Electronic Supplementary Material (ESI) for Green Chemistry
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Supporting Information

CeO_2-catalysed one-pot selective synthesis of esters from nitriles and alcohols

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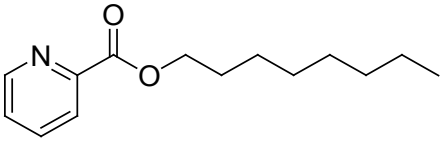
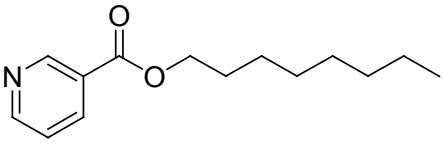
Characterization of the compounds (GC-MS data)

Picolinic Acid Octyl Ester (Table2-1)



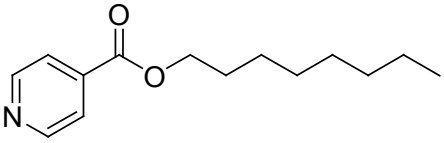
GC-MS: *m/z* (% rel. inten.) 235(M^+, 0.03), 207(41), 124(76), 106(63), 79(100), 78(98).

Nicotinic Acid Octyl Ester (Table2-3)



MS: *m/z* (relative intensity) 235(M^+, 0.99), 124(100), 106(79), 78(59).

Isonicotinic Acid Octyl Ester (Table2-4)



MS: *m/z* (relative intensity) 235(M^+, 1.17), 124(100), 106(79), 78(69).

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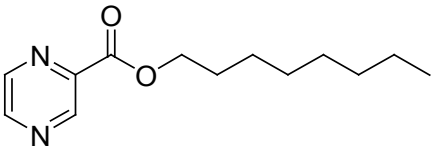
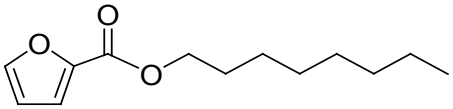
Pyrazinecarboxylic Acid Octyl Ester (Table2-5)



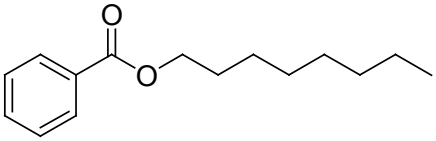
MS: *m/z* (relative intensity) 236(M^+, 4.62), 125(100), 107(59), 80(81).

2-Furoic Acid Octyl Ester (Table2-6)



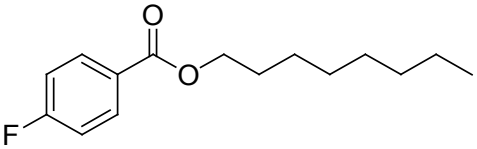
MS: *m/z* (relative intensity) 224(M^+, 4.86), 113(100), 95(81).

Benzoic Acid Octyl Ester (Table2-7)



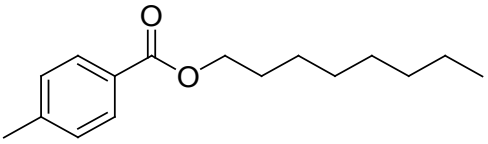
MS: *m/z* (relative intensity) 234(M^+, 1.55), 123(100), 105(99.9), 77(97).

4-Fluorobenzoic Acid Octyl Ester (Table2-8)



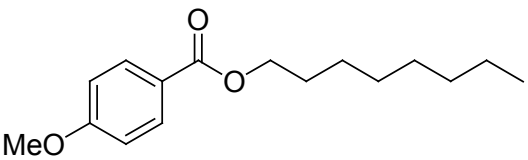
MS: *m/z* (relative intensity) 252(M^+, 0.58), 141(93), 123(100), 112(23), 95(58).

4-Methylbenzoic Acid Octyl Ester (Table2-9)



MS: *m/z* (relative intensity) 248(M^+, 1.55), 137(100), 119(99.9), 91(73).

4-Methoxybenzoic Acid Octyl Ester (Table2-10)



MS: *m/z* (relative intensity) 264(M^+, 14.84), 152(100), 135(93), 107(13).

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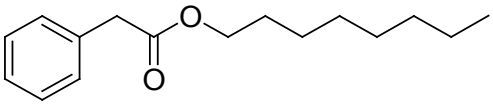
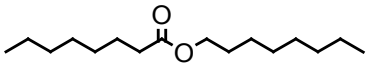
Phenylacetic Acid Octyl Ester (Table2-11)



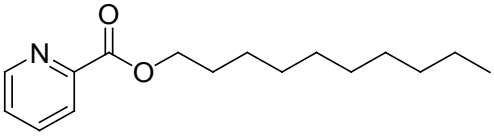
MS: *m/z* (relative intensity) 248(M^+, 0.73), 157(18), 136(31), 91(100).

n-Octanoic Acid Octyl Ester (Table2-12)



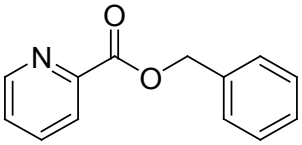
MS: *m/z* (relative intensity) 256(M^+, 0.13), 145(56), 127(29), 112(37), 57(100).

Picolinic Acid Dodecyl Ester (Table3-1)



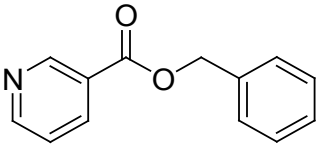
MS: *m/z* (relative intensity) 263(M^+, 0.06), 124(100), 106(82), 79(73).

Picolinic Acid Benzyl Ester (Table3-3)



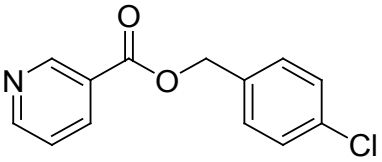
MS: *m/z* (relative intensity) 213(M^+, 0.47), 107(35), 79(100).

Nicotinic Acid Benzyl Ester (Table3-4)



MS: *m/z* (relative intensity) 213(M^+, 86), 106(73), 91(100), 78(30).

Nicotinic Acid 4-Chlorobenzyl Ester (Table3-5)



MS: *m/z* (relative intensity) 247(M^+, 49.41), 125(100), 106(93), 89(40).

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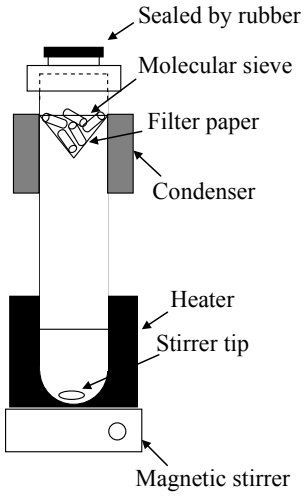

Fig. S1 Reaction apparatus for the one-pot esterification.

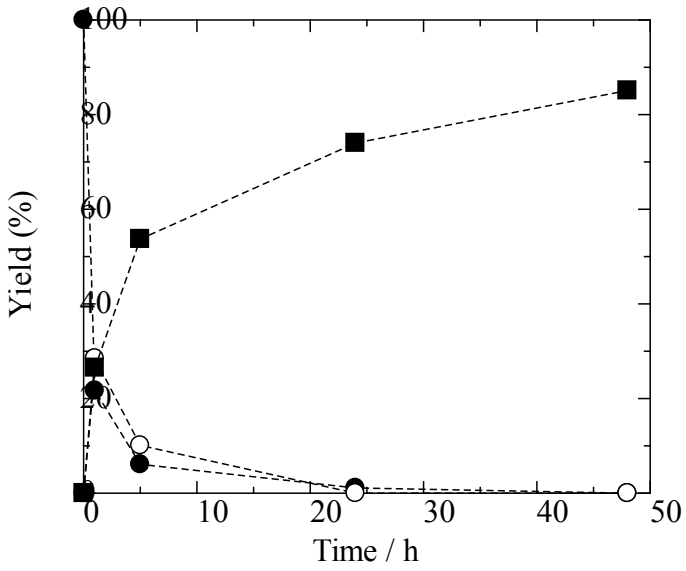

Fig. S2 Time-yield diagram for ester formation from benzonitrile with n-octanol by CeO_2. ●: benzonitrile, ○: benzamide, ■: benzoic acid octyl ester. Reaction conditions: benzonitrile (1.0 mmol), *n*-octanol (10.0 mmol), H_2O (1.0 mmol), CeO_2 (50 mg), molecular sieve (1 g), T = 160 ^{o}C, N_2.

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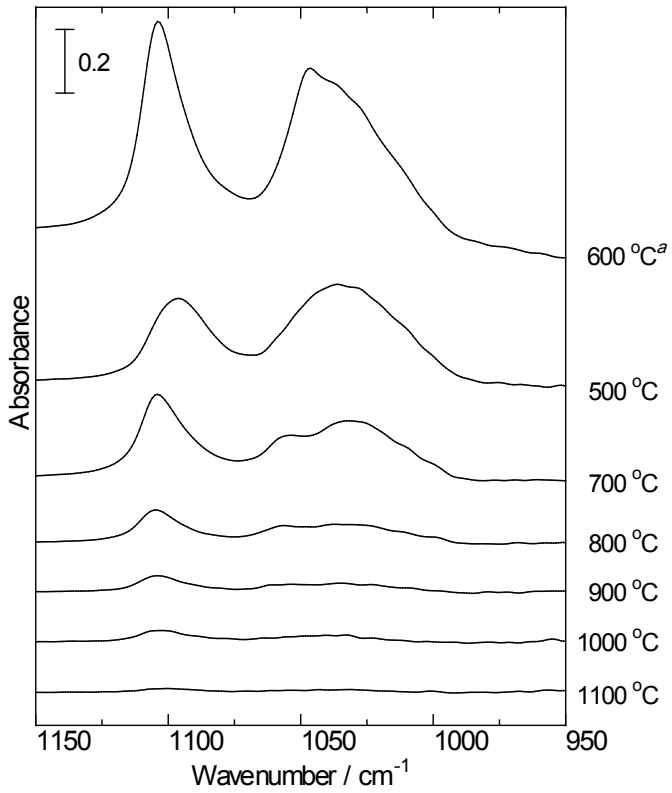

Fig. S3 Spectra of methanol complexes adsorbed to CeO_2 at different calcination temperature. Numbers in the graph are calcination temperatures ([a] JRC-CEO3).