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## Novel One-Pot Synthesis of Imidazolinones from Ester: A Concise

Synthesis of GSK2137305

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## 1.Study on the possible synthetic pathway of Imidazolinone

A 25ml sealed tube was charged with CuI (10 mol%), Methyl 2-(4-bromophenyl) acetate (0.37 mmol),  $(NH_4)_2CO_3$  (7.4 mmol), and MeOH (2 mL), the mixture was stirred at 100°C for 10h and intermediate F was detected by LC-MS([M+H]+:226.9). Then acetone(0.37 mmol) was added and the mixture was stirred at 100°C for another 1h,5-(4-bromophenyl)-2,2-dimethyl-2,3-dihydro - 4*H*-imidazol-4-one was detected by TLC.



## 2.Crystal data

Crystal data of 2,2-dimethyl-5-phenyl-2,3-dihydro-4H-imidazol-4-one (CCDC 1855758)



Empirical formula	$C_{11}H_{12}N_2O$
Formula weight	188.23
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/n

Unit cell dimensions	a = 5.9234(10) Å	α= 90°.
	b = 9.2189(14) Å	β=92.203(4)°.
	c = 19.396(3) Å	γ=90°.
Volume	1058.4(3) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.181 Mg/m <sup>3</sup>	
Absorption coefficient	0.078 mm <sup>-1</sup>	
F(000)	400	
Crystal size	0.210 x 0.170 x 0.130 mm <sup>3</sup>	
Theta range for data collection	2.102 to 26.000°.	
Index ranges	-7≤h≤4, -11≤k≤11, -23≤l≤23	
Reflections collected	6167	
Independent reflections	2090 [R(int) = 0.0335]	
Completeness to theta = $25.242^{\circ}$	100.0 %	
Absorption correction	Semi-empirical from equiv	valents
Max. and min. transmission	0.7456 and 0.6589	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2090 / 0 / 133	
Goodness-of-fit on $F^2$	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0435, wR2 = 0.1057	
R indices (all data)	R1 = 0.0581, wR2 = 0.1133	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.119 and -0.150 e.Å <sup>-3</sup>	

spectra















































































