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TD-DFT calculations, electronic structure, natural bond orbital analysis, nonlinear optical properties electronic absorption spectra and antimicrobial activity application of new *bis*-spiropipridinon/pyrazole derivatives

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ABSTRACT

A new *bis*-spiropipridinon/pyrazole compound and some of its derivatives are characterized in terms of several theoretical parameters such as density of states (DOS), molecular electrostatic potentials (MEPs), non-linear optical (NLO) properties and electrophilicity. The electronic structure and nonlinear optical properties of the studied compounds 1-5 are investigated theoretically at the DFT-B3LYP/6-311G(d,p) level of theory. The effect of substituents of different strengths on the geometry and energetic are analyzed and discussed. The static dipole moment (μ), polarizability (α), anisotropy polarizability ($\Delta\alpha$), and first order hyperpolarizability (β_{tot}), are parameters for NLO of the studied compounds have been calculated at the same level of theory and compared with the prototype *para*-nitro-aniline (PNA). The electronic absorption spectra of the studied compounds are recorded in the UV-VIS region, in both ethanol and dioxane solvents. The theoretical spectra computed at a new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP) at the 6-311G(d,p) bases set in gas phase and with the polarizable continuum model (PCM) in dioxane and ethanol indicate a good agreement with the observed spectra. The antimicrobial activity for studied compounds was investigated. The antimicrobial activity results revealed that compound 4 has a good potency against Gram positive bacteria (*E. coli*) and Gram negative bacteria (*P. vulgaris*) in comparison with doxymycin standard. The structure activity relationship SAR has been studied for the studied compounds by DFT calculations, moreover, confirmed practical antimicrobial activity results.

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Supplementary Materials

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Table S1. Theoretical and experimental UV spectra of compound **1**, calculated at CAM-B3LYP/6-311G(d,p).

TD-Theoretical												
Gas phase					**Dioxane**				**Ethanol**			
State	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**
I	180-183	0.597	0.210	336.2	180-183	0.592	0.216	337.7	180-183	0.597	0.214	336.2
	181-183	-0.240			181-183	-0.263			181-183	-0.245		
	181-184	0.167			181-184	0.168			181-184	0.170		
	182-184	-0.130							182-184	-0.120		
II	180-183	-0.100	0.225	323.6	180-184	-0.128	0.360	320.4	180-185	-0.124	0.254	322.8
	180-185	-0.120			180-185	-0.138			181-184	-0.115		
	181-184	-0.100			181-184	0.231			182-184	-0.345		
	182-184	-0.380			181-185	-0.125			182-185	0.526		
	182-185	0.503			182-184	0.118			182-186	-0.141		
	182-186	-0.140			182-185	0.568						
					182-186	0.129						
III	180-184	0.172	0.101	318.2	180-183	-0.161	0.373	315.8	180-184	0.179	0.095	317.0
	181-184	-0.160			180-184	-0.212			181-184	-0.184		
	181-185	-0.100			181-184	0.420			181-185	-0.104		
	182-183	-0.190			181-185	-0.113			182-183	-0.189		
	182-184	0.506			182-183	0.102			182-184	0.528		
	182-185	0.325			182-184	-0.397			182-185	0.271		
					182-185	-0.131						
IV	180-183	-0.120	0.440	305.4	181-184	0.346	0.199	303.1	180-183	-0.119	0.439	305.3
	180-184	-0.220			182-183	-0.137			180-184	-0.210		
	181-184	0.532			182-184	0.507			181-184	0.524		
	181-185	0.163			182-185	-0.250			181-185	0.157		
	182-184	0.141							182-184	0.170		
	182-185	0.235							182-185	0.248		
V	169-183	0.103	0.114	290.8	169-183	0.134	0.221	290.7	169-183	0.106	0.127	290.7
	180-185	-0.270			180-184	0.107			180-185	-0.284		
	181-185	-0.150			180-185	0.363			181-185	-0.154		
	182-186	0.547			181-184	0.114			182-186	0.535		
	182-195	0.100			181-185	0.157						
					182-186	0.452						
					182-190	0.121						
VI	180-184	-0.120	0.391	283.1	165-183	-0.143	0.182	281.1	180-184	-0.123	0.356	282.9
	180-185	0.420			169-183	-0.241			180-185	0.410		
	181-184	-0.150			180-185	-0.219			181-184	-0.137		
	181-185	0.324			181-183	-0.116			181-185	0.324		
	182-185	0.182			181-184	-0.118			182-185	0.187		
	182-186	0.287			181-186	0.116			182-186	0.298		
	182-187	-0.120			182-185	-0.183			182-187	-0.123		
					182-186	0.418						
					182-187	-0.112						

Table S2. Theoretical and experimental UV spectra of compound **2**, calculated at CAM-B3LYP/6-311G(d,p).

TD-Theoretical													**Experimental**
Gas phase					**Dioxane**				**Ethanol**				**Dioxane, Ethanol**
State	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**$\lambda_{,nm}$, $\lambda_{,nm}$**
I	196-199	0.607	0.132	336.1	196-199	0.598	0.269	336.3	196-199	0.591	0.281	335.4	343, 339
	197-199	0.252			197-199	0.236			197-199	0.207			
	197-200	-0.120			197-200	-0.175			197-200	-0.172			
					198-200	-0.112			198-200	-0.152			
									198-201	0.137			
II	196-200	0.116	0.292	320.8	196-200	0.117	0.327	320.0	196-199	-0.172	0.213	325.3	
	196-201	-0.110			196-201	-0.122			196-201	-0.115			
	197-200	0.182			197-200	0.157			197-200	0.116			
	198-200	-0.180			197-201	0.122			198-200	-0.321			
	198-201	0.590			198-200	-0.223			198-201	0.524			
	198-204	-0.110			198-201	0.563			198-202	0.109			
					198-204	-0.103							
III	196-199	0.120	0.344	303.6	196-199	0.153	0.384	304.2	196-199	0.115	0.400	303.5	
	196-200	0.228			196-200	0.262			196-200	0.239			
	197-200	0.451			197-200	0.428			197-200	0.490			
	197-201	0.166			197-201	0.188			197-201	0.194			
	198-200	0.344			198-200	0.351			198-200	-0.185			
									198-201	-0.244			
IV	187-199	0.129	0.262	291.8	185-199	0.112	0.177	292.1	196-201	0.250	0.117	292.3	295, 298
	196-201	0.274			196-200	-0.116			197-201	-0.160			
	197-200	0.276			196-201	0.319			198-200	0.102			
	198-199	0.167			197-200	0.100			198-202	0.528			
	198-200	-0.170			197-201	-0.166			198-203	-0.129			
	198-201	-0.100			198-200	0.136			198-204	0.117			
	198-202	0.373			198-202	0.450			198-211	0.104			
	198-203	0.132			198-204	-0.142							
	198-204	-0.130											
	198-206	-0.120											
V	181-199	-0.130	0.149	273.2	181-199	-0.169	0.188	276.3	181-199	0.222	0.141	274.1	
	187-199	-0.200			185-199	-0.273			183-199	-0.114			
	196-200	0.103			185-202	0.108			184-199	0.123			
	196-201	-0.270			196-201	-0.182			185-199	0.377			
	197-199	-0.100			197-199	-0.149			185-202	-0.137			
	197-200	-0.140			197-200	-0.126			197-199	0.184			
	197-202	-0.130			197-202	-0.202			197-201	0.211			
	198-201	-0.130			198-201	-0.127			197-202	0.184			
	198-202	0.378			198-202	0.331			198-202	-0.129			
	198-203	0.125			198-204	-0.111							
	198-204	-0.170											

Table S3. Theoretical and experimental UV spectra of compound **3**, calculated at CAM-B3LYP/6-311G(d,p).

TD-Theoretical													**Experimental**
Gas phase					**Dioxane**				**Ethanol**				**Dioxane, Ethanol**
State	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**$\lambda_{,nm}$, $\lambda_{,nm}$**
I	188-191	0.604	0.100	339.7	188-191	0.599	0.199	339.4	188-191	0.606	0.203	337.4	348, 344
	189-191	-0.260			189-191	-0.257			189-191	-0.234			
	189-192	0.106			189-192	0.159			189-192	0.166			
									190-192	-0.110			
II	188-192	-0.130	0.282	313.7	188-192	-0.133	0.346	311.4	188-192	0.200	0.234	314.6	
	188-193	-0.110			188-193	-0.126			189-192	-0.208			
	189-192	0.284			189-192	0.236			189-193	0.117			
	190-193	0.571			189-193	-0.126			190-191	-0.184			
	190-196	-0.110			190-192	0.148			190-192	0.489			
					190-193	0.560			190-193	-0.306			
					190-197	0.115							
III	188-191	-0.130	0.362	306.6	189-192	0.327	0.198	302.2	188-191	-0.116	0.444	305.8	
	188-192	-0.170			190-191	-0.134			188-192	-0.209			
	189-192	0.423			190-192	0.510			189-192	0.513			
	189-195	-0.110			190-193	-0.271			189-193	-0.134			
	190-191	0.108							190-192	0.178			
	190-192	-0.360							190-193	-0.272			
	190-193	-0.200											
IV	173-191	-0.140	0.219	288.3	179-191	0.118	0.209	289.9	188-193	-0.286	0.172	289.3	297, 293
	179-191	-0.230			188-192	0.112			189-193	-0.174			
	188-193	-0.240			188-193	0.357			190-194	0.453			
	189-191	-0.100			189-193	0.171			190-195	-0.219			
	189-192	-0.180			190-194	-0.307			190-197	0.176			
	189-193	0.106			190-195	0.273			190-198	0.113			
	190-191	0.155			190-196	-0.130							
	190-194	0.183			190-197	0.138							
	190-195	0.293			190-198	0.134							
	190-196	0.179											
	190-198	0.155											

Table S4. Theoretical and experimental UV spectra of compound **4**, calculated at CAM-B3LYP/6-311G(d,p).

TD-Theoretical													**Experimental**
Gas phase					**Dioxane**				**Ethanol**				**Dioxane, Ethanol**
State	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**λ_{nm}, λ_{nm}**
I	202-205	0.433	0.116	348.3	202-205	0.369	0.167	349.9	202-205	0.467	0.210	347.4	355, 358
	202-207	-0.270			202-207	0.200			202-207	0.318			
	203-205	0.223			203-205	0.200			203-205	0.221			
	204-205	0.181			204-205	0.217			204-205	-0.140			
	204-206	-0.220			204-206	0.247			204-207	0.146			
	204-207	0.206			204-207	-0.329			204-209	-0.122			
	204-208	-0.110			204-208	0.129			204-211	-0.147			
II	202-208	0.107	0.273	321.9	202-205	-0.114	0.325	324.9	202-205	0.158	0.261	323.9	
	203-206	-0.100			202-209	-0.119			202-209	-0.107			
	203-208	0.134			203-208	-0.146			203-208	0.116			
	204-208	-0.340			204-207	-0.115			204-207	0.135			
	204-209	0.453			204-208	0.139			204-209	0.466			
	204-210	0.209			204-209	0.486			204-211	0.354			
	204-214	-0.120			204-211	-0.303			204-214	-0.111			
					204-214	0.128							
III	202-205	0.101	0.267	311.7	202-205	-0.112	0.305	313.5	202-207	-0.155	0.344	310.5	
	203-206	-0.260			202-207	-0.112			202-208	0.153			
	203-207	-0.240			202-208	0.154			203-205	0.138			
	203-208	0.225			203-206	-0.165			203-206	-0.226			
	203-209	0.238			203-207	-0.180			203-207	-0.218			
	204-208	0.388			203-208	0.304			203-208	0.427			
	204-214	0.115			204-207	0.109			203-209	0.112			
					204-208	0.425			203-211	0.122			
					204-210	-0.144			204-208	-0.173			
					204-214	0.109			204-209	-0.132			
									204-211	-0.107			
IV	202-206	0.102	0.155	290.0	202-209	0.164	0.160	292.5	202-208	-0.108	0.352	291.1	298, 295
	203-206	0.133			203-205	0.120			202-209	0.360			
	203-208	0.308			203-206	-0.118			202-211	0.283			
	203-209	0.189			204-208	-0.216			203-207	-0.213			
	204-209	-0.250			204-209	0.155			203-209	-0.278			
	204-210	0.224			204-212	-0.327			203-211	-0.174			
	204-212	-0.280			204-213	-0.164			204-209	0.128			
	204-213	0.177			204-214	0.348			204-214	0.129			
	204-214	-0.100											
V	202-208	0.182	0.133	273.8	202-209	0.170	0.158	274.3	202-206	0.297	0.064	273.6	
	202-209	-0.220			202-211	-0.108			203-206	0.175			
	202-210	-0.130			203-209	0.329			203-207	0.321			
	203-209	-0.330			203-211	-0.147			203-208	0.239			
	203-212	-0.110			203-212	-0.116			203-210	-0.169			
	203-213	-0.120			203-213	-0.152			203-211	-0.122			
	203-214	0.387			203-214	0.426			204-214	-0.101			
					203-219	0.102							

Table S5. Theoretical and experimental UV spectra of compound **5**, calculated at CAM-B3LYP/6-311G(d,p).

TD-Theoretical													**Experimental**
Gas phase					**Dioxane**				**Ethanol**				**Dioxane, Ethanol**
State	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**Config.**	**Coef.**	**f**	**λ, nm**	**λ_{nm}, λ_{nm}**
I	196-199	0.601	0.118	343.5	196-199	0.597	0.191	342.9	196-199	0.604	0.194	340.6	353, 349
	197-199	0.270			197-199	0.264			197-199	0.242			
	197-200	-0.100			197-200	-0.152			197-200	-0.162			
									198-200	-0.102			
II	196-200	-0.130	0.294	313.5	196-199	0.145	0.401	311.1	196-200	0.197	0.226	315.3	
	196-201	-0.100			196-200	0.205			197-200	0.202			
	197-200	-0.280			197-200	0.417			197-201	0.119			
	198-201	0.572			197-201	0.116			198-199	-0.180			
	198-206	-0.110			198-200	0.395			198-200	0.473			
					198-201	-0.135			198-201	0.329			
III	196-199	0.120	0.353	306.3	197-200	-0.330	0.184	303.5	196-199	0.113	0.455	306.0	
	196-200	0.164			198-199	-0.118			196-200	0.206			
	197-200	0.413			198-200	0.499			197-200	0.516			
	197-204	0.133			198-201	0.266			197-201	0.145			
	198-199	-0.100							198-200	-0.165			
	198-200	0.375							198-201	-0.269			
	198-201	0.205											
IV	181-199	-0.130	0.229	290.3	187-199	0.128-	0.197	292.6	196-200	-0.121	0.266	293.3	298, 295
	187-199	-0.210			196-200	0.116			196-201	0.351			
	196-200	0.102			196-201	-0.320			197-200	0.131			
	196-201	0.219			197-200	-0.136			197-201	-0.297			
	197-200	-0.230			197-201	0.125			198-201	0.206			
	197-201	0.110			198-199	0.104			198-203	0.346			
	198-199	-0.160			198-202	0.341			198-204	0.196			
	198-202	0.261			198-203	0.204			198-205	0.109			
	198-203	0.121			198-204	0.192							
	198-204	0.150			198-206	-0.229							
	198-205	0.124											
	198-206	-0.230											
V	181-199	0.155	0.083	273.8	181-199	0.121	0.197	276.8	196-201	0.218	0.108	275.6	
	187-199	0.235			187-199	0.180			197-201	-0.194			
	196-201	-0.170			196-201	0.260			198-202	0.431			
	197-201	0.242			197-200	0.100			198-203	-0.357			
	198-202	0.368			197-201	-0.127			198-204	-0.127			
	198-203	0.255			198-201	0.123			198-205	-0.226			
					198-202	0.504							

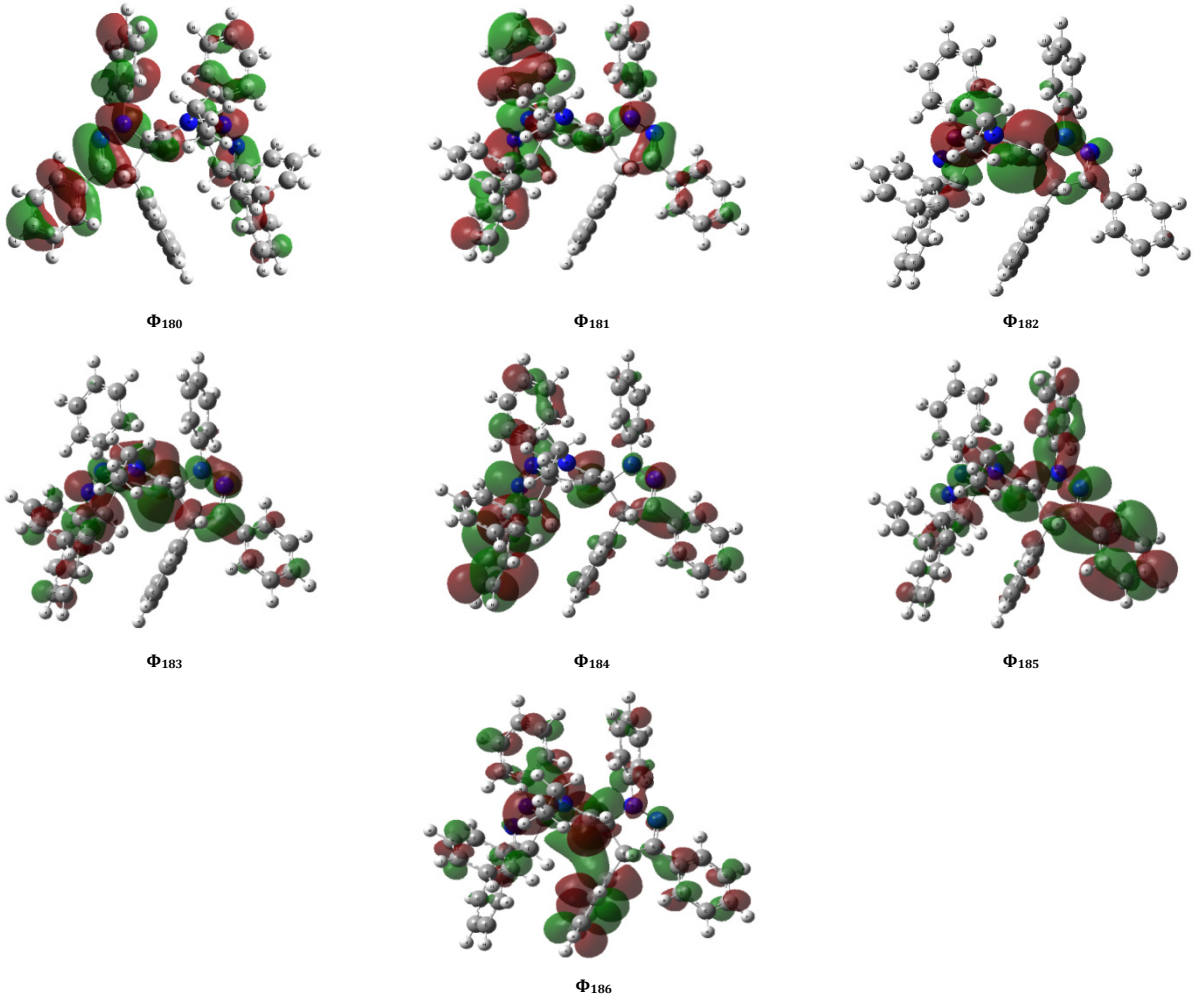

Figure S1. Electron density contours of the studied compound **1**.

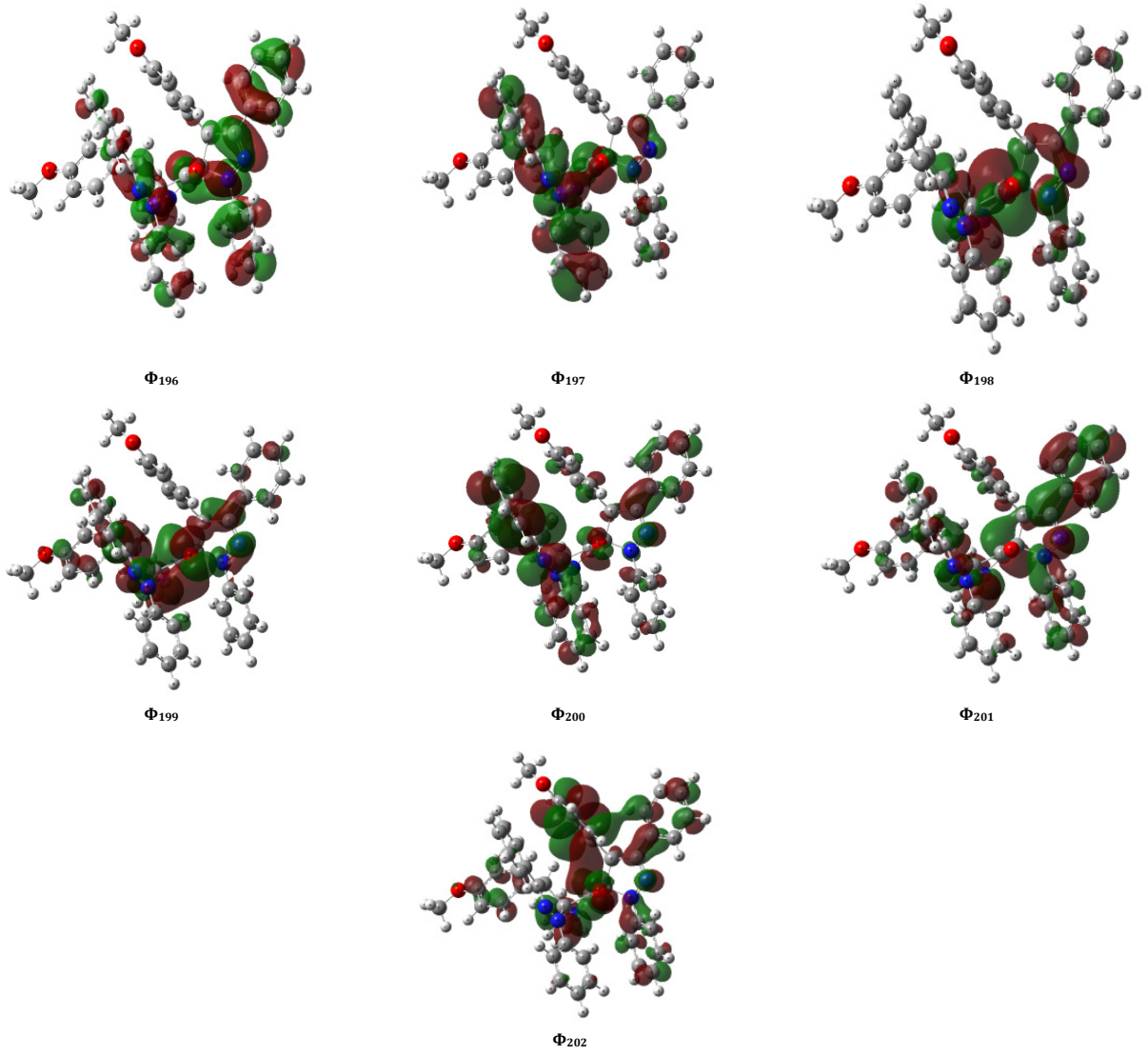

Figure S2. Electron density contours of the studied compound **2**.

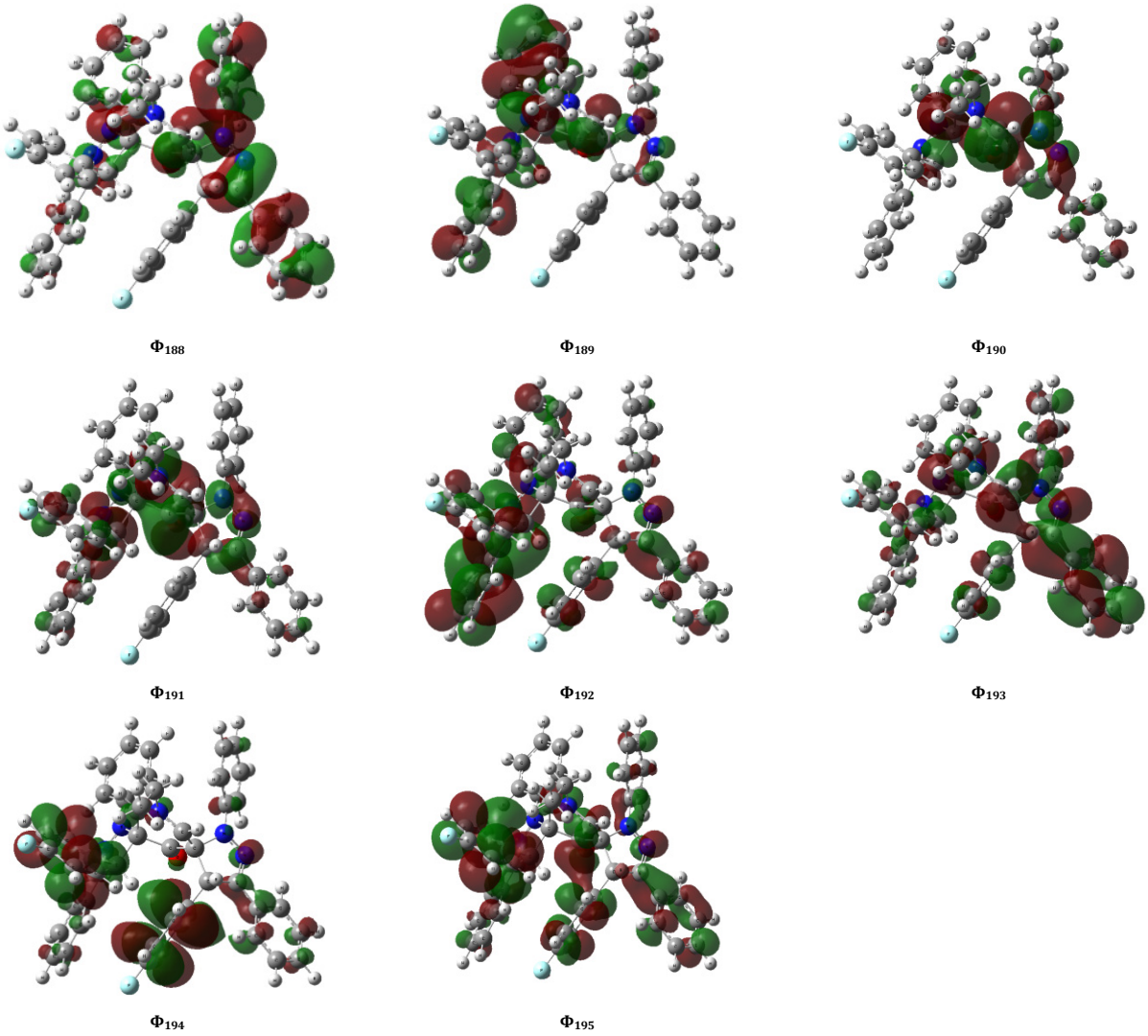

Figure S3. Electron density contours of the studied compound **3**.

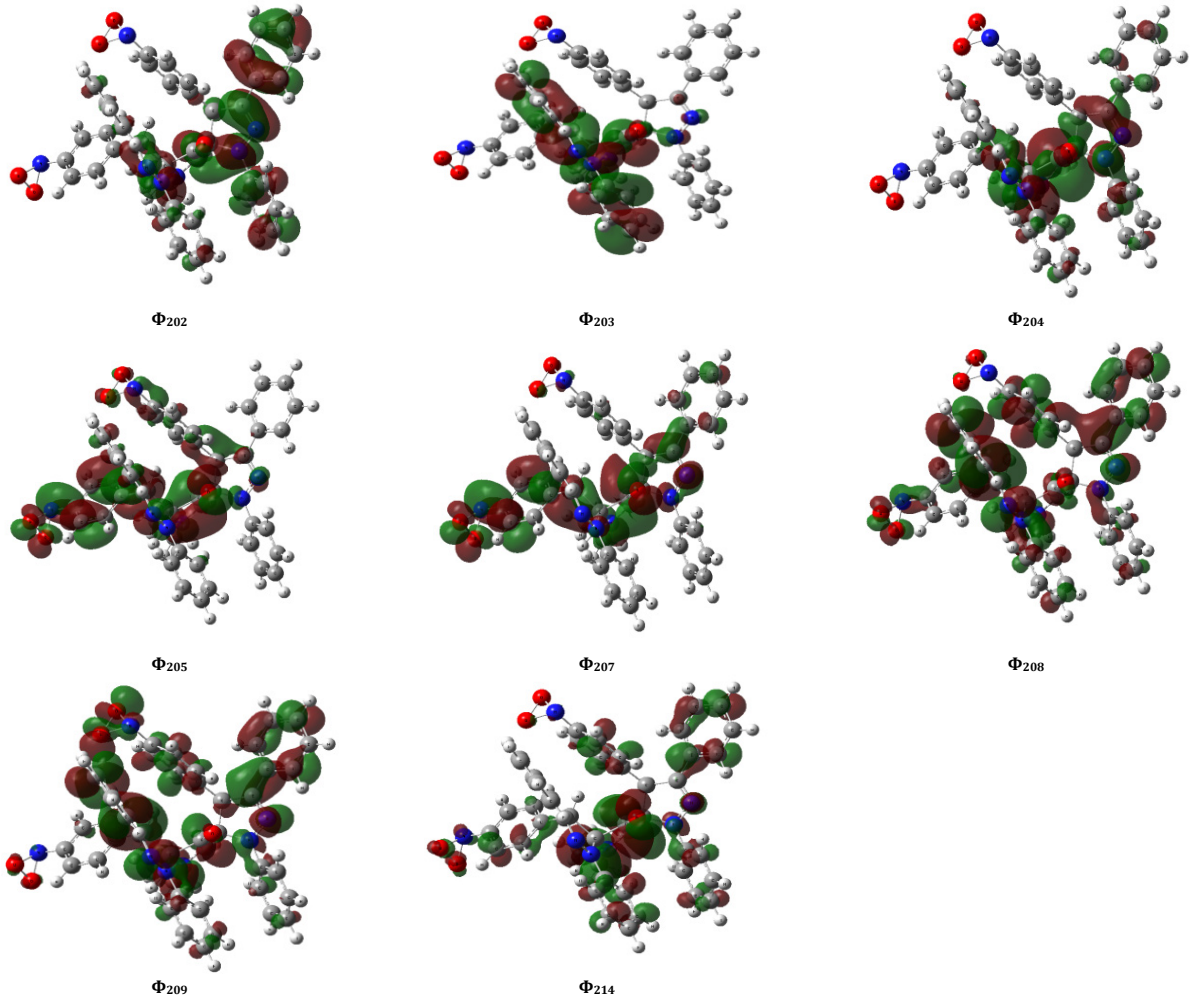

Figure S4. Electron density contours of the studied compound **4**.

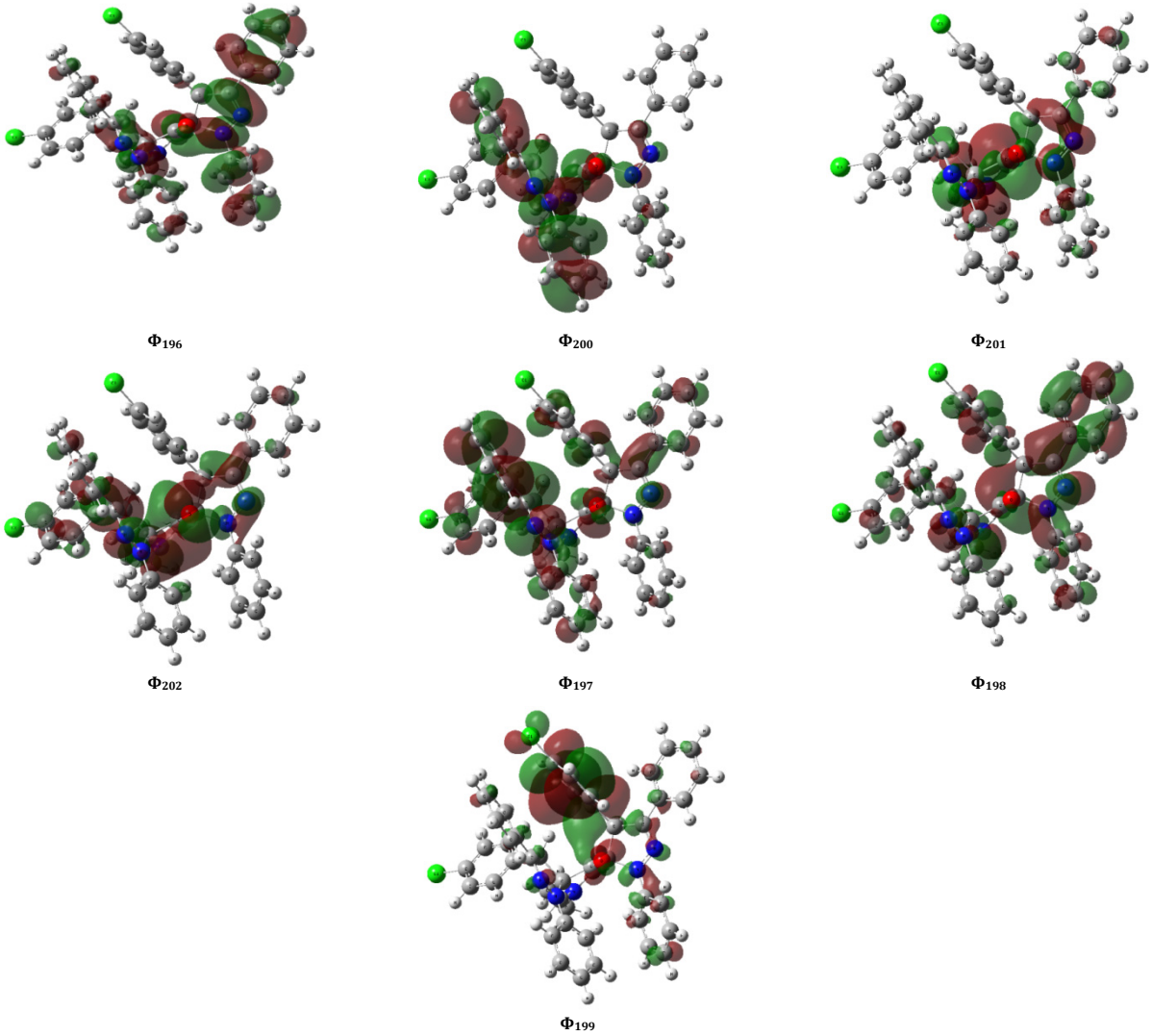

Figure S5. Electron density contours of the studied compound **5**.