## **Supplementary Material**

## Iron nitrate/TEMPO-catalyzed oxidative Passerini reaction of alcohols in air

Shivalinga Kolle,<sup>a</sup> Shashikant U. Dighe,<sup>a</sup> and Sanjay Batra<sup>\*a,b</sup>

<sup>a</sup> Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, BS-10/1, Sector 10, Jankipuram Extension, Sitapur Road, Lucknow 226031, India <sup>b</sup> Academy of Scientific and Innovative Research, New Delhi 110025, India E-mail: <u>batra\_san@yahoo.co.uk</u>, <u>s\_batra@cdri.res.in</u>

Dedicated to Dr. Jhillu Singh Yadav on the occasion of his 65<sup>th</sup> anniversary

## Contents

1. Copies of <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of CompoundsS-2

## Copies <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of Compounds:



Figure S1. <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl benzoate (4aAa).



Figure S2. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl benzoate (4aAa).



**Figure S3.** <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl benzoate (**4aAb**).



Figure S4. <sup>13</sup>C-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl benzoate (4aAb).



Figure S5. <sup>1</sup>H-NMR spectrum of 2-((2-ethoxy-2-oxoethyl)amino)-2-oxo-1-phenylethyl benzoate (4aAc).



Figure S6. <sup>13</sup>C-NMR spectrum of 2-((2-ethoxy-2-oxoethyl)amino)-2-oxo-1-phenylethyl benzoate (4aAc).



**Figure S7.** <sup>1</sup>H-NMR spectrum of 2-((2-morpholinoethyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAd**).



**Figure S8.** <sup>13</sup>C-NMR spectrum of 2-((2-morpholinoethyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAd**).



**Figure S9.** <sup>1</sup>H-NMR spectrum of 2-((2,6-dimethylphenyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAe**).



**Figure S10.** <sup>13</sup>C-NMR spectrum of 2-((2,6-dimethylphenyl)amino)-2-oxo-1-phenylethyl benzoate (**4aAe**).



Figure S11. <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl benzoate (4bAa).



Figure S12. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl benzoate (4bAa).



Figure S13. <sup>1</sup>H-NMR spectrum of 1-(4-bromophenyl)-2-(*tert*-butylamino)-2-oxoethyl benzoate (4cAa).



Figure S14. <sup>13</sup>C-NMR spectrum of 1-(4-bromophenyl)-2-(*tert*-butylamino)-2-oxoethyl benzoate (4cAa).



**Figure S15.** <sup>1</sup>H-NMR spectrum of 1-(4-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl benzoate (**4cAb**).







**Figure S17.** <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (**4dAa**).



Figure S18. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (4dAa).



**Figure S19.** <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (**4dAb**).



Figure S20. 13C-NMR spectrum of 2-(cyclohexylamino)-1-(4-nitrophenyl)-2-oxoethyl benzoate (4dAb).



**Figure S21.** <sup>1</sup>H-NMR spectrum of (*E*)-1-(*tert*-butylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (**4eAa**).



**Figure S22.** <sup>13</sup>C-NMR spectrum of (*E*)-1-(*tert*-butylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (**4eAa**).



**Figure S23.** <sup>1</sup>H-NMR spectrum of (*E*)-1-(cyclohexylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (**4eAb**).



**Figure S24.** <sup>13</sup>C-NMR spectrum of (*E*)-1-(cyclohexylamino)-1-oxo-4-phenylbut-3-en-2-yl benzoate (**4eAb**).



Figure S25. <sup>1</sup>H-NMR spectrum of 1-(*tert*-butylamino)-3-methyl-1-oxobutan-2-yl benzoate (4fAa).



Figure S26. <sup>13</sup>C-NMR spectrum of 1-(*tert*-butylamino)-3-methyl-1-oxobutan-2-yl benzoate (4fAa).



**Figure S27.** <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (**4gAa**).



Figure S28. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (4gAa).



**Figure S29.** <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (**4gAb**).



Figure S30. <sup>13</sup>C-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-(pyridin-2-yl)ethyl benzoate (4gAb).



**Figure S31.** <sup>1</sup>H-NMR spectrum of methyl 1-(1-(benzoyloxy)-2-(*tert*-butylamino)-2-oxoethyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate (**4hAa**).







**Figure S33.** <sup>1</sup>H-NMR spectrum of methyl 1-(1-(benzoyloxy)-2-(cyclohexylamino)-2-oxoethyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate (4hAb).

<sup>©</sup>ARKAT-USA, Inc.





<sup>©</sup>ARKAT-USA, Inc.



**Figure S35.** <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl nicotinate (**4aBa**).



Figure S36. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl nicotinate (4aBa).



Figure S37. <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl nicotinate (4aBb).



Figure S38. <sup>13</sup>C-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl nicotinate (4aBb).



**Figure S39.** <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl 3-nitrobenzoate (**4aCb**).



Figure S40. <sup>13</sup>C-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl 3-nitrobenzoate (4aCb).



Figure S41. <sup>1</sup>H-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl cinnamate (4aDb).



Figure S42. <sup>13</sup>C-NMR spectrum of 2-(cyclohexylamino)-2-oxo-1-phenylethyl cinnamate (4aDb).



Figure S43. <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl 2-(3-chlorophenyl)acetate (4aEa).



Figure S44. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-2-oxo-1-phenylethyl 2-(3-chlorophenyl)acetate (4aEa).



Figure S45. <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (4bEa).



Figure S46. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-1-(2-chlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (4bEa).



**Figure S47.** <sup>1</sup>H-NMR spectrum of 2-(*tert*-butylamino)-1-(2,3-dichlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (**4iEa**).



Figure S48. <sup>13</sup>C-NMR spectrum of 2-(*tert*-butylamino)-1-(2,3-dichlorophenyl)-2-oxoethyl 2-(3-chlorophenyl)acetate (4iEa).