Supplementary Materials: A Computational Study of Structure and Reactivity of *N*-Substitued-4-Piperidones Curcumin Derivatives and Their Radical Anions

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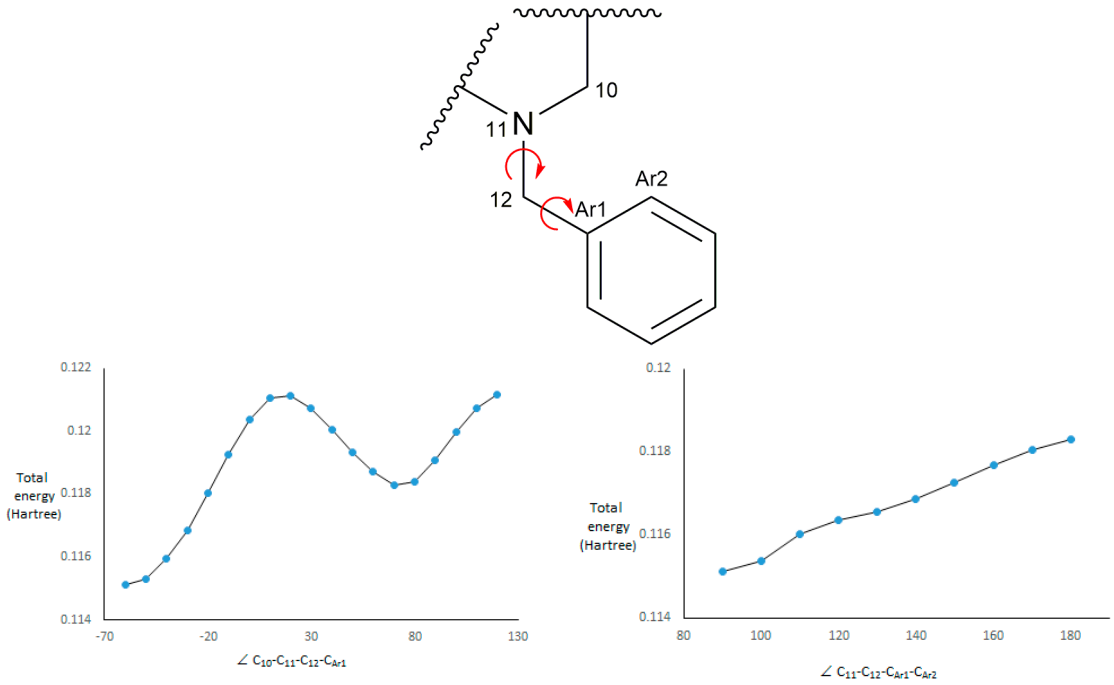
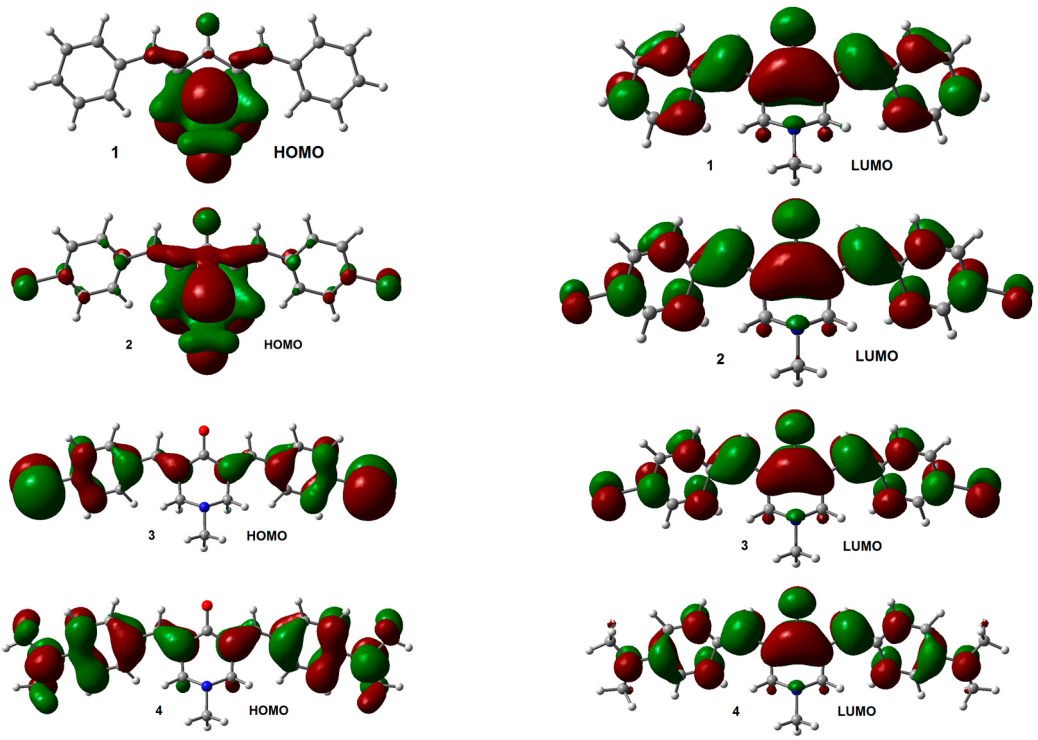


Figure S1. Energy profile for rotation around N_{11}–C_{12} and C_{12}–CAr_1 bonds of compound **7**.



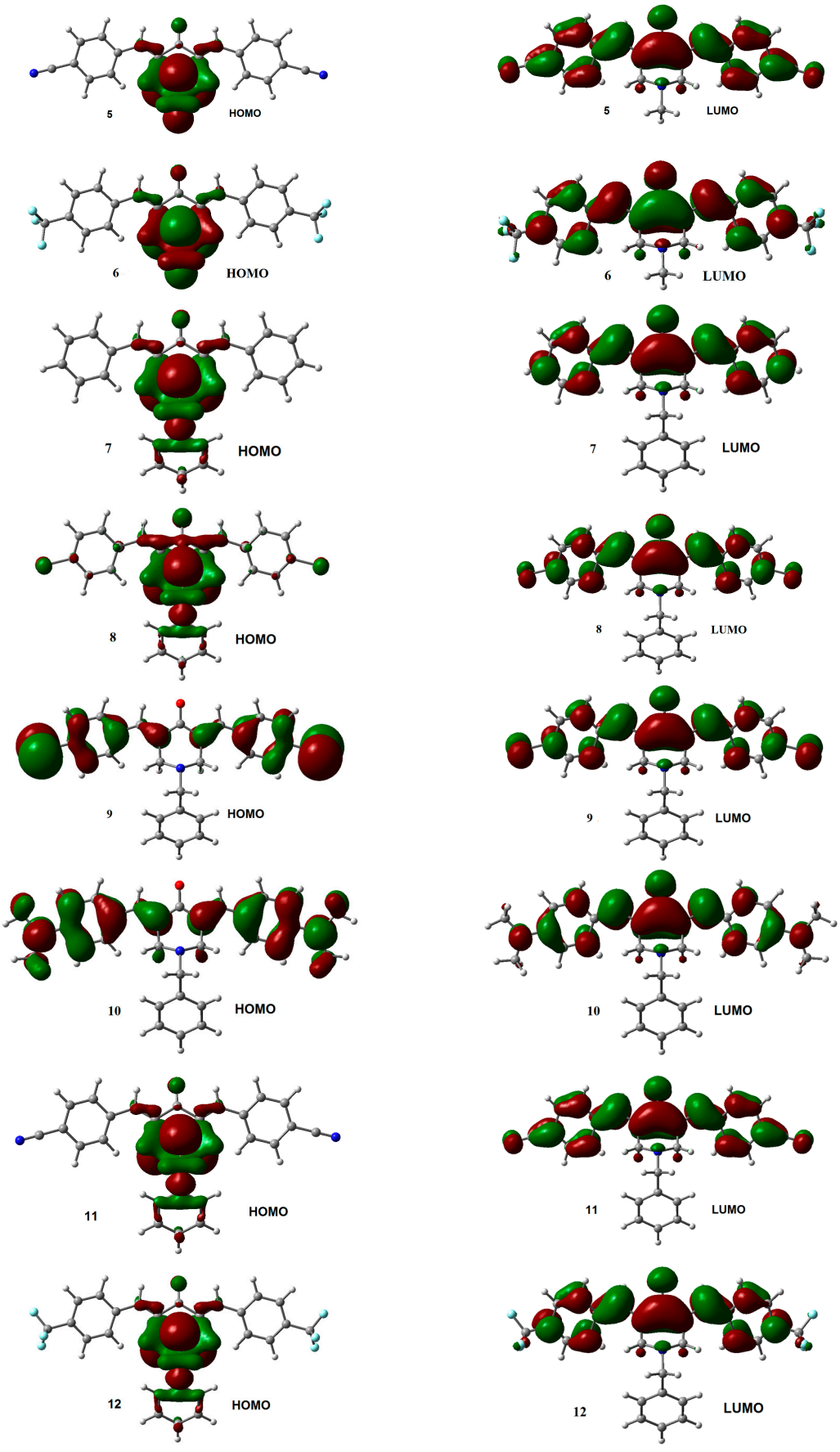
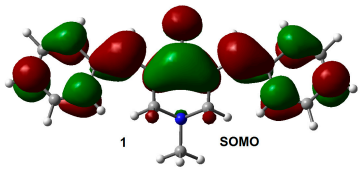


Figure S2. Frontier Molecular Orbitals (FMO) for neutral molecules. Isosurface value = 0.02 e/Å^3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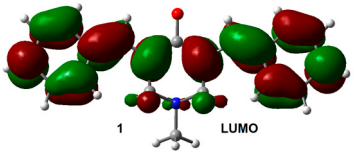
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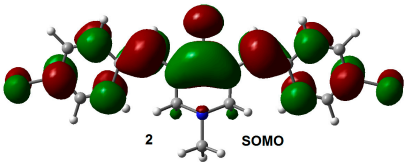
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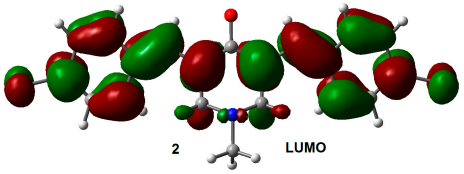
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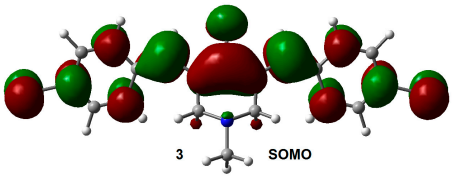
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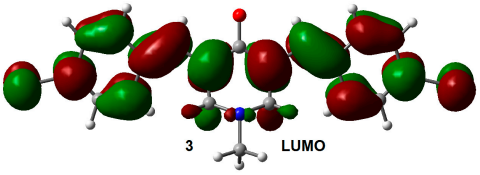
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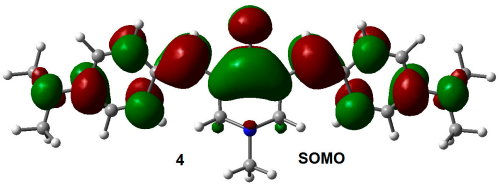
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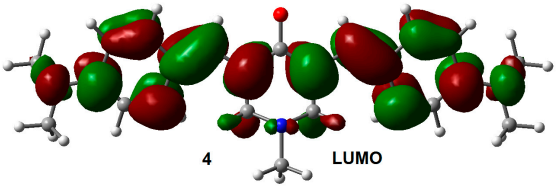
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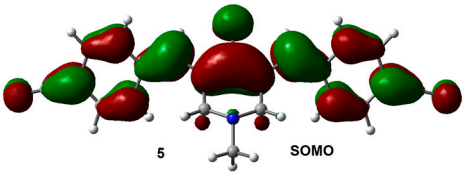
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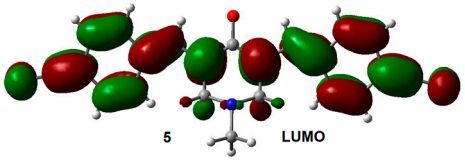
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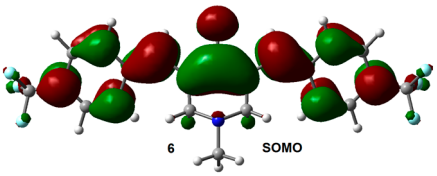
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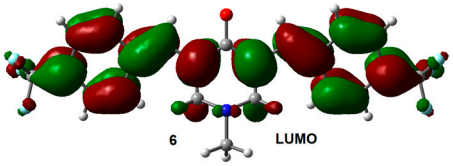
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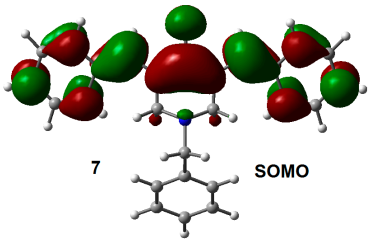
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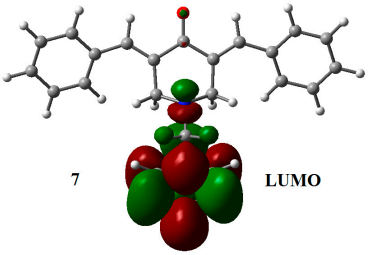
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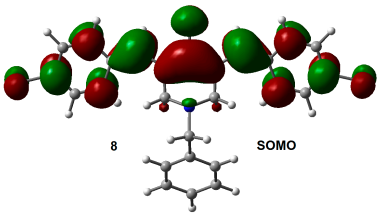
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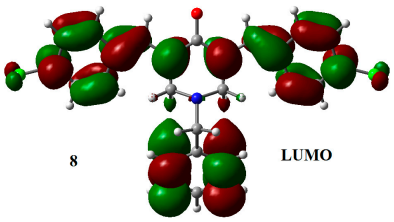
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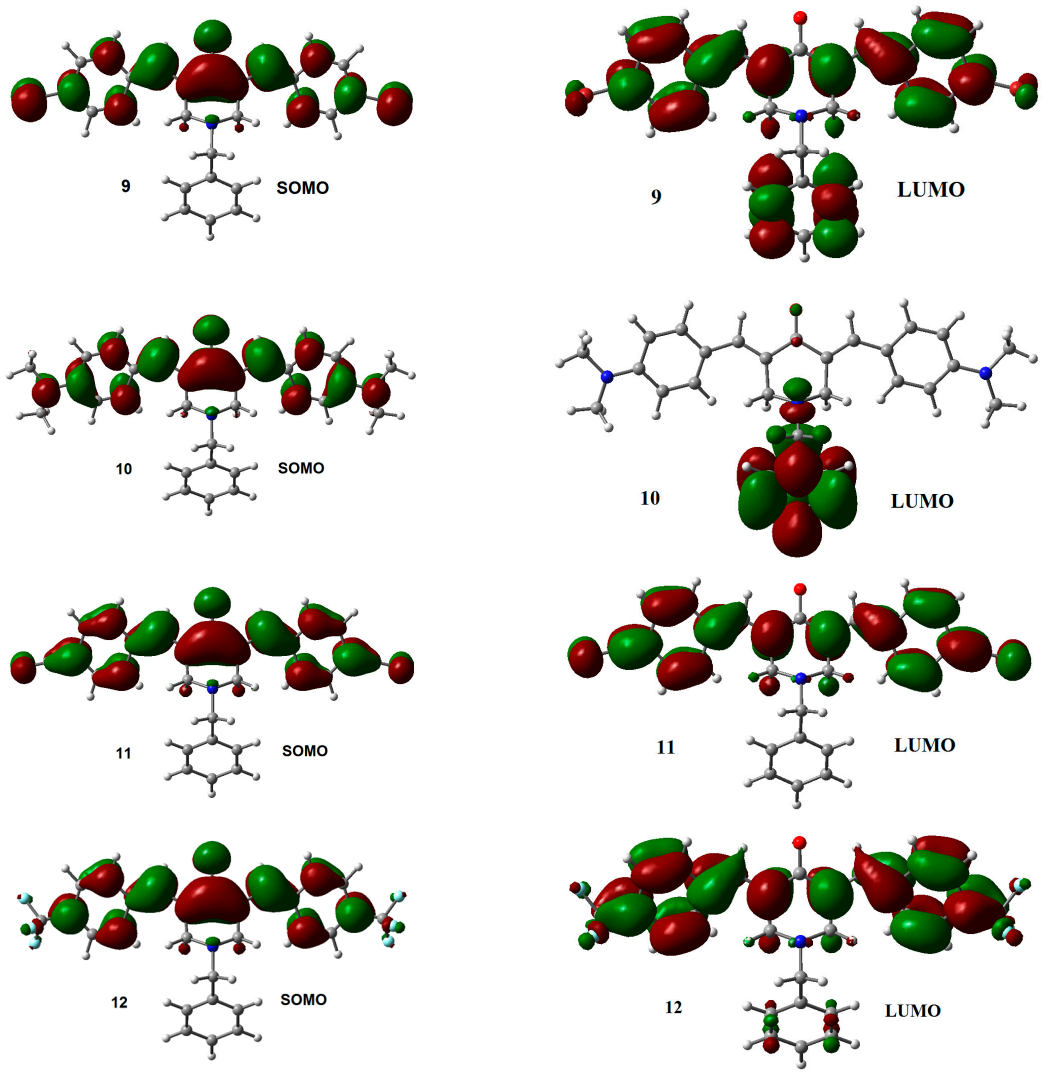

Figure S3. Frontier Molecular Orbitals (FMO) for vertical radical anions (equals to adiabatic, except LUMO for **7**–**12**). Isosurface value = 0.02 e/Å^3.

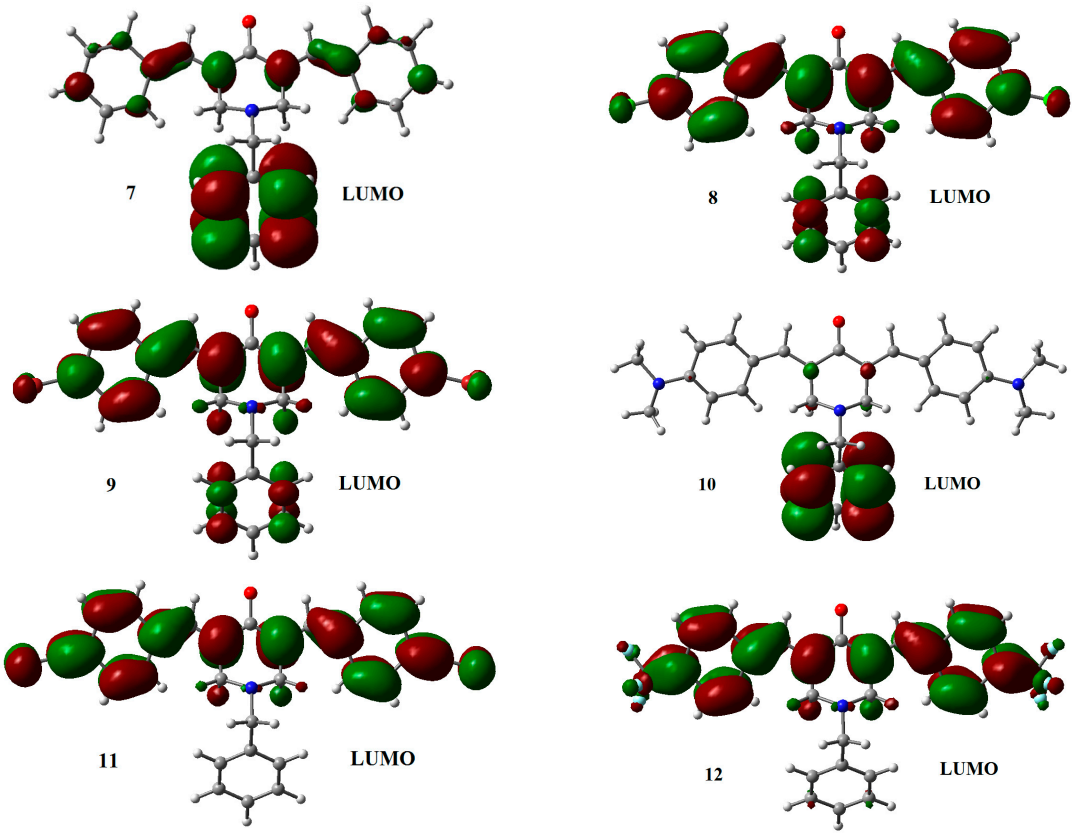

Figure S4. LUMO for adiabatic radical anions **7**–**12**. Isosurface value = 0.02 e/Å^3.

Table S1. Main geometrical parameters for the neutral molecules.

Compounds	C_1–C_2	C_2–C_3	C_3–C_4	C_1–C_7	C_7=C_8	C_9=O_9	N_{11}–C_{12}
1	1.410	1.391	1.397	1.463	1.353	1.230	1.455
2	1.410	1.390	1.395	1.462	1.353	1.230	1.455
3	1.410	1.390	1.395	1.462	1.353	1.230	1.455
4	1.411	1.385	1.416	1.456	1.356	1.234	1.453
5	1.411	1.387	1.406	1.463	1.353	1.228	1.456
6	1.410	1.389	1.398	1.464	1.352	1.229	1.456
7	1.410	1.391	1.397	1.464	1.353	1.230	1.470
8	1.410	1.390	1.395	1.463	1.353	1.230	1.470
9	1.410	1.390	1.395	1.463	1.353	1.230	1.471
10	1.411	1.385	1.416	1.456	1.356	1.233	1.468
11	1.411	1.387	1.406	1.463	1.353	1.228	1.472
12	1.410	1.390	1.398	1.464	1.352	1.229	1.471

Table S2. Main geometrical parameters for radical anions of **1–12**.

Compounds	C_1–C_2	C_2–C_3	C_3–C_4	C_1–C_7	C_7=C_8	C_9=O_9	N_{11}–C_{12}
1	1.424	1.388	1.402	1.445	1.377	1.262	1.448
2	1.424	1.387	1.398	1.443	1.377	1.261	1.449
3	1.424	1.387	1.397	1.443	1.377	1.261	1.449
4	1.424	1.383	1.410	1.444	1.377	1.263	1.448
5	1.426	1.380	1.415	1.439	1.376	1.256	1.450
6	1.425	1.383	1.406	1.441	1.376	1.259	1.449
7	1.423	1.388	1.402	1.445	1.377	1.262	1.461
8	1.423	1.387	1.398	1.443	1.377	1.261	1.462
9	1.424	1.387	1.397	1.443	1.376	1.261	1.462
10	1.420	1.387	1.413	1.445	1.377	1.264	1.461
11	1.426	1.380	1.415	1.439	1.375	1.256	1.464
12	1.410	1.390	1.398	1.464	1.352	1.229	1.471

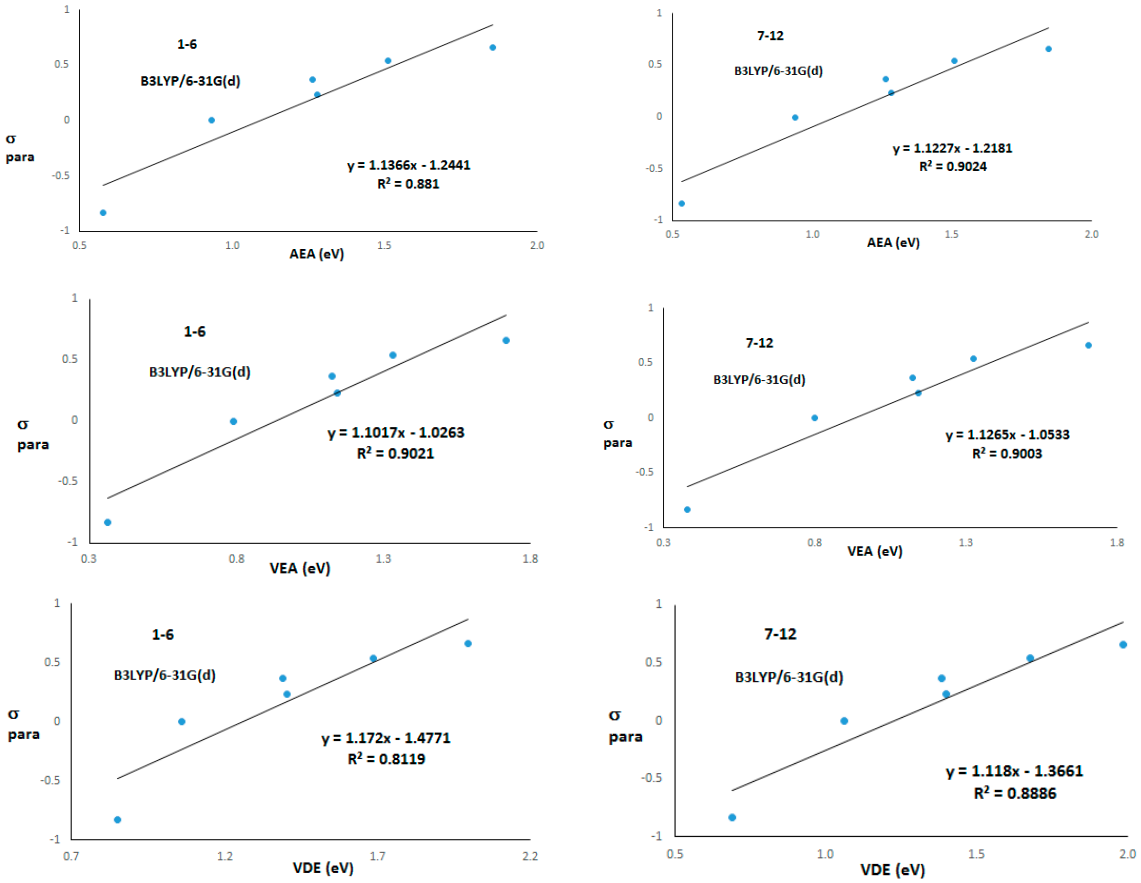

Figure S5. Correlation among AEAs, VEAs and VDEs with Hammett sigma constant at B3LYP/6-31G(d).

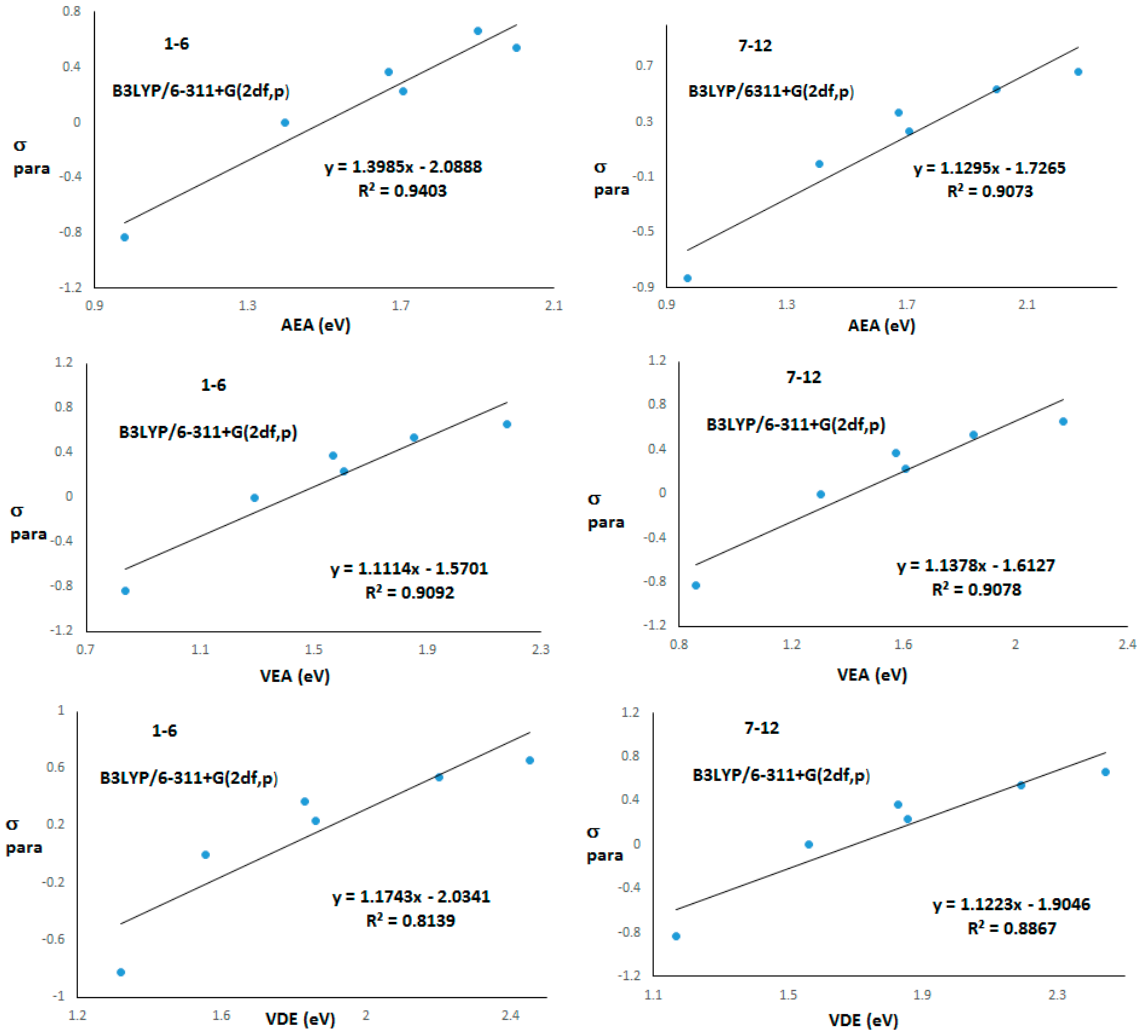

Figure S6. Correlation among AEAs, VEAs and VDEs with Hammett sigma constant at B3LYP/6-311+G(2df,p)//B3LYP/6-31G(d).