

## Supplementary file 1

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### Thiazolo-pyridopyrimidines: An *in silico* evaluation as a lead for CDK4/6 inhibition, synthesis and cytotoxicity screening against breast cancer cell lines

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**Table S1.** Physiochemical properties of synthesized compounds

Compound	Colour	% yield	Melting point (°C)	Solubility	R <sub>f</sub> value	λ <sub>max</sub> (nm)
4a	Yellow	86	>260	Acetone, DMF, DMSO	0.73	289
4c	Dark Brown	47	>260	Acetone, DMF, DMSO	0.65	279
4d	Off white	84	>260	Acetone, DMF, DMSO	0.61	296
4g	Brown	84	>260	Acetone, DMF, DMSO	0.83	284

**Table S2.** Percentage inhibition and IC<sub>50</sub> of compounds against MCF-7 cells by SRB assay

Compounds	Percentage Inhibition					IC <sub>50</sub>
	10μM	20μM	30μM	40μM	50μM	
4a	12.771±0.222	29.453±0.424	43.135±0.295	62.381±0.472	80.486±0.347	32.597±0.12
4c	20.018±0.346	34.162±0.343	53.987±0.538	74.331±0.745	91.738±0.602	27.086±0.194
4d	9.754±0.355	23.142±0.443	39.143±0.661	54.958±0.339	71.694±0.311	36.604±0.052
4g	8.59±0.375	21.698±0.167	37.267±0.468	51.875±0.778	65.111±0.143	39.154±0.194
Dox(1-5 μM)	43.157± 0.402	59.250± 0.463	70.79 0.463	82.874 ±0.036	95.141 ±0.043	1.413 ±0.031

**Table S3.** Percentage inhibition and IC<sub>50</sub> of compounds against MDAMB-231 cells by SRB assay

<b>Compounds</b>	<b>Percentage Inhibition</b>					
<b>Concentration</b>	<b>10μM</b>	<b>20μM</b>	<b>30μM</b>	<b>40μM</b>	<b>50μM</b>	<b>IC<sub>50</sub></b>
4a	13.31±0.491	26.577±0.529	42.755±0.394	59.278±0.514	73.819±0.349	34.468±0.114
4c	19.15±0.245	30.821±0.259	50.681±0.948	67.964±0.139	89.167±0.332	29.133±0.116
4d	9.277±0.809	20.617±0.803	37.907±1.451	51.548±1.196	69.648±0.894	38.061±0.607
4g	6.843±0.206	19.254±0.483	36.092± 0.557	48.9±0.168	61.099±0.635	41.271±0.199
Dox(1-5 μM)	43.157± 0.402	59.250± 0.463	70.795± 0.463	82.874 ±0.036	95.141 ±0.043	1.413 ±0.031