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SUPPORTING INFORMATION

Molecular Architecture 2.[1] Synthesis and Metal Complexation of Heptacyclic Terpyridyl Molecular Clefts.

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Peak assignments for ^1H NMR spectra:

8-Butyltricyclo[7.3.1.0^{2,7}]tridec-2(7)-en-13-one (8). ^{1}H NMR (80 MHz, $CDCl_3$) δ 2.5 (m, 1 H, C=C-CHC=O), 1.9 - 2.3 (m, 6 H, other CH, allylic CH_2), 1.1 - 1.9 (m, 16 H, other CH_2), 0.89 (t, J = 6, 3 H, CH_3).

9-Butyl-2,3,5,6,7,8-hexahydroacridin-4(1H)-one (13). ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.01 (m, 2 H, H3), 2.92 (t, J = 6 Hz, 2 H, H5), 2.75 (m, 4 H, H1,8), 2.61 (t, J = 6 Hz, 2 H, CH_2-Pr), 2.15 (m, 2 H, H2), 1.85 (m, 4 H, H6,7), 1.45 (m, 4 H, CH_2CH_2Me), 0.98 (t, J = 7 Hz, 3 H, CH_3).

9-Butyl-3-hydroxymethylene-2,3,5,6,7,8-hexahydroacridin-4(1H)-one (16). ^{1}H NMR (80 MHz, $CDCl_3$) δ 9.85 (bs, 1 H, C=CH), 2.5-3.0 (m, 10 H, H1,2,5,8, CH_2-Pr), 1.7 - 1.9 (m, 4 H, H6,7), 1.3 - 1.5 (m, 4 H, CH_2CH_2Me), 0.97 (t, J = 6 Hz, 3 H, CH_3).

5,11-Dibutyl-1,2,3,4,6,7,9,10,12,13,14,15-dodecahydroacridino[4,3-b]benzo[j]-[1,10]phenanthroline (20). ^{1}H NMR (80 MHz, $CDCl_3$) δ 7.70 (s, 1 H, C=CH), 3.10 (s, 6 H, NCH_3), 2.5 - 3.4 (m, 10 H, H1,2,5,8, CH_2-Pr), 1.7 -1.9 (m, 4 H, H6,7), 1.3 - 1.5 (m, 4 H, CH_2CH_2Me), 0.96 (t, J = 6 Hz, 3 H, CH_3).

5-Benzylidene-9-butyl-1,2,3,4,5,6,7,8-octahydroacridin-4-ol hydrobromide (22•HBr). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.52 (s, 1 H, C=CH), 7.36 - 7.62 (m, 5 H, ArH), 6.29 (d, J = 5 Hz, 1 H, OH), 5.56 (m, 1 H, C*H*OH), 2.71 - 2.95 (m, 8 H, H1,6,8, CH_2-Pr), 1.92 - 2.18 (m, 6 H, H2,3,6), 1.46 - 1.49 (m, 4 H, CH_2CH_2Me), 1.01 (t, J = 7 Hz, 3 H, CH_3).

5-Benzylidene-9-butyl-1,2,3,4,5,6,7,8-octahydroacridin-4-ol (22). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (s, 1 H, C=CH), 7.35 - 7.43 (m, 4 H, *o,m*-ArH), 7.31 (t, J = 6 Hz, 1 H, *p*-ArH), 4.66 (dd, J = 5, 9 Hz, 1 H, H4), 4.59 (s, 1 H, OH), 2.74 - 2.89 (m, 6 H, H1,6,8), 2.55 (m, 2 H, CH_2Pr), 2.35 (m, 1 H, H3), 2.06 (m, 1 H, H3′), 1.80-1.87 (m, 4 H, H2,7), 1.43 (m, 4 H, CH_2CH_2Me), 0.98 (t, J = 6 Hz, 3 H, CH_3).

5-Benzylidene-9-butyl-2,3,5,6,7,8-hexahydroacridin-4(1H)-one (23). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 (s, 1 H, C=CH), 7.31-7.39 (m, 4 H, *o,m*-ArH), 7.23 (t, J = 7 Hz, 1 H, *p*-ArH), 2.97 (t, J = 6.2 Hz, 2 H, H3), 2.82-2.88 (m, 4 H, H1,8), 2.76 (t, J = 6.3 Hz, 2 H, H6), 2.66 (m, 2 H, CH_2-Pr), 2.16 (m, 2 H, H2), 1.84 (m, 2 H, H7), 1.45 (m, 4 H, CH_2CH_2Me), 0.98 (t, J = 7 Hz, 3 H, CH_3).

5-Benzylidene-9-butyl-3-(N,N-dimethylaminomethyl)-2,3,5,6,7,8-hexahydroacridin-4(1H)-one hydrochloride (27•HCl). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (s, 1 H, C=CH), 7.3-7.4 (m, 4 H, *o,m*-ArH), 7.17 (t, J = 6.3, *p*-ArH), 3.81 (dd, J = 5, 13 Hz, 1 H, CH_2NMe_2), 3.27 (dd, J = 5, 10 Hz, 1 H, H3), 3.03-3.13 (m, 3 H, H1, CH_2NMe_2), 2.87 (s, 6 H, NCH_3), 2.52-2.63 (m, 4 H, H8, CH_2-Pr), 1.94 (m, 2 H, H2), 1.77 (m, 2 H, H7), 1.36 (m, 4 H, CH_2CH_2Me), 0.90 (t, J = 6 Hz, 3 H, CCH_3).

5-Benzylidene-9-butyl-3-(*N,N*-dimethylaminomethyl)-2,3,5,6,7,8-hexahydroacridin-4(1H)-one (27). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (s, 1 H, C=CH), 7.20-7.43 (m, 5 H, ArH), 3.07 (m, 1 H, CH_2NMe_2), 2.93 (m, 1 H, CH_2NMe_2), 2.86 (m, 4 H, H1,6), 2.80 (m, 1 H, H3), 2.78 (m, 2 H, H8), 2.65 (t, J = 6 Hz, 2 H, H10), 2.44 (m, 1 H, H2), 2.28 (s, 6 H, NCH_3), 1.96 (m, 1 H, H2′), 1.84 (m, 2 H, H7), 1.46 (m, 4 H, CH_2CH_2Me), 0.98 (t, J = 6 Hz, 3 H, CCH_3).

5-Benzylidene-9-butyl-3-methylene-2,3,5,6,7,8-hexahydroacridin-4(1H)-one (29). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (s, 1 H, C=CHPh), 7.33-7.44 (m, 4 H, *o,m*-ArH), 7.24 (t, J = 6 Hz, 1 H, *p*-ArH), 6.28 (s, 1 H, (**Z**)-HC=CCO), 5.48 (s, 1 H, (**E**)-HC=CO), 3.00 (t, J = 6 Hz, 2 H, H1), 2.88 (m, 6 H, H2,6,8), 2.67 (m, 2 H, CH_2Pr), 1.86 (m, 2 H, H7), 1.46 (m, 4 H, CH_2CH_2Me), 0.99 (t, J = 7 Hz, 3 H, CH_3).

1,15-Dibenzylidene-5,11-dibutyl-1,2,3,4,6,7,9,10,12,13,14,15-dodecahydroacridino[4,3-b]benzo[j][1,10]phenanthroline (26). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 (s, 2 H, C=CH), 7.41 (s, 1 H, H8), 7.24 (m, 4 H, *m*-ArH), 7.11 (m, 6 H, *o,p*-ArH), 2.94 (s, 8 H, H6,7,8,10), 2.78-2.86 (m, 8 H, H2,4,12,14), 2.67 (t, J = 6 Hz, 4 H, CH_2Pr), 1.83 (quin, J = 6 Hz, 4 H, H3,13), 1.45 (m, 8 H, CH_2CH_2Me), 0.97 (t, J = 6 Hz, 6 H, CH_3).

1,11-Dibenzylidene-5,15-dibutyl-1,2,3,4,6,7,11,12,13,14,16,17-dodecahydroacridino[3,4-c]benzo[j][1,10]phenanthroline (33). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1 H, C=CH), 8.21 (s, 1 H, C=CH), 8.04 (s, 1 H, H8), 7.21-7.45 (m, 10 H, ArH), 3.79 (t, J = 6 Hz, 2 H, H17), 2.88-2.92 (m, 14 H, H2,4,6,7,12,14,16), 2.70-2.72 (m, 4 H, CH_2-Pr), 1.84-1.97 (m, 4 H, H3,13), 1.47-1.49 (m, 8 H, CH_2CH_2Me), 0.96-1.00 (m, 6 H, CH_3).

3,4-(5-Benzylidene-9-butyl-1,2,5,6,7,8-hexahydroacridino[4,3-c])-8,9-(8-benzylidene-4-butyl-5,6,7,8-tetrahydroquino[8,9-f])-2-oxaspiro[5.5]undecane-3,8-dien-7-one (31). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 1H, C=CHPh), 7.71 (s, 1 H, C=CHPh′), 7.2-7.4 (m, 10 H, ArH), 3.55 (m, 1 H, OCH), 2.0-3.0 (m, 23H, OCH′, $ArCH_2$, CH_2C=C, CH_2CC=O), 1.80 (m, 4 H, CH_2CC=C), 1.31-1.41 (m, 8 H, CH_2CH_2Me), 0.94 (m, 6 H, CH_3).

5,11-Dibutyl-2,3,4,6,7,9,10,12,13,14-decahydroacridino[4,3-b]benzo[j][1,10]phenanthroline-1,15-dione (6). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 (s, 1 H, H8), 4.46 (s, 2 H, H_2O), 2.95-3.03 (m, 12 H, H2,6,7,9,10,14), 2.76 (m, 8 H, H4,12, CH_2Pr), 2.19 (m, 4 H, H3,13), 1.47 (m, 8 H, CH_2CH_2Me), 0.98 (t, J = 7 Hz, 6 H, CH_3).

6•Na(picrate). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.41 (s, 2 H, picrate), 7.43 (s, 1 H, H8), 3.0-3.15 (m, 12 H, H2,6,7,9,10,14), 2.8-2.9 (m, 4 H, H4,12), 2.75 (m, 4 H, CH_2Pr), 2.28 (m, 4 H, H3,13), 1.45-1.60 (m, 8 H, CH_2CH_2Me), 1.03 (t, J = 7 Hz, 6 H, CH_3).

6•K(picrate). ^{1}H NMR (300 MHz $CDCl_3$) δ 8.46 (s, 2 H, picrate), 7.44 (s, 1 H, H8), 7.36 (s, 2 H, benzene), 2.9-3.1 (m, 12 H, H2,6,7,9,10,14), 2.82 (t, J = 6 Hz, 4 H, H4,12), 2.73 (m, 4 H, CH_2Pr), 2.25 (m, 4 H, H3,13), 1.45-1.60 (m, 8 H, CH_2CH_2Me), 1.02 (t, J = 7 Hz, 6 H, CH_3).

$(6)_2Ca(CF_3SO_3)_2$. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 (s, 1 H, H8), 3.26 (s, 8 H, H6,7,9,10), 2.80-2.95 (m, 8 H, H4,12, CH_2Pr), 2.13 (t, J = 6 Hz, 4 H, H2,14), 1.72 (m, 4 H, H3,13), 1.4-1.6 (m, 8 H, CH_2CH_2Me), 1.01 (t, J = 7 Hz, 6 H, CH_3).

2,6-Bis(3-dimethylaminopropenoyl)pyridine (36). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (d, J = 7.5 Hz, 2 H, H3,5), 7.92 (d, J = 12 Hz, 2 H, $CHNMe_2$), 7.89 (t, J = 7.5 Hz, 1 H, H4), 6.61 (d, J = 12 Hz, 2 H, CHC=O), 3.18 (s, 6 H, CH_3), 2.99 (s, 6 H, CH_3).

2,6-Bis(5,6,7,8-tetrahydroquinol-2-yl)pyridine (37). ^{1}H NMR (300 MHz, $CDCl_3$) 8.37 (d, J = 8 Hz, 2 H, quin-H3), 8.31 (d, J = 8 Hz, 2 H, quin-H4), 7.85 (t, J = 8 Hz, 1 H, py-H4), 7.49 (d, J = 8 Hz, 2 H, py-H3,5), 3.01 (t, J = 6 Hz, 4 H, quin-H8), 2.83 (t, J = 6 Hz, 4 H, quin-H5), 1.79-1.98 (m, 8 H, quin-H6,7).