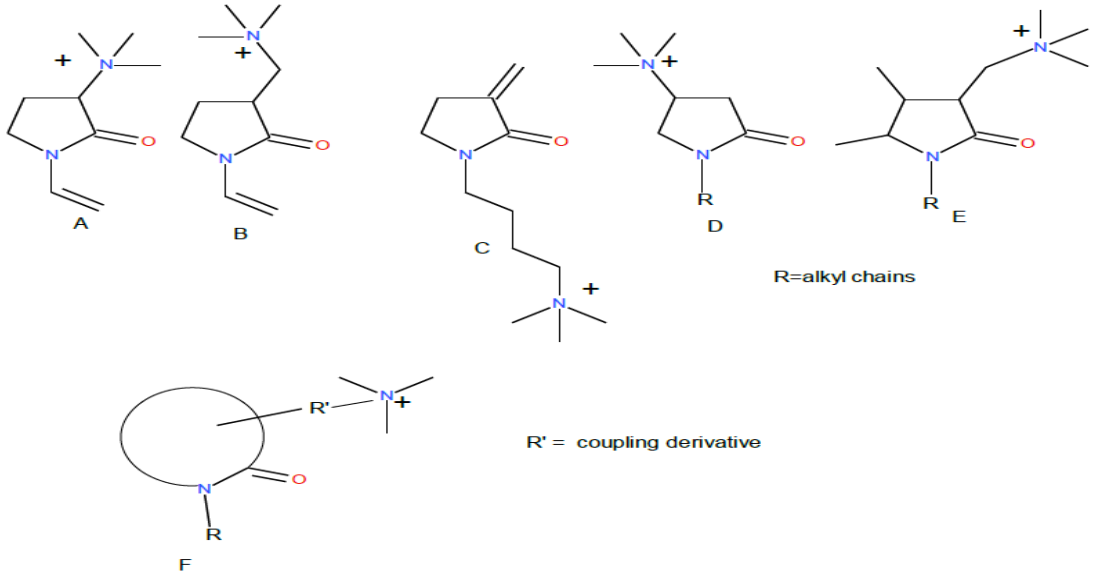
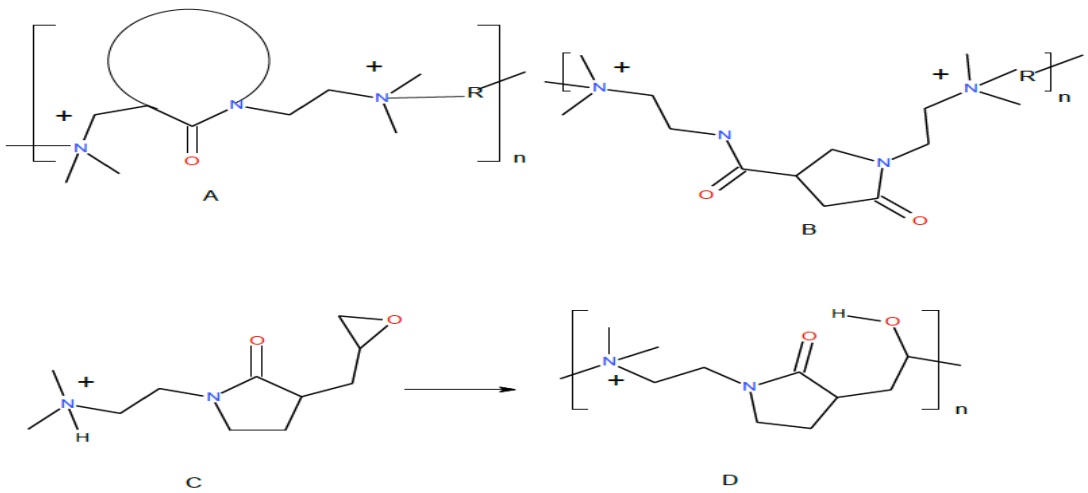
Lactam Quaternary Derivatives

By: Robert B. Login rloginconsulting.com

My idea is to use various lactams derivatized with quaternary ammonium groups as potential biologically active germacidal compounds. Both monomeric and polymeric structures are possible. For example:



Scheme 1: Possible examples of monomeric pyrrolidone and a generalized lactam quat.

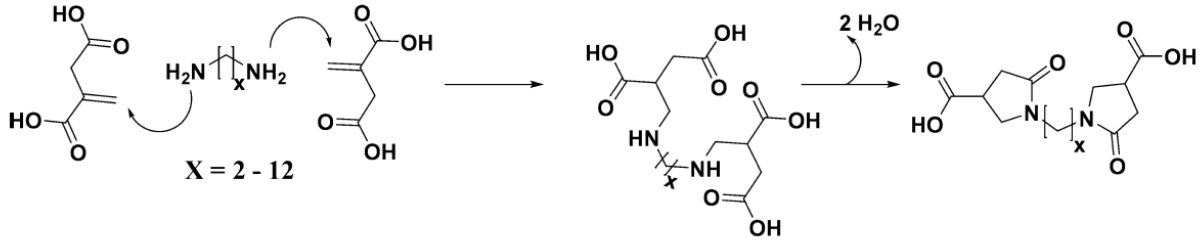


Scheme 2: Various ideas for polymeric quats. B is an example of a polyquat derived from itaconic acid.

Qi, P., Chen, H. L., Nguyen, H. T. H., Lin, C. C., & Miller, S. A. (2016). Synthesis of bio renewable and water-degradable polylactam esters from itaconic acid. *Green Chemistry*, *18*(15), 4170-4175.

Teleky, B. E., & Vodnar, D. C. (2019). Biomass-derived production of itaconic acid as a building block in specialty polymers. *Polymers*,*11*(6), 1035.

Scheme 2. Aza-Michael Addition of Various Diamines with Itaconic Acid, Followed by Intramolecular Cyclization[a]

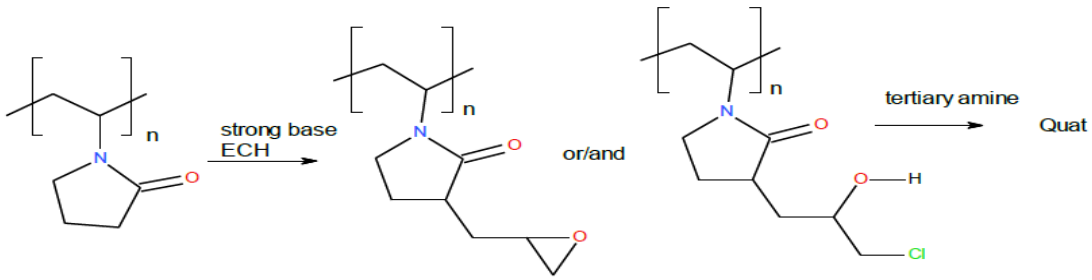


[a]The ensuing monomers are abbreviated as BP-C_x, where x stands for the number of methylene groups in the used diamine spacer. For example, the *N,N′*-octamethylene-bis(pyrrolidone-4-carboxylic acid) monomer based on 1,8-diaminooctane is named BP-C_8.

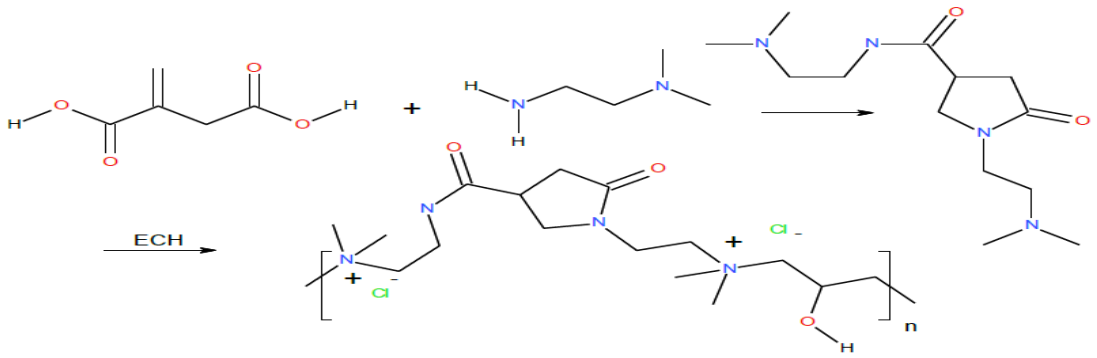
Teleky, B. E., & Vodnar, D. C. (2019). Biomass-derived production of itaconic acid as a building block in specialty polymers. *Polymers*, *11*(6), 1035.

They employ the above dimer to prepare polyesters. Using two equivalents of the diamine affords the polyamide. Both are water soluble to some extent.

Ali, M. A., Tateyama, S., Oka, Y., Kaneko, D., Okajima, M. K., & Kaneko, T. (2013). Syntheses of high-performance biopolyamides derived from itaconic acid and their environmental corrosion. *Macromolecules*, *46*(10), 3719-3725.



Scheme 3: Partially derivatised PVP. I think that a few percent of a PVP polymer might be enough to form an effective quat derivative after reaction with a tertiary amine. So if this worked you would have PVP with a few percent of a quat randomly scattered along the PVP backbone.



Scheme 4: Itaconic based polyquat. I have not found references to such

ECH(epichlorohydrin) derived polymers.

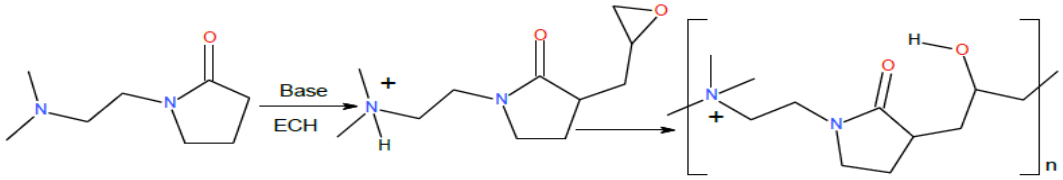
You could stop at the diquat by not employing a difunctional alkylating compound.

https://pubchem.ncbi.nlm.nih.gov/compound/N_N_-dimethylethane-1_2-diamine

Bis-quaternary ammonium compounds USP 4,734,277

Abstract

"A method of preparing certain bis-quaternary ammonium compounds and mixtures is disclosed. The method involves contacting a tertiary amine with a suitable amount of neutralizing acid, e.g. HCl, and subsequently contacting the resulting mixture with a suitable epoxide, e.g. epichlorohydrin, at an elevated temperature and in an amount that e.g. 2-hydroxypropylene-bis-1,3-(dimethyl stearyl ammonium chloride) is obtained in almost stoichiometric yields."



Scheme 5: Another polyquat possible synthesis.

Iodophors:

Can iodine be combined with quat polymers to afford two methods to kill pathogens in one compound?
Can a powder of one of the above quat polymers be milled with iodine to generate an iodophor(this is one synthesis method). Like PVPHI3 said iodophor would dissolve in water to release the active iodophor and the polyquat. Polyquats are known to kill pathogens by attaching to cell walls and disrupting them. They might carry the iodophor to where it would have the maximum inpact.

"Three methods are used to obtain povidone–iodine: exposing the polymer to iodine vapors[36], mixing PVP and iodine solutions [37], and heating dry PVP and iodine samples at 80–90°C until the titrated iodine concentration is constant [35]."

"The interaction of the polymer with iodine proceeds through two steps. First, iodine, which has pronounced acceptor properties, forms a bond with the lone electron pair of an oxygen atom of a pyrrolidone ring. Second, dissociation of the complex yields iodine atoms, which interact with iodine molecules to produce triiodide ions,"

Makhayeva, D. N., Irmukhametova, G. S., & Khutoryanskiy, V. V. (2020). Polymeric Iodophors: Preparation, Properties, and Biomedical Applications. *Review Journal of Chemistry*, *10*(1), 40-57."

Since polymers with pyrrolidone in the backbone instead of being pendent should also form iodophors, and also containing polyquats would be a new idea.

Obviously pyrrolidone backbone polymers without quats might also form interesting iodophors. Please look at my previous ideas for such polymers:

Pyrrolidone Backbone Polymers

PVP, one of the most lucrative specialty polymers has dominated its market for eighty years, but is it the best way to obtain it's outstanding properties? Please take a look at my ideas for an improved competitor.

Thank you for reading these proposals.
Dr. Robert B. Login rloginconsulting.com