Saligenin derivative borocryptands: synthesis and structural analysis of new type lithium borocryptate

M. Toğrul[a]*, M. Sünkür[a], F. B. Kaynak[b], H. Hosgören[a] and S. Özbey[b]

[a]*Department of Chemistry, Faculty of Science, Dicle University, 21280 Diyarbakır, Turkey*

[b]*Deparment of Engineering Physics, Faculty of Engineering, Hacettepe University, 06532 Beytepe, Ankara, Turkey*

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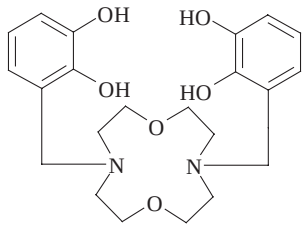
A new lithium receptor based on the combination of the [11] macrocyclic core and two 4-*tert*-butyl saligenin units was designed and prepared.

Keywords: borocryptate, lithium, Li-selective receptor, peristatic chirality, boron compounds

Due to the role played by lithium in science, medicine and technology,[1] the design of Li-selective complexing agents is still an active area of research. The complexation of lithium by a variety of synthetic receptor molecules has been investigated.[2] Among many structural features screened, cryptands[3] appeared to be the most appropriate and selective receptors for lithium. Based on structural aspects of boromycin[4] and aplasmomycin,[5] natural antibiotics bearing a spiroborate group, and of cryptands, a new family of artifical receptors for alkaline metal cations has been designed.[6-9] The early design of borocryptands was based on the double functionalisation, at both nitrogen centers, of the [11] macrocyclic core by two catechol units[10] leading thus to the receptor molecule **L1**. Probably due to the strong basic of its macrocyclic core promoting an intramolecular proton transfer from catechol moieties to the tertiary amino groups and thus generating the catecholate ammonium zwitterion **L1** was found to be extremely sensitive to oxidation and it should be stored in the absence of dioxygen.



L1

In the present contribution new lithium receptors based on the combination of the [11] macrocyclic core and two saligenin units instead of catechol moieties as in the case of **L2** was designed. The design of **L2** as a precursor of a selective lithium receptor is based on the shirinking of the size of the cavity of the borocryptand.

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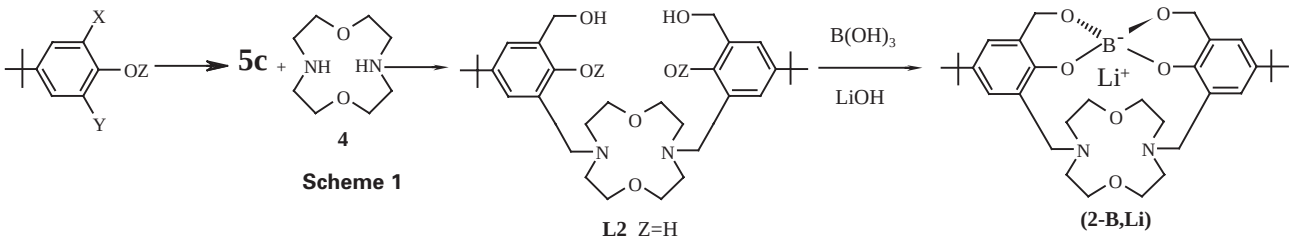

Scheme 1

L2 Z=H
L3 Z=Bn

(2-B,Li)

5 X=H; Y=H; Z=H
5a X=CH_2OH; Y=CH_2OH; Z=H
5b X=CH_2OH; Y=CH_2OH; Z=Bn
5c X=CH_2OH; Y=CH_2Cl; Z=Bn
5d X=CH_2Cl; Y=CH_2Cl; Z=Bn

* To receive any correspondence. E-mail: mtogrul@dicle.edu.tr

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