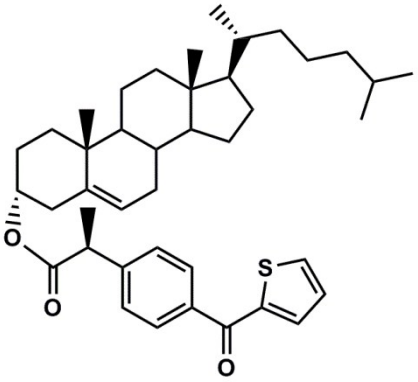
ELECTRONIC SUPPLEMENTARY INFORMATION

Steric shielding *vs* σ–π orbital interactions in triplet-triplet energy transfer

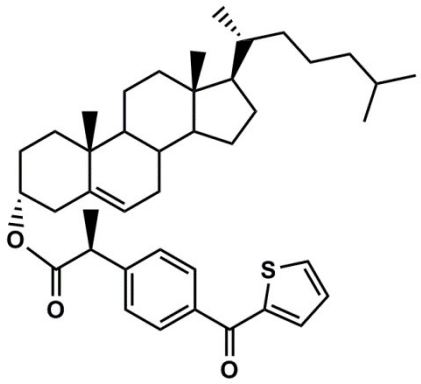
Inmaculada Andreu,[a] Isabel Morera,[b] Fabrizio Palumbo,[c] Germán Sastre,[c] Francisco Bosca,[c,] * and Miguel A. Miranda[c,] *

Table of Contents



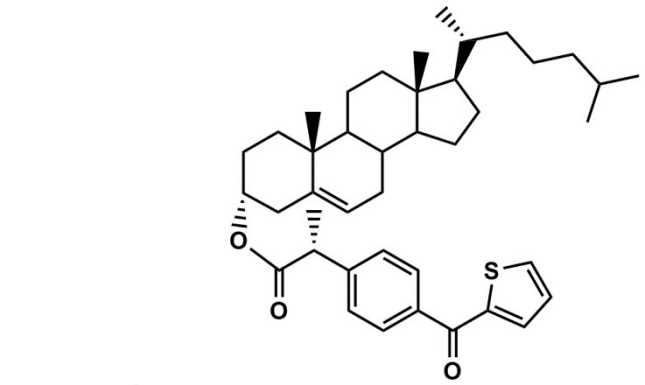
(*S*)-SUP-α-Ch

($CDCl_3$, 300 MHz)



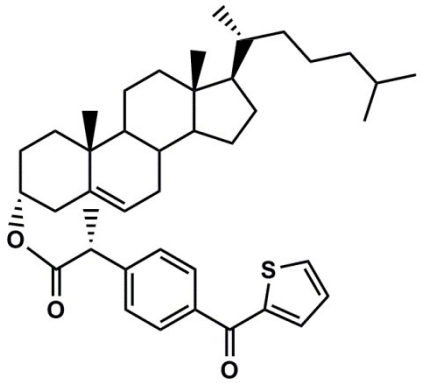
(*S*)-SUP-α-Ch

($CDCl_3$, 75 MHz)



(*R*)-SUP-α-Ch

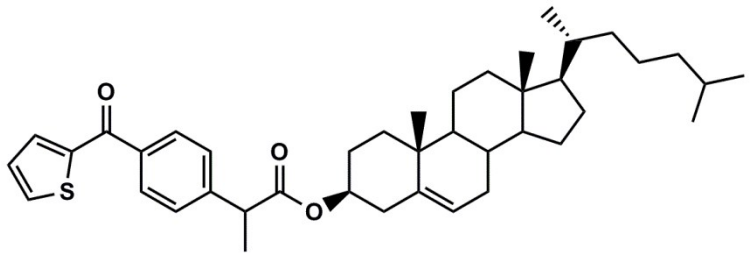
($CDCl_3$, 300 MHz)



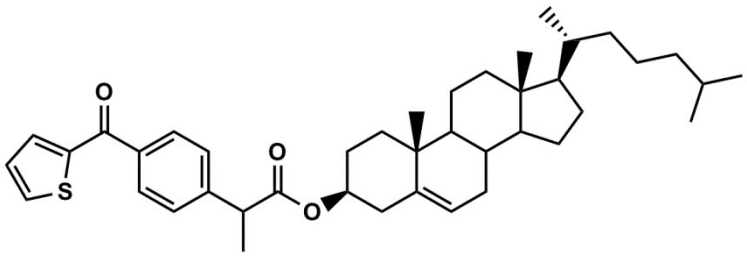
(*R*)-SUP-α-Ch

($CDCl_3$, 75 MHz)

($CDCl_3$, 300 MHz)



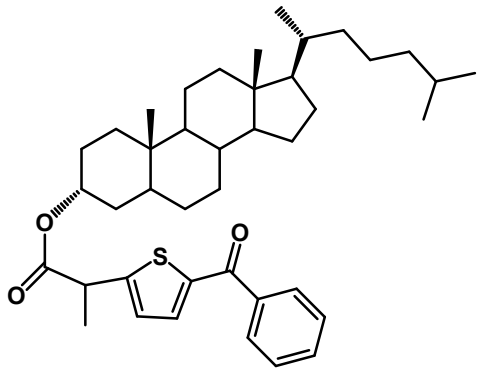
SUP-β-Ch



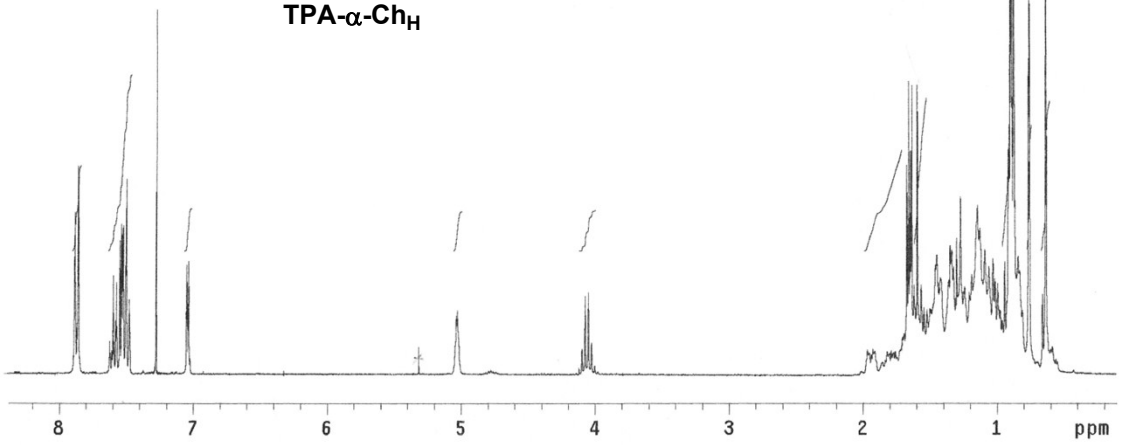
($CDCl_3$, 75 MHz)

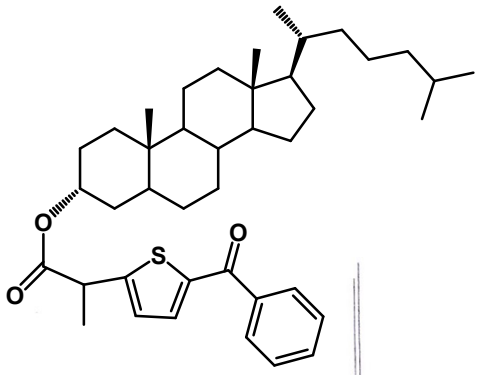
SUP-β-Ch

($CDCl_3$, 300 MHz)



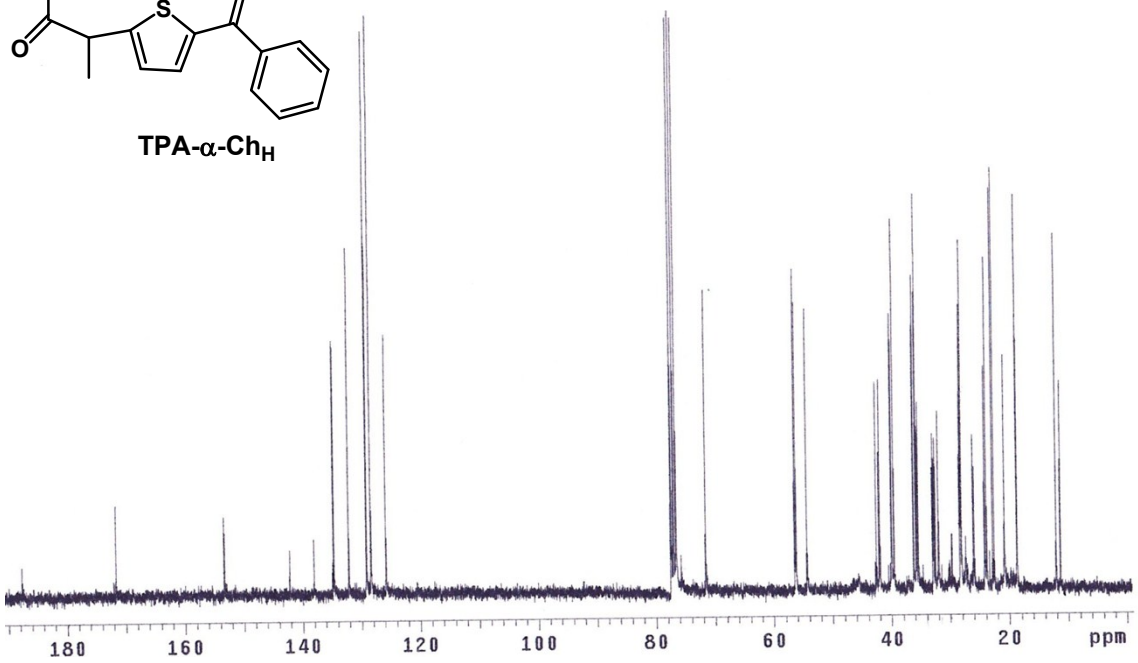
TPA-α-Ch_H

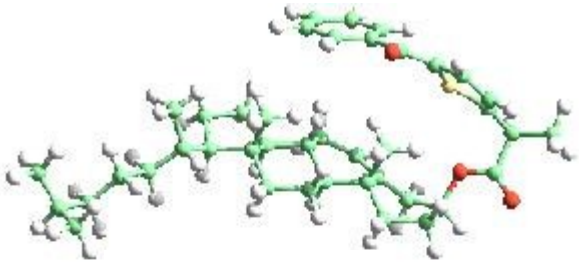




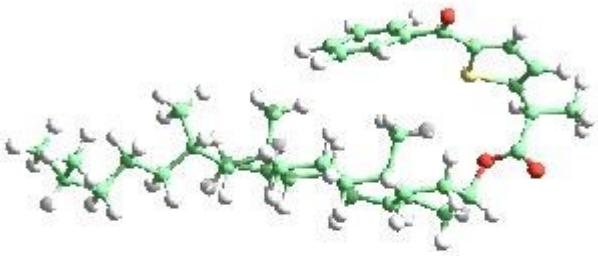
TPA-α-Ch_H

($CDCl_3$, 75 MHz)

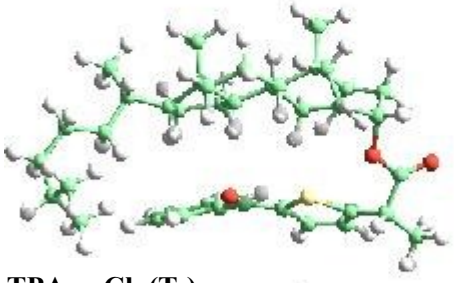




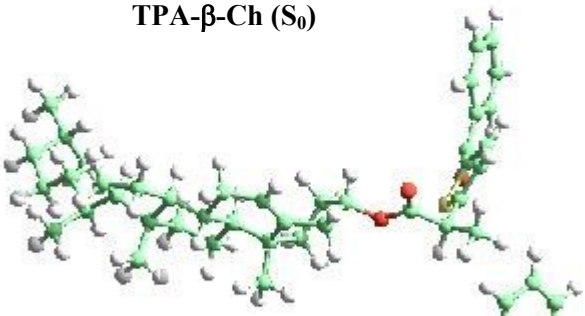
TPA-β-Ch (T_1)



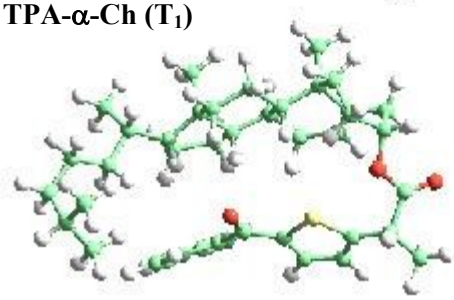
TPA-β-Ch (S_0)



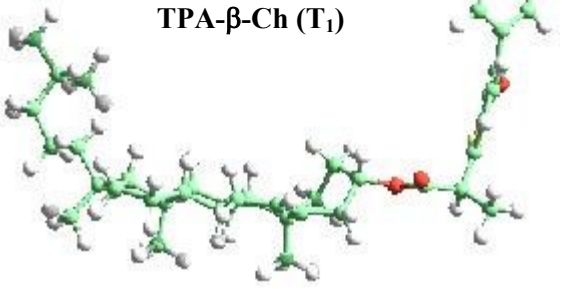
TPA-α-Ch (T_1)



TPA-β-Ch (T_1)

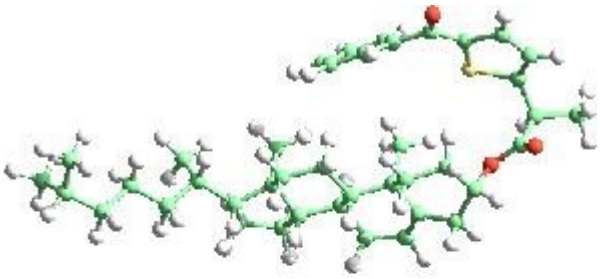


TPA-α-Ch (S_0)

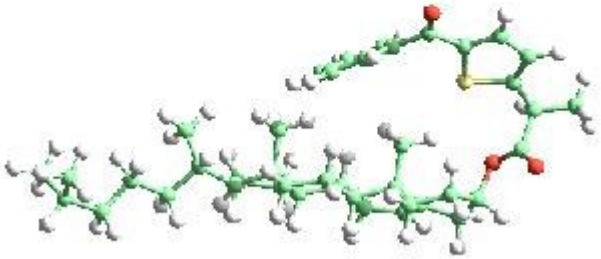


TPA-β-Ch (S_0)

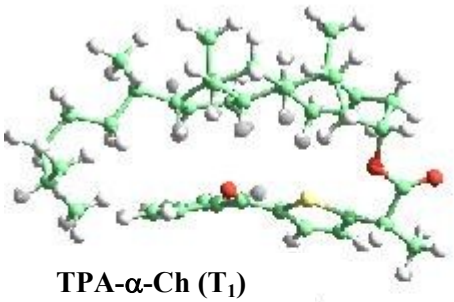
Optimized geometries of ground state (S_0) and triplet excited state (T_1) of TPA-α-Ch and TPA-β-Ch using PBE-D3 functional. The effect of solvent has not been included, but the geometries have also been optimized using dichloromethane as solvent with very similar results. In TPA-β-Ch, folded and unfolded have similar energies and for this reason both conformations have been calculated.



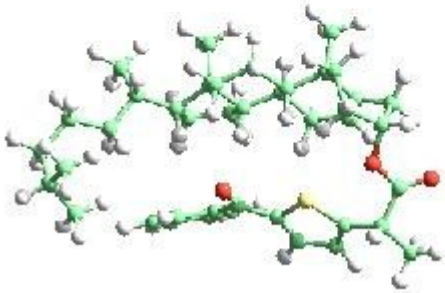
TPA-β-Ch (T_1)



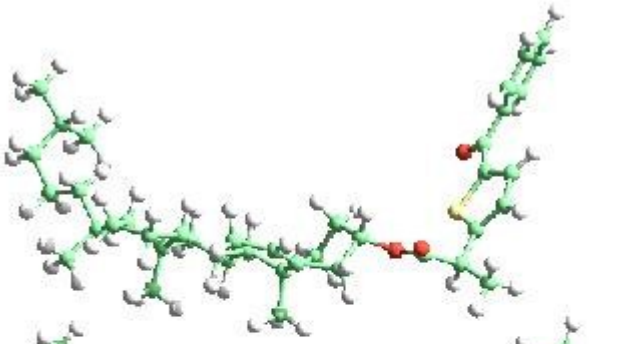
TPA-β-Ch (S_0)



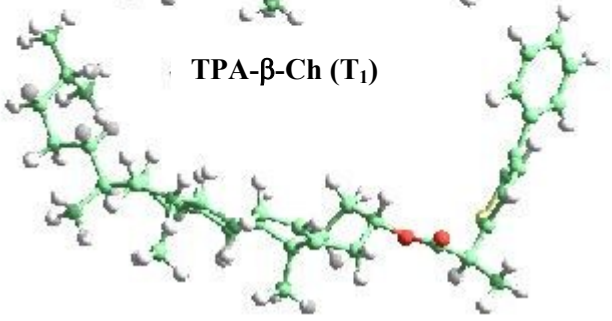
TPA-α-Ch (T_1)



TPA-α-Ch (S_0)

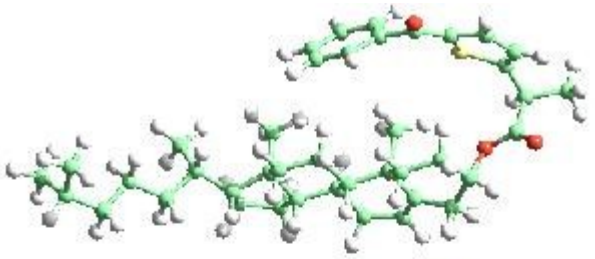


TPA-β-Ch (T_1)

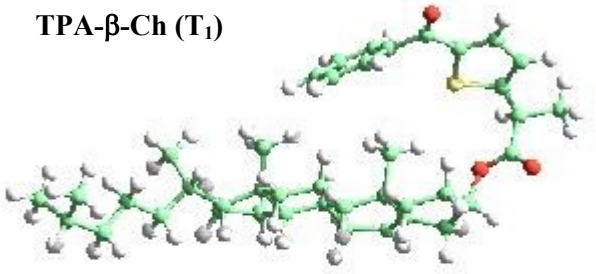


TPA-β-Ch (S_0)

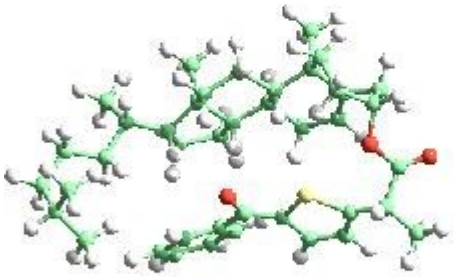
Optimized geometries of ground state (S_0) and triplet excited state (T_1) of TPA-α-Ch and TPA-β-Ch using M062X-D3 functional. The effect of solvent has not been included, but the geometries have also been optimized using dichloromethane as solvent with very similar results. In TPA-β-Ch, folded and unfolded have similar energies and for this reason both conformations have been calculated.



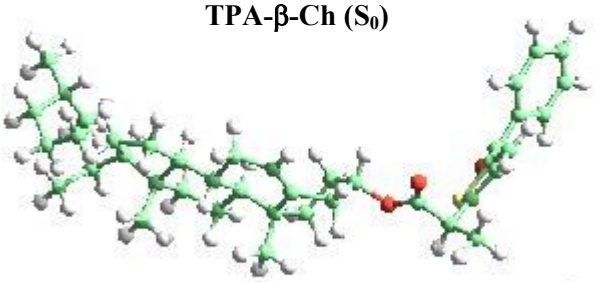
TPA-β-Ch (T_1)



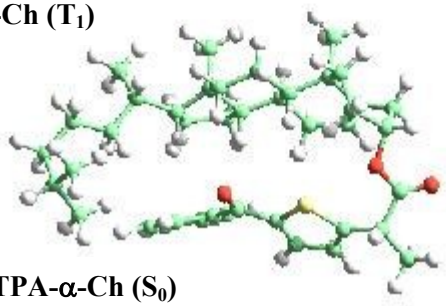
TPA-β-Ch (S_0)



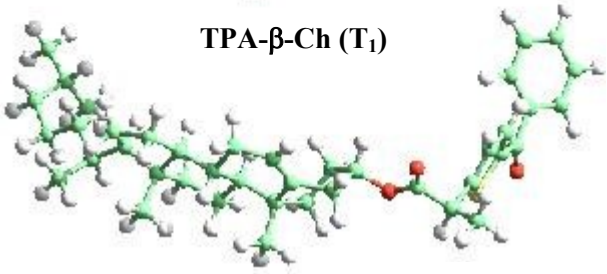
TPA-α-Ch (T_1)



TPA-β-Ch (T_1)



TPA-α-Ch (S_0)



TPA-β-Ch (S_0)

Optimized geometries of ground state (S_0) and triplet excited state (T_1) of TPA-α-Ch and TPA-β-Ch using wB97XD functional. The effect of solvent has not been included, but the geometries have also been optimized using dichloromethane as solvent with very similar results. In TPA-β-Ch, folded and unfolded have similar energies and for this reason both conformations have been calculated.