Supporting Information

New Ru(II) Complexes Containing dmso and pyrazolyl Ligands as Catalysts for Nitrile Hydration in environmentally friendly media

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Keywords: catalysis / Hydration / Ruthenium complexes / dmso complexes / Pyrazolyl ligands / recyclability.

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Table S1. Crystallographic Data for Complex **2**.

	2
Empirical formula	$C_{24}H_{40}Cl_4N_6O_5Ru_2S_4$
Formula weight	964.80
Crystal system	Monoclínic
Space group	C2/c
a [Å]	24.7647(10)
b [Å]	11.7498(5)
c [Å]	14.0980(5)
α [°]	90
β [°]	116.3070(10)
γ [°]	90
V [Å^3]	3677.4(3)
Formula Units/ cell	4
Temp. [K]	300(2)
ρ_{calc}, [Mg/m^{-3}]	1.743
μ [mm^{-1}]	1.382
Final R indices, [I>2σ(I)]	R1=0.0224 wR2 = 0.0663
R indices [all data]	R1=0.0243 wR2 = 0.0675

$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

$wR_2 = [\Sigma\{w(F_o^2-F_c^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$, where $w = 1/[\sigma^2(Fo^2) + (0.0042P)^2]$ and $P=(F_o^2+2F_c^2)$

Table S2. Selected Bond Lengths (Å) and Angles (°) for Complex **2**.

Ru(1)-N(3)	2.0313(15)
Ru(1)-N(1)	2.1237(15)
Ru(1)-S(2)	2.2432(5)
Ru(1)-S(1)	2.2558(5)
Ru(1)-Cl(1)	2.4103(5)
Ru(1)-Cl(2)	2.4277(5)
N(3)-Ru(1)-N(1)	76.92(6)
N(3)-Ru(1)-S(2)	90.03(4)
N(1)-Ru(1)-S(2)	92.89(4)
N(3)-Ru(1)-S(1)	96.74(4)
N(1)-Ru(1)-S(1)	171.61(5)
S(2)-Ru(1)-S(1)	92.595(19)
N(3)-Ru(1)-Cl(1)	171.27(4)
N(1)-Ru(1)-Cl(1)	94.66(4)
S(2)-Ru(1)-Cl(1)	92.735(19)
S(1)-Ru(1)-Cl(1)	91.413(19)
N(3)-Ru(1)-Cl(2)	86.95(4)
N(1)-Ru(1)-Cl(2)	83.49(4)
S(2)-Ru(1)-Cl(2)	175.728(18)
S(1)-Ru(1)-Cl(2)	90.75(2)
Cl(1)-Ru(1)-Cl(2)	89.83(2)

Table S3. Selected Bond Lengths (Å) and Angles (°) for Complex **3**.

	3
Empirical formula	$C_9H_{22}Cl_2N_2O_3RuS_3$
Formula weight	474.44
Crystal system	Monoclínic
Space group	P21
a [Å]	8.531(7)
b [Å]	13.122(11)
c [Å]	8.953(8)
α [°]	90
β [°]	116.997(13)
γ [°]	90
V [Å^3]	893.1(13)
Formula Units/ cell	4
Temp, [K]	300(2)
ρcalc, [Mg/m^{-3}]	1.764
μ [mm^{-1}]	1.533
Final R indices, [I>2σ(I)]	R1=0.0521 wR2 = 0.1475
R indices [all data]	R1=0.0729 wR2 = 0.2150

$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$

$wR_2 = [\Sigma\{w(F_o^2-F_c^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$, where $w = 1/[\sigma^2(Fo^2) + (0.0042P)^2]$ and $P=(F_o^2+2F_c^2)$

Table S4. Selected Bond Lengths (Å) and Angles (°) for Complex **3**.

Ru(1)-N(1)	2.145(9)
Ru(1)-S(1)	2.295(3)
Ru(1)-S(2)	2.309(3)
Ru(1)-S(3)	2.316(4)
Ru(1)-Cl(1)	2.429(4)
Ru(1)-Cl(2)	2.447(3)
N(1)-Ru(1)-S(1)	94.4(3)
N(1)-Ru(1)-S(2)	89.8(3)
S(1)-Ru(1)-S(2)	91.51(13)
N(1)-Ru(1)-S(3)	170.6(3)
S(1)-Ru(1)-S(3)	92.16(14)
S(2)-Ru(1)-S(3)	96.78(14)
N(1)-Ru(1)-Cl(1)	84.4(3)
S(1)-Ru(1)-Cl(1)	89.39(12)
S(2)-Ru(1)-Cl(1)	174.14(14)
S(3)-Ru(1)-Cl(1)	88.97(13)
N(1)-Ru(1)-Cl(2)	87.6(3)
S(1)-Ru(1)-Cl(2)	176.63(14)
S(2)-Ru(1)-Cl(2)	91.24(12)
S(3)-Ru(1)-Cl(2)	85.57(14)
Cl(1)-Ru(1)-Cl(2)	88.08(13)

Figure S1.

a)

b)

Figure S2.

a)

b)

c)

Espectre 2D COSY 1H-1H

d)

NOESY

e)

Espectre 2D 1H-13C HMBC
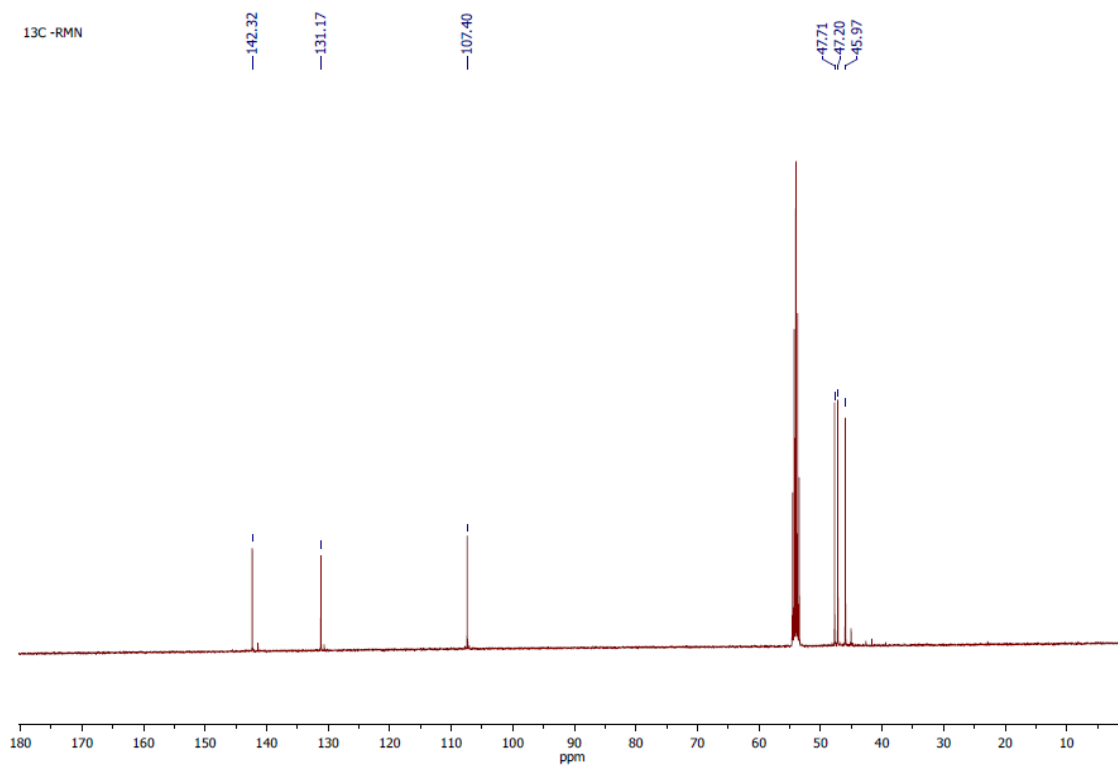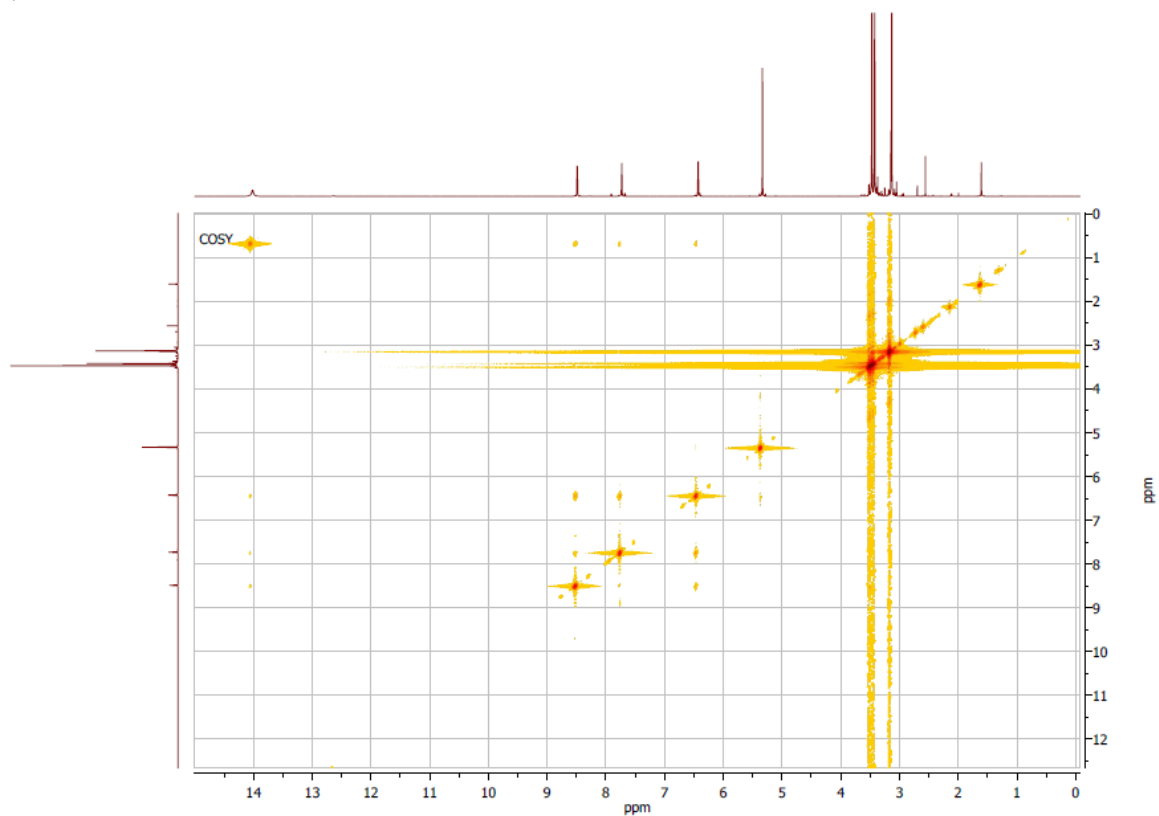Optimitzat 8 Hz

f)

Espectre 2D1H-13C HSQC
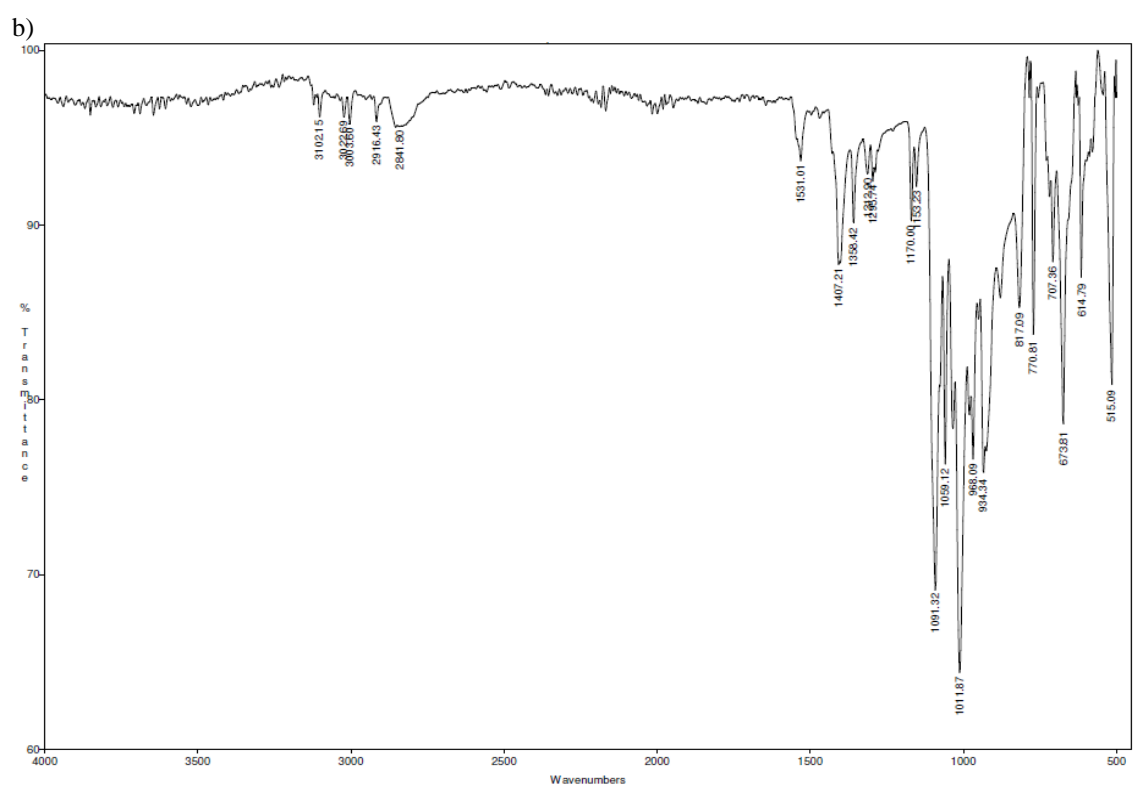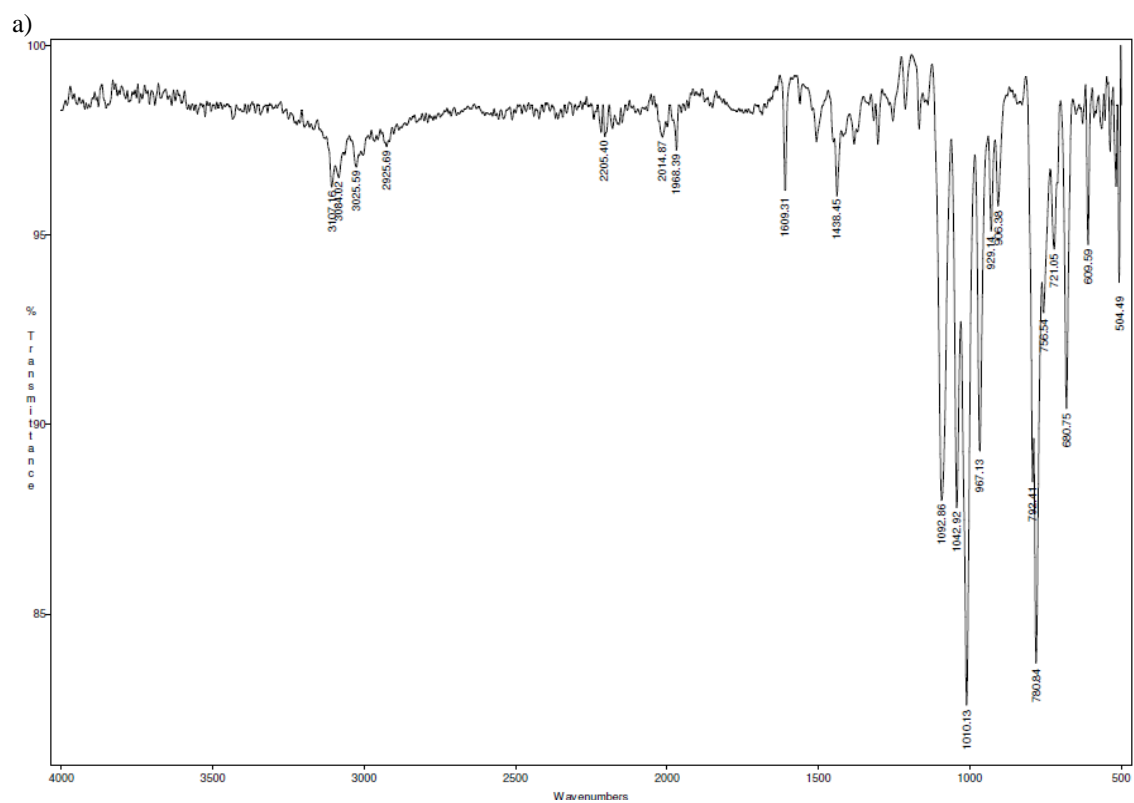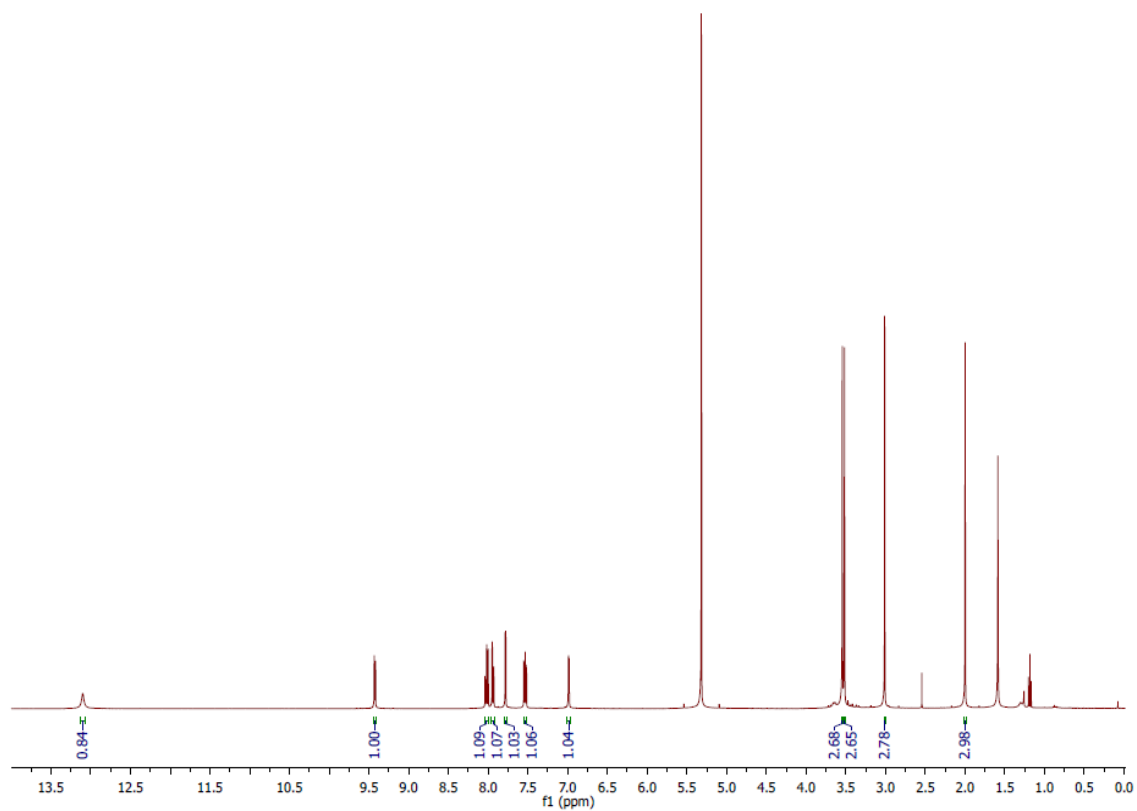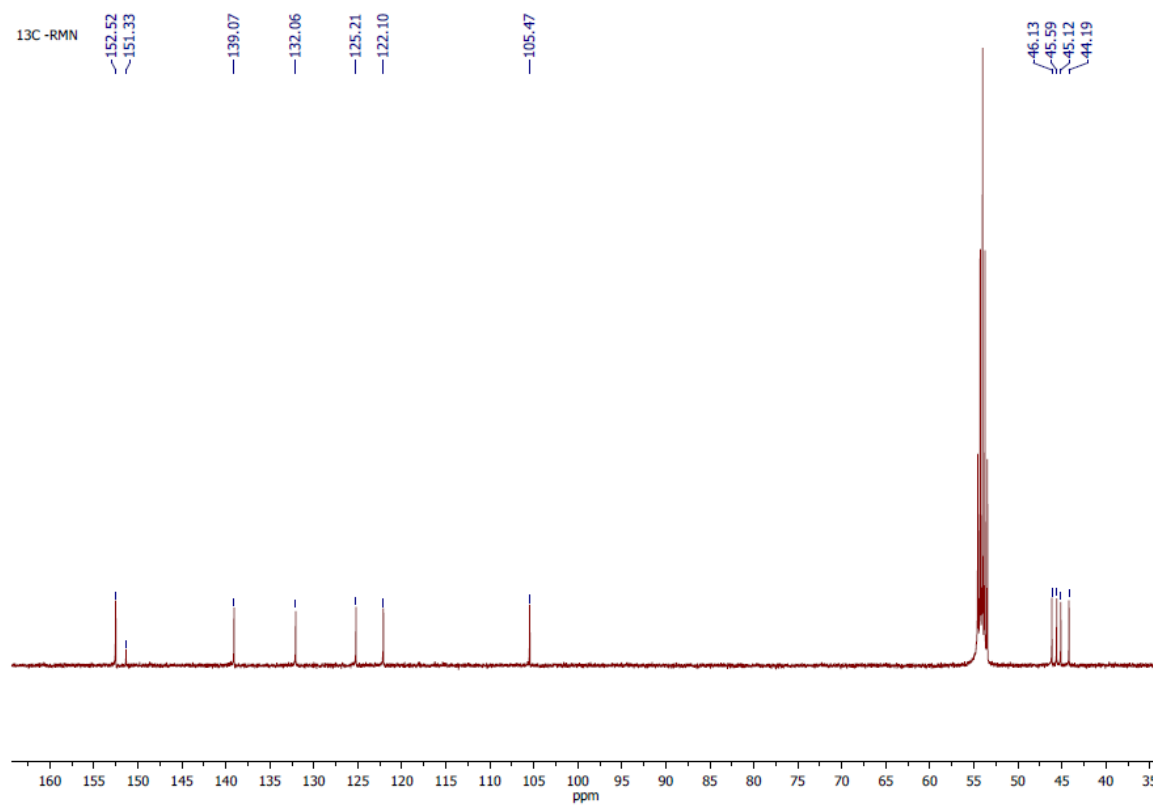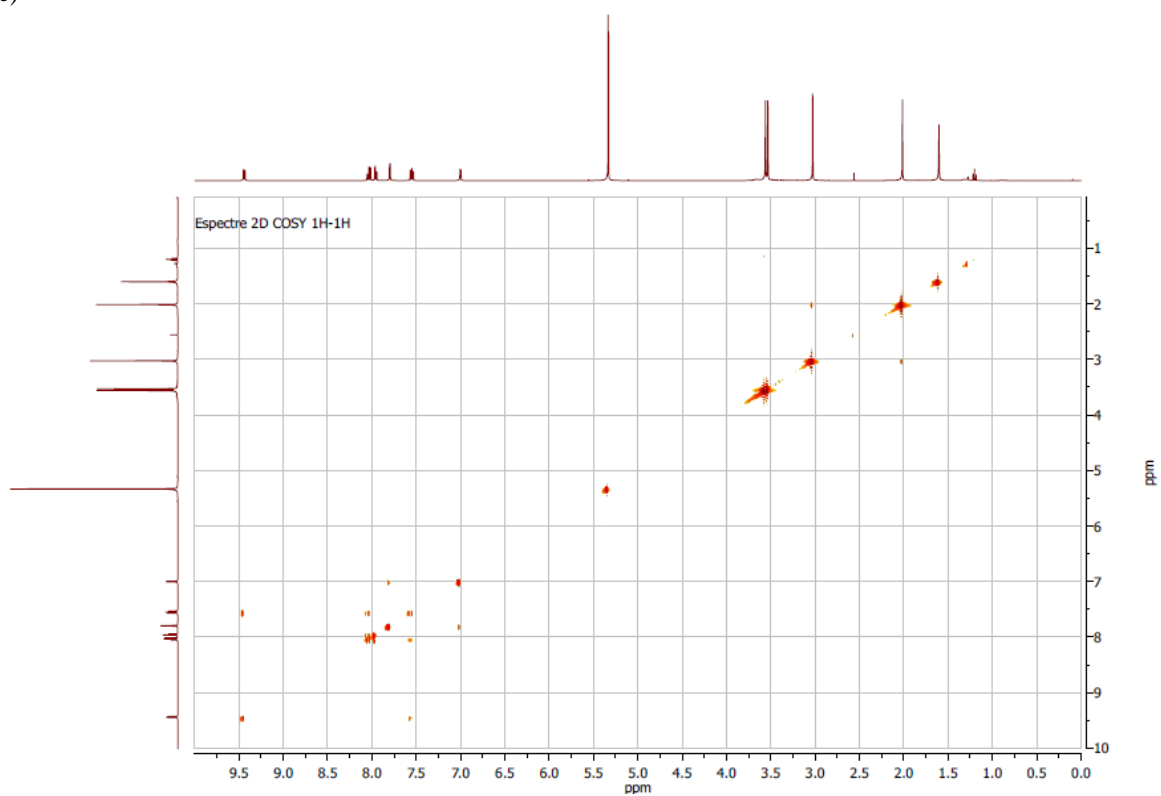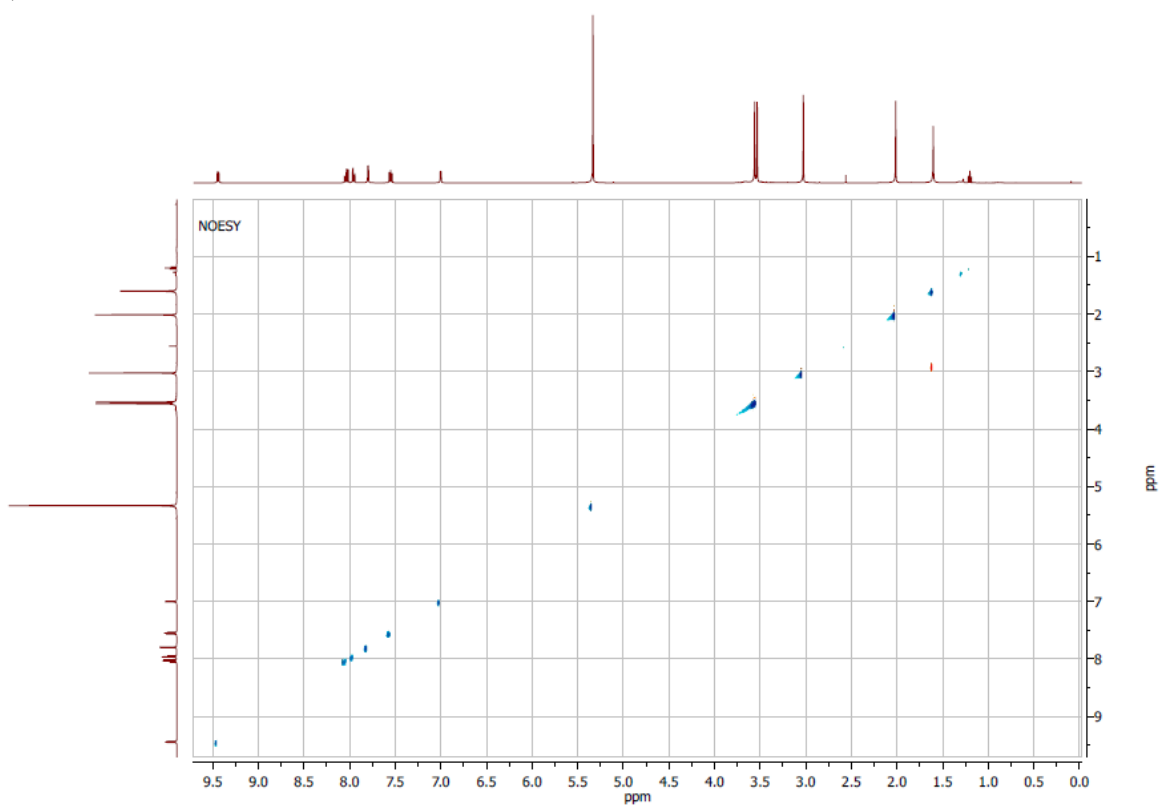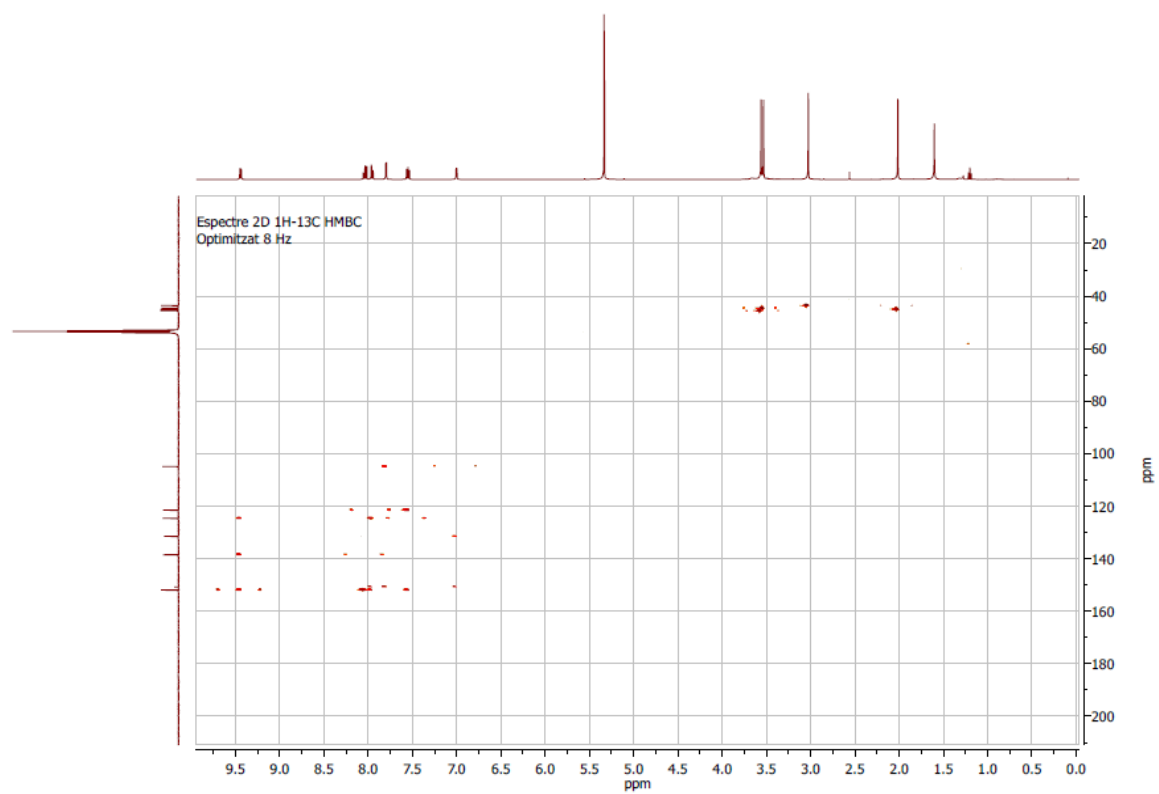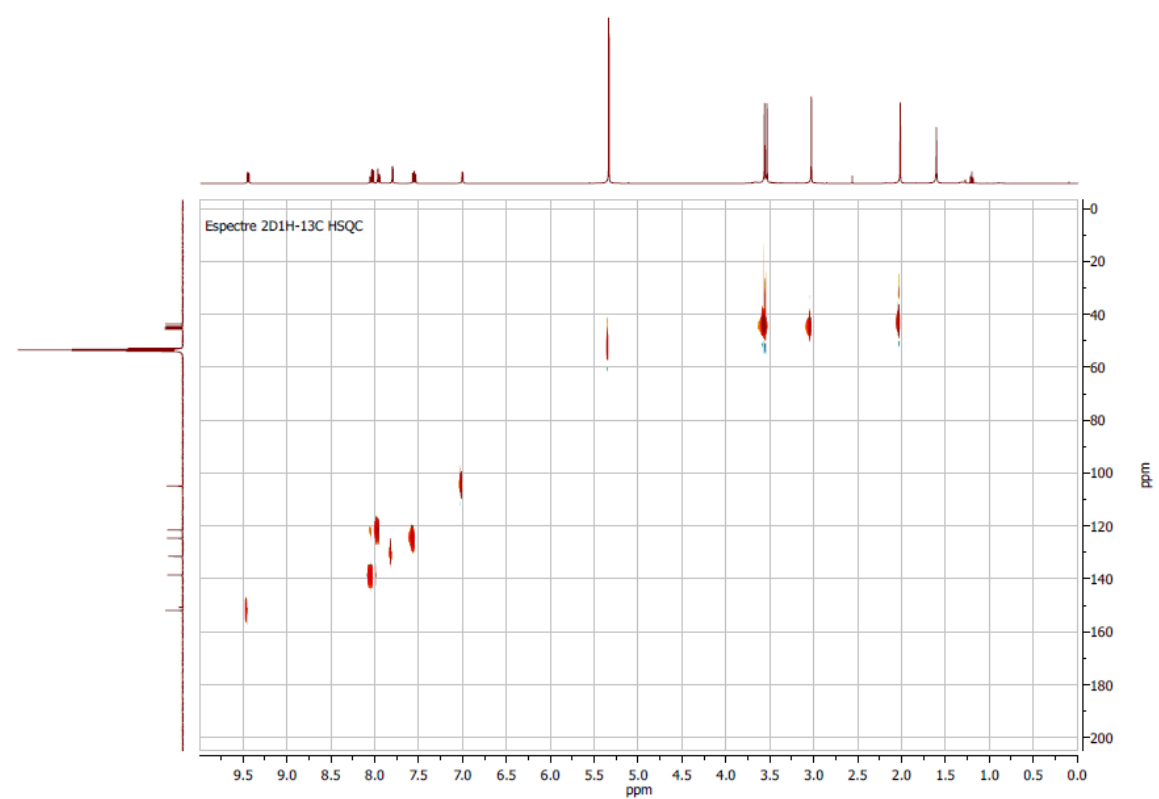
Figure S3.

a)
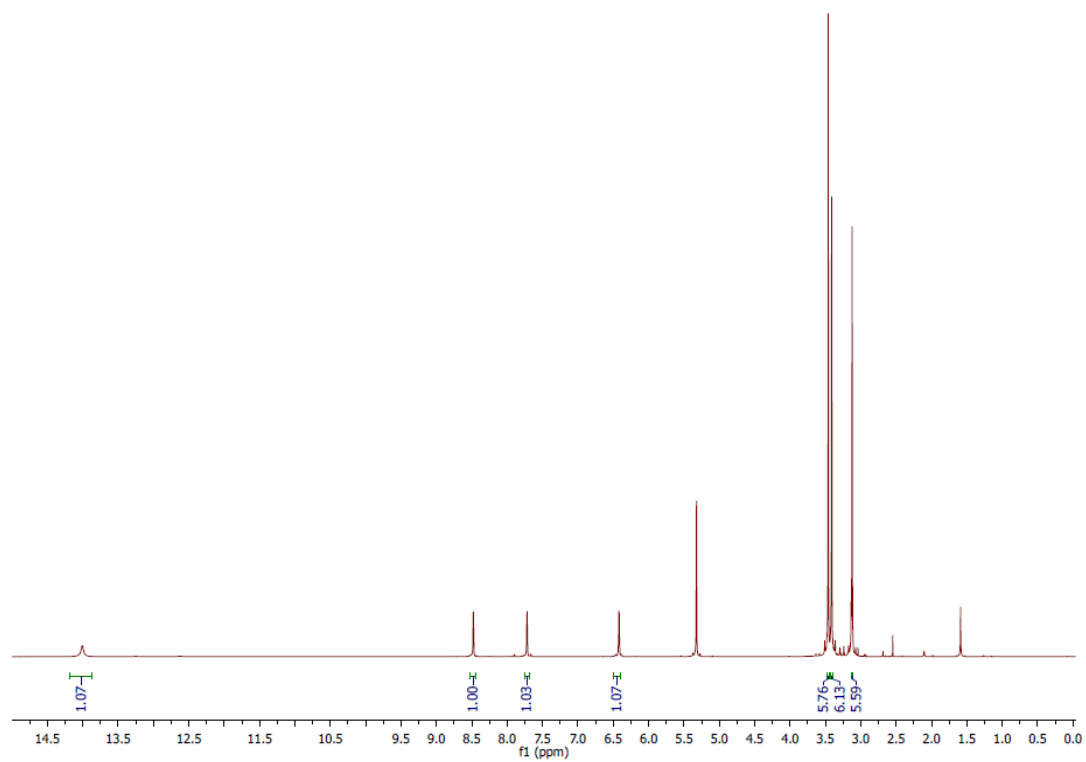
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c)

d)
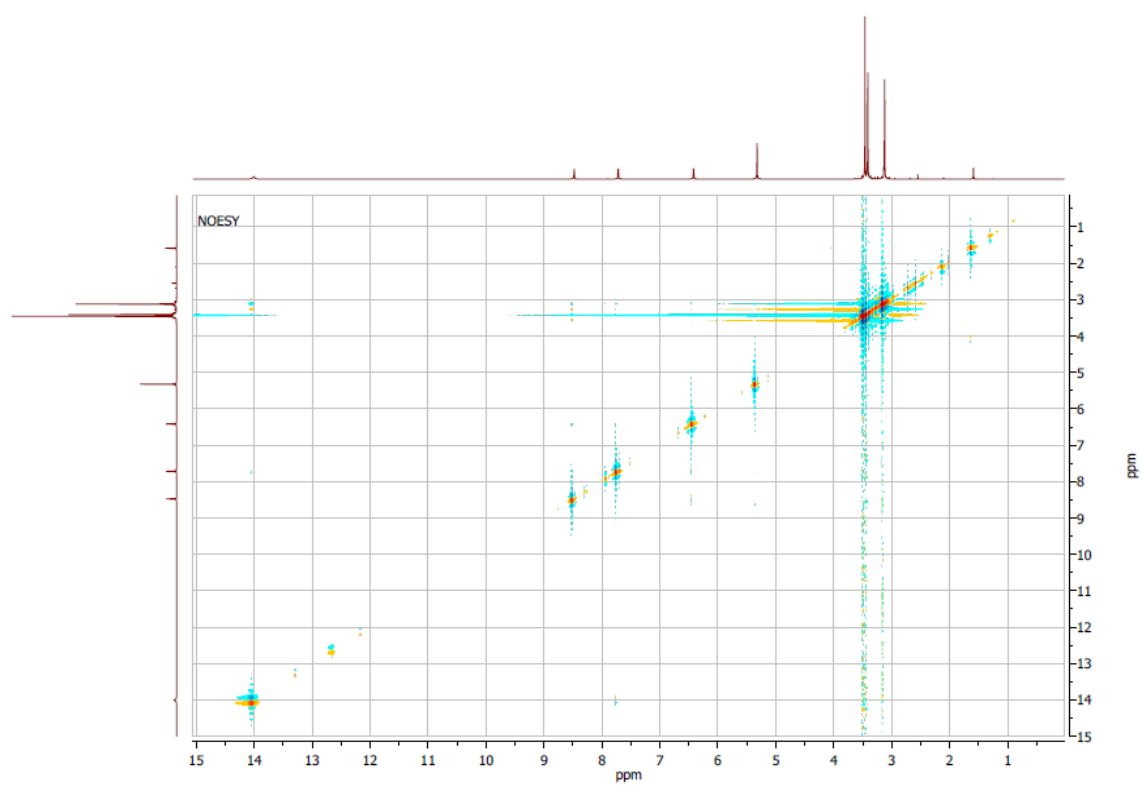
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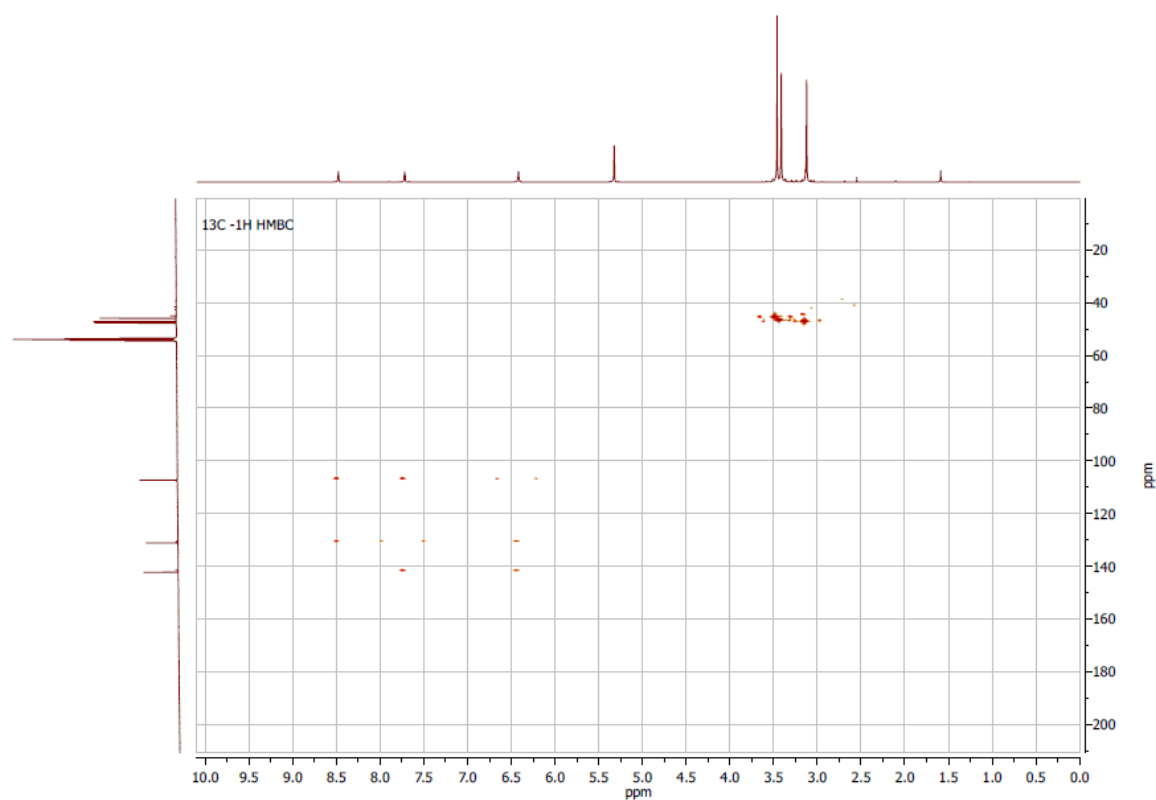
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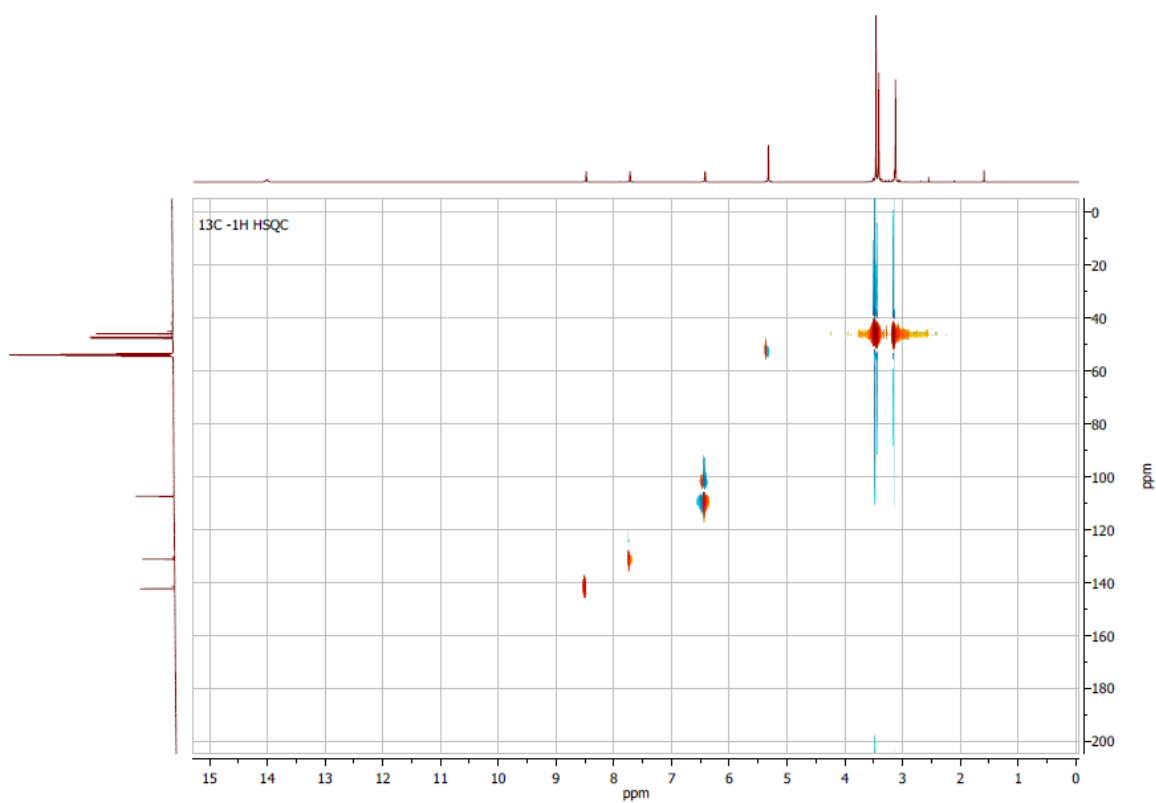
Figure S4.
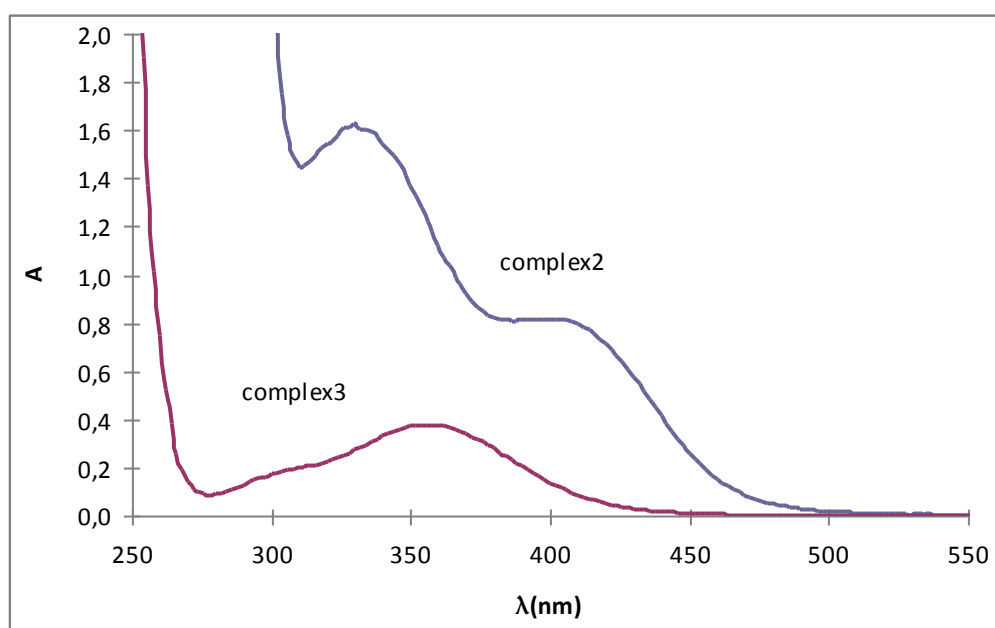
Figure S5.

Figure S6.

Figure S7.