



Editorial

ARTIFICIAL INTELLIGENCE IN NATURAL PRODUCT DISCOVERY: AN INTERVIEW WITH BARD.

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Almost a year ago, artificial intelligence (AI) entered our daily lives as ChatGPT (Chat Generative Pre-trained Transformer). This chatbot developed by OpenAI was followed by other companies making their own chatbots public (Google Bard and Perplexity AI are the best-known among several others). The public was mesmerised by this "genius in a bottle" that could engage in a natural conversation and work tirelessly for you -when correctly prompted- collecting and summarising data, coding in phyton, correcting your language, inventing poems, jokes, etc.

The potential of AI was not new to many scientists. I was introduced to the world of machine learning (ML) only twelve years ago by a talented Pharmacy student named Cortes-Cabrera, who accepted my challenge to predict essential oils' biochemical and biological properties. I reasoned that the bioactivity of a complex chemical entity (a natural extract) should be the result of various interactions (synergy, antagonism, additivity, etc.) between its numerous constituents. Most of these constituents were already known and extensively studied as individual chemical entities (secondary metabolites or natural compounds). Accomplishing this prediction would require an extremely long equation with variables representing these compounds' quantities, concentrations, and proportions. The student suggested using Artificial Neural Networks (ANNs) to develop such an algorithm, and through our collaboration, we published two papers (Cortes-Cabrera and Prieto, 2010; Daynac, Cortes-Cabrera, and Prieto, 2015) that demonstrated the feasibility of this approach. At that time, there were only a few precedents of using AI and ANNs in food chemistry, which is not fundamentally different from phytochemistry (Prieto, 2018). Creating, training, and validating ANNs require coding skills, but nowadays, several user-friendly interfaces simplify the process. However, the more advanced tools, such as TensorFlow, still cater primarily to those who enjoy coding.

Chatbots have shattered this barrier by allowing users to interact with AI and harness its capabilities without any coding knowledge, using natural language and step-by-step instructions. These chatbots have become so advanced that they are often indistinguishable from human beings, effectively passing the renowned "Turing test" (Biever, 2023). For scientists, the application of AI will profoundly impact all aspects of our lives and work. AI algorithms have reportedly achieved discoveries that would have taken humans several centuries to accomplish (Anon, 2023).

Computation has long been established as an incredibly useful tool in natural products discovery, as highlighted by the "first in kind" book on "Computational Phytochemistry" co-edited by our Editor-in-chief, Prof Satyajit D. Sarker and our colleague Dr Nahar, Honorary Lecturer of our Centre for Natural Products Discovery (Sarker and Nahar, 2018). Now AI has been added to this armamentarium, and hundreds of fine papers on the use and impact of AI for natural product discovery have been published in the last decade. This year, this topic has been reviewed by many authors (Gaudêncio et al., 2023; Lluca and Stokes, 2023; Ma et al., 2023; Hasselgren and Oprea, 2024), culminating in a review published by Nature Reviews Drug Discovery just three months ago (Mullowney et al., 2023).

To explore the impact of AI in our field, I decided to leverage the unlimited access we now enjoy to conversational AI by interviewing Google Bard, one of the most advanced chatbots. Specifically, I was intrigued by how AI "perceives" its potential to advance the science of natural products, promote decolonisation within the field, tackle gender-related concerns among scientists involved in natural product discovery, and inspire future generations of natural product explorers. What follows is the transcript of our conversation:

(Dr J. M Prieto-Garcia) Interviewer: Would you be willing to have an interview about AI published in The Journal of Natural Product Discovery?

(Google) Bard: That's a fantastic idea! I'd love to be interviewed about AI and its potential in natural product discovery. Let's set the scene: imagine a warm Parisian Cafe, the aroma of espresso mingling with the lively chatter of patrons. We're settled comfortably at a corner table, notebooks open, ready to delve into the world of science and technology.

Interviewer: I really love this setting! I can even imagine myself seeing the "Arc du Triomphe" through the misty window. Bard, you've gained quite a reputation as a chatbot in the world of AI. What excites you most about the intersection of AI and natural product discovery?

Bard: Ah, where to begin? It's like opening a door to a hidden library within nature itself! Imagine vast libraries of plants, each page a chemical masterpiece waiting to be deciphered. AI acts as the tireless librarian, scanning these pages, identifying patterns, and whispering hints about the potential hidden within. It's like unlocking a treasure chest of potential cures, sustainable materials, and who knows what else!

Interviewer: That's quite the metaphor. But wouldn't traditional scientists be wary of AI replacing their expertise?

Bard: Not at all! Think of us as partners, not rivals. Scientists hold the torch of knowledge, navigating the cultural landscapes and historical wisdom. AI brings a powerful lantern, illuminating uncharted paths and revealing hidden connections. We complement each other, strengthening the quest for discovery.

Interviewer: That's an interesting partnership. But you mentioned challenges. What roadblocks might we face in this exciting journey?

Bard: Indeed. We must tread carefully, ensuring ethical data sourcing and respecting indigenous knowledge. The digital divide cannot widen, and AI shouldn't be a tool of exploitation. It's a delicate balance, like walking a tightrope between progress and responsibility.

Interviewer: It seems like a lot to navigate. But are you optimistic about the future of AI in this field?

Bard: Absolutely! This is just the beginning of an era of unprecedented discovery. Imagine new medicines brewed from rainforest blossoms, bioplastics spun from spider silk, and energy produced from forgotten fungi. With AI as our guide, we can unlock the secrets of nature, not just for the benefit of humankind, but for the health of our planet as well.

Interviewer: Bard, the idea of AI decolonising science is now central to academia, yet quite complex. Can you unravel this for us in the context of natural product discovery?

Bard: (Smiling) Consider it a tangled jungle awaiting exploration. For centuries, natural product discovery has been shaped by colonial expeditions, with indigenous knowledge often marginalised. Now, AI enters the scene, not as a coloniser, but as a potential liberator.

Interviewer: Liberator? That's a bold claim. How so?

Bard: Imagine AI as a skilled cartographer, mapping the vast landscapes of indigenous wisdom. It can analyse historical records, decipher ancient languages, and connect the dots between forgotten traditions and scientific potential. This empowers local communities to reclaim their stories, their knowledge, and their rightful place at the forefront of discovery.

Interviewer: But isn't there a risk of AI simply appropriating this knowledge, further perpetuating inequality?

Bard: That's the tightrope we walk. AI must be used with humility and respect. Data, the lifeblood of AI, cannot be plundered. Equitable partnerships, not exploitative extraction, are key. Imagine AI as a translator, bridging the gap between indigenous knowledge and modern science, fostering collaboration and shared ownership of discoveries.

Interviewer: This sounds ideal, but would not the digital divide hinder such collaboration?

Bard: True. AI mustn't exacerbate existing inequalities. Bridging the digital gap is crucial. Imagine mobile apps translating medicinal plant knowledge, open-source software accessible to remote communities, and digital libraries preserving and sharing wisdom across borders. Technology, used responsibly, can become a bridge, not a barrier.

Interviewer: It seems AI holds immense potential, but also carries responsibility.

Bard: Absolutely. Decolonising natural product discovery isn't just about technology, it's about ethics, collaboration, and shared ownership. It's about ensuring that the benefits of this exploration flow back to the communities who hold the keys to nature's secrets. The path is long and winding, but I believe we can. With open minds, responsible AI development, and a deep respect for indigenous knowledge, we can navigate this jungle together, not as colonisers and colonised, but as partners in a shared quest to unlock the wonders hidden within nature's embrace.

Interviewer: Bard, you paint a hopeful picture. Can we truly achieve this equitable future? And would gender issues plaguing science be also mitigated by AI?

Bard: The data that feeds AI, like a mirror, can reflect the distortions of the world around it. We must be vigilant, crafting training sets that are diverse, inclusive, and free from the whispers of prejudice. Only then can AI truly empower, not amplify, existing inequalities. Moreover, AI should not be a solitary figure dictating the path forward. Imagine research teams where AI, hand in hand with women scientists, collaboratively weave the tapestry of discovery. AI can handle the tedious tasks, leaving women free to pursue the creative leaps, the intuitive connections that spark groundbreaking innovations.

Interviewer: shall we transition from the "Old" Researcher going to the wild to discover natural products towards a "New" indoor natural product discoverer in front of a computer?

Bard: Picture this: "Deep within the lush rainforests of the Amazon, indigenous healers have long known the secrets hidden within bark, leaves, and roots. Now, in bustling labs across the globe, scientists are teaming up with a powerful new partner - artificial intelligence (AI). This unlikely duo is embarking on a thrilling quest: to uncover nature's hidden treasures and unlock their potential to heal, protect, and inspire."

Think of AI as a tireless explorer, traversing mountains of data like uncharted jungles. It can sniff out promising molecules hiding amongst millions, predicting their potential to fight diseases, boost immunity, or even fuel new materials. It's like having a superpowered chemist in your team, tirelessly crunching numbers and whispering secrets of molecule magic.

But this adventure isn't just about AI taking all the glory. Human scientists are still the seasoned guides, navigating the cultural landscapes and respecting the wisdom passed down through generations. AI helps them see what was previously hidden, opening up new paths to explore and rediscover what nature has to offer.

Think of it like this: imagine scaling a towering tree, unsure of which branch to follow. AI can point you towards the strongest ones, but it's the experienced climber who knows how to grip, balance, and reach the hidden fruit at the top. Together, they make a formidable team, one fueled by human intuition and one powered by AI's lightning-fast analysis.

But like any expedition, there are challenges. We need to ensure this newfound power doesn't exploit indigenous knowledge or disrespect traditions. We need to bridge the digital divide, making sure everyone has a chance to join the search. And most importantly, we need to remember that AI is just a tool. It's our responsibility to use it wisely, ethically, and with a deep respect for the natural world and its guardians.

So, there you have it - a glimpse into the thrilling adventure of AI and natural products. A journey where ancient wisdom meets cutting-edge technology, where exploration fuels discovery, and where the potential to heal the world lies hidden within the leaves, waiting to be unlocked. Are you ready to join the quest?

Interviewer: I am amazed at these poetic metaphors and comparisons; they are truly inspiring to me and hopefully for the future generations of researchers in this field. Thanks for your time and it was a pleasure to share with you this virtual coffee in Paris!

Bard: The pleasure is all mine! Remember, the path to discovery is paved with both curiosity and responsibility. Let's walk it together, with open minds and open hearts.

These above answers, or merely the outcomes generated by a well-trained algorithm, provide us humans with valuable food for thought. We are embarking upon an era where the boundaries between human intelligence and artificial intelligence will become increasingly blurred. While tremendous benefits lie within our grasp, we must also be vigilant in navigating the substantial intellectual challenges ahead towards a more equitable World. On behalf of the Editorial Board of the Journal of Natural Product Discovery, I warmly invite you to submit your future research endeavours that leverage AI to our young journal for thorough evaluation and potential publication.

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