6th Commonwealth Chemistry Posters
Building Networks to Address the Goals
1-2 October 2025

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GOAL 3: GOOD HEALTH AND WELL-BEING | ENSURE HEALTHY LIVES AND PROMOTE WELL-BEING FOR ALL AT ALL AGES

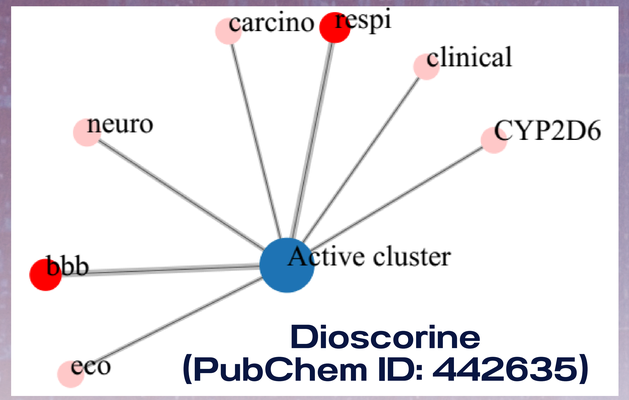
Toxic or Not? ProTox-3.0 Prediction of Dioscorine & Diosgenin in *Dioscorea hispida*

LD_{50}
1,890 mg/kg BW (Class 4)

Prediction accurarcy
68.07%

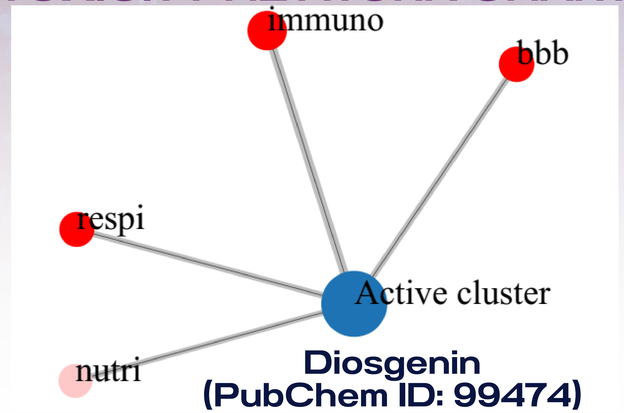
65.51%
Average similarity

221.30 g/mol
Molecular weight



Dioscorine (PubChem ID: 442635)

TOXICITY NETWORK CHART



Diosgenin (PubChem ID: 99474)

Results

Average similarity
100%

Molecular weight
414.62 g/mol

8,000 mg/kg BW (Class 6)
LD_{50}

100%
Prediction accurarcy

Results & Discussion

Acute toxicity: Dioscorine = moderate (Class 4); Diosgenin = very low (Class 6).

Risk profile: Diosgenin → respiratory + immunotoxicity; long-term safety important.

Shared risk: Both show respiratory toxicity.

CNS risk: Both may cross BBB → possible neurological effects.

Prediction confidence: Diosgenin = high; Dioscorine = lower, needs validation.

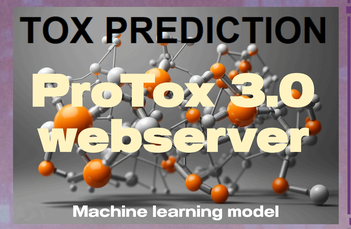
Toxicity targets: None predicted → effects likely indirect/ systemic.

Research gap: Experimental confirmation needed, especially for dioscorine.

Conclusion

Dioscorine has moderate toxicity; **diosgenin** is safer but with respiratory and immune risks. Findings stress dosage control, toxicity awareness, and computational screening for safe, evidence-based use of *D. hispida*, supporting SDG 3.

Prediction tool used (Input: SMILES)



Introduction

Traditional uses
Skin disorders
Inflammation
Digestive problem
High blood glucose
Analgesic
Diuretic
Detoxifying

Reference: https://tox.charite.de/protox3/index.php?site=home

Acknowledgement: We would like to thank the Director General of Health Malaysia for granting permission to present this poster.