Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Material. Mechanism of non-phenolic substrate oxidation by fungal laccase Type 1 Copper site from *Trametes versicolor*. The case of benzo[a]pyrene and anthracene

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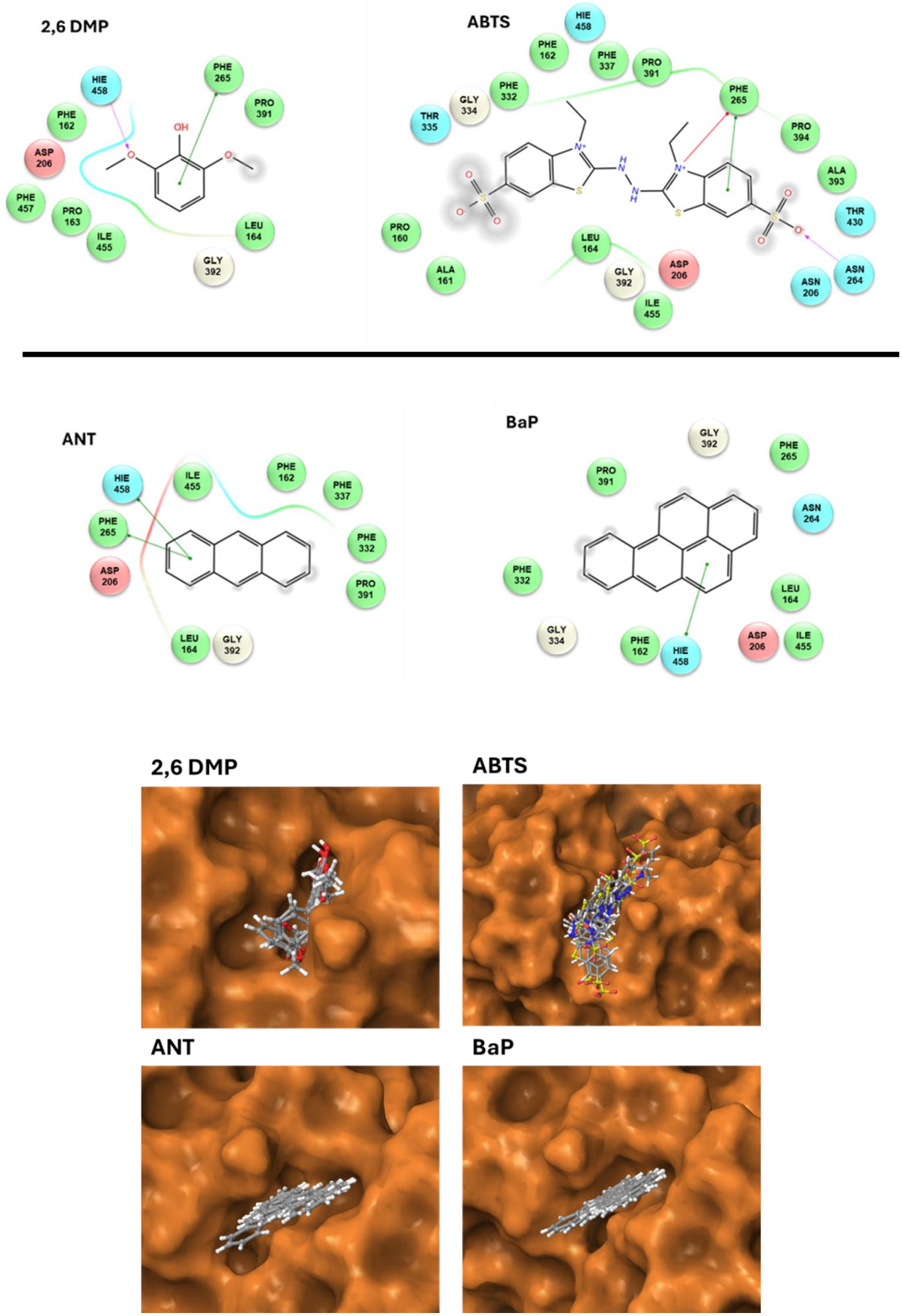
Table S1. Summary of docking results for 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid (ABTS) and 2,6-dimethoxyphenol (2,6 DMP), Anthracene (ANT) and benzo[a]pyrene (BaP). Distance from T1 has been calculated with respect to the substrate barycenter.

Substrate	**Distance from T1 (Å)**	**H-Bonds**	**π-CAT**	**π-π**	**Docking scores (kcal/mol)**	**Best pose Docking (kcal/mol)**
2,6 DMP	3.08	His 458	no	Phe 265	-3.61 / -4.96	-4.96
ABTS	7.07	Asn 264	Phe 265	Phe 265	-3.58 / -4.90	-4.90
ANT	6.78	no	no	His 458 - Phe 265	-2.92 / -3.61	-3.61
BaP	7.20	no	no	His 458	-3.00 / - 4.07	-4.07

Figure S1. Interaction diagrams of the best pose obtained for each substrate to TvL. Below are reported the positions of each ligand in the TvL binding pocket.



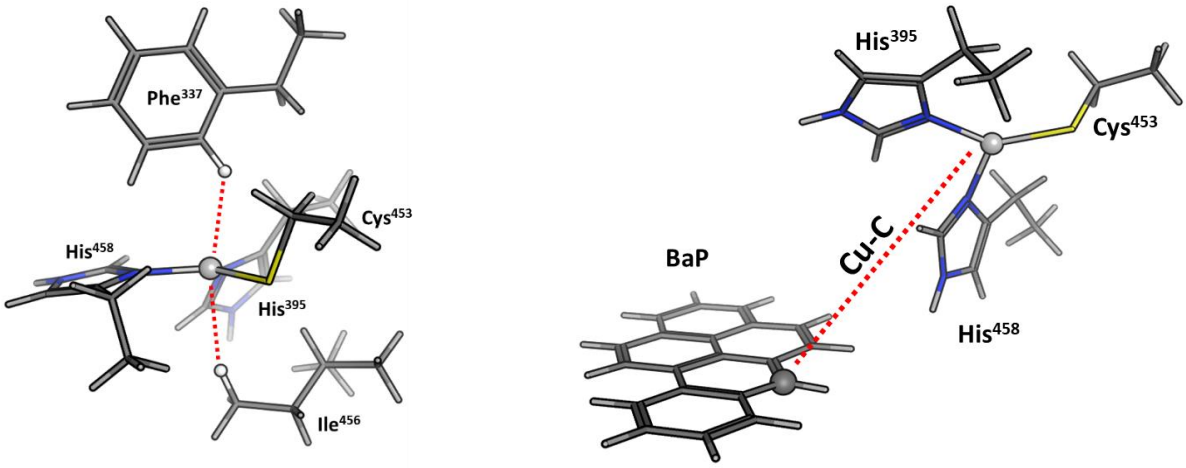


Table S2. Large model optimized T1 Cu coordination sphere Cu-ligand bond distances (in Å) for the reactant R-Cu(II) at BP86/TZVP/D3/Cosmo and PBE0/TZVP/D3/Cosmo level of theory; for the Int-Cu(I) at BP86/TZVP/D3/Cosmo. The Cu-H_{Phe} and Cu-H_{Ile} distances refer to the distances between copper (Cu) and the hydrogen (H) atoms of the side chains of hydrophobic residues, specifically phenylalanine (Phe) and isoleucine (Ile), within the first coordination sphere of T1 copper. These distances are calculated based on the shortest distance between one of the hydrogen atoms within the side chain (see figure above).

	R-Cu(II) ANT		**R-Cu(II) BaP**		**ANT Intermediate Cu(I)**	**BaP Intermediate Cu(I)**
	BP86	**PBE0**	**BP86**	**PBE0**	**BP86**	**BP86**
Cu-N_{His}	1.974	1.965	1.972	1.959	1.990	1.992
Cu-N_{His}	1.975	1.979	1.978	1.976	2.067	2.067
Cu-S_{Cys}	2.155	2.142	2.151	2.139	2.192	2.192
Cu-H_{Phe}	2.567	2.604	2.630	2.635	2.541	2.539
Cu-H_{Ile}	2.708	2.801	2.720	2.824	2.725	2.715
Cu-C	8.210	8.674	8.385	8.614	8.505	8.740

NBO spin population (in electrons) for R-Cu(II) large models computed at BP86 and PBE0 level using optimized BP86/TZVP/D3/Cosmo geometries.

	R-Cu(II)				**Int-Cu(I)**			
	ANT		**BaP**		**ANT**		**BaP**	
	BP86	**PBE0**	**BP86**	**PBE0**	**BP86**	**PBE0**	**BP86**	**PBE0**
Cu	0.43	0.50	0.43	0.49	0.12	0.00	0.13	0.00
S_{Cys}	0.45	0.43	0.45	0.43	0.08	0.00	0.09	0.00
N_{Hi}	0.03	0.03	0.04	0.03	0.00	0.00	0.00	0.00
N_{Hi}	0.03	0.03	0.03	0.03	0.00	0.00	0.00	0.00
Ligand	0.00	0.00	0.00	0.00	0.80	1.02	0.75	1.01

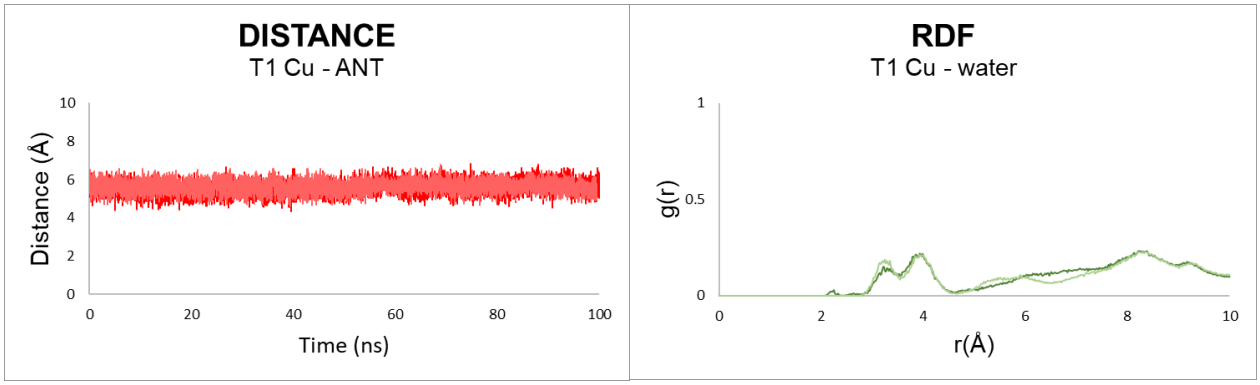


Figure S2. Analysis of MD simulations (two replicas) of the enzyme-substrate complex (taking ANT as an example), performed starting from the best docking pose. Left: Distance calculation between ANT and T1 Cu. During both simulations, the substrate maintains essentially the same positioning within the pocket and a distance from T1 Cu similar to the initial conformation. Right: RDF analysis for the T1 Cu and water molecules, calculated for each replica along the entire simulations. This result confirms the presence of water molecules in the first hydration sphere of T1 Cu (2 - 4 Å) in between the metal and the substrate.

MD details: two replicas of 100 ns were performed for the protein in complex with ANT, starting from the best docking pose. By using AmberTools23, the 3D system was placed in a 10 Å cubic box containing a neutralized water buffer with counterions. The system was described by the model from the general Amber force field (GAFF) and ff99SB in combination with the TIP3P water model; proper restraints have been added to maintain a proper coordination in T1 Cu. Using the GROMACS 2020 package *S. Pronk, et al.*, the system was relaxed by applying harmonic positional constraints on all atoms (50 kcal mol-1 Å 2) using 5000 steps of steepest descent (SD), followed by 5000 steps of conjugate gradient (CG). The system was progressively heated for 10 ns at 300 K using the Langevin thermostat in the NVT ensemble. The system was maintained at constant pressure with the NPT ensemble at 1 bar pressure using the Berendsen barostat with a time constant τp = 2.0 ps. The 100 ns MDs were produced with an integration step of 2 fs and a cutoff radius of 10.0, with the SHAKE algorithm coupling the Particle Mesh Ewald (PME) summation method. The stability of the complex was verified by monitoring the T1 Cu - ANT distance, calculated with respect to the barycenter of the latter. In order to verify the presence of water molecules in the proximity of T1 Cu, the radial distribution function (RDF) was also calculated.

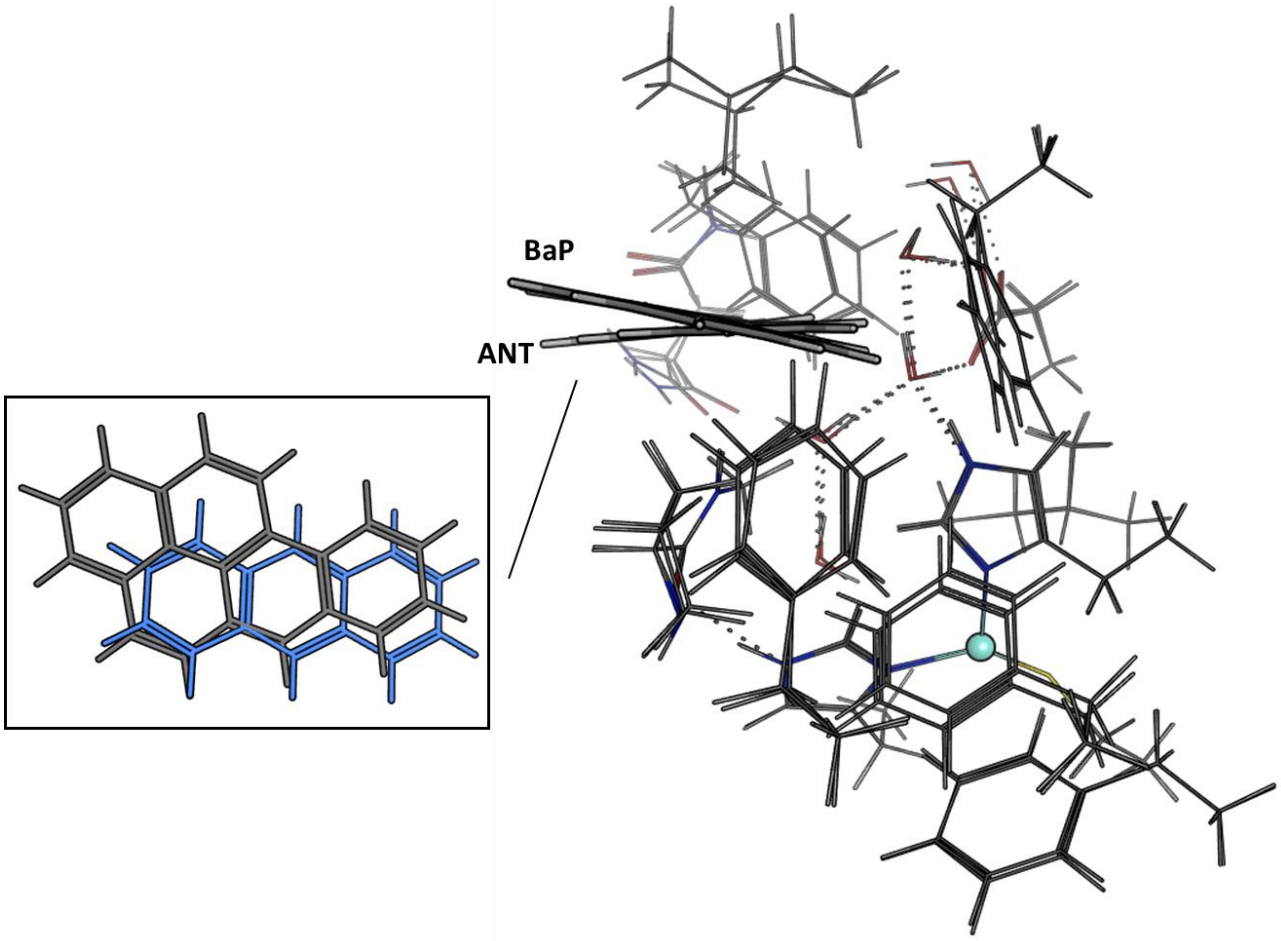


Figure S3. Comparison of ANT and BaP geometries, optimized using BP86/TZVP/D3 COSMO ε=80 DFT, within a large cluster model comprising 14 side chain residues (Cα position are fixed at the crystallographic positions form 1KYA pdb), the ligand, and five water molecules. The inset depicts a top view of the ligands, highlighting a slight twisting between the two ligands.

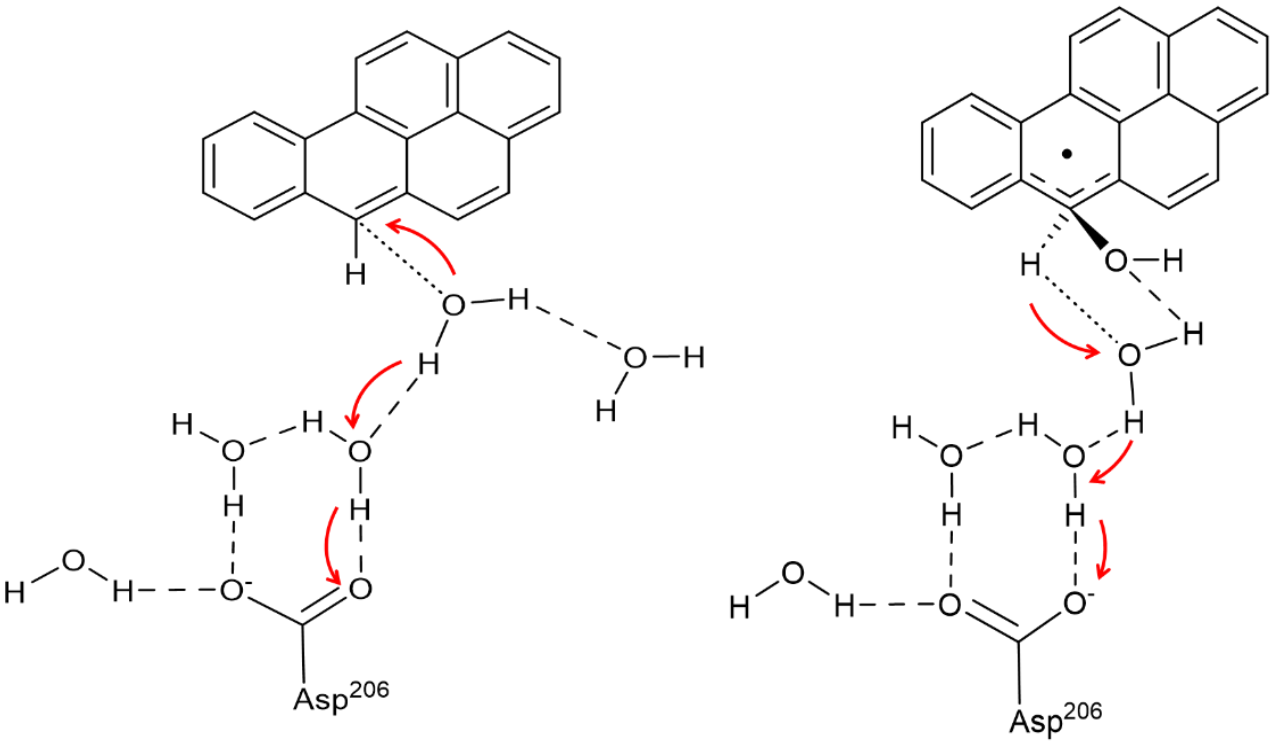


Figure S4. Molecular motions along the reaction coordinates for the first (left) and second (right) oxidation steps of BaP. The observed atomic displacements in BaP are equally observed in ANT. The dotted line indicates the interatomic distance explored in the PES scan. The red arrows indicate the atomic displacements observed during the PES scan.

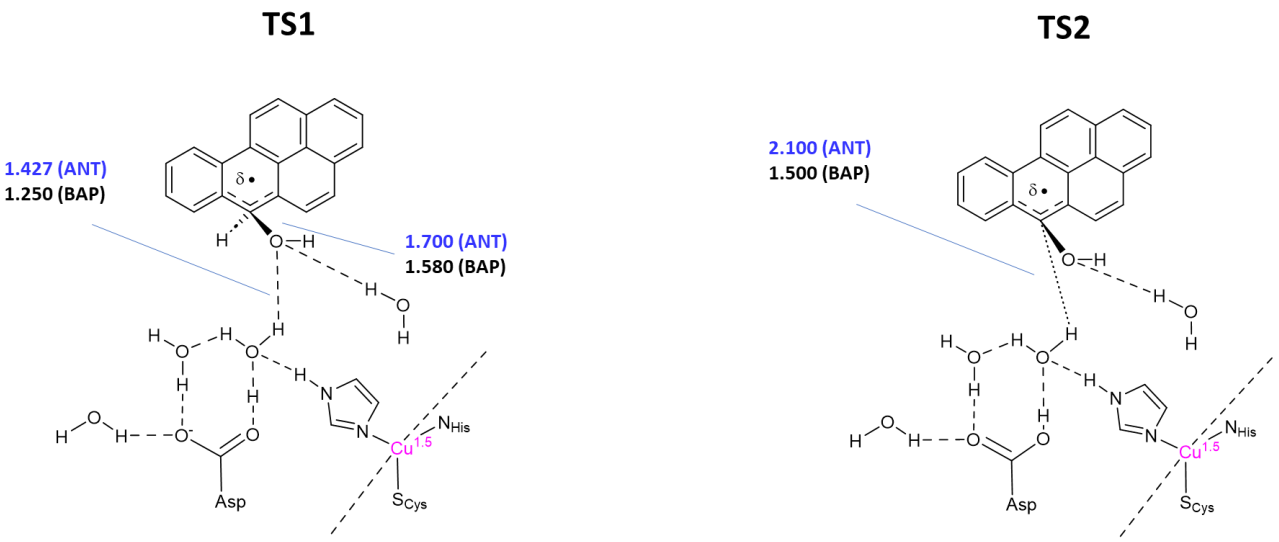


Figure S5. Geometries of the first and second transition state (TS1 and TS2) along the reaction coordinates for the first and second oxidation steps. In both cases the NBO spin population computed at PBE0/TZVP/D3 COSMO $\sum$=80 DFT level of the copper ion is compatible with the $Cu^{1.5}$ redox state. In the case of TS1 for BaP, a spin population of 0.6 is observed on the ligand, indicating that Cu is slightly more reduced compared to ANT.

Table S3. Transition state Cu-X (in Å) optimized bond distances at BP86/TZVP/D3/COSMO level.

	TS1		**TS2**	
	ANT	**BaP**	**ANT**	**BaP**
$Cu\text{-}N_{His}$	2.002	1.996	2.001	1.972
$Cu\text{-}N_{His}$	2.007	2.047	2.017	1.977
$Cu\text{-}S_{Cys}$	2.184	2.193	2.186	2.156
$Cu\text{-}H_{Phe}$	2.594	2.630	2.532	2.608
$Cu\text{-}H_{Ile}$	2.702	2.814	2.612	2.673

Table S4. Reaction energy barriers (in kcal/mol) computed at BP86/TZVP/D3/Cosmo level and PBE0/TZVP/D3/Cosmo level from BP86/TZVP/D3/Cosmo level optimized geometries. $\otimes E_1^{\#}$ and $\otimes E_2^{\#}$ are the energy barrier between the R-Cu(II) and Int-Cu(I) ($\otimes E_1^{\#}$) and between Int-Cu(II)/P-Cu(I).

Level of theory	**BP86** TZVP/D3/Cosmo		**PBE0** TZVP/D3/Cosmo	
	ANT	**BaP**	**ANT**	**BaP**
$\otimes E_1^{\#}$	31.1	29.1	29.7	30.3
$\otimes E_{r,1ox}$	26.4	20.1	18.1	14.8
$\otimes E_2^{\#}$	19.3	28.1	27.9	30.5
$\otimes E_{r,2ox}$	-48.8	-31.7	-46.8	-27.5

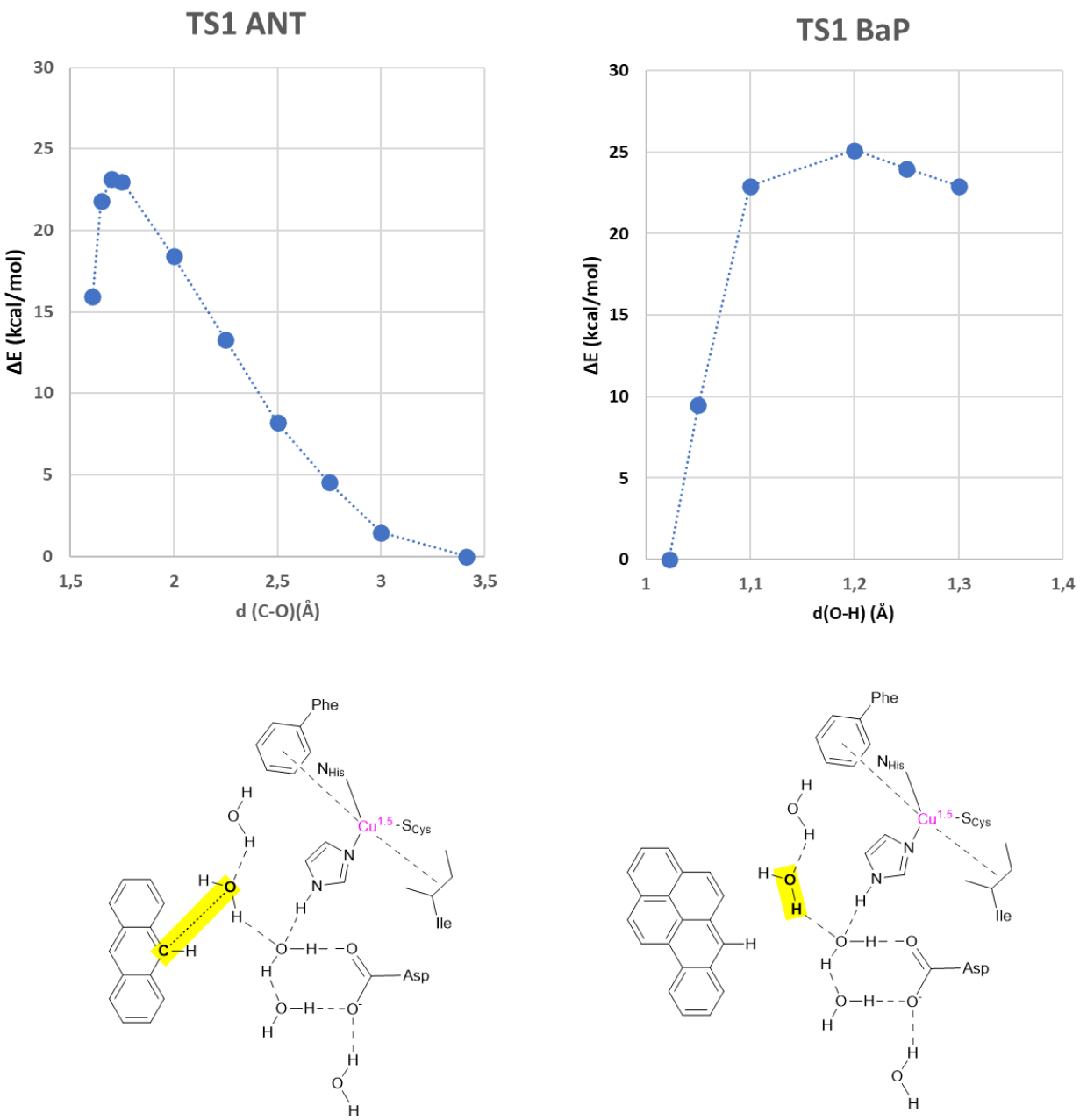


Figure S6. Potential energy surface scans along the reaction coordinate for the first oxidation step at BP86/SV-P/D3/COSMO level. The interatomic distances evidenced in yellow are those considered to implement the energy scan. In the main text are then reported the energy barrier of the transition state structure obtained from these scans upon re-optimization at BP86/TZVP/D3 COSMO level and single-point energy calculation at PBE0/TZVP/D3 COSMO level on BP86/TZVP/D3/COSMO optimized saddle points.

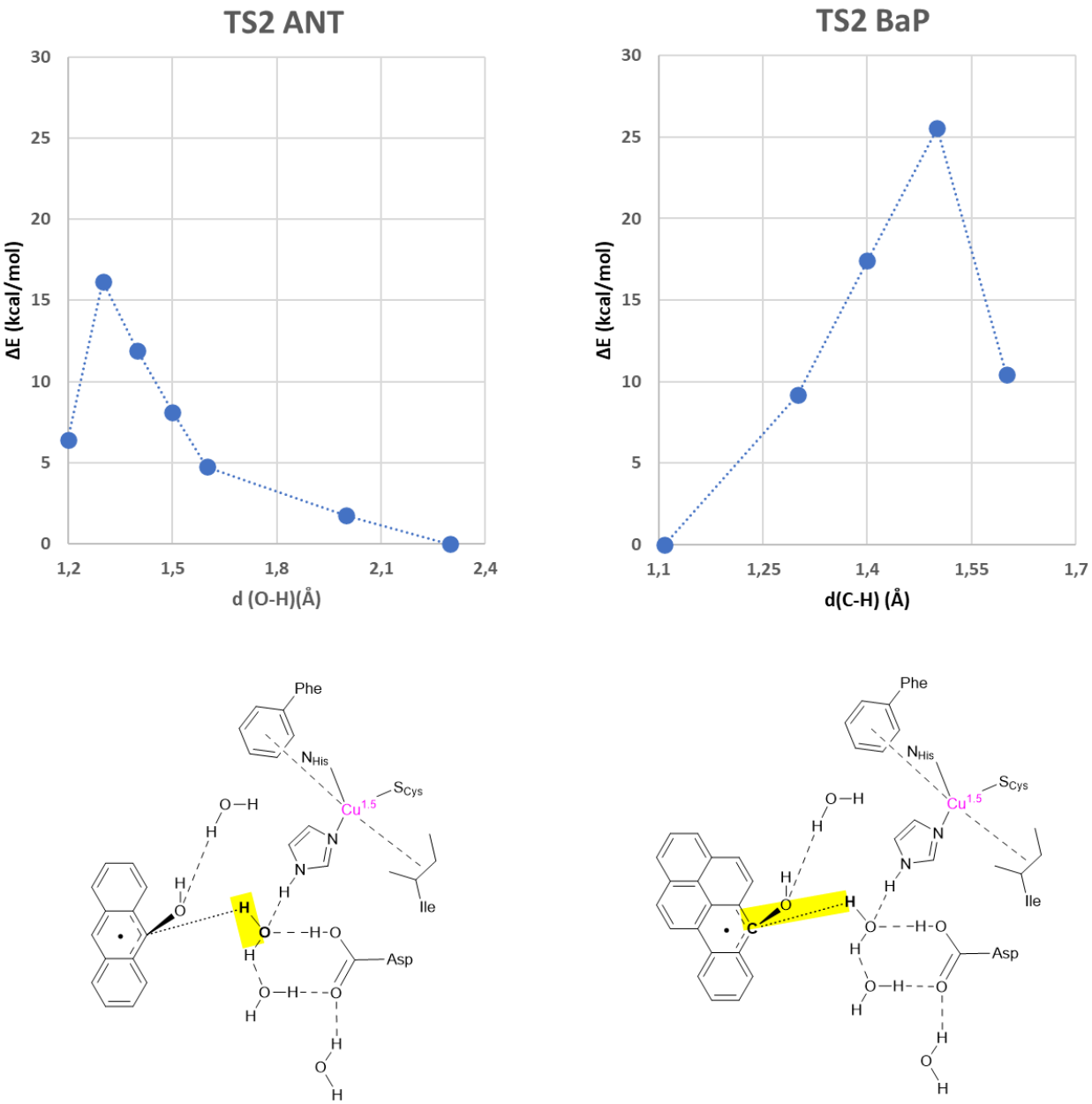


Figure S7. Potential energy surface scans along the reaction coordinate for the second oxidation step at BP86/SV-P/D3/COSMO level. The interatomic distances evidenced in yellow are those considered to implement the energy scan. In the main text are then reported the energy barrier of the transition state structure obtained from these scans upon re-optimization at BP86/TZVP/D3 COSMO level and single-point energy calculation at PBE0/TZVP/D3 COSMO level on BP86/TZVP/D3/COSMO optimized saddle points.

Table S5. Summary of the ANT and BaP oxidation experiment with fungal laccases in absence of mediator. % ox refers to the percentage of oxidized quinone product with respect to the control without enzyme.

Organism	Experimental condition with no mediator	% ox ANT	% ox BaP	Reference
Trametes versicolor	27 °C, pH=5, Tween80, 24h	85%	<2%	(Collins et al. 1996)
Trametes versicolor	pH 5.0, RT, 72h	18%	19%	(Majcherczyk, Johannes, and Hüttermann 1998)
Marasmius quercophilus	pH 4.5	30%		(Farnet et al. 2009)
Trametes versicolor	pH 4.5, Tween80	73.8%	5.3%	(Johannes and Majcherczyk 2000)
Pycnoporus cinnabarinus	pH 5, Tween80	65%		(Cañas et al. 2007)
Trametes versicolor	Immobilized enzyme, pH 4.5, Tween80	17%	19%	(Dodor, Hwang, and Ekunwe 2004)
Rigidoporus lignosus	pH 4.5, 30°C, 72h	9%		(Cambria et al. 2008)
Pleurotus ostreatus D1	pH 4.5	0%		(Natalia N. Pozdnyakova et al. 2006)
yellow laccase from *Pleurotus ostreatus D1*	pH 6, Tween80	95%		(N. N. Pozdnyakova, Rodakiewicz-Nowak, and Turkovskaya 2004)

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Cartesian Coordinates (in atomic units) of the BP86/TZVP/D3/Cosmo DFT-optimized extended cluster for the starting species R-Cu(II)/ANT and R-Cu(II)/BaP and the product P-Cu(I)/ANT e P-Cu(I)/BaP. Fixed atoms are marked with the symbol “f”.

R-CU(II) **ANT**

-48.62454312528049	-2.58136589752179	115.32809616387793	c f
-49.79936980145420	-1.66951448820772	117.83190802995601	c
-52.02147432706082	0.04407077776889	117.48716050803256	c
-51.80864434553546	2.67144566687051	117.33532165587451	n
-54.54435978667052	-0.55791984805873	117.23665495498402	c
-54.14983569444591	3.59381750789823	117.03191018313379	c
-55.83983885020042	1.69092480710952	116.95737331204930	n
-40.66501665356616	2.74199261881707	120.61554988369195	c f
-43.36507019703377	3.76361235623186	120.63696202929532	c
-44.82486488046185	3.47371398507148	117.46913186694732	s
-46.66300739934519	13.67783774982629	119.18880665336330	c f
-47.67516728702713	10.96349886626535	119.06748655273307	c
-49.20436758576646	10.43633283945634	116.75526187178613	c
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-50.09400046771768	12.07692104387321	114.93762405880192	c
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-57.77631022691608	1.90355487414921	116.61568826910698	h
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-39.82098784553700	2.94647293942363	122.50588260589804	h
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-49.24900877893113	10.61267775539542	105.06414385563239	o
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-48.93921655902469	4.59068629495802	109.80065875545883	h
-40.94274642134098	8.06786468483022	110.11690663161306	h
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-48.360889210268470	6.104287376608740	122.400736745780510	h
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-44.708107290077410	8.200786744718950	129.865815660925140	h
-45.068758158703900	8.253988452433890	125.026447503284980	h
-47.360789678188130	10.626977747204680	125.263695471900180	h
-46.893550009054862	10.748466499366530	129.994502258780790	h
-43.931055006614590	11.171474732440550	128.491717174507950	h
-62.505866565194440	5.548350862002410	119.885925340528600	n
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-61.467155425657240	4.742045580145860	115.498135320546910	c
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-55.392103174967100	-1.934818294192140	97.102705884073460	c
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-66.52508639313493	8.88876121456657	108.51653712192727	c
-63.91146980415754	9.10821399099856	107.86855492062602	c
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-56.10138386204327	10.11630199145001	103.89955628633592	h
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-58.03071564820971	15.05722962898971	113.54019729354198	h
-57.20684102652910	7.22855680420051	102.41549012783024	h
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