
1-Alkyl-2-methyl-5-nitroimidazoles represent a very important group of chemotherapeutics known as anti-protozoal and antibacterial agents [1—4]. Among them, 1-(2-hydroxypropyl)-2-methyl-5-nitroimidazole (sécnidazole) and its derivatives are reported as compounds exhibiting good antiamebic and trichomonacidal activity [5—7]. Antiparasitic activity of these derivatives was also described [8].

Recently, we have found [9, 10] that some nitrogen heterocycles substituted with a longer alkyl chain exhibit remarkable antibacterial activity, especially against gram-positive bacteria. Therefore, in our previous paper [11] we have studied in this respect some 1-(3-alkylthio-2-hydroxypropyl)-2-methyl-5-nitroimidazoles. This paper deals with corresponding 1-(3-alkylamino) analogues.

Several 1-(3-alkylamino-2-hydroxypropyl)-2-methyl-5-nitroimidazoles were prepared by the ring-opening displacement reaction of 1-(2,3-epoxypropyl)-2-methyl-5-nitroimidazole with some amines. The structure of the prepared compounds was confirmed on the basis of IR, mass, NMR spectral data and elemental analysis. Antimicrobial activity of these compounds against selected bacteria and fungi was also determined. No significant effects were found in this respect.

1-Alkyl-2-methyl-5-nitroimidazoles represent a very important group of chemotherapeutics known as anti-protozoal and antibacterial agents [1—4]. Among them, 1-(2-hydroxypropyl)-2-methyl-5-nitroimidazole (sécnidazole) and its derivatives are reported as compounds exhibiting good antiamebic and trichomonacidal activity [5—7]. Antiparasitic activity of these derivatives was also described [8].

Recently, we have found [9, 10] that some nitrogen heterocycles substituted with a longer alkyl chain exhibit remarkable antibacterial activity, especially against gram-positive bacteria. Therefore, in our previous paper [11] we have studied in this respect some 1-(3-alkylthio-2-hydroxypropyl)-2-methyl-5-nitroimidazoles. This paper deals with corresponding 1-(3-alkylamino) analogues.

Starting from 1-(2,3-epoxypropyl)-2-methyl-5-nitroimidazole (I), prepared from 1-(3-chloro-2-hydroxypropyl)-2-methyl-5-nitroimidazole (ornidazole) by alkaline dehydrohalogenation [12], we have synthesized several 1-(3-alkylamino-2-hydroxypropyl)-2-methyl-5-nitroimidazoles II—XXXII (Scheme 1). The yields of ring-opening displacement reaction of I with amine nucleophiles depend on the basicity of corresponding amine. Generally, very basic starting amines afforded lower yields of desired products. When primary amines were used as reactants, the main products represented monoalkylated amines with minority of corresponding dialkylated amines. Secondary starting amines afforded exclusively monoalkylated products. Reaction of I with piperazine (in the mole ratio 1:1) gave a mixture (x = 1 : 1) of mono- and dialkylated products (XXXI, XXXII). This mixture was separated by preparative TLC and both compounds were isolated and characterized. When

\[
\begin{align*}
\text{I} & \quad \text{II—XXXII} \\
\text{O} & \quad \text{O} \\
\text{N} & \quad \text{N} \\
\text{CH}_3 & \quad \text{CH}_3 \\
\text{CH}_2 & \quad \text{CH}_2 \\
\text{CHCH}_2 & \quad \text{CHCH}_2 \\
\text{OH} & \quad \text{N—X} \\
& \quad \text{Y}
\end{align*}
\]

Scheme 1
the mole ratio of \( I \) and piperazine was 2 : 1, only 
\( XXXII \) was isolated. The survey and characterization 
of the prepared compounds is summarized in Table 1. Their structure was confirmed on the basis of

<table>
<thead>
<tr>
<th>Compound X</th>
<th>Y</th>
<th>Formula</th>
<th>( M_r )</th>
<th>( \frac{w_{(\text{calc})}}{w_{(\text{found})}} % )</th>
<th>Yield ( % )</th>
<th>M.p. ( ^\circ \text{C} )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>II</strong> Isopropyl</td>
<td>H</td>
<td>( \text{C}_5\text{H}_8\text{N}_4\text{O}_3 )</td>
<td>242.32</td>
<td>49.56 7.50 23.13</td>
<td>71</td>
<td>68–69</td>
</tr>
<tr>
<td><strong>III</strong> Isobutyl</td>
<td>H</td>
<td>( \text{C}<em>{11}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>256.35</td>
<td>51.54 7.88 21.86</td>
<td>77</td>
<td>73–74</td>
</tr>
<tr>
<td><strong>IV</strong> 2,2-Diethoxyethyl</td>
<td>H</td>
<td>( \text{C}<em>{13}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>316.41</td>
<td>49.34 7.66 17.71</td>
<td>89</td>
<td>109–110</td>
</tr>
<tr>
<td><strong>V</strong> 2-Methoxyethyl</td>
<td>H</td>
<td>( \text{C}<em>{10}\text{H}</em>{18}\text{N}_4\text{O}_3 )</td>
<td>258.32</td>
<td>46.49 7.04 21.69</td>
<td>84</td>
<td>86–87</td>
</tr>
<tr>
<td><strong>VI</strong> 2-Dimethylaminoethyl</td>
<td>H</td>
<td>( \text{C}<em>{11}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>271.37</td>
<td>48.68 7.82 25.81</td>
<td>79</td>
<td>95–96</td>
</tr>
<tr>
<td><strong>VII</strong> 3,3-Dimethoxypropyl</td>
<td>H</td>
<td>( \text{C}<em>{12}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>302.38</td>
<td>47.66 7.35 18.53</td>
<td>82</td>
<td>113–114</td>
</tr>
<tr>
<td><strong>VIII</strong> 3-Dimethylaminopropyl</td>
<td>H</td>
<td>( \text{C}<em>{12}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>285.40</td>
<td>50.50 8.14 24.54</td>
<td>78</td>
<td>98–99</td>
</tr>
<tr>
<td><strong>IX</strong> Benzyl</td>
<td>H</td>
<td>( \text{C}<em>{14}\text{H}</em>{19}\text{N}_4\text{O}_3 )</td>
<td>280.36</td>
<td>57.91 6.26 19.30</td>
<td>80</td>
<td>101–102</td>
</tr>
<tr>
<td><strong>X</strong> Furfuryl</td>
<td>H</td>
<td>( \text{C}<em>{12}\text{H}</em>{18}\text{N}_4\text{O}_3 )</td>
<td>280.32</td>
<td>51.41 5.76 19.99</td>
<td>81</td>
<td>104–105</td>
</tr>
<tr>
<td><strong>XI</strong> Hexyl</td>
<td>H</td>
<td>( \text{C}<em>{13}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>284.41</td>
<td>54.90 8.52 19.70</td>
<td>78</td>
<td>90–91</td>
</tr>
<tr>
<td><strong>XII</strong> Heptyl</td>
<td>H</td>
<td>( \text{C}<em>{14}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>298.44</td>
<td>56.34 8.80 18.78</td>
<td>79</td>
<td>92–93</td>
</tr>
<tr>
<td><strong>XIII</strong> Octyl</td>
<td>H</td>
<td>( \text{C}<em>{16}\text{H}</em>{30}\text{N}_6\text{O}_3 )</td>
<td>312.47</td>
<td>57.65 9.05 17.93</td>
<td>78</td>
<td>86–87</td>
</tr>
<tr>
<td><strong>XIV</strong> Nonyl</td>
<td>H</td>
<td>( \text{C}<em>{18}\text{H}</em>{32}\text{N}_6\text{O}_3 )</td>
<td>326.50</td>
<td>58.85 9.28 17.16</td>
<td>78</td>
<td>89–91</td>
</tr>
<tr>
<td><strong>XV</strong> Decyl</td>
<td>H</td>
<td>( \text{C}<em>{17}\text{H}</em>{32}\text{N}_6\text{O}_3 )</td>
<td>340.53</td>
<td>58.81 9.30 17.12</td>
<td>79</td>
<td>92–94</td>
</tr>
<tr>
<td><strong>XVI</strong> Dodecyl</td>
<td>H</td>
<td>( \text{C}<em>{19}\text{H}</em>{36}\text{N}_6\text{O}_3 )</td>
<td>368.59</td>
<td>61.91 9.86 15.20</td>
<td>77</td>
<td>95–97</td>
</tr>
<tr>
<td><strong>XVII</strong> Piperidino*</td>
<td>H</td>
<td>( \text{C}<em>{12}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>268.36</td>
<td>53.70 7.53 20.88</td>
<td>72</td>
<td>123–124</td>
</tr>
<tr>
<td><strong>XVIII</strong> 2-Ethylpiperidino*</td>
<td>H</td>
<td>( \text{C}<em>{14}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>296.42</td>
<td>56.72 8.18 19.91</td>
<td>70</td>
<td>117–118</td>
</tr>
<tr>
<td><strong>XIX</strong> Morpholino*</td>
<td>H</td>
<td>( \text{C}<em>{11}\text{H}</em>{19}\text{N}_4\text{O}_3 )</td>
<td>270.33</td>
<td>56.77 8.23 18.86</td>
<td>74</td>
<td>137–138</td>
</tr>
<tr>
<td><strong>XX</strong> Ethyl</td>
<td>Ethyl</td>
<td>( \text{C}<em>{11}\text{H}</em>{20}\text{N}_6\text{O}_3 )</td>
<td>256.35</td>
<td>51.54 7.68 21.86</td>
<td>70</td>
<td>75–76</td>
</tr>
<tr>
<td><strong>XXI</strong> 2-Hydroxyethyl</td>
<td>Methyl</td>
<td>( \text{C}<em>{10}\text{H}</em>{18}\text{N}_4\text{O}_3 )</td>
<td>258.32</td>
<td>46.49 7.04 21.69</td>
<td>73</td>
<td>97–98</td>
</tr>
<tr>
<td><strong>XXII</strong> 2-Cyanoethyl</td>
<td>Methyl</td>
<td>( \text{C}<em>{11}\text{H}</em>{20}\text{N}_6\text{O}_3 )</td>
<td>267.33</td>
<td>49.42 6.42 26.20</td>
<td>75</td>
<td>91–92</td>
</tr>
<tr>
<td><strong>XXIII</strong> Butyl</td>
<td>Methyl</td>
<td>( \text{C}<em>{12}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>270.38</td>
<td>53.30 8.22 20.73</td>
<td>71</td>
<td>86–87</td>
</tr>
<tr>
<td><strong>XXIV</strong> 2-Hydroxyethyl</td>
<td>2-Hydroxyethyl</td>
<td>( \text{C}<em>{11}\text{H}</em>{20}\text{N}_6\text{O}_3 )</td>
<td>288.35</td>
<td>45.82 7.01 19.43</td>
<td>74</td>
<td>103–104</td>
</tr>
<tr>
<td><strong>XXV</strong> Propyl</td>
<td>Propyl</td>
<td>( \text{C}<em>{13}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>284.41</td>
<td>54.90 8.52 19.70</td>
<td>71</td>
<td>78–79</td>
</tr>
<tr>
<td><strong>XXVI</strong> Allyl</td>
<td>Allyl</td>
<td>( \text{C}<em>{12}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>280.37</td>
<td>55.69 7.20 19.99</td>
<td>73</td>
<td>73–74</td>
</tr>
<tr>
<td><strong>XXVII</strong> Benzyl</td>
<td>Methyl</td>
<td>( \text{C}<em>{15}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>304.39</td>
<td>55.75 7.19 19.95</td>
<td>75</td>
<td>91–92</td>
</tr>
<tr>
<td><strong>XXVIII</strong> Hexyl</td>
<td>Hexyl</td>
<td>( \text{C}<em>{19}\text{H}</em>{36}\text{N}_6\text{O}_3 )</td>
<td>368.59</td>
<td>61.91 9.86 15.20</td>
<td>75</td>
<td>139–141</td>
</tr>
<tr>
<td><strong>XXIX</strong> 2-Hydroxypropyl</td>
<td>Octyl</td>
<td>( \text{C}<em>{18}\text{H}</em>{34}\text{N}_6\text{O}_3 )</td>
<td>370.56</td>
<td>58.34 9.27 15.12</td>
<td>76</td>
<td>71–73</td>
</tr>
<tr>
<td><strong>XXX</strong> 2-Hydroxypropyl</td>
<td>Dodecyl</td>
<td>( \text{C}<em>{22}\text{H}</em>{42}\text{N}_6\text{O}_3 )</td>
<td>426.68</td>
<td>61.92 9.94 13.13</td>
<td>75</td>
<td>78–80</td>
</tr>
<tr>
<td><strong>XXXI</strong> 1-Piperaziny l*</td>
<td>H</td>
<td>( \text{C}<em>{11}\text{H}</em>{19}\text{N}_5\text{O}_3 )</td>
<td>269.35</td>
<td>49.05 7.12 26.01</td>
<td>34</td>
<td>111–112</td>
</tr>
<tr>
<td><strong>XXXII</strong> 4-[3-(5-nitro-2-methyl-1-imidazolyl)-2-hydroxypropyl]-1-piperaziny l*</td>
<td>H</td>
<td>( \text{C}<em>{18}\text{H}</em>{26}\text{N}_6\text{O}_3 )</td>
<td>452.54</td>
<td>47.77 6.25 24.77</td>
<td>36</td>
<td>132–133</td>
</tr>
</tbody>
</table>

a) Substituent represents NXY part of the molecule; b) when the mole ratio of reactants is 1 : 1; c) when the mole ratio of \( I \) and piperazine is 2 : 1.

Chem. Papers 48 (1) 54–57 (1994)
elemental analysis and IR, mass, $^1$H and $^{13}$C NMR spectral data.

In the IR spectra of the prepared compounds strong absorption bands in the region of $\tilde{v} = 1324$ cm$^{-1}$, 1434 cm$^{-1}$, and 1465 cm$^{-1}$ (stretching vibrations of the imidazole ring), $\tilde{v} = 1265$ cm$^{-1}$ (deformation vibrations of C–H bond of imidazole ring), and $\tilde{v} = 1368$ cm$^{-1}$ and 1525 cm$^{-1}$ (stretching vibrations of the nitro group) were observed. In the case of secondary amines $II$–$XVI$ the bands in the region of $\tilde{v} = 3328$–3360 cm$^{-1}$ corresponding to the stretching vibrations of N–H bonds were registered.

Mass spectra of the prepared compounds $II$–$XXXII$ did not exhibit the peaks of molecular ions [M]$^+$. The base peaks ($I_r = 100\%$) corresponded to the ions XYN$^+$$=\text{CH}_2$ formed by $\alpha$-cleavage. Further significant peaks ($I_r = 63$–96\%) were registered for [M – NO$_2$]$^+$ fragments. Surprisingly, like in the case of analogical alkylthio derivatives [11], no rearrangement with elimination of an aldehyde or ketone, characteristic of 1-alkyl-5-nitroimidazoles [13], was observed.

Characteristic NMR data of selected compounds [11], the results of antimicrobial activity testing revealed only low efficiency against selected microorganisms. Mostly, the values of minimum inhibitory concentration (MIC) were about 1000 ppm excepting compounds $XI$–$XV$ exhibiting MIC about 10 ppm against Staphylococcus aureus, Staphylococcus epidermidis, and Bacillus subtilis (Table 2). This fact is in accordance with our previous observations [9, 10], where hexyl, heptyl, and octyl derivatives exhibited the best activity against some gram-positive bacteria.

**EXPERIMENTAL**

Starting 1-(2,3-epoxypropyl)-2-methyl-5-nitroimidazole ($I$) was prepared according to the known method [12]. Ornidazole as well as the other used chemicals were commercially available products (Lachema, Brno; Fluka, Buchs; Merck, Darmstadt).

Melting points were determined on a Kofler hot-stage. IR spectra (in KBr pellets) were obtained on a Perkin–Elmer G-983 instrument. Mass spectra (70 eV) were measured on a Jeol JMS-100D spectrometer at an emission current of 300 $\mu$A, applying direct sample-introduction technique. $^1$H and $^{13}$C NMR spectra were obtained on a Bruker AM-

**Table 2. Antimicrobial Activity (MIC/(μg cm$^{-3}$)) of the Prepared Compounds**

<table>
<thead>
<tr>
<th>Compound</th>
<th>Staphylococcus aureus</th>
<th>Staphylococcus epidermidis</th>
<th>Bacillus subtilis</th>
<th>Streptococcus faecalis</th>
<th>Escherichia coli</th>
<th>Pseudomonas aeruginosa</th>
<th>Salmonella typhimurium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$II$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$III$</td>
<td>1000</td>
<td>1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$IV$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$V$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$VI$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$VII$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$VIII$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$IX$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$X$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XI$</td>
<td>&lt;10</td>
<td>&lt;10</td>
<td>10</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XII$</td>
<td>&lt;10</td>
<td>&lt;10</td>
<td>&lt;10</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XIII$</td>
<td>10</td>
<td>10</td>
<td>&lt;10</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XIV$</td>
<td>10</td>
<td>10</td>
<td>&lt;100</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XV$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XVI$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XVII$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XVIII$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XIX$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XX$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXI$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXII$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXIII$</td>
<td>1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXIV$</td>
<td>1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXV$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXVI$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXVII$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXVIII$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXIX$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXX$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXXI$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>$XXXII$</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
</tbody>
</table>

Chem. Papers 48 (1) 54–57 (1994)
300 spectrometer operating at 300.13 MHz or 75.46 MHz working frequencies in CDCI$_3$ or DMSO-d$_6$ solutions with TMS as an internal standard. For the assignment of signals in $^{13}$C NMR spectra DEPT and semiselective INEPT techniques were used. (Note: Comma index refers to the positions of 2-hydroxy-propyl grouping; positions of the furan ring are two-comma indexed). Elemental analyses were performed on a Perkin—Elmer 240 analyzer.

MIC was determined by using the suspension method on solid cultivation media [9]. [1-(Ethoxy-carbonyl)pentadecyl]trimethylammonium bromide (Septonex), an antiseptic agent usually applied in practice, was used as a standard [14].

1-(3-Heptylamino-2-hydroxypropyl)-2-methyl-5-nitroimidazole (XII)

A mixture of epoxide I (1.83 g; 0.01 mol) and heptylamine (1.15 g; 0.01 mol) in dry methanol (30 cm$^3$) was heated under reflux for 3 h. Then the solvent was evaporated under diminished pressure and cold dry ether (20 cm$^3$) was added to the residue. Separated solid was filtered off and after decolourizing using charcoal it was recrystallized in heptyl, 56.3 (C-3'), 50.4 (C-1'), 47.1 (CH$_3$ in ethyls), 14.8 (CH$_3$ in imidazole), 11.9 (CH$_3$ in ethyls).

Compound XVIII: $^1$H NMR spectrum (CDCl$_3$), $\delta$: 7.96 (s, 1H, H-4 in imidazole), 4.56 (dd, 1H, H$_a$-'1', $J$ = 13.5 Hz and 1.4 Hz), 4.03 (dd, 1H, H$_b$-'1', $J$ = 8.4 Hz and 13.5 Hz), 3.95 (m, 1H, H-2'), 2.57 (s, 3H, CH$_3$ in imidazole), 2.32—2.54 (m, 4H, CH$_2$ in butyl), 0.92 (t, 3H, CH$_3$ in butyl). $^{13}$C NMR spectrum (CDCl$_3$), $\delta$: 152.0 (C-2), 138.2 (C-5), 133.1 (C-4), 67.2 (C-2'), 60.5 (the first CH$_3$ in butyl), 57.6 (C-3'), 50.4 (C-1'), 42.0 (N—CH$_3$), 29.3 and 20.3 (the second and the third CH$_2$ in butyl), 14.8 (CH$_3$ in imidazole), 14.0 (CH$_3$ in butyl).

Acknowledgements. The authors thank Dr. M. Kačuráková, A. Gembická, A. Karovičová, and K. Paule (Institute of Chemistry, Slovak Academy of Sciences, Bratislava) for measurements of IR, mass, and NMR spectra and for elemental analyses.

REFERENCES