Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Understanding the interaction of SARS-CoV-2 with UVC light:

An insight from quantum chemical calculation-based findings

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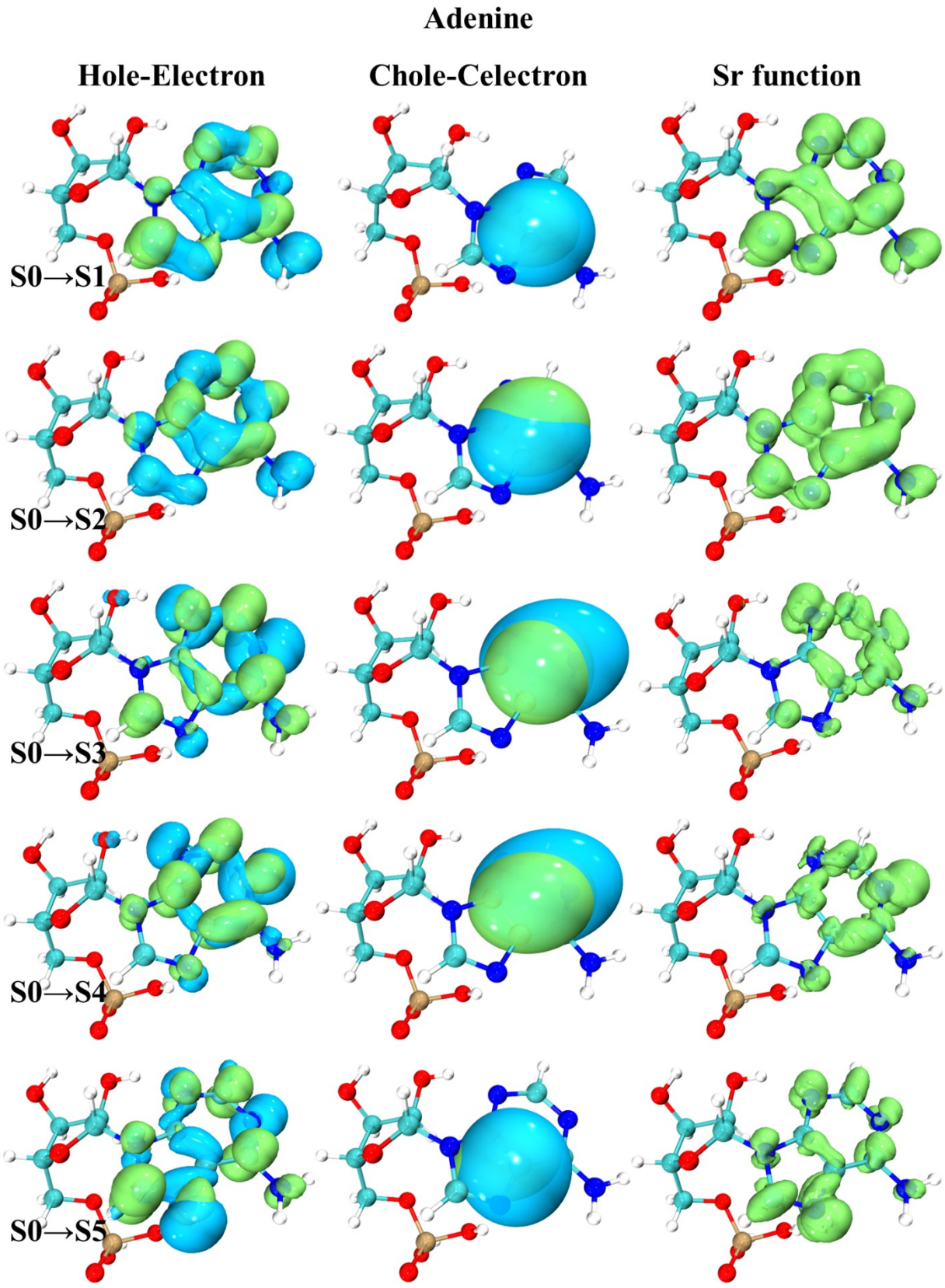

Figure S1. The illustration of hole-electron, Chole-Celectron, and Sr function of S1 to S5 of adenine. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

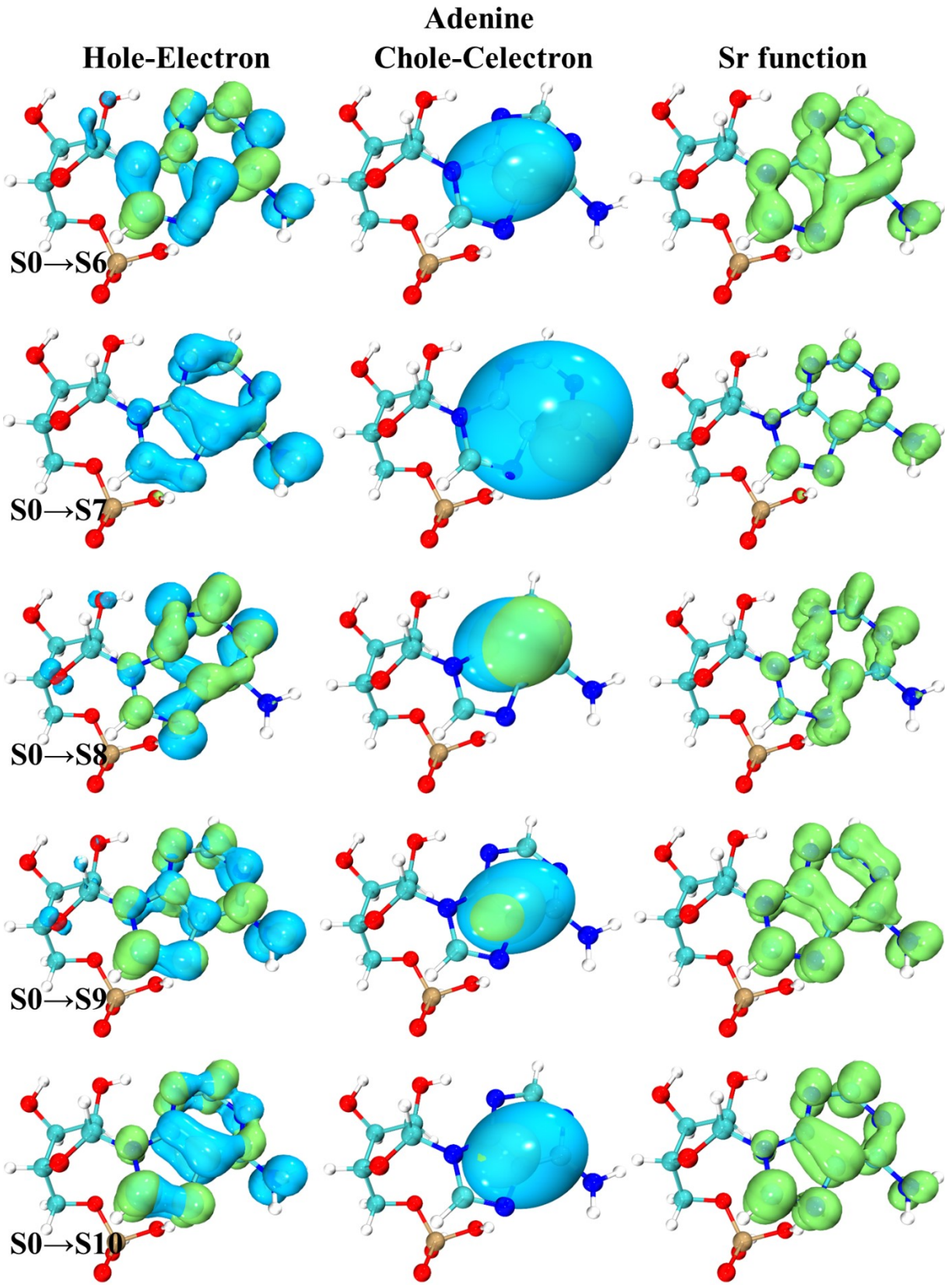

Figure S2. The illustration of hole-electron, Chole-Celectron, and Sr function of S6 to S10 of adenine. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

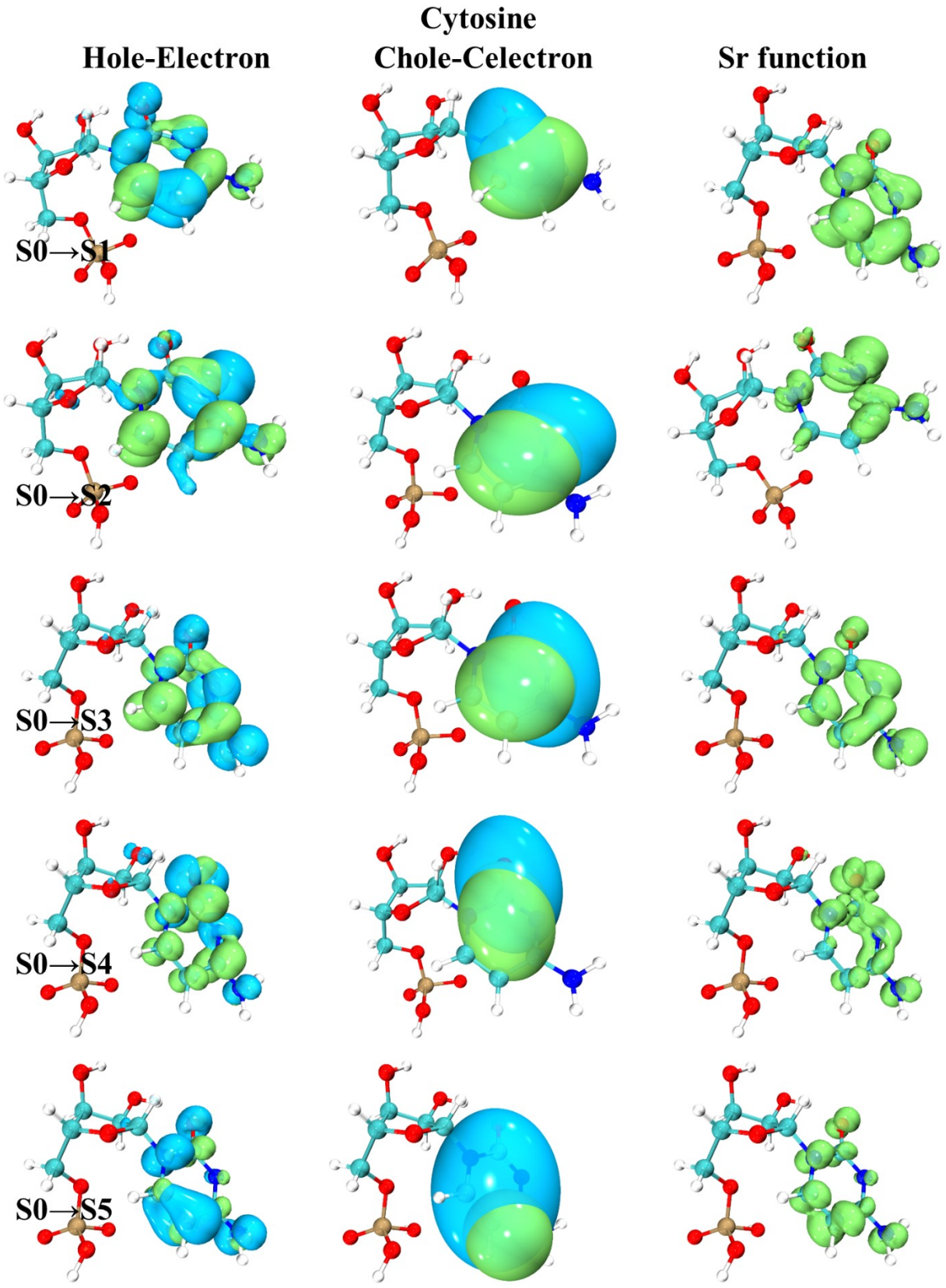

Figure S3. The illustration of hole-electron, Chole-Celectron, and Sr function of S1 to S5 of cytosine. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

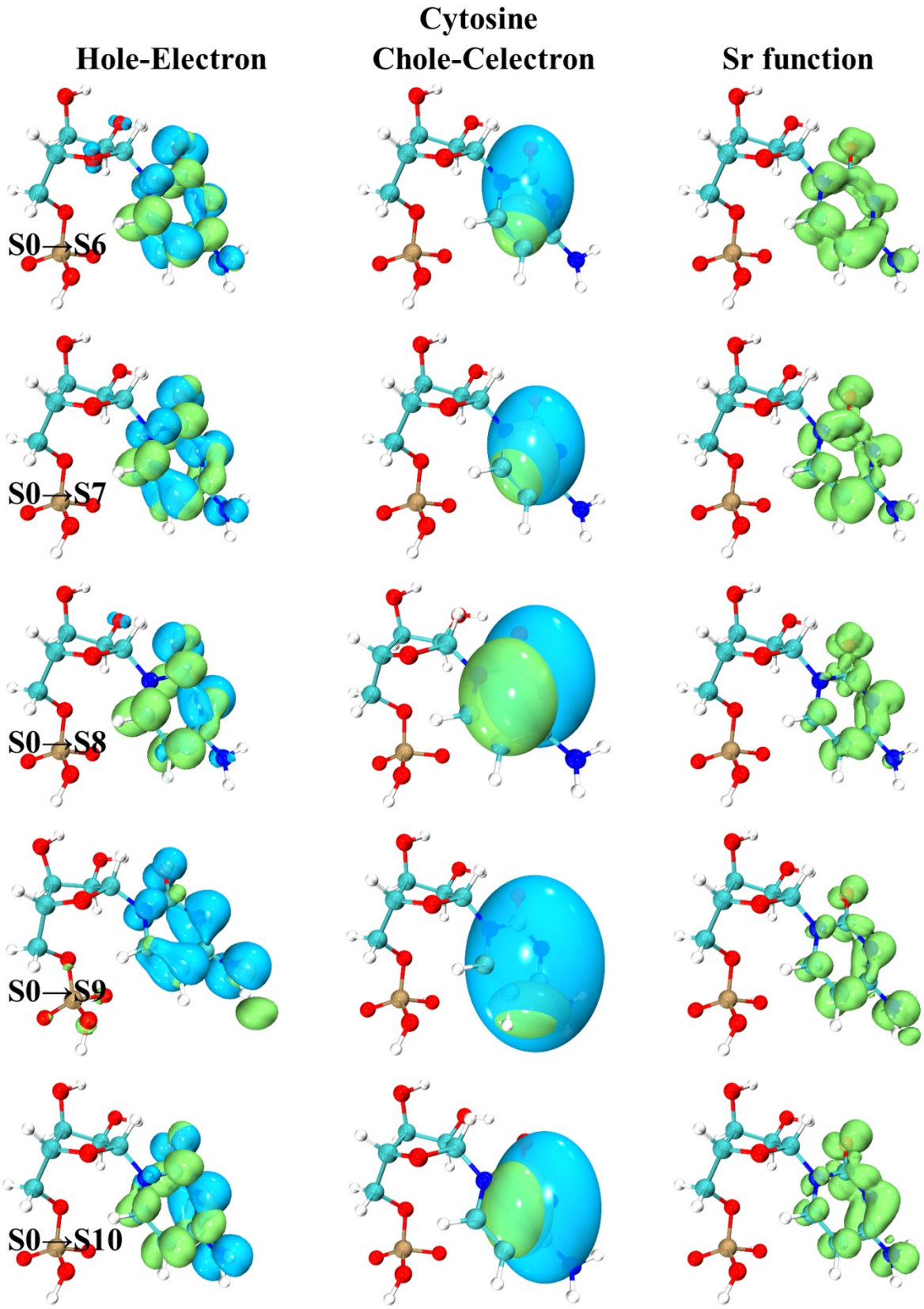

Figure S4. The illustration of hole-electron, Chole-Celectron, and Sr function of S6 to S10 of cytosine. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

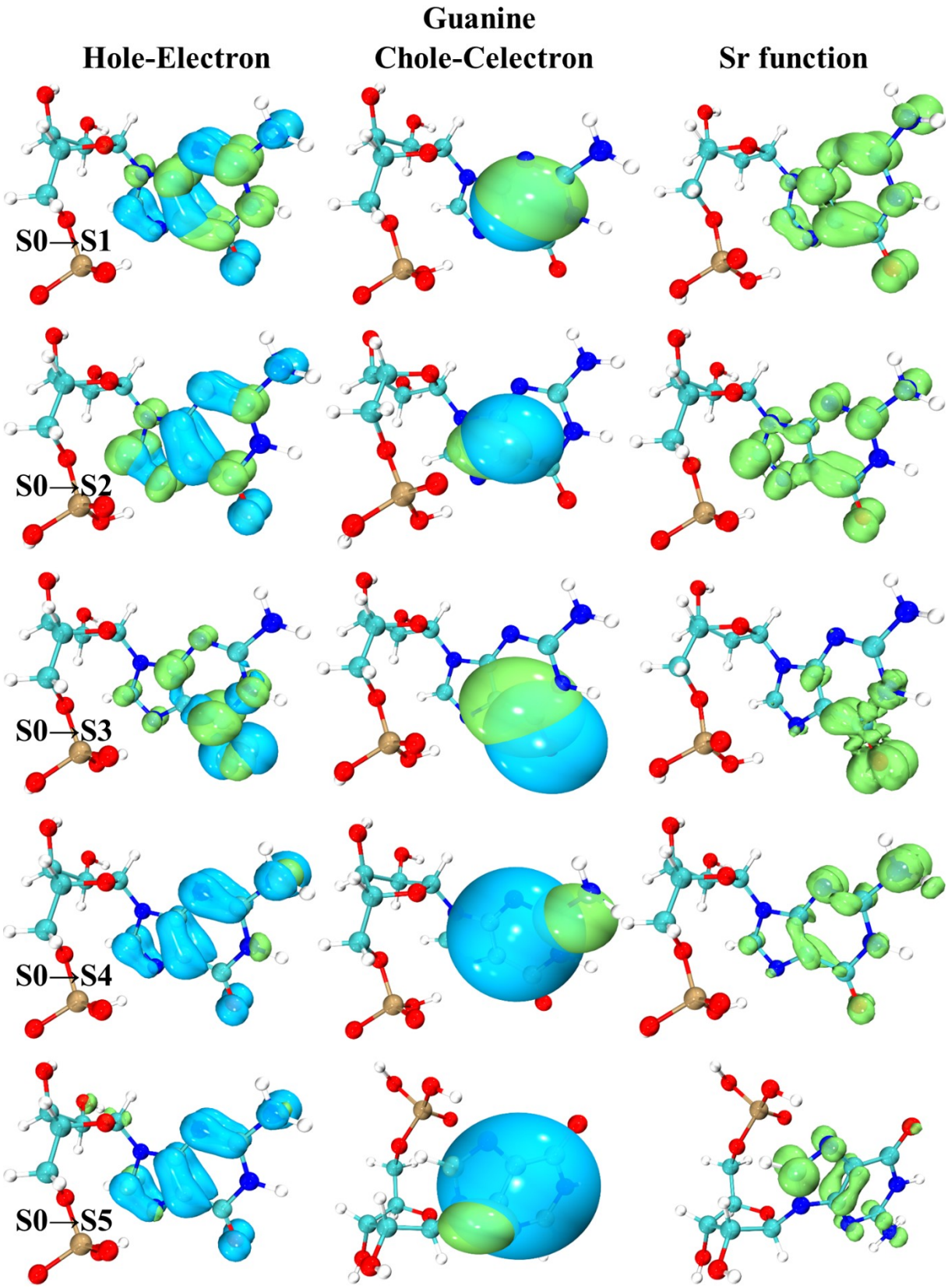

Figure S5. The illustration of hole-electron, Chole-Celectron, and Sr function of S1 to S5 of guanine. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

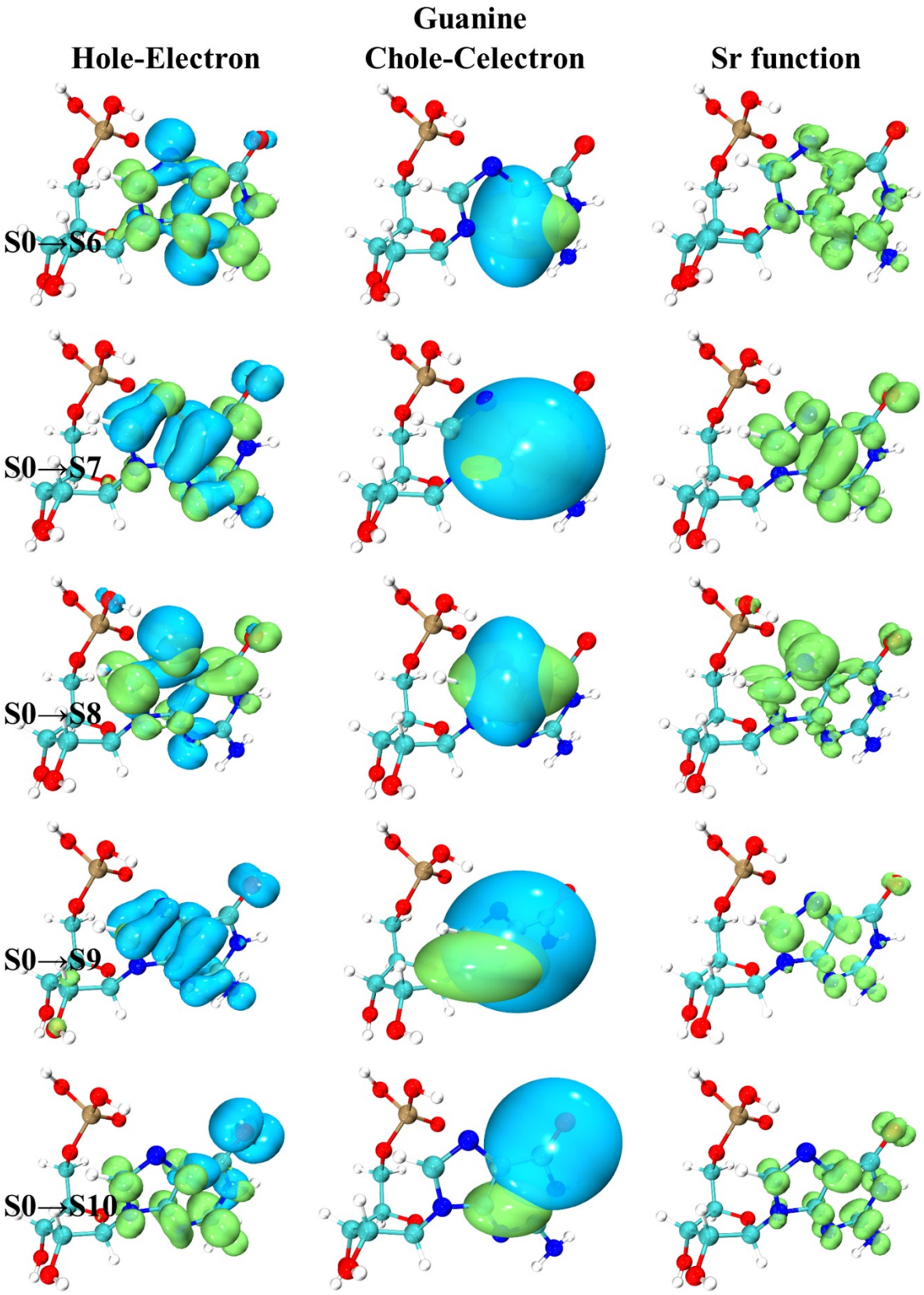

Figure S6. The illustration of hole-electron, Chole-Celectron, and Sr function of S6 to S10 of guanine. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

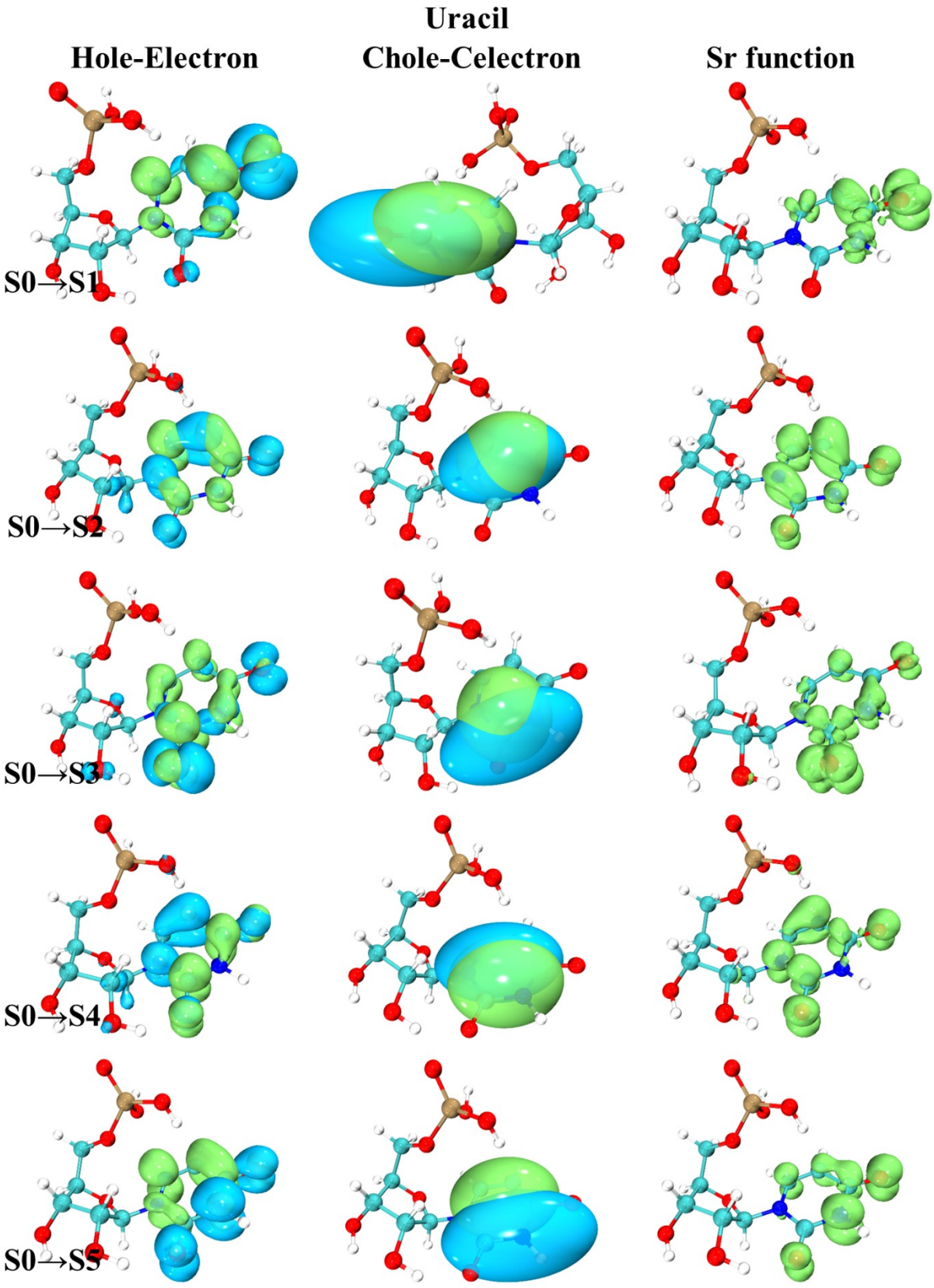

Figure S7. The illustration of hole-electron, Chole-Celectron, and Sr function of S1 to S5 of uracil. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

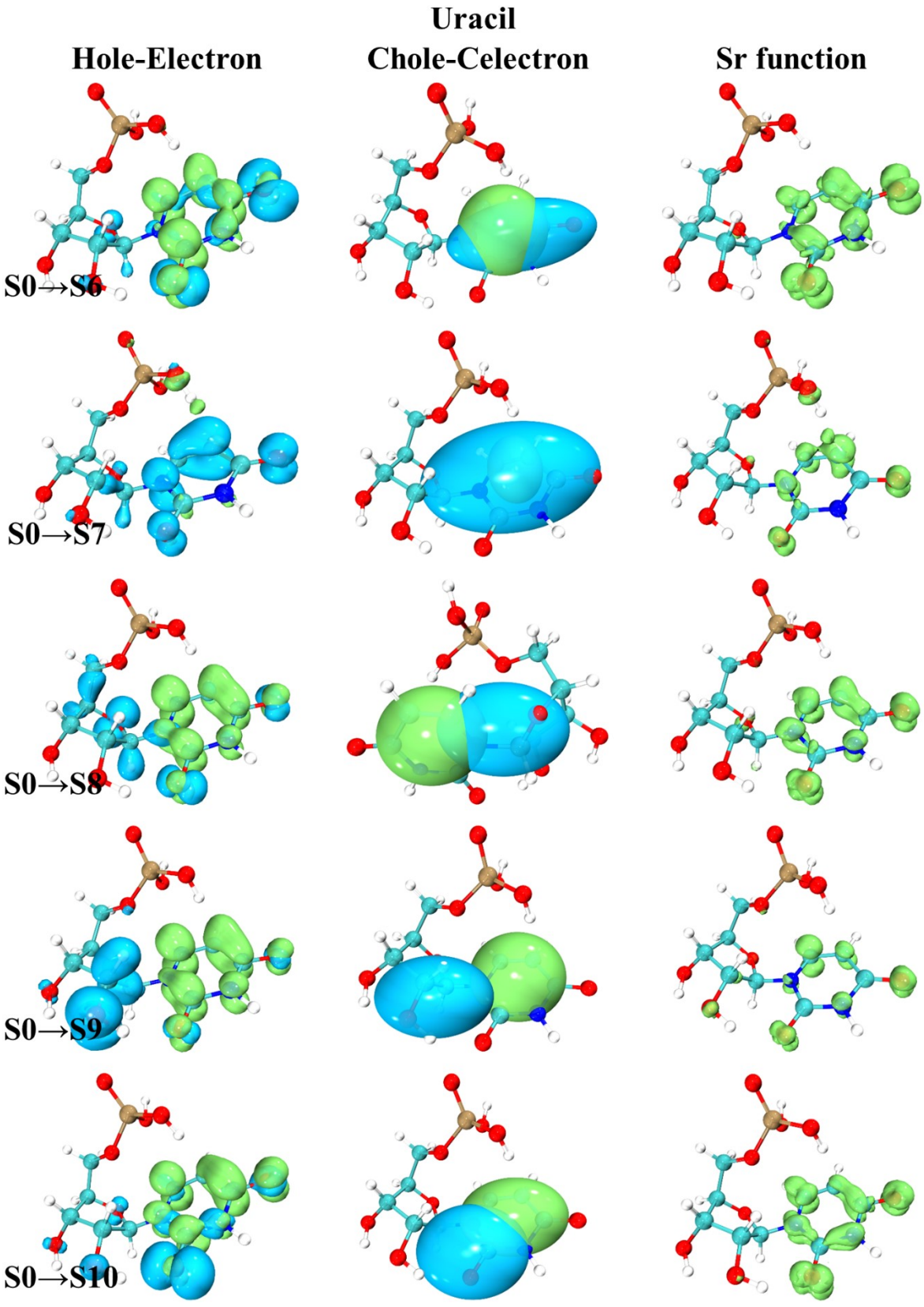

Figure S8. The illustration of hole-electron, Chole-Celectron, and Sr function of S6 to S10 of uracil. The isovalues of hole and electron are 0.003 au for hole-electron, while they are set to 0.002 au for Chole-Celectron and Sr function. Green and blue are denoted as electron and hole distributions, respectively.

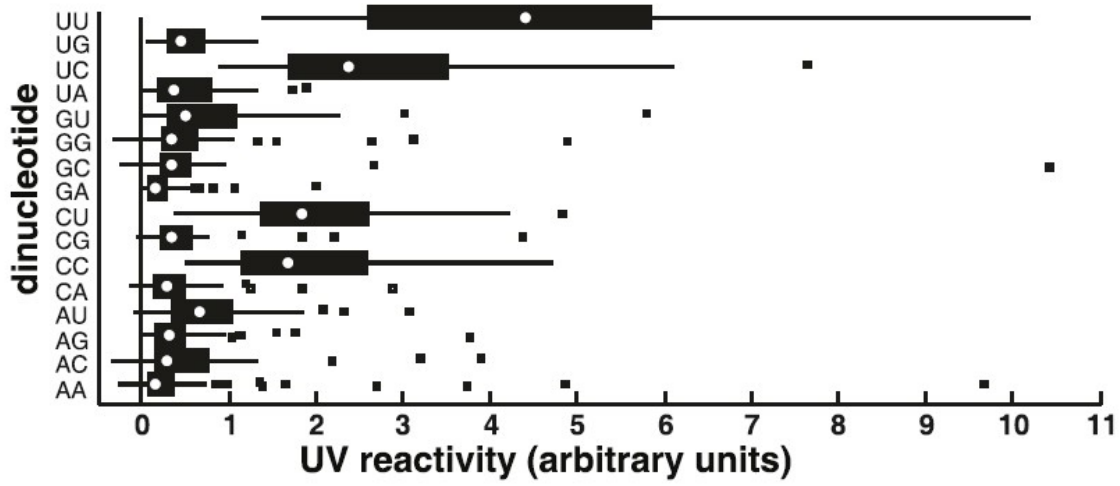

Figure S9. Box plot of reactivities across all dinucleotide types.[1]

References

1. W. Kladwang, J. Hum and R. Das, *Scientific reports*, 2012, **2**, 1-7.