

Table S1: The ProTox-II normal cell toxicity prediction of Dactyloquinone B

Classification	Target	Prediction	Probability
Organ toxicity	Hepatotoxicity	Inactive	0.78
Toxicity endpoints	Carcinogenicity	Active	0.51
Toxicity endpoints	Immunotoxicity	Active	0.97
Toxicity endpoints	Mutagenicity	Inactive	0.83
Toxicity endpoints	Cytotoxicity	Inactive	0.66
Tox21-Nuclear receptor signaling pathways	Aryl hydrocarbon Receptor (AhR)	Inactive	0.97
Tox21-Nuclear receptor signaling pathways	Androgen Receptor (AR)	Inactive	0.58
Tox21-Nuclear receptor signaling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	Inactive	0.88
Tox21-Nuclear receptor signaling pathways	Aromatase	Active	0.56
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Alpha (ER)	Inactive	0.74
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	Inactive	0.82
Tox21-Nuclear receptor signaling pathways	Peroxisome Proliferator-Activated Receptor Gamma (PPAR-Gamma)	Inactive	0.99
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/ antioxidant responsive element (nrf2/ARE)	Inactive	0.92
Tox21-Stress response pathways	Heat shock factor response element (HSE)	Inactive	0.92
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	Inactive	0.67
Tox21-Stress response pathways	Phosphoprotein (Tumor Suppressor) p53	Inactive	0.87
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	Inactive	0.91

Table S2: The ProTox-II normal cell toxicity prediction of Dactyloquinone C

Classification	Target	Prediction	Probability
Organ toxicity	Hepatotoxicity	Inactive	0.78
Toxicity endpoints	Carcinogenicity	Active	0.51
Toxicity endpoints	Immunotoxicity	Active	0.98
Toxicity endpoints	Mutagenicity	Inactive	0.83
Toxicity endpoints	Cytotoxicity	Inactive	0.66
Tox21-Nuclear receptor signaling pathways	Aryl hydrocarbon Receptor (AhR)	Inactive	0.97
Tox21-Nuclear receptor signaling pathways	Androgen Receptor (AR)	Inactive	0.58
Tox21-Nuclear receptor signaling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	Inactive	0.88
Tox21-Nuclear receptor signaling pathways	Aromatase	Active	0.56
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Alpha (ER)	Inactive	0.74
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	Inactive	0.82
Tox21-Nuclear receptor signaling pathways	Peroxisome Proliferator-Activated Receptor Gamma (PPAR-Gamma)	Inactive	0.99
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	Inactive	0.92
Tox21-Stress response pathways	Heat shock factor response element (HSE)	Inactive	0.92
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	Inactive	0.67
Tox21-Stress response pathways	Phosphoprotein (Tumor Suppressor) p53	Inactive	0.87
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	Inactive	0.91

Table S3: The ProTox-II normal cell toxicity prediction of Dactyloquinone C

Classification	Target	Prediction	Probability
Organ toxicity	Hepatotoxicity	Inactive	0.74
Toxicity endpoints	Carcinogenicity	Active	0.53
Toxicity endpoints	Immunotoxicity	Active	0.99
Toxicity endpoints	Mutagenicity	Inactive	0.81
Toxicity endpoints	Cytotoxicity	Inactive	0.73
Tox21-Nuclear receptor signaling pathways	Aryl hydrocarbon Receptor (AhR)	Inactive	0.97
Tox21-Nuclear receptor signaling pathways	Androgen Receptor (AR)	Inactive	0.50
Tox21-Nuclear receptor signaling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	Inactive	0.81
Tox21-Nuclear receptor signaling pathways	Aromatase	Inactive	0.60
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Alpha (ER)	Inactive	0.79
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	Inactive	0.87
Tox21-Nuclear receptor signaling pathways	Peroxisome Proliferator-Activated Receptor Gamma (PPAR-Gamma)	Inactive	0.98
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	Inactive	0.91
Tox21-Stress response pathways	Heat shock factor response element (HSE)	Inactive	0.91
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	Inactive	0.74
Tox21-Stress response pathways	Phosphoprotein (Tumor Suppressor) p53	Inactive	0.87
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	Inactive	0.90

Table S4: The ProTox-II normal cell toxicity prediction of Dysidavarone D

Classification	Target	Prediction	Probability
Organ toxicity	Hepatotoxicity	Inactive	0.82
Toxicity endpoints	Carcinogenicity	Active	0.55
Toxicity endpoints	Immunotoxicity	Active	0.98
Toxicity endpoints	Mutagenicity	Inactive	0.81
Toxicity endpoints	Cytotoxicity	Active	0.70
Tox21-Nuclear receptor signaling pathways	Aryl hydrocarbon Receptor (AhR)	Inactive	0.89
Tox21-Nuclear receptor signaling pathways	Androgen Receptor (AR)	Inactive	0.67
Tox21-Nuclear receptor signaling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	Inactive	0.73
Tox21-Nuclear receptor signaling pathways	Aromatase	Inactive	0.76
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Alpha (ER)	Inactive	0.54
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	Inactive	0.92
Tox21-Nuclear receptor signaling pathways	Peroxisome Proliferator-Activated Receptor Gamma (PPAR-Gamma)	Inactive	0.99
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/ antioxidant responsive element (nrf2/ARE)	Inactive	0.81
Tox21-Stress response pathways	Heat shock factor response element (HSE)	Inactive	0.81
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	Inactive	0.78
Tox21-Stress response pathways	Phosphoprotein (Tumor Suppressor) p53	Inactive	0.94
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	Inactive	0.97

Table S5: The ProTox-II normal cell toxicity prediction of Smenohaimien F

Classification	Target	Prediction	Probability
Organ toxicity	Hepatotoxicity	Inactive	0.82
Toxicity endpoints	Carcinogenicity	Active	0.53
Toxicity endpoints	Immunotoxicity	Active	0.89
Toxicity endpoints	Mutagenicity	Inactive	0.73
Toxicity endpoints	Cytotoxicity	Inactive	0.68
Tox21-Nuclear receptor signaling pathways	Aryl hydrocarbon Receptor (AhR)	Inactive	0.97
Tox21-Nuclear receptor signaling pathways	Androgen Receptor (AR)	Inactive	0.76
Tox21-Nuclear receptor signaling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	Inactive	0.85
Tox21-Nuclear receptor signaling pathways	Aromatase	Inactive	0.67
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Alpha (ER)	Inactive	0.67
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	Inactive	0.74
Tox21-Nuclear receptor signaling pathways	Peroxisome Proliferator-Activated Receptor Gamma (PPAR-Gamma)	Inactive	0.97
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	Inactive	0.90
Tox21-Stress response pathways	Heat shock factor response element (HSE)	Inactive	0.90
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	Inactive	0.69
Tox21-Stress response pathways	Phosphoprotein (Tumor Suppressor) p53	Inactive	0.82
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	Inactive	0.93

Table S6: The ProTox-II normal cell toxicity prediction of Sollasin E

Classification	Target	Prediction	Probability
Organ toxicity	Hepatotoxicity	Inactive	0.75
Toxicity endpoints	Carcinogenicity	Inactive	0.61
Toxicity endpoints	Immunotoxicity	Inactive	0.78
Toxicity endpoints	Mutagenicity	Inactive	0.76
Toxicity endpoints	Cytotoxicity	Inactive	0.78
Tox21-Nuclear receptor signaling pathways	Aryl hydrocarbon Receptor (AhR)	Inactive	0.97
Tox21-Nuclear receptor signaling pathways	Androgen Receptor (AR)	Inactive	0.89
Tox21-Nuclear receptor signaling pathways	Androgen Receptor Ligand Binding Domain (AR-LBD)	Inactive	0.95
Tox21-Nuclear receptor signaling pathways	Aromatase	Inactive	0.70
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Alpha (ER)	Inactive	0.66
Tox21-Nuclear receptor signaling pathways	Estrogen Receptor Ligand Binding Domain (ER-LBD)	Inactive	0.78
Tox21-Nuclear receptor signaling pathways	Peroxisome Proliferator-Activated Receptor Gamma (PPAR-Gamma)	Inactive	0.97
Tox21-Stress response pathways	Nuclear factor (erythroid-derived 2)-like 2/antioxidant responsive element (nrf2/ARE)	Inactive	0.84
Tox21-Stress response pathways	Heat shock factor response element (HSE)	Inactive	0.84
Tox21-Stress response pathways	Mitochondrial Membrane Potential (MMP)	Inactive	0.80
Tox21-Stress response pathways	Phosphoprotein (Tumor Suppressor) p53	Inactive	0.91
Tox21-Stress response pathways	ATPase family AAA domain-containing protein 5 (ATAD5)	Inactive	0.98