

Cryptoids May Interfere with the Binding of Rocuronium Macrocycle Complexes

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Introduction: Cryptoids are unwanted ligands that become encapsulated and buried inside the lipophilic cores of macrocyclic molecular nests(carcerand).They displace molecules from their hosts. Cyclodextrins have high affinity toward steroid based compounds, cucurbiturils toward tertiary amines. A fishing expedition was performed using isothermal titration calorimetry (ITC) to test the affinity of dexamethasone and other cryptoids for sugammadex. Over 150 molecules were screened and found to have low affinity, in contrast to tightly bound rocuronium(1) . Calabadiion is being tested as a reversal agent for rocuronium and cisatracurium(2). Do cryptoids exist for acyclic cucurbiturils?

Methods: Using ITC(isothermal titration calorimetry), the affinity constants , K_a 's, of a series of narcotic based compounds to an acyclic cucurbituril, were measured.

Results: Both fentanyl and dextrophan have high affinity for acyclic cucurbituril

Discussion: reversing a rocuronium- based neuromucular block with Calabadiion may also decrease blood narcotic levels and interfere with post operative analgesia, a phenomenon not seen with sugammadex , a selective carcerand.

References: (1) Zweirs,Clin Drug Investig 2011:31,101-111 (2)
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