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**Tunable N-Substitution in Zwitterionic Benzoquinonemonoimines :
Straightforward Synthesis, Metal Coordination
and Supramolecular Structures**

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Solid-state structures of Compounds $4 \cdot \text{H}_2\text{O}$ and $5 \cdot \text{H}_2\text{O}$

$4 \cdot \text{H}_2\text{O}$ forms intermolecular interactions in the solid state with π - π stacking and strong hydrogen bonding generating a 3-D supramolecular network (Figure S1). This is consistent with the very poor solubility of **4** in almost all the solvents. The molecule show head-to-head π - π stacking model with two intermolecular C(4)···C(4) distances of 3.654 Å. The hydrogen bonds are complicated in the solid state owing to the presence of water molecule and two more H-donor. There are four types of bonds which originated from interaction of water and four zwitterions with O(3)···N(1), O(3)···N(1), O(3)···O(1) and O(3)···O(2) distances of 3.005, 2.867, 2.854 and 2.814 Å, respectively. The last type of hydrogen bond is formed between N(2) and O(2) of two zwitterions with distance of 2.906 Å.

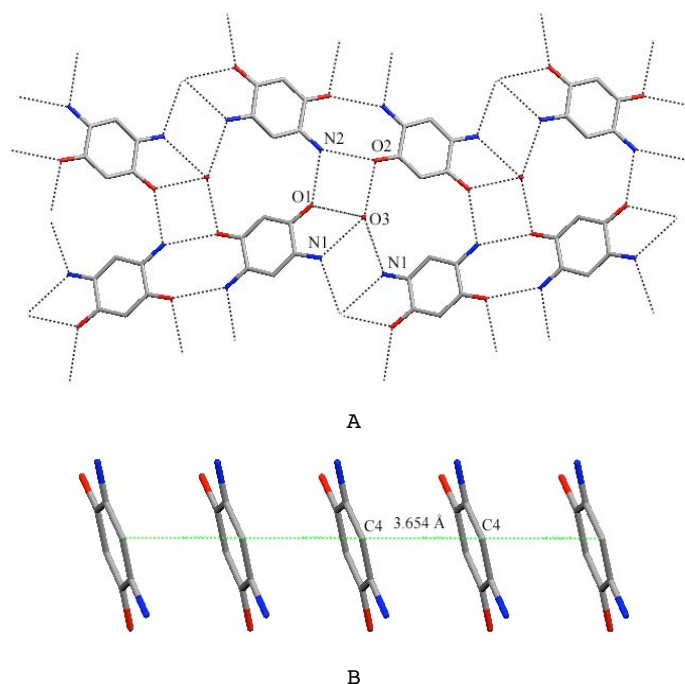


Figure S1. A) View of the supramolecular array generated by $4 \cdot \text{H}_2\text{O}$ in the solid state. B) View of the head-to-head π - π stacking arrangement generated by $4 \cdot \text{H}_2\text{O}$ in the solid state. Color coding: nitrogen, blue; oxygen, red.

Compound **5**·H₂O forms a two-dimensional parallel layers in the solid state connected by head-to-tail π - π interactions with intermolecular C(1)···C(4) distances of 3.934 Å and hydrogen bonding (Figure S2). There are four types of hydrogen bonds in the solid states. Three of them are arising from the interaction of water molecule and three molecules **5** with O(3)···N(2), O(3)···O(1) and O(3)-O(2) distances of 2.895 Å, 2.817 Å and 2.887 Å, respectively. The last hydrogen bond results from interaction between two zwitterions with N(1)-O(2) distance of 2.948 Å.

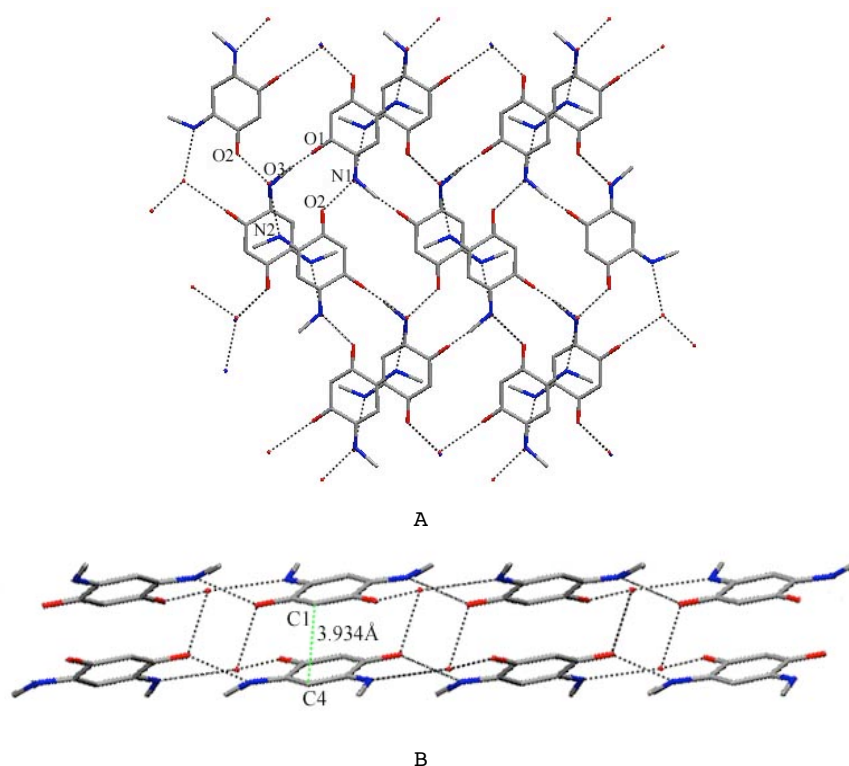


Figure S2. View of the supramolecular array generated by **5**·H₂O in the solid state, A) plane view and B) side view. Color coding: nitrogen, blue; oxygen, red.