

10,14-Dibenzyl-6,18-dimethyl-1,5,10,14,19,20-hexaaza-tricyclo[14.2.1.1^{5,8}]eicosa-6,8(20),16(19),17-tetraen-12-ol

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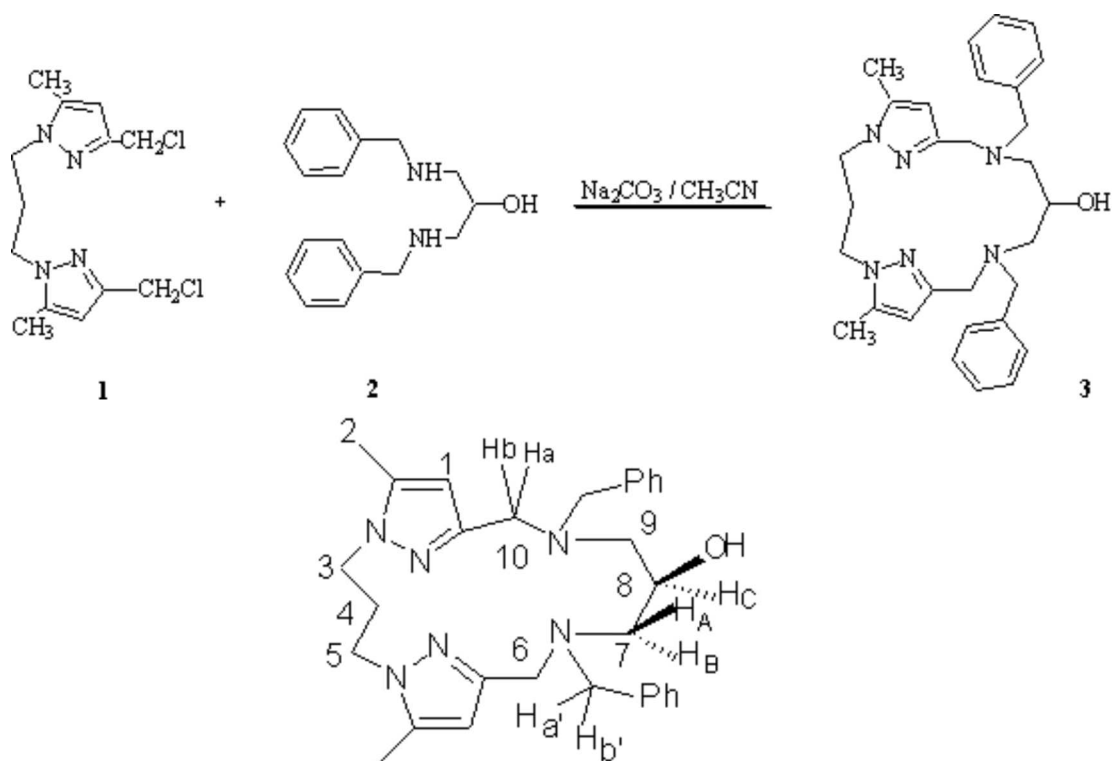
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Received: Received: 27 June 2005 / Accepted: 10 August 2005 / Published: 1 November 2005

Keywords: macrocyclic compounds, macrocyclic cavity, pyrazole

Macrocyclic chemistry is one of the fastest growing fields in chemistry. Studies of molecular recognition, transport biological aspects, selective catalysis the macrocycle containing the mixed sites of coordination, complexing with Ru (II) gives catalytic properties of SOD type and catalase [1,2], inclusion phenomena, organic synthesis and industrial applications of macrocyclic compounds are all burgeoning in many directions. In this work we describe the synthesis of new macrocyclic ligand containing pyrazole and aminic coordination sites.



A suspension of sodium carbonate (12 g, 120 mmol) in acetonitrile (250 mL) was refluxed under magnetic stirring, then a solution of 1,3-bis(3-chloromethyl-5-methylpyrazolyl)propane 1 (2.1 g, 7 mmol) [1] and 1,3-Bis-benzylamino-propan-2-ol 2 (1.9 g, 7 mmol) [3] in acetonitrile (50 mL) was added dropwise. The solution was refluxed under stirring for two hours, filtered and the solvent was removed in vacuum, the residue was purified on alumina column with (CH₂Cl₂/MeOH: 95/5) as eluent to give the 2.62 g (75% yield) macrocycle 3 as an oily substance.

¹H-NMR (250 MHz; CDCl₃): δ = 7.3-7.8 (m, H Ph); 5.85 (e, 2H, H¹); 4.06 (t, 4H, H^{3,5}); 3.96 (m, 1H, H^C)

$J_{BC}=3,33\text{ Hz}$ $J_{AC}=4,99\text{ Hz}$); 3.77 (d, 2H, H^a $J=9,09\text{ Hz}$); 3.67 (d, 2H, H^b $J=9,09\text{ Hz}$); 3.58 (d, 1H, $H^{a'}$, $J=9,08\text{ Hz}$); 3.48 (d, 1H, $H^{b'}$, $J=9,08\text{ Hz}$); 2.58 (q, 2H, H^B $J_{AB}=8,33\text{ Hz}$ $J_{BC}=3,33\text{ Hz}$); 2.49 (q, 2H, H^A $J_{AB}=8,33\text{ Hz}$ $J_{AC}=4,99\text{ Hz}$); 2.34 (t, 2H, H^4); 2.20 (d, 6H, H^2).

MS (FAB; m/z): 499 $[M+H]^+$.

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Sample Availability: Available from MDPI.

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