

Modeling the Selective Binding Behavior of Yervin's Compound C

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Yervin's recent discovery of compound C, [Tetra-t-amylperoxypropylpyromellitate ($C_{30}H_{46}O_{12}$)], raises hopes of a cure for victims of spider bites. These hopes are based on past experimental studies that prove that compound C binds to spider toxin, deactivating the toxin and preventing it from doing neurological damage to the bite victim. However, for this to work as a cure, compound C must bind only to the spider toxin and not to other chemicals in the patient's blood. The computer modeling studies reported here suggest that compound C may bind to a large family of chemical compounds. The chemical formula for the spider toxin is shown in Figure 1. The studies presented here suggest that compound C will bind to any chemical that has the structural unit shown in the box of Figure 1. This structural unit consists of a phenyl (benzene) ring with a hydroxyl (-OH) and amine (-NH₂) group in para positions relative to one another (i.e. on opposite sides of the ring).

Figure 1: Spider Toxin (with box around binding region)

