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Docking- and *In Silico* Screening for Identification of Micromolar Inhibitors of Tropomyosin-related Kinase A from Natural Origin

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First published: 12 January 2017

<https://doi.org/10.1002/bkcs.11064>

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Abstract

Tropomyosin- β -casein-related kinase A (TrkA) serves as a promising target protein for the development of anticancer medicines. We report new TrkA inhibitors of natural origin identified from the structure-based virtual and biochemical screening. A proper molecular hydration term was implemented into the original free energy function to perform virtual screening with an improved accuracy. As a consequence, four natural TrkA inhibitors were found with IC_{50} values ranging from 3 to 70 μ M. The good biochemical efficacies and structural simplicities of these new inhibitors signifies that they deserve to be further studied for optimization of the anticancer activity through the structure-activity relationship analysis. The detailed analysis of binding modes indicates that the micromolar biochemical efficacy of the new inhibitors could be achieved by the simultaneous establishment of multiple hydrogen bonds and hydrophobic interactions in the ATP-binding site of TrkA.

[Volume38, Issue2](#)

February 2017

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```

```
var _prum=[[['id','59e8fecb3847311aab7b23c6'],['mark','firstbyte',(new  
Date()).getTime()]];function(){var s=document.getElementsByTagName('script')[0],p=document.creat  
eElement('script');p.async='async';p.src='//rum-  
static.pingdom.net/prum.min.js';s.parentNode.insertBefore(p,s);})();
```