

## عنوان مقاله:

A TD-DFT Study Of the Thermodynamic Properties of Bropiramine Anti-Cancer Drug

## محل انتشار:

سومین کنفرانس سراسری نوآوری های اخیر در شیمی و مهندسی شیمی (سال: 1395)

تعداد صفحات اصل مقاله: 3

## نویسندگان:

A.S Ghasemi - Dept. of Chemistry, Payame Noor University

F.S Fallah - Dept. of Chemistry, Payame Noor University

## خلاصه مقاله:

One of the major causes of cancer deaths worldwide. Despite the progress of science and technology, mankind still has failed to cure this disease. In this work, investigated, geometric parameter anti-cancer drug Bropiramine at the PBE1PBE level of theory with 6-311++G (2d,2p) basis set in gas phase and water , ethanol solution phase in ground and excited state. Thermodynamic properties, the relative energy, dipole moment, Structural parameters, gap energy, .Molecular orbital of HOMO and LUMO, thermodynamic was obtained

## کلمات کلیدی:

Bropiramine, PBE1PBE, Excited state

## لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/569313>

