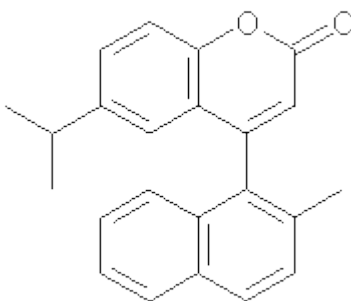


# COMPUTED ECD OF A COUMARIN WITH AXIAL CHIRALITY

It's been a while since I blogged about the use of computed spectra to determine the structure or configuration of a compound. Well, here's a nice example of the use of computed electronic circular dichroism to determine the configuration of a coumarin that displays axial chirality.

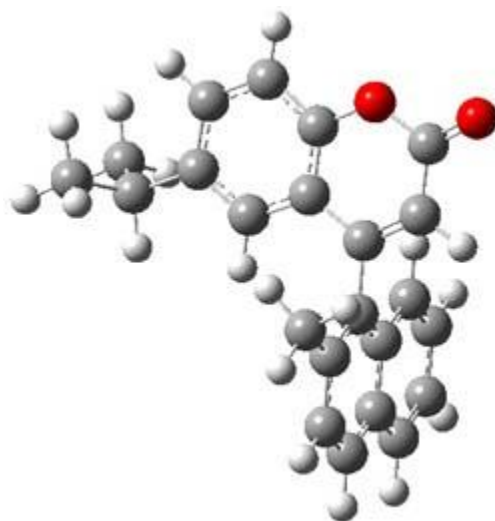
Mazzanti and coworkers have synthesized a series of coumarins,<sup>1</sup> obtained their ECD and computed their structures, stereo-interconversion barriers (at B3LYP/6-31G(d)) and ECD (at TD-DFT/B3LYP/6-311++G(2d,p)//B3LYP/6-31G(d)). I will mention explicitly here just one example, compound **1**, which elutes off a chiral column in two mirror image forms, both of which do not stereomutate over time.



**1**

The computed structure of **1** is shown in Figure 1 and the barrier for stereomutation is predicted to be quite large, 35.7 kcal mol<sup>-1</sup>.

This explains the lack of stereomutation. The computed ECD of **1M** matches very well with the experimental ECD of the first eluted isomer, making the second eluted isomer **1P**.



**1**

**Figure 1.** B3LYP/6-31G(d) optimized structure of **1**.

Source: <http://comporgchem.com/blog/?p=1120>