

Supporting Information

In Silico and In Vitro Study of Antioxidant Potential of Urolithins

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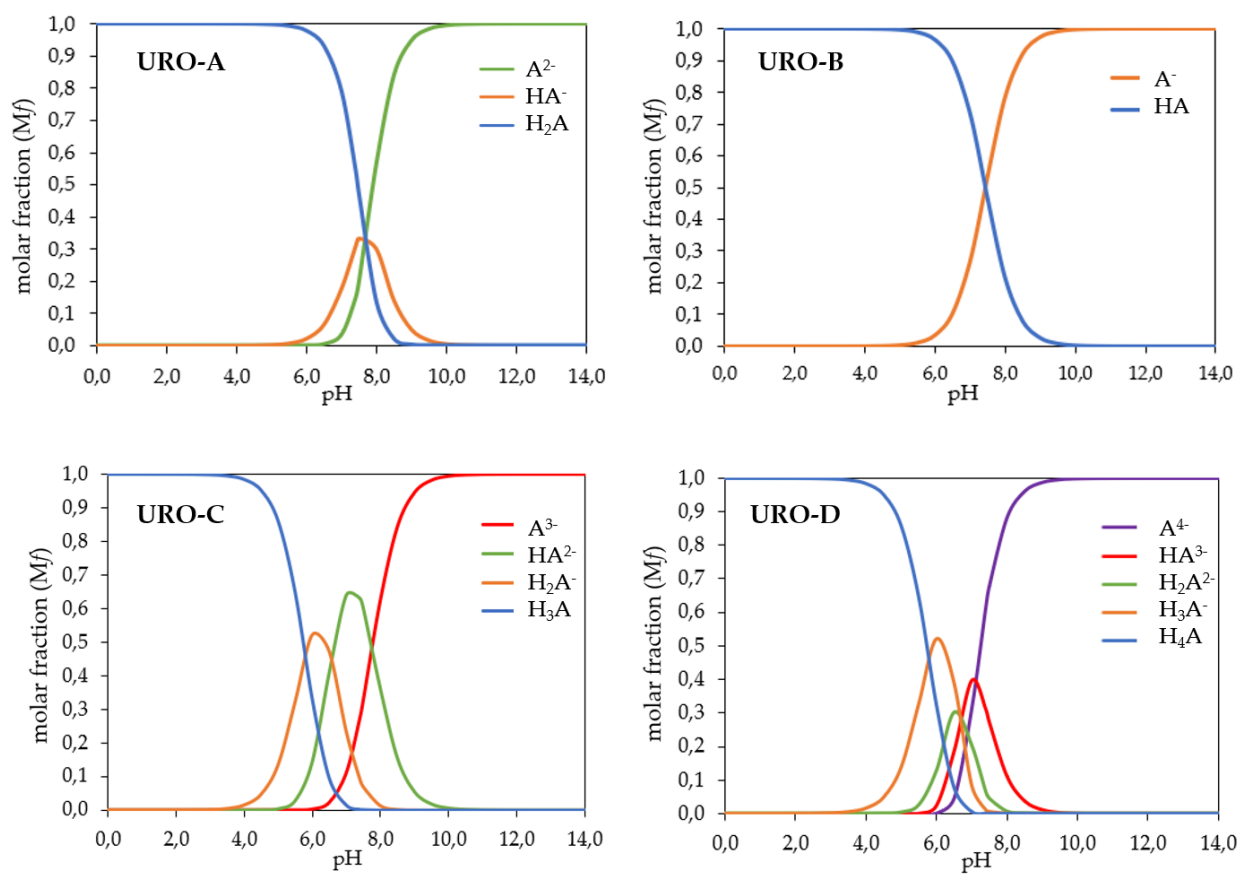


Figure S1. Distribution diagrams of UROs as function of pH.

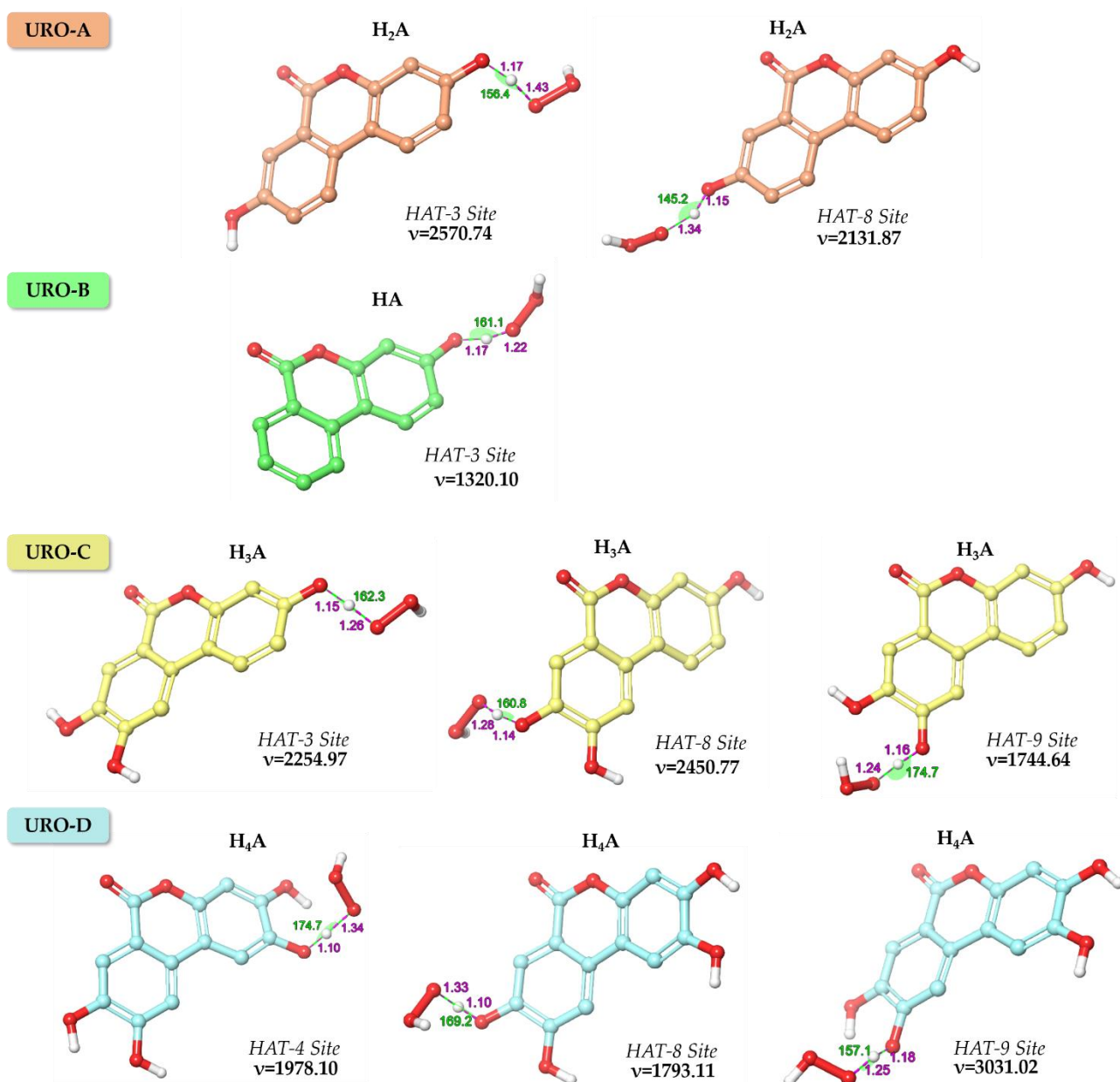


Figure S2. Geometries of the transition states of URO-A, URO-B, URO-C and URO-D obtained for the HAT reaction pathways in pentyl ethanoate (PE). Bond lengths (\AA), angles (degrees) and imaginary frequencies (ν) are reported in \AA , degrees and cm^{-1} , respectively.

Table S1. Nuclear organization term (λ) for the calculation of the barrier of reaction in SET mechanism, computed using the Marcus theory.

	specie	ΔG°	ΔE	λ	ΔG^\ddagger
URO-A	HA ⁻	-10.83	29.83	40.66	5,47
URO-B	HA	-5.03	89.66	94.69	21.23
URO-C	H ₂ A ⁻	-7.70	34.61	42.31	7.08
	H ₃ A ⁻	-25.04	19.89	44,93	2.20
URO-D	HA ³⁻	-16.73	-4.43	12,30	0,40
	A ⁴⁻	-22.20	-10.38	11.82	2.28

Table S2. Rate Constants (k_{app}), expressed in $M^{-1} s^{-1}$, in pentyl ethanoate and branching ratios (Γ) computed at M05-2X level of theory at 298.15 K.

	Mechanism	site	k_{app}	$\Gamma(\%)$
URO-A	HAT	3	1.72×10^{-10}	~0.00
	HAT	8	4.27×10^{-6}	100.00
URO-B	HAT	3	4.97×10^{-8}	100.00
URO-C	HAT	3	6.15×10^{-11}	0.04
	HAT	4	5.70×10^{-12}	~0.00
	HAT	8	1.48×10^{-7}	99.95
URO-D	HAT	4	6.30×10^1	96.06
	HAT	8	2.62×10^{-2}	0.04
	HAT	9	2.56×10^1	3.90

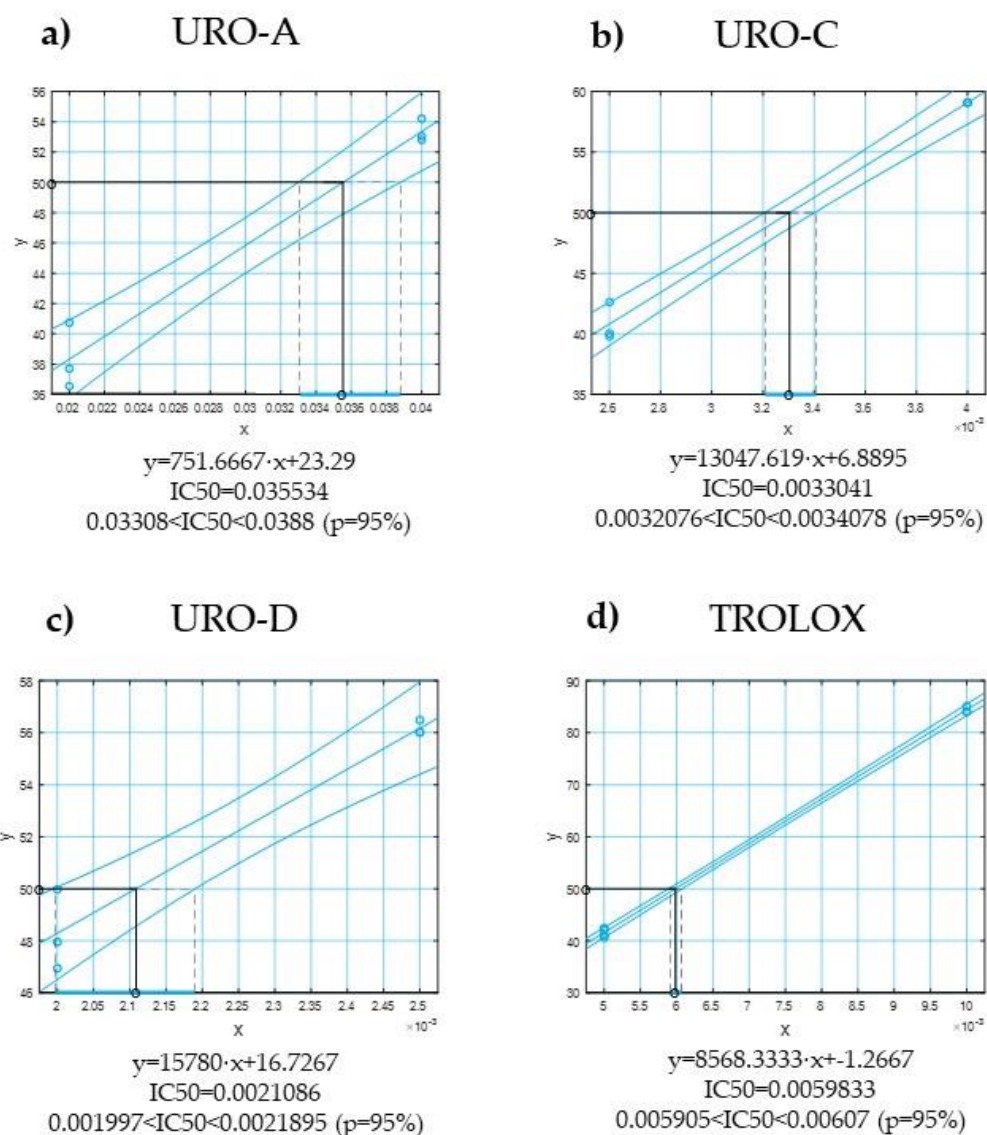


Figure S3. Regression lines for the calculation of the IC_{50} values.

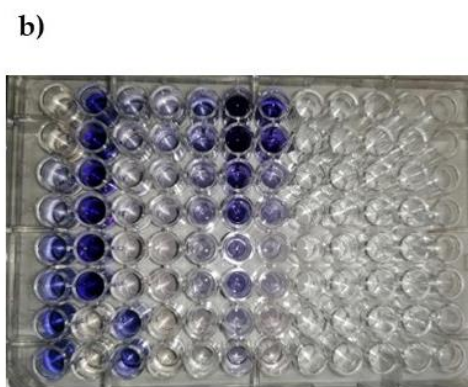
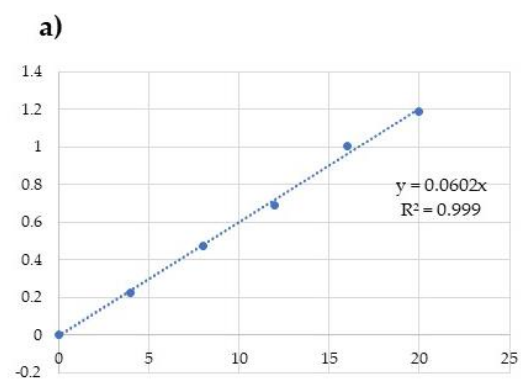


Figure S4. (a) Calibration curve of FRAP assay; (b) The microplate containing standards and samples at different concentrations.