OP-5

In silico Drug Designing of Natural Coumarins

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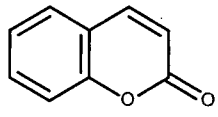
The term in-silico drug designing can be defined as the study of drugs by computational means. Coumarnis are benzopyranones having the structure as shown below. Plenty of coumarins are isolated from natural source, mainly plant source having diverse biological activity.



These coumarins are secondary metabolites from the plant source and may have some adverse / toxic activity. Hence there is a great demand for the screening of these natural coumarins for its druggability. In the present study, we have identified around 1500 natural coumarins which are reported in literature. These coumarins were screened for druggability and later, its biological activity was predicted. The results indicate that out of 1500 natural coumarins, only 500 molecules exhibit druggable properties. The paper describes all these results in detail.