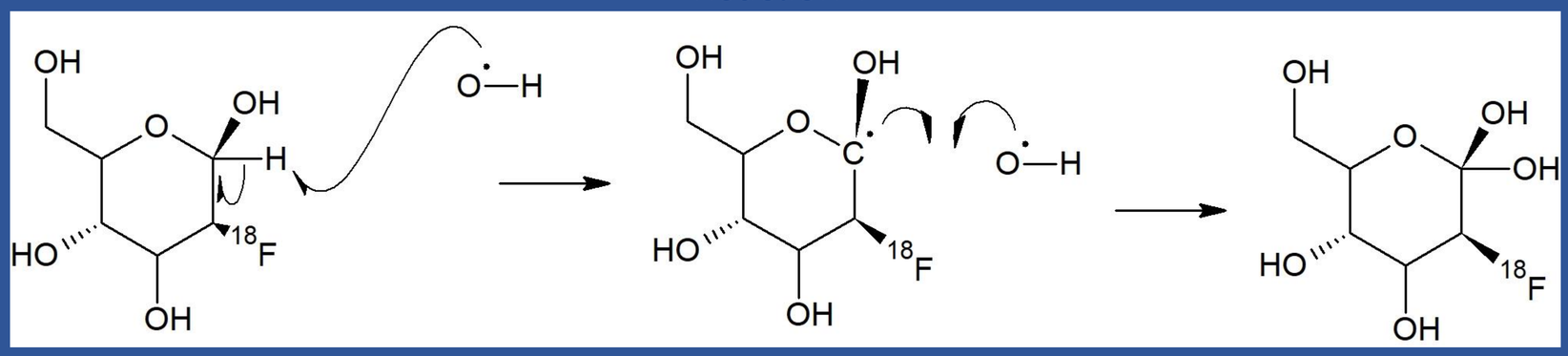
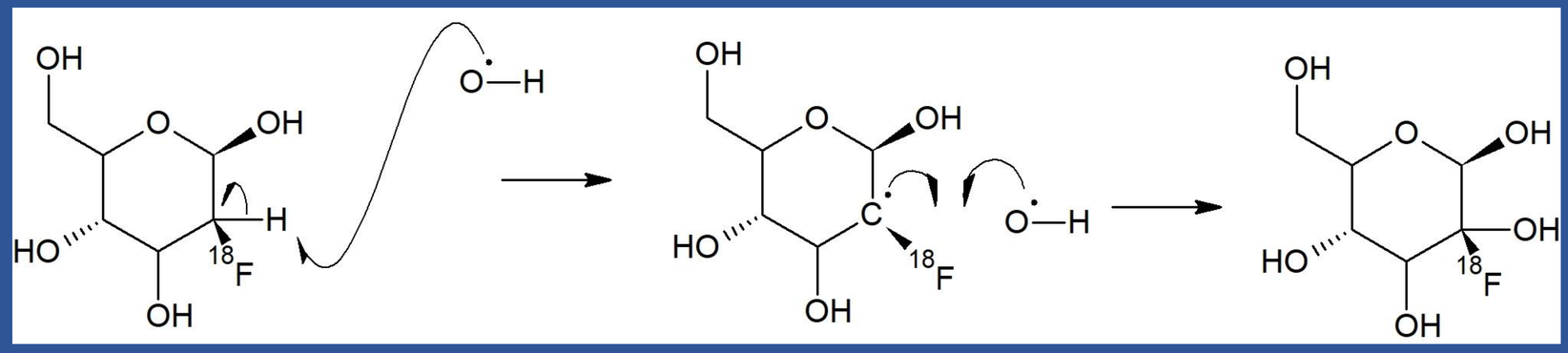
Density Functional Theory Calculations for the Radiolytic Stability of [18F]Fluorodeoxyglucose

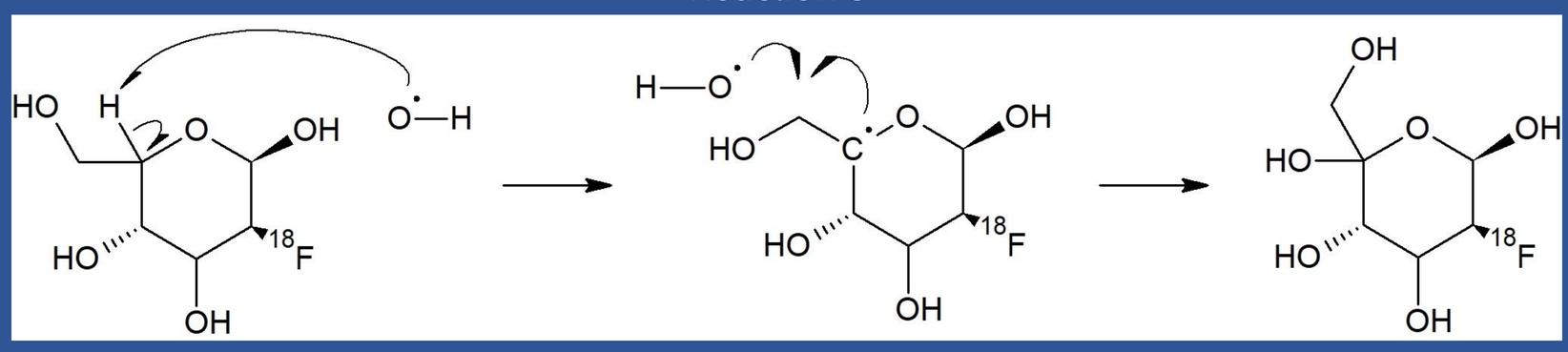
Reaction 1



Reaction 2



Reaction 3



DFT calculations show that reaction 1 (see above) is the most energetically favorable case for [18F] FDG radiolytic degradation

INTRODUCTION

- [18F] Fluorodeoxyglucose has had a profound impact in neurosciences since its development in 1976.
- An important property of any radiopharmaceutical, however, is its radiolytic stability.
- In this study, we perform initial calculations involving the radiolytic stability of FDG using density functional theory.

METHODS

- The Becke, 3-parameter, Lee–Yang–Parr (B3LYP) hybrid functional was used with valence triple-zeta polarization basis sets from the Karlsruhe group.
- All calculations were performed using ORCA ver. 5.0.4 while output files were visualized using Avogadro 1.2.0, and Chemcraft 1.8.
- Since [18F] FDG can exist in both chain and ring forms, reaction energies associated with both forms were also calculated

RESULTS

Reaction Number	Reaction Energy (kcal/mol) (Chain)	Reaction Energy (kcal/mol) (Ring)
Reaction 1	-119.7810231	-130.7304359
Reaction 2	-113.2765404	-113.9856062
Reaction 3	-112.9509981	-121.8316904

DISCUSSIONS AND CONCLUSION

- Results show that H abstraction at C1 site is the most energetically favorable reaction
- Based on the calculations, Rxn 3 is now more favorable vs. Rxn 2 in this case, illustrating how the initial structure influences the reaction energies
- Additional work needs to be done to further apply ab-initio computational techniques to modelling neuroimaging, and neurodegenerative systems.

Vincent Munar[1*], and Noel Oquendo[2]

[1]Universidad Politécnica de Madrid, [2]Ateneo de Manila University

*vincent.munar@alumnos.upm.es

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