Chiral Recognition in HPLC by Computer Simulations

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Chiral high performance liquid chromatography (HPLC) is very important in the pharmaceutical industry. However, the method can be expensive to implement. In order to help drive down the costs, we have been developing simulation methods to help identify how to optimise the chiral discrimination. These methods are based on a free energy sampling scheme to estimate the free energy differences in the interaction of two enantiomers with the stationary phase.

We report the results of molecular dynamics simulations on dimers of a linked dimeric carbohydrate and benzoin dissolved in tetrahydrofuran. A subset of the results have been used in our previous study [*JML*,**101**/1−3(2002) 261−272] and has shown that the prediction in an early stage of the simulation is difficult and unreliable. Therefore, we include a large set of the simulations and give an account of the chiral discrimination that arises.