Electronic Supplementary Material (ESI) for RSC Advances.

Mode of Inhibitory Binding of Epigallocatechin Gallate to the Ubiquitin-Activating Enzyme Uba1 via Accelerated Molecular Dynamics

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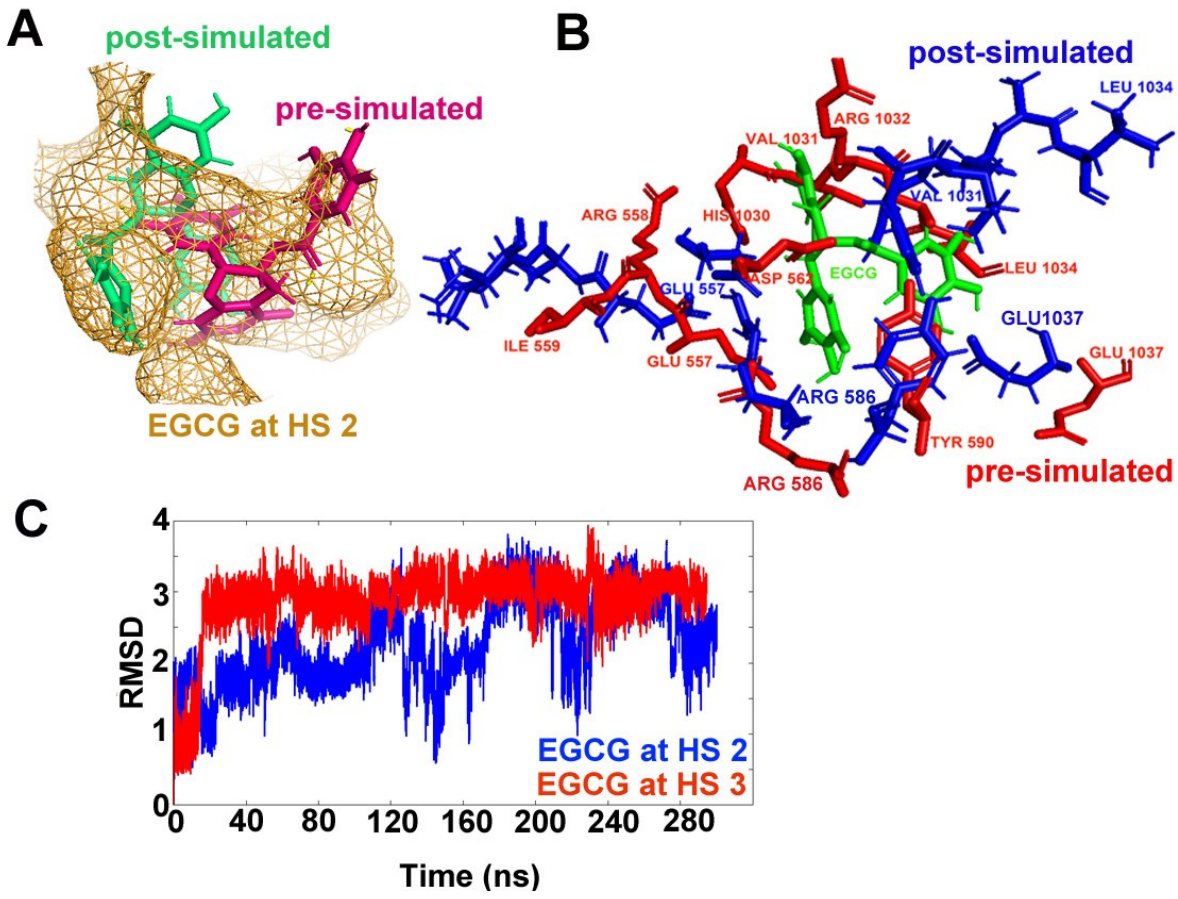
Supplementary Figure 1. Structural dynamics observed for hUba1 upon EGCG binding (A) A comparative snapshot of the binding pose of EGCG at HS2 before and after aMD simulations. (B) A comparative snapshot of the change in binding pocket upon EGCG binding. (C) The root-mean-square deviation in Å calculated for EGCG when bound at HS2 (in blue) and at HS3 (in red).



Supplementary Figure 2. Comparison of pre- and post-simulation poses of Uba1 with EGCG bound at HS 2 (A) Uba1~Ub interface 1; small difference observed in the positions of Uba1 Phe926 from Ub Leu8 (in red) (B) Uba1~Ub interface 2; ~20 Å shift in position of Uba1 Arg239 from Ub Asp32-Glu34 patch and (C) Uba1 Gln243 from Ub Thr12 (D) Uba1~Ub interface 3; similar shift in position observed for Uba1 Ser621 and Asp623 of the crossover loop from Ub C-terminal Arg72 (E) crossover loop; shift in position observed for Uba1 Glu626 from Ub C-terminal Arg74 leading to disruption of salt-bridge formation (F) crossover loop; ~15 Å shift in position observed for Uba1 Asp623 from Ub Arg42 leading to disruption of salt-bridge formation.