Table S1. The 10 ER agonists/antagonists with the highest predicted IC$_{50}$s, as predicted by the regression model. The names of the compounds are given along with their targets and original energy scores from eHiTS.

ranking from regression model	predicted IC50 from regression model (nM)	ER agonist/antagonist	ER targets in BindingDB	original eHiTS energy score (pKi)
1	18	GSK 5182	ERa, E-RRg	-10.40
2	23	4-hydroxytamoxifen 4-OHT analog, 16	ERa, E-RRg	-9.64
3	25	4-hydroxytamoxifen 4-OHT analog, 6	ERa, E-RRg	-11.73
4	29	4-hydroxytamoxifen 4-OHT analog, 5	ERa, E-RRg	-11.73
5	29	4-hydroxytamoxifen 4-OHT analog, 11	ERa, E-RRg	-11.73
6	34	4-hydroxytamoxifen 4-OHT analog, 4	ERa, E-RRg	-11.69
7	38	4-hydroxytamoxifen 4-OHT analog, 12	ERa, E-RRg	-10.21
8	46	4-hydroxytamoxifen 4-OHT analog, 9	ERa, E-RRg	-9.71
9	54	4-hydroxytamoxifen 4-OHT analog, 10	ERa, E-RRg	-11.72
10	58	4-hydroxytamoxifen 4-OHT analog, 14	ERa, E-RRg	-11.74

Table S2. The 10 most highly ranked ER agonists/antagonists, as predicted by the classification model. The names of the compounds are given along with their targets and original energy scores from eHiTS.

ranking from classification model	ER agonist/antagonist	ER targets in BindingDB	original eHiTS energy score (pKi)
1	piperidine derivative, 38c	ERa, ERb	-11.74
2	GSK 5182	ERa, E-RRg	-10.40
3	4-hydroxytamoxifen 4-OHT analog, 16	ERa, E-RRg	-9.64
4	pyrazolo[1,5-a]pyrimidine, 12c	ERa, ERb	-11.74
5	piperazine derivative, 47	ERa, ERb	-11.74
6	4-hydroxytamoxifen 4-OHT_analog, 5	ERa, E-RRg	-11.73
7	piperazine derivative, 49	ERa, ERb	-11.74
8	4-hydroxytamoxifen 4-OHT analog, 4	ERa, E-RRg	-11.69
9	tetrahydroisoquinoline derivative, 19e	ERa, ERb	-11.74
10	4-hydroxytamoxifen 4-OHT analog, 14	ERa, E-RRg	-11.74