

Supporting Information for

Reaction Pathways and Energetics of the Deconstruction of Lignin Carbohydrate Complexes (LCCs) in Lignocellulosic Biomass

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Figure S.1, S.2 and S.3 show the molecular structures of the product compounds resulting from the C₆ – O₁, C₂ – OH and C₃ – OH bond breaking pathways, respectively.

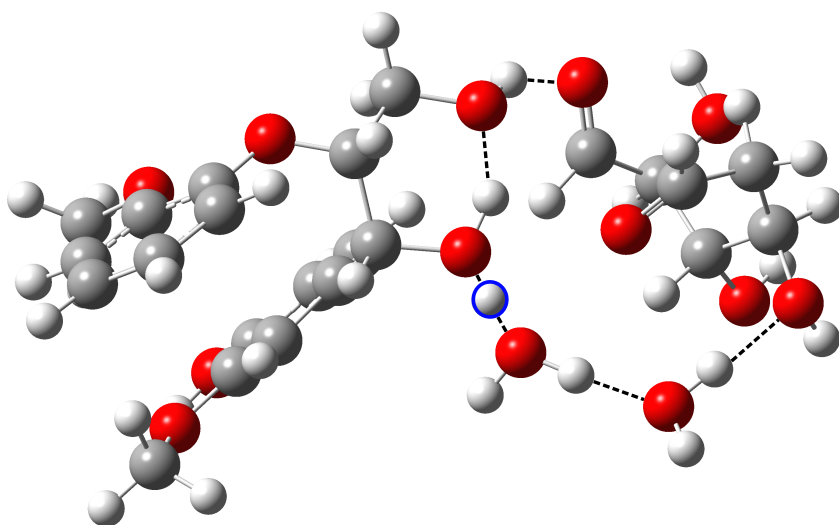


Figure S.1: The product structure resulting from the C₆ – O₁ bond breaking pathway. Carbon, oxygen and hydrogen are colored in gray, red and white, respectively. The approximate location of the positive charge is highlighted in a blue circle and the hydrogen bonds are depicted with black dashed lines.

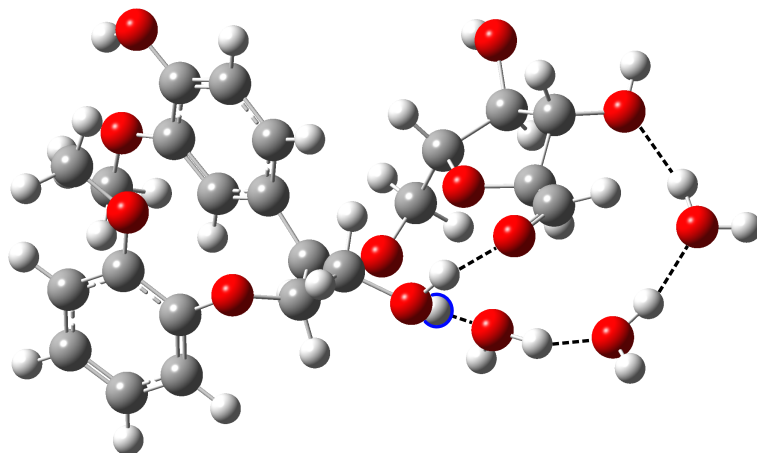


Figure S.2: The product structure resulting from the $C_2 - OH$ bond breaking pathway. Carbon, oxygen and hydrogen are colored in gray, red and white, respectively. The approximate location of the positive charge is highlighted in a blue circle and the hydrogen bonds are depicted with black dashed lines.

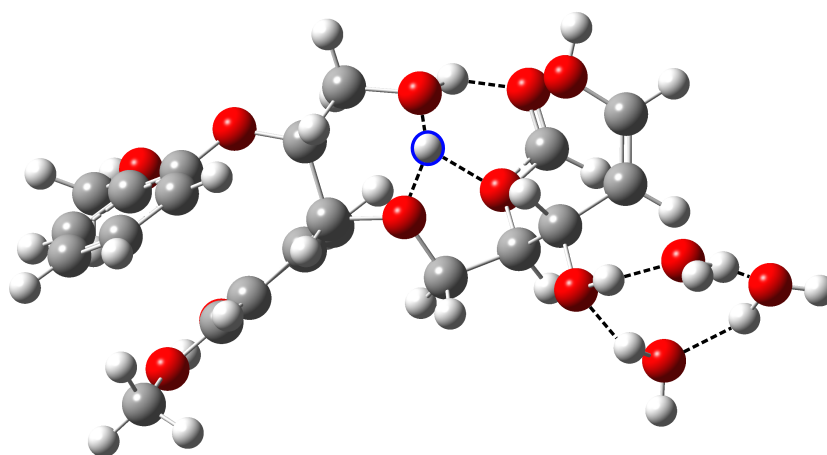


Figure S.3: The product structure resulting from the $C_3 - OH$ bond breaking pathway. Carbon, oxygen and hydrogen are colored in gray, red and white, respectively. The approximate location of the positive charge is highlighted in a blue circle and the hydrogen bonds are depicted with black dashed lines.