Supplementary materials

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Supplement G. ProTox toxicity prediction outcome of selected alkaloids.

Compound	Predicted LD50	Class	Toxicity Targets (Probability)
Cryptolepine	1190 mg/kg	Class 4	Hepatotoxicity (0.69), Neurotoxicity (0.87), Respiratory toxicity (0.98), Immunotoxicity (0.96), Ecotoxicity (0.73), Aromatase (1.00), Estrogen Receptor Alpha (0.99), ER-LBD (1.00)
Vindolinine	325 mg/kg	Class 4	Neurotoxicity (0.65), Respiratory toxicity (0.94), Carcinogenicity (0.50), BBB (0.92), Ecotoxicity (0.64), Clinical toxicity (0.61), AChE (0.61), CYP2D6 (0.72)
Harman	1000 mg/kg	Class 4	Neurotoxicity (0.57), Mutagenicity (0.85), BBB (0.93), Ecotoxicity (0.75), AhR (0.92), p53 (0.56), CYP1A2 (1.0), CYP2C9 (0.59), CYP2D6 (0.89), CYP3A4 (0.98)
Palmatine	200 mg/kg	Class 3	Neurotoxicity (0.55), Respiratory toxicity (0.81), Carcinogenicity (0.50), Immunotoxicity (0.96), Mutagenicity (0.57), Cytotoxicity (0.56), BBB (0.78), Ecotoxicity (0.62), AhR (0.52), MMP (0.84), CYP2C19 (0.51), CYP2C9 (0.54), CYP2D6 (0.79)
Jatrorrhizine	200 mg/kg	Class 3	Neurotoxicity (0.51), Respiratory toxicity (0.84), Immunotoxicity (0.98), Mutagenicity (0.52), BBB (0.68), AhR (0.50), MMP (0.73), CYP2D6 (0.76)
Magnoflorine	401 mg/kg	Class 4	Respiratory toxicity (0.92), Immunotoxicity (0.94), BBB (0.84), CYP2D6 (0.64)
Groenlandicine	200 mg/kg	Class 3	Neurotoxicity (0.52), Nephrotoxicity (0.57), Respiratory toxicity (0.81), Carcinogenicity (0.54), Immunotoxicity (0.99), Mutagenicity (0.58), BBB (0.75), AhR (0.73), MMP (0.66), AChE (0.74), CYP2C19 (0.52), CYP2D6 (0.86), CYP3A4 (0.51)
Galegine	112 mg/kg	Class 3	Respiratory toxicity (0.56), BBB (0.77), Ecotoxicity (0.58)
Radicamine B	1751 mg/kg	Class 4	Respiratory toxicity (0.71), Nephrotoxicity (0.56)
Vindoline	150 mg/kg	Class 3	Neurotoxicity (0.51), Nephrotoxicity (0.58), Respiratory toxicity (0.93), Carcinogenicity (0.53), Immunotoxicity (0.99), BBB (0.52), Clinical toxicity (0.74), AChE (0.52)
Norharmane	260 mg/kg	Class 3	Neurotoxicity (0.64), Mutagenicity (0.53), BBB (0.92), Ecotoxicity (0.75), AhR (1.0), p53 (0.66), CYP1A2 (0.99), CYP2C9 (0.60), CYP2D6 (0.75), CYP3A4 (0.84)
Berberine	200 mg/kg	Class 3	Neurotoxicity (0.55), Respiratory toxicity (0.76), Carcinogenicity (0.56), Immunotoxicity (0.99), Mutagenicity (0.62), Cytotoxicity (0.96), BBB (0.85), Ecotoxicity (0.55), AhR (0.87), MMP (0.87), CYP1A2 (0.69), CYP2C19 (0.76), CYP2D6 (0.93), CYP3A4 (0.70)
Catharanthine	2100 mg/kg	Class 5	Neurotoxicity (0.65), Respiratory toxicity (0.94), BBB (0.86), Ecotoxicity (0.65), Clinical toxicity (0.60), GABA receptor (0.53), AChE (0.67), CYP2D6 (0.80), CYP3A4 (0.53)
Casuarine	3500 mg/kg	Class 5	Nephrotoxicity (0.55), Respiratory toxicity (0.68), BBB (0.52), Clinical toxicity (0.53)
Tembetarine	700 mg/kg	Class 4	Respiratory toxicity (0.93), Immunotoxicity (0.99), BBB (0.84), CYP2D6 (0.65)
Mahanimbine	4000 mg/kg	Class 5	Respiratory toxicity (0.64), Immunotoxicity (0.97), BBB (0.93), Ecotoxicity (0.72), GABA receptor (0.50), PXR (0.52), CYP2C9 (0.62)
Echinulin	400 mg/kg	Class 4	Neurotoxicity (0.61), Respiratory toxicity (0.81), Immunotoxicity (0.86), BBB (0.73), Clinical toxicity (0.71), Nutritional toxicity (0.66), PXR (0.61), CYP2C9 (0.54)
Radicamine A	400 mg/kg	Class 4	Nephrotoxicity (0.61), Respiratory toxicity (0.74), Clinical toxicity (0.51)
Tecostanine	200 mg/kg	Class 3	Neurotoxicity (0.55), Respiratory toxicity (0.74), BBB (0.92)
Vasicine	290 mg/kg	Class 3	Neurotoxicity (0.69), Respiratory toxicity (0.93), BBB (0.85), Clinical toxicity (0.63), GABA receptor (0.54), AChE (0.59), CYP2D6 (0.84)
Vasicinol	100 mg/kg	Class 3	Neurotoxicity (0.69), Respiratory toxicity (0.93), BBB (0.78), Clinical toxicity (0.66), GABA receptor (0.51), AChE (0.55), CYP2D6 (0.78)
Epiberberine	200 mg/kg	Class 3	Neurotoxicity (0.55), Respiratory toxicity (0.76), Carcinogenicity (0.56), Immunotoxicity (0.98), Mutagenicity (0.62), Cytotoxicity (0.96), BBB (0.85), Ecotoxicity (0.55), AhR (0.87), MMP (0.87), CYP1A2 (0.69), CYP2C19 (0.76), CYP2D6 (0.93), CYP3A4 (0.70)
Coptisine	200 mg/kg	Class 3	Neurotoxicity (0.54), Nephrotoxicity (0.52), Respiratory toxicity (0.73), Carcinogenicity (0.55), Immunotoxicity (0.87), Mutagenicity (0.55), Cytotoxicity (0.55), BBB (0.81), Ecotoxicity (0.54), AhR (0.66), CYP1A2 (0.70), CYP2C19 (0.65), CYP2D6 (0.86), CYP3A4 (0.67)
Conophylline	280 mg/kg	Class 3	Nephrotoxicity (0.59), Respiratory toxicity (0.93), Carcinogenicity (0.61), Immunotoxicity (0.98), Cytotoxicity (0.65), Clinical toxicity (0.81), Nutritional toxicity (0.69), AChE (0.57), PXR (0.53)
Physostigmine	2 mg/kg	Class 1	Neurotoxicity (0.74), Respiratory toxicity (0.92), BBB (0.99), Ecotoxicity (0.68), Clinical toxicity (0.55), Nutritional toxicity (0.86), AChE (0.86), CYP2D6 (0.78)
Sanguinarine	700 mg/kg	Class 4	Neurotoxicity (0.55), Respiratory toxicity (0.63), Carcinogenicity (0.54), Immunotoxicity (0.98), Mutagenicity (0.66), BBB (0.84), Ecotoxicity (0.54), AhR (1.0), ER-LBD (1.0), nrf2/ARE (1.0), HSE (1.0), CYP1A2 (0.94), CYP2C19 (0.98), CYP2D6 (0.77), CYP3A4 (0.91)
Capsaicin	47 mg/kg	Class 2	Nephrotoxicity (0.55), Respiratory toxicity (0.79), Carcinogenicity (0.71), Immunotoxicity (0.86), Mutagenicity (0.51), BBB (0.68), Clinical toxicity (0.63), Aromatase (1.0), CYP1A2 (0.93), CYP2C19 (0.94), CYP2C9 (0.76), CYP2D6 (0.70), CYP3A4 (0.99)

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Compound	Predicted LD50	Class	Toxicity Targets (Probability)
Pinoline	787 mg/kg	Class 4	Neurotoxicity (0.74), Respiratory toxicity (0.84), Immunotoxicity (0.88), BBB (0.86), Clinical toxicity (0.54), AChE (0.58), CYP1A2 (0.92)
Lupinine	227 mg/kg	Class 4	Neurotoxicity (0.62), Respiratory toxicity (0.80), BBB (0.92), Ecotoxicity (0.50), Clinical toxicity (0.50), NMDAR (0.54), AChE (0.51), CYP2D6 (0.72)
Matrine	243mg/kg	Class 3	Neurotoxicity (0.64), Respiratory toxicity (0.69), BBB (0.98), Ecotoxicity (0.56), Clinical toxicity (0.66), NMDAR (0.71), AChE (0.61), CYP2D6 (0.57)