Title: Design, Synthesis and Evaluation of 4,5,6,7-Tetrahydrobenzo[*d*]thiazole-Based Novel Dual Kinase Inhibitors of CK2 and GSK3β

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Authors: Triveni R. Pardhi[a], Manishkumar S. Patel[b], V. Sudarsanam[c], Kamala K. Vasu[a,c,*]

Affiliations:

[a]Department of Natural Products, National Institute of Pharmaceutical Education and Research (NIPER)-Ahmedabad, Gandhinagar-382355, Gujarat, India

[b]Department of Biotechnology, National Institute of Pharmaceutical Education and Research (NIPER)-Ahmedabad, Gandhinagar-382355, Gujarat, India

[c]Department of Medicinal Chemistry, B. V. Patel Pharmaceutical Education & Research Development (PERD) Centre, Ahmedabad-380054, Gujarat, India.

***Corresponding Author e-mail address:** kamalav@perdcentre.com, triveni.pardhi@gmail.com

Supplementary file 1: Fit values of synthesized structural analogs of the lead on common feature pharmacophore model (pharm18)[34] and 3DQSAR pharmacophore model (Hypo1).[34]

Compound	Pharm18 (CFP model)	Hypo1 (3DQSAR model)	Compound	Pharm18 (CFP model)[a]	Hypo1 (3DQSAR model)
CK2 inhibitor[38]	3.71	8.24	**3b**	3.06	8.66
GSK3β inhibitor[39]	2.60	7.83	**3c**	2.99	8.53
1a	2.98	8.52	**3d**	3.63	10.59
1b	3.10	9.51	**3e**	3.81	9.22
1c	3.01	8.74	**3f**	3.76	8.56
1d	3.70	10.19	**3g**	3.69	10.39
1e	3.60	8.87	**3h**	3.88	9.87
1f	2.82	8.54	**4a**	3.71	8.59
1g	3.91	11.24	**4b**	3.65	8.71
1h	3.80	10.81	**4c**	3.68	9.37
2a	3.41	8.59	**4d**	3.76	9.73
2b	3.56	8.61	**4e**	3.84	9.90
2c	3.42	8.56	**4f**	3.50	9.28
2d	3.50	9.10	**4g**	3.58	8.59
2e	3.59	9.13	**4h**	3.61	8.61
2f	3.47	8.78	**4i**	3.48	8.60
2g	3.89	11.06	**4j**	3.49	8.86
2h	3.48	9.79	**4k**	3.60	9.57
3a	2.98	8.56	**4l**	3.46	9.49

[a]CFP model: Common feature pharmacophore model