CORRECTION

Correction to: Theoretical investigation on the water-assisted excited-state proton transfer of 7-azaindole derivatives: substituent effect

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The original version of this article unfortunately contained a mistake in Table 3. This correct Table 3 is given below.

Reference

1. Yi J, Fang H (2017). Photochem. Photobiol. <https://doi.org/10.1111/php.12839>

Table 3 Reaction energies (ΔE) and barrier heights (ΔV) for excited-state proton transfer in 2RAI-H₂O (R=H, OH, OCH₃; CN, CHO, NO₂) complexes in water

Complex	ΔV	ΔE
7AI-H ₂ O ^a	10.6(6.86)	-13.6(-13.2)
2(OH)AI-H ₂ O	9.43(6.20)	-15.9(-15.4)
2(OCH ₃)AI-H ₂ O	9.38(5.86)	-15.4(-14.8)
2(NO ₂)AI-H ₂ O	15.6(12.8)	0.10(-0.10)
2(CN)AI-H ₂ O	10.2(7.30)	-13.4(-13.1)
2(CHO)AI-H ₂ O	19.7(15.6)	-2.90(-2.70)

The numbers in parentheses include zero-point energies. Energies are in kcal/mol.

^a Data from Ref [1]

The online version of the original article can be found at <https://doi.org/10.1007/s00894-017-3487-5>

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