

## Wiener Index and the Number of Subtrees

Abstract: The Wiener index of a tree is the sum of all pairwise distances between vertices. The Wiener index is one of the main descriptors that correlate a chemical compound's molecular graph with experimentally gathered data regarding the compound's characteristics. We characterize binary trees with  $n$  leaves, which have the greatest number of subtrees (leaf-containing subtrees). These binary trees coincide with those which were shown to minimize the Wiener index by Fischermann et al. and Jelen and Triesch. Our results also give an exact value of the number of "acceptable residue configurations", which was used in Knudsen's multiple parsimony alignment.