Electronic Supplementary Material (ESI) for RSC Advances.

Anticancer and antimicrobial properties of novel η^6-*p*-cymene ruthenium(II) complexes containing a *N,S*-type ligand, and their structural and theoretical characterization

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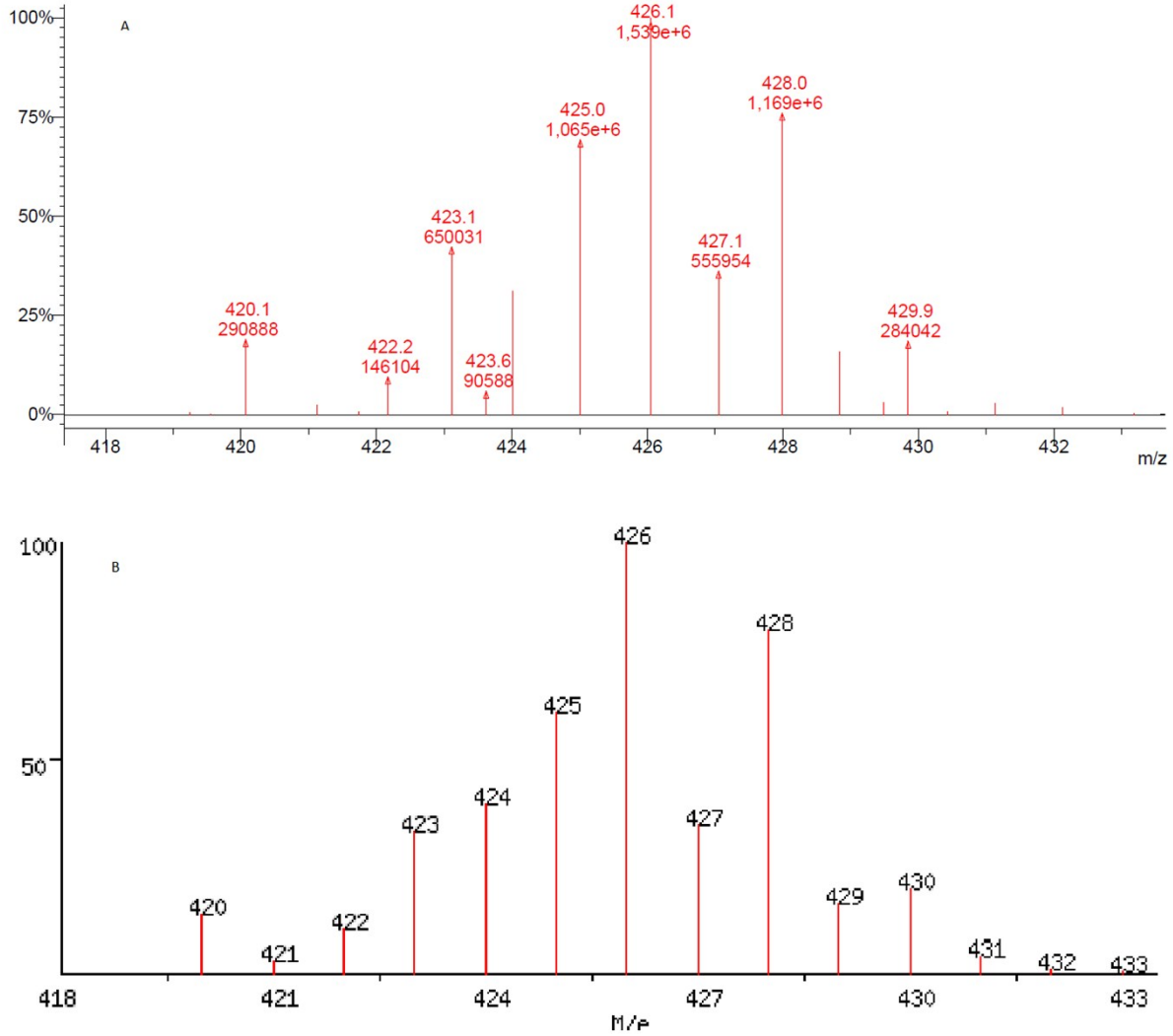

Fig. 1S Isotope profiles of complexes **2a** observed by ESI-MS (spectrum A) and simulated isotope patterns of the corresponding $[C_{16}H_{23}Cl_1N_3SRu]+$ (spectrum B).

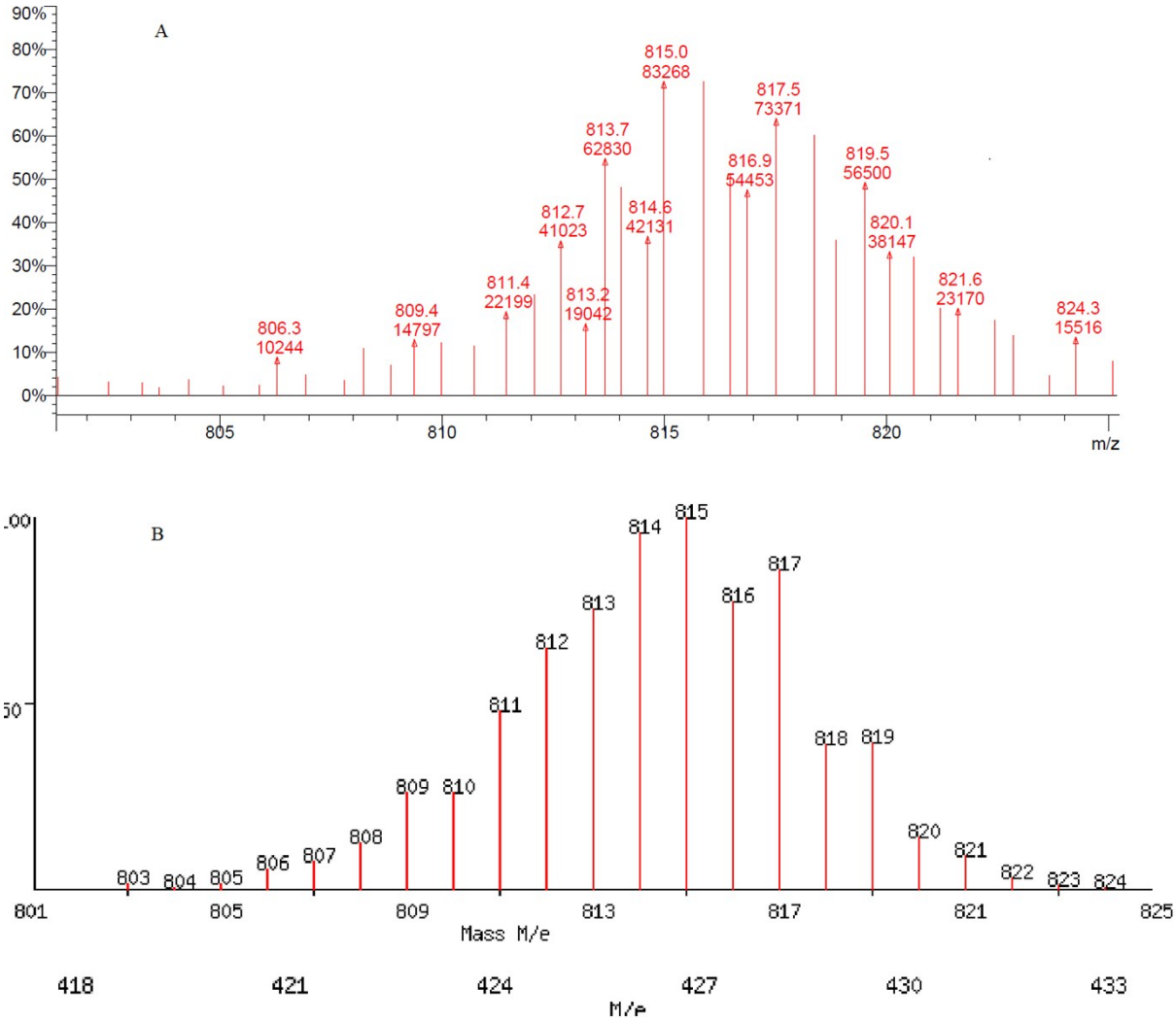

Fig. 2S Isotope profiles of half-sandwich Ru(II) complexes for **2a** observed by ESI-MS (spectrum A) and simulated isotope patterns of the corresponding [C32H44Cl1N6S2Ru2]+ (spectrum B).

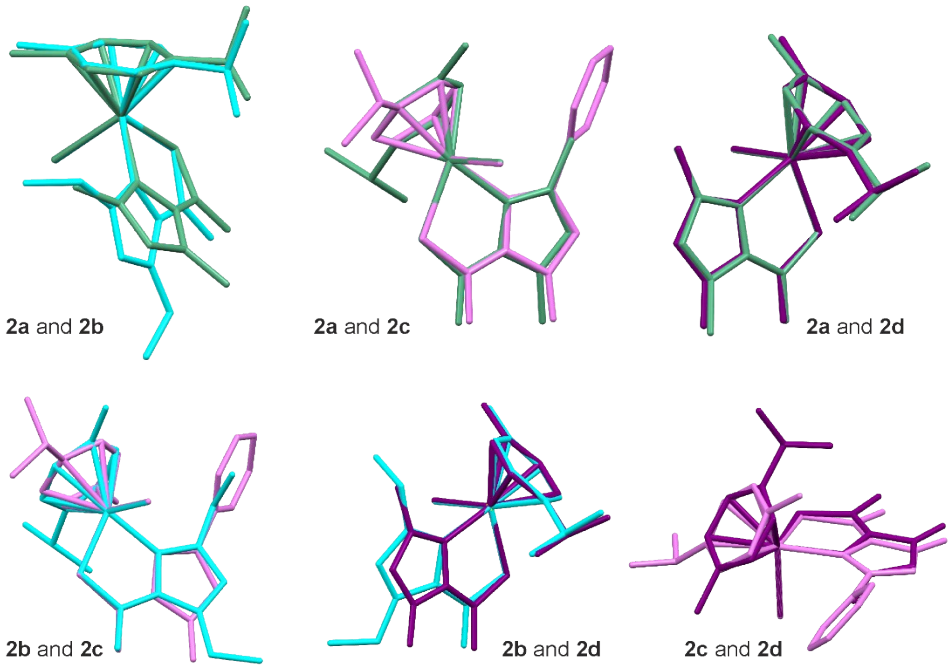

Fig. 3S Overlays of structures of **2a – 2d**. Colours: **2a** – green; **2b** –cyan, **2c** – violet, **2d** - purple.

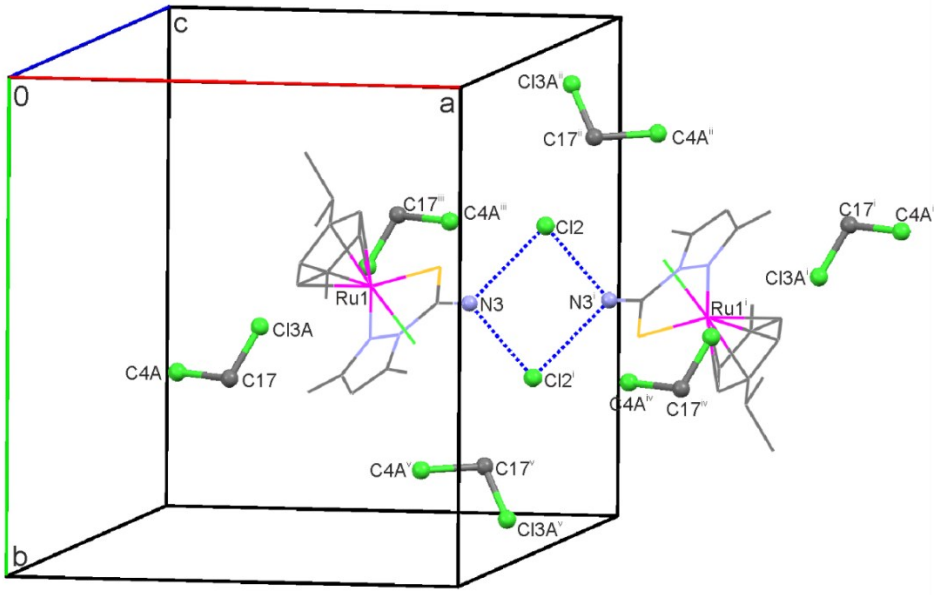

Fig. 4S Crystal packing of **2a**. Hydrogen bonds indicated by the dashed lines. Only one position of disordered dichloromethane molecule is shown. Symmetry operations: i (2-x, 1-y, 1-z), ii (1.5-x, -0.5+y, z), iii (1-x, 1-y, 1-z), iv (1+x, y, z), v (0.5+x, 1.5-y, 1-z).

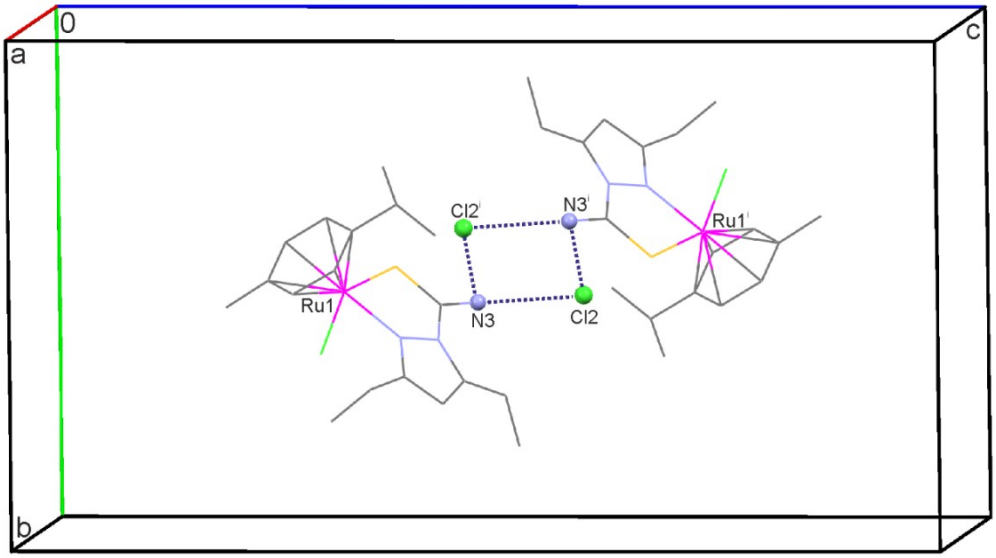

Fig. 5S Crystal packing of **2b**. Hydrogen bonds indicated by the dashed lines. Symmetry operation: i (–x, 1-y, 1-z).

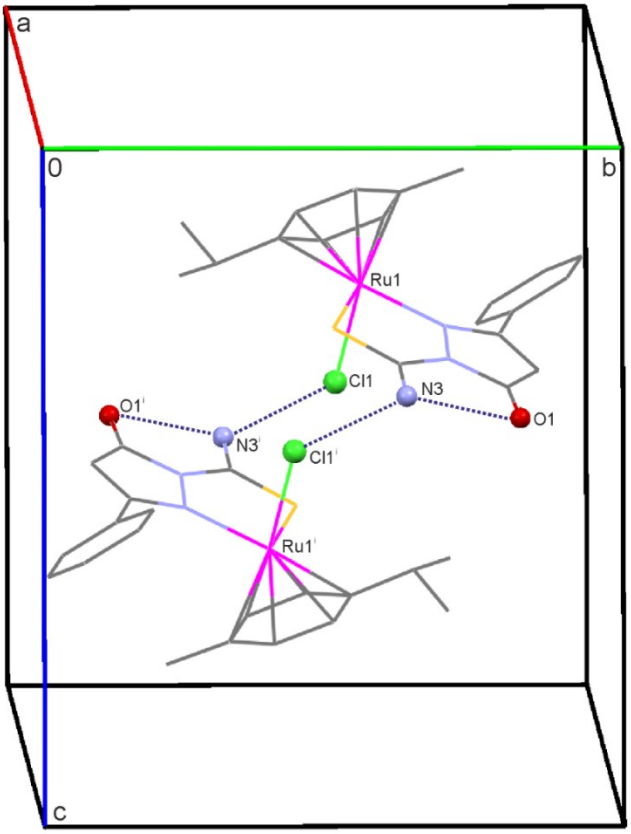

Fig. 6S Crystal packing of **2c**. Hydrogen bonds indicated by the dashed lines. Symmetry operation: i (1-x, 1-y, 1-z).

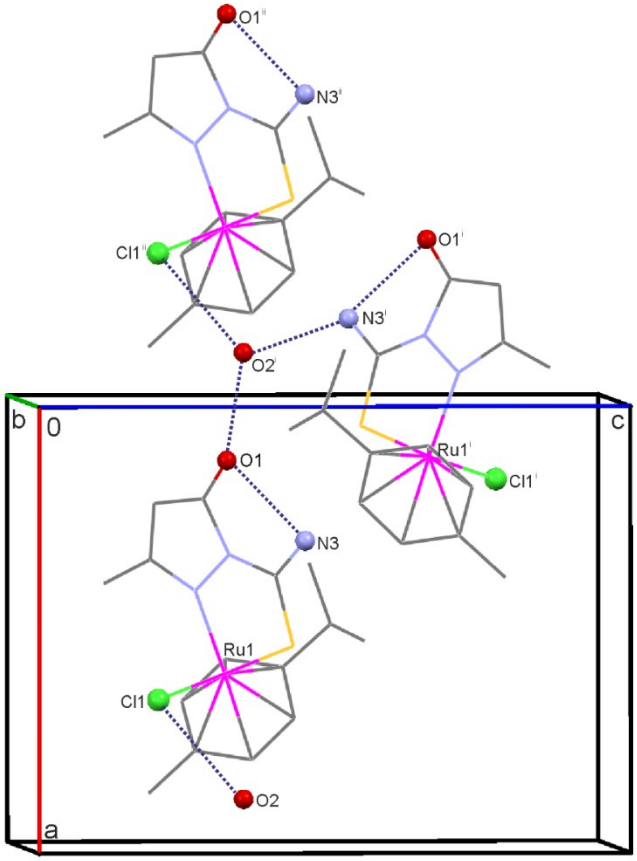

Fig. 7S Crystal packing of **2d**. Hydrogen bonds indicated by the dashed lines. Symmetry operation: i (-0.5+x, 0.5-y, 1-z), ii (-1+x, y, z).

Table 1S. Hydrogen bonds for **2a**-**2d** [Å and °].

D-H...A	d(D-H) [Å]	d(H...A) [Å]	d(D...A) [Å]	<(DHA) [°]
2a				
N3-H3A...Cl2^{i}	0.86(8)	2.45(9)	3.241(9)	153(10)
N3-H3B...Cl2	0.96(8)	2.13(9)	3.096(10)	175(11)
2b				
N3-H3A...Cl2	0.90(4)	2.26(4)	3.103(3)	157(3)
N3-H3B...Cl2^{ii}	0.83(3)	2.35(4)	3.177(3)	178(3)
2c				
N3-H3A...O1	0.86	1.96	2.643(5)	135.7
N3-H3B...Cl1^{iii}	0.86	2.41	3.222(4)	157.9
2d				
O2-H2A...O1^{iv}	0.85	1.87	2.718(9)	171.4
O2-H2B...Cl1	0.85	2.35	3.186(7)	170.1
N3-H3A...O1	0.86	2.03	2.690(11)	132.5
N3-H3B...O2^{v}	0.86	1.89	2.726(11)	163.9

Symmetry transformations used to generate equivalent atoms: ^{i} -x+2,-y+1,-z+1; ^{ii} -x,-y+1,-z+1; ^{iii} -x+1,-y+1,-z+1; ^{iv} x+1,y,z ; ^{v} x-1/2,-y+1/2,-z+1

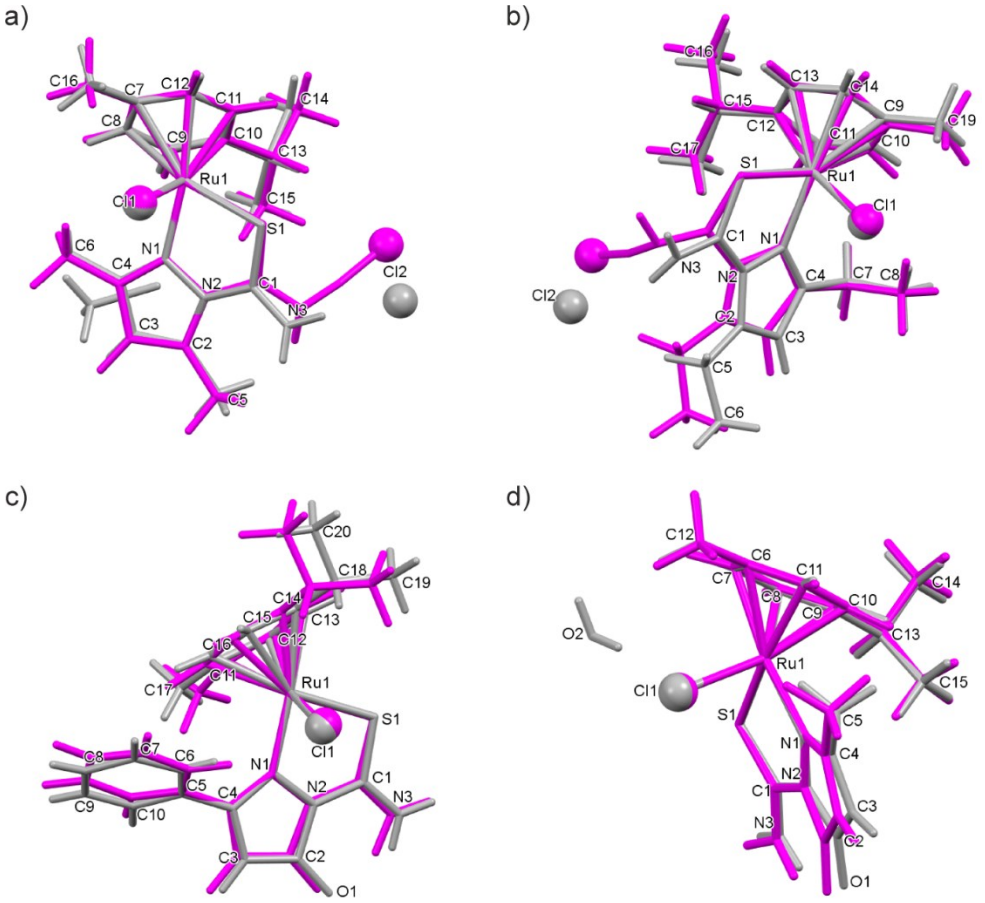

Fig. 8S The overlays of calculated DFT BP86-D/TZP (magenta) and experimental X-ray (grey) structures of: a) **2a**; b) **2b**; c) **2c**; d) **2d.** The overlays of Ru1, Cl1 and S1 atoms for each pair of molecules were prepared in Mercury 4.1.0.

Table S2 The comparison of selected experimental (X-ray) and calculated (DFT BP86-D/TZP) bond lengths in the studied complexes **2a** – **2d**.

Bond	**2a**		**2b**		**2c**		**2d**	
	Exp.	Calcd.	Exp.	Calcd.	Exp.	Calcd.	Exp.	Calcd.
Ru1-N1	2.101(8)	2.084	2.104(2)	2.103	2.109(4)	2.097	2.087(6)	2.088
Ru1-CPC	1.704	1.727	1.691	1.720	1.683	1.706	1.688	1.714
Ru1-S1	2.357(3)	2.366	2.3260(7)	2.363	2.3635(12)	2.387	2.369(2)	2.387
Ru1-Cl1	2.411(3)	2.404	2.4144(7)	2.403	2.4393(11)	2.423	2.429(2)	2.402
S1-C1	1.693(10)	1.711	1.686(3)	1.713	1.688(4)	1.714	1.703(10)	1.715
N2-N1	1.385(10)	1.384	1.401(3)	1.391	1.410(5)	1.389	1.404(9)	1.392