

## MS33-P17 | DIRECT STRUCTURE DETERMINATION OF VOLATILE ODOR COMPOUNDS VIA CRYSTALLINE SPONGE METHOD

Kikuchi, Takashi (Rigaku Corporation, Tokyo, JPN)

Three-dimensional structure determination of odor compounds leads to elucidating cause of natural odor and developing artificial flavors or aromas. Single crystal X-ray analysis (SCX), the most powerful tool to determine 3D molecular structure, has rarely been applicable to odor compounds, because they are usually gaseous or volatile liquid compounds, which never crystallize under ambient conditions. Recently, Fujita's group reported that incorporation of analyte compound in a porous coordination polymer, crystalline sponge (CS), enabled SCX of a sub-microgram scale of non-crystalline compounds. Here we present direct 3D structure analysis of volatile odor compounds contained in daily commodities, foods, and aroma oils by SCX assisted by the CS method. Several drops of lime-flavored kitchen detergent were sealed in a capped vial besides a small vial containing one CS crystal and the vial was kept for 1 day at room temperature. The resultant crystal afforded good X-ray diffraction, and structure analysis directly revealed the 3D structure of a compound absorbed in the pore of CS, d-limonene. Although the detergent sample and the CS crystal were spatially separated, vapor of the odor compound diffused into CS to form the inclusion complex. Interestingly, only d-limonene was selectively incorporated in CS from the flavor mixture containing several other terpenoids, presumably because of majority rule or best affinity to the CS pore. We have also tested food samples, wasabi and garlic, and mint oils, and achieved direct structure elucidation of the volatile odor compounds.