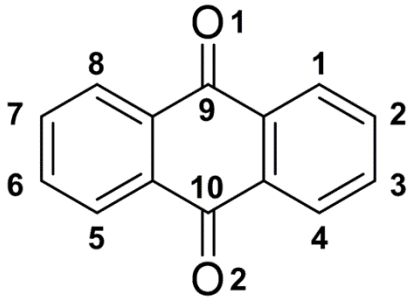


Compound	Substituents	Compound	Substituents
1	2-NMe_2	7	1-OH
2	1-NMe_2	8	1,5-diOH
3	1,5-diNH_2	9	1,8-diOH
4	1,4-diNH_2	10	1,2-diOH
5	1,4-diNHEt	11	1,2-diOMe
6	1-NPhMe	12	1,4-diOH

FIGURE 1 Chemical structures of anthraquinones

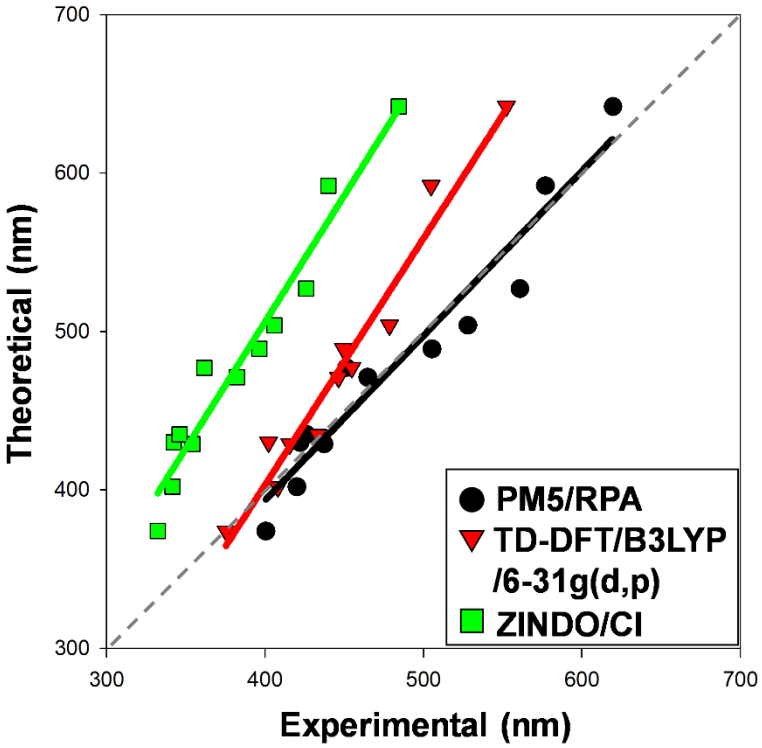


FIGURE 2 Comparison between experimental and theoretical absorption wavelength for AQ dyes. The theoretical values are obtained from TD-DFT, PM5/RPA and ZINDO using X-ray structure

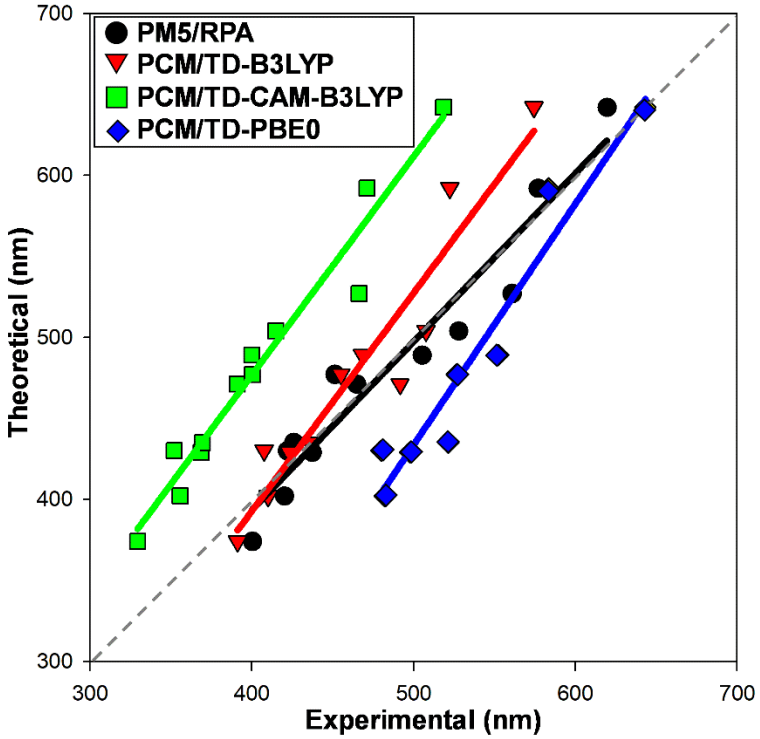


FIGURE 3 Comparison between experimental and theoretical absorption wavelength for AQ dyes. The theoretical values are obtained from PM5/RPA, PCM(EtOH)/TD-B3LYP/6-31g(d,p), PCM(EtOH)/TD-CAM-B3LYP/6-31g(d,p), PCM(EtOH)/TD-PBE0/6-31g(d,p) methods using X-ray structure

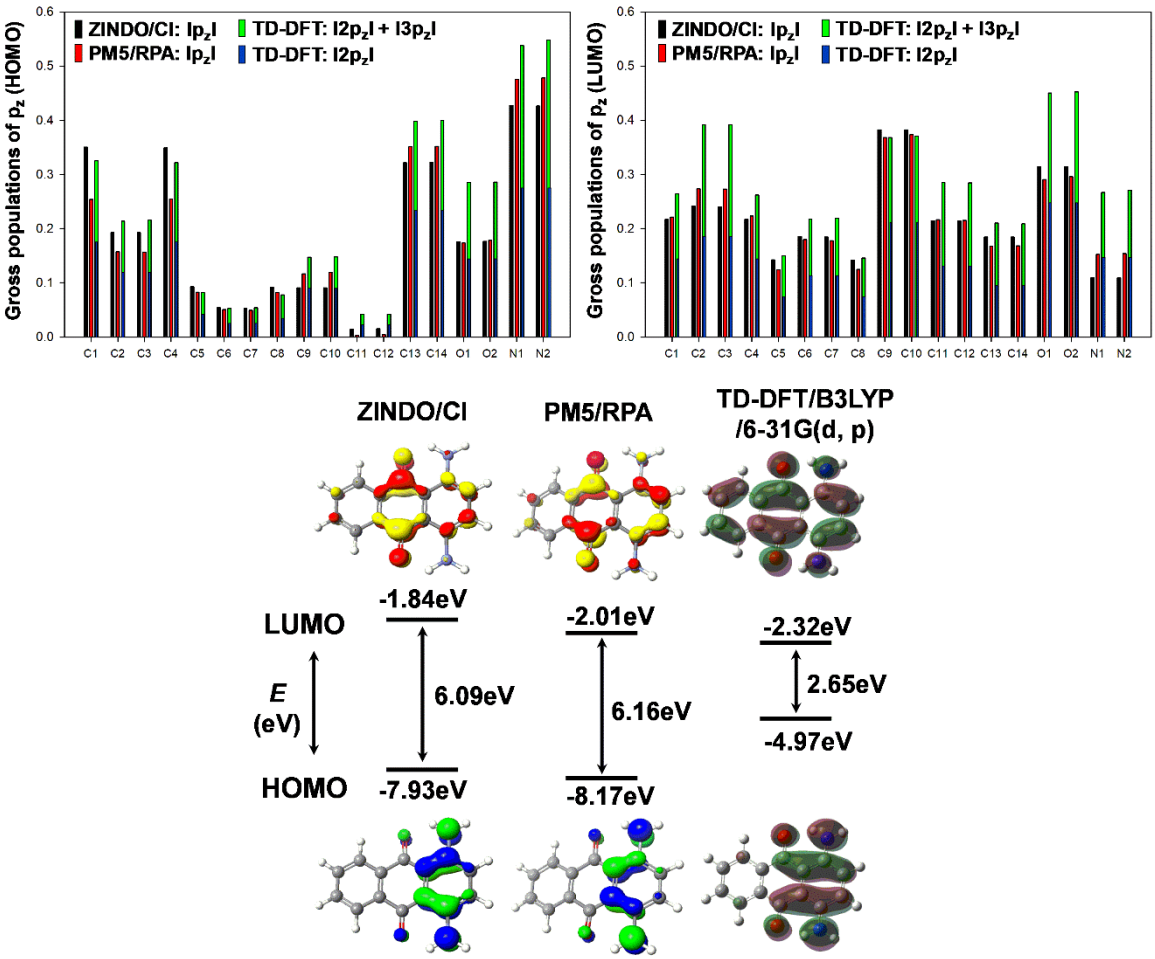
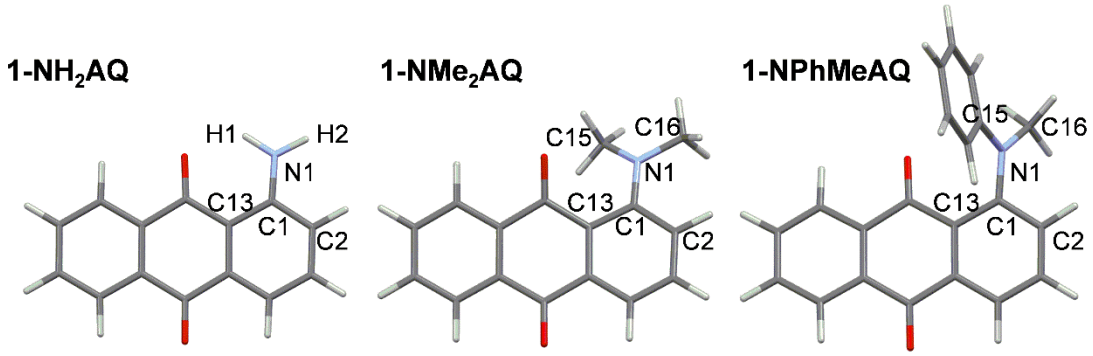
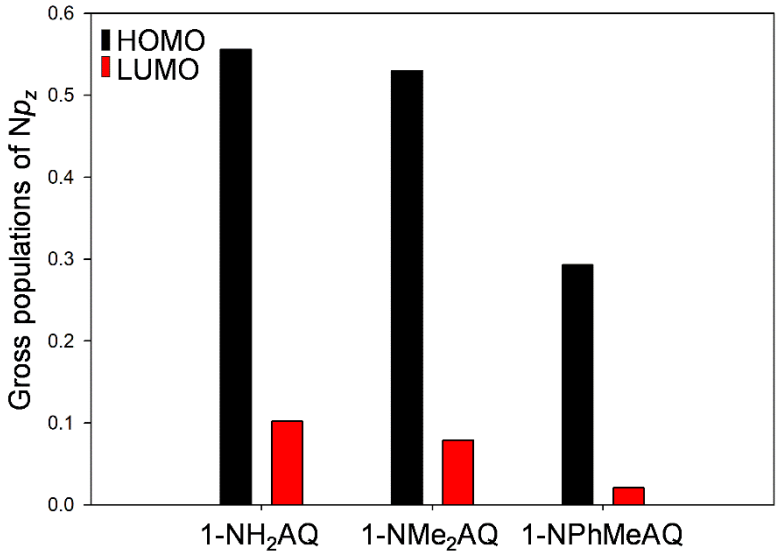


FIGURE 4 Comparison of HOMO and LUMO of 1,4-diNH_2AQ by ZINDO/CI, PM5/RPA, TD-DFT/B3LYP/6-31G(d,p) methods and differences in gross populations of p_z orbitals; $|p_z|$ is the absolute value. The isosurface values are 0.06 (ZINDO/CI, PM5/RPA) a.u. and 0.02 (TD-DFT) a.u., respectively



	Torsion angles (°)		$\lambda_{max.obs.(nm)}$ (EtOH)	$\lambda_{.max.calc.(nm)}$ (PM5/RPA)	$\varepsilon(M^{-1}\cdot cm^{-1})$ (EtOH)	Oscillator strength (*f*)
1-NH_2AQ	C13-C1-N1-H1 C2-C1-N1-H2	0.8 0.1	465	479	6300	0.152
1-NMe_2AQ	C13-C1-N1-C15 C2-C1-N1-C16	32.8 13.1	504	528	5370	0.092
1-NPhMeAQ	C13-C1-N1-C15 C2-C1-N1-C16	58.1 59.0	527	560	3300	0.024

FIGURE 5 PM5/RPA-calculated torsion angle and oscillator strength of 1-NH_2AQ, 1-NMe_2AQ and 1-NPhMeAQ dyes



	HOMO (Np_z)	LUMO (Np_z)	*f*
1-NH_2AQ	0.556	0.102	0.152
1-NMe_2AQ	0.530	0.079	0.126
1-NPhMeAQ	0.293	0.021	0.069

FIGURE 6 PM5/RPA-calculated Np_z and torsion angle of 1-NH_2AQ, 1-NMe_2AQ and 1-NPhMeAQ dyes