

**Table S2.** Comparison ( $\Delta G_{bin}$ , kcal/mol) of chalcones-1,4-Naphthoquinone/Hydroquinone hybrids with kinase proteins overexpressed in cancer.

Compounds	Target proteins						cLogP
	EGFR	HER2	c-MET	TRKA	MEK1	TPK	
4a	-10.9	-10.5	-9.7	-10.1	-10.3	-10.2	6.11
4b	-10.6	-9.8	-9.9	-10.3	-9.8	-10.0	6.04
4c	-11.1	-9.9	-10.4	-10.4	-9.8	-10.6	6.45
4d	-11.2	-10.0	-10.3	-10.4	-10.2	-10.7	7.32
4e	-10.5	-9.5	-9.3	-9.7	-9.0	-9.0	5.90
4f	-10.0	-9.4	-9.4	-9.1	-10	-8.4	5.90
5a	-8.8	-9.4	-9.6	-9.7	-9.5	-9.3	6.77
5'b	-9.2	-9.7	-9.4	-10.1	-9.3	-8.8	6.37
5'c	-9.2	-10.1	-10.2	-10.4	-10.2	-9.7	6.78
5'd	-9.3	-10	-9.9	-10.3	-9.9	-9.6	7.65
5e	-7.2	-8.3	-9.8	-8.9	-9.2	-8.6	6.56
5f	-7.4	-8.6	-9.7	-9.1	-8.7	-8.2	6.56
6a	-10.6	-10.8	-10.3	-10.5	-10.5	-10.3	5.53
6b	-10.6	-10.2	-10.3	-10.7	-9.8	-10.3	5.46
6c	-11.1	-10.4	-10.6	-11.0	-10.2	-10.4	5.87
6d	-11.2	-10.6	-10.4	-11.0	-10.4	-10.6	6.74
6e	-10.0	-10.2	-9.8	-9.6	-9.9	-9.9	5.32
6f	-8.6	-9.5	-10.4	-9.1	-10.2	-9.5	5.32

Proteins with their respective (PDB) entries: **EGFR**: Epidermal growth factor receptor (5GTY); **HER2**: Epidermal growth factor receptor 2 (7JXH); **c-MET**: Mesenchymal-epithelial transition factor (3RHK); **TRKA**: Tropomyosin receptor kinase A (6PL2); **MEK1**: MAPK/ERK kinase (4AN3); **TPK**: Tyrosine-protein kinase (4EHZ).