

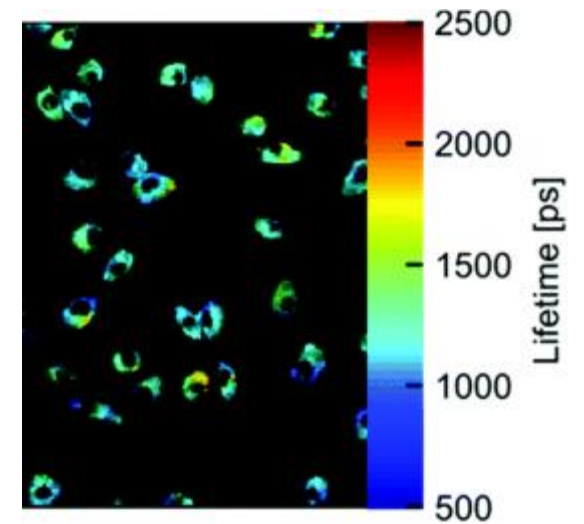
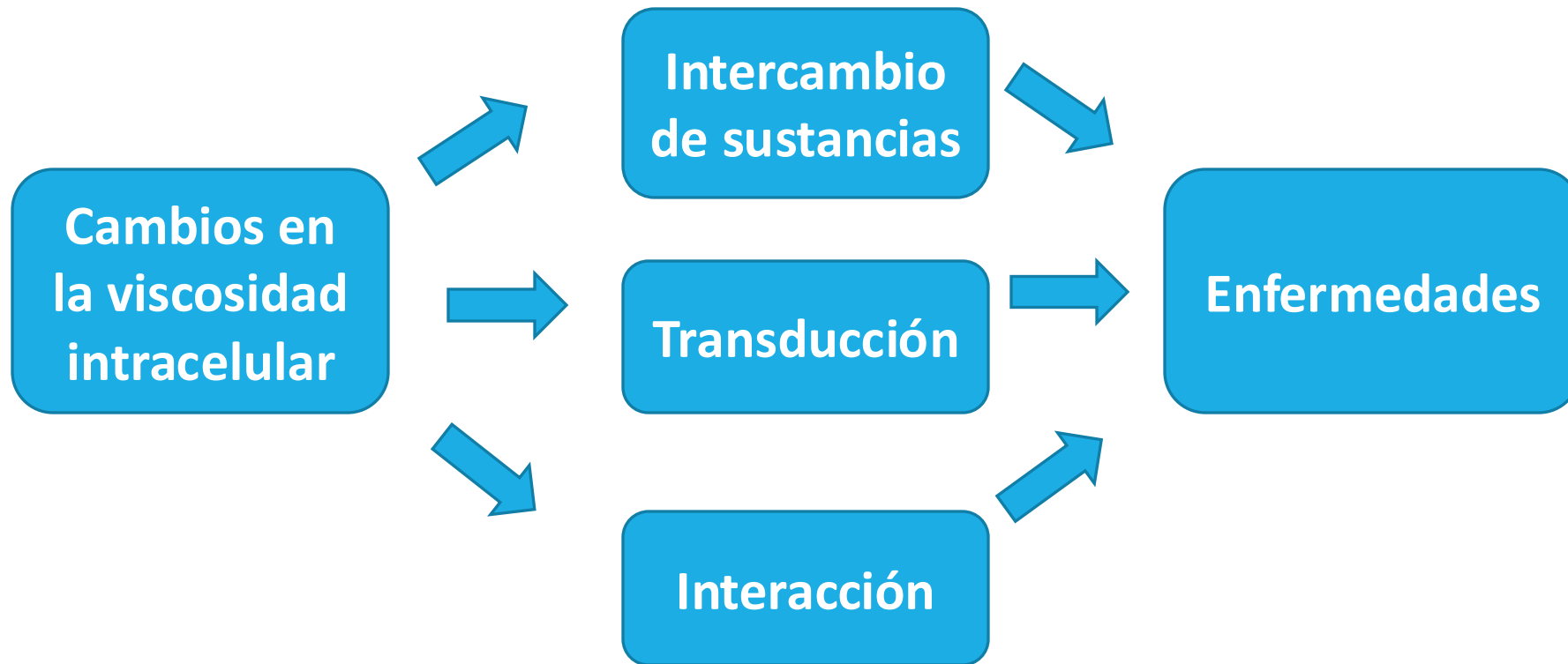
Estudio de ortodiestirilbencenos como sensores de viscosidad

Antonio Cuesta Casas

Química Orgánica Farmacéutica



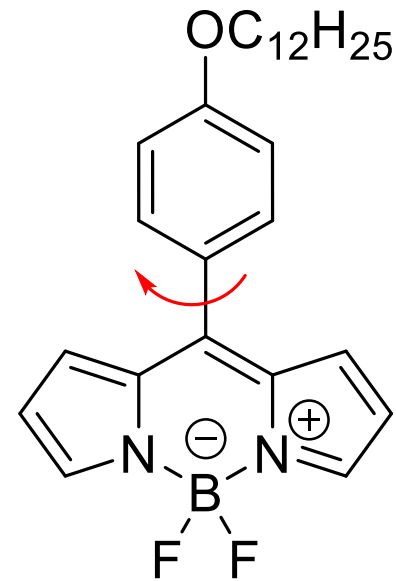
Viscosidad



Rotores moleculares como sensores de viscosidad

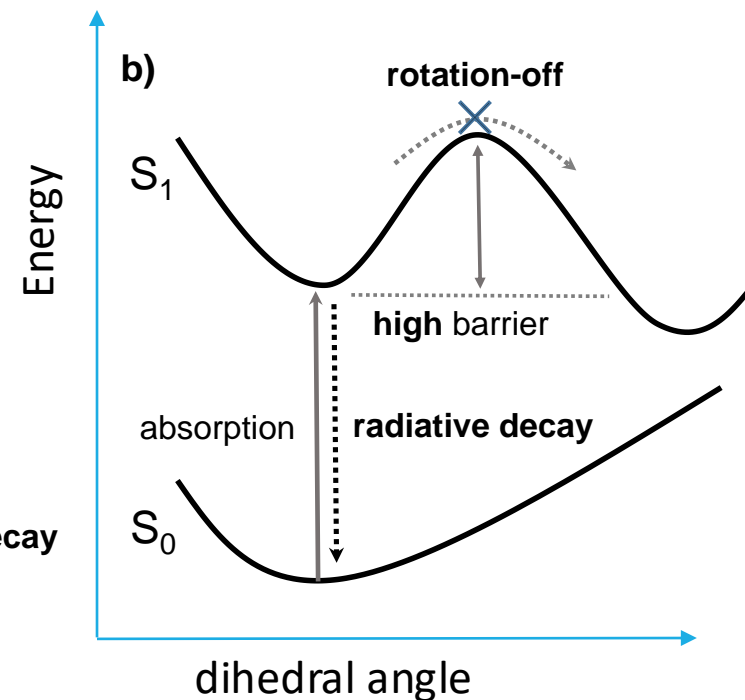
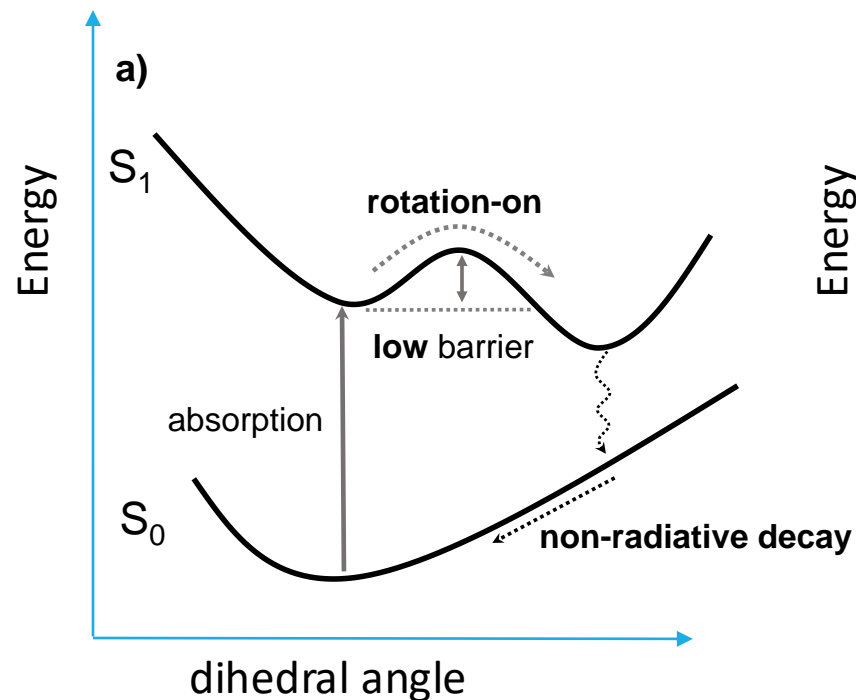
$$\log \Phi = C + x \log \eta$$

$$\log \tau = C + x \log \eta$$



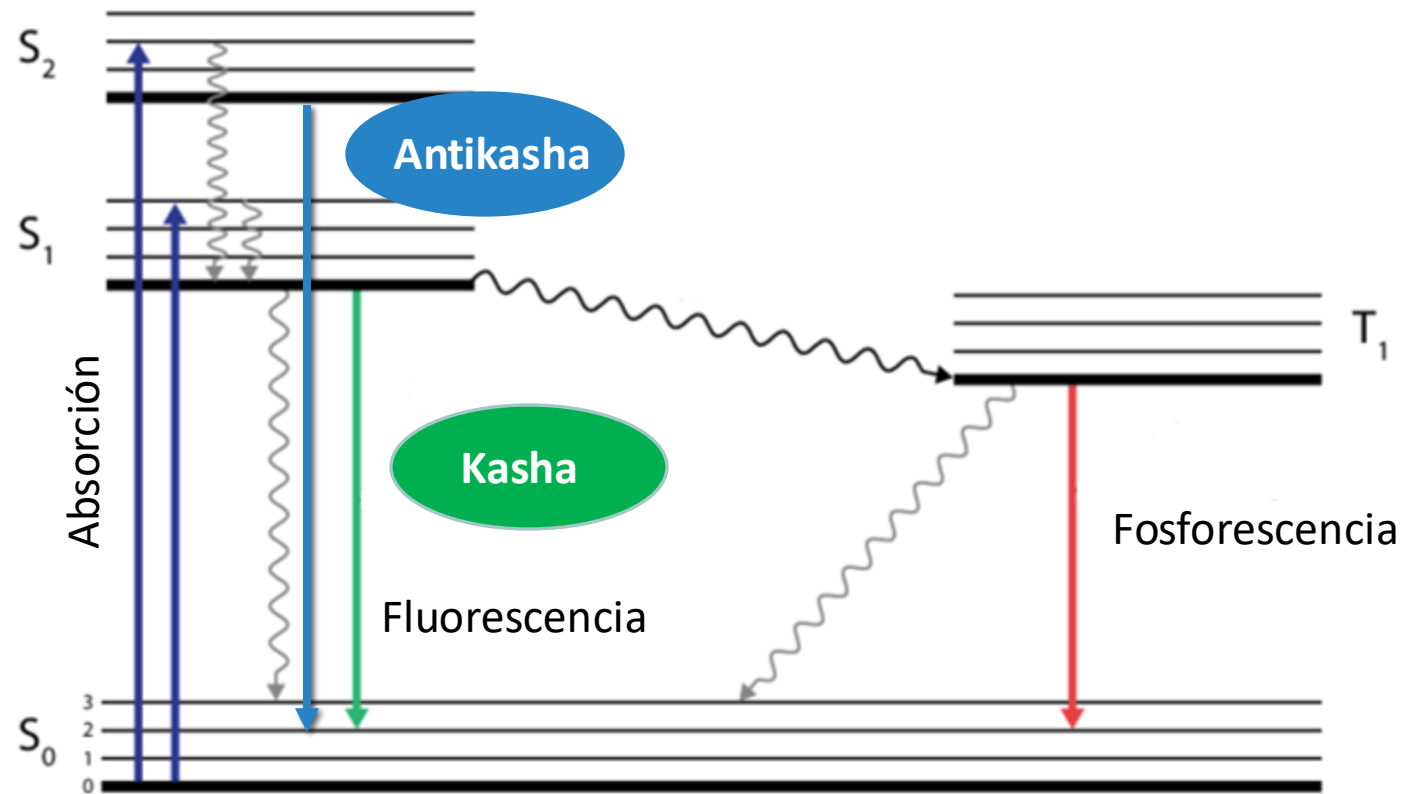
Rotores moleculares como sensores de viscosidad

Baja energía de barrera
Reduce la emisión
Mejora la sensibilidad a la viscosidad

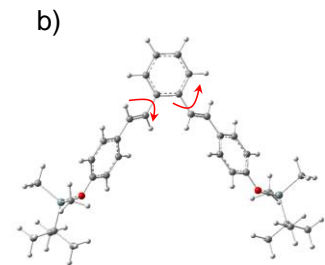
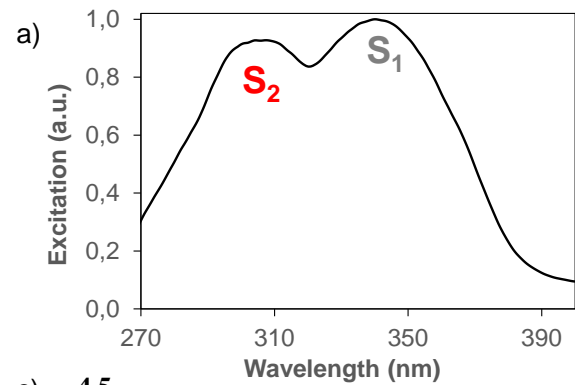


Barrera de alta energía
Aumenta la emisión
Reduce la sensibilidad a la viscosidad

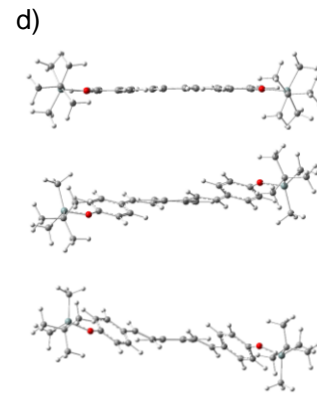
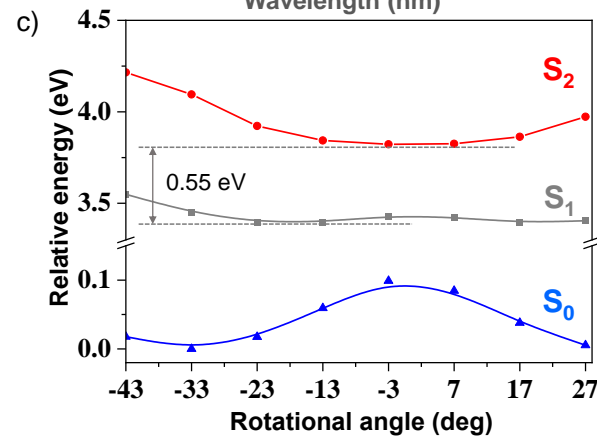
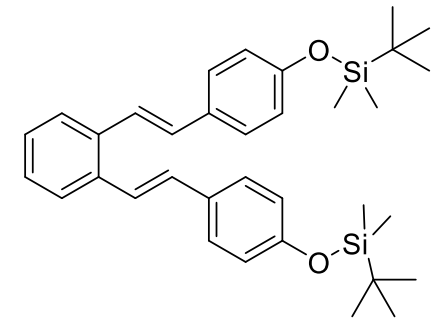
Antikasha



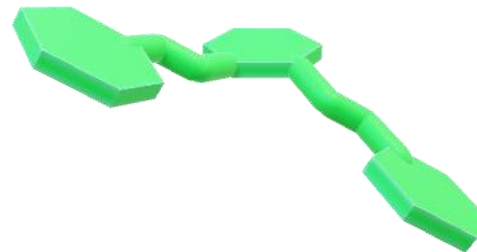
Ortodiestirilbencenos



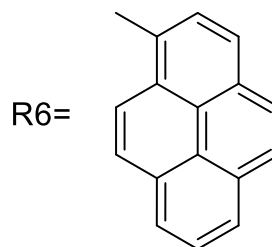
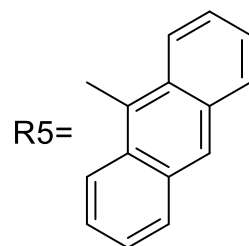
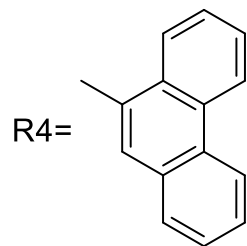
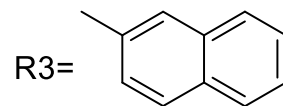
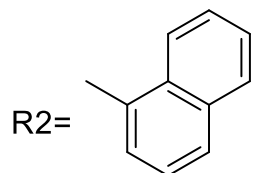
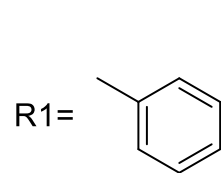
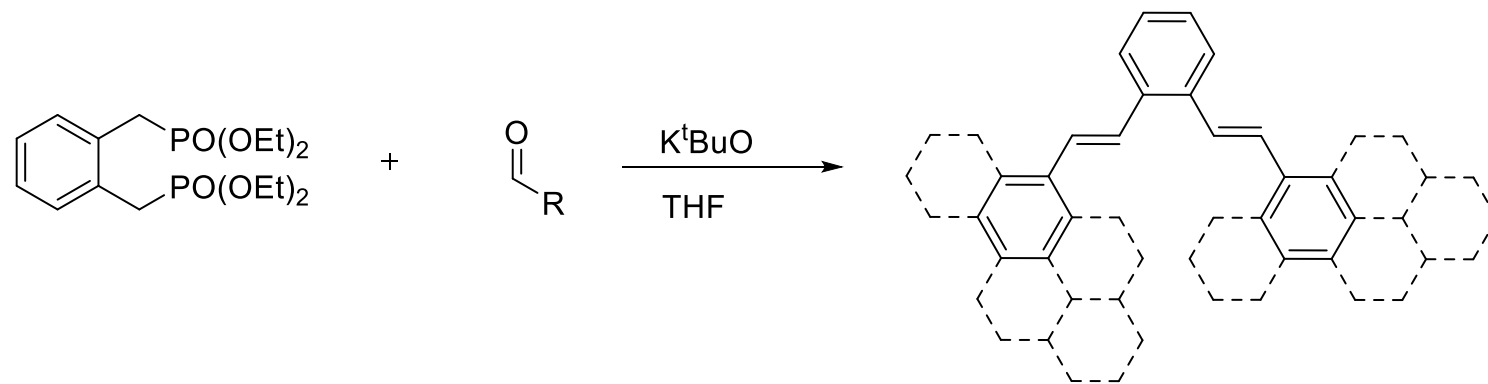
S_2

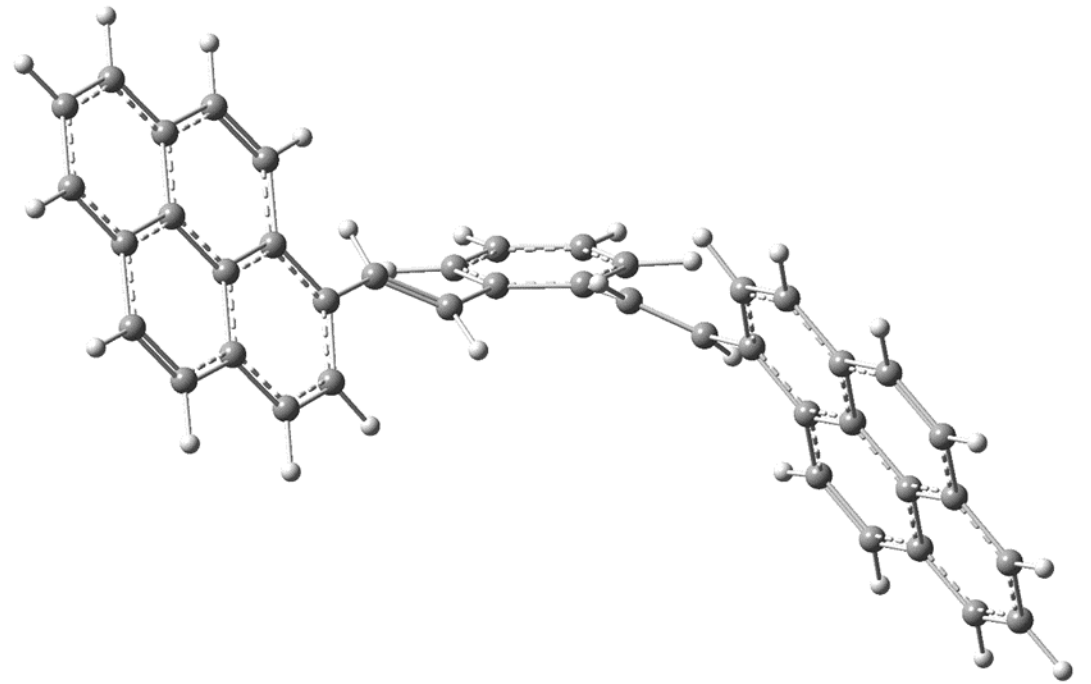
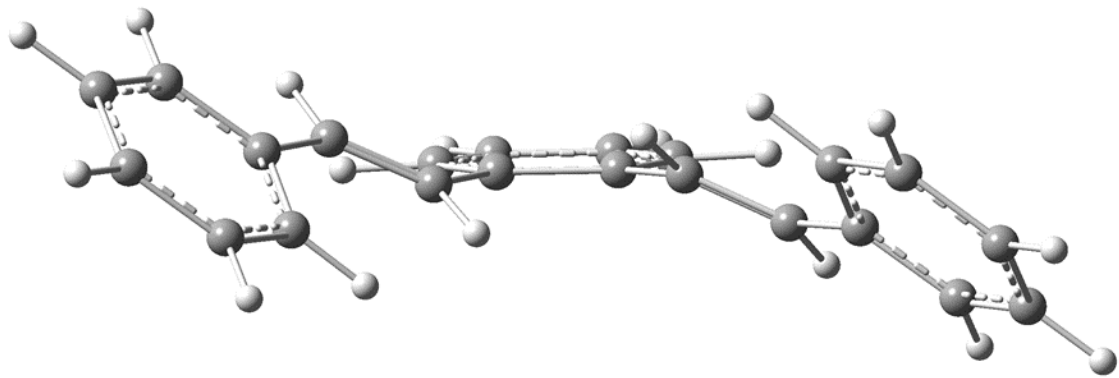


S_0

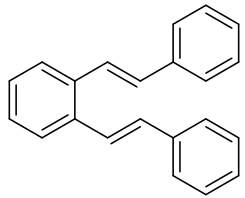


Síntesis



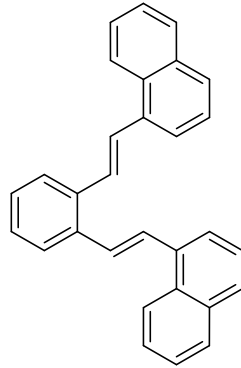


Caracterización



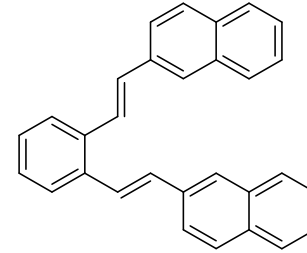
1

$\lambda_{\text{abs}}=288\text{nm}$
 $\lambda_{\text{em}}=422\text{nm}$
 $\phi=90$
 $\tau=9\text{ns}$



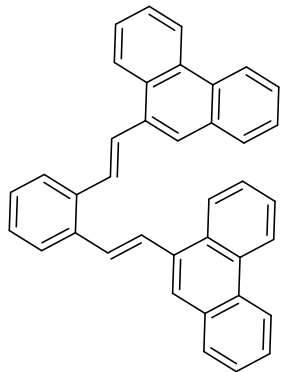
2

$\lambda_{\text{abs}}=328\text{nm}$
 $\lambda_{\text{em}}=466\text{nm}$
 $\phi=75$
 $\tau=4,6\text{ns}$



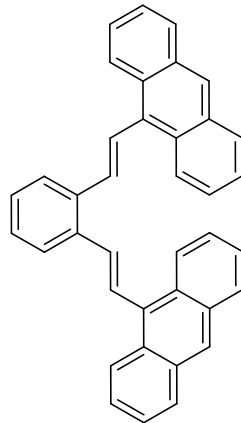
3

$\lambda_{\text{abs}}=314\text{nm}$
 $\lambda_{\text{em}}=444\text{nm}$
 $\phi=90$
 $\tau=3,8\text{ns}$



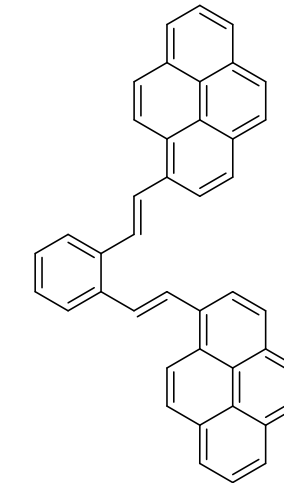
4

$\lambda_{\text{abs}}=324\text{nm}$
 $\lambda_{\text{em}}=482\text{nm}$
 $\phi=90$
 $\tau=5,1\text{ns}$



5

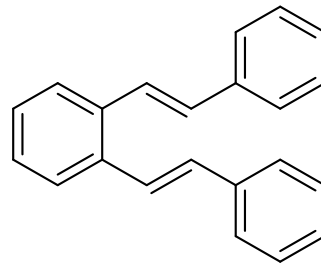
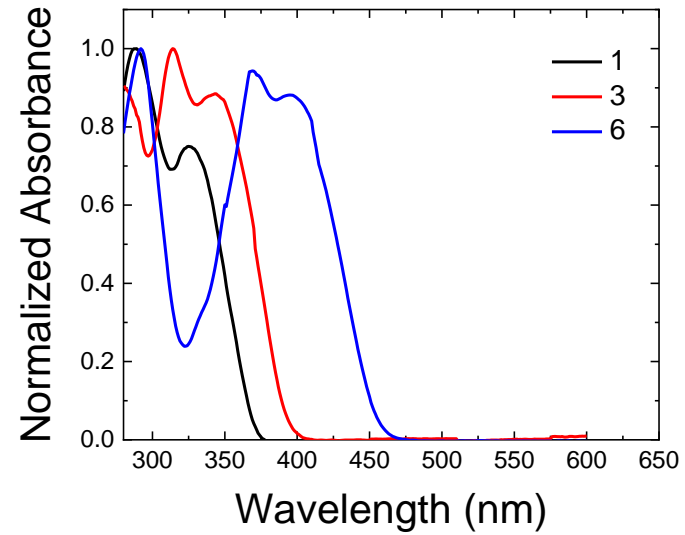
$\lambda_{\text{abs}}=392\text{nm}$
 $\lambda_{\text{em}}=494\text{nm}$
 $\Phi<1$
 $\tau=2,8\text{ns}$



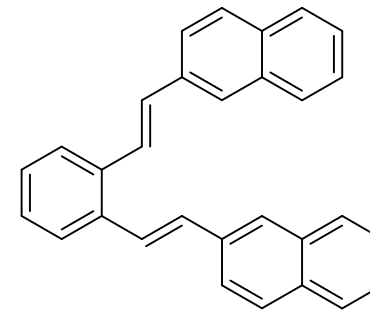
6

$\lambda_{\text{abs}}=371\text{nm}$
 $\lambda_{\text{em}}=525\text{nm}$
 $\phi=90$
 $\tau=2,9\text{ns}$

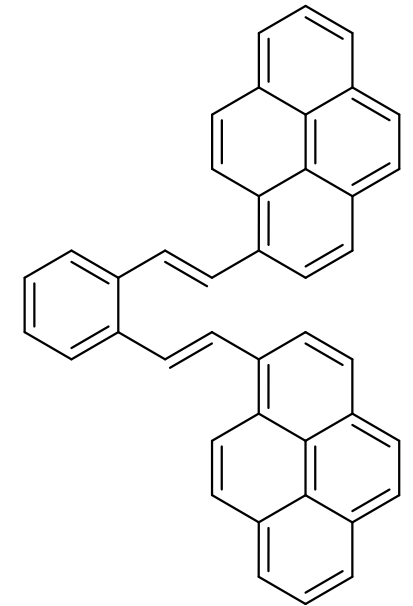
Caracterización



1

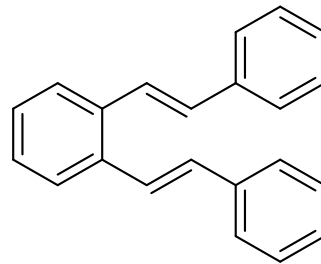
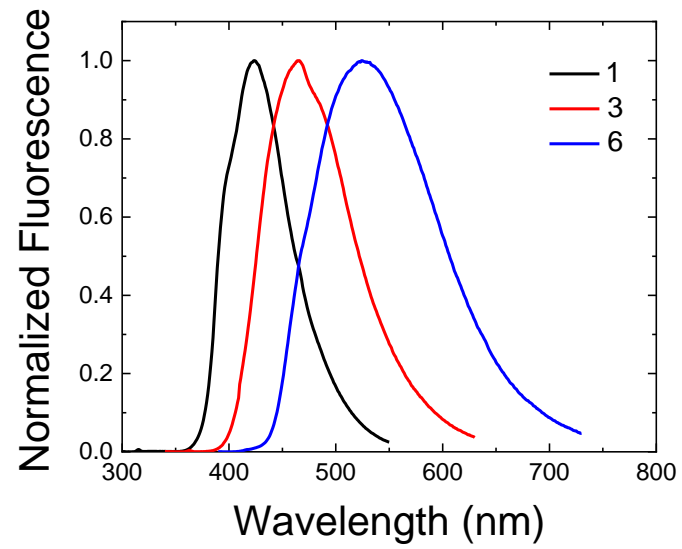


3

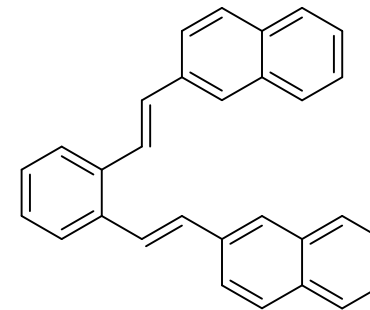


6

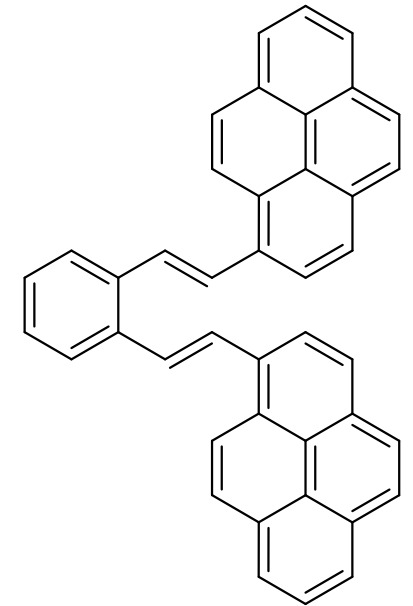
Caracterización



1



3



6

Cálculos químico cuánticos

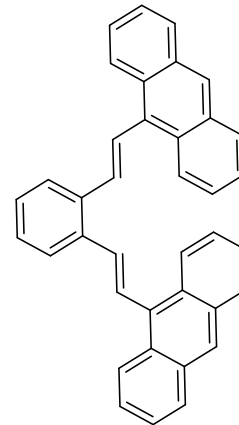
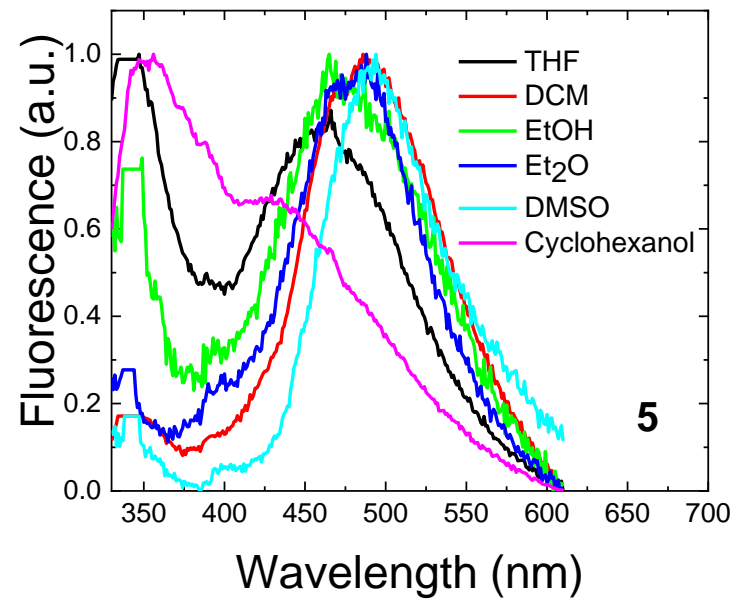
Comp.	S ₀	S ₁	S ₂	$\Delta E (S_2-S_1)$ (eV)
1	-848.844451	-848.725576	-848.703808	0.59
2	-1156.018732	-1155.907193	-1155.887154	0.55
3	-1156.025096	-1155.909937	-1155.887602	0.61
4	-1463.204174	-1463.093134	-1463.073526	0.53
5	-1463.179689	-1463.079838	-1463.079838	0.00
6	-1615.624254	-1615.523635	-1615.507658	0.43

Comp.	μ_{S_0} (D)
1	0.34
2	0.13
3	0.46
4	0.16
5	0.32
6	0.21

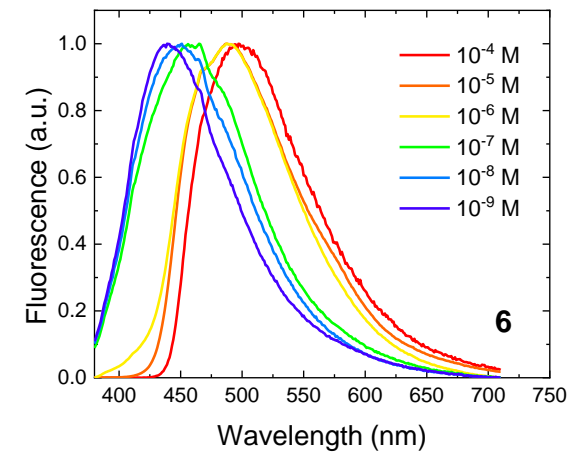
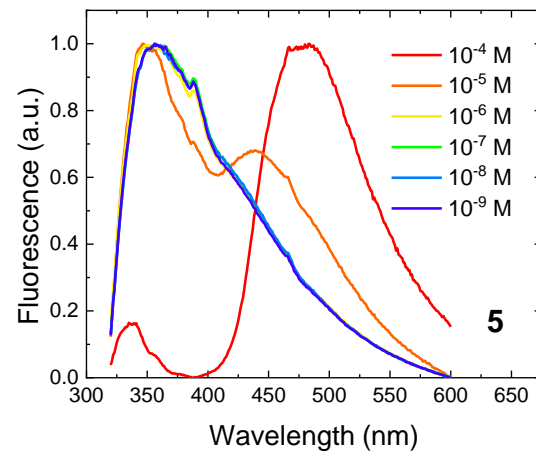
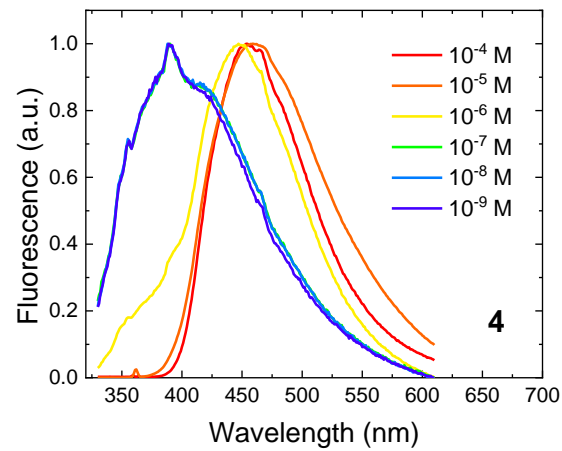
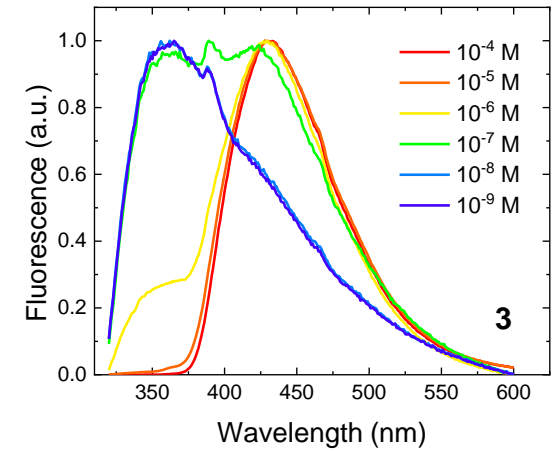
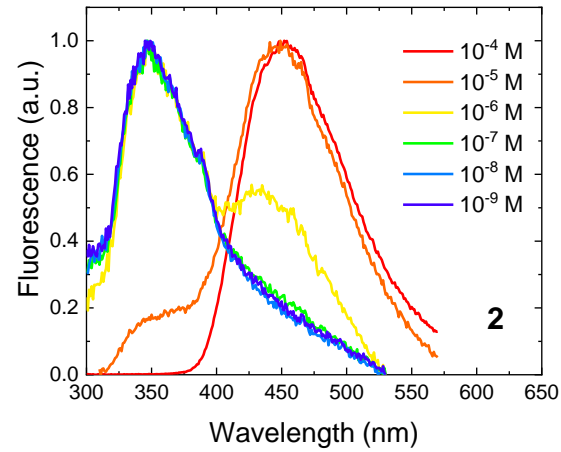
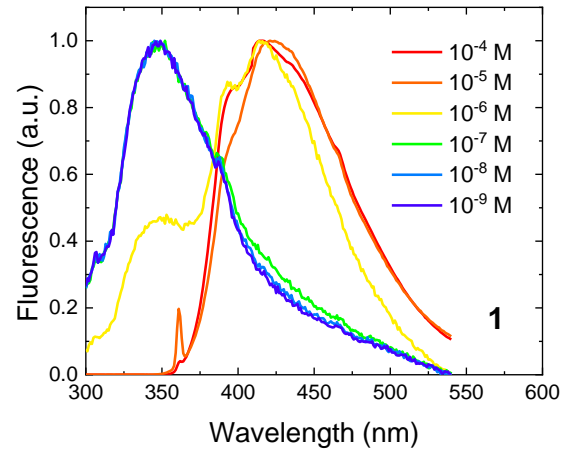
Cálculos químico cuánticos

Comp	$\lambda_{\text{em}}^{\text{exp}}$	Φ_{F}	$\lambda_{\text{vert-em}}^{\text{calc}}$ (S_1-S_0)	f	% Contr.	$\lambda_{\text{vert-em}}^{\text{calc}}$ (S_2-S_0)	f	% Contr.
1	422 (2.94)	100	407 (3.05)	1.18	H \rightarrow L (96)	338 (3.67)	0.88	H \rightarrow L+1 (73), H-1 \rightarrow L (25)
2	466 (2.66)	75	446 (2.78)	1.18	H \rightarrow L (95)	349 (3.55)	0.97	H \rightarrow L+1 (57), H-1 \rightarrow L (40)
3	444 (2.79)	100	422 (2.94)	1.82	H \rightarrow L (95)	336 (3.69)	1.08	H \rightarrow L+1 (71), H-1 \rightarrow L (23)
4	466 (2.66)	91	452 (2.75)	1.03	H \rightarrow L (96)	352 (3.53)	1.66	H \rightarrow L+1 (55), H-1 \rightarrow L (43)
5	490 (2.53)	<1	537 (2.31)	0.66	H \rightarrow L (99)	537 (2.31)	0.66	H \rightarrow L (99)
6	525 (2.36)	100	490 (2.53)	2.09	H \rightarrow L (93)	377 (3.29)	0.74	H-1 \rightarrow L (52), H \rightarrow L+1 (45)

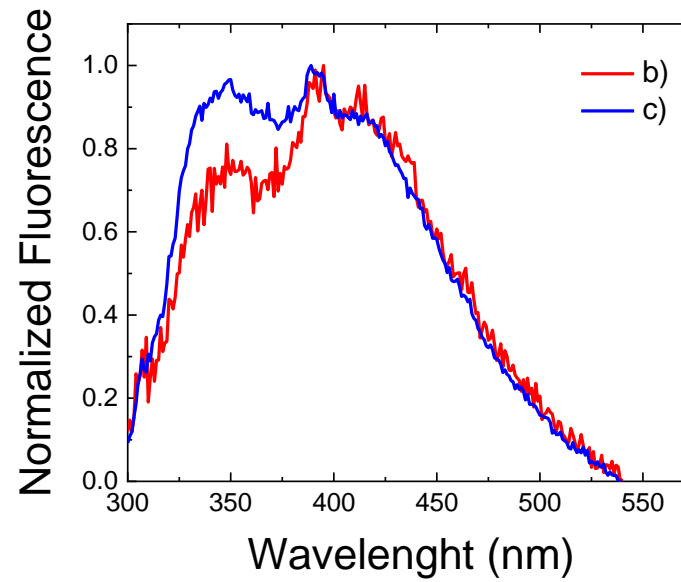
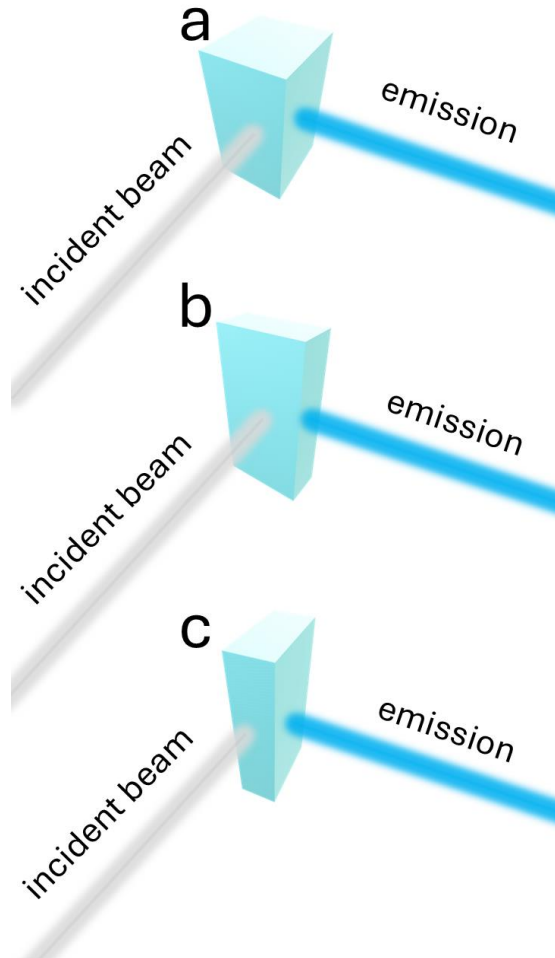
¿Antikasha?



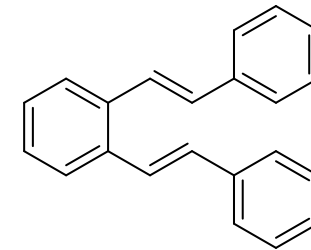
¿Antikasha?



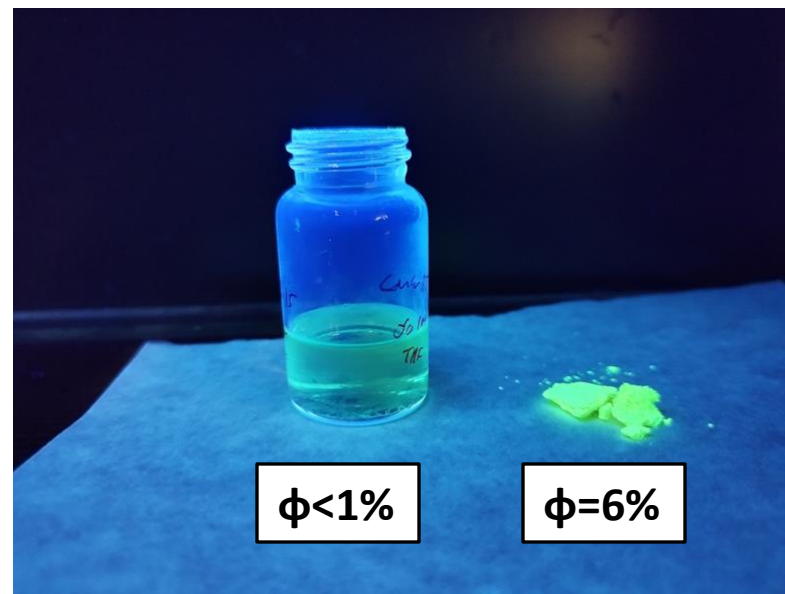
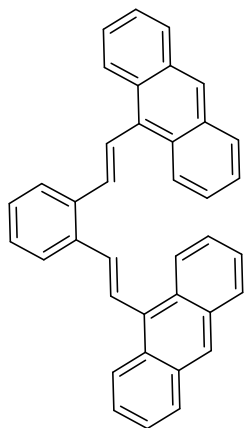
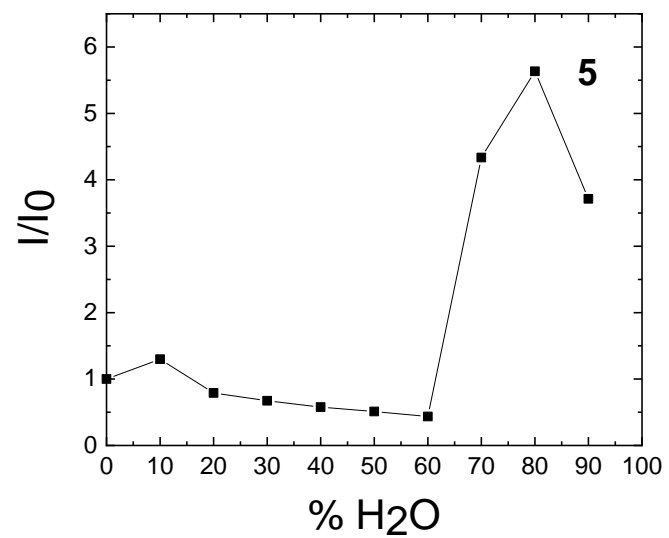
Estudio autoabsorción



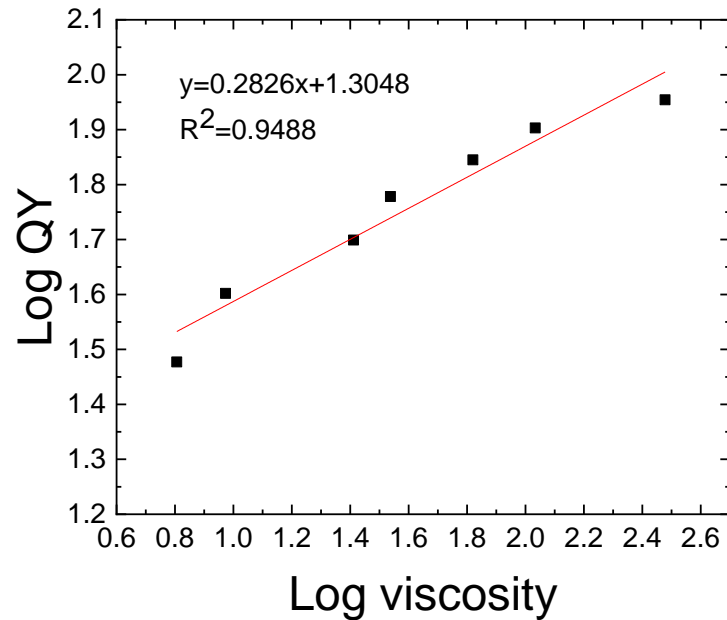
10^{-7} M



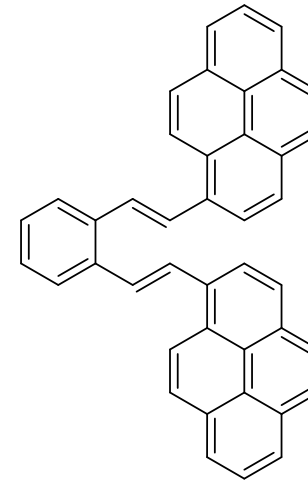
AIE



Estudio rotor molecular

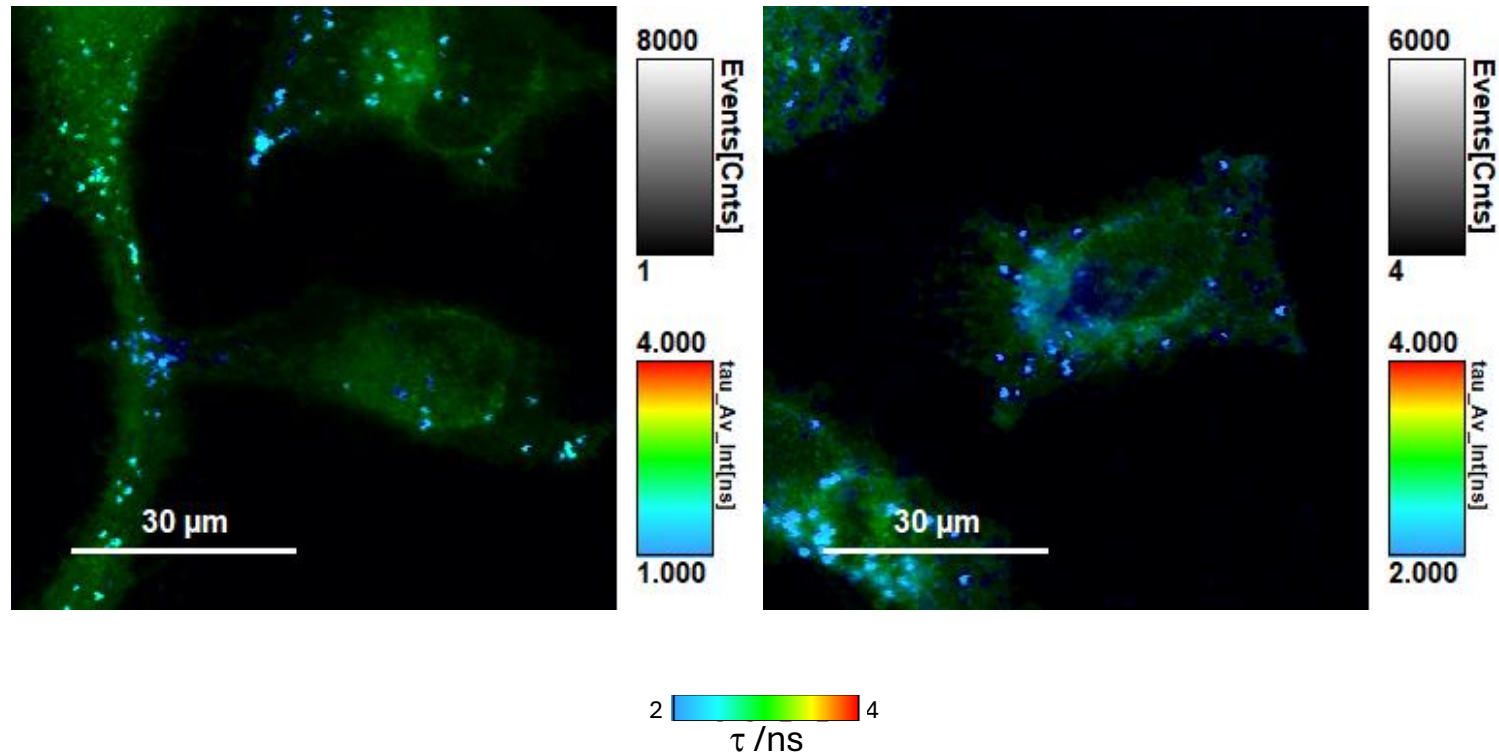


$$\log \Phi = C + x \log \eta$$



6

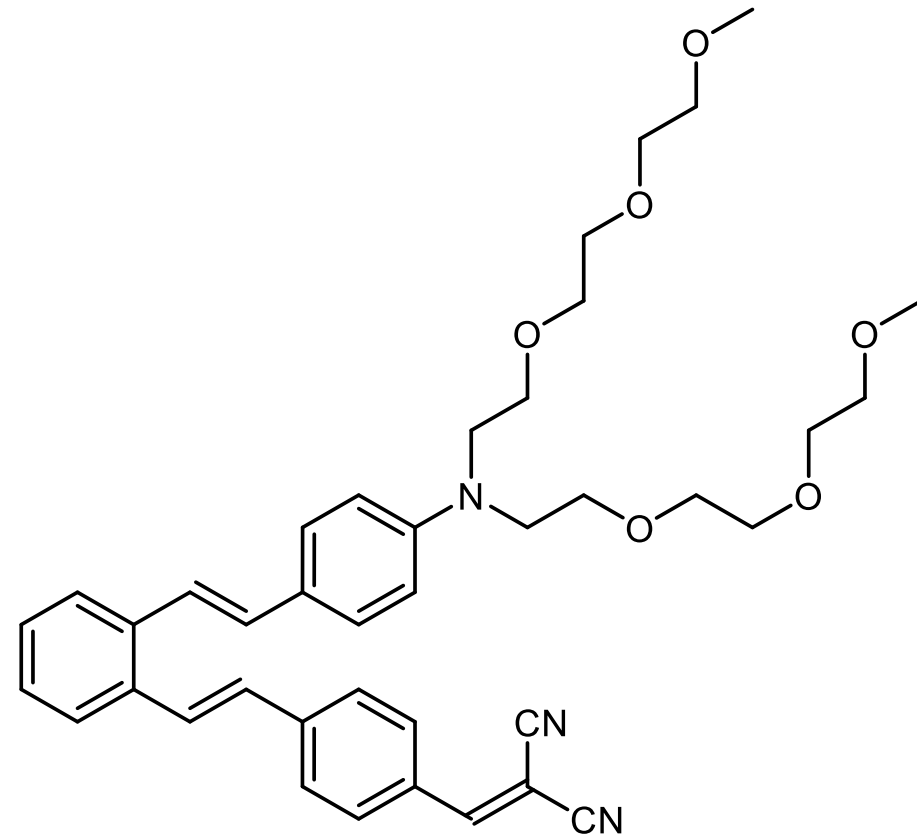
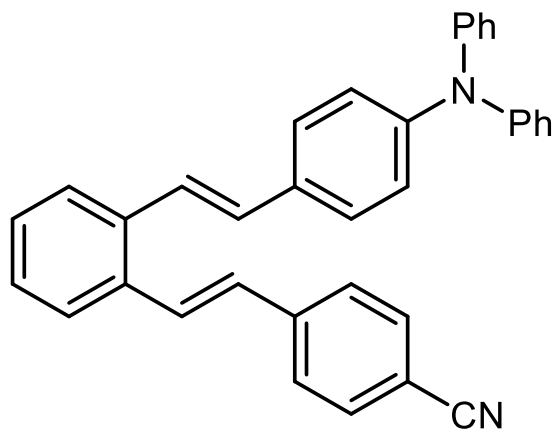
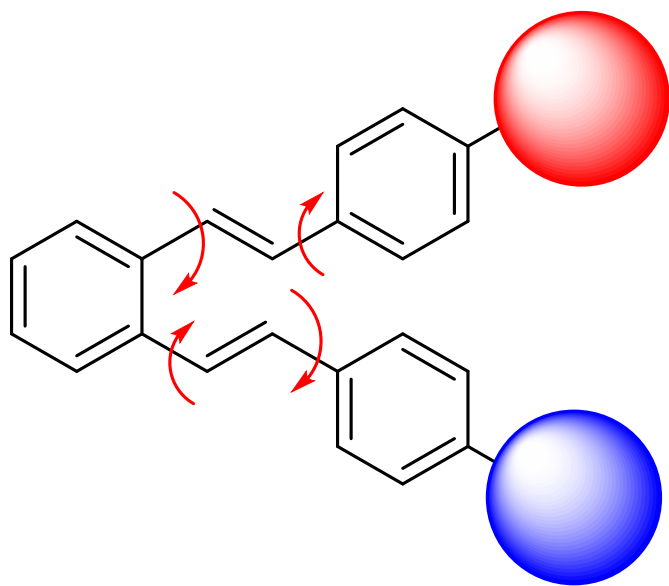
Medidas en FLIM



Conclusiones

1. Se ha comprobado que los compuestos derivados de ortodiestirilbencenos son compuestos antikasha.
2. El compuesto 6 se ajusta a un rotor molecular.

Trabajos futuros



Cálculos químico cuánticos

Compuesto	μ_{S_0} (D)	ΔE ($S_2 - S_1$)
o4e	3.68	0.82
o4d	5.05	0.54
o3d	5.49	0.66
o3p	6.01	0.00
o1e	6.46	0.62
o1b	7.24	0.69
o4b	7.72	0.67
o1b-b	8.18	0.63
o4b-b	8.19	0.62
o2f	8.20	0.73
o5b-b	9.78	0.50
o2j	9.82	0.00
o2e	10.05	0.60
o5j	10.24	0.39
o5b	10.38	0.53
o5e	11.11	0.72
o2c	11.38	0.66
o2b	11.61	0.00
o2p	11.66	0.78
o5g	12.1	0.87
o5p	12.62	0.91
o2b-b	12.79	0.71



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QUÍMICOS

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Universidad de Granada
FQM247 - Photochemistry and Photobiology
Nanoscopy Lab
Ángel Orte



Castilla-La Mancha

SBPLY/21/180501/000042

**Gracias por su
atención**

