Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Exploring the Nature of Clopidogrel-Bromocresol Green-Interaction via Spectrophotometric Measurements and Quantum Chemical Calculations

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Figures

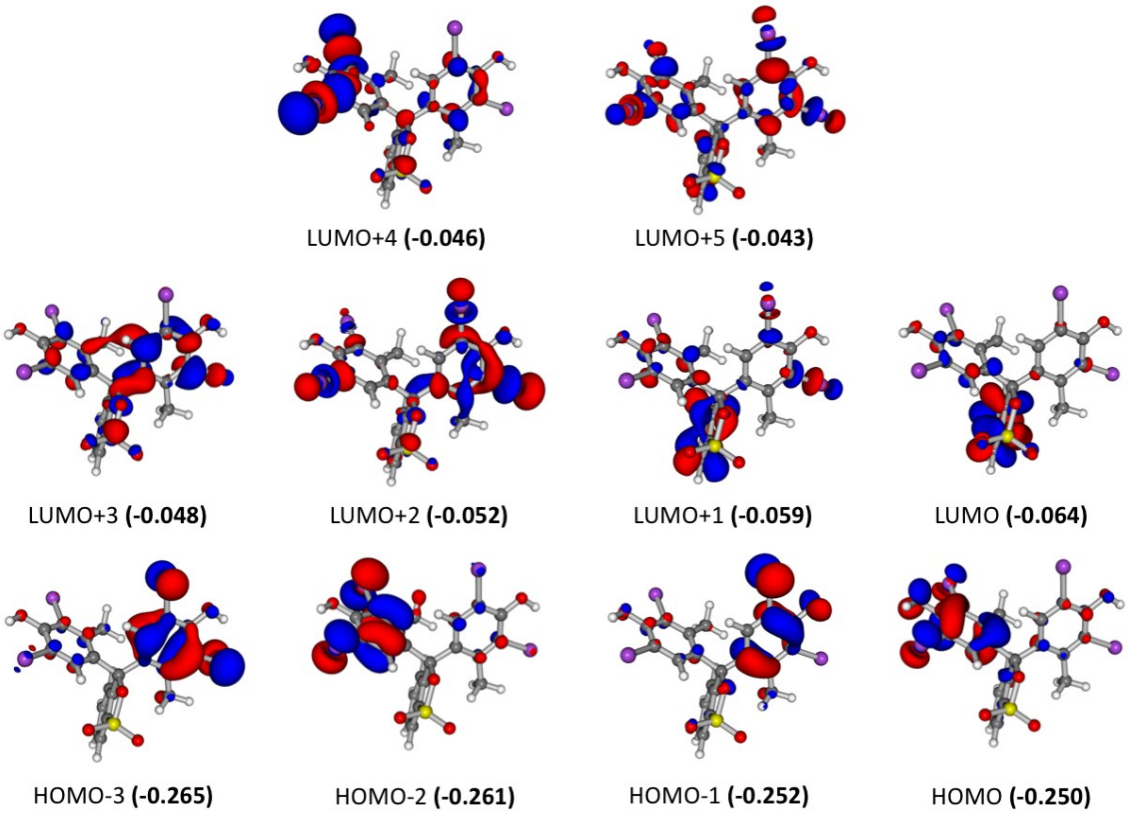

Fig. S1. Frontier molecular orbitals for the optimized geometry of BCG at the B3LYP/6–31+G(d,p)+Lanl2dz level of theory and using CPCM. Values in parentheses are the electronic energies in a.u. of the corresponding frontier molecular orbitals. Band gap = 0.186 a.u.

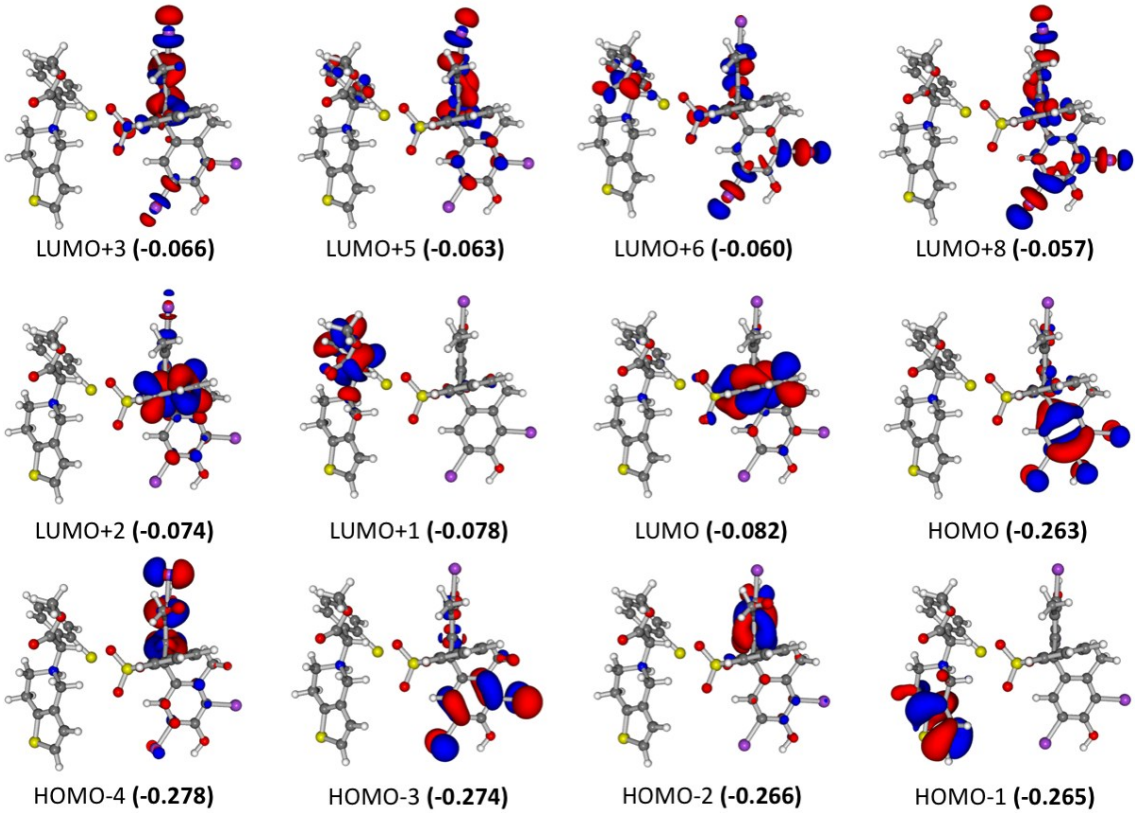

Fig. S2. Frontier molecular orbitals for the optimized geometry of BCG–$CLOP^{+}$ ion-pair at the B3LYP/6–31+G(d,p)+Lanl2dz level of theory and using CPCM. Values in parentheses are the electronic energies in a.u. of the corresponding frontier molecular orbitals. Band gap = 0.181 a.u.

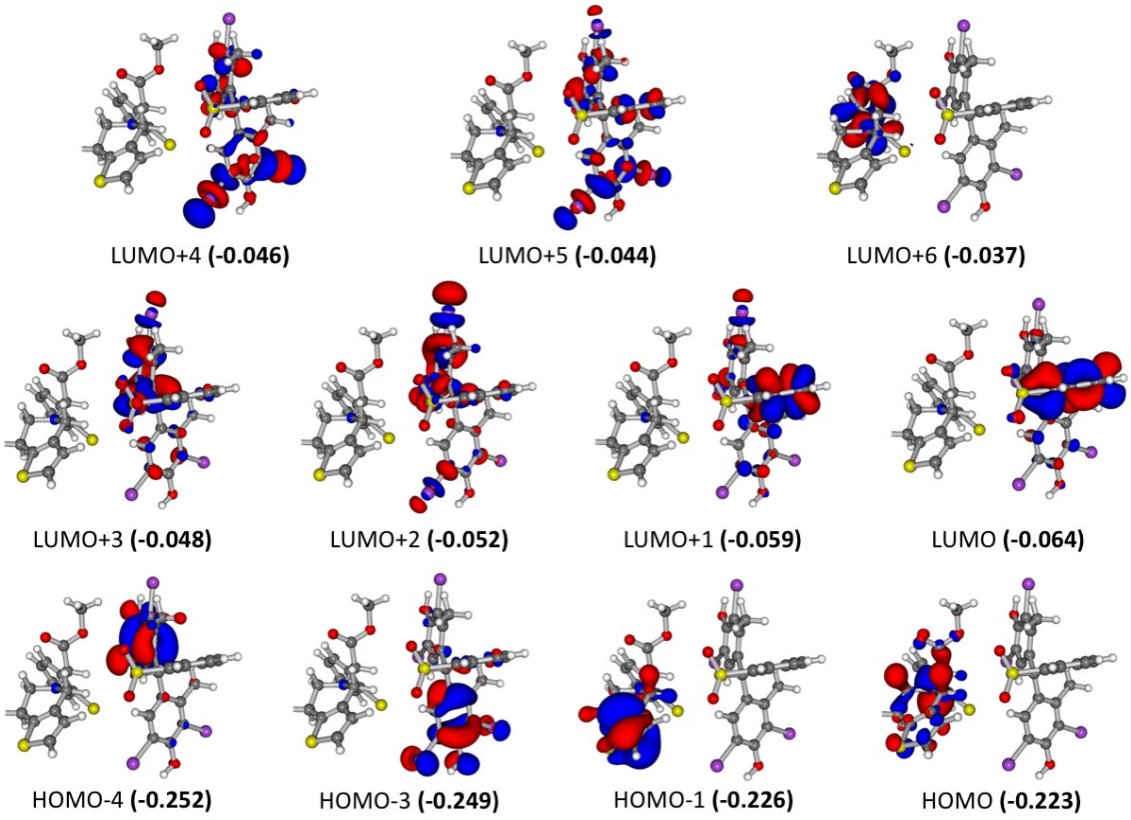

Fig. S3. Frontier molecular orbitals for the optimized geometry of BCG–CLOP ion-pair at the B3LYP/6–31+G(d,p)+Lanl2dz level of theory and using CPCM. Values in parentheses are the electronic energies in a.u. of the corresponding frontier molecular orbitals. Band gap = 0.159 a.u.

Tables

TableS1. Possible excited states,their oscillator strength values, and most contributed electronic transitions to every excited state calculated for BCGat the B3LYP6–31+G(d,p)+Lanl2dz level of theory and using CPCM.

Excitation	Oscillator strength	Transitions	Contributions [%]
excited state 1 (282.65 nm)	0.0098	HOMO-1 → LUMO	18.6
		HOMO-1 → LUMO+1	25.0
		HOMO-1 → LUMO+2	23.2
		HOMO → LUMO	13.7
excited state 2 (280.35 nm)	0.0304	HOMO → LUMO	40.3
		HOMO → LUMO+2	19.0
		HOMO → LUMO+4	20.4
excited state 3 (274.68 nm)	0.0060	HOMO → LUMO	30.5
		HOMO → LUMO+1	30.2
		HOMO → LUMO+2	8.7
		HOMO → LUMO+4	10.6
excited state 4 (268.78 nm)	0.0033	HOMO-1 → LUMO	64.3
excited state 5 (266.71 nm)	0.0038	HOMO-3 → LUMO	11.7
		HOMO-3 → LUMO+1	12.9
		HOMO-3 → LUMO+2	25.6
		HOMO-1 → LUMO+1	16.0
excited state 6 (266.10 nm)	0.0314	HOMO-2 → LUMO	21.5
		HOMO → LUMO	11.0
		HOMO → LUMO+1	14.3
		HOMO → LUMO+3	10.0
		HOMO → LUMO+4	17.1
excited state 7 (263.27 nm)	0.0083	HOMO-2 → LUMO	10.1
		HOMO-1 → LUMO+3	10.1
		HOMO → LUMO+1	31.0
excited state 8 (260.60 nm)	0.0477	HOMO-3 → LUMO+1	12.9
		HOMO-3 → LUMO+3	9.2
		HOMO-1 → LUMO+1	10.21
		HOMO-1 → LUMO+3	4.7
excited state 9 (258.19 nm)	0.0091	HOMO-1 → LUMO+1	31.2
		HOMO-1 → LUMO+2	27.1
		HOMO-1 → LUMO+5	13.7
excited state 10 (257.29 nm)	0.0214	HOMO-2 → LUMO+4	26.1
		HOMO → LUMO+3	27.0
excited state 11 (255.46 nm)	0.0065	HOMO-2 → LUMO	8.5
		HOMO → LUMO+2	35.6
		HOMO → LUMO+3	18.2
		HOMO → LUMO+4	21.1
excited state 12 (253.27 nm)	0.0295	HOMO-2 → LUMO	47.5
		HOMO-2 → LUMO+1	29.2

TableS2. Possible excited states, their oscillator strength values, and most contributed electronic transitions to every excited state calculated for BCG–$CLOP^{+}$ion-pair at the B3LYP/6–31+G(d,p)+Lanl2dz level of theory and using CPCM.

Excitation	**Oscillator strength**	**Transitions**	**Contributions [%]**
excited state 1 (287.27 nm)	0.0471	HOMO → LUMO	89.7
excited state 2 (282.74 nm)	0.0045	HOMO-2 → LUMO	52.9
		HOMO-2 → LUMO+2	16.5
excited state 3 (277.77 nm)	0.0102	HOMO → LUMO+2	49.1
		HOMO → LUMO+3	9.5
		HOMO → LUMO+6	10.4
		HOMO → LUMO+8	13.3
excited state 4 (274.78 nm)	0.0024	HOMO-2 → LUMO	43.3
		HOMO-2 → LUMO+2	20.4
		HOMO-2 → LUMO+5	8.3
excited state 5 (270.99 nm)	0.0093	HOMO-3 → LUMO	32.2
		HOMO → LUMO+3	8.3
		HOMO → LUMO+5	8.9
		HOMO → LUMO+6	8.5
excited state 6 (270.53 nm)	0.0011	HOMO-1 → LUMO	38.4
		HOMO-1 → LUMO+1	60.9
excited state 7 (267.69 nm)	0.0005	HOMO-1 → LUMO	61.0
		HOMO-1 → LUMO+1	37.9
excited state 8 (267.22 nm)	0.0231	HOMO-4 → LUMO+3	11.4
		HOMO-3 → LUMO	20.4
		HOMO-2 → LUMO+2	8.4
		HOMO → LUMO+2	15.9
excited state 9 (265.78 nm)	0.0051	HOMO-4 → LUMO+3	12.6
		HOMO-2 → LUMO+5	20.1
		HOMO → LUMO+2	14.5
excited state 10 (264.16 nm)	0.0001	HOMO-2 → LUMO+1	32.5
		HOMO → LUMO+1	64.8
excited state 11 (262.30 nm)	0.0302	HOMO-4 → LUMO	19.0
		HOMO-4 → LUMO+2	15.6
		HOMO-2 → LUMO+5	11.8
excited state 12 (261.38 nm)	0.0002	HOMO-2 → LUMO+1	64.2
		HOMO → LUMO+1	31.5

TableS3. Possible excited states, their oscillator strength values, and most contributed electronic transitions to every excited state calculated for BCG–CLOP ion-pair at the B3LYP/6–31+G(d,p)+Lanl2dz level of theory and using CPCM.

Excitation	Oscillator strength	Transitions	Contributions [%]
excited state 1 (313.76 nm)	0.0000	HOMO → LUMO	98.7
excited state 2 (305.62 nm)	0.0001	HOMO-1 → LUMO	98.6
excited state 3 (302.57 nm)	0.0001	HOMO → LUMO+1	98.3
excited state 4 (294.50 nm)	0.0006	HOMO → LUMO+2 HOMO → LUMO+6	18.8 59.8
excited state 5 (294.42 nm)	0.0000	HOMO-1 → LUMO+1	90.6
excited state 6 (291.63 nm)	0.0002	HOMO → LUMO+2	70.6
excited state 7 (285.17 nm)	0.0003	HOMO → LUMO+3	85.4
excited state 8 (283.46 nm)	0.0069	HOMO-4 → LUMO HOMO-4 → LUMO+1 HOMO-4 → LUMO+2 HOMO-3 → LUMO	22.3 27.8 21.9 11.4
excited state 9 (282.19 nm)	0.0004	HOMO-1 → LUMO+2	89.1
excited state 10 (280.84 nm)	0.0346	HOMO-3 → LUMO HOMO-3 → LUMO+2 HOMO-3 → LUMO+4	51.4 10.6 12.1
excited state 11 (280.49 nm)	0.0034	HOMO → LUMO+4	81.0
excited state 12 (275.88 nm)	0.0006	HOMO-1 → LUMO+3 HOMO → LUMO+5	54.2 36.4