



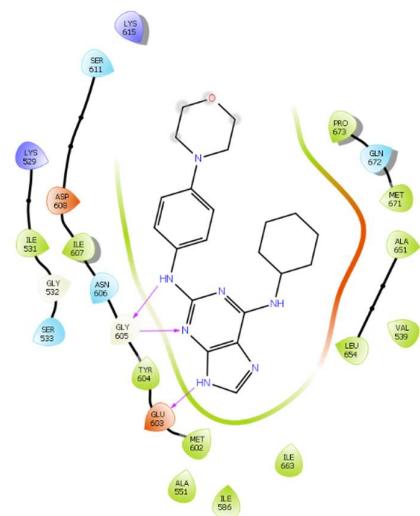
## Support Information

# The dynamics of Mps1 kinase molecular interactions with iso-flavones revealed a chemical scaffold with potential to develop new therapeutics for the treatment of cancer

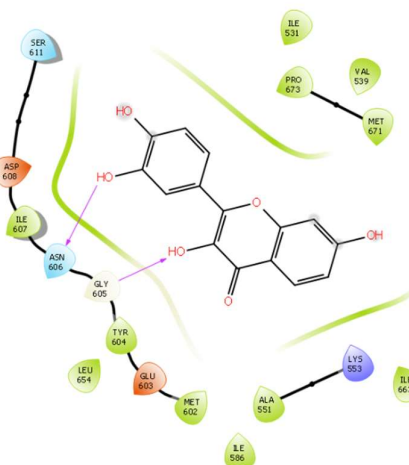
Lauren Pugh<sup>1</sup>, Alisha Pancholi<sup>1</sup>, Priscila Celeste Purat<sup>1</sup>, Sandra Agudo-Alvarez<sup>2</sup>, Raúl Benito-Arenas<sup>2</sup>, Agatha Bastida<sup>2\*</sup>, Victor M. Bolanos-Garcia<sup>1\*</sup>

**Figure S1.** 2D structure of Reversine (A), Fisetin (B), Genistein (C), Daidzein (D) and Glycitein (E) bound to Mps1 (PDB ID 5ljy).

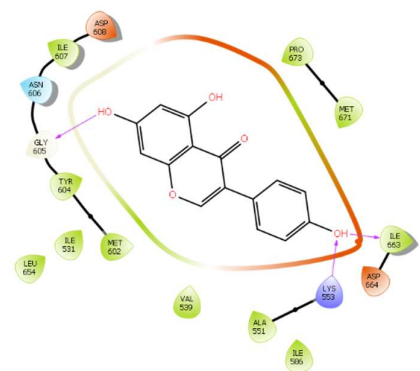
A



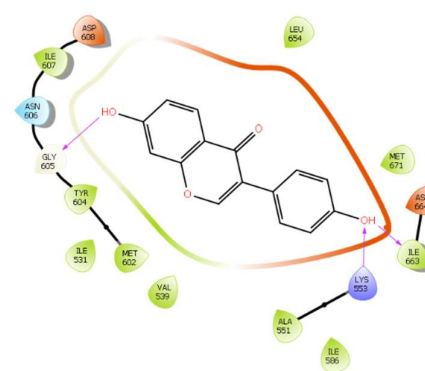
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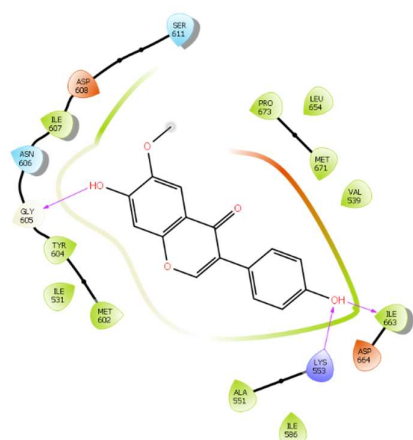
C



D



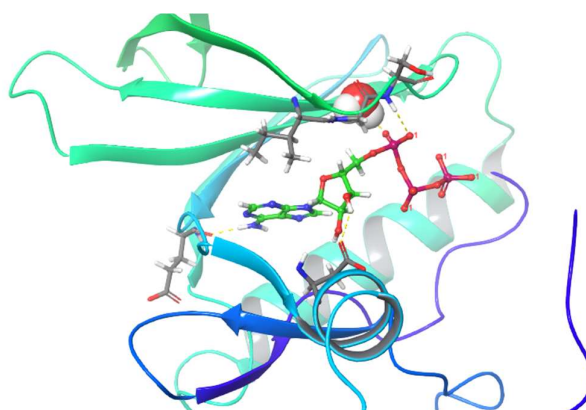
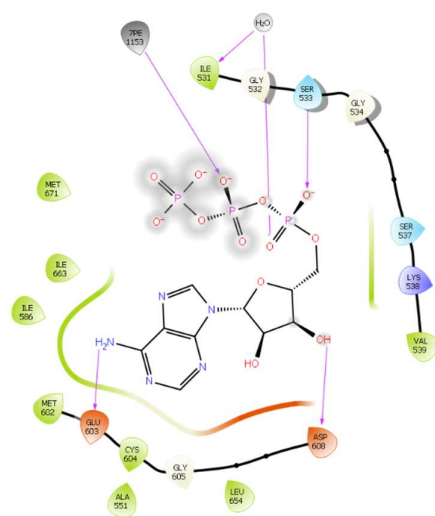
E



**Figure S2.-** (A) 2D-structure of the nucleotide binding pocket (ATP) of the Mps1; (B) 3-D representation of the Mps1-ATP complex (PDB ID 3hmn).

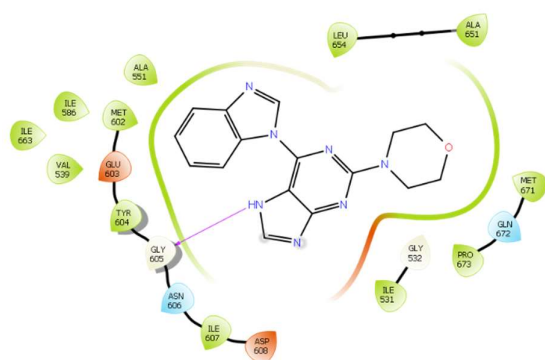
A

B

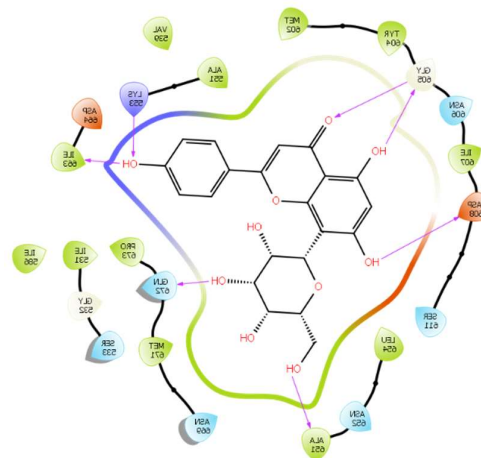


**Figure S3.** 2D structures of new isoflavoids bound to human Mps1 kinase domain. (A) CID 68916574; (B) CID 5378180; (C) CID 11810419; (D) CID 24039298.

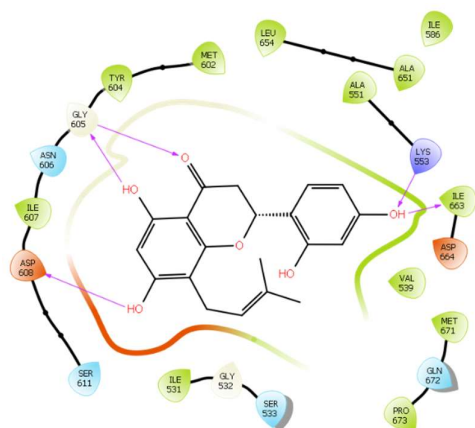
A



B



C



D

