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Supporting information for article:

The effect of cation–π interactions on the stability and electronic properties of anticancer drug Altretamine: a theoretical study

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Table S1

The geometrical parameters (bond lengths (d) is in Å), interaction energy (ΔE, in kJ mol^{-1}), selected topological parameters of complexes (in a.u.), the stabilizing energies ($E^{(2)}$, in kcal mol^{-1}), the charge transfers (Δq_{CT} in e) and dipole moment (μ°, in Deby) calculated in water and CCl_4 solutions.

°μ	$q_{CT}\Delta$	$E^{(2)}$	$\nabla^2\rho_{ion\text{-}N}$	$\rho_{ion\text{-}N}$	ΔE	$d_{ion-\pi}$ [c]	$d_{C2\text{-}N7}$ [b]	$d_{C2\text{-}N3}$ [a]		Media
14.42	0.028-	0.82	0.0053	0.0011	2.86	3.240	1.361	1.341	Li^+	Water
14.46	0.005-	0.42	0.0058	0.0011	0.48	3.204	1.359	1.342	^+Na	
10.79	0.089-	0.84	0.0263	0.0068	1.58	2.990	1.354	1.344	^+K	
5.38	1.487	7.63	0.2591	0.0648	101.30-	1.375	1.306	1.383	$^+Be^2$	
30.35	0.024-	0.51	0.0048	0.0044	4.41	3.560	1.359	1.342	$^+Mg^2$	
30.12	0.010-	0.41	0.0046	0.0024	0.50-	3.760	1.359	1.341	$^+Ca^2$	
11.57	0.006-	0.90	0.0086	0.0018	21.63-	3.074	1.359	1.344	^+Li	CCl_4
11.97	0.002	0.48	0.0082	0.0016	24.71-	3.351	1.360	1.344	^+Na	
8.08	0.091-	1.36	0.0424	0.0105	40.30-	2.765	1.353	1.346	^+K	
2.44	1.818	10.67	0.3114	0.0693	564.07-	1.281	1.295	1.398	$^+Be^2$	
9.20	1.088	3.71	0.1436	0.0308	200.82-	1.919	1.315	1.377	$^+Mg^2$	
25.42	0.005	0.48	0.0063	0.0031	43.29-	3.603	1.355	1.347	$^+Ca^2$	

[a] The C-N bond length of cyclic

[b] The C-N bond length of exocyclic

[c] Distance between the ion and the center of ALT ring