**Supplementary**

**Table S1** Reactivity descriptors and their equations.

|  |  |  |
| --- | --- | --- |
| **Reactivity descriptor** | **Symbol** | **Equation** |
| Electron affinity  Ionization potential  Global hardness  Electrophilicity index  Electronegativity  Fraction of transferred electrons | A  I  η  ω  χ  ΔN |  |

**Table S2** Quantum chemical reactivity descriptors of protonated molecules at B3LYP/6-31g(d).

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Electronic properties** | **Compounds** | | | | | | | |
| **(2)** | **(3)** | **(4)** | **(5)** | **(6)** | **(7)** | **(8)** | **(9)** |
| EHOMO (eV)  ELUMO (eV)  ΔE (eV)  χ (eV)  η (eV)  ΔN | -6.328  -1.447  4.881  3.888  2.441  0.638 | -6.327  -1.247  5.081  3.787  2.540  0.632 | -6.327  -0.956  5.371  3.642  2.686  0.625 | -6.327  -0.995  5.332  3.661  2.666  0.626 | -6.329  -0.863  5.465  3.596  2.733  0.623 | -6.131  -1.691  4.440  3.911  2.220  0.696 | -6.326  -1.749  4.578  4.038  2.289  0.647 | -6.230  -1.105  5.125  3.667  2.562  0.650 |