Supporting Information for

Quantitative evaluation of H-donating abilities of C(sp^3)-H bonds of nitrogen-containing heterocycles in hydrogen atom transfer reaction

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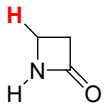
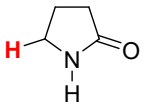
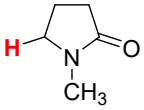
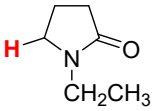
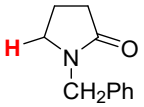
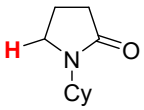
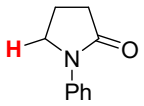
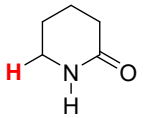
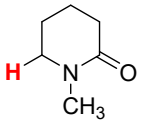
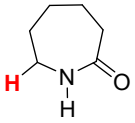
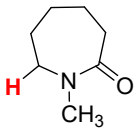
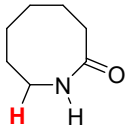
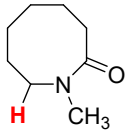
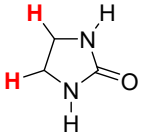
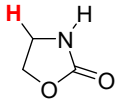
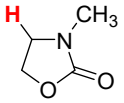
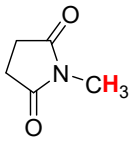
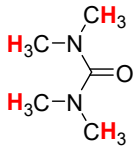
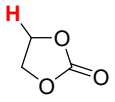
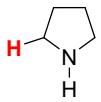
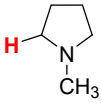
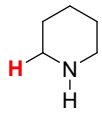
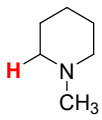
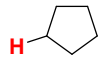
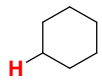
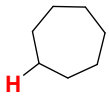
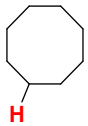
SI. Kinetic studies of the HAT reactions from C(sp^3)-H bonds of nitrogen-containing heterocycles and other H-donors to CumO• radical in literatures

The second-order rate constants k_2 and activation free energies $\Delta G^{\neq}_{XH/Y}$ which were obtained by Eyring equation [$k_2 = (k_B T/h)\exp(-\Delta G^{\neq}/RT)$] of HAT reactions from C(sp^3)-H bonds of nitrogen-containing heterocycles and other H-donors to CumO• radical in acetonitrile (MeCN) at 298 K are listed in Table S1.

Table S1. Second-order rate constants (k_2), activation free energies ($\Delta G^{\neq}_{XH/CumO•}$) of HAT reactions (XH/CumO•) and the references in MeCN at 298 K.

Entry	XH	k_2 ($M^{-1}s^{-1}$) [a]	$\Delta G^{\neq}_{XH/CumO•}$ (kcal/mol) [b]	Ref.
1H		3.60×10^5	9.87	S1
2H		2.27×10^6	8.78	S1
3H		4.53×10^6	8.37	S1
4H		4.60×10^6	8.36	S1
5H		2.34×10^6	8.76	S1
6H		3.80×10^6	8.47	S1
7H		1.90×10^6	8.88	S1
8H		2.76×10^6	8.66	S1
9H		3.75×10^6	8.48	S1
10H		8.90×10^5	9.33	S1

11H		2.45×10^6	8.73	S1
12H		6.44×10^5	9.52	S1
13H		1.14×10^6	9.19	S1
14H		9.20×10^6	7.95	S1
15H		3.20×10^7	7.21	S1
16H		8.90×10^5	9.33	S1
17H		2.02×10^6	8.85	S1
18H		1.00×10^5	10.63	S1
19H		6.00×10^6	8.20	S1
20H		4.00×10^4	11.17	S1
21H		1.24×10^8	6.41	S2
22H		1.91×10^8	6.15	S2

23H		1.07×10^8	6.50	S2
24H		1.22×10^8	6.42	S2
25H		9.54×10^5	9.29	S3
26H		1.10×10^6	9.21	S4
27H		2.20×10^6	8.80	S5
28H		3.20×10^6	8.57	S6

[a] The uncertainty of date is smaller than 5%. [b] The date of $\Delta G^{\neq}_{XH/Y}$ are derived from Eyring equation $k_2 = (k_B T/h)\exp(-\Delta G^{\neq}/RT)$.

SII. The brief introduction of Applied Photophysics SX.18MV-R stopped-flow

SX.18MV-R stopped-flow is a fast dynamic measuring device with high sensitivity produced by Applied Photophysics Limited Company. The system has a detection wavelength range of 200 ~ 900 nm and a movable sample cell of 20ul, 5ul and 2ul to suit different determination needs. The Dead-Time of the system is less than 500 us (far less than the Dead-Time of the general stopped-flow device about 4 ms), and the rate constant can be measured up to 3000 s^{-1}; High sensitivity, low noise (0.0001AU); Temperature control range (-20 to 60 ℃). RISC OS3.11 operating system, fast and simple, and can directly analyze the dynamics curve to give the corresponding dynamics parameters. The picture of the Applied Photophysics SX.18MV-R stopped-flow is shown below.

References

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