



Belinda Akpa



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Integrated Synthetic and
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Emrlab.org

Integrative Mathematical Modeling of Dynamic Physiological Processes

Research emphasis:

The EMRLab develops mathematical models to connect molecular events to dynamic physiological outcomes. Of particular interest is the challenge of using numerical simulations to bridge length-scales in integrated computational and experimental investigations – with the aim of accelerating the translation of molecular and cellular level findings to medical applications. The models we develop involve mechanistic representations of biophysical, biochemical, and physiological events thought to underlie medical outcomes. Integrated with experimental data, they become valuable tools in hypothesis testing, identification of experimentally inaccessible causal mechanisms, and experimental design.

Application:

- Systems pharmacology
- Cell signaling pathways
- Host-pathogen interactions
- Molecular toxicology

Collaboration potential:

- Translational systems biology/physiology
- Synthesis of evidence from knock-out experiments and interrogation of systems-level consequences
- Computationally-driven experiment design

Selected publications:

Ayee M.A.A., Roth C., and Akpa B. S.† Structural perturbation of a dipalmitoylphosphatidylcholine (DPPC) bilayer by warfarin and its bolaamphiphilic analogue: A molecular dynamics study. *Journal of Colloid and Interface Science*. 468:227-237 (2016)

Fettiplace M.R., Lis K., Ripper R., Kowal K., Pichurko A., Vitello D., Schwartz D., Rubinstein I., Akpa B.S. †, and Weinberg G.L. † Multi-modal contributions to detoxification of acute pharmacotoxicity by a triglyceride micro-emulsion. *Journal of Controlled Release*. 198:62-70 (2015)

Kuo I., Akpa B.S.† Validity of the lipid sink as a mechanism for reversal of local anesthetic systemic toxicity: A physiologically based pharmacokinetic model study. *Anesthesiology*. 118(6):1350-1361 (2013)

Graf von der Schulenburg D.A., Akpa B.S., Gladden L.F., Johns M.L. Non-invasive mass transfer measurements in complex biofilm-coated structures. *Biotechnology and Bioengineering*. 101(3):602-608 (2008)