Supporting Information

NHC/Iron Cooperative Catalysis: Aerobic Oxidative Esterification of Aldehydes with Phenols

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General Remarks

Dioxane was freshly distilled over sodium. All reactions were performed in oven-dried glassware under air or N₂. Preparative thin layer chromatography plates were prepared with silica gel 60 GF254 MercK (Ref. 1.07730.1000). Reaction mixtures were analysed by TLC using ALUGRAM® SIL G/UV254 from MN (Ref. 818133, silica gel 60), and visualisation of TLC spots was effected using UV and KMnO₄ solution. NMR spectra were recorded in a Bruker AMX 400 using CDCl₃ as solvent and (CH₃)₄Si (1H) as internal standard. All coupling constants are expressed in Hz. Iron sources: Fe(TfO)₂ (Solchemar, >99.5 %); carbonyl iron metal powder (Aldrich, 99.5 %, low trace metals). NHC ligands used were prepared following reported procedures: 1,3-bis(*tert*-butyl) imidazolium chloride¹, 1,3-bis(2,6diisopropylphenyl) imidazolium chloride and 1,3-bis(2,6-diisopropylphenyl) imidazolinium chloride², were prepared according to literature procedures, except 1,3-bis(2,4,6-trimethy-phenyl) imidazolinium chloride which was purchased from Aldrich. The aldehydes and phenols were purchased from Aldrich and used without further purification. Potassium *tert*-butoxide was purchased from Aldrich and purified by sublimation prior to use.

Preparation of iron (II) triflate:

To an oven dried round bottom flask previously washed with HNO₃/HCl to remove metal traces, freshly distilled methanol (2 ml) and Fe powder (60 mg, 1.1 mmol) were added under N₂. Then, freshly distilled trifluoromethanesulfonic acid (180 μ l, 2 mmol) was slowly added with stirring. The mixture was stirred at room temperature overnight, excess iron filtered out and the solvent removed at reduced pressure. The solvated salt was dried under vacuum at 120 °C until constant weight. Iron (II) triflate was obtained in approximately quantitative yield and kept stored under N₂

General procedures for oxidative esterification:

¹ Arduengo A. J. III, Dias H. V. R., Harlow R. L., Kline M., J. Am. Chem. Soc., 1992, 114, 5530.

² Arduengo A. J. III; Krafczyk R.; Schmutzer R. Tetrahedron, 1999, 55, 14523.

Method A: To a round bottom flask under N_2 were added freshly dried dioxane over sodium (1.5 mL), NHC ligand precursor (20 mol%) and sublimed KO'Bu (0.247 mmol). The mixture was allowed to react at room temperature for 20 min., after which Fe(TfO)₂ (20 mol%) was also added. The mixture was left reacting 5 min. at room temperature and then the phenol (0.25 mmol) and the aldehyde (0.25 mmol) were sequentially added. The N₂ atmosphere was removed and the mixture was heated at 90 °C. Typically, after a reaction time of 24 h the volatiles were removed under reduced pressure and the product isolated by preparative thin layer chromatography (Hexanes:AcOEt).

 $3b^{3}$, $(3c, 3d)^{4}$, $(3e, 3f, 3g, 3n)^{5}$, $3h^{6}$, $3i^{7}$, $3j^{8}$, $3s^{9}$.

Method B: To a round bottom flask under N_2 were added freshly dried dioxane over sodium (1.5 mL), NHC ligand precursor (20 mol%) and dried K₂CO₃ (0.247 mmol). The mixture was allowed to react at room temperature for 20 min., after which anhydrous FeCl₃ (20 mol%) was also added. The mixture was left reacting 5 min. at room temperature and then the aldehyde (0.25 mmol) and the phenol (0.25 mmol) were sequentially added. The N₂ atmosphere was removed, a drying tube filled with blue silica gel was fitted and the mixture was heated at 90 °C. Typically, after a reaction time of 24 h the volatiles were removed under reduced pressure and the product isolated by flash column chromatography (Hexanes:AcOEt).

 $(3t, 3v)^{10}, 3u^{11}, 3v^{12}, 3w^{13}$

phenyl benzoate (3a)

The title compound was prepared according to method A, in 84% yield.

Yellow crystals, m.p. 69-70 °C; IR (CHCl3): v 1728 (C=O) cm⁻¹, v 1077 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) 8.19-8.20 (d, 2H), 7.65-7.70 (t, 1H)7.53-7.57 (t, 2H), 7.44-7.50 (t, 2H), 7.29-7.34 (t, 1H), 7.23-7.26 (d, 2H); ¹³C NMR (100 MHz, CDCl₃) 165.2, 151.0, 133.6, 130.2, 129.5, 129.6, 128.6, 125.9, 121.7

phenyl 4-chlorobenzoate (3b)

The title compound was prepared according to method A, in 77% yield.

White crystals, m.p. 104-105 °C; IR (CHCl3): v 1734 (C=O) cm⁻¹, v 1077 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.17 (2H, d, J = 8.4 Hz), 7.52 (2H, d, J = 8.4 Hz), 7.46 (2H, t, J = 7.8 Hz), 7.31 (1H, t, J= 7.8 Hz), 7.23 (2H, d, J = 7.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.4, 150.8, 140.2, 131.6, 129.6, 129.0, 128.0, 126.1, 121.6.

2-naphtyl 4-methoxybenzoate (3c)

The title compound was prepared according to method A, in 62% yield.

³ Liu J.; Chen J.; Xia C., J. of Catalysis, 2008, 253, 50.

⁴ Shintou T., Fukumoto K., Mukaiyama T., Bull. Chem. Soc. of Japan, 2004, 77, 1569.

⁵ Qin C.; Wu H.; Chen J.; Liu M.; Cheng J.; Su W.; Ding J. Org. Lett., 2008, 10, 1537.

Graffner-Nordberg M., Sjodin K., Tunek A., Hallberg A., Chem. Pharm. Bull., 1998, 46, 591.

⁷ Chen C.-T., Munot Y. S., J. Org. Chem., 2005, 70, 8625.

Zhang L., Zhang J. Y., *J. Comb. Chem.*, **2006**, *8*, 361. Krause M., Rouleau A., Stark H., Garbarg M., Schwartz J.C., Schunack W., *Pharmazie*, **1996**, *51*, 720.

¹⁰ Ruiz, Diego M.; Romanelli, Gustavo P.; Autino, Juan C.; Vazquez, Patricia G., Appl. Cat. A: Gen., 2010, 374 (1-2), 110.

¹¹ Bairwa, R.; Kakwani, M.; Tawari, N. R.; Lalchandani, J.; Ray, M.K.; Rajan, M.G.R.; Degani, M.S.; Bioorg Med Chem Lett., 2010, 20, 1623.

² Dave, J. S.; Lohar, J. M.; J. Indian Chem. Soc., 1989, 66, 25.

¹³ Magens, S.; Plietker, B., J. Org. Chem., **2010**, 75, 3715.

¹⁴ Correia, V. R.; Cuccovia, I. M.; Chaimovich, H. J.Phys. Org. Chem. 1991, 4, 13.

White crystals, m.p. 107-108 °C; IR (CHCl₃): v 1734 (C=O) cm⁻¹, v 1070 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.23 (2H, d, J = 8.8 Hz), 7.92 (1H, d, J = 8.9 Hz), 7.87 (2H, m), 7.71 (1H, d, J = 2.3 Hz), 7.52 (2H, m), 7.38 (1H, dd, J_1 = 8.9 Hz, J_2 = 2.3 Hz), 7.03 (2H, d, J = 8.8 Hz), 3.94 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 165.2, 164.0, 148.7, 133.9, 132.4, 131.5, 129.4, 127.8, 127.7, 126.5, 125.6, 121.9, 121.4, 118.8, 113.9, 55.6.

phenyl 4-bromobenzoate (3d)

The title compound was prepared according to method A, in 59% yield.

White crystals, m.p. 104-105 °C; IR (CHCl₃): v 1727 (C=O) cm⁻¹, v 1076 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.09 (2H, d, J = 8.4 Hz), 7.68 (2H, d, J = 8.4 Hz), 7.46 (2H, t, J = 7.8 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.23 (2H, d, J = 7.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.5, 150.8, 132.0, 131.7, 129.6, 128.9, 128.5, 126.1, 121.6.

phenyl 4-fluorobenzoate (3e)

The title compound was prepared according to method A, in 82% yield.

White crystals, m.p. 59-60 °C; IR (CHCl₃): v 1721 (C=O) cm⁻¹, v 1064 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.25 (2H, dd, $J_{\text{HH}} = 8.7$ Hz, $J_{\text{HF}} = 5.6$ Hz), 7.46 (2H, t, J = 7.8 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.23 (2H, d, J = 7.8 Hz), 7.21 (2H, t, $J_{\text{HH}} = J_{\text{HF}} = 8.7$ Hz); ¹³C NMR (100 MHz, CDCl₃) δ 166.2 (d, $J_{\text{CF}} = 255.4$ Hz), 164.3, 150.8, 132.8 (d, $J_{\text{CF}} = 9.7$ Hz), 129.6, 126.0, 125.8 (d, $J_{\text{CF}} = 2.8$ Hz), 121.7, 115.8 (d, $J_{\text{CF}} = 22.1$ Hz).

phenyl 4-cyanobenzoate (3f)

The title compound was prepared according to method A, in 55% yield.

Brown crystals, m.p. 165-166 °C; IR (CHCl₃): v 1728 (C=O) cm⁻¹, v 1070 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.34 (2H, d, J = 7.8 Hz), 7.85 (2H, d, J = 7.8 Hz), 7.48 (2H, t, J = 7.8 Hz), 7.33 (1H, t, J = 7.8 Hz), 7.24 (2H, d, J = 7.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 163.6, 150.5, 133.4, 132.4, 130.7, 129.7, 126.4, 121.5, 117.9, 117.0.

phenyl 4-methylbenzoate (3g)

The title compound was prepared according to method A, in 85% yield.

White crystals, m.p. 76-77 °C; IR (CHCl₃): v 1727 (C=O) cm⁻¹, v 1077 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.15 (2H, d, J = 8.1 Hz), 7.47 (2H, t, J = 7.8 Hz), 7.35 (2H, d, J = 8.1 Hz), 7.31 (1H, t, J = 7.8 Hz), 7.26 (2H, d, J = 7.8 Hz), 1.55 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 165.3, 151.1, 144.5, 130.3, 129.5, 129.3, 126.8, 125.8, 121.8, 21.8.

phenyl 2-naphthenate (3h)

The title compound was prepared according to method A, in 89% yield.

White crystals, m.p. 94-95 °C; IR (CHCl₃): v 1728 (C=O) cm⁻¹, v 1077 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.8 (1H, s), 8.24 (1H, d, *J* = 8.6 Hz), 8.04 (1H, d, *J* = 8.1 Hz), 7.98 (1H, d, *J* = 8.8 Hz), 7.95

(1H, d, *J* = 8.6 Hz), 7.64 (2H, m), 7.50 (2H, t, *J* = 7.4 Hz), 7.32 (3H, m); ¹³C NMR (100 MHz, CDCl₃) δ 165.4, 148.6, 133.8, 133.7, 131.5, 130.2, 129.6, 129.5, 128.6, 127.8, 127.7, 126.6, 125.8, 121.3, 118.7.

2-naphtyl benzoate (3i)

The title compound was prepared according to method A, in 83% yield.

White crystals, m.p. 108-109 °C; IR (CHCl₃): v 1734 (C=O) cm⁻¹, v 1051 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.33 (2H, d, J = 8.2 Hz), 7.96 (1H, d, J = 9.0 Hz), 7.91 (2H, m), 7.76 (1H, d, J = 2.3 Hz), 7.70 (1H, t, J = 7.5 Hz), 7.59 (2H, d, J = 7.9 Hz), 7.57-7.53 (2H, m), 7.43 (1H, dd, J_1 = 8.8 Hz, J_2 = 2.3 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 165.4, 151.1, 135.8, 132.5, 132.0, 129.6, 129.5, 128.7, 128.4, 127.9, 126.9, 126.8, 126.0, 125.5, 121.8.

4-methylphenyl 4-bromobenzoate (3j)

The title compound was prepared according to method A, in 65% yield.

white crystals, m.p. 118-119 °C; IR (CHCl₃): v 1727 (C=O) cm⁻¹, v 1077 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.08 (2H, d, J = 8.3 Hz), 7.67 (2H, d, J = 8.3 Hz), 7.25 (2H, d, J = 8.2 Hz), 7.10 (2H, d, J = 8.2 Hz), 2.40 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 164.7, 148.5, 135.7, 131.9, 131.7, 130.1, 128.7, 128.6, 121.3, 21.0.

4-chlorophenyl benzoate (3k)

The title compound was prepared according to method A, in 82% yield.

White crystals, m.p. 86-88 °C; IR (CHCl₃): v 1734 (C=O) cm⁻¹, v 1058 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.22 (2H, d, J = 8.0 Hz), 7.68 (1H, t, J = 7.4 Hz), 7.55 (2H, t, J = 7.6 Hz), 7.42 (2H, d, J = 8.8 Hz), 7.19 (2H, d, J = 8.7 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 165.0, 149.4, 133.8, 131.3, 130.2, 129.6, 129.2, 128.7, 123.1.

4-nitrophenyl benzoate (3l)

The title compound was prepared according to method A, in 88% yield.

Pale Yellow crystals, m.p. 129-130 °C; IR (CHCl₃): v 1741 (C=O) cm⁻¹, v 1058 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.36 (2H, d, J = 9.1 Hz), 8.23 (2H, d, J = 8.0 Hz), 7.71 (1H, t, J = 7.5 Hz), 7.57 (2H, t, J = 7.7 Hz), 7.45 (2H, d, J = 9.2 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.2, 155.7, 145.4, 134.3, 130.3, 128.8, 128.5, 125.3, 122.7.

2,4-dichlorophenyl benzoate (3m)

The title compound was prepared according to method A, in 51% yield.

White crystals, m.p. 91-92 °C; IR (CHCl₃): v 1740 (C=O) cm⁻¹, v 1050 (C-O) cm⁻¹, ¹H NMR (400 MHz, CDCl₃) δ 8.24 (2H, d, J = 7.8 Hz), 7.69 (1H, t, J = 7.4 Hz), 7.55 (2H, t, J = 7.7 Hz), 7.52 (1H, d, J = 2.4 Hz), 7.33 (1H, dd, J_I = 8.7 Hz, J_2 = 2.4 Hz), 7.25 (1H, d, J = 9.0 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.1, 146.0, 134.1, 132.0, 130.4, 130.2, 128.7, 128.5, 128.0, 124.7.

4-fluorophenyl benzoate (3n)

The title compound was prepared according to method A, in 86% yield.

White crystals, m.p. 55-56 °C; IR (CHCl₃): v 1734 (C=O) cm⁻¹, v 1050 (C-O) cm⁻¹, ¹H NMR (400 MHz, CDCl₃) δ 8.22 (2H, d, *J* = 7.6 Hz), 7.67 (1H, t, *J* = 7.4 Hz), 7.54 (2H, t, *J* = 7.7 Hz), 7.21 (2H, dd, *J*_{HH} = 9.1 Hz, *J*_{HF} = 4.6 Hz)), 7.14 (2H, t, *J*_{HH} = *J*_{HF} = 8.6 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 165.2, 160.3 (d, *J*_{CF} = 244.2 Hz), 146.8 (d, *J*_{CF} = 2.9 Hz), 133.8, 130.2, 129.3, 128.6, 123.1 (d, *J*_{CF} = 8.5 Hz), 116.2 (d, *J*_{CF} = 23.5 Hz).

4-bromophenyl benzoate (30)

The title compound was prepared according to method A, in 87% yield.

White crystals, m.p. 103-105 °C; IR (CHCl₃): v 1728 (C=O) cm⁻¹, v 1058 (C-O) cm⁻¹, ¹H NMR (400 MHz, CDCl₃) δ 8.22 (2H, d, J = 7.7 Hz), 7.68 (1H, t, J = 7.1 Hz), 7.57 (2H, d, J = 8.0 Hz), 7.54 (2H, t, J = 7.3 Hz), 7.14 (2H, d, J = 8.5 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.9, 150.0, 133.8, 132.6, 130.2, 129.2, 128.7, 123.6, 119.0.

4-(trifluoromethyl)-phenyl benzoate (3p)

The title compound was prepared according to method A, in 81% yield.

White solid, m.p. 107-108.5 °C; IR (CHCl₃): v 1734 (C=O) cm⁻¹, v 1058 (C-O) cm⁻¹, ¹H NMR (400 MHz, CDCl₃) δ 8.24 (2H, d, J = 7.4 Hz), 7.74 (2H, d, J = 8.4 Hz), 7.70 (1H, t, J = 7.4 Hz), 7.56 (2H, t, J = 7.7 Hz), 7.38 (2H, d, J = 8.4 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.7, 153.5, 134.0, 130.3, 129.0, 128.7, 128.0, 126.9 (q, J_{CF} = 3.7 Hz), 122.3.

phenyl 2-chlorobenzoate (3q)

The title compound was prepared according to method A, in 15% yield.

White crystals, IR (CHCl₃): v 1740 (C=O) cm⁻¹, v 1032 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.07 (1H, dd, $J_1 = 7.7$ Hz, $J_2 = 1.3$ Hz), 7.63-7.38 (5H, m), 7.32 (1H, J = 7.6 Hz), 7.27 (2H, J = 7.0 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.1, 150.7, 134.4, 133.2, 131.9, 131.4, 129.6, 129.4, 126.8, 126.1, 121.6.

4-cyanophenyl benzoate (3r)

The title compound was prepared according to method A, in 86% yield.

White crystals, m.p. 90-92 °C; IR (CHCl₃): v 1741 (C=O) cm⁻¹, v 1064 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.22 (2H, d, *J* = 8.0 Hz), 7.78 (2H, d, *J* = 8.4 Hz), 7.70 (1H, t, *J* = 6.9 Hz), 7.56 (2H, t, *J* = 7.6 Hz), 7.40 (2H, d, *J* = 8.4 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 164.3, 154.3, 134.2, 133.8, 130.3, 128.8, 128.6, 123.0, 118.3, 109.8.

4-fluorophenyl cyclohexanecarboxylate (3s)

The title compound was prepared according to method A, in 32% yield.

White crystals, m.p. 195-196 °C; IR (CHCl₃): v 1753 (C=O) cm⁻¹, v 1121 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.10-7.02 (4H, m), 2.57 (1H, tt, $J_1 = 11.2$ Hz, $J_2 = 3.6$ Hz), 2.07 (2H, d, J = 11.0 Hz), 1.87-1.81 (2H, m), 1.74-1.70 (1H, m), 1.65-1.55 (2H, m), 1.43-1.28 (3H, m); ¹³C NMR (100 MHz,

CDCl₃) δ 174.6, 160.1 (d, J_{CF} = 242.5 Hz), 146.7 (d, J_{CF} = 2.8 Hz), 122.9 (d, J_{CF} = 8.5 Hz), 116.0 (d, J_{CF} = 23.3 Hz), 43.1, 28.9, 25.7, 25.4.

Phenyl cynnamate (3t)

The title compound was prepared according to method A, in 46% yield, or method B, in 89% yield. White crystals, m.p. 74.5-75.5 °C; IR (CHCl₃): v 1728 (C=O) cm⁻¹, v 1638 (C=C) cm⁻¹, v 1140 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.92 (1H, d, *J* = 16.0 Hz), 7.62 (2H, m), 7.47-7.43 (5H, m), 7.29 (1H, t, *J* = 7.6 Hz), 7.21 (2H, d, *J* = 8.0 Hz), 6.68 (1H, d, *J* = 16.0 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 165.5, 150.8, 146.6, 134.2, 130.7, 129.5, 129.0, 128.3, 125.8, 121.7, 117.3.

Phenyl 4-methoxycynnamate (3u)

The title compound was prepared according to method B, in 55% yield.

White crystals, m.p. 74-75 °C; IR (CHCl₃): v 1721 (C=O) cm⁻¹, v 1600 (C=C) cm⁻¹, v 1140 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.76 (1H, d, J = 15.9 Hz), 7.48 (2H, d, J = 8.8 Hz), 7.34 (2H, t, J = 7.9 Hz), 7.18 (2H, t, J = 7.4 Hz), 7.10 (2H, d, J = 7.5 Hz), 6.87 (2H, d, J = 8.8 Hz), 6.43 (1H, d, J = 15.9 Hz), 3.79 (3H, s). ¹³C NMR (100 MHz, CDCl₃) δ 165.9, 161.8, 151.0, 146.4, 130.2, 129.6, 127.0, 125.8, 121.8, 114.8, 114.6, 55.6.

4-Bromophenyl cynnamate (3v)

The title compound was prepared according to method B, in 87% yield.

Colorless solid, m.p. 104-105.5 °C; IR (CHCl₃): v 1734 (C=O) cm⁻¹, v 1593 (C=C) cm⁻¹, v 1141 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ ¹H NMR (400 MHz, CDCl₃) δ 7.86 (1H, d, *J* = 16 Hz), 7.57-7.62 (2H, m), 7.43 (2H, d, J= 8.8 Hz), 7.25 – 7.38 (3H m), 7.06 (2H, d, J = 8.9 Hz), 6.60 (1H, d, *J* = 16.0 Hz); ¹³C NMR (100 MHz, CDCl₃), δ (ppm): 117.1, 119.1, 123.7, 128.6, 129.3, 131.1, 132.7, 134.3, 147.3,150.1, 165.3.

4-Chlorophenyl cynnamate (3w)

The title compound was prepared according to method B, in 73% yield.

White crystals, m.p. 99.5-101 °C; IR (CHCl₃): v 1741 (C=O) cm⁻¹, v 1632 (C=C) cm⁻¹, v 1134 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ ¹H NMR (400 MHz, CDCl₃) δ 7.87 (1H, d, *J* = 16.0 Hz), 7.64 – 7.55 (2H m), 7.48 – 7.40 (3H, m), 7.37 (2H, d, *J* = 8.8 Hz), 7.13 (2H, d, *J* = 8.8 Hz), 6.62 (1H, d, *J* = 16.0 Hz). ¹³C NMR (100 MHz, CDCl₃) δ 165.3, 149.4, 147.2, 134.2, 131.3, 131.0, 129.6, 129.2, 128.5, 123.2, 117.0.

4-Chlorophenyl 4-methoxycynnamate (3x)

The title compound was prepared according to method B, in 71% yield.

White crystals, m.p. 99-100 °C; IR (CHCl₃): v 1728 (C=O) cm⁻¹, v 1600 (C=C) cm⁻¹, v 1141 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.83 (1H, d, J = 15.9 Hz), 7.54 (2H, d, J = 8.2 Hz), 7.36 (2H, d, J = 8.2 Hz), 7.11 (2H, d, J = 8.2 Hz), 6.94 (2H, d, J = 8.2 Hz), 6.48 (1H, d, J = 15.9 Hz), 3.86 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 165.6, 162.0, 149.5, 146.8, 131.1, 130.2, 129.6, 126.9, 123.2, 114.6, 114.3, 55.6.

4-Fluorophenyl cynnamate (3y)

The title compound was prepared according to method B, in 90% yield.

White crystals, m.p. 73-74.5 °C; IR (CHCl₃): v 1728 (C=O) cm⁻¹, v 1638 (C=C) cm⁻¹, v 1153 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.87 (1H, d, *J* = 16.0 Hz), 7.63-7.56 (2H, m), 7.47-7.38 (3H, m), 7.18-7.05 (4H, m), 6.62 (1H, d, *J* = 16.0 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 165.6, 160.4 (d, *J*_{CF} = 244.2 Hz), 147.0, 146.7 (d, *J*_{CF} = 2.9 Hz), 134.2, 131.0, 129.2, 128.5, 123.2 (d, *J*_{CF} = 8.5 Hz), 117.1, 116.2 (d, *J*_{CF} = 23.4 Hz).

3-Methylphenyl cynnamate (3z)

The title compound was prepared according to method B, in 84% yield.

Yellow crystals, m.p. 53.5-55 °C; IR (CHCl₃): v 1728 (C=O) cm⁻¹, v 1632 (C=C) cm⁻¹, v 1150 (C-O) cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.80 (1H, d, J = 16.0 Hz), 7.57 – 7.46 (2H, m), 7.40 – 7.33 (3H, m), 7.22 (1H, t, J = 7.8 Hz), 7.00 (1H, d, J = 7.5 Hz), 6.95-6.86 (2H, m), 6.56 (1H, d, J = 16.0 Hz), 2.31 (3H, s). ¹³C NMR (100 MHz, CDCl₃) δ 165.7, 150.8, 146.6, 139.8, 134.3, 130.8, 129.3, 129.1, 128.4, 126.8, 122.4, 118.7, 117.5, 21.5.

Computational details

All calculations were performed using the GAUSSIAN 03 software package,¹⁴ and the PBE1PBE functional, without symmetry constraints. That functional uses a hybrid generalized gradient approximation (GGA), including 25 % mixture of Hartree-Fock¹⁵ exchange with DFT¹⁶ exchange-correlation, given by Perdew, Burke and Ernzerhof functional (PBE).¹⁷ The optimized geometries were obtained with a standard 6-31G(d,p) basis set.¹⁸ Frequency calculations were performed confirming the stationary points as minima. The energy values reported result from single point calculations using a standard 6-311++G(d,p) basis set.¹⁹ and the geometries optimized at the PBE1PBE/6-31G(d,p) level. Solvent (1,4-dioxane) effects were considered in the PBE1PBE/6-311++G(d,p)//PBE1PBE/6-31G(d,p)

¹⁴ Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.

¹⁵ Hehre, W. J.; Radom, L.; Schleyer, P. v.R.; Pople, J. A. Ab Initio Molecular Orbital Theory, John Wiley & Sons, NY, 1986.

¹⁶ Parr, R. G.; Yang, W. in Density Functional Theory of Atoms and Molecules; Oxford University Press: New York, 1989.

¹⁷ (a) Perdew, J. P.; Burke, K.; Ernzerhof, M. Phys. Rev. Lett. 1997, 78, 1396. (b) Perdew, J. P. Phys. Rev. B 1986, 33, 8822.

 ¹⁸ (a) Ditchfield, R.; Hehre W. J.; Pople, J. A. J. Chem. Phys. 1971, 54, 724. (b) Hehre, W. J.; Ditchfield R.; Pople, J. A. J. Chem. Phys. 1972, 56, 2257. (c) Hariharan, P. C.; Pople, J. A. Mol. Phys. 1974, 27, 209. (d) Gordon, M. S. Chem. Phys. Lett. 1980, 76, 163. (e) Hariharan, P. C.; Pople, J. A. Theor. Chim. Acta 1973, 28, 213.

 ¹⁹ (a) McClean, A. D.; Chandler, G. S. J. Chem. Phys. **1980**, 72, 5639. (b) Krishnan, R.; Binkley, J. S.; Seeger, R. Pople, J. A. J. Chem. Phys. **1980**, 72, 650. (c) Wachters, A. J. H. J. Chem. Phys. **1970**, 52, 1033. (d) Hay, P. J. J. Chem. Phys. **1977**, 66, 4377. (e) Raghavachari, K.; Trucks, G. W. J. Chem. Phys. **1989**, 91, 1062. (f) Binning Jr., R. C.; Curtiss, L. A. J. Comp. Chem., **1990**, 11, 1206. (g) McGrath, M. P.; Radom, L. J. Chem. Phys. **1991**, 94, 511. (h) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. v. R. J. Comp. Chem. **1983**, 4, 294. (i) Frisch, M. J.; Pople, J. A.; Binkley, J. S. J. Chem. Phys. **1984**, 80, 3265.

energy calculations using the Polarizable Continuum Model (PCM) initially devised by Tomasi and coworkers²⁰ as implemented on Gaussian 03.²¹ The molecular cavity was based on the united atom topological model applied on UAHF radii, optimized for the HF/6-31G(d) level. The parameters used for 1,4-dioxane were: $\varepsilon = 2.2094$, $\varepsilon_{\infty} = 2.0232$, r = 2.53 Å, $\rho = 1.0337$.



Figure S1. Energy balance (kcal/mol, italics) calculated for the catalytic cycles with NHC from precursors 4 (top left), 5 (top right), 8 (bottom left) and 9 (bottom right).

²⁰ (a) Cancès, M. T.; Mennucci, B.; Tomasi, J. J. Chem. Phys. **1997**, 107, 3032. (b) Cossi, M.; Barone, V.; Mennucci, B.; Tomasi, J. Chem. Phys. Lett. **1998**, 286, 253. (c) Mennucci B.; Tomasi, J. J. Chem. Phys. **1997**, 106, 5151.

 ²¹ (a) Tomasi, J.; Mennucci, B.; Cammi, R. Chem. Rev. 2005, 105, 2999. (b) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V. J. Chem. Phys. 2002, 117, 43.



- 500

400

300

- 200

L-100

0

- 100

Appendix A - Spectra

- 1100

- 1000

- 900

.800

- 700

009.















S

ß

40

40

33

98

22



Ę

-20

-10

φ







Appendix A - Spectra





R ង់ 무 ĥ 2 មុ φ ស្រ ស៊ ŧł. 4 Ŕ Ŗ Ŕ 8 տ P IN A REAL PROPERTY. 멹 8 В 4 ន 9 2 22'92n SE'LL 8 00 f1 (ppm) B 110 120 29'121---29 121 80'921 29'121 29'121 29'121 29'121 29'121 29'121 29'121 130 ₽<u></u>___ 140 Appendix A - Spectra 'n 5 92.051-0...= 09172040RSR22B RSR22**B** Ń 160 `œॅ≌ 170
















































Appendix A - Spectra







-8000 -7500 -7000 -6000 -1000 -6500 -5500 5000 -4500 4000 -3500 3000 -2500 -2000 -1500 -200 9 dial a in he has no been a start with the start is a start in the start and a start and a start is a start in the start as a start in the start is a start in the 9 8 a second seco Θ 40 90'67ß and the second state of the ball of the second s 99 20 \$8.92-91 22 84'22-8 90 f1 (ppm) 10 110 120 SZ' 821-LL 821-62' 621 89' 621 62' 021 130 19.151-0° 140 4 150 ES'6#1ò 240640JR130A 24062010JR130A 7 0..= 160



009-20 -450 -400 900--200 -150 -100 -550 -350 -250 22 ធុ 9 7.35 mont 7.40 54'2 94'2-94'2-94'2-94'2-54'2 5-54'2-54'2-54'2-54'2 7,45 -112 7.50 7,55 55'2-25'2-65'2--20'2 7,60 7.65 7.70 69'2~ 122-222~ -00'T 7.75 7,80 7.85 7.95 7.90 f1 (ppm) 8.00 8.05

Appendix A - Spectra

10<u></u> 22'8 // 8'54 8'54 11 200410RSR17 % ក្ល ក្ល អូ អ្ 200410 RSR 17% % % % % % 0.0 0.0= 1

8.10

8.15

8.20

8.25

8,30

8.35

8,40

8.45

-10'Z

-00'Z

-5500 -5000 -4500 -3000 -2500 -1000 -4000 -3500 -2000 -1500 500 9 9 20 贸 4 ß 99 2 \$8.927 84.77 8 90 f1 (ppm) - 8 110 120 82 221 25' 521 99' 821 25' 20 25' 10 130 140 45' SP I ò 150 0542010R0917 0.0= 160



165



05142010RSRA7 RSR17 0.

0.0=

Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is © The Royal Society of Chemistry 2011





Appendix A - Spectra















-30000 -25000 -20000 -15000-10000 -5000 9 0 9 20 8 6 8 Man Line 99 2 \$\$'92 91'22 \$\$'48) f1 (ppm) 6 10 110 11.011-120 29' EZI — 92'821 92'621 99'33 99'33 7133'66 130 140 11 Ö 150 80'051-0.0= 2805401137c JR132c 160 NAMES OF TAXABLE PARTY. Ē 170







-550

20

-400

-350

-300

-450



-200

-250

-150

-100

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P

8

2.0





-1100



Appendix A - Spectra



-1100 -1000 008--200 -100 06-700 -60 -500 -400 90e-9 -9 Land Andrews and a fait before the 20 8 And Mail 6 3 99 20 \$8'9Z~ 91'22 87'22 8 90 f1 (ppm) 10 110 120 156 54 156 54 156 24 152 85 152 10 01.751 01.751 02.151 130 and the second second in the second \mathbf{c} 140 1191 Ò « 150 62 0ST-⊡**≌** 0.0= 150910R\$R31A 11 160 RSR 1A




























- 1300 1200 - 1100 1000 -400 - 100 906 800 700 600 500 300 200 0-2.0 2.4 2.8 3.2 3.6 3.16 4.0 4.4 4.8 f1 (ppm) 5.2 5.6 6.0 <u>_</u> 🗠 4= 6.4 22.9 84.9 2 **1**860 ~ 6.8 0111128417896441 318209577777556595 318209577777556595 °0 7.0 0₽ Appendix A - Spectra 7.2][1.93 2.02 2.02 2.02 2.02 7.4 7.6 7.8 ┝ 1.900



Appendix A - Spectra

Appendix A - Spectra







-450 99.99 ----78.97 -87.*TT -*\ f1 (ppm) ۲۵.411 ۲۹.78 - 151 83 - 152 83 - 152 02 - 153 02 - 130 18 _ ---_____ Ŵ Lt[.]97L ----10.131 **8111병**R209 JR월09년 | | °5 °H °H °H

۲<u>۲</u>, ۶۲ ۲۱۹, ۶۶ 121.83 £8[.]521 — 50.721 ----f1 (ppm) 146.41 10.121 ----ю<mark>е</mark> 58'191 — **珠**209 JR 209 近



°5°−å0



- 150

0_

2.0



-40 - 20 0-لمرج الشاليل علما اللامة للم فرودان المتعادلة للمتعالك والمحالي المتعادل والمتعادلة والمعالمات للتلا . 1.4 ما 11 ما 14 \$8.97 -84.77 f1 (ppm) 86.911 123.17 05'821 81'621 91'52' 20'121 7 7 7 7 7 91'421 <u>ö</u> `0₽ 145.39 145.39 O**⊨**= 190181JR205II JR 20511

Appendix A - Spectra



Appendix A - Spectra

280

- 1100 1000 006 500 400 300 200 100 800 700 009 0 2.0 2.4 2.8 3.2 3.6 3.02 98.6 ----Ϊ 4.0 4.4 5.2 4.8 f1 (ppm) 5.6 6.0 ū₽ 6.4 9†[.]9 ~ - 6 -26.0 <u>//</u> 6.8 ١ 2.00-1 7.2 7.0 °0₽ 0₽= Appendix A - Spectra 2.05 7.4 # Ń -90[.]2 7.6 01232011JR 2313 7.8 -00.r °5^{−30} 8.2



⊢ 1500 1400 1300 1200 1100 1000 - 100 906 800 700 009 500 400 300 200 0 structure in the production of the sector is a sector of the sector of the sector of the sector of the sector of 30 40 50 NAM NUMBER <u> 75.85 –</u> _ 60 70 **⊅**8`9L ¬ 87.*TT* -/ and a second 80 90 100 f1 (ppm) 110 ×114.30 120 12.21 -°⊒ - 133 31 - 159.60 - 130.22 - 130.22 130 _//° // 140 `r 0₽= 98.94r -146[.]50 150 Ń 012320119R213 JR21쐁 - 161 - - - -160 °5°−3° 170

⊢ 1500 1400 1300 1200 - 1100 1000 - 100 906 800 700 009 500 400 300 200 0 author (M **WWW** 114 - 114[.]30 _ _ 118 Authors in the particular 122 123.21 -126 structure in the second of the second proceed by the second of the second of the structure - 156.90 ___ — 156'26 — 130'52 — 131'14 130 ___ _ 134 138 142 f1 (ppm) 146 97. 146.85 _ 09[.]671 — 150 ū≈ ო 154 1 °05 158 0₽= // 162 86.161 -Ĥ 01232011J**R**213 JR213 ទ្រ 166 ္ကိုင္ငံုခဲ့၀

Appendix A - Spectra

650 600 -450 400 - 150 550 500 350 300 250 200 100 50 0 6.5 6.6 09.9 --66'0 79.9 — 6.7 20'2 60'2 11'2 11'2 21'2 51'2 51'2 51'2 51'2 91'2 -62.4 \langle 92.7 ----7.4 2743 472 5772 2743 -+0.5 7.5 5 85'2 65'2 09'2 19'2 7.6 -20.2 шç 7.7 <u>/</u>/ 7.8 °0¢ Appendix A - Spectra 0 == 58°Z -----00.1 12282010JR204 JR204 7.9 8.0

6.8 6.9 7.0 7.1 7.3 7.2 f1 (ppm)

₩92 91.77 84.77 84.77 21.911 25.911 80.711 173'13 шę S 146.70 146.73 147.02 Ĩ\, `0₽ \parallel -

Appendix A - Spectra

-450

f1 (ppm)



Appendix A - Spectra









Atomic coordinates of all optimised species

O_2				С	-0.392897	-2.485753	1.947649
0	0.000000	0.000000	0.003688	С	-0.096506	-3.759755	2.437939
0	0 000000	0 000000	1 206312	C	0 336372	-4 767038	1 590514
0	0.000000	0.000000	1.200512	G	0.330372	1.707030	0.004504
				C	0.482889	-4.50/318	0.234504
OH⁻				C	0.195261	-3.254251	-0.312705
0	0.000000	0.00000	-0.023270	С	0.074448	2.607459	-2.311090
н	0.00000	0.00000	0.953270	С	0.492036	3.869698	-2.739667
	0.000000	0.000000	0.935270	c	0 702005	1 969669	1 007750
				C	0.793095	4.000009	-1.02//32
C ₆ H ₅ C	СНО			C	0.684810	4.611975	-0.467597
С	-0.300098	1.015370	-0.268429	С	0.267064	3.370342	0.018698
C	0 237798	-0 225974	0 063181	С	0.228896	3,194055	1.529686
a	0.237790	1 200102	0.000101	c	0.210045	1 524700	2 242442
C	-0.599108	-1.306163	0.349629	C	-0.219043	1.554780	-3.343442
С	-1.976022	-1.145749	0.304658	C	-0.834316	-1.405307	2.917637
С	-2.520627	0.099023	-0.027841	C	0.432389	-3.077745	-1.805480
С	-1.680327	1.176973	-0.313735	С	-2.165201	-1.759934	3.586024
Ċ	2 005525	0 276726	0 077247	C	0 251/3/	-1 120440	3 958772
C	-3.905525	0.2/0/30	-0.077347	c	1 0.231434	-1.120440	5.550772
0	-4.791911	-0.597121	0.154786	C	1.700154	-2.260872	-2.081660
Η	0.355953	1.851714	-0.490305	C	-0.771322	-2.558205	-2.595130
Н	1.316016	-0.354270	0.099032	С	-1.112864	2.721406	2.093960
U	0 170791	2 270240	0 607229	C	1 397995	2 336116	2 027513
11	-0.170781	-2.270349	0.007238	G	1 415400	1 010200	4 000054
н	-2.656006	-1.964240	0.521774	C	-1.415429	1.912362	-4.220854
Η	-2.114699	2.140792	-0.571231	C	1.016918	1.228205	-4.193385
Η	-4.317566	1.303258	-0.351409	Н	-2.641194	1.435198	-0.792907
				н	-2 752982	-1 226056	-0 017820
спо) -			11	0.000406	2.057200	2 501001
C ₆ H ₅ C	J			п	-0.203496	-3.95/360	3.501001
0	2.495195	-0.279957	-0.747900	Н	0.563421	-5.753854	1.983874
С	1.287250	-0.153154	-0.410298	H	0.829721	-5.295697	-0.428725
C	0 451816	0 948137	-0 838637	н	0.585599	4.065458	-3.804426
c	0.451010	1.000001	0.050057	11	1 110007	F 04C400	2 172400
C	-0.8/4418	1.0//984	-0.461842	п	1.110207	5.040499	-2.1/3499
С	-1.500943	0.139874	0.368876	Н	0.929514	5.393512	0.247274
С	-0.731781	-0.944845	0.809313	Н	0.383171	4.203887	1.932944
С	0.595926	-1.093959	0.444736	Н	-0.476051	0.616023	-2.810155
U	0 017006	1 600705	1 495790	н	-0 984448	-0 483422	2 350021
п	0.91/990	1.090705	-1.485780	11	0.001110	0.400422	2.330021
Н	-1.446363	1.936208	-0.823125	н	0.620722	-4.092437	-2.181230
Η	-2.543341	0.249299	0.659863	H	-2.488604	-0.950700	4.249177
Н	-1.190437	-1.694768	1,458520	Н	-2.952755	-1.926145	2.844277
ч	1 17/099	-1 946603	0 800171	н	-2 080062	-2 670264	4 189442
11	1.1/4000	-1.940003	0.0001/1	11	0.050000	0.007665	4 (12150
				п	-0.056009	-0.29/665	4.013139
C ₆ H ₅ C	COOC ₆ H ₅			Н	1.192057	-0.839896	3.476715
С	4.582130	0.289684	0.633741	Н	0.442890	-1.994025	4.591362
Ċ	5 250038	-0 920931	0 462847	н	1.871388	-2.181139	-3.161297
c	1.5200005	0.920951	0.402047	л. Ц	2 574476	2 7/2006	1 624071
C	4.539895	-2.0/1059	0.123298	п	2.5/44/0	-2.743090	-1.034071
С	3.162970	-2.010565	-0.044282	Н	1.622195	-1.255734	-1.654477
С	2.490675	-0.797371	0.126089	Н	-0.566904	-2.640745	-3.668052
C	3 203947	0 355585	0 465822	Н	-1.670898	-3.144599	-2.380466
a	1 010700	0.001567	0.405022	 ц	0 002050	1 511104	2 270567
C	1.018/68	-0.801567	-0.064161	п	-0.993030	-1.511104	-2.3/950/
0	0.496351	0.441956	0.106097	Н	-1.940270	3.332459	1.718317
0	0.366685	-1.779292	-0.337883	Н	-1.325622	1.678957	1.849365
С	-0.865848	0.663705	-0.026347	Н	-1.100643	2.810008	3.185637
c	1 227110	1 007202	0 720012	н	1 371190	2 258127	3 120421
C	-1.22/110	1.00/393	-0.729012	11	2.371190	2.200127	1 740011
C	-2.571989	2.143421	-0.840680	н	2.354358	2.105968	1./42811
С	-3.545036	1.338965	-0.254331	Н	1.362513	1.331183	1.594233
С	-3.165294	0.198451	0.448285	H	-1.635273	1.111010	-4.934163
C	-1.823532	-0.148851	0.572340	Н	-2.313023	2.086418	-3.619179
	E 127202	1 10/555	0.000000	 U	-1 218520	2 824202	-4 795160
н	5.137283	1.184555	0.898666	11	-1.210520	2.024205	-4.755102
Ĥ	6.327307	-0.968097	0.594587	Н	U.804103	0.410345	-4.890107
Η	5.061503	-3.014057	-0.009848	H	1.860601	0.930344	-3.564667
Н	2.584220	-2.890133	-0.307385	Н	1.326006	2.096132	-4.785856
л. Ц	2 674715	1 202702	0 506972				
11	2.0/4/13	1.292795	0.550075	CID. (from mroourcor F)		
н	-0.449913	2.418347	-1.176591	SIFF (nom precursor 5)		
Η	-2.857283	3.036398	-1.388795	C	-1.919422	0.816254	-0.167970
Н	-4.595169	1.599639	-0.343644	С	-1.994118	-0.593199	0.414049
н	-3,919670	-0.432523	0.908909	Ν	-0.565536	-0.955287	0.504779
11 TT	1 525205	1 020202	1 110004		0 280760	0 070040	0 217000
н	-1.525285	-1.039322	1.110634	L	0.200/00	0.0/2240	0.31/923
				N	-0.484311	1.128707	-0.009556
UIPr	(from precursor 4)			C	0.014396	2.402804	-0.424489
C	-1.861224	0.739499	-0.524521	С	-0.190619	-2.246671	0.991066
ĉ	_1 016040	-0 556330	_0 1/0105	C	-0 249160	-2 491248	2 376494
C	-1.910049	-0.556520	-0.142133		0.249100	2.771270	2.3/0404
N	-0.601110	-0.949544	0.074156	C	0.040134	-3.//4629	2.846055
С	0.301673	0.055757	-0.140214	C	0.389983	-4.792114	1.972848
Ν	-0.516687	1.089064	-0.506329	С	0.469980	-4.528069	0.612219
C	-0 042864	2 376116	-0 929378	С	0.184794	-3.264216	0.089414
c	-0.042004	2.3/0140	-0.929370	C	0 01 5000	2.201210	_1 700201
C	-U.25U/51	-2.250548	0.569006	C	0.213200	2.000004	- + • • 20201

C	0 625347	3 906542	-2 211918	н	1 020807	3 706975
c	0.025547	4 0100042	1 202706	11 U	1 2620007	1 000670
C	0.645526	4.919694	-1.292/96	н	1.203023	1.990070
C	0.6/23/0	4.664689	0.060869	H	-0.366487	2.633079
C	0.257180	3.414823	0.527337	Н	0.106365	1.874620
C	0.174733	3.232194	2.035350	Н	-1.218641	1.343687
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Ċ	-1 8/8528	-1 714711	1 170961	ц	-2 387738	1 369747
c	0 606600	1 1/2520	4.216920	и Ц	-2 514863	-1 235962
C	0.606608	-1.143526	4.316630	н	-2.514803	-1.235962
C	1.647448	-2.268317	-1.702206	Н	-0.022245	-4.045400
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п	-2.541450	1.556546	0.300039	н	1.526124	-1.9/200/
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Н	-0.002694	-3.972504	3.913935	Н	1.920026	-6.548066
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и 11	-0.255204	0 631835	-2 319460	SIMes	(from precursor 9)	
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~	U./30/91	J.023900	1 (50000	н 	0.777300	- 1.000094
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-	-0.704306	-1.842224	4.182527
Η	-1.832741	-1.297275	2.935275
Ŧ	-2 387738	1 369747	-0 666304
-	2.507750	1.005060	0.000304
1	-2.514863	-1.235962	0.2/8206
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7	1.041711	-6.138779	2.348989
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Η	1.284051	-3.673031	-1.980602
Ŧ	1 528124	-1 972687	-1 508537
	1.520124	1.572007	1.500557
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Ŧ	0 214799	-6 840052	2 184595
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1	1.24/066	-6.122613	3.4229/3
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	-0.239175 -0.548753 0.801258	-4.617282 -3.331956 2.582286	-0.024405 -0.474205 -1.817330
	-0.239175 -0.548753 0.801258	-4.617282 -3.331956 2.582286	-0.024405 -0.474205 -1.817330 -2.096336
	-0.239175 -0.548753 0.801258 1.327444	-4.617282 -3.331956 2.582286 3.841416	-0.024405 -0.474205 -1.817330 -2.096336
	-0.239175 -0.548753 0.801258 1.327444 1.059818	-4.617282 -3.331956 2.582286 3.841416 4.950869	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512
() () () () () ()	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536
(1) (1) (1) (1) (1) (1) (1) (1) (1) (1)	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536
() () () () () () () ()	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401
() () () () () () () ()	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476
בו בו בו בו בו בו בו בו	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326
() () () () () () () () () ()	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 2.102528	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.8522874
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846
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	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538 1.753929 0.200704	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538 1.753929 0.200704 1.611765	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538 1.753929 0.200704 1.611765	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146 -2.131622
0000000000000000000000	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538 1.753929 0.200704 1.611765 0.601139	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567 -1.654109	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146 -2.131622 3.639618
000000000000000000000000000000000000000	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538 1.753929 0.200704 1.611765 0.601139 -0.686053	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567 -1.654109 -0.761701	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146 -2.131622 3.639618 2.812760
	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.961556 -2.192538 1.753929 0.200704 1.611765 0.601139 -0.686053 -2.57101	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567 -1.654109 -0.761701 1.603853	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146 -2.131622 3.639618 2.812760
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H H H H H H H H H H H H H H H H H H H	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538 1.753929 0.200704 1.611765 0.601139 -0.686053 -2.657101 -2.213956 0.742111 0.581573 -0.353882 1.964882 1.614795 0.053636 0.972491 -0.657832 -0.655951 -2.111781 0.171966	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567 -1.654109 -0.761701 1.603853 0.983293 -3.921004 -6.239403 -5.453975 3.959047 6.303991 5.615305 -0.588336 -3.924123 -2.168021 -3.116348 -7.000094	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146 -2.131622 3.639618 2.812760 -0.122474 -1.723323 3.132813 1.724769 -0.710862 -2.970566 -1.639834 0.483352 2.258995 -2.536058 -2.281553 -1.957667 1.054793
	$\begin{array}{c} -0.239175\\ -0.548753\\ 0.801258\\ 1.327444\\ 1.059818\\ 0.255798\\ -0.286537\\ -1.120116\\ 1.113777\\ 0.253230\\ -1.016758\\ -0.869705\\ -0.961556\\ -2.192538\\ 1.753929\\ 0.200704\\ 1.611765\\ 0.601139\\ -0.686053\\ -2.657101\\ -2.213956\\ 0.742111\\ 0.581573\\ -0.353882\\ 1.964882\\ 1.614795\\ 0.053636\\ 0.972491\\ -0.657832\\ -0.655951\\ -2.111781\\ 0.171966\\ 0.202625\end{array}$	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567 -1.654109 -0.761701 1.603853 0.983293 -3.921004 -6.303991 5.615305 -0.588336 -3.924123 -2.168021 -3.116348 -7.000094 -6.436746	-0.024405 -0.474205 -1.817330 -2.096336 -1.292512 -0.170536 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.81846 -3.535034 -3.120146 -2.131622 3.639618 2.812760 -0.122474 -1.723323 3.132813 1.724769 -0.710862 -2.970566 -1.639834 0.483352 2.258995 -2.536058 -2.281553 -1.957667 1.054793 2.732555
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C C C C C C C C C C C F F F F F F F F F	-0.239175 -0.548753 0.801258 1.327444 1.059818 0.255798 -0.286537 -1.120116 1.113777 0.253230 -1.016758 -0.869705 -0.961556 -2.192538 1.753929 0.200704 1.611765 0.601139 -0.686053 -2.657101 -2.213956 0.742111 0.581573 -0.353882 1.964882 1.614795 0.053636 0.972491 -0.657832 -0.655951 -2.111781 0.171966 0.202625 1.668686	-4.617282 -3.331956 2.582286 3.841416 4.950869 4.769087 3.524362 3.366938 1.410220 -1.306906 -3.121666 4.136946 2.386547 3.462303 1.711967 0.969915 0.620567 -1.654109 -0.761701 1.603853 0.983293 -3.921004 -6.239403 -5.453975 3.959047 6.303991 5.615305 -0.588336 -3.924123 -2.168021 -3.116348 -7.000094 -6.436746 -6.377695	-0.024405 -0.474205 -1.817330 -2.096336 0.159636 0.154401 1.394476 -2.702326 2.663515 -1.886258 2.128874 1.852287 1.181846 -3.535034 -3.120146 -2.131622 3.639618 2.812760 -0.122474 -1.723323 3.132813 1.724769 -0.710862 -2.970566 -1.639834 0.483352 2.258995 -2.536058 -2.281553 -1.957667 1.054793 2.732555 1.756098
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