Supporting Information for

Markovnikov addition of imidazole derivatives with vinyl esters Catalyzed by lipase TL IM from *Thermomyces lanuginosus*/K_2CO_3 in a Continuous-Flow Microreactor

Li-Hua Du,[*a] Bing-Zhuo Cheng,[a]Wen-Jun Yang[a] Liang-Liang Xu[a]and Xi-Ping Luo,[a, b]

[a]*College of Pharmaceutical Science, ZheJiang University of Technology, Hangzhou，310014, China*

[b]*Department of Environmental Science and Technology, ZheJiang A&F University, Hangzhou, 311300, China.*

∗ Corresponding author. Fax: +86 571 88320903. E-mail: orgdlh@gmail.com; orgdlh@zjut.edu.cn.

Materials

Unless otherwise stated, all chemicals were obtained from commercial sources and used without further purification. Lipozyme TL IM from *Thermomyces lanuginosus* was purchased from Novo Nordisk. Imidazole, vinyl esters and all other chemicals were of the highest purity commercially available and without further purification. Harvard Apparatus PHD 2000 syringe pumps were purchased from Harvard apparatus.

Thin-Layer Chromatography

Analytical TLC was performed on silica gel 60 plates (Merck) using ethyl acetate/ hexane (2:1, by vol) as eluent. Spots were detected by ultraviolet irradiation at 254 nm.

High Performance Liquid Chromatography (HPLC)

The reaction was monitored by HPLC analysis using a Shim-Pack VP-ODS column (4.6×150 mm) and a UV detector (285 nm). MeOH/NaH_2PO_4 solution (7.5×10^{-3} M) (25:75) was used as eluant at 1.0 mL min^{-1} for imidazole and vinyl acetate.

MeOH/H_2O (30:70) was used as eluant at 1.0 mL min^{-1} for 4-nitroimidazole and vinyl acetate. The yield was defined as the ratio between the molar concentration of *N*-substituted imidazole derivatives and the initial molar concentration of the imidazole derivatives used.

Experimental setup

The enzymatic Markovnikov addition of imidazole derivatives with vinyl esters was performed in microreactor. The equipment configuration that was used for the enzymatic Markovnikov addition of imidazole derivatives with vinyl esters starting from 4-nitroimidazole and vinyl acetate is described in Figure 1. Harvard Apparatus PHD 2000 syringe pumps were used to deliver reagents from syringes to the reactor. On the syringe pump, a 10 mL syringe with the 4-nitroimidazole solution and a 10 mL syringe with vinyl acetate in DMSO were mounted. Lipozyme TL IM (catalyst reactivity: 260 IUN/g) from *Thermomyces lanuginosus*/K_2CO_3 were full mixed and filled in silica gel tubing (inner diameter ID = 2.0 mm, length = 1 m). The result of the void volume was about 965 mm^3. The temperature of this reaction was controlled by water bath, just immersed the tubing in water and controlled the temperature of water. Streams **1** and **2** were mixed together at a flow rate of 10.4 μL min^{-1} in a Y-mixer at 50 °C and the resulting stream (20.8 μL min^{-1}) was connected to a sample vial which was used to collect the final mixture.

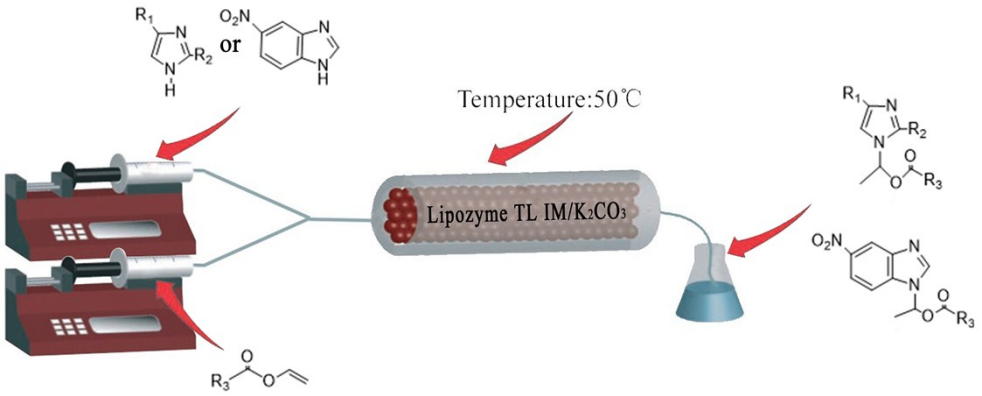


Figure 1. Experimental setup for Markovnikov addition of imidazole derivatives with vinyl esters in the continuous flow microreactor catalyzed by lipase TL IM/K_2CO_3.

General Procedure for Markovnikov addition reaction in Continuous Flow Microreactors

Method B: 1 mmol of the 4-nitroimidazole was dissolved in 10 mL DMSO (feed 1, ~0.1 M) and 6 mmol vinyl acetate were dissolved in 10 mL DMSO (feed 2; ~0.6 M). Lipozyme TLIM (0.80 g) and K_2CO_3 (41.4 mg) were weighed and mixed thoroughly, then filled the silica gel tubing with the mixed catalyst. (inner diameter ID: 2.0 mm, length: 1 m). Streams **1** and **2** were mixed together at a flow rate of 10.4 μL min^{-1} in a Y-mixer at 50 °C and the resulting stream (20.8μL min^{-1}) was connected to a sample vial which was used to collect the final mixture. The final mixture was then evaporated, and the residue was submitted to column chromatography on silica gel (200–300 mesh). The products were eluted with a gradient of normal hexane/ethyl acetate (5:1, by vol). The purification was monitored by TLC. The fractions containing the main products were pooled, the solvent evaporated, and the residue analyzed by ^{1}H NMR, ^{13}C NMR and ESI-MS.

General Procedure for Markovnikov addition reaction under Shaker Conditions.

Method A: 4-nitroimidazole (0.25 mmol) and vinyl acetate (1.5 mmol) were added to 5 mL DMSO. The biocatalyst lipozyme TL IM (40 mg/mL, 0.20 g) and K_2CO_3 (1.5 $\times 10^{-2}$ mmol/mL, 10.70 mg) was then added and the suspension maintained at 50 °C for 24 h～48 h under Shaker Conditions. The reactions were performed in the presence of 3 Å molecular sieves. Aliquots were withdrawn at different times, analyzed by TLC and HPLC. When the conversion of 4-nitroimidazole to acetic acid 1-(4-nitro-imidazol-1-yl)-ethyl ester reached the maximum value (determined by TLC and HPLC), the mixture was cooled and filtered. Then evaporated under reduced pressure and the residue was submitted to column chromatography on silica gel (200–300 mesh). The products were eluted with a gradient of normal hexane/ethyl acetate (5:1, by vol). The purification was monitored by TLC. The fractions containing the main products were pooled, the solvent evaporated, and the residue analyzed by ^{1}H NMR, ^{13}C NMR and ESI-MS.

In order to examine the reproducibility of the method, we repeated the reaction five times, the result are illustrate in Figure S1.

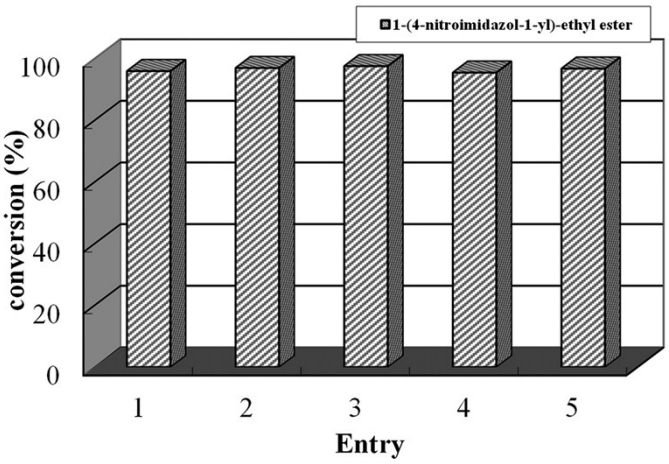


Figure S1. The reproducibility of the reaction on the conversion of acetic acid 1-(4-nitro-imidazol-1-yl)-ethyl ester catalysed by Lipozyme TL IM / K_2CO_3 in a flow microreactor.

The structure of the Markovnikov acceptor and donor can affect the results of the enzymatic Markovnikov reaction. With respect to the acceptor structure, the longer the vinyl esters carboxyl group chain, the lower the conversion. Figure S2 shows the effect of acceptor structure effect on the Markovnikov addition reaction. When 4-nitroimidazole was used as Markovnikov donor, the decrease of yields was detected with the increase of carboxyl group chain. such as vinyl acetate and vinyl laurate.

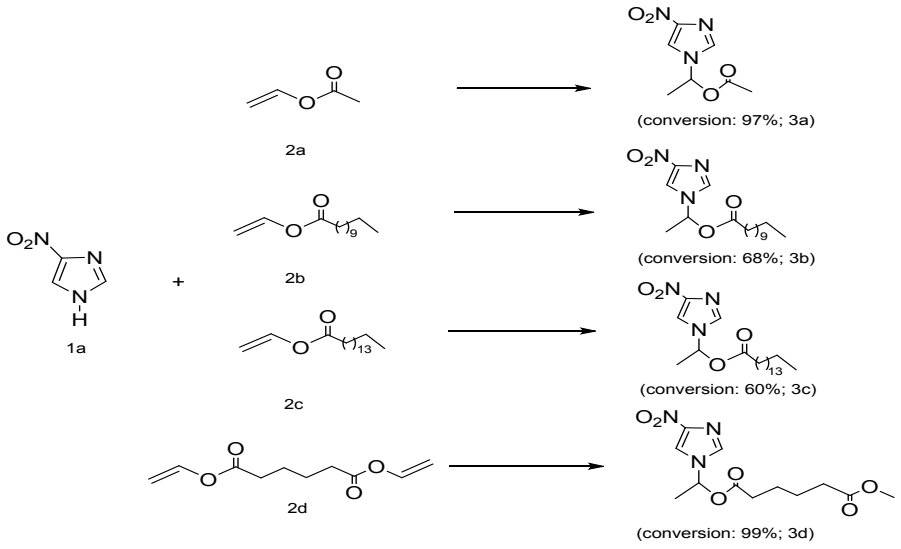
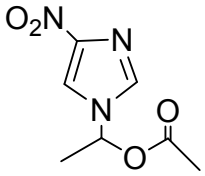
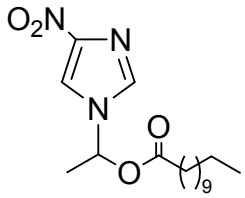


Figure S2. Acceptor structure effect on the Markovnikov addition performance.

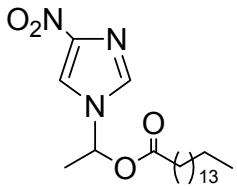
Experimental Procedures for Examples Described in Table 1



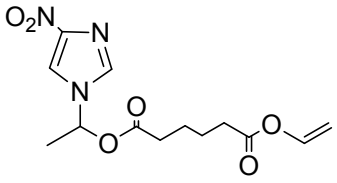
Acetic acid 1-(4-Nitro-imidazol-1-yl)-ethyl ester (3a)*[1-2]*: White crystals; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.66 (s, 1H, N=CHN), 8.10 (s, 1H, NCH=C), 6.77 (q, 1H, J = 6.25 Hz, $CH_3C\underline{H}O$), 2.06 (s, 3H, $COCH_3$),1.78 (d, 3H, J = 6.25 Hz, $CHC\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 169.78 (CO), 147.80 (C4), 137.24 (C2), 120.13 (C5), 77.34 ($CH_3\underline{C}HO$), 21.13 ($CO\underline{C}H_3$), 20.18 ($CH\underline{C}H_3$). ESI-MS: m/z = 200 (M+1).



Lauric acid 1-(4-Nitro-imidazol-1-yl)- ethyl ester(3b): Yellow liquid oil; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.65 (s, 1H, N=CHN), 8.09 (s, 1H, NCH=C), 6.80 (q, 1H, J = 6.15 Hz, $CH_3C\underline{H}O$), 2.32 (t, 2H, J = 7.30 Hz, $COC\underline{H}_2CH_2$), 1.78 (d, 3H, J = 6.25 Hz, $C\underline{H}_3CHO$), 1.48 (m, 2H, $O{=}CCH_2C\underline{H}_2$), 1.18 (m, 16H, $(C\underline{H}_2)_8CH_3$), 0.84 (t, 3H, J = 6.70 Hz, $CH_2C\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 171.78 (CO), 147.40 (C4), 136.58 (C2), 119.31 (C5), 76.79 ($CH_3\underline{C}HO$), 33.25 ($O{=}C\underline{C}H_2$), 31.36 ($\underline{C}H_2CH_2CH_3$), 28.78 ($(\underline{C}H_2)_6CH_2CH_2CH_3$), 24.13 ($COCH_2\underline{C}H_2$), 22.04 ($\underline{C}H_2CH_3$), 19.72 ($OCH\underline{C}H_3$), 13.88 ($CH_2\underline{C}H_3$). ESI-MS: m/z = 340 (M+1). HR-MS: m/z calculated for $C_{17}H_{29}N_30_4$ [M+1]: 340.2231 found 340.2230.

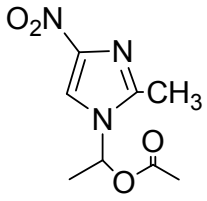


Palmitic acid 1-(4-Nitro-imidazol-1-yl)-ethyl ester (3c): White crystals; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.67 (s, 1H, N=CHN), 8.10 (s, 1H, NCH=C), 6.79 (q, 1H, J = 6.15 Hz, $CH_3C\underline{H}O$), 2.31(t, 2H, J = 7.20 Hz, $O{=}C\underline{C}H_2$), 1.77 (d, 3H, J = 6.15 Hz, $C\underline{H}_3CH$), 1.48 (m, 2H, $COCH_2C\underline{H}_2$), 1.20 (m, 24H, $(C\underline{H}_2)_{12}CH_3$), 0.85 (t, 3H, J = 6.70 Hz, $CH_2C\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 171.81 (CO), 147.42 (C4), 136.69 (C2), 119.37 (C5), 76.83 ($CH_3\underline{C}HO$), 33.22 ($CO\underline{C}H_2$), 31.38 ($\underline{C}H_2CH_2CH_3$), 28.81 ($(\underline{C}H_2)_{10}CH_2CH_2CH_3$), 24.12 ($O{=}CCH_2\underline{C}H_2$), 22.06 ($\underline{C}H_2CH_3$), 19.76 ($OCH\underline{C}H_3$), 13.93 ($CH_2\underline{C}H_3$). ESI-MS: *m/z* = 396 (M+1). HR-MS: *m/z* calculated for $C_{21}H_{37}N_30_4$ [M+1]: 396.2855 found 396.2994.

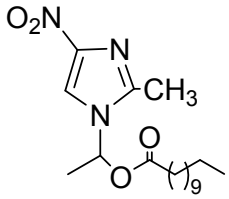


Adipic acid vinyl 1-(4-Nitro-imidazol-1-yl)-ethyl ester (3d) [3]***:*** Yellow liquid oil; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.65 (s, 1H, N=CHN), 8.10 (s, 1H, NCH=C), 7.20 (m, 1H, $OC\underline{H}{=}CH_2$), 6.79 (q, 1H, J = 6.19 Hz, $CH_3C\underline{H}O$), 4.89, 4.64 (m, 2H, $CH{=}C\underline{H}_2$), 2.42-2.36 (m, 4H, $O{=}CCH_2$), 1.78 (d, 3H, J = 6.20 Hz, $CHC\underline{H}_3$), 1.53 (t, 4H, $COCH_2(C\underline{H}_2)_2$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 172.00, 170.65 (CO), 147.80 (C4), 141.66 ($O\underline{C}H{=}CH_2$), 137.08 (C2), 119.94 (C5), 98.46 ($OCH{=}\underline{C}H_2$), 77.29 ($CH_3\underline{C}HO$), 33.19, 33.02 ($CO\underline{C}H_2CH_2CH_2\underline{C}H_2$), 23.76, 23.70 ($COCH_2\underline{C}H_2\underline{C}H_2CH_2$), 20.15 ($CH\underline{C}H_3$). ESI-MS: *m/z* = 312 (M+1). HR-MS: *m/z* calculated for

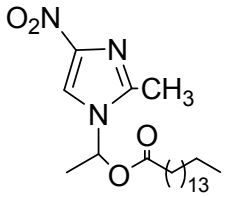
$C_{13}H_{17}N_30_6$ [M+1]: 312.1190 found 312.1181.



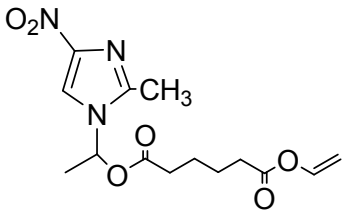
Acetic acid 1-(2-Methyl-4-nitro-imidazol-1-yl)-ethyl ester(3e) [4]***:*** White crystals; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.63 (s, 1H, NCH=C), 6.77 (q, 1H, *J* = 6.10 Hz, $CH_3C\underline{H}O$), 2.46 (s, 3H, $N{=}CCH_3$), 2.07 (s, 3H, $O{=}CCH_3$), 1.75 (d, 3H, *J* = 6.20 Hz, $CHC\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6) δ = 169.74 (CO), 148.48 (C4), 146.79 (C2), 119.62 (C5), 76.26 ($CH_3\underline{C}HO$), 21.05 ($CO\underline{C}H_3$), 20.05 ($CH\underline{C}H_3$), 13.48 ($NC\underline{C}H_3$). ESI-MS: *m/z* = 214 (M+1).



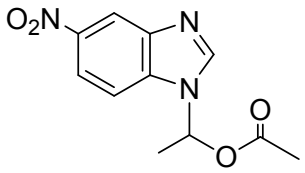
Lauric acid 1-(2-Methyl-4-nitro-imidazol-1-yl)-ethyl ester(3f): yellow liquid oil; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.60 (s, 1H, NCH=C), 6.69 (q, 1H, *J* = 6.15 Hz, $CH_3C\underline{H}O$), 2.46 (s, 3H, $N{=}CCH_3$), 2.32 (t, 2H, *J* = 3.35 Hz, $COC\underline{H}_2$), 1.74 (d, 3H, *J* = 6.15 Hz, $C\underline{H}_3CH$), 1.49 (m, 2H, $COCH_2C\underline{H}_2$), 1.20 (m, 16H, $(C\underline{H}_2)_8CH_3$), 0.85 (t, 3H, *J* = 6.80 Hz , $CH_2C\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 170.60 (CO), 146.30 (C4), 144.79 (C2), 118.72 (C5), 75.65 ($CH_3\underline{C}HO$), 33.09 ($CO\underline{C}H_2CH_2$), 31.24 ($\underline{C}H_2CH_2CH_3$), 28.65 ($COCH_2CH_2(\underline{C}H_2)_6$), 24.05 ($COCH_2\underline{C}H_2$), 22.02 ($\underline{C}H_2CH_3$), 19.94($CH\underline{C}H_3$), 13.81($CH_2\underline{C}H_3$), 12.86 ($NC\underline{C}H_3$). ESI-MS: *m/z* = 354 (M+1). HR-MS: *m/z* calculated for $C_{18}H_{31}N_30_4$ [M+1]: 354.2387 found 354.2421.



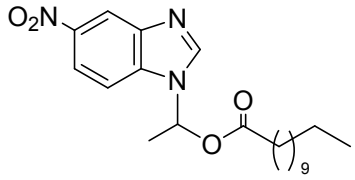
Palmitic acid 1-(2-Methyl-4-nitro-imidazol-1-yl)-ethyl ester(3g): Yellow liquid oil; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.63 (s, 1H, C=CHN), 6.69 (q, 1H, J = 6.10 Hz, $CH_3C\underline{H}O$), 2.46 (s, 3H, $NCCH_3$), 2.32 (t, 2H, J = 5.6 Hz, $COC\underline{H}_2CH_2$), 1.74 (d, 3H, J = 6.20 Hz, CH_3CH), 1.48 (m, 2H, $COCH_2C\underline{H}_2$), 1.21 (m, 24H, $(C\underline{H}_2)_{12}CH_3$), 0.86 (t, 3H, J = 6.70 Hz, $CH_2C\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 170.62 (CO), 146.31 (C4), 144.92 (C2), 118.74 (C5), 75.67 ($CH_3\underline{C}HO$), 33.11 ($CO\underline{C}H_2$), 31.25 ($\underline{C}H_2CH_2CH_3$), 28.66 ($COCH_2CH_2(\underline{C}H_2)_{10}$), 24.04 ($COCH_2\underline{C}H_2$), 22.06 ($\underline{C}H_2CH_3$), 19.98 ($CH\underline{C}H_3$), 13.87 ($CH_2\underline{C}H_3$), 12.88 ($NC\underline{C}H_3$). ESI-MS: m/z = 410 (M+1). HR-MS: m/z calculated for $C_{22}H_{39}N_30_4$ [M+1]: 410.3045 found 410.3185.



Adipic acid vinyl 1-(2-Methyl-4-nitro-imidazol-1-yl)-ethyl ester(3h) [4]***:*** Yellow liquid oil; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.62 (s, 1H, C=CHN), 7.19 (m, 1H, $OC\underline{H}=CH_2$), 6.69 (q, 1H, J = 6.10 Hz, $CH_3C\underline{H}O$), 4.88, 4.64 (m , 2H, $OCH=C\underline{H}_2$), 2.46 (s, 3H, $N=CCH_3$), 2.42-2.38 (m, 4H, $COC\underline{H}_2CH_2CH_2C\underline{H}_2$), 1.74 (d, 3H, J = 6.20 Hz, $CHC\underline{H}_3$), 1.53-1.52 (m, 4H, $COCH_2C\underline{H}_2C\underline{H}_2$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 171.78, 171.35 (CO), 147.32 (C4), 140.66 ($O\underline{C}H=CH_2$), 138.16 (C2), 119.64 (C5), 98.37 ($OCH=\underline{C}H_2$), 77.18 ($CH_3\underline{C}HO$), 33.08, 32.97 ($CO\underline{C}H_2CH_2CH_2\underline{C}H_2$), 23.66, 23.57 ($COCH_2\underline{C}H_2\underline{C}H_2CH_2$), 20.07 ($CH\underline{C}H_3$), 13.26 ($NCCH_3$). ESI-MS: m/z = 326 (M+1). HR-MS: m/z calculated for $C_{14}H_{19}N_30_6$ [M+1]: 326.1346 found 326.1371.

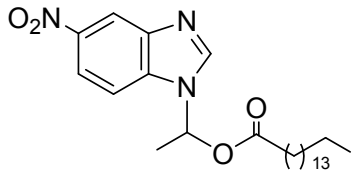


Acetic acid 1-(6-Nitro-benzimidazol-1-yl)-ethyl ester(3q): White crystals; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.83 (s, 1H, C5-H, 6-nitro-benzimidazole), 8.56 (d, 1H, J = 2.20 Hz, C2-H, 6-nitro-benzimidazole), 8.23 (dd, 1H, J_1 = 2.20 Hz, J_2 = 9.05 Hz, C7-H, 6-nitro-benzimidazole), 7.93 (d, 1H, J = 9.0 Hz, C8-H, 6-nitro-benzimidazole), 7.12 (q, 1H, J = 6.30 Hz, $CH_3C\underline{H}O$), 2.04 (s, 3H, CH_3CO), 1.91 (d, 3H, J = 4.40 Hz, $C\underline{H}_3CH$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 169.41 (CO), 147.10 (C6), 143.02 (C2), 136.07 (C4), 131.86 (C9), 118.13 (C7), 112.30 (C5), 108.47 (C8), 75.50 ($CH_3\underline{C}HO$), 20.53 ($CO\underline{C}H_3$), 19.64 ($CH\underline{C}H_3$). ESI-MS: m/z = 250 (M+1).

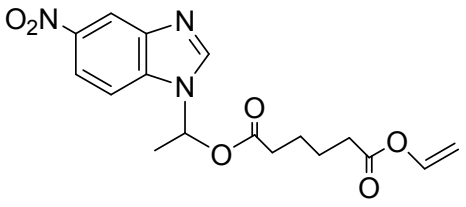


Lauric acid 1-(6-Nitro-benzimidazol-1-yl)-ethyl ester(3r): Yellow liquid oil; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.83 (s, 1H, C5-H, 6-nitro-benzimidazole), 8.56 (d, 1H, J = 2.15 Hz, C2-H, 6-nitro-benzimidazole), 8.23 (dd, 1H, J_1 = 2.20 Hz, J_2 = 8.90 Hz, C7-H, 6-nitro-benzimidazole), 7.93(d, 1H, J = 9.20 Hz, C8-H, 6-nitro-benzimidazole), 7.15 (q, 1H, J = 6.25 Hz, $CH_3C\underline{H}O$), 2.31 (t, 2H, J = 7.05 Hz, $COCH_2$), 1.91 (d, 3H, J = 3.10 Hz, $C\underline{H}_3CHO$), 1.42 (m, 2H, $COCH_2C\underline{H}_2$), 1.12-1.25 (m, 16H, $(C\underline{H}_2)_8CH_3$), 0.84 (t, 3H, J = 6.95 Hz, $CH_2C\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 171.58 (CO), 146.18 (C6), 143.18 (C2), 141.87 (C4), 136.35 (C9), 118.23 (C7), 115.48 (C5), 112.17 (C8), 74.43($CH_3\underline{C}HO$), 33.18($CO\underline{C}H_2$), 31.16 ($\underline{C}H_2CH_2CH_3$), 28.63

($COCH_2CH_2(\underline{C}H_2)_6$), 24.09 ($COCH_2\underline{C}H_2$), 22.03 ($\underline{C}H_2CH_3$), 19.37 ($CH\underline{C}H_3$), 13.82 ($CH_2\underline{C}H_3$). ESI-MS: *m/z* = 390 (M+1). HR-MS: *m/z* calculated for $C_{21}H_{31}N_30_4$ [M+1]: 390.2387 found 390.2405.



Palmitic acid 1-(6-Nitro-benzimidazole-1-yl)-ethyl ester(3s): Yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.82 (s, 1H, C5-H, 6-nitro-benzimidazole), 8.56 (d, 1H, *J* = 2.20 Hz, C2-H, 6-nitro-benzimidazole), 8.23 (dd, 1H, J_1 = 2.20 Hz, J_2 = 8.95 Hz, C7-H, 6-nitro-benzimidazole), 7.93 (d, 1H, *J* = 8.95 Hz, C8-H, 6-nitro-benzimidazole), 7.15 (q, 1H, *J* = 6.30 Hz, $CH_3C\underline{H}O$), 2.31 (t, 2H, *J* = 7.20 Hz, $COCH_2$), 1.91 (d, 3H, *J* = 6.30 Hz, $C\underline{H}_3CH$), 1.42 (m, 2H, $COCH_2C\underline{H}_2$), 1.03-1.23 (m, 24H, $(C\underline{H}_2)_{12}CH_3$), 0.85 (t, 3H, *J* = 6.70 Hz, $CH_2C\underline{H}_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 171.78 (CO), 146.36 (C6), 143.36 (C2), 142.77 (C4), 136.55 (C9), 118.43 (C7), 115.76 (C5), 112.20 (C8), 74.45 ($CH_3\underline{C}HO$), 33.20 ($CO\underline{C}H_2$), 31.21 ($\underline{C}H_2CH_2CH_3$), 28.66($COCH_2CH_2(\underline{C}H_2)_{10}$), 24.13 ($COCH_2\underline{C}H_2$), 22.00 ($\underline{C}H_2CH_3$), 19.44 ($CH\underline{C}H_3$), 13.84 ($CH_2\underline{C}H_3$). ESI-MS: *m/z* = 446 (M+1). HR-MS: *m/z* calculated for $C_{25}H_{39}N_30_4$ [M+1]: 446.3011 found 446.3169.



Adipic acid vinyl 1-(6-Nitro-benzimidazole-1-yl)-ethyl ester(3t): Yellow liquid oil; ^{1}H NMR (500

MHz, DMSO-d_6): δ = 8.84 (s, 1H, C5-H, 6-nitro-benzimidazole), 8.57 (d, 1H, J = 1.95 Hz, C2-H, 6-nitro-benzimidazole), 8.23 (dd, 1H, J_1 = 2.00 Hz, J_2 = 10.95 Hz, C7-H, 6-nitro-benzimidazole), 7.94 (d, 1H, J = 9.0 Hz, C8-H, 6-nitro-benzimidazole), 7.24 (m, 1H, OC<u>H</u>=CH_2), 7.15 (q, 1H, J = 6.20 Hz, CH_3C<u>H</u>O), 4.86, 4.63 (m, 2H, OCH=C<u>H_2</u>), 2.36-2.34 (m, 4H, CO<u>CH_2</u>CH_2CH_2<u>CH_2</u>CO), 1.92 (d, 3H, J = 3.30 Hz, CHC<u>H_3</u>), 1.46 (m, 4H, $COCH_2$C<u>H_2</u>C<u>H_2</u>). ^{13}C NMR (125 MHz, DMSO-d_6): δ = 171.63，171.56 (CO), 147.05 (C6), 142.34 (C2), 136.56 (C4), 131.73 (C9), 118.02 (C7), 112.15 (C5), 108.33 (C8), 97.95 (OCH=<u>C</u>H_2), 75.43 (CH_3<u>C</u>HO), 33.73, 32.87 (CO<u>C</u>$H_2CH_2CH_2$<u>C</u>H_2), 23.17, 23.35 ($COCH_2$<u>C</u>H_2<u>C</u>H_2), 19.57 (CH<u>C</u>H_3). ESI-MS: *m/z* = 362 (M+1). HR-MS: *m/z* calculated for $C_{17}H_{19}N_30_5$ [M+1]: 362.1346 found 362.1356.

Notes and references

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