

Structure-Based Drug Design

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Our research is to screen and design several series of compounds showing activity to Aurora A in vitro. To elucidate their interaction with the target protein, structural biology study is performed to solve the ligand-protein complex structure and furthermore, to design more specific and potent Aurora A agonist. Crystals of Aurora A were separated by four series 1A1957, 1A2346, 1K0025, 1K0224

and grew important co-crystals with compounds 1A1957, 1A2346, 1K0025, 1K0224 and 1K0231. All dataset were collected on a CCD detector. The data collection parameters for these datasets are summarized in table 1. All datasets have been processed by HKL2000 in the station. The data process results are shown in table2.

Table 1. The summary of data collection parameters

Sample	Series	Distance (mm)	Wavelength (Å)	Oscillation range(°)	Beam position (x,y)	Total frames	Station/CCD
Aurora with 1A1957	1A1957	160	1.0	0.5	(94.388, 93.798)	267	SP12B2/Q4R
Aurora with 1A2346	1A2346	220	0.97315	0.5	(104.45,105.3)	500	13C1/Q210
Aurora with 1K0025	1K0025	190	1.0	0.5	(104.9,104.9)	273	13B1/Q210
Aurora with 1K0224	1K0224	300	1.0	0.5	(157.30,157.30)	110	13B1/Q315
Aurora with 1K0231	1K0224	300	1.0	0.5	(157.30,157.30)	80	13B1/Q315

Table 2 . The summary of data process results

Data collection statistics	Aurora with 1A1957	Aurora with 1A2346	Aurora with 1K0025	Aurora with 1K0224	Aurora with 1K0231
Space group, P6122 ($\alpha=\gamma=90^\circ$ $\beta=120^\circ$)	a=81.571 b=81.571 c=170.043	a=83.043 b=83.043 c=172.318	a=83.053 b=83.053 c=170.894	a=82.275 b=82.275 c=171.839	a=83.322 b=83.322 c=172.062
Resolution range(Å)	30-2.3	30.0-2.66	30.0-2.3	30.0-2.35	30.0-2.4
Completeness(%)	99.5	96.6	97.9	97.9	96.4
R_{merge} (%)	4.3	4.1	3.0	4.3	4.1
I/σ(I)	59.9	44.6	67.26	36.48	30.3