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# SUPPORTING INFORMATION

**Title:**
**Author(s):**
**Ref. No.:** I

## Preparations of Schiff Bases

**Compound 1b:** A mixture of *p*-nitrobenzaldehyde (75.6 mg, 0.50 mmol) and *p*-(hexadecyloxy)aniline (167 mg, 0.50 mmol) in absolute ethanol (1 mL) as solvent was heated to reflux and stirred for 2 h. The Schiff base **1b** that separated on cooling at 0 °C was filtered off and washed with cold ethanol. The crude product was purified by recrystallization from ethanol to give an analytically pure compound in 95% yield (222 mg). IR (KBr): ν(CH=N) = 1626 cm$^{-1}$. $^1$H NMR ($CDCl_3$): δ = 0.87 (m, 3H, Me), 1.25–1.46 (m, 26H, $(CH_2)_{13}$), 1.80 (qnt, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2CH_2$), 3.98 (t, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2$), 6.94 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_4$), 7.29 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_3$), 8.04 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_2$), 8.30 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_1$) and 8.57 (s, 1H, CH=N) ppm. $^{13}$C NMR ($CDCl_3$): δ = 14.24, 22.79, 26.12, 29.34, 29.44, 29.48, 29.66, 29.68, 29.74, 29.77, 32.00, 68.34 ($C_{16}H_{33}$), 115.01, 122.52, 123.90, 128.95, 141.88, 143.20, 148.83, 154.40 (Ar) and 158.73 (CH=N). FAB MS: *m/z* = 467 [M$^+$]. $C_{29}H_{42}N_2O_3$ (467): calcd. C 74.64, H 9.07, N 6.00; found C 74.52, H 8.98, N 5.88.

**Compound 2a:** 9-Anthraldehyde (103 mg, 0.50 mmol) and *p*-anisidine (61.5 mg, 0.50 mmol) were combined in ethanol (1 mL) and the mixture was then refluxed for 2 h. After cooling, the title compound was filtered and a pure sample of **2a** can be obtained upon recrystallization from ethanol with an isolated yield of 93% (145 mg). IR (KBr): ν(CH=N) = 1625 cm$^{-1}$. $^1$H NMR ($CDCl_3$): δ = 3.88 (s, 3H, Me), 7.04 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_{11}$), 7.45 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_{10}$), 7.49–7.59 (m, 4H, $H_{2,3,6,7}$), 8.03 (d, $J_{HH}$ = 7.8 Hz, 2H, $H_{4,5}$), 8.52 (s, 1H, CH=N), 8.72 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_{1,8}$) and 9.67 (s, 1H, $H_9$) ppm. $^{13}$C NMR ($CDCl_3$): δ = 55.58 (Me), 114.41, 122.22, 124.70, 125.21, 126.94, 127.54, 128.85, 130.13, 130.38, 131.19, 145.40, 157.56 (Ar) and 158.38 (CH=N) ppm. FAB MS: *m/z* = 312 [M$^+$]. $C_{22}H_{17}NO$ (312): calcd. C 84.86, H 5.50, N 4.50; found C 84.65, H 5.36, N 4.33.

**Compound 2b:** Similar as above, this compound was obtained from a mixture of 9-anthraldehyde (103 mg, 0.50 mmol) and *p*-(hexadecyloxy)aniline (167 mg, 0.50 mmol) in refluxing ethanol (1 mL). The yield is 92% (240 mg). IR (KBr): ν(CH=N) = 1624 cm$^{-1}$. $^1$H NMR ($CDCl_3$): δ = 0.87 (m, 3H, Me), 1.25–1.49 (m, 26H, $(CH_2)_{13}$), 1.82 (qnt, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2CH_2$), 4.02 (t, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2$), 7.02 (d, $J_{HH}$ = 7.8 Hz, 2H, $H_{11}$), 7.44 (d, $J_{HH}$ = 7.8 Hz, 2H, $H_{10}$), 7.47–7.58 (m, 4H, $H_{2,3,6,7}$), 8.04 (d, $J_{HH}$ = 8.4 Hz, 2H, $H_{4,5}$), 8.54 (s, 1H, CH=N), 8.70 (d, $J_{HH}$ = 8.1 Hz, 2H, $H_{1,8}$) and 9.69 (s, 1H, $H_9$) ppm. $^{13}$C NMR ($CDCl_3$): δ = 14.23, 22.78, 26.15, 29.40, 29.44, 29.51, 29.67, 29.69, 29.73, 29.78, 32.00, 68.39 ($C_{16}H_{33}$), 115.04, 122.22, 124.77, 125.25, 126.96, 127.66, 128.87, 130.10, 130.42, 131.25, 145.20, 157.40 (Ar) and 158.03 (CH=N) ppm. FAB MS: *m/z* = 522 [M$^+$]. $C_{37}H_{47}NO$ (522): calcd. C 85.17, H 9.08, N 2.68; found C 85.02, H 8.83, N 2.40.

**General Procedures for the Mercuration Reactions.** A mixture of the Schiff base (**1a**, **1b**, **2a** or **2b**, 0.40 mmol) and an equimolar amount of mercuric acetate was charged in a reaction flask containing MeOH and the mixture was stirred under reflux for 4 h. In a typical run, **2b** (208 mg, 0.40 mmol) and mercuric acetate (152 mg, 0.40 mmol) in MeOH (4 mL) were used. At the end of the reaction, the mixture was allowed to cool down to room temperature. A solution of LiCl (42.4 mg, 1.00 mmol) in hot MeOH was subsequently added dropwise and the resulting slurry mixture was further stirred for about 10 min. The precipitate was then filtered and recrystallized from a $CHCl_3$/hexane solvent mixture to give a yellow solid of the corresponding orthomercurated derivative in good yield.

**Compound 3b**: Yellow solid. Yield 56% (157 mg). IR (KBr): ν  CH=N) = 1622 cm$^{-1}$. $^1$H NMR ($CDCl_3$): δ = 0.87 (m, 3H, Me), 1.25–1.55 (m, 26H, $(CH_2)_{13}$), 1.80 (qnt, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2CH_2$), 3.99 (t, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2$), 6.93 (dd, $J_{HH}$ = 2.7, 8.9 Hz, 1H, $H_4$), 7.00 (d, $J_{HH}$ = 2.7 Hz, 1H, $H_5$), 7.47 (d, $J_{HH}$ = 8.9 Hz, 1H, $H_3$), 8.05 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_2$), 8.34 (d, $J_{HH}$ = 8.9 Hz, 2H, $H_1$) and 8.71 (s, 1H, CH=N) ppm. $^{13}$C NMR ($CDCl_3$): δ = 14.23, 22.78, 26.09, 29.26, 29.44, 29.45, 29.64, 29.68, 29.73, 29.77, 32.00, 68.60 ($C_{16}H_{33}$), 116.42, 117.15, 121.22, 124.10, 128.97, 141.18, 145.58, 148.99, 153.20, 154.23 (Ar) and 159.08 (CH=N) ppm. FAB MS: *m/z* = 701 [M$^+$]. $C_{29}H_{41}N_2ClHgO_3$ (701): calcd. C 49.64, H 5.89, N 3.99, found C 49.44, H 5.68, N 3.70.

**Compound 4a**: Yellow powder. Yield 92% (201 mg). IR (KBr): ν(CH=N) = 1623 cm$^{-1}$. $^1$H NMR (DMSO-$d_6$): δ = 3.81 (s, 3H, Me), 7.00 (dd, $J_{HH}$ = 2.4, 8.9 Hz, 1H, $H_{11}$), 7.31 (m, 1H, $H_{12}$), 7.56–7.68 (m, 4H, $H_{2,3,6,7}$), 7.77 (d, $J_{HH}$ = 8.9 Hz, 1H, $H_{10}$), 8.17 (d, $J_{HH}$ = 8.1 Hz, 2H, $H_{4,5}$), 8.77 (s, 1H, CH=N), 8.96 (d, $J_{HH}$ = 8.6 Hz, 2H, $H_{1,8}$) and 9.88 (s, 1H, $H_9$) ppm. FAB MS: *m/z* = 547 [M$^+$]. $C_{22}H_{16}NClHgO$ (547): calcd. C 48.36, H 2.95, N 2.56; found C 48.20, H 2.85, N 2.42.

**Compound 4b**: Yellow solid. Yield 72% (218 mg). IR (KBr): ν(CH=N) = 1625 cm$^{-1}$. $^1$H NMR ($CDCl_3$): δ = 0.89 (m, 3H, Me), 1.28  1.49 (m, 26H, $(CH_2)_{13}$), 1.80 (qnt, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2CH_2$), 3.95 (t, $J_{HH}$ = 6.5 Hz, 2H, $OCH_2$), 6.89  6.92 (m, 2H, $H_{11,12}$), 7.41–7.57 (m, 5H, $H_{2,3,6,7,10}$), 7.99 (d, $J_{HH}$ = 8.1 Hz, 2H, $H_{4,5}$), 8.46 (s, 1H, CH=N), 8.72 (d, $J_{HH}$ = 8.6 Hz, 2H, $H_{1,8}$) and 9.69 (s, 1H, $H_9$) ppm. $^{13}$C NMR ($CDCl_3$): δ = 14.23, 22.77, 23.24, 26.11, 29.33, 29.44, 29.51, 29.68, 29.71, 29.73, 29.78, 31.99, 68.48 ($C_{16}H_{33}$), 116.39, 117.04, 121.42, 124.65, 125.25, 126.49, 127.13, 128.95, 130.56, 130.67, 131.13, 148.08, 156.54, 157.85 (Ar) and 176.95 (CH=N) ppm. MS (FAB): *m/z* = 757 [M$^+$]. $C_{37}H_{46}NClHgO$ (757): calcd. C 58.72, H 6.13, N 1.85; found C 58.65, H 5.99, N 1.60.

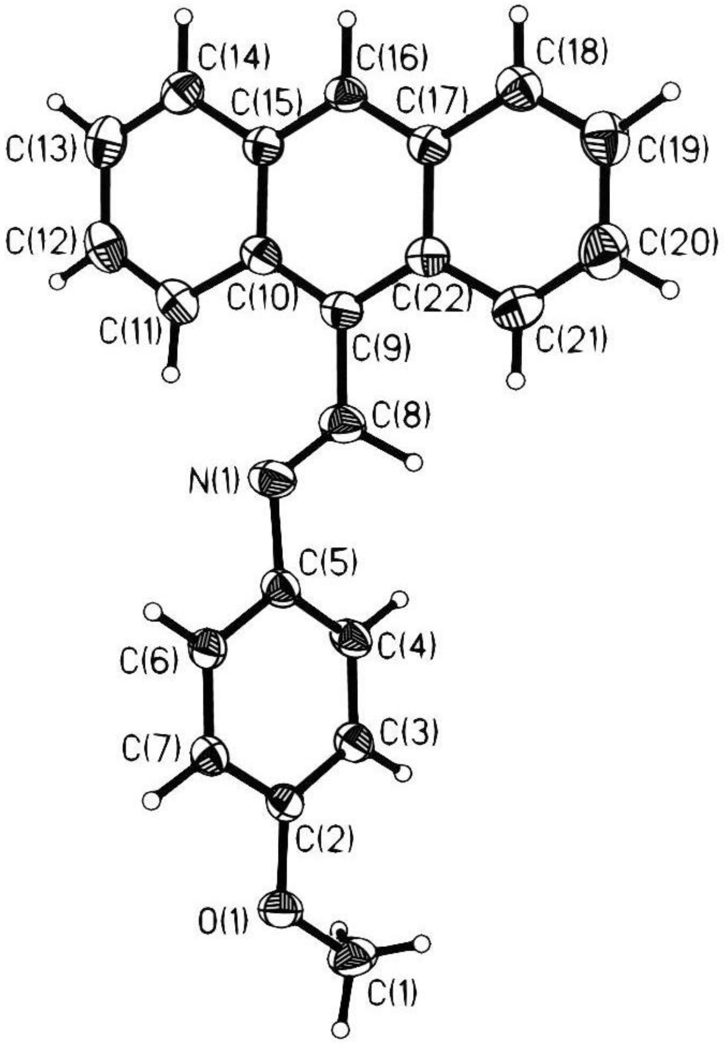

Figure S1  Perspective view of one molecule of **2a**, with thermal ellipsoids shown at the 25% probability level.

Table 1. Crystal data and structure refinement for **2a**

| | |
|---|---|
| Identification code | wy0061wm |
| Empirical formula | $C_{22}H_{17}NO$ |
| Formula weight | 311.37 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Triclinic |
| Space group | $P\bar{1}$ |
| Unit cell dimensions | $a$ = 9.3972(6) Å alpha = 88.6270(10)°<br>$b$ = 10.6793(7) Å beta = 75.5300(10)°<br>$c$ = 17.0900(11) Å gamma = 85.5900(10)° |
| Volume, Z | 1655.73(19) $Å^3$, 4 |
| Density (calculated) | 1.249 $Mg/m^3$ |
| Absorption coefficient | 0.076 $mm^{-1}$ |
| F(000) | 656 |
| Crystal size | 0.36 x 0.28 x 0.21 mm |
| θ range for data collection | 1.91 to 27.52° |
| Limiting indices | $-10 \le h \le 11$, $-13 \le k \le 13$, $-22 \le l \le 18$ |
| Reflections collected | 9773 |
| Independent reflections | 7075 ($R_{int}$ = 0.0119) |
| Completeness to θ = 27.52° | 92.8 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7075 / 0 / 569 |
| Goodness-of-fit on $F^2$ | 1.050 |
| Final R indices [$I>2\sigma(I)$] | R1 = 0.0446, wR2 = 0.1375 |
| R indices (all data) | R1 = 0.0643, wR2 = 0.1542 |
| Largest diff. peak and hole | 0.312 and -0.200 $eÅ^{-3}$ |