Supporting Information

Iron-catalyzed oxidative decarbonylative α-alkylation of acylsubstituted furans with aliphatic aldehydes as the alkylating agents

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I. Copies of ¹H and ¹³C NMR spectra of starting materials and products





Figure S-2. ¹³C{¹H} NMR spectrum of (2a) (CDCl₃, 100 MHz) *N*-methyl-*N*-phenylfuran-2-carboxamide

96	93 22	93 93	92 03	9
9.4	7.1 4.3	9.6 7.9 1.4	6.3 1.0	.55
15	$14\\14$	12 12 12	11	30 30
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Figure S-3. ¹H NMR spectrum of (2b) (CDCl₃, 400 MHz) *N*,*N*-dimethylfuran-2-carboxamide







Figure S-4. ¹³C{¹H} NMR spectrum of (**2b**) (CDCl₃, 100 MHz) *N*,*N*-dimethylfuran-2-carboxamide



Figure S-5. ¹H NMR spectrum of (2c) (CDCl₃, 400 MHz) *N*,*N*-diethylfuran-2-carboxamide



Figure S-6. ¹³C{¹H} NMR spectrum of (**2c**) (CDCl₃, 100 MHz) *N*,*N*-diethylfuran-2-carboxamide



Figure S-7. ¹H NMR spectrum of (2d) (CDCl₃, 400 MHz) *N*-(2-bromophenyl)-*N*-methylfuran-2-carboxamide



Figure S-8. ¹³C{¹H} NMR spectrum of (2d) (CDCl₃, 100 MHz) *N*-(2-bromophenyl)-*N*-methylfuran-2-carboxamide



Figure S-9. ¹H NMR spectrum of (2e) (CDCl₃, 400 MHz) *N*-(3-methoxyphenyl)-*N*-methylfuran-2-carboxamide



Figure S-10. ¹³C{¹H} NMR spectrum of (2e) (CDCl₃, 100 MHz) *N*-(3-methoxyphenyl)-*N*-methylfuran-2-carboxamide

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	$\int 147.086$ $\int 145.363$ $\int 144.343$		147.086 145.363 144.343 -130.328 -130.328 119.715 116.357 111.051 111.051	7147.086 145.363 144.343 -130.328 -130.328 -130.328 -119.715 119.715 111.051 -55.522









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Figure S-12. ¹³C{¹H} NMR spectrum of (2f) (CDCl₃, 100 MHz) furan-2-yl(pyrrolidin-1-yl)methanone



Figure S-13. ¹H NMR spectrum of (2g) (CDCl₃, 400 MHz) furan-2-yl(piperidin-1-yl)methanone



Figure S-14. ¹³C{¹H} NMR spectrum of (2g) (CDCl₃, 100 MHz) furan-2-yl(piperidin-1-yl)methanone



Figure S-15. ¹H NMR spectrum of (2h) (CDCl₃, 400 MHz) *N*-methoxy-*N*-methylfuran-2-carboxamide



Figure S-16. ¹³C{¹H} NMR spectrum of (**2h**) (CDCl₃, 100 MHz) *N*-methoxy-*N*-methylfuran-2-carboxamide



Figure S-17. ¹H NMR spectrum of (2l) (CDCl₃, 400 MHz) furan-2-yl(phenyl)methanone



Figure S-18. ¹³C{¹H} NMR spectrum of (**2**I) (CDCl₃, 100 MHz) **furan-2-yl(phenyl)methanone**



Figure S-19. ¹H NMR spectrum of (20) (CDCl₃, 400 MHz) 1-(furan-2-yl)-2,2-dimethylpropan-1-one





Figure S-20. ¹³C{¹H} NMR spectrum of (20) (CDCl₃, 100 MHz) 1-(furan-2-yl)-2,2-dimethylpropan-1-one

10

Figure S-21. ¹H NMR spectrum of (2p) (CDCl₃, 400 MHz) 2-phenylfuran



Figure S-22. ¹³C{¹H} NMR spectrum of (2p) (CDCl₃, 100 MHz) 2-phenylfuran



Figure S-23. ¹H NMR spectrum of (2s) (CDCl₃, 400 MHz) *N*-methyl-*N*-phenylfuran-3-carboxamide



Figure S-24. ¹³C{¹H} NMR spectrum of (2s) (CDCl₃, 100 MHz) *N*-methyl-*N*-phenylfuran-3-carboxamide

-163.361	∕_145.807 144.232 √142.003		-111.114	-38.309
1	$\leq 1 \geq$	$\leq P >$	1	





Figure S-25. ¹H NMR spectrum of (3c) (CDCl₃, 400 MHz) 1-methylcyclohexanecarboxaldehyde







Figure S-27. ¹³C{¹H} NMR spectrum of (1a) (CDCl₃, 100 MHz) 5-(*tert*-butyl)-*N*-methyl-*N*-phenylfuran-2-carboxamide



Figure S-28. ¹H NMR spectrum of (1b) (CDCl₃, 400 MHz) 5-(*tert*-butyl)-N, N-dimethylfuran-2-carboxamide



Figure S-29. ¹³C{¹H} NMR spectrum of (1b) (CDCl₃, 100 MHz) 5-(*tert*-butyl)-*N*, *N*-dimethylfuran-2-carboxamide



Figure S-30. ¹H NMR spectrum of (1c) (CDCl₃, 400 MHz) 5-(*tert*-butyl)-*N*, *N*-diethylfuran-2-carboxamide



Figure S-31. ¹³C{¹H} NMR spectrum of (1c) (CDCl₃, 100 MHz) 5-(*tert*-butyl)-*N*, *N*-diethylfuran-2-carboxamide



Figure S-32. ¹H NMR spectrum of (1d) (CDCl₃, 400 MHz) N-(2-bromophenyl)-5-(*tert*-butyl)-N-methylfuran-2-carboxamide







Figure S-34. ¹H NMR spectrum of (1e) (CDCl₃, 400 MHz) 5-(tert-butyl)-N-(3-methoxyphenyl)-N-methylfuran-2-carboxamide






Figure S-36. ¹H NMR spectrum of (1f) (CDCl₃, 400 MHz) (5-(*tert*-butyl)furan-2-yl)(pyrrolidin-1-yl)methanone



Figure S-37. ¹³C{¹H} NMR spectrum of (1f) (CDCl₃, 100 MHz) (5-(*tert*-butyl)furan-2-yl)(pyrrolidin-1-yl)methanone



Figure S-38. ¹H NMR spectrum of (1g) (CDCl₃, 400 MHz) (5-(*tert*-butyl)furan-2-yl)(piperidin-1-yl)methanone



Figure S-39. ¹³C{¹H} NMR spectrum of (1g) (CDCl₃, 100 MHz) (5-(*tert*-butyl)furan-2-yl)(piperidin-1-yl)methanone



Figure S-40. ¹H NMR spectrum of (1h) (CDCl₃, 400 MHz) 5-(*tert*-butyl)-N-methoxy-N-methylfuran-2-carboxamide







Figure S-42. ¹H NMR spectrum of (1i) (CDCl₃, 400 MHz) methyl 5-(*tert*-butyl)furan-2-carboxylate





Figure S-43. ¹³C{¹H} NMR spectrum of (1i) (CDCl₃, 100 MHz) methyl 5-(*tert*-butyl)furan-2-carboxylate

Figure S-44. ¹H NMR spectrum of (1j) (CDCl₃, 400 MHz) ethyl 5-(*tert*-butyl)furan-2-carboxylate



Figure S-45. ¹³C{¹H} NMR spectrum of (1j) (CDCl₃, 100 MHz) ethyl 5-(*tert*-butyl)furan-2-carboxylate



Figure S-46. ¹H NMR spectrum of (1k) (CDCl₃, 400 MHz) isopropyl 5-(*tert*-butyl)furan-2-carboxylate



Figure S-47. ¹³C{¹H} NMR spectrum of (1k) (CDCl₃, 100 MHz) isopropyl 5-(*tert*-butyl)furan-2-carboxylate



Figure S-48. ¹H NMR spectrum of (11) (CDCl₃, 400 MHz) (5-(*tert*-butyl)furan-2-yl)(phenyl)methanone



 $\label{eq:Figure S-49.} Figure S-49. \ ^{13}C\{^{1}H\} \ NMR \ spectrum \ of \ (1l) \ (CDCl_{3}, \ 100 \ MHz) \ (5-(\textit{tert-butyl})\textit{furan-2-yl}) \ (phenyl) \ methanone$



Figure S-50. ¹H NMR spectrum of (1m) (CDCl₃, 400 MHz) 5-(*tert*-butyl)furan-2-carbaldehyde







Figure S-52. ¹H NMR spectrum of (1n) (CDCl₃, 400 MHz) 1-(5-(*tert*-butyl)furan-2-yl)ethanone



Figure S-53. ¹³C{¹H} NMR spectrum of (1n) (CDCl₃, 100 MHz) 1-(5-(*tert*-butyl)furan-2-yl)ethanone



Figure S-54. ¹H NMR spectrum of (10) (CDCl₃, 400 MHz) 1-(5-(*tert*-butyl)furan-2-yl)-2,2-dimethylpropan-1-one



Figure S-55. ¹³C{¹H} NMR spectrum of (10) (CDCl₃, 100 MHz) 1-(5-(*tert*-butyl)furan-2-yl)-2,2-dimethylpropan-1-one



Figure S-56. ¹H NMR spectrum of (1p) (CDCl₃, 400 MHz) 2-(*tert*-butyl)-5-phenylfuran



Figure S-57. ¹³C{¹H} NMR spectrum of (1p) (CDCl₃, 100 MHz) 2-(*tert*-butyl)-5-phenylfuran







Figure S-58. ¹H NMR spectrum of (1r) (CDCl₃, 400 MHz) 2-(*tert*-butyl)benzofuran



Figure S-59. ¹³C{¹H} NMR spectrum of (1r) (CDCl₃, 100 MHz) 2-(*tert*-butyl)benzofuran



Figure S-60. ¹H NMR spectrum of (1s) (CDCl₃, 400 MHz) 2,5-di-tert-butyl-N-methyl-N-phenylfuran-3-carboxamide



Figure S-61. ¹³C{¹H} NMR spectrum of (1s) (CDCl₃, 100 MHz) 2,5-di-*tert*-butyl-*N*-methyl-*N*-phenylfuran-3-carboxamide





Figure S-62. ¹H NMR spectrum of (1t) (CDCl₃, 400 MHz) 5-(1-methylcyclohexyl)- *N*-methyl-*N*-phenylfuran-2-carboxamide



Figure S-63. ¹³C{¹H} NMR spectrum of (1t) (CDCl₃, 100 MHz) 5-(1-methylcyclohexyl)- *N*-methyl-*N*-phenylfuran-2-carboxamide

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	-					1 4 2	0 4
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Figure S-64. ¹H NMR spectrum of (1u) (CDCl₃, 400 MHz) 5-(1-(4-isopropylphenyl)propan-2-yl)-*N*-methyl-*N*-phenylfuran-2-carboxamide







Figure S-66. ¹H NMR spectrum of (1v) (CDCl₃, 400 MHz) 5-(1-(4-(tert-butyl)phenyl)propan-2-yl)-N-methyl-N-phenylfuran-2-carboxamide



Figure S-67. ¹³C{¹H} NMR spectrum of (1v) (CDCl₃, 100 MHz) 5-(1-(4-(tert-butyl)phenyl)propan-2-yl)-*N*-methyl-*N*-phenylfuran-2-carboxamide



Figure S-68. ¹H NMR spectrum of (1w) (CDCl₃, 400 MHz) 5-cyclohexyl-*N*-methyl-*N*-phenylfuran-2-carboxamide





Figure S-69. ¹³C{¹H} NMR spectrum of (1w) (CDCl₃, 100 MHz) 5-cyclohexyl-*N*-methyl-*N*-phenylfuran-2-carboxamide

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Figure S-70. ¹H NMR spectrum of (1x) (CDCl₃, 400 MHz) 5-cyclopentyl-*N*-methyl-*N*-phenylfuran-2-carboxamide


Figure S-71. ¹³C{¹H} NMR spectrum of (1x) (CDCl₃, 100 MHz) 5-cyclopentyl-*N*-methyl-*N*-phenylfuran-2-carboxamide



Figure S-72. ¹H NMR spectrum of (1y) (CDCl₃, 400 MHz) 5-(cyclohex-3-en-1-yl)-*N*-methyl-*N*-phenylfuran-2-carboxamide



~162.449 ~159.678 <145.786
<144.756</pre> 26.920 129.521 127.471 .403 -105.299~38.566 733.316 729.419 ~26.919 ~24.650 5.47Ме Ö 90 8 fl (ppm)



Figure S-74. ¹H NMR spectrum of (1z) (CDCl₃, 400 MHz) 5-isopropyl-*N*-methyl-*N*-phenylfuran-2-carboxamide





Figure S-75. ¹³C{¹H} NMR spectrum of (1z) (CDCl₃, 100 MHz) 5-isopropyl-*N*-methyl-*N*-phenylfuran-2-carboxamide

Figure S-76. ¹H NMR spectrum of (1aa) (CDCl₃, 400 MHz) 5-(heptan-3-yl)-N-methyl-N-phenylfuran-2-carboxamide







Figure S-78. ¹H NMR spectrum of (1ab) (CDCl₃, 400 MHz) *N*-methyl-5-(pentan-3-yl)-*N*-phenylfuran-2-carboxamide







Figure S-80. ¹H NMR spectrum of (1ac) (CDCl₃, 400 MHz) *N*-methyl-5-(pentan-2-yl)-*N*-phenylfuran-2-carboxamide



Figure S-81. ¹³C{¹H} NMR spectrum of (1ac) (CDCl₃, 100 MHz) *N*-methyl-5-(pentan-2-yl)-*N*-phenylfuran-2-carboxamide



Figure S-82. ¹H NMR spectrum of (1ad) (CDCl₃, 400 MHz) 5-(sec-butyl)-N-methyl-N-phenylfuran-2-carboxamide





Figure S-83. ¹³C{¹H} NMR spectrum of (1ad) (CDCl₃, 100 MHz) 5-(sec-butyl)-N-methyl-N-phenylfuran-2-carboxamide

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Figure S-84. ¹H NMR spectrum of (1ae) (CDCl₃, 400 MHz) *N*-methyl-*N*-phenyl-5-propylfuran-2-carboxamide

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4 1 1 2 1 6 0	8071	S	765	0 1 0 00 0 1
0 8 9 4 7 0 0 6	4 6 0 1	-	400	0.0 m - 0.0 - 0.0
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Figure S-85. ¹³C{¹H} NMR spectrum of (1ae) (CDCl₃, 100 MHz) *N*-methyl-*N*-phenyl-5-propylfuran-2-carboxamide

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Figure S-86. ¹H NMR spectrum of (1af) (CDCl₃, 400 MHz) (1af) 5-isobutyl-*N*-methyl-*N*-phenylfuran-2-carboxamide



Figure S-87. ¹³C{¹H} NMR spectrum of (1af) (CDCl₃, 100 MHz) 5-isobutyl-*N*-methyl-*N*-phenylfuran-2-carboxamide



Figure S-88. ¹H NMR spectrum of (1ag) (CDCl₃, 400 MHz) 5-butyl-*N*-methyl-*N*-phenylfuran-2-carboxamide



Figure S-89. ¹³C{¹H} NMR spectrum of (1ag) (CDCl₃, 100 MHz) 5-butyl-*N*-methyl-*N*-phenylfuran-2-carboxamide



II. Control experiments



Figure S-90. the product of alkyl radical trapping (4a)



