Conformational studies on 2-guanidinylthiazole, famotidine and some analogues

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Conformational analysis of famotidine (FAMO) and some analogues have been performed using AM1 calculations. In addition, conformational analysis were done on the 2-guanidinylthiazole moiety in order to see the effect of the N-sulfamoyl fragment and the methylthioethyl chain of FAMO on the thiazole ring. The results revealed that the N6H form (the guanidinium cation) was the most stable and might therefore be the best candidate for interacting with the histamine H2-receptor. The calculations for the N6H forms of FAMO and analogues showed a strong hydrogen bond anchoring the guanidine chain in the same plane as the thiazole ring, in agreement with X-ray diffraction and 1H NMR studies.