

Title: Design, Synthesis and Evaluation of 4,5,6,7-Tetrahydrobenzo[d]thiazole-Based Novel Dual Kinase Inhibitors of CK2 and GSK3 β

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Supplementary file 2: Molecular docking of synthesized structural analogs of the lead on CK2 and GSK3 β receptor proteins

Compound	CK2	GSK3 β	Compound	CK2	GSK3 β
CK2 inhibitor	160.1		3b	145.8	132.3
GSK3β inhibitor		116.5	3c	141.7	131.4
Hit15	140.7	130.8	3d	157.9	146.5
1a	141.8	133.0	3e	166.3	136.9
1b	143.1	130.6	3f	151.2	131.5
1c	141.7	130.2	3g	160.0	145.7
1d	160.5	142.4	3h	160.5	134.5
1e	144.7	137.2	4a	150.1	133.9
1f	135.9	129.8	4b	156.6	137.3
1g	174.7	148.9	4c	157.6	134.1
1h	163.7	143.4	4d	162.9	138.4
2a	147.5	134.3	4e	161.3	130.7
2b	155.1	135.5	4f	155.9	135.2
2c	152.9	131.7	4g	154.7	139.9
2d	155.8	136.1	4h	153.1	141.3
2e	157.4	135.3	4i	154.7	142.4
2f	155.3	129.8	4j	161.7	142.5
2g	168.6	148.6	4k	158.7	139.7
2h	168.3	136.3	4l	157.6	137.5
3a	139.2	130.9			