Matrix Performance for *MALDI-MS* has been shown to be related to *Absorbance at Laser Wavelength* and *Proton Transfer* but *these are not the only Factors!*

DFT and TD-DFT Studies of Some Aminoacridines as Matrices in MALDI-MS

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INTRODUCTION

- ✓ ***MALDI,*** Matrix-Assisted Laser Desorption/Ionization, is one of the most successful **"soft" ionization** methods in **Mass Spectrometry, MS**.
- ✓ ***Matrix*** should have enough **absorbance at laser wavelength** and the tendency to participate in **proton transfer** reactions.
- ✓ ***Computational Chemistry*** can give insights about the role of these factors in matrix performance.

MATRICES and METHODS

- ✓ Matrices: 2-, 3-, and 9-Aminoacridines (**2-AA, 3-AA and 9AA**), *Fig. 1*.
- ✓ Absorbance: Vertical electronic transitions at **TD-CAM-B3LYP/6-31+G(d,p)** level of theory
- ✓ Ground- and excited-state gas-phase basicities (**GB and GB***): the **G4MP2 method** and **Förster cycle**.

RESULTS and DISCUSSION

- ✓ Based on **preliminary experimental** MALDI-MS results, **3-AA** has the **best performance**.
- ✓ Based on calculated absorbance at laser wavelength, *Fig. 2*, **9-AA** has the **highest absorption coefficient**.
- ✓ Based on calculated basicity results, *Fig. 3*, **9-AA** and **2-AA** have the **highest GB** and **GB*, respectively**.

COUNCLUSIONS

- ✓ Having **good absorbance** is essential for a matrix but is **not the most important factor**.
- ✓ Having **highest GB or GB*** is also **not sufficient** for having the **best performance**.
- ✓ **Other factors** are contributing to the observed experimental performance which are under investigation by our group.

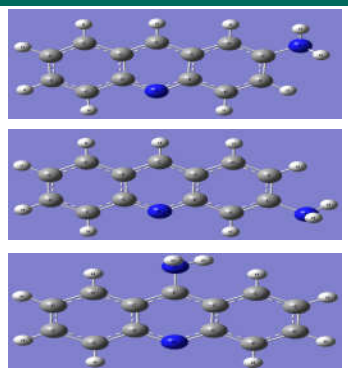

Fig 1.

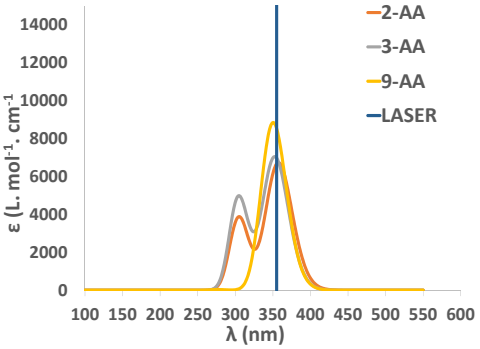

Fig2.

$\varepsilon_{\lambda=355}$(9-AA) > $\varepsilon_{\lambda=355}$ (3-AA) > $\varepsilon_{\lambda=355}$ (2-AA)

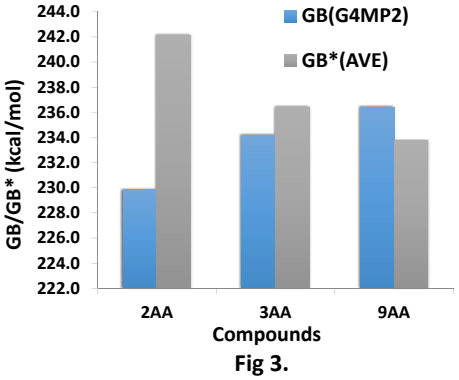

Fig 3.

GB(9-AA) > GB(3-AA) > GB(2-AA)
GB*(2-AA) > GB*(3-AA) > GB*(9-AA)

Please take a picture to download the abstract, the poster and my CV.

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