Supplementary Materials

Synthesis, Characterization, and Anticancer Activities Evaluation of Compounds Derived from 3,4-Dihydropyrimidin-2(1*H*)-one

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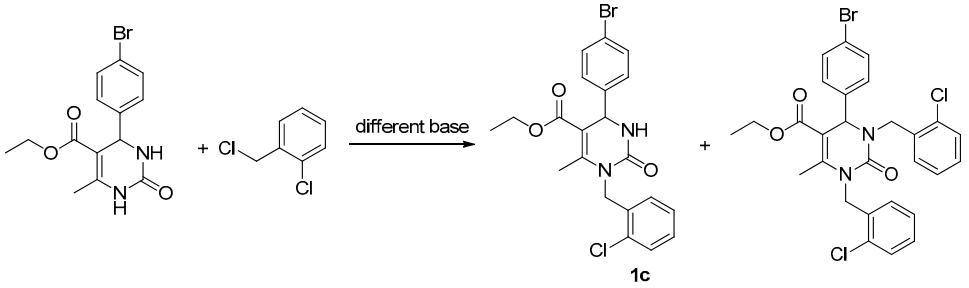
Table S1. Results of N^1-alkylation of DHPMs reaction with different bases.



Entry	Base	Additive	Reaction time (h)	Temperature (°C)	N1-alkylation Yield[a] (%)	N1 and N3-dialkylation Yield (%)
1	potassium carbonate	KI TBA	24	r.t.[b]	\	\
2	cesium carbonate	KI TBA	22	r.t.	25	27
3	lithium hydroxide	KI TBA	22	r.t	12	31
4	sodium hydride	\	1.5	0-5 then r.t.	9	18
5	triethylamine	KI TBA	22	r.t.	\	\
6	1,8-diazabicyclo[5.4.0]undec-7-ene	KI TBA	22	r.t.	\	\
7	tetramethylguanidine	KI TBA	22	r.t.	\	\
8	tetrabutylammonium hydroxide	KI TBA	22	r.t.	23	NA
9	potassium tert-butoxide	KI TBA	16	r.t.	13	20

[a] The separation yield.

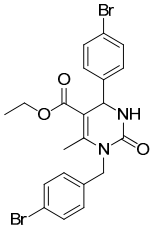
[b] Room temperature.

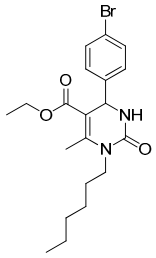
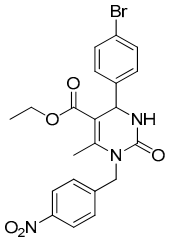
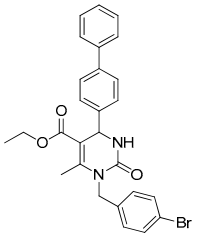
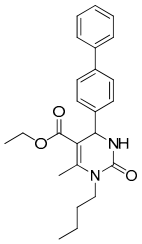
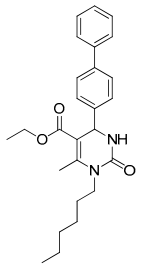
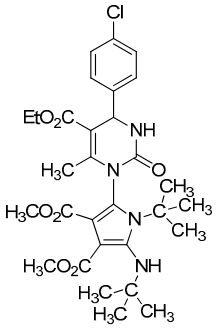
Table S2. Orthogonal tests for N1-alkylation of DHPMs in tetrabutylammonium hydroxide system.

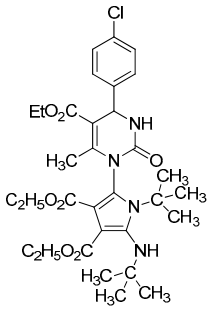
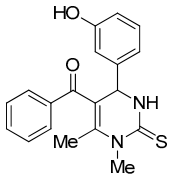
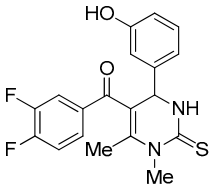
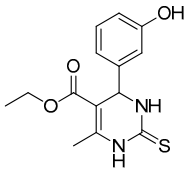
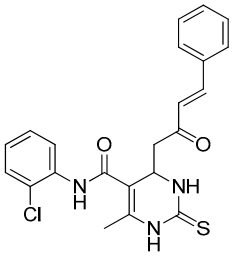
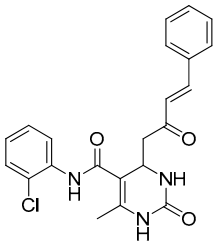
Entry	Mole ratio of halohydrocarbons	Mole equivalent of base	Temperature (°C)	Reaction time (h)	interval time[a] (h)	Phase transfer catalyst	Amount of solvent (ml/g)	N1-alkylation Yield (%)	N3-dialkylation Yield (%)
1	1.5	1.7	15	24	1.5	TBA	20	17.2	NA
2	1.8	1.7	45	24	0.5	TBA	10	21.9	NA
3	1.5	2.0	45	24	1.5	\	10	21.2	NA
4	1.8	2.0	15	24	0.5	\	20	11.3	NA
5	1.5	1.7	45	16	0.5	\	20	21.6	NA
6	1.8	1.7	15	16	1.5	\	10	19.0	NA
7	1.5	2.0	15	16	0.5	TBA	10	15.4	NA
8	1.8	2.0	45	16	1.5	TBA	20	35.1	NA
Sum of low dose yields	77.5	79.7	62.9	91.1	70.2	89.6	77.5		
Sum of high dose yields	85.2	83.0	99.8	71.6	92.5	73.1	85.2		
Range(R)	11.9	3.3	36.9	19.5	22.3	16.5	7.7		

[a] interval time between compound **1** and compound **2**.

Table S3. Dataset used for Pharmacophore analysis.

Cpd.	Structure	In Vitro Cell Viability
1d		9.72 [a]

1h		9.30 [a]
1j		39.31 [b]
3d		6.36 [a]
3g		7.32 [a]
3h		48.79 [b]
1		10.36 [a]

2		9.90 [a]
3		0.68 [a]
4		0.48 [a]
5		1.41 [a]
6		71 [b]
7		79 [b]

[a] Compounds **1d**, **1h**, **3d**, **3g, 1, 2, 3, 4** and **5** were IC_{50} values (μM). [b] Compounds **1j**, **3h, 6** and **7** were cytotoxic activity (%).