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# An isotope metallomics characterization of samples from the Australian Imaging, Biomarker & Lifestyle Flagship Study of Ageing, and *ab initio* calculations of K isotope fractionation in biological systems.

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Biometals are inherent to both healthy and diseased brain functioning, notably with respect to neurodegenerative diseases like Alzheimer's (AD). In AD, the brain accumulates certain metals (e.g. Ca, Fe, Cu, Zn), yet may also experience deficits in other such as K. The natural stable isotope compositions of these metals have shown potential in differentiating between healthy and diseased states in both organ and blood media, making them potential crux parameters in novel diagnostic tools. While the bibliography of research on metals and their isotopes in relation to AD in natural systems continues to grow, our theoretical understanding of metal isotope fractionation in the context of AD, especially for more recent target isotope systems such as for K, remains limited.

The Australian Imaging, Biomarker & Lifestyle Flagship Study of Ageing—AIBL—is one of the largest and most comprehensive longitudinal studies of AD. It includes cohort information on biomarker development (e.g. blood amyloid beta), neuropsychological assessments, vital signs, medical history, and lifestyle factors. Moreover, all participants have undergone magnetic resonance imaging (MRI) and positron emission tomography (PET). As such, AIBL cohort samples are richly characterized and represent an ideal cohort biobank for isotope metallomics characterization.

Here, we present major/trace element data and the first stable metal isotope data from AIBL human blood serum samples. This is a first glimpse into an ongoing study aiming to comprehensively characterize both healthy and AD-afflicted cohort samples for isotopic systems of biological and diagnostic relevance.

Additionally, we report the first *ab initio* calculations of K isotope fractionation between biologically relevant bonding environments, including hydrated $K^+$ ("free K"), K bound to aspartate glutamate (as in Na/K-ATPase), and $K_x$-EDTA (a common anti-coagulant and likely contaminant source).