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Extraction and Molecular Modeling of Phytohormones from Medicinal Plants

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ABSTRACT

In recent decades, phytohormones came up as suitable alternate for various severe diseases but as amount of phytohormone present and less availability of medicinal plants has made extraction as well as molecular modeling and chemical synthesis of the drug like molecule with the help of protein bioinformatics, modeling techniques and molecular dynamics simulation. Current review article focuses a brief insight on the process and possible step associated with it.

INTRODUCTION

Phytohormones are the plant growth substances, which actually controls compete growth and form of a plant. These regulators plays vital role in growth of leaves, stems, sex differentiation of flowers and senescence of leaves, or fruit. They are present in a plant with very low concentration. These are mostly concerned with higher plants, but their presence cannot be ignored in lower plants like algae, fungi and even microorganisms like bacteria. But in these cases, these do not play a significant role in direct physiological activities and hence termed as secondary metabolite [1-8].

Medicinal Aspect

Modern molecular and genetic analysis gives us an idea about understanding of techniques and possible application of these phytohormones. These phytohormones are biomolecules possessing same kind of effect to alter physiological activities at cellular level. These molecules resemble with many drug like molecules or in most of the cases almost same structure compatible to target sites [9,10].

Review of literature

Melatonin is known to be produced by plants and to exert numerous effects, which overlap with actions of known phytohormones, including auxins, ethylene, abscisic, jasmonic and salicylic acids. It exhibits growth effects, alleviates stress by heat, cold, drought, and toxic chemicals, counteracts infections by bacterial or fungal pathogens, favours wound healing, delays senescence and acts as an antioxidant and photoprotectant. Stressors and intense radiation frequently induce substantial increases in melatonin. High levels are particularly found in oily seeds. The criteria are discussed which have to be fulfilled before melatonin might be classified as a phytohormone. These include, in particular, the identification of high-affinity binding sites, of components of signal transduction pathways, the determination of freely movable melatonin and its movements within the organism [11-17].

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Abiotic stresses, primarily drought, salinity, heat, cold, flooding and ultra-violet rays are causing widespread crop losses worldwide. Because of the complexity of the stress-tolerance traits, conventional breeding techniques have met with little success in fulfilling the world food demands. Therefore, to face the abiotic stresses, novel and potent approaches should be devised and engineering of phytohormones could be a method of choice to increase the crop productivity [18-21].

Development of more advanced and functional biomaterials has been an ongoing challenge in the last decades towards the benefit of millions of patients worldwide that need to be treated with biomaterial-based therapies. The ability of individual polymers to respond to changes in pH, temperature, electric or magnetic fields, together with the possibility of combining different polymers, is a strategy largely pursued in the field [22-25].

This review examines contemporary views of the role of plant hormones in the control of physiological processes. Past and present difficulties with nomenclature encapsulate the problems inherent in using the 'classic' hormone concept in plants, with their distinctive multicellular organization. Chemical control may be a more relevant notion. However, control may also reside in the responding tissue via changes in sensitivity, or as combined control, where response is dictated by both sensitivity and concentration [26-29].

While animals and plants appear to have coinherited homologueous intracellular signalling systems, at the whole organism level modes of hormone action may diverge. It is postulated that the synthesis-transport-action mechanism of action may be just one of several possible ways that phytohormones could control physiological processes. Twelve separate roles are discussed, and it is suggested that some of these could operate simultaneously to the plant's advantage [30-36].

Molecular modeling

Molecular modeling is one of the basic and preliminary steps for target based drug designing or medicinal research. In this step we need to model a ligand molecule according to the target site compatibility. The designed chemical formula is first exposed to 2-D formulation and structure, after that we convert that two-dimensional structure to 3-D models. After determination of chemical molecules structure in 3-D, the process of rotation starts, where we check most stable conformation space where binding with molecule would be most thermodynamic stable in terms of free energy [37-41].

Another aspect would be computation al chemistry calculation where we check compatibility according to the quantum mechanics as well as classical mechanics. During which quantum mechanics can be based on the method like ab ignition, density functional theory or semi-Emperical method, while classical mechanics would be primarily based on molecular mechanic and molecular dynamics study or monte carlo methods [42-56].

After all, prediction of molecular property would be based on mainly structural, chemical, physical and biological. So, that we can easily understand, explain and predict about chemical process [47]. Next step we go for a force field calculation, which differs from molecule to molecule. Force fields are mathematical expression that describes the dependence of the energy of a molecule on the coordinates of the atoms in the molecule **(Table 1).**

MM2/MM3/MM4	Molecular Mechanic Force field for small organic molecules
CHARMM	Chemistry at Harvard Macromolecular Mechanics
AMBER	Assisted Model Building with Energy Refinement
OPLS	Optimized Parameters for Liquid Simulation
CFF	Consistent Force Field
CVFF	Valence Consistent Force Field
MMFF94	Merck Molecular Force Field 94
DREIDING	Generic rules based force field
UFF	Universal Force Field
ReaxFF	Speciality force-field to allow bond breaking

Table 1. Common Force Fields.

Force Fields differ in their parameters, terms and the method of development, according to that we may classify them as below:

1. Class I - simple functional form with data fitted to quantum mechanical calculations and/or experiment (AMBER, CHARMM)
2. Class II - more complicated functional form using cross terms and data fitted to quantum mechanical calculations and/or experiment (CFF, PCFF)
3. Class III - new generation force fields that incorporate polarizability (AMOEBA, AMBER ff02, CHARMM Drude)
4. Rules Based - covers most of the periodic table – UFF, DREIDING
5. Fundamental quantities are derived for each atom type: electronegativity, hardness, atomic radius
6. Forcefield parameters are derived at runtime using a series of theoretically or empirically derived rules Specialist - developed for a particular family of compounds fluorinated polymers, zeolites
7. Reaction Forcefields - ReaxFF

Energy minimization strategies and methods

Energy minimization strategies and methods can be implemented and understand at two different levels of local minima and global minima. Minimization methods mainly optimize the molecule and provide the closest local minimum possible **(Figure 1).** To find global minimum we may use systematic conformational searches, but it is very time consuming and nearly impossible to imply with smaller molecules. Another method may be molecular dynamics, Monte Carlo method, random sampling [57-77].

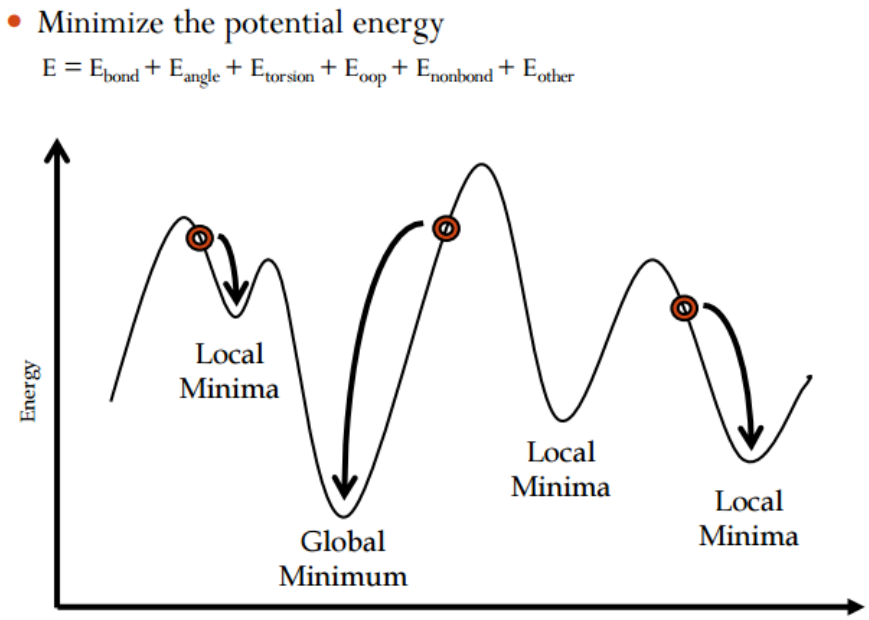

Figure 1. Energy minimization in terms of potential energy.

Molecular dynamic simulation

Molecular dynamics can also be better understood in terms of high temperature dynamics, which can be checked under simulated annealing and quench dynamics. Molecular Dynamics Variations can also be measured on basis of three basic classifications as

- Constant Volume - Constant Temperature (NVT)
- Constant Volume - Constant Energy (NVE)
- Constant Pressure – Constant Temperature (NPT)

Most simulations are on the order of picoseconds (10-12 s) or nanoseconds (10-9 s) while running on system. Overall during process we prepare the model, them minimization process is done, heating would also be implement and checked for equilibrium with NVE and simulation would be run for all NVT, NVE, and NPT.

After this process solvation test would be performed for both explicit as well as dielectric models. Next would be informatics searches and bioinformatics implementation to the study [78-95].

We would make a cross check with already available databases for phytohormones and on the basis of structure, properties and activities. After that we can go for Combinatorial Chemistry and start comparing structure with modeled molecules. Protein bioinformatics and QSAR- Quantitative Structure Activity Relationships will also play major role in designing with help of comparative studies of biological activity and structural similarity along with conformational stability and structural compatibility [96-100].

Conclusion

Molecular modeling and molecular dynamics simulation plays a driving role in designing and extraction from medicinal plants. We cannot rely much on the extraction, as number of plants is very less and moreover the amount of phytohormones getting extracted also is very low. Mostly we go for a molecular modeling for higher amount of these chemical molecules at production level.

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