

Table S1. Crystallographic data for compounds 4 and 8.

Parameter	Compound	
	4	8
Empirical formula	C ₂₀ H ₁₉ BrClF ₃ O ₂ Ru	C ₁₂ H ₈ N ₂ O ₄ RuS ₂
Formula weight	564.78	409.39
Crystal system	orthorhombic	triclinic
Space group	<i>P b c a</i>	<i>P</i> $\bar{1}$
<i>T</i> [K]	150.00(10)	150.05(10)
λ [Å]	0.71073	0.71073
<i>a</i> [Å]	9.1573(3)	7.4914(4)
<i>b</i> [Å]	20.5173(7)	9.8535(6)
<i>c</i> [Å]	21.4528(7)	10.1047(5)
α [°]	90	85.849(4)
β [°]	90	74.188(4)
γ [°]	90	85.560(4)
<i>V</i> [Å ³]	4030.6(2)	714.49(7)
<i>Z</i>	8	2
<i>D</i> _{calc} [g/cm ³]	1.861	1.903
μ [mm ⁻¹]	2.933	1.404
<i>F</i> (000)	2224	404
Size [mm ³]	0.5×0.3×0.08	0.2×0.15×0.04
Collected reflections	20571	7311
Unique reflections	5525	3741
Observed reflections	4384	3195
<i>R</i> _{int}	0.0377	0.0302
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0350	0.0281
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.0763	0.0568
<i>R</i> ₁ (all data)	0.0525	0.0378
<i>wR</i> ₂ (all data)	0.0850	0.0602

Table S2. Relevant bond lengths and angles in compound 4.

Bonds [Å]		
Ru1–Cl1		2.4024(8)
Ru1–O1		2.0810(19)
Ru1–O2		2.0862(19)
Ru1–C21		2.193(3)
Ru1–C22		2.176(3)
Ru1–C23		2.158(3)
Ru1–C24		2.201(3)
Ru1–C25		2.159(3)
Ru1–C26		2.164(3)
Angles [°]		
O1–Ru1–Cl1		84.31(6)
O1–Ru1–O2		87.19(7)
O1–Ru1–C21		126.59(10)
O1–Ru1–C22		163.73(10)
O1–Ru1–C23		145.27(10)
O1–Ru1–C24		108.32(9)
O1–Ru1–C25		87.96(9)
O1–Ru1–C26		95.83(9)
O2–Ru1–Cl1		84.88(6)
O2–Ru1–C21		145.15(10)
O2–Ru1–C22		108.97(10)
O2–Ru1–C23		88.51(10)
O2–Ru1–C24		96.38(9)
O2–Ru1–C25		127.64(10)
O2–Ru1–C26		165.18(10)
C21–Ru1–Cl1		89.85(8)
C21–Ru1–C24		81.92(11)
C22–Ru1–Cl1		98.68(9)
C22–Ru1–C21		37.95(11)
C22–Ru1–C24		68.95(11)
C23–Ru1–Cl1		129.56(8)
C23–Ru1–C21		68.66(12)
C23–Ru1–C22		37.92(11)
C23–Ru1–C24		38.15(11)
C23–Ru1–C25		67.88(11)
C23–Ru1–C26		80.73(11)
C24–Ru1–Cl1		167.34(8)
C25–Ru1–Cl1		146.17(8)
C25–Ru1–C21		68.77(11)
C25–Ru1–C22		80.66(11)
C25–Ru1–C24		37.55(11)
C25–Ru1–C26		38.36(11)
C26–Ru1–Cl1		109.83(9)
C26–Ru1–C21		37.72(11)
C26–Ru1–C22		68.06(11)
C26–Ru1–C24		68.88(11)

Table S3. Relevant bond lengths and angles in compound 8.

Bonds [Å]		
Ru1–S1		2.3711(6)
Ru1–S2		2.3598(6)
Ru1–O1		2.0859(16)
Ru1–O2		2.1023(16)
Ru1–C30		1.860(3)
Ru1–C40		1.856(3)
Angles [°]		
S2–Ru1–S1		167.08(2)
O1–Ru1–S1		83.32(4)
O1–Ru1–S2		85.76(4)
O1–Ru1–O2		84.84(6)
O2–Ru1–S1		88.71(5)
O2–Ru1–S2		83.43(5)
C30–Ru1–S1		97.52(8)
C30–Ru1–S2		93.08(8)
C30–Ru1–O1		177.26(9)
C30–Ru1–O2		92.56(9)
C40–Ru1–S1		92.17(8)
C40–Ru1–S2		94.99(8)
C40–Ru1–O1		91.37(9)
C40–Ru1–O2		175.98(9)
C40–Ru1–C30		91.21(11)

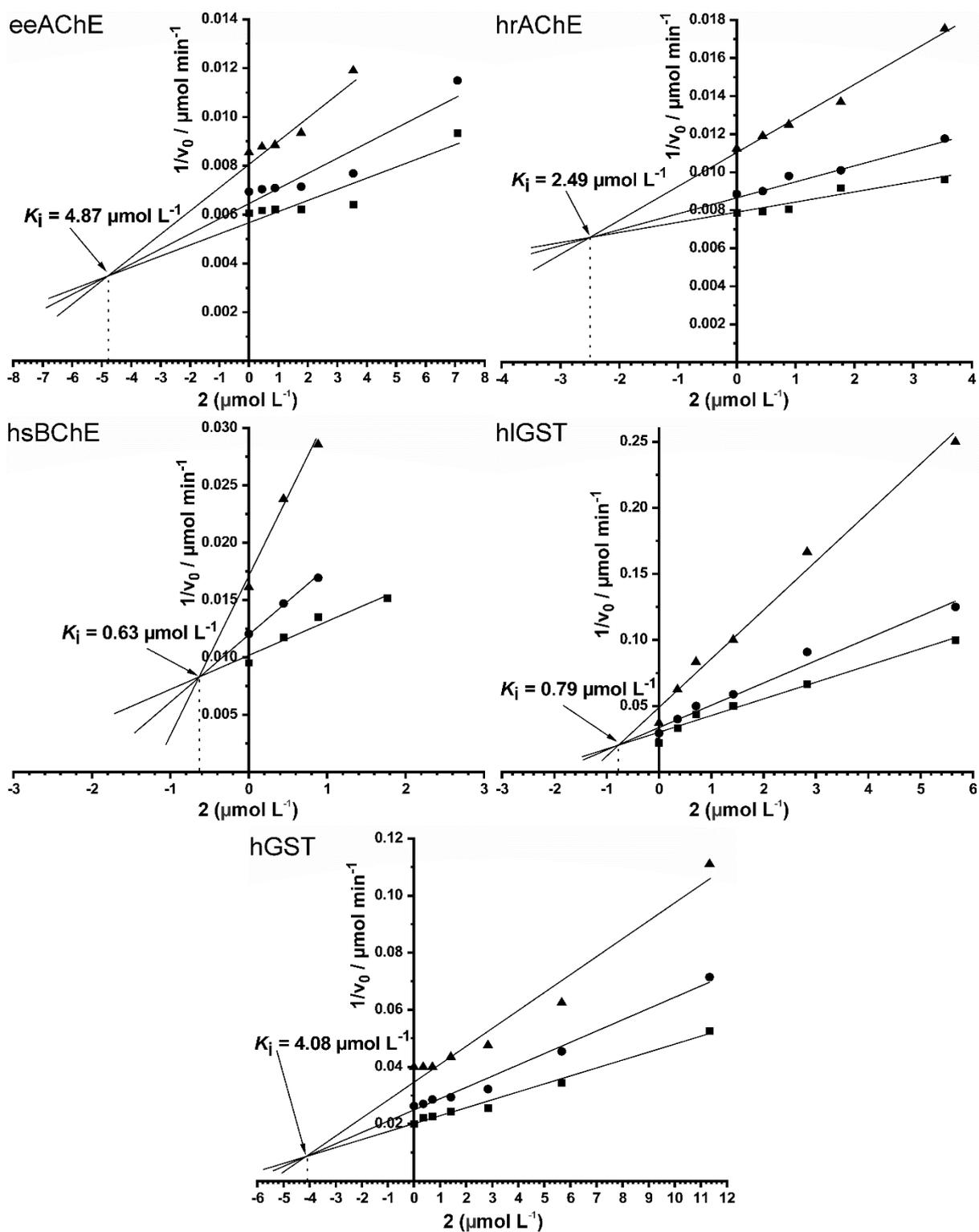


Figure S1. Dixon plots for determination of type of inhibition and inhibition constants (K_i) for compound 2 against electric eel acetylcholinesterase (eeAChE), human recombinant acetylcholinesterase (hrAChE), horse serum butyrylcholinesterase (hsBChE), horse liver glutathione S-transferase (hIGST) and human placenta glutathione S-transferase (hGST). Substrate concentrations: acetylthiocholine (eeAChE, hrAChE, hsBChE), 0.125 mM (\blacktriangle), 0.25 mM (\bullet), 0.5 mM (\blacksquare); 1-chloro-2,4-dinitrobenzene (hIGST, hGST), 200 μM (\blacktriangle), 400 μM (\bullet), 800 μM (\blacksquare).

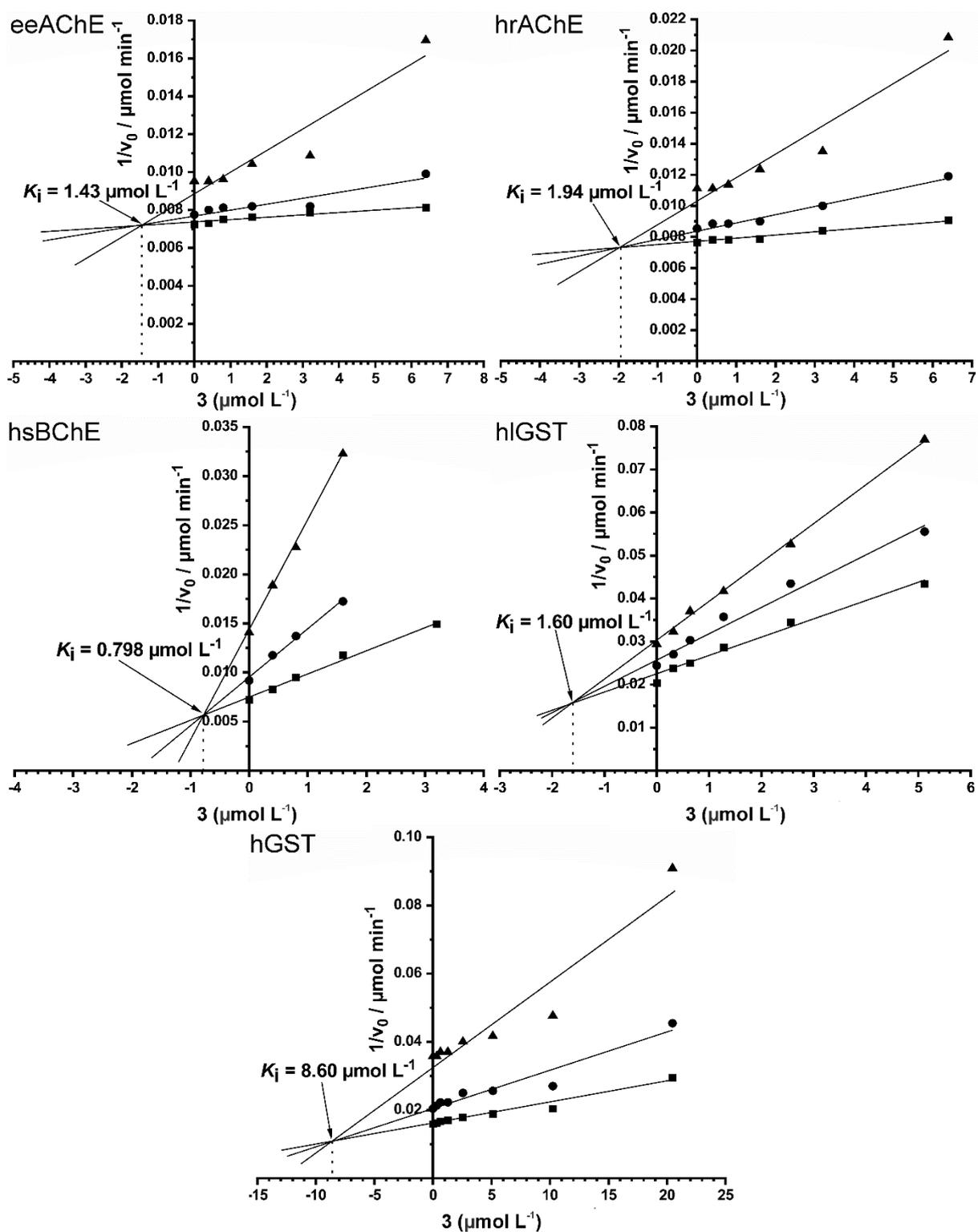


Figure S2. Dixon plots for determination of type of inhibition and inhibition constants (K_i) for compound 3 against electric eel acetylcholinesterase (eeAChE), human recombinant acetylcholinesterase (hrAChE), horse serum butyrylcholinesterase (hsBChE), horse liver glutathione S-transferase (hIGST) and human placenta glutathione S-transferase (hGST). Substrate concentrations: acetylthiocholine (eeAChE, hrAChE, hsBChE), 0.125 mM (\blacktriangle), 0.25 mM (\bullet), 0.5 mM (\blacksquare); 1-chloro-2,4-dinitrobenzene (hIGST, hGST), 200 μM (\blacktriangle), 400 μM (\bullet), 800 μM (\blacksquare).

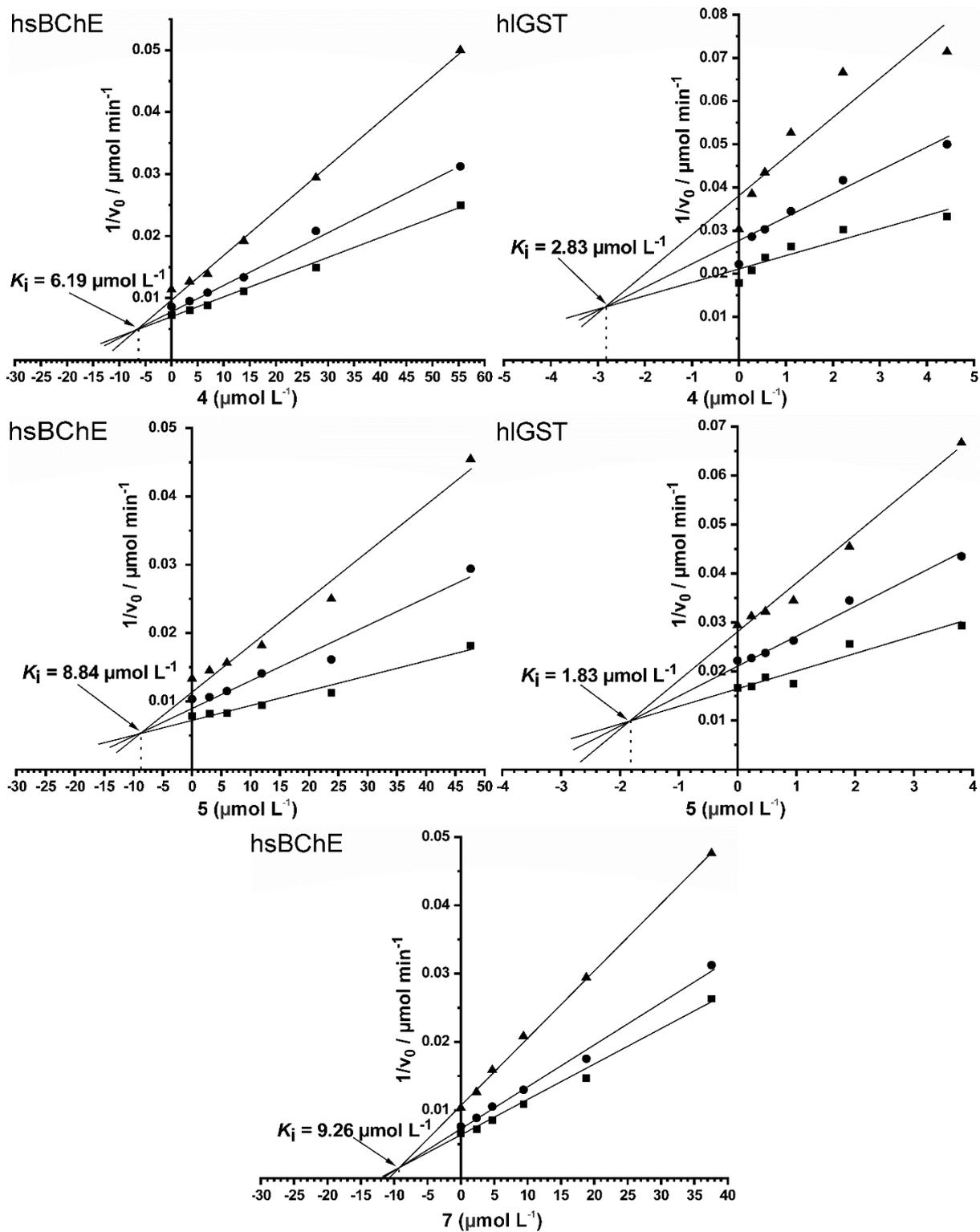


Figure S3. Dixon plots for determination of type of inhibition and inhibition constants (K_i) for compounds 4, 5 and 7 against horse serum butyrylcholinesterase (hsBChE) and horse liver glutathione S-transferase (hIGST). Substrate concentrations: acetylthiocholine (hsBChE), 0.125 mM (\blacktriangle), 0.25 mM (\bullet), 0.5 mM (\blacksquare); 1-chloro-2,4-dinitrobenzene (hIGST), $200 \mu\text{M}$ (\blacktriangle), $400 \mu\text{M}$ (\bullet), $800 \mu\text{M}$ (\blacksquare).

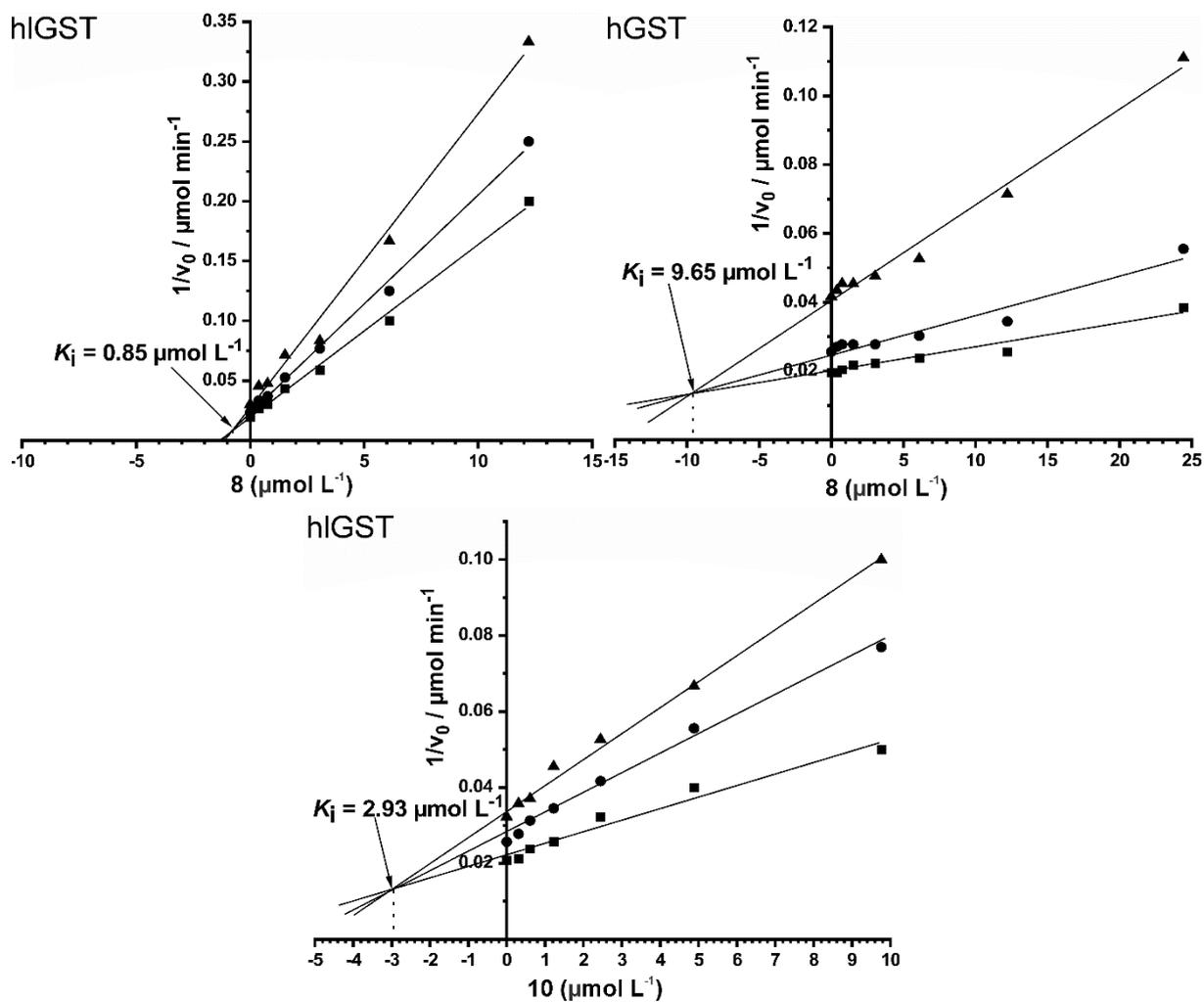


Figure S4. Dixon plots for determination of type of inhibition and inhibition constants (K_i) for precursor 10 and compound 8 against horse liver glutathione S-transferase (hGST). Substrate concentrations: 1-chloro-2,4-dinitrobenzene, 200 μM (▲), 400 μM (●), 800 μM (■).