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Comparison of Physiological, Biochemical, and Enzymatic Traits in PyMol Evaluation

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Abstract

A comparative synthesis of the structural data for all nine biomolecules, as summarized in Table 1, demonstrates a coherent coordination between three-dimensional architecture and biological function. The specific spatial arrangements in chlorophyll, carotenoids, metabolites (proline, carbohydrates, antioxidants), and antioxidant enzymes (APX, POD, CAT) collectively support essential processes such as light harvesting, energy transfer, osmotic balance, and peroxide neutralization. This integrated molecular framework provides a structural rationale for the physiological improvements observed under SNP treatment in our accompanying experimental data. The structural resilience and predicted functional efficiency of these key molecules form a coordinated defense network. SNP likely upregulates the biosynthesis or stabilizes the structures of these components, thereby enhancing photosynthesis, ROS scavenging, and osmotic adjustment in a synergistic manner (according to advisory consultations, 2025).

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1 A comparative synthesis of the structural data for all nine biomolecules, as summarized in Table 1, demonstrates a coherent coordination between three-dimensional architecture and biological function. The specific spatial arrangements in chlorophyll, carotenoids, metabolites (proline, carbohydrates, antioxidants), and antioxidant enzymes (APX, POD, CAT) collectively support essential processes such as light harvesting, energy transfer, osmotic balance, and peroxide neutralization. This integrated molecular framework provides a structural rationale for the physiological improvements observed under SNP treatment in our accompanying experimental data. The structural resilience and predicted functional efficiency of these key molecules form a coordinated defense network. SNP likely upregulates the biosynthesis or stabilizes the structures of these components, thereby enhancing photosynthesis, ROS scavenging, and osmotic adjustment in a synergistic manner (according to advisory consultations, 2025).

2 Table 1. Comparison between physiological, biochemical and enzymatic traits (chlorophyll, carotenoids, carbohydrates, proline, protein, antioxidants, ascorbate peroxidase, peroxidase and catalase) in the evaluation of Pymol

3 Chlorophyll - Physiological Trait: Structural Features (PyMOL): 1. Porphyrin ring, 2. Central magnesium, 3. Symmetric ring arrangement. Molecular and Biochemical Function: 1. Stabilizes photosynthetic performance and light absorption. Relation to Seedling Response: 1. Changes in chlorophyll content under SNP treatment align with spatial structure.

4 Carotenoid - Biochemical Trait: Structural Features (PyMOL): 1. Long hydrocarbon chains, 2. Conjugated double bonds. Molecular and Biochemical Function: 1. Light absorption and energy transfer, 2. Enhanced molecular stability. Relation to Seedling Response: 1. Strengthens antioxidant defense in seedlings.

5 Carbohydrate - Biochemical Trait: Structural Features (PyMOL): 1. Long chains, 2. Geometric arrangement, 3. Arrangement of functional groups. Molecular and Biochemical Function: 1. Energy transfer, 2. Biochemical interactions. Relation to Seedling Response: 1. Supports energy supply and cellular balance under cold stress.

6 Proline - Biochemical Trait: Structural Features (PyMOL): 1. Specific side chains, 2. Spatial arrangement of functional groups. Molecular and Biochemical Function: 1. Mitigates oxidative stress, 2. Absorbs energy. Relation to Seedling Response: 1. Key role in seedling response to cold stress.

7 Protein - Biochemical Trait: Structural Features (PyMOL): 1. Multiple hydrogen bonds, 2. α-helix arrangement. Molecular and Biochemical Function: 1. Molecular stabilization, 2. Biochemical function. Relation to Seedling Response: 1. Functional changes under SNP treatment are consistent with spatial structure.

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No.	Trait	Trait Type	Structural Features (PyMOL)	Molecular and Biochemical Function	Relation to Seedling Response
6	Antioxidant	Biochemical	1. Long hydrocarbon chains 2. Conjugated bonds	1. Reduces free radicals 2. Enhances defense activity	1. Protects membranes and photosynthetic system under cold stress
7	Ascorbate Peroxidase (APX)	Enzymatic	1. α-helices 2. β-sheets 3. hydrogen bonds	1. Neutralizes peroxides 2. Protects cells	1. Enhances antioxidant defense efficiency under cold stress
8	Peroxidase (POD)	Enzymatic	1.Organized α-helices and β-sheets 2, hydrogen-bond network	1. Neutralizes free radicals 2. Protects cells	1. Strengthens enzyme activity in reducing oxidative damage
9	Catalase (CAT)	Enzymatic	1. α-helices and β-sheets 2. Optimized active site	1. Decomposes hydrogen 2. Peroxide, protects cells	1. Reduces free radical damage and maintains metabolic integrity

Fig. 1 Plate layout for compounds stock solutions in acetonitrile.