SUPPLEMENTARY MATERIAL TABLE A. Free energies of binding (ΔG) In silico in kcal/mol in trypanothione and glutathione reductases by both Q and NADPH sites.

Molecule	Trypanothione Reductase		Glutathione Reductase	
	ΔG In silico (Q site)	ΔG In silico (NADPH site)	ΔG In silico (Q site)	ΔG In silico (NADPH site)
Naphthoquinones				
Nq-a	-10.08		-10.5	
Nq-b	-11.7	-10.0	-11.1	-10.8
Nq-c	-11.6	-9.7	-11.4	-10.1
Nq-d	-11.0		-11.8	
Nq-e	-12.5	-9.7	-12.6	-11.6
Nq-f	-12.1		-11.9	
Nq-g	-12.2	-6.2	-10.9	-10.7
Nq-h	-13.4	-7	-11.6	-12.4
Nq-i	-12.1	-8.6	-11.7	-10.6
Nq-j	-9.97	-8.5	-11.2	-11.0
Furanquinones				
Fq-a	-11.1	-8.2	-12.2	-10.1
Fq-b	-12.8	-9.3	-13.1	-10.1
Fq-c	-11.3	-8.5	-12.5	-10.2
Quinolinquinones				
Qq-b	-11.7		-10.7	
Qq-c	-12.0	-9.0	-10.9	-10.8
Qq-d	-12.7	-10.0	-12.1	-10.7
Qq-e	-11.2	-10.0	-11.5	-10.7
Qq-g	-12.7	-5.2	-11.8	-9.8
Qq-i	-12.5	-9.1	-12.2	-10.3