Supporting Information for

From Peptides to Non-Peptide Peptidomimetics: Design and Synthesis of New Piperidine Inhibitors of Aspartic Peptidases

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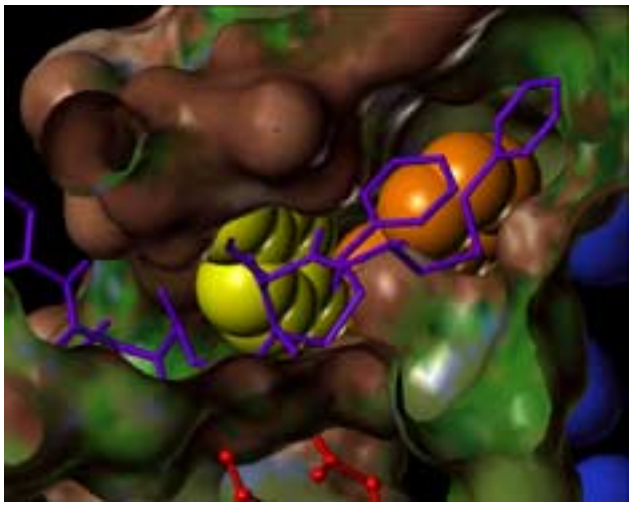

Figure 2. X-ray structure of **6** bound in porcine pepsin active site. Flap, light brown; **6**, purple; Asp32 & Asp215, red; Try75, yellow; Trp39, orange**.**

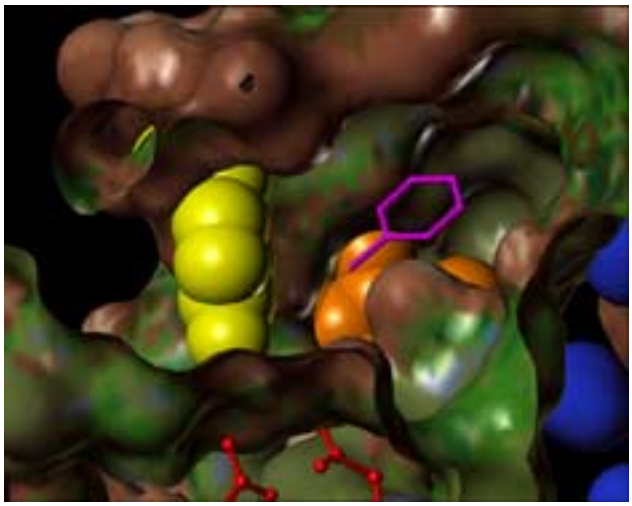

Figure 7. Active site of porcine pepsin after flap opening and rotating Tyr75 and Trp39 side-chains. Flap, light brown; S-Benzyl **7**, pink; Asp32 & Asp215, red; Try75, yellow; Trp39, orange.

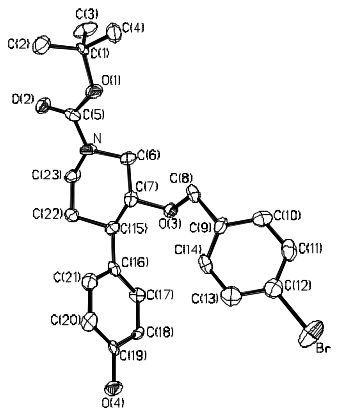

Figure 8. X-ray structure of Phenol **23**.

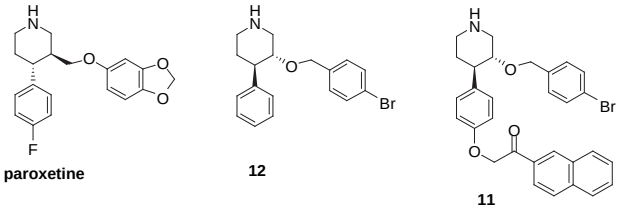

Figure 9. Comparison of piperidine inhibitors **11** & **12** with paroxetine.

Experimentals

A. General

All reactions were carried out under an atmosphere of argon using flame or oven dried glassware. A Buchi rotary evaporator equipped with a water condenser, a dry ice trap, and a water aspirator was used for the concentrated *in vacuo* steps. Tetrahydrofuran (THF) was distilled from Na/benzophenone. Dichloromethane (DCM) was distilled from calcium hydride. All other solvents and reagents were purchased from Aldrich and used without further purification.

^{1}H NMR spectra were taken on a 300 MHz Bruker Aspect 3000 system at ambient temperature. Chemical shifts were reported in ppm (δ units) downfield from tetramethylsilane (TMS) as the internal standard except for MeOH-d_4 where solvent peaks were used as the internal standard. Electron Impact mass spectra (EIMS) was determined on a ?? spectrometer. Fast atom bombardment (FAB) mass spectra was determined on a ?? Spec spectrometer.

Liquid chromatography was performed by flash chromatography using Merck grade 60 silica gel (230-400 mesh). Analytical thin layer chromatography (TLC) was run on Merck Kiesselgel 60F_{254} precoated plates of 0.25 mm thickness. For visualization, either ultraviolet light, polyphosphomolybdic acid and cerium sulfate in EtOH with H_2SO_4,or ninhydrin in EtOH with H_2SO_4 was used.

B. Procedures

tert-Butyl 4-phenyl-3,6-dihydro-2H-pyridine-1-carboxylate (**13**). To a stirred solution of 4-phenyl-1,2,3,6-tetrahydropyridine hydrochloride (5.17 g, 26.4 mmol) in CH_3CN (200 mL) was added triethylamine (7.36 mL, 52.8 mmol). After stirring 15 min a solution of Boc_2O (6.92 g, 31.7 mmol) in CH_3CN (10 mL) and DMAP (0.16 g, 1.3 mmol) was added. The reaction mixture was allowed to stir overnight. The solvent was removed under reduced pressure. The resulting residue was dissolved in CH_2Cl_2 (150 mL), washed with 1N HCl (3 x 75 mL), dried (Na_2SO_4), and concentrated *in vacuo*. Purification via flash column chromatography (CH_2Cl_2) afforded 6.33 g (93%) of **13** as a light yellow solid. TLC R_f = 0.60 (100% DCM); ^{1}H NMR ($CDCl_3$) δ 7.29-7.37 (m, 5H), 5.90 (bs, 1H), 3.96 (d, J= 2.1Hz, 2H), 3.52 (t, J= 5.6Hz, 2H), 2.40 (bs, 2H), 1.40 (s, 9H);^{13}C NMR ($CDCl_3$) δ 154.91, 140.71,135.41, 128.43, 124.92, 79.66, 43.72, 39.90, 28.52, 27.41; EI-MS: Calculated for [$C_{23}H_{23}NO_4$] 259.1562 found 259.1572.

(R, R)-tert-Butyl-3,4-dihydroxy-4-phenyl-piperidine-1-carboxylate (**14**). To a stirred solution of AD-mix-α (26.99 g) in *t*BuOH (95 mL) and H_2O (95 mL) was added $CH_3SO_2NH_2$ (1.83 g, 19.3 mmol). The reaction mixture was cooled to 0^o C followed by addition of **13** (5.00 g, 19.3 mmol). The reaction was stirred at 0^o C for 30 min and allowed to stir overnight at rt. To the reaction mixture was added Na_2SO_3 (28.95 g) followed by stirring for 1 h then addition of CH_2Cl_2 (180 mL). The layers were separated and the aqueous layer washed with CH_2Cl_2 (4 x 70 mL). The combined organics were washed with 2N KOH (150 mL), dried (Na_2SO_4), and concentrated *in vacuo*. Purification via flash column chromatography (hexanes/ EtOAc 7:3) afforded 5.34 g (95%) of **8** as white foam. TLC R_f = 0.31 (30% EtOAc-hexane); ^{1}H NMR (CD_3OD) δ 7.46 (m, 2H), 7.29 (m, 2H), 7.18 (m, 1H), 4.00 (m, 2H), 3.84 (dd, J=10.5, 5.1 Hz, 2H), 3.26 (m, 2H), 1.83 (m, 1H), 1.63 (m, 1H), 1.48 (s, 9H);^{13}C NMR (CD_3OD) δ 156.50, 147.28, 129.08, 127.72, 126.45, 81.85, 75.19, 72.00, 46.24, 40.03, 39.37, 28.71; ESI-MS: Calculated for $[C_{16}H_{24}NO_4]^+$ 294.1705 found 294.1703.

(R, R)-tert-Butyl-3-hydroxy-4-phenyl-piperidine-1-carboxylate (**15**). To a vigorously stirred solution of **14** (5.34 g, 18.2 mmol) in EtOH (180 mL) was added approx. 1 g Raney-Nickel (50/50 water slurry). The stirred suspension was heated to reflux for 5 h. The reaction mixture was allowed to cool to rt, filtered over a celite pad, and rinsed with copious amounts of EtOH. (**Note**: Caution must be taken as Raney-Nickel will ignite if allowed to dry). The solvent was removed *in vacuo* and purification via flash column chromatography (hexanes/ EtOAc 7:3) afforded 4.08 g (81%) of **15** as a white foam. TLC R_f = 0.51 (30% EtOAc-hexane); ^{1}H NMR ($CDCl_3$) δ 7.35 (m, 2H), 7.26 (m, 3H), 4.38 (m, 1H), 4.19 (m, 1H),

3.67 (m, 1H), 2.76 (m, 1H), 2.63 (m, 1H), 2.52 (m, 1H), 1.81-1.60 (m, 2H), 1.48 (s, 9H);^{13}C NMR (CD_3OD) δ 156.16, 144.01, 129.37, 128.90, 127.49, 81.11, 71.03, 52.00, 45.38, 44.63, 33.89, 28.74; ESI-MS: Calculated for $[C_{16}H_{24}NO_3]^+$ 278.1756 found 278.1757.

(R, R)-tert-Butyl-3-(4-bromo-benzyloxy)-4-phenyl-piperidine-1-carboxylate (**16**). To a stirred suspension of NaH (0.035 g of a 60% suspension, 8.65 mmol) in DMF (4 mL) at 0° C was added **15** (0.20 g, 7.21 mmol) in DMF (6 mL) via canula. Following stirring for 1 h at 0° C *p*-bromobenzyl bromide (0.69 g, 4.0 mmol) was added to the reaction mixture. The reaction was stirred at 0° C for 1 h and allowed to stir overnight at rt. To the reaction mixture was added Et_2O (50 mL) and the mixture washed with H_2O (2 x 25 mL) and brine (20 mL). The organic layer was dried (Na_2SO_4) and concentrated *in vacuo*. Purification via flash column chromatography (hexanes/ EtOAc 4:1) afforded 0.25 g (77%) of **16** as a white solid. TLC R_f = 0.48 (20% EtOAc-hexane); ^{1}H NMR ($CDCl_3$) δ 7.26 (m, 7H), 6.7 (d, J= 8.4 Hz, 2H), 4.50-4.07 (m, 4H), 3.37 (m, 1H), 2.76 (m, 1H), 2.27 (m, 2H), 1.80-1.61 (m, 2H), 1.48 (s, 9H);^{13}C NMR ($CDCl_3$) δ 160.60, 142.65, 137.09, 131.83, 131.24, 130.01, 129.30, 128.42, 127.10, 126.71, 79.92, 78.25, 75.05, 71.06, 64.86, 49.76, 32.17, 28.45; ESI-MS: Calculated for $[C_{23}H_{29}NO_3Br]^+$ 446.1331 found 446.1310.

(R, R)-3-(4-bromo-benzyloxy)-4-phenyl-piperidine-hydrochloride (**12**). To a stirred solution of **12** (0.035 g, 0.08 mmol) was added 4N HCl-dioxane (1 mL). Tituration with Et_2O afforded 0.026 g (87%) of **12** used without further purification. ^{1}H NMR (CD_3OD) δ 7.34-7.25 (m, 7H), 6.7 (d, J= 8.4 Hz, 2H), 4.35 (d, J=11.7 Hz, 1H), 4.13 (d, J= 12.0 Hz, 1H), 3.97 (ddd, J= 15.0, 10.5, 4.8 Hz, 1H), 3.78-3.65 (m, 1H), 3.52-3.39 (m, 2H), 2.93-2,69 (m, 2H), 2.07-1.97 (m, 2H); FAB-MS: Calculated for $[C_{18}H_{21}NOBr]^+$ 346.0807 found 346.0790.

tert-Butyl 1,2,3,6-Tetrahydro-4-[(trifluoromethyl)sulfonyloxy]-pyridine-1-carboxylate (**17**). A solution of t-butyl 4-oxypiperidine-1-carboxylate (3.25, 16.3 mmol) in THF (25 mL) was added dropwise over 25 min to a stirred solution of LDA (1.5 M in hexanes, 12.0 mL, 17.9 mmol) in THF (25 mL) at -78° C. After stirring for 20 min, a solution of N-phenyltrifluoromethanesulfonamide (6.24 g, 17.5 mmol) in THF (25 mL) was added. The mixture was stirred for 3.5 h at 0° C. The reaction was concentrated *in vacuo* and filtered over a pad of alumina (hexanes/ EtOAc 9:1) to afford 4.9 (91%) g of **17** as an pale yellow oil used without further purification.

4-phenoxy-tert-butyl-dimethyl-silane boronic acid (**18**). A solution of *n*-BuLi (2.5 M in hexanes, 10.4 mL, 26.1 mmol) was added dropwise to a stirred solution of (4-Bromo-phenoxy)-*tert*-butyl-dimethyl-

silane (6.0 g, 21.0 mmol) in THF (50 mL) at –78˚ C. The reaction mixture was stirred for 30 min at –78˚ C and triisopropyl borate (4.7 mL, 41.8 mmol) was added rapidly. The mixture was stirred for 30 min at –78˚ C and rt for 1 h. The reaction mixture was partitioned between 10% aqueous HCl (100 mL) and EtOAc (200 mL). The organic layer was washed with brine (2 x 50 mL), dried (Na_2SO_4), and concentrated in vacuo to afford 4.9 g (92%) of **18** as an off white solid used without further purification.

tert-Butyl 4-[4-(tert-butyl-dimethyl-silanoxy-phenyl]-3,6-dihydro-2H-pyridine-1-carboxylate (**19**). A three neck flask was charged with triflate **17** (3.81 g, 11.8 mmol), boronic acid **18** (4.03 g, 16.0 mmol), LiCl (1.50 g, 35.5 mmol), aq Na_2CO_2 (16.56 mL of a 2N solution), 1,2-dimethoxyethane (DME, 35 mL) and $Pd(PPh_3)_4$ (0.68 g, 0.59 mmol). The reaction mixture was heated to reflux for 2 h followed by cooling to rt and concentration under reduced pressure. The resulting residue was partitioned between CH_2Cl_2 (125 mL), aqueous 2N Na_2CO_2 (100 mL), and concentrated NH_4OH (6 mL). The layers were separated and the aqueous layer extracted again with CH_2Cl_2 (3 x 125 mL). The combined organics were dried (Na_2SO_4) and concentrated *in vacuo*. The resulting black residue was purified via flash column chromatography (hexanes/ CH_2Cl_2/ EtOAc 9:1:1) to afford 2.3 g (52%) of **19** as a light yellow oil. TLC R_f = 0.59 (30% EtOAc-hexane);^{1}H NMR ($CDCl_3$) δ 7.30 (d, J= 8.4 Hz, 2H), 6.80 (d, J= 8.4 Hz, 2H), 5.95 (bs, 1H), 4.01 (d, J= 2.2Hz, 2H), 3.59 (t, J= 5.7Hz, 2H), 2.46 (bs, 2H), 1.50 (s, 9H), 0.98 (s, 9H), 0.19 (s, 6H); ^{13}C NMR ($CDCl_3$) δ 155.01, 134.72, 133.76, 125.82, 119.92, 119.07, 79.56, 43.68, 41.03, 28.48, 27.35, 25.66, 18.20, -4.43. EI-MS: Calculated for [$C_{22}H_{35}NO_3Si$] 389.2393 found 389.2386

tert-Butyl 4-[4-(tert-butyl-dimethyl-silanoxy-phenyl]-3,4-dihydroxy-piperidine-1-carboxylate (**20**). To a stirred solution of AD-mix-α (7.94 g) in *t*BuOH (20 mL) and H_2O (20 mL) was added $CH_3SO_2NH_2$ (0.54 g, 5.67 mmol). The reaction mixture was cooled to 0^o C followed by the addition of **19** (2.21 g, 5.67 mmol) with *t*BuOH (9 mL) and H_2O (9 mL). The reaction was stirred at 0^o C for 30 min and allowed to stir overnight at rt. To the reaction mixture was added Na_2SO_3 (8.51 g) followed by stirring for 1 h then addition of CH_2Cl_2 (60 mL). The layers were separated and the aqueous layer washed with CH_2Cl_2 (4 x 30 mL). The combined organics were washed with 2N KOH (50 mL), dried (Na_2SO_4), and concentrated *in vacuo*. Purification via flash column chromatography (hexanes/ EtOAc 7:3) afforded 2.20 g (92%) of **20** as a white foam. TLC R_f = 0.43 (30% EtOAc-hexane); ^{1}H NMR (CD_3OD) δ 7.38 (d, J= 8.6 Hz, 2H), 6.82 (d, J= 8.6 Hz, 2H), 4.04, (dd, J= 12.3, 4.8 Hz, 1H), 3.91-3.82 (m, 2H), 3.17-3.06 (m, 2H), 1.88 (ddd, J= 18.4, 13.6, 4.6, 1 H), 1.73-1.68 (m, 1 H), 1.49 (s, 9H), 1.00 (s, 9H), 0.19 (s, 6H);^{13}C NMR (CD_3OD) δ 156.49, 155.66, 140.19, 127.67, 120.57, 81.15, 74.91, 71.99, 46.68, 40.58,

39.46, 28.72, 26.19, 19.03, -4.28; FAB-MS: Calculated for $[C_{22}H_{37}NO_5SiNa]^+$ 446.2339 found 446.2337.

(R, R)-tert-Butyl 3-hydroxy-4-(4-hydroxy-phenyl)-piperidine-1-carboxylate (**21**). To a solution of **20** (2.0 g, 4.7 mmol) in THF at 0˚C was added TBAF (1.0 M in THF, 9.44 mL, 9.4 mmol). The reaction mixture was stirred at 0° C for 1 h and 1 h at rt. To the reaction mixture was added acetic acid (1 mL) and EtOAc (200 mL). The reaction mixture was washed with NH_4Cl (2 x 60 mL) and brine (60 mL), dried (Na_2SO_4), and concentrated *in vacuo* to afford a tan colored oil. This residue was dissolved in EtOH (200 mL) and approx. 1 g of Raney-Nickel (50/50 water slurry) was added with vigorous stirring. The stirred suspension was heated to reflux for 4 h. The reaction mixture was allowed to cool to rt, filtered over a celite pad, and rinsed with EtOH (300 mL). (**Note**: Caution must be taken as Raney-Nickel will ignite if allowed to dry). The solvent was removed *in vacuo* and purification via flash column chromatography (CH_2Cl_2/ MeOH 95:5) afforded 1.10 g (80%) of **21** as a white foam. TLC R_f = 0.47 (93% DCM-MeOH); ^{1}H NMR ($CDCl_3$) δ 7.05 (d, J= 8.3 Hz, 2H), 6.80 (d, J= 8.3 Hz, 2H), 5.30 (s, 1H), 4.33-4.10 (m, 3H), 3.48 (m, 1H), 2.74 (m, 1H), 2.66 (m, 1H), 2.42 (m, 1H), 1.80-1.62 (m, 2H), 1.49 (s, 9H);^{13}C NMR ($CDCl_3$) δ 156.18, 144.23, 129.48, 128.73, 127.49, 81.11, 71.12, 52.23, 45.78, 44.63, 33.89, 28.52; FAB-MS: Calculated for $[C_{16}H_{23}NO_4Na]^+$ 316.1525 found 316.1532.

(R,R)-tert-Butyl3-(4-bromo-benzyloxy)-4-(4-triisopropylsilanyloxy-phenyl)-piperidine-1-carboxylate (**22**). To a stirred solution of **21** (0.58 g, 1.98 mmol) and imidazole (0.30 g, 4.35 mmol) in CH_2Cl_2 (20 mL) at 0° C was added TIPS-Cl (0.53 mL, 2.47 mmol). The reaction was stirred at 0° C for 30 min and allowed to stir overnight at rt. The reaction mixture was washed with H_2O (25 mL), brine (25 mL), dried (Na_2SO_4), and concentrated *in vacuo*. Purification via flash column chromatography (hexanes/ EtOAc 4:1) afforded 0.80 g (90%) of the protected phenol as a white foam. TLC R_f = 0.29 (98% DCM-MeOH); ^{1}H NMR ($CDCl_3$) δ 7.10 (d, J= 8.5 Hz, 2H), 6.81 (d, J= 8.5 Hz, 2H), 4.39-4.16 (m, 2H), 3.59 (m, 1H), 2.73-2.61 (m, 2H), 2.45 (m, 1H), 1.77 (m, 3H), 1.48 (s, 9H);^{13}C NMR ($CDCl_3$) δ 155.23, 154.67, 133.41, 128.67, 120.20, 79.78, 71.05, 50.75, 49.78, 43.58, 31.97, 28.42, 17.89, 12.63; ESI-MS: Calculated for $[C_{25}H_{44}NO_4Si]^+$ 450.3039 found 450.3022.

To a stirred suspension of NaH (0.10 g of a 60% suspension, 2.4 mmol) in THF (350 mL) at 0° C was added the alcohol (0.90 g, 2.0 mmol). Following stirring for 1 h at rt *p*-bromobenzyl bromide (0.69 g, 4.0 mmol) was added. The reaction mixture was heated to 50° C and allowed to stir overnight. To the reaction mixture was added EtOAc (100 mL) and H_2O (25 mL). The layers were separated and the organic layer dried (Na_2SO_4), and concentrated *in vacuo*. Purification via flash column chromatography (hexanes/ EtOAc 5:1) afforded 0.84 g (67%) of **22** as a white solid. TLC R_f = 0.57 (20% EtOAc-

hexane); ^{1}H NMR ($CDCl_3$) δ 7.31 (d, J= 8.6 Hz, 2H), 7.05 (d, J= 8.6 Hz, 2H), 6.83 (overlapping doublets, J= 8.0 Hz, 4H), 4.43-4.11 (m, 4H), 3.32 (m, 1H), 2.74 (m, 1H), 2.59 (m, 2H), 1.17 (m, 2H), 1.48 (s, 9H), 1.26 (m, 6H), 1.12 (d, J= 6.8, 18H); ^{13}C NMR ($CDCl_3$) δ 154.81, 154.64, 137.16, 135.03, 131.26, 129.27, 128.63, 121.33, 119,76, 79.83, 78.47, 71.20, 48.95, 47.95, 44.14, 32.26, 28.45, 17.94, 12.68; ESI-MS: Calculated for $[C_{32}H_{49}NO_4Si]^+$ 618.2614 found 618.2625.

(R, R)-tert-Butyl 3-(4-bromo-benzyloxy)-4-(4-hydro-phenyl)-piperidine-1-carboxylate (**23**). A solution of TBAF (1.0 M in THF, 2.67 mL, 2.67 mmol) was added semi-dropwise to a stirred solution of **22** (0.83 g, 1.34 mmol) in THF (80 mL) at 0° C. The reaction mixture was stirred at 0° C for 1 h then 8 h at rt. To the reaction mixture was added acetic acid (1 mL) and EtOAc (200 mL). The reaction mixture was washed with NH_4Cl (2 x 60 mL) and brine (60 mL), dried (Na_2SO_4), and concentrated *in vacuo*. Purification via flash column chromatography (hexanes/ EtOAc 4:1) afforded 0.53 g (86%) of **23** as a white foam. TLC R_f = 0.23 (20% EtOAc-hexane); ^{1}H NMR ($CDCl_3$) δ 7.31 (d, J= 7.9 Hz, 2H), 7.05 (d, J= 8.5 Hz, 2H), 6.77 (overlapping doublets, J= 8.5 Hz, 4H), 5.17 (s, 1H), 4.32-4.09 (m, 4H), 3.31 (m, 1H), 2.75 (m, 1H), 2.59 (m, 2H), 1.79-1.6 (m, 3H), 1.49 (s, 9H); ^{13}C NMR ($CDCl_3$) δ 154.76, 154.68, 137.06, 134.42, 131.20, 129.25, 128.85, 121.30, 115.19, 80.18, 78.32, 71.02, 48.72, 47.54, 44.07, 32.23, 28.43; ESI-MS: Calculated for $[C_{23}H_{29}NO_4Br]^+$ 462.1280 found 462.1286.

(R, R)-tert-Butyl-3-(4-bromo-benzyloxy)-4-[4-(2-naphthalen-1-yl-2-oxo-ethoxy)-phenyl]-piperidine-1-carboxylate (**24**). A stirred suspension of K_2CO_3 (0.038g, 0.27 mmol) and **23** (0.025 g, 0.054 mmol) in acetone (5 mL) was heated to reflux. 2-Bromo-2'-acetonaphthone (0.016 g, 0.065 mmol) was added with acetone (1 mL) and stirred at reflux overnight. To the reaction mixture was added DCM (10 mL) and the mixture washed with H_2O (2 x 5 mL) and brine (5 mL). The organic layer was dried (Na_2SO_4) and concentrated *in vacuo*. Purification via flash column chromatography (hexanes/ EtOAc 4:1) afforded 0.026 g (76%) of **24** as a clear oil. TLC R_f = 0.24 (20% EtOAc-hexane); ^{1}H NMR ($CDCl_3$) δ 8.58 (s, 1H), 8.08-7.88 (m, 4H), 7.63 (m, 2H), 7.30 (d, J= 8.1 Hz, 2H), 7.10 (d, J= 8.7 Hz, 2H), 6.92 (d, J= 8.7Hz, 2H), 6.77 (d, J= 8.1 Hz, 1H), 5.43 (s, 2H), 4.40-4.07 (m, 4H), 3.30 (m, 1H), 2.78 (m, 1H) 2.56 (m, 2H), 1.81-1.62 (m, 2H), 1.48 (s, 9H);^{13}C NMR ($CDCl_3$) δ 194.53, 156.84, 154.58, 137.02, 135.89, 135.71, 132.24, 131.22, 129.96, 129.62, 129.30, 128.88, 128.83, 128.77, 128.68, 128.58, 127.87, 127.02, 123.60, 114.68, 79.87, 78.20, 71.02, 70.97, 48.79, 47.98, 43.95, 32.15, 28.41; ESI-MS: Calculated for $[C_{35}H_{37}NO_5Br]^+$ 630.1855 found 630.1886.

(R, R)-3-(4-bromo-benzyloxy)-4-[4-(2-naphthalen-1-yl-2-oxo-ethoxy)-phenyl]-piperidine-hydrochloride (**11**). To **24** (0.020 g, 0.03 mmol) was added 4N HCl-dioxane (1 mL). Tituration with Et_2O afforded

0.014 g (83%) of **11** used without further purification. ^{1}H NMR (CD_3OD_3) δ 8.72 (s, 1H), 8.10-7.94 (m, 4H), 7.71-7.61 (m, 2H), 7.32 (d, J= 8.2 Hz, 2H), 7.16 (d, J= 8.6 Hz, 2H), 6.97 (d, J= 8.6 Hz, 2H), 6.81 (d, J= 8.5 Hz, 2H), 5.61 (s, 2H), 4.34 (d, J=12.1 Hz, 1H), 4.11 (d, J=12.2 Hz, 1H), 3.58 (m, 2H), 3.31 (m, 1H), 2.79-2.54 (m, 3H), 1.81-1.62 (m, 2H); EI-MS: Calculated for $[C_{30}H_{29}NO_3Br]^+$ 530.1331 found 530.1341

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