

L15 Deuterium Labeled Compounds in Drug Discovery Process

Vijaykumar Hulikal

Bioorganics and Applied Materials Pvt Ltd.
B64/1, Licross, III Stage, PIA, Peenya
Bangalore-560 058
email: vijay.hulikal@bioorganics.biz

Abstract

Stable isotope-labeled compounds have been synthesized and utilized by scientists from various areas of biomedical research during the last several decades. Compounds labeled with stable isotopes, such as deuterium and carbon-13, have been used effectively by drug metabolism scientists and toxicologists to gain better understanding of drugs' disposition and their potential role in target organ toxicities. The combination of stable isotope-labeling techniques with mass spectrometry and nuclear magnetic resonance (NMR) spectroscopy, which allows rapid acquisition and interpretation of data, has promoted greater use of these stable isotope-labeled compounds in absorption, distribution, metabolism, and excretion (ADME) studies.

A molecule can be labeled by the direct exchange of a hydrogen atom (bonded to a carbon atom) by a deuterium atom. Since these exchange reactions can often be carried out directly on the target molecule or a late intermediate in the synthesis, and deuterium-containing reagents derived from Heavy water can be used as the deuterium source, this method is particularly efficient for the synthesis of deuterated organic compounds. Deuterium can be inserted into a molecule by halogen/deuterium exchange, reductive deuteration, and several other methods. In recent years the development of laboratory microwave apparatus has resulted in a plethora of studies on the preparation of deuterated substances by H/D exchange. Examples of the H/D exchange reactions and deuterium labeled drug entities will be presented.



Vijaykumar Hulikal is a product of Dr. Sukh Dev's school of chemistry. After a stint of 7 years abroad with prof. Guy Ourisson and prof. Vaseela, Hulikal joined Astrazeneca in the year 1992 and joined Biorganics in the year 2005 as managing director. Vijaykumar Hulikal has more than 20 years of experience in organic synthesis and Medicinal chemistry. He has three patents to his credit from AstraZeneca. He has worked in the field of microwave chemistry and in the development of small organic molecule libraries using microwave chemistry. He has developed techniques for deuterium labeling and using this technique he has synthesized deuterium labeled metabolites, APIs and manufacturing impurities.