Supporting Information

Design and synthesis of 1-indol-1-yl-propan-2-ones as inhibitors of human cytosolic phospholipase $A_2\alpha$

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Supporting Information Contents:

2-(4-Octylphenoxy)methyloxirane[26] (7)

^{1}H-NMR ($CDCl_3$): δ 0.90 (t, 3H), 1.28-1.32 (m, 10H), 1.57-1.60 (m, 2H), 2.55 (t, 2H), 2.76 (dd, 1H), 2.91 (dd, 1H), 3.34-3.37 (m, 1H), 3.95 (dd, 1H), 4.19 (dd, 1H), 6.84 (d, 2H), 7.09 (d, 2H). MS (EI): m/z (%) 262 (31) [M^+], 163 (100).

1-Bromo-3-(4-octylphenoxy)propan-2-ol (8)

^{1}H-NMR ($CDCl_3$): δ 0.89 (t, 3H), 1.27-1.31 (m, 10H), 1.54-1.61 (m, 2H), 2.55 (t, 2H), 2.59 (br s, 1H), 3.59 (dd, 1H), 3.66 (dd, 1H), 4.05 (dd, 1H), 4.10 (dd, 1H), 4.16-4.21 (m, 1H), 6.84 (d, 2H), 7.10 (d, 2H). MS (EI): m/z (%) 344 (20) and 342 (20) [M^+], 107 (100).

[1-Bromo-3-(4-octylphenoxy)propan-2-yl]acetate (9)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.27-1.31 (m, 10H), 1.55-1.59 (m, 2H), 2.13 (s, 3H), 2.54 (t, 2H), 3.63 (dd, 1H), 3.71 (dd, 1H), 4.12 (dd, 1H), 4.18 (dd, 1H), 5.28-5.33 (m, 1H), 6.82 (d, 2H), 7.09 (d, 2H). MS (EI): m/z (%) 386 (1), 384 (1) [M^+], 179 (100).

***tert*-Butyl 1-[2-acetoxy-3-(4-octylphenoxy)propyl]indole-2-carboxylate (10)**

^{1}H-NMR ($CDCl_3$): δ 0.89 (t, 3H), 1.28-1.32 (m, 10H), 1.57-1.61 (m, 2H), 1.62 (s, 9H), 1.81 (s, 3H), 2.56 (t, 2H), 4.16-4.17 (m, 2H), 4.83 (dd, 1H), 5.07 (dd, 1H), 5.55-5.60 (m, 1H), 6.84 (d, 2H), 7.09 (d, 2H), 7.11-7.15 (m, 1H), 7.26 (s, 1H), 7.30-7.34 (m, 1H), 7.57 (d, 1H), 7.64 (d, 1H). MS (EI): m/z (%) 521 (31) [M^+], 260 (100).

***tert*-Butyl 1-[2-hydroxy-3-(4-octylphenoxy)propyl]indole-2-carboxylate (11)**

^{1}H-NMR ($CDCl_3$): δ 0.89 (t, 3H), 1.27-1.32 (m, 10H), 1.57-1.61 (m, 2H), 1.63 (s, 9H), 2.57 (t, 2H), 3.62 (br s, 1H), 3.99 (dd, 1H), 4.04 (dd, 1H), 4.39-4.44 (m, 1H), 4.76 (dd, 1H), 4.81 (dd, 1H), 6.86 (d, 2H), 7.10 (d, 2H), 7.12-7.16 (m, 1H), 7.27 (s, 1H), 7.27-7.31 (m, 1H), 7.48 (d, 1H), 7.69 (d, 1H). MS (EI): m/z (%) 479 (61) [M^+], 217 (100).

***tert*-Butyl 1-[3-(4-octylphenoxy)-2-oxopropyl]indole-2-carboxylate (12)**

^{1}H-NMR ($CDCl_3$): δ 0.89 (t, 3H), 1.27-1.31 (m, 10H), 1.56-1.61 (m, 11H), 2.57 (t, 2H), 4.73 (s, 2H), 5.57 (s, 2H), 6.87 (d, 2H), 7.13 (d, 2H), 7.14-7.18 (m, 2H), 7.28-7.32 (m, 2H), 7.68 (d, 1H). MS (EI): m/z (%) 477 (27) [M^+], 216 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-2-carboxylic acid (13)

^{1}H-NMR (DMSO-d_6): δ 0.83 (t, 3H), 1.22-1.25 (m, 10H), 1.48-1.52 (m, 2H), 2.48 (t, 2H), 4.99 (s, 2H), 5.60 (s, 2H), 6.86 (d, 2H), 7.07 (d, 2H), 7.10-7.13 (m, 1H), 7.26 (s, 1H), 7.28-7.31 (m, 1H), 7.54 (d, 1H), 7.68 (d, 1H). MS (EI): m/z (%) 421 (76) [M^+], 174 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-3-carboxylic acid (14)

^{1}H-NMR (DMSO-d_6): δ 0.84 (t, 3H), 1.23-1.26 (m, 10H), 1.50-1.53 (m, 2H), 2.49 (t, 2H), 5.00 (s, 2H), 5.46 (s, 2H), 6.88 (d, 2H), 7.10 (d, 2H), 7.15-7.21 (m, 2H), 7.43-7.46 (m, 1H), 7.97 (s, 1H), 7.99-8.01 (m, 1H). MS (EI): m/z (%) 421 (49) [M^+], 107 (100).

***tert*-Butyl 1-[2-hydroxy-3-(4-octylphenoxy)propyl]indole-4-carboxylate (15)**

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.27-1.31 (m, 10H), 1.56-1.64 (m, 2H), 1.67 (s, 9H), 2.38 (br s, 1H), 2.55 (t, 2H), 3.83 (dd, 1H), 3.92 (dd, 1H), 4.34-4.38 (m, 2H), 4.47 (dd, 1H), 6.79 (d, 2H), 7.08 (d, 2H), 7.13 (d, 1H), 7.20-7.24 (m, 1H), 7.27 (d, 1H), 7.57 (dd, 1H), 7.86 (d, 1H). MS (EI): m/z (%) 479 (1) [M^+], 174 (100).

***tert*-Butyl 1-[3-(4-octylphenoxy)-2-oxopropyl]indole-4-carboxylate (16)**

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.27-1.31 (m, 10H), 1.56-1.60 (m, 2H), 1.67 (s, 9H), 2.57 (t, 2H), 4.61 (s, 2H), 5.22 (s, 2H), 6.82 (d, 2H), 7.14 (d, 2H), 7.16 (d, 1H), 7.20-7.22 (m, 2H), 7.24-7.28 (m, 1H), 7.88 (dd, 1H). MS (EI): m/z (%) 477 (1) [M^+], 174 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-4-carboxylic acid (17)

^{1}H-NMR ($CDCl_3$): δ 0.89 (t, 3H), 1.28-1.32 (m, 10H), 1.56-1.63 (m, 2H), 2.58 (t, 2H), 4.64 (s, 2H), 5.26 (s, 2H), 6.84 (d, 2H), 7.15 (d, 2H), 7.22 (d, 1H), 7.25-7.29 (m, 1H), 7.31 (d, 1H), 7.35 (d, 1H), 8.02 (d, 1H). MS (EI): m/z (%) 421 (6) [M^+], 107 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-5-carboxylic acid (18)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.27-1.32 (m, 10H), 1.56-1.61 (m, 2H), 2.58 (t, 2H), 4.66 (s, 2H), 5.25 (s, 2H), 6.71 (d, 1H), 6.85 (d, 2H), 7.11-7.16 (m, 4H), 7.96 (d, 1H), 8.49 (s, 1H). MS (EI): m/z (%) 421 (12) [M^+], 174 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-6-carboxylic acid (19)

^{1}H-NMR (DMSO-d_6): δ 0.83 (t, 3H), 1.21-1.27 (m, 10H), 1.48-1.62 (m, 2H), 2.48 (t, 2H), 5.00 (s, 2H), 5.48 (s, 2H), 6.55 (dd, 1H), 6.86 (d, 2H), 7.08 (d, 2H), 7.46 (d, 1H), 7.58-7.62 (m, 2H), 8.06-8.07 (m, 1H). MS (EI): m/z (%) 421 (64) [M^+], 174 (100).

1-Indol-1-yl-3-(4-octylphenoxy)propan-2-one (20)

^{1}H-NMR ($CDCl_3$): δ 0.90 (t, 3H), 1.28-1.31 (m, 10H), 1.57-1.61 (m, 2H), 2.55 (t, 2H), 4.59 (s, 2H), 5.16 (s, 2H), 6.60 (d, 1H), 6.81 (d, 2H), 7.05 (d, 1H), 7.12-7.16 (m, 4H), 7.19-7.23 (m, 1H), 7.65 (d, 1H). MS (EI): m/z (%) 377 (13) [M^+], 130 (100).

1-(5-Methylindol-1-yl)-3-(4-octylphenoxy)propan-2-one (21)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.27-1.31 (m, 10H), 1.55-1.59 (m, 2H), 2.44 (s, 3H), 2.56 (t, 2H), 4.57 (s, 2H), 5.12 (s, 2H), 6.51 (d, 1H), 6.79 (d, 2H), 7.00-7.02 (m, 3H), 7.11 (d, 2H), 7.42-7.43 (m, 1H). MS (EI): m/z (%) 391 (12) [M^+], 144 (100).

1-(5-Chloroindol-1-yl)-3-(4-octylphenoxy)propan-2-one (22)

^{1}H-NMR ($CDCl_3$): δ 0.89 (t, 3H), 1.28-1.32 (m, 10H), 1.56-1.60 (m, 2H), 2.57 (t, 2H), 4.61 (s, 2H), 5.17 (s, 2H), 6.52 (dd, 1H), 6.82 (d, 2H), 6.99 (d, 1H), 7.05 (d, 1H), 7.12-7.15 (m, 3H), 7.60 (d, 1H). MS (EI): m/z (%) 413 (2), and 411 (4) [M^+], 164 (100).

1-(5-Methoxyindol-1-yl)-3-(4-octylphenoxy)propan-2-one (23)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.27-1.31 (m, 10H), 1.55-1.57 (m, 2H), 2.56 (t, 2H), 3.85 (s, 3H), 4.56 (s, 2H), 5.12 (s, 2H), 6.51 (dd, 1H), 6.80 (d, 2H), 6.86 (dd, 1H), 7.01 (d, 1H), 7.02 (d, 1H), 7.10 (d, 1H), 7.12 (d, 2H). MS (EI): m/z (%) 407 (3) [M^+], 160 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-5-carbonitrile (24)

^{1}H-NMR ($CDCl_3$): δ 0.89 (t, 3H), 1.28-1.32 (m, 10H), 1.58-1.62 (m, 2H), 2.59 (t, 2H), 4.67 (s, 2H), 5.27 (s, 2H), 6.67 (dd, 1H), 6.85 (d, 2H), 7.11 (d, 1H), 7.14 (d, 1H), 7.16 (d, 2H), 7.41 (dd, 1H), 7.99 (dd, 1H). MS (EI): m/z (%) 402 (2) [M^+], 155 (100).

Methyl 1-[3-(4-octylphenoxy)-2-oxopropyl]indole-5-carboxylate (25)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.27-1.31 (m, 10H), 1.57-1.60 (m, 2H), 2.57 (t, 2H), 3.92 (s, 3H), 4.63 (s, 2H), 5.22 (s, 2H), 6.67 (dd, 1H), 6.83 (d, 2H), 7.08-7.10 (m, 2H), 7.14 (d, 2H), 7.89 (dd, 1H), 8.39 (m, 1H). MS (EI): m/z (%) 435 (7) [M^+], 188 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-5-carbaldehyde (26)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.28-1.32 (m, 10H), 1.59-1.63 (m, 2H), 2.58 (t, 2H), 4.67 (s, 2H), 5.26 (s, 2H), 6.74 (dd, 1H), 6.85 (d, 2H), 7.12 (d, 1H), 7.15 (d, 2H), 7.16 (d, 1H), 7.76 (dd, 1H), 8.16-8.17 (m, 1H), 10.02 (s, 1H). MS (EI): m/z (%) 405 (1) [M^+], 158 (100).

1-[2-Hydroxy-3-(4-octylphenoxy)propyl]indole-5-carboxamide (27)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.26-1.30 (m, 10H), 1.55-1.58 (m, 2H), 2.52 (m, 3H), 3.85 (dd, 1H), 3.94 (dd, 1H), 4.32-4.39 (m, 2H), 4.46 (dd, 1H), 5.40-6.28 (br s, 2H), 6.59 (d, 1H), 6.80 (d, 2H), 7.09 (d, 2H), 7.23 (d, 1H), 7.42 (d, 1H), 7.66 (d, 1H), 8.12 (s, 1H). MS (EI): m/z (%) 422 (2) [M^+], 173 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indol-5-carboxamide (28)

^{1}H-NMR (DMSO-d_6): δ 0.84 (t, 3H), 1.23-1.26 (m, 10H), 1.49-1.53 (m, 2H), 2.47-2.51 (m, 2H), 4.97 (s, 2H), 5.39 (s, 2H), 6.54 (d, 1H), 6.85 (d, 2H), 7.07-7.10 (m, 3H), 7.33 (d, 1H), 7.38 (d, 1H), 7.65 (d, 1H), 7.83 (br s, 1H), 8.13 (s, 1H). MS (EI): m/z (%) 420 (61) [M^+], 215 (100).

***tert*-Butyl 3-chloroindole-5-carboxylate (30)**

^{1}H-NMR ($CDCl_3$): δ 1.64 (s, 9H), 7.22 (d, 1H), 7.35 (d, 1H), 7.90 (d, 1H), 8.33 (d, 1H), 8.39 (s, 1H). MS (EI): m/z (%) 251 (21) [M^+], 195 (100).

***tert*-Butyl 3-formylindole-5-carboxylate (31)**

^{1}H-NMR (DMSO-d_6): δ 1.55 (s, 9H), 7.56 (dd, 1H), 7.81 (dd, 1H), 8.39 (d, 1H), 8.67 (d, 1H), 9.94 (br s, 1H), 12.40 (br s, 1H). MS (EI): m/z (%) 245 (11) [M^+], 188 (100).

***tert*-Butyl 3-cyanoindole-5-carboxylate (33)**

^{1}H-NMR (DMSO-d_6): δ 1.55 (s, 9H), 7.62 (dd, 1H), 7.82 (dd, 1H), 8.16 (s, 1H), 8.37 (m, 1H), 12.49 (br s, 1H). MS (EI): m/z (%) 242 (14) [M^+], 186 (100).

5-*tert*-Butyl 3-methylindole-3,5-dicarboxylate (34)

^{1}H-NMR ($CDCl_3$): δ 1.58 (s, 9H), 3.94 (s, 3H), 7.42 (d, 1H), 7.92 (d, 1H), 7.99 (d, 1H), 8.84 (d, 1H), 9.36 (br s, 1H). MS (EI): m/z (%) 275 (36) [M^+], 219 (100).

Methyl 3-acetylindole-5-carboxylate (36)

^{1}H-NMR (DMSO-d_6): δ 2.49 (s, 3H), 3.87 (s, 3H), 7.53 (dd, 1H), 7.82 (dd, 1H), 8.43 (d, 1H), 8.85 (d, 1H), 12.23 (br s, 1H). MS (EI): m/z (%) 217 (42) [M^+], 202 (100).

3-Acetylindole-5-carboxylic acid (37)

^{1}H-NMR (DMSO-d_6): δ 2.47 (s, 3H), 7.50 (dd, 1H), 7.86 (dd, 1H), 8.41 (d, 1H), 8.82 (d, 1H), 12.17 (br s, 1H), 12.57 (br s, 1H). MS (EI): m/z (%) 203 (49) [M^+], 188 (100).

***tert*-Butyl 3-acetylindole-5-carboxylate (38)**

^{1}H-NMR (DMSO-d_6): δ 1.56 (s, 9H), 2.46 (s, 3H), 7.50 (d, 1H), 7.76 (d, 1H), 8.40 (s, 1H), 8.78 (s, 1H), 12.17 (br s, 1H). MS (EI): m/z (%) 259 (29) [M^+], 188 (100).

3-*tert*-Butyl-1-[3-(4-octylphenoxy)-2-oxopropyl]indole-5-carboxylic acid (39)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.26-1.30 (m, 10H), 1.46 (s, 9H), 1.56-1-60 (m, 2H), 2.57 (t, 2H), 4.62 (s, 2H), 5.15 (s, 2H), 6.82 (m, 3H), 7.09 (d, 1H), 7.14 (d, 2H), 7.93 (dd, 1H), 8.65 (s, 1H). MS (EI): m/z (%) 477 (23) [M^+], 107 (100).

3-Chloro-1-[3-(4-octylphenoxy)-2-oxopropyl]indole-5-carboxylic acid (40)

^{1}H-NMR ($CDCl_3$): δ 0.88 (t, 3H), 1.28 (m, 10H), 1.62 (m, 2H), 2.58 (t, 2H), 4.68 (s, 2H), 5.22 (s, 2H), 6.91 (d, 2H), 7.09 (m, 2H), 7.16 (d, 2H), 7.97 (d, 1H), 8.47 (s, 1H). MS (ESI): m/z (%) 465 $[M-H]^-$.

3-Cyano-1-[3-(4-octylphenoxy)-2-oxopropyl]indole-5-carboxylic acid (41)

^{1}H-NMR (DMSO-d_6): δ 0.83 (t, 3H), 1.22-1.25 (m, 10H), 1.51 (m, 2H), 2.47-2.49 (m, 2H), 5.01 (s, 2H), 5.57 (s, 2H), 6.89 (d, 2H), 7.10 (d, 2H), 7.68 (d, 1H), 7.88 (dd, 1H), 8.22 (s, 1H), 8.28 (m, 1H). MS (ESI): m/z (%) 445 $[M-H]^-$.

3-Formyl-1-[3-(4-octylphenoxy)-2-oxopropyl]indole-5-carboxylic acid (42)

^{1}H-NMR (DMSO-d_6): δ 0.83 (t, 3H), 1.24 (m, 10H), 1.51 (m, 2H), 2.51 (t, 2H), 5.03 (s, 2H), 5.58 (s, 2H), 6.90 (d, 2H), 7.11 (d, 2H), 7.60 (d, 1H), 7.86 (dd, 1H), 8.29 (s, 1H), 8.74 (d, 1H), 9.97 (s, 1H). MS (ESI): m/z (%) 449 $[M-H]^-$.

3-Acetyl-1-[3-(4-octylphenoxy)-2-oxopropyl]indole-5-carboxylic acid (43)

^{1}H-NMR (DMSO-d_6): δ 0.83 (t, 3H), 1.23 (m, 10H), 1.51 (m, 2H), 2.47 (m, 2H), 2.51 (s, 3H), 5.03 (s, 2H), 5.53 (s, 2H), 6.89 (d, 2H), 7.10 (d, 2H), 7.56 (d, 1H), 7.81 (dd, 1H), 8.33 (s, 1H), 8.83 (d, 1H), 12.72 (br s, 1H). MS (ESI): m/z (%) = 463 $[M-H]^-$.

3-Methylhydrogen 1-[3-(4-octylphenoxy)-2-oxopropyl]indole-3,5-dicarboxylate (44)

^{1}H-NMR (DMSO-d_6): δ 0.83 (t, 3H), 1.22 (m, 10H), 1.50 (m, 2H), 2.53 (m, 2H), 3.83 (s, 3H), 5.00 (s, 2H), 5.52 (s, 2H), 6.88 (d, 2H), 7.09 (d, 2H), 7.57 (d, 1H), 7.80 (dd, 1H), 8.16 (s, 1H), 8.65 (d, 1H). MS (ESI): m/z (%) = 479 $[M-H]^-$.

Dimethyl indole-3,5-dicarboxylate (46)

^{1}H-NMR (DMSO-d_6): δ 3.82 (s, 3H), 3.86 (s, 3H), 7.56 (d, 1H), 7.83 (dd, 1H), 8.21 (d, 1H), 8.67 (m, 1H), 12.25 (br s, 1H). MS (EI): m/z (%) 233 (69) $[M^+]$, 202 (100).

Dibenzyl indole-3,5-dicarboxylate (47)

^{1}H-NMR ($CDCl_3$): δ 5.40 (s, 4H), 7.27-7.45 (m, 11H), 7.98-8.02 (m, 2H), 8.97 (br s, 1H), 8.98 (m, 1H). MS (EI): m/z (%) 385 (41) $[M^+]$, 278 (100).

Dibenzyl 1-[2-hydroxy-3-(4-octylphenoxy)propyl]indol-3,5-dicarboxylate (48)

^{1}H-NMR ($CDCl_3$): δ 0.86 (t, 3H), 1.22-1.28 (m, 10H), 1.55 (m, 2H), 2.51 (t, 2H), 2.54 (br s, 1H), 3.88 (dd, 1H), 3.93 (dd, 1H), 4.29-4.33 (m, 2H), 4.39 (dd, 1H), 5.30 (s, 2H), 5.36 (s, 2H), 6.76 (d, 2H), 7.08 (d, 2H), 7.28-7.46 (m, 11H), 7.92-7.96 (m, 2H), 8.94 (s, 1H).). MS (EI): m/z (%) 647 (6) $[M^+]$, 91 (100).

Dibenzyl 1-[3-(4-octylphenoxy)-2-oxopropyl]indole-3,5-dicarboxylate (49)

^{1}H-NMR ($CDCl_3$): δ 0.86 (t, 3H), 1.26-1.30 (m, 10H), 1.56 (m, 2H), 2.55 (t, 2H), 4.67 (s, 2H), 5.26 (s, 2H), 5.38 (s, 4H), 6.84 (d, 2H), 7.07 (d, 1H), 7.14 (d, 2H), 7.31-7.37 (m, 8H), 7.44 (m, 2H), 7.81 (s, 1H), 7.98 (d, 1H), 8.97 (m, 1H).). MS (EI): m/z (%) 645 (6) $[M^+]$, 354 (100).

1-[3-(4-Octylphenoxy)-2-oxopropyl]indole-3,5-dicarboxylic acid (50)

^{1}H-NMR (DMSO-d_6): δ (ppm) = 0.82 (t, J = 7 Hz, 3H), 1.21-1.23 (m, 10H), 1.49-1.51 (m, 2H), 2.48 (m, 2H), 5.00 (s, 2H), 5.51 (s, 2H), 6.68 (d, 2H), 7.09 (d, 2H), 7.53 (d, 1H), 7.78 (dd, 1H), 8.07 (s, 1H), 8.68 (d, 1H). MS (ESI): m/z (%) 464 $[M-H]^-$.

1-[3-(4-Decyloxyphenoxy)-2-oxopropyl]indole-5-carboxylic acid (54)

^{1}H-NMR ($CDCl_3$): δ (ppm) = 0.89 (t, 3H), 1.28-1.33 (m, 12H), 1.43-1.49 (m, 2H), 1.75-1.82 (m, 2H), 3.93 (t, 2H), 4.63 (s, 2H), 5.25 (s, 2H), 6.72 (dd, 1H), 6.84-6.89 (m, 4H), 7.12 (d, 1H), 7.14 (d, 1H), 7.97 (dd, 1H), 8.50 (d, 1H). MS (EI): m/z (%) 465 (13) [M^+], 174 (100).

5-*tert*-Butyl-3-methyl 1-[3-(4-decyloxyphenoxy)-2-hydroxypropyl]indole-3,5-dicarboxylate (55)

^{1}H-NMR ($CDCl_3$): δ 0.86 (t, 3H), 1.26-1.34 (m, 12H), 1.39-1.45 (m, 2H), 1.60 (s, 9H), 1.73 (quin, 2H), 2.57 (s, 1H), 3.81-3.92 (m, 7H), 4.31-4.48 (m, 2H), 4.45 (m, 1H), 6.79 (m, 4H), 7.39 (d, 1H), 7.88 (dd, 1H), 7.93 (s, 1H), 8.77 (s, 1H). MS (EI): m/z (%) 582 (14) [M^+], 385 (100).

5-*tert*-Butyl-3-methyl 1-[3-(4-decyloxyphenoxy)-2-oxopropyl]indole-3,5-dicarboxylate (56)

^{1}H-NMR ($CDCl_3$): δ 0.86 (t, 3H), 1.24-1.29 (m, 14H), 1.60 (s, 9H), 1.75 (m, 2H), 3.81-3.92 (m, 5H), 4.63 (s, 2H), 5.25 (s, 2H), 6.85-6.87 (m, 4H), 7.06 (d, 1H), 7.78 (s, 1H), 7.90 (dd, 1H), 8,82 (m, 1H). MS (EI): m/z (%) 579 (22) [M^+], 383 (100).

3-Methylhydrogen 1-[3-(4-decyloxyphenoxy)-2-oxopropyl]indole-3,5-dicarboxylate (57)

^{1}H-NMR (DMSO-d_6): δ 0.83 (t, 3H), 1.24-1.29 (m, 14H), 1.64-1.66 (m, 2H), 3.83 (s, 3H), 3.88 (t, 2H), 4.96 (s, 2H), 5.52 (s, 2H), 6.83-6.85 (m, 4H), 7.57 (d, 2H), 7.81 (dd, 1H), 8.16 (s, 1H), 8.66 (m, 1H). MS (ESI): m/z (%) 523 [M-H]$^+$.

{1-[3-(4-Octylphenoxy)-2-oxopropyl]indol-3-yl}acetic acid (59)

^{1}H-NMR (DMSO-d_6): δ 0.84 (t, 3H), 1.22-1.26 (m, 10H), 1.47-1.53 (m, 2H), 2.50 (t, 2H), 3.65 (s, 2H), 4.97 (s, 2H), 5.30 (s, 2H), 6.86 (d, 2H), 7.04-7.12 (m, 4H), 7.18 (s, 1H), 7.26 (d, 1H), 7.53 (d, 1H). MS (EI): m/z (%) 435 (13) [M^+], 188 (100).

High resolution MS

Apparatus: MicroTof, Bruker Daltronics (Bremen, Germany);
Ionization: ESI negative mode; calibration was performed with sodium formiate clusters immediately before measuring the samples.

Compound	$[M-H]^+$	Calculated	Measured
42	$C_{27}H_{30}NO_5^-$	448.21186	448.21433
43	$C_{28}H_{32}NO_5^-$	462.22748	448.22882
44	$C_{28}H_{32}NO_6^-$	478.22241	478.22366
54	$C_{28}H_{34}NO_5^-$	464.24313	464.24442
57	$C_{30}H_{36}NO_7^-$	522.24863	522.25243

Purity of the target compounds
Purity was determined by two different HPLC systems.

Compound	Cyano-Phase[a]	Amino-Phase[b]
13	>99%	>99%
14	97%	97%
17	98%	>99%
18	99%	>99%
19	97%	>99%
20	98%	99%
21	99%	>99%
22	99%	>99%
23	>99%	>99%
24	98%	98%
25	97%	>99%
26	99%	99%
28	99%	>99%
39	98%	>99%
40	98%	>99%
41	95%	99%
42	99%	98%
43	>99%	>99%
44	98%	99%
50	96%	99%
54	99%	99%
57	98%	99%
59	97%	98%

a:
Column: LiChrospher 100 CN, 5 µm, 3.0 mm (I.D.) x 250 mm, Merck, Darmstadt
Mobile phase: isohexane/THF containing 0.1% trifluoroacetic acid, gradient elution
Flow rate: 0.5 mL/min
Detection: UV absorbance at 254 nm

b:
Column: Spherisorb NH_2, 5 µm, 4.0 mm (I.D.) x 250 mm, Latek, Heidelberg
Mobile phase: isohexane/THF, gradient elution
Flow rate: 0.75 mL/min
Detection: UV absorbance at 254 nm