Quantum Computational Biology - Evolution

Prior to the review of this article, following our discovery of the role of inorganic elements as constituents of cytokines (refer to the following) it was necessary to develop a novel model of the periodic table that will allow for assessment of interactions of elements and minerals that support epigenetic activity.

https://www.mcfip.net/upload/Cell%20Surface%20Signaling%20Molecule%20Formation%207-2017.pdf

Lacking an existing format of the periodic table that would meet our needs, more than 100,000 hours of combined efforts were required to develop an algorithmic model that would allow for identification of the interactions between the inorganic elements (agonistic - antagonistic and transitional states) to enable research to optimize the evolving discipline of metalloendocrinology.

In essence, dependent on the disciple and objectives, the “standard” model of the periodic system does not provide the crucial information for nanoparticle interactions that are critical for the application of epigenetics in cellular physiology.

The following are provided for discussion with computational biology professionals to explain the formation of nutrients on the surface of cells and to highlight of how they are transported in the cytoplasm to provide the nutrients require for survival.

https://www.mcfip.net/upload/Quantum%20Biology%20MCFIP%20Discoveries%20(1).pdf https://www.mcfip.net/upload/Quantum%20Biology%20-%20Gene%20Constituents.pdf

https://www.mcfip.net/upload/Quantum%20Biology%20-%20Physical%20Chemistry.pdf

Outcomes from the application of Quantum Computational Biology (QCB) modeling are provide in the Cancer, Cardiology and Neurodegenerative Disease tabs on the website www.MCFIP.net.

Note: MCFIP is a healthcare modeling entity. The aforementioned findings are provided for use by the research community.

Refer to the document affixed to this article to understand the new sub - discipline in chemistry; i.e. metalloendocrinology.

https://phys.org/news/2019-06-hidden-periodic.html

JUNE 17, 2019

The hidden structure of the periodic system

by Max Planck Society

The periodic table of elements that most chemistry books depict is only one special case. This tabular overview of the chemical elements, which goes back to Dmitri Mendeleev and Lothar Meyer and the approaches of other chemists to organize the elements, involve different forms of representation of a hidden structure of the chemical elements. This is the conclusion reached by researchers at the Max Planck Institute for Mathematics in the Sciences in Leipzig and the University of Leipzig in a recent paper. The mathematical approach of the Leipzig scientists is very general and can provide many different periodic systems depending on the principle of order and classification—not only for chemistry, but also for many other fields of knowledge.

It is an icon of natural science and hangs in most chemistry classrooms: the periodic table of elements, which is celebrating its 150th birthday this year. The tabular overview is closely linked to Dmitri Mendeleev and Lothar Meyer—two researchers who, in the 1860s, created an arrangement of elements based on their atomic masses and similarities. Today they are sorted by atomic number (which indicates the number of protons in the atomic nucleus) from the light hydrogen (one proton) to the synthetic oganesson (118 protons). The elements are also classified into groups: Atoms in the same column usually have the same number of electrons in their outer shell.

Periodic table in different variants

At first glance, the periodic table seems to have brought an unambiguous and final order to the currently known 118 elements. But appearances can be deceptive because many things still remain controversial: Scientists do not agree on exactly which elements belong in the third group below scandium and yttrium. For example, the correct position of lanthanum and actinium is debated. If one takes a closer look, one will discover slightly different variants of the periodic table in classrooms, lecture halls, and textbooks.

Guillermo Restrepo and Wilmer Leal from the Max Planck Institute for Mathematics in the Sciences and the University of Leipzig are not surprised. For them, there is no unambiguously correct arrangement of the elements; depending on the criterion applied for classification, a different periodic table results. The atoms can be subdivided according to the electron configuration (i.e. the number and arrangement of their electrons), their chemical behavior, their solubility, or their occurrence in geological deposits. It is now widely accepted that the chemical elements should be arranged according to their atomic number and divided into groups according to their electron configuration. But even for this periodic table, there are numerous different forms of representation. For example: as a spiral with various bulges, pyramid-shaped, or as a three-dimensional flower.

A common structure behind the periodic tables

Guillermo Restrepo and Wilmer Leal have now systematically investigated the ambiguity of the periodic table. This has led to findings that are also of considerable importance beyond chemistry. Accordingly, all forms of representation of the chemical elements are based on a common structure, which mathematicians refer to as an ordered hypergraph. The venerable periodic table of Mendeleev and Meyer thus offers only a representation of the general structure, which Guillermo Restrepo and Wilmer Leal now postulate. New arrangements can also be derived from this at any time. Guillermo Restrepo therefore compares the order of the chemical elements with a sculpture on which light falls from different directions. "The various shadows that the figure casts are the periodic tables. That's why there are so many ways to create these tables. In a way, the period tables are projections. Projections of the internal structure of the periodic table."

The scientists from Leipzig are now trying to determine the hidden mathematical structure on which the known periodic tables of chemistry are based. For the time being, they have defined three conditions that must be met in order to establish a periodic table. First, one needs objects that are to be ordered. For Mendeleev, Meyer and the creators of the other known periodic tables of chemistry, these are the chemical elements. These objects must be arranged according to some properties such as the atomic mass or the atomic number (i.e. the number of protons). Finally, one criterion is required to group the objects in classes. Mendeleev and Meyer used the chemical similarity for this.

Periodic table of chemical bonds

"If these three conditions are met, periodic tables can also be created for other chemical objects and even for objects outside chemistry," says Guillermo Restrepo. He and Wilmer Leal show this by looking at the chemical bonds between atoms of 94 elements and different conjugates. The polarizability of 94 single-covalent bonds, where bonds are arranged according to the electronegativity and atomic radius of one of the bonded atoms. For example, fluorine, chlorine, or oxygen are highly electronegative and assume relatively small atomic radii in compounds. The bonds are then classified based on how much they resemble each other.

"We have investigated almost 5,000 substances consisting of two elements in different proportions," explains Guillermo Restrepo. "We then looked for similarities within this data. For example, sodium and lithium are similar because they combine with the same elements in the same proportions (e.g. with oxygen or chlorine, bromine, and iodine). We thus found patterns we can use to classify the elements."

A periodic table as a network instead of a matrix

In the 44 classes of chemical elements, there are some similarities with the main groups of Mendeleev's and Meyer's periodic table. For example, the alkali metals sodium and lithium are found in one group because they form the same simple salts with halogens such as chlorine or fluorine. Like the elements themselves, the bonds of the four halogens (fluorine, chlorine bromine, and iodine) are also found in the same group. However, there are also classifications that differ significantly from those in the conventional periodic table. For example, carbon and silicon are no longer in the same class because they form very different compounds.

The representation of the periodic table of chemical bonds also has nothing to do with the familiar matrix-like arrangement of the classical periodic tables of the elements. Instead, the 94 covalent bonds are represented in a network of differently colored circles. Each circle represents a chemical bond, and the colou symbolizes belonging to one of the 44 groups. Because now two criteria are used for the sorting, there is no longer any clear order of the atoms (like in the tables of Mendeleev and Meyer)—mathematicians speak of a partial order. The circles are therefore connected to other circles by one or more arrows, thereby creating an ordered hypergraph.

Periodic tables in other scientific fields

The chemical elements and their compounds can also be represented in completely different periodic tables—depending on the underlying order and classification principle. What's more: The objects of numerous other scientific fields and their applications can also be arranged in periodic tables. For example, ordered hypergraphs are used in information systems and web mining. Possible periodic systems also emerge when countries are considered; these can be classified according to social or economic indicators as well as geographical proximity or cultural similarity. Other examples can be found in engineering, environmental sciences, sociology, and many other disciplines. The scientists not only study periodic systems because of their importance for chemistry, but, above all, because of their applications in many other disciplines.

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These researchers are not using the principles of metalloendocrinology being developed by the chemistry team at UC Davis. Simply, based on the fundamentals of inorganic chemistry, agonistic and antagonistic relationships can occur.

The What We Have tab of the website www.MCFIP.net provides 4 links for Quantum Computation Biology (QCB) that can be used to verify the underlying scientific principles of metalloendocrinology.

https://phys.org/news/2019-06-technique-sensory-nanoparticles-disease.html

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Innovative technique uses sensory nanoparticles to detect disease

by Brigham and Women's Hospital

Investigators from Brigham and Women's Hospital are taking advantage of a unique phenomenon of nanoparticles to develop a test for early detection of different types of diseases, including cancer.

Through previous investigations, Morteza Mahmoudi, Ph.D., now a biomedical investigator in the Department of Anesthesiology, Perioperative and Pain Medicine, and colleagues have shown that biomolecules in the blood of healthy individuals and patients form various corona profiles around nanoparticles. Like dipping a donut hole in powdered sugar, nanoparticles collect a unique coating of proteins from the blood. In a new study published in the *Royal Society of Chemistry's* peer-reviewed journal *Nanoscale Horizons*, Mahmoudi and the team present evidence that these coronas are personalized and precise, with different compositions or patterns in people with cancers. They have developed a sensor array that has been tested on blood samples, both from people diagnosed with five different types of cancer as well as purportedly healthy people who went on to have a cancer diagnosis several years later. The team's goal is to develop an early detection test that could be used in the clinic to identify those at risk of cancer and other diseases.

"For cancer and many other catastrophic diseases, the earlier you can diagnose, the more likely you can treat and extend survival and attain better quality of life," said Mahmoudi, the paper's corresponding author. Mahmoudi is the former director of the nanobio interactions laboratory at Tehran University of Medical Sciences where he began this work in 2014. "The goal here is to develop a strategy to help people get better information about their health. Today, in the clinic, we have ways to measure lipids and predict risk of cardiovascular disease, but limited ways for cancer. If everything goes well, we hope our work will lead to a screening test for the earliest signs of cancer."

To carry out their investigation, the team combined the concepts of disease-specific protein coronas with sensor array technology. Sensor arrays can identify a wide variety of interacting chemical and biological compounds all at once rather than in isolation. To test blood samples for early patterns of disease, the team developed a sensor array that consisted of three different cross-reactive liposomes—fatty molecules that caused protein coronas to form around them. The team tested samples from five patients, each with a different form of cancer: lung cancer, glioblastoma, meningioma, myeloma, and pancreatic cancer. The team found that the selected pattern of corona composition, through advanced classification techniques detected by the nanoparticle sensor array, provided a unique "fingerprint" for each type of cancer. The team also tested the tool using blood from 15 people who were subsequently diagnosed with brain, lung, and pancreatic cancer up to eight years later, finding that their approach could identify and discriminate the cancers at the very early stages.

Although promising, as with other diagnostic approaches, the team's preliminary results will need to be validated in a larger number of people to make sure the test not only works but also provides accurate diagnostic information. Mahmoudi and his colleagues are also interested in applying the technology beyond cancer to diagnose other diseases at an early stage.

"The only reason I'm in science is to do something that can help patients," said Mahmoudi. "When I see predictions about cancer, the number of new cases each year and its global burden, it excites me to think that our multidisciplinary expertise in nanobio interfaces, sensor array, and advanced statistics may offer a way to help. There is so much potential here and we are working to tap into it."