**Supporting information**

# Preparation of RHgCl and $R_2Hg$ (R = 8-quinolyl) via Transmetallation of (8-quinolyl)$SnMe_3$

Sem Raj Tamang, Jung-Ho Son, James D. Hoefelmeyer

*Department of Chemistry, University of South Dakota, 414 E. Clark St., Vermillion, SD 57069*

jhoefelm@usd.edu

Contents

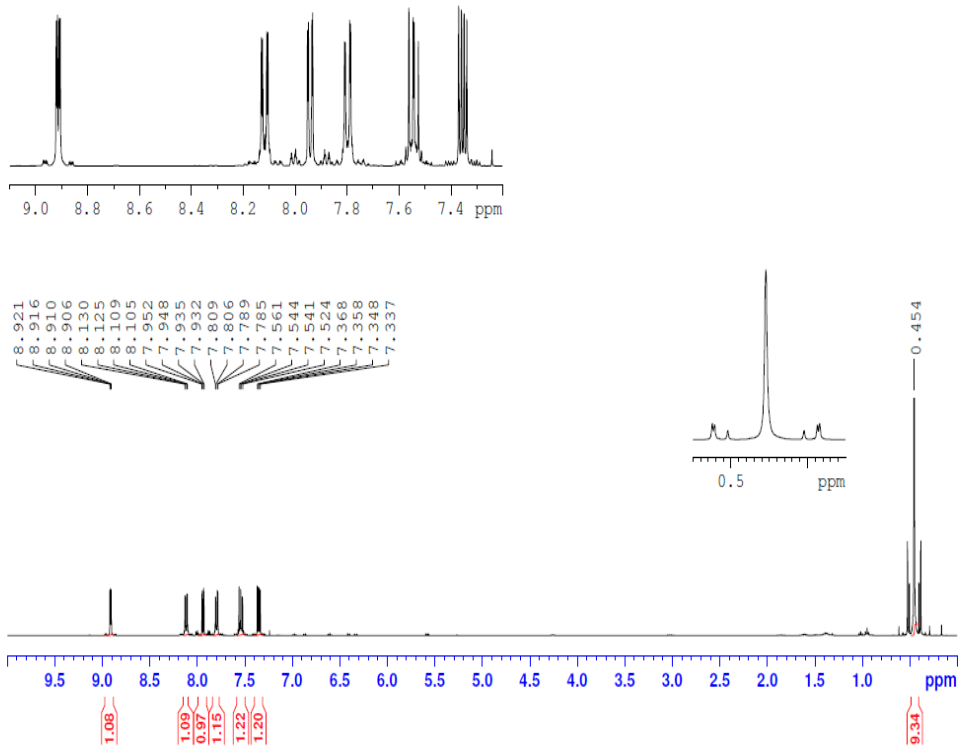


**Figure S1** $^{1}$H of 8-trimethyltinquinoline (**1**).

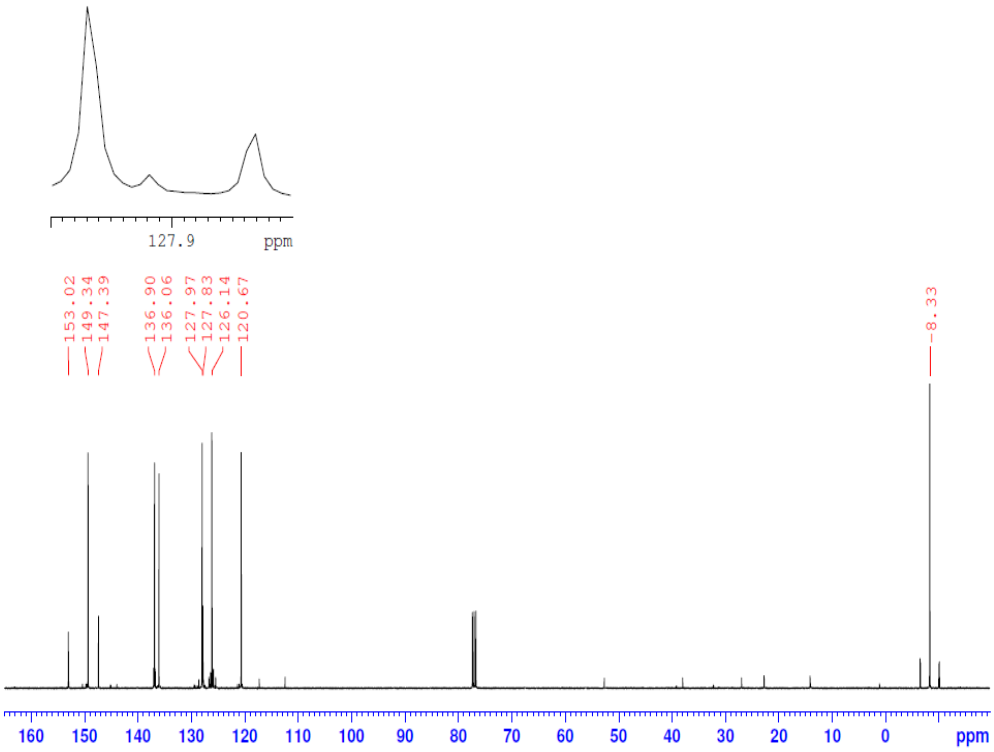


**Figure S2** $^{13}$C of 8-trimethyltinquinoline (**1**).

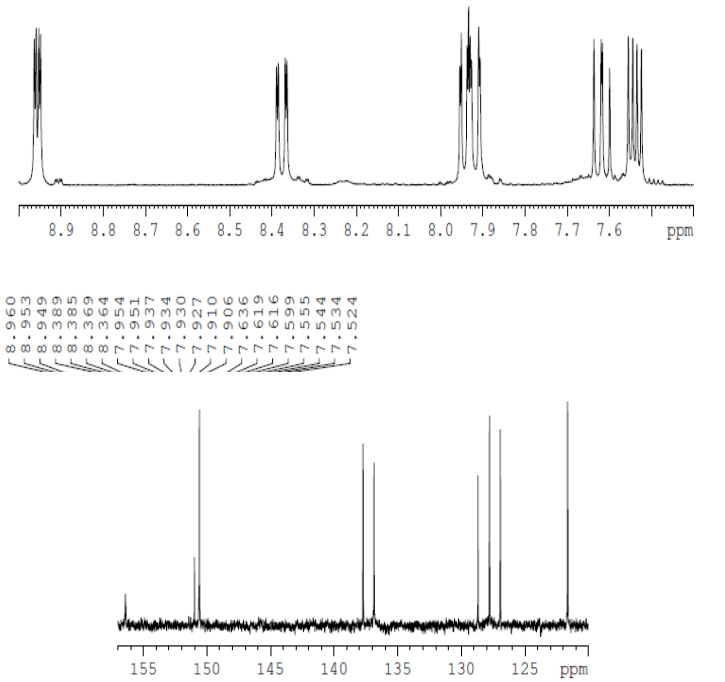


**Figure S3** $^{1}$H of chloro-8-quinolylmercury(II) (**2**).

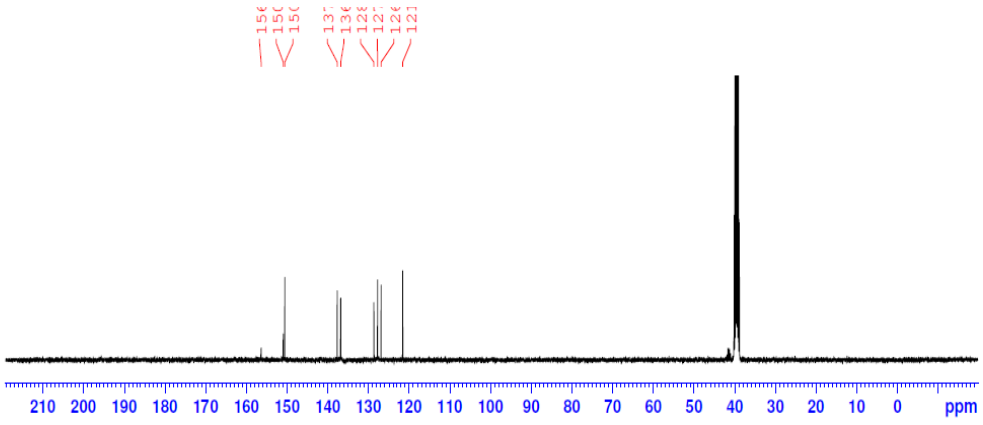


**Figure S4** $^{13}$C of chloro-8-quinolylmercury(II) (**2**).

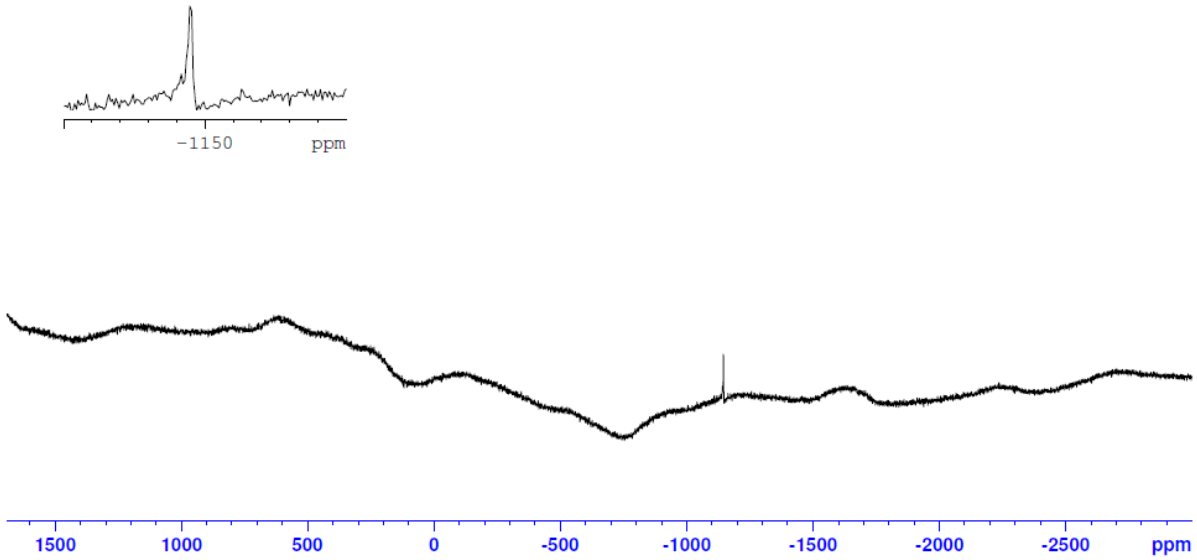


**Figure S5** $^{199}$Hg of chloro-8-quinolylmercury(II) (**2**).

\

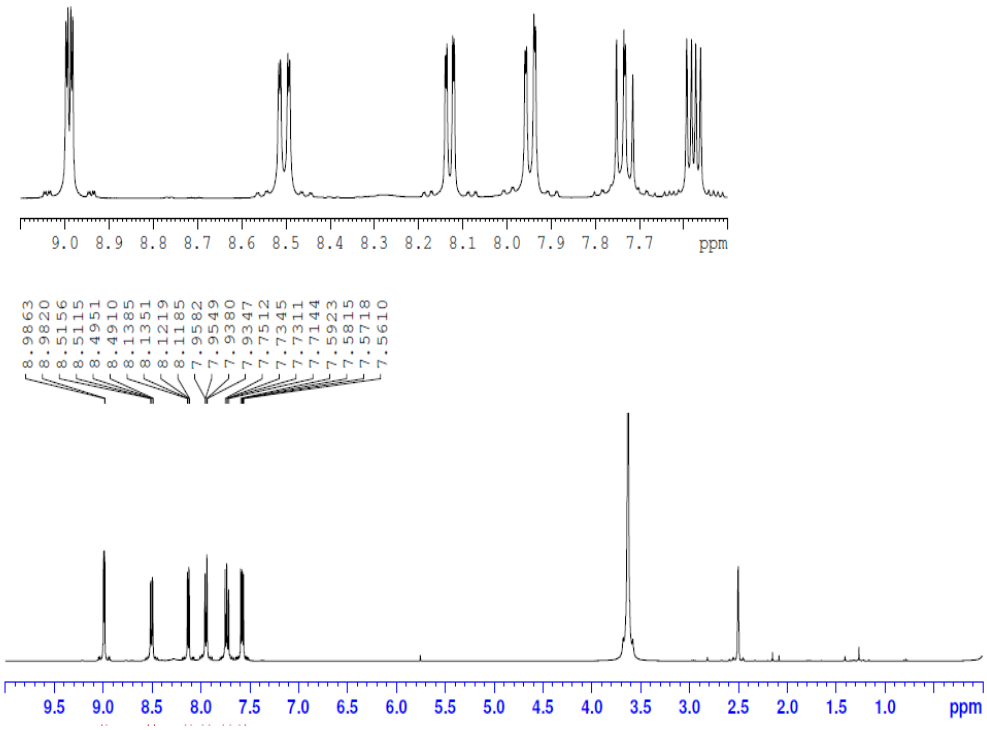


**Figure S6** $^{1}$H of bis (8-quinolyl)mercury (II) (bent (**3**) and linear (**4**)).

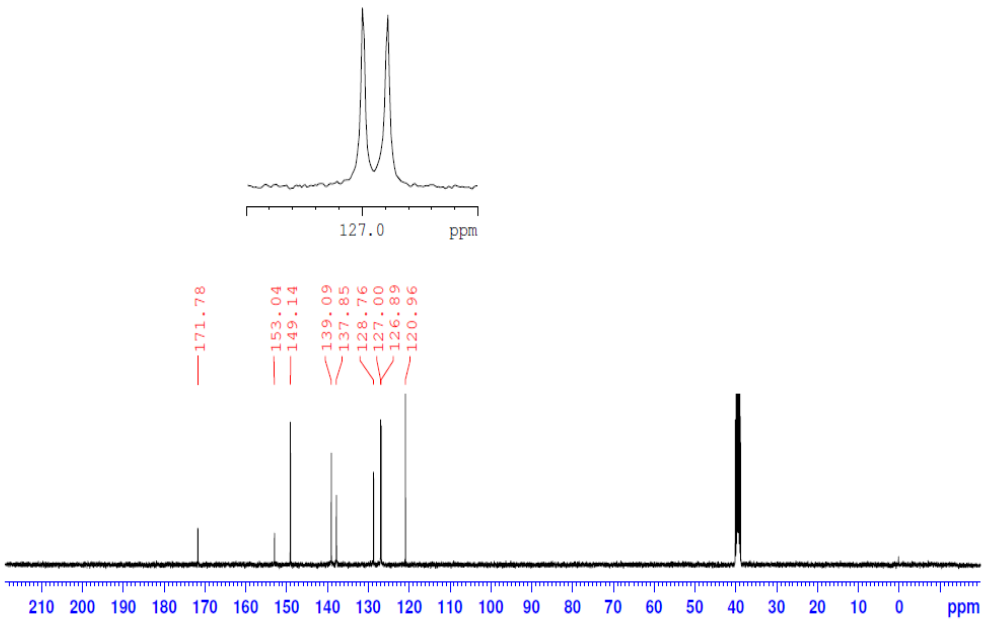
127.0
ppm
171.78
153.04
149.14
139.09
137.85
128.76
127.00
126.89
120.96
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

**Figure S7** $^{13}C$ of bis(8-quinolyl)mercury (II) (bent (**3**) and linear (**4**)).

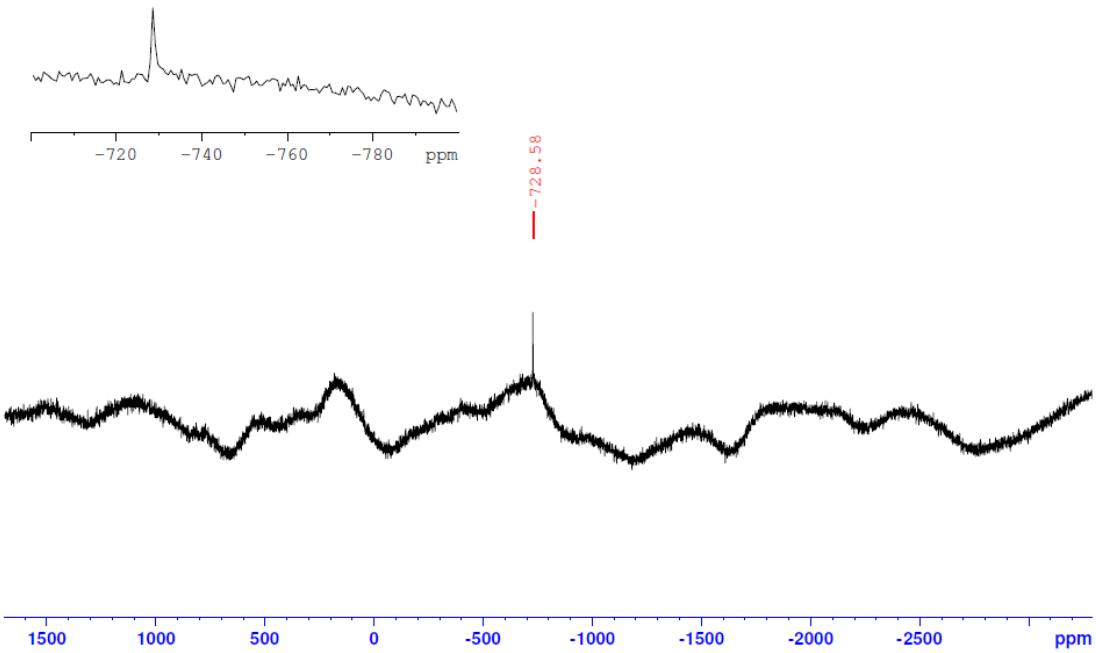


**Figure S8** $^{199}Hg$ of bis(quinolyl)mercury (II) (bent (**3**) and linear (**4**)).

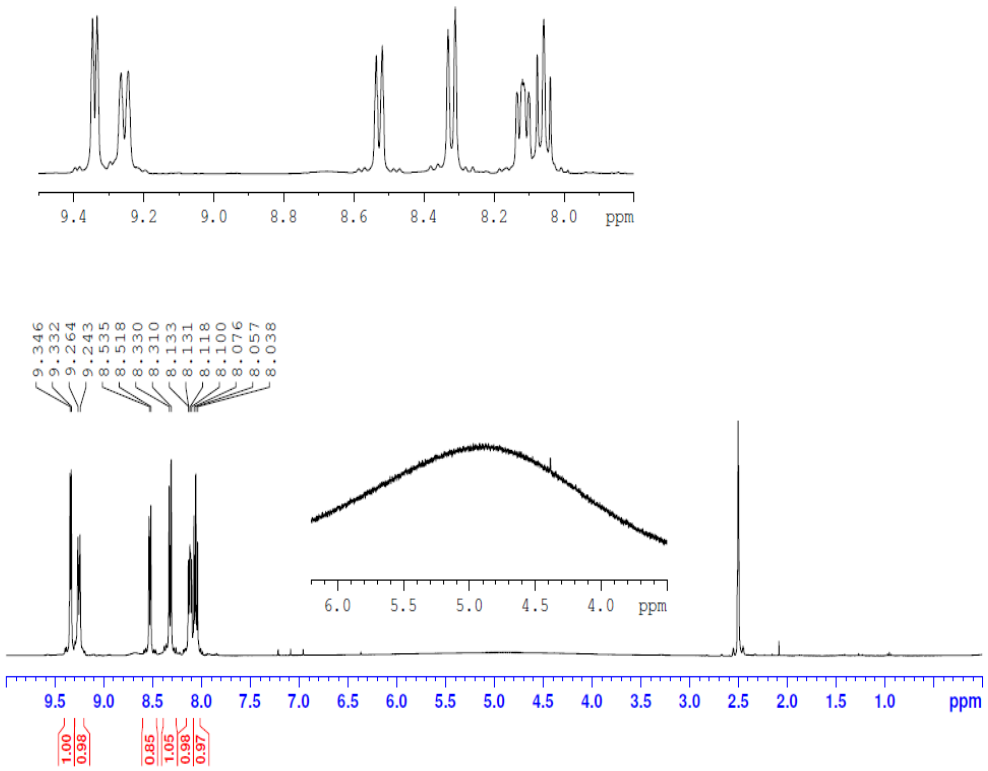


**Figure S9** $^{1}H$ of bis(8-quinolyl)mercury (II)[ $SCN]^{-}_{2}$ (**5**).

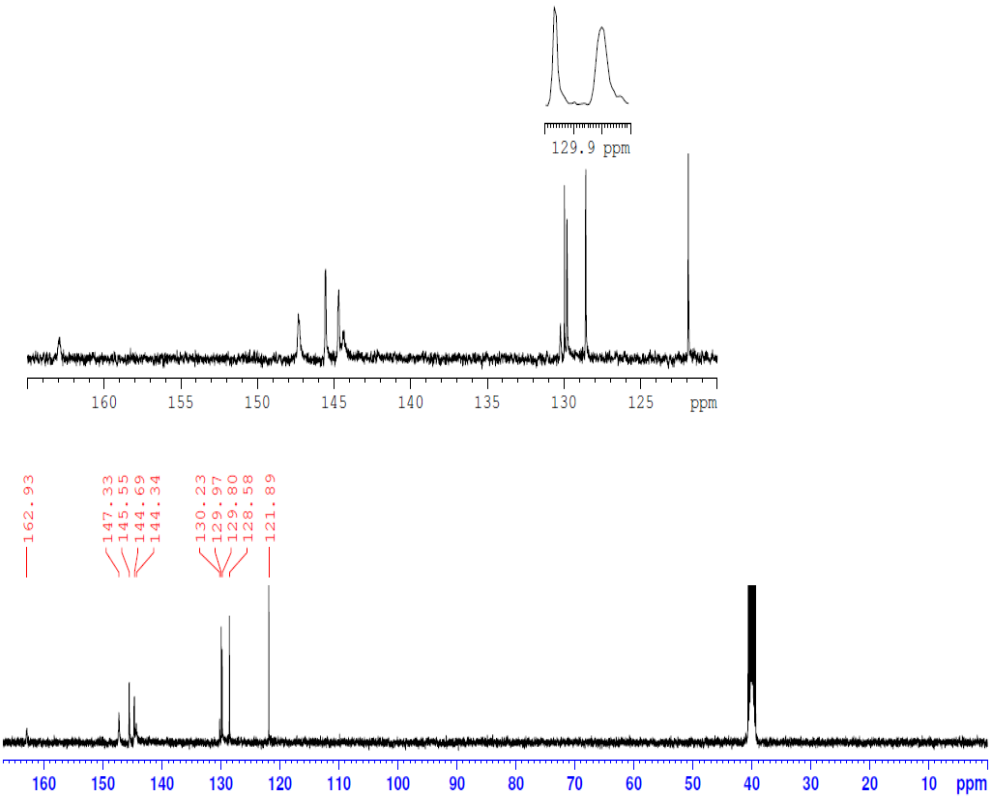


**Figure S10** $^{13}C$ of bis(8-quinolyl)mercury (II)[ $SCN]^{-}_{2}$ (**5**).

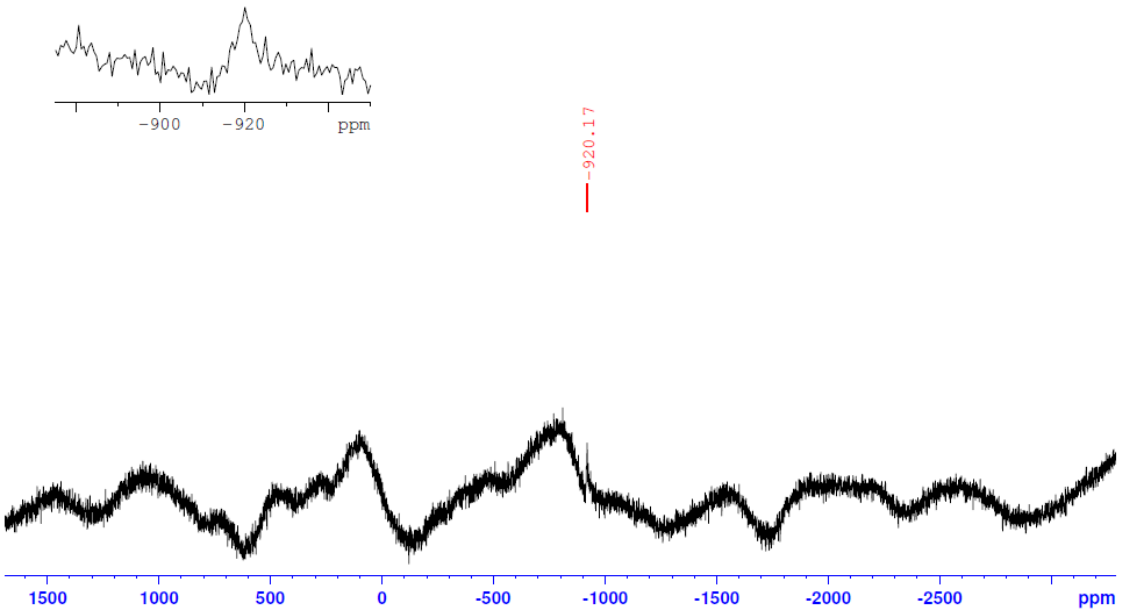


**Figure S11** $^{199}$Hg of bis(8-quinolyl)mercury (II)$[SCN]^-_2$ (**5**).

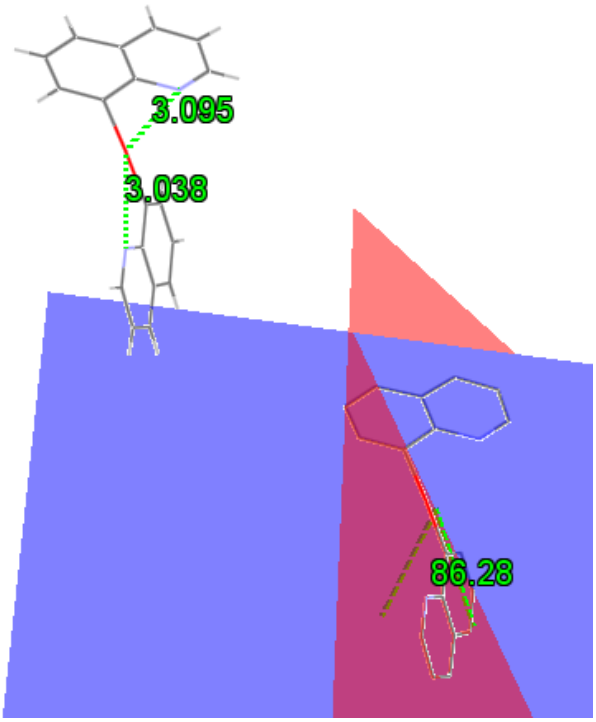


**Figure S12** Dihedral angel between the two quinolyl planes in (**3**).

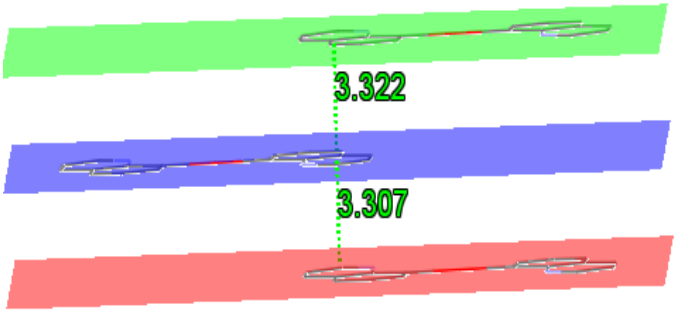

**Figure S13** Intermolecular π-π interaction between the planes in (**5**).

**Table 1** Crystallographic data for 2-5**.**

| | 2 | 3 | 4 | 5 |
|---|---|---|---|---|
| Formula | $C_9H_6NHgCl$ | $C_{18}H_{12}N_2Hg$ | $C_{18}H_{12}N_2Hg$ | $[C_{18}H_{14}N_2Hg]\cdot[SCN]_2$ |
| Formula Wt. | 364.19 | 456.89 | 456.89 | 575.06 |
| Cryst. Syst. | Monoclinic | Monoclinic | Monoclinic | Triclinic |
| space group | P 21/c | P 21/c | C2 | P-1 |
| *a*(Å) | 10.133(5) | 4.7776(3) | 14.1731(17) | 6.860(3) |
| *b*(Å) | 4.048(5) | 11.4357(9) | 6.2064(8) | 8.202(4) |
| *C*(Å) | 21.799(5) | 25.3031(2) | 10.469(19) | 9.116(4) |
| $\alpha$ | 90 | 90 | 90 | 107.127(5) |
| $\beta$ | 91.253(5) | 90.326 | 131 | 110.701(5) |
| $\gamma$ | 90 | 90 | 90 | 94.266(5) |
| V ($Å^3$) | 893.9(12) | 1382.4(2) | 694.89 | 449.2(4) |
| Z | 4 | 4 | 2 | 1 |
| T(K) | 100(2) | 100(2) | 100(2) | 100 |
| D ($g/cm^3$) | 2.706 | 2.195 | 2.184 | 2.126 |
| R(Int) | 0.0254 | 0.0473 | 0.0198 | 0.0423 |
| $\mu(mm^{-1})$ | 17.453 | 11.127 | 11.068 | 8.811 |
| F(000) | 656 | 856 | 428 | 274 |
| θ range | 2.72-25.42 | 2.40-28.35 | 2.58-25.37 | 2.53-25.23 |
| Index ranges | ±12, ±4, ±26 | ±6, ±14,±32 | ±16, ±7, ±12 | ±8, ±9, ±10 |
| Reflections collected | 8065 | 16608 | 3449 | 4152 |
| Independent reflections | 1402 | 2769 | 1279 | 1529 |
| Observed reflections | 1612 | 3458 | 1279 | 1529 |
| Data/ restr./ param. | 1612/0/109 | 3458/0/190 | 1279/3/97 | 1529/1/128 |
| Min/Max trans. | 0.049, 0.175 | 0.408, 0.573 | 0.276, 0.408 | 0.020, 0.071 |
| R(>2σ) | 0.0255 | 0.0246 | 0.018 | 0.0495 |
| $R_w$ | 0.065 | 0.0472 | 0.0461 | 0.1298 |
| GOOF | 1.059 | 1.016 | 1.087 | 1.094 |