

Supporting Information

ESIPT-PET based triphenylamine-anthraquinone probe for the detection of phosgene: DFT studies, real time application in soil samples and test strips

Ramakrishnan AbhijnaKrishna^a and Sivan Velmathi^{a,*}

*^aDepartment of Chemistry, National Institute of Technology, Tiruchirapalli, 620015, India
velmathis@nitt.edu*

Table of Contents

Fig No	Supplementary Figures	Page No.
S1	¹ H NMR spectrum (DMSO) of TPAAQ	S3
S2	¹³ C NMR spectrum (DMSO) of TPAAQ	S3
S3	HR-Mass spectrum of TPAAQ	S4
S4	HR-Mass spectrum of TPAAQ + phosgene	S4
S5	Absorption study of TPAAQ and TPAAQ + phosgene in different solvents	S5
S6	Emission study of TPAAQ and TPAAQ + phosgene in different solvents	S5
S7	Selectivity plot of TPAAQ (30 μM) in UV-Vis spectroscopy with 3 equiv. addition of analytes (90 μM) in 1,4-dioxane solvent	S6
S8	Titration plot of TPAAQ (30 μM) in UV-Vis spectroscopy with addition of phosgene (0-117 μM) in 1,4-dioxane solvent	S6
S9	Fluorescence titration plot of TPAAQ (30 μM) with addition of phosgene (0-117 μM) in 1,4-dioxane solvent	S7
S10	Fluorescence change of TPAAQ (30 μM) at 533 nm with and without phosgene as time increases.	S7
S11	DFT Optimized structures of TPAAQ, TPAAQ' and TPAAQ + Phosgene	S8
S12	Images of probe solution containing soil treated without (I,III, and V) and with phosgene (II,IV and VI)	S8
S13	Emission changes of the probe at 533nm with different concentration of phosgene pre- treated soil	S9

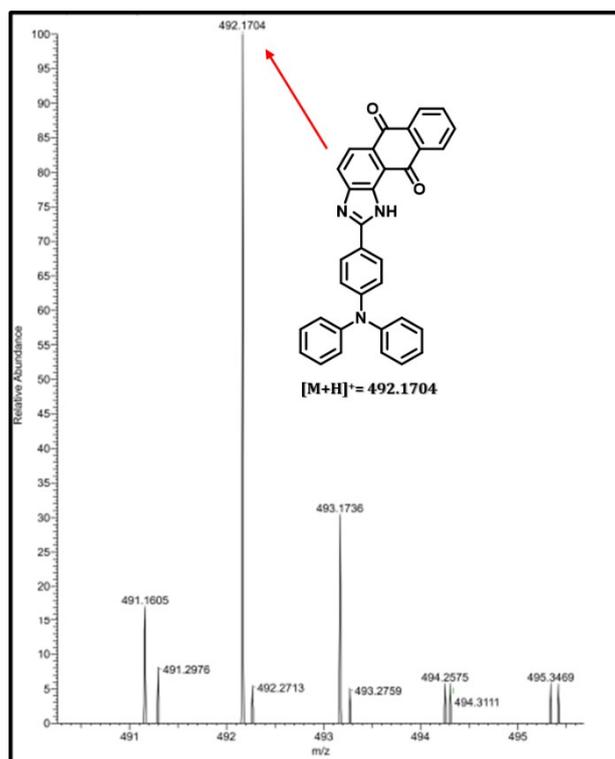


Figure S3. HR-Mass spectrum of TPAAQ

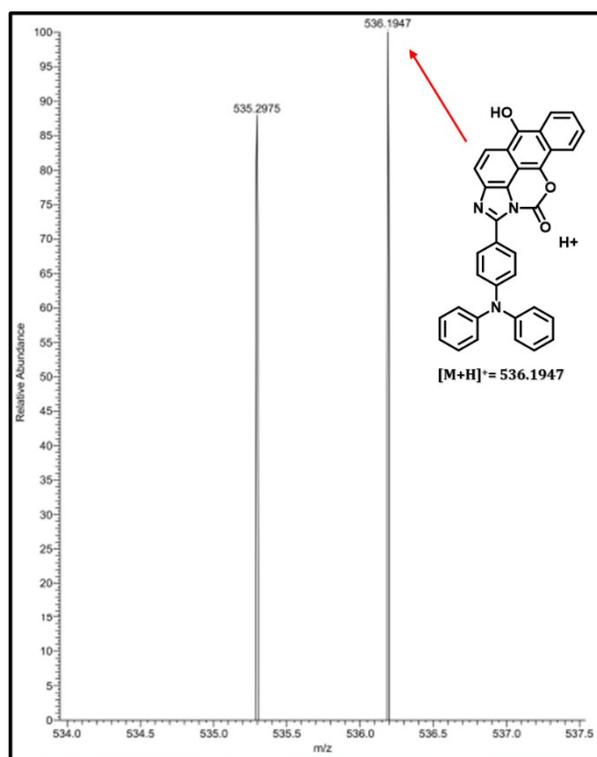


Figure S4. HR-Mass spectrum of TPAAQ + Phosgene

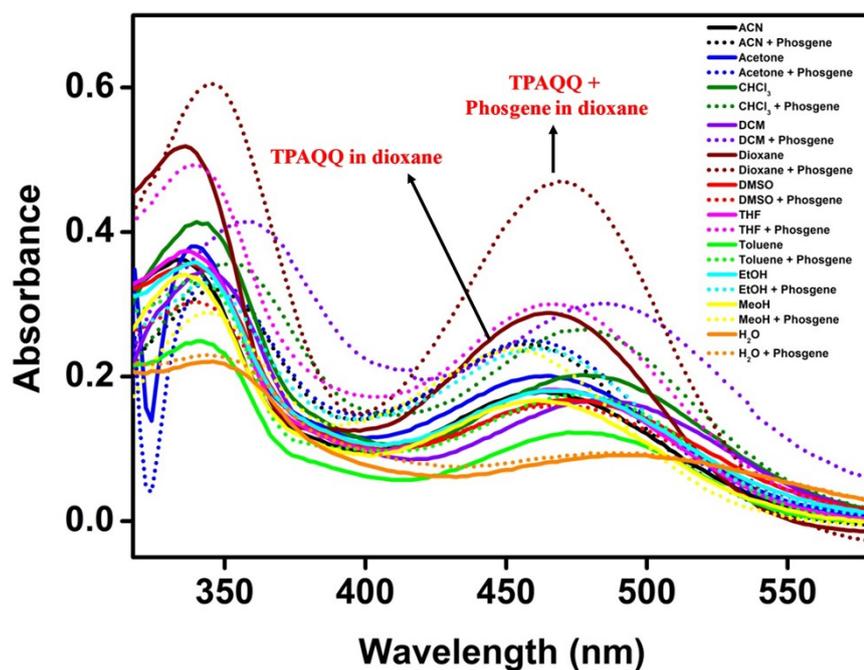


Figure S5. Absorption study of TPAQQ and TPAQQ + Phosgene in different solvents

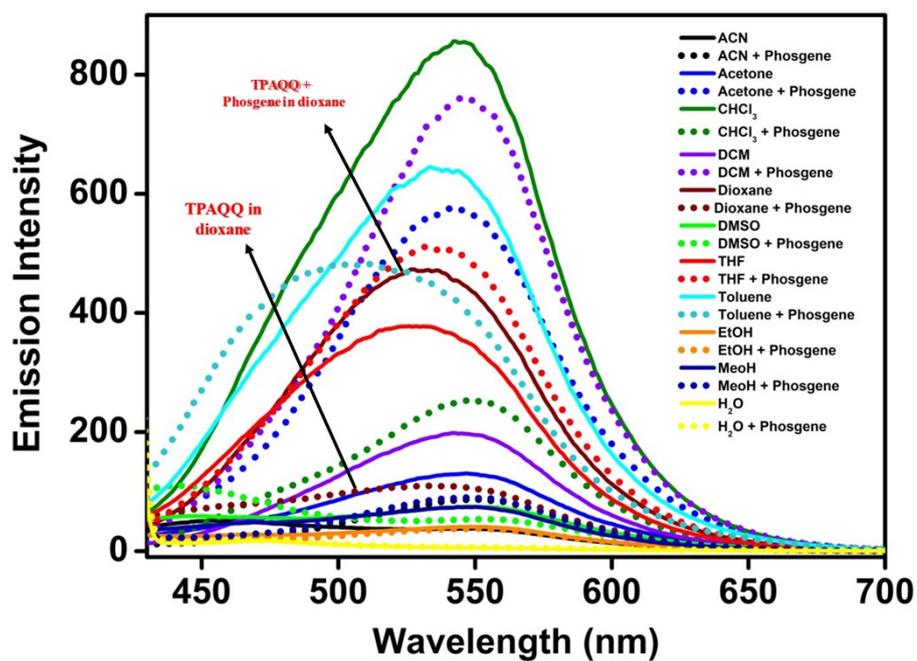


Figure S6. Emission study of TPAQQ and TPAQQ + Phosgene in different solvents

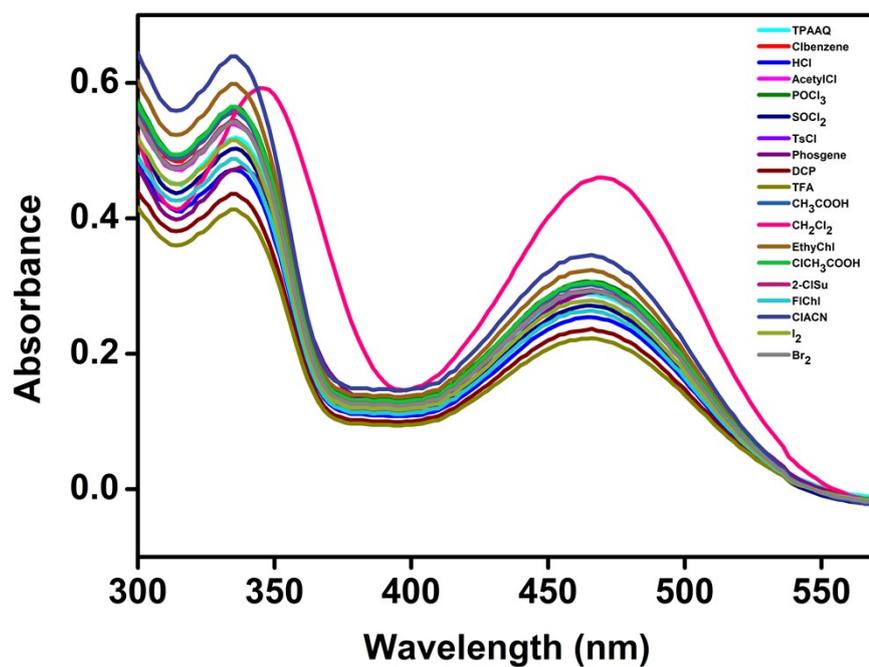


Figure S7. Selectivity plot of TPAAQ (30 μM) in UV-Vis spectroscopy with 3 equiv. addition of analytes (90 μM) in 1,4-dioxane solvent

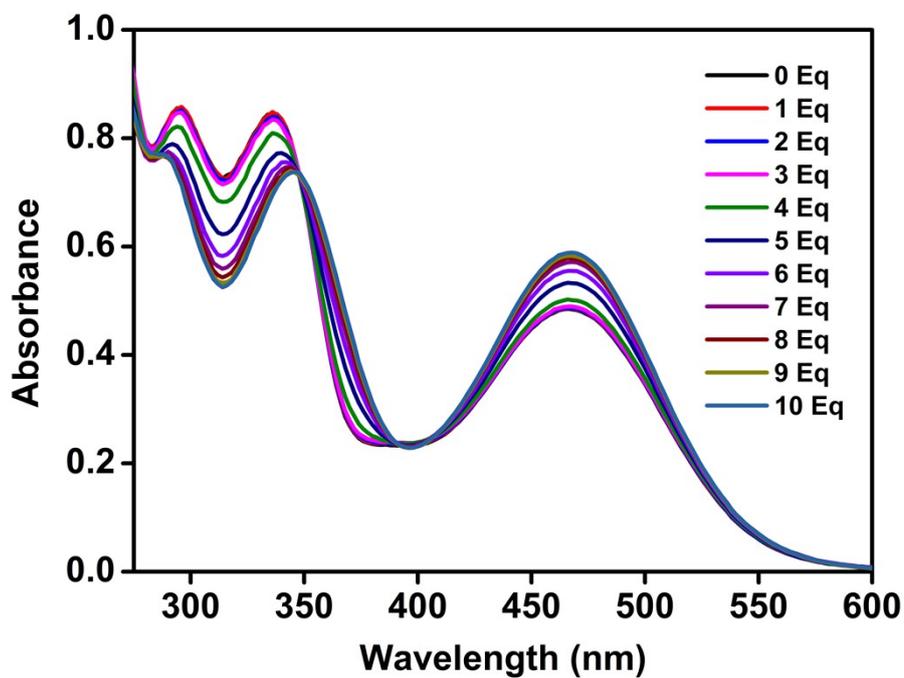


Figure S8. Titration plot of TPAAQ (30 μM) in UV-Vis spectroscopy with addition of phosgene (0-117 μM) in 1,4-dioxane solvent

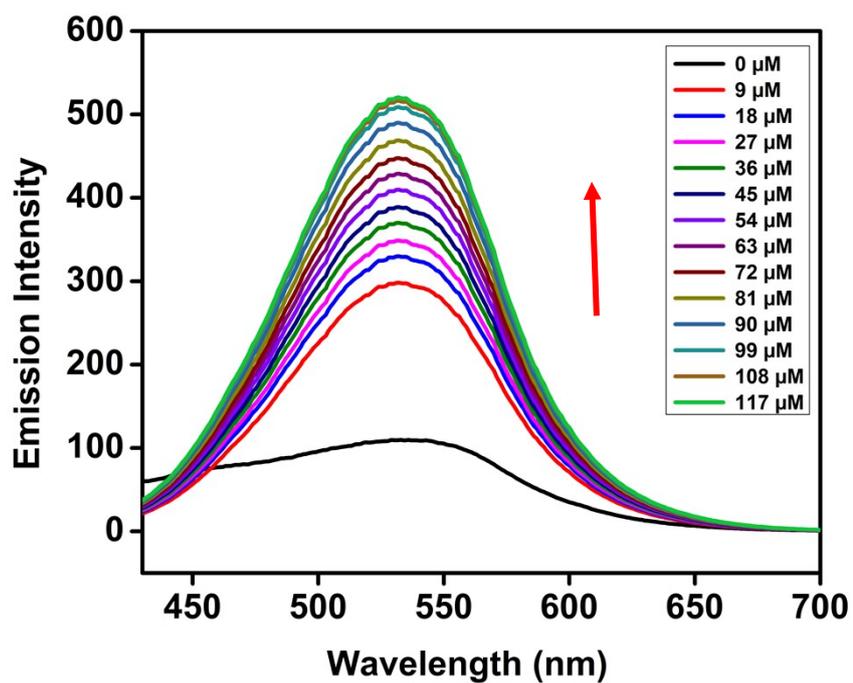


Figure S9. Fluorescence titration plot of TPAAQ (30 μM) with addition of phosgene (0-117 μM) in 1,4-dioxane solvent

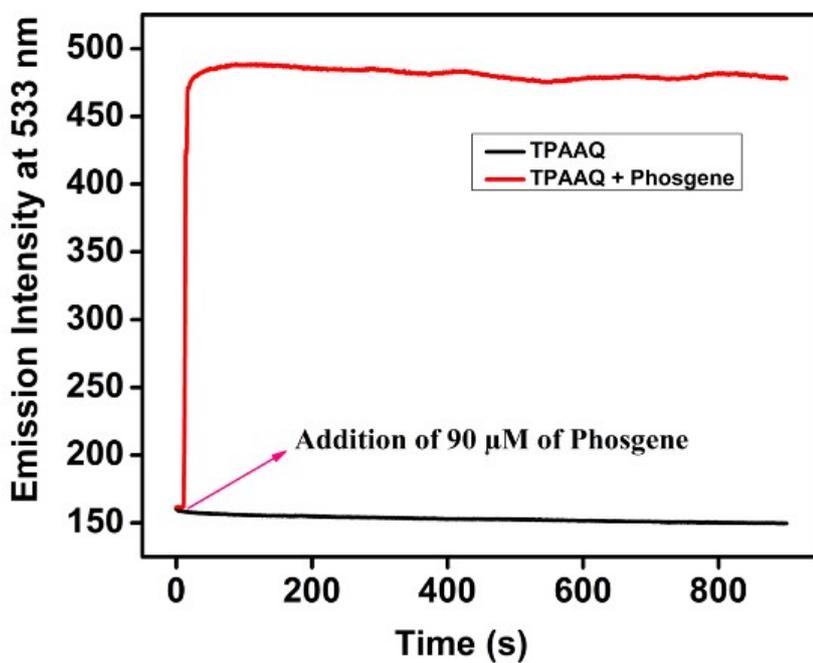


Figure S10. Fluorescence change of TPAAQ (30 μM) at 533 nm with and without phosgene as time increases.

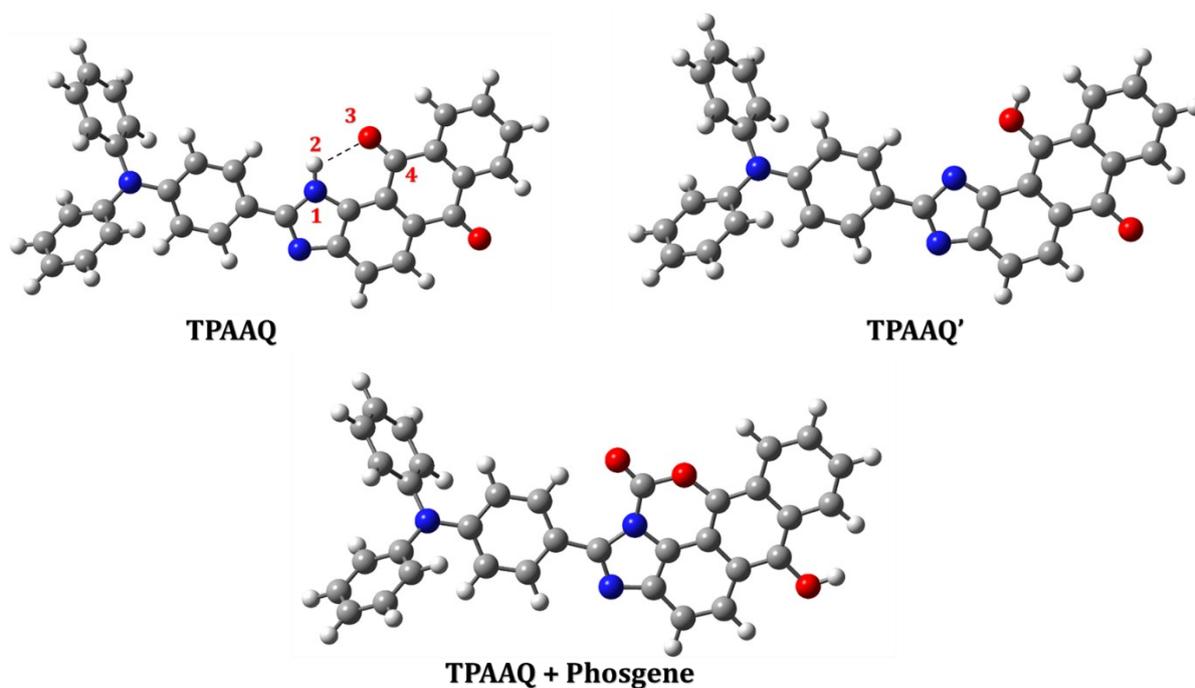


Figure S11. DFT Optimized structures of TPAAQ, TPAAQ' and TPAAQ + Phosgene

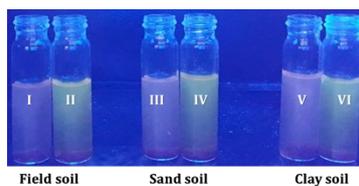


Figure S12. Images of probe solution containing soil treated without (I,III, and V) and with phosgene (II,IV and VI)

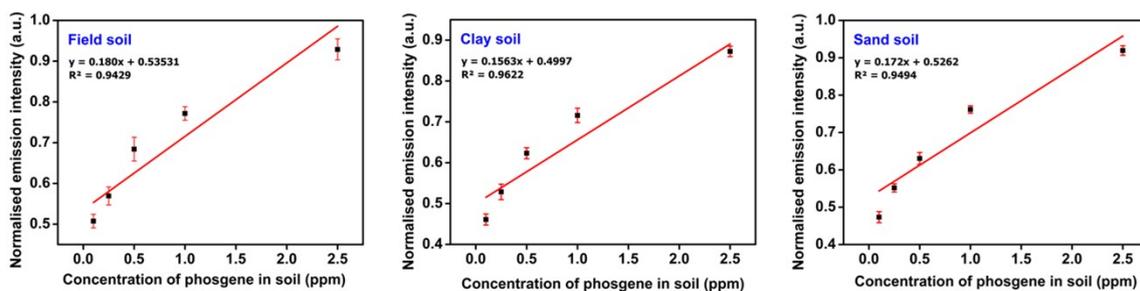


Figure S13. Emission changes of the probe at 533nm with different concentration of phosgene pre-treated soil