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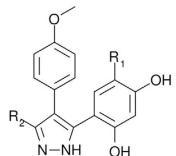
Corrigendum: Kinetics of protein-ligand unbinding via smoothed potential molecular dynamics simulations

Luca Mollica, Sergio Decherchi, Syeda Rehana Zia, Roberto Gaspari, Andrea Cavalli & Walter Rocchia

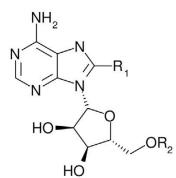
Scientific Reports 5:11539; doi: 10.1038/srep11539; published online 23 June 2015; updated on 06 May 2016

This Article contains an error in Fig. 1: in panel C groups R2 of compounds 4g and 4h were incorrectly stated as OH. The correct Fig. 1 appears below.

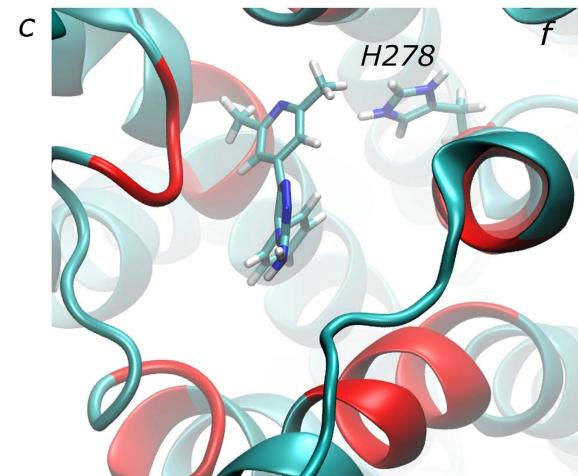
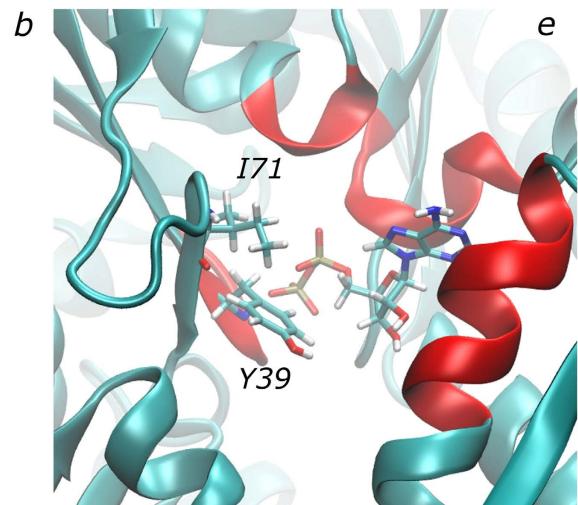
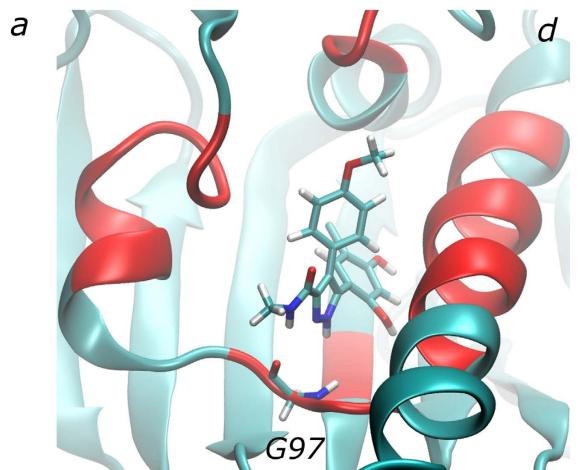
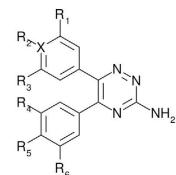
	R_1	R_2	k_{off}	t_{comp}
BS1	Cl	CONHCH ₃	1.1E-2	21.5
BS2	Br	CONHCH ₂ CH ₃	6.1E-3	32.3
BS3	Br	CH ₃	2.2E-2	18.9
BSM	Cl	CONHCH ₂ CH ₃	6.9E-3	30.7



	R_1	R_2	k_{off}	t_{comp}
L01 (ADP)	H	P2O ₆ ³⁻	5E-3	12.0
L02	NH ₂	H	~1	2.8
L10		H	4E-1	5.8
L14			4E-2	8.4



	X	R_1	R_2	R_3	R_5	R_{4-6}	k_{off}	t_{comp}
4a	C	H	H	H	H	H	~1	25.3
4e	C	Cl	OH	H	H	H	1.01E-3	37.8
4g	N	CH ₃		CH ₃	H	H	1.15E-2	31.8
4h	N	CH ₃		CH ₃	F	H	1.15E-1	26.5

**Figure 1.**

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