26G-ISMS07 **Development and Construction of an Original Compound Library for CNS Drug Discovery: Combining Computational and Wet Data to Enhance CNS Drug-likeness**

○ Daiju HASEGAWA[1]

[1]Medicinal Chemistry, Neurology Tsukuba Research Department, Discovery, Medicine Creation, Neurology Business Group, Eisai Co., Lid.

High quality HTS hits are important for drug discovery programs to accelerate medchem campaign to clinical candidate and improve the overall success rate in the drug development. To provide such high quality HTS hits, sophisticatedly designed compound libraries play an important role in HTS strategy. In addition, a compound library with enhanced CNS drug-likeness (good brain penetrability and good oral availability) should improve the productivity of drug discovery programs in the neuroscience area. Against this background, we have been constructing a CNS-focused compound library by:

- Innovative design to improve the probability of the compounds reaching the CNS.
- Extensive *in vitro*, *in vivo* and physicochemical characterization of library members to eliminate structures with inherent liabilities.
- Newly-designed compounds based on structurally novel scaffolds.

In this poster, we describe our strategy for constructing a CNS-focused compound library utilizing the combination of a computational scoring system and in vitro/in vivo DMPK data. In addition, we also describe how we gathered our original scaffold collection to emphasize structural novelty in the library.