PROSPECTIVE FLUORESCENT PLANT GROWTH REGULATORS AND THEIR RESPONSE IN PLANTS

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The development of environmentally friendly plant growth regulators (PGRs) has become a necessity for sustainable agriculture. Our research provides the synthesis, structural and physico-chemical characterization, as well as biological assessment of new fluorescent compounds based on non-toxic components or natural metabolites as alternatives to classical PGRs [1-3]. Crystallographic studies reveal the versatility of alkanolamine-substituted benzoic acid systems, which generate various supramolecular assemblies guided by different non-covalent interactions [4, 5].

Molecular properties

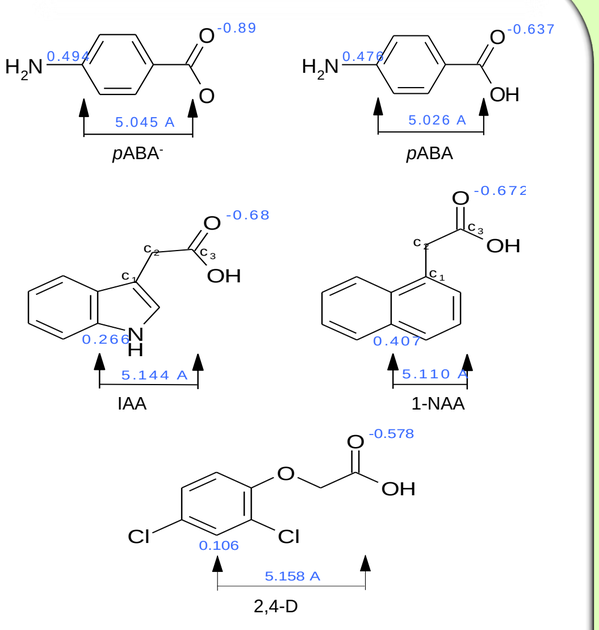

Figure 1. Optimal distance calculation for *p*ABA$^-$ (*p*-aminobenzoate anion), *p*ABA (*p*-aminobenzoic acid) and classical auxin molecules (IAA, 1-NAA, 2,4-D)

Molecular modeling and ligand binding

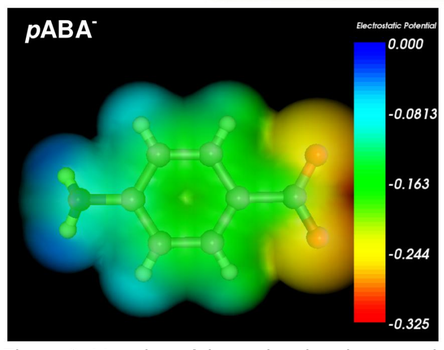

Figure 2. Mapping of the molecular electrostatic potential onto *p*ABA$^-$ accessible surface area.

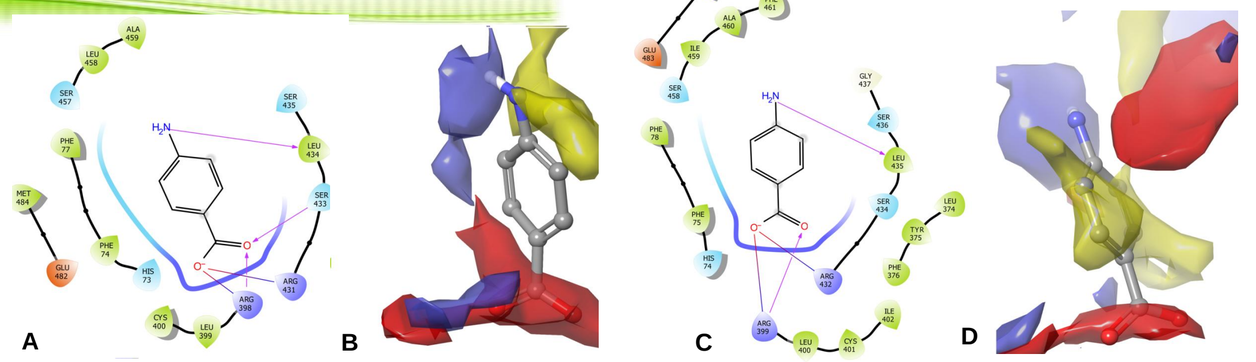

Figure 3. Binding model of HEA-*p*ABA (ethanolammonium *p*-aminobenzoate) in the auxin binding site of the TIR1 from *C. sativus* - CsTIR1 (A, B) and *S. lycopersicum* - SlTIR1 (C,D). The blue mesh is favorable for occupancy by functional groups that act as hydrogen-bond donors, the red mesh for hydrogen bond acceptor groups and the yellow areas can easily accommodate hydrophobic parts of a potential ligand.

Table 1. Interactions of IAA in AtTIR1, CsTIR1, and SlTIR1 binding sites

Interaction type	***AtTIR1***	***CsTIR1***	***SlTIR1***
Salt bridge (COO-)	Arg403; Arg 436	Arg431; Arg398	Arg399; Arg432
Hydrogen bond (COO-)	Arg406; Ser438	Arg398; Ser433	Arg399; Ser434
Hydrogen bond (NH)	Leu439	Leu434	Leu435
π- alkyl (pyrrole ring)	Cys405	Cys400	Cys401
π - alkyl (phenyl ring)	Ala464	Ala459	Ala460
π - cation (phenyl ring)	Arg489	-	-

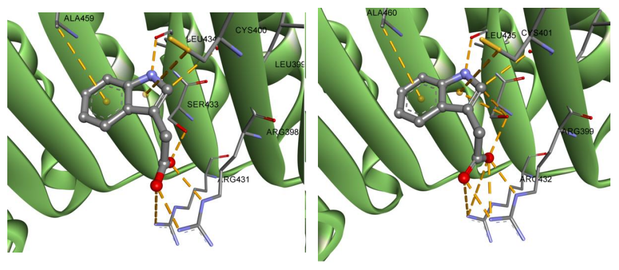

Figure 4. IAA (indole-3-acetic acid0 in the CsTIR1 (B) and SlTIR1 (C) binding site. All interactions are shows as orange dash lines.

Synthesis / Characterization / Fluorescence properties

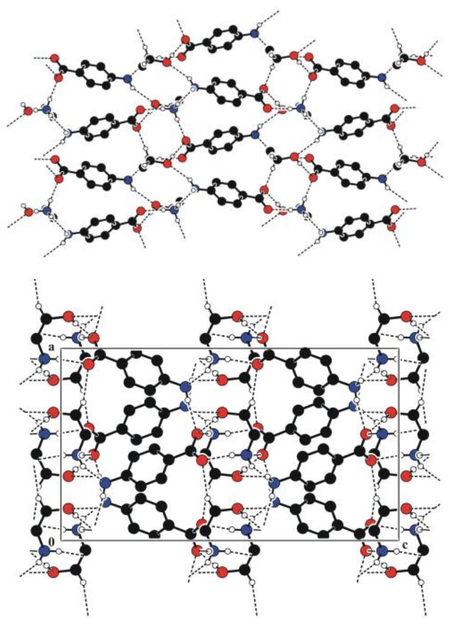

Figure 5. Crystal packing of HEA-*p*ABA

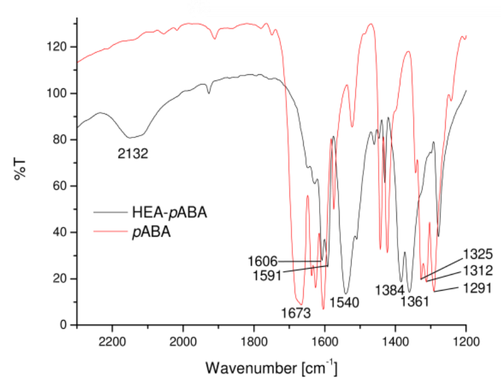

Figure 6. FT-IR spectra of HEA-*p*ABA and *p*ABA

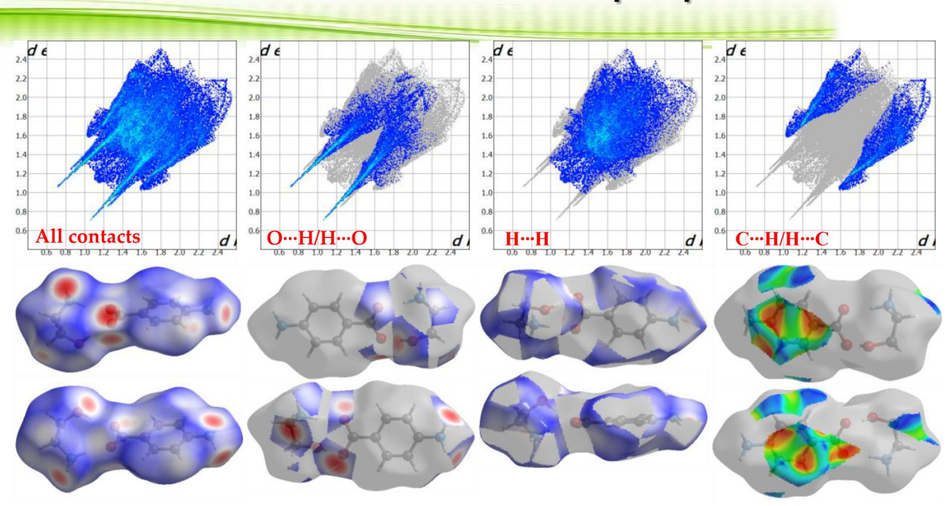

Figure 7. 2D fingerprint plots (left) and Hirshfeld surfaces (right) of the different interactions (for all contacts, O···H/H···O, H···H and C···H/H···C) in HEA-*p*ABA, in two orientations.

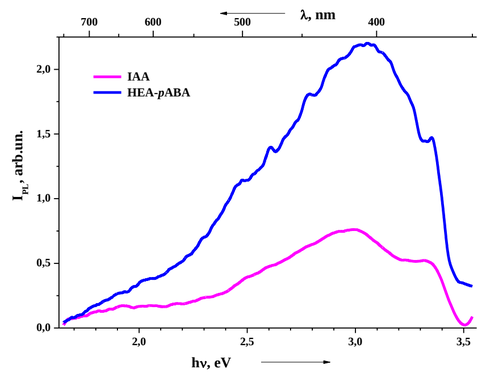

Figure 8. Emission spectra of HEA-*p*ABA and IAA

- HEA-*p*ABA exhibits hydrogen-bonded supramolecular network architecture *via* ionic N-H···O and normal O-H···O hydrogen bonds.
- HEA-*p*ABA has higher fluorescence intensity than classical IAA (3.04 eV band, emitting violet light)
- 2D fingerprint plots of Hirshfeld surface indicate different distribution of interactions in the crystal structures

Seed germination test

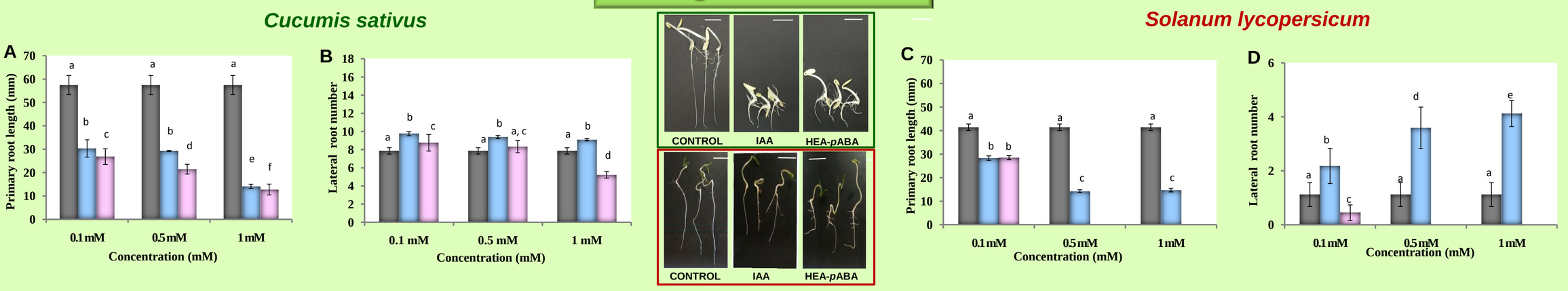

Figure 9. Effect of HEA-*p*ABA (blue), IAA (pink) different concentrations and control (grey) on primary root length and lateral root number of *C. sativus* (A, B) and *S. lycopersicum* (C, D)

Auxins act as signaling molecules to regulate almost every process of a plant's life, from germination to plant development. They regulate growth, particularly by inhibition of primary root elongation and promoting the initiation of lateral roots.

- HEA-*p*ABA inhibits primary root length in commercial vegetables such as cucumber (*C. sativus* L.) and tomato (*S. lycopersicum* L.).
- HEA-*p*ABA promotes lateral roots initiation in all tested plants.

Conclusion

Both experimental and theoretical results highlight HEA-*p*ABA as a fluorescent compound with auxin-like activity, more potent and effective when compared with natural auxin IAA in studied plants. Therefore, HEA-*p*ABA can be considered promising PGR with great potential to be efficiently used in sustainable vegetable crops.

References

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