

# Structure-Activity Relationship of Taxol Inferring from Docking Taxol Analogues to Microtubule Binding Site

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In order to find the minimal structural requirements to maintain microtubule binding, 12 taxol analogues have been docked to the taxol binding site of tubulin. By comparing the interactions of each analogue with  $\alpha$ -tubulin, the structure-activity relationships are summarized as follow: C-2 benzoyl and taxane ring systems are the essential groups for microtubule binding, the improvements of bioactivity and bioavailability are dependent on the substituents at positions C-1, C-4, C-7, C-9, C-10, and C-14, whereas the C-13 side chain mainly provides a specific binding.

*Key words:* Molecular Docking, Structure-Activity Relationship, Taxol, Tubulin