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Approaches of Virtual Screening in Drug Discovery

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Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | Virtual screening has become an integral part of the drug discovery process. Through the two main streams of VS, ligand based and structure based, various interesting new scaffolds could be defined. Many interesting detailed studies were implemented in this field of research. A comparative computational study of pharmacophore model generation was explored, mentioning the advantage and disadvantage of each method. Also, an employed comparison between the two main streams was mentioned using CDK-2 as representative example with detection of the most acceptable pharmacophore model. A promising linking between the direct (ligand docking) and indirect (pharmacophore model) methods to identify the successful scaffold was explored. This linking approach using pharmacophore post filtering aims to increase the hit rates with minimizing the time used in VS process. Further, different programs that handled direct ligand docking approach was mentioned with mapping of their algorithm. | Format: Paperback | Language/Sprache: english | 121 gr | 220x150x4 mm | 68 pp.

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