

Spectroscopic study, Quantum Chemical Investigations, *In silico* and Drug Likeness of 4-Chloro-6,7-dimethoxyquinazoline: A potent study of new anti-alzheimer agent

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Supplementary Tables

Table 1 — Mulliken and Natural bond orbital (NBO) charges for 4-chloro-6,7-dimethoxyquinazoline calculated using B3LYP/6-311++G(d,p)

Atoms	MullikenCharges		NBO Charges	
	In gas phase	In Water	In gas phase	In Water
N1	-0.023015	-0.09277	-0.477	-0.639
C2	0.113486	0.123142	0.45	0.584
N3	0.054406	-0.00876	-0.665	-0.948
C4	-1.83975	-1.82436	0.927	1.345
C5	-1.66535	-1.70338	-0.081	-0.110
C6	-0.52152	-0.47049	0.438	0.598
C7	0.194454	0.253287	0.599	0.854
C8	-0.65072	-0.72794	-0.172	-0.264
C9	-0.14309	-0.09865	0.303	0.458
C10	3.044383	3.108411	-0.271	-0.386
Cl11	0.59688	0.569319	-0.38	-0.523
O12	-0.13719	-0.16724	-0.932	-1.242
C13	-0.26538	-0.26503	0.529	0.672
O14	-0.12678	-0.15678	-0.868	-1.188
C15	-0.26471	-0.26939	0.522	0.660
H16	0.177827	0.194482	0.08	0.104
H17	0.239263	0.256617	0.025	0.028
H18	0.220129	0.228098	0.073	0.088
H19	0.142073	0.153342	-0.027	-0.034
H20	0.165284	0.178519	-0.01	-0.012
H21	0.196142	0.198725	0.005	0.006
H22	0.188637	0.190685	0.001	-0.002
H23	0.165462	0.178819	-0.01	-0.013
H24	0.139078	0.151331	-0.027	-0.033

Table 2 — Second-order perturbation theory analysis of Fock matrix for 4-chloro-6,7-dimethoxyquinazoline

Donor(i)	ED (i) (e)	Acceptor (j)	ED (j) (e)	Stabilization energy E(2) (Kcal/mol)	Energy difference E (j) -E (i) (arb. units)	Fock matrix element F(i,j) (arb. units)
π (N1-C2)	1.79059	π^* (N3-C4)	0.35231	9.53	0.31	0.05
π (N1-C2)	1.79059	π^* (C9-C10)	0.46085	20.92	0.34	0.08
σ (C2-N3)	1.97497	σ^* (C4-C111)	0.07123	6.67	0.94	0.071
σ (C2-H17)	1.98123	σ^* (N1-C9)	0.02222	5.26	1.02	0.065
π (N3-C4)	1.79223	π^* (N1-C2)	0.27009	24.49	0.34	0.083
π (N3-C4)	1.79223	π^* (C9-C10)	0.46085	8.36	0.36	0.052
π (C5-C6)	1.72803	π^* (C7-C8)	0.27224	17.62	0.3	0.065
π (C5-C6)	1.72803	π^* (C9-C10)	0.46085	16.01	0.3	0.065
π (C7 -C8)	1.71579	π^* (C5-C6)	0.27427	16.8	0.3	0.063
π (C7-C8)	1.71579	π^* (C9-C10)	0.46085	18.28	0.3	0.069
σ (C9-C10)	1.96141	σ^* (C4-C111)	0.07123	5.22	0.82	0.059
π (C9-C10)	1.53640	π^* (N1-C2)	0.27009	12.31	0.27	0.054
π (C9-C10)	1.53640	π^* (N3-C4)	0.35231	28.27	0.25	0.077
π (C9-C10)	1.53640	π^* (C5-C6)	0.27427	17.59	0.28	0.066
π (C9-C10)	1.53640	π^* (C7-C8)	0.27224	14.03	0.28	0.059
σ (O14-C15)	1.98017	σ^* (C15-H24)	0.01666	16.17	3.8	0.221
σ (C15-H23)	1.99131	σ^* (C15-H24)	0.01666	9.27	3.53	0.162
σ (C15-H24)	1.99592	σ^* (C15-H22)	0.01724	5.05	1.12	0.067
σ (C15-H24)	1.99592	σ^* (C15-H24)	0.01666	24.6	3.53	0.264
LP (1)N1	1.91245	σ^* (C2-N3)	0.03721	11.97	0.83	0.09
LP(1)N1	1.91245	σ^* (C9-C10)	0.04412	9.87	0.87	0.084
LP(1)N3	1.89370	σ^* (N1-C2)	0.02380	9.56	0.92	0.086
LP(1)N3	1.89370	σ^* (C4-C10)	0.04700	10.87	0.86	0.088
LP(1)N3	1.89370	σ^* (C4-C111)	0.07123	5.11	0.48	0.045
LP(2)C111	1.96587	σ^* (N3-C4)	0.02560	5.8	0.88	0.064
LP(3)C111	1.90449	π^* (N3-C4)	0.35231	16.41	0.31	0.068
LP(1)O12	1.94915	σ^* (C6-C7)	0.05262	6.47	0.98	0.071
LP(2)O12	1.90865	π^* (C7-C8)	0.27224	8.58	0.42	0.056
LP(1)O14	1.94838	σ^* (C6-C7)	0.05262	6.1	0.99	0.069
LP(2)O14	1.91404	σ^* (C5-C6)	0.02433	5.02	0.97	0.063
LP(2)O14	1.91404	π^* (C5-C6)	0.27427	7.36	0.41	0.052
π^* (N1-C2)	0.27009	π^* (C9-C10)	0.46085	155.87	0.02	0.074
π^* (N3-C4)	0.35231	π^* (N1-C2)	0.27009	146.02	0.02	0.078
π^* (N3-C4)	0.35231	π^* (C9-C10)	0.46085	97.75	0.03	0.079