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Scheme S1. Chemical diagrams of studied phenazines 15–22, respectively.

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Scheme S2. Chemical diafram of the organometallics of type I–III, from the corresponding strarting aniline reagents; Most stable molecular geometry and the theoretical $q_X(NBO)$ data, here X = Ag, Cl, C, O and N, respectively.

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Scheme S3. Most stable conformation of the N,N-diethyl-p-phenylenediamine, N,N-dimethyl-p-phenylenediamine, and N-cyclohexyl-3-pyridyl carbaldehyde; Theoretical $q_X(NBO)$ values, were the X = C, N and O; The H-atoms are omitted.



Figure S1. ESI–MS spectra of 4 and 5, respectively.