Supplementary Materials: Prediction of Drug-Drug Interactions with Bupropion and Its Metabolites as CYP2D6 Inhibitors Using a Physiologically-Based Pharmacokinetic Model

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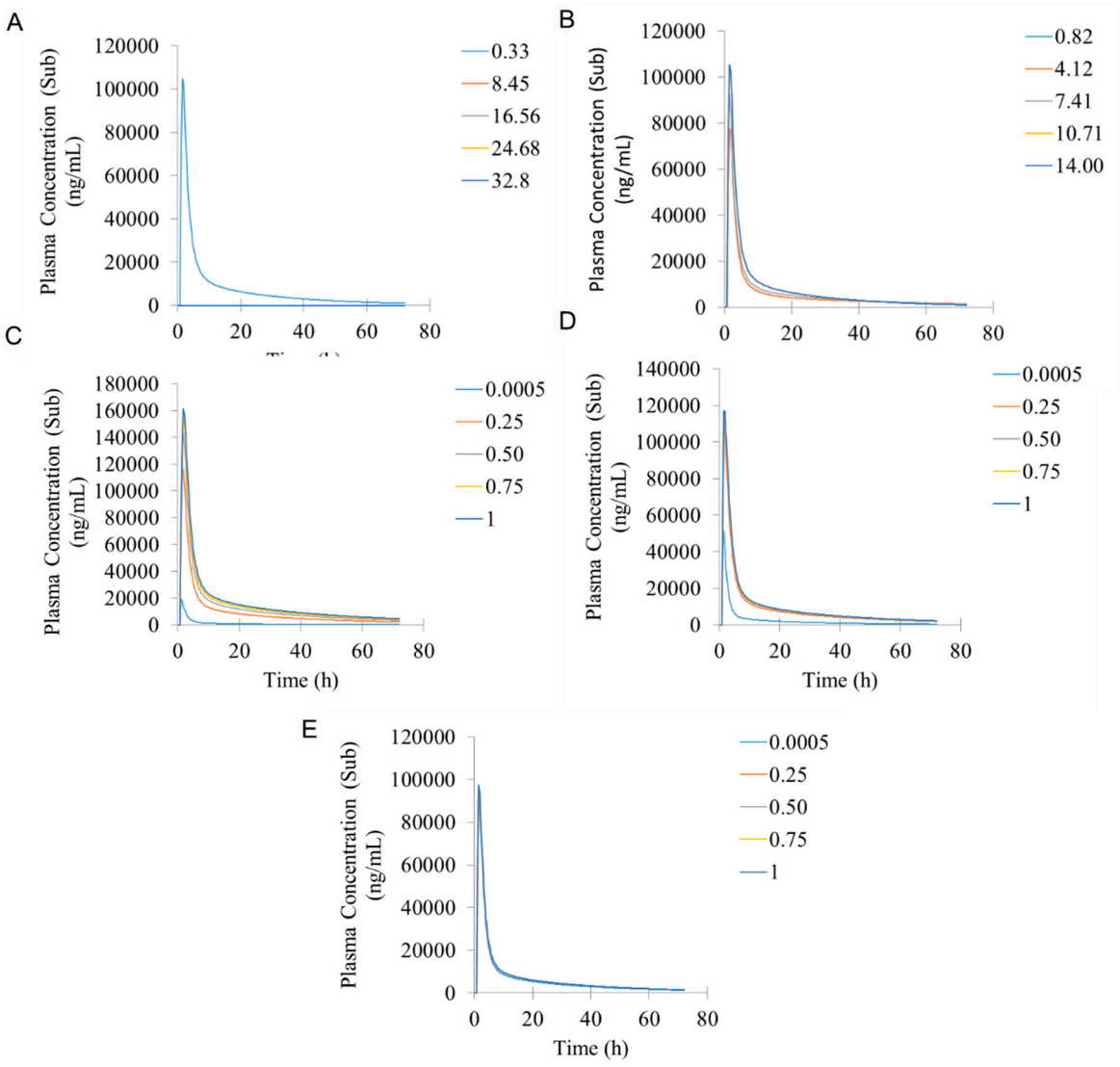

Figure S1. Sensitivity analysis results expressed as plasma concentration-time profiles from Simcyp PBPK model simulations: (**A**) logP; (**B**) pKa; (**C**) $f_{u,mic}$ for formation of hydroxybupropion, (**D**) $f_{u,mic}$ for formation of threohydrobupropion, (**E**) $f_{u,mic}$ for formation of erythrohydrobupropion. The parameter ranges assessed were logP, 0.33–32.8, pKa, 0.82–14.00, $f_{u,mic}$, 0.0005–1.