

## Poster Presentation

MS65.P02

### *Charge Density Studies on Anti-Alzheimer Agents*

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The average age of people is increasing continuously thanks to the progress in the medicinal sciences and further social advances. As a consequence, however, diseases which affect people more likely at a higher age also increase. In this course Alzheimer's disease (AD) and related brain disorders distribute rapidly and have to be taken more serious. One of the most frequently applied drugs against AD is donepezil®. Its function is a reversible inhibition of acetylcholinesterase (AChE), thereby reducing the deficit of acetylcholine associated with the occurrence of AD. As one result from the charge density (CD) of the small-molecule structure containing the donepezilium cation comparable electronic interactions were identified as in the macromolecular TcAChE-donepezil complex which were made visible by electrostatic potential and Hirshfeld surfaces.[1] Two newer developments of Alzheimer agents are bexarotene and methylene blue. For the first one a therapeutic effect on AD in a mouse model was recently reported. From a comparative CD study on bexarotene and its disila analogue differences in the electrostatic potentials were identified, while the spherical structures showed no significant differences. The second one, methylene blue, targets the abnormal tangle type tau protein aggregation inside the nerve cells in the brain and stops its spread. The molecule is positively charged with various counterions. From the CD an answer to the not yet understood question is expected whether the formal positive charge is localized or delocalized.

[1] P. Luger, M. Weber, B. Dittrich, *Future Med. Chem.*, 2012, 4, 1399-1404

**Keywords:** Alzheimer, Drug research, charge density