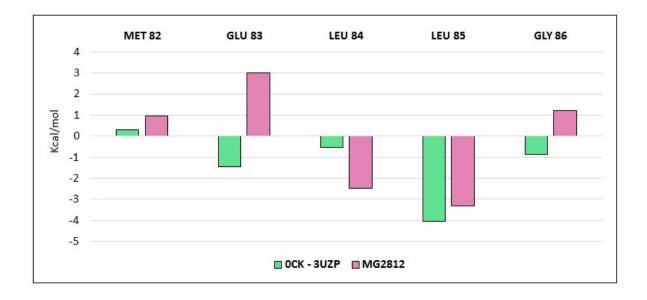
## Scaffold repurposing of in-house chemical library toward the identification of new Casein kinase 1 $\delta$ inhibitors.

Eleonora Cescon<sup>[a,b]</sup>, Giovanni Bolcato<sup>[a]</sup>, Stephanie Federico<sup>[b]</sup>, Maicol Bissaro<sup>[a]</sup>, Alice Valentini<sup>[a]</sup>, Maria Grazia Ferlin<sup>[a]</sup>, Gianpiero Spalluto<sup>[b]</sup>, Mattia Sturlese<sup>[a]</sup>, Stefano Moro<sup>[a]\*</sup>

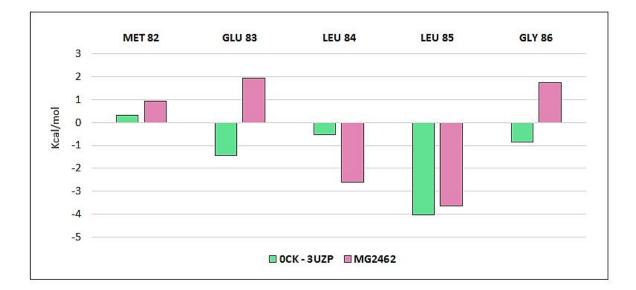
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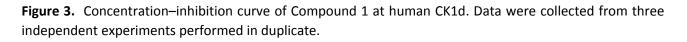
[a] Department of Pharmaceutical and Pharmacological Sciences, University of Padova, via Marzolo 5, 35131 Padova, Italy

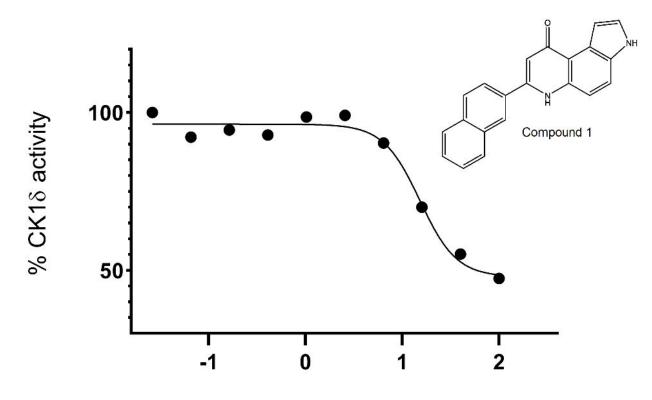
[b] Department of Chemical and Pharmaceutical Sciences, University of Trieste, Piazzale Europa,1 34127 Trieste, Italia **Figure 1.** The plot displays the comparison of the electrostatic contributions to the interaction energy of OCK (3UZP ligand) and Compound 1.



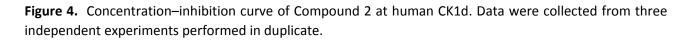
**Figure 2.** The plot displays the comparison of the electrostatic contributions to the interaction energy of OCK (3UZP ligand) and Compound 2.

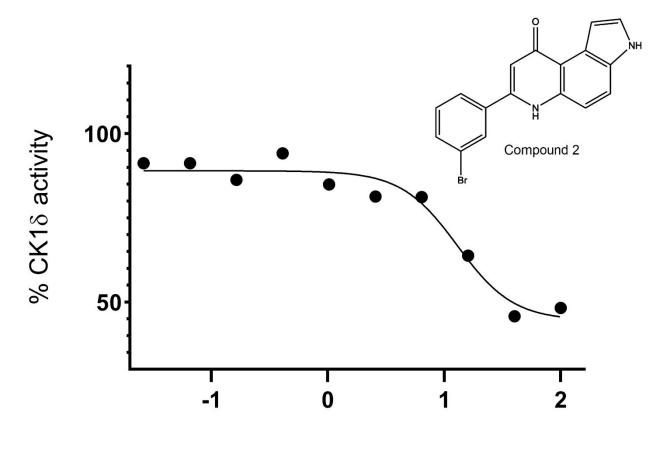






Log [Compound 1]  $\mu M$ 





Log [Compound 2]  $\mu M$