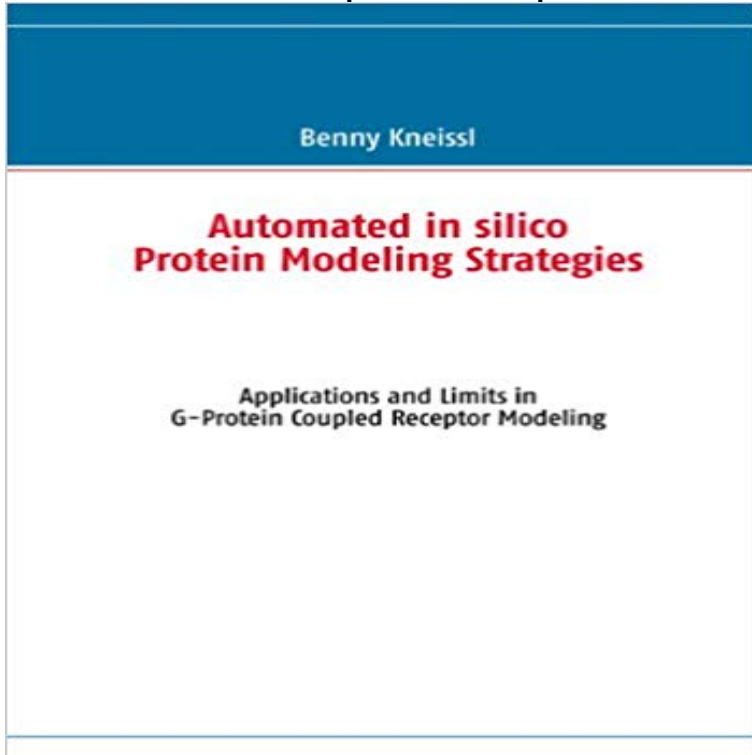


Automated in silico Protein Modeling Strategies: Applications and Limits in G-Protein Coupled Receptor Modeling



Im 21. Jahrhundert sind computergestützte Methoden zu einem etablierten Werkzeug in der Pharmaindustrie geworden. Da viele Proteinstrukturen nur mit großem Aufwand experimentell aufgeklärt werden können, wurden diverse in silico Methoden entwickelt, um ihre dreidimensionale Struktur aus der dazugehörigen Sequenz zu modellieren. Leider muss der Modellierungsprozess häufig an das Zielprotein angepasst oder die automatisch generierten Modelle von den Anwendern auf Basis ihres Fachwissens verfeinert werden, um letztendlich vernünftige Resultate zu erhalten. Das Ziel dieser Arbeit ist die Untersuchung der Anwendbarkeit automatischer in silico Modellierungsstrategien am Beispiel der G-Protein gekoppelten Rezeptoren (GPCRs). Zunächst analysieren wir bis zu welchem Grad verfügbare Proteinstruktur-Vorhersagemethoden für die automatische Modellierung von GPCRs angepasst werden können. Anschließend entwickeln wir unser eigenes Verfahren und zeigen, dass dieses im Vergleich zu anderen modernen Methoden verbesserte Ergebnisse erzielt. Hervorzuheben ist dabei, dass unser Ansatz keinerlei Interaktion vom Anwender benötigt und somit auf alle GPCRs angewendet werden kann. Des Weiteren stellen wir eine neue sequenzbasierte Methode zur Vorhersage von so genannten Kinks in α -Helices vor. Auch diese Methode übertrifft die Vorhersagegenauigkeit vergleichbarer Ansätze.

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