

# Development of drug design for therapy

**Keywords:** chemical, salted water, drug design, chronic disease, antibiotics

## Editorial

In our imaginary, for every kind of illness, there should exist a pill, whose immediate effect would heal our sorrow. The above is so true that in many cases a placebo, just a pill with no drug, would have some beneficial effect (and anyway the placebo is composed by something, even being sugar or magnesium, thus providing some chemical, not to mention the water usually used to take the pill, itself quite a healing chemical, being ourselves mainly salted water, even without thinking of the religious meaning of water). Of course this is not enough in most serious circumstances, not for who is professionally or economically

engaged in drug design: our goal should instead be to identify the very origin of the illness (not just the symptoms when possible) and then design how to provide the proper chemical in order to bring back the steady health state where it was compromised, either by acute or even chronic disease, for which a permanent administration could be devised.

Such ability is not yet possible for every illness: this is why at least symptomatic drugs exist in order to at least minimize the effect of the symptoms when the underlying illness is anyway treated or at least treated in a different way: it would be dangerous to silence symptoms while not curing the real problem!

Even when the proper chemical is found and known, and favorably compared with possible competitors in terms of efficacy, adverse effects, cost, the problem is still how to administrate the proper dose at the very target place, without intoxicating too much the rest of the body while also wanting an useful chemical that in the very end will anyway pollute our world while not even creating resistance like antibiotics in bacterial. Administrating such right amount directly at the very target is usually not even possible, and anyway not easy. The standard must tolerate, but at the same time less direct, way is to ingest a pill, who has to pass the digestive compartment before entering the blood, then diffuse to blood everywhere in the body to also arrive at target: pharmacokinetics and pharmacodynamics come to understand how much and how often to administrate in order to get the desired effect at target when the proper cover is found for the very molecule in order to arrive safe at target.

Parenteral administration does not look much different except that a different transfer compartment is used to reach blood in order to bypass the digestive one when the active principle would not stand it without being transformed in a not anymore useful way. Direct injection in blood do appear more easy for the drug, avoiding the

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previous compartment, but it is less comfortable for the ambulatory patient, needing a professional help for administration: the search of new drugs is intended in improving such strategy, trying to embed the same particle of drug in such a way that it could be chemically preserved by interaction while travelling in blood to target and may be physically driven to target in a more controlled and fast and direct way, for instance through magnetism.

No matter of which of the recalled administration methods is chosen, but of course taking into account of the choice, the key necessary point is anyway to discover the very molecule, specific, more useful than already existing competitors and possibly less obstructive in adverse effects. Several tool do exist nowadays besides the necessary intuition of the researcher. On one side machine learning help to predict characteristic of the new molecule with respect to important behavior, like for instance hydrophily versus hydrophobic behavior, while molecular simulation through systems of coupled Schrödinger equations for every single atom could help in understanding very subtle modification deriving by just few atoms substitution in a family of known molecules.

As often, no one approach is really always better than another, but the whole increasing and refining portfolio helps to better and better control the discovery process, helping the researcher, and more often the often interdisciplinary teams, to better improve their already deep skills in the process.

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## Conflict of interest

Author declares that there is no conflict of interest.

# Drug Design Development And Therapy Call For Papers

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## **Table of Contents Drug Design Development And Therapy Call For Papers**

1. Understanding the eBook Drug Design Development And Therapy Call For Papers
  - The Rise of Digital Reading Drug Design Development And Therapy Call For Papers
  - Advantages of eBooks Over Traditional Books
2. Identifying Drug Design Development And Therapy Call For Papers
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Drug Design Development And Therapy Call For Papers
  - User-Friendly Interface
4. Exploring eBook Recommendations from Drug Design Development And Therapy Call For Papers
  - Personalized Recommendations
  - Drug Design Development And Therapy Call For Papers User Reviews and Ratings
  - Drug Design Development And Therapy Call For Papers and Bestseller Lists
5. Accessing Drug Design Development And Therapy Call For Papers Free and Paid eBooks
  - Drug Design Development And Therapy Call For Papers Public Domain eBooks
  - Drug Design Development And Therapy Call For Papers eBook Subscription Services

- Drug Design Development And Therapy Call For Papers Budget-Friendly Options
- 6. Navigating Drug Design Development And Therapy Call For Papers eBook Formats
  - ePub, PDF, MOBI, and More
  - Drug Design Development And Therapy Call For Papers Compatibility with Devices
  - Drug Design Development And Therapy Call For Papers Enhanced eBook Features
- 7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Drug Design Development And Therapy Call For Papers
  - Highlighting and Note-Taking Drug Design Development And Therapy Call For Papers
  - Interactive Elements Drug Design Development And Therapy Call For Papers
- 8. Staying Engaged with Drug Design Development And Therapy Call For Papers
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Drug Design Development And Therapy Call For Papers
- 9. Balancing eBooks and Physical Books Drug Design Development And Therapy Call For Papers
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Drug Design Development And Therapy Call For Papers
- 10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
- 11. Cultivating a Reading Routine Drug Design Development And Therapy Call For Papers
  - Setting Reading Goals Drug Design Development And Therapy Call For Papers
  - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Drug Design Development And Therapy Call For Papers
  - Fact-Checking eBook Content of Drug Design Development And Therapy Call For Papers
  - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
  - Utilizing eBooks for Skill Development
  - Exploring Educational eBooks
- 14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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