

## Supplementary Material

# Assessment of a Diverse Array of Nitrite Scavengers in Solution and Solid State: A Study of Inhibitory Effect on the Formation of Alkyl-Aryl and Dialkyl *N*-Nitrosamine Derivatives

Miha Homšak <sup>1,†</sup>, Marko Trampuž <sup>1,†</sup>, Klemen Naveršnik <sup>1</sup>, Zoran Kitanovski <sup>1</sup>, Mateja Žnidarič <sup>1</sup>, Markus Kiefer <sup>2</sup> and Zdenko Časar <sup>1,3,\*</sup>

<sup>1</sup> Sandoz Development Center Slovenia, Lek Pharmaceuticals d.d., Kolodvorska cesta 27, 1234 Mengeš, Slovenia; miha.homsak@sandoz.com (M.H.); marko.trampuz@sandoz.com (M.T.); klemen.naversnik@sandoz.com (K.N.); zoran.kitanovski@sandoz.com (Z.K.); mateja.znidaric@novartis.com (M.Ž.)

<sup>2</sup> Global Manufacturing Science & Technology, Novartis Technical Operations, Fabrikstrasse 2, Novartis AG, 4056 Basel, Switzerland; mk.kiefer@outlook.com

<sup>3</sup> Faculty of Pharmacy, University of Ljubljana, Aškerčeva cesta 7, 1000 Ljubljana, Slovenia

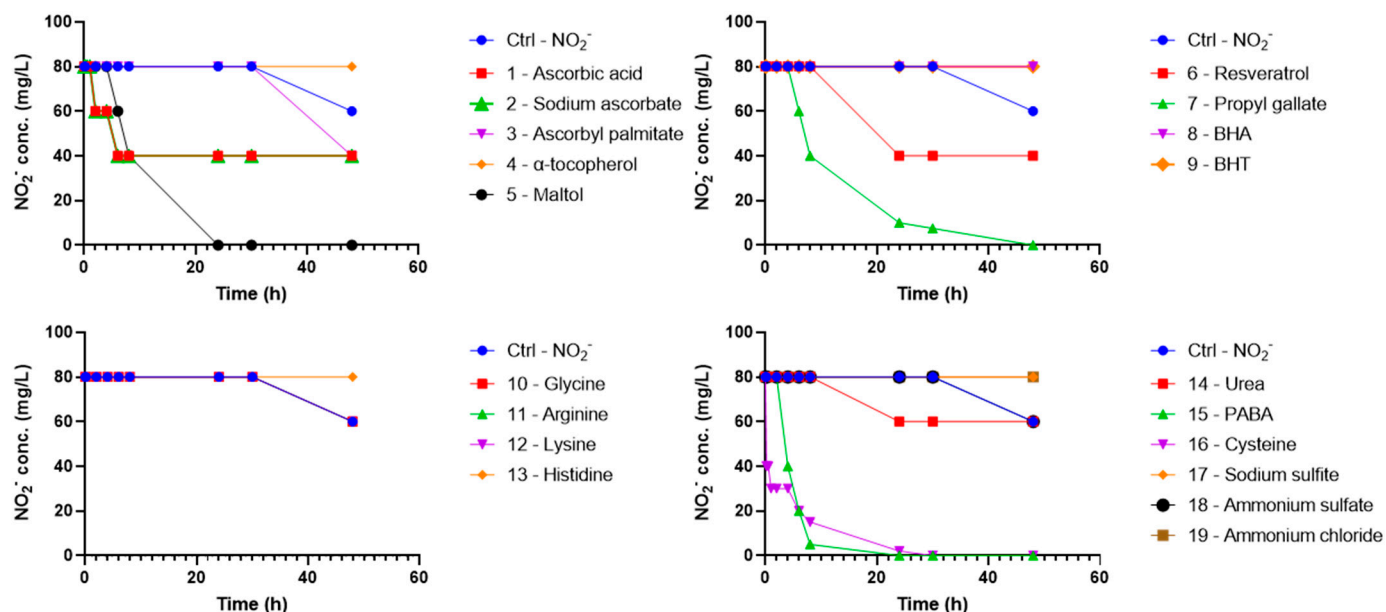
\* Correspondence: zdenko.casar@sandoz.com or zdenko.casar@ffa.uni-lj.si; Tel.: +386-1-5802079

† These authors contributed equally to this work.

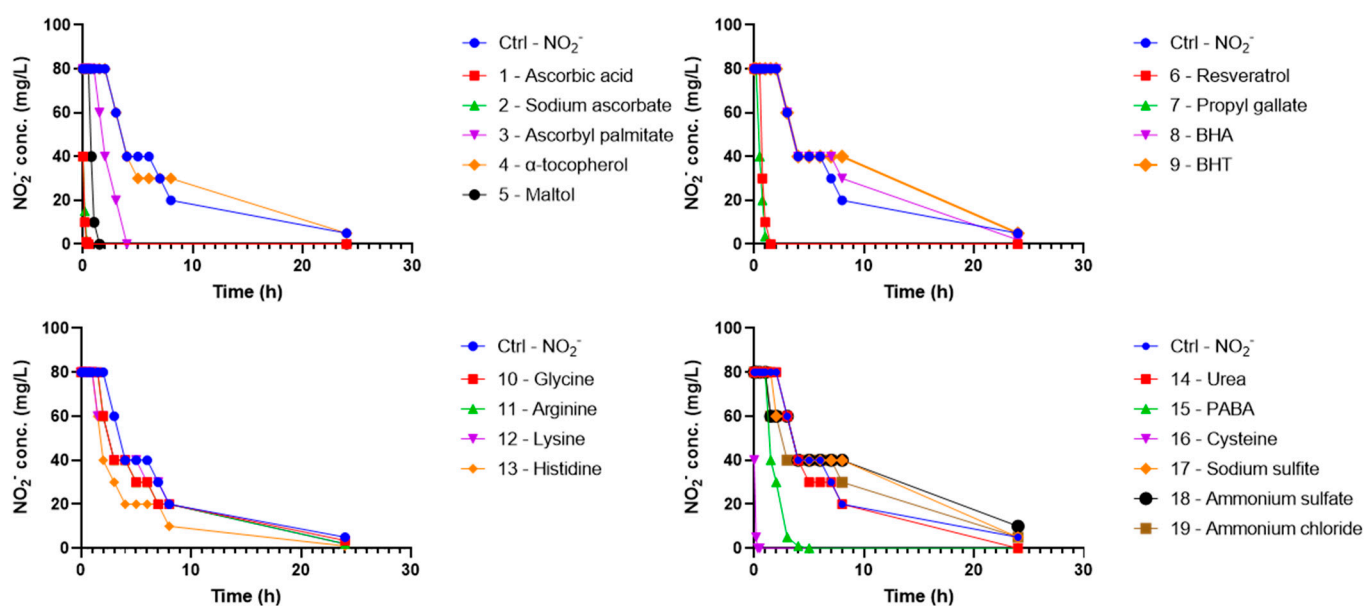
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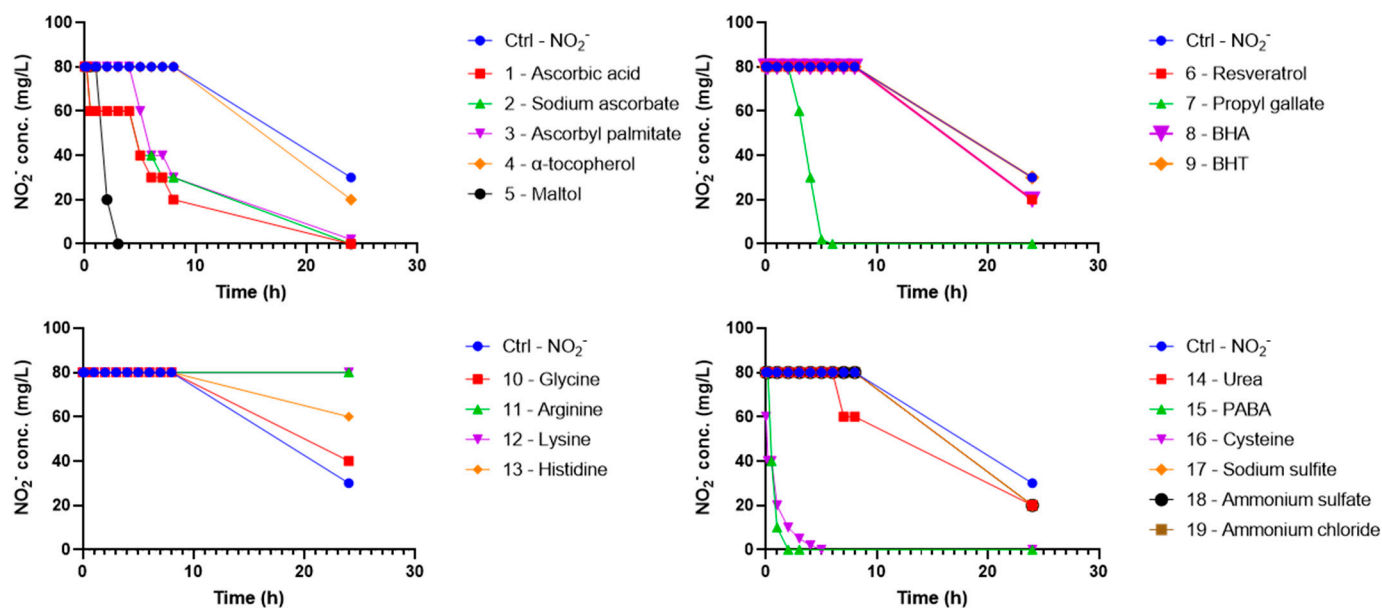
## 1. Scavenger screening experiments



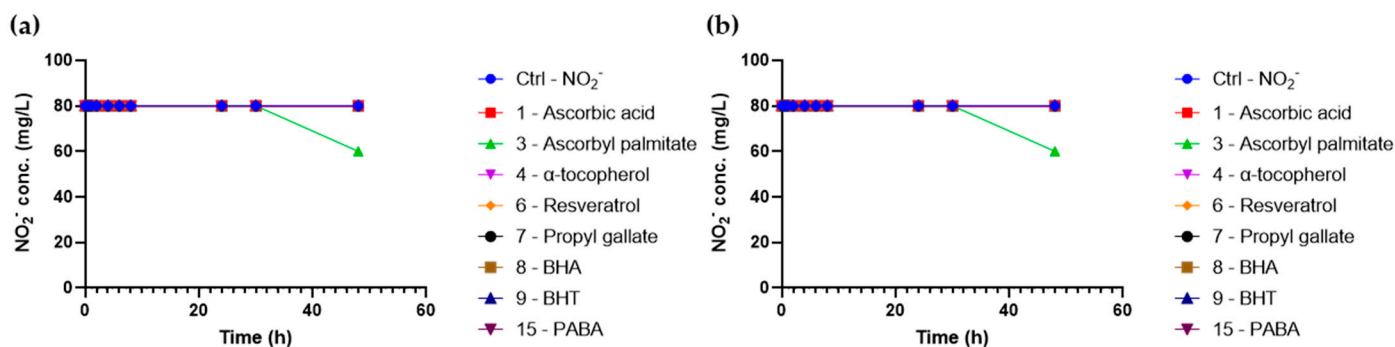
**Figure S1:** The result of the screening experiment with the 19 shortlisted scavengers. Nitrite : scavenger 1 : 10, all reactions carried out at 20 °C in pH 5.0 phosphate buffer.



**Figure S2:** The result of the screening experiment with the 19 shortlisted scavengers. Nitrite : scavenger 1 : 10, all reactions carried out at 50 °C in pH 3.0 phosphate buffer.

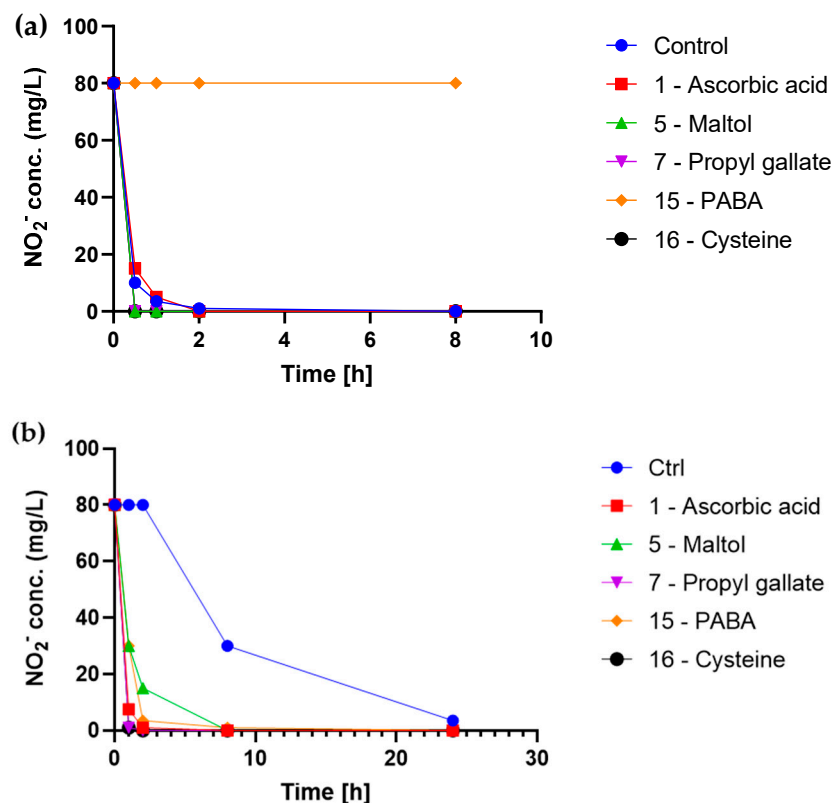


**Figure S3:** The result of the screening experiment with the 19 shortlisted scavengers. Nitrite : scavenger 1 : 10, all reactions carried out at 50 °C in pH 5.0 phosphate buffer.

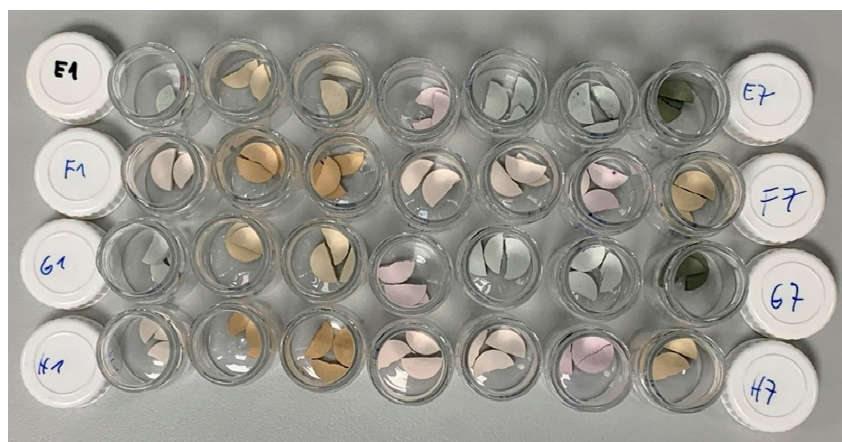


**Figure S4:** The result of the screening experiment with the 8 water-insoluble scavengers in 75 % v/v DMSO in pH 3.0 (a) or pH 5.0 (b) phosphate buffer. Nitrite : scavenger 1 : 10, all reactions carried ran at 20 °C for the first 24 h and at 50 °C for the remaining 24 h.

## 2. Scavenger evaluation experiments

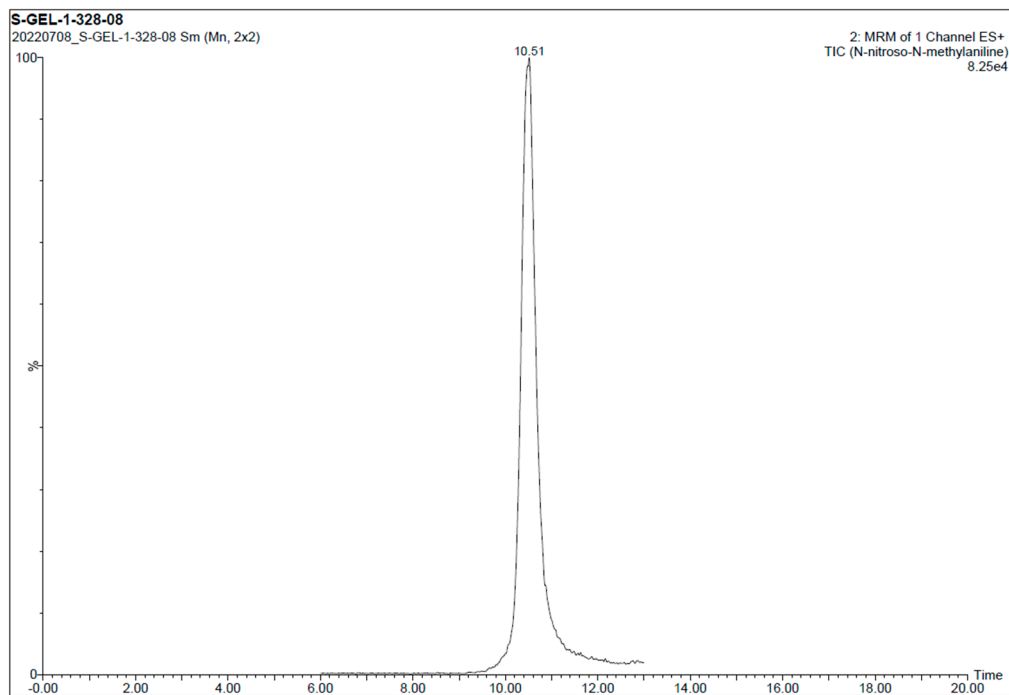


**Figure S5:**  $\text{NO}_2^-$  concentrations during experiments for evaluation of *N*-nitrosation inhibitory activity of selected nitrite scavengers 1, 5, 7, 15, and 16. (a) Experiments with MA as model API; (b) Experiments with PP as model API.

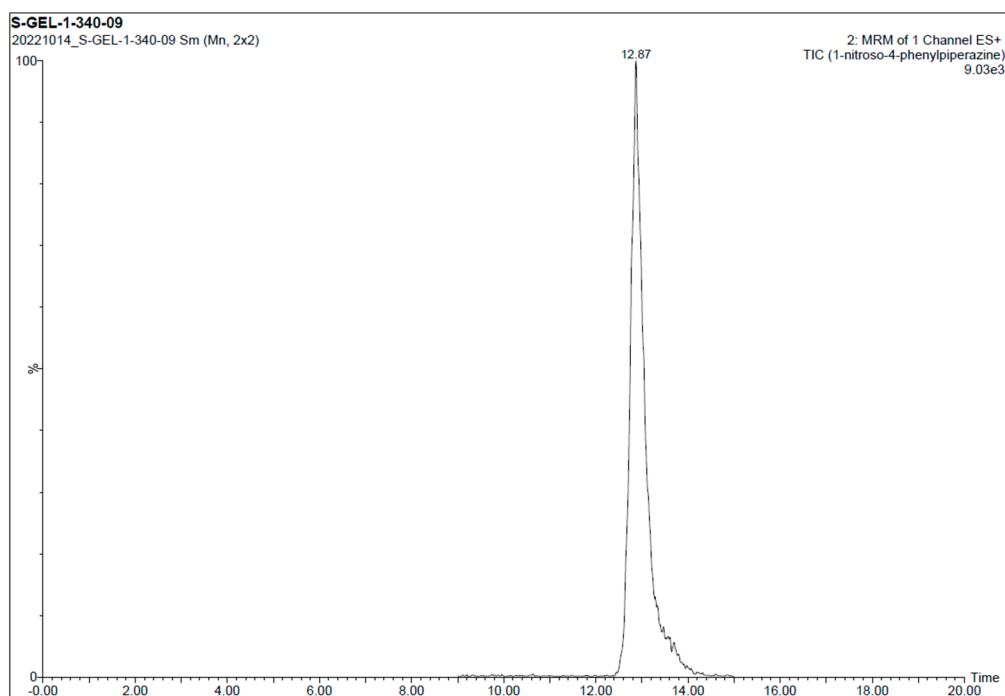


**Figure S6:** Tablets after 28-day stress testing at 50 °C and 75% RH. Rows are marked from E to H with E non-spiked tablets with MA×HCl, F non-spiked tablets with PP×HCl, G nitrite-spiked tablets with MA×HCl and H nitrite-spiked tablets with PP×HCl. Columns are marked from 1 to 7, with 1 control (no scavenger), 2 ascorbic acid, 3 sodium ascorbate, 4 cysteine, 5 maltol, 6 propyl gallate, and 7 PABA. Please note that the numbers are different to the scavenger numbering in the manuscript.

### 3. Representative chromatograms



**Figure S7:** Representative LC chromatograms for the determination of NMA.



**Figure S8:** Representative LC chromatograms for the determination of NPP.