

Interactions of Uranyl Ion with Bidentate Eudistomin Ligands

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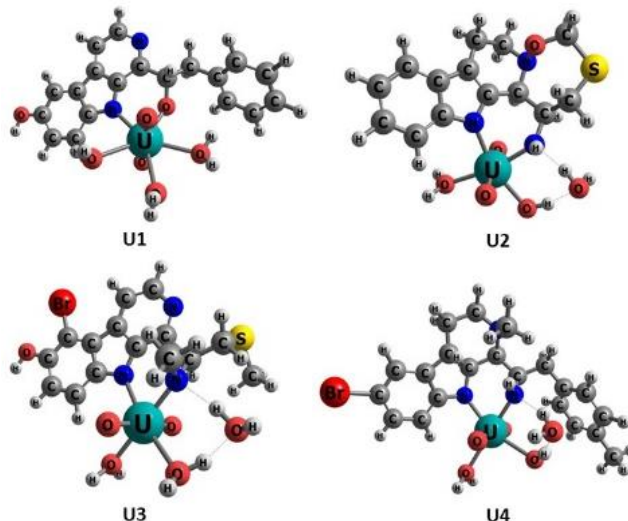
Can Eudistomins help in the enrichment of Uranium in Ascidians?

INTRODUCTION

- Ascidians are known to concentrate various unusual metals in their bio-systems, including Uranium¹
- Eudistomins are β -carboline derivatives, and are known to form complexes with Iron²
- Four simple bidentate Eudistomins from literature were chosen for this work^{3,4}
- Our work has been done using The Amsterdam Density Functional (ADF) software⁵

COMPUTATIONAL DETAILS

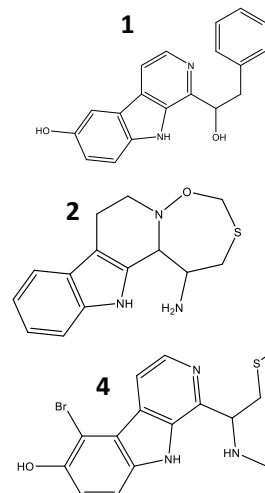
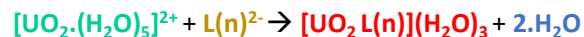
- Amsterdam Density Functional (v.2017)
- GGA: PBE – D3
- TZ2P
- Scalar ZORA (small frozen core)
- COSMO (for solvation)



RESULTS

L(n)	ΔG (gas-phase) (kcal/mol)	ΔG (solvation-phase) (kcal/mol)
1	-401.03	-73.35
2	-410.19	-82.39
3	-402.54	-89.35
4	-396.01	-78.31

MODEL



n =

- 1 = Eudistomin W
 - 2 = Debromoeudistomin K
 - 3 = Eudistomidin B
 - 4 = Eudistomidin C
- Complexes are labelled as U1, U2, U3, & U4 respectively

REFERENCES

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3. Cao, R. *et al.* *Curr. Med. Chem.* 14, 479-500 (2007).
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CONCLUSIONS

- Our initial model shows Uranyl ions are capable of forming complexes with Eudistomins
- In our further work, we are exploring sulphate based models, to mimic realistic conditions

