



Next Generation Chemical Preservatives: Protecting People, Products, and our Planet

Heather L. Buckley,^a Adam P. Byrne,^b William M. Hart-Cooper^a and Jiawen Liao^c (University of California Berkeley, ^aCollege of Chemistry, ^bDepartment of Civil and Environmental Engineering, ^cSchool of Public Health)
Email: hbuckley@berkeley.edu, abyrne@berkeley.edu, hartcoop@berkeley.edu, fredliao@berkeley.edu

1. Hazards of Conventional Preservatives

- Home and personal care products provide a nutrient-rich medium for microbial growth.
- Preservatives used to prevent microbial growth in consumer products include isothiazolinones (MIT/BIT), quaternary ammonium salts, and formaldehyde releasers.
- Widely used antimicrobials may induce acute or chronic toxicity endpoints such as irritation, sensitization, or cancer.



Source: soapqueen.com

2. Partner Organizations

- Partner organizations Seventh Generation and Beautycounter helped us understand the home and personal care industries and develop relevant recommendations for current product formulations.



Seventh Generation

- Dish liquid
- Auto dish gel
- Laundry detergent



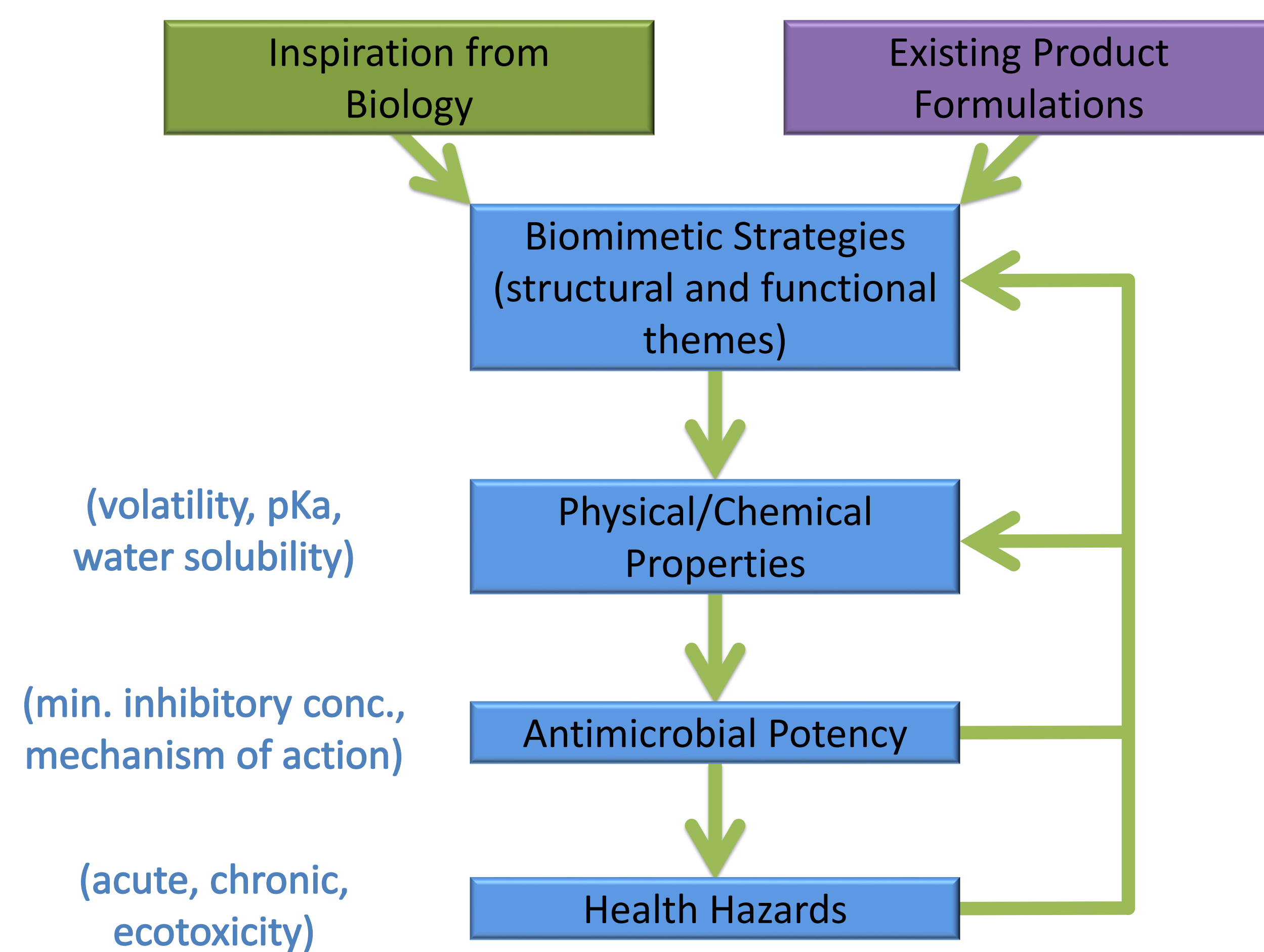
Beautycounter

- Sunscreen
- Kids' shampoo
- Face cream

- Primary considerations: safety, efficacy, biodegradability, cost.

3. Biomimetic Approach

- Working with Biomimicry 3.8, we identified antimicrobial strategies used in natural systems:
 - Amphiphilicity for membrane disruption
 - Synergy
 - Nutrient limitation
- These served as inputs to an iterative analysis of industrially relevant approaches.



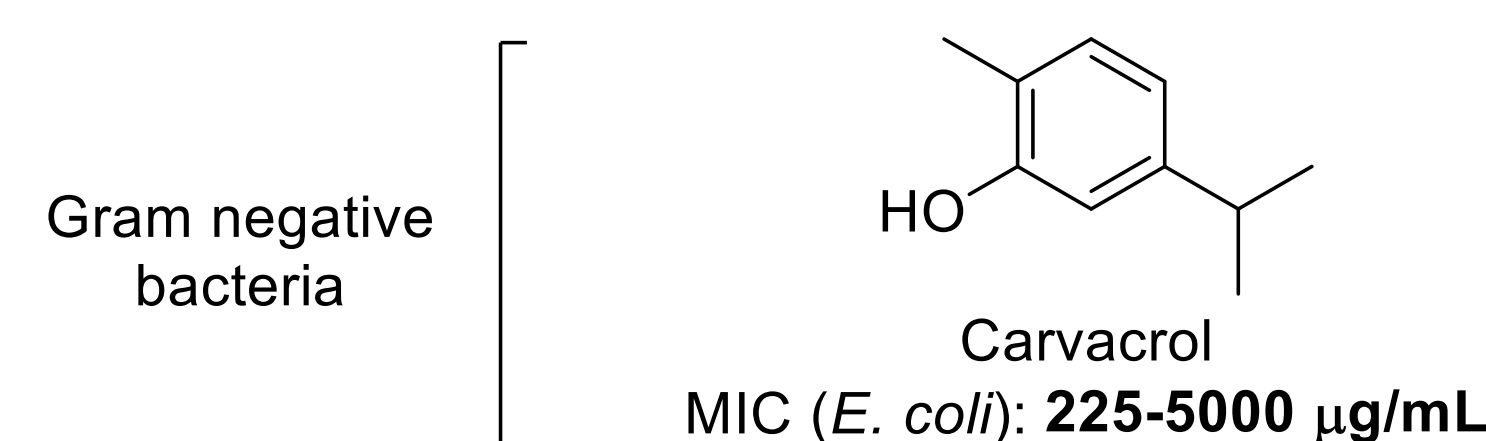
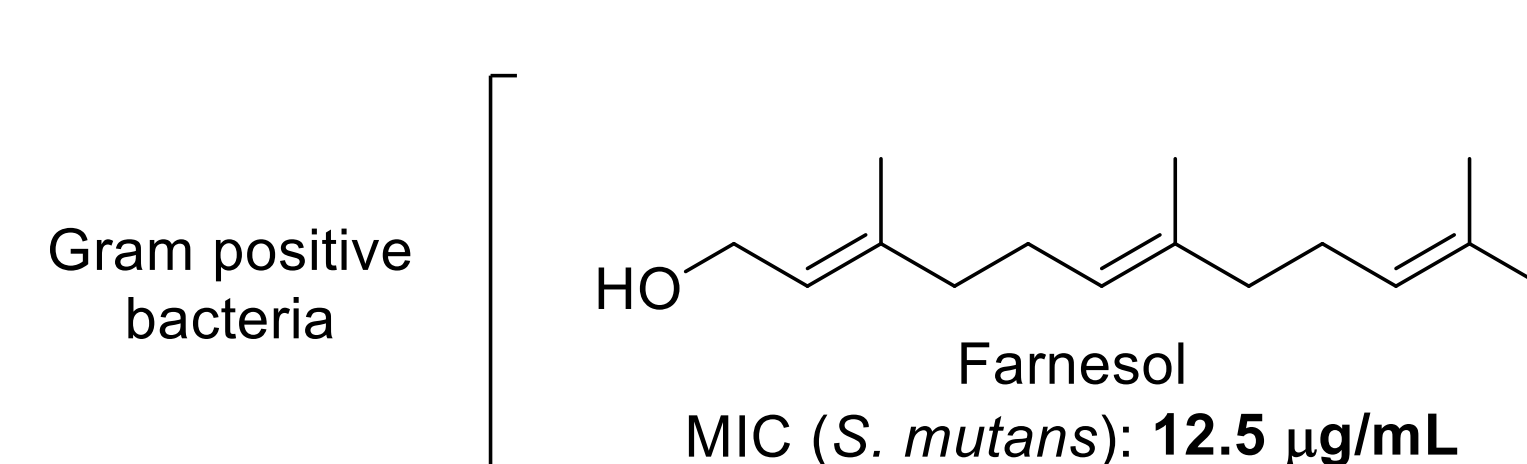
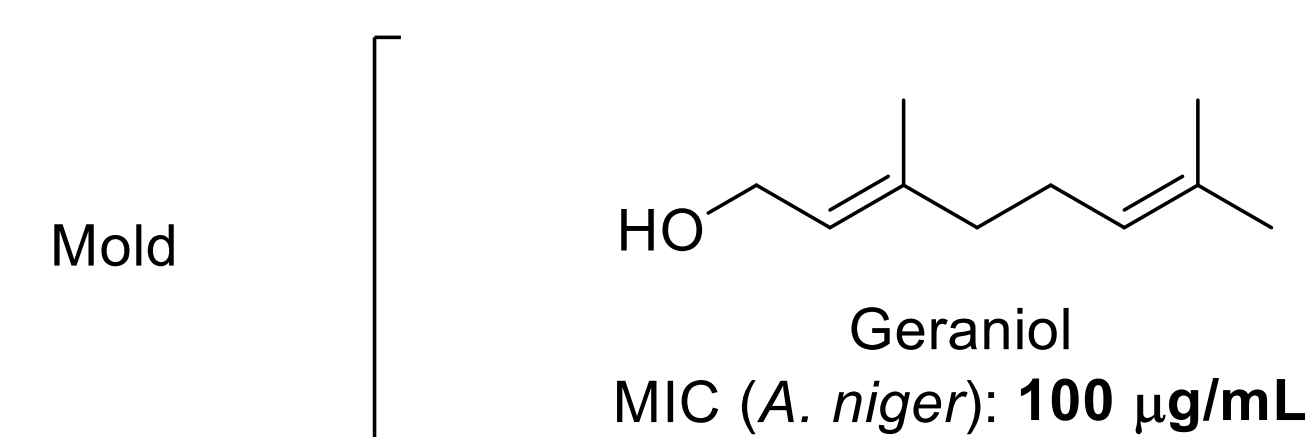
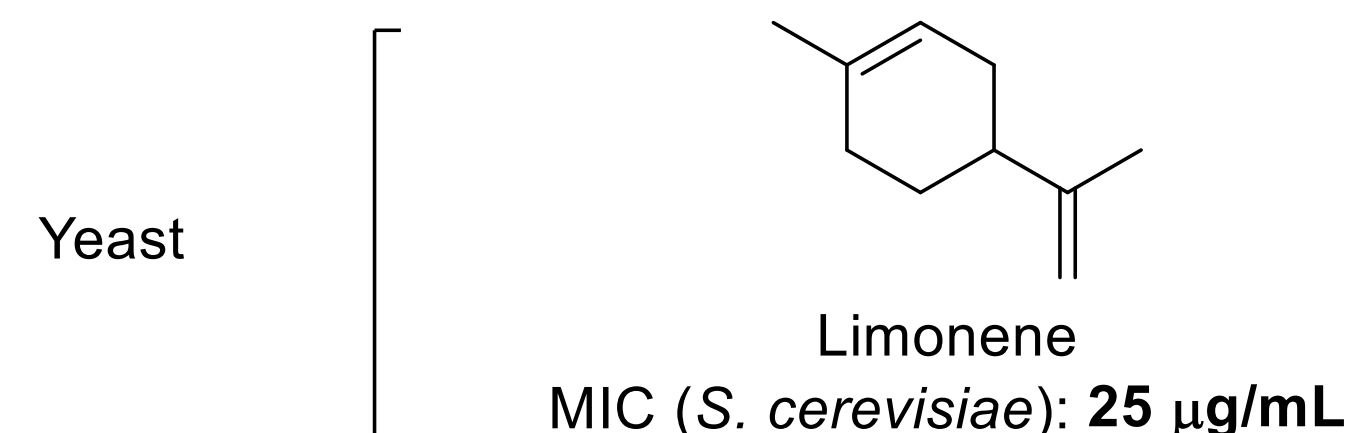
- From this analysis, we identified four classes of compounds for further study.

4. Bioinspired Chemical Preservatives

Terpenoid Antimicrobials

- Naturally sourced, biodegradable
- Color: light yellow to colorless
- Distinctive scents to unscented
- Cost: \$10+/kg
- Hazards: some are irritants, sensitizers

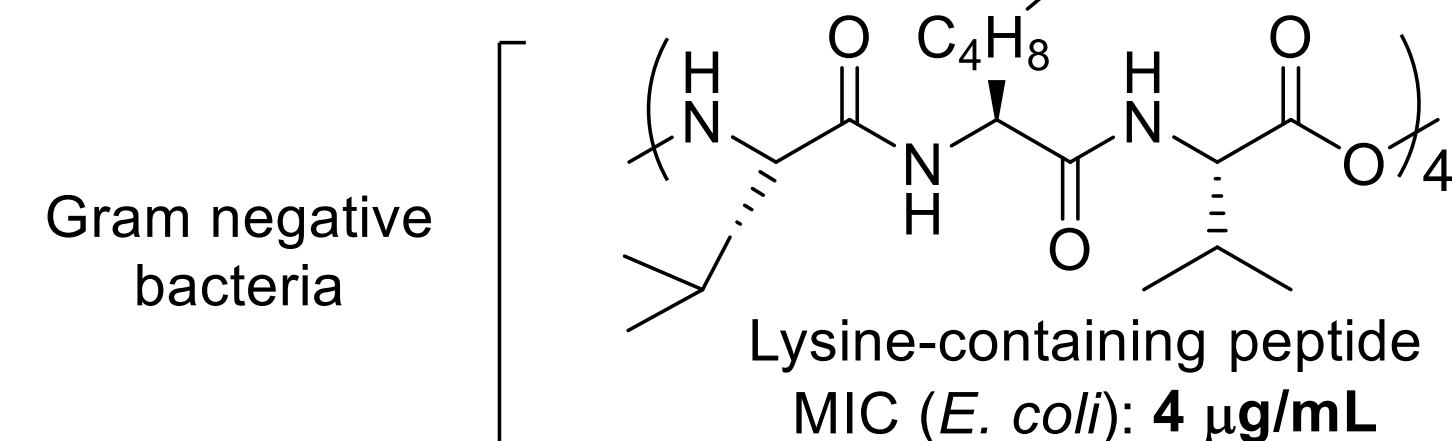
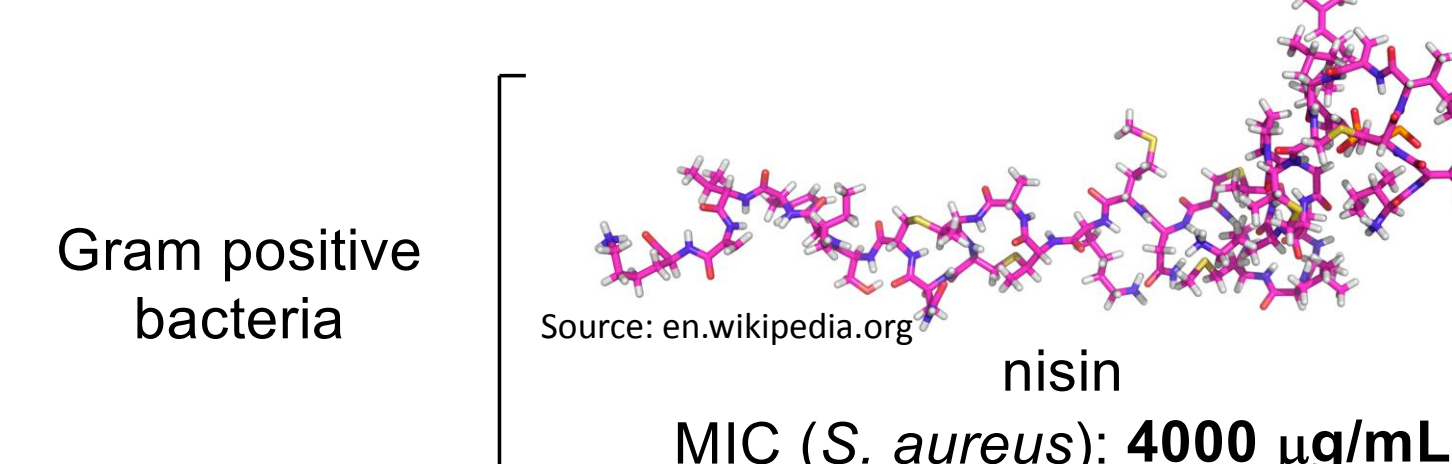
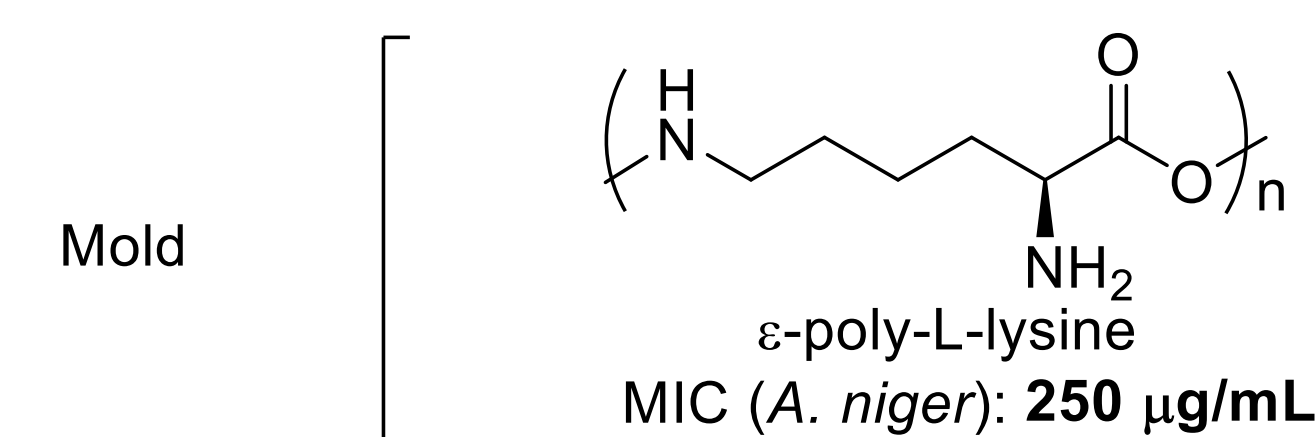
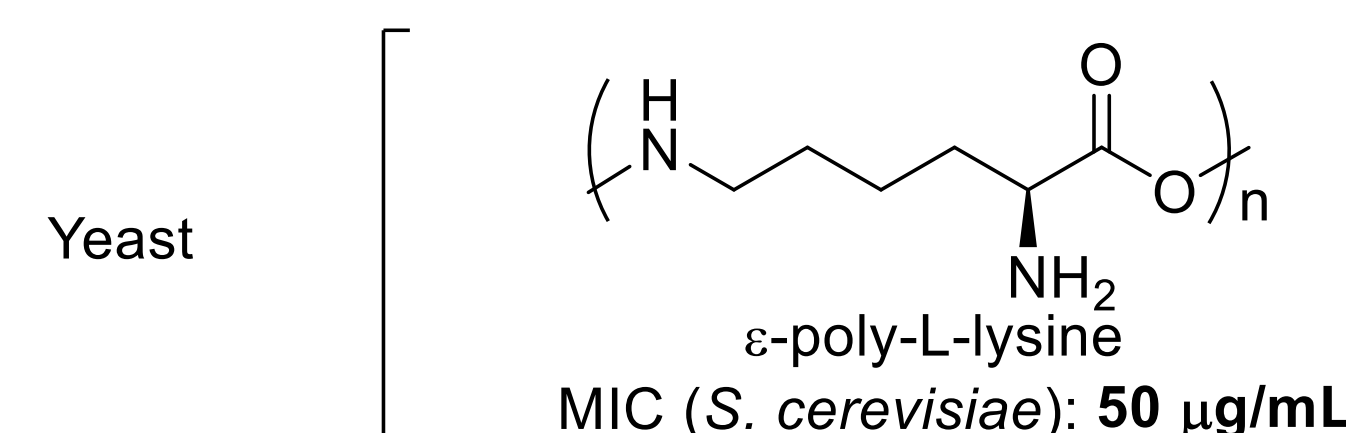
Potency against:



Antimicrobial Peptides

- Prepared through chemical or biosynthesis
- Low volatility
- Cost: \$1-10/kg or prohibitively expensive
- Easily biodegradable, low hazard
- Used as alternative preservatives in food

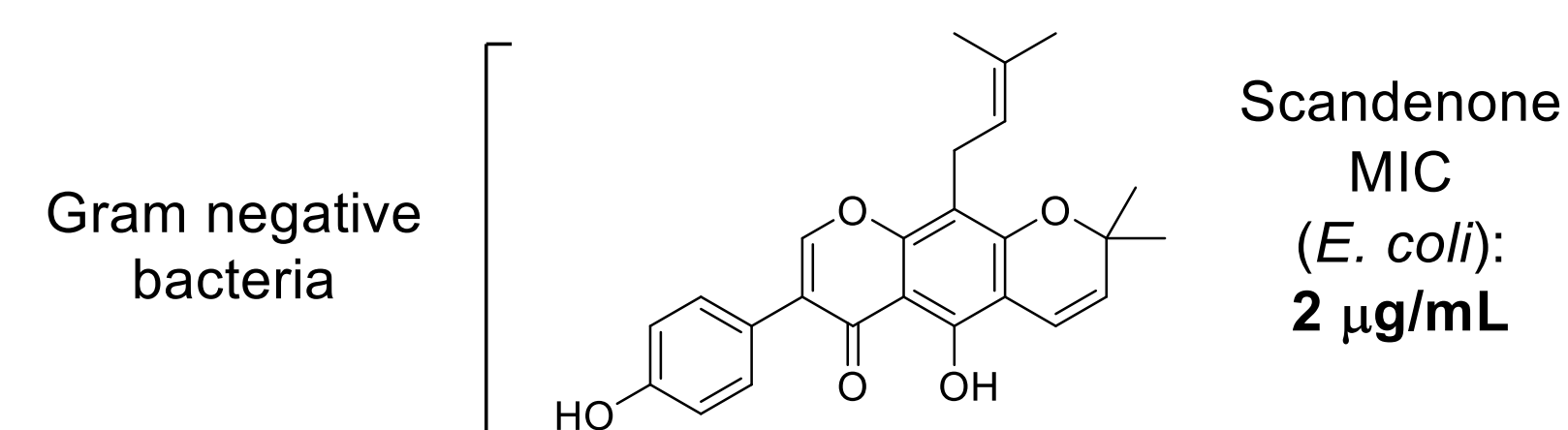
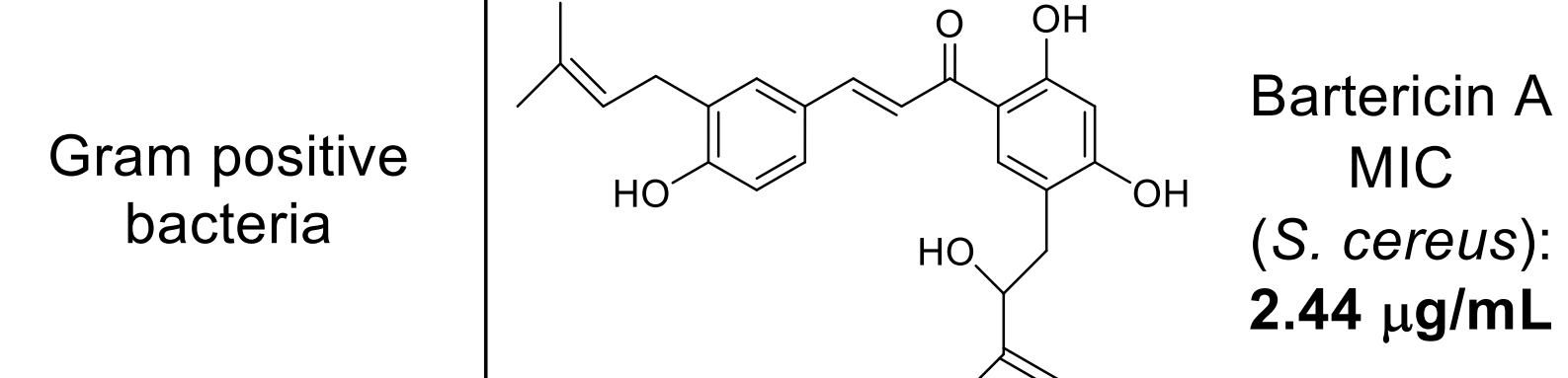
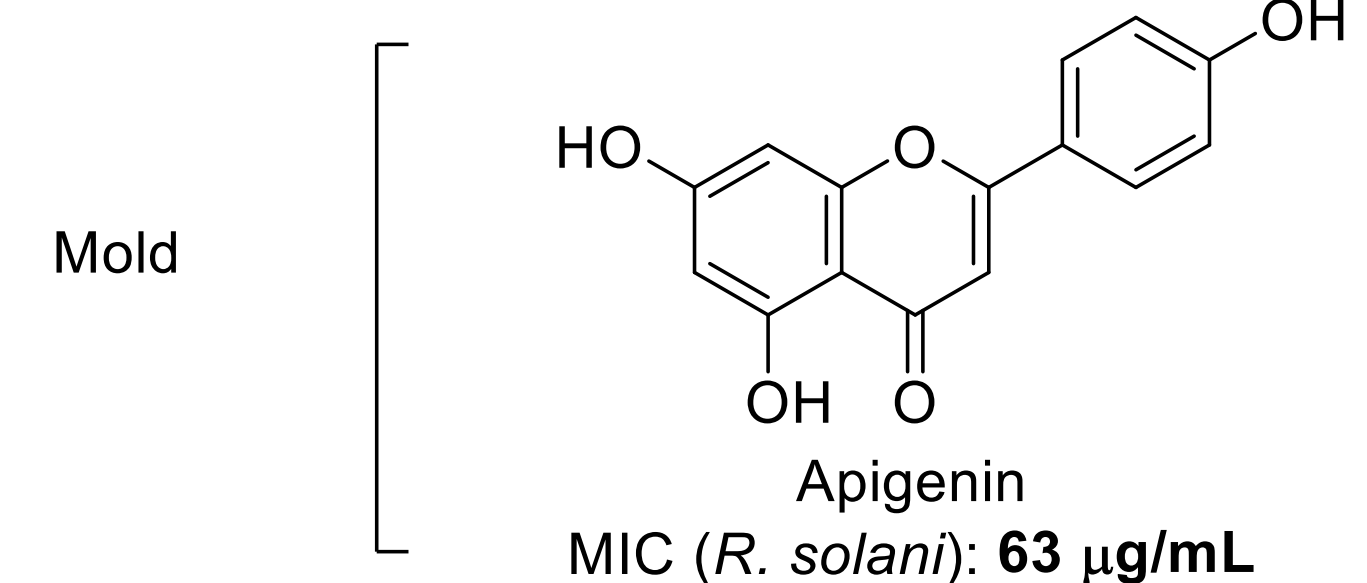
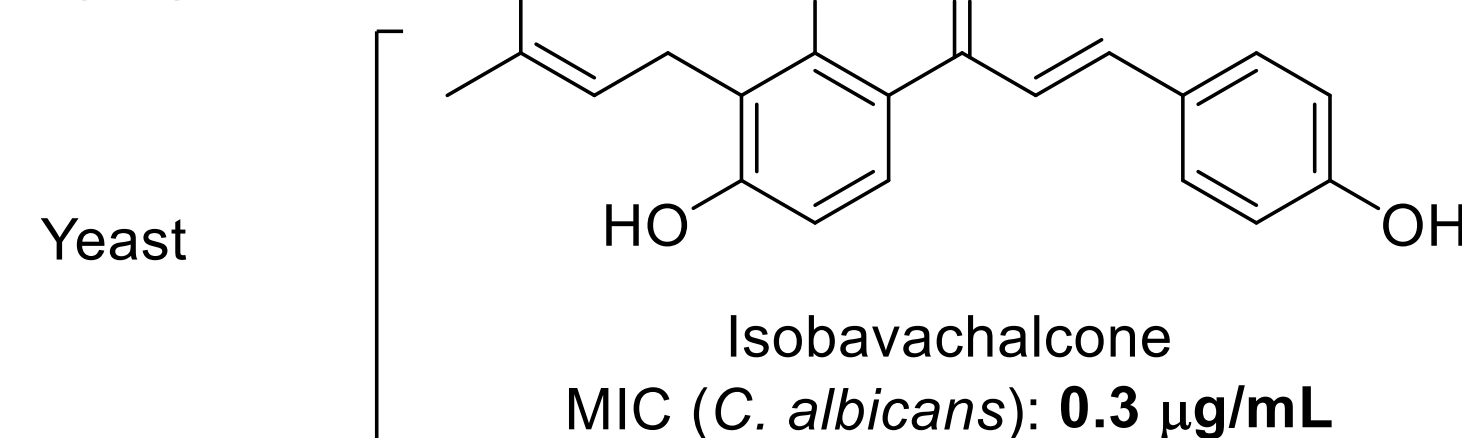
Potency against:



Flavonoid Antimicrobials

- Naturally sourced, biodegradable
- Nutraceutical and pharmaceutical features
- Cost: \$10/kg (Plant extracts)
- Hazards: some are estrogenic

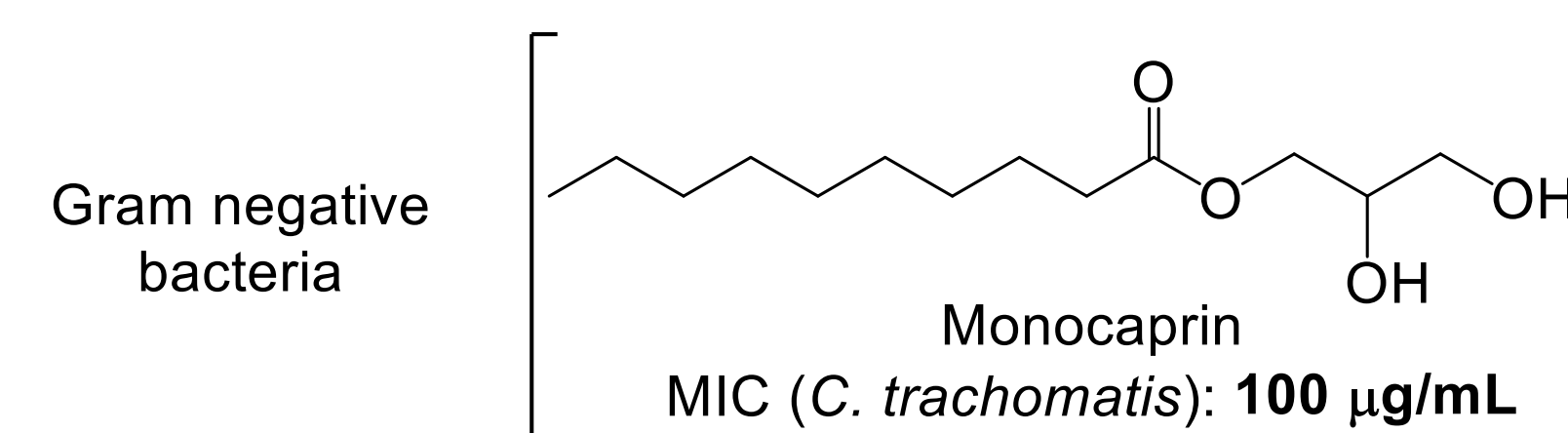
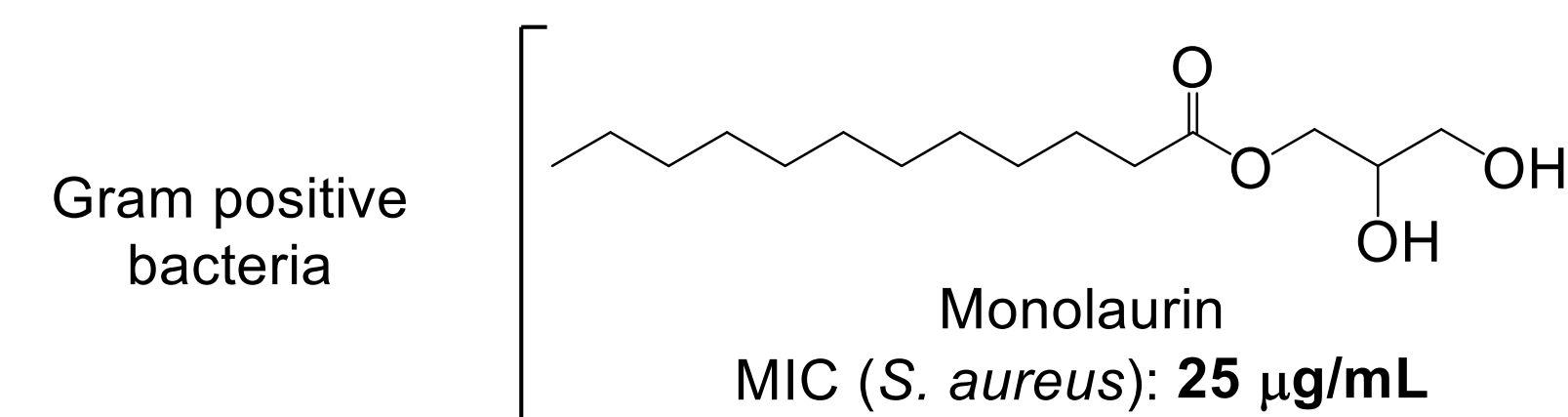
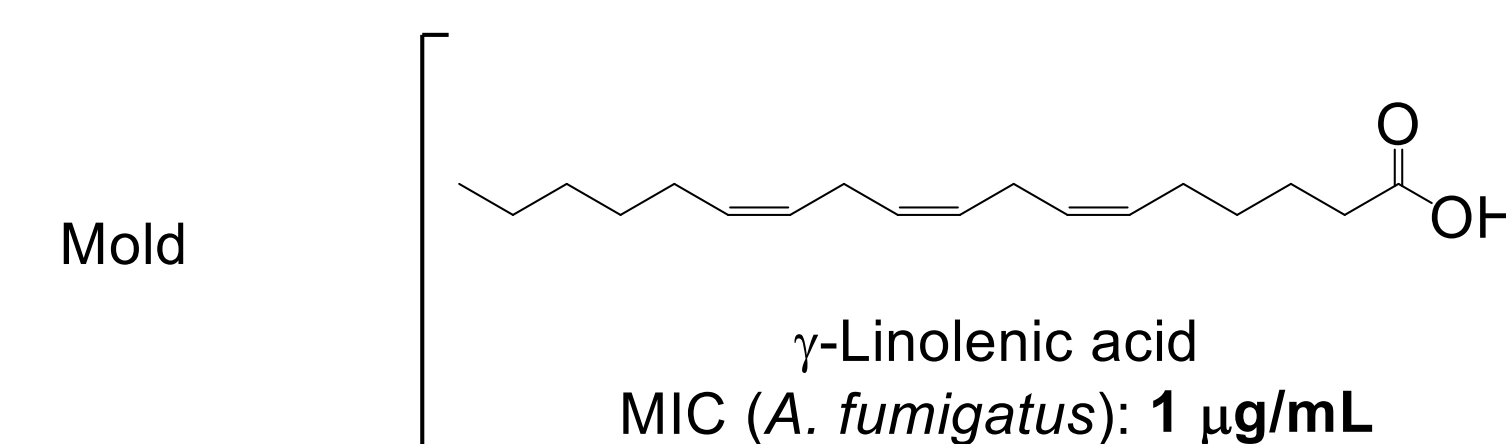
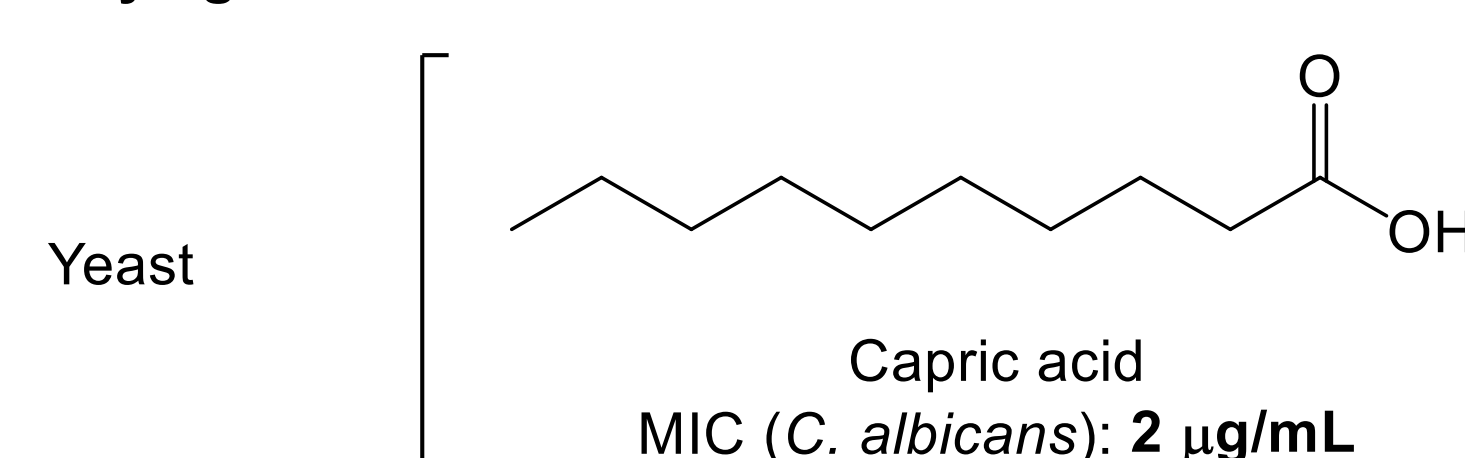
Potency against:



Antimicrobial Fatty Acids

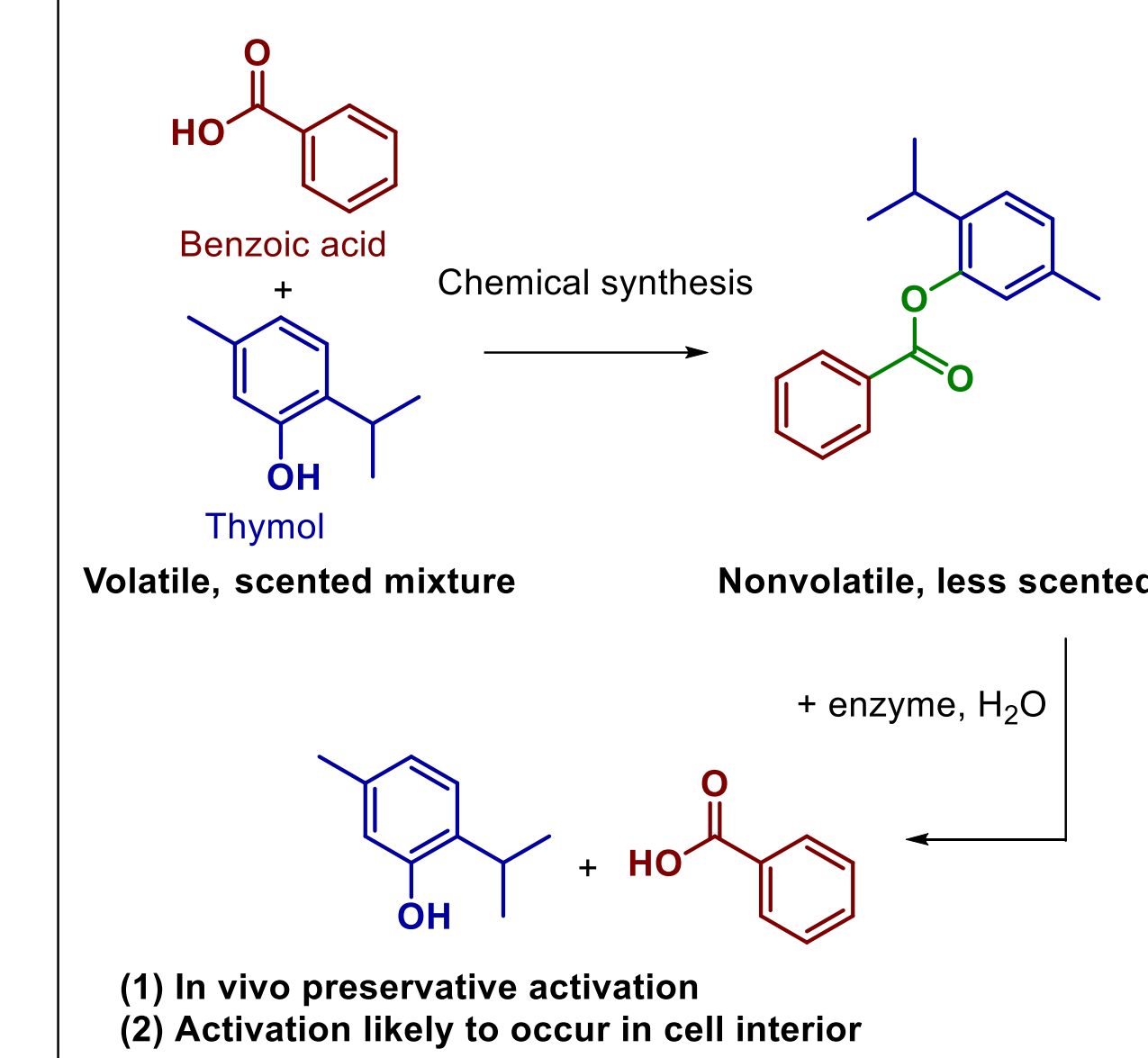
- Naturally sourced, biodegradable
- Natural anti-infective on human skin surface
- Limited effectiveness against Gram-negative organisms
- Cost: \$1-20/kg
- Hazards: skin and eye irritation, skin sensitization

Potency against:



5. Formulation Strategies

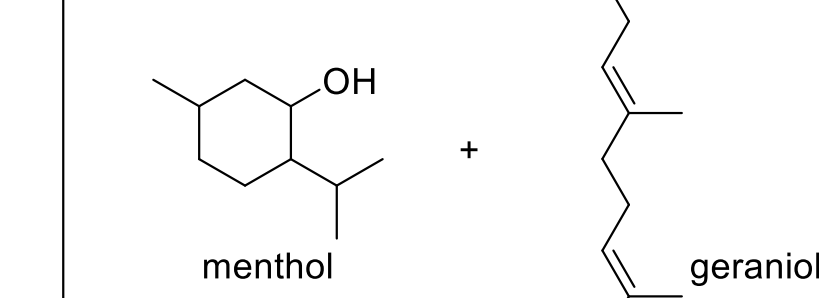
Preservative Activation by Microbial Enzymes



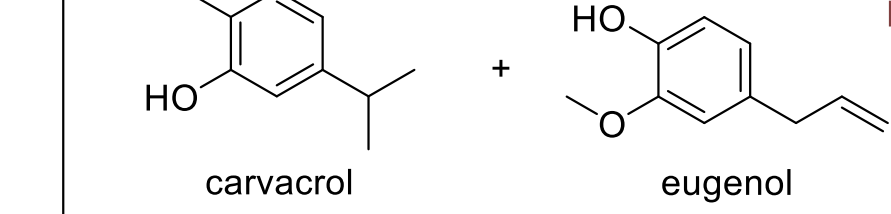
Synergism and Antagonism

1. FIC = (A/MIC A) + (B/MIC B)

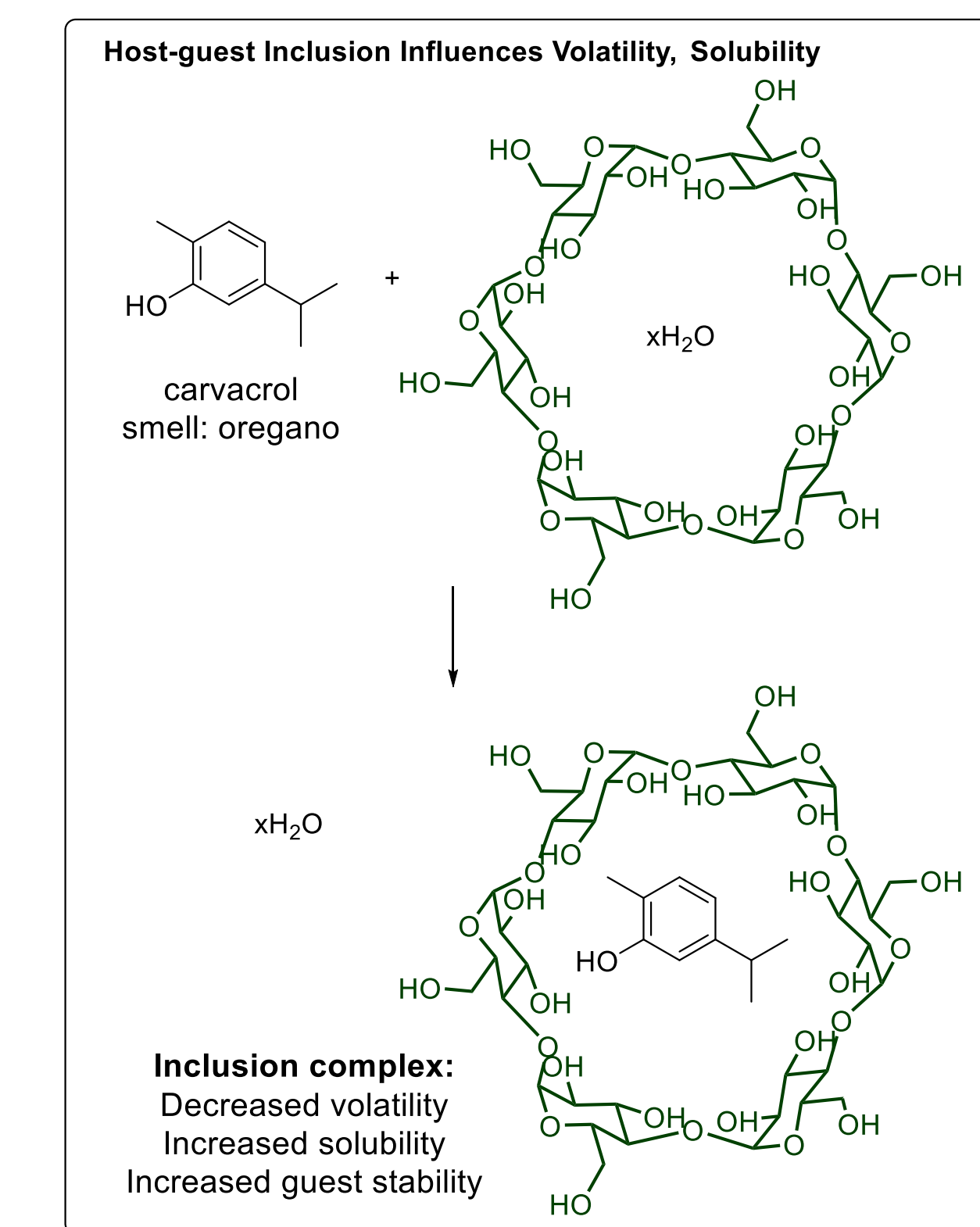
2. Synergism



3. Antagonism



- Considering a full product—including performance, scent, aesthetics, and how a consumer interacts with it—leads to strategies beyond single chemicals.
- Hybrid strategies present more opportunities for innovation and safety.



6. Conclusions

- Terpenoids, peptides, flavonoids, and fatty acids are promising alternative preservatives that are:
 - Safe** – adverse health effects often occur at much higher exposure levels than are needed for product preservation
 - Effective** – biostatic or biocidal against a range of pathogens
 - Biodegradable** – unlikely to accumulate in the environment

- Synergistic and antagonistic effects are poorly understood and can significantly influence the antimicrobial efficacy of a formulation.

For more information, see our full report: bcgc.berkeley.edu/greenersolutions

7. Acknowledgements

- Meg Schwarzman and Marty Mulvihill (Berkeley Center for Green Chemistry)
- Mia Davis (Beautycounter) and Lauren Armstrong (Northwest Cosmetics labs)
- Chantal Bergeron, Clement Choy and Martin Wolf (Seventh Generation)
- Mark Dorfman (Biomimicry 3.8)
- Larry Weiss (AoBiome)
- Kaj Johnson and Ryan Williams (Method)

8. References

MIC Data: **Terpenes:** Himejima *et al.*, *J. Chem. Ecol.* 1992, 18, 1809–1818. Moleyar & Narasimham, *Food Microbiol.* 1986, 3, 331–336. Kubo *et al.*, *J. Agric. Food Chem.* 1993, 41, 2447–2450. <http://antibiotics.toku-e.com/> and references therein. **Peptides:** US Patent US7563764 B2, 2009. Feng *et al.*, *Sci. China. Ser. B. Chem.* 2007, 50, 291. Tippayatum *et al.*, *Nat. Sci.* 2007, 41, 319–323. **Flavonoids:** Basile *et al.*, *J. Med. Food.* 2010, 13, 189. Kuete *et al.*, *J. Ethnopharmacol.* 2007, 112, 271. Mbaveng *et al.*, *J. Ethnopharmacol.* 2008, 116, 483. Ozcelik *et al.*, *Z. Naturforsch., C, J. Biosci.* 2006, 61, 632. **Fatty Acids:** Clément *et al.*, *FEMS Yeast Res.* 2007, 7, 276; *J. Dairy Sci.* 2008, 91, 2535. Kabara *et al.*, *Antimicrob. Agents Chemother.* 1972, 2, 23. Bergsson *et al.*, *Antimicrob. Agents Chemother.* 1998, 42, 2290.