

Supporting Information

File 1. Spectral data of products

Diethyl-2,6-dimethyl-4-phenyl-1,4-dihydropyridin-3,5-dicarboxylate (1)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3329, 1721, 1488.

^1H NMR (400 MHz; CDCl_3 ; Me_4Si): δ 1.21-1.25 (t, 6H, 2x $-\text{CH}_2\text{CH}_3$), 2.31 (s, 6H, 2x $-\text{CH}_3$), 4.06-4.15 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 5.00 (s, 1H, C-4H), 5.68 (bs, 1H, $-\text{NH}$), 7.14-7.32 (m, 5H, Ar-H).

^{13}C NMR (100 MHz; CDCl_3 ; Me_4Si): δ 14.29, 19.62, 39.63, 60.58, 104.20, 127.83, 128.02, 128.37, 143.82, 147.75, 167.74.

MS (ESI): 352 (M+1).

Diethyl-4-(4-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (2)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3332, 1708, 1340.

^1H NMR (400 MHz; CDCl_3 ; Me_4Si): δ 1.24-1.29 (t, 6H, 2x $-\text{CH}_2\text{CH}_3$), 2.30 (s, 6H, 2x $-\text{CH}_3$), 4.03-4.10 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 4.94 (s, 1H, C-4H), 5.63 (bs, 1H, $-\text{NH}$), 7.42-7.44 (d, 2H, Ar-H), 8.01-8.05 (d, 2H, Ar-H).

^{13}C NMR (100 MHz; CDCl_3 ; Me_4Si): δ 14.29, 19.70, 39.22, 59.64, 103.61, 122.72, 126.30, 144.92, 146.34, 150.60, 167.47.

MS (ESI): 375 (M+1).

Diethyl-4-(2-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (3)

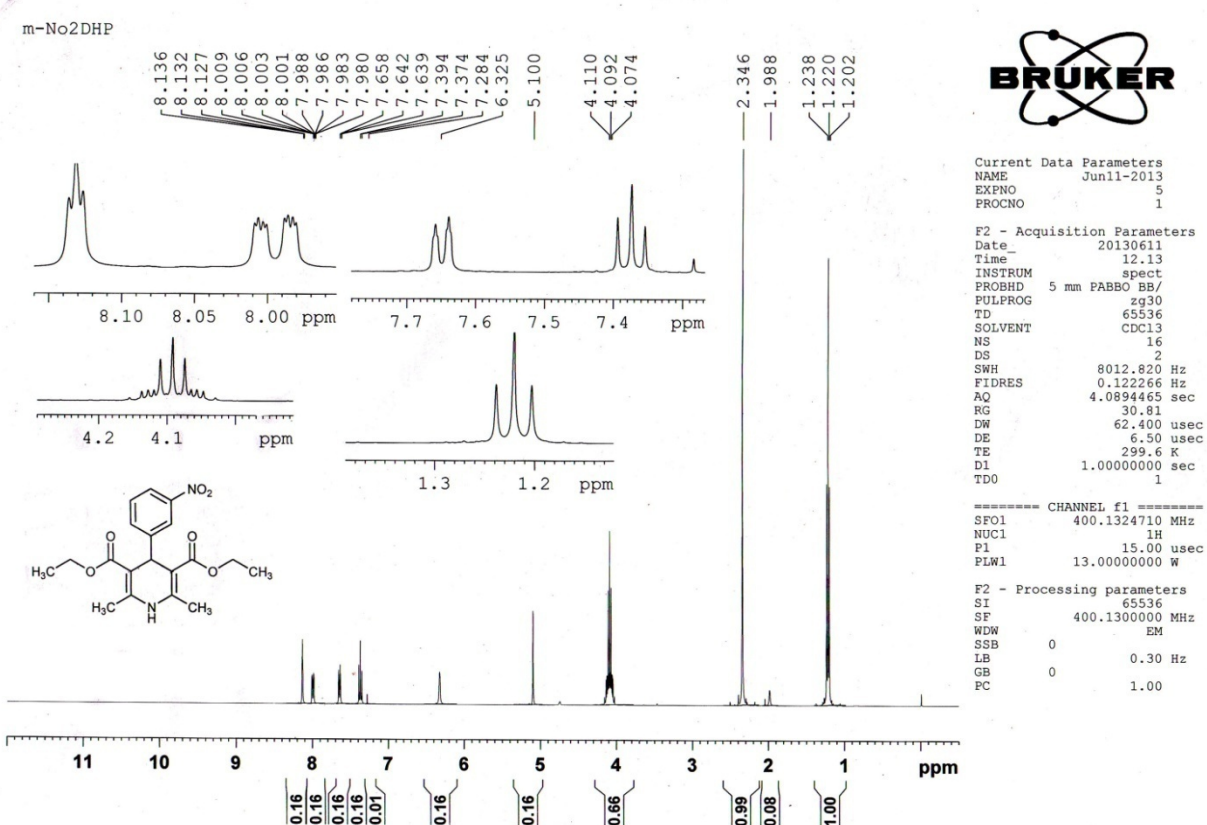
IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3369, 1754, 1431.

^1H NMR (400 MHz; CDCl_3 ; Me_4Si): δ 1.21 (t, 6H, 2x $-\text{CH}_2\text{CH}_3$), 2.35 (s, 6H, 2x $-\text{CH}_3$), 4.11 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 4.82 (s, 1H, C-4H), 5.57 (bs, 1H, $-\text{NH}$), 7.34-8.15 (m, 4H, Ar-H).

^{13}C NMR (100 MHz; CDCl_3 ; Me_4Si): δ 14.20, 19.85, 35.16, 60.70, 102.25, 121.13, 126.17, 129.60, 131.54, 133.48, 147.98, 150.37, 167.27.

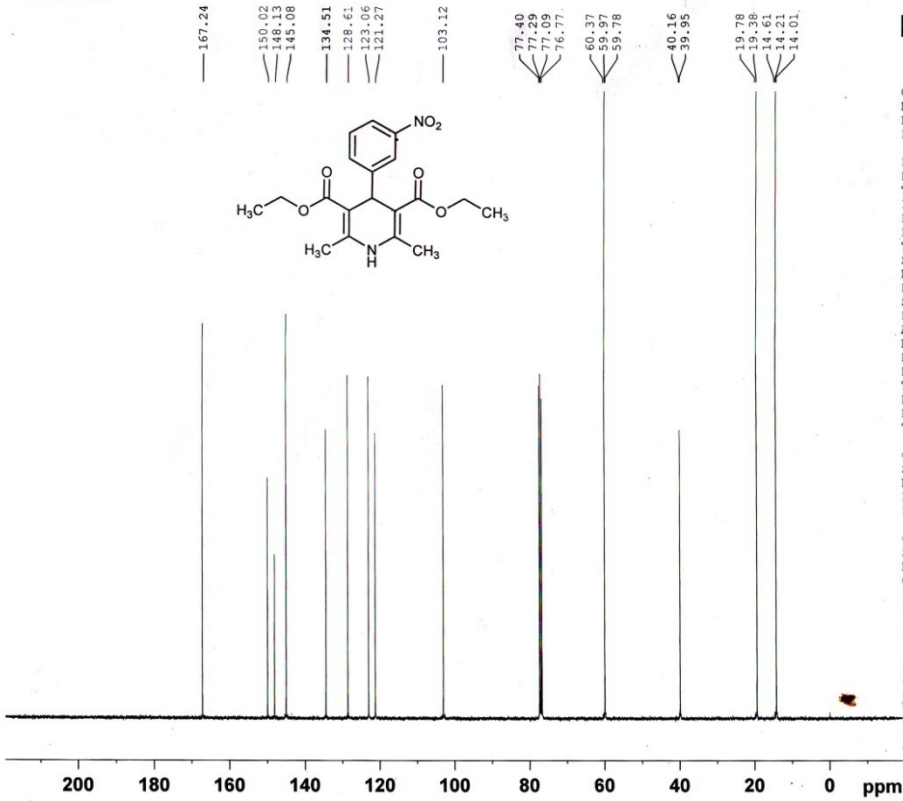
MS (ESI): 375 (M+1).

Diethyl-4-(3-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4)



¹H NMR of Diethyl-4-(3-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4)

m-No2DHP



Current Data Parameters
NAME Jun11-2013
EXPNO 6
PROCNO 1

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Time_ 13.05
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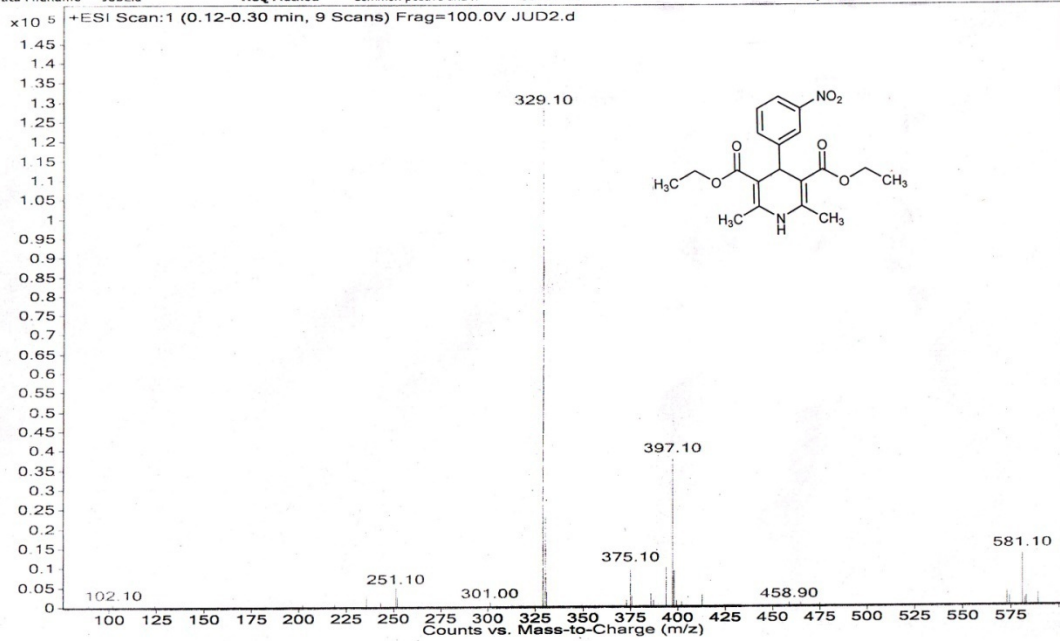
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NUC2 1H
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PLW2 13.00000000 W
PLW12 0.36111000 W
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F2 - Processing parameters
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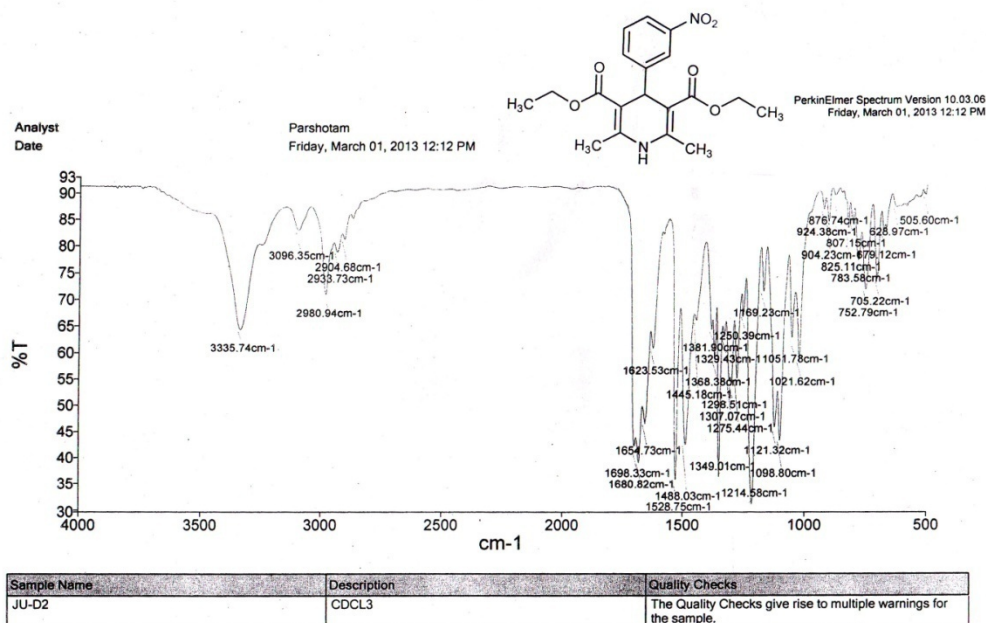
¹³C NMR of Diethyl-4-(3-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4)

Sample Name JUD2 Position Vial 38 Instrument Name SG11351102 User Name
Inj Vol 0.05 InjPosition Sample Type Sample IRM Calibration Status Not Applicable
Data Filename JUD2.d ACQ Method Common positive and n Comment Acquired Time 3/8/2013 1:57:58 PM



Mass spectra of *Diethyl-4-(3-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate*

(4)



IR of *Diethyl-4-(3-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4)*

Diethyl-4-(3-nitrophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (4)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3335, 1698, 1488.

$^1\text{H NMR}$ (400 MHz; CDCl_3 ; Me_4Si): δ 1.20-1.23 (t, 6H, 2x $-\text{CH}_2\text{CH}_3$), 2.34 (s, 6H, 2x $-\text{CH}_3$), 4.07-4.11 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 5.1 (s, 1H, C-4H), 6.32 (bs, 1H, $-\text{NH}$), 7.28-7.39 (t, Ar-H), 7.63-7.65 (d, Ar-H), 7.98-8.00 (d, Ar-H), 8.13 (s, Ar-H).

$^{13}\text{C NMR}$ (100 MHz; CDCl_3 ; Me_4Si): δ 14.21, 19.56, 39.95, 60.00, 103.12, 121.27, 123.06, 128.61, 134.51, 145.08, 148.13, 150.02, 167.24.

MS (ESI): 375 (M+1).

Diethyl-4-(4-chlorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (5)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3352, 1704, 1295.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.22-1.26 (t, 6H, 2x -CH₂CH₃), 2.32 (s, 6H, 2x -CH₃), 4.03-4.11 (q, 4H, 2x -OCH₂CH₃), 4.98 (s, 1H, C-4H), 5.52 (bs, 1H, -NH), 7.15-7.17 (d, 2H, Ar-H), 7.28-7.29 (d, 2H, Ar-H).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.21, 19.76, 39.23, 59.86, 103.88, 127.97, 129.46, 131.54, 144.00, 146.29, 167.76.

MS (ESI): 365 (M+1), 366 (M+2).

Diethyl-4-(4-methylphenyl)-2,6-dimethyl-1,4-dihydropyridin-3,5-dicarboxylate (6)

IR (KBr, ν_{max}/cm⁻¹): 3362, 1698, 1487.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.21-1.26 (t, 6H, 2x -CH₂CH₃), 2.36 (s, 6H, 2x -CH₃), 2.24 (s, 3H, -CH₃), 3.78 (s, 3H, -OCH₃), 4.09-4.18 (q, 4H, 2x -OCH₂CH₃), 4.95 (s, 1H, C-4H), 5.74 (bs, 1H, NH), 7.01-7.04 (d, 2H, Ar-H), 7.09-7.10 (d, 2H, Ar-H).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.38, 19.52, 22.01, 38.72, 59.42, 102.81, 126.96, 128.46, 132.51, 144.12, 146.48, 167.89.

MS (ESI): 344 (M+1).

Diethyl-4-(4-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridin-3,5-dicarboxylate (7)

IR (KBr, ν_{max}/cm⁻¹): 3345, 1744, 1497.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.21-1.25 (t, 6H, 2x -CH₂CH₃), 2.19 (s, 6H, 2x -CH₃), 3.90 (s, 3H, -OCH₃), 4.07-4.13 (q, 4H, 2x -OCH₂CH₃), 4.94 (s, 1H, C-4H), 5.68 (bs, 1H, -NH), 7.17-7.28 (m, 5H, Ar-H).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.26, 19.62, 30.93, 39.26, 59.81, 103.93, 127.94, 129.43, 131.69, 143.93, 146.32, 167.41.

MS (ESI): 360 (M+1).

Diethyl-4-(2-furyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (8)

IR (KBr, ν_{max}/cm⁻¹): 3342, 1695, 1487.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.27-1.30 (t, 6H, 2x -CH₂CH₃), 2.35 (s, 6H, 2x -CH₃), 4.11-4.25 (q, 4H, 2x -OCH₂CH₃), 5.22 (s, 1H, C-4H), 5.83 (bs, 1H, -NH), 5.86 (d, 1H, Ar-H), 6.22-6.23 (t, 1H, Ar-H), 7.27 (d, 1H, Ar-H).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.37, 19.39, 59.82, 101.55, 104.44, 109.99, 140.86, 145.04, 158.67, 167.47.

MS (ESI): 320 (M+1).

Diethyl-4-(2-thienyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (9)

IR (KBr, ν_{max}/cm⁻¹): 3346, 1699, 1489.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.29-1.34 (t, 6H, 2x -CH₂CH₃), 2.37 (s, 6H, 2x -CH₃), 4.11-4.21 (q, 4H, 2x -OCH₂CH₃), 5.34 (s, 1H, C-4H), 6.41 (bs, 1H, -NH), 6.79-6.80 (d, 1H, Ar-H), 6.83-6.85 (t, 1H, Ar-H), 7.04-7.06 (d, 1H, Ar-H).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.74, 19.34, 34.37, 59.96, 103.29, 123.09, 126.94, 144.96, 151.65, 167.56

MS (ESI): 336 (M+1).

Diethyl-1,4-dihydro-4-(4-hydroxy-3-methoxyphenyl)-2,6-dimethylpyridin-3,5-dicarboxylate (10)

IR (KBr, ν_{max}/cm⁻¹): 3349, 2948, 1639, 1481.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.24 (t, 6H, 2x -CH₂CH₃), 2.18 (s, 6H, 2x -CH₃), 3.72 (s, 3H, -OCH₃), 4.59 (s, 1H, C-4H), 5.34 (bs, 1H, -OH), 5.7 (bs, 1H, -NH) and 6.6-6.8 (m, 3H, ArH).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.22, 19.81, 39.52, 59.91, 61.93, 101.53, 114.35, 116.71, 122.28, 134.85, 141.69, 151.25, 151.32, 167.24

MS (ESI): 376 (M+1).

Diethyl-4-(2-phenylvinyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (11)

IR (KBr, ν_{max}/cm⁻¹): 3332, 1753, 1445.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.27-1.31 (t, 6H, 2x -CH₂CH₃), 2.35 (s, 6H, 2x -CH₃), 4.13-4.24 (q, 4H, 2x -OCH₂CH₃), 4.64 (s, 1H, C-4H), 5.72 (bs, 1H, -NH), 6.17-6.19 (d, 1H, =CH), 6.18-6.23 (dd, 1H, =CH), 7.15-7.34 (m, 5H, Ar-H).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.46, 19.42, 35.54, 59.81, 101.28, 126.23, 126.87, 128.05, 128.39, 131.85, 137.78, 145.25, 167.76.

MS (ESI): 356 (M+1).

Diethyl-4-(4-bromophenyl)-2,6-dimethyl-1,4-dihydropyridin-3,5-dicarboxylate (12)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3382, 1712, 1291.

^1H NMR (400 MHz; CDCl_3 ; Me_4Si): δ 1.18-1.25 (t, 6H, 2x $-\text{CH}_2\text{CH}_3$), 2.28 (s, 6H, 2x $-\text{CH}_3$), 4.0-4.10 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 4.91 (s, 1H, C-4H), 5.46 (bs, 1H, $-\text{NH}$), 7.09-7.15 (d, 2H, Ar-H), 7.25-7.27 (d, 2H, Ar-H).

^{13}C NMR (100 MHz; CDCl_3 ; Me_4Si): δ 14.17, 19.69, 39.18, 59.81, 103.82, 127.92, 129.36, 131.39, 143.10, 146.29, 167.68.

MS (ESI): 410 (M+1), 411 (M+2).

Diethyl-4-(2-methoxyphenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (13)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3361, 1744, 1426.

^1H NMR (400 MHz; CDCl_3 ; Me_4Si): δ 1.23 (t, 6H, 2x $-\text{CH}_2\text{CH}_3$), 2.33 (s, 6H, 2x $-\text{CH}_3$), 3.94 (s, 3H, $-\text{OCH}_3$), 4.14 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 4.84 (s, 1H, C-4H), 5.59 (bs, 1H, $-\text{NH}$), 7.39-8.18 (m, 4H, Ar-H).

^{13}C NMR (100 MHz; CDCl_3 ; Me_4Si): δ 14.18, 19.65, 35.19, 60.79, 102.34, 121.18, 126.22, 129.65, 131.34, 133.39, 147.87, 150.31, 166.89.

MS (ESI): 360 (M+1).

Diethyl-4-(2-Chlorophenyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (14)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3381, 1764, 1439.

^1H NMR (400 MHz; CDCl_3 ; Me_4Si): δ 1.26 (t, 6H, 2x $-\text{CH}_2\text{CH}_3$), 2.35 (s, 6H, 2x $-\text{CH}_3$), 4.16 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 4.81 (s, 1H, C-4H), 5.63 (bs, 1H, $-\text{NH}$), 7.36-8.16 (m, 4H, Ar-H).

^{13}C NMR (100 MHz; CDCl_3 ; Me_4Si): δ 14.21, 19.69, 35.26, 61.08, 102.50, 120.97, 125.83, 130.07, 131.45, 133.33, 147.92, 150.38, 167.00.

MS (ESI): 365 (M+1), 366 (M+2).

Diethyl-2,4,6-trimethyl-1,4-dihydropyridine-3,5-dicarboxylate (15)

IR (KBr, $\nu_{\max}/\text{cm}^{-1}$): 3364, 1736, 1436.

^1H NMR (400 MHz; CDCl_3 ; Me_4Si): δ 1.21 (s, 3H, $-\text{CH}_3$), 1.21 (t, 6H, 2x $-\text{OCH}_2\text{CH}_3$), 2.19 (s, 6H, 2x $-\text{CH}_3$), 4.11 (q, 4H, 2x $-\text{OCH}_2\text{CH}_3$), 4.78 (s, 1H, C-4H), 5.51 (bs, 1H, $-\text{NH}$).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.13, 15.89, 18.4, 37.06, 62.12, 106.13, 149.89, 167.30.

MS (ESI): 268 (M+1).

Diethyl-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (16)

IR (KBr, ν_{max}/cm⁻¹): 3385, 1731, 1424.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 1.26 (t, 6H, 2x -OCH₂CH₃), 2.23 (s, 6H, 2x -CH₃), 4.17 (q, 4H, 2x -OCH₂CH₃), 3.19 (s, 2H, C-4H), 5.49 (bs, 1H, -NH).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 14.18, 16.49, 36.26, 61.8, 100.60, 150.20, 166.92.

MS (ESI): 254 (M+1).

Diethyl-4-ethyl-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (17)

IR (KBr, ν_{max}/cm⁻¹): 3370, 1724, 1440.

¹H NMR (400 MHz; CDCl₃; Me₄Si): δ 0.71 (t, 3H, -CH₂CH₃), 1.21 (t, 6H, 2x -OCH₂CH₃), 1.35 (q, 2H, -CH₂CH₃), 2.19 (s, 6H, 2x -CH₃), 4.11 (q, 4H, 2x -OCH₂CH₃), 4.78 (s, 1H, C-4H), 5.51 (bs, 1H, -NH).

¹³C NMR (100 MHz; CDCl₃; Me₄Si): δ 12.2, 14.18, 16.49, 22.4, 36.26, 61.8, 105.90, 149.97, 167.02.

MS (ESI): 282 (M+1).