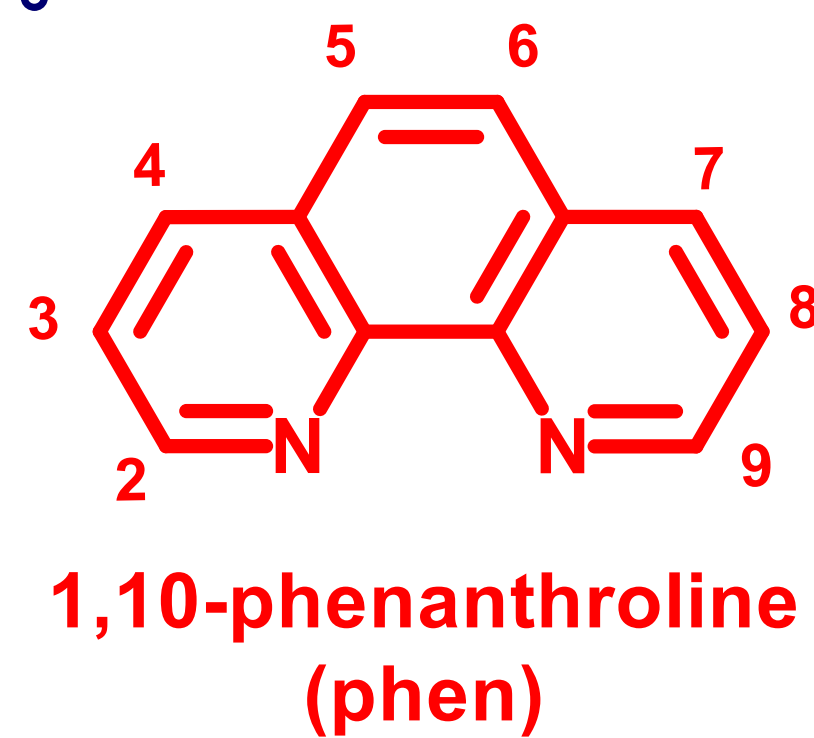
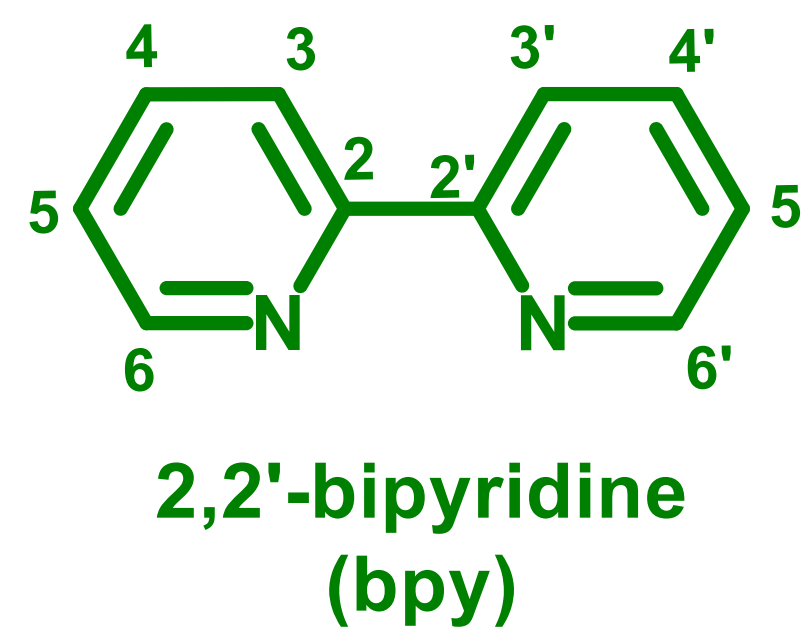
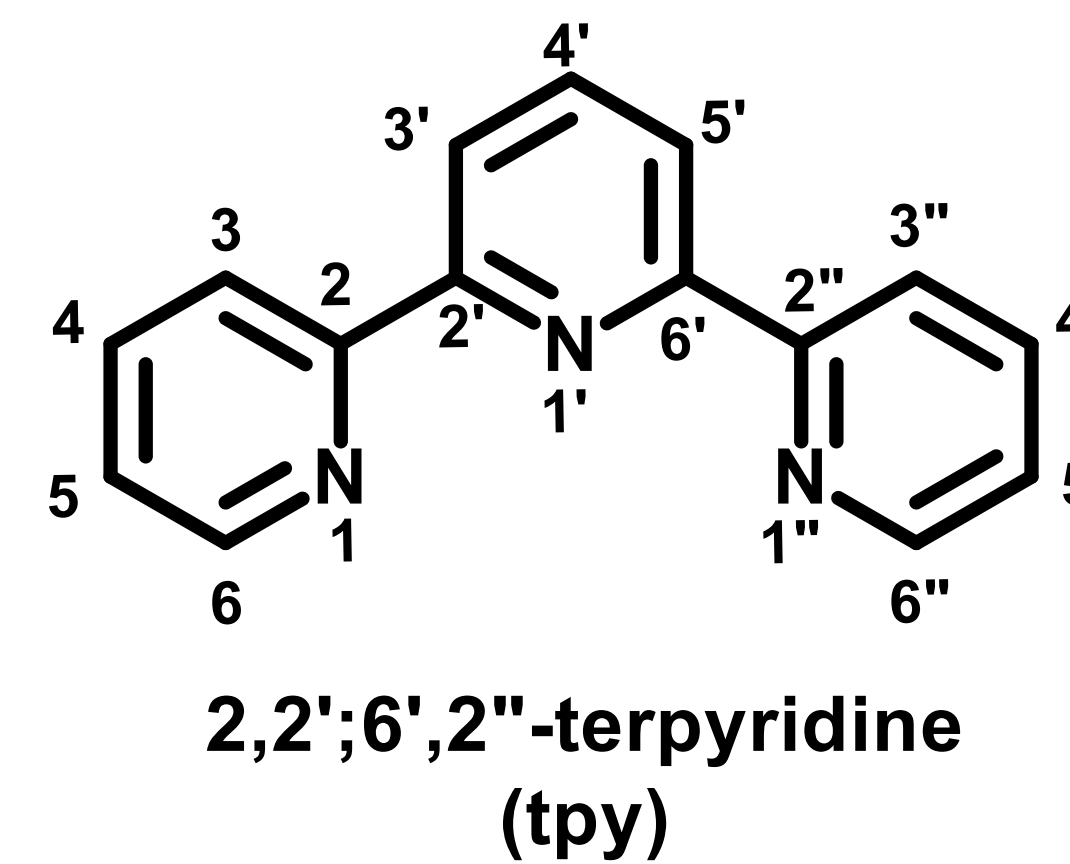




CV and DFT of terpyridine ligands

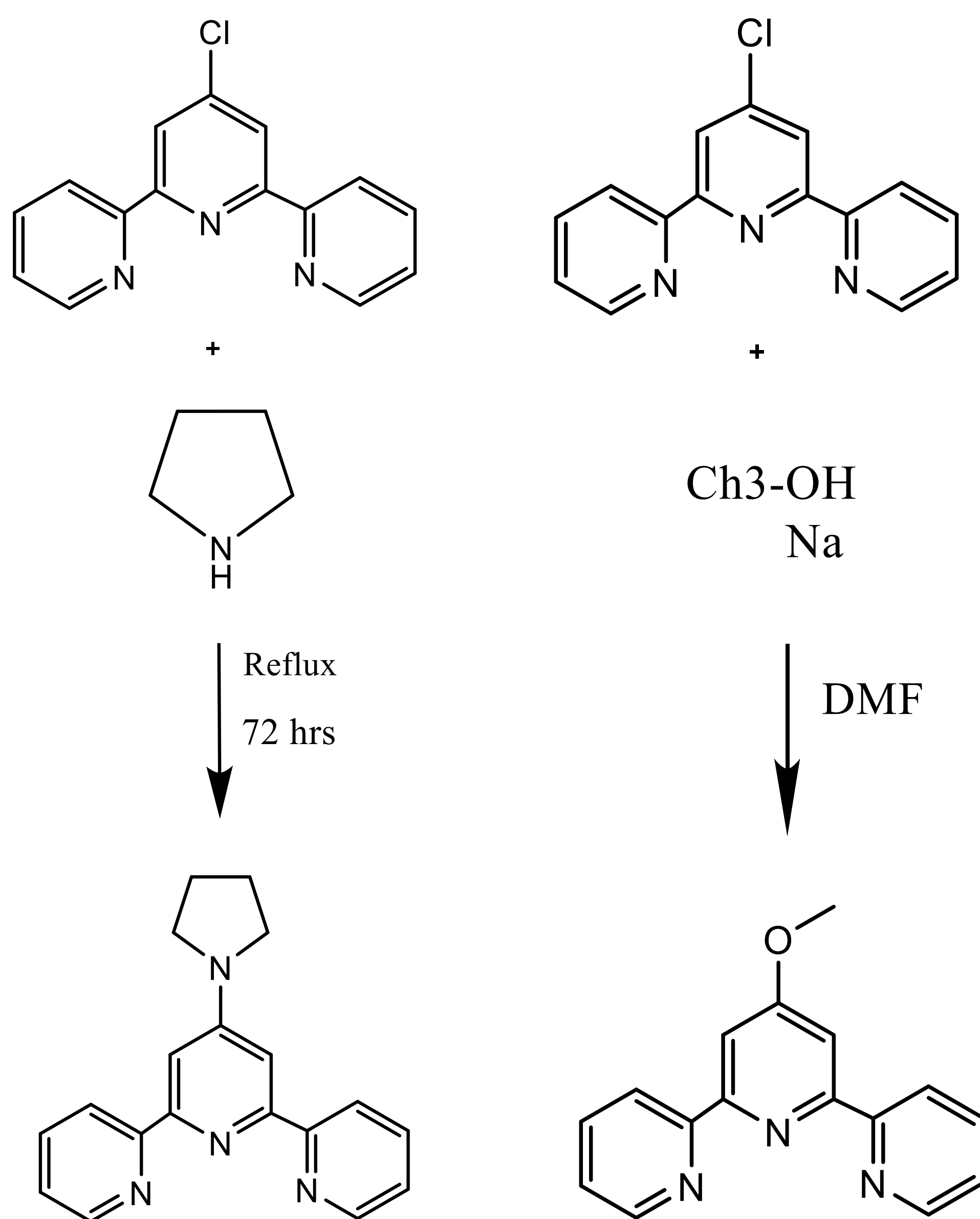
Nandisiwe Ghandi Sibongile Mateyise, Jeanet Conradie , Marrigje Marianne Conradie

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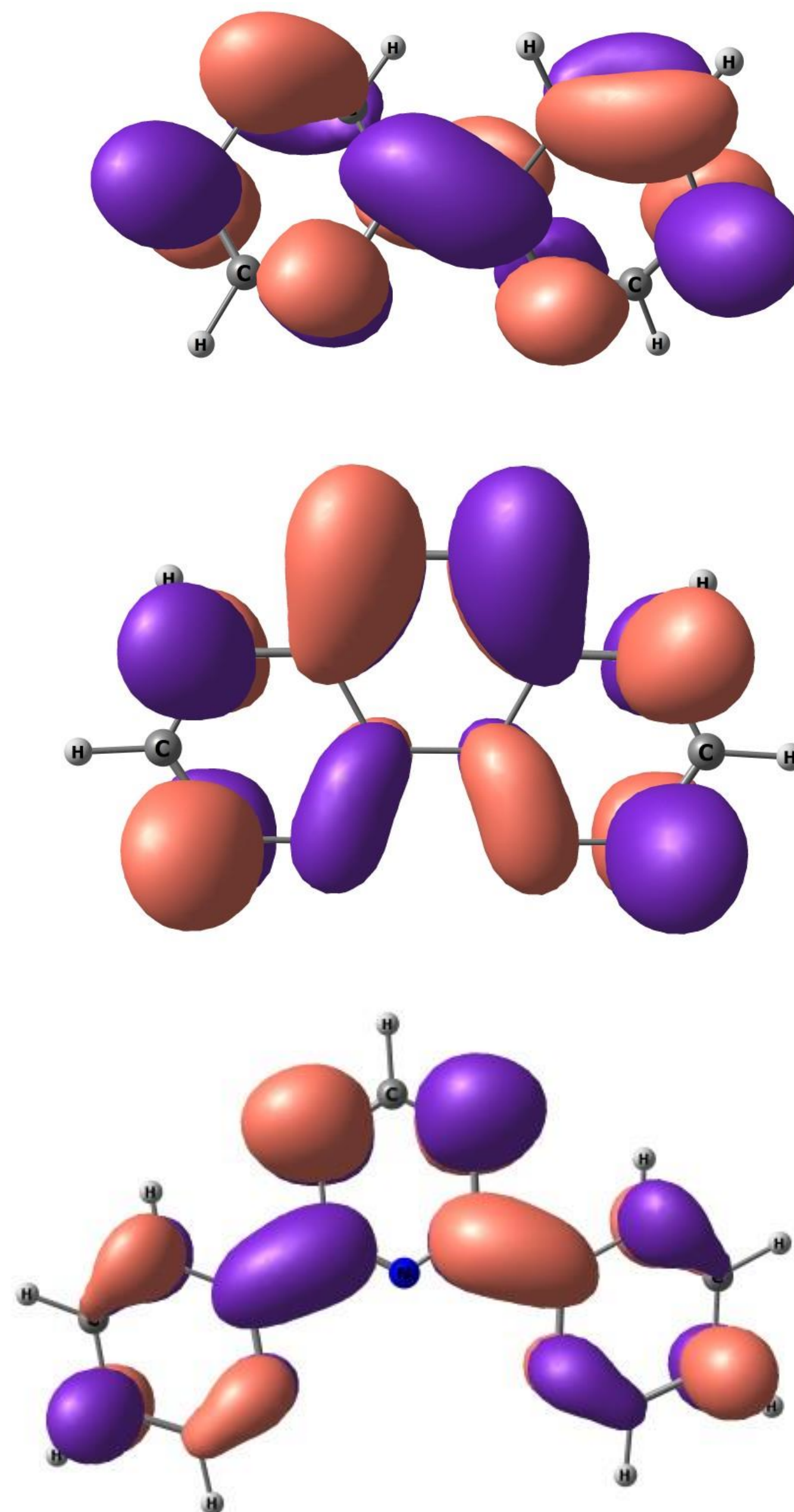
- Reactivity of metal complexes are related to the properties of the ligands attached to the metal, including the redox activity of the ligands.
- Aim is to identify theoretical methods that can be used to predict the redox potentials and thus the expected reactivity of the metal-ligand
- This study on substituted terpyridine, including substituted bipyridines and phenanthrolines

- Cyclic voltammetry (CV) shown irreversible reduction peak(s).
- Locus of lowest unoccupied molecular orbital (LUMO) show reduction centre.
- Reduction potential of tpys give linear trend with DFT calculated LUMO energies, following the same trend than substituted phens and substituted bpys.

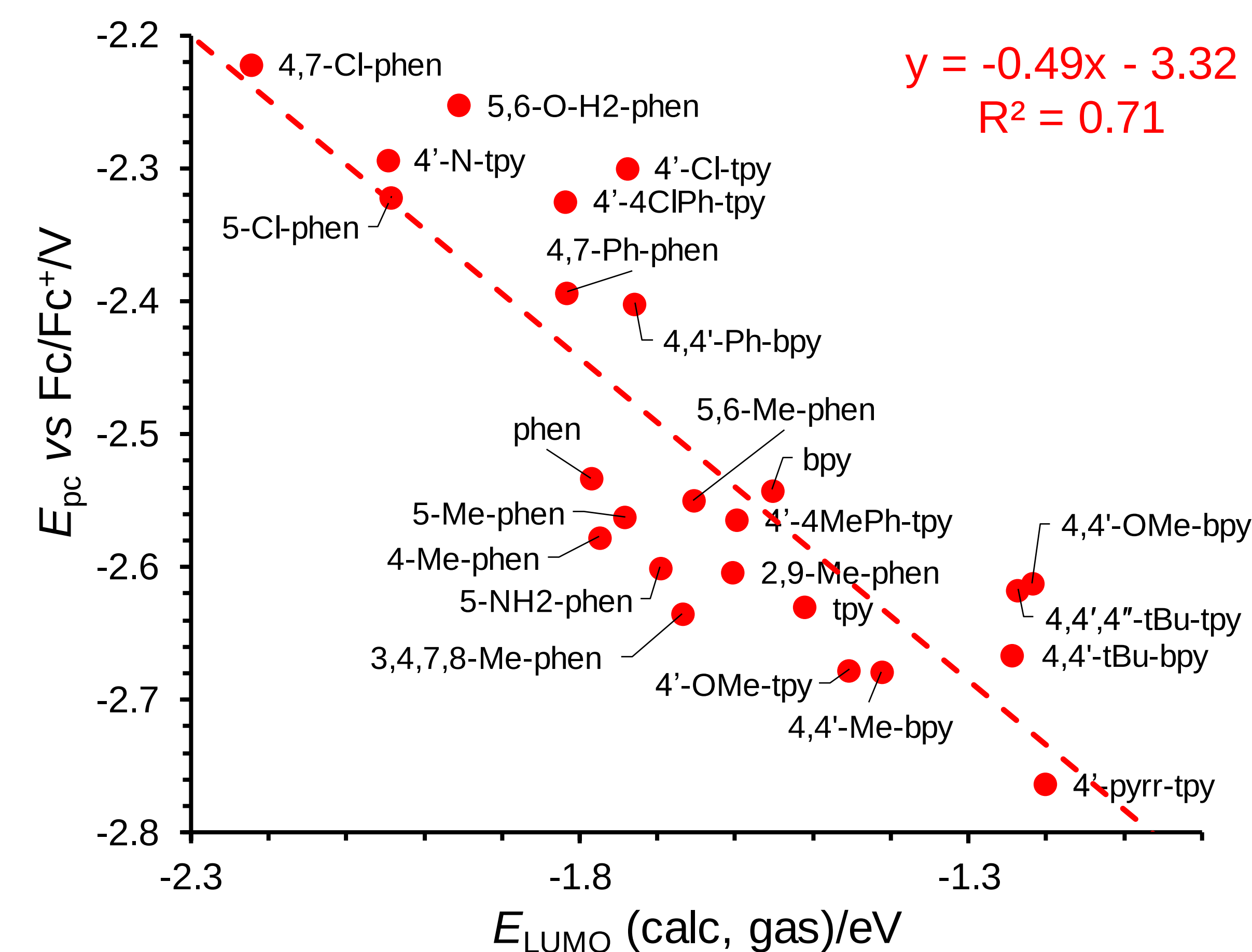
Synthesis tpys



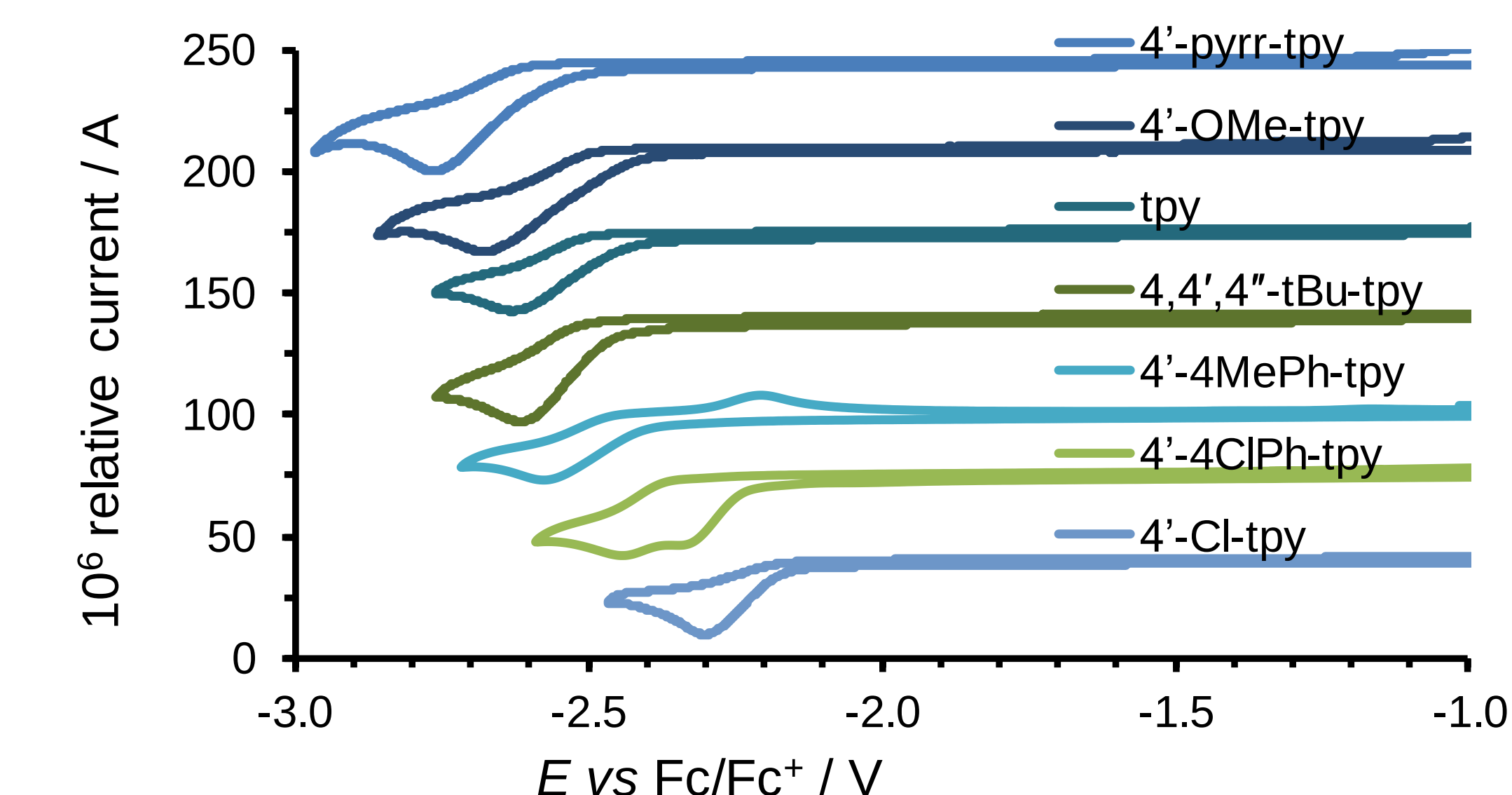
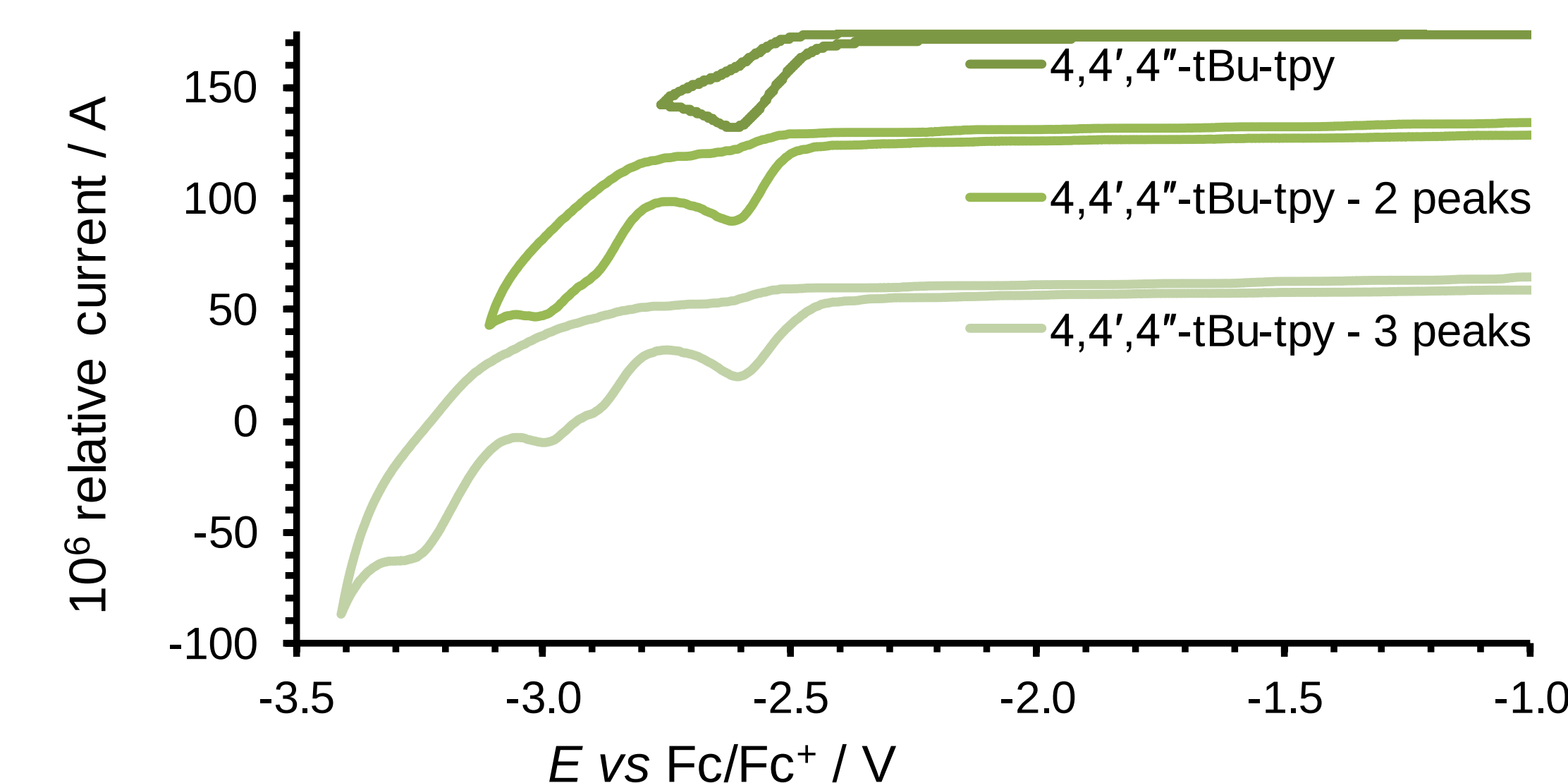
DFT LUMO



Relationship involving data of phens, bpys and tpys



CVs of tpys



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