

Supplementary Information

Figure S1. Superposition of glutathione transferase A1 (GSTA1) monomer with or without OTB-SG conjugate (A2). Free/ligand protein structure is colored in cyan.



Figure S2. Superposition of glutathione transferase A1 (GSTA1) monomer with or without OTB-SG conjugate (B1). Free/ligand protein structure is colored in cyan.



Figure S3. Superposition of glutathione transferase A1 (GSTA1) monomer with or without OTB-SG conjugate (B2). Free/ligand protein structure is colored in cyan.



Table S1. Calculated total potential energy (kcal/mol) of optimized conjugates A1, A2, B1 and B2.

Structure	Total potential energy (kcal/mol)
A1	-7879.17
A2	-8268.93
B1	-7760.40
B2	-8019.00