**A Review on**

**Artificial intelligence in drug discovery: recent advances and future perspectives**

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Deep learning, a subset of machine learning that makes use of artificial neural networks, has drawn a lot of interest in the drug discovery space because of its capacity to automatically extract features from data and model complex, nonlinear relationships. This is in addition to conventional machine learning techniques that use molecular descriptors created by humans. The comeback of deep learning in drug discovery has sped up the creation of new models and applications that will help a number of chemical science fields. The article demonstrates the following:

**How deep learning has enhanced;**

**1. QSAR/QSPR and Structure-Based Modeling**

* Automatic Feature Extraction, removing the need for manual feature engineering. This enables them to capture complex, nonlinear relationships that conventional QSAR/QSPR methods might overlook.
* Graph Neural Networks, allowing them to learn complex interactions between atoms and bonds. Valuable for predicting biological activity and other properties derived from molecular structures.
* Multitask Learning, allowing a single model to predict multiple related outcomes at once. This maximizes data efficiency and can enhance predictive accuracy across different tasks.

**2. De Novo Chemical Design**

* Generative Models like VAEs and GANs can create new molecular structures by learning from the distribution of existing compounds. This enables the design of novel candidates that fulfill specific requirements.
* Rule-Free Design of bioactive molecules that enables the exploration of a wider chemical space by not being restricted to predefined synthetic rules, fostering the discovery of novel compounds.
* Optimization of multiple Properties simultaneously such as potency and selectivity, through multitask learning.

**3. Synthesis Prediction**

* Automated Synthesis Planning which predicts feasible synthetic pathways for new compounds, and is essential for confirming that designed molecules can be practically synthesized.
* Data-Driven Insights which allows for the identification of patterns in chemical reactions and synthesis pathways, leading to more informed predictions about the feasibility of synthesizing new compounds
* Enhanced Predictive Performance which is essential for the practical application of de novo designs in drug discovery

**Current Shortcomings of AI Tools in Drug Discovery**

1. Data Quality and Availability
2. Interpretability
3. Integration with Existing Workflows
4. Limited Understanding of Complex Biological Systems
5. Ethical and Regulatory Concerns

**Future Transformations in Computer-Assisted Drug Discovery**

1. Enhanced Data Sharing and Management
2. Enhanced Interpretability
3. Integration of Multi-Omics Data
4. Hybrid Approaches
5. Ethical Frameworks and Guidelines
6. Accelerated Drug Development