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# The Effect of Solvents on the Solvation Shell of $[Tb(DPA)_3]^{3-}$ with the Addition of a Mixture of L-/D-Serine Through the Utilization of Circularly Polarized Luminescence Spectroscopy

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## Abstract

**Chirality is an important part of medicine and pharmaceuticals** because drugs need to be able to selectively bind and to be compatible with the different proteins in the body in order to help the body resist and overcome sickness. Hence, drug molecules are often defined as chiral compounds.

The focus of our research is to use $[Tb(DPA)_3]^{3-}$ (where DPA = 2,6-pyridinedicarboxylate)to probe and identify the chirality amino acids. Thus, we investigated the effect of different solvents have on the mixture of L-/D-serine when this mixture interacts with the $[Tb(DPA)_3]^{3-}$.

**The solvent environment was changed by adding varying the proportion of selected solvent relative to water. We were interested in the effect this would have on the association of the mixture of L-/D-serine to $[Tb(DPA)_3]^{3-}$ and how this would in turn effect the magnitude of the circularly polarized luminescence (CPL) signal.**

Our study suggests that the CPL technique is well suited for recognition of chiral biological molecules, because of its high sensitivity to changes in the surrounding chiral environment.

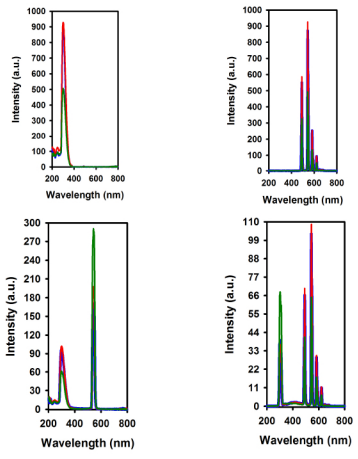
## Project Activities or Findings

Our preliminary results suggest that:

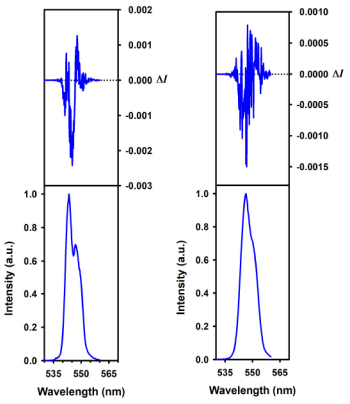
- The solvent environment has a direct influence on the formation of the $[Tb(DPA)_3]^{3-}$:L-/D-serine adduct,
- A higher percentage of 1,4-dioxane resulted in a greater CPL activity, thus a greater perturbation for the mixture of L-/D-serine at physiological pH,
- Methanol does not have much perturbation compared to the 1,4-dioxane solvent,
- Hydrophobic groups are essential in the mechanism of perturbation of $[Tb(DPA)_3]^{3-}$, and
- The CPL technique is well suited for projects aimed at probing specific chiral structural changes and/or for recognition of chiral biological molecules, because of its high sensitivity to changes in the surrounding chiral environment.

## Preliminary Findings

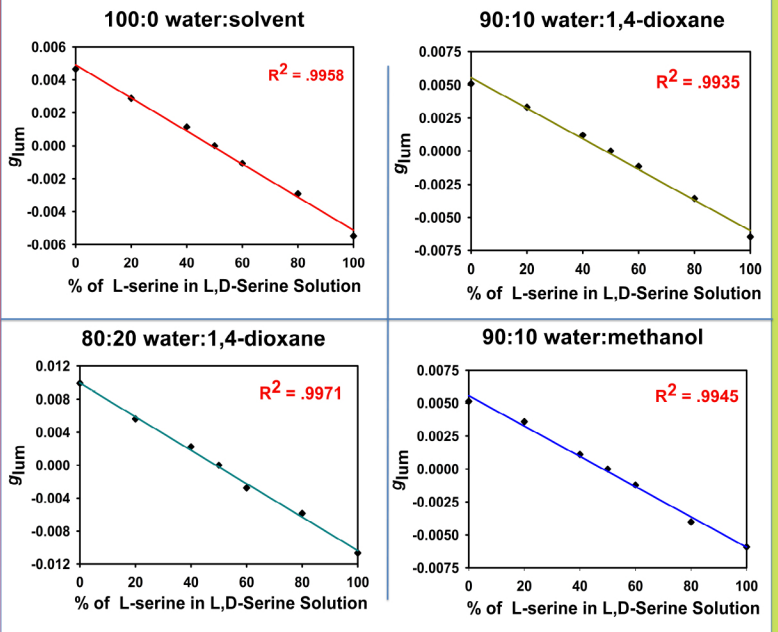
**Time-resolved (top) and steady-state (bottom) excitation (left) and emission (right) spectra of 0.005 M $[Tb(DPA)_3]^{3-}$ after addition of 40 equiv. of 80:20 L-:D-serine in 100:0 (blue), 90:10 (red), and 80:20 (green) water:1,4-dioxane at RT and pH 7.00 ($\lambda_{exc}$ = 300.00 nm and $\lambda_{em}$ = 545.00 nm)**




**CPL (top curves) and total luminescence (lower curves) spectra for the $^5D_4 \rightarrow {}^7F_5$ transition of 0.005 M $[Tb(DPA)_3]^{3-}$ after addition of 40 equiv. of 80:20 L-:D-serine in 100:0 (top) and 80:20 (bottom) water:1,4-dioxane at RT and pH 7.00 ($\lambda_{exc}$ = 300.00 nm)**




## Preliminary Findings




## Research Questions

- How will the Pfeiffer effect play a role in determining the perturbation for the mixture of L-/D-serine with different solvents?
- Which solvent will have the greatest perturbation on the mixture of L-/D-serine?
- Which enantiomer of the L-/D-serine will have the greatest contribution for the perturbation?
- How much of a difference will the solvents 1,4-dioxane and methanol have on the perturbation?

## Citations

1. J. L. Lunkley, N. M. Nguyen, K. M. Tuminaro, D. Margittai, G. Muller, *The Importance of Solvent Effects on the Mechanism of the Pfeiffer Effect, Inorganics,* **2018,** *6*, 87-112.
2. A. Moussa, C. Pham, S. Bommireddy, G. Muller, *Importance of Hydrogen-Bonding Sites in the Chiral Recognition Mechanism Between Racemic $D_3$ Terbium(III) Complexes and Amino Acids, Chirality*, **2009**, *21*, 497-506.
3. J. Neugebauer, *Induced Chirality in Achiral Media: How Theory Unravels Mysterious Solvent Effects, Angew. Chem. Int. Ed.*, **2007**, *46*, 7738-7740.