SUPPORTING INFORMATION FOR:

Correlation Analysis of the Substituent Electronic Effects on the Allylic H-Abstraction in Cyclohexene by Phthalimide-*N*-oxyl Radicals: a DFT Study

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Figure S1 Optimized structures (side-view) for compounds 1~11. Definition of compounds 1~11 is shown in [Figure 1](#).

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Figure S2 The optimized structures (side view) of the radicals corresponding to compounds 1~11. Definition of compounds 1~11 is shown in [Figure 1](#).

Figure S3 The allylic H-abstraction activation energies as a function of the spin density of the active O atom, concerning the solvent effects using the default Gaussian 03 implementation of the polarizable continuum model (PCM). Definition of compounds **1~11** is shown in [Figure 1](#).

Figure S4 The bond dissociation energy (BDE) of O-H bond as a function of the spin density on the active O atom, using B3LYP/6-311++G** method. Definition of compounds **1~11** is shown in [Figure 1](#).