Supporting Information

MS Title: Reaction modes and mechanism in indolizine photooxygenation reactions Author: Yun Li, Hua-You Hu, Jian-Ping Ye, Hoong-Kun Fun, Hong-Wen Hu, Jian-Hua Xu*

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1. General Experimental Conditions

Melting points were measured on a Yanaco microscopic melting point apparatus and uncorrected. ¹HNMR spectra were recorded on a Bruker spectrometer at 300MHz with CDCl₃ or d_6 -DMSO as solvent and internal standard. *J*-Values are give in Hz. IR spectra were taken with a Shimadzu IR 440 spectrometer in KBr pellets. Mass spectra were recorded with a VG ZAB-HS spectrometer. Elemental analyses were obtained using a Perken-Elmer 240 C analyzer. Fluorescence and phosphorescence spectra were recorded on a HITACHI F-4500 Fluorescence Spectrophotometer. Acetonitrile (AR grade) was distilled from Phosphorus pentoxide, methanol was treated by magnesium and distilled before use. Other reagents were CP or AR grade and were used as received without further purification. Petroleum ether refers to the fraction with boiling point in the range 60-90 °C.

2. Crystallgraphic structure of 2a, 3a, 3b, 5a, 6d and 9f



3b



Crystal Structures of compounds **3a** (*Acta Cryst.* (2002). E**58**, 790), **5a** (*Acta Cryst.* (2002). E**58**, 1400), **6d** (*Acta Cryst.* (2002). E**58**, 1060) and **9f** (*Acta Cryst.* (2002). E**58**,1427) have been published.

3. Analytical and spectroscopic data for all compounds 2-9 (a-f)

E-3-Benzoyl-3-(6-methyl-2-pyridinyl)-2-phenylacrylic acid methyl ester (2a). Colorless crystals from petroleum ether – ethyl acetate, mp 86-88 °C; IR (KBr) 3090, 2980, 1721, 1666, 1580, 1492, 1449, 1299,1244, 1209, 1161, 946, 786, 738, 696; ¹H NMR (300 MHz, CDCl₃) δ 2.61 (s, 3H, Me), 3.83 (s, 3H, OMe), 7.11 (d, *J* = 7.7 Hz, 1H), 7.16- 7.39 (m, 8H, ArH), 7.45 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 2H); MS *m/z* 357 (M⁺, 5.68), 342 (8.27), 325 (67.81), 296 (12.46), 270 (35.86), 105 (base), 66 (60.67). Anal. Calcd for C₂₃H₁₉NO₃: C, 77.31; H, 5.32; N, 3.92. Found: C, 77.29; H, 5.35; N, 3.98.

Z-3-Benzoyl-3-(6-methyl-2-pyridinyl)-2-phenylacrylic acid methyl ester (3a). Colorless crystals from petroleum ether – ethyl acetate, mp 138-140 °C; IR (KBr) 3050, 2952, 1720, 1684, 1584, 1455, 1319, 1230, 1101, 1021, 789, 762, 700; ¹H NMR (300 MHz, CDCl₃) δ 2.62 (s, 3H, Me), 3.51 (s, 3H, OMe), 7.22-7.61 (m, 10H, ArH), 7.78 (br, 1H), 8.34 (d, *J* = 6.7 Hz, 2H); MS *m/z* 357 (M⁺,15.62), 342 (21.17), 329 (40.81), 328 (37.38), 325 (21.10), 313 (20.68), 298 (20.71), 296 (22.34), 270 (92.87), 105 (base), 77 (85.67). Anal. Calcd for C₂₃H₁₉NO₃: C, 77.31; H, 5.32; N, 3.92. Found: C, 77.29; H, 5.36; N, 3.95.

Dihydro-3,5-diphenyl-4-(6-methyl-2-pyridinyl)-5-hydroxyfuran-2-one (4a). Colorless crystals from petroleum ether – ethyl acetate, mp 148-150 °C; IR (KBr) 3054, 2745, 2575, 1745, 1589, 1570, 1492, 1448, 1384, 1267, 1200, 1088, 975, 918, 810, 787, 746, 722, 701; ¹H NMR (300 MHz, CDCl₃) δ 2.56 (s, 3H, Me), 6.99 (d, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 7.8 Hz, 1H), 7.29-7.55 (m, 11H), 7.99 (br, 1H); MS *m*/*z* 343 (M⁺, 15.62), 342 (21.17), 329 (40.81), 328 (37.48), 325 (21.10), 313 (20.68), 298 (20.71), 296 (22.34), 270 (92.87), 105 (base), 77 (85.67). Anal. Calcd for C₂₂H₁₇NO₃: C, 76.96; H, 4.96; N, 4.08. Found: C, 76.91; H, 4.98; N, 4,11.

1-(6-Methyl-2-pyridinyl)-2-phenylthanedione (5a). Colorless crystals from petroleum ether – ethyl acetate, mp 80-82 °C; IR KBr) 3069, 1699, 1589, 1477, 1317, 1216, 987, 930, 847, 757, 684; ¹H NMR (300 MHz, CDCl₃) δ 2.5 (s, 3H, Me) , 7.37 (d, J = 7.7, 1H), 7.51 (t, J = 7.7 Hz, 2H), 7.63 (td, J = 7.4, 1.1 Hz, 1H), 7.81 (t, J = 7.7 Hz, 1H), 7.94 (d, J = 8.3 Hz, 2H), 8.01 (d, J = 7.5 Hz, 1H); MS *m/z* 225 (M⁺,10.93), 196 (30.39), 169 (19.17), 105 (base), 92 (25.51), 77 (58.29). Anal. Calcd for C₁₄H₁₁NO₂: C, 74.65; H, 4.89; N, 6.22. Found: C, 74.62; H, 4.91; N, 6.15.

3-Benzoyl-3-(6-methyl-2-pyridinyl)-2-phenyl-2-oxiranecaboxaldehyde (6a). White crystals from ether, mp130-132°C (dec.). This compound decomposes slowly on silica gel column at room temperature or when crystallized from ethyl acetate. It was separated by thin layer chromatography on silica gel plates at temperatures below 5 °C. IR (KBr) 3062, 2968, 2926, 1726, 1689, 1594, 1576, 1450, 1252, 1210, 1180, 1096, 1027, 799, 768, 696; ¹H NMR (300 MHz, CDCl₃) δ 2.59 (s, 3H, Me), 7.13 (d, *J* = 7.8 Hz, 1H), 7.16-7.58 (m, 10H), 7.91 (dd, *J* = 1.3, 8.3 Hz, 2H), 9.70 (s, 1H, CHO), MS *m/z* 315 (M⁺ 28, 15.75), 314 (M⁺ CHO, 63.28), 270 (9.75), 238

(12.43), 223 (7.75), 106 (7.69), 105 (base), 92 (19.44), 77 (63.21). Anal. Calcd for $C_{22}H_{17}NO_3$: C,

77.0; H, 4.96; N, 4.08. Found: C, 76.9; H, 4.94; N, 4.10.

E-3-(4-Methoxybenzoyl)-3-(6-methyl-2-pyridinyl)-2-phenylacrylic acid methyl ester (2b). White crystals from petroleum ether – ethyl acetate, mp 118-120 °C (dec); IR (KBr) 2949, 2840, 1724, 1665, 1594, 1509, 1447, 1424, 1318, 1247, 1161, 1024, 952, 921, 849, 806, 745, 705; ¹H NMR (300 MHz, CDCl₃) δ 2.66 (s, 3H, Me), 3.80 (s, 3H, OMe), 3.81 (s, 3H, OMe), 6.80 (d, *J* = 8.8 Hz, 2H), 7.18-7.41 (m, 7H, ArH), 7.59 (br, 1H), 7.95 (d, *J* = 6.9 Hz, 2H); MS *m/z* 387 (M⁺, 3.58), 372 (9.30), 358 (25.87), 344 (26.12), 328 (14.32), 326 (20.10), 300 (63.71), 135 (base), 107 (21.48), 92 (47.19), 77 (58.91). Anal. Calcd for C₂₄H₂₁NO₄: C, 74.42; H, 5.43; N, 3.62. Found: C, 74.41; H, 5.46; N, 3.65.

Z-3-(4-Methoxybenzoyl)-3-(6-methyl-2-pyridinyl)-2-phenylacrylic acid methyl ester (3b). White crystals from petroleum ether – ethyl acetate, mp 140-142 °C (dec); IR (KBr) 3015, 2951, 1708, 1668, 1597, 1509, 1447, 1320, 1251,1162, 1016, 795, 775, 758, 697; ¹H NMR (300 MHz, CDCl₃) δ 2.33 (s, 3H, Me), 3.58 (s, 3H, OMe), 3.86 (s, 3H, OMe), 6.86 (t, *J* = 6.6 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 7.20-7.32 (m, 6H), 8.05 (d, *J* = 8.8 Hz, 2H); MS *m/z* 387 (M⁺), 372 (9.30), 358 (18.33), 344 (13.28), 326 (12.22), 300 (52.59), 191 (11.29), 165 (11.42), 135 (base), 107 (22.18), 92 (50.20), 77 (62.15). Anal. Calcd for C₂₄H₂₁NO₄: C, 74.42; H, 5.43; N, 3.62. Found: C, 74.40; H, 5,42; N, 3.63.

3-(4-Methoxybenzoyl)-3-(6-methyl-2-pyridinyl)-2-phenylacrylic acid (4b) White crystals from petroleum ether – ethyl acetate, mp 118-120 °C; IR (KBr) 3385, 3100, 2955, 1755, 1610, 1519, 1456, 1307, 1255, 1176, 1034, 970, 845, 790, 742, 69; ¹H NMR (300 MHz, CDCl₃) δ 2.68 (s, 3H, Me), 3.79 (s, 3H, OMe), 6.84 (d, *J* = 8.8 Hz, 2H), 6.91 (d, *J* = 7.7 Hz, 2H), 7.35-7.47 (m, 7H), 7.63 (S, 1H); MS *m/z* 373 (M⁺, 2.68), 328 (22.24), 317 (29.91), 300 (base), 266 (25.77), 238 (85.79),

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194 (84.19), 193 (29.97), 165 (19.16), 152 (20.58), 135 (78.19), 92 (41.76), 77 (44.08). Anal. Calcd for C₂₃H₁₉NO₄: C, 73.99; H, 5.09; N, 3.75. Found: C, 73.95; H, 5.07; N, 3.72.

1-(6-Methyl-2-pyridinyl)-2-(4-methoxyphenyl)ethanedione (5b) White crystals from petroleum ether – ethyl acetate, mp 106 -108 °C; IR (KBr) 3080, 2938, 1693, 1658, 1603, 1573, 1510, 1459, 1425, 1265, 1218, 1172, 1030, 984, 914, 749; ¹H NMR (300 MHz, CDCl₃) δ 2.62 (s, 3H, Me), 3.91 (s, 3H, OMe), 6.98 (dt, *J* = 7.0, 2.3 Hz, 2H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.90 (t, *J* = 7.7 Hz, 1H), 7.96 (dt, *J* = 7.0, 2.3 Hz, 2H), 8.03 (d, *J* = 7.6 Hz, 1H); MS *m/z* 255 (M⁺, 9.22), 135 (base), 92 (14.04), 77 (12.11). Anal. Calcd for C₁₅H₁₃NO₃ : C, 70.60; H, 5.10; N, 5,49. Found: C, 70.58; H, 5.08; N, 5.46.

3-(4-Methoxybenzoyl)-3-(6-methyl-2-pyridinyl)-2-phenyl-2-oxiranecarboxaldehyde (6b) Acquired from silica gel column as oil, after dissolving the oil in etherand evaporation of the ether in vacuo, yellow solid was obtained, mp 184-186°C; IR (KBr) 3067, 2926, 2843, 1726, 1679, 1598, 1510, 1454, 1261, 1170, 1024, 847, 793, 753, 699; ¹H NMR (300 MHz, CDCl₃) δ 2.60 (S, 3H, Me), 3.81 (s, 3H, OMe), 6.80 (d, *J* = 8.8 Hz, 2H), 7.13 (d, *J* = 7.7 Hz, 1H), 7.20-7.22 (m, 3H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.53-7.62 (m, 3H), 7.93 (d, *J* = 8.8 Hz, 2H), 9.70 (s, 1H, CHO); MS *m/z* 373 (M⁺, 7.63), 344 (base), 300 (19.44), 253 (28.74), 135 (23.25), 105 (87.14), 92 (18.60), 77 (43.78). Anal. Calcd for C₂₃H₁₉NO₄: C, 73.99; H, 5.09; N, 3.75. Found: C, 73.95; H, 5.06; N, 3.73.

E-3-(6-Methyl-2-pyridinyl)-3-(4-nitrophenyl)-2-phenylacrylic acid methyl ester (2c). Not fully separated from 3c. ¹H NMR (300 MHz, CDCl₃) δ2.57 (s, 3H, Me), 3.82 (s, 3H, OMe), 7.06 (d *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.16-7.19 (m, 2H), 7.30-7.40 (m, 3H), 7.56 (t, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 8.9 Hz, 2H), 8.12 (d, *J* = 8.8 Hz, 2H).

Z-3-(6-Methyl-2-pyridinyl)-3-(4-nitrophenyl)-2-phenylacrylic acid methyl ester (3c).

Colorless crystals from petroleum ether – ethyl acetate, mp 106 - 108 °C; IR (KBr) 3105, 3067, 2951, 1726, 1679, 1586, 1526, 1451, 1346, 1232, 1101, 1018, 845, 803, 761, 699; ¹H NMR (300 MHz, CDCl₃) δ 2.31 (s, 3H, Me), 3.62 (s, 3H, OMe), 6.74 (d, *J* = 7.8 Hz, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 7.26-7.30 (m, 3H), 7.33-7.36 (m, 3H), 8.21 (d, *J* = 8.8 Hz, 2H), 8.31 (d, *J* = 8.9 Hz, 2H); MS *m*/*z* 402 (M⁺, 48.58), 387 (24.52), 374 (44.62), 373 (59.98), 371 (39.29), 359 (33.92), 343 (42.67), 315 (base), 314 (24.22), 252 (25.39), 150 (74.84), 104 (82.08), 76 (51.68). Anal. Calcd for C₂₃H₁₈N₂O₅ : C, 68.66; H, 4.48; N, 6.97. Found; C, 68.63; H, 4.49; N, 6.99.

3-Phenyl-4-(6-methyl-2-pyridinyl)-5-hydroxy-5-(4-nitrophenyl)furan-2-one (4c). Colorless crystals from petroleum ether – ethyl acetate, mp 178 -180 °C; IR (KBr) 3359 (br), 3123, 3082, 1732 (br), 1650, 1586, 1522, 1494, 1434, 1379, 1351, 1277, 1215, 1176, 1073, 995, 861, 843, 785, 748, 701; ¹H NMR (300 MHz, CDCl₃) δ2.60 (s, 3H, Me), 7.03 (d, *J* = 7.7 Hz, 1H), 7.19 (d, *J* = 7.9 Hz, 1H), 7.46-7.51 M, 6H), 7.72 (d, *J* = 8.7 Hz, 2H), 8.17 (d, *J* = 8.6 Hz, 2H); MS *m/z* 388 (M⁺, 36.81), 369 (22.30), 322 (28.84), 315 (43.26), 266 (31.34), 238 (38.99), 194 (base), 92 (26.08). Anal. Calcd for C₂₂H₁₆N₂O₅: C, 68.04; H, 4.12; N, 7.22. Found: C, 68.01; H, 4.10; N, 7.20.

1-(6-Methyl-2-pyridinyl)-2-(4-nitrophenyl)ethanone (5c). Colorless crystals from petroleum ether – ethyl acetate, mp 160 -162 °C; IR (KBr) 3135,3110, 1699, 1679, 1594, 1526, 1459, 1351, 1324, 1257, 1213, 987, 925, 843, 806, 775, 752, 721, 704; ¹H NMR (300 MHz, CDCl₃) δ 2.52 (s, 3H, Me), 7.45 (d, *J* = 7.7 Hz, 1H), 7.89 (t, *J* = 7.7 Hz, 1H), 8.05 (d, *J* = 7.7 Hz, 1H), 8.12 (d, *J* = 8.9 Hz, 2H), 8.37 (d, *J* = 8.9 Hz, 2H); MS *m/z* 270 (M⁺, 13.91), 241 (15.46), 214 (9.20), 150 (13.49), 120 (32.24), 104 (18.80), 92 (base), 76 (16.51). Anal. Calcd for C₁₄H₁₀N₂O₄ : C, 62.22; H, 3.70; N, 10.37. Found: C, 62.20; H, 3.72; N, 10.35.

3-(6-Methyl-2-pyridinyl)-3-(4-nitrobenzoyl)-2-phenylacrolein (6c). White solid mp 172

-17 4 °C; IR (KBr) 1677, 1653, 1601, 1591, 1523, 1344, 1247, 1221, 855, 785, 734, 695; ¹H NMR (300 MHz, CDCl₃) δ 2.62 (s, 3H, Me), 7.21 (d, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 8.05 (d, *J* = 7.6 Hz, 2H), 8.16 (d, *J* = 8.7 Hz, 2H), 8.29 (d, *J* = 8.7 Hz, 2H), 8.38 (s, 1H, CHO); ¹³C NMR (75 MHz, CDCl₃) δ 24.91, 76.99, 77.42, 77.84, 120.77, 124.44, 125.54, 129.25, 129.30, 129.81, 134.27, 137.15, 137.89, 141.32, 150.65, 151.04, 159.96, 189.19, 196.63; MS *m*/*z* 372 (M⁺, 74.56), 315 (12.73), 295 (13.00), 267 (38.58), 239 (base), 222 (45.27), 194 (24.63), 193 (24.96), 150 (28.09), 120 (15.53), 105 (87.73), 92 (37.72), 77 (94.29). Anal. Calcd for C₂₂H₁₆N₂O₄ : C, 70.78; H, 5.88; N, 7.53. Found: C, 70.76; H, 5.85; N, 7.56.

E-3-Benzoyl-3-(2-pyridinyl)-3-phenylacrylic acid methyl ester (2d). White crystals from petroleum ether – ethyl acetate, mp 96 - 98 °C; IR (KBr) 3054, 3003, 2950, 1725, 1671, 1581, 1468, 1431, 1257, 1157, 1021, 938, 785, 745, 711, 697; ¹H NMR (300 MHz, CDCl₃) δ 3.78 (s, 3H, Me), 7.17-7.20 (m, 3H), 7.27-7.46 (m, 6H, ArH), 7.68 (t, *J* = 7.7 Hz, 1H), 7.92 (dd, *J* = 1.3, 8.4 Hz, 3H), 8.66 (m, 1H); MS *m*/*z* 343 (M⁺, 27.04), 314 (59.55), 300 (18.64), 284 (18.45), 256 (65.02), 179 (14.15), 127 (10.82), 105 (base), 77 (94.84). Anal. Calcd for C₂₂H₁₇NO₃ : C, 54.50; H, 4.96; N, 4.08%. Found: C, 54.48; H, 4.93; N, 4.09.

2-Benzoyl-2-(2-pyridinyl)-3-phenyl-3-phenylglyoxyloxirane (6d). Colorless crystals from petroleum ether – ethyl acetate, mp 142 - 144 °C; IR (KBr) 3057, 1705, 1689, 1665, 1583, 1489, 1470, 1296, 1213, 1177, 1123, 1101, 838, 769, 725, 687; ¹H NMR (300 MHz, CDCl₃) δ 7.14-7.25 (m, 5H), 7.41 (t, *J* = 7.7 Hz 2H), 7.52-7.61 (m, 4H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.71-7.74 (m, 2H), 7.96 (d, *J* = 4.7 Hz, 1H), 7.99 (dd, *J* = 1.4, 8.5 Hz, 2H), 8.31 (dd, *J* = 1.4, 8.5 Hz 2H); MS *m/z* 433 (M⁺, 0.22), 328 (10.87), 300 (base), 256 (5.92), 105 (93.74), 77 (55.53). Anal. Calcd for

C₂₈H₁₉NO₄ : C, 77.60; H, 4.39; N, 3,23%. Found: C, 77.56; H, 4.37; N, 3.23.

Z-3-(2-Pyridinyl)-2-phenylacrylic acid methyl ester (2e). Oil; IR (KBr) 3056, 2946, 1729, 1625, 1583, 1495, 1471, 1429, 1365, 1281, 1212, 1097, 1011, 939, 833, 779, 744, 693; ¹H NMR (300 MHz, CDCl₃) δ 3.94 (s, 3H, OMe), 6.97 (s, 1H), 7.16 (br, 1H), 7.28-7.44 (m, 4H), 7.57 (dd, *J* = 7.8, 1.5 Hz, 2H), 7.66 (m, 1H), 8.59 (m, 1H); MS *m/z* 239 (M⁺, 31.56), 238 (base), 180 (33.21), 152 (10.67), 78 (20.15), 77 (9.09). Anal. Calcd for C₁₅H₁₃NO₂ : C, 75.31; H, 5.44; N, 5.86. Found: C, 75.29; H, 5.46; N, 5.84.

2-Phenyl-3-(2-pyridinyl)oxiranecarboxylic acid (6e). White solid, mp 178-180 °C (dec); IR (KBr) 3037, 2493 (br), 1725, 1647, 1618, 1496, 1410, 1303, 1231, 977, 865, 773, 684, 655,624; ¹H NMR (300 MHz, DMSO-d₆) δ 7.12 (s, 1H), 7.30 (m, 1H), 7.36-7.47 (m, 3H), 7.52-7.60 (m, 3H), 7.83 (td, *J* = 5.5 1.5 Hz, 1H), 8.56 (d, *J* = 4.5 Hz, H); MS *m*/*z* 224 (M-OH, 6.11), 208 (6.56), 181 (25.30), 180 (base), 179 (5.64), 178 (5.16), 152 (8.41), 102 (4.02), 90 (3.84), 79 (6.09), 78 (8.85), 77 (4.87), 52 (6.34), 51 (8.35). Anal. Calcd for C₁₄H₁₁NO₃ : C, 69.71; H, 4.56; N, 5.81.Found: C, 69.69; H, 4.62; N, 5.79.

2-(2-Pyridinyl)maleic acid dimethyl ester (7f) or (8f) Oil; IR (KBr) 3004, 2953, 1741, 1721, 1634, 1582, 1435, 1357, 1297, 1250, 1028, 1007, 892, 791, 750; ¹H NMR (300 MHz, CDCl₃) δ 3.73 (s, 3H, OMe), 3.92 (s, 3H, OMe), 6.84 (s, 1H), 7.21-7.26 (ddd, J = 0.9, 4.8, 7.6 Hz, 1H), 7.39 (d, J = 7.9 Hz, 1H), 7.66 (td, J = 7.8, 1.8 Hz, 1H), 8.58 (m, 1H); MS *m*/*z* 221 (M⁺, 12.54), 206 (25.59), 190 (57.06), 162 (34.68), 133 (17.19), 130 (65.56), 117 (57.72), 105 (44.31), 104 (90.03), 103 (73.85), 91 (25.20), 78(base), 76 (75.00), 59 (41.81). Anal. Calcd for C₁₁H₁₁NO₄ : C, 59.73; H, 4.98; N, 6.33. Found: C, 59.75; H, 4.99; N, 6.31.

3-Benzoyl-5-methoxyl-6-hydroxyindolizine-1-carboxylic acid methyl ester (9f) Yellow crystals

from petroleum ether – ethyl acetate mp 162 - 164 °C; IR (KBr) 3017, 1667, 1627, 1597, 1514, 1452, 1410, 1279, 1235, 1036, 909, 776, 755, 726, 702, 671; ¹H NMR (300MHz, CDCl₃) δ 3.82 (s, 3H, OMe), 3.92 (s, 3H, OMe), 6.19 (d, *J* = 8.3 Hz, 1H), 6.81 (d, *J* = 8.3 Hz, 1H), 7.50-7.60 (m, 4H), 7.81 (dd, *J* = 1.5, 8.6 Hz, 2H), 11.1 (s, 1H); MS *m/z* 325 (M⁺, 50.63), 293 (16.62), 278 (base), 250 (22.71), 177 (30.83), 105 (20.27), 77 (30.95). Anal. Calcd for C₁₈H₁₅NO₅ : C, 66.46; H, 4.61; N, 4.31. Found: C, 66.43; H, 4.59; N, 4.29.



3. ¹HNMR (300MHz, CDCl₃) of compounds 2-9(a-f)

2b





.



2d



2e





3b



3c



4a





5a

-8 15 -



5b





6a











9f







5. UV spectra of 1a, 1b and CTC spectra of 1a in :





UV spectra of **1a** in oxygen free and oxygen saturated acetonitrile solution ([**1a**]~0.028 mol/L)

6. Phosphorescence spectra of **1b**, **1d** and **1f** in glassy acetonitrile at 77K:





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