**Responses to Reviewers' Comments on Manuscript egusphere-2025-1662**

(Acid-catalyzed hydrolysis kinetics of organic hydroperoxides: Computational strategy and structure-activity relationship)

***Reviewer 4***

**Reviewer: General comment**

*This study focuses on improving our representation of acid-catalyzed hydrolysis of ROOHs. The authors appear to have a strong understanding of the computational models employed in this study and do a good job of explaining the chemical reasoning behind the modeled behavior. Additionally, the figures are clear, helpful, and well-made. I recommend this paper for publication after very minor changes.*

**Response:** We sincerely appreciate your positive comment and have further refined the manuscript based on your valuable suggestions.

**Reviewer: Special Suggestions and Comments**

**Reviewer:** 1) *In Section 2.2, it would be helpful to have more background on why those 4 compounds were chosen. In the introduction you describe the importance of alpha-HHs and alpha-AHs, and it would be good in Section 2.2 to include a brief description and/or references to explain why these specific 4 were chosen.*

**Response:** Thanks for the comment. The four ROOHs were chosen due to the availability of experimental kinetic data under different pH conditions. These compounds also represent typical structures of α-AHs and α-HHs highlighted in the introduction. We have added these explanations and supporting references in Section 2.2. Please see lines 107 - 108 in the revised manuscript.

**Reviewer:** 2) *Consider expanding the discussion of future work in the Conclusions section. Do you think that more modelling studies, laboratory validation studies, or both would be helpful*

*to expand on and utilize this work?*

**Response:** We appreciate the reviewer's insightful comment and fully agree that both further modelling and laboratory validation studies are necessary to expand our findings. Accordingly, we have developed quantitative structure-activity relationship models linking Taft ($\sigma^*$) constants to the logarithms of the acid-catalyzed hydrolysis second-order rate constants (log $k_A$). In the revised manuscript, we emphasize the importance of laboratory validation in the Conclusions section. Please see lines 118 - 124, 268 - 278, 329 - 331 in the revised manuscript, and Figs. S15 and S16 in the SI.

**Reviewer:** 3) *There are some minor grammatical errors throughout the paper. I recommend having a native English speaker review the paper.*

**Response:** Thanks for the suggestion. The revised manuscript has been professionally reviewed by a native English speaker to address grammatical issues throughout.

**Reviewer:** 4) *Specify the pH that was used to calculate the enhancement factors in Figure 3 b-f. Or are these enhancement factors constant across pH?*

**Response:** Thanks for the comment. The enhancement factors remain constant across different pH values because the predicted acid-catalyzed hydrolysis rate constants of ROOHs show a linear dependence on the concentration of protonated water clusters, and thus on pH. We have added the corresponding description in the revised manuscript (see lines 179 - 180).