Supporting Information

Structure-Activity Relationships of Truncated C2- or C8-Substituted Adenosine Derivatives as Dual Acting A_{2A} and A_3 Adenosine Receptor Ligands

Xiyan Hou,[1] Mahesh S. Majik,[1] Kyunglim Kim,[1] Yuna Pyee,[2] Yoonji Lee,[1] Varughese Alexander,[1] Hwa-Jin Chung,[2] Hyuk Woo Lee,[1] Girish Chandra,[1] Jin Hee Lee,[1] Seul-gi Park,[1] Won Jun Choi,[1,3] Hea Ok Kim,[1] Khai Phan,[4] Zhan-Guo Gao,[4] Kenneth A. Jacobson,[4] Sun Choi[1] Sang Kook Lee,[2] and Lak Shin Jeong[1,*]

[1]Laboratory of Medicinal Chemistry, College of Pharmacy and Department of Bioinspired Science, Ewha Womans University, Seoul 120-750, Korea, [2]College of Pharmacy, Seoul National University, Seoul 151-742, Korea, [3]College of Pharmacy, Dongguk University, Kyungki-do 410-774, Korea, and [4]Molecular Recognition Section, Laboratory of Bioorganic Chemistry, National Institute of Diabetes, and Digestive and Kidney Disease, National Institutes of Health, Bethesda, Maryland 20892, USA

e-mail: lakjeong@ewha.ac.kr

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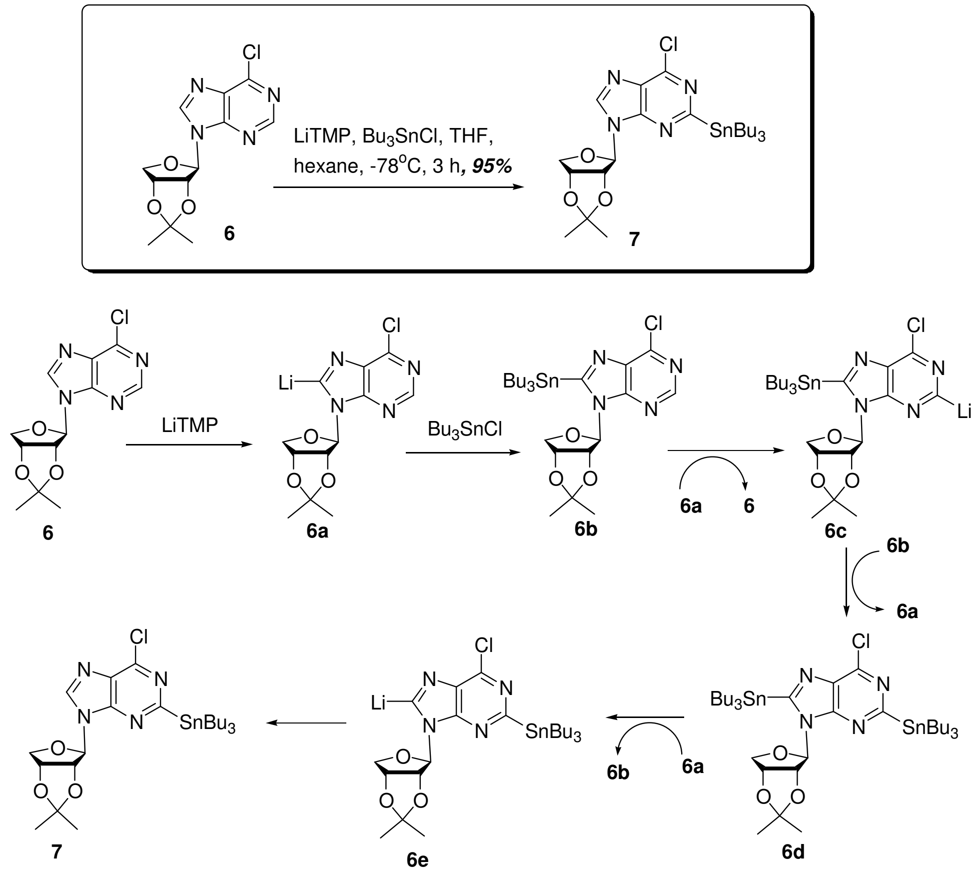
Scheme 1S. Mechanism for lithiation mediated stannyl transfer of 6-chloropurine nucleoside



The possible reaction mechanism is depicted in Scheme 1S which can be summarized as follows: The initial lithiation (LiTMP) occurs at the C8-position of purine moiety to give **6a** which was trapped with Bu_3SnCl to give C8-stannylated derivative **6b**. Further, the **6b** undergoes lithiation at the C2-position with **6a** (or with lithiating agent) to give **6c**. The reaction between **6c** and **6b** (C8-stannylated derivative) gave the 2,8-bis stannylated compound **6d** and the regeneration of **6a** simultaneously. Finally, stannyl transfer from **6d** (2,8-bis stannylated derivative) to **6a** furnish **6e** which is stable under the lithiation condition and thus get accumulated in the reaction mixture to give **7** as a sole product in regioselective manner. (Kato, K.; Hayakawa, H.; Tanaka, H.; Kumamoto, H.; Shindoh, S.; Shuto, S.; Miyasaka, T. *J. Org. Chem.* **1997**, *62*, 6833–6841).