

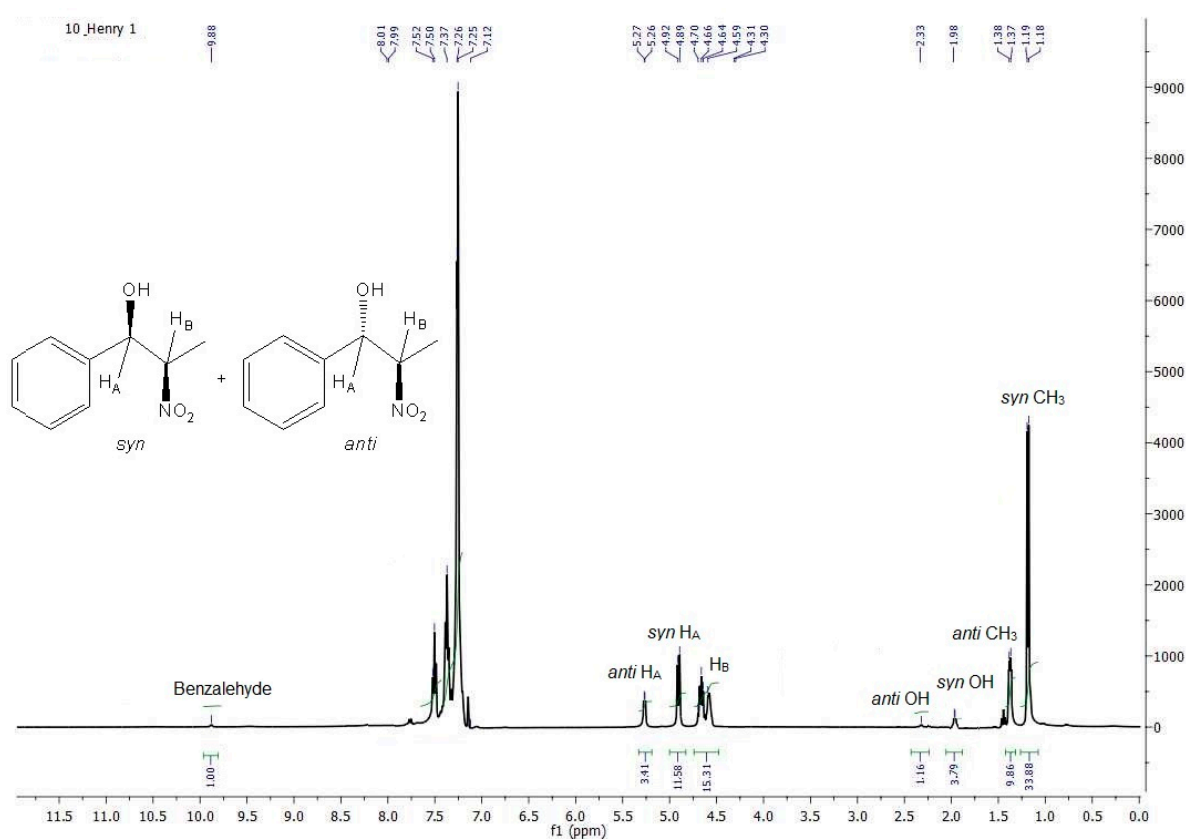
Electronic Supplementary Information

Ni(II)-aroylhydrazone complexes as catalyst precursors
towards

efficient solvent-free nitroaldol condensation reaction

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Figure S1. ¹H NMR spectrum for the nitroaldol product of nitroethane and benzaldehyde in CDCl₃ (Table 3, entry 10).



¹H NMR spectrum for the determination of the nitroaldol products (Table 3, Entry 10); ¹H NMR (400 MHz, CDCl₃) δ 7.56-7.26 (m, 5H), 5.27 (d, *J* = 3.6 Hz, 3.41H) (*anti*), 4.92 (d, *J* = 8.8 Hz, 11.58H) (*syn*), 4.70-4.59 (m, 15.31H), 2.33 (b, 1.16H) (*anti*), 1.98 (b, 3.79H) (*syn*), 1.38 (d, *J* = 6.8 Hz, 9.86H) (*anti*), 1.19 (d, *J* = 6.8 Hz, 33.88H) (*syn*).

Calculation of the yield and selectivity

$$\begin{aligned} \text{Total amount of compounds} &= \text{benzaldehyde} + \text{anti} + \text{syn} \\ &= 1 + 3.4 + 11.6 = 16 \text{ (100\%)} \end{aligned}$$

$$\text{Unreacted benzaldehyde} = (1/16) \times 100 = 6.2\%$$

$$\text{Yield of } \beta\text{-nitroalkanols} = 100 - 6.2 = 94\%$$

$$\text{Yield of } \textit{syn} = (11.6/16) \times 100 = 72.5\%$$

$$\text{Yield of } \textit{anti} = (3.4/16) \times 100 = 21.3\%$$

Selectivity:

$$(\textit{syn} + \textit{anti}) = 72.5 + 21.3 = 93.8 \text{ (100\%)}$$

$$\text{Selectivity of } \textit{syn} = (72.5/93.8) \times 100 = 77\%$$

$$\text{Selectivity of } \textit{anti} = (21.3 / 93.8) \times 100 = 23\%$$

References

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