Computing New Medicines

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Computing is used more and more now to discover and expedite new medicine therapies from masses of previously stored digital data. This new capability will continue to be employed given recent successes.

Some topics are so exciting that we don't want to wait; we think computing *new* drug therapies is one. So, let's glance at it.

For thousands of years, and with minimal resources and no computers, scientists studied the medicinal value of plants and minerals on human ailments and disease. Some example discoveries were from mimosa trees (1665), where the bark could be used to treat forms of depression (still used to this day), or a fern plant (Middle Ages) to treat kidney stones.

"Modern" medications began to be discovered in the early 1800s by scientists analyzing plants, minerals, and animals in their individual labs. Drug discoveries were not quick due to the absence of today's computing power.

Antibiotics were introduced only in the 1940s. Access to medicines was limited; there was no Dr. Google or Alexa, M.D.; and thus, home remedies were employed before seeking a doctor. Examples include whiskey-drizzled warm toast for stomachaches and onions in socks for fever reduction.

Moving forward to today's traditional clinical trial designs, where human participants and data collection are the focus, there are signs of bias and selective publishing.[4] Further, clinical trials are costly and have relatively low success rates.[5]

Fortunately, the future is bright for drug and vaccine discovery because of high-performance computing (HPC), artificial intelligence (AI), and big data (BD). Medicine development is evolving due to "ever-expanding past data" that included "large-scale biological experiments, clinical trials, and medical records."[6] AI enables quick identification of the drug molecules that reduce/eliminate viruses, hypothesize scenarios, and compare/repurpose other drugs—all at speeds that were not before available.

Repurposing, the process of employing existing drug therapies to treat other diseases, is now a greater possibility thanks to AI and BD, and is transforming drug discovery. Repurposing occurs when AI technologies are used

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with BD to reveal and extract patterns in the mounds of available biomedical data. This process speeds up treatments and provides additional safety since these medications already have known safety profiles.

Great potential for drug repurposing exists with the use of real-world data along with AI and deep learning.[1] A current example of repurposing is applying AI-based assistive tools to find an existing drug that can treat COVID-19.[7] Repurposing was explored for the treatment of COVID-19, and the results pointed to an antiviral medication, Remdesivir, that is used as part of the treatment for hepatitis C.[3]

The great news is that researchers now have many tools and methodologies to leverage new computational methodologies that are continuing to transform drug discovery. More effective insights are possible given so much existing digital data. With improved data resources, AI can drive predictive power beyond current traditional clinical trial success rates.[2] Moving from traditional clinical trials to the integration of BD, AI, and HPC will continue to transform drug development with speed, repurposing, and improved success.

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Expect to see much more on this topic in *Computer* as well as discussions on how computing is greatly impacting agrifood technology. The two might seem unrelated, but they aren't.

Stay tuned!

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REFERENCES

1. Y. Cha et al., "Drug repurposing from the perspective of pharmaceutical companies," *Brit. J. Pharmacol.*, vol. 175, no. 2, pp. 168–180, Jan. 2018, doi: 10.1111/bph.13798.
2. Glicksberg, L. Li, R. Chen, J. Dudley, and B. Chen, "Leveraging big data to transform drug discovery," in *Bioinformatics and Drug Discovery. Methods in Molecular Biology*, vol. 1939, R. Larson and T. Oprea, Eds. New York, NY, USA: Humana Press, 2019, pp. 91–118.
3. R. T. Eastman et al., "Remdesivir: A review of its discovery and development leading to emergency use authorization for treatment of COVID-19," *ACS Central Sci.*, vol. 6, no. 5, pp. 672–683, May 27, 2020, doi: 10.1021/acscentsci.0c00489. Erratum in: ACS Central Sci., vol. 6, no. 6, p. 1009, Jun. 24, 2020, doi: 10.1021/acscentsci.0c00489.
4. S. Every-Palmer and J. Howick, "How evidence-based medicine is failing due to biased trials and selective publication," *J. Eval. Clin. Pract.*, vol. 20, no. 6, pp. 908–914, 2014, doi: 10.1111/jep.12147.
5. A. Mullard, "Parsing clinical success rates," *Nature Rev. Drug Discovery*, vol. 15, no. 7, pp. 447–448, 2016, doi: 10.1038/nrd.2016.136.
6. T. Qian, S. Zhu, and Y. Hoshinda, "Use of big data in drug development for precision medicine: An update," *Expert Rev. Precis. Med. Drug Develop.*, vol. 4, no. 3, pp. 189–200, 2019, doi: 10.1080/23808993.2019.1617632.
7. Y. Zhou, F. Wang, J. Tang, R. Nussinov, and F. Cheng, "Artificial Intelligence in COVID-19 drug repurposing," *Lancet Digit. Health*, vol. 2, no. 12, pp. e667–e676, Dec. 1, 2020, doi: 10.1016/S2589-7500(20)30192-8.

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