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Supplementary material

SUPPLEMENTARY MATERIAL TO

Synthesis, characterization and biological activity of new Ni(II), Pd(II) and Cr(III) complex compounds with chlorhexidine

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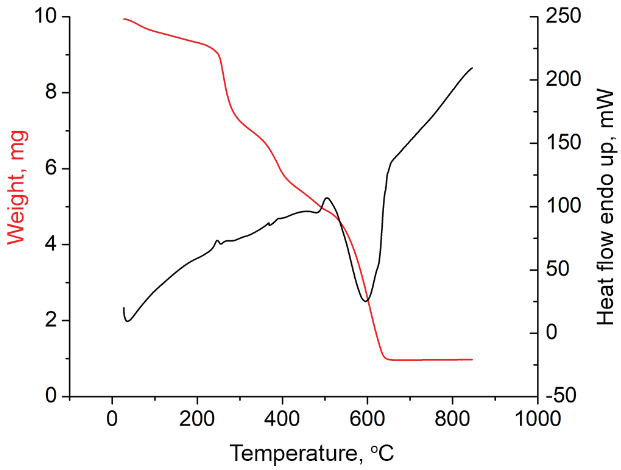

Fig. S-1. TG and DTA curves for $[Ni(CHX)]Cl_2\cdot 2H_2O$ (**1**).

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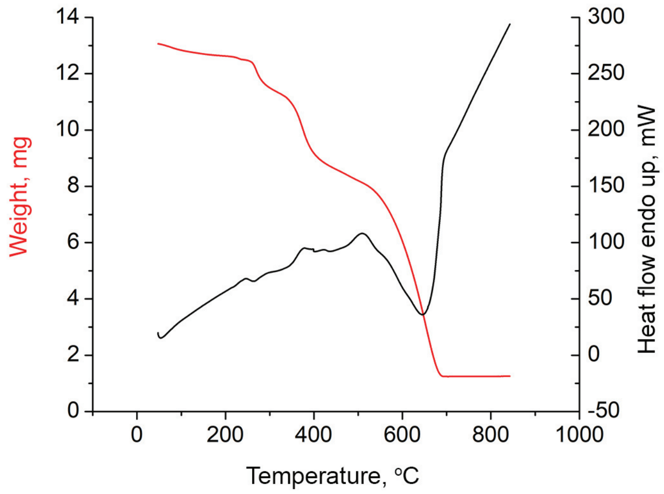

Fig. S-2. TG and DTA curves for $[Ni(CHX)]Br_2 \cdot 2H_2O$ (**2**).

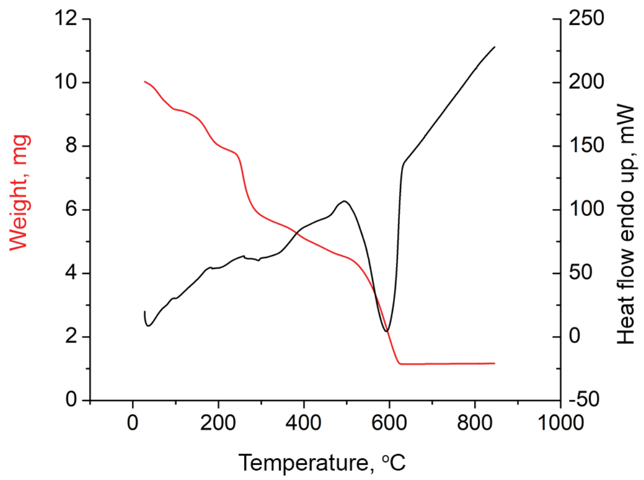

Fig. S-3. TG and DTA curves for $[Ni(CHX)](CH_3COO)_2 \cdot C_2H_5OH$ (**3**).

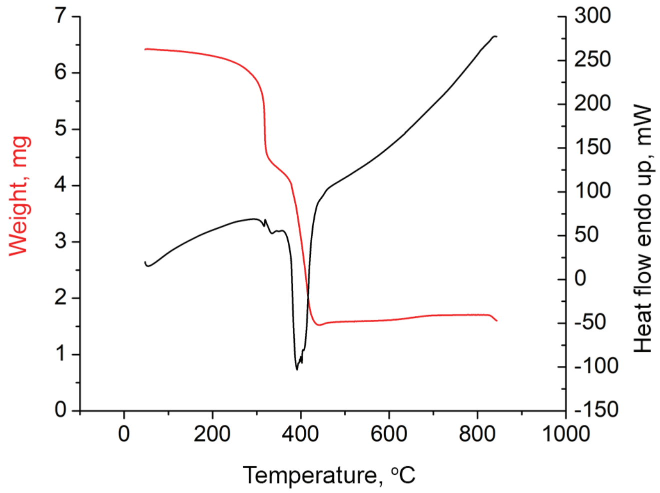

Fig. S-4. TG and DTA curves for $[Pd(CHX)][PdCl_4]\cdot 2H_2O$ (**4**).

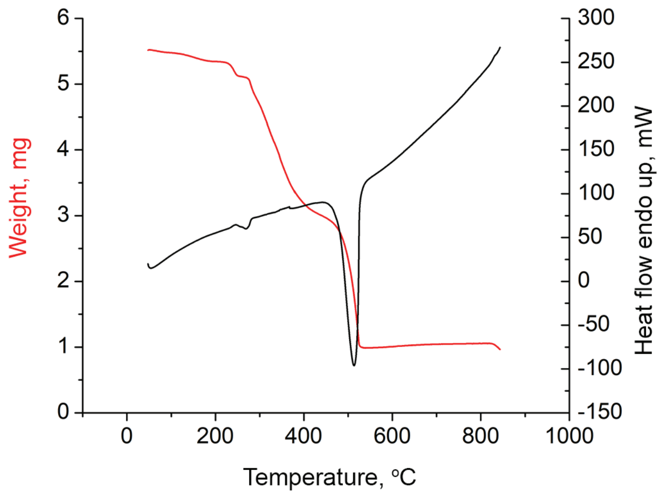

Fig. S-5. TG and DTA curves for $[Pd(CHX)](CH_3COO)_2$ (**5**)

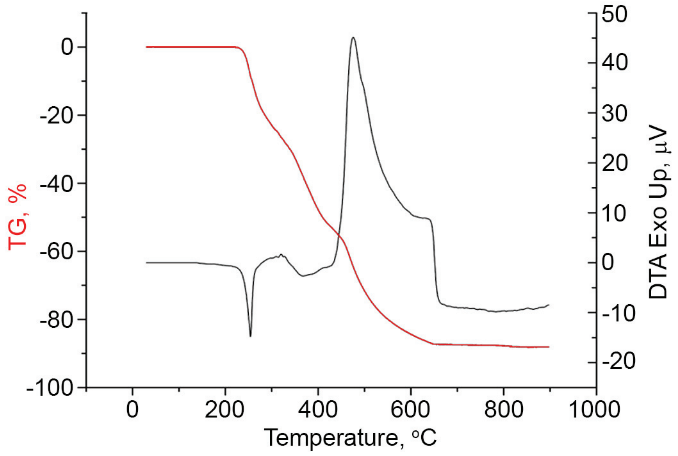

Fig. S-6. TG and DTA curves for $[Cr(CHX)Cl_2](CH_3COO)$ (**6**).

NMR DATA

Chlorhexidine diacetate monohydrate. ^{1}H-NMR (300 MHz, DMSO-d_6 δ / ppm): 1.25 (4H, *bs*, $2CH_2$), 1.45 (4H, *bs*, $2CH_2$), 1.71 (6H, *s*, $2CH_3COO$), 3.03 (4H, *bs*, $2NCH_2$), 7.26, 7.43 (8H, *2d*, J = 8.5 Hz, Ar-H), 7.45–7.80, 8.20–8.60 (*bs*, NH); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 24.7 ($2CH_3$), 25.9 ($2CH_2$), 28.8 ($2CH_2$), 40.5 ($2CH_2N$), 122.1, 125.8, 128.8, 139.9 (4C, Ar-C), 155.1, 159.6 (C=NH), 175.9 (COO).

*[Ni(CHX)]Br$_2$·2H$_2$O (**2**)*. ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 1.27 (4H, *bs*, $2CH_2$), 1.40 (4H, *bs*, $2CH_2$), 3.06 (4H, *bs*, $2NCH_2$), 7.29–7.36 (8H, *m*, Ar-H), 7.70, 8.80 (2*bs*, NH); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 26.0 ($2CH_2$), 28.7 ($2CH_2$), 39.5 ($2CH_2N$), 122.0, 128.4, 128.9, 137.5 (4C, Ar-C), 153.3, 154.8, 160.2 (C=NH).

*[Pd(CHX)][PdCl$_4$]·2H$_2$O (**4**)*. ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 1.30 (4H, *bs*, $2CH_2$), 1.46 (4H, *bs*, $2CH_2$), 3.11 (4H, *bs*, $2NCH_2$), 7.35 (8H, *bs*, Ar-H), 9.56 (1*bs*, NH); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 25.8 ($2CH_2$), 28.1 ($2CH_2$), 41.6 ($2CH_2N$), 122.2, 125.3, 128.5, 129.9, 135.4 (4C, Ar-C), 148.5, 150.0, 160.6 (C=NH).