Benzoquinone-imidazole hybrids as selective colorimetric sensors for cyanide in aqueous, solid and gas phases

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Figure S1. The packing diagram of (A) R5 and (B) R5-CN⁻.



Figure S2. Color changes observed in DMF solution of **R1-R4** (6.25x10⁻⁴ M) upon addition of various anions.



Figure S3. Color changes observed for **R5** at different pH values: A) free **R5** and B) after the addition of cyanide ion.



Figure S4. UV-Vis spectra of R1 (6.25×10^{-4} M) with the incremental addition of TBACN (0 - 6.25×10^{-7} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).



Figure S5. UV-Vis spectra of R2 (6.25×10^{-4} M) with the incremental addition of TBACN (0 - 6.25×10^{-6} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).



Figure S6. UV-Vis spectra of R3 (6.25×10^{-4} M) with the incremental addition of TBACN (0 - 6.25×10^{-6} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).



Figure S7. UV-Vis spectra of R4 (6.25×10^{-4} M) with the incremental addition of TBACN (0 - 6.25×10^{-6} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).



Figure S8. UV-Vis absorption changes of R5 with cyanide ion in presence of other anions.



Figure S9. UV-Vis absorption changes of **R5** (6.25×10^{-4} M) upon addition of 1 eqv. of Ag⁺, Ca²⁺, Cu²⁺, Fe³⁺, Mg²⁺, Co²⁺, Zn²⁺ and Ni²⁺.



Figure 10. Job's plots for the receptor-cyanide complexes.



Figure S11. Fluorescence emission spectra of **R1** (6.25×10^{-4} M) with incremental addition of TBACN (0 - 6.25×10^{-6} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).



Figure S12. Fluorescence emission spectra of **R2** (6.25×10^{-4} M) with incremental addition of TBACN (0 - 6.25×10^{-6} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).



Figure S13. Fluorescence emission spectra of **R3** (6.25×10^{-4} M) with incremental addition of TBACN (0 - 6.25×10^{-6} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).



Figure S14. Fluorescence emission spectra of **R4** (6.25×10^{-4} M) with incremental addition of TBACN (0 - 6.25×10^{-6} M) in aq. HEPES buffer-DMF (9:1 v/v) medium (pH = 7.26).

Receptor	δ _{N-H} in free receptor	$\delta_{\text{N-H}}$ in complex [*]	Δδ (ppm)
R1	14.324	14.466	0.142
R2	14.276	14.379	0.103
R3	14.213	14.316	0.103
R4	14.132	14.245	0.113
R5	13.400	13.534	0.134

Table S1. ¹H NMR spectral data for the interaction of the receptors with CN⁻

* After the addition of 0.5 equivalents of CN^{-} ion.



Figure S15. ¹H NMR spectrum of **R1** with addition of 0.5 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S16. ¹H NMR spectrum of **R1** with addition of 2.0 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S17. ¹H NMR spectrum of **R2** with addition of 0.5 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S18. ¹H NMR spectrum of **R2** with addition of 2.0 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S19. ¹H NMR spectrum of **R3** with addition of 0.5 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S20. ¹H NMR spectrum of **R3** with addition of 2.0 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S21. ¹H NMR spectrum of **R4** with addition of 0.5 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S22. ¹H NMR spectrum of **R4** with addition of 2.0 eqv. of CN^{-1} ion in DMSO-d₆.



Figure S23. Correlation between association constant (K_A) and chemical shift (δ_H).



Figure S24. CV response of receptor R1 with CN^{-1} ion.



Figure S25. CV response of receptor R2 with CN^{-1} ion.



Figure S26. CV response of receptor R3 with CN^{-1} ion.



Figure S27. CV response of receptor $\mathbf{R4}$ with \mathbf{CN}^{-} ion.









Figure S28. Optimized structure for receptors R1-R5 and its Cyanide complexes.

So 0

R5-CN-

-0 0



Figure S29. Molecular orbitals (HOMO–LUMO) of receptors R1-R5.























Figure S30. Molecular orbitals (HOMO –LUMO) of receptors–CN⁻ complexes.

Receptor	Free receptor			Receptor-CN ⁻ complex		
	E _{HOMO}	E _{LUMO}	ΔΕ	E _{HOMO}	E _{LUMO}	ΔΕ
R1	-6.3305	-3.3908	2.9397	-6.720	-5.6951	1.0569
R2	-6.2472	-3.3932	2.8540	-6.8257	-5.7136	1.1121
R3	-6.0975	-3.3818	2.7157	-6.3136	-5.3343	0.9793
R4	-6.3990	-3.3897	3.0093	-6.9245	-5.7152	1.2093
R5	-6.8004	-3.2738	3.5266	-7.9955	-6.4872	1.5083
R1 R2 R3 R4 R5	-6.3305 -6.2472 -6.0975 -6.3990 -6.8004	-3.3908 -3.3932 -3.3818 -3.3897 -3.2738	2.9397 2.8540 2.7157 3.0093 3.5266	-6.720 -6.8257 -6.3136 -6.9245 -7.9955	-5.6951 -5.7136 -5.3343 -5.7152 -6.4872	1.0569 1.1121 0.9793 1.2093 1.5083

Table S2. Energies (in eV) of the MOs in free receptors and in receptor- CN^{-} complexes



Figure S31. ¹H NMR spectrum of 1



Figure S32. ¹³C NMR spectrum of 1



Figure S33. LCMS spectrum of 1



Figure S34. ¹H NMR spectrum of R1.



Figure S35. LCMS spectrum of R1.



Figure S36. ¹H NMR spectrum of R2.



Figure S37. LCMS spectrum of R2.



Figure S38. ¹H NMR spectrum of R3.



Figure S39. LCMS spectrum of R3.



Figure S40. ¹H NMR spectrum of R4.



Figure S41. LCMS spectrum of R4.



Figure S42. ¹H NMR spectrum of R5.



Figure S43. LCMS spectrum of R5.