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Addition, Retraction, Correction

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Correction to Discovery of a Potent and Selective DDR1 Receptor Tyrosine Kinase Inhibitor

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In the reported X-ray cocrystal structure of the DDR1 kinase domain in complex with the inhibitor DDR1-IN-1 (PDB code 4BKI), the indolin-2-one moiety was modeled with two hydrogen bonds to the kinase hinge residues Met704 and Asp702. Subsequent analysis of the electron density has revealed that the indolin-2-one group is flipped allowing only a single hydrogen bond to Met704. The amended coordinates have been released with the new PDB code 4CKR. The corrected Figure 2A is shown, together with the

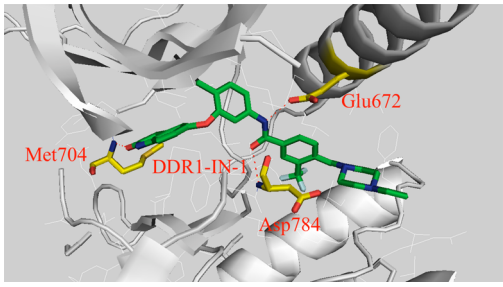

Figure 2. Binding information of DDR1-IN-1/2 against DDR1. (A) X-ray cocrystal structure of DDR1-IN-1 with DDR1 kinase.

updated refinement statistics (Table 5) reported in Supporting Information Table 5 of the original paper. This change does not otherwise affect the scientific integrity of the article. We thank Oliver Smart, Global Phasing Ltd., for drawing our attention to the error.

Table 5. Data Processing and Refinement Statistics. Values in Parentheses Refer to the Highest Resolution Shell

	DDR1 with DDR1-IN-1
Data	
wavelength (Å)	0.9795
resolution range (Å)	49.44−2.2 (2.278−2.199)
space group	$P4_12_12$
unit cell (Å)	59.3, 59.3, 178.5
unit cell (deg)	90, 90, 90
total reflections	183798 (14101)
unique reflections	17062 (1526)
multiplicity	11 (9.2)
completeness (%)	100 (100.00)
$I/\sigma(I)$	17.5 (2.4)
Wilson B-factor (Å^2)	36.2
R-merge	0.1 (0.956)
R-meas	0.109 (1.071)
$CC_{1/2}$	0.999 (0.720)
Refinement	
R-work/R-free	0.1982/0.2470
no. of atoms	2422
macromolecules	2324
ligands	60
water	38
protein residues	301
RMS(bonds) (Å)	0.01
RMS(angles) (°)	1.3
Ramachandran favored (%)	96.2
Ramachandran outliers (%)	0.34
Clashscore	1.49
avg B-factor (Å^2)	48.3
macromolecules	48.8
ligands	33.1
solvent	37.3
PDB ID	4CKR

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