



Elise Bezold

Roche Award

Ph.D. Candidate, Chemistry
Second Year ARCS Scholar

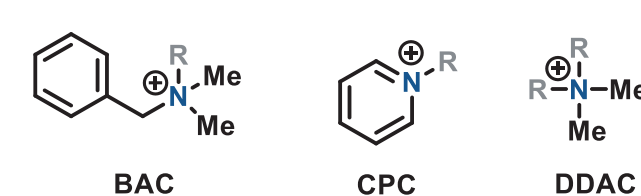


EMORY
UNIVERSITY

Leveraging novel disinfectants to combat antimicrobial resistance

Disinfectants serve as our first line of defense against pathogenic bacteria. Using a multidisciplinary approach, we are designing new antimicrobial agents with a novel mechanism of action to combat highly-resistant pathogens.

QACs are found in our everyday life

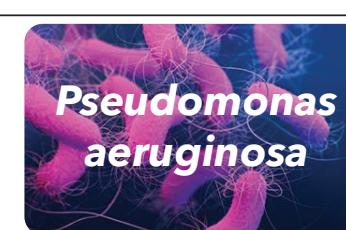


Resistance to QAC disinfectants first reported in the **1980s**

Overuse and misuse of QAC disinfectants has exacerbated bacterial resistance mechanisms towards these agents

Carden et al. *ChemMedChem*. 2020, 15 (21), 1974. Mahoney et al. *iScience*. 2021, 24 (4).

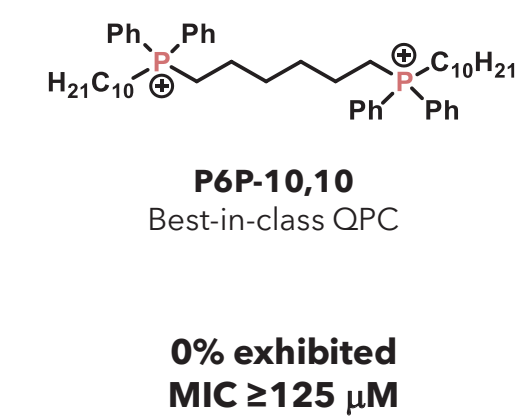
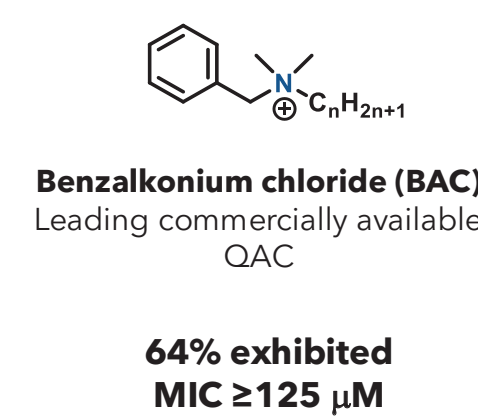
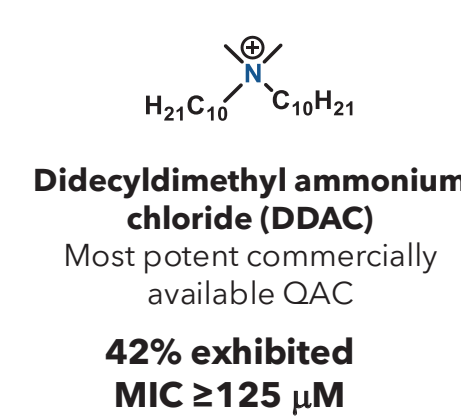
Pseudomonas aeruginosa and disinfectants



Panel of 50 highly resistant clinical isolates from military hospitals

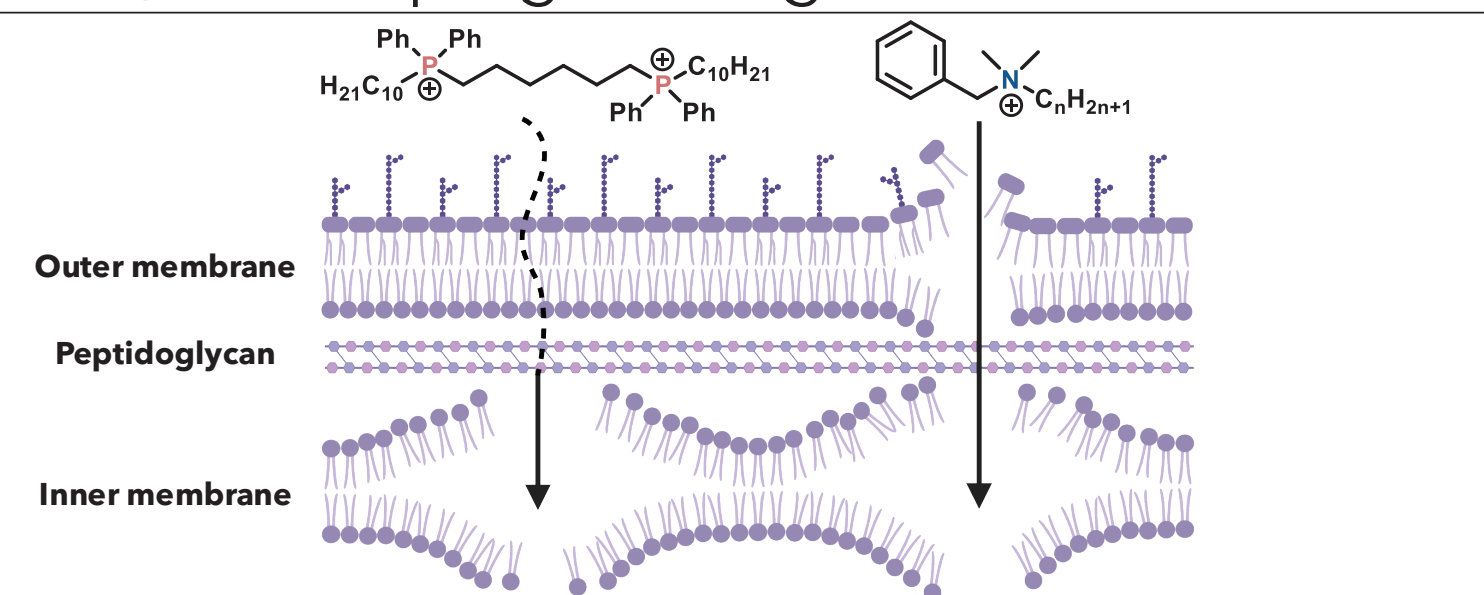
- **Serious** threat classified by CDC and WHO
- Isolated between 2022 to 2023 from military hospitals in Texas and Hawaii
- Persisted on surfaces after treatment with peroxide or QAC-based disinfectants

When the strain can grow at concentrations above 63 μM , we classify these as biocide resistant.



Michaud et al. *ACS Infect. Dis.* 2022, 8 (2), 387-397. MIC screen is unpublished work.

P6P-10,10 disrupts gram-negative inner membrane

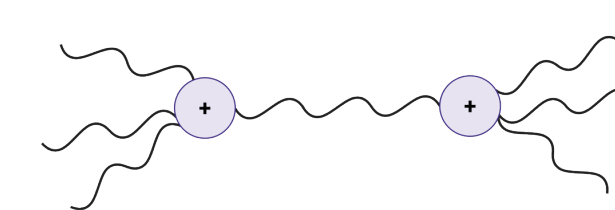


We hope our results can act as a catalyst for the design of novel disinfectants that can prevent the spread of highly-resistant bacteria.

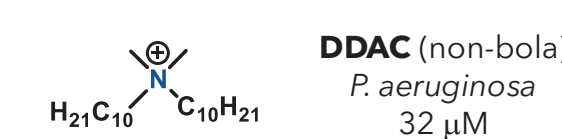
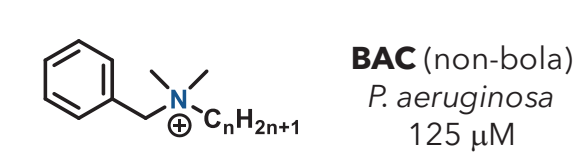
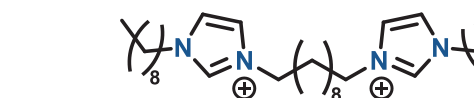
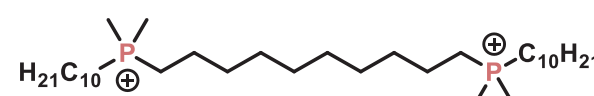
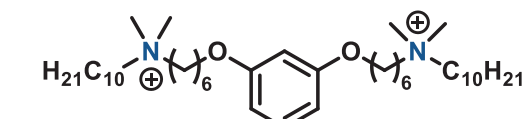
Sanchez, C.A. et al. *ACS Infect. Dis.* 2024, 10, 3868-3879.

Harnessing the bolaamphiphilic structure

- Bolaamphiphilic structure:**
- Two cations separated by a short carbon linker.
 - Inner membrane targeting



Our novel bolaamphiphiles show 6-fold better activity than BAC and DDAC.

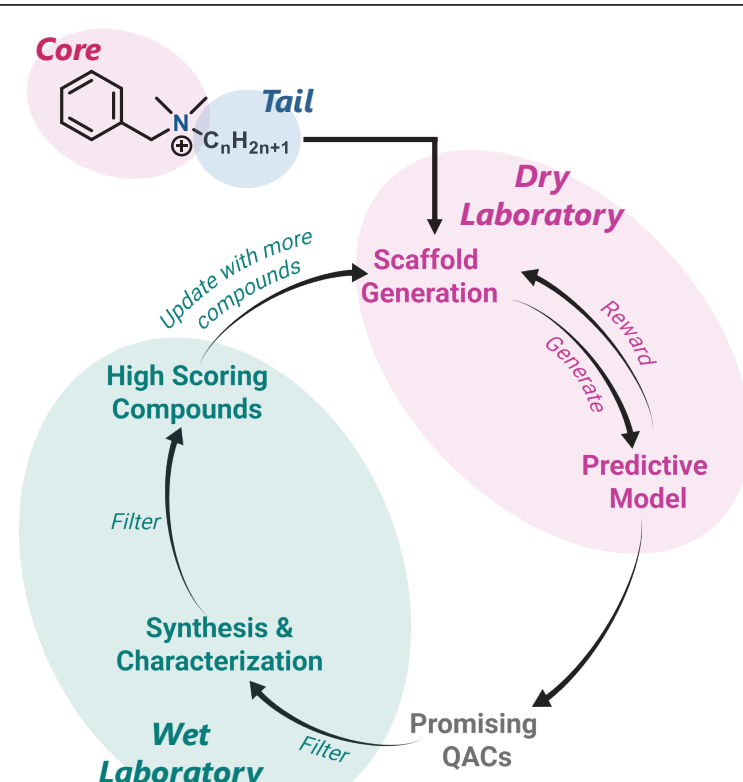


Asante et al. *ChemMedChem*. 2025, e202400932. Alkyl BisQPCs submitted to RSC Med. Chem. Imidazole QACs unpublished work.

Designing disinfectants with AI to fight superbugs

- Chemical space for molecular discovery is vast.
- Deep-learning frameworks in AI can help design molecules faster and smarter.
- Coupling models that generate molecules with those that predict bioactivity can help us focus on compounds that have high bioactivity.

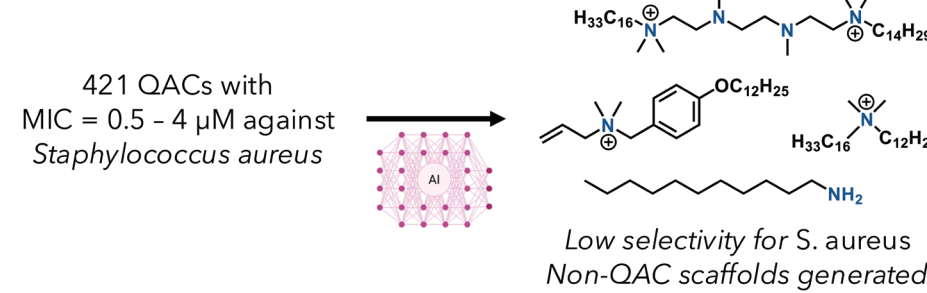
Using both AI and lab experiments, we hope to accelerate the discovery of powerful disinfectants and showing AI-driven design can help tackle antimicrobial resistance.



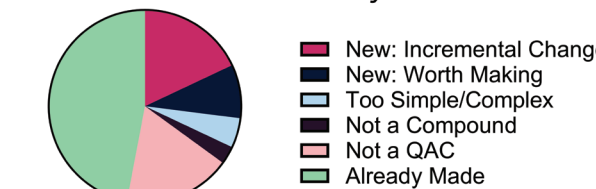
Pan et al. In *Proceedings of the 31st ACM SIGKDD Conference*. p. 4740-4750.

Designing disinfectants with AI to fight superbugs

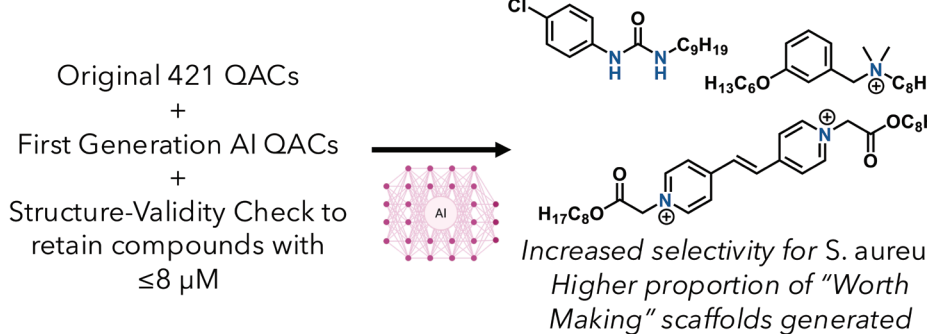
First Generation AI QACs



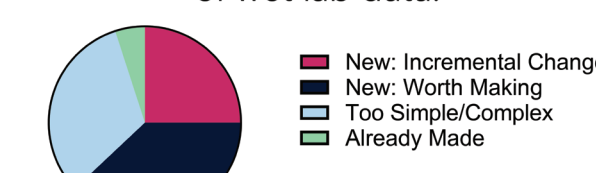
31% of compounds were classified as "Top Compounds" based on predicted bioactivity.



Second Generation AI QACs



This rose to **37%**, demonstrating model refinement through iterative incorporation of wet lab data.



Ghaemi et al. Submitted to *J. Chem. Inf. Model*. Pan et al. In *Proceedings of the 31st ACM SIGKDD Conference*. p. 4740-4750.

Scholar Awards Celebration
November 12, 2025



Igniting
Innovation
in Georgia