Abstract

The fragmentation patterns of cholic acid in electron impact mass spectrometry were studied using Gaussian09 software. The fragments that were most likely to be generated from the parent molecule were theorized using principles of molecular rearrangements and ionic fragmentations. The structures were optimized both as ground state molecules, and as radical cations. The frequency calculations of these optimized structures yielded energies that represented a theoretical saddle-point for the energetic gradient. The resulting pairs of molecules were evaluated according to their thermodynamic stability to provide thermodynamic justification for the mass spectrometry data. The results showed that the thermodynamically favorable B3 (273) fragmentation pathway has the thermodynamic potential to yield the most prominent M/Z peak from the NIST data.