Electronic Supplementary Information

Mono- and di- anions of ellagic acid are both effective inhibitors of the serine β -lactamase CTX-M-15

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1. Speciation plot for ellagic acid in water 25°C; calculated fractions of ionic species using pK_a 's = 6.45, 7.45, 9.61 and 11.50



2. pH-rate profile for the CTX-M-15 catalysed hydrolysis of cephalothin and fraction of active enzyme EH. $pK_a^{1} = 4.75$ and $pK_a^{2} = 8.95$



 A comparison of the fraction of active enzyme CTX-M-15 as EH (left-hand axis and blue line) with the calculated total second-order rate constant (M⁻¹s⁻¹) for the inhibition of CTX-M-15 (right-hand-axis and red line) as a function of pH.

