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RSMD (Root Mean Square Deviation) is a measure of the difference between two molecular structures. It is calculated as the square root of the average of the squared distances between corresponding atoms in the two structures. RSMD is a common metric for comparing molecular structures, and it is used in many applications, including molecular docking, molecular dynamics simulations, and molecular recognition. In this paper, we use RSMD to compare the structures of the ligands and the protein, and to evaluate the accuracy of the docking results. The RSMD values are calculated for each ligand-protein complex, and they are used to rank the complexes according to their structural similarity. The results show that the docking results are highly accurate, and that the RSMD values are very low, indicating a high degree of structural similarity between the docked ligands and the protein.



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**Statement in accordance with s.519 of the Companies Act 2006 to Careersite.biz Limited – Company Number 04147019 on ceasing to hold office as auditors**

Yours sincerely

Wang

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