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Computational chemistry for the study and design of used drugs and their pharmacological effects

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Abstract
The design and development of new pharmaceutical compounds and the manufacture and development of new chemical compounds to suit therapeutic uses is a topic of great importance in the sense of increasing their therapeutic effect and reducing side effects by determining the type of disease and the appropriate treatment for the disease. For this, many chemical and technical techniques are used, as well as new computer chemistry applications. To study the drugs used and their biological effects, the most important of these techniques are: the structure-effect relationship (SAR) and the structure-effect relationship (QESAR). The compounds that are used as medicines are usually organic compounds, which are divided into small organic molecules such as atorvastatin and clopidogrel, and biological substances such as infliximab and insulin. Specifically, pharmaceutical chemistry focuses on small organic molecules, some aspects of natural products, biochemistry, and enzymology, and aims to discover and develop drugs in these areas.

Keywords: chemical drug, drug chemistry, computational chemistry, nano medical, nano polymer, drug carrier

Introduction

Currently, the most common use of smart polymers in biomedicine is specifically targeted drug delivery. Since the advent of timed drugs, scientists have faced the problem of finding ways to deliver drugs to a specific site in the body without first breaking down in the highly acidic environment of the stomach. Prevention of harmful effects to healthy bone and tissue is also an important consideration. Researchers have devised ways to use smart polymers to control drug release until the delivery system reaches its target [1, 2]. This release is controlled by either a chemical or physiological trigger. Linear and matrix smart polymers exist with a variety of properties that depend on the reactive functional groups and side chains. These groups may respond to pH, temperature, ionic strength, electric or magnetic fields, and light. Some polymers are inversely linked via unequal bonds that can break and depend on external conditions. Nanotechnology has been instrumental in the development of some nanopolymers such as dendrimers and fullerenes, which have been applied to drug delivery. Conventional drug encapsulation has been using lactic acid polymers. Recent advances have seen the formation of hair-like matrices that maintain the incorporation of the drug of interest or wrap between the polymer strands [3-6].

Smart polymer matrices release drugs via a chemical or physiological reaction to alter the structure, often a hydrolysis reaction that results in cleavage of bonds and drug release as the matrix breaks down into biodegradable components. The use of natural polymers has given way to synthetic polymers such as polyanhydrides, polyesters, polyacrylic acids, poly (methyl methacrylates) and polyurethanes. It has been found that aqueous, amorphous, low molecular weight polymers containing heterocyclic atoms (ie atoms other than carbon) degrade faster. Scientists control the rate of drug delivery by changing these properties and thus adjusting the rate of degradation [6-9]. The bait and block copolymer are two different polymers that have been grafted together. There are already a number of patents for different groups of polymers with different reactive groups. The product exhibits properties of each of the individual components that add a new dimension to a smart polymer structure, and may be useful in some applications. Crosslinked hydrophobic and hydrophilic polymers result in the formation of mixel-like structures that can effectively aid drug delivery through an aqueous medium until conditions at the target site cause both polymers to collapse simultaneously.

The graft and block approach may be useful in solving the problems encountered in the use of a common biopolymer, polyacrylic acid (PAAc). PAAc adheres to mucosal surfaces but swells and degrades rapidly at pH 7.4, resulting in the rapid release of drugs trapped in the matrix [10-13]. A combination of PAAc with another polymer less sensitive to changes in neutral pH may increase residence time and slow drug release, thus improving bioavailability and efficacy. Hydrogels are polymer networks that do not dissolve in water but swell or collapse in changing aqueous environments. They are useful in biotechnology for phase separation because they are reusable or recyclable. New ways to control the flow, or capture and release of target compounds, in hydrogels, are being investigated. Highly specialized hydrogels have been developed to deliver and release drugs in specific tissues. Hydrogels made with PAAc are especially popular due to their bioadhesive properties and

tremendous absorbency [14, 15]. Enzyme immobilization in hydrogels is a fairly well-established process. Reversibly cross-linked polymer networks and hydrogels can similarly be applied to a biological system where response and drug release are triggered from the same target molecule. Alternatively, the response may be turned on or off by an enzyme reaction product. This is often done by incorporating an enzyme, receptor or antibody, which binds to the molecule of interest, into the hydrogel. Once it occurs, a chemical reaction occurs that leads to the reaction of the hydrogel. The trigger could be oxygen, the sensation using oxidoreductase enzymes, or a response to pH sensing. An example of the latter is the combination of glucose oxidase effusion and insulin in a pH responsive hydrogel. In the presence of glucose, the formation of glucagon acid by enzyme catalysts releases insulin from the hydrogel. Two criteria for this technique to work effectively are enzyme stability and rapid kinetics (rapid response to the trigger and recovery after the trigger is removed) [16-20]. Several strategies have been tested in type 1 diabetes research, which include using similar types of smart polymers that can detect changes in blood glucose levels and trigger production or release of insulin. Similarly, there are many possible applications [22-26] for similar hydrogels as drug delivery agents for other conditions and diseases.

Computational Design of Drugs

Pharmaceutical chemistry is by nature an interdisciplinary science, and its professionals have a strong background in organic chemistry, which must be linked to broad biological concepts specific to drug targets at the cellular level. Most training systems include a two-year post-doctoral fellowship study (Ph.D) in chemistry. However, there are also job opportunities for master's degree holders in the pharmaceutical industry. At the master's and doctoral level there are opportunities to work in the academic field. Postgraduate programs in pharmaceutical chemistry are often found in faculties of pharmacy and some departments of chemistry. Most of the modern workers in the field of pharmaceutical chemistry, especially in the United States of America, have not received formal training in this field, but they receive the required background in pharmaceutical chemistry and pharmacology after employment in pharmaceutical companies [27-30].

Smart polymers as a drug delivery

Its properties make it particularly suitable for bioseparations. The time and costs involved in purifying proteins may be significantly reduced by using smart polymers that undergo rapid reversible changes in response to a change in intermediate properties. Paired regimens have been used for many years in physical separation, kinship and immunogenicity [31-33]. Microscopic changes in the polymer composition are manifested in the form of precipitate formation, which can be used to help separate the trapped proteins from the solution. These systems operate when the protein or other molecules that are separated from the mixture, form a bio conjugate with the polymer, and precipitate with the polymer when their environment undergoes change. The precipitate is removed from the media, thus separating the desired constituent in the conjugate from the rest of the mixture. Removal of this component from the union depends on the recovery of the polymer and its return to its original state, and therefore hydrogels are very useful for such processes. Another approach to controlling biological interactions using smart polymers is the preparation of recombinant proteins with polymer-integrated binding sites close to gene or cell binding sites. This technique has been used to control ligand and cell binding activity, based on a variety of stimuli including temperature and light. Smart polymers play an integral role in self-adapting wound dressing technology. The design of the dressing offers synthetic, super-absorbent smart polymers embedded in a 3D fiber matrix with an added wetting function achieved by including a hydrogel in the core of the material. The modus operandi of the dressing is based on the ability of polymers to simultaneously sense and adapt to changing moisture and fluid content in all areas of the wound, automatically and reversing from absorption to hydration. The smart polymer action ensures the dressing material's active simultaneous response to changes in and around the wound to support an optimum moist healing environment at all times [34-36].

Determining Treatment through Computer Technology

Pharmaceutical compounds and their properties, as well as the methods of calibrating them and determining their identity, are divided into an organic branch and an inorganic section. Reference books for this science should include a comprehensive classification of the huge numbers of drugs available in the commercial market according to pharmacological or chemical groups, highlighting the so-called structure-effect relationship for members of each particular group. These references should provide information such as physical and chemical properties, use, side effects and dosage With the exception of this information, there are wide differences between every reference book and another in the field of pharmaceutical chemistry, as some of them go to the interest in studying drugs in terms of dissolution, binding to proteins, absorption and elimination, and some of them go to interest in studying the analytical methods of these drugs. Teaching pharmacy and the first of these trends started from the concept of interest in medicine to interest in the patient’s medicine fate to interest in clinical case medicine to interest in the synthesis and manufacture of medicine of biological origin. And other directions adopted by pharmacy schools around the world in which new effective chemical compounds are identified., They are called "views". It is discovered while using pre-existing medicines for therapeutic purposes for various diseases, and by witnessing the biological effect of a new or pre-existing natural substance extracted(37-40) from bacteria, fungi or plants., Figure (1).

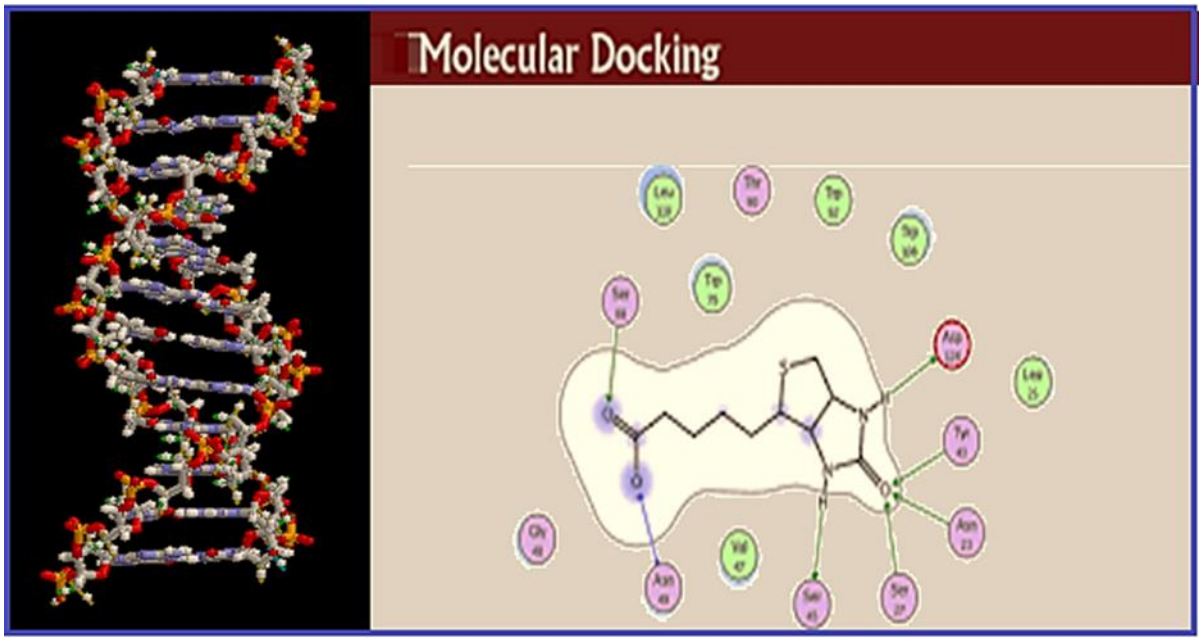

Fig 1: Computational Chemistry for The study and Design of Drugs

Conclusion

It is worth noting that such polymers used in the medical field must be animal compatible and not elicit an inflammatory response, must have appropriate mechanical and processing properties, and most importantly, the decomposition products must be harmful and must be easily reabsorbed or excreted, and for these reasons it is important to test each substance appropriately. Sufficient before use in the human body.

References

1. Gupta AK, Gupta M. "Synthesis and surface engineering of iron oxide nanoparticles for biomedical applications". Biomaterials,2005:26(18):3995-4021. doi:10.1016/j.biomaterials.2004.10.012. PMID 15626447.
2. Nagham Mahmood Aljamali, Khudheyer Abbas Aziz Alnomani, Maysaa A Alhar. Review on Computational Biology and Computational Chemistry Applications. International Journal of Cheminformatics Research,2021:7(2):1-10. http://chemical.journalspub.info/index.php? journal= JAWCM& page=article&op=view&path%5B%5D=1159
3. LaVan DA, McGuire T, Langer R. Small-scale systems for in vivodrug delivery, Nat Biotechnol,2013:21(10):1184-1191. doi:10.1038/nbt876. PMID 14520404.
4. Cavalcanti A, Shirinzadeh B, Freitas RA Jr, Hogg T. Nanorobot architecture formedical target identification, Nanotechnology,2008:19(1):015103(15). Doi:10.1088/0957- 4484/19/01/01510.
5. Nagham Mahmood Aljamali. "Synthesis and Biological Study of Hetero (Atoms and Cycles) Compounds", Der Pharma Chemica,2016:8(06):40-48.
6. Nagham Mahmood Aljamali. Synthesis and Chemical Identification of Macro Compounds of (Thiazol and Imidazol)".,Research J. Pharm. and Tech,2005:8(1):78-84., DOI: 10.5958/0974-360X.2015.00016.5.
7. Aviram A. Molecular Rectifier, Chemical Physics Letters,1974:29:277. Doi:10.1016/0009-2614(74)85031-1.
8. Nagham Mahmood Aljamali. Creation of Innovated Macrocyclic Sulfazan-Formazan Compounds and Linear Sulfazan-Formazan for the first Time Globally with their Assay as Antifungal. Biomedical Journal of Scientific & Technical Research,2021:40(3):32266-32272. DOI: 10.26717/BJSTR.2021.40.006453
9. Nagham Mahmood Aljamali. Review on (Azo, Formazane, Sulfazane)-Compounds, International Journal of Innovations in Scientific Engineering.,2019:10:19-45.
10. Nagham Mahmood Aljamali, Imd Kam. Development of Trimethoprim Drug and Innovation of Sulfazane-Trimethoprim Derivatives as Anticancer Agents, Biomedical & Pharmacology Journal,2020:13(2):613-625. http://dx.doi.org/10.13005/bpj/1925.
11. Imd Kam, Hsanen Kudhair Abdulabas, Nagham Mahmood Aljamali. Invention of (Gluta. Sulfazane-Cefixime) Compounds as Inhibitors of Cancerous Tumors., Journal of Cardiovascular Disease Research,2020:11(2):44-55. DOI: 10.31838/jcdr.2020.11.02.09 .
12. Nagham Mahmood Aljamali. “Inventing of Macrocyclic Formazan Compounds and Studying Them Against Breast Cancer for The first Time Globally” Annals of pharma research,2021:9(7):525-533., Available at:https://www.annalsofpharmaresearch.com/index.php?journal=apr&page=article&op=view&path%5B%5D=38
13. Aviram A. Molecules for memory, logic, and amplification, Journal of the American Chemical Society,1988:110(17):5687-5692, Doi:10.1021/ja00225a017.

14. Jensen K. Nanotube Radio, Nano Lett.,2007:7(11):3508-3511, Doi:10.1021/nl0721113.
15. Nagham Mahmood Aljamali, Ahmed Kareem Thamer, Aryaf Mahmood Sabea. Review on Electronic Instruments and Its Nano-Skill Solicitations, Journal of Electrical and Power System Engineering,2021:7(3):11-19, Available at: http://matjournals.in/index.php/JOEPSE/article/view/7246.
16. Amen Abdul, Nagham Mahmood Aljamali, Triazole-Anil, Triazol-Azo. Reagents (Creation, Spectral Categorization, Scanning Microscopy, Thermal Analysis)., NeuroQuantology,2021:19(11):84-94 ., DOI Number: 10.14704/nq.2021.19.11.NQ21178 .
17. Pliskin NH, Meyer GJ, Dolske MC, Heilbronner RL, Kelley KM, Lee RC. Neuropsychiatric aspects of electrical injury: a review of neuropsychological research, Annals of the New York Academy of Sciences,1994:720(1):219-223, DOI: https://doi.org/10.1111/j.1749-6632.1994.tb30450.x
18. Grigorovich A, Gomez M, Leach L, Fish J. Impact of posttraumatic stress disorder and depression on neuropsychological functioning in electrical injury survivors, Journal of Burn Care & Research,2013:34(6):659-665. DOI: https://doi.org/10.1097/BCR.0b013e31827e5062.
19. Nagham Mahmood Aljamali, Widad Hashim Yahya Almuhana. Review on Biomedical Engineering and Engineering Technology in Bio-Medical Devices, Journal of Advances in Electrical Devices,2021:6(2):18-24. Available at: https://www.researchgate.net/publication/352414547Review_ on_Biomedical_ Engineering_and_Engineering_Technology_in_Bio-_Medical_Devices.
20. Nagham Mahmood Aljamali, Jhan Razq Molim. Review on Engineering Designs for Laboratory Chemical Devices and Displays, Journal of Control and Instrumentation Engineering,2021:7(2):38-46, Available at: http://matjournals.in/index.php/JOCIE/article/view/7068.
21. Halliday D, Resnick R, Krane KS. Physics, 2, Wiley Custom Learning Solutions, 2015.
22. Griffiths DJ, Colleger R. Introduction to Electrodynamics Prentice Hall Upper Saddle River, New Jersey, 1999, 7458.
23. Hsanen Kdhair Abdulabas, Aseel Mahmood Jawad, Nagham Mahmood Aljamali. Synthesis of drugs derivatives as inhibitors of cancerous cells., Biochem. Cell. Arch, 2020, 20(2). DocID: https://connectjournals.com/03896.2020.20.5315.
24. Abdmajed, Nagham Mahmood Aljamali MN. Preparation of Benzothiazole-Formazane Reagents and Studying of (Spectral, Thermal, Scanning Microscopy, Biological Evaluation)., International Journal of Pharmaceutical Research,2021:13(1):4290-4300.
25. Aseel Mahmood Jawad, Nagham Mahmood Aljamali. "Innovation, Preparation of Cephalexin Drug Derivatives and Studying of (Toxicity & Resistance of Infection)"., International Journal of Psychosocial Rehabilitation,2020:24(4):3754-3767 .
26. Hssein Ahmd, Nagham Mahmood Aljamali., Preparation, Characterization, Antibacterial Study, Toxicity Study of New Phenylene diamine- Formazan Derivatives., Indian Journal of Forensic Medicine & Toxicology, 2021, 15(2).
27. Nagham Mahmood Aljamali, Husin Mebel Azez. Synthesis and Characterization of Some New Formazan - Cefixime and Study of Against Breast Cancer Cells., Annals of the Romanian Society for Cell Biology,2021:25(4):8562–8578. Retrieved from https://www.annalsofrscb.ro/index.php/journal/article/view/2400
28. Nagham Mahmood Aljamali, Asmaa Kefah Mahdi., Synthesis, Identification and Anticancer Studying of Heterocyclic- Mefenamic Drug via Thiosemicarbazide., Annals of the Romanian Society for Cell Biology, 8521–8537.,2021:25(4):8521-8537. Retrieved from https://www.annalsofrscb.ro/index.php/journal/article/view/2398
29. Jawad F, Nagham Mahmood Aljamali, Preparation, Investigation and Study of Biological Applications of Tyrosine Derivatives against Breast Cancer Cells., NeuroQuantology,2021:19(9):117-125. doi: 10.14704/nq.2021.19.9.NQ21144
30. Haus HA, Melcher JR. Electromagnetic fields and energy, Englewood Cliffs, NJ: Prentice-Hall, 1989, 107.
31. Nagham Mahmood Aljamali, HS H. Review on Engineering Applications of Designed Polymers to Protect Electrical Equipment, Journal of Power Electronics and Devices,2021:7(2):26-32, Available at: https://www.researchgate.net/profile/Nagham-Aljamali.
32. Pasa André Avelino. Chapter 13: Metal Nanolayer-Base Transistor, Handbook of Nanophysics: Nanoelectronics and Nanophotonics, 2010, 1-13, ISBN 9781420075519.
33. Nagham Mahmood Aljamali, Jad F. Preparation, Diagnosis and Evaluation of Cyclic-Tryptophan Derivatives as Anti Breast Cancer Agents. Biomed Pharmacol J.,2021:14(4):1983-1991., Available from: DOI : https://dx.doi.org/10.13005/bpj/2296
34. Ding Y, Hayes MJ, Widhalm M. Measuring economic impacts of drought: A review and discussion, Disaster Prevention and Management,2011:20(4):434-446, doi:10.1108/09653561111161752.
35. Dai A. Drought under global warming: A review, Wiley Interdisciplinary Reviews: Climate Change,2011:2:45-65, doi:10.1002/wcc.81.
36. Nagham Mahmood A. Origination of Macrocyclic Formazan with Macrocyclic Sulfazan and Triazan as Innovated Compounds and Compared Their efficiency Against Breast Cancer. Open Access Journal of Biomedical Science, 2022, 4(1). OAJBS.ID.000383. DOI: 10.38125/OAJBS.000383
37. Julie Brigham-Grette; et al. Petroleum Geologists' Award to Novelist Crichton Is Inappropriate, Eos,2006:87(36):364. Doi:10.1029/2006EO360008.

38. Gu BK, Ismail YA, Spinks GM, Kim SI, So I, Kim SJ. A linear actuation of the polymeric Nano fibrous bundle for artificial muscles, Chemistry of Materials,2009:21(3):511-515, Available at https://pubs.acs.org/doi/abs/10.1021/cm802377d.
39. Nagham Mahmood Aljamali. Designation of Macrocyclic Sulfazan and Triazan as Innovated Compounds with Their Estimation in Nano-Activities by the Scanning Microscope., International Journal of Convergence in Healthcare,2022:02:25-34. Available at: https://www.ijcih.com/index.php/ijcih/article/view/21
40. Carney R, Warner J, Iliffe S, Van Haselen R, Griffin M, Fisher P. Effect: a randomized, controlled trial, BMC medical research methodology,2007:7(2):4-9. Available at: https://bmcmedresmethodol. biomedcentral.com/articles/10.1186/1471-2288-7-42.
41. Nagham Mahmood Aljamali. Inventing of Macrocyclic Formazan Compounds with Their Evaluation in Nano- Behavior in the Scanning Microscope and Chromatography. Biomedical Journal of Scientific & Technical Research, 2022, 41(3). P: 32783-32792.; BJSTR. MS.ID.006616.; DOI: 10.26717/BJSTR.2022.41.006616
42. Pearson K. X. On the criterion that a given system of deviations from the probable in the case of a correlated system of variables is such that it can be reasonably supposed to have arisen from random sampling, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science,1900:50(302):157-175. DOI: https://doi.org/10.1080/14786440009463897.
43. Nagham Mahmood Aljamali. Synthesis Innovative Cyclic Formazan Compounds for the First Time and Evaluation of Their Biological Activity. International Journal of Polymer Science & Engineering,2021:7(2):5-14. DOI: https://doi.org/10.37628/ijpse.v7i2.830.; Available at: http://materials.journalspub.info/ index.php?journal=JPMSE&page=article&op=view&path%5B%5D=830
44. Jahinpoor Mohsen. ed. Ionic Polymer Metal Composites (IPMCs): Smart Multi-Functional Materials and Artificial Muscles, Royal Society of Chemistry, 2016, 2, Available at https://pubs.rsc.org/en/content/ebook/978-1-78262-728-3.
45. Hingh Simon. The codebook the science of secrecy from ancient Egypt to quantum cryptography (Anchor Books), New York, Anchor Books, 2002. ISBN 972-0-385-49532-5, Available at: http://www.accessdata.fda.gov/scripts/cdrh/cfdocs/cfres/res.cfm.,doi:10.1038/ 015492 a0.