Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supporting Information for:

8-Quinoline Based Ligands and Their Metallic Derivatives: A Structural and Statistical Investigation of Quinoline π – π stacking Interactions†

Radu F. Semeniuc,* Thomas J. Reamer and Mark D. Smith

Correspondance of the Figures with the Schemes within the article:

Scheme 1 → see Fig. S1

Scheme 2 → see Fig. S1

Scheme 3 → see Fig. S1

Scheme 4 → see Fig. S1

Scheme 5 → see Fig. S1

Scheme 6 → see Fig. S1

Scheme 7 → see Fig. S1

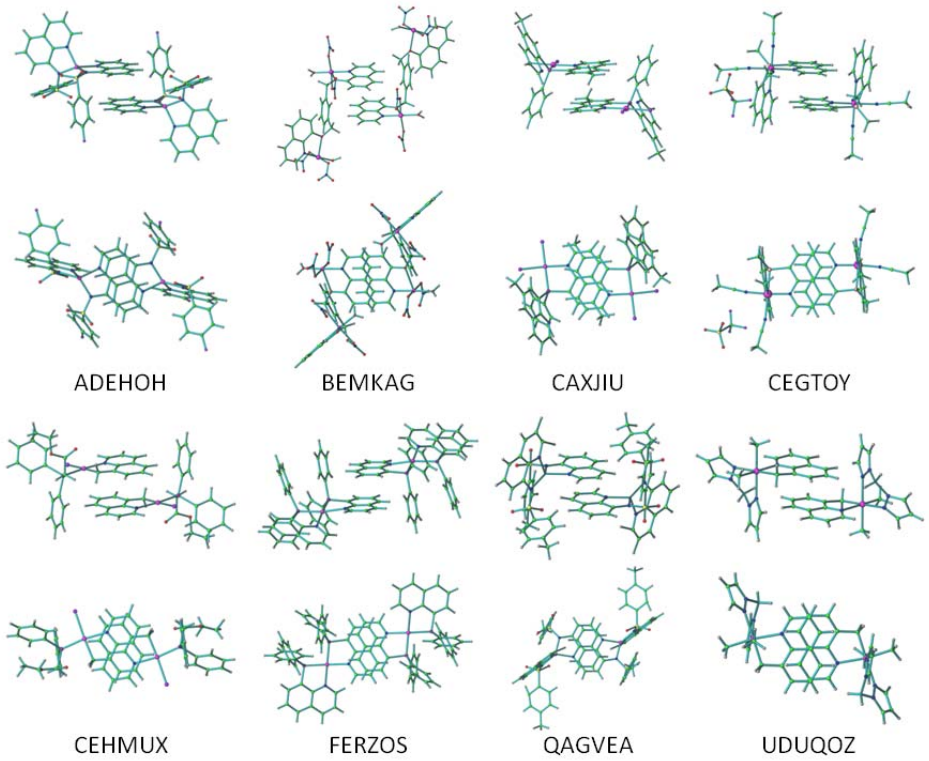

Fig. S1. ADEHOH: Ct-Ct = 3.6 Å, ⊥ = 3.5 Å, β = 18°, H-Ct = 2.74 Å, C-H-Ct = 153°, H-O = 2.71 Å, C-H-O = 162°; BEMKAG: Ct-Ct = 3.9 Å, ⊥ = 3.5 Å, β = 6°, H-Ct = 2.72 Å, C-H-Ct = 156°; CAXJIU: Ct-Ct = 3.7 Å, ⊥ = 3.7 Å, β = 6°, H-Ct = 2.76 Å, C-H-Ct = 145°; CEGTOY: Ct-Ct = 3.7 Å, ⊥ = 3.6 Å, β = 20.8°, H-Ct = 2.93 Å, C-H-Ct = 165°, H-Ct = 2.55 Å, C-H-Ct = 169°; CEHMUX: Ct-Ct = 3.7 Å, ⊥ = 3.6 Å, β = 21.1°, H-Ct = 2.88 Å, C-H-Ct = 166°; FERZOS: Ct-Ct = 3.7 Å, ⊥ = 3.5 Å, β = 19.0°, H-Ct = 2.69 Å, C-H-Ct = 164°; QAGVEA: Ct-Ct = 3.56 Å, ⊥ = 3.4 Å, β = 18.5°, H-Ct = 2.75 Å, C-H-Ct = 141°; UDUQOZ: Ct-Ct = 3.7 Å, ⊥ = 3.5 Å, β = 22.6°, H-Ct = 2.66 Å, C-H-Ct = 175°.

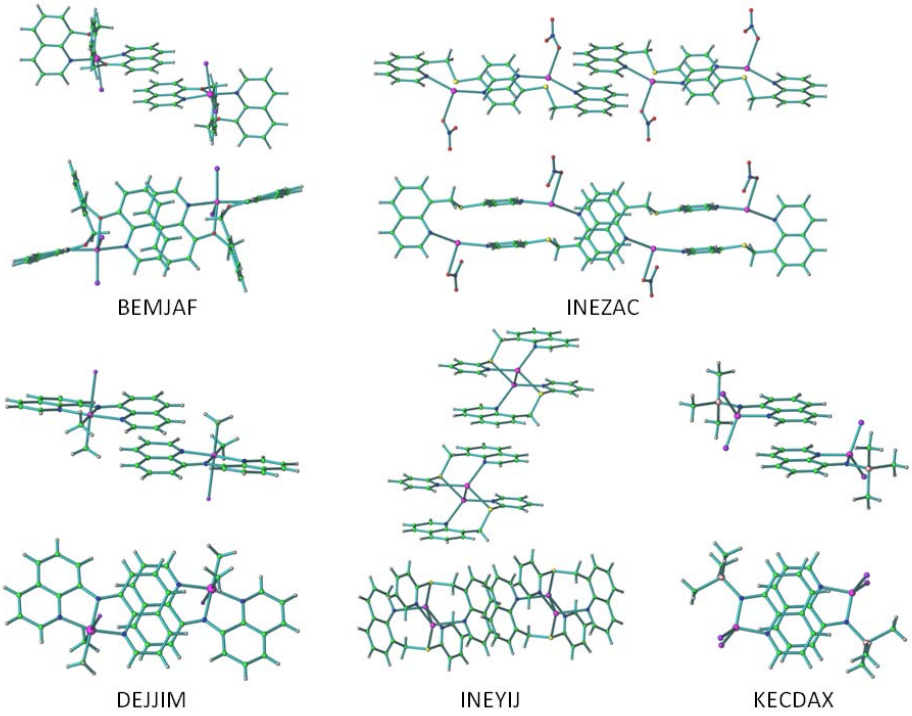

Fig. S2. BEMJAF; Ct-Ct = 3.7 Å, ⊥ = 3.4 Å, β = 28.8°, H-Cl = 2.91 Å, C-H-Cl = 144°, H-Cl = 2.73 Å, C-H-Cl = 150°; INEZAC; Ct-Ct = 3.7 Å, ⊥ = 3.6 Å, β = 19.6°, H-O = 2.6 Å, C-H-O = 140°, H-O = 2.7 Å, C-H-O = 146°; DEJJIM; Ct-Ct = 3.7 Å, ⊥ = 3.4 Å, β = 23.9°; INEYIJ; Ct-Ct = 3.8 Å, ⊥ = 3.5 Å, β = 24.5°; KECDAX; Ct-Ct = 3.4 Å, ⊥ = 3.3 Å, β = 15.3°.

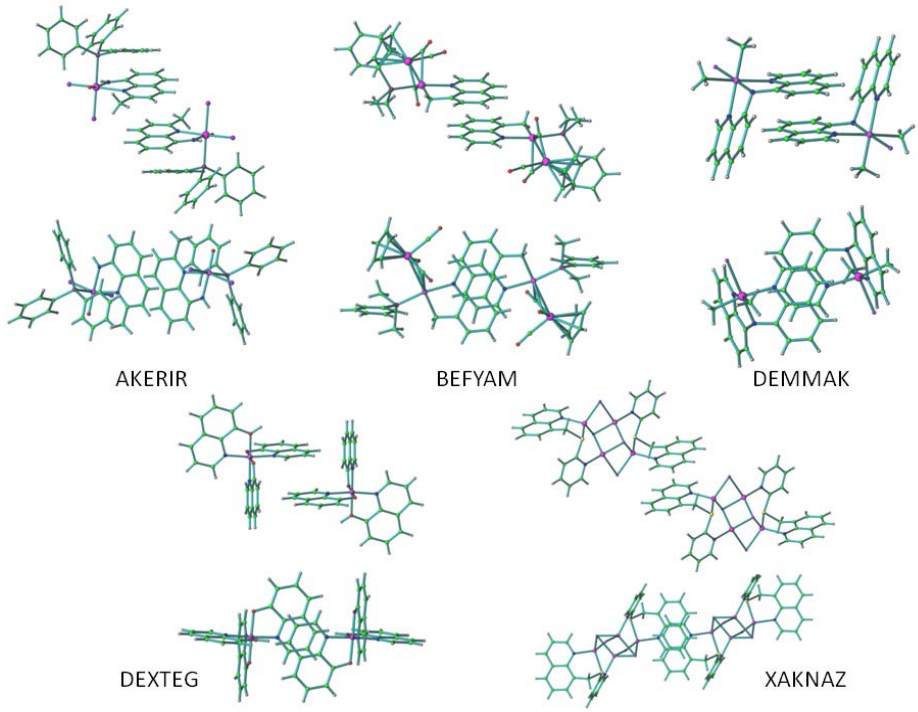

Fig. S3. AKERIR; Ct-Ct = 3.6Å, ⊥ = 3.5 Å, β = 20.1°, H-Cl = 3.1 Å, C-H-Cl = 139°, H-Cl = 2.9 Å, C-H-Cl = 144°; BEFYAM; Ct-Ct = 3.6 Å, ⊥ = 3.4 Å, β = 21.4°, H-O = 2.6 Å, C-H-O = 143.8°; DEMMAK; Ct-Ct = 3.4 Å, ⊥ = 3.4 Å, β = 16°, H-Ct = 2.7 Å, C-H-Ct = 171°; DEXTEG; Ct-Ct = 3.6 Å, ⊥ = 3.4 Å, β = 20.2°, H-Ct = 2.5 Å, C-H-Ct = 165°; XAKNAZ; Ct-Ct = 3.7 Å, ⊥ = 3.4 Å, β = 23.1°

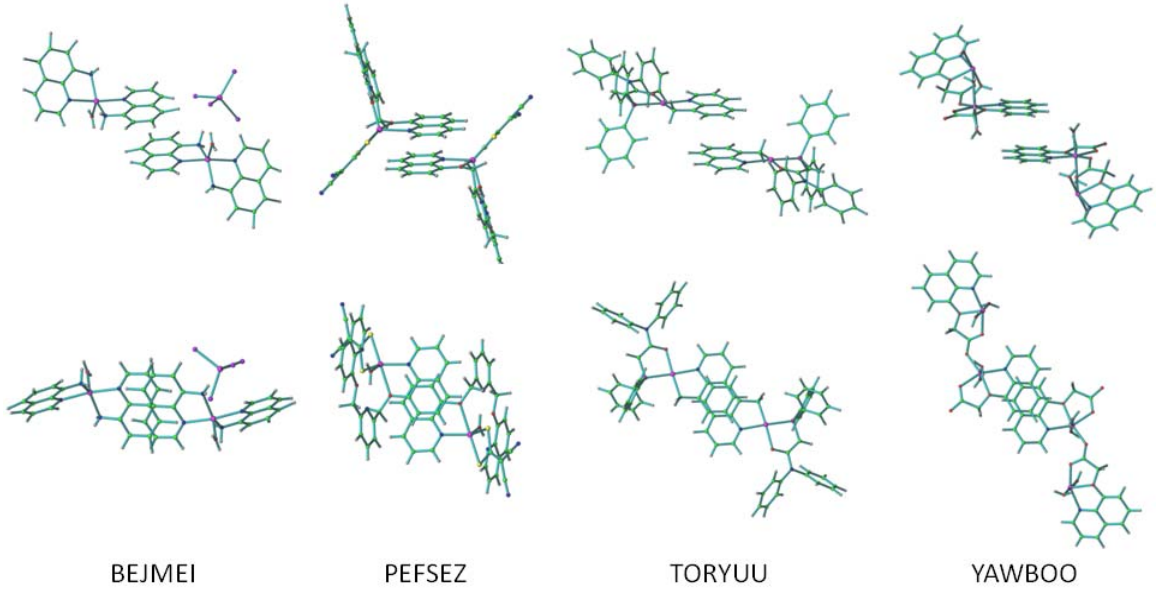

Fig. S4. BEJMEI; Ct-Ct = 3.7 Å, ⊥ = 3.5 Å, β = 21.7°, H-Cl = 2.89 Å, C-H-Cl = 178°; PEFSEZ; Ct-Ct = 3.5 Å, ⊥ = 3.4 Å, β = 15.4°; TORYUU; Ct-Ct = 3.6 Å, ⊥ = 3.5 Å, β = 12.7°; YAWBOO; Ct-Ct = 3.7 Å, ⊥ = 3.5 Å, β = 19.9°.

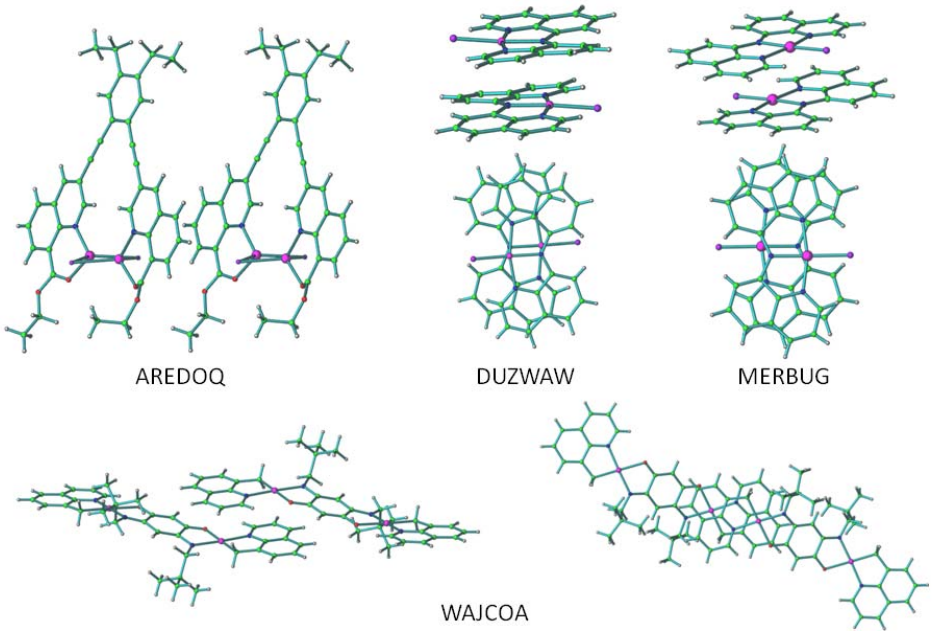

Fig. S5. AREDOQ; Ct-Ct = 3.6 Å, ⊥ = 3.4 Å, β = 20.2°; DUZWAW; Ct-Ct = 4.5 Å, ⊥ = 3.5 Å, β = 39.5 °; MERBUG; Ct-Ct = 3.6 Å, ⊥ = 3.3 Å, β = 22.7°; WAJCOA; no quinoline interaction observed; Ct-Pd = 3.7 Å, ⊥ Pd-Arene distance = 3.5 Å.

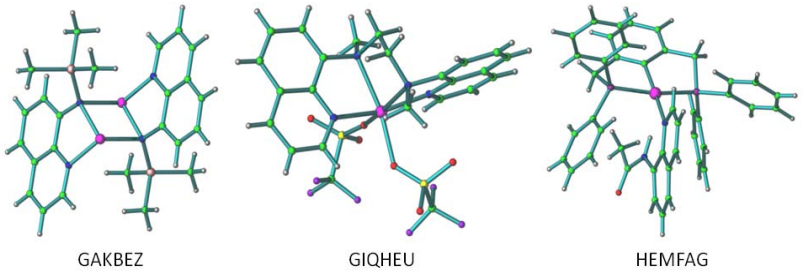

Fig. S6. Selected examples of quinoline based compounds with no π-π stacking interactions: left, CSD refcode: GAKBEZ; middle, CSD refcode: GIQHEU; right, CSD refcode: HEMFAG.

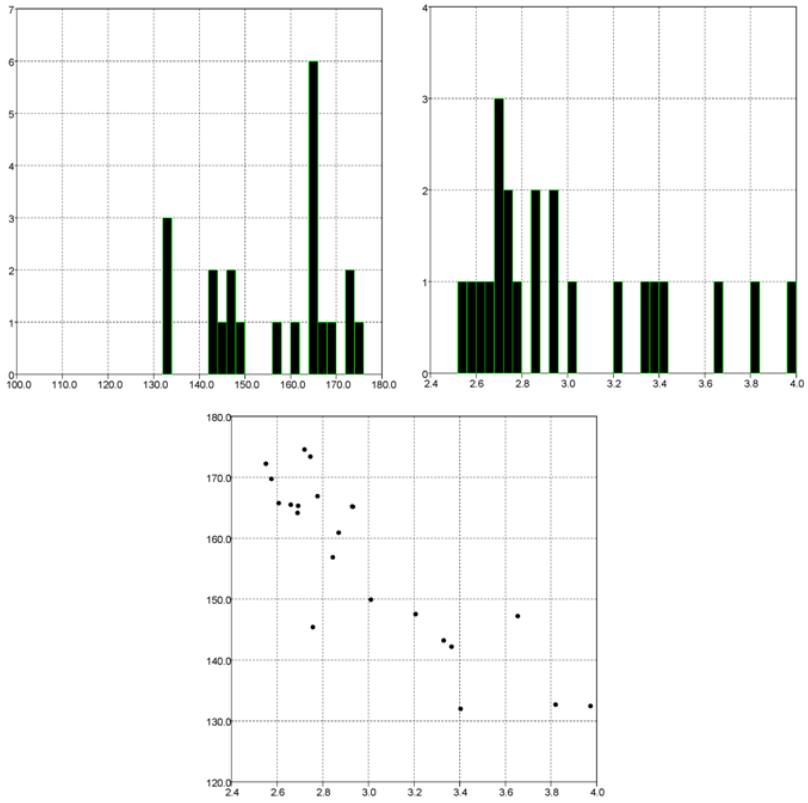

Fig. S7. Statistical analysis of the Q_NM_Ph case: top-left: histogram for the C-H-Ct angle (^{o}); top-right: histogram for the H-Ct distance; bottom: scattergram for a correlation between the C-H-Ct angle and H-Ct distance.

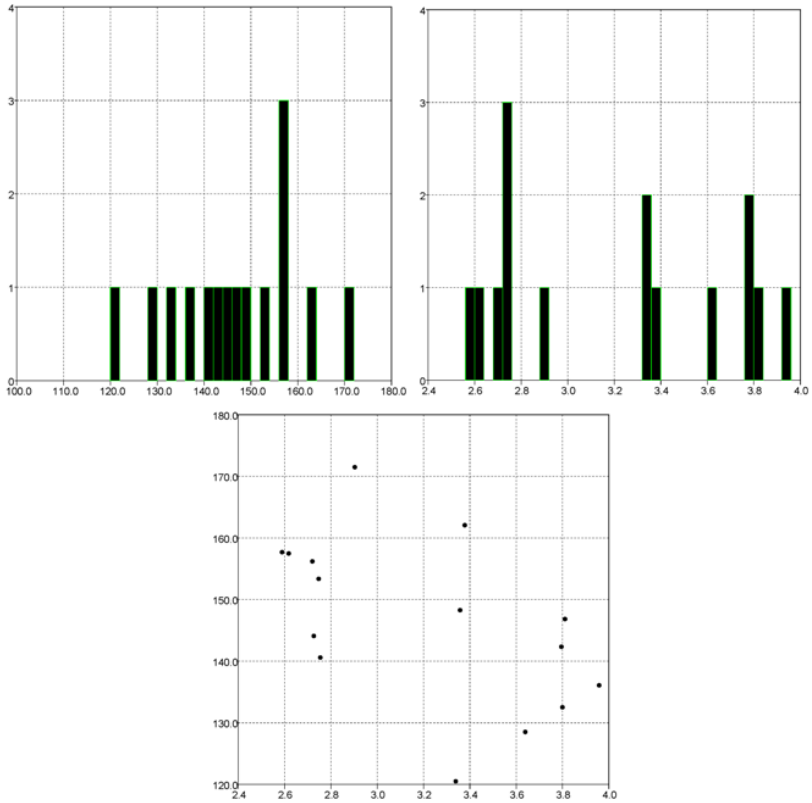

Fig. S8. Statistical analysis of the Q_NM_NM_Ph case: top-left: histogram for the C-H-Ct angle (^{o}); top-right: histogram for the H-Ct distance; bottom: scattergram for a correlation between the C-H-Ct angle and H-Ct distance.