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SUPPLEMENTARY MATERIAL TO

Synthesis and characterization of palladium(II) complexes with glycine coumarin derivatives

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CHARACTERIZATION DATA FOR THE SYNTHESIZED COMPOUNDS

*2-([1-{2,4-Dioxochroman-3-ylidene}ethyl]amino)acetate (**HL[1]**).* Yield: 0.56 g (83 %); m.p.: 152 °C; Anal. Calcd. for $C_{14}H_{13}NO_5$ (FW: 275.26): C, 61.09; H, 4.76; N, 5.09 %. Found: C, 61.13; H, 4.85; N, 5.01 %; IR (KBr, cm^{-1}): 3406 (*w*), 3109 (*w*), 2961 (*w*), 2911 (*w*), 1748 (*s*), 1720 (*s*), 1617 (*s*), 1577 (*s*), 1486 (*m*), 1467 (*s*), 1428 (*m*), 1365 (*m*), 1332 (*m*), 1232 (*m*), 1215 (*s*), 1158 (*m*), 1113 (*m*), 1027 (*w*), 985 (*m*), 955 (*m*), 899 (*m*), 766 (*m*), 740 (*w*), 731 (*w*); ^{1}H-NMR (200 MHz, $CDCl_3$, δ / ppm): 2.70 (3H, *s*, H2′), 3.86 (3H, *s*, H3″), 4.32 (2H, AB_q, J_{ABq} = 12.99 Hz, H1″), 7.23 (2H, *m*, H6 & H7), 7.55 (1H, *dd*, ^3J = 8.10 Hz & ^4J = 2.11 Hz, H8), 8.07 (1H, *dd*, ^3J = 7.99 Hz & ^4J = 1.90 Hz, H5), 12.51 (0.25H, *bs*, OH), 14.65 (0.75 H, *bs*, NH) from enolic and enaminic tautomer, respectively; ^{13}C-NMR (50 MHz, $CDCl_3$, δ / ppm): 18.9 (C2′), 45.4 (C1″), 52.9 (C3″), 98.8 (C3), 116.4 (C8), 123.5 (C5), 126.2 (C6), 128.2 (C10), 133.9 (C7), 153.6 (C9), 162.5 (C2), 167.8 (C2″), 177.5 (C1′), 182.2 (C4).

*2-([1-{2,4-Dioxochroman-3-ylidene}ethyl]amino)acetic acid (**H_2L^2**).* Yield: 0.47 g (73 %); m.p.: 132 °C; Anal. Calcd. for $C_{13}H_{11}NO_5$ (FW: 261.23): C, 59.77; H, 4.24; N, 5.36 %. Found: C, 59.46; H, 4.07; N, 5.28 %; IR (KBr, cm^{-1}): 3502 (*w*), 3072 (*w*), 2917 (*w*), 1740 (*m*), 1650 (*m*), 1604 (*s*), 1560 (*m*), 1490 (*m*), 1463 (*m*), 1421 (*m*), 1359 (*m*), 1326 (*m*), 1293 (*w*), 1224 (*m*), 1144 (*w*), 1106 (*w*), 1039 (*w*), 989 (*w*), 904 (*w*), 756 (*w*), 717 (*w*), 673 (*w*), 645 (*w*), 576 (*w*), 519 (*w*), 450 (*w*); ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 2.60 (3H, *s*, H2′), 4.50 (2H,

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AB_q, J_{ABq} = 5.00 Hz, H1″), 7.42 (2H, *m*, H6 & H7), 7.81 (1H, *dd*, ^3J = 8.10 Hz & ^4J = 2.11 Hz, H8), 8.00 (1H, *dd*, ^3J = 8.00 Hz & ^4J = 2.00 Hz, H5), 13.74 (1H, *bs*, NH & OH); ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm: 19.2 (C2′), 45.9 (C1″), 95.5 (C3), 116.4 (C8), 123.9 (C5), 125.5 (C6), 125.9 (C10), 134.4 (C7), 153.2 (C9), 159.5 (C2), 169.5 (C2″), 176.5 (C1′), 178.1 (C4).

*Chlorido(methyl 2-[{1-(2,4-dioxochroman-3-ylidene)ethyl}amino]acetate)-palladium(II) complex (**1**)*. Yield: 0.030 g (47 %); Anal. Calcd. for $C_{14}H_{12}ClNO_5Pd$ (FW: 416.12): C, 40.41; H, 2.91; N, 3.37 %. Found: C, 39.99; H, 2.71; N, 3.62 %; IR (KBr, cm^{-1}) 2962 (*w*), 1676 (*s*), 1606 (*m*), 1566 (*m*), 1483 (*m*), 1454 (*w*), 1402 (*w*), 1366 (*w*), 1291 (*w*), 1250 (*w*), 1216 (*w*), 1115 (*w*), 1084 (*w*), 1021 (*w*), 994 (*w*), 945 (*w*), 909 (*w*), 878 (*w*), 751 (*w*), 684 (*w*), ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 2.97 (3H, *s*, H2′), 3.15 (3H, *s*, H3″), 4.47 (2H, *s*, H1″), 7.30 (2H, *m*, H6 & H7), 7.65 (1H, *t*, ^3J = 8.00 Hz, H8), 7.89 (1H, *d*, ^3J = 8.00 Hz, H5).

*Dimethylamine(2-[{1-(2,4-dioxochroman-3-ylidene)ethyl}amino]acetato)palladium(II) complex (**2**)*. Yield 86 %; Anal. Calcd. for $C_{15}H_{16}N_2O_5Pd{\cdot}H_2O$ (FW: 428.74): C, 42.02; H, 4.23; N, 6.53 %. Found: C, 41.34; H, 4.46; N, 6.47 %; IR (KBr, cm^{-1}): 3227 (*m*), 3071 (*w*), 3020 (*w*), 2986 (*w*), 2936 (*w*), 1690 (*s*), 1660 (*s*), 1601 (*m*), 1573 (*m*), 1482 (*m*), 1440 (*w*), 1403 (*m*), 1348 (*m*), 1292 (*w*), 1269 (*w*), 1245 (*w*), 1214 (*w*), 1141 (*w*), 1108 (*w*), 1081 (*w*), 1064 (*w*), 1026 (*w*), 986 (*w*), 939 (*w*), 903 (*w*), 759 (*m*), 684 (*w*), 617 (*w*), 580 (*w*), 530 (*w*); ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 2.35 (3H, *s*, H2′), 2.40 (6H, *s*, CH_3 from dimethylamine), 2.52 (1H, *s*, NH from dimethylamine), 4.41 (2H, H1″), 7.27 (2H, *m*, H7), 7.31 (2H, *m*, H6), 7.63 (1H, *td*, ^3J = 8.00 Hz & ^4J = 2.00 Hz, H8), 7.98 (1H, *dd*, ^3J = 8.00 Hz & ^4J = 1.50 Hz, H5); ^{13}C-NMR (125 MHz, DMSO-d_6, δ / ppm): 19.8 (C2′), 41.0 (CH_3 from dimethylamine), 60.3 (C1″), 102.6 (C3), 115.8 (C7), 118.0 (C10), 123.9 (C6), 126.0 (C5), 133.6 (C8), 151.8 (C9), 161.5 (C2), 165.8 (C2″), 170.2 (C1′), 178.8 (C4).

NMR abbreviations: *s* – singlet, *d* – doublet, *dd* – doublet of doublets, *td* – triplet of doublets, *m* – multiplet, *bs* – broadened singlet.

TABLE S-I. Crystal data and structure refinement for **2**

Empirical formula	$C_{15}H_{18}N_2O_6Pd$
Formula weight	428.71
Temperature, K	293.15
Crystal system	monoclinic
Space group	$P2_1/n$
a / Å	14.425(5)
b / Å	6.913(2)
c / Å	15.918(5)
α / °	90
β / °	102.100(6)
γ / °	90

TABLE S-I. Continued

V / Å^3	1552.1(9)
Z	4
ρ_{calc} / g cm^{-3}	1.835
μ / mm^{-1}	1.231
F(000)	864
Crystal size, mm^3	0.35 × 0.2 × 0.012
Radiation	MoKα (λ = 0.71073 Å)
2θ range for data collection, °	3.466 – 64.286
Index ranges	$-20 \leq h \leq 20$, $-10 \leq k \leq 10$, $-23 \leq l \leq 23$
Reflections collected	23580
Independent reflections	5123 [R_{int} = 0.0910, R_{sigma} = 0.0875]
Data / restraints/parameters	5123 / 0/247
Goodness-of-fit on F^2	0.894
Final R indexes [$<I> = 2\sigma(I)$]	R_1 = 0.0548, wR_2 = 0.1338
Final R indexes (all data)	R_1 = 0.1347, wR_2 = 0.1746
Largest F max / min, e Å^{-3}	0.69 / –0.77