**Supplementary**

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

|  |  |  |
| --- | --- | --- |
| **Reactivity descriptor** | **Symbol** | **Equation** |
| Electron affinityIonization potentialGlobal hardnessElectrophilicity indexElectronegativityFraction of transferred electrons | AIηωχΔN | $$-E\_{HOMO}$$$$-E\_{LUMO}$$$$\frac{I-A}{2}$$$$\frac{μ^{2}}{2η}$$$$\frac{I+A}{2}$$$$\frac{[χ\_{Fe}- χ\_{inh}] }{2 (η\_{Fe}- η\_{inh})}$$ |

**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 | -6.328-1.4474.8813.8882.4410.638 | -6.327-1.2475.0813.7872.5400.632 | -6.327-0.9565.3713.6422.6860.625 | -6.327-0.9955.3323.6612.6660.626 | -6.329-0.8635.4653.5962.7330.623 | -6.131-1.6914.4403.9112.2200.696 | -6.326-1.7494.5784.0382.2890.647 | -6.230-1.1055.1253.6672.5620.650 |