Synthesis of Some Novel Organic Nitrates and Comparative in Vitro Study of Their Vasodilator Profile

This is the author's manuscript

Original Citation:

Availability:
This version is available http://hdl.handle.net/2318/57836 since

Published version:
DOI:10.1021/jm9002236

Terms of use:
Open Access
Anyone can freely access the full text of works made available as "Open Access". Works made available under a Creative Commons license can be used according to the terms and conditions of said license. Use of all other works requires consent of the right holder (author or publisher) if not exempted from copyright protection by the applicable law.

(Article begins on next page)
SUPPORTING INFORMATION

Synthesis of some novel organic nitrates and comparative in vitro study of their vasodilator profile.

Konstantin Chegaev,1 Loretta Lazzarato,1 Paolo Marcarino,1 Antonella Di Stilo,1 Roberta Fruttero,1 Nicolas Vanthuyne,2 Christian Roussel,2 and Alberto Gasco*1

1 Dipartimento di Scienza e Tecnologia del Farmaco, Università degli Studi di Torino, Via Pietro Giuria 9, 10125 Torino, Italy

2 UMR ISM2, Chirosciences Université Paul Cézanne Aix-Marseille III Case A62, 13397 Marseille, CEDEX 20, France

Table of contents (total of 9 pages), page S1

Elemental analyses, page S2

IR spectras, page S3-S5

Supplementary figures, page S6-S9
Elemental analyses

<table>
<thead>
<tr>
<th>Compound</th>
<th>Formula</th>
<th>Calculated</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>% C</td>
<td>% H</td>
</tr>
<tr>
<td>5a</td>
<td>C_{10}H_{11}N_{3}O_{9}</td>
<td>37.86</td>
<td>3.50</td>
</tr>
<tr>
<td>5b</td>
<td>C_{10}H_{11}N_{3}O_{9}</td>
<td>37.86</td>
<td>3.50</td>
</tr>
<tr>
<td>7</td>
<td>C_{10}H_{12}N_{2}O_{5}</td>
<td>46.89</td>
<td>4.72</td>
</tr>
</tbody>
</table>
Figure S1. IR spectra of rac 4-phenylbutane-1,2-diyldinitrate (7).
Figure S2. IR spectra of rac erythro-4-phenylbutane-1,2,3-triyl trinitrate (5a).
Figure S3. IR spectra of rac \textit{neo}-4-phenylbutane-1,2,3-triyl trinitrate (Sb).
Figure S4. Concentration-response curves of (−)5a in the absence and in the presence of inhibitors (1 μM benomyl or 1 μM ODQ) or in GTN tolerant vessels.

Figure S5. Concentration-response curves of (+)5a in the absence and in the presence of inhibitors (1 μM benomyl or 1 μM ODQ) or in GTN tolerant vessels.

Figure S6. Concentration-response curves of (−)5b in the absence and in the presence of inhibitors (1 μM benomyl or 1 μM ODQ) or in GTN tolerant vessels.
Figure S7. Concentration-response curves of (+)5b in the absence and in the presence of inhibitors (1 μM benomyl or 1 μM ODQ) or in GTN tolerant vessels.

Figure S8. Concentration-response curves of (+)7 in the absence and in the presence of inhibitors (1 μM benomyl, 1mM chloral hydrate (CH) or 1 μM ODQ) or in GTN tolerant vessels.

Figure S9. Concentration-response curves of (-)7 in the absence and in the presence of inhibitors (1 μM benomyl, 1mM chloral hydrate (CH) or 1 μM ODQ) or in GTN tolerant vessels.
Figure S10. Concentration-response curves of 9 in the absence and in the presence of inhibitors (1 μM benomyl, 1mM chloral hydrate (CH) or 1 μM ODQ) or in GTN tolerant vessels.

Figure S11. Concentration-response curves of (-)1a in the absence and in the presence of inhibitors (1 μM benomyl or 1 μM ODQ) or in GTN tolerant vessels.

Figure S12. Concentration-response curves of (+)1a in the absence and in the presence of inhibitors (1 μM benomyl or 1 μM ODQ) or in GTN tolerant vessels.
Figure S13. Concentration-response curves of (+)1b in the absence and in the presence of inhibitors (1 μM benomyl or 1 μM ODQ) or in GTN tolerant vessels

Figure S14. Concentration-response curves of (-)2 in the absence and in the presence of inhibitors (1 μM benomyl, 1mM chloral hydrate (CH) or 1 μM ODQ) or in GTN tolerant vessels

Figure S15. Concentration-response curves of 8 in the absence and in the presence of inhibitors (1 μM benomyl, 1mM chloral hydrate (CH) or 1 μM ODQ) or in GTN tolerant vessels