Electronic Supplementary Information Material

N-(4-hydroxyphenyl)acetamide against di-iodine towards polyiodide dianion

Christina N. Banti[a]*, Nikolaos Kourkoumelis[b], Catherine P. Raptopoulou [c], Vassilis Psycharis[c], Sotiris K. Hadjikakou[a]*

[a] Section of Inorganic and Analytical Chemistry, Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece;

[b] Medical Physics Laboratory, Medical School, University of Ioannina, Greece;

[c] NCSR "Demokritos", Institute of Nanoscience and Nanotechnology, 15310, Aghia Paraskevi Attikis, Greece.

*All correspondence should be addressed to:

Dr. C.N. Banti (Post Doctoral Fellow); email: cbanti@cc.uoi.gr

Dr S.K. Hadjikakou (Professor); e-mail: shadjika@uoi.gr;

tel. xx30-26510-08374

fax xx30-26510-08786

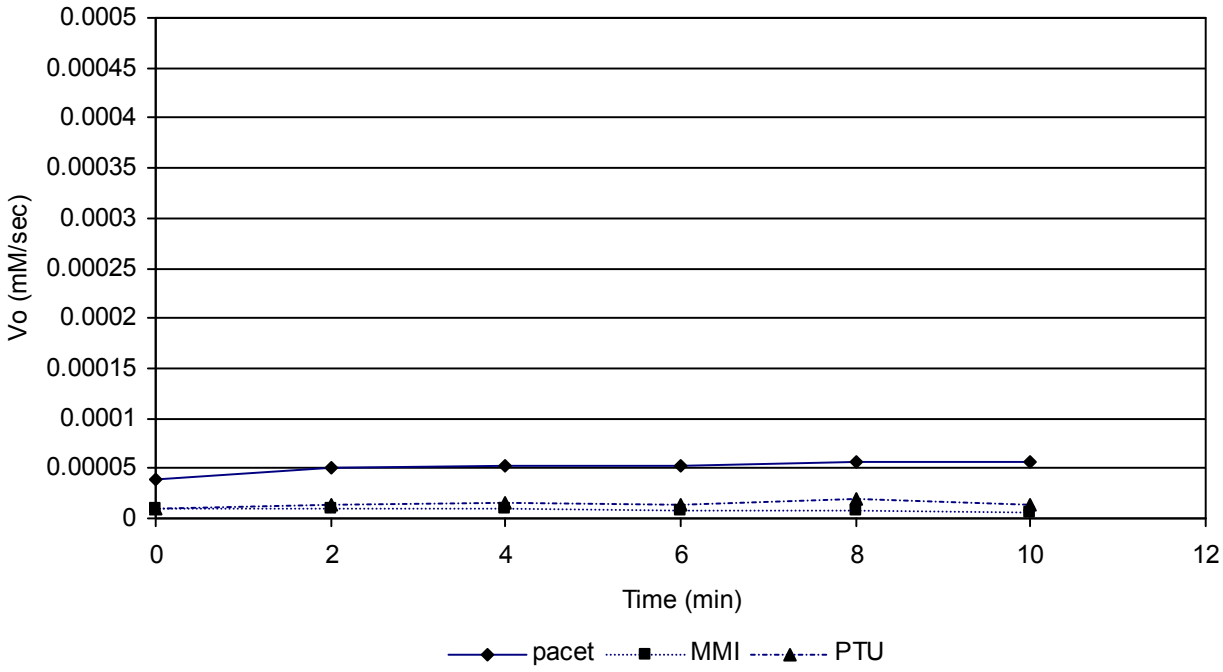


Figure S1. Initial rate (V_o) of the peroxidase-catalysed iodide oxidation vs incubation time in the presence of constant concentration of the inhibitors.

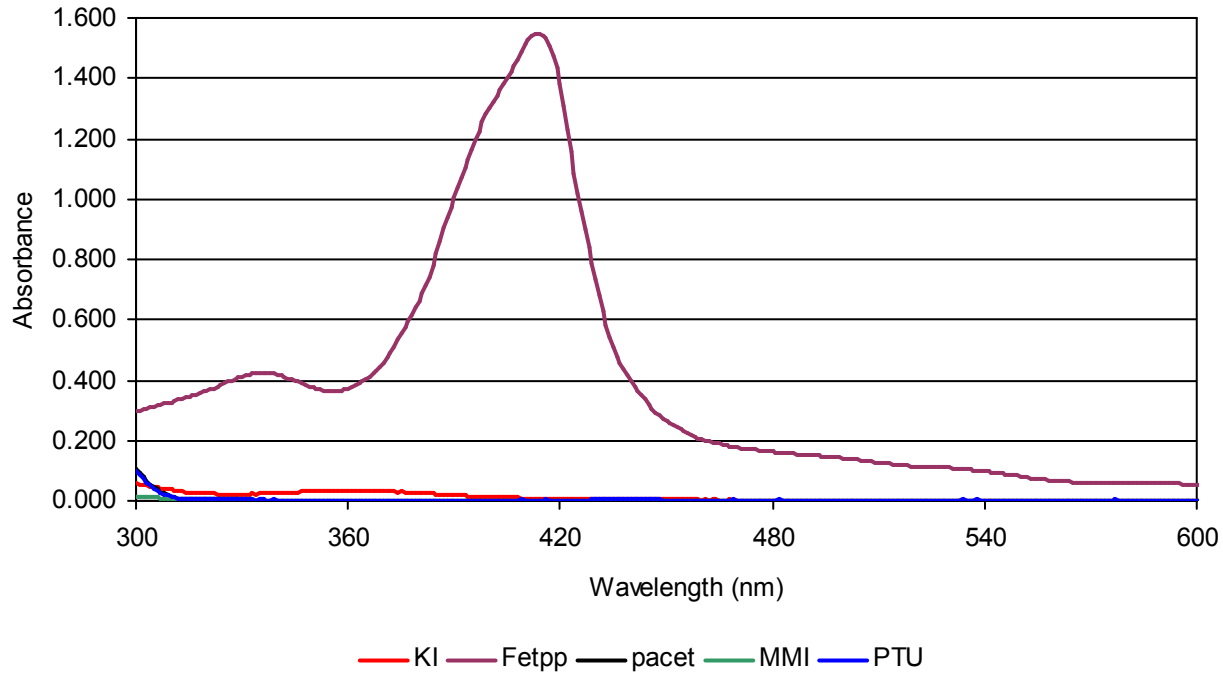
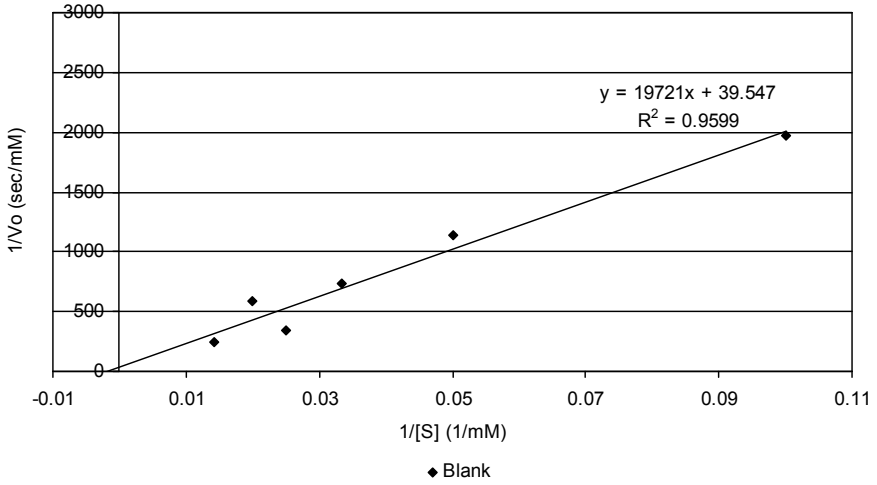
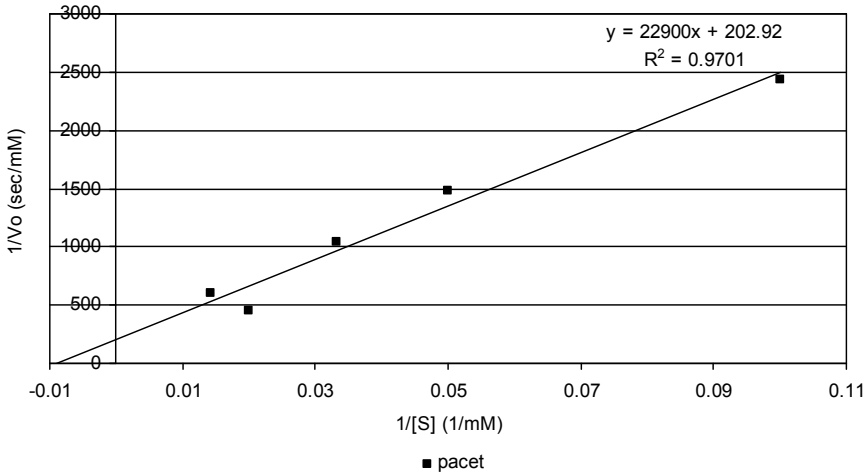


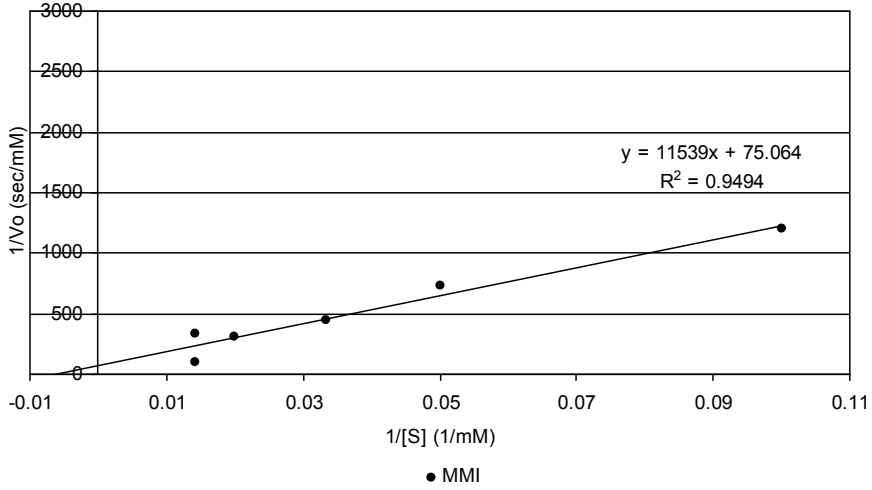
Figure S2. UV spectra of KI, Fetpp, pacet, MMI and PTU



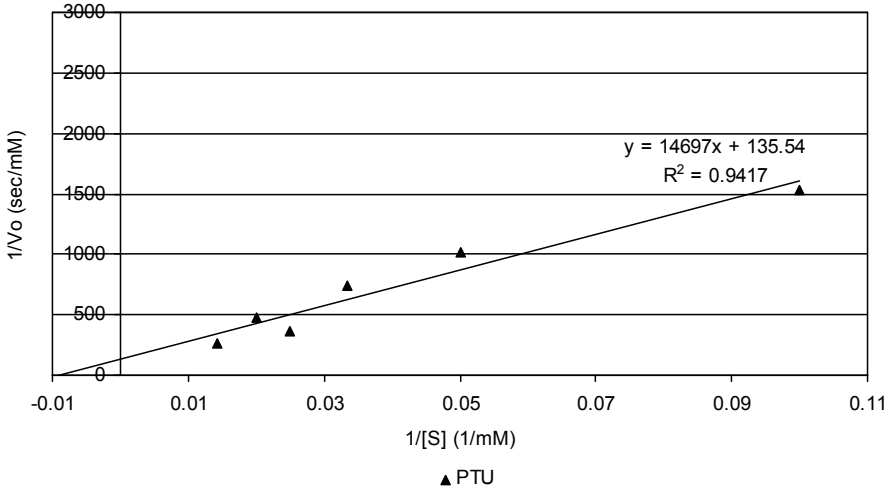
(A)



(B)



(C)



(D)

Figure S3 Lineweaver–Burk plots for determination of Km and Vmax of HRP in the absence (A) and presences of the inhibitors PACET (B), MMI (C) and PTU (D)

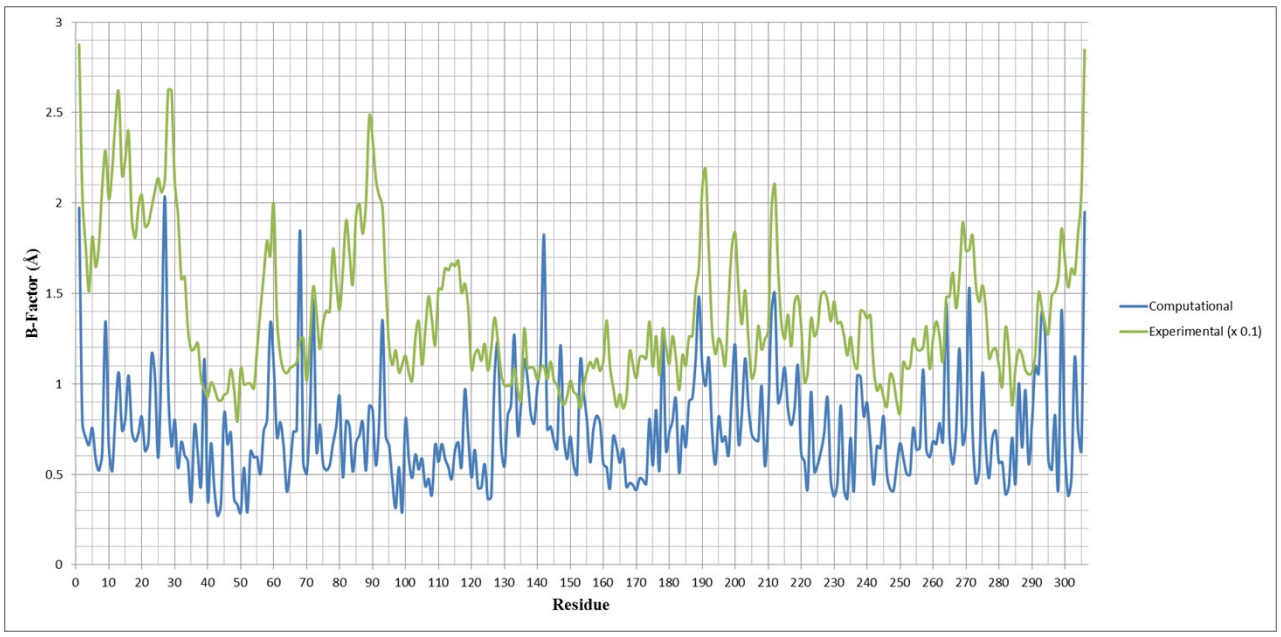


Figure S4 depicts the root mean square fluctuation (RMSF) of backbone Ca atoms for the unbound structure (1H5G) vs. the calculated RMSF with experimental crystallographic temperature factors (B-factors x 0.1). The good correlation confirms the validity of the MD simulations protocol being able to approximate the behavior of the real protein.