## **Supporting Information**

## Discovery of 3-hydroxy-3-pyrrolin-2-one-based mPGES-1 inhibitors using a multi-step virtual screening protocol

Gianluigi Lauro,<sup>a</sup> Vincenza Cantone,<sup>a</sup> Marianna Potenza,<sup>a</sup> Katrin Fischer,<sup>b</sup> Andreas Koeberle,<sup>b</sup> Oliver Werz,<sup>b</sup> Raffaele Riccio,<sup>a</sup> and Giuseppe Bifulco<sup>a,\*</sup>

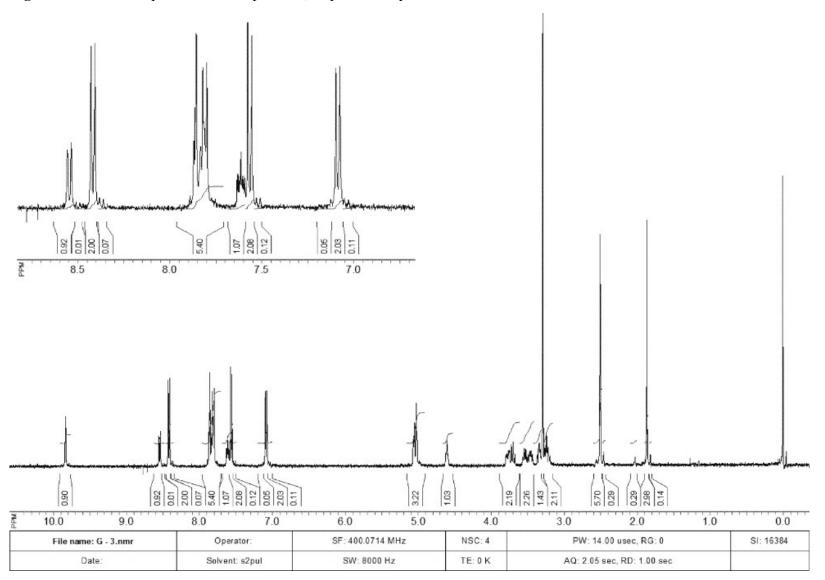
<sup>a</sup>Department of Pharmacy, University of Salerno, via Giovanni Paolo II 132, 84084 Fisciano, Italy <sup>b</sup>Department of Pharmaceutical/Medicinal Chemistry, Institute of Pharmacy, Friedrich-Schiller-University Jena, Philosophenweg 14, D-07743 Jena, Germany

\*To whom correspondence should be addressed: <u>bifulco@unisa.it</u>, Telephone: +39 (0)89 969741

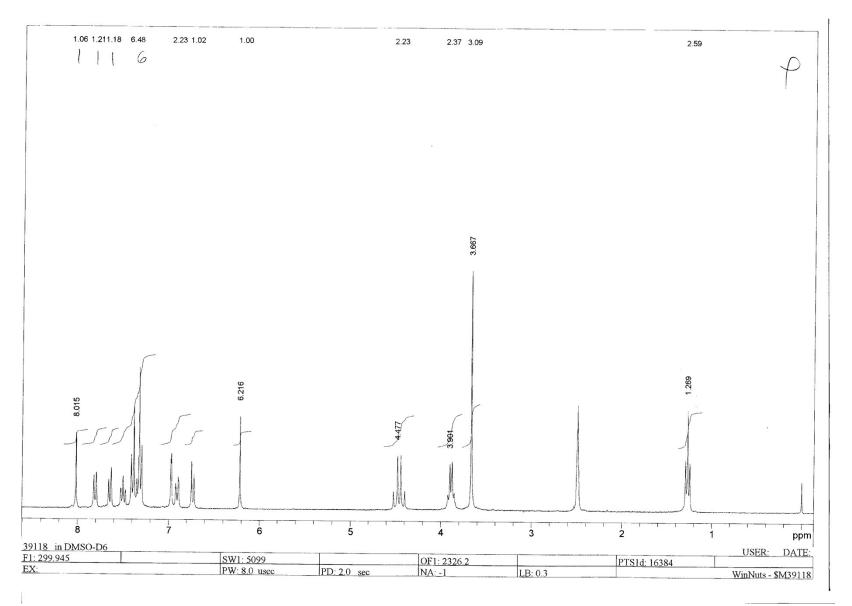
## **List of Contents**

**Figure S9** Analytical reversed-phase HPLC of compounds **2** (A) and **3** (B).... S10

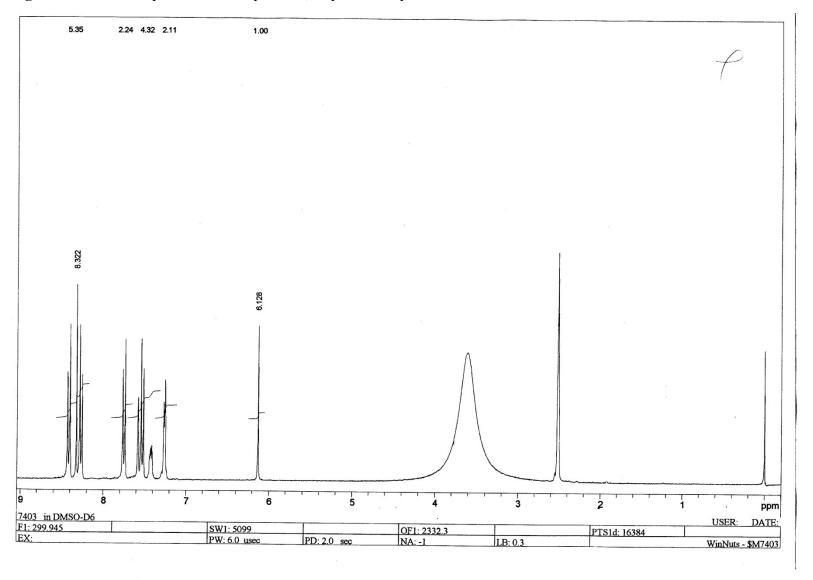
**Figure S1.** <sup>1</sup>H NMR spectrum of compound **1**, as provided by Otava Ltd.



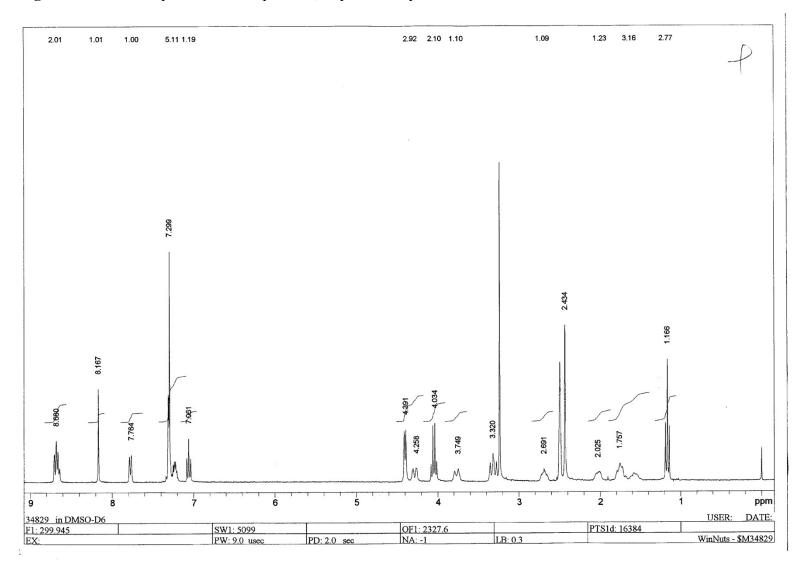
**Figure S2.** <sup>1</sup>H NMR spectrum of compound **2**, as provided by Otava Ltd.



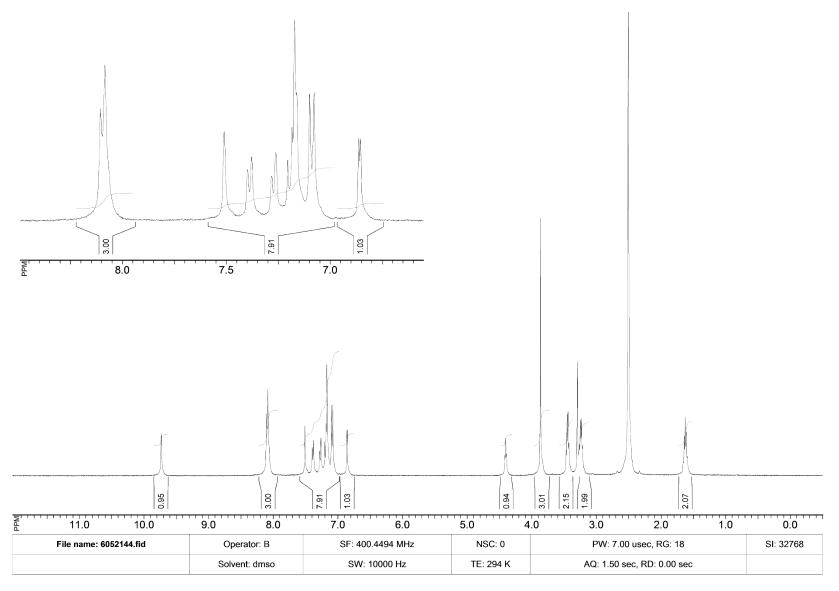
**Figure S3.** <sup>1</sup>H NMR spectrum of compound **3**, as provided by Otava Ltd.



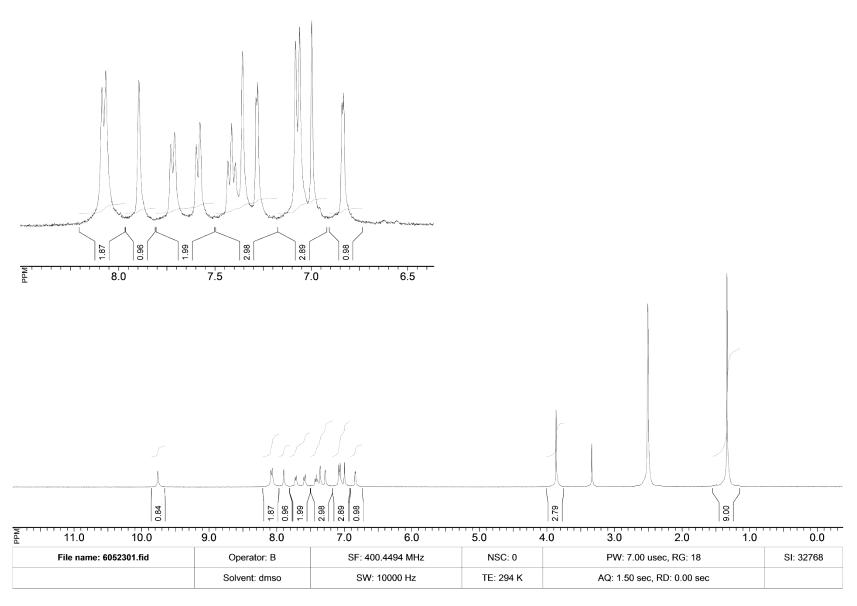
**Figure S4.** <sup>1</sup>H NMR spectrum of compound **4**, as provided by Otava Ltd.



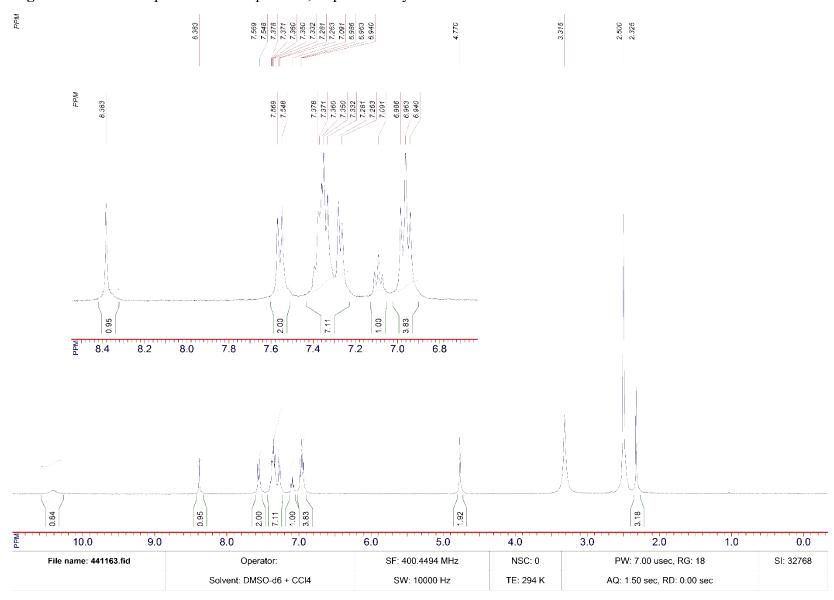
**Figure S5.** <sup>1</sup>H NMR spectrum of compound **5**, as provided by Otava Ltd.



**Figure S6.** <sup>1</sup>H NMR spectrum of compound **6**, as provided by Otava Ltd.



**Figure S7.** <sup>1</sup>H NMR spectrum of compound 7, as provided by Otava Ltd.



**Figure S8.** <sup>1</sup>H NMR spectrum of compound **8**, as provided by Otava Ltd.

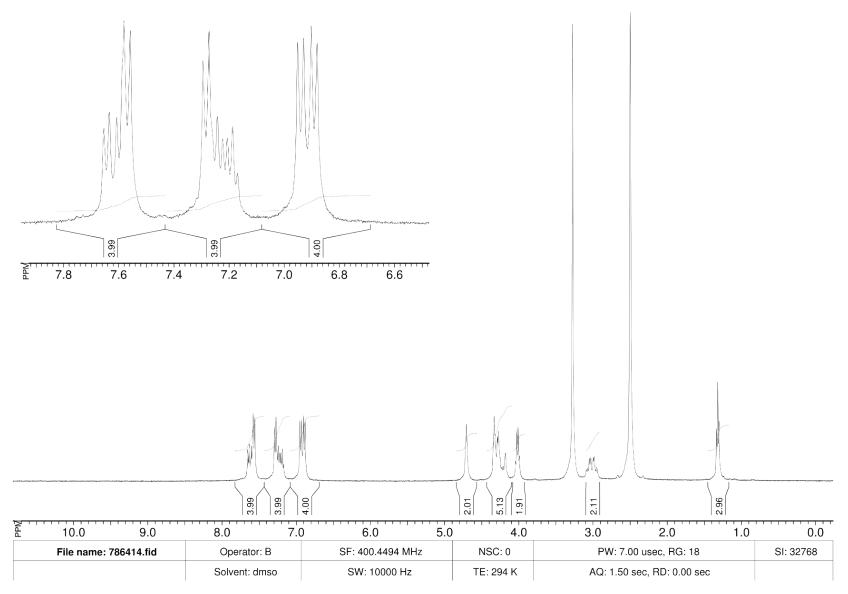


Figure S9. Analytical reversed-phase HPLC of compounds 2 (A) and 3 (B).



