

*Supplementary materials for:*

# **Discovery of a novel trifluoromethyl diazirine inhibitor of SARS-CoV-2 M<sup>pro</sup>**

**Andrea Citarella,<sup>1</sup> Davide Moi,<sup>2</sup> Martina Pedrini,<sup>1</sup> Helena Pérez-Peña,<sup>1</sup> Stefano Pieraccini,<sup>1</sup> Claudio Stagno,<sup>3</sup> Nicola Micale,<sup>3</sup> Tanja Schirmeister,<sup>4</sup> Giulia Sibille,<sup>5</sup> Giorgio Gribaldo,<sup>5</sup> Alessandra Silvani,<sup>1</sup> Daniele Passarella<sup>1</sup> and Clelia Giannini,<sup>\*1</sup>**

<sup>1</sup> Department of Chemistry, University of Milan, Via Golgi 19, 20133, Milano, Italy

<sup>2</sup> Dipartimento di Scienze Chimiche e Geologiche, University of Cagliari, Cittadella Universitaria - S.S. 554 bivio per Sestu, Monserrato (CA), 09042, Italy

<sup>3</sup> Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Viale Ferdinando Stagno D'Alcontres 31, I-98166 Messina

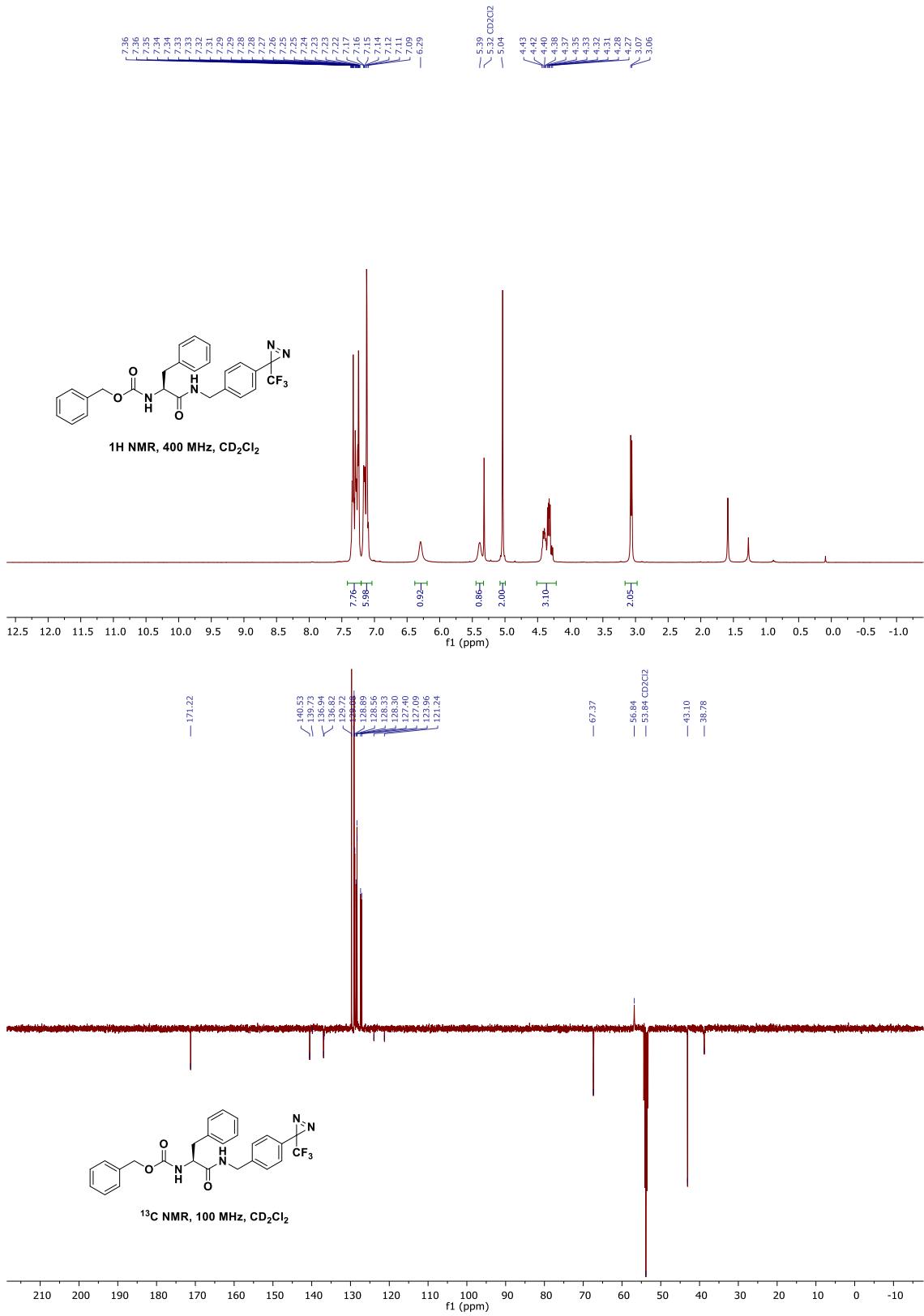
<sup>4</sup> Department of Medicinal Chemistry, Institute of Pharmaceutical and Biomedical Sciences, Johannes Gutenberg University, Staudinger Weg 5, 55128 Mainz, Germany

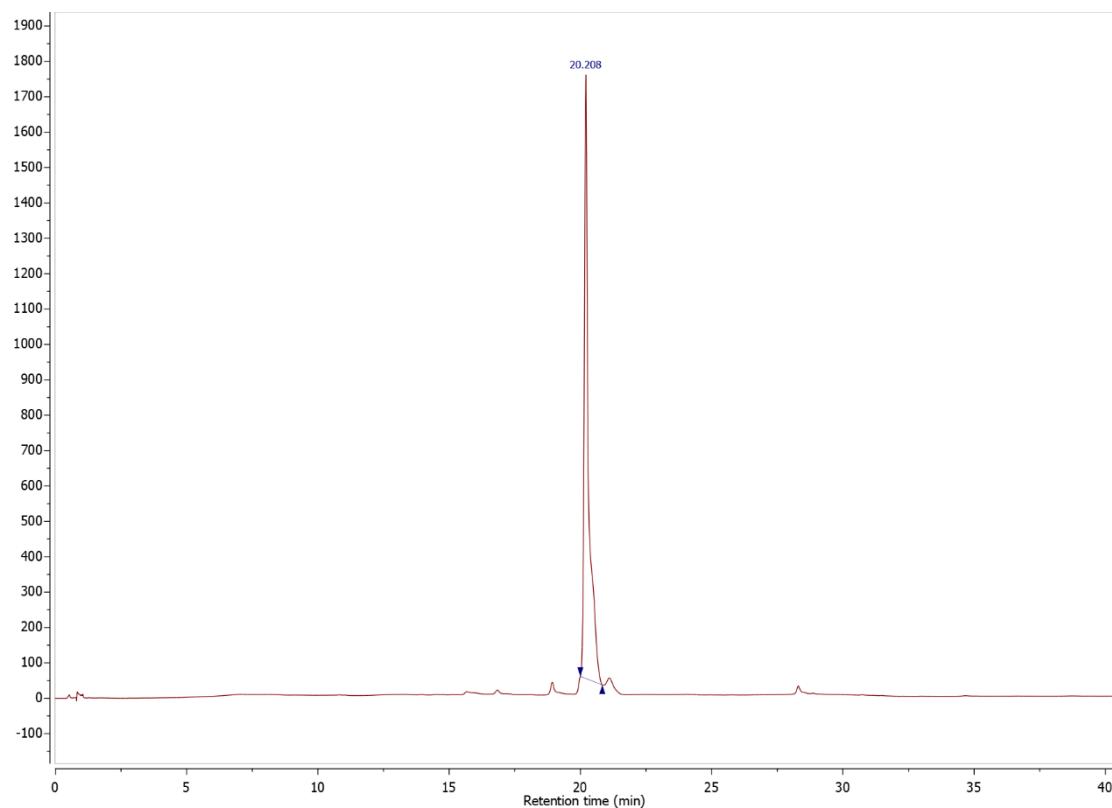
<sup>5</sup> Department of Life Sciences and Systems Biology, University of Turin, Via Accademia Albertina 13, 10123, Torino, Italy

Correspondence: clelia.giannini@unimi.it

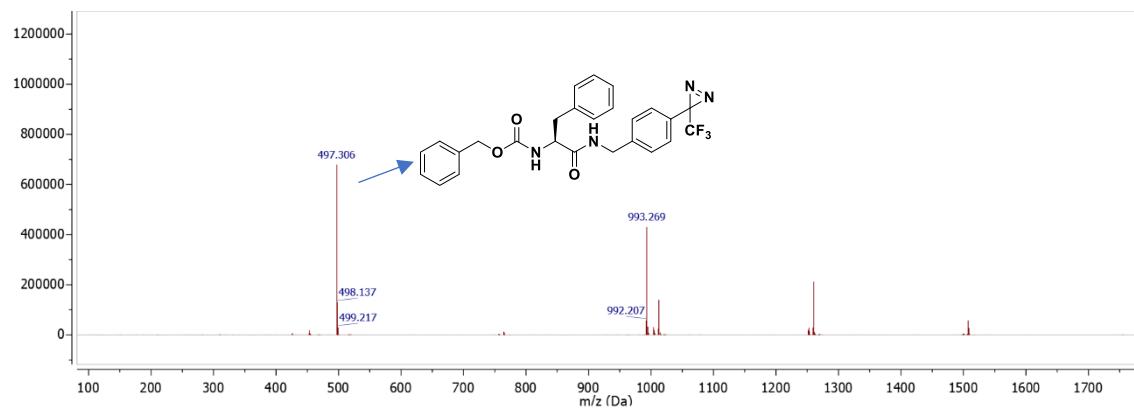
## **Table of contents**

<b>1. <sup>1</sup>H- and <sup>13</sup>C- NMR Spectra of MPD112</b>	<b>1</b>
<b>2. HPLC trace (Figure S1) and MS Spectra (Figure S2) of MPD112</b>	<b>2</b>
<b>3. Dose-response curve of MPD112 (Figure S3)</b>	<b>3</b>



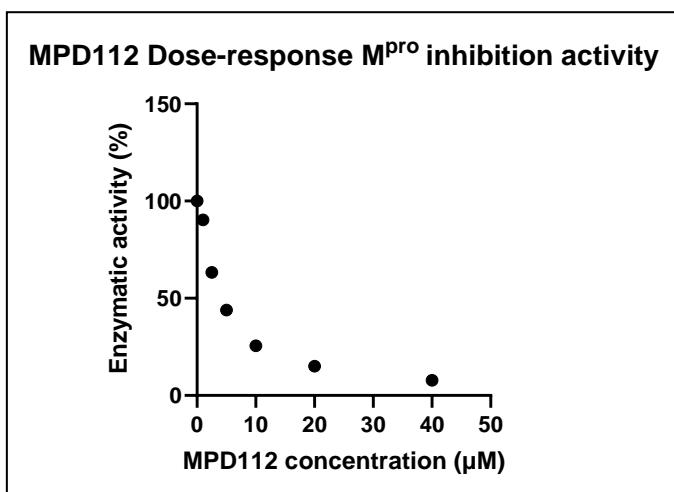


**Figure S1.** HPLC trace of MPD112.



**Figure S2.** MS spectra of MPD112.

Predicted  $m/z$  [M+H] $^+$ : 497.179, found 497.306.



**Figure S3.** Dose-response curve of MPD112.