

Table S1. The binding free energy for 1b/Erastin-SLC7A11 (kcal/mol)

system	Polar contributions		Non-polar contributions		ΔG_{bind}
	ΔG_{ele}	$\Delta G_{\text{ele,sol}}$	ΔG_{vdw}	$\Delta G_{\text{nonpol,sol}}$	
1b-SLC7A11	-23.133	36.688	-46.067	-5.671	-38.183
Erastin-SLC7A11	-2.667	18.139	-38.525	-4.928	-27.981