SUPPORTING INFORMATION

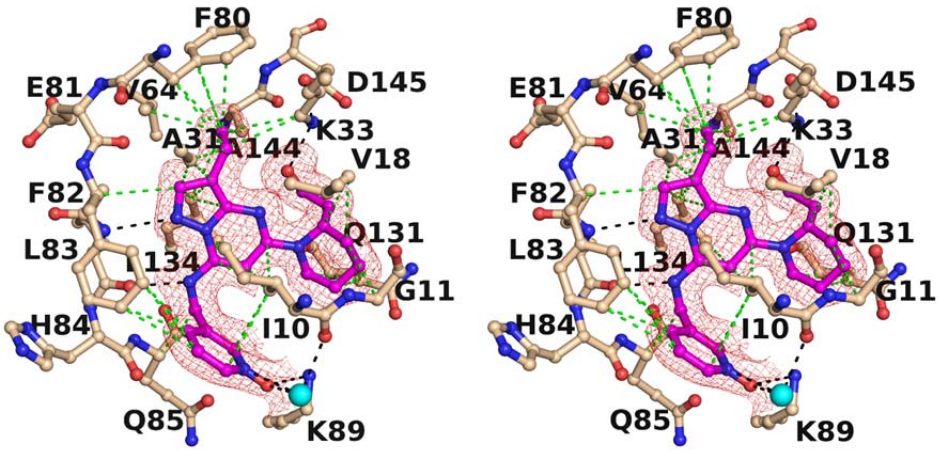
The cyclin-dependent kinase inhibitor dinaciclib interacts with the acetyl-lysine recognition site of bromodomains.

Mathew P. Martin[1], Sanne H. Olesen[1], Gunda I. Georg[2], and Ernst Schönbrunn[1*]

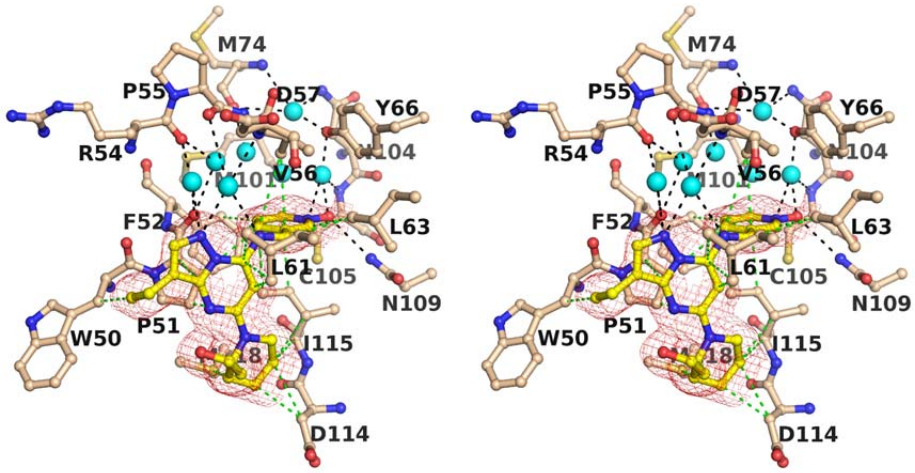
Supplementary Table 1. Summary of data collection and structure refinement[a].

Structure (PDB ID)	(4KD1) CDK2-Dinaciclib	(4KCX) BRDT-Dinaciclib
Data Collection		
X-ray	SER-CAT 22-ID	SER-CAT 22-ID
Wavelength (Å)	1.0	1.0
Space group	$P2_12_12_1$	$P2_1$
Unit cell dimensions (Å)	a=53.69 b=71.89 c=72.40	a=64.72 b=29.95 c=71.38 β=94.12
Resolution range	20-1.7 (1.8-1.7)	20-2.0 (2.1-2.0)
Unique reflections	31460 (4879)	18535 (2488)
Completeness (%)	99.9 (100)	97.8 (98.1)
I/σI	24.9 (4.8)	7.7 (3.3)
R_{sym}[a] (%)	4.8 (37.9)	12.7 (62.4)
Structure refinement		
Protein atoms **Average B-factor (Å^2)**	2398 25	1780 (dimer) 42
Ligand atoms **Average B-factor (Å^2)**	29 20	58 28
Solvent molecules **Average B-factor (Å^2)**	216 29	137 41
other atoms **Average B-factor (Å^2)**	4 34	1 20
r.m.s.d.[b] bonds (Å)	0.016	0.008
r.m.s.d.angles (°)	1.2	1.2
R_{cryst}[c] (%)	19.4	21.1
R_{free}[d] (%)	23.2	25.3
R_{free} reflection set size	1007 (3.2 %)	927 (5.0 %)
Coordinate error (Å) (ML method from PHENIX)	0.23	0.23

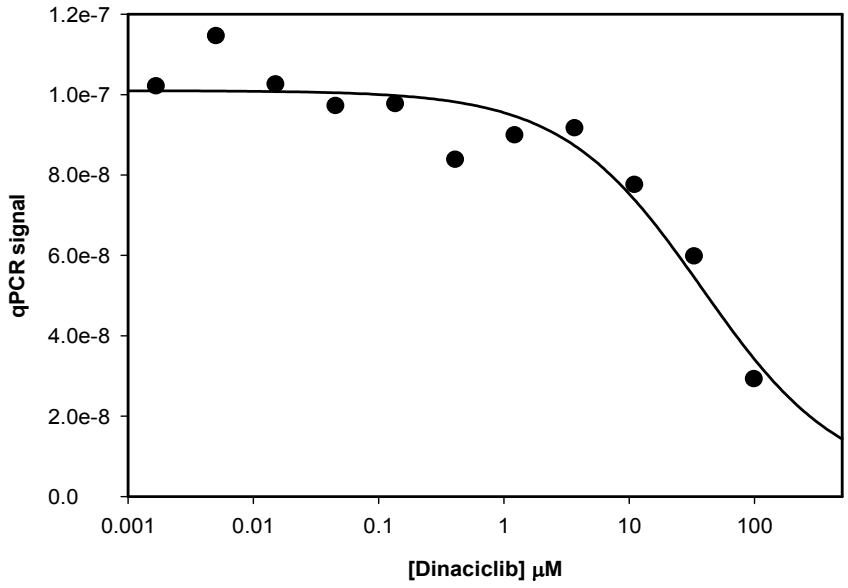
[a] R_{sym} = SUM (ABS(I - <I>)) / SUM (I)
[b] r.m.s.d. = root mean square deviation from ideal values.
[c] R_{cryst} = 100 x □ | F_{obs}-F_{model} | / F_{obs} where F_{obs} and F_{model} are observed and calculated structure factor amplitudes, respectively.
[d] R_{free} is R_{cryst} calculated for randomly chosen unique reflections, which were excluded from the refinement.



Supplementary Figure 1. Crystal structure of dinaciclib bound to CDK2 (Stereo presentations of the binding interactions). The Fo-Fc electron density map of the omitted inhibitor is contoured at 2.5 σ and shown as red mesh. Potential hydrogen bonding and van der Waals interactions are indicated as black and green dotted lines, respectively.



Supplementary Figure 2. Crystal structure of dinaciclib bound to BRDT (Stereo presentations of the binding interactions). The Fo-Fc electron density map of the omitted inhibitor is contoured at 2.5 σ and shown as red mesh. Potential hydrogen bonding and van der Waals interactions are indicated as black and green dotted lines, respectively.



Supplementary Figure 3. K_d determination of dinaciclib interaction with BRDT (performed by DiscoveRx Corp.).