamics in antamanide using the Charmm force-field. *J. Am. Chem. Soc.* **115**, 9747-9756.
5. Mitra, B., Gerlt, J.A., Babbitt, P.C., Koo, C.W., Kenyon, G.L., **Joseph, D.**, Petsko, G.A. (1993) A novel structural basis for membrane-association of a protein: Construction of a chimeric soluble mutant of S-mandelate dehydrogenase from pseudomonas putida. *Biochemistry* **32**, 12959-12967.
6. **Joseph-McCarthy, D.**, Lolis, E., Komives, E.A., Petsko, G.A. (1994) Crystal structure of the K12M/G15A triosephosphate isomerase double mutant and electrostatic analysis of the active site. *Biochemistry* **33**, 2815-2823.
7. **Joseph-McCarthy, D.**, Rost, L.E., Komives, E.A., Petsko, G.A. (1994) Crystal structure of the mutant yeast triosephosphate isomerase in which the catalytic base glutamic acid 165 is changed to aspartic acid. *Biochemistry* **33**, 2824-2829.
8. **Joseph-McCarthy, D.**, Petsko, G.A., Karplus, M. (1995) Use of a minimum perturbation approach to predict TIM mutant structures. *Prot. Engng.* **8**, 1103-1115.
9. **Joseph-McCarthy, D.**, Fedorov, A.A., Almo, S.C. (1996) Comparison of experimental and computational functional group mapping of an RNase A structure: Implications for computer-aided drug design. *Prot. Engng*. **9**, 773-780.
10. Fedorov, A.A., **Joseph-McCarthy, D.**, Fedorov, E., Sirakova, D., Graf, I., Almo, S.C. (1996) Ionic interactions in crystalline bovine pancreatic ribonuclease A. *Biochemistry* **35**, 15962-15979.
11. Wu, Q., Gao, J., **Joseph-McCarthy, D.**, Sigal, G.B., Bruce, J.E., Whitesides, G.M., Smith, R.D. (1997) Carbonic anhydrase-inhibitor binding: From solution to the gas phase. *J. Am. Chem. Soc.*, **119**, 1157-1158.
12. **Joseph-McCarthy, D.**, Hogle, J.M., Karplus, M. (1997) Use of multiple copy simultaneous search to design of a new class of picornavirus capsid binding drugs. *Proteins*, **29**, 32-58.
13. MacKerell, A.D., Jr., *et al.* (1998) All-atom empirical potential for molecular modeling and dynamics studies of protein. *J. Phys. Chem. B*, **102**, 3586-3616.
14. **Joseph-McCarthy, D.** (1999) Computational approaches to structure-based ligand design, *Pharmacol.Therapeut.*, **84**, 179-191.
15. Somoza, J.R., Schmidt, H., Menon, S., **Joseph-McCarthy, D.**, Dessen, A., Stahl, M.L., Somers, W.S., Sullivan, F.X. (2000) Structural and kinetic analysis of E. coli GDP-mannose 4,6-dehydratase provides insights into the enzyme's catalytic mechanism and regulation by GDP-fucose. *Structure*, **8**, 123-135.
16. Thomas, B.E., IV, **Joseph-McCarthy, D.**, Alvarez, J.C. (2000) Pharmacophore-based molecular docking. In O.F. Guner (Ed.). Pharmacophore perception, development, and use in drug design. La Jolla: International University Line, 351-367.
17. Elkin, C.D., Zuccola, H., Hogle, J.M., **Joseph-McCarthy, D.** (2000) Computer-aided design of D-peptide inhibitors of hepatitis delta antigen dimerization, *J. Comp. Aided Mol. Design*, **14**, 705-718.
18. Tsang, S.K., Cheh, J., Isaacs, L., **Joseph-McCarthy, D.**, Choi, S.-K., Pevear, D.C., Whitesides, G.M., Hogle, J.M. (2000) A structurally biased combinatorial approach for discovering new anti-picornaviral compounds, *Chem. & Biol*., **50**, 1-13.
19. **Joseph-McCarthy, D.** (2001) Structure-based combinatorial library design and screening: Application of the Multiple Copy Simultaneous Search method. In A.K. Ghose and V.N. Viswanadhan (Eds.). Combinatorial library design and evaluation for drug discovery: Principles, methods, software tools and applications. New York: Marcel Dekker, Inc., 503-530.
20. Bitetti-Putzer, R., **Joseph-McCarthy, D.**, Hogle, J.M., Karplus, M. (2001) Functional group placement in protein binding sites: A comparison of the GRID and MCSS*, J. Comp. Aided Mol. Design*, **15**, 935-960.
21. **Joseph-McCarthy, D.**, Tsang, S.K., Filman, D.J., Hogle, J.M., Karplus, M. (2001) Use of MCSS to design small targeted libraries–Application to picornavirus ligands, *J. Am. Chem. Soc*., **123**, 12758-12769.
22. **Joseph-McCarthy, D.** (2002) An overview of in silico design and screening: Toward efficient drug discovery*, Curr. Drug Disc.*, March, 20-23.

23. **Joseph-McCarthy, D.**, Thomas, B.E., IV, Belmarsh, M., Moustakas, D., Alvarez, J.C. (2003) Pharmacophore-based molecular docking to account for ligand flexibility, *Proteins*, **51**, 172-188.
24. **Joseph-McCarthy, D.**, Alvarez, J.C. (2003) Automated generation of MCSS-derived pharmacophoric DOCK site points for searching multi-conformation databases, *Proteins*, **51**, 189-202.
25. McKew, J.C., Lovering, F., Clark, J.D., Bemis, J., Xiang, Y., Shen, M., Zhang, W., Alvarez, J.C., **Joseph-McCarthy, D.** (2003) Structure-activity relationships of indole cytosolic phospholipase $A_2\alpha$ inhibitors: Substrate mimetics. *Bioorg. Med. Chem. Lett.*, **13**, 4501-4.
26. Gilbert, A.M., Kirisits, M., Toy, P., Failli, A., Dushin, E.G., Novikova, E., Peter J. Petersen, P.J., **Joseph-McCarthy, D.**, McFadyan, I.J., Fritz, C.C. (2004) Anthranilate 4H-oxazol-5-ones: Novel small molecule antibacterial acyl carrier protein synthase (AcpS) inhibitors, *Bioorg. Med. Chem. Lett*., **14**, 37-41.
27. Xu, Z.-B., Chaudhary, D., Olland, S., Wolfrom, S., Czerwinski, R., Malakian, K., Lin, L., Stahl, M. L., **Joseph-McCarthy**, D., Benander, C., Fitz, L., Greco, R., Somers, W. S., Mosyak, L. (2004) Catalytic domain crystal structure of protein kinase C-theta (PKCθ), *J. Biol. Chem.*, **279**, 50401-50409.
28. Venkatesan, A.M., Davis, J. M., Grosu, G. T., Baker, J., Levin, J. I., Ellingboe, J., Skotnicki, J. S., DiJoseph, J. F., Sung, A., Jin, G., Xu, W., **Joseph-McCarthy, D.**, Barone, D. (2004) Synthesis and structure activity relationships of 4-alkynyloxy phenyl sulfanyl, sulfinyl and sulfonyl alkyl hydroxamates as Tumor Necrosis Factor-α Converting Enzyme (Tace) and matrix metalloproteinase inhibitors, *J. Med. Chem.*, **47**, 6255-6269.
29. **Joseph-McCarthy, D.**, McFadyen, I.J., Zou, J., Walker, G., Alvarez, J.C. (2005) Pharmacophore-based molecular docking: A practical guide. In J.C. Alvarez and B.K. Shoichet (Eds.). Virtual screening in drug discovery. New York: CRC Press, 317-334.
30. **Joseph-McCarthy, D.** (2005) Structure-based lead optimization. *Annu. Rep. Comp. Chem.*, **1**, 169-183.
31. **Joseph-McCarthy, D.**, Parris, K.; Huang, A., Failli, A., Quagliato, D., Dushin, E. G., Novikova, E., Severina, E., Tuckman, M., Petersen, P. J., Dean, C., Fritz, C. C., Meshulam, T., DeCenzo, M., Dick, L., McFadyen, I. J., Somers, W. S., Lovering, F., Gilbert, A. M. (2005) Use of structure-based drug design approaches to obtain novel anthranilic acid acyl carrier protein synthase inhibitors, *J. Med. Chem.*, **48***,* 7960-7969.
32. Moretto, A.F., Kirincich, S.J., Xu, W.X., Smith, M.J., Wan, Z.-K., Wilson, D.P., Follows, B.C., Binnun, E., **Joseph-McCarthy, D.**, Foreman, K., Erbe, D.V., Zhang, Y.L., Tam, S.K., Tam, S.Y., Lee, J. (2006) Bicyclic and tricyclic thiophenes as protein tyrosine phosphatase 1B inhibitors, *Bioorg. Med. Chem.*, **14**, 2162-2177.
33. Gopalsamy, A., Yang, H., Ellingboe, J.W., McKew, J.C., Tam, S**., Joseph**-**McCarthy,** D., Zhang, W., Shen, M., Clark, J.D. (2006) 1,2,4-Oxadiazolidin-3,5-diones and 1,3,5-triazin-2,4,6-triones as cytosolic phospholipase A2alpha inhibitors, *Bioorg. Med. Chem. Lett.*, **16**, 2978-2981.
34. Katz, S.L., Andino, R**., Joseph-McCarthy, D.**, Modlin, J.F., Nathanson, N., Whitley, R.J., Wimmer. E. (2006) Exploring the role of antiviral drugs in the eradication of polio: Workshop report, Committee on Development of a Polio Antiviral and Its Potential Role in Global Poliomyelitis Eradication, National Research Council of the National Academies, Washington, D.C.
35. Wan, Z.-K., Lee, J., Xu, W.X., Erbe, D.V., **Joseph-McCarthy, D.**, Follows, B.C., Zhang, Y.L. (2006) Monocyclic thiophenes as protein tyrosine phosphatase 1B inhibitors: Capturing interactions with Asp48**,** *Bioorg. Med. Chem. Lett.*, **16**, 4941-4945.
36. Condon, J. S., **Joseph-McCarthy, D.**, Levin, J. I., Lombart, H.-G., Lovering, F. E., Sun, L., Wang, W., Xu, W., Zhang, Y. (2007) Identification of potent and selective TACE inhibitors via the S1 pocket, *Bioorg. Med. Chem. Lett.* **17**, 34-39.
37. Wan, Z.-K., Follows, B., Kirincich, S., Wilson, D., Binnun, E., Xu, W., **Joseph-McCarthy, D.**, Wu, J., Smith, M., Zhang, Y.-L., Tam, M., Erbe, D., Tam, S., Saiah, E., Lee, J. (2007) Probing acid replacements of thiophene PTP1B inhibitors, *Bioorg. Med. Chem. Lett.* **17**, 2913-2920.
38. **Joseph-McCarthy, D.**, Baber, J.C., Feyfant, E., Thompson, D.C., Humblet C. (2007) Lead optimization via high-throughput molecular docking, *Curr. Opin. Drug Discovery Dev.*, **10**, 264-274.
39. Lombart, H.-G., Feyfant, E., **Joseph-McCarthy, D.**, Huang, A., Lovering, F., Sun, L.H., Zhu, Y., Zeng, C., Zhang, Y., Levin, J. (2007) Design and synthesis of 3,3-piperidine hydroxamate analogs as selective TACE inhibitors, *Bioorg. Med. Chem. Lett.*, **17**, 4333-4337
40. Huang, A., **Joseph-McCarthy, D.**, Lovering, F., Sun, L., Wang, W., Xu, W., Zhu, Y., Cui, J., Zhang, Y., Levin, J. I. (2007) Structure-based design of TACE selective inhibitors: Manipulations in the S1'-S3' pocket, *Bioorg. Med. Chem.*, **15**, 6170-6181.
41. Evensen, E., **Joseph-McCarthy, D**., Weiss, G.A., Schreiber, S.L., Karplus, M. (2007) Ligand design by a combinatorial approach based on modeling and experiment: Application to HLA-DR4, *J. Comp. Aided Mol. Design*, **21**, 395-418.

42. Wilson, D. P., Wan, Z.-K., Xu, W.-X., Kirincich, S. J., Follows, B. C., **Joseph-McCarthy, D.**, Foreman, K., Moretto, A., Wu, J., Zhu, M., Binnun, E., Zhang, Y.-Li., Tam, M., Erbe, D. V., Tobin, J., Xu, X., Leung, L., Shilling, A., Tam, S. Y., Mansour, T. S., Lee, J. (2007) Structure-Based Optimization of Protein Tyrosine Phosphatase 1B Inhibitors: From the Active Site to the Second Phosphotyrosine Binding Site, *J. Med. Chem.*, **50**, 4681-4698.
43. Green, N., Hu, Y., Janz, K., Li, H.-Q., Kaila, N., Guler, S., Thomason, J., **Joseph-McCarthy, D.**, Tam, S. Y., Hotchandani, R., Wu, J., Huang, A., Wang, Q., Leung, L., Pelker, J., Marusic, S., Hsu, S., Telliez, J-B., Hall, J. P., Cuozzo, J. W., Lin, L.-L. (2007) Inhibitors of Tumor Progression Loci-2 (Tpl2) Kinase and Tumor Necrosis Factor a (TNF-a) Production: Selectivity and in Vivo Antiinflammatory Activity of Novel 8-Substituted-4-anilino-6-aminoquinoline-3-carbonitriles, *J. Med. Chem.*, **50**, 4728-4745.
44. Mosyak, L., Xu, Z., **Joseph-McCarthy, D.**, Brooijmans, N., Somers, W., Chaudhary, D. (2007) Structure-based optimization of PKCθ inhibitors, *Biochemical Society Transactions*, **35**, 1027-1031.
45. Thompson, D.C., Humblet, C., **Joseph-McCarthy, D.** (2008) Investigation of MM-PBSA Re-scoring of Docking Poses, *J. Chem. Inf. Model.*, **48**, 1081-1091.
46. Williams, G., Wood, A., Williams, E.-J., Gao, Y., Mercado, M.L., Katz, A., **Joseph-McCarthy**, D., Bates, B., Ling, H.-P., Aulabaugh, A., Zaccardi, J., Xie, Y., Pangalos, M.N., Walsh, F.S., and Doherty, P. (2008) Ganglioside inhibition of neurite outgrowth requires Nogo receptor function, identification of interaction sites and development of novel antagonists**,** *J. Biol. Chem.*, **283**, 16641-16652.
47. Cole, D.C., Asselin, M., Brennan, A., Czerwinski, R., Ellingboe, J.W., Fitz, L., Greco, R., Huang, X., **Joseph-McCarthy, D.**, Kirisits, M., Lee, J., Li, Y., Morgan, P., Stock, J.R., Tsao, D.H.H., Wissner, A., Yang, X., Chaudhary, D. (2008) Identification, Characterization and Initial Hit-to-Lead Optimization of a Series of 4-Arylamino-3-Pyridinecarbonitrile as Protein Kinase C theta (PKCθ) Inhibitors, *J. Med. Chem.*, **51**, 5958-5963.
48. Thompson, D.C., Denny, A., Humblet, C., **Joseph-McCarthy, D.**, Feyfant, E, (2008) CONFIRM: Connecting fragments in receptor molecules, *J. Comp. Aided Mol. Design*, **22**, 761-772.
49. Wan, Z.-K., Lee, J., Hotchandani, R., Moretto, A., Binnun, E., Wilson, D.P., Kirincich, S.J., Follows, B.C., Ipek, M., Xu, W., **Joseph-McCarthy, D.**, Zhang, Y.-L., Tam, M., Erbe, D.V., Tobin, J.F., Li, W., Tam, S.Y., Mansour, T.S., Wu, J. (2008) Structure-based optimization of protein tyrosine phosphatase-1 B inhibitors: capturing interactions with arginine 24, *Chem. Med. Chem.*, **3**, 1525-1529.
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58. Campbell, A.J., Lamb, M.L., **Joseph-McCarthy, D.** (2014) Ensemble-Based Docking Using Biased Molecular Dynamics, *J. Chem. Inf. Model.*, 54, 2127-38.

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61. Basu, S., Hochberg, N. S., Senior, B. A., **Joseph-McCarthy, D.**, & Chakravarty, A. (2021) Computational projection of virion transmission rates to the lower airway from the initial SARS-CoV-2 infection at the Nasopharynx, *Journal of Aerosol Medicine and Pulmonary Drug Delivery*, A8-A9.
62. Van Egeren, D., Novokhodko, A., Stoddard, M., Tran, U., Zetter, B., Rogers, M., Pentelute, B.L., Carlson, J.M., **Joseph-McCarthy, D.** & Chakravarty, A. (2021) Risk of rapid evolutionary escape from biomedical interventions targeting SARS-CoV-2 spike protein, *PloS One*, 16, e0250780.
63. Van Egeren, D., Novokhodko, A., Stoddard, M., Tran, U., Zetter, B., Rogers, M. S., **Joseph-McCarthy, D.** & Chakravarty, A. (2021) Controlling long-term SARS-CoV-2 infections can slow viral evolution and reduce the risk of treatment failure, *Scientific Reports*, 11, 1-9.
64. Van Egeren, D., Stoddard, M., Novokhodko, A., Rogers, M. S., **Joseph-McCarthy, D.,** Zetter, B., & Chakravarty, A. (2021) Rapid relaxation of pandemic restrictions after vaccine rollout favors growth of SARS-CoV-2 variants: A model-based analysis, *PloS One*, 16, e0258997.
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69. Walker, K.C., Shwarts, M., Demidkin, S., Chakravarty, A., **Joseph-McCarthy, D.** (2023) Machine learning for the identification of respiratory viral attachment machinery from sequences data, *PloS One*, 18, e0281642.
70. Akash, M.M.H, Lao, Y., Balivada, P.A., Ato, P., Ka, N.K., Mituniewicz, A., Silfen, Z., Suman, J.D., Chakravarty, A., **Joseph-McCarthy, D**., Basu, S. (2023) On a model-based approach to improve intranasal spray targeting for respiratory viral infections, *Front. Drug Deliv*., 3, 1164671.
71. Lazou, M., Hutton, J.R., Chakravarty, A., **Joseph-McCarthy, D.** (2024) Identification of a druggable site on GRP78 at the GRP78-SARS-CoV-2 interface and virtual screening of compounds to disrupt that interface, *J. Comp. Aided Mol. Design,* in press.
72. Bekar-Cesaretli, A., Khan, O., Nguyen, T., Kozakov, D., **Joseph-Mccarthy, D**., Vajda, S. (2024) Conservation of Hot Spots and Ligand Binding Sites in Protein Models by AlphaFold2, *J. Chem. Inf. Model.*, accepted.

Patents

Joseph-McCarthy, D.M., Bermudez, L., "Antibiotic potentiation for nontuberculous mycobacterial disease", published application **US 17/617,711** (2022).

Joseph-McCarthy, D.M., Koeva, M.I., "Aminoglycoside potentiation for treatment of pulmonary bacterial infection", published application **WO 2018107020** (2018), US 18/135, 907 (2023).

Cole, D. C., Boschelli, D. H., Wang, Y. D., Asselin, M., Joseph-McCarthy, D. M., Prashad, A. S., Wissner, A., Dushin, R., Wu, B., Tumey, L. N., Niu, C. S., Chen, J. "Substituted 3-cyanopyridines as protein kinase inhibitors", **US 7,781,591** (2010).

Lee, J., Smith, M.J., Moretto, A.F., Wan, Z.-K., Binnun, E.D., Xu, W., Foreman, K.W., Joseph-McCarthy, D.M., Erbe, D.V., Tam, S.Y., "PTP1B inhibitors", **US 7,674,822** (2010).

Olland, A., Strand, J., Fleming, M., Joseph-Mccarthy, D., Krykbaev, R. "High resolution crystal structures of acidic mammalian chitinases and their uses", published application **WO 2009076621** (2009).

Lee, J., Kirincich, S.J., Smith, M.J., Wilson, D.P., Follows, B.C., Wan, Z.-K., Joseph-McCarthy, D., Erbe, D.V., Zhang, Y.-L., Xu, W., Tam, S. Y., "Inhibitors of protein tyrosine phosphatase 1B", published application **US 20050203081** (2005).

Tsang, S.K., Joseph-McCarthy, D., Hogle, J.M. "Method for identifying new antipicornaviral compounds", **US 6,558,899** (2003).

Hogle, J.M., Joseph-McCarthy, D., Isaacs, L., Cheh, J., Whitesides, G.M., Karplus, M. "Antipicornaviral ligands via a combinatorial computational and synthetic approach", **US 6,416,762** (2002).

Hogle, J.M., Karplus, M., Joseph-McCarthy, D. "Structure-based design of capsid stabilizing or antiviral agents", **US 5,637,708** (1997).

Invited Talks

"Structure-Guided Computational Approaches for Viral Mitigation Strategies":
- Modeling of Protein Interactions Conference, The University of Kansas, May 2023
- Precision In Drug Discovery & Preclinical Summit, June 2023

"COVID-19 Predictions for Mitigation Strategies":
- Research on Tap: Pandemic Preparedness and Response, Boston University, September 2021.

"Analysis of Big Data for Novel Target Identification":
- Bioinformatics Strategy Meeting USA, Panel Discussion, November 2018.

"An Anti-Persister Aminoglycoside-Potentiator Combination for Treating Chronic *Pseudomonas* Infections":
- Discovery on Target, Re-entering Antibacterial Discovery & Development Summit, September 2018.
- Dartmouth Cystic Fibrosis Retreat, March 2018.

"EnBiotix's Systems Biology Platform: Artificial Intelligence for Drug Discovery":
- AI for Drug Discovery, **JLABs QuickFire Challenge Finalist**, December 2017.

"Candidate Selection Strategies: Where are we now":
- Translating Molecules into Medicines, Think Tank, December 2017.

"Bioinformatics for Complex Biological Systems":
- Bioinformatics Strategy Meeting USA, **Keynote Presentation**, November 2017.

"EBX-001: A Tobramycin-Potentiator Combination Focused on Bacterial Persisters":
- Boston Area Antibiotic Resistance Network (BAARN) Annual Meeting, November 2017.
- European Cystic Fibrosis Society Conference, September 2017.

"A Novel Combination of Tobramycin with a Potentiator for the Treatment of Chronic *P. aeruginosa* Infections":
- Dartmouth Cystic Fibrosis Retreat, March 2016.

"Fragment-Based Lead Discovery and Design: A Multipronged Approach":
- ZING Fragment-Based Drug Discovery Conference, July 2014.

"MINE: A Novel Computational Approach for Gene Network Identification":
- Bio-IT World Conference, April 2014.

"Computational Approaches for Effective Drug Discovery: One Chemists Career Path":
- Bryn Mawr College, Summer Science Research Program, June 2014.
- Women in Chemistry Seminar Series, Boston University, October 2013.
- Research Experience for Undergraduates Seminar Series, Boston University, June 2013.

"Computational Target Evaluation and Lead Generation Strategies":
- CCG North American UGM & Conference, June 2012.
- Structure-Based Drug Design, Cambridge Healthtech Conference, June 2012.
- Cresset UGM, May 2012.

"Fragment-Based Generation of Inhibitors":
- 51st ICAAC, September 2011, presenter and co-convener of the Meet-the-Experts session "Computational Approaches for Designing Antibacterial Agents", Talk 1640.

"Fragment Screening Paradigm for Drug Discovery":
- The 240th ACS National Meeting, August 2010, *Abstracts of the ACS* **240**, 214-COMP.

"Fragments for Drug Discovery":
- Petsko-Ringe 30th Anniversary Symposium, Brandeis University, June 2010.

"Fragment-Based Lead Discovery and Design":
- Gordon Research Conference on Biomolecular Interactions, January 2010.

"Fragment-Based De Novo Design: Past to Present":
- Fragment-Based Lead Discovery (FBLD) Conference, University of York, September 2009.

"Fragment Screening for Drug Discovery":
- Gordon Research Conference on Bioorganic Chemistry, June 2009.
- Sanibel Symposium, February 2009.

"Virtual Screening for Drug Discovery":

- The 236th ACS National Meeting, August 2008; *Abstracts of the ACS* **236**, 267-MEDI.
- Symposium Organizer, "Computational Approaches for Fragment Screening", The 236th ACS National Meeting, August 2008.

"Pharmacophores for Drug Discovery":

- Computer-Aided Drug Design, Keystone, March 2008.

"Strategies for Screening "Fragment" vs. Lead-like Molecules":

- The 234th ACS National Meeting, August 2007; *Abstracts of the ACS* **234**, 162-COMP.
- Session Chair, "Drug Discovery", The 234th ACS National Meeting, August 2007.
- Wyeth-Columbia Workshop, Columbia University, May 2007.

"Strategies for Docking and Scoring: How Can We Do Better?":

- Boston Area Group for Informatics and Modeling, Wyeth Research, September 2006.

"Case Presentation of Strategies for High-Throughput Molecular Docking":

- Structure-Based Drug Design, Cambridge Healthtech Conference, June 2006.

"Lead Optimization via High-throughput Molecular Docking":

- The 230th ACS National Meeting, August 2005; *Abstracts of the ACS* **230**, 115-COMP.

"Virtual Screening for Lead Discovery and Optimization":

- Biomolecular Simulations: from prediction to practice, MGMS International Meeting, September 2005.
- Virtual Screening, Cambridge Healthtech Conference, March 2005.

"Virtual Screening for Drug Discovery ":

- Wyeth Discovery Research Retreat, May 2005.

"High-Throughput Molecular Docking for Lead Discovery":

- The 228th ACS National Meeting, August 2004; *Abstracts of the ACS* **228**, 075-CINF.
- Validation and Results from Virtual Screening, Cambridge Healthtech Conference, June 2004.

"High-Throughput Ligand Docking for Lead Discovery":

- High Throughput Screening for Drug Discovery, Marcus Evans Conference, July 2002.
- New England Bioinformatics Group Seminar, Boston University, May 2002.

"Pharmacophoric Ensembles for Virtual Screening":

- Intelligent Drug Discovery, Cambridge Healthtech Conference, May 2002.

"Docking of Flexible Ligands Using Pharmacophoric Ensembles":

- Boston University, Biomolecular Seminar Series, November 2001.
- The 222nd ACS National Meeting, August 2001; *Abstracts of the ACS* **222**, 013-COMP.

"Pharmacophore-Based Molecular Docking that Accounts for Ligand Flexibility":

- Structure-Based Drug Design, Cambridge Healthtech Conference, April 2001.
- The 221st ACS National Meeting, April 2001; *Abstracts of the ACS* **221**, 063-CINF.

"Developing Methods for Pharmacophore-Based Molecular Docking":

- The 220th ACS National Meeting, August 2000; *Abstracts of the ACS* **220**, 063-CINF.
- IIR Computational Drug Design Conference, July 2000.

"Computational Structure-Based Drug Design: Connecting the Dots":

- MIT Women in Chemistry Series, June 2000.
- MIT Alumni Seminar Series, December 1999.

"Various Docking Strategies that Account for Ligand Flexibility":

- The 218th ACS National Meeting, August 1999; *Abstracts of the ACS* **218**, 068-COMP.
- The 217th ACS National Meeting, March 1999; *Abstracts of the ACS* **217**, 192-COMP.

"Combinatorial Computational Ligand Design for Large Biological Systems":

- WITI Regional Conference, "Innovations in Drug Research" Symposium, October 1998.
- Department of Biomedical Engineering, Boston University, September 1998.
- The 216th ACS National Meeting, August 1998; *Abstracts of the ACS* **216**, 033-COMP.

"A Combinatorial Computational Approach to Ligand Design for Large Biological Systems":

- Center for Bioinformatics, University of Pennsylvania, April 1998.
- Genetics Institute, February 1998.
- Program in Molecular Medicine, University of Massachusetts Medical Center, February 1998.
- Department of Biochem. and Biophys. Sci., University of Houston, February 1998.
- Vertex Pharmaceuticals, November 1997.
- The 214th ACS National Meeting, September 1997; *Abstracts of the ACS* **214**, 229-COMP.
- Fox Chase Cancer Center, April 1997.

"Computational Approaches to Ligand Design for Large Biological Systems":

- Department of Chemistry, College of the Holy Cross, January 1997.

"Application of MCSS/HOOK to Ligand Design for Large Biological Systems":

- Department of Macromolecular Structure, Bristol-Myers Squibb (NJ & CT sites), January 1997.

"Use of MCSS/HOOK to Design New Picornavirus Capsid-Binding Drugs":

- The 212th ACS National Meeting, August 1996; *Abstracts of the ACS* **212**, 188-COMP.

"Design of New Structure-Based Drugs for Poliovirus and Related Viruses through the Use of Computational Methods":

- Department of Chemistry, University of Pennsylvania, January 1996.
- Department of Physiology, Boston University Medical School, October 1995.
- The Radcliffe Bunting Institute Seminar Series, February 1995.

"The Design of New Drugs for Poliovirus and Related Viruses":

- Harvard-Radcliffe Science Alliance Program for Radcliffe freshman, September 1994.

Poster Presentations

- ASM Microbe, June 2018 (2 posters)
- North American Cystic Fibrosis Conference, October 2017.
- ASM/ESCMID Conference on Drug Development, September 2017.
- North American Cystic Fibrosis Conference, October 2016.
- ASM Microbe, June 2016 (2 posters).
- Boston Area Antibiotic Resistance Network (BAARN) Symposium, June 2016.
- Advances in Drug Discovery to Combat Bacterial Resistance, Merck Series, April 2015.
- Boston Area Antibiotic Resistance Network (BAARN) Symposium, March 2015.
- Martin Karplus 75th Birthday Symposium, April 2005.
- Computer-Aided Drug Design Gordon Conference, July 2003.
- Computational Chemistry Gordon Conference, July 2002.
- NetSci Computational and Structural Chemistry Conference, March 2000.
- Computational Chemistry Gordon Conference, July 1998.
- The Protein Society Meeting, July 1997.
- Harvard University Chemical Biology/Structural Biology Retreat, July 1997.
- Harvard Medical School, Biological Chemistry & Molecular Pharmacology Retreat, January 1997.
- Harvard University Chemical Biology/Structural Biology Retreat, July 1996.
- Computational Chemistry Gordon Conference, July 1996.
- Harvard University Chemical Biology/Structural Biology Retreat, July 1995.
- The ASBMB/ACS-DBC satellite Computers and Structure-Based Drug Design Meeting, May 1995; *FASEB J.* **9**, C13 (1995).
- The 208th ACS National Meeting, August 1994; *Abstracts of the ACS* **208**, 40-BIOL.
- Computational Chemistry Gordon Conference, July 1994.
- Biopolymers Gordon Conference, June 1994.
- *FASEB J.* **6**, A143 (1992).
- Computational Chemistry Gordon Conference, June 1992.
- The 203rd ACS National Meeting, April 1992, as an Eli Lilly Travel Award recipient; *Biochemistry* **31**, 2199 (1992).
- *Biophys. J.* **47**, 509a (1985).

SELECT GRANT FUNDING

- **NSF Predictive Intelligence for Pandemic Prevention (PIPP) Phase I: Predicting and Preventing Epidemic to Pandemic Transitions Proposal** (NSF-2200052); co-PI leading the effort on therapeutics and vaccines related to mitigation and response strategies
- **Gates Foundation Grand Challenges Explorations Award,** 2016; PI developing a fully integrated systems biology approach to study the effect of phage therapy on the host immune system and the microbiome.
- **Massachusetts Life Science Center Cooperative Research Matching Grant,** 2015; Enbiotix PI working in collaboration with Massachusetts General Hospital on anti-persisters platform.