Electronic Supplementary Information

Impact of resonance effects on the protonation of aminobenzoic acid derivatives†

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1. Time-of-Flight Mass Spectra of Aminobenzoic Acids (ABAs) and Their Ethyl Esters (ABEs)

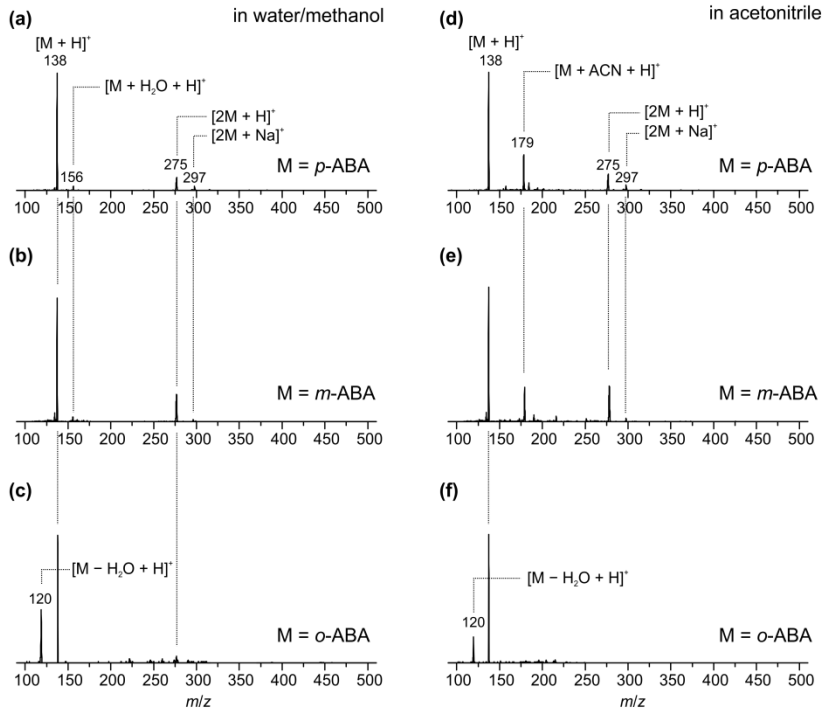

Figure S1. Nano-electrospray ion mobility-TOF mass spectra of (a,d) *p*-, (b,e) *m*-, and (c,f) *o*-aminobenzoic acids (ABAs) in (a,b,c) water/methanol and (d,e,f) acetonitrile. Drift gas was He.

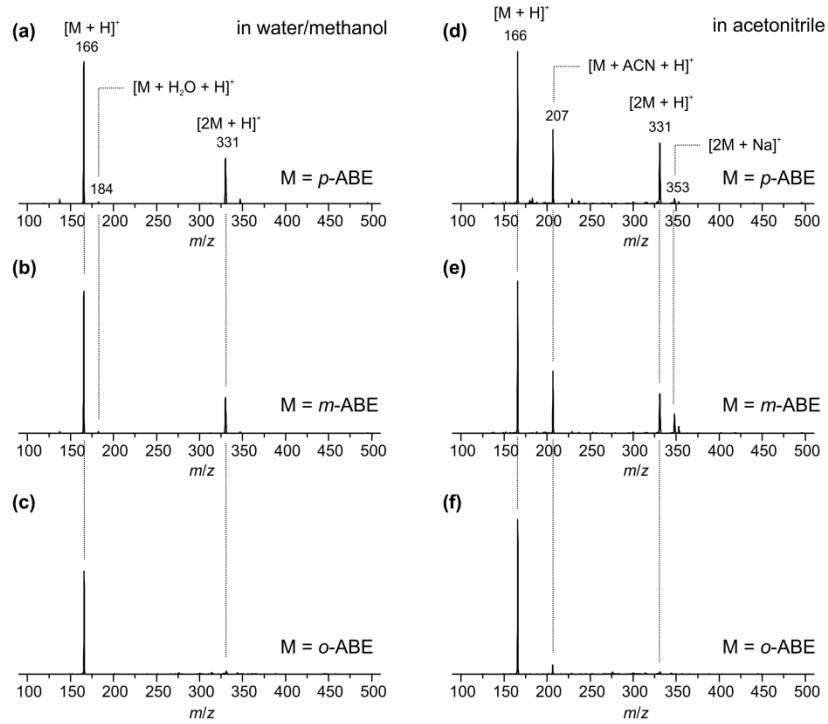

Figure S2. Nano-electrospray ion mobility-TOF mass spectra of (a,d) *p*-, (b,e) *m*-, and (c,f) *o*-aminobenzoic acid ethyl esters (ABEs) in (a,b,c) water/methanol and (d,e,f) acetonitrile. Drift gas was He.

2. Optimized Geometries of ABAs and ABEs

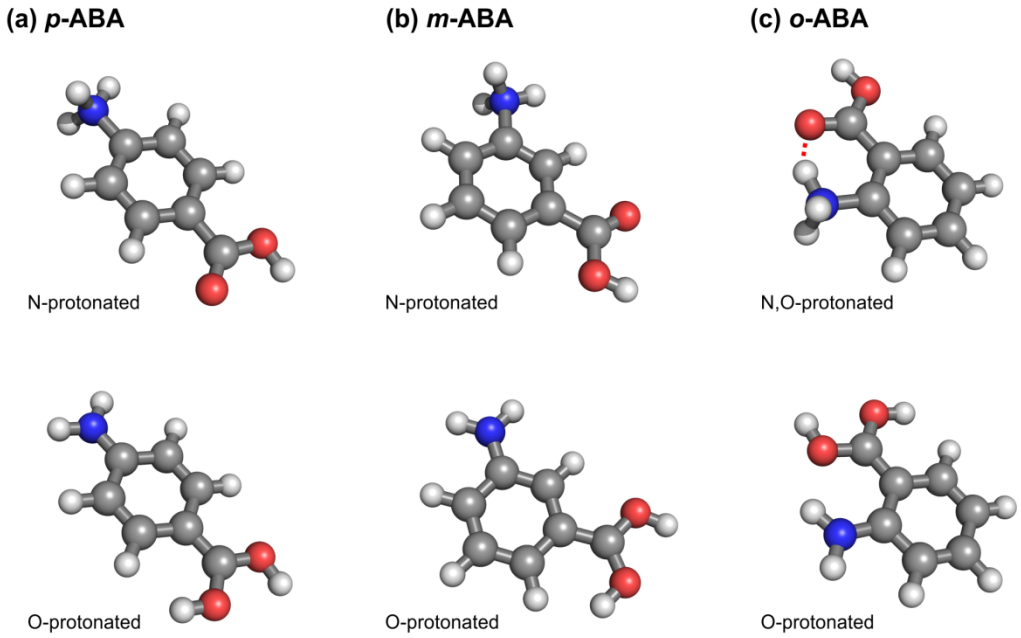

Figure S3. Optimized geometries of protonated (a) *p*-, (b) *m*-, and (c) *o*-aminobenzoic acids (ABAs).

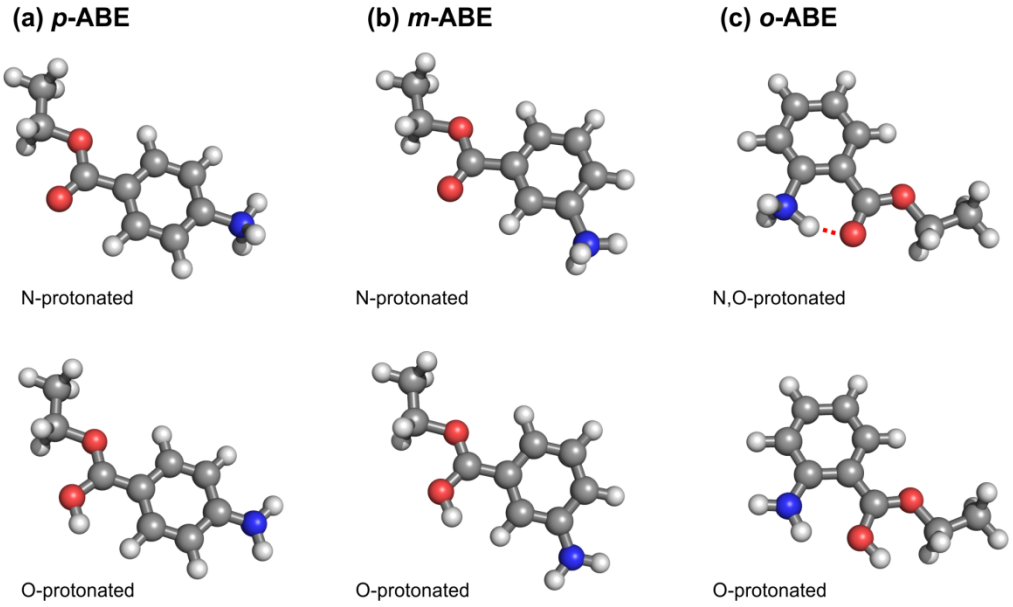

Figure S4. Optimized geometries of protonated (a) *p*-, (b) *m*-, and (c) *o*-aminobenzoic acids ethyl esters (ABEs).

3. Optimized Geometries of Protonated ABE-Acetonitrile complex

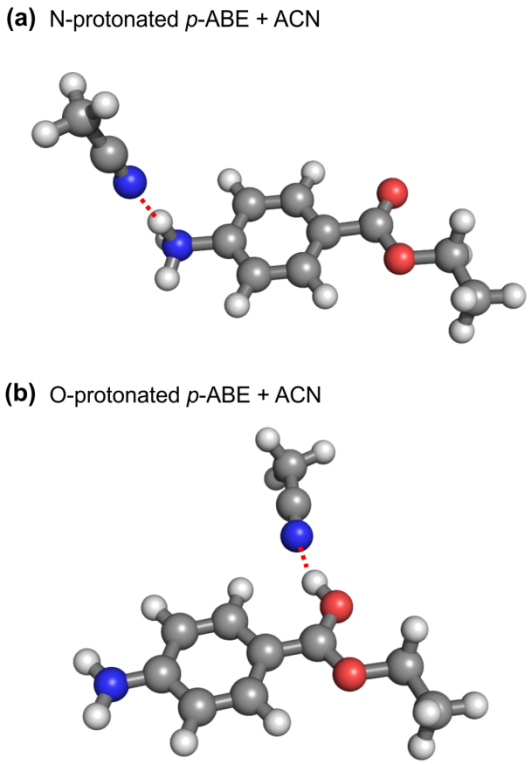

Figure S5. Optimized geometries of acetonitrile-bound complexes of (a) N- and (b) O-protonated *p*-ABEs.

4. Potential Energy Surface for Intramolecular Proton Migration

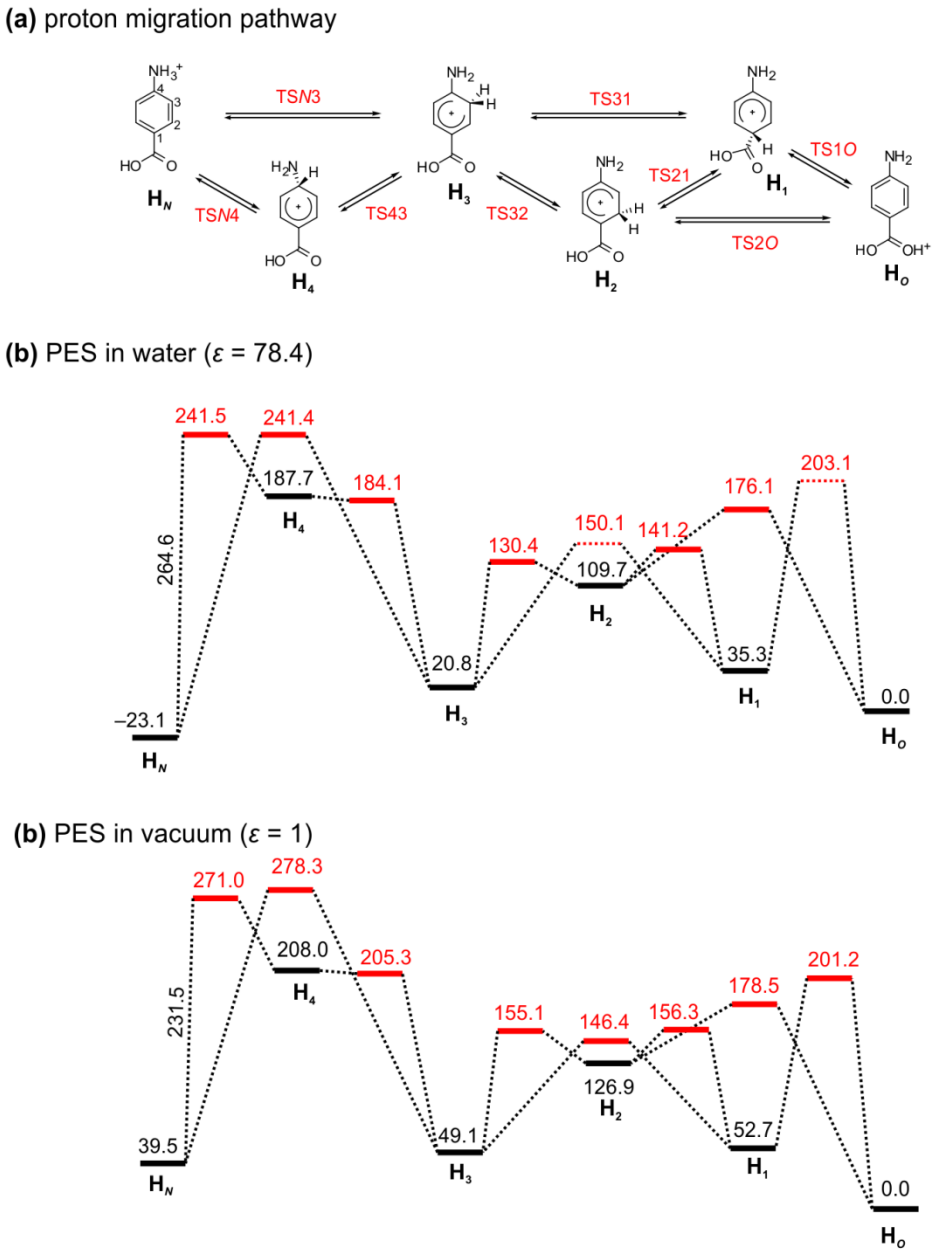

Figure S6. (a) Pathway for the intramolecular proton migration from N-protonated to O-protonated *p*-ABA, and calculated potential energy surface (a) in water and (b) in vacuum. All energies are in kJ mol^{-1}.

5. Optimized Geometries of Proton-Bound Dimers

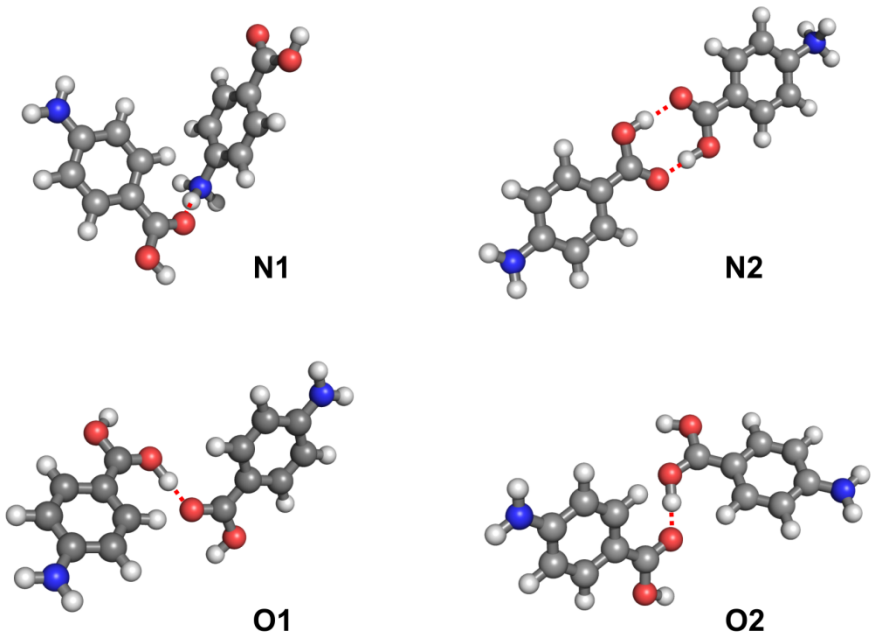

Figure S7. Optimized geometries of proton-bound dimers of *p*-aminobenzoic acid.

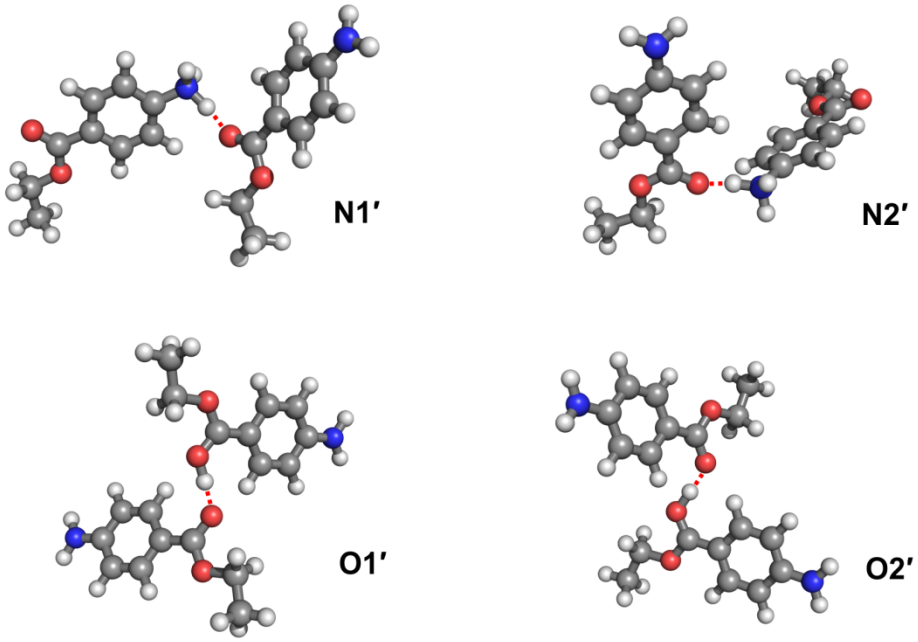

Figure S8. Optimized geometries of proton-bound dimers of *p*-aminobenzoic acid ethyl ester.