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Corrigendum

Corrigendum to "Structure–function relationship between soluble epoxide hydrolases structure and their tunnel network" [Comput. Struct. Biotechnol. J. 20 (2022) 193–205]

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The authors regret that during the revision process of the follow-up paper (reference 15 Bzówka et al. 'Evolution of tunnels in α/β-hydrolases fold proteins – what can we learn from studying epoxide hydrolases?' – previously published as a preprint), the multiple sequence alignment (MSA) used for calculating the tunnels' variability was not adequately post-processed. After verifying all the results, the variability of the tunnels changed and almost all identified tunnels can be described as conserved features. These findings do not call into question the results presented in the article 'Structure–function relationship between soluble epoxide hydrolases structure and their tunnel network' published in the Computational and Structural Biotechnology Journal but they influenced the results presented in the reference 15. After introducing the changes, the preprint has been updated and has also been approved for publication in the Plos Computational Biology Journal. Taking responsibility for our work and the quality of the article published in the Computational and Structural Biotechnology Journal, we would like to provide a corrigendum note. We marked the changed text bold, so the changes can be easier to follow.

We would like to introduce the following changes:

Introduction section:

Second paragraph:

Original text: "However, in our other study [15] we elucidate that in the case of the soluble epoxide hydrolases (sEHs) most of their tunnels should be considered **as variable structural features with only one exception – the tunnel located at the border between the main and cap domains. These counterintuitive** findings has inspired the investigation of the structure–function relationship of sEHs in more detail."

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Discussion section:

Second paragraph:

Original text: "In our other study [15], sEHs were employed as a sample system in order to investigate the evolution of tunnels. It was determined that most tunnels should be considered as **variable** structural features of proteins. **Tc/m tunnel was found to be the only exception, located between the cap and main domains.** We proposed that insertion of the cap domain defined the buried active site cavity and the tunnel linking it with the environment. Such structural arrangement was preserved in most of the EHs which supports the hypothesis regarding the origin of the positioning of the active site between both domains.

Changed text: "In our other study [15], sEHs were employed as a sample system in order to investigate the evolution of tunnels. It was determined that most tunnels should be considered as **conserved** structural features of proteins **with Tc/m tunnel identified in all analyzed structures, between the cap and main domains.** We proposed that insertion of the cap domain defined the buried active site cavity and the tunnel linking it with the environment. Such structural arrangement was preserved in most of the EHs which supports the hypothesis regarding the origin of the positioning of the active site between both domains".

Fourth paragraph:

Original text: "Mammalian (hsEH and msEH) and fungal (TrEH) structures were assigned to group I. Members of this group shared common features such as relatively long back-loop and cap-loop. Enzymes in this group primarily utilize two main tunnels – Tc/m, and Tm1. In all sEHs from the group I, T/cm tunnel was found conserved [15]. This was also the case for Tm1 tunnel, **but only in the case of msEH** [15]. The results of the structure flexibility analysis (Fig. 5) showed significant differences between sEHs that represent mammalian and fungal families."

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served. This was also the case for the Tm1 tunnel [15]. The results of the structure flexibility analysis (Fig. 5) showed significant differences between sEHs that represent mammalian and fungal families."

Fifth paragraph:

Original text: "Similar to mammalian and fungal sEHs, plant sEHs structures had relatively long cap-loop and back-loop, however, the enzymes predominantly utilize the Tm1 tunnel, which was identified **as a variable feature in StEH1 structure** [15]. The flexibility analysis results of plant sEHs showed that the most flexible regions were distant to the tunnel entries and, therefore, the conformational changes were only limited to slight effect on for catalytic efficiency (if any).

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Sixth paragraph:

Original text: "This observation supported the hypothetical origin of sEHs via insertion resulting in active site positioning between cap and main domains. **Surprisingly, in the case of IIb group enzymes the Tc/m tunnel was found to be a variable feature [15]. This could be due a small number of residues lining the walls of the tunnel, which was significantly shorter in comparison to Tc/m tunnels in other sEHs.**"

Changed text: "This observation supported the hypothetical origin of sEHs via insertion resulting in active site positioning between cap and main domains. **In the case of IIb group enzymes the Tc/m tunnel was found to be a conserved structural feature [15].**"

The authors would like to apologise for any inconvenience caused.