

Supplementary Information

Design, synthesis, crystal structure, photophysics and aggregation-induced emission of a novel pyrene scaffold multifunctional Schiff base ligand: Inhibition of digestive enzymes and docking studies

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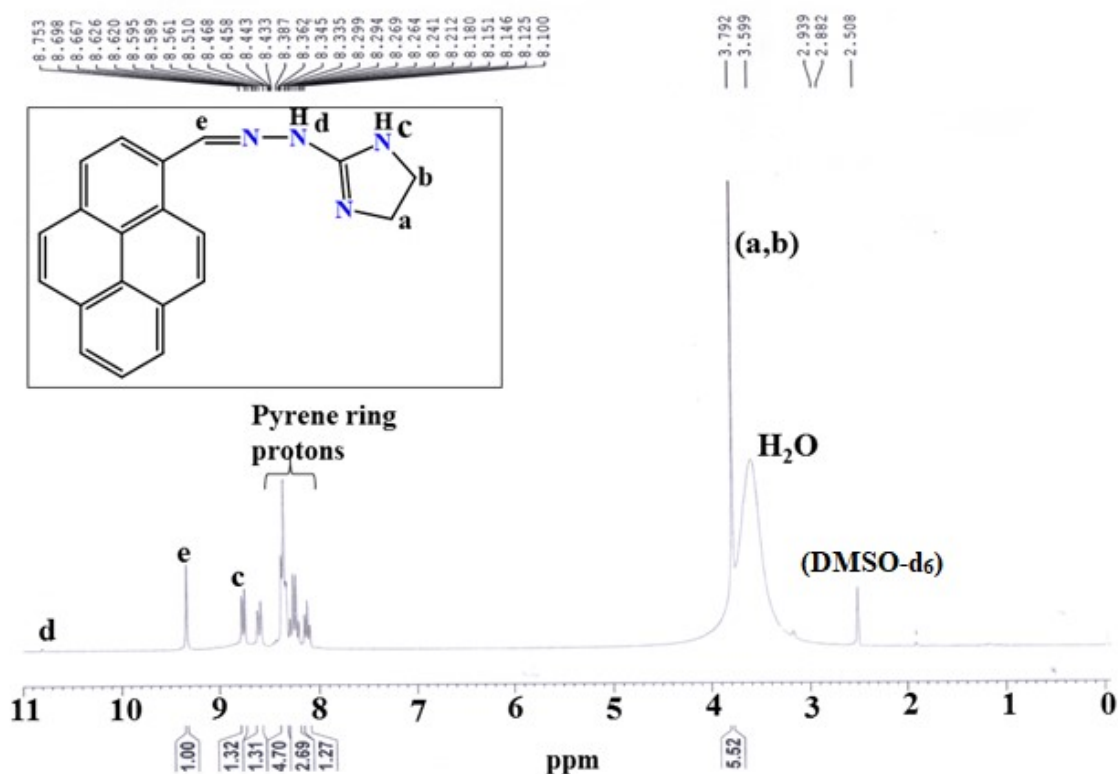


Figure S1. ¹H NMR spectrum of PI.

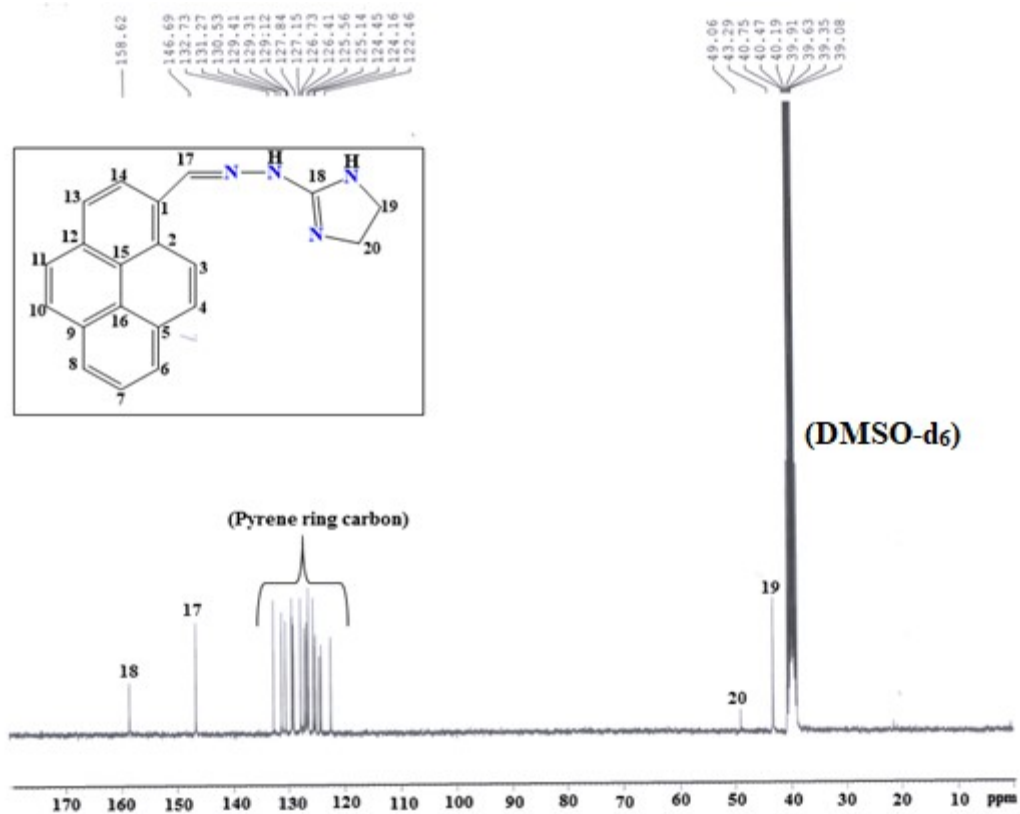


Figure S2. ¹³C NMR spectrum of PI.

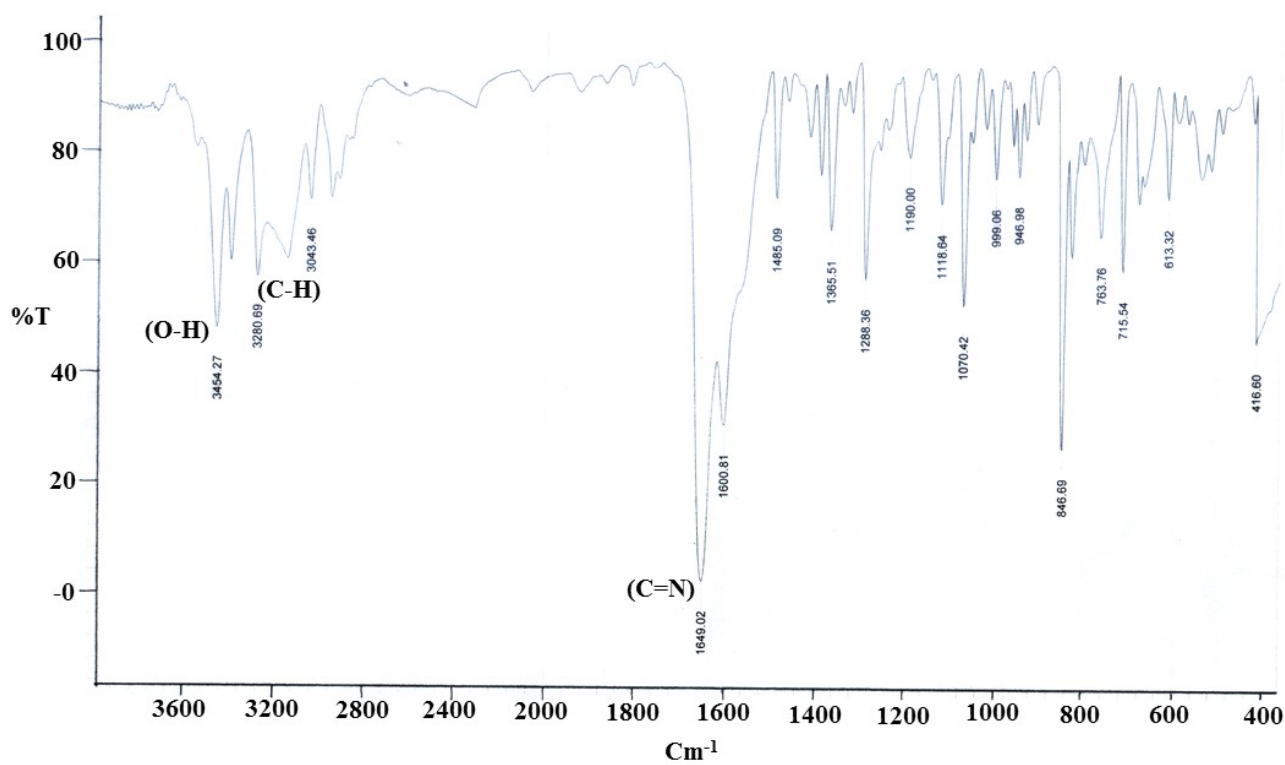


Figure S3. FT-IR spectrum of PI.

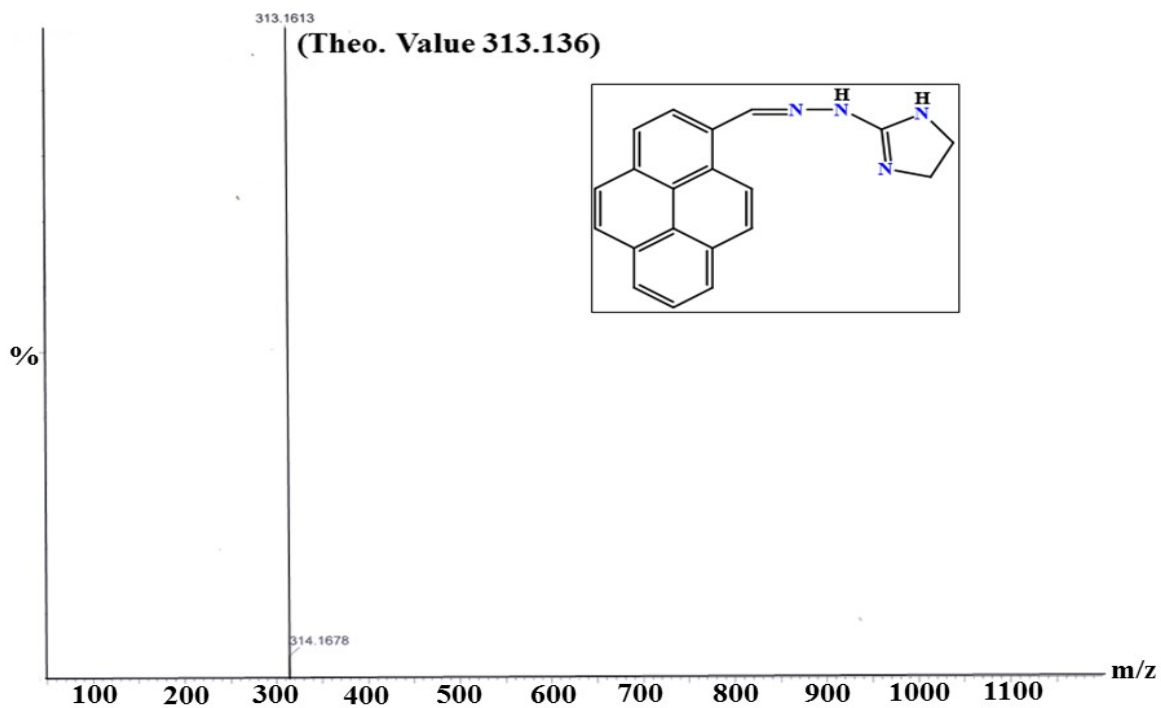


Figure S4. ESI-MS spectrum of PI.

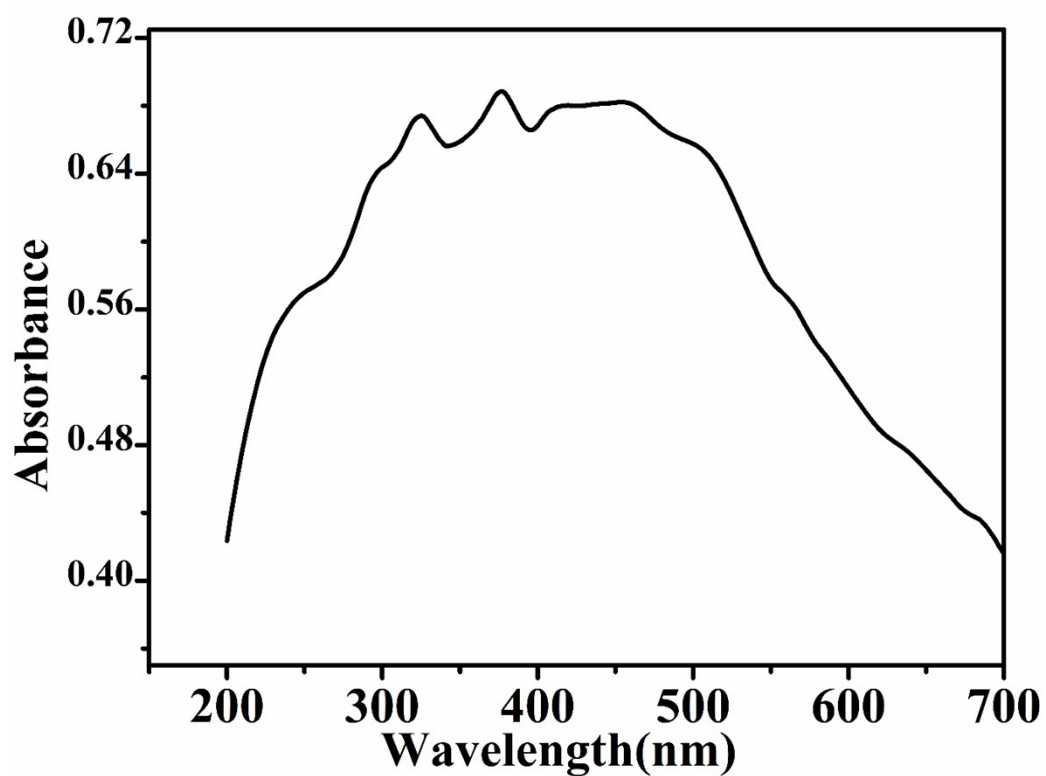


Figure S5. Solid state diffuse reflectance spectrum of PI.

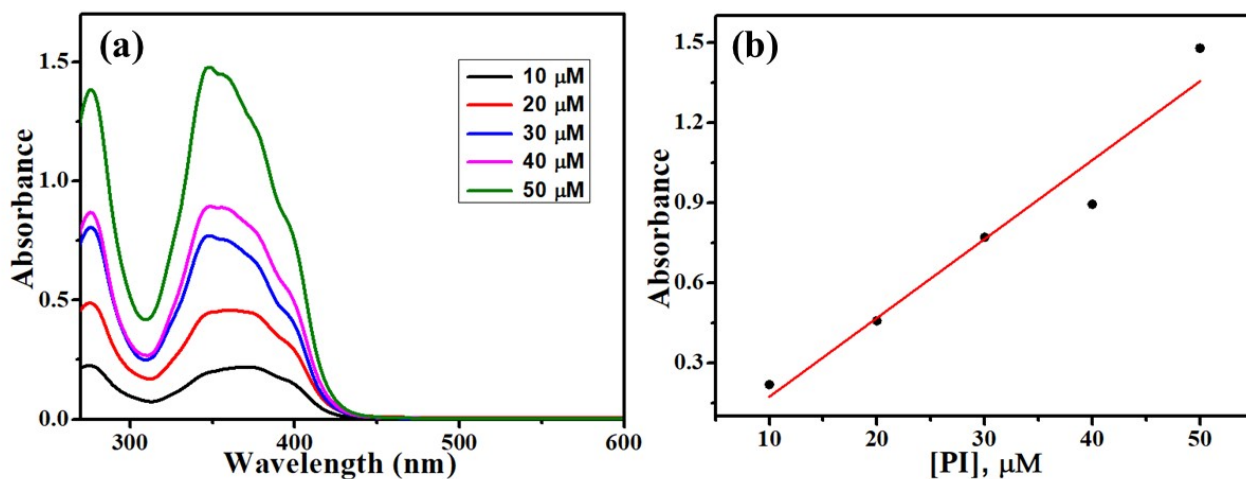


Figure S6. (a) Absorption spectra of PI ($1-5 \times 10^{-5}$ M) in methanol (b) Beer-Lambert plot of PI in methanol.

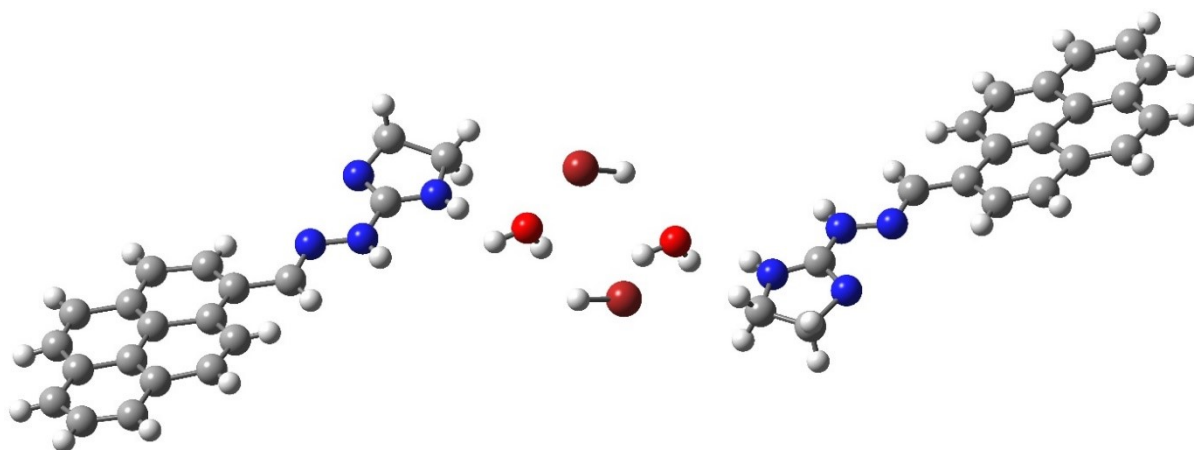


Figure S7. Geometry optimized structure of PI (N: blue, O: red, C: grey and H: white shed).

Table S1. PI in methanol with increasing percentage of water.

Sl. No.	PI/MeOH (mL) [#]	Water (mL)	Total volume (mL)	Percentage of water
1	2.5		2.5	0 %
2	2.25	0.25	2.5	10 %
3	2	0.5	2.5	20 %
4	1.75	0.75	2.5	30 %
5	1.50	1	2.5	40 %
6	1.25	1.25	2.5	50 %
7	1	1.5	2.5	60 %
8	0.75	1.75	2.5	70 %

9	0.5	2	2.5	80 %
10	0.25	2.25	2.5	90 %

taken from stock solution (10 μ M)