

*Supplementary material*

## **Synthesis, Docking and Biological Evaluation of a Novel Class of Imidazothiazoles as IDO1 Inhibitors**

**Marta Serafini <sup>1,†</sup>, Enza Torre <sup>1,†</sup>, Silvio Aprile <sup>1</sup>, Alberto Massarotti <sup>1</sup>, Silvia Fallarini <sup>1</sup> and Tracey Pirali <sup>1,\*</sup>**

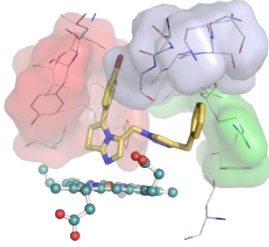
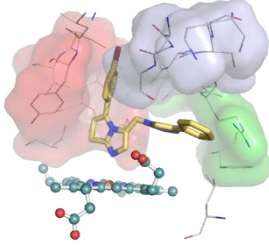
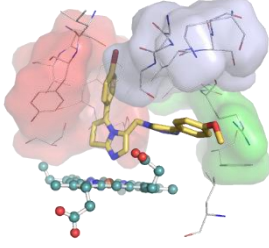
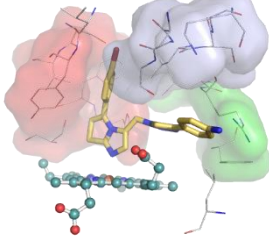
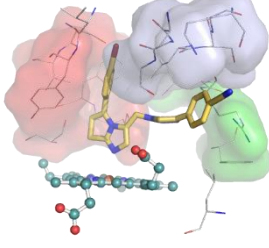
<sup>1</sup> Department of Pharmaceutical Sciences; Università del Piemonte Orientale, Largo Donegani 2, 28100, Novara, Italy;

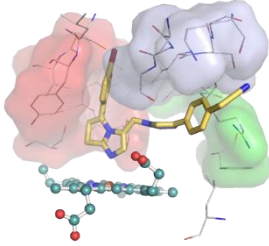
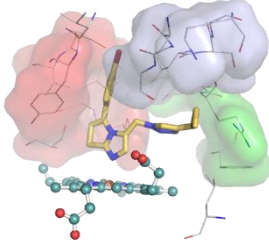
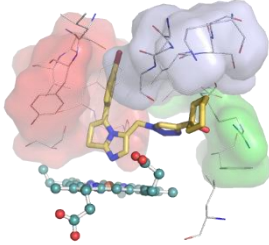
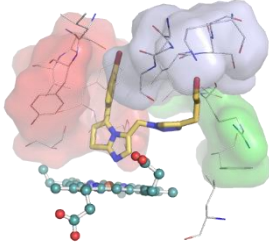
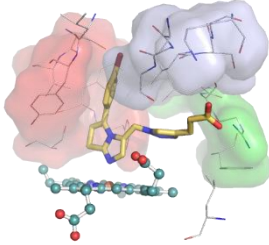
marta.serafini@uniupo.it (M.S.)

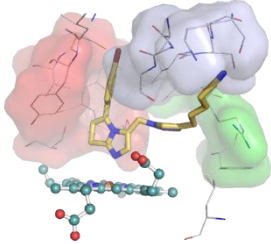
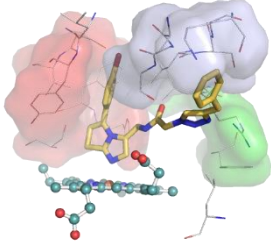
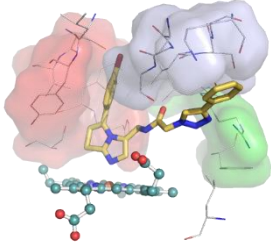
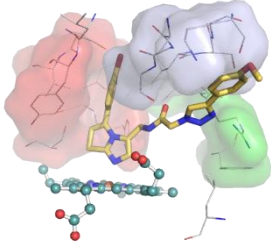
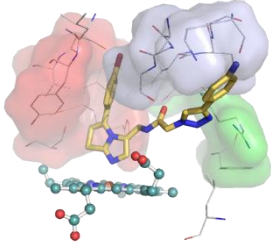
\* Correspondence: tracey.pirali@uniupo.it; Tel.: +39-0321-375-852 (T.P.)

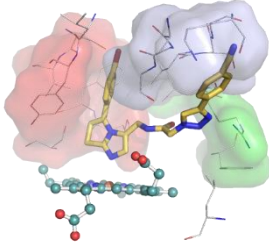
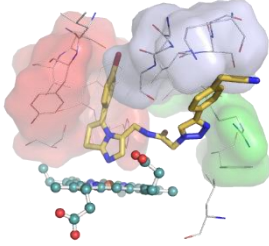
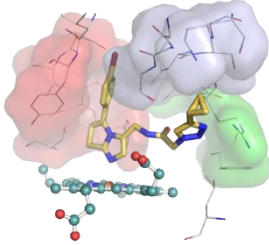
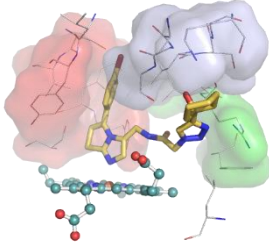
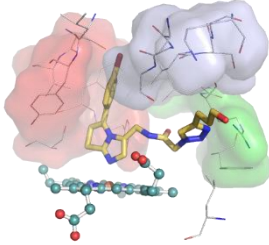
† These authors contributed equally to this work.

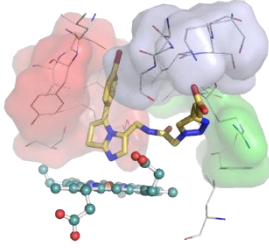
**Table S1.** Structure and biological profile of compounds evaluated by molecular docking. Structures of docking poses are depicted as gold sticks, while heme is depicted as cyan sticks. Aminoacids of pocket A, B and C are depicted as red, green and blue shape, respectively.

Cpd	FRED Chemgauss4 score	Docking pose
11a	-15.45	
11b	-13.56	
11c	-13.99	
11d	-13.97	
11e	-14.89	

Cpd	FRED Chemgauss4 score	Docking pose
11f	-14.36	
11g	-14.86	
11h	-14.40	
11i	-14.67	
11j	-14.18	

Cpd	FRED Chemgauss4 score	Docking pose
11k	-14.35	
12a	-11.98	
12b	-11.70	
12c	-12.38	
12d	-12.39	

Cpd	FRED Chemgauss4 score	Docking pose
12e	-12.74	
12f	-14.46	
12g	-14.87	
12h	-15.99	
12i	-15.16	

Cpd	FRED Chemgauss4 score	Docking pose
12j	-15.31	
12k	-15.37	