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In keeping with our interest in elucidating the mechanism of tryptanthrin (indolo[2,1-b]quinazolin-6,12-dione) and its analogues against parasitic micro-organisms, we have employed scanning tunneling microscopy (STM) as a method to study the electronic and conformational behaviors of these alkaloids at the molecular level. Our ability to image and study individual molecules at submolecular resolution has opened possibilities and new methodologies for the refinement QSAR modeling and the potential identification of pharmacophores and toxicophores. Presented herein is progress on applying STM, and Density Functional Theory (DFT), as a theoretical framework, to study how various tryptanthrin analogues may interact with DNA and other biological systems.