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SUPPLEMENTARY MATERIAL TO

Synthesis and properties of new fused pyrrolo-1,10-phenanthroline type derivatives

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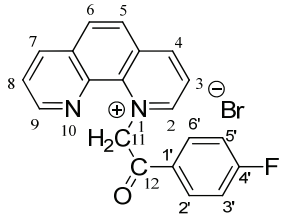
PHYSICAL AND SPECTRAL DATA FOR THE SYNTHESIZED COMPOUNDS

*1-(2-(4-fluorophenyl)-2-oxoethyl)-1,10-phenanthrolin-1-ium bromide (**3a**)*



Pink powder, mp = 277-279 ºC, yield: 65%. Spectral data are in accordance to the literature.[40] Obtained by general procedure, at room temperature in acetone. Pink powder, mp = 277-279 ºC, yield: 65 %. IR (KBr): 3062, 3027; 2986, 2916 1687 1595, 1531, 1230 cm^{-1}. ^1H NMR (500 MHz, DMSO-d6, δ(ppm)): 9.66 (1H, dd, J = 6.0, 1.0 Hz, H-2), 9.61 (1H, dd, J = 8.5, 1.0 Hz, H-4), 8.78 (1H, dd, J = 8.0, 1.5 Hz, H-9), 8.63 (1H, dd, J = 8.5, 6.0 Hz, H-3), 8.50 (3H, m, H-7, H-5, H-6,), 8.30 (2H, m, H-2', 6'), 7.91 (1H, dd, J = 8.0, 4.0 Hz, H-8), 7.60 (2H, m, H-3', 5'), 7.29 (2H, as, H-11). ^{13}C RMN (125 MHz, DMSO-d6, δ(ppm)): 189.4 C-12, 165.5 (d, $J_{C,F}$ = 251.0 Hz, C-4'), 152.1 C-2, 148.8 C-9, 148.2 C-4, 138.4 C-10a, 138.0 C-7, 136.2 C-10b, 132.0 C-4a, 131.5 C-6a, 131.3 (d, $J_{C,F}$ = 10 Hz, C-2', C-6'), 131.0 (d, $J_{C,F}$ = 2.5 Hz, C-1'), 130.7 C-5, 127.0 C-6, 125.5 C-8, 124.3 C-3, 116.4 (d, $J_{C,F}$= 22.5 Hz, C-3', C-5'), 69.5 C-11. Combustion analysis for $C_{20}H_{14}BrFN_2O$: Calculated. C 60.47, H 3.55, N 7.05; found C 60.49, H 3.53, N 7.08.

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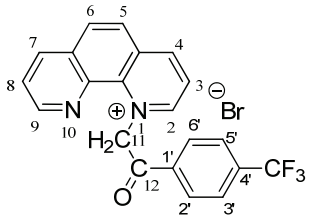
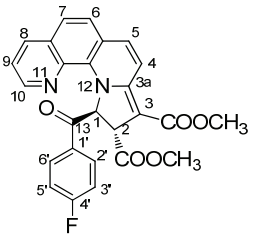
*1-(2-oxo-2-(4-(trifluoromethyl)phenyl)ethyl)-1,10-phenanthrolin-1-ium bromide (**3b**)*



Obtained by general procedure, at room temperature in acetone. Pink powder, mp = 212-215 ºC, yield: 80 %. IR (KBr): 2988, 2918, 1691, 1630, 1585, 1321, 1230, 1175, 1126, 1065 cm^{-1}. ^1H NMR (500 MHz, DMSO-d6, δ(ppm)): 9.65 (1H, d, *J* = 5.5 Hz, H-2), 9.62 (1H, dd, *J* = 8.5, 1.0 Hz, H-4), 9.20 (1H, dd, *J* = 4.5, 1.5 Hz, H-9), 8.80 (1H, dd, *J* = 8.5, 1.5 Hz, H-7), 8.64 (1H, dd, *J* = 8.5, 6.0 Hz, H-3), 8.51 (1H, d, *J* = 9.0 Hz, H-6), 8.49 (1H, d, *J* = 9.0 Hz, H-5), 8.40 (2H, d, *J* = 8.0 Hz, H-2', 6'), 8.13 (2H, d, *J* = 8.0 Hz, H-3', 5'), 8.00 (1H, dd, *J* = 8.5, 4.5 Hz, H-8), 7.30 (2H, bs, H-11). ^{13}C RMN (125 MHz, DMSO-d6, δ(ppm)): 190.0 C-12, 152.1 C-2, 148.7 C-9, 148.3 C-4, 138.2 C-10a, 138.1 C-7, 137.6 C-1', 136.1 C-10b, 133.3 (q, $J_{C,F}$ = 31.3 Hz, C-4'), 132.1 C-4a, 131.5 C-6a, 130.8 C-5, 129.1 (C-2', C-6'), 127.1 C-6, 124.9 C-3, 124.6 C-8, 123.8 (q, $J_{C,F}$ = 270.0 Hz, CF_3), 126.4 (q, $J_{C,F}$= 3.8 Hz, C-3',C-5'), 69.6 C-11. Combustion analysis for $C_{21}H_{14}BrF_3N_2O$: Calculated. C 56.39, H 3.16, N 6.26; found C 56.40, H 3.14, N 6.28.

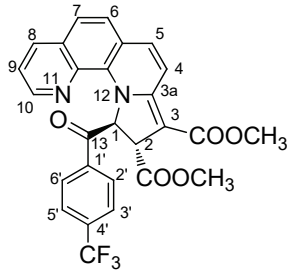
*Dimethyl 11-(4-fluorobenzoyl)-10,11-dihydropyrrolo[1,2-a][1,10]phenanthroline-9,10-dicarboxylate (**4a**)*



Crystallized from methanol-chloroform 1:1, (v/v). Red crystals, mp = 235-237 ºC, yield: 30 %. IR (KBr): 3070, 2954, 2920, 1749, 1688, 1627, 1592, 1566, 1497, 1230, 1119, 1047 cm^{-1}. ^1H-NMR (500 MHz, $CDCl_3$, δ(ppm)): 8.13 (2H, m, H-2', H-6'), 7.96 (1H, d, *J* = 4.5 Hz, H-10), 7.92 (1H, d, *J* =7.5 Hz, H-4), 7.79 (1H, d, *J* = 8.5 Hz, H-8), 7.56 (1H, d, *J* = 5.0 Hz, H-1), 7.26 (1H, d, *J* = 7.5 Hz, H-5), 7.25 (2H, bs, H-6, H-7), 7.19 (2H, m, H-3', H-5'), 7.13 (1H, dd, *J* = 8.5; 4.5 Hz, H-9), 4.00 (1H, d, *J*= 5.0 Hz, H-2), 3.72 (3H, s, CH_3), 3.62 (3H, s, CH_3). ^{13}C-RMN (125 MHz, $CDCl_3$, δ(ppm)): 189.3 C-13, 173.9 CO_{ester}, 166.1 CO_{ester}, 166.0 (d, $J_{C,F}$= 253.75 Hz, C-4'), 155.3 C-3a, 146.5 C-10, 137.6 C-7, 136.6 C-4, 135.8 C-11b, 132.0 (d, $J_{C,F}$= 8.75 Hz, C-2', C-6'), 130.1 (d,

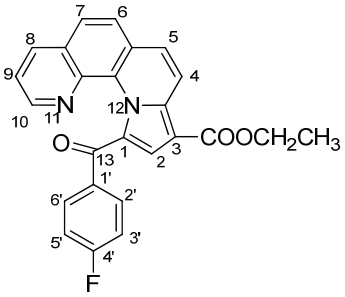
$J_{C,F}$= 3.75 Hz, C-1'), 126.9 C-6, 126.1 C-7a, C-11a, 125.6 C-5a, 122.0 C-9, 121.0 C-5, 119.7 C-8, 116.2 (d, J_{C-F}= 21.25 Hz, C-3', C-5'), 88.2 C-3, 71.3 C-1, 52.9 CH_3, 50.6 CH_3, 49.6 C-2. Combustion analysis for $C_{26}H_{19}FN_2O_5$: Calculated. C 68.12, H 4.18. N 6.11; found C 68.15, H 4.15, N 6.14.

*Dimethyl 11-(4-(trifluoromethyl)benzoyl)-10,11-dihydropyrrolo[1,2-a][1,10]phenanthroline-9,10-dicarboxylate (**4b**)*



Crystallized from methanol-chloroform 1:1, (v/v). Red crystals, mp = 225-226 ºC, yield: 55 %. IR (KBr): 3022, 2953, 1728, 1690, 1630, 1585, 1547, 1463, 1230, 1115, 1065 cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$, δ(ppm)): 8.29 (2H, d, *J* = 8.0 Hz, H-2', H-6'), 8.02 (1H, d, *J* = 8.0 Hz, H-4), 7.97 (1H, d, *J* = 4.5 Hz, H-10), 7.85-7.89 (3H, overlapped signals, H-3', H-5', H-8), 7.62 (1H, d, *J* = 4.0 Hz, H-1), 7.44-7.48 (2H, overlapped signals, H-6, H-7), 7.37 (1H, d, *J* = 8.5 Hz, H-5), 7.23 (1H, dd, *J* = 7.5; 4.0 Hz, H-9), 4.07 (1H, d, *J* = 4.5 Hz, H-2), 3.79 (s, 3H, CH_3), 3.70 (s, 3H, CH_3). ^{13}C-RMN (125 MHz, $CDCl_3$, δ(ppm)): 189.23 C-13, 173.7 CO_{ester}, 166.0 CO_{ester}, 155.1 C-3a, 146.5 C-10, 137.4 C-7, 136.8 C-4, 136.6 (C-1'), 135.6 C-11b, 134.8 (q, $J_{C,F}$= 31.3 Hz, C-4'), 130.5 C-7a, 129.8 (C-2', C-6'), 127.0 (C-6, C-5a), 126.0 (C-3', C-5', C-11a), 122.1 C-9, 123.76 (q, $J_{C,F}$= 271.3 Hz, CF_3), 121.1 C-5, 119.8 C-8, 88.2 C-3, 71.3 C-1, 53.0 CH_3, 50.6 CH_3, 49.5 C-2. Combustion analysis for $C_{27}H_{19}F_3N_2O_5$: Calculated. C 63.78, H 3.77, N 5.51; found C 63.80, H 3.76, N 5.53.

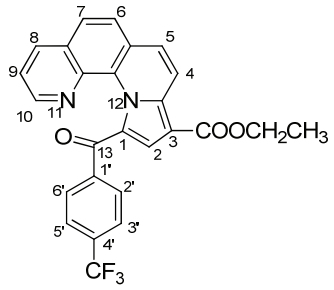
*Ethyl 11-(4-fluorobenzoyl) pyrrolo[1,2-a][1,10]phenanthroline-9-carboxylate (**5a**)*



Crystallized from methanol-chloroform 1:1, (v/v). Yellow crystals, mp = 162-164 °C, yield: 40 %. IR (KBr): 2981, 1697, 1645, 1596, 1226, 1121 cm^{-1}.

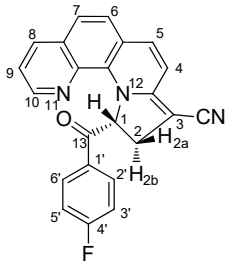
^{1}H-NMR (500 MHz, $CDCl_3$, δ(ppm)): 8.58 (1H, d, J = 9.5 Hz, H-4), 8.33 (1H, bs, H-8), 8.44 (1H, bs, H-10), 8.15 (2H, bs, H-2', H-6'), 7.94 (1H, d, J = 8.5 Hz, H-7), 7.87 (1H, d, J = 8.5 Hz, H-6), 7.72 (1H, d, J = 9.5 Hz, H-5), 7.50 (1H, m, H-9), 7.53 (1H, s, H-2), 7.21 (2H, at, J = 8.5 Hz, H-3', H-5'), 4.40 (2H, q, J = 7.0 Hz, CH_2), 1.42 (3H, t, J = 7.0 Hz, CH_3). ^{13}C-RMN (125 MHz, $CDCl_3$, δ(ppm)): 191.4 C-13, 164.6 CO_{ester}, 165.2 (d, $J_{C,F}$ = 252.5 Hz, C-4'), 157.4 C-3a, 145.9 C-10, C-11b, 137.4 C-8, 134.9 (d, $J_{C,F}$ = 3.75 Hz, C-1'), 131.9 (d, $J_{C,F}$ = 8.75 Hz, C-2', C-6'), 127.4 C-7, 127.9 C-7a, C-11a, 125.7 C-5, 125.1 C-5a, 125.0 C-6, 122.8 C-9, 121.0 C-4, C-2, 115.7 (d, J_{C-F} = 21.25 Hz, C-3', C-5'), 107.3 C-1, 104.5 C-3, 60.3 CH_2, 14.7 CH_3. Combustion analysis for $C_{25}H_{17}FN_2O_3$: Calculated. C 72.81, H 4.15, N 6.79; found C 72.83, H 4.12, N 6.81.

*Ethyl 11-(4-(trifluoromethyl)benzoyl)pyrrolo[1,2-a][1,10]phenanthroline-9-carboxylate (**5b**)*



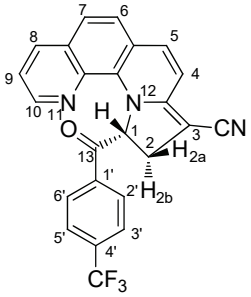
Crystallized from methanol-chloroform 1:1, (v/v). Yellow powder, mp = 220-221 °C, yield: 45 %. IR (KBr): 3072, 2986, 1697, 1651, 1584, 1236, 1126 cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$, δ(ppm)): 8.60 (1H, d, J = 9.0 Hz, H-4), 8.25-8.33 (4H, overlapped signals, H-8, H-10, H-2', H-6'), 7.93 (1H, d, J = 8.5 Hz, H-7), 7.82-7.85 (3H, overlapped signals, H-6, H-3', H-5'), 7.75 (1H, d, J = 9.0 Hz, H-5), 7.54 (1H, s, H-2), 7.43 (1H, dd, J = 7.5; 5.5 Hz, H-9), 4.40 (2H, m, CH_2), 1.42 (3H, t, J = 7.0 Hz, CH_3). ^{13}C-RMN (125 MHz, $CDCl_3$, δ(ppm)): 192.9 C-13, 164.6 CO_{ester}, 157.4 C-3a, 146.1 C-10, 141.2 C-11b, 138.4 (C-1'), 136.9 C-8, 133.8 (q, $J_{C,F}$ = 31.3 Hz, C-4'), 130.3 (C-2', C-6'), 128.0 C-7a, C-11a, 127.1 C-7, 125.8 C-5a, 125.7 C-5, 125.6 (q, $J_{C,F}$ = 2.5 Hz, C-3', C-5'), 125.2 C-6, 124.0 (q, $J_{C,F}$ = 271.3 Hz, CF_3), 122.8 C-9, 121.6 C-2, 120.6 C-4, 106.9 C-1, 104.4 C-3, 60.3 CH_2, 14.7 CH_3. Combustion analysis for $C_{26}H_{17}F_3N_2O_3$: Calculated. C 67.53, H 3.71, N 6.06; found: C 67.56, H 3.68, N 6.05.

*11-(4-fluorobenzoyl)-10,11-dihydropyrrolo[1,2-a][1,10]phenanthroline-9-carbonitrile (**6a**)*



Crystallized from ethanol-chloroform 1:1, (v/v). Red solid, mp = 213-215 °C, yield: 40 %. IR (KBr): 3060, 2962, 2917, 2160, 1695, 1594, 1458, 1192 cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$, δ(ppm)): 7.99 (2H, m, H-2', H-6'), 7.88 (2H, overlapped signals, H-10, H-8), 7.12-7.27 (7H, overlapped signals, H-5, H-3', H-5', H-4, H-6, H-1, H-9), 6.77 (1H, s, H-7), 3.38 (1H, t, J = 13.5; 11.5 Hz, H-2a), 2.85 (1H, dd, J = 15.0; 6.0 Hz, H-2b). ^{13}C-RMN (125 MHz, $CDCl_3$, δ(ppm)): 190.2 C-13, 165.9 (d, $J_{C,F}$ = 253.75 Hz, C-4'), 157.4 C-11a, 146.4 C-10, 137.1 C-3a, 136.6 C-11b, 136.4 C-8, 135.8 C-7a, 131.5 (d, $J_{C,F}$ = 8.75 Hz, C-2', C-6'), 130.6 (d, $J_{C,F}$ = 3.75 Hz, C-1'), 126.9 C-6, C-5, C-5a, 122.1 C-9, 120.6 C-4, 120.2 CN, 118.0 C-7, 116.3 (d, J_{C-F} = 21.25 Hz, C-3', C-5'), 69.4 C-3, 68.0 C-1, 33.0 C-2. Combustion analysis for $C_{23}H_{14}FN_3O$: Calculated. C 75.19, H 3.84, N 11.44; found C 75.18, H 3.81, N 11.46.

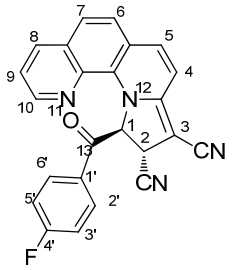
*11-(4-(trifluoromethyl)benzoyl)-10,11-dihydropyrrolo[1,2-a][1,10]phenanthroline-9-carbonitrile (**6b**)*



Crystallized from methanol-chloroform 1:1, (v/v). Red crystals, mp = 240-242 °C, yield: 40 %. IR (KBr): 2995, 2943, 2243, 2172, 1680, 1639, 1595, 1452, 1128 cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$, δ(ppm)): 8.15 (2H, d, J = 7.5 Hz, H-2', H-6'), 7.99 (1H, d, J = 7.5 Hz, H-8), 7.85-7.88 (3H, overlapped signals, H-10, H-3', H-5'), 7.20-7.37 (5H, overlapped signals, H-5, H-4, H-6, H-1, H-9), 6.86 (1H, bs, H-7), 3.47 (1H, t, J = 14.0 Hz, H-2a), 2.93 (1H, dd, J = 14.5; 6.5 Hz, H-2b). ^{13}C-RMN (125 MHz, $CDCl_3$, δ(ppm)): 190.1 C-13, 157.4 C-11a, 155.1 C-3a, 146.3 C-10, 136.8 C-8, 135.8 C-11b, 130.6 C-7a, 129.3 (C-2', C-6'), 137.4 (C-1'), 134.79 (q, $J_{C,F}$ = 31.3 Hz, C-4'), 126.9 C-6, C-5, C-5a, 126.2 (C-3',

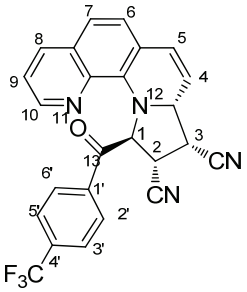
C-5'), 123.7 (q, $J_{C,F}$ = 271.3 Hz, CF_3), 122.2 C-9, 120.9 C-4, 120.7 CN, 118.0 C-7, 67.9 C-1, 66.8 C-3, 32.9 C-2. Combustion analysis for $C_{24}H_{14}F_3N_3O$: Calculated. C 69.06, H 3.38, N 10.07; Found C 69.08, H 3.35, N 10.09.

*11-(4-fluorobenzoyl)-8a,9-dihydropyrrolo[1,2-a][1,10]phenanthroline-9,10-dicarbonitrile (**7a**)*



Crystallized from ethanol-chloroform 1:1, (v/v). Orange solid, mp = 238-240 °C, yield: 52 %. IR (KBr): 3062, 2978, 2925, 2225, 2175, 1691, 1596, 1460, 1153cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$, δ(ppm)): 8.17 (2H, m, H-2', H-6'), 8.05-8.09 (2H, overlapped signals, H-10, H-8), 7.74 (1H, d, J = 5.0 Hz, H-1), 7.50-7.53 (2H, overlapped signals, H-4, H-7), 7.34 (2H, t, J = 8.5 Hz, H-3', H-5'), 7.30 (1H, dd, J = 8.5; 4.5 Hz, H-9), 7.26 (1H, d, J = 9.5 Hz, H-5), 6.99 (1H, d, J = 8.5 Hz, H-6), 4.13 (1H, d, J = 5.0 Hz, H-2). ^{13}C-RMN (125 MHz, $CDCl_3$, δ(ppm)): 187.2 C-13, 166.6 (d, $J_{C,F}$ = 253.75 Hz, C-4'), 158.2 C-3a, 147.2 C-10, 137.8 C-7, 137.0 C-8, C-11b, 135.2 C-11a, 131.8 (d, $J_{C,F}$ = 10.0 Hz, C-2', C-6'), 130.7 C-7a, 129.1 (d, $J_{C,F}$ = 3.75 Hz, C-1'), 127.0 C-4, 125.9 C-5a, 122.6 C-9, 122.2 C-6, 122.1 C-5, 118.0 CN, 117.5 CN, 117.0 (d, $J_{C\text{-}F}$= 22.5 Hz, C-3', C-5'), 71.2 C-1, 63.0 C-3, 35.6 C-2. Combustion analysis for $C_{24}H_{13}FN_4O$: Calculated. C 73.46, H 3.34, N 14.28; found C 73.44, H 3.31, N 14.30.

*11-(4-(trifluoromethyl)benzoyl)-8a,9,10,11-tetrahydropyrrolo[1,2-a][1,10]phenanthroline--9,10-dicarbonitrile (**7b**)*



Crystallized from methanol-chloroform 1:1, (v/v). Orange solid, mp = 230-232 °C, yield: 68 %. IR (KBr): 2996, 2914, 2365, 2249, 1688, 1647, 1454, 1126 cm^{-1}. ^{1}H-NMR (500 MHz, DMSO-d6, δ(ppm)): 8.36 (2H, d, J = 8.0 Hz,

H-2', H-6'), 8.09 (1H, dd, *J* = 8.0; 1.5 Hz, H-8), 8.04 (2H, d, *J* =8.0 Hz, H-3', H-5'), 7.53 (1H, dd, *J* = 4.5; 1.5 Hz, H-10), 7.28 (1H, d, *J* = 8.5 Hz, H-6), 7.18-7.21 (2H, overlapped signals, H-7, H-9), 6.72-6.77 (2H, overlapped signals, H-5, H-1), 5.88 (1H, dd, *J* = 10.0; 2.0 Hz, H-4), 5.40 (1H, dd, *J* = 4.5; 1.5 Hz, H-3a), 4.33 (1H, dd, *J* = 7.0; 5.0 Hz, H-3), 4.08 (1H, t, *J* = 7.0 Hz, H-2). ^{13}C-RMN (125 MHz, DMSO-d6, δ(ppm)): 192.6 C-13, 145.0 C-10, 138.3 C-1', 137.3 C-11b, 136.5 C-8, 136.3 C-11a, 132.6 (q, $J_{C,F}$= 32.5 Hz, C-4'), 129.8 (C-2', C-6'), 129.5 C-7a, 128.3 C-5, 126.8 C-6, 126.0 (d, J_{C-F}= 3.8 Hz, C-3', C-5'), 123.5 (q, $J_{C,F}$= 271.3 Hz, CF_3), 121.1 C-7, 119.9 C-4, 118.7 C-5a, 117.8 CN, 117.3 CN, 116.8 C-9, 65.7 C-1, 63.6 C-3a, 39.5 C-3, 32.9 C-2. Combustion analysis for $C_{25}H_{15}F_3N_4O$: Calculated. C 67.57, H 3.40, N 12.61; found C 67.59, H 3.38, N 12.62.

TABLE S-I. Crystallographic data and refinement details

Compound	**4b** (4719)	**6a** (4665)	**6b** (4819)	**7b** (4833)
Empirical formula	$C_{27}H_{19}F_3N_2O_5$	$C_{23}H_{14}FN_3O$	$C_{24}H_{14}F_3N_3O$	$C_{25}H_{15}F_3N_4O$
Formula weight	508.44	367.37	417.38	444.41
Temperature/K	200	293	200	140
Crystal system	triclinic	monoclinic	triclinic	monoclinic
Space group	*P*-1	*C*2/*c*	*P*-1	$P2_1/c$
a / Å	7.5236(5)	26.468(2)	5.4429(5)	9.2761(4)
b / Å	9.5486(7)	6.2708(4)	9.7038(8)	11.1990(4)
c / Å	17.3690(12)	22.8898(19)	18.6668(14)	20.0050(9)
α / °	77.052(6)	90	75.239(7)	90
β / °	87.591(6)	113.351(11)	82.490(7)	91.083(4)
γ / °	70.374(6)	90	80.305(7)	90
Volume, Å^3	1144.66(15)	3488.0(5)	935.77(14)	2077.81(15)
Z	2	8	2	4
ρ_{calc}g / cm^3	1.475	1.399	1.481	1.421
μ / mm^{-1}	0.119	0.095	0.113	0.108
Crystal size, mm^3	0.3×0.15 0.15	0.15×0.10×0.10	0.3×0.15×0.15	0.30×0.25×0.20
2*θ* / °	4.646 to 50.046	3.352 to 57.404	4.384 to 50.052	4.072 to 50.038
Reflections collected	9201	9862	8106	11269
Independent reflections	4009 [R_{int}= 0.0361]	3942 [R_{int}= 0.0735]	3306 [R_{int}= 0.0311]	3668 [R_{int}= 0.0409]
Data/restraints/parameters	4009/0/336	3942/0/253	3306/81/277	3668/70/299
R_1[a]	0.0667	0.0671	0.0841	0.050
R_2[b]	0.1561	0.1827	0.2286	0.2300
GOF[c]	1.091	0.994	1.050	1.055
Largest diff. peak/hole, e Å^{-3}	0.28/-0.29	0.17/-0.23	0.82/-0.79	0.50/-0.48

[a]$R_1=\Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b]$wR_2=\{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. [c]$GOF=\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$, where *n* is the number of reflections and *p* is the total number of parameters refined.

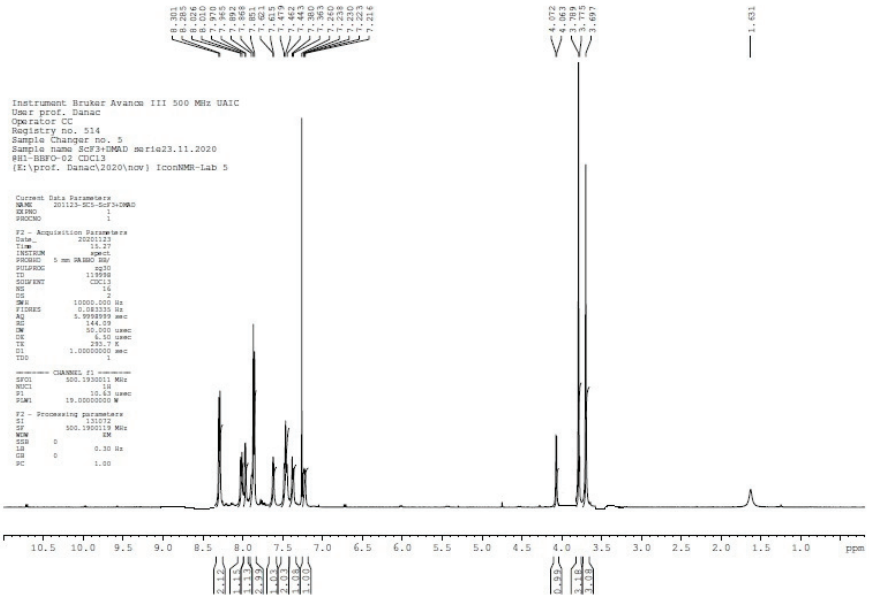


Fig. S-1. ^{1}H NMR spectrum of compound **4b**.

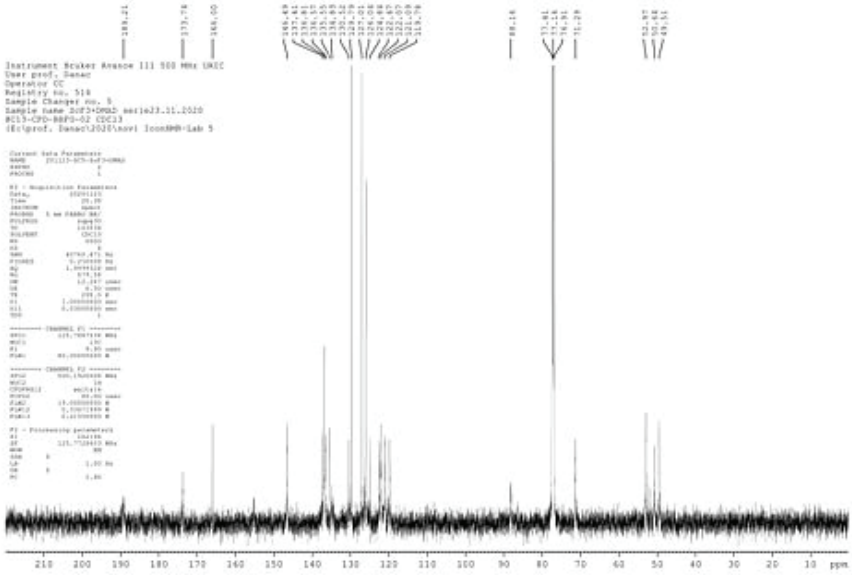


Fig. S-2. ^{13}C NMR spectrum of compound ^{13}C NMR of **4b**.

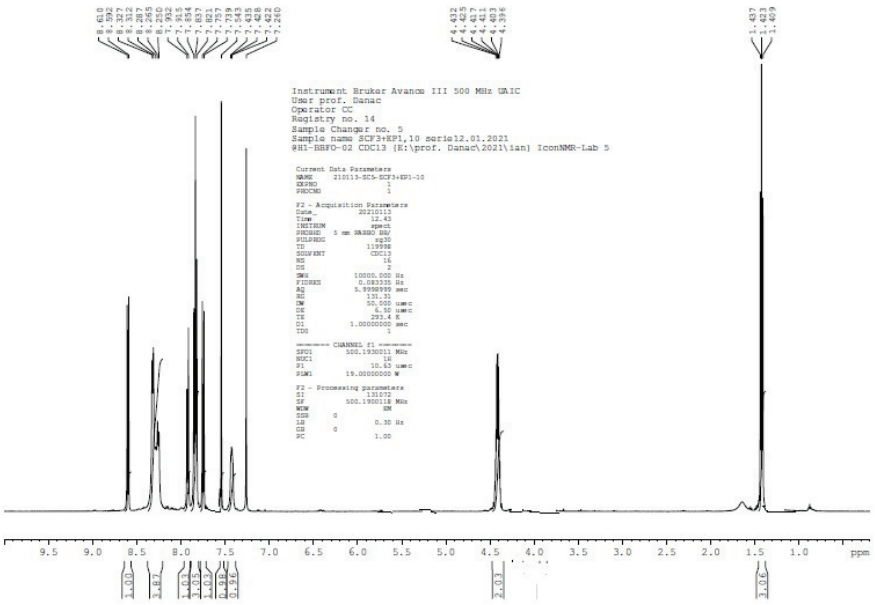


Fig. S-3. ^{1}H NMR spectrum of compound **5b**.

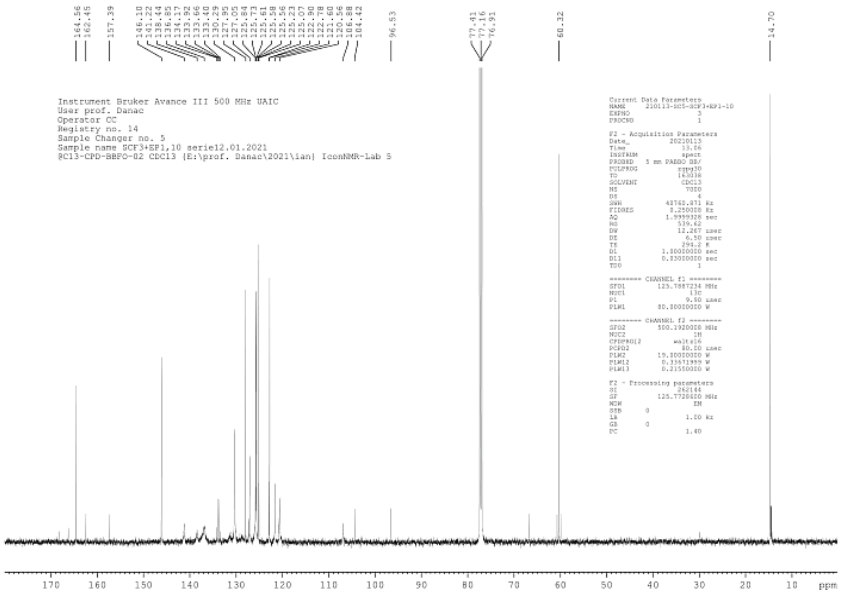


Fig. S-4. ^{13}C NMR spectrum of compound ^{13}C NMR of **5b**.

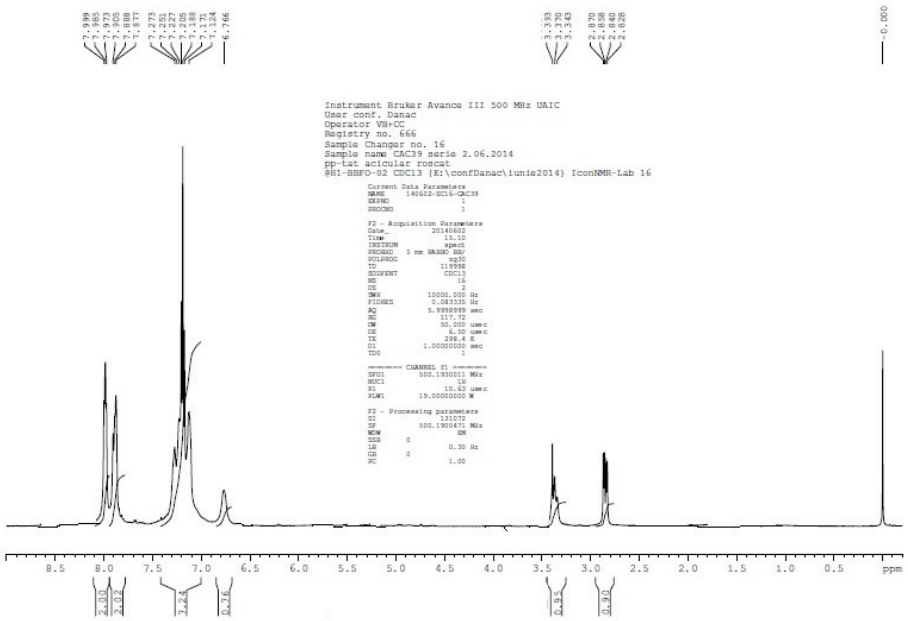


Fig. S-5. ^{1}H NMR spectrum of compound **6a**.

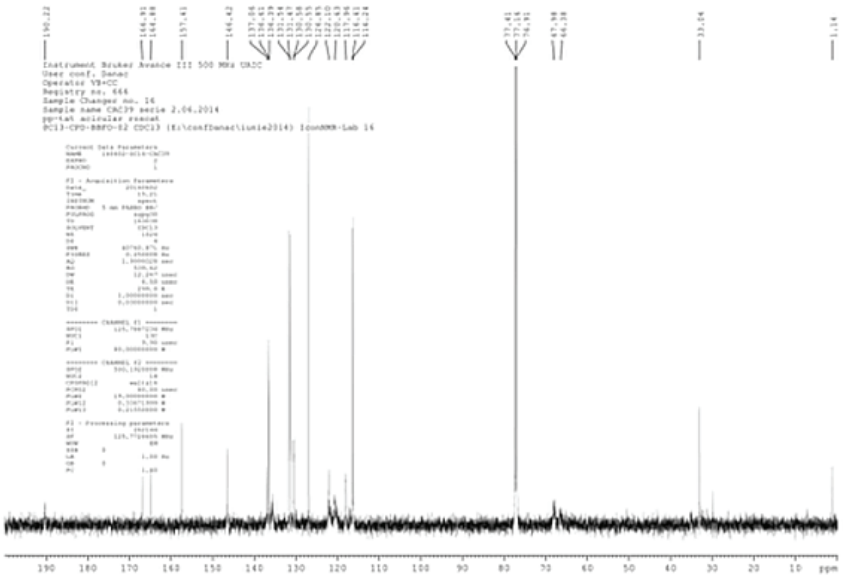


Fig. S-6. ^{13}C NMR spectrum of compound ^{13}C NMR of **6a**.

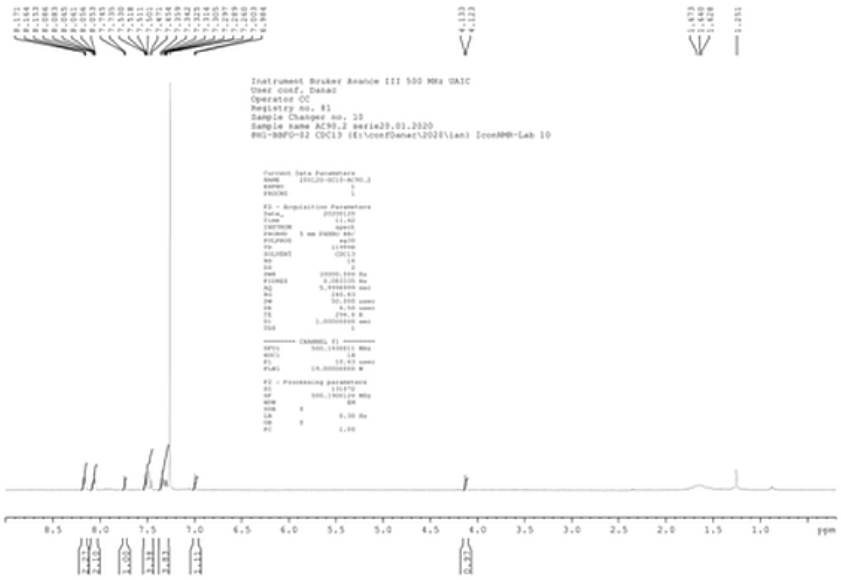


Fig. S-7. ^{1}H NMR spectrum of compound **7a**.