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## PUBLICATION LIST

### A. Publications with peer review process

#### 1. **Coupling Quantum Interpretative Techniques: Another Look at Chemical Mechanisms in Organic Reactions.**

Gillet, N.; Chaudret, R.; Contreras-García, J.; Yang, W.; Silvi, B.; Piquemal, J.-P. *J. Chem. Theory Comput.* **8**:3993-3997 (2012).

#### 2. **Investigation of the Molecular Mechanism of Electronic Decoherence within a Quinone Cofactor.**

Narth, C.; Gillet, N.; Lévy, B.; Demachy, I.; de la Lande, A. *Canadian Journal of Chemistry* **91**:628-636 (2013).

#### 3. **Electron and hydrogen atom transfers in the hydride carrier protein EmoB**

Gillet, N.; Lévy, B.; Moliner, V.; Demachy, I.; de la Lande, A. *J. Chem. Theory Comput.* **10**:5036–5046 (2014).

#### 4. **Entasis Through Hook-and-Loop Fastening in a Glycoligand with Cumulative Weak Forces Stabilizing CuI**

Garcia, L.; Cisnetti, F.; Gillet, N.; Guillot, R.; Aumont-Nicaise, M. Piquemal, J.-P.; Desmadril, M.; Lambert, F.; Policar, C. *JACS* **137**:1141-1146 (2015).

#### 5. **Electron transfer, decoherence and protein dynamics. Insights from atomistic simulations**

Narth, C. ; Gillet, N.; Cailliez, F.; Lévy, B.; de la Lande, A. *Acc. Chem. Res.* **48**:1090-1097 (2015).

#### 6. **Progress and Challenges in Simulating and Understanding Electron Transfer in Proteins**

de la Lande, A.; Gillet, N.; Chen S.; Salahub D. R. *Arch Biochem Biophys.* **582**:28-41 (2015).

#### 7. **L-lactate oxidation by Flavocytochrome *b*<sub>2</sub>**

Gillet, N.; Ruiz-Pernia, J.; Demachy, I.; Lévy, B.; Lederer F.; de la Lande, A.; Moliner, V. *Phys Chem Chem Phys* **18**:15609 - 15618 (2016)

#### 8. **Electronic Coupling Calculations for Bridge-Mediated Charge Transfer Using CDFT and Effective Hamiltonian approaches at DFT and FODFTB level**

Gillet, N.; Berstis, L.; Wu, X.; Gajdos, F.; Heck, A.; de la Lande, A.; Blumberger, J.; Elstner, M. *J. Chem. Theory Comput.* **12**:4793-4805 (2016).

#### 9. **Theoretical Estimation of Redox Potential of Biological Quinone Cofactors**

Gillet, N.; Lévy, B.; Moliner, V.; Demachy, I.; de la Lande, A. *J. Comput. Chem.* (2017) DOI: 10.1002/jcc.24802

### B. Submitted publications with peer review process

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**Functional Role of an Unusual Tyrosine Residue in the Electron Transfer Chain of a Prokaryotic (6-4) Photolyase**

Holub, D; Lamparter, T.; Elstner, M.; Gillet, N. (*submitted*)