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SUPPORTING INFORMATION

Mechanisms of reactions of Ru(III)-based drug NAMI-A and its aquated products with DNA purine bases: A DFT Study

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Table S1: Gibbs free barrier energy (kcal/mol) and rate constant (s^{-1}) of the first hydrolysis step of NAMI-A.

Level of Theory	Barrier Energy	Rate constant
Gas Phase		
M062X/6-31G(d,p)+LanL2DZ	25.68	9.04×10^{-7}
M062X/6-311+G(d,p)+LanL2DZ	28.88	4.06×10^{-9}
Aqueous Media		
M062X/6-311+G(d,p)+LanL2DZ	24.01	1.51×10^{-5}

Table S2: Important geometrical parameters (Å, degree) of stationary points involved in the reaction of NAMI-A and guanine.

Geometrical Parameters	RC	TS	PC
Ru-Cl1	2.4426	3.1447	6.8428
Ru-Cl2	2.4342	2.5290	2.4143
Ru-Cl3	2.4089	2.4096	2.4297
Ru-Cl4	2.4215	2.4362	2.4122
Ru-S	2.4418	2.4432	2.4307
Ru-N1	2.0972	2.0651	2.0703
Ru-N7(Guanine)	5.0383	2.4999	2.1096
Cl1-Ru-Cl2	88.770	128.297	102.665
Cl1-Ru-Cl3	179.548	141.885	156.372
Cl1-Ru-Cl4	89.581	68.950	72.874
Cl1-Ru-S	89.864	71.174	73.591
Cl1-Ru-N1	90.429	109.232	109.578
Cl2-Ru-Cl3	91.088	81.156	90.392
Cl2-Ru-Cl4	178.333	161.883	175.534
Cl2-Ru-S	88.273	85.862	90.302
Cl2-Ru-N1	89.249	94.292	91.624
Cl3-Ru-Cl4	90.563	80.871	93.880
Cl3-Ru-S	89.703	90.430	86.906
Cl3-Ru-N1	89.998	88.891	89.356
Cl4-Ru-S	91.971	96.527	88.628
Cl4-Ru-N1	90.516	83.101	89.731
S-Ru-N1	177.498	179.269	175.80

Table S3: Important geometrical parameters (Å, degree) of stationary points involved in the reaction of NAMI-A(mono-aquated) and guanine.

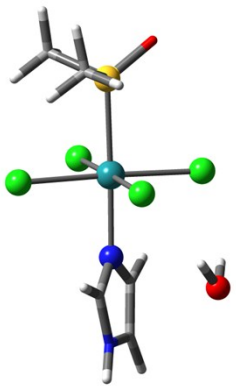
Geometrical Parameters	RC	TS	PC
Ru-Cl1	2.3975	2.4298	2.3837
Ru-Cl2	2.3673	2.3449	2.3993
Ru-Cl3	2.4053	2.4839	2.4446
Ru-O1(water)	2.1458	2.6023	4.1903
Ru-S	2.4030	2.5639	2.4428
Ru-N1	2.0718	2.0730	2.0686
Ru-N7(Guanine)	3.9295	2.6923	2.1377
Cl1-Ru-Cl2	95.334	86.771	92.166
Cl1-Ru-Cl3	169.803	172.784	172.844
Cl1-Ru-O1	87.474	116.570	125.143
Cl1-Ru-S	90.492	92.395	90.529
Cl1-Ru-N1	89.566	89.330	91.361
Cl2-Ru-Cl3	94.841	87.820	94.482
Cl2-Ru-O1	176.795	145.728	137.571
Cl2-Ru-S	89.235	83.785	86.734
Cl2-Ru-N1	92.476	84.930	89.655
Cl3-Ru-O1	82.373	70.404	49.816
Cl3-Ru-S	88.979	82.269	87.209
Cl3-Ru-N1	90.660	94.947	91.327
O1-Ru-S	92.291	117.543	109.755
O1-Ru-N1	85.990	71.477	71.916
S-Ru-N1	178.276	68.467	175.98

Table S4: Important geometrical parameters (Å,deg) of stationary point involved in the reaction of NAMI-A (di-aquated) and guanine.

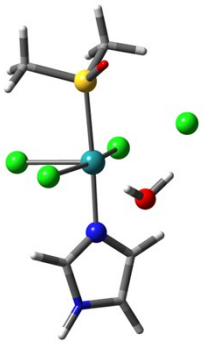
Geometrical Parameters	RC	TS	PC
Ru-O1(water)	2.0464	2.3867	6.3563
Ru-O2(water)	2.1807	2.1399	2.2057
Ru-Cl1	2.3707	2.3969	2.3638
Ru-Cl2	2.3736	2.5062	2.3942
Ru-S	2.4416	2.3888	2.4618
Ru-N1	2.0740	2.0980	2.0940
Ru-N7(Guanine)	3.7969	2.6167	2.0539
O1-Ru-O2	179.182	145.346	146.316
O1-Ru-Cl1	95.848	138.580	120.629
O1-Ru-Cl2	94.727	71.394	70.488
O1-Ru-S	83.763	84.295	70.082
O1-Ru-N1	89.390	91.512	110.511
O2-Ru-Cl1	84.931	75.873	84.636
O2-Ru-Cl2	84.507	73.964	82.217
O2-Ru-S	96.485	92.191	89.304
O2-Ru-N1	90.349	89.657	88.703
Cl1-Ru-Cl2	169.156	149.616	166.526
Cl1-Ru-S	90.890	92.096	90.593
Cl1-Ru-N1	90.682	92.918	91.722
Cl2-Ru-S	87.873	85.502	86.321
Cl2-Ru-N1	91.828	90.491	90.919
S-Ru-N1	173.097	174.945	176.793

Table S5: Important geometrical parameters (Å, degree) of stationary points involved in the reaction of NAMI-A(mono-aquated) and adenine.

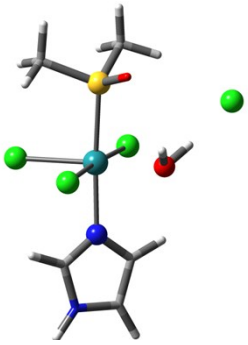
Geometrical Parameters	RC	TS	PC
Ru-Cl1	2.3946	2.4099	2.3811
Ru-Cl2	2.3518	2.3207	2.3744
Ru-Cl3	2.4145	2.4536	2.4545
Ru-O1(water)	2.1589	2.8729	3.8541
Ru-S	2.3904	2.4331	2.4493
Ru-N1	2.1005	2.0928	2.0803
Ru-N7(Adenine)	3.9191	2.9365	2.1538
Cl1-Ru-Cl2	96.388	87.356	96.136
Cl1-Ru-Cl3	167.972	173.210	174.367
Cl1-Ru-O1	85.976	120.193	119.341
Cl1-Ru-S	89.893	90.498	86.345
Cl1-Ru-N1	90.201	89.617	89.927
Cl2-Ru-Cl3	95.588	86.525	89.496
Cl2-Ru-O1	177.637	148.275	129.554
Cl2-Ru-S	89.569	88.100	87.589
Cl2-Ru-N1	90.132	90.968	89.020
Cl3-Ru-O1	82.050	66.517	56.258
Cl3-Ru-S	89.079	86.361	93.937
Cl3-Ru-N1	90.889	93.426	90.148
O1-Ru-S	90.455	105.688	62.511
O1-Ru-N1	89.842	75.052	122.764
S-Ru-N1	179.695	179.054	174.66



(a) **RC**



(b) **PC**



(c) **TS**

Fig. S1: Structures of reactant complex (RC), transition state (TS) and product complex (PC) involved in the first hydrolysis reaction of NAMI-A where a chloride anion is replaced by a water molecule.