Selective Sensing of nitric oxide by 9,10-phenanthroquinone-pyridoxal based fluorophore

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Fig.S1. ¹H-NMR spectrum of PQPY in DMSO-d₆.



Fig.S2. Mass spectrum of PQPY in MeCN.



Fig.S3. Simulated mass spectrum of PQPY in MeCN.



Fig.S4. IR spectrum of ligand (PQPY)



Fig.S5. Normalized emissions of probe PQPY upon reaction with NO in different solvent (7:3 hepes buffer:solvent) of different polarity.



Fig.S6. ¹H-NMR spectrum of PQPY-NO in DMSO-d₆.



Fig.S7. IR spectrum of PQPY-NO



Fig.S8. Determination of LOD of PQPY+ NO.



Fig.S9. Emission profile of the probe at different pH.

Bond Lengths (Å)				
N24-H26	1.429	N23-C25	1.345	
C7-N24	1.393	C10-C23	1.384	
C25-N24	1.237	C7-C10	1.390	
Bond Angles (°)				
N24-C7-C10	105.49	N24-C25-N23	110.36	
C25-N23-C10	105.93	C25-N24-N26	122.23	

Table-S1 : List of some selected bond lengths of Probe (PQPY) in the ground state calculated at B3LYPLevels.

Bond Lengths (Å)				
N24-C25	1.429	N23-C25	1.310	
C24-N44	1.393	C10-C23	1.406	
N44-O45	1.237	C7-C10	1.390	
Bond Angles (°)				
N24-C7-C10	103.33	N24-N44-O45	117.46	
C25-N23-C10	106.67	C25-N24-C7	107.19	
C25-N24-C44	114.95			

Table-S2 : Some selected geometrical parameters for NO product (PQPY-NO) in the ground state calculated at B3LYP Levels.