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STRUCTURE-BASED DESIGN FOR BINDING PEPTIDES IN ANTI-CANCER THERAPY

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The conventional anticancer therapeutics usually lack cancer specificity, leading to damage of normal tissues that patients find hard to tolerate. Ideally, anticancer therapeutics carrying payloads of drugs equipped with cancer targeting peptides can act like "guided missiles" with the capacity of targeted delivery toward many types of cancers. Peptides are amenable for conjugation to nano drugs for functionalization, thereby improving drug delivery and cellular uptake in cancer-targeting therapies. Peptide drugs are often more difficult to design through molecular docking and *in silico* analysis than small molecules, because peptide structures are more flexible, possess intricate molecular conformations, and undergo complex interactions. In this report, the development and application of strategies for structure-based design of cancer-targeting peptides against GRP78 are discussed. The author will also cover topics related to peptide pharmacokinetics and targeting delivery, including molecular docking studies, features that provide advantages for *in vivo* use, and properties that influence the cancer-targeting ability. Some advanced technologies and special peptides that can overcome the pharmacokinetic challenges have also been included.