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Rigidochromism by imide functionalisation of an aminomaleimide fluorophore†

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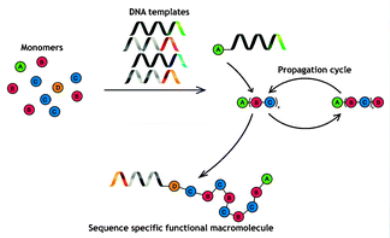
Rachel K. O'Reilly

Rachel O'Reilly是伯明翰大学工程与物理科学学院化学系主任。从2018 年 8 月1日起，她成为化学学院院长。她被公认为英国皇家化学学会的175 位化学名人之一。她担任《Science》杂志的评论编辑，并且是她所在领域的主要期刊Macromolecules的副主编。她的团队的工作获得了无数国家和国际奖项，其中包括来自皇家化学学会 (RSC) 的四项独特奖项，以及来自美国化学学会 (ACS)和国际化学联合会的年轻研究员奖章。

课题组研究领域



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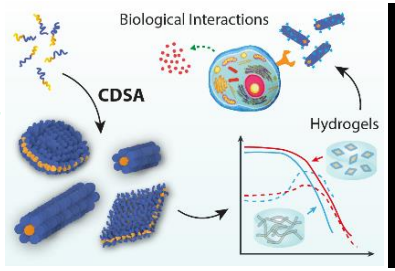

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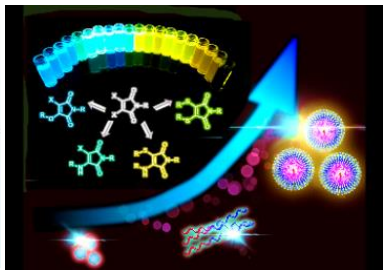

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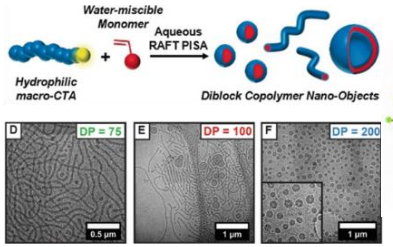

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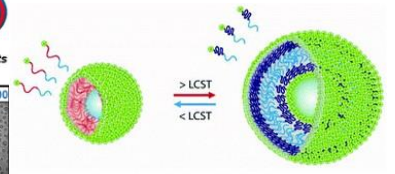
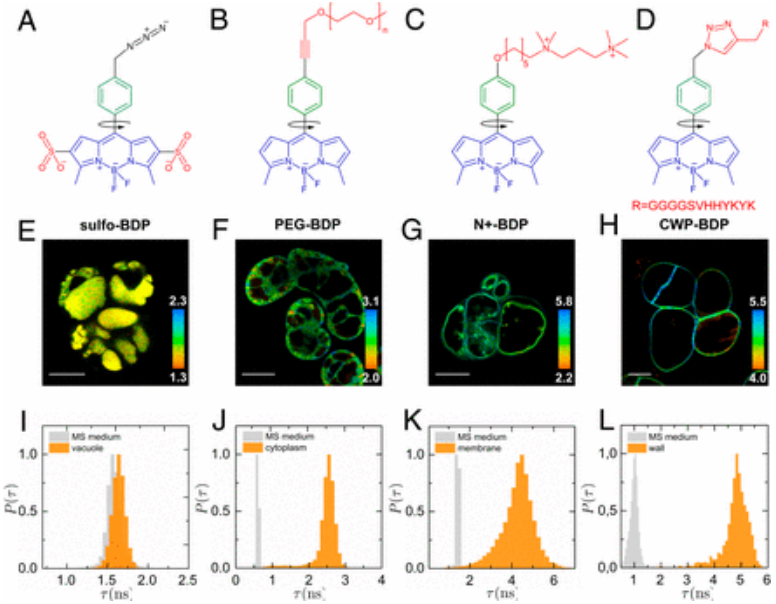
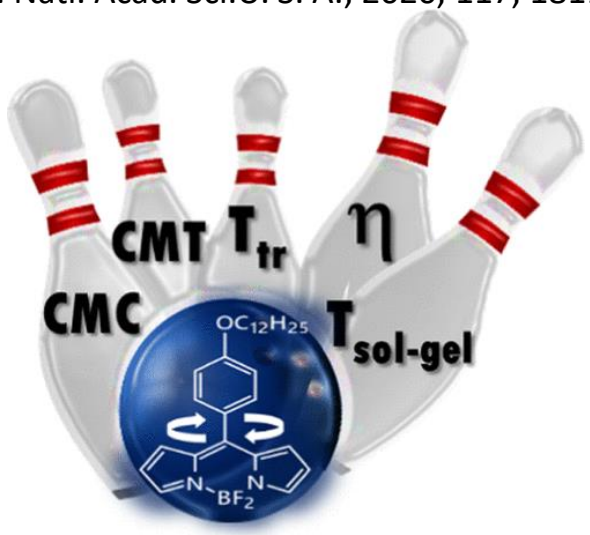


响应粒子

Introduction



Proc. Natl. Acad. Sci.U. S. A., 2020, 117, 18110–18118.



Macromolecules, 2021, 54, 655–664

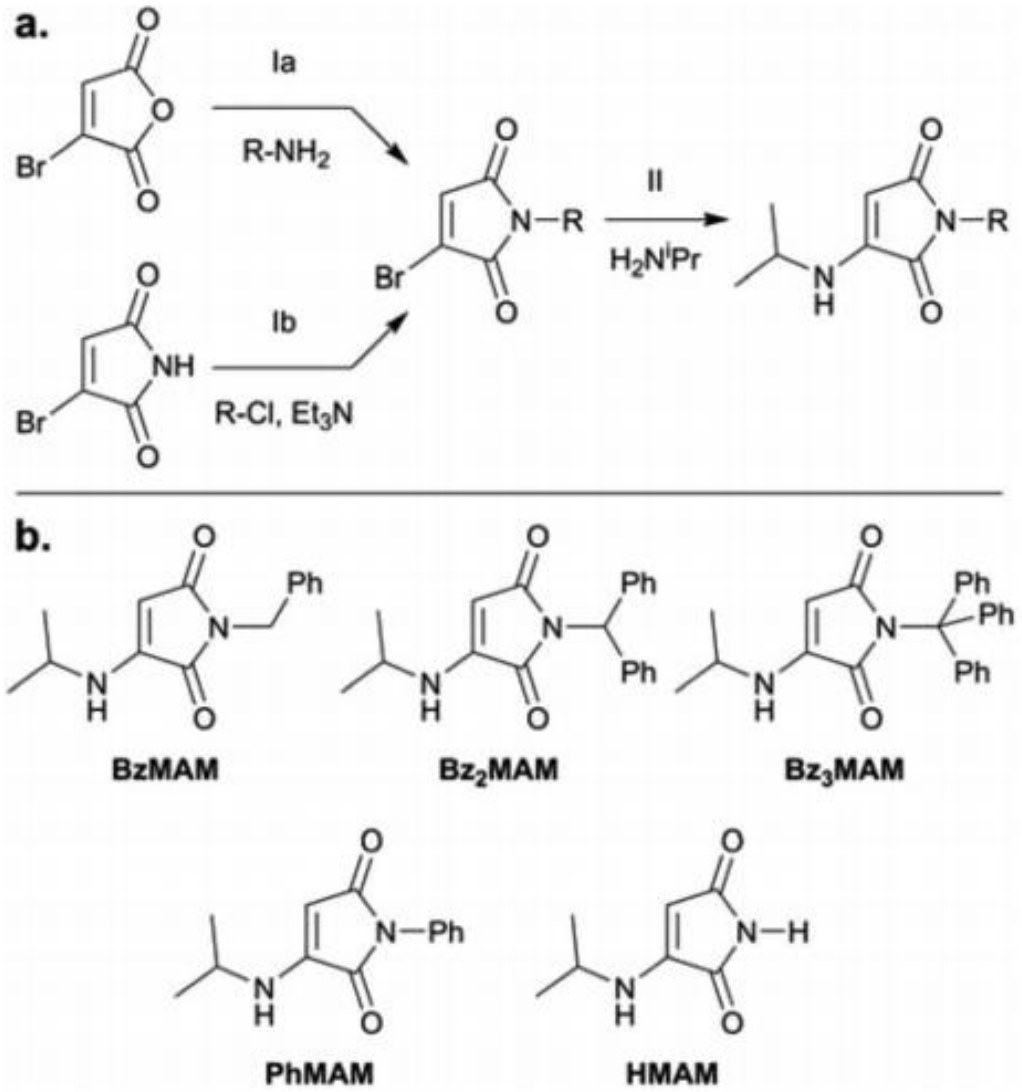


Fig. 1 (a) Synthetic routes for the dye series.
(b) Structures of the series of dyes used in this work

Results and discussion

Table 1 Excitation and emission maxima for the dye series in a range of solvents

非极性 蓝移

	$\lambda_{ex}/\lambda_{em}$ (nm)						
	MeOH	DMSO	Dioxane	THF	Toluene	Et_2O	Solid state[b]
HMAM	369/489	357/469	346/452	346/447	341/443	341/441	–/486
PhMAM	—[a]	370/505	361/503	360/501	358/502	359/500	–/488
BzMAM	370/491	371/490	362/478	361/472	355/471	357/469	–/477
Bz_2MAM	367/499	370/484	359/464	359/462	355/460	353/456	–/498
Bz_3MAM	364/488	363/476	352/459	352/465	352/465	348/450	–/472

[a] Not recordable. [b] Solid state excitation spectra were very broad, so extraction of λ_{ex} was not possible.

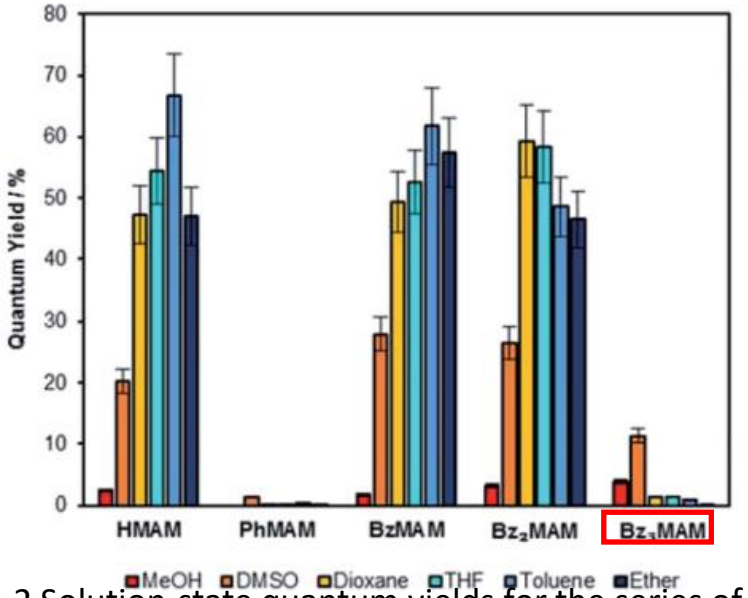


Fig. 2 Solution-state quantum yields for the series of dyes in a range of different solvents, calculated via a reference method.

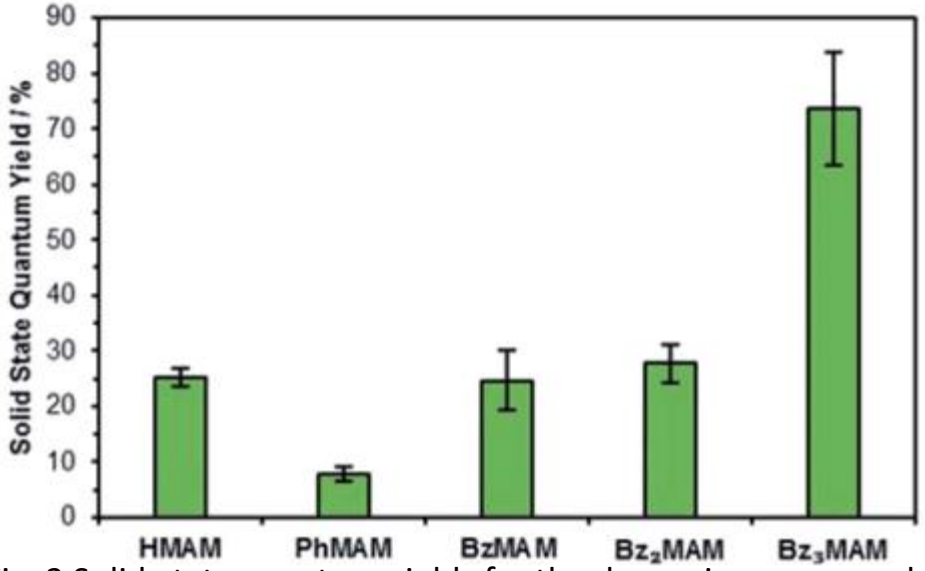


Fig. 3 Solid-state quantum yields for the dye series, measured by an absolute method using an integrating sphere.

Results and discussion

Table 2 Maleimide crystal packing distances and angles for the benzyl MAM series

	Ring plane angle[a]	Ring centroid distance[a] Å^{-1}	Inter plane distance[b] Å^{-1}
HMAM	9.8° (±0.14)	3.649 (±0.001)	3.520 (±0.001)
BzMAM	0.0° (±0.07)	4.053 (±0.001)	3.519 (±0.002)
Bz_2MAM (N101 *etc.*)	0.0° (±0.05)	5.042 (±0.003)	2.764 (±0.009)
Bz_3MAM	13.0° (±0.3)	6.464 (±0.004)	5.885 (±0.007)

[a] Measured distance and angle between ring centroid of N1C1C2C3C4 and $N1_iC1_iC2_iC3_iC4_i$ (**HMAM** $i = 1 - X, +Y, -1/2 + Z$. **BzMAM** $i = 1 - X, 1 - Y, 1 - Z$. **Bz_2MAM** $i = 1 - X, 1 - Y, -Z$. **Bz_2MAM** (N101 *etc.*) $i = -X, 2 - Y, 1 - Z$ **Bz_3MAM** $i = +Y, +X, 1 - Z$). [b] Measured distance between ring centroid of N1C1C2C3C4 and plane of $N1_iC1_iC2_iC3_iC4_i$. See ESI 4.3 for more parameters and further details.

非共价相互作用 (NCI)

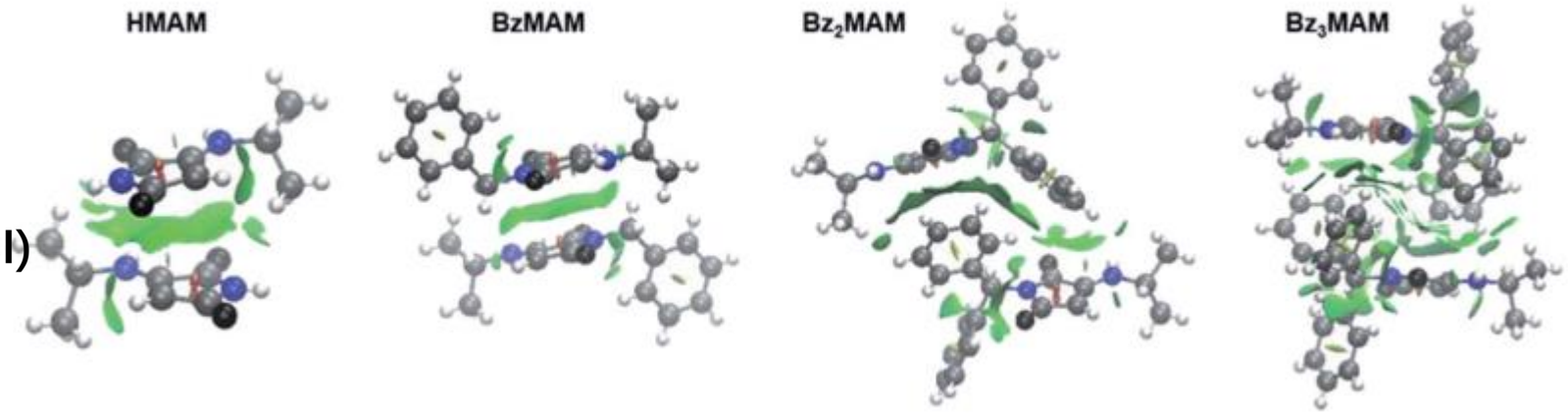


Fig. 4 Crystal structures of HMAM, BzMAM, Bz2MAM, and Bz3MAM overlaid with CAM-B3LYP/6-311G(d,p) gradient isosurfaces with s = 0.5 and a blue–green–red colour scale from 0.05 <p sign(λ_2) <0.05 au

Results and discussion

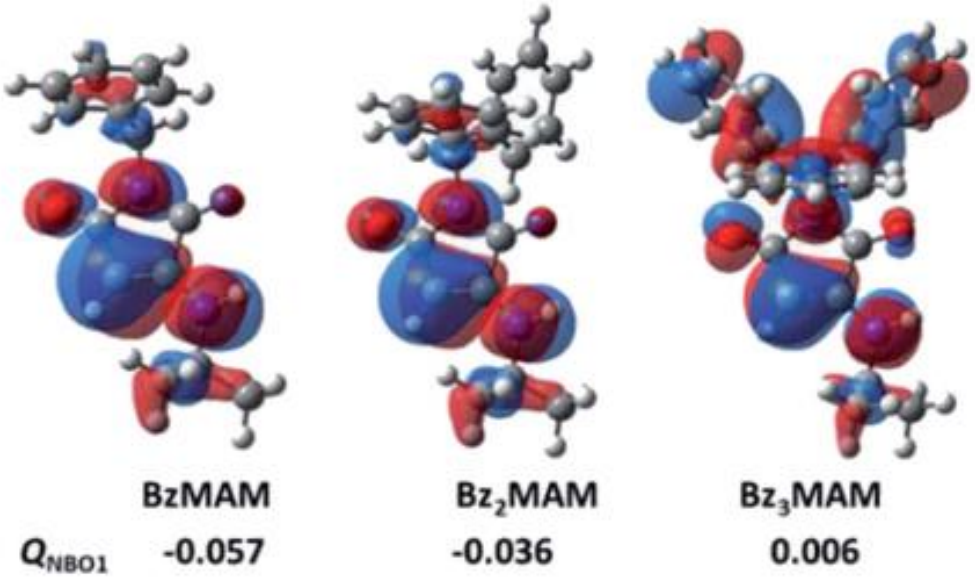


Fig. 5 **HOMO isosurfaces** of the benzyl MAM dye series and the sum of the **natural population charges** of the p-conjugated structure in the aminomaleimide ring (QNBO1).

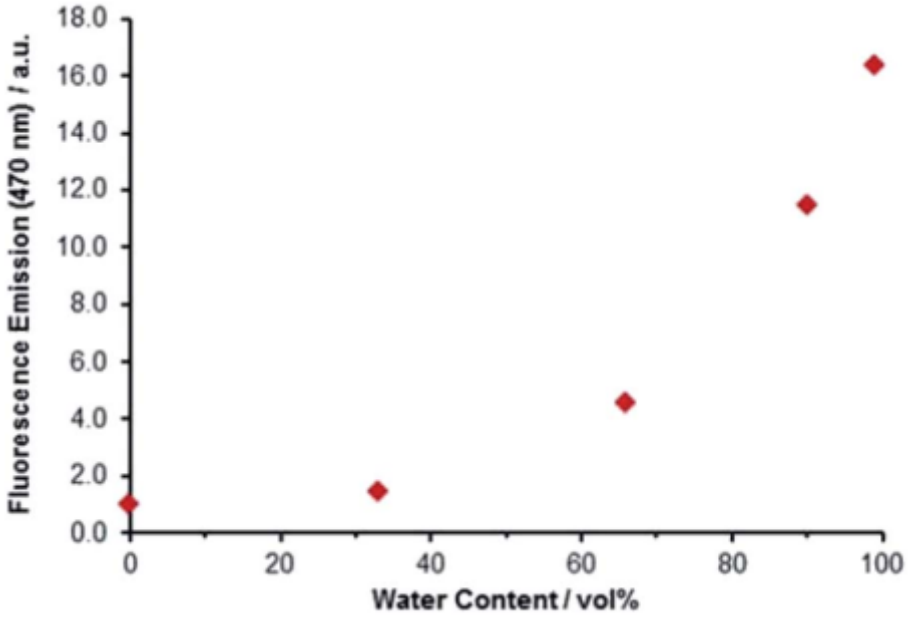


Fig. 6 A solution of
Bz3MAM in dioxane was titrated with water, resulting in an increase in fluorescence upon precipitation of the dye molecule.

三苯甲基电荷密度分布

Results and discussion

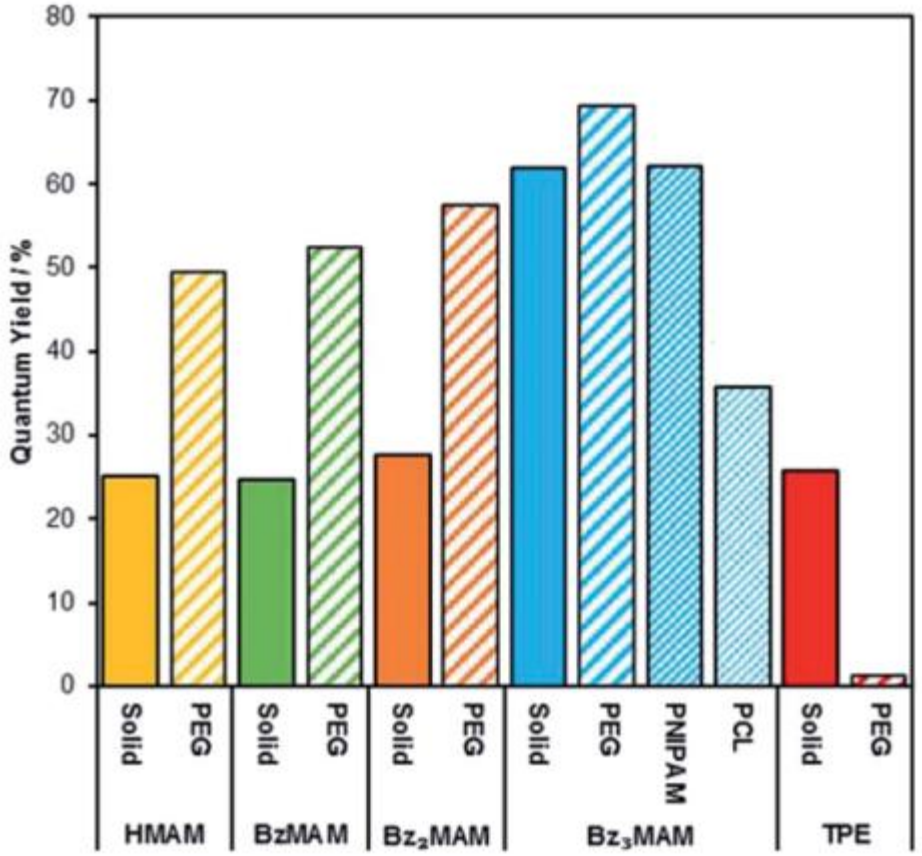


Fig. 7 Solid-state quantum yields of the dyes before and following incorporation into different polymer matrices.

每种染料聚乙二醇 (PEG) 滴铸形成染料掺杂粉末

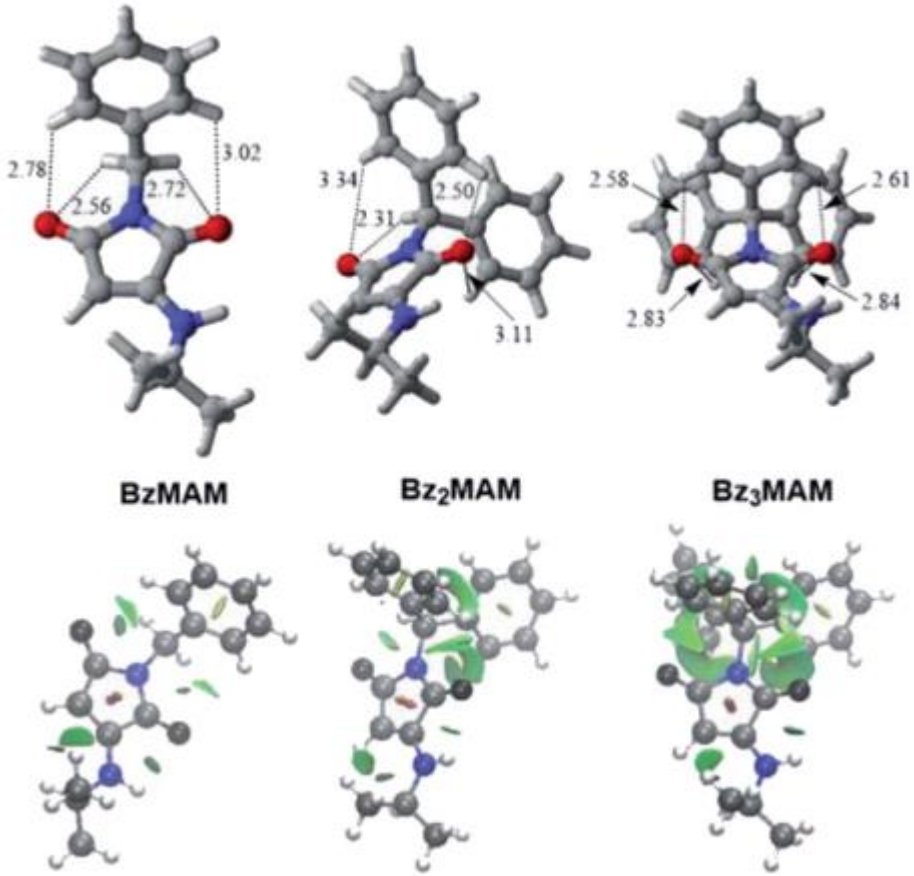


Fig. 8 Visualisations of carbonyl–phenyl interactions for the dye series.

Results and discussion

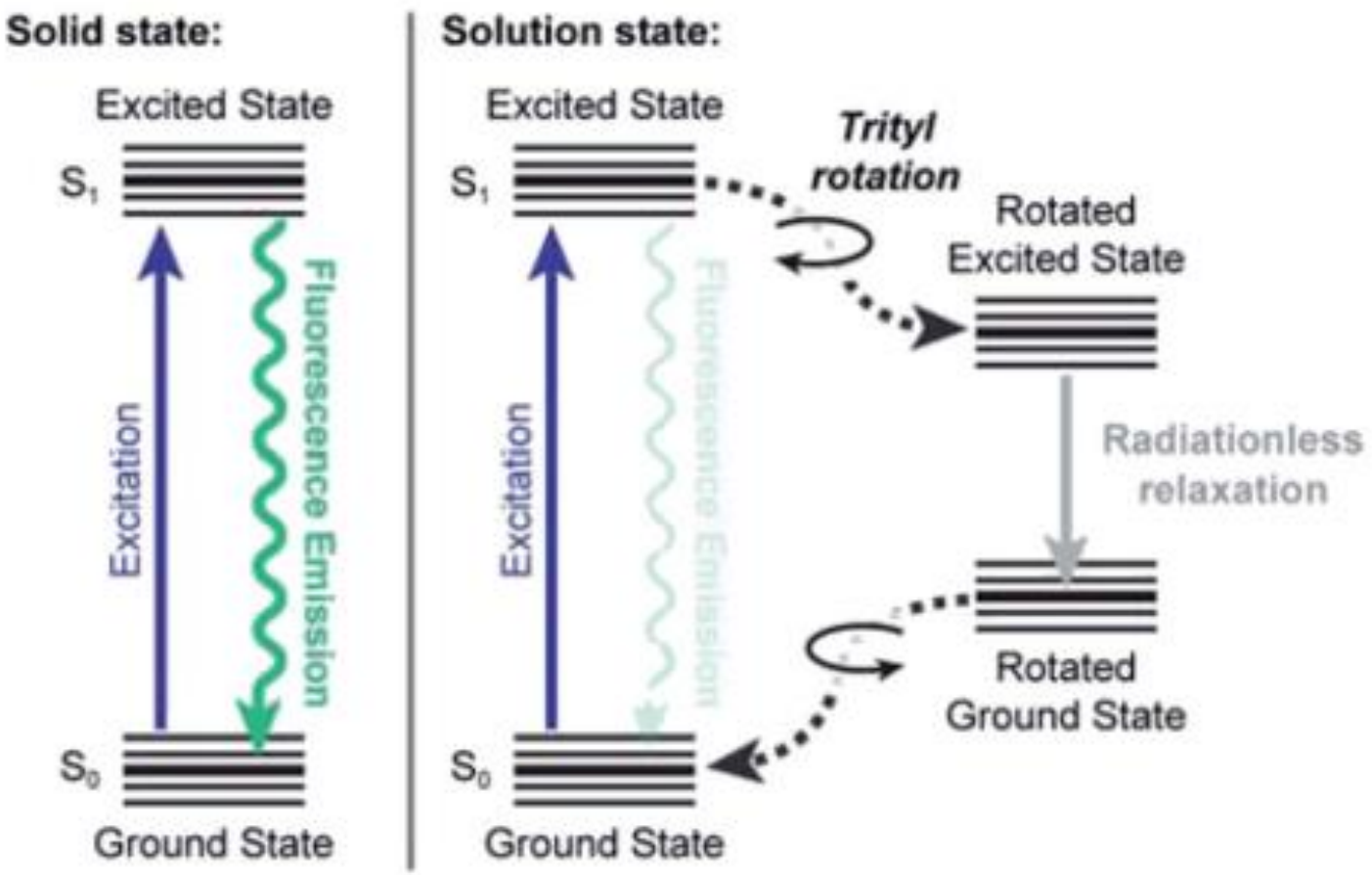


Fig. 9 Jablonski diagram showing proposed mechanism allowing rigidochromic behaviour in Bz3MAM.

Results and discussion

Thank you!