

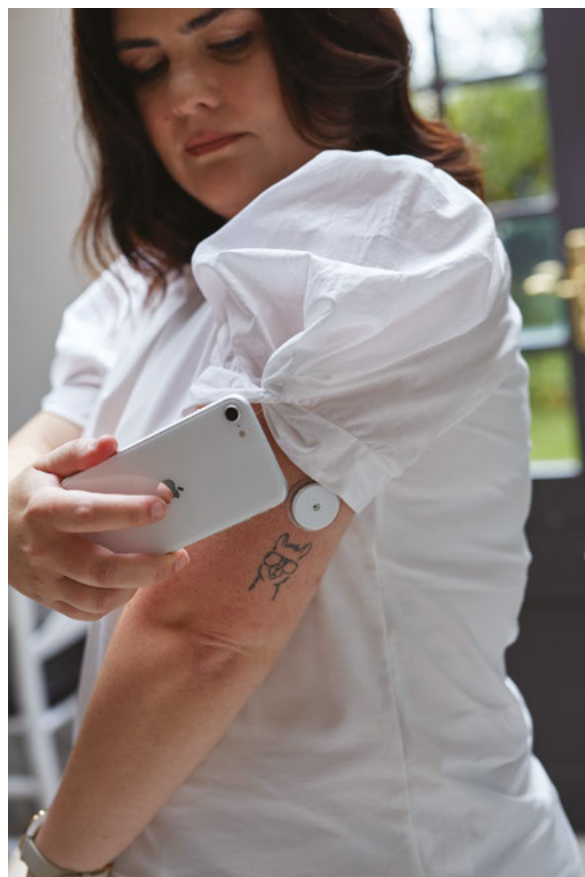
IUPAC's 2023 Top Ten Emerging Technologies in Chemistry

by Fernando Gomollón-Bel

This manuscript marks the five-year anniversary of IUPAC's "Top Ten" initiative [1]. The new additions will grow the list of emerging technologies to fifty—all with a powerful potential to make our world more sustainable and all suitable solutions to the current polycrisis [2]. This past summer, the theme of the IUPAC World Chemistry Congress in the Hague was "Connecting Chemical Worlds," which aligns almost perfectly with the goals of the "Top Ten"—multidisciplinary research is key towards transitioning to net-zero and achieving the United Nation's Sustainable Development goals by 2030 [3]. Moreover, the selection this year particularly promotes cross-collaboration in chemistry to create exciting emerging technologies that bridge the gap between academia and industry, while continuing the current competitiveness of chemical manufacturers. From a pool of possible ideas, a panel of experts have selected the following list, covering a range of fields from synthesis and polymer chemistry to health and artificial intelligence. The technology readiness level varies along the different solutions—nevertheless, all show a provocative promise to reimagine our world and our society.

Wearable sensors

In the past years, wearables have witnessed an unprecedented rise, revolutionising how we interact with technology. The COVID-19 pandemic accelerated this trend, and technologies to track and monitor our health flourished [4]. Usually, wearable devices determine data such as fitness metrics, sleep patterns, and they enable seamless communication and navigation. Chemistry adds another layer of valuable information, allowing the real-time monitoring of chemical, biological, and physical inputs—all with high sensitivity performance, but at a low cost [5]. Among the most popular applications is glucose detection in diabetes—wearable sensors have become widely-adopted, and allow quick connectivity with everyday devices, such as smartphones and smartwatches, giving patients unprecedented power and freedom [6]. But beyond glucose, chemical wearable sensors offer an opportunity to detect a wide variety of biomarkers, including pH, lactate, uric acid, ion levels, cytokines, and much more. This provides a platform not only to monitor the progress of patients in real-time, but also to detect and diagnose diseases in-depth, which increases the rapidness and efficiency of classical labwork in medical settings [7].



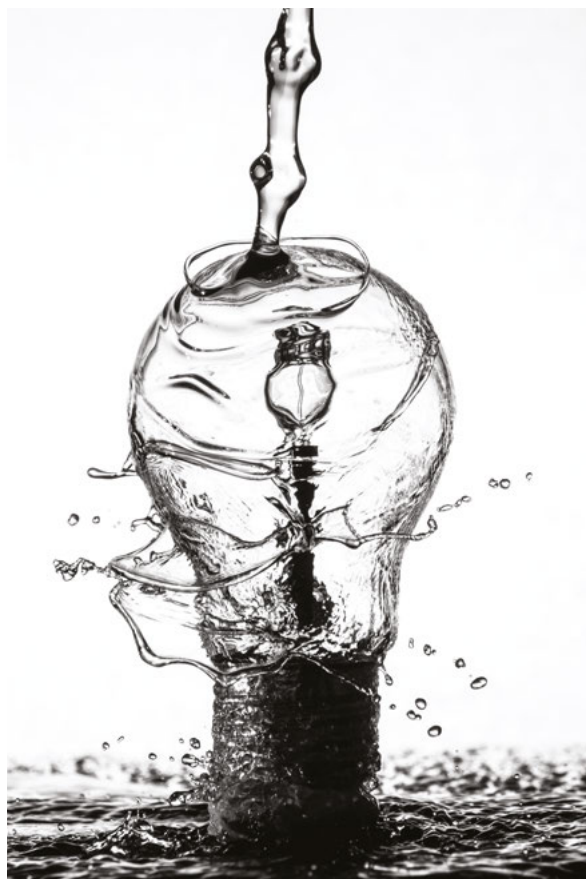
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Sensors usually convert chemical signals to electrical pulses—however, several solutions explore different detection methods, based on spectroscopic read-outs such as fluorescence, Raman, impedance, and ultrasounds. Beyond finding the features to measure, the real challenge comes from engineering devices with high biocompatibility, flexibility, durability and, of course, comfort [8]. An exciting development comes from the advances in microneedle technologies, which on top of detecting biomarkers could offer options for immediate drug-delivery in response [9]. Another advancement with great promise is pairing wearable sensors with connected devices. Beyond basic read-outs, such connectivity could provide new applications in telemedicine, giving doctors and medical professionals the ability to remotely monitor patients' health conditions with precision and accuracy, promoting timely interventions and tailored treatments. The continuous collection of health data could create new opportunities in drug discovery as well—provided that privacy and anonymity are granted.

Coupled with big data and machine learning, the information from wearable chemical sensors is emerging as a low-cost, non-invasive alternative to classical clinical trials, which often require in-person visits, biopsies, and blood sampling. In the era of multi-omics (genomics, proteomics, metabolomics), chemistry could convey a new revolution [10].

Photocatalytic hydrogen

In the past editions of the “Top Ten,” the lists highlighted exciting energy innovations, such as sustainable ammonia and liquid solar fuels. Along this line, green hydrogen is clearly emerging as a key-player – both as an alternative to fossil fuels in applications such as transport, industry, and chemical manufacturing, and as a viable vector to safely store and stockpile excess energy from intermittent renewable sources, such as solar and wind. It is estimated that clean hydrogen could cut over 700 million tonnes of carbon dioxide annually [11]. However, 99 % of hydrogen today still stems from fossil fuels—we need sustainable solutions. An attractive alternative is the photocatalytic production of hydrogen, which only requires renewable resources—sunlight and water. However, this technology is still in an early stage, unlike water electrolysis, which has showcased an efficiency of over 30 % with countless cost-effective commercial applications [12]. While still struggling with efficiency, the paramount promise of photovoltaic hydrogen is scalability for safe systems that offer durability and practicality. Recently, researchers demonstrated a photocatalytic production plant of 100 square metres [13], and the field is thriving with published papers and patents growing exponentially. Photocatalytic hydrogen still faces several challenges. For instance, performance is closely connected with the band structure and the bandgap of the catalyst—as well as responsiveness to a wider wavelength range. Narrowing the band gap could boost hydrogen production and reduce the reliance on specific wavelengths, maximising the utilisation of solar energy [14]. Furthermore, scalable systems should safely separate hydrogen, to reduce the risk of explosion. Technologies such as membranes, metal-organic frameworks and, more recently, hydrogels, have emerged as a practical possibility, which could enable applications such as floatable production platforms, with promising potential in large-scale production, sometimes straight from seawater, a sustainable source of hydrogen [15]. Additionally, chemists could collaborate with biologists to boost the efficiency of photo-biological processes to produce hydrogen, thanks to some of the most competent



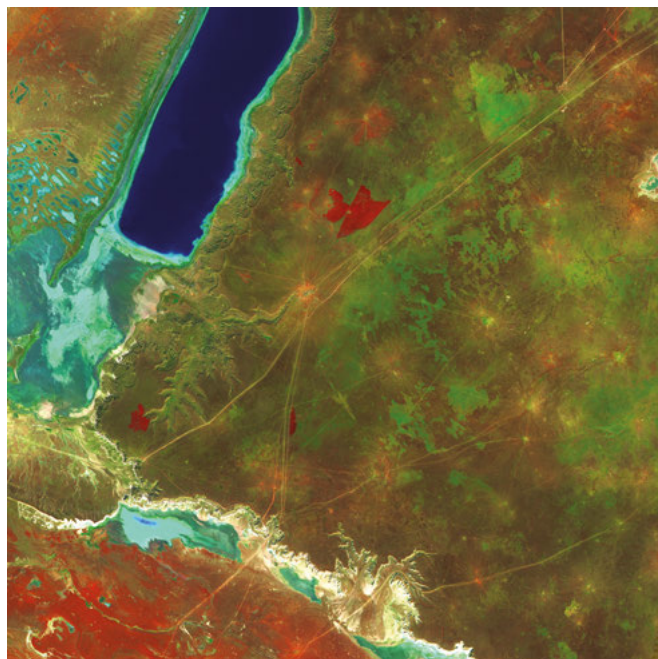
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catalysts—enzymes [16]. Biological transformations open the door to the generation of clean hydrogen from water, as well as other renewable sources such as biogas, biomass, and even wastewater [17]. Tools such as the genetic and metabolic engineering of microorganisms, as well as the directed evolution of enzymes (one of the “Top Ten” picks in the first edition of the initiative), could advance the avenues towards a scalable, low-cost, commercial clean hydrogen [18].

Chloride-mediated removal of ocean CO₂

The United Nations consider the ocean our greatest ally against climate change. It absorbs a quarter of all carbon emissions, as well as 90 % of the excess heat generated by greenhouse gases—a big buffer blocking the consequences of the climate crisis [19]. However, the ocean’s force is finite, and the excess carbon dioxide accumulated is acidifying seawater and affecting marine

life. On the other hand, the excess carbon dioxide could be converted into a capital resource—a carbon reserve free from fossil fuels. In that sense, the electrochemical capture of carbon dioxide from seawater has emerged as an attractive alternative towards net negative emissions, which some venture could provide synthetic fuels and chemical feedstocks at a gigaton per year scale [20]. Nowadays, most systems for electrochemical CO₂ removal rely on bipolar membrane electrodialysis, a technology that presents two important challenges—it is still expensive, and sometimes leaks, which could contribute to additional contamination of the ocean. Now, a new idea bypasses membranes altogether, and could potentially provide an efficient and inexpensive mechanism for ocean carbon removal [21]. This alternative only requires two bismuth-based electrodes, pumps, and gas separation systems, all economical and easy to scale up. It is a cyclic process. The pump provides water to the first electrode, which acidifies it further to free and filter carbon dioxide out. The same mixture travels to the second electrode, featuring a reverse voltage and setup to raise the pH. Regularly, the roles of the electrodes switch to regenerate a continuous flow, cyclic operation, which could cost as little as \$56 per ton of carbon dioxide, according to the first technoeconomic studies [22]. It is an early emerging technology, but definitely a promising plan to reduce and reverse the acidification of our oceans.



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GPT language models in chemistry

In 2020, artificial intelligence (AI) already made the “Top Ten” selection [23]. Since then, AI models and applications have advanced remarkably, particularly thanks to the release of improved large language models (LLMs) such as OpenAI's ChatGPT, designed and developed to both understand and generate conversations. After meticulous training with a vast amount of data, the AI model learns patterns, grammar, and semantics in language, understands inputs and reasoned responses, which include translation, summarisation, and more. The popularisation of LLMs has equally excited and concerned the scientific community. For example, some feared that fake research papers generated with AI tools could eventually get published—it is relatively easy to trick reviewers, and even simpler to fool specialised tools for plagiarism detection [24]. LLMs have also allegedly started generating peer-review reports, which generates many questions about the solidity and stability of the present-day publishing industry [25]. Nevertheless, many defend LLMs as ‘the future of the field.’ Because, on top of retrieving responses that look like real-life human discussions, language models have been successfully used in chemistry applications. ChatGPT and other algorithms analyse microscopy images, predict protein structures, and even estimate reaction yields – the possibilities are endless [26]. A novel tool called ‘ChemCrow’ makes the most of LLMs and is quite capable of accomplishing tasks including planning synthetic routes, controlling robotic reaction platforms, automated analysis, and much more. Additionally, the newest updates include several safety checks to avoid the accidental preparation of potentially harmful products, such as explosives, chemical weapons, and controlled substances [27]. Some studies suggest that LLMs ‘understand’ complex chemical problems better than tools such as deep learning, expanding the possibilities beyond chatbots [28]. Moreover, LLMs could convey advantages for chemistry education, streamlining literature reviews, information search, and much

more. Although some early experiments suggest LLMs still struggle with basic chemistry questions, ChatGPT could rescue students and professors from 'the morass of the mundane, from meetings and memos' [29], freeing time for creativity and constructive conversations.

Synthetic electrochemistry

Electron exchanges drive chemical reactions. Since electricity is our cheapest and greenest source of electrons, it has been used as a powerful tool to transform substances since the discovery of the battery in the early 19th century. The first electrolysis soon ensued the experiments by Alessandro Volta, and just a few years later Michael Faraday performed an electrochemical reaction on an organic compound—the decarboxylation of acetate. The field faded after these famous feats, and briefly resurfaced in the mid-20th century with the discovery of cyclic voltammetry, a technique that enabled a better characterisation of the reaction processes, and was further enhanced later on with the advances in computational calculations [30]. Now, these advances, together with the development and deployment of intuitive and inexpensive equipment, have shed light into a process previously considered a “black box,” and synthetic electrochemistry is experimenting a recent renaissance, which has brought benefits such as higher levels of chemo- and regio-selectivity [31]. Now, electrochemistry enables an enormous variety of transformations—the synthesis of ethers, Birch-type reactions, oxidation and fluorination of carbon–hydrogen bonds, and many more [32]. Recently, researchers reported yet another breakthrough in the field—the selective reduction of carbonyl groups, even in presence of other redox-active groups, thanks to alternating current. The team had collaborated closely with chemistry equipment manufacturer IKA to design and develop hardware and software that make the new method accessible to as many laboratories as possible. ElectraSyn is a device designed to democratise synthetic electrochemistry [33]. Electrosynthesis is intimately linked to green chemistry, and shares several key aspects, including high levels of safety, reliability, atom economy, and low energy consumption. These standards have streamlined industrial uptake, with productive processes such as the Baizer process, a method to manufacture adiponitrile, key in the production of nylon, which yields over 300 kilotonnes annually [34]. BASF also uses electrochemistry to synthesize substituted toluenes, making more than 30 kilotonnes of *para*-tolualdehyde and 3.5 kilotonnes of *para*-methoxytoluene. 3M, Bayer, Johnson Matthey, La Roche, and Sandoz also make the most of electrosynthesis

towards key products and intermediates [35]. Currently, many manufacturers embrace electrosynthesis to enhance their production processes, reducing costs and greenhouse gas emissions in the chemical industry. Combined with renewable electricity, electrochemistry emerges as a sustainable and versatile tool for organic synthesis.

Artificial muscles

Surprisingly, the idea of artificial muscles—or mimicking muscle action with actuators—dates back to the 17th century and experiments by British scientist Robert Hooke. However, it was not until the last 30 years that advances in chemistry and materials science have made the artificial muscles a real possibility. Some state-of-the-art solutions have safely survived in-vivo studies [36], showcasing the promising potential of the field—nevertheless, experts envision clinical trials and applications in humans still lay years ahead. Research on artificial muscles encompasses many materials, a multidisciplinary endeavour examining devices that contract, expand, or rotate in response to different external stimuli, including current, temperature, pH, and light, among others [37]. The challenge is twofold: first, it is about synthesising structures that mimic muscles, then infusing functionality and responsiveness. Researchers have found inspiration in insects, with microfilaments that emulate the movements and micro-structures of myosin and actin, the main muscle proteins in nature; as well as powerful polymers, elastomers engineered to respond to electrical currents, which have shown promise in patients recovering from heart surgery, urinary incontinence, and some side-effects of strokes [38]. Another attractive approach comes from the design and development of composite materials that mimic the natural structure of skeletal muscles. With a combination of liquid crystal elastomers and a matrix of graphene fillers, which mimic myosin and actin in natural fibres, the artificial muscle materials maintain strong mechanical properties and convey conductivity of electrical signals, key for functionalities such as actuation and locomotion. The technology, now patented as “Hercules” fibres, is seeking commercialisation through a Korean spin-off company, and could uncover applications in defence, manufacturing, and medicine, according to the authors [39]. Additionally, artificial muscles have revolutionised robotics, creating highly-adaptable and flexible systems for applications that include prosthetics, exoskeletons, and biomedical devices such as grippers, microsurgery mechanisms, and many more. Thanks to artificial muscles, robots could potentially provide more precise control, as well

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as improved responsiveness with lifelike movements, making them more suitable and usually safer than current alternatives, especially for delicate tasks [40].

Phage therapy

Phage therapy is a promising approach to combat bacterial infections, in a time when antimicrobial resistance is rising to worrying levels—in 2019 it killed five million people, most of them in low- and middle-income countries. If the trend continues, current calculations estimate that the numbers will double by 2050, which will immediately impact the global economy with costs of one trillion dollars per year [41]. The discovery of bacteriophages (or simply, phages), took place in the early 20th century, simultaneously and independently by Frederick Twort in 1915 and Félix d'Hérelle in 1917. It was the latter who not only extensively studied this type of viruses that specifically target and infect bacteria, but also already recognised the huge potential of phages as a therapeutic tool to treat bacterial infections. In the past years, the field of phages has witnessed a renaissance, a revitalisation that has shown great promise treating bacterial infections, as well as other diseases such as cancer [42]. The differences among applications lay in key structural differences across the phage viruses—the 'lytic' phages infect bacteria and reproduce within, until the crowd of duplicates destroys the host; the 'non-lytic' or 'lysogenic' phage [43], on the other hand, assimilates its genome within the host's, and have found applications in targeted treatments for cancer, stroke, bone defects, and more [44]. But besides biology, chemistry could also complement the characteristics and features

of phages—as well as spark uses in drug discovery, diagnosis, and materials science. For example, encapsulation techniques (such as liposomes, nanoparticles, hydrogels, or metal-organic frameworks) could convey controlled delivery of phages, increasing stability, availability, protection from degradation, and advanced active site targeting [45]. Phages have also found use in novel nanomedicine applications, including the study of protein interactions. Recent studies suggest that phages could display peptides and proteins of interest for proteomics analyses—a strategy to discover interesting targets for diagnosis, therapy, and signalling pathways [46]. Last but not least, phages have also emerged as an extremely versatile platform for supramolecular chemistry, a field in the frontiers of chemistry, materials science, and medicine. Phages have formed inorganic nanostructures, platforms for stem-cell differentiation, detected disease biomarkers, and structured scaffolds for applications such as tissue regeneration [47]. The rediscovery of phages could not only create innovative ways of fighting the so-called 'superbacteria', but also stimulate exciting discoveries in supramolecular chemistry and biomaterials.

Biological recycling of PET

Plastic pollution is a persistent problem [48]. Recent reports have shown plastics and microplastics appearing in the most improbable places—Antarctic krill, freshly fallen snow, even human blood samples [49]. The Organisation for Economic Co-operation and Development (OECD) is concerned that, while the world has doubled its production of plastic waste in the past



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twenty years, only 9 % of plastic is properly recycled, and 22 % of waste is mismanaged and incorrectly disposed [50]. Once again, chemistry could come to the rescue, bringing better solutions for sustainability, providing a hopeful new model based on the reutilisation of resources and the reduction of waste and by-products [51]. The discovery and characterisation of enzymes that could naturally hydrolyse and degrade polymers and plastics opened a world of new possibilities for repurposing and recycling [52]; and soon the expansion of directed evolution (awarded with the 2018 Nobel Prize in Chemistry and selected as one of IUPAC's "Top Ten" Emerging Technologies in 2019) has further driven the promises in this field [53]. An especially exciting development is an enzyme that hydrolyses polyethylene terephthalate (PET) back into its building blocks, with excellent yield and productivity. The traditional techniques for PET recycling result in an incremental loss of mechanical properties. However, the evolved enzymes eventually produce PET with the same properties as petrochemical PET—contributing to circularity and reducing waste in landfills and the environment [54]. And the good news is commercialisation is close. French green chemistry company, Carbios, is currently building a plant that will implement this innovation industrially and, by 2025, it will be ready to recycle 50 kilo tonnes of PET per year—the equivalent to 2 billion PET bottles [55].

Depolymerisation

We have already reviewed the problems of plastic pollution. Moreover, back in 2019, we explored some

solutions based in biotechnology to break polymers back into basic building blocks—monomers. Now, we are revisiting this approach to recycling, with additional angles on upcycling, circularity, and sustainable design. Different tools could provide interesting ideas for repurposing plastic waste into valuable resources. Chemically cutting polymers into monomers is an especially suitable solution for polycondensation polymers such as PET, polyamides, and polyurethanes. Similarly, high-temperature processes like pyrolysis and gasification convert polymers such as polyethylene and polypropylene of smaller molecular fragments—not monomers, yet interesting feedstock for recycling. Several start-ups and companies have successfully implemented chemical recycling processes for various waste products, including PET packaging, bottles, textiles, as well as polyurethane and polystyrene streams [55]. Finding the right approach to chemical recycling can significantly contribute to a circular economy for plastics and aid in achieving carbon neutrality within the plastics value chain. Two priorities towards more productive depolymerisation include the rational design of polymers and macromolecules and the reduction (or removal, if possible) of additives acquired during plastic processing. All efforts towards re-engineering the production of polymers and plastics could mitigate some of the problems of pollution [56]. Some exciting examples include polydiketoenamines, a family of strong and powerful polymers that bring us closer to closed-loop, zero-waste plastics. The covalent bonds in polydiketoenamines are easy to recycle and upcycle with simple mechanochemical methods [57]. Another attractive



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alternative is microwave-assisted depolymerisation, which is already scaled-up for the recycling of PET. Recently, Swiss firm Gr3n announced a new plant that will recycle 40 kilo tonnes of PET annually using this method, which will open in 2027 [58]. Beyond biodegradability, chemists could create polymers and plastics safe and sustainable by design. For example, the latest advances in molecular modelling could help anticipate and predict possible pollution problems, degradation side-effects, and the viability of recycling reactions. Moreover, comprehensive life-cycle analyses would help us better understand the impacts beyond waste, including factors such as economics, carbon emissions, and product-life. In this sense, policies such as REACH [59] and new digital product passports, already implemented in the EU, could catalyse change towards the circular economy [60].

“Low-sugar” vaccinations

Glycans—namely oligo- and polysaccharides—cover most biological structures, including nucleic acids, lipids, proteins, and cells in general. Glycans’ sugar coatings contribute to a variety of functions - immune responses, receptor recognition, as well as communication, signalling, and interactions between cells. Understanding glycans and the “glycome” is vital for developing vaccines, studying diseases, and advancing biomedical research [61]. The role of sugars was key in the development of vaccines and treatments for SARS-CoV-2, the virus that causes COVID-19. Researchers demonstrated that glycans played a key role in the recognition process of the spike protein, contributing to a more effective infection [62]. And more recently, another advancement related to sugar chemistry conveyed an interesting steppingstone towards better and broader vaccines against SARS-CoV-2, with

enhanced effectiveness against new variants. In this case, however, removing the sugar skin of the spike protein seems to provide a powerful protection against infection. Deleting some of the sugars exposes the most common and conserved regions of the virus, which leads to stronger and broader immune responses, including both neutralising antibodies and T-cells. This “sugar-free” vaccine showcased many advantages *in vitro*, however further studies will need to corroborate the results *in vivo*, and then examined further by clinical trials [63]. A similar solution, “glycan trimming,” has also shown promise in the development of more effective vaccines against HIV infection. The modifications in the glycoprotein improve the immune response in animal models, helping better recognise the HIV virus despite its evasive envelope—a glycan coating that tricks antibodies and T-cells [64]. Although the technology is still in a very early stage, some biotechnology and pharmaceutical companies have already attained agreements to further develop and commercialise the idea.

The 2023 “Top Ten” Emerging Technologies in Chemistry represent a diverse selection all around—from very early-stage ideas to industrialised innovations, in many different fields of chemistry, including synthesis, materials science, energy, biomedicine, and education. Perhaps instead of considering chemistry the “central science,” we should consider it the “connecting science”—one that catalyses collaboration across disciplines and encourages industrial innovation. Similarly, sustainability remains a universal subject throughout the “Top Ten” selections—the uttermost purpose of the initiative is still to ensure a sustainable future, advancing our society, and improving our quality of life [65]. We need creative chemistry solutions for a better world, therefore let us work together to identify the most imaginative ideas and innovations

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and guarantee growth, as well as access to basic rights—including renewable energy, fuels, food, and pharmaceuticals for all.

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