Electronic Supplementary Material (ESI) for Analytical Methods

Supporting Information

Determination of paracetamol degradation process with online UV spectroscopic and Multivariate Curve Resolution -Alternating Least Squares methods: comparative validation by HPLC

*Xinwei Feng, Qinghua Zhang, Peisheng Cong, Zhongliang Zhu**

Department of Chemistry, Tongji University, Shanghai, 200092, P.R. China.
* Email: zhuzl@tongji.edu.cn.

Ab initio calculation methods

The energetic of the reaction pathways for the studied reaction can be investigated using ab initio method on the perspective of potential energy surface. The calculation results evaluate that whether the reaction channels are energetically accessible. The geometries of the reactant, product and various intermediates were optimized using Density Functional Theory (DFT) calculations at the B3LYP /6-31+G level. Vibrational frequency analysis was performed to confirm whether the optimized structures are stationary points at the B3LYP/6-31+G level. To confirm that the transition state connecting designated intermediates, the intrinsic reaction coordinate (IRC) computations were carried out at the B3LYP/6-31+G level as well. All quantum chemical calculations were completed using Gaussian 09 program package.

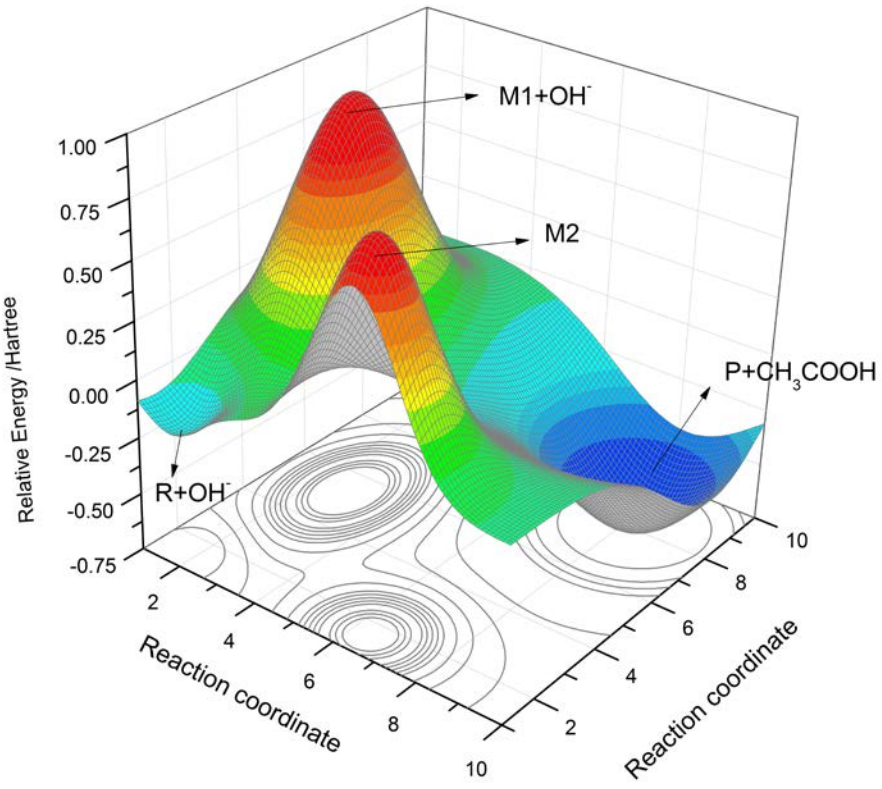

Fig. S1 Schematic potential energy surface for the Paracetamol+OH^- reaction. (R: reactant; M1: intermediate I; M2: intermediate II; P: product)

Table S1 Total energies (including ZPE corrections) of the reactants, of the products, and of the intermediates for the Paracetamol+OH^- reaction calculated at B3LYP/6-31G level with the optimized geometry are given in units of (Hartree).

Species	B3LYP/6-31G	Zero point energy	Total energy
R	-512.167	0.022	-512.145
OH^-	-75.312	0.005	-75.307
R+OH^-			**-587.452**
M1	-510.937	0.026	-510.911
M1+OH^-			**-586.218**
M2	-586.989	0.025	**-586.964**
P	-360.451	0.015	-360.436
CH_3COOH	-227.701	0.002	-227.699
P+CH_3COOH			**-588.135**