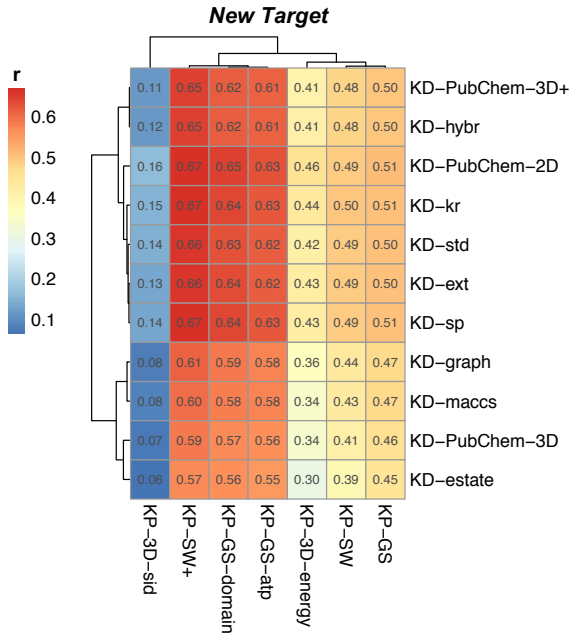
(a)



(b)

	Abbreviation	Description	
Drug compounds	KD-PubChem-2D	881-bit fingerprint based on 2D substructures defined by PubChem	Fingerprint-based linear kernels
	KD-PubChem-3D	PubChem's descriptor based on up to 10 calculated 3D conformers	
	KD-PubChem-3D+	PubChem's descriptor based on up to 10 calculated 3D conformers, additionally including information on acceptor count, hydrophobe count and ring count	
	KD-estate	79-bit fingerprint corresponding to EState substructures	
	KD-ext	1024-bit path-based, hashed fingerprint taking into account ring systems	
	KD-graph	1024-bit path-based, hashed fingerprint considering connectivity	
	KD-hybr	1024-bit path-based, hashed fingerprint considering hybridization states	
	KD-kr	4860-bit fingerprint defined by Klekota and Roth	
	KD-maccs	166-bit fingerprint based on MACCS structural keys	
	KD-sp	1024-bit fingerprint based on the shortest paths between pairs of atoms taking into account ring systems and charges	
	KD-std	1024-bit path-based, hashed fingerprint	
Protein targets	KP-SW	Amino acid sequence-based linear kernel	
	KP-SW+	Amino acid sequence and extended target profile-based linear kernel	
	KP-3D-energy	Protein structure-based linear kernel (using absolute value of the energy needed to align proteins)	
	KP-3D-sid	Protein structure-based linear kernel (using sequence identity)	
	KP-GS	Generic String kernel applied to full protein sequences	
	KP-GS-domain	Generic String kernel applied to kinase domain sequences	
	KP-GS-atp	Generic String kernel applied to ATP binding pocket sequences	

S7 Fig. (a) Leave-target-out cross-validation results. The prediction accuracy was evaluated with Pearson correlation (r) between binding affinities (pK_i) from the study by Metz *et al*. and those predicted using KronRLS algorithm with different pairs of drug (rows) and protein (columns) molecular descriptors encoded as kernel matrices **(b)**.