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Polyathia longifolia: Redox potential of a cellulose nanocrystal derivative and ADMET predictions of selected compounds

Chiagoziem AnariochiOtuechere[a] AdewaleAdewuyi[b] TiOluwani BamideleSalau[a] Netra PrasadNeupane[c] Olusegun LateefAdebayo[a] MotunrayoEgunjobi[a] AmitaVerma[c]

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Highlights

- Cellulose nanocrystal from *Polyathia longifolia* (PCN) was synthesized by green method.
- In vivo assays revealed no effects on albumin, cortical and cerebellar catalase, and glutathione S-transferase levels.
- PCN significantly elevated aspartate aminotransferase and cortical and cerebellar reduced glutathione.
- Histology did not show any adverse effects on neurons, hippocampus, and Purkinje layers.
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5-hydroxy-2 (5H)-furanone, a bioactive ingredient of *P. longifolia* showed good promise of frug-likeness.

Abstract

Cellulosic biomass, endowed with several hydroxyl groups, has been the source of nanomaterials and functionalized derivatives for biomedical applications. However, the effect of green-synthesized cellulose nanocrystals from *Polyathia longifolia* (PCN) on redox parameters in the rat cortex and cerebellum has not been evaluated. In the present study, eighteen male albino rats were randomly grouped as control, PCN-50 and PCN-100, and administered distilled water, 50, and 100 mg/kg body weight PCN once a day *(per os)* for 14 consecutive days. Growth performance, biochemical, histological analyses were performed to monitor treatment-related parameters. PCN, at both doses, did not significantly ($p > 0.05$) alter the body weights, absolute organ weights, albumin, cortical and cerebellar catalase, and glutathione S-transferase levels. However, PCN significantly elevated aspartate aminotransferase, cortical and cerebellar glutathione, and lipid peroxidation levels. Interestingly, histological observations revealed normal-appearing neurons, hippocampus, and Purkinje layers. Furthermore, *in silico* absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties of nine ligands from *Polyalthia longifolia* established oral drug-like behavior. They showed 5-hydroxy-2 (5H)-furanone as the safest compound among all selected ligands. Our data provide insight into the redox potential of green synthesized cellulose nanocrystals in rat sub-brain