1–13 Cause of Radioactivity Concentration in Mushrooms
—Cesium Selectivity Evaluation of Mushroom Pigment Norbadione A—

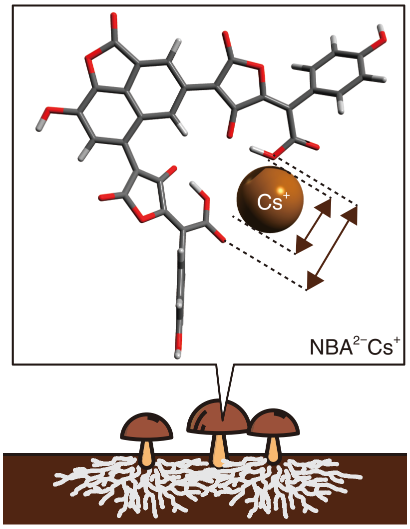

Fig.1-26 Radioactive cesium concentration mechanism in mushrooms
The brown pigment norbadione A, a scissor-like molecule, binds cesium ions. The binding becomes more stable when the scissor spacing matches the cesium ion diameter.

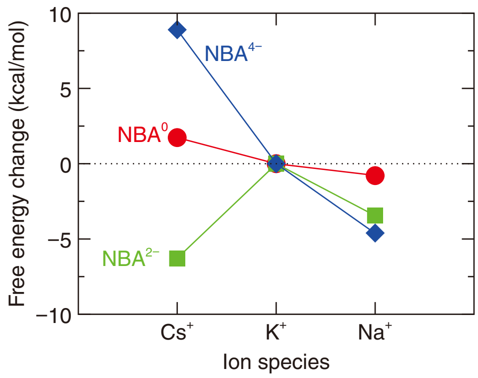

Fig.1-27 Free energy change for alkali-metal ion exchange of norbadione A in water
The change in free energy ΔG_{aq}^{exc} associated with replacing potassium bound with norbadione A to with cesium and or sodium. Three forms are were considered: NBA^0 with no dissociated hydrogen ions (H^+), NBA^{2-} with two dissociated H^+, and NBA^{4-} with four dissociated H^+. A negative ΔG_{aq}^{exc} indicates a transformation to a more stable form.

Radiocesium (Cs) released by the accident at the TEPCO's Fukushima Daiichi Nuclear Power Station has been reported to be partly retained in fungi, lichens, and trees in forests, and particularly concentrated in mushrooms. The concentration of Cs in mushrooms was noticed after the Chernobyl nuclear plant accident, with high concentrations observed around the pigments contained in the mushroom cups. One representative mushroom pigment molecule is norbadione A (NBA; $C_{35}H_{18}O_{15}$), which is the predominant pigment of the Bay Boletus in Europe and the Pisolithus arrhizus in Japan's pine forests. Norbadione A is known to bind with Cs (see Fig.1-26), and has been investigated experimentally and via molecular dynamics simulations to clarify its selective binding mechanism. Here, the selective binding mechanism was attributed to the scissor-like molecular structure of norbadione A.

In this study, state-of-the-art quantum chemical computational techniques were used to calculate the structure of norbadione A, the free energy of formation of the binding between norbadione A and Cs, and the binding free energy binding between norbadione A and Cs, which characterizes the binding strength in a living body (i.e., in water). As potassium is generally abundant in living bodies and binds with norbadione A, the possibility of cesium concentration can be evaluated by calculating the free energy change associated with replacing a potassium ion with a Cs ion. The results demonstrated that NBA^{2-}, norbadione A with two dissociated hydrogen ions, binds more stably with a Cs ion than with potassium or sodium ions (Fig.1-27). This indicates that cesium is selectively bound with norbadione A. For most other biomolecules, potassium binding is more stable than Cs binding, whereas Cs binding is more stable than potassium binding for norbadione A. This anomality is likely owing to the scissor-like molecular structure of norbadione A; the scissor spacing matches the cesium ion diameter, as shown in Fig.1-26. Several mushroom pigments are known to have scissor-like molecular structures such as norbadione A and badione A; their characteristic scissor-like structures may be one reason for the high concentration of Cs in mushrooms.

This research was conducted using the supercomputer SGI ICE X in the JAEA.

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Reference

Suno, H. et al., Quantum Chemical Calculations for the Norbadione A Complexes with Cs^+, K^+, and Na^+ in Gas and Aqueous Phases, Chemical Physics Letters, vol.730, 2019, p.26–31.