Supporting Information

Maleic Anhydride Derivatives as Catalysts for *N*-oxidation of Pyridine using Hydrogen Peroxide

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SI-1: ***^{1}H NMR and ^{13}C NMR chemical shifts of N-Oxide products:***

Pyridine N-Oxide: δ ^{1}H NMR (500 MHz, CDCl3): 7.35-7.37 (3H, m, Ar-H), 8.25-8.27 (2H, m, Ar-H) ppm. δ ^{13}C NMR (125 MHz, CDCl3): 125.26, 125.53, 138.49 ppm.

2-Methylpyridine N-Oxide: δ ^{1}H NMR (500 MHz, CDCl3): 2.53 (3H, s, -CH3), 7.20-7.32 (3H, m, Ar-H), 8.29-8.30 (1H, d, J = 5.5 Hz, Ar-H); δ ^{13}C NMR (500 MHz, $CDCl_3$): 17.31, 123.20, 125.53, 126.15, 138.85, 148.51 ppm.

Quinoline N-Oxide: δ ^{1}H NMR (500 MHz, CDCl3): 7.29-7.32 (1H, dd, J=6.0, 8.5 Hz, Ar-H), 7.62-7.65 (1H, t, J=7.5 Hz, Ar-H), 7.74-7.77 (2H, m, Ar-H), 7.86-7.87 (1H, d, J=8.5 Hz, Ar-H), 8.54-8.56 (1H, d, J=6 Hz, Ar-H), 8.73-8.75 (1H, d, J= 9Hz, Ar-H) ppm; δ ^{13}C NMR (500 MHz, $CDCl_3$): 119.37, 120.73, 126.18, 127.93, 128.55, 130.21, 130.29, 135.44, 141.10 ppm.

2-Chloropyridine N-Oxide: δ ^{1}H NMR (500 MHz, CDCl3): 7.28-7.32 (2H, m, Ar-H), 7.55-7.58 (1H, m, Ar-H), 8.40-8.41 (1H, m, Ar-H) ppm; δ ^{13}C NMR (500 MHz, CDCl3 w/ DMSO): 123.78, 126.02, 126.04, 140.26, 141.46 ppm.

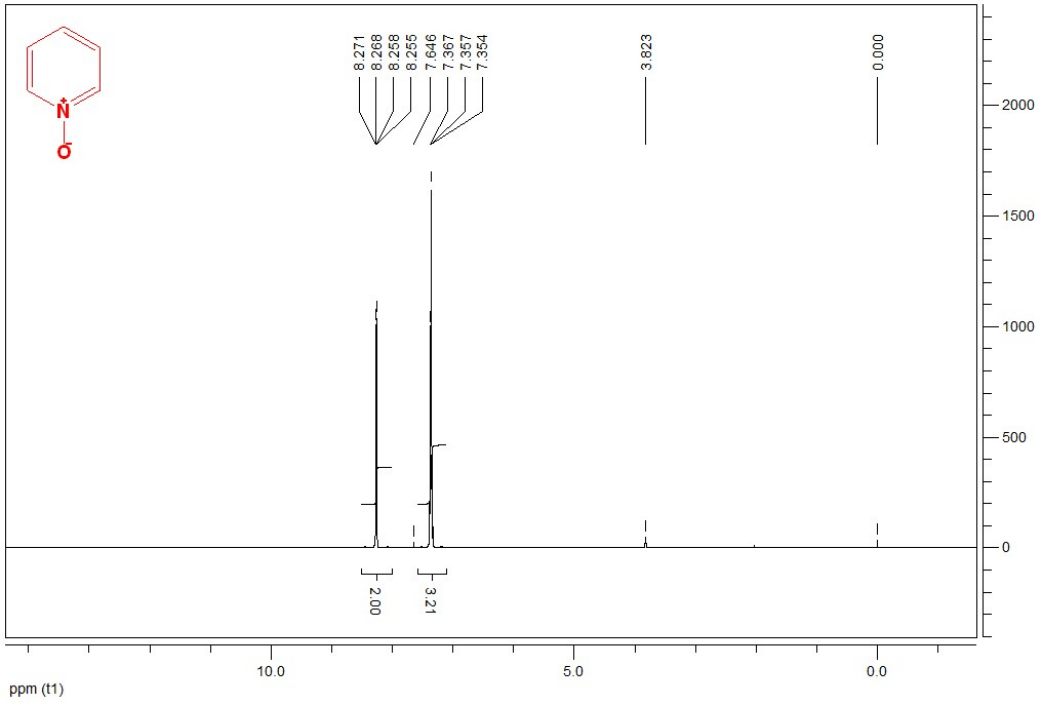
2-carboxypyridine N-Oxide: δ ^{1}H NMR (500 MHz, DMSO): 7.88-7.95 (2H, m, Ar-H), 8.30-8.32 (1H, dd, J=2.5 Hz, 7.5 Hz, Ar-H), 8.73-8.74 (1H, m, Ar-H) ppm; δ ^{13}C NMR (500 MHz, DMSO): 128.63, 130.10, 132.84, 135.90, 138.99, 160.93 ppm.

Nicotinic N-Oxide: δ ^{1}H NMR (500 MHz, DMSO): 7.53-7.55 (1H, dd, J=6.8, 7.5 Hz, Ar-H), 7.76-7.78 (1H, d, J=8 Hz, Ar-H), 8.42-8.44 (1H, dd, J=0.7, 6.4 Hz, Ar-H), 8.48 (1H, s, Ar-H) ppm; δ ^{13}C NMR (500 MHz, DMSO): 126.11, 127.18, 131.06, 139.41, 142.58, 164.67 ppm.

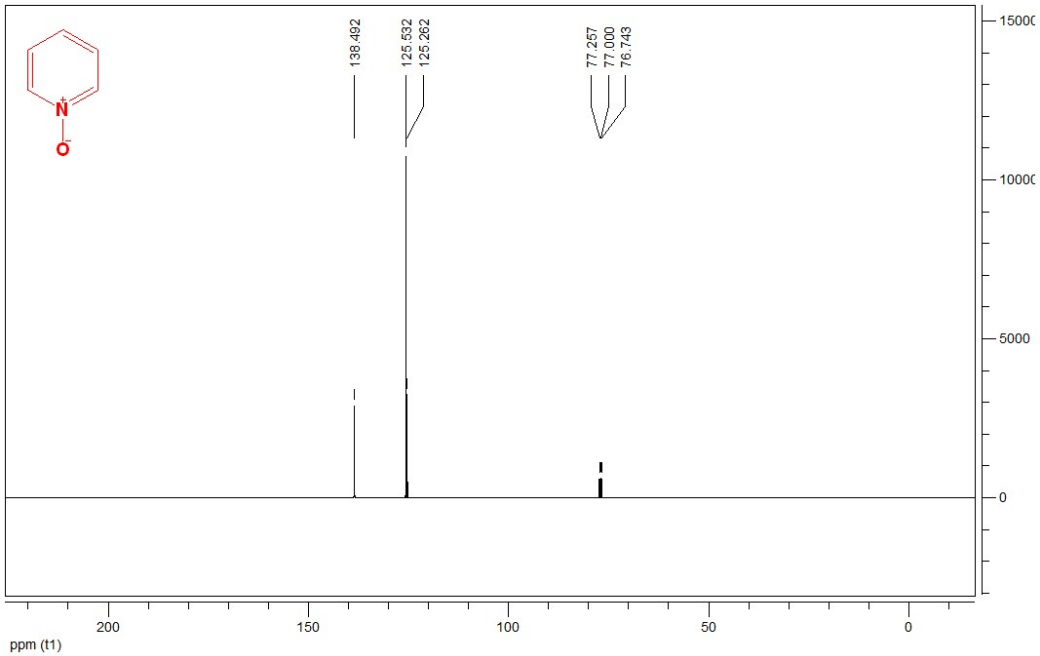
Isonicotinic N-oxide: δ ^{1}H NMR (500 MHz, DMSO): 7.81-7.82 (2H, d, J=6.5 Hz, Ar-H), 8.28-8.29 (2H, d, J=7 Hz, Ar-H).

2,6-Lutidine N-Oxide: δ ^{1}H NMR (500 MHz, $CDCl_3$): 2.55 (6H, s, 2 x $-CH_3$), 7.08-7.11 (1H, dd, J=6.5 Hz, 8.5 Hz), 7.15-7.17 (2H, d, 7.5 Hz)

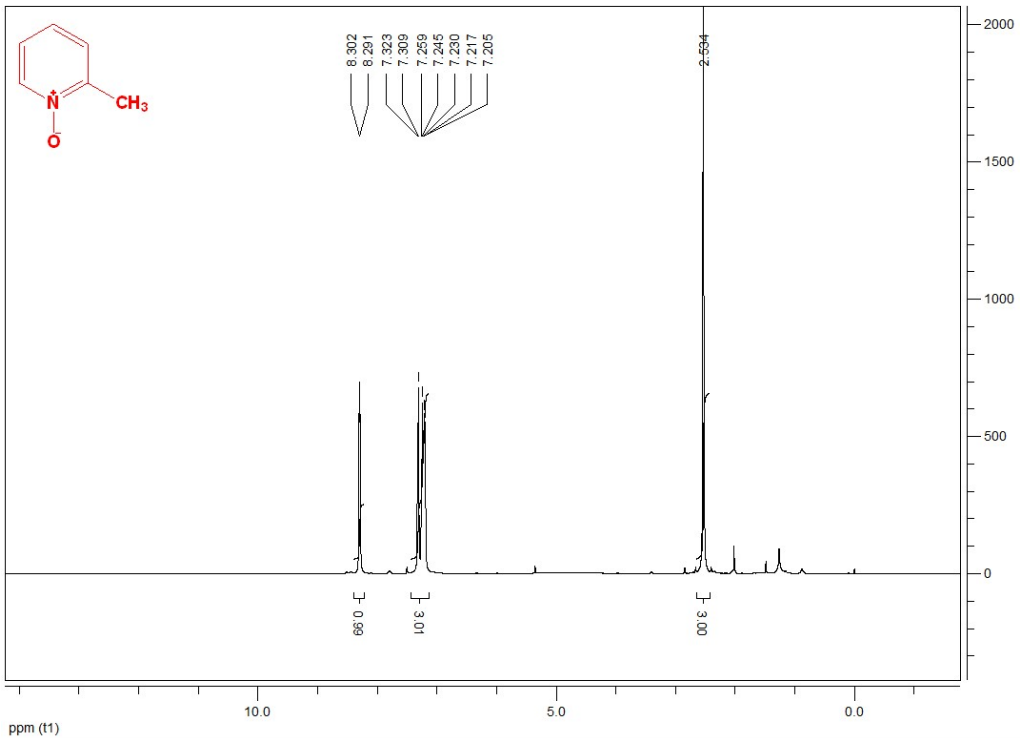
[1]H NMR and [13]C NMR spectra of N-Oxide products:



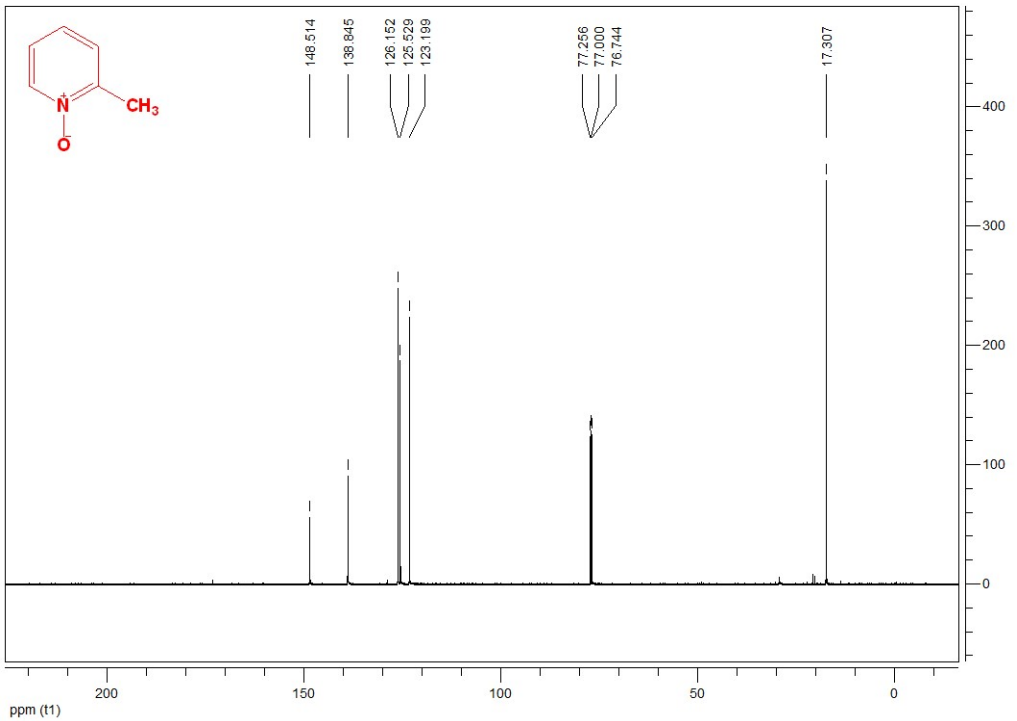
SI-1A. ^{1}H NMR spectrum of Pyridine N-Oxide in $CDCl_3$.



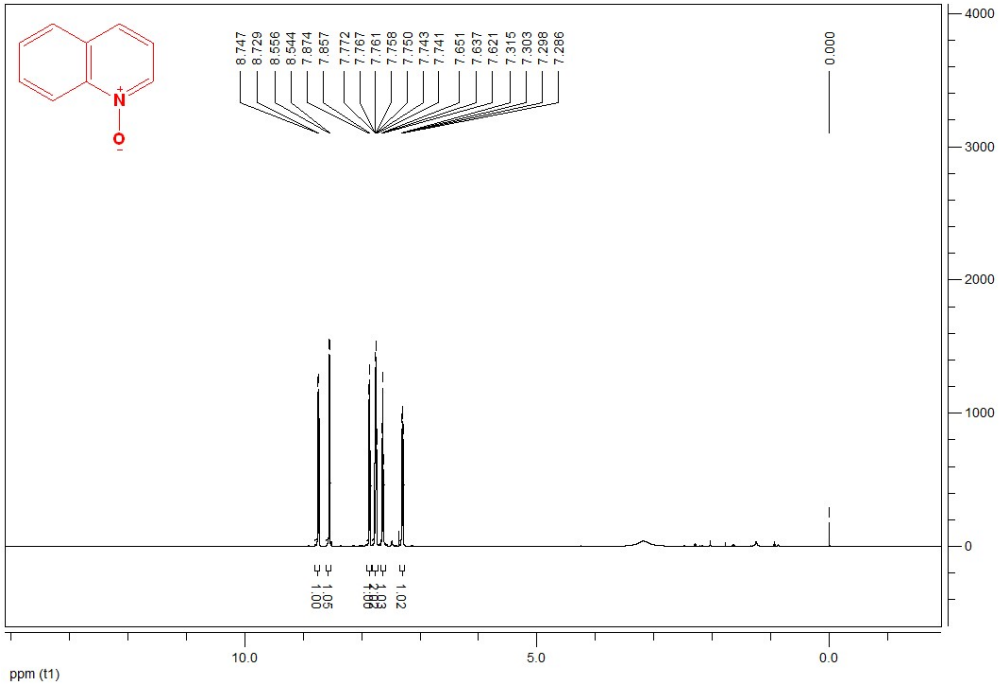
SI-1A-1. ^{13}C NMR spectrum of Pyridine N-Oxide in $CDCl_3$.



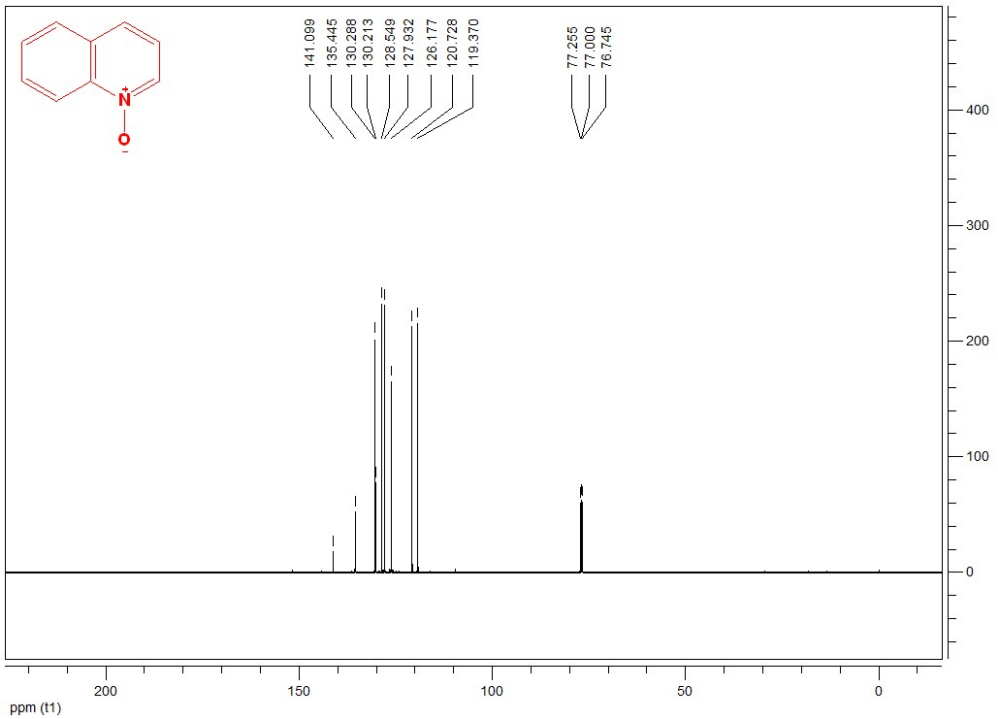
SI-1B. ^{1}H NMR spectrum of 2-Methylpyridine N-Oxide in $CDCl_3$.



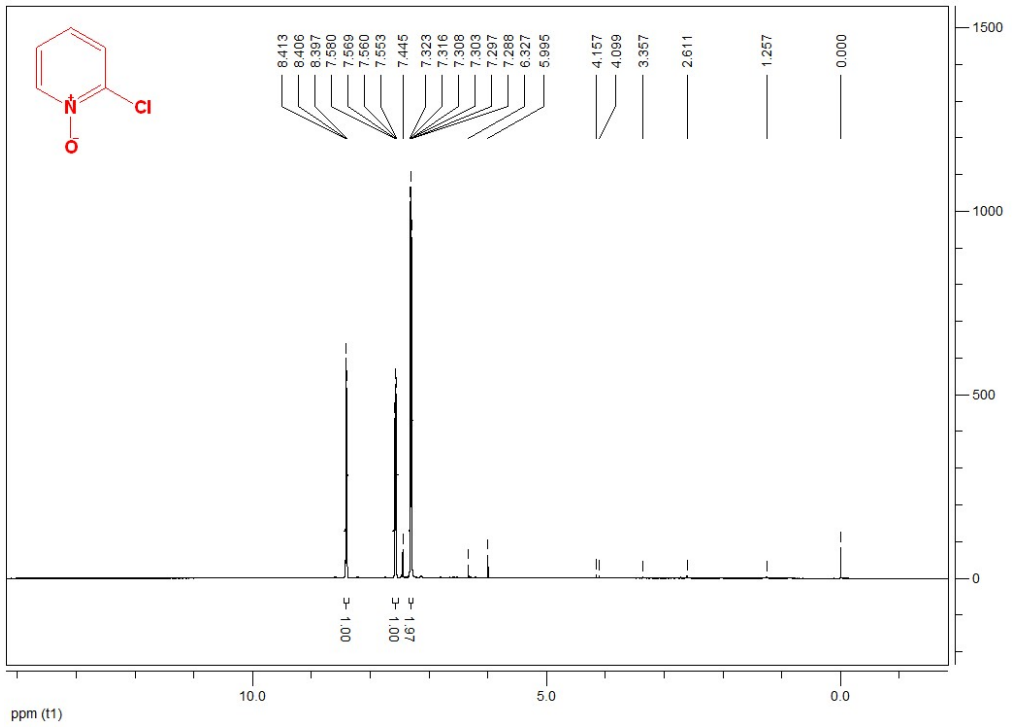
SI-1B-1. ^{13}C NMR spectrum of 2-Methylpyridine N-Oxide in $CDCl_3$.



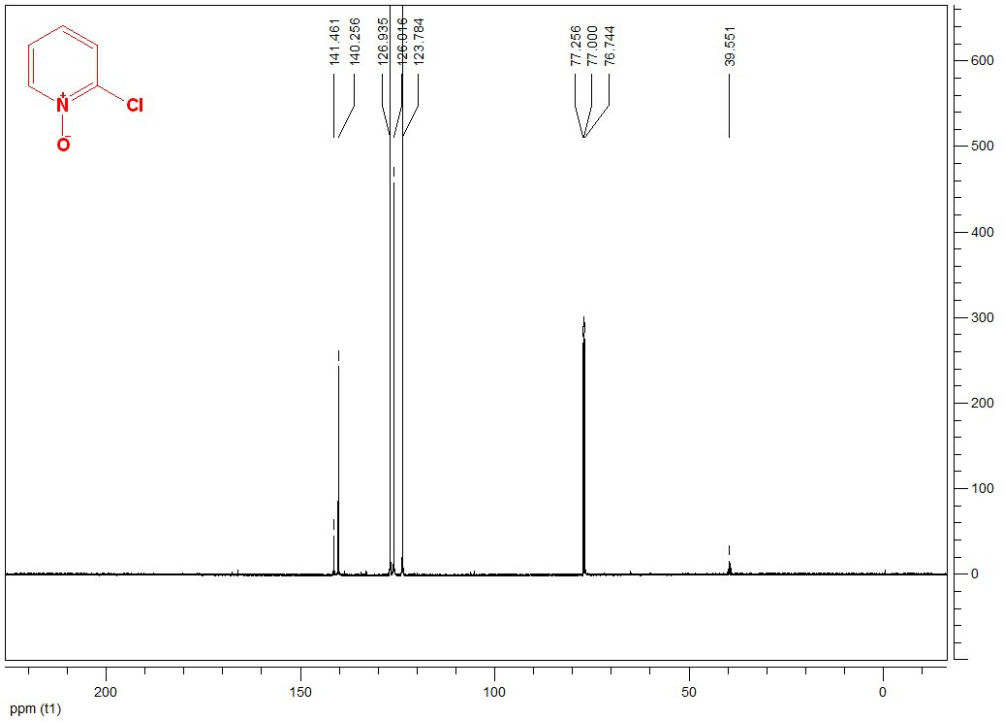
SI-1C. ^{1}H NMR spectrum of Quinoline N-Oxide in $CDCl_3$.



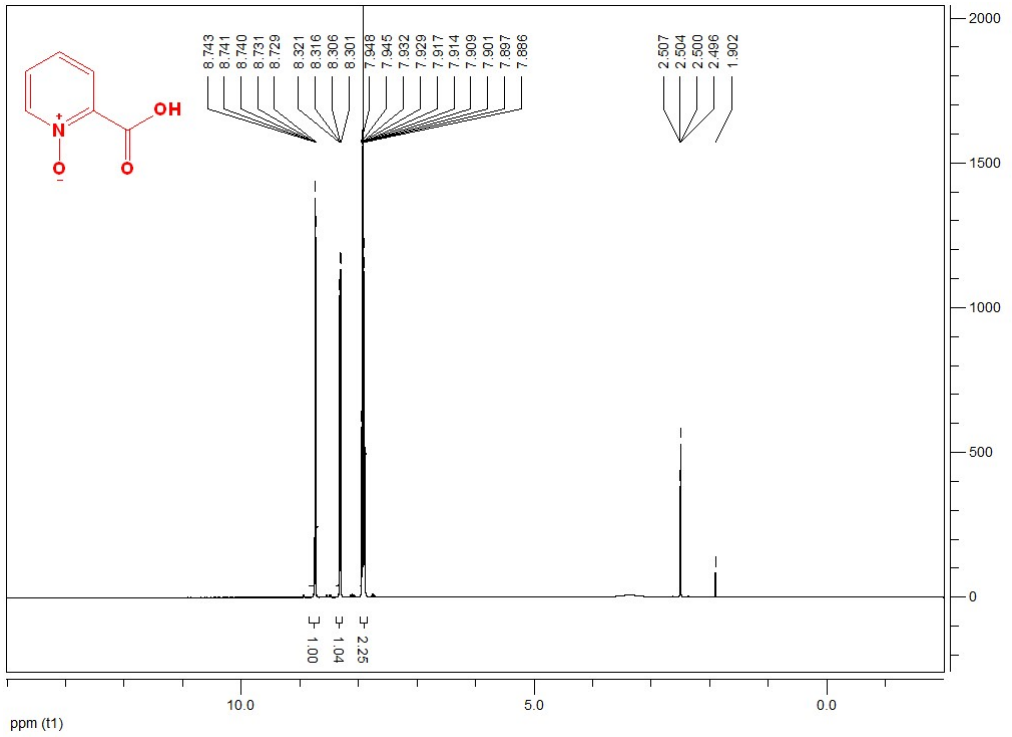
SI-1C-1. ^{13}C NMR spectrum of Quinoline N-Oxide in $CDCl_3$.



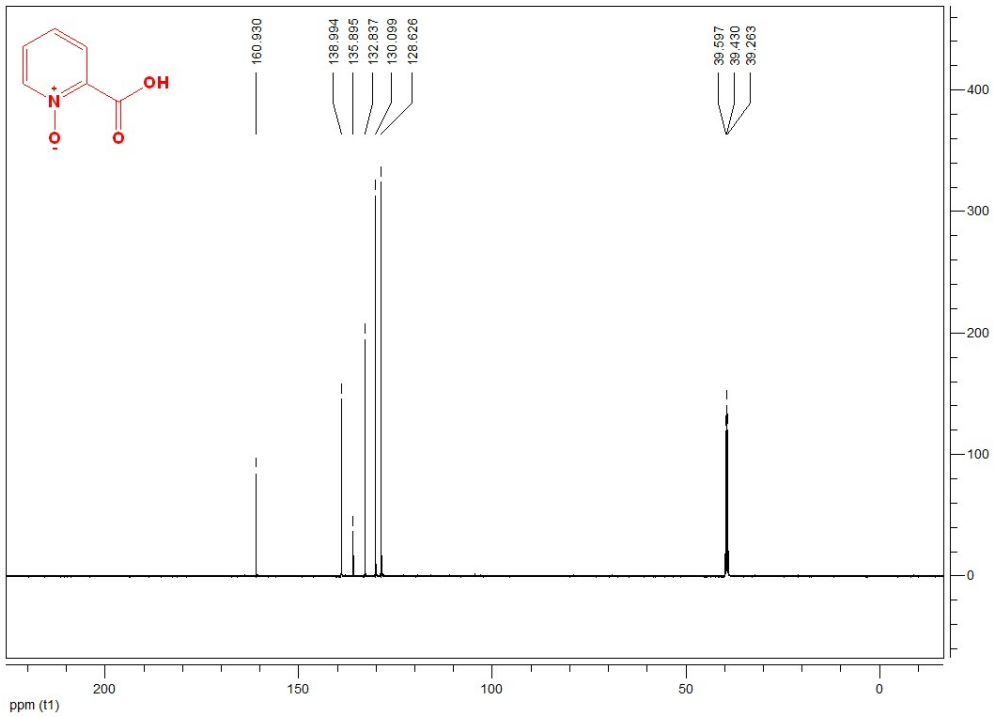
SI-1D. ^{1}H NMR spectrum of 2-Chloropyridine N-oxide in $CDCl_3$.



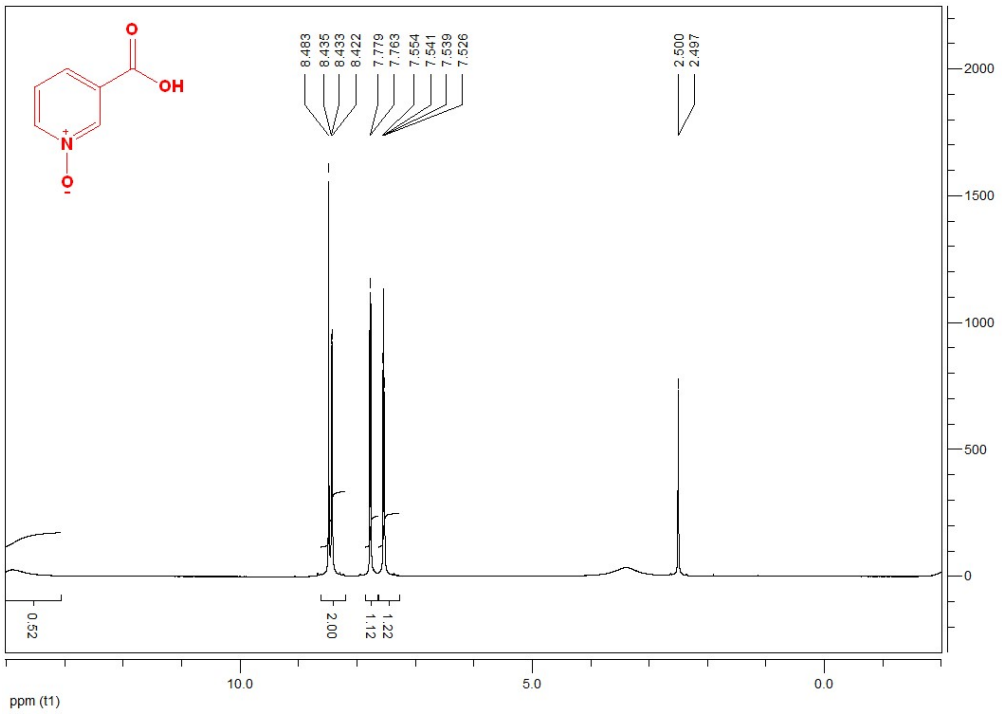
SI-1D-1. ^{13}C NMR of 2-Chloropyridine N-oxide in $CDCl_3$ (with a drop of DMSO).



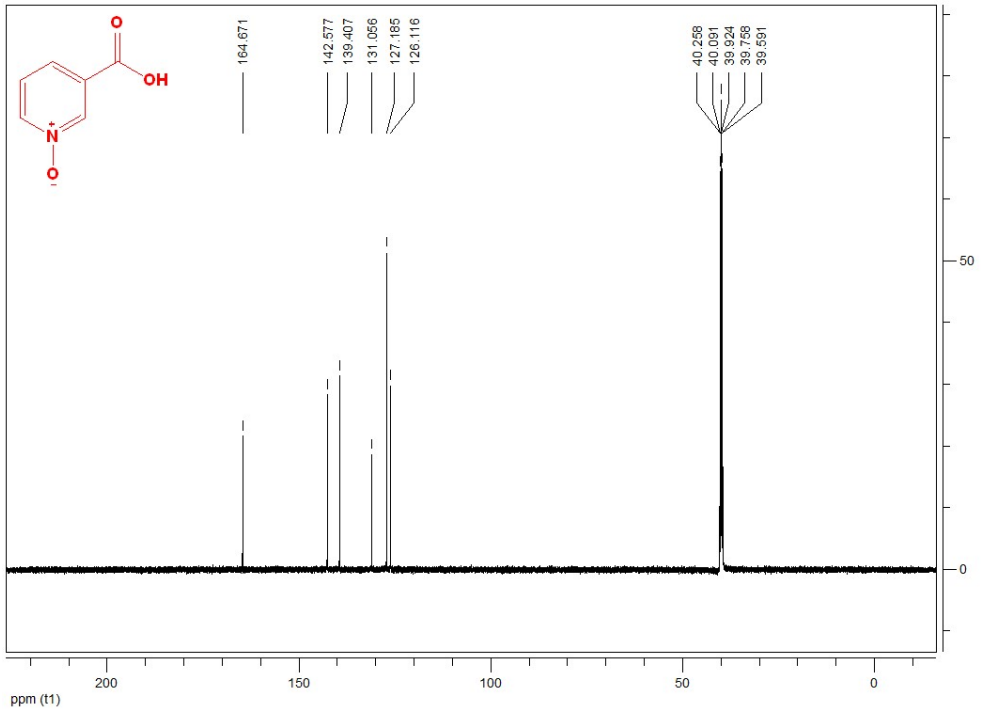
SI-1E. ^{1}H NMR spectrum of 2-Carboxypyridine N-Oxide in DMSO.



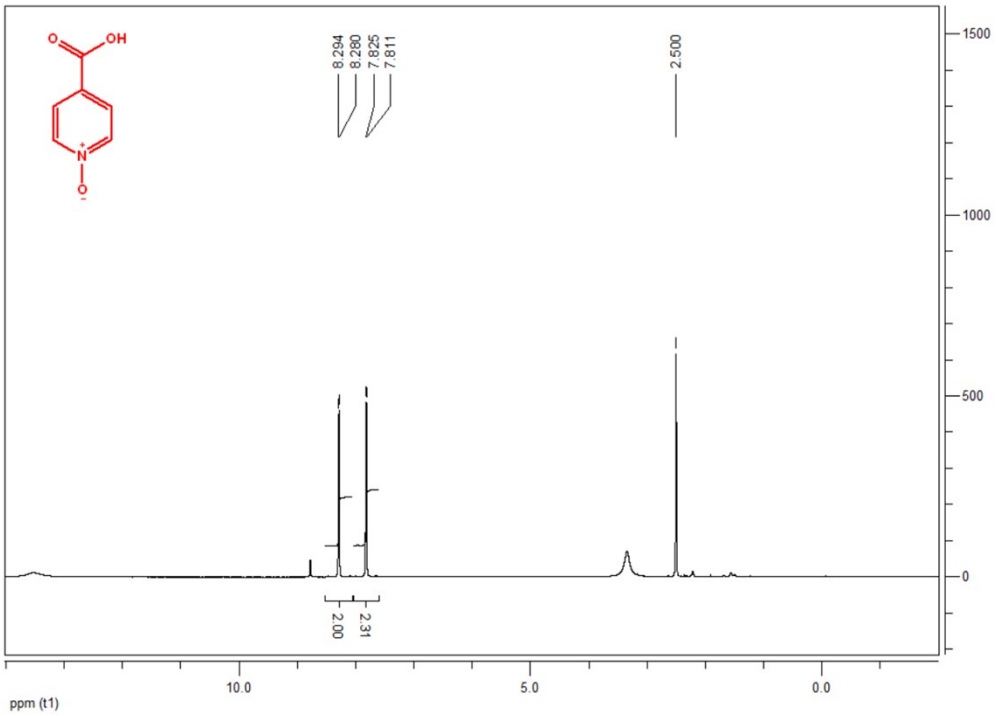
SI-1E-1. ^{13}C NMR spectrum of 2-Carboxypyridine N-Oxide in DMSO.



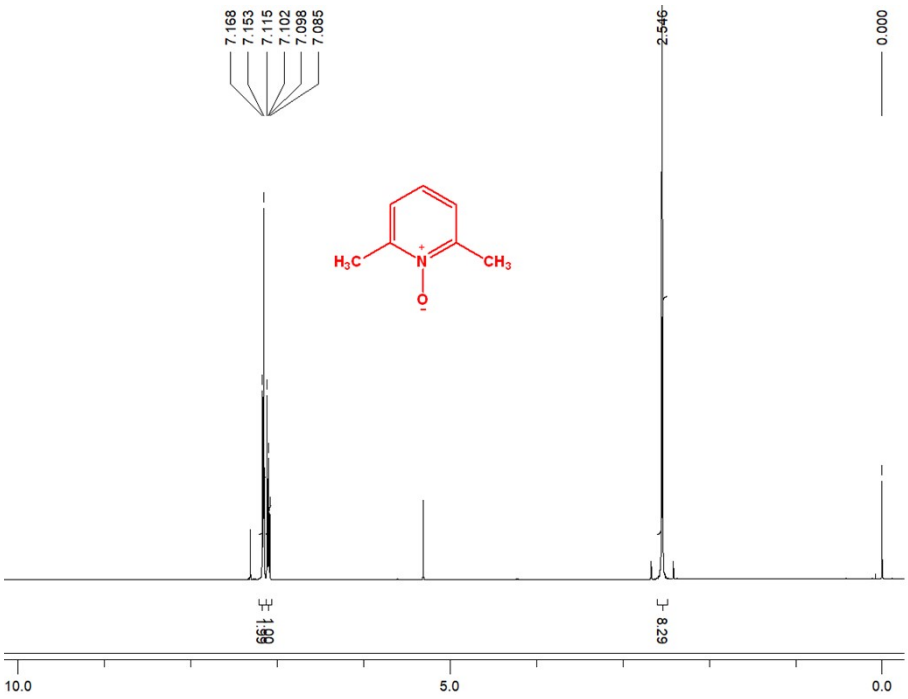
SI-1F. ^{1}H NMR spectrum of Nicotinic N-Oxide in DMSO.



SI-1F-1. ^{13}C NMR spectrum of Nicotinic N-Oxide in DMSO.

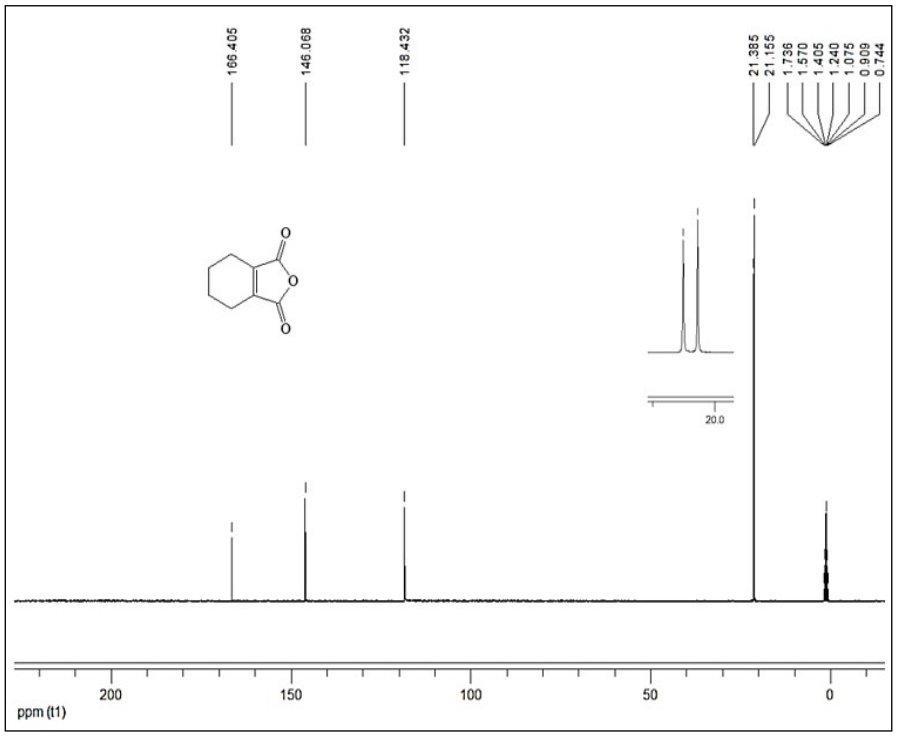


SI-1G. ^{1}H NMR spectrum of Isonicotinic N-Oxide in DMSO.

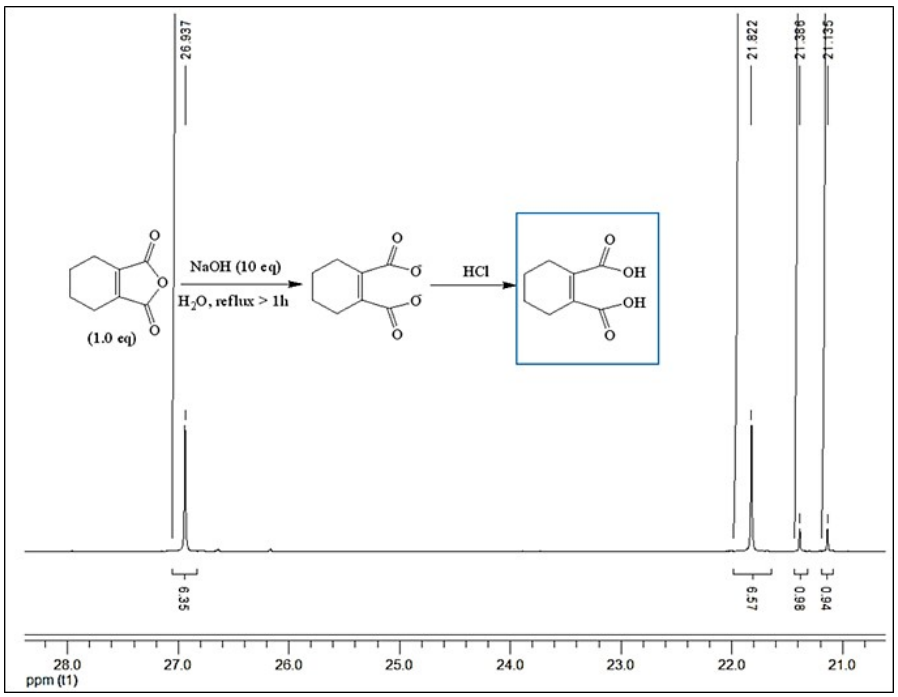


SI-1H. ^{1}H NMR spectrum of 2,6-Lutidine N-Oxide in $CDCl_3$.

SI-2: ^{13}C NMR spectra for perhydrolysis of CHMA with H_2O_2 in CD_3CN.



SI-2A. ^{13}C NMR of **CHMA** in CD_3CN.



SI-2B. ^{13}C NMR of CHMA-diacid in CD_3CN. It was initially synthesized from CHMA by hydrolysis: contains 15% anhydride

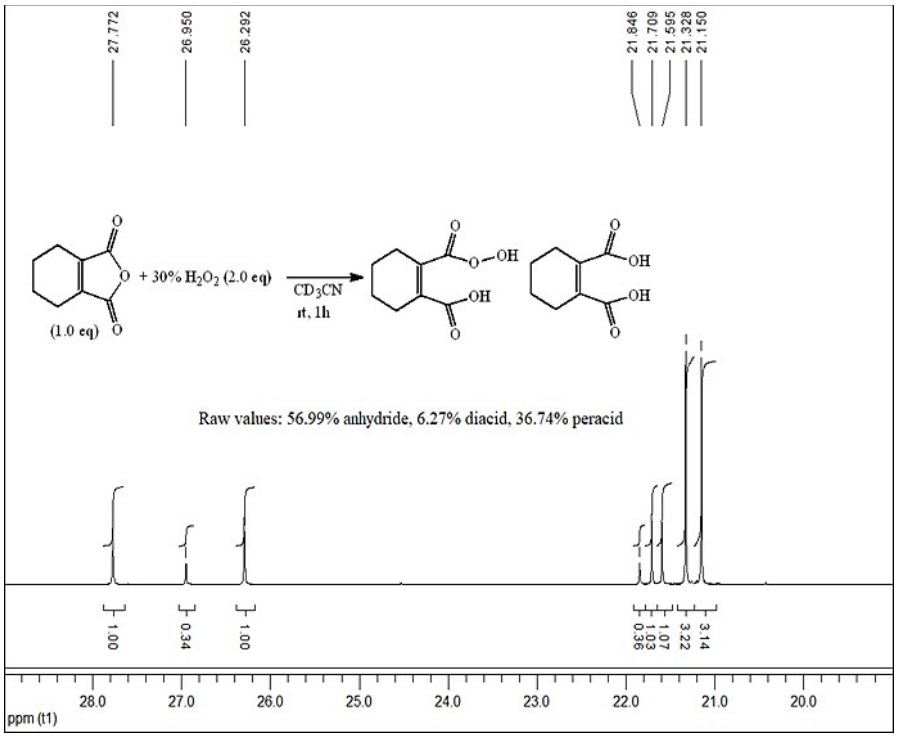


Figure SI-2C. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 1 h.

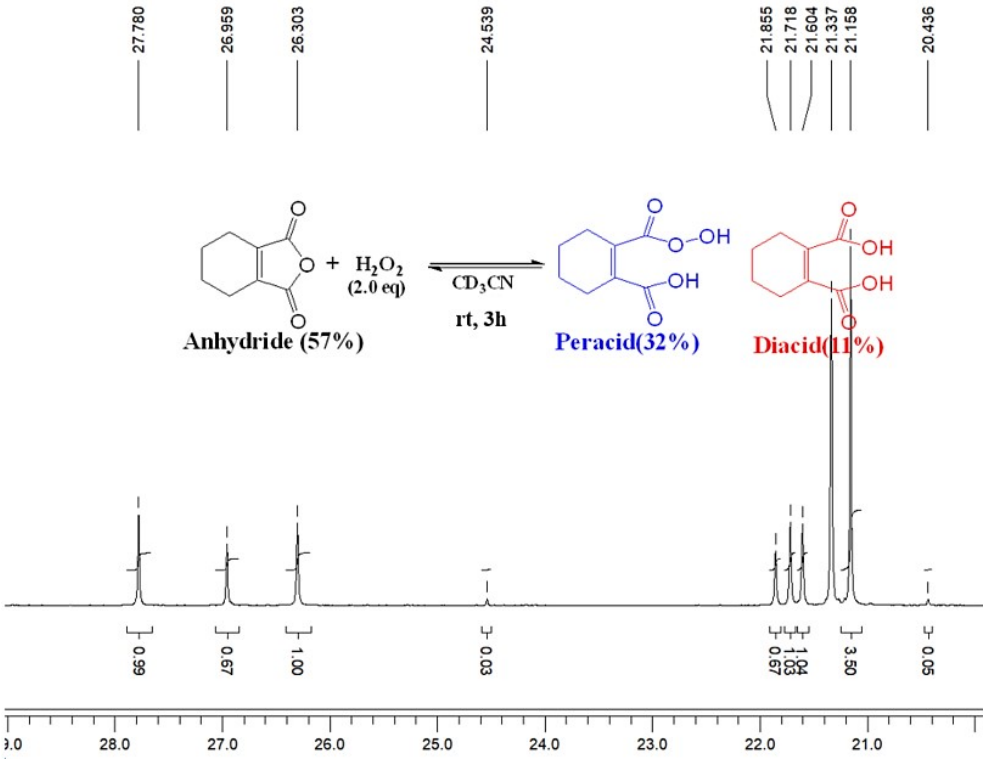
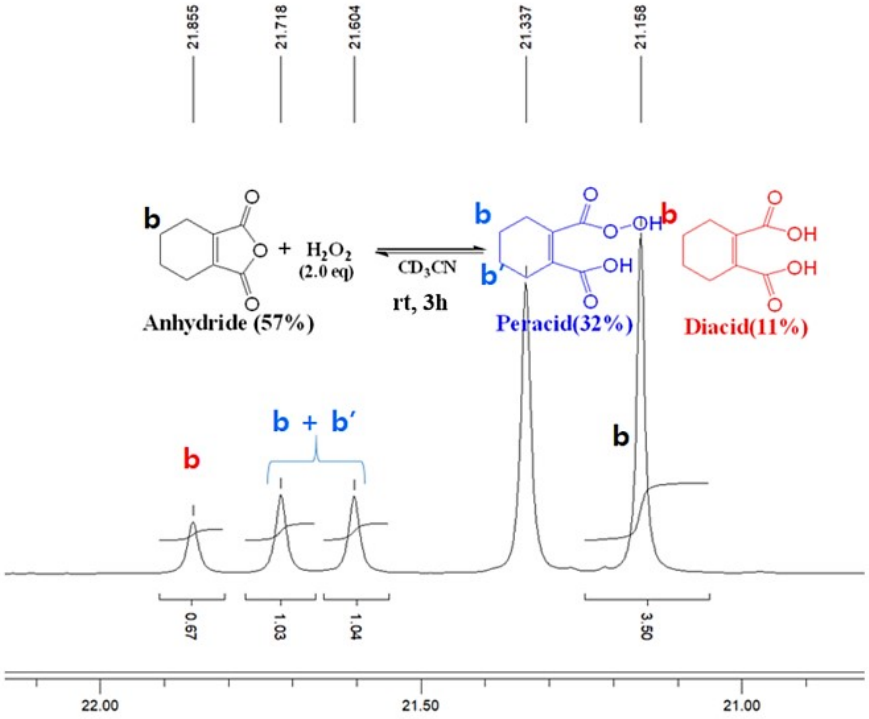
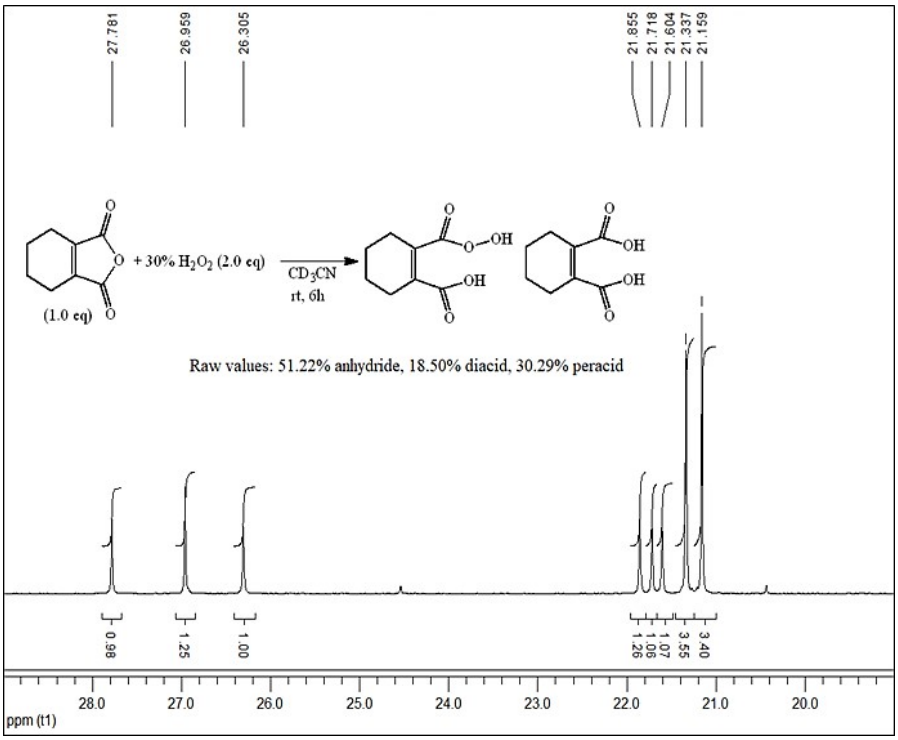


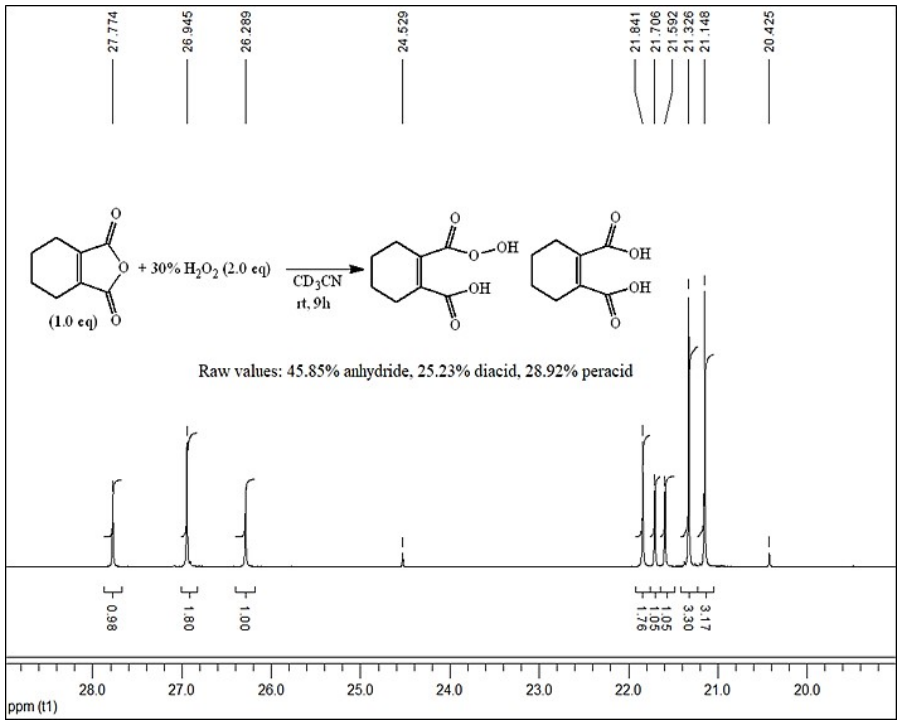
Figure SI-2D. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2 (2 eq), rt, 3 h.



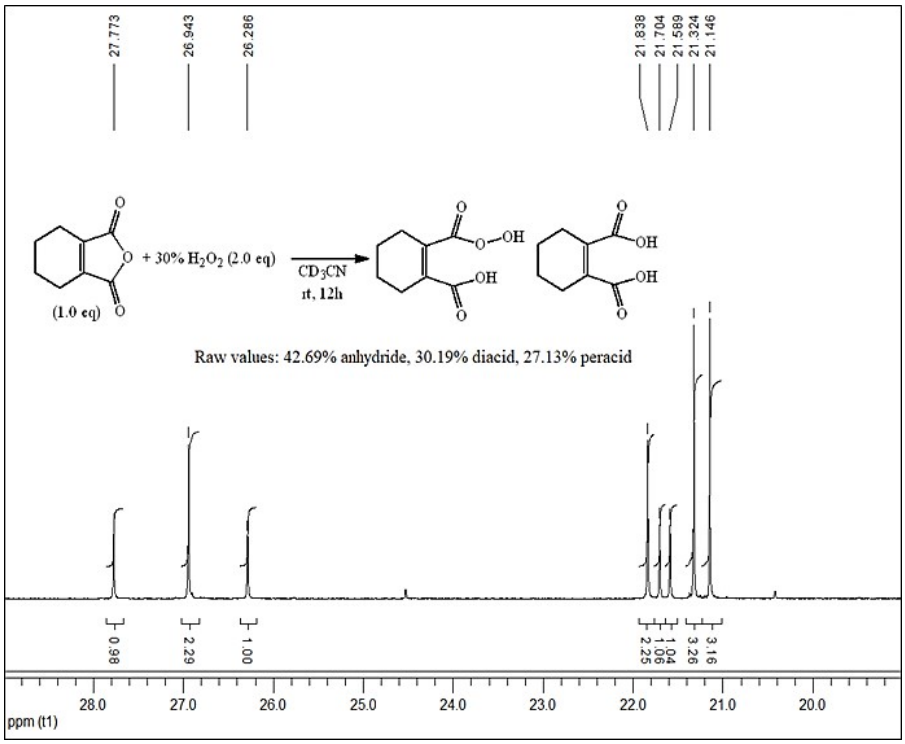
SI-2D-1. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 3 h



SI-2E. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 6 h.



SI-2F. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 9 h.



SI-2G. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 12 h.

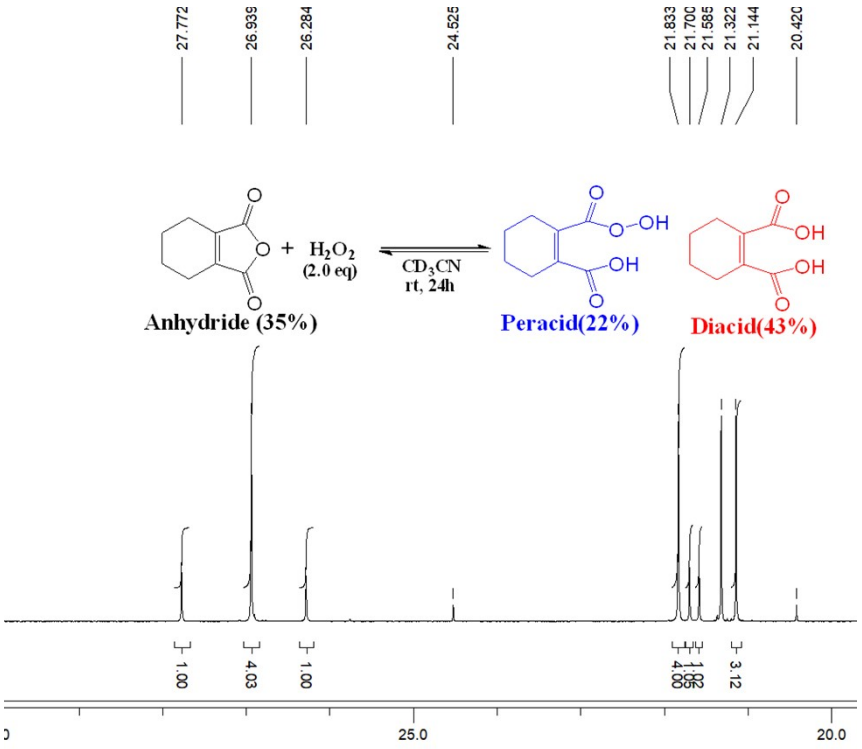
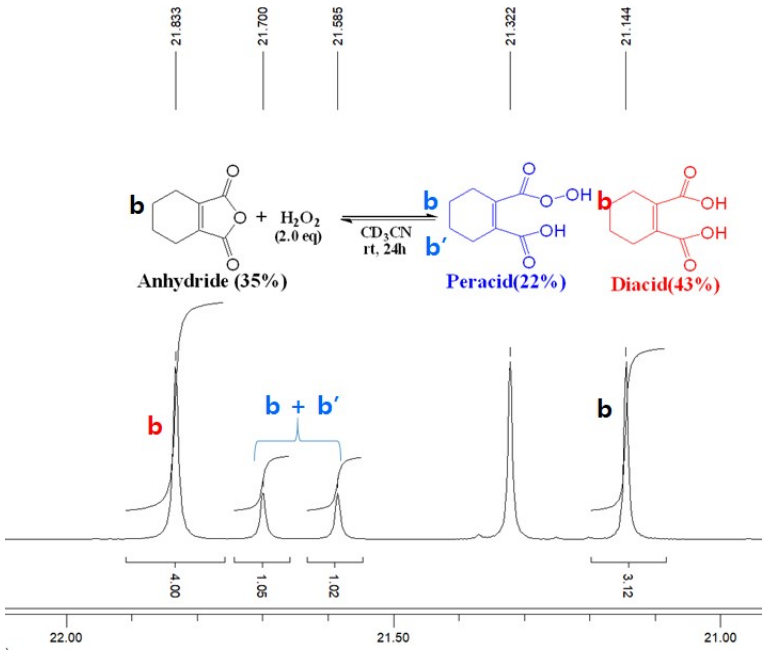
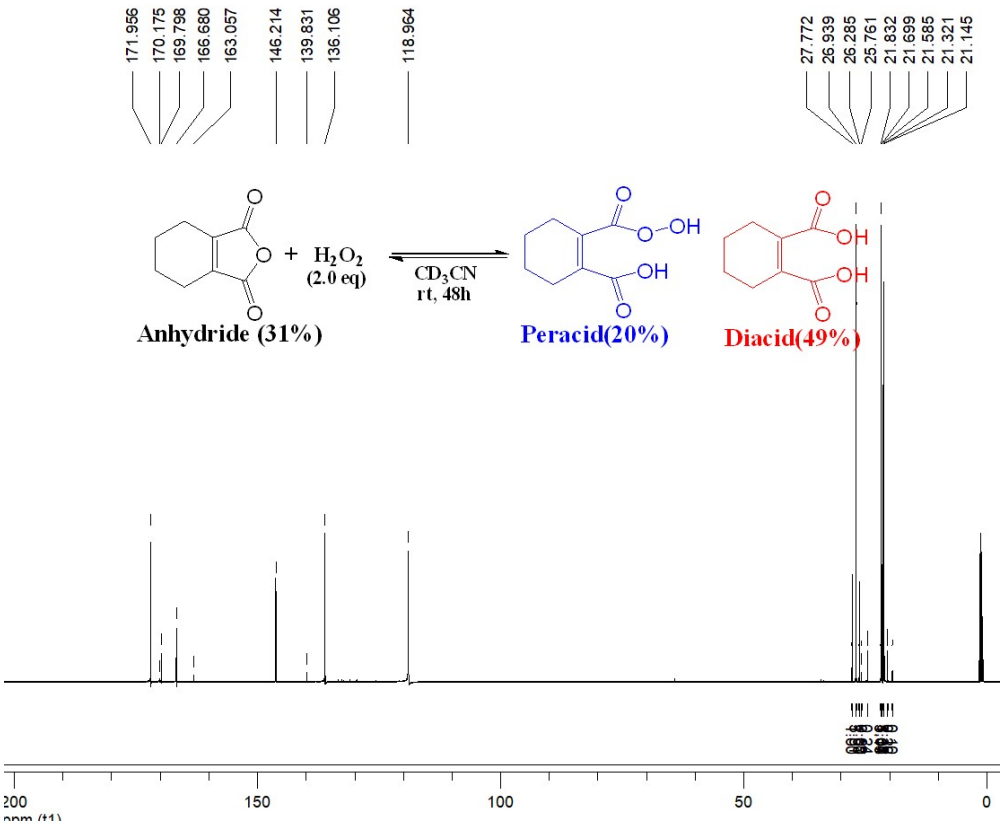


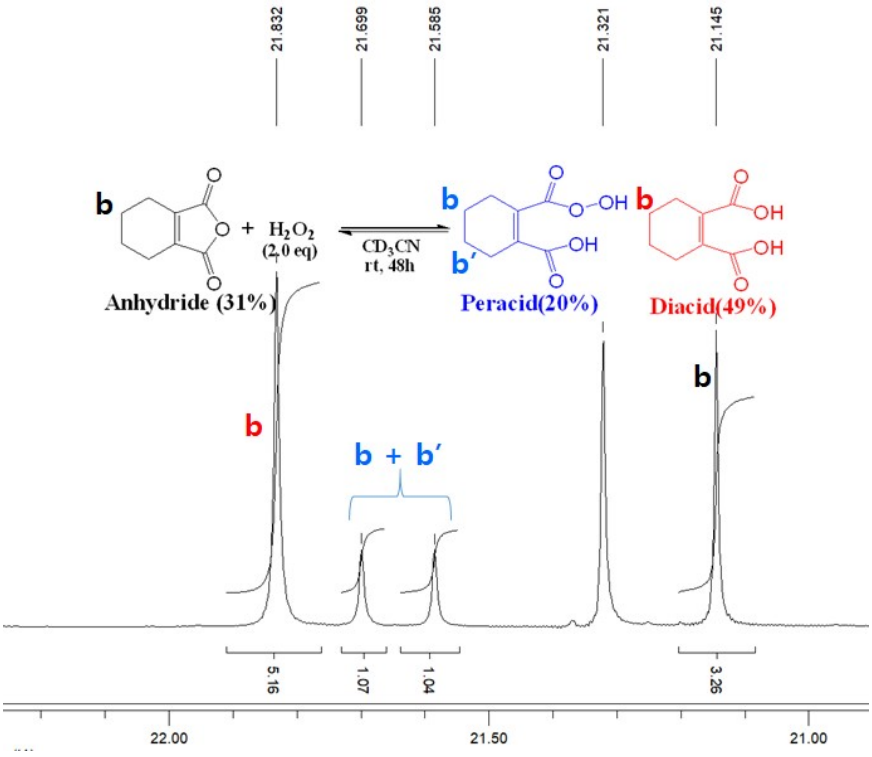
Figure SI-2H. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 24 h.



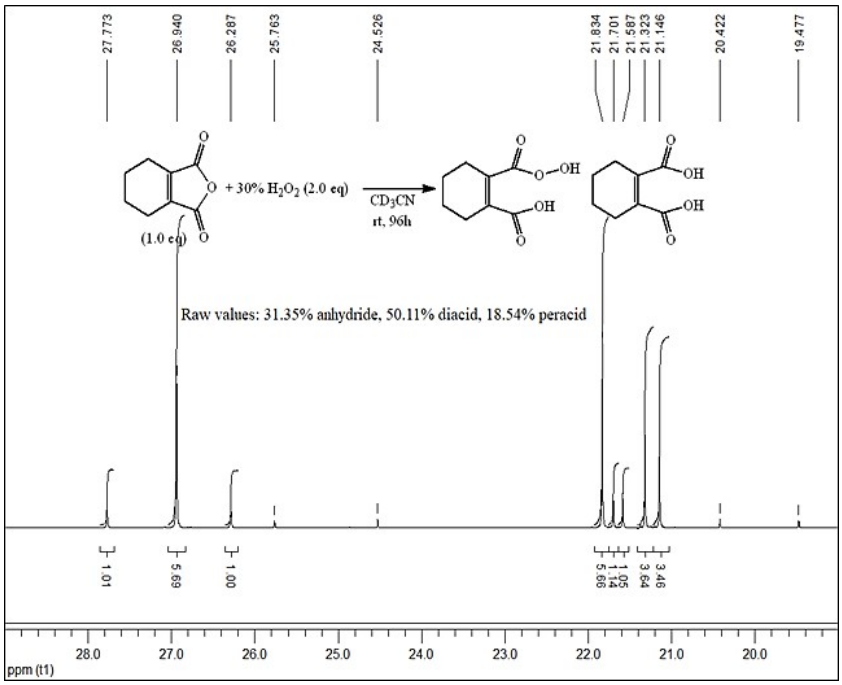
SI-2H-1. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 24 h.



SI-2I. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 48 h.



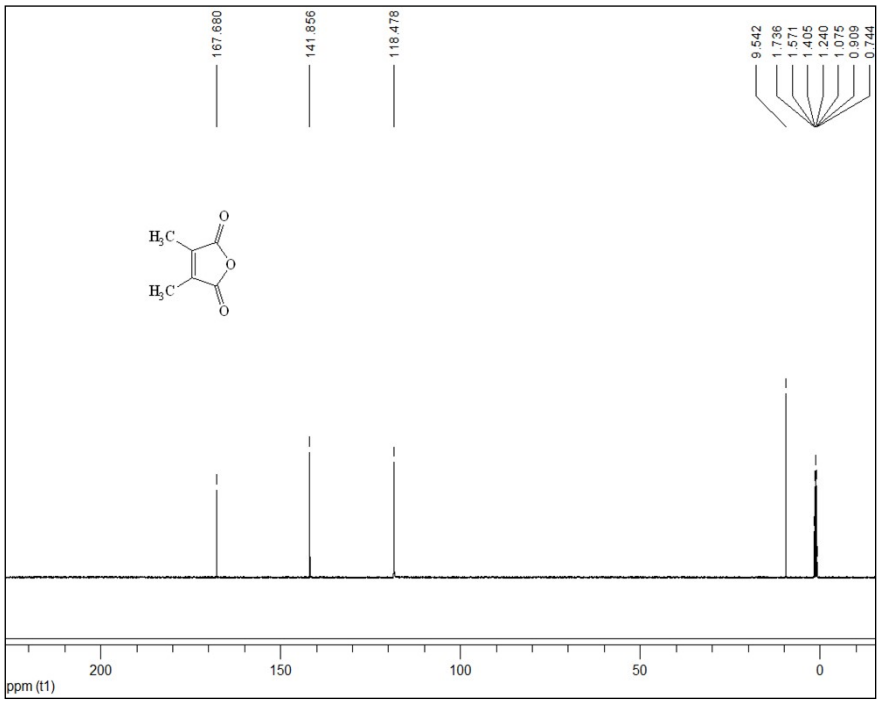
SI-2I-1. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 48 h.



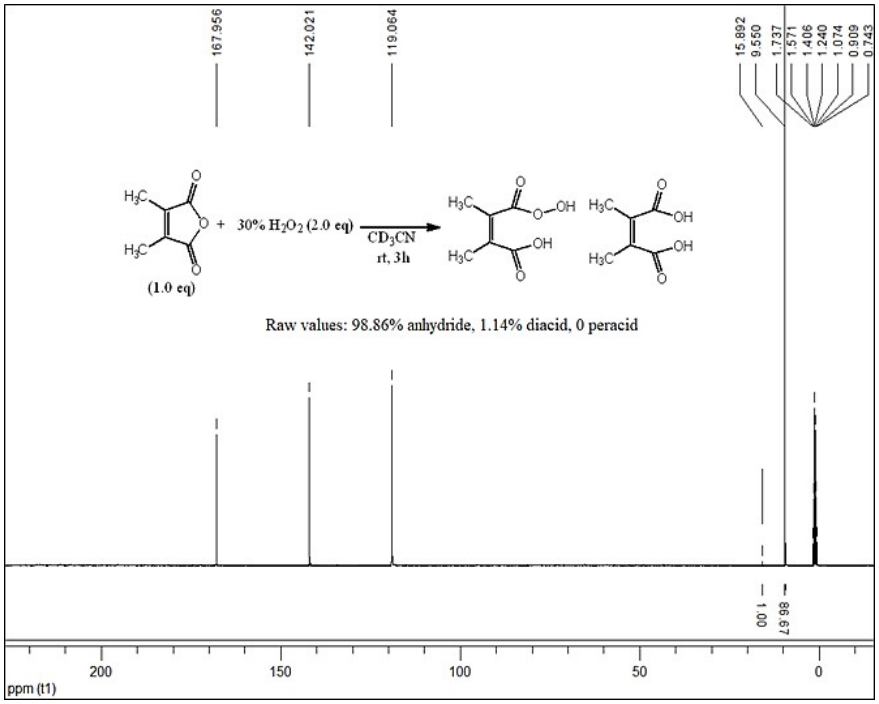
SI-2J. ^{13}C NMR of **CHMA** in CD_3CN + 30% H_2O_2, rt, 96 h.

SI-3: ^{13}C NMR spectra for perhydrolysis of DMMA in H_2O_2.

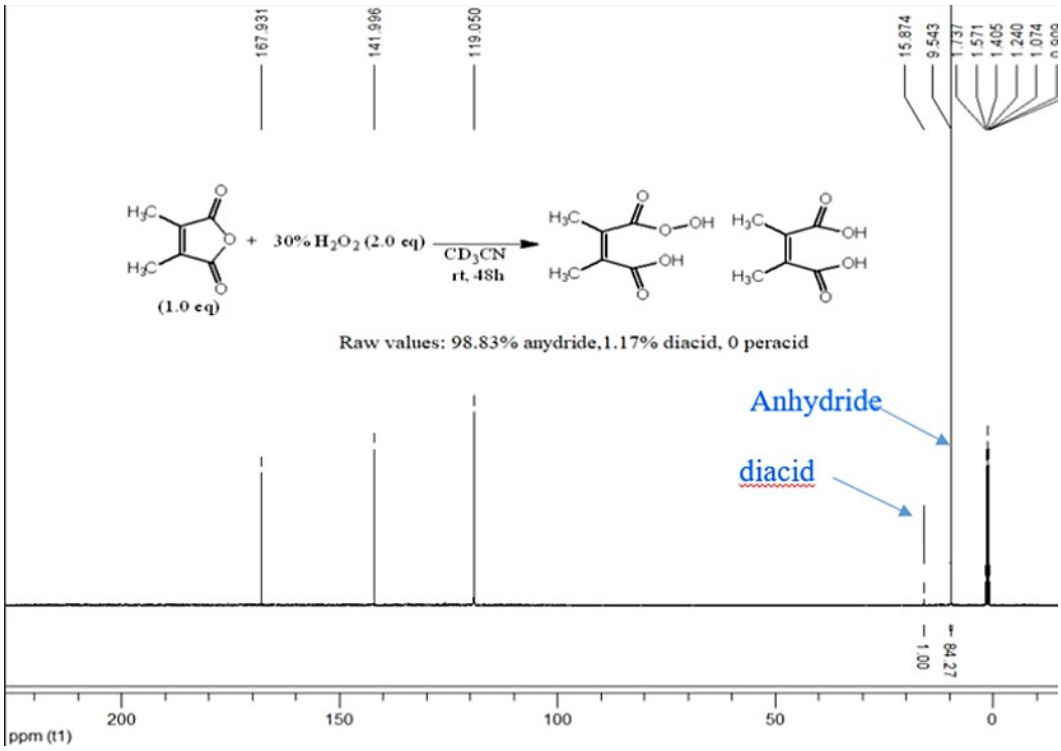
Perhydrolysis of DMMA



SI-3A. ^{13}C NMR of **DMMA** in CD_3CN.



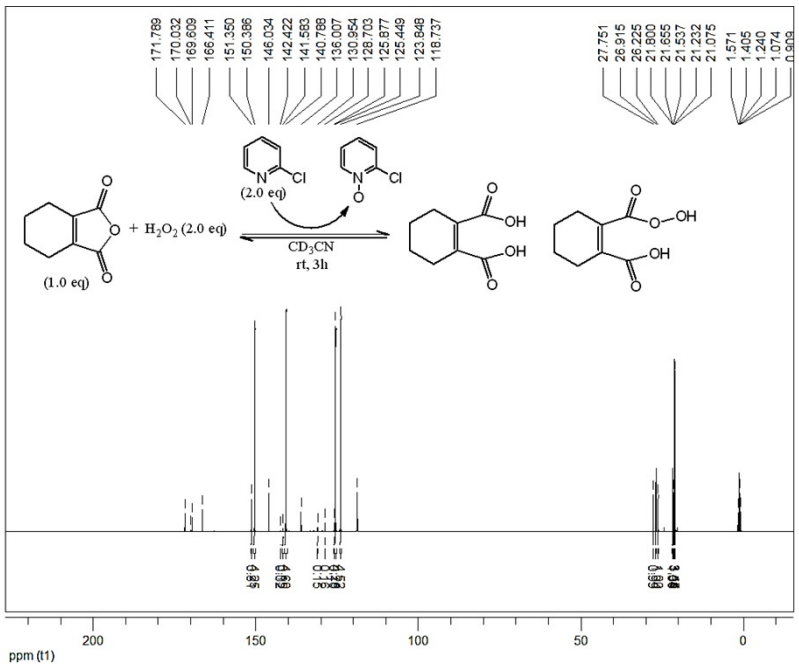
SI-3B. ^{13}C NMR of **DMMA** in CD_3CN + 30% H_2O_2, rt, 3 h.



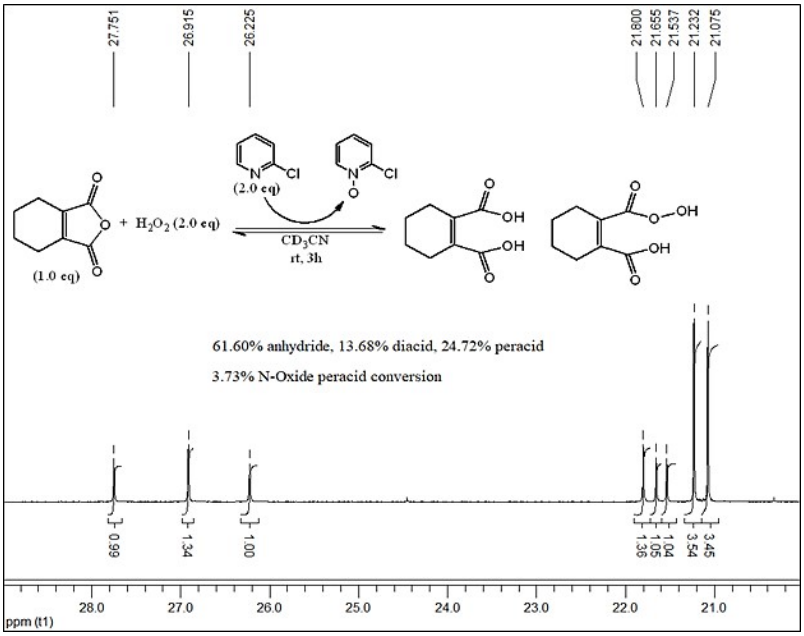
SI-3C. ^{13}C NMR of **DMMA** in CD_3CN + 30% H_2O_2, rt, 48 h.

SI-4: ^{13}C NMR study for the determination of the equilibrium species of CHMA in the presence of quinoline and 2-chloropyridine.

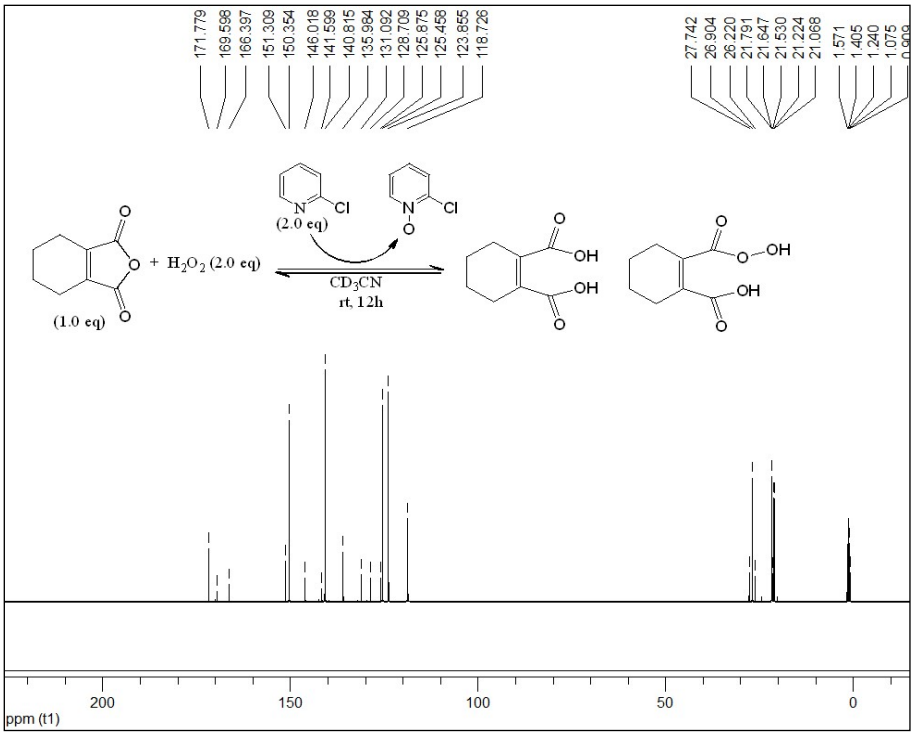
CHMA in H_2O_2 with 2-Chloropyridine



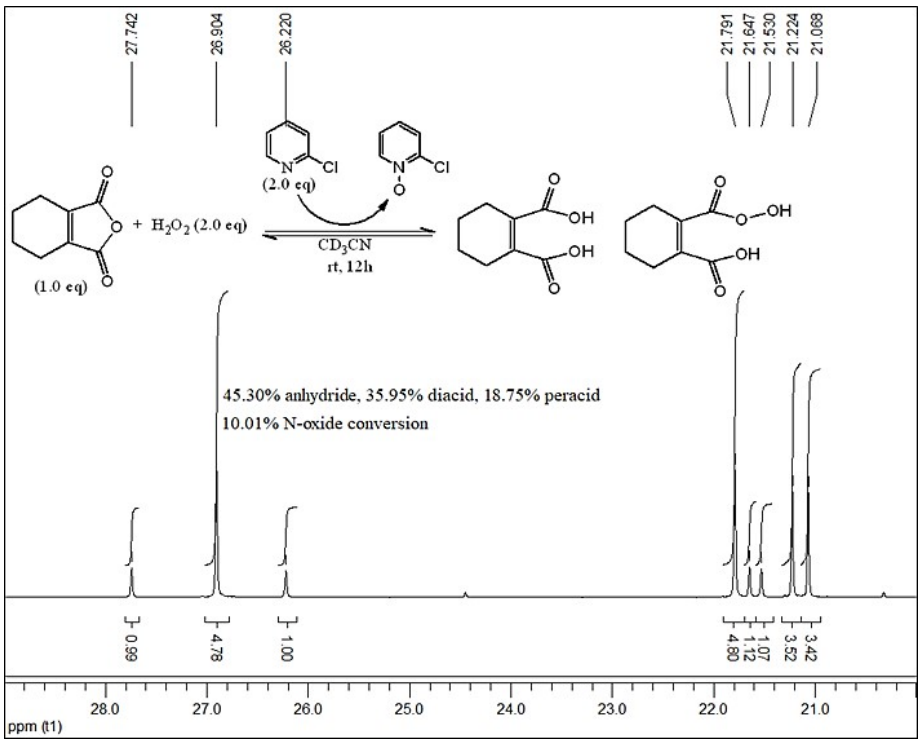
SI-4A. ^{13}C NMR full spectrum of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of 2-chloropyridine at rt, 3 h (peracid determination).



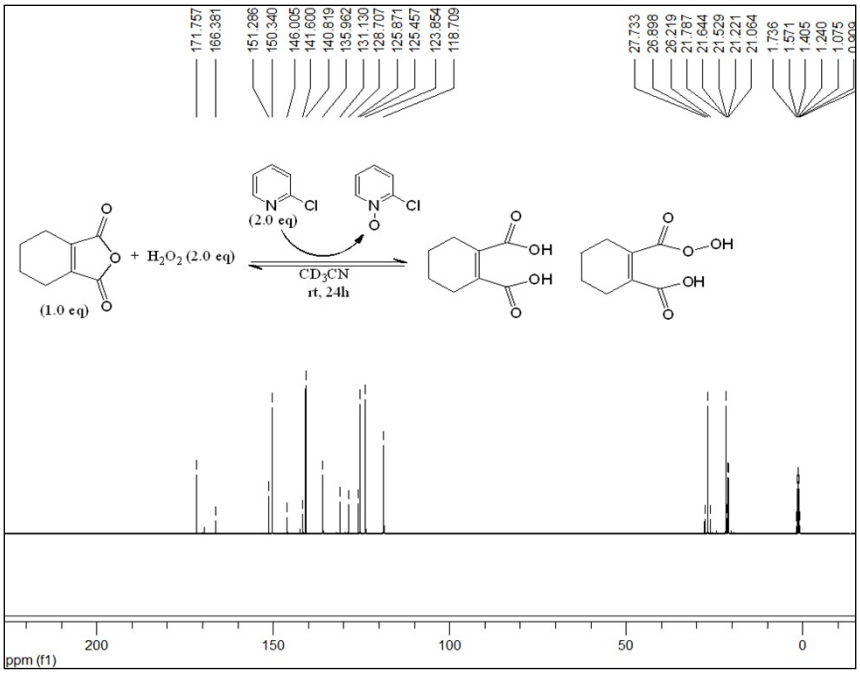
SI-4A-1. ^{13}C NMR of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of 2-chloropyridine at rt, 3 h (peracid determination).



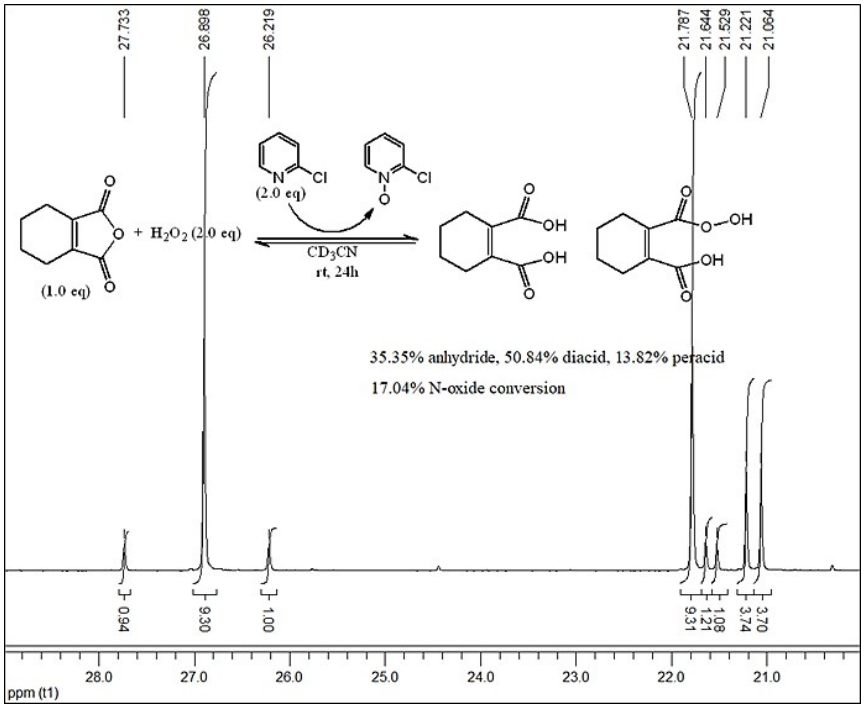
SI-4B. ^{13}C NMR full spectrum of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of 2-chloropyridine at rt, 12 h (peracid determination).



SI-4B-1. ^{13}C NMR of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of 2-chloropyridine at rt, 12 h (peracid determination).

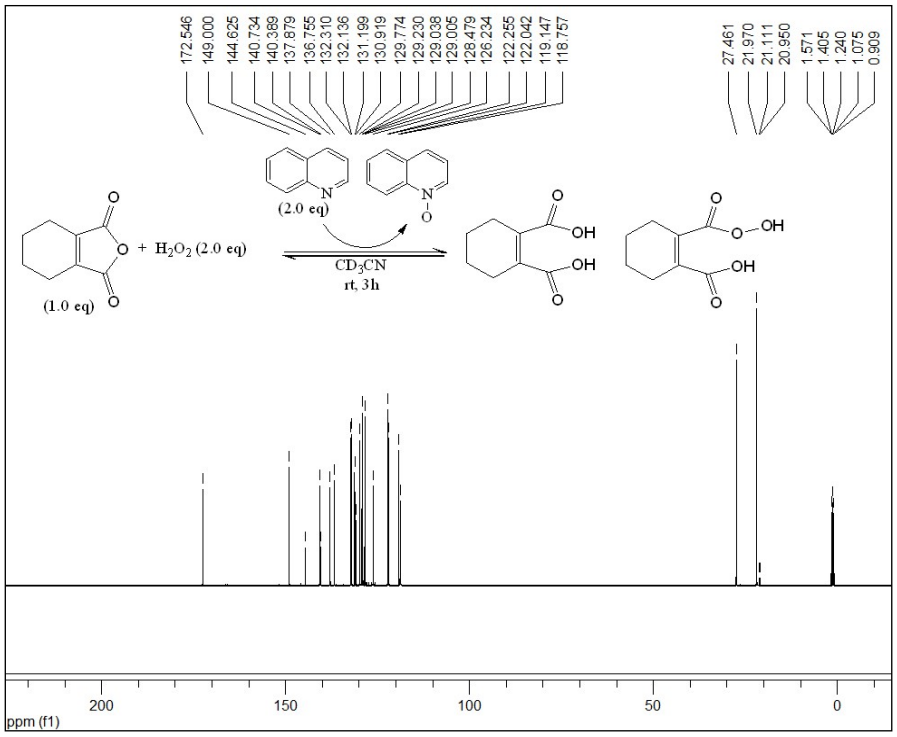


SI-4C. ^{13}C NMR full spectrum of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of 2-chloropyridine at rt, 24 h (peracid determination).

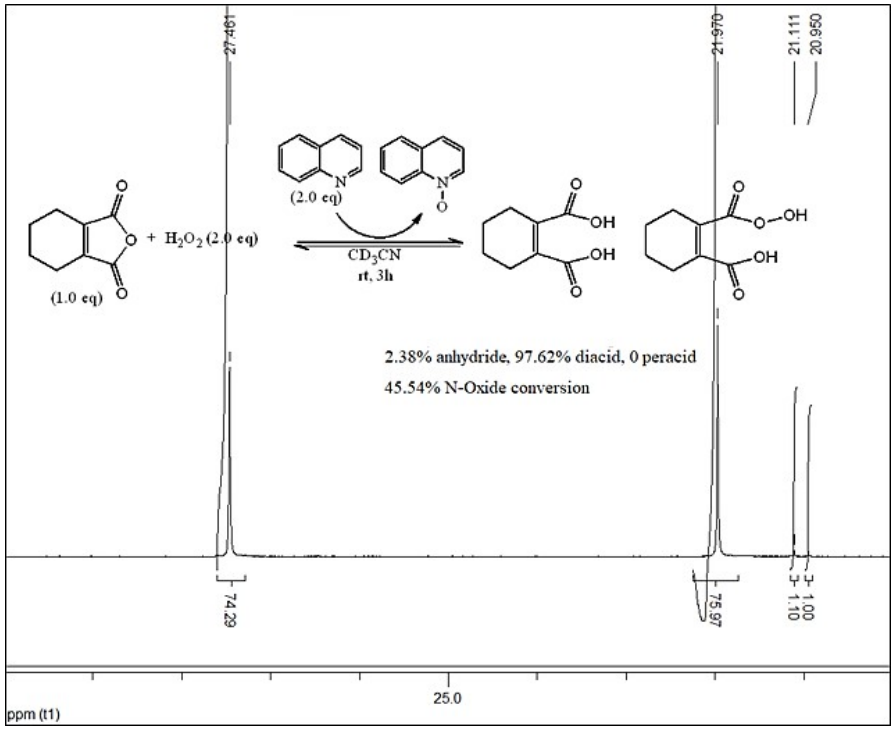


SI-4C-1. ^{13}C NMR of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of 2-chloropyridine at rt, 24 h (peracid determination).

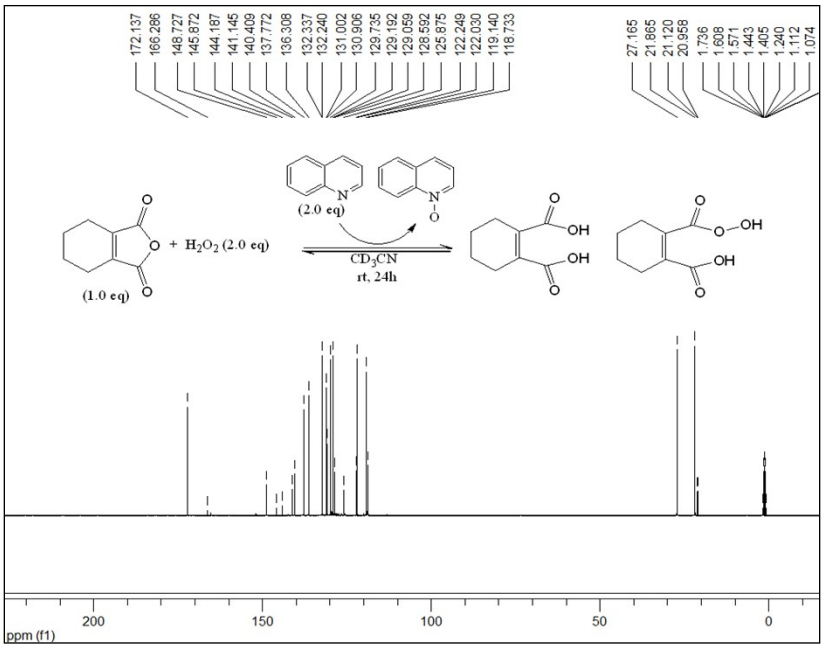
CHMA in H_2O_2 with quinoline



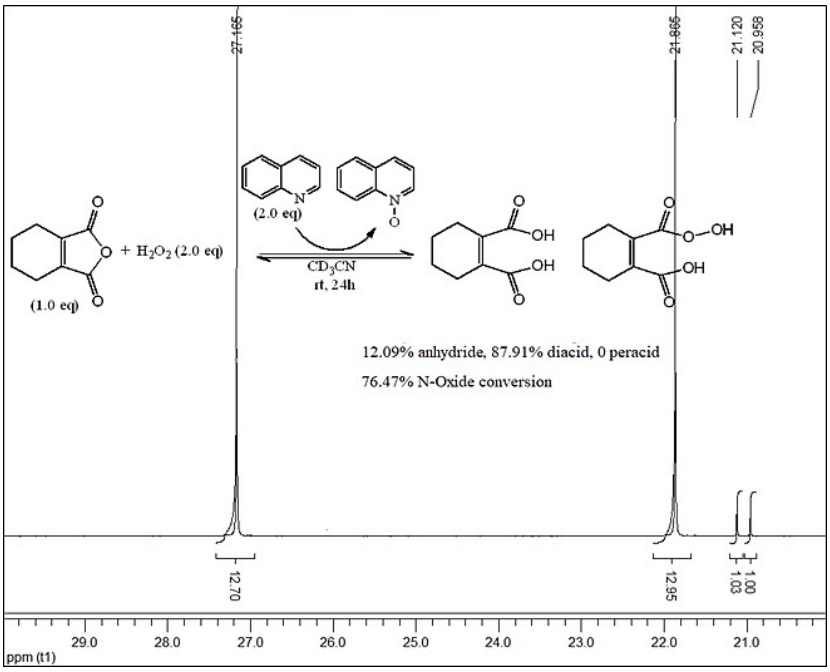
SI-4D. ^{13}C NMR full spectrum of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of quinoline at rt, 3 h (peracid determination).



SI-4D-1. ^{13}C NMR of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of quinoline at rt, 3 h (peracid determination).



SI-4E. ^{13}C NMR full spectrum of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of quinoline at rt, 24 h (peracid determination).



SI-4E-1. ^{13}C NMR spectrum of the perhydrolysis of CHMA with H_2O_2 in CD_3CN in the presence of quinoline at rt, 24 h (peracid determination).