Supplementary Information for:

Supramolecular architectures based on p-cymene/ruthenium complexes functionalized with nucleobases

Fabio Sce,[a,b] Garikoitz Beobide,[,a] Oscar Castillo,*[,a] Imanol de Pedro,[b] Sonia Pérez-Yáñez[a] and Efraim Reyes[c]*

[a]Departamento de Química Inorgánica, Facultad de Ciencia y Tecnología, Universidad del País Vasco/Euskal Herriko Unibertsitatea, UPV/EHU, Apartado 644, E-48080 Bilbao, Spain.

[b]CITIMAC, Facultad de Ciencias, Universidad de Cantabria, 39005 Santander, Spain.

[c]Departamento de Química Orgánica II, Facultad de Ciencia y Tecnología, Universidad del País Vasco/Euskal Herriko Unibertsitatea, UPV/EHU, Apartado 644, E-48080 Bilbao, Spain.

Table S1. Most relevant coordination bonds (Å) and angles (º) for compounds **1**-**4**.

Compound **1**			
	Bonds		Angles
Ru1-C11/C16	2.155(3)-2.195(3)	Cl1-Ru1-Cl2	87.23(3)
Ru1-Cl1	2.429(1)	Cl1-Ru1-N4	90.72(7)
Ru1-Cl2	2.443(1)	Cl2-Ru1-N4	86.93(7)
Ru1-N4	2.100(2)		
Compound **2**			
	Bonds		Angles
Ru1-C31/C36	2.164(7)-2.205(7)	Cl1-Ru1-Cl2	87.12(6)
Ru1-Cl1	2.417(2)	Cl1-Ru1-S12	88.17(6)
Ru1-Cl2	2.431(2)	Cl2-Ru1-S12	93.13(7)
Ru1-S12	2.411(2)		
Ru2-C41/C46	2.171(7)-2.208(7)	Cl3-Ru2-Cl4	85.80(6)
Ru2-Cl3	2.430(2)	Cl3-Ru2-S22	92.86(6)
Ru2-Cl4	2.428(2)	Cl4-Ru2-S22	90.11(6)
Ru2-S22	2.406(2)		
Compound **3**			
	Bonds		Angles
Ru1-C11/C16	2.155(2)-2.211(2)	Cl1-Ru1-Cl2	87.81(2)
Ru1-Cl1	2.426(1)	Cl1-Ru1-N9	86.61(5)
Ru1-Cl2	2.435(1)	Cl2-Ru1-N9	83.55(4)
Ru1-N9	2.138(2)		
Compound **4**			
	Bonds		Angles
Ru1-C11/C16	2.168(3)-2.199(3)	Cl1-Ru1-Cl2	88.31(2)
Ru1-Cl1	2.406(1)	Cl1-Ru1-N5	81.89(6)
Ru1-Cl2	2.427(1)	Cl2-Ru1-N5	82.10(6)
Ru1-N5	2.165(2)		
Compound **5**[a]			
	Bonds		Angles
Ru1-C11/C16	2.088(10)-2.226(10)	N1-Ru1-N3^{i}	87.70(14)
Ru1-N1^{i}	2.119(4)	N1-Ru1-O2^{i}	84.22(12)
Ru1-N3	2.092(4)	N3-Ru1-O2	61.90(13)
Ru1-O2	2.145(3)		

[a]Symmetry codes: (i) *– y + 1/2, x, – z + 3/2.*

Table S2. Structural parameters (Å, º) for non-covalent interactions in compound **1**.[a]

D–H···A[b]	H···A	D···A	D–H···A
N1-H1···O2^{i}	1.94	2.782(3)	164.7
N3-H3···Cl1	2.41	3.079(3)	135.2
N3-H3···Cl2	2.77	3.335(2)	124.2
N4-H4···Cl2^{ii}	2.57	3.424(2)	176.2
C6-H6···Cl2^{iii}	2.78	3.640(3)	154.0
C17-H17···O2^{ii}	2.44	3.353(4)	158.0

π-π interactions[c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
cyt–cyt^{iv}	0.0	3.78	31.2	3.23	1.96

[a]Symmetry codes: (i) *– x + 2*, *– y*, *– z + 2*; (ii) *x – 1*, *y*, *z;* (iii) *x – 1, y – 1*, z; (iv) *– x +1, – y –1, –z + 2*. [b]D:donor, A: acceptor. [c]Angle: dihedral angle between the planes (°), DC: distance between the centroids of the rings (Å), α: angle between the normal to the first ring and the DC vector (°), DZ: interplanar distance (Å), DXY: lateral displacement (Å). [d]cyt: aromatic ring of the cytosine.

Table S3. Structural parameters (Å, º) for non-covalent interactions in compound **2**.[a]

D–H···A[b]	H···A	D···A	D–H···A
N11-H11···Cl1^{i}	2.29	3.132(6)	167.9
N13-H13···Cl2	2.28	3.080(6)	154.5
N21-H21···Cl3^{ii}	2.72	3.347(7)	130.6
N21-H21···Cl4^{ii}	2.43	3.192(6)	148.3
N23-H23···Cl3	2.40	3.122(6)	142.2
N23-H23···Cl4	2.63	3.194(6)	124.7
C25-H25···O24^{iii}	2.49	3.419(11)	173.0
C26-H26···O24^{ii}	2.58	3.472(9)	162.0

π-π interactions[c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
thiur–cym^{iv}	6.26	3.62	19.3	3.42	0.0

[a]Symmetry codes: (i) *x + 1*, *y*, *z* ; (ii) *x – 1*, *y*, *z*; (iii) *–x, -y – 1, -z + 2*; (iv) *–x + 1, -y, -z + 1*. [b]D:donor, A: acceptor. [c]Angle: dihedral angle between the planes (°), DC: distance between the centroids of the rings (Å), α: angle between the normal to the first ring and the DC vector (°), DZ: interplanar distance (Å), DXY: lateral displacement (Å). [d]thiur: aromatic ring of the 2-thiouracil, cym: aromatic ring of p-cymene.

Table S4. Structural parameters (Å, º) for non-covalent interactions in compound **3**.[a]

D–H···A[b]	H···A	D···A	D–H···A
N1-H1···Cl2[i]	2.40	3.206(2)	155.4
N7-H7···O6[ii]	1.90	2.723(2)	158.4

π-π interactions[c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
hypo–hypo[i]	0.02	3.45	23.4	3.17	1.37

[a] Symmetry codes: (i) *-x, -y, -z + 1* ; (ii) *-x + 1, -y, -z + 2*. [b] D:donor, A: acceptor. [c]Angle: dihedral angle between the planes (°), DC: distance between the centroids of the rings (Å), α: angle between the normal to the first ring and the DC vector (°), DZ: interplanar distance (Å), DXY: lateral displacement (Å). [d] hypo: pyrimidinic ring of the hypoxhantine.

Table S5 Structural parameters (Å, º) for non-covalent interactions in compound **4**.[a]

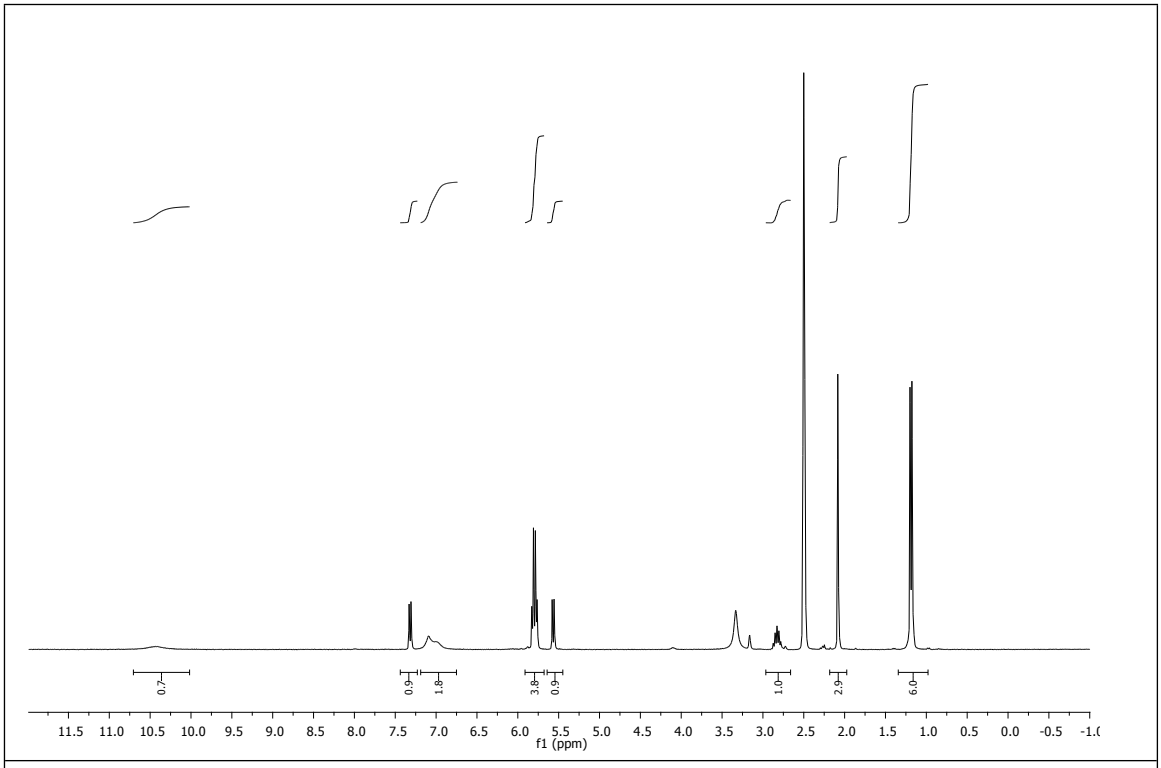
D–H···A[b]	H···A	D···A	D–H···A
N1-H1···O2[i]	1.91	2.758(3)	166.6
N3-H3···O4[ii]	1.91	2.766(3)	173.8
N5-H5A···Cl2[iii]	2.46	3.281(2)	151.0

[a]Symmetry codes: (i) *-x + 2, -y, -z +2* ; (ii) *-x + 2, -y +1, -z +2 ;* (iii) *-x + 1, -y, -z +1*. [b]D:donor, A: acceptor.

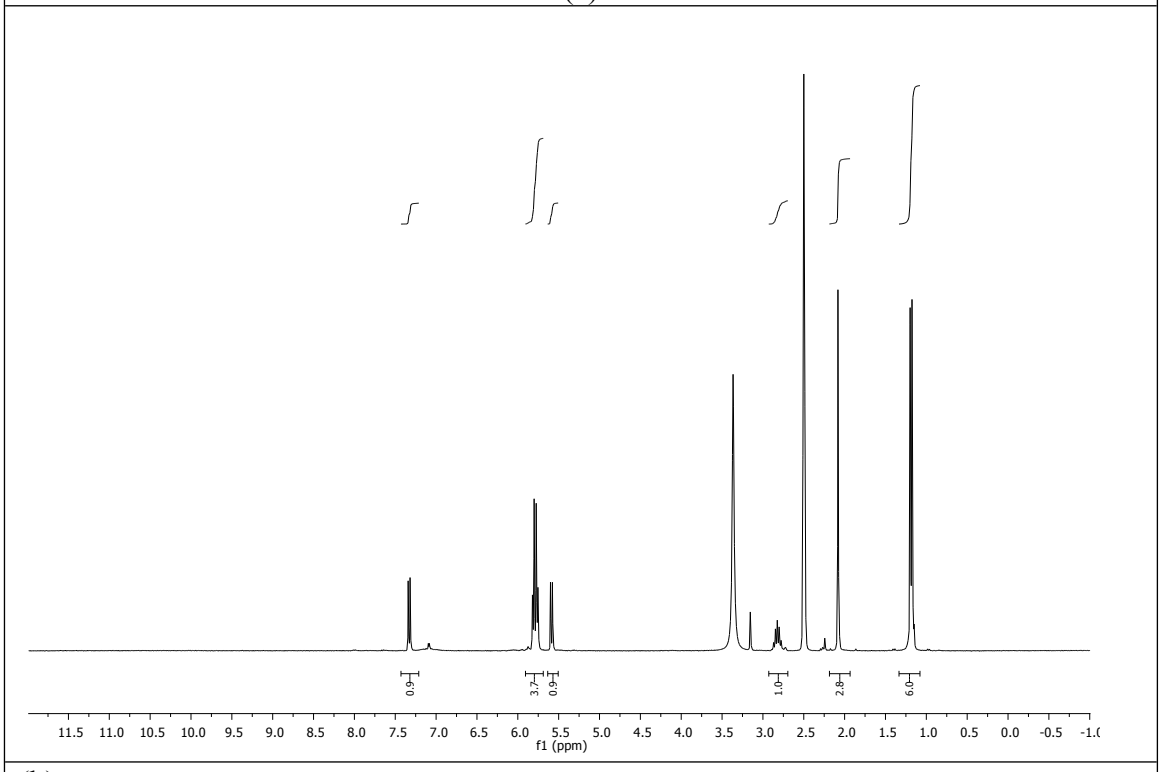
Table S6. Supramolecular parameters (Å, º) for hydrogen bonding interactions in compound **5**.[a]

D–H···A[b]	H···A	D···A	D–H···A
N4-H4A···O11B[i]	2.02	2.87(1)	174.5
N4-H4A···O12A[i]	2.21	2.89(1)	135.5
N4-H4B···O13A	2.21	2.90(1)	138.2
N4-H4B···O13B	2.28	3.07(1)	152.6

[a] Symmetry codes: (i) *–x + 1, -y + 1, -z + 2.* [b] D:donor, A: acceptor.



(a)



(b)

Figure S1. H1-NMR of compound 1 (a) in DMSO and (b) in DMSO/D2O. δ (ppm): 10.44 (sa, 1H, NH), 7.32 (d, *J* = 7.0 Hz, 1H, CytosineCH), 7.09 (s, 2H, NH and NH), 5.82 (d, *J* = 6.1 Hz, 2H, CymeneCH), 5.77 (d, *J* = 6.3 Hz, 2H, CymeneCH), 5.57 (d, *J* = 7.0 Hz, 1H, CytosineCH), 2.92 – 2.74 (m, 1H, Cymene*i*Pr), 2.08 (s, 3H, CymeneCH_3), 1.19 (d, *J* = 6.9 Hz, 6H, Cymene*i*Pr).