Supplementary Material:

Binding Energies and Hydrogen Bonds Effects on DNA-cisplatin Interactions: A DFT-xTB Study

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In this file we present tables with bond distances and their differences in relation to experimental values. Additionally, geometric figures of the structures studied in this work are also presented.

Table 1 Bond Distances (Å) for Guanine-Cytosine in gas phase and water solvent.

	gas		solvent [1]		Experimental
Distance	CAM-B3LYP	xTB	CAM-B3LYP	xTB	
O20-C19	1.233 (0.003)	1.222 (0.014)	1.246 (0.010)	1.236 (0.000)	1,236
N21-C22	1.334 (0.016)	1.329 (0.011)	1.340 (0.022)	1.336 (0.018)	1,318
C25-C24	1.350 (0.009)	1.351 (0.010)	1.352 (0.011)	1.351 (0.010)	1,341
O7-C6	1.237 (0.031)	1.230 (0.024)	1.243 (0.037)	1.238 (0.032)	1,206
C9-N11	1.319 (0.043)	1.316 (0.046)	1.324 (0.038)	1.321 (0.041)	1,362
C12-C5	1.392 (0.034)	1.401 (0.043)	1.391 (0.033)	1.402 (0.043)	1,358
N4-C3	1.301 (0.019)	1.292 (0.028)	1.307 (0.013)	1.297 (0.023)	1,32
C9-N10	1.347 (0.016)	1.336 (0.005)	1.342 (0.011)	1.329 (0.002)	1,331
C9-N8	1.370 (0.012)	1.366 (0.016)	1.373 (0.009)	1.370 (0.012)	1,382
C6-N8	1.397 (0.007)	1.390 (0.000)	1.390 (0.000)	1.385 (0.005)	1,39
C6-C5	1.427 (0.025)	1.425 (0.027)	1.423 (0.029)	1.422 (0.030)	1,452
N4-C5	1.384 (0.013)	1.392 (0.005)	1.387 (0.010)	1.376 (0.021)	1,397
C3-N2	1.384 (0.023)	1.374 (0.013)	1.376 (0.015)	1.369 (0.008)	1,361
C12-N2	1.367 (0.012)	1.359 (0.020)	1.365 (0.014)	1.358 (0.021)	1,379
C12-N11	1.348 (0.002)	1.342 (0.008)	1.348 (0.002)	1.340 (0.010)	1,35
N23-C22	1.331 (0.004)	1.321 (0.006)	1.333 (0.006)	1.321 (0.006)	1,327
C24-C22	1.442 (0.003)	1.438 (0.007)	1.434 (0.011)	1.434 (0.011)	1,445
C25-N18	1.359 (0.002)	1.350 (0.007)	1.359 (0.002)	1.352 (0.005)	1,357
C19-N18	1.398 (0.004)	1.405 (0.011)	1.383 (0.011)	1.391 (0.003)	1,394
C19-N21	1.353 (0.003)	1.337 (0.008)	1.352 (0.007)	1.336 (0.009)	1,345
			Hydrogen Bonds		
N23-O7	2.745 (0.165)	2.680 (0.230)	2.853 (0.057)	2.789 (0.121)	2,91
N21-N8	2.893 (0.057)	2.819 (0.131)	2.908 (0.042)	2.849 (0.101)	2,95
O20-N10	2.881 (0.021)	2.799 (0.061)	2.830 (0.030)	2.809 (0.051)	2,86
$\frac{\sum \lvert X_i - X_{exp.} \rvert}{N}$	0.023	0.032	0.018	0.025	

[1]Implicit solvation conductor-like polarizable continuum (C-PCM) and analytical linearized Poisson-Boltzmann (ALPB) models were used for DFT em xTB calculations.

Table 2 Bond Distances (Å) in Adenine-Thymine in gas phase and water solvent.

	gas		solvent [1]		Experimental
Distance	CAM-B3LYP	xTB	CAM-B3LYP	xTB	
N2-C3	1.377 (0.027)	1.368 (0.018)	1.370 (0.020)	1.365 (0.015)	1.35
C3-N5	1.305 (0.024)	1.296 (0.033)	1.311 (0.018)	1.299 (0.030)	1.329
N5-C6	1.383 (0.014)	1.372 (0.003)	1.384 (0.015)	1.373 (0.004)	1.369
C6-C15	1.390 (0.031)	1.404 (0.045)	1.392 (0.033)	1.404 (0.045)	1.359
C6-C7	1.410 (0.001)	1.411 (0.000)	1.410 (0.001)	1.413 (0.002)	1.411
C7-N11	1.346 (0.015)	1.343 (0.018)	1.350 (0.011)	1.412 (0.051)	1.361
N11-C12	1.344 (0.018)	1.329 (0.033)	1.341 (0.021)	1.327 (0.035)	1.362
C12-N14	1.324 (0.022)	1.314 (0.032)	1.326 (0.020)	1.316 (0.030)	1.346
N14-C15	1.340 (0.022)	1.336 (0.026)	1.345 (0.017)	1.342 (0.020)	1.362
C7-N8	1.339 (0.019)	1.331 (0.027)	1.338 (0.020)	1.327 (0.031)	1.358
C25-O26	1.231 (0.048)	1.224 (0.055)	1.238 (0.041)	1.230 (0.049)	1.279
C25-N27	1.380 (0.008)	1.372 (0.000)	1.381 (0.009)	1.374 (0.002)	1.372
C25-C20	1.462 (0.042)	1.460 (0.040)	1.452 (0.032)	1.453 (0.033)	1.42
C20-C21	1.496 (0.022)	1.494 (0.020)	1.497 (0.023)	1.493 (0.019)	1.474
C20-C18	1.347 (0.012)	1.346 (0.011)	1.350 (0.015)	1.349 (0.014)	1.335
C18-N17	1.375 (0.017)	1.365 (0.007)	1.372 (0.014)	1.364 (0.006)	1.358
N17-C29	1.383 (0.022)	1.384 (0.023)	1.370 (0.009)	1.369 (0.008)	1.361
C29-O30	1.219 (0.002)	1.208 (0.013)	1.230 (0.009)	1.223 (0.002)	1.221
			Hydrogen Bonds		
O26-N8	2.891 (0.058)	2.809 (0.141)	2.903 (0.047)	2.868 (0.082)	2.95
N11-N27	2.802 (0.018)	2.691 (0.129)	2.858 (0.038)	2.728 (0.092)	2.82
$\frac{\sum \lvert X_i - X_{exp.} \rvert}{N}$	0.023	0.035	0.022	0.030	

[1]Implicit solvation conductor-like polarizable continuum (C-PCM) and analytical linearized Poisson-Boltzmann (ALPB) models were used for DFT em xTB calculations.

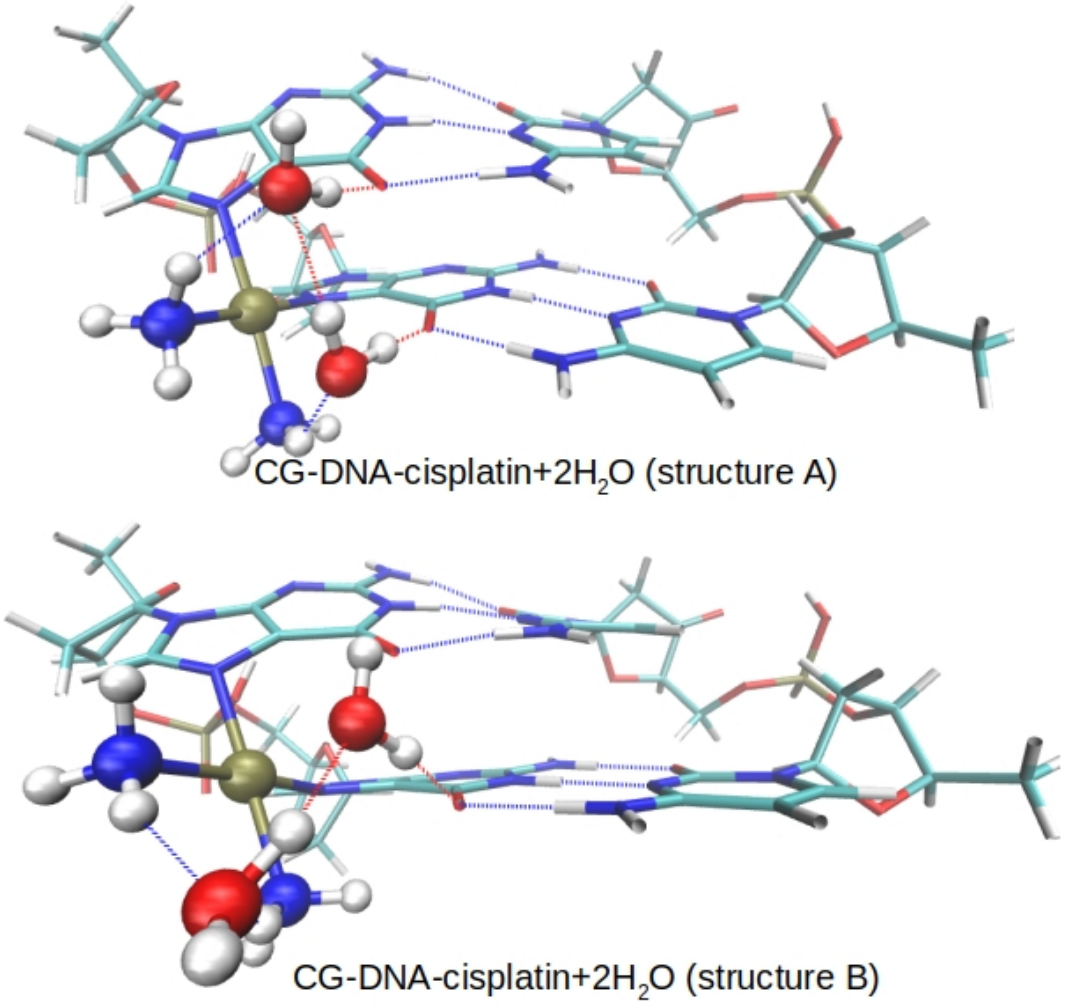

Fig. 1 Minimum CG-cisplatin structures and additional explicit water molecules obtained at the xTB calculation.

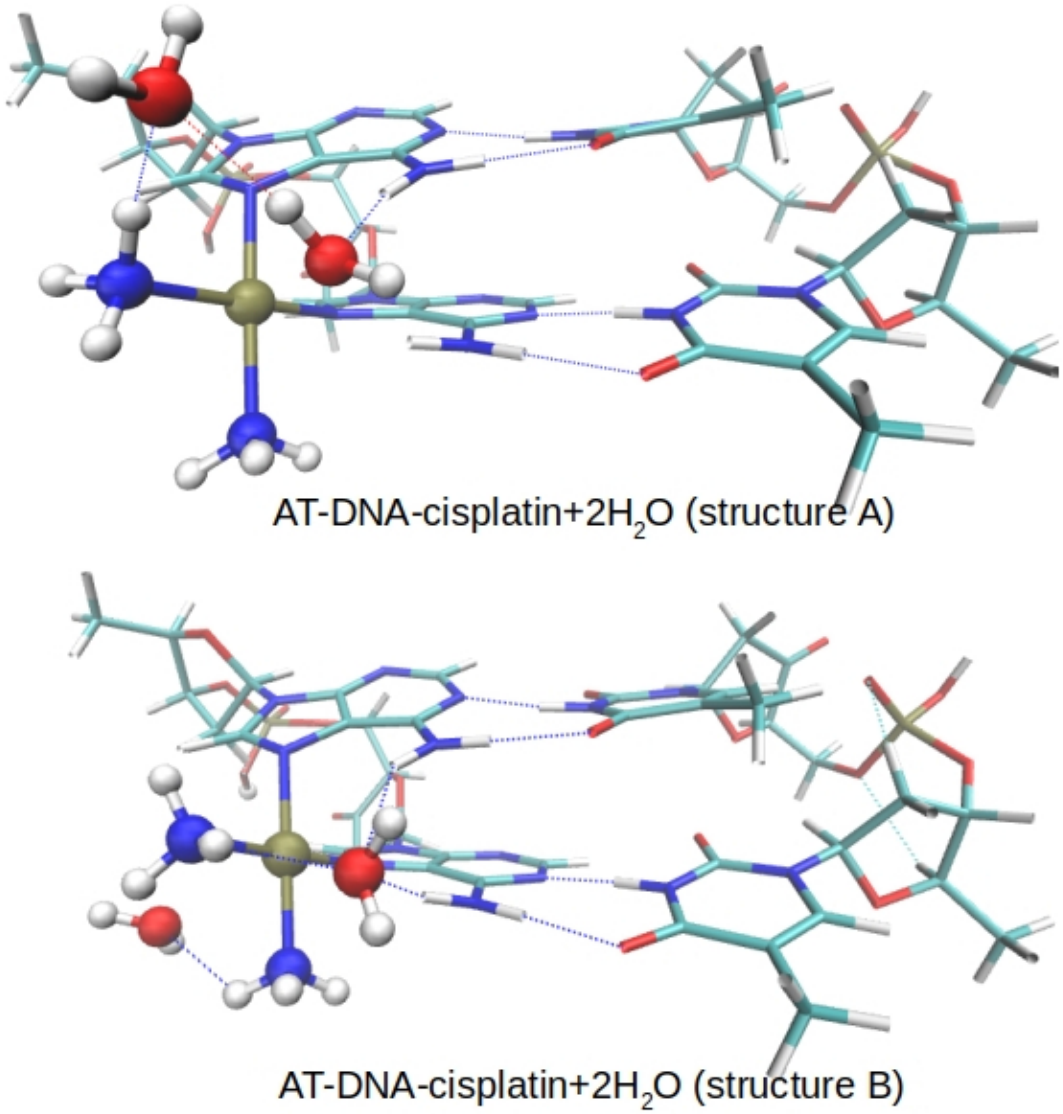

Fig. 2 Minimum AT-cisplatin structures and additional explicit water molecules obtained at the xTB calculation.

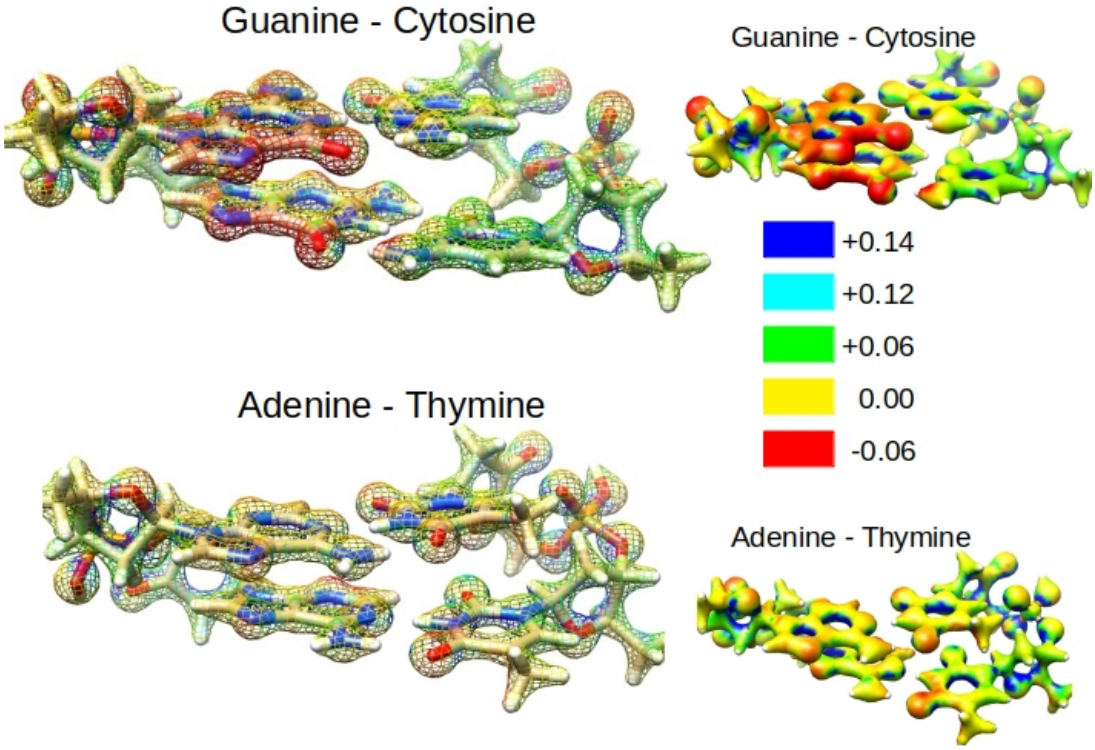

Fig. 3 Surface of electrostatic potential of the GC-DNA structure (in top) and AT-DNA structure (in botton). Colors ware used to show the regions of the values in the electrostatic potential.