Abstract

A family of 18 molecules based on octathio[8]circulene was defined and modeled, including circulenes with different combinations of heteroatoms (S, Se, As, P and N), and different numbers of rings (8, 10 and 12).

In order characterize them, several of their properties were studied and discussed: bond lengths, ring strain, nucleus-independent magnetic shielding (NICS), and Raman and electronic spectra.

Then, they were used as substrates to adsorb the marine toxin saxitoxin (STX).

This resulted in an enhancement of its electronic properties, which allowed us to study its electronic and Raman spectra and propose viable detection conditions based on resonance Raman (RR).

Universidade Vigo