

Two-photon absorption in nitrofuran derivatives: promising compounds for photochemotherapy

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² EMBRAPA Instrumentação

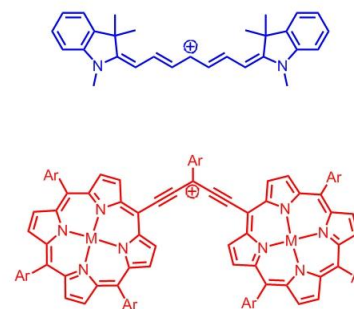
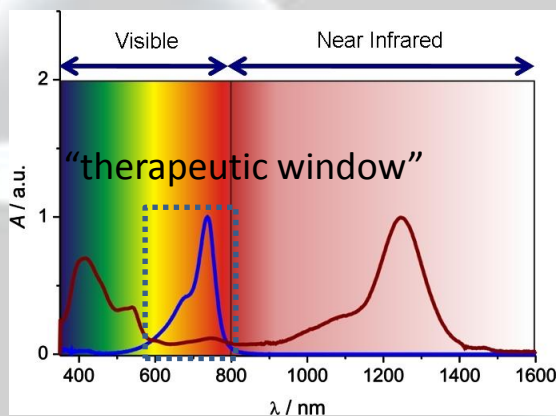
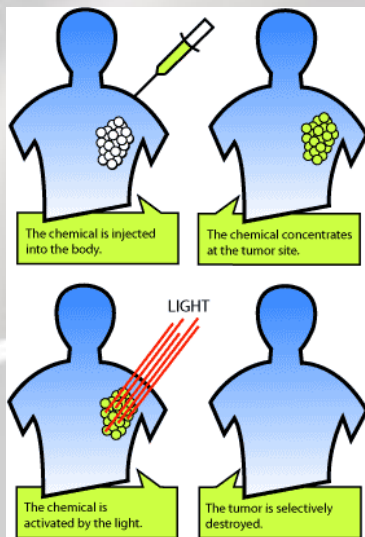
³ Instituto de Física, Universidade de São Paulo

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Motivation

Photochemotherapy



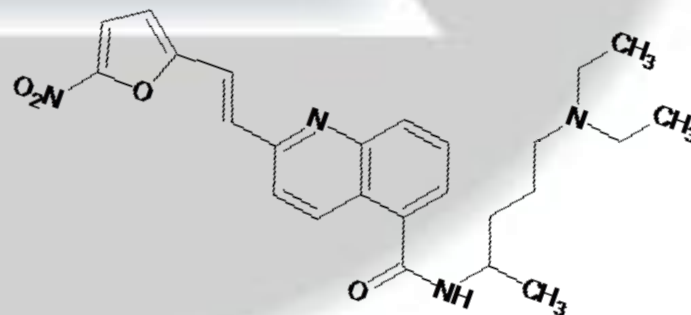
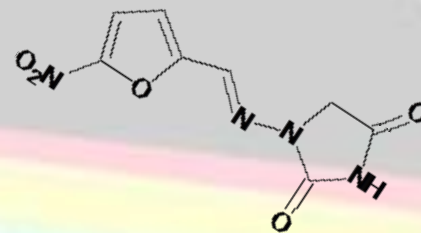
Sources : <http://www.photochembgsu.com/applications/therapy.html>

<http://hla.chem.ox.ac.uk/research.shtml>

- ✕ Multi-photon absorption (can go deeper into the tumor)
- ✕ Find new molecules (low toxicity)
- ✕ Excited state life time (depends on the process)

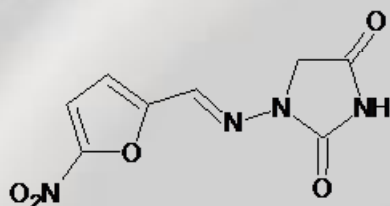
Outline

- ✕ Samples
- ✕ Two-photon Background
- ✕ Experimental setup
- ✕ Experimental and theoretical results
- ✕ Conclusion



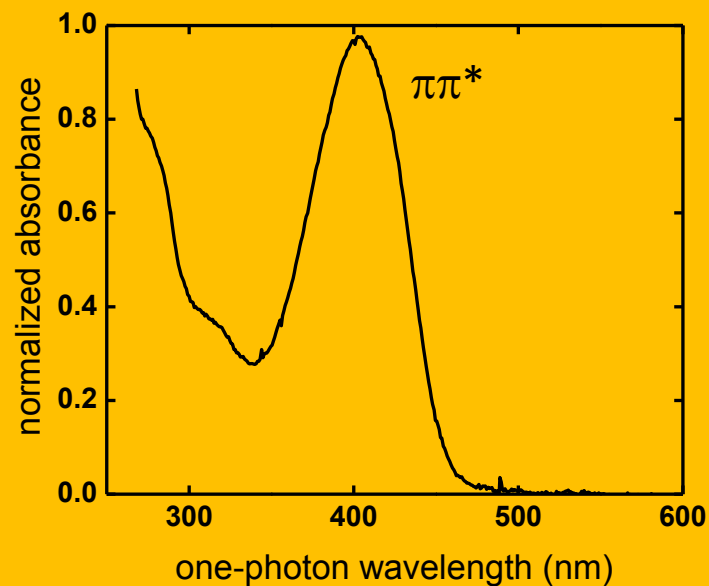
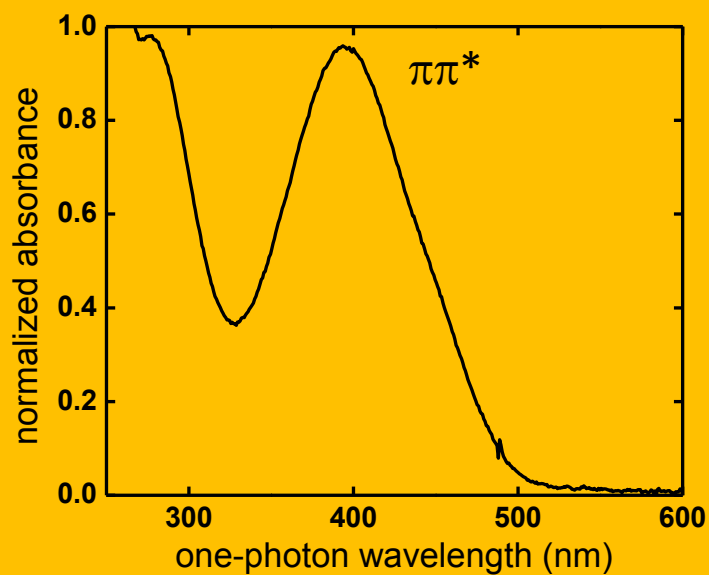
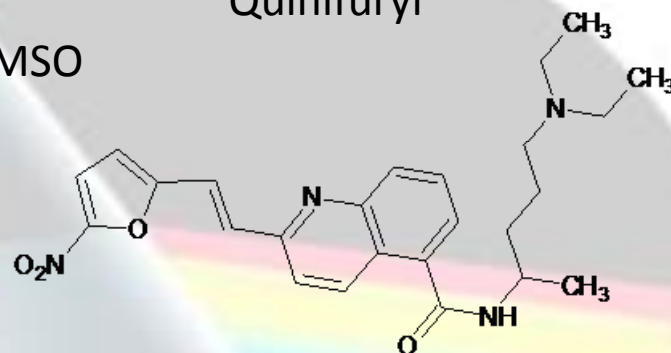
Samples

Nitrofurantoin

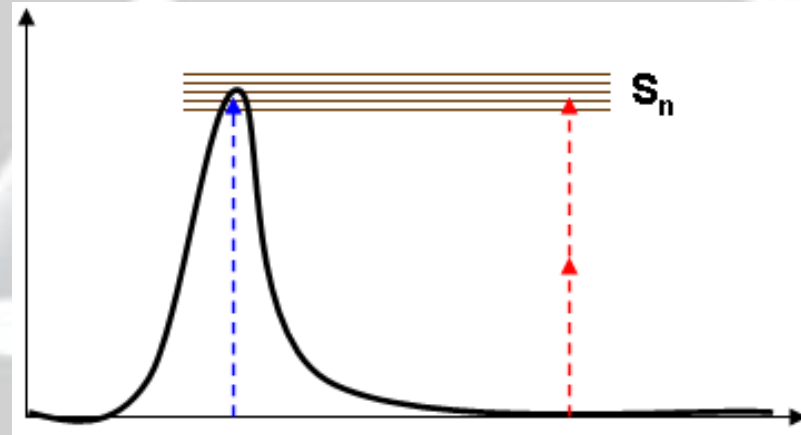
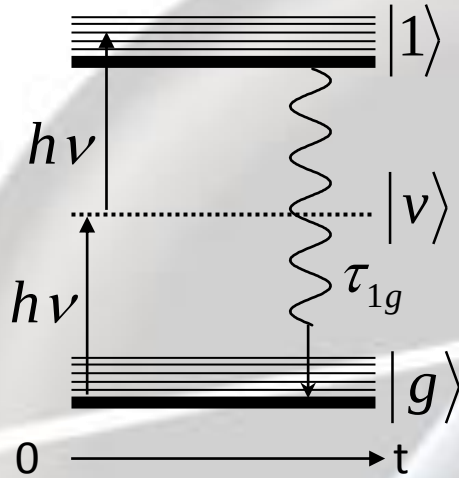


Solvent DMSO

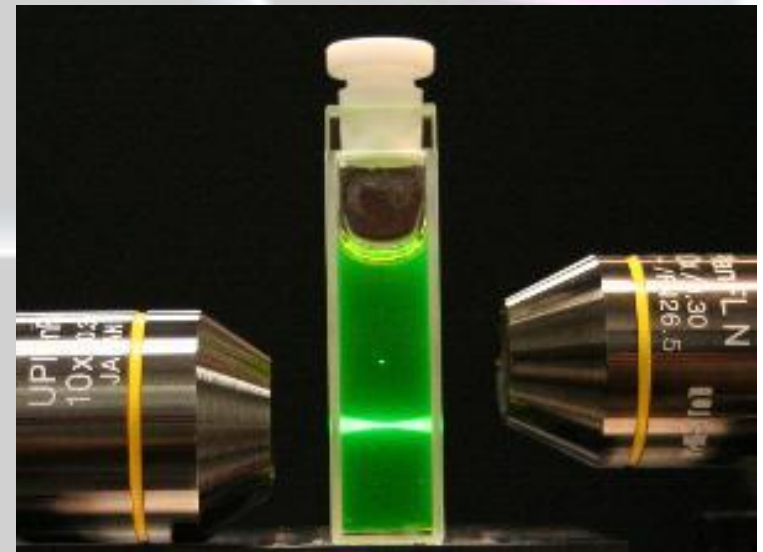
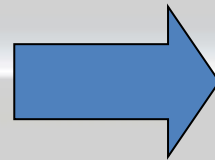
Quinifuryl



Two-photon introduction



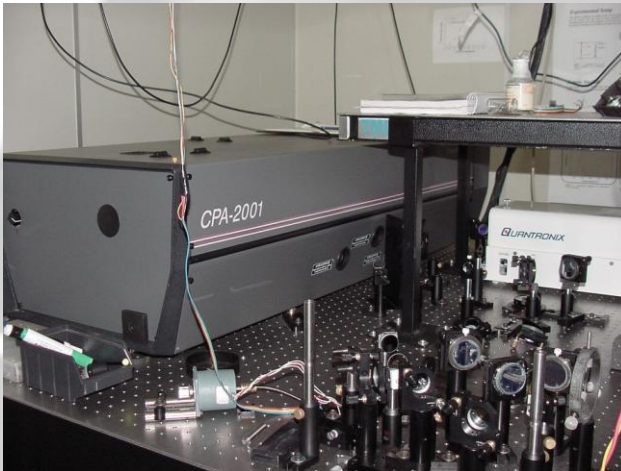
$$\frac{dI}{dz'} = -\cancel{\alpha}I - \beta I^2$$



✖ Multi-photon absorption (can go deeper into the tumor)

Experimental setup

Laser System



✓ *Ti:sapphire chirped pulse amplified system (CPA-2001)*

✓ 775 nm

✓ 150 fs

✓ 800 μ J



✓ *Optical parametric amplifier (TOPAS)*

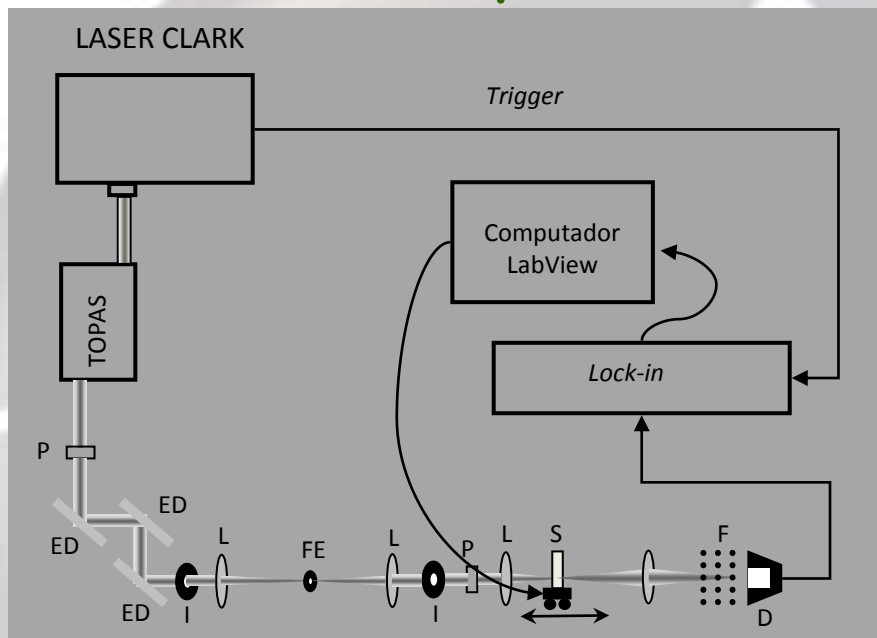
✓ 460 - 2600 nm

✓ $\approx$ 120 fs

✓ 20-60 μ J

Experimental setup

Z-scan technique

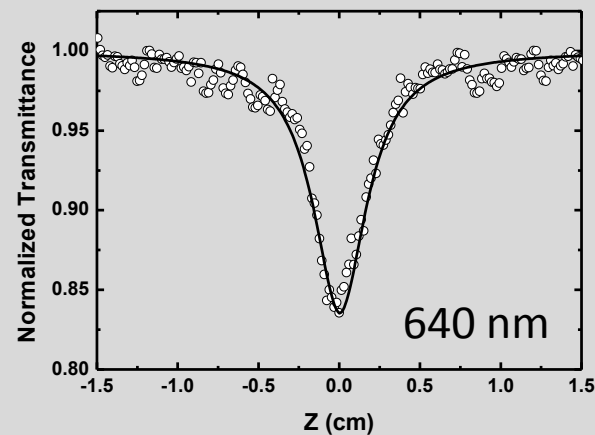
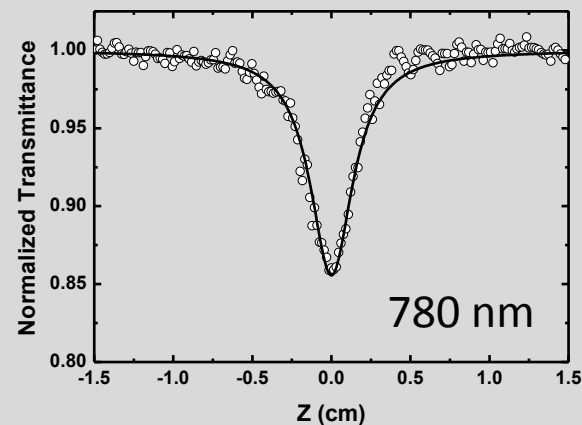
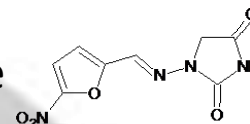


$$T = \frac{1}{\sqrt{\pi} q_0(z,0)} \int_{-\infty}^{\infty} \ln[1 + q_0(z,0)e^{-\tau^2}] d\tau$$

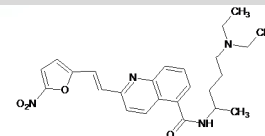
$$q_0(z,t) = \frac{\beta I_0(t)L}{1 + z^2/z_0^2}$$

$$\beta = \frac{N}{h\nu} \delta$$

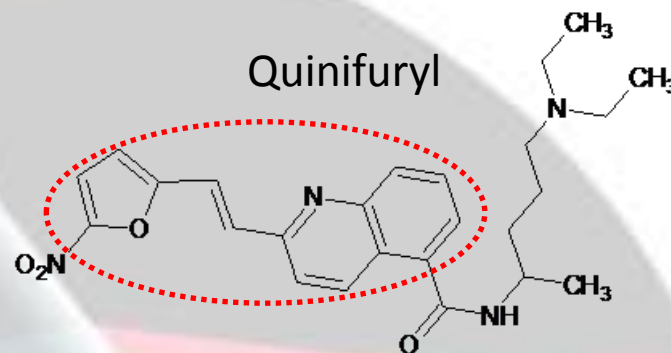
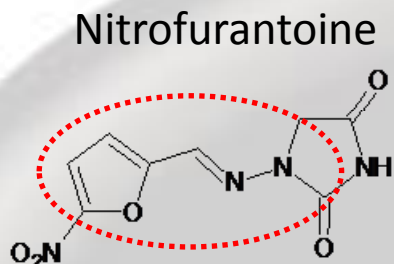
Nitrofurantoin



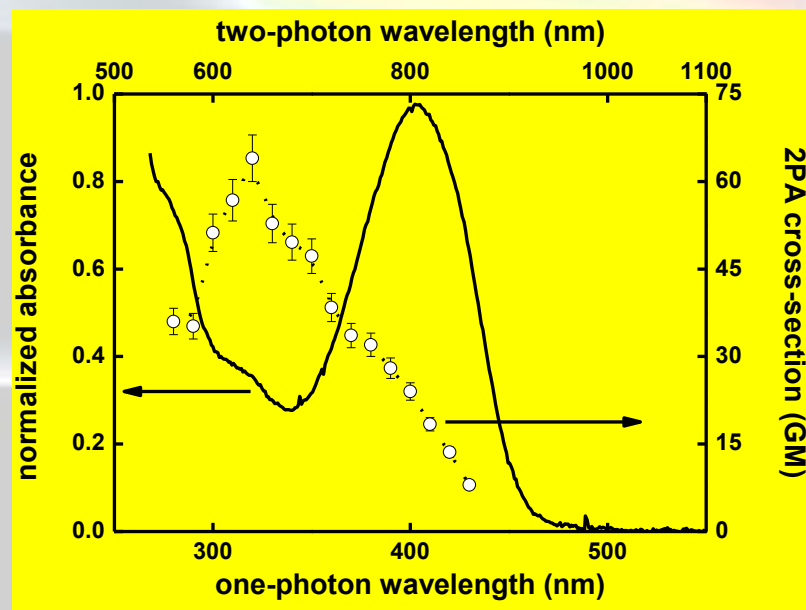
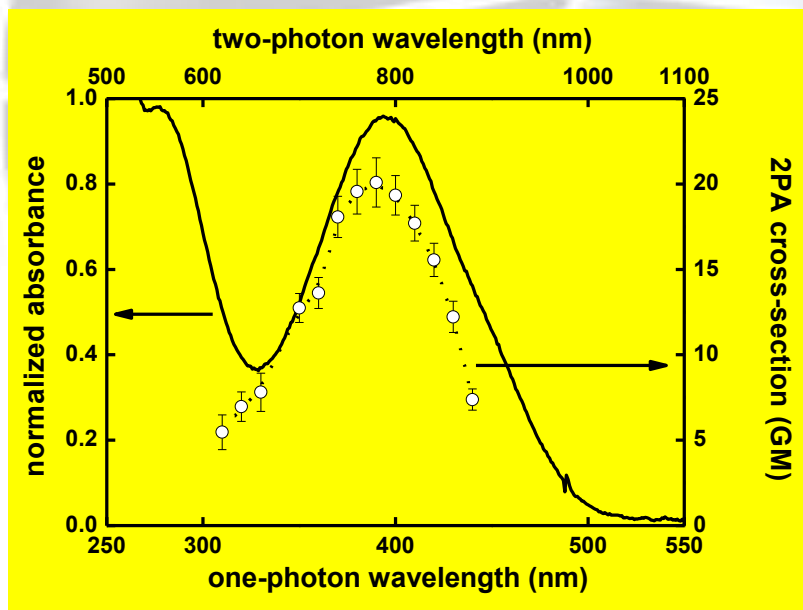
Quinifuryl



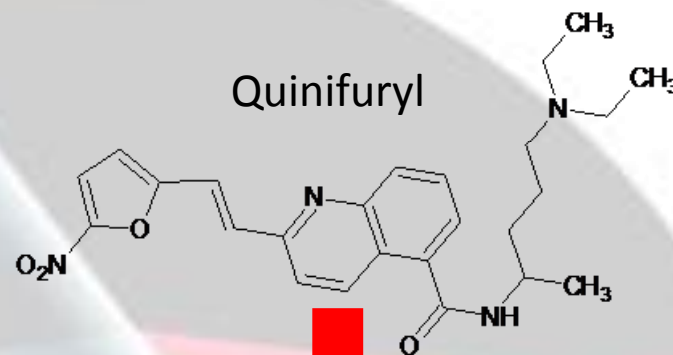
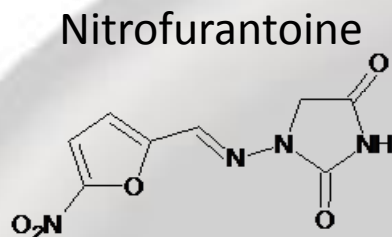
Two-photon absorption spectra



π -conjugated systems

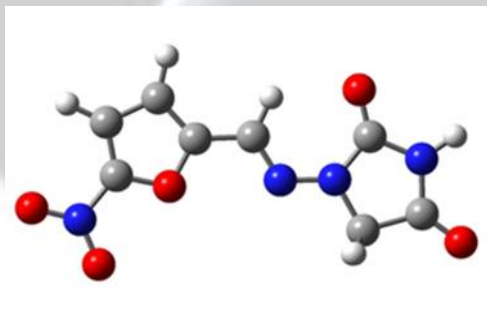


Theoretical calculations

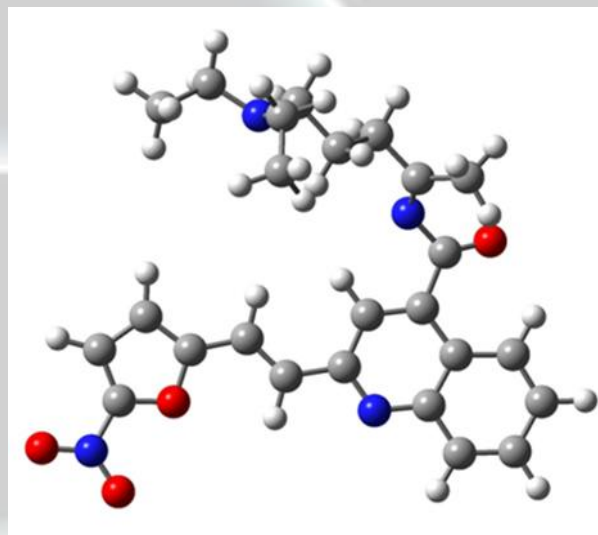


Optimized geometry
Density Functional Theory (DFT)
Gaussian 3

equilibrium geometry of the molecules



planar



Theoretical calculations

Nitrofurantoin

Quinifuril

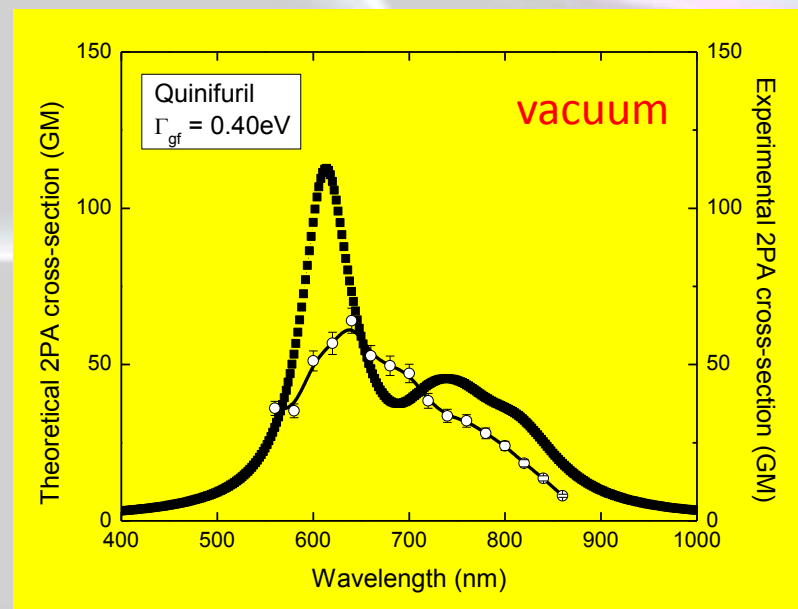
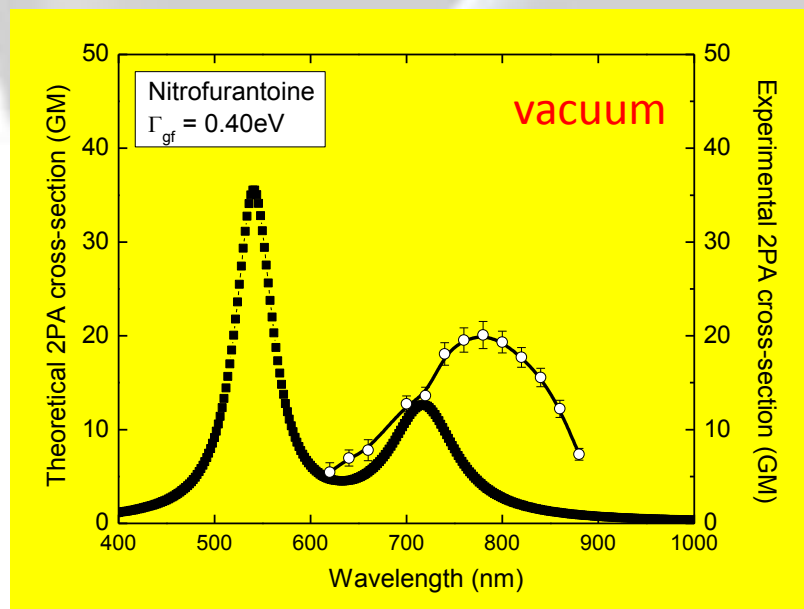
One- and Two-photon allowed transitions,
probabilities and oscillator strength

Density Functional Theory (DFT)

B3LYP and 6-31G(d)

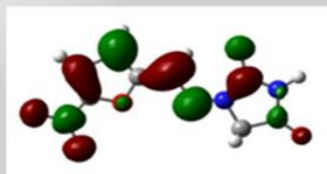
DALTON.

$$\sigma_{\text{eff}}(\omega/2) = \left(1,89679 \left[\text{GM} / \text{u.a.} \right] \right) \times 16 \pi^3 \alpha^2 \frac{\omega^2 [\text{u.a.}]}{\pi \left(\Gamma_{\text{eff}} [\text{u.a.}] / 2 \right)} \left\langle \delta_{\text{eff}} [\text{u.a.}] \right\rangle.$$

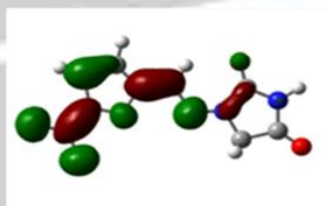


Theoretical calculations

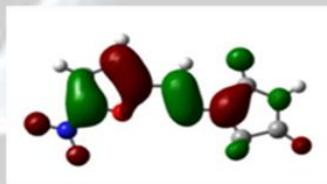
Nitrofurantoin



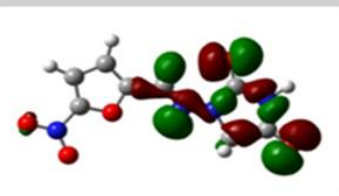
LUMO +1



LUMO

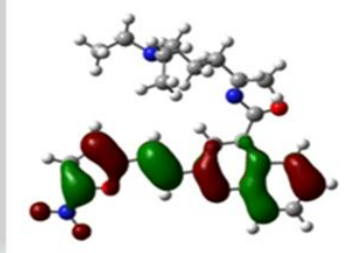
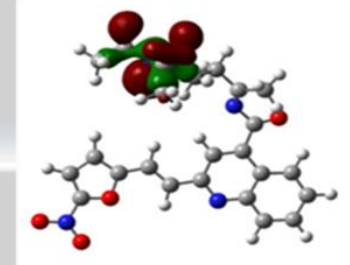
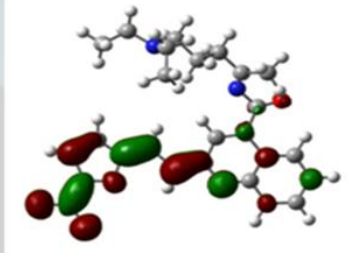
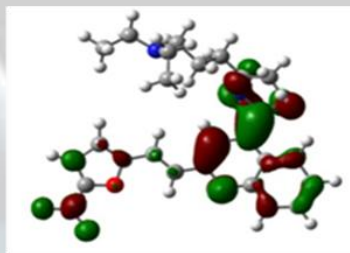


HOMO



HOMO -1

Quinifurlyl



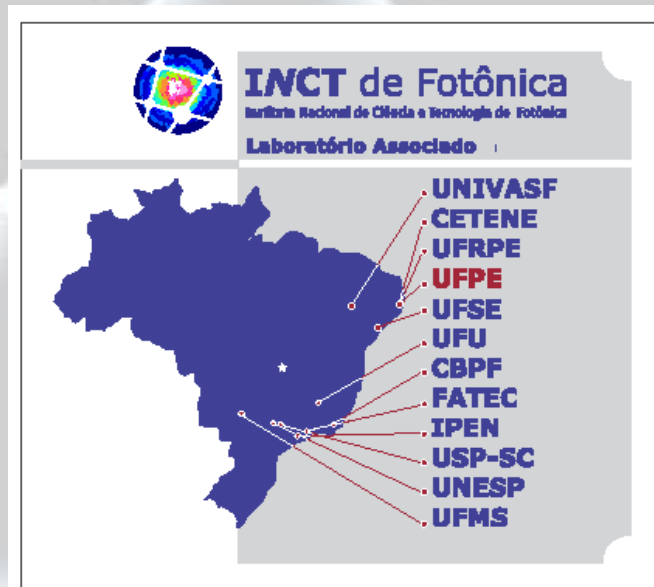
Conclusions

Samples

- ✓ *Two-photon absorptions with considerable values*
- ✓ *Two-photon absorptions occurs in the therapeutic windows*
- ✓ *Two-photon absorptions is higher for quinifuryl because of the conjugation length is also higher*
- ✓ *The quantum chemistry calculation have presented a good agreement with the experimental results*

Position and magnitude of the spectra

Acknowledgements



Thank you