Supporting Information

Inhibition of thyroid hormone sulfotransferase activity by brominated flame retardants and halogenated phenolics

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Figures

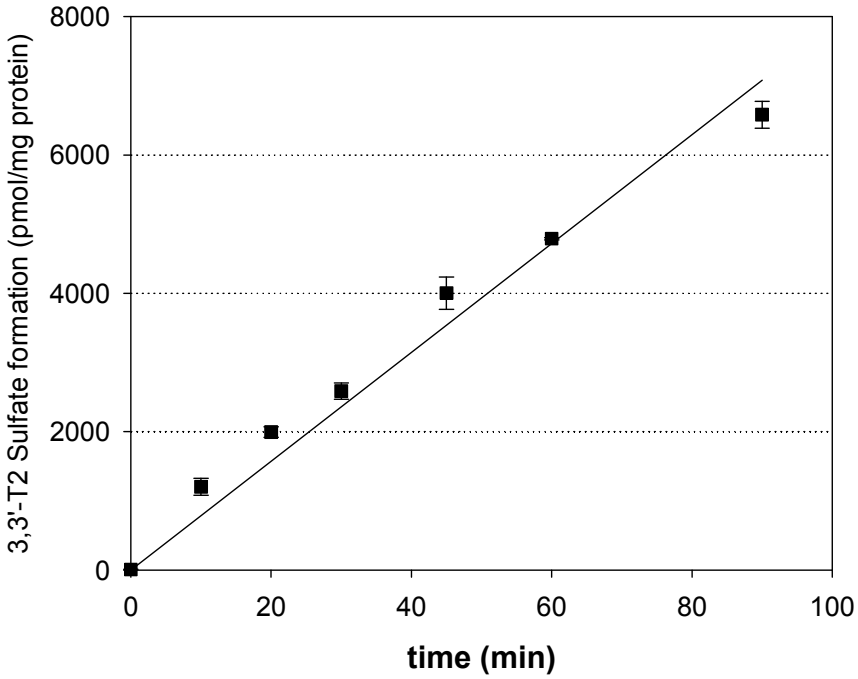
Figure S1. Formation rate (pmol/mg protein) of 3,3'-T2 sulfate resulting from the incubation of 1 μM 3,3'-T2 in 0.25 mg protein/ml of pooled human liver cytosol as a function of time. Line of best fit obtained by linear regression analysis. Each data point represents the mean (n=3) and error bars represent 1 standard error.

Figure S2. Formation rate (pmol/min) of 3,3'-T2 sulfate resulting from the incubation of 1 μM 3,3'-T2 in pooled human liver cytosol for 30 min as a function of protein concentration. Line of best fit obtained by linear regression analysis. Each data point represents the mean (n=3) and error bars represent 1 standard error.

Figure S3. IC_{50} concentration (nM) versus A) number of bromines, B) OH-group substitution, C) number of bromines adjacent to OH-group and D) pKa for OH-BDEs for incubation of 1 μM 3,3'-T2 in pooled human liver cytosol.

Figure S4. Interaction energy (kJ/mol) versus A) number of bromines ($r^2 = 0.40$, $p<0.05$), B) OH-group substitution, C) number of bromines adjacent to OH-group and D) pKa ($r^2 = 0.45$, $p<0.01$) for SULT1A1 binding of OH-BDEs as determined by docking simulation.

Figure S5. IC_{50} concentration (nM) versus interaction energy (kJ/mol) for 3,3'-T2 sulfotransferase inhibition by OH-BDEs. Regression line excludes 4'-OH BDE49, 4'-OH BDE 101, 4'-OH BDE 201.



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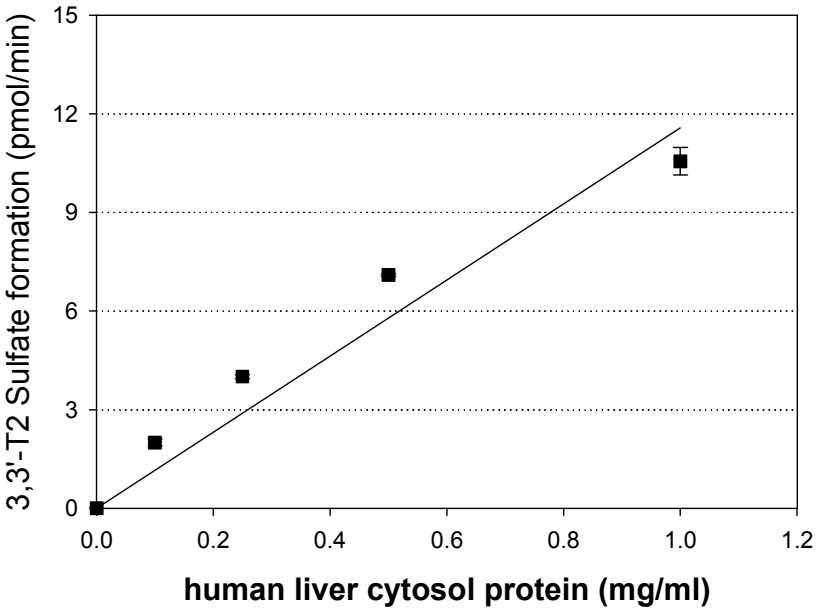

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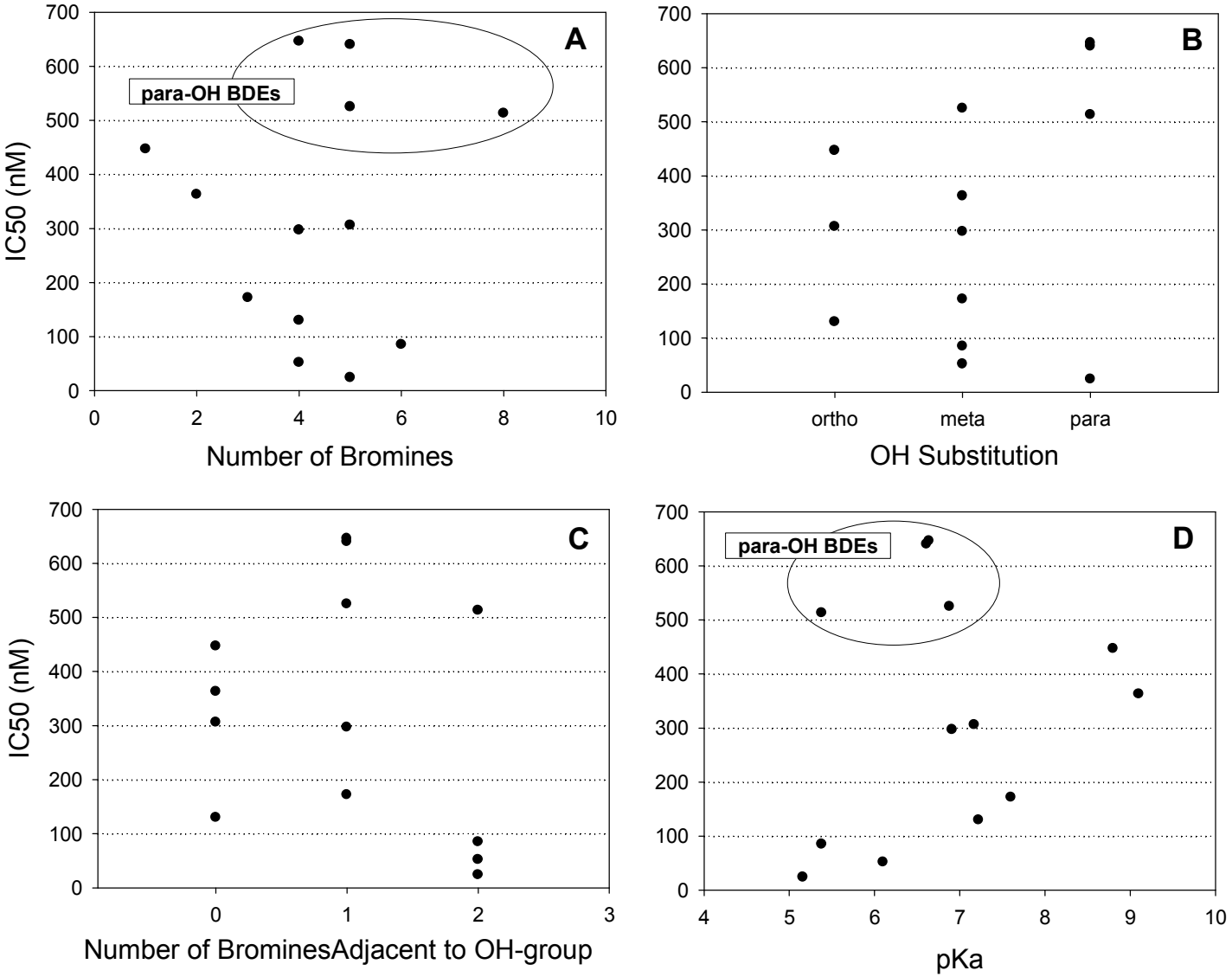

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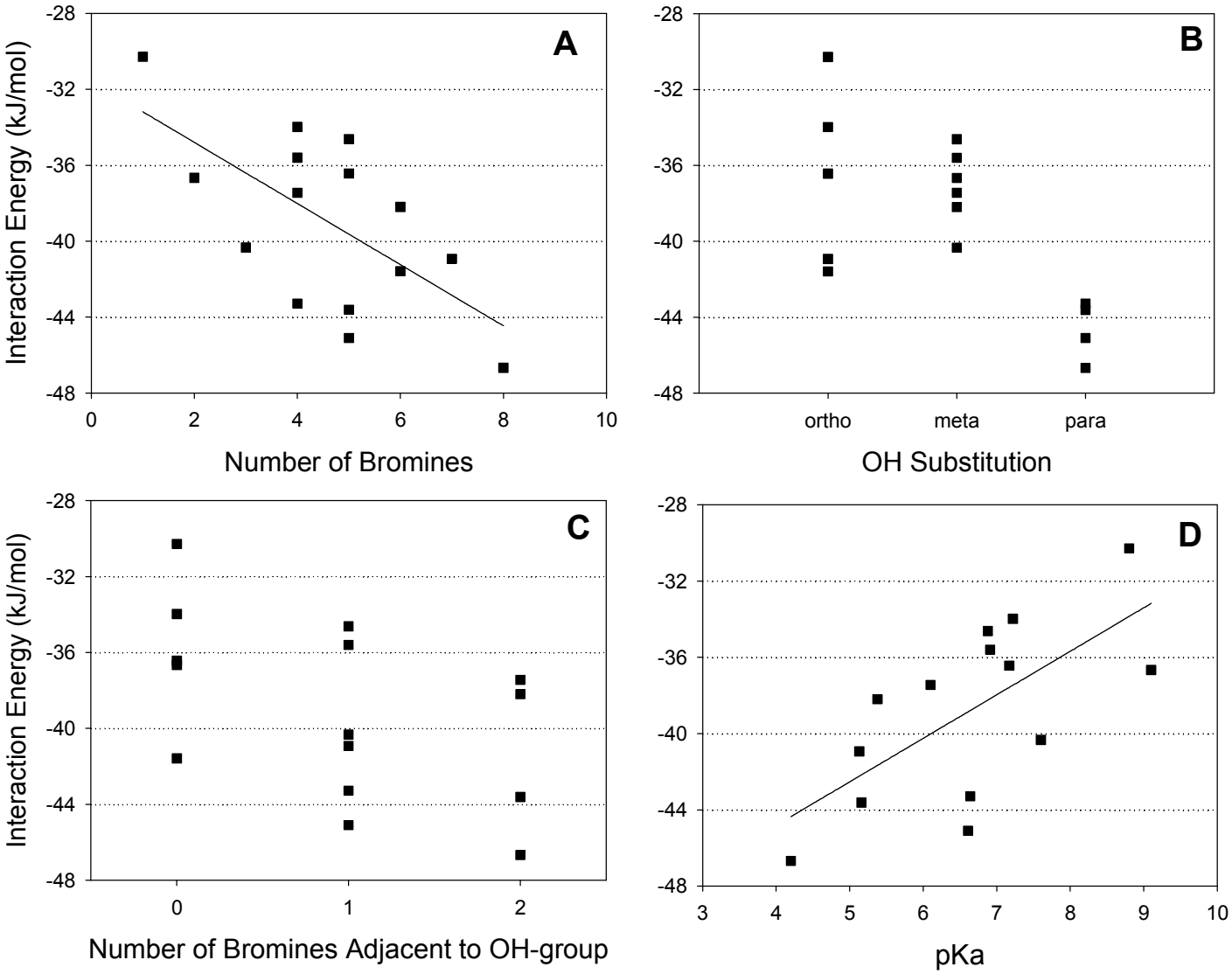

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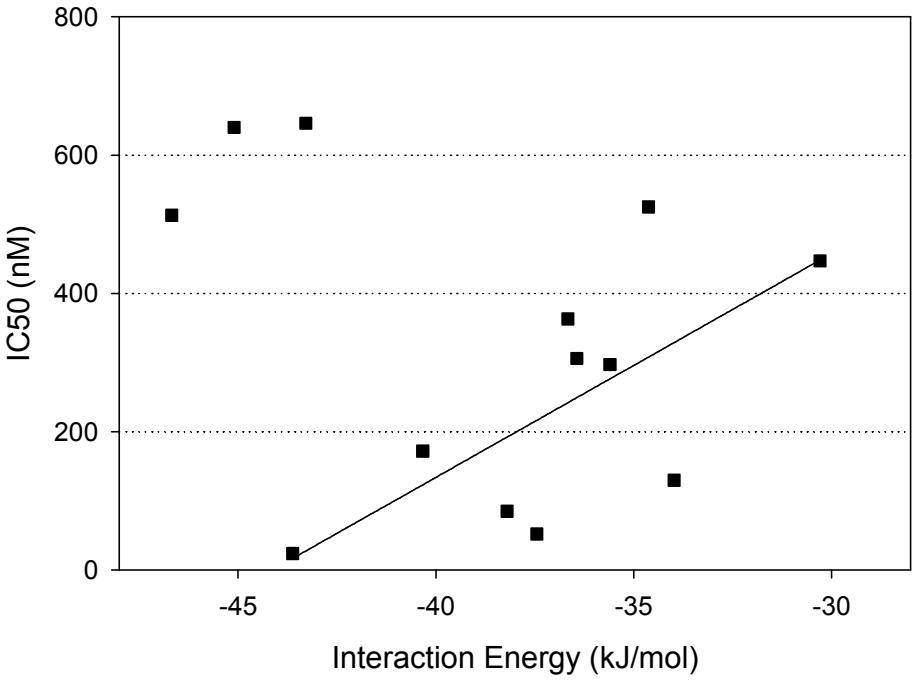

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