Supporting Information for: Catalytic, Asymmetric α-Fluorination of Acid Chlorides: Dual Metal-Ketene-Enolate Activation

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General.

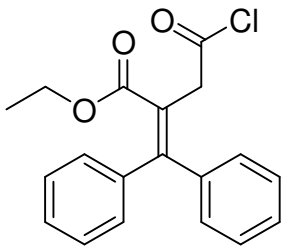
Unless otherwise stated, all reactions were carried out under anhydrous, air-free conditions. All solvents were dried and distilled by standard procedures. The ^{1}H (300 or 400 MHz) and ^{13}C (75 or 101 MHz) and ^{19}F (282 MHz) chemical shifts are given in parts per million (•) with respect to internal TMS or trichlorofluoromethane standards or residual chloroform. Optical rotations were recorded at room temperature. Enantiomeric ratios were obtained by HPLC using DIACEL Chiracel OD and Regis Technologies (*R,R*)-Whelk-01 chiral phase columns. Diasteromeric ratios were determined by proton-decoupled ^{19}F NMR or HPLC. Masses were determined by dissolving all samples in 1:1 THF:MeOH with NaCl and analyzed by positive ion electrospray on a Bruker 12 Tesla APEX-Qe FTICR-MS with an Apollo II ion source. Benzoylquinidine was formed from quinidine and benzoyl chloride according to the method of Pracejus.[1]

General procedure for the synthesis of reported products:

Benzoylquinidine (0.04 mmol) and *trans*-bis-triphenylphosphine palladium(II) chloride (0.012 mmol) were placed into a 10 mL round bottom flask equipped with a magnetic stir bar and 1 mL THF was added. The reaction mixture was cooled to -78 ˚C and Hünig's base (0.4 mmol) was added followed by *N*-Fluorobenzenesulfonimide (0.4 mmol) as a solution in 1 mL THF. The acid chloride (0.4 mmol) was added dropwise as a solution in 1 mL THF and the reaction was kept at -78 ˚C for 6-8 hours. The reaction was quenched with 3 mL methanol and allowed to warm to

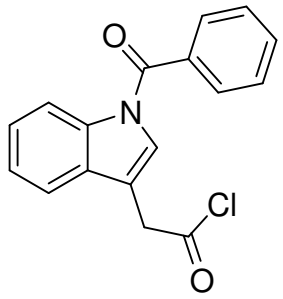
room temperature overnight. The reaction mixture was concentrated and purified by flash chromatography using EtOAc/hexanes.

Procedure for the synthesis of ethyl 4-chloro-2-(diphenylmethylene)-4-oxobutanoate:



3-(Ethoxycarbonyl)-4,4-diphenylbut-3-enoic acid (7.3g, 23.5 mmol) was dissolved in 50 mL CH_2Cl_2 with DMF (cat.) under a drying tube. The mixture was cooled to 0 ºC before oxalyl chloride (3.6g, 28.2 mmol) was added and allowed to warm to room temperature overnight. The reaction mixture was then concentrated and placed under high vacuum for several hours before being used in the above general reaction procedure to yield product **2l**. ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.36-7.33 (m, 3H), 7.29-7.27 (m, 3H), 7.14-7.11 (m, 4H), 3.99-3.94 (m, 4H), 0.88 (t, 3H); ^{13}C NMR ($CDCl_3$) δ 171.9, 167.9, 155.1, 141.3, 140.1, 128.7, 128.6, 128.5, 128.4, 128.2, 128.1, 123.1, 60.9, 49.8, 13.3.

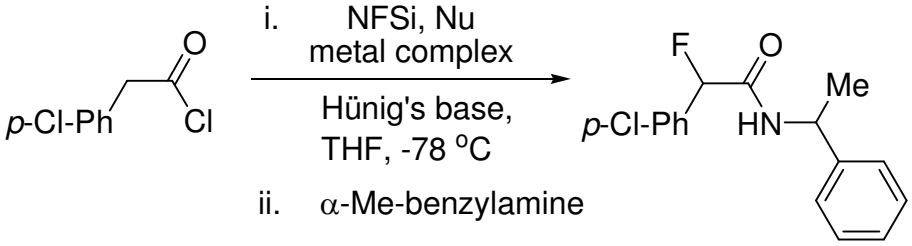
Procedure for the synthesis of 2-(1-benzoyl-1H-indol-3-yl)acetyl chloride:



2-(1-Benzoyl-1H-indol-3-yl)acetic acid (3.67g, 13.1 mmol) was suspended in 30 mL of CH_2Cl_2 under N_2. The mix was cooled to 0 ºC and oxalyl chloride (1.18 mL, 13.8 mmol) was added dropwise, followed by 2 drops of dimethylformide. The reaction mixture was allowed to warm to room temperature overnight, during which time all solids dissolved. The solvents were removed in vacuo to give a thick brown residue which was combined with a small amount of diethyl ether, then diluted with hexanes. The cloudy, white, top layer was separated from the brown residue by decantation and the process was repeated three times. The combined decanted

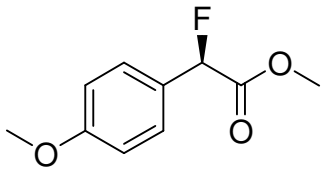
layers were evaporated to give a light brown oil which was recrystallized from ethyl acetate/hexanes in the freezer over 2 days to give light brown crystals (0.307g, 8% yield). ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 8.41 (d, 1H), 7.79-7.71 (m, 2H), 7.67-7.60 (m, 1H), 7.59-7.50 (m, 3H), 7.47-7.35 (m, 3H), 4.24 (s, 2H); ^{13}C NMR ($CDCl_3$) δ 171.2, 168.5, 136.3, 134.3, 132.3, 129.7, 129.3, 128.9, 127.1, 125.8, 124.3, 118.7, 116.8, 112.2.

Absolute configuration was confirmed from products **2e** and **2f** by optical rotation. In addition, we correlate these α-fluorination products with our previous results for α-chlorination and α-bromination – each instance agrees that the BQd consistently gives the sense of induction observed here (see reference 5 of the Communication manuscript). Finally, the following correlation was also shown:

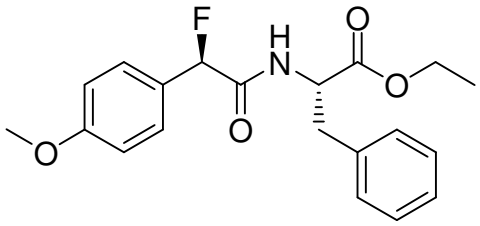


All four diastereomers were confirmed by comparison of the crude ^{19}F NMR with those values obtained by Barrelle and Hamman[2], when α-methylbenzylamine of known absolute configuration was used.

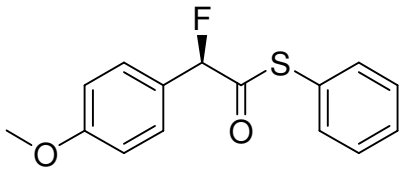
For instance, the shift-difference δ_f(RR) - δ_f(RS) = -1.34 ppm (lit = -1.36 ppm).



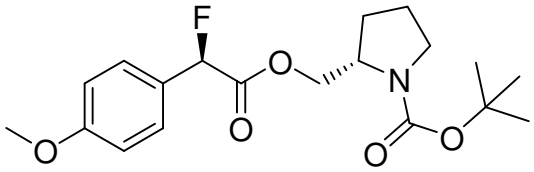
(R)-methyl 2-fluoro-2-(4-methoxyphenyl) acetate (2a): white solid: % yield = 83, %ee = 99; mp = 27 ºC; $[\bullet]_D$ = -115º (c = 0.35, $CHCl_3$); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.38 (d, 2H), 6.91 (d,2H), 5.22 (d, 1H, J = 47.5 Hz), 3.81 (s, 3H), 3.72 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 169.5, 169.2, 160.8, 160.7, 128.7, 128.6, 126.4, 126.2, 114.3, 90.4, 87.9, 55.3, 52.6; ^{19}F NMR ($CDCl_3$) δ -175.0 (d, J = 47.6 Hz); IR (CH_2Cl_2) 1761, cm^{-1}; HRMS (ESI+) calc for $C_{10}H_{11}FO_3Na^+$: 221.058444, found: 221.057723; HPLC (Whelk-01, 3% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 14.8 min, (S) = 10.2 min.



(S)-ethyl 2-((R)-2-fluoro-2-(4-methoxyphenyl)acetamido)-3-phenylpropanoate (2b): white solid: % yield = 68, % de = >99; mp = 100-103 ºC; $[\bullet]_D$ = -12.9º (c = 0.30, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.38-7.28 (m, 5H), 7.16 (d, 2H), 6.95 (m, 1H), 6.90 (d, 2H), 5.67 (d, 1H, J = 48.6 Hz), 4.99 (q, 1H) 4.16 (q, 2H), 3.76 (s, 3H), 3.16 (m, 2H), 1.21 (t, 3H); ^{13}C NMR ($CDCl_3$) δ 170.8, 168.4, 168.1, 160.5, 135.4, 129.1, 128.9, 128.8, 128.5, 127.0, 126.7, 126.5, 114.0, 92.7, 90.2, 76.6, 61.5, 55.1, 52.6, 37.6, 13.9; ^{19}F NMR ($CDCl_3$) δ -170.6 (d, J = 48.6); IR (CH_2Cl_2) 1740, 1688 cm^{-1}; HRMS (ESI+) calc for $C_{20}H_{22}FNO_4Na^+$: 382.142507, found: 382.142193; proton-decoupled ^{19}F NMR: (R,S)= δ -170.9, (S,S) = δ -173.0.

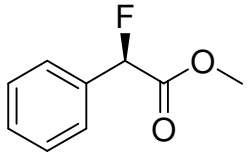


(R)-S-phenyl 2-fluoro-2-(4-methoxyphenyl)ethanethioate (2c): colorless oil: % yield = 67, % ee = 99; $[\bullet]_D$ = +116º (c = 0.35, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.37-7.44 (m, 7H), 6.94 (d, 2H), 5.84 (d, 1H, J = 47.3 Hz), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 196.5, 196.1, 160.7, 134.8, 129.7, 129.3, 128.3, 128.2, 126.2, 125.9, 125.8, 114.3, 96.6, 94.1, 55.5; ^{19}F NMR ($CDCl_3$) δ -175.4 (d, J = 47.5 Hz); IR (CH_2Cl_2) 1705 cm^{-1}; HRMS (ESI+) calc for $C_{15}H_{13}FO_2SNa^+$: 299.051801, found: 299.051406; HPLC (Whelk-01, 20% CH_2Cl_2/hexanes, 1.0 mL/min) (R) = 12 min, (S) = 6 min.

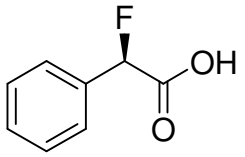


(S)-tert-butyl 2-(((R)-2-fluoro-2-(4-methoxyphenyl)acetoxy)methyl)pyrrolidine-1-carboxylate (2d): pale yellow oil: % yield = 90, % de = >99; $[\bullet]_D$ = -174º (c = 0.30, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.35 (d, 2H), 6.90 (d, 2H), 5.66 (d, 1H, J = 47.6 Hz), 4.23-4.14 (m, 2H), 3.98-3.86 (m, 1H), 3.75 (s, 3H), 3.25 (m, 1H), 3.09 (m, 1H), 1.82 (m, 1H), 1.67 (m, 3H), 1.34 (s, 9H); ^{13}C NMR ($CDCl_3$) δ

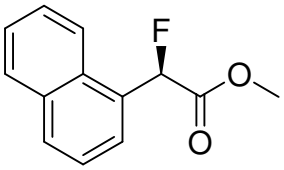
168.6, 168.2, 160.5, 154.3, 154.0, 130.1, 128.4, 128.3, 126.5, 126.2, 125.9, 114.1, 113.8, 90.0, 87.7, 79.7, 79.3, 65.4, 55.2, 55.1, 46.5, 46.3, 28.6, 28.2, 27.6, 25.1, 22.7, 22.5; ^{19}F NMR ($CDCl_3$) δ -174.7 (d, J= 47.7 Hz), -175.5 (d, J = 47.4 Hz), rotameric mixture; IR (CH_2Cl_2) 1757, 1686, 1610 cm^{-1}; HRMS (ESI+) calc for $C_{19}H_{26}FNO_5Na^+$: 390.168722, found: 390.168254; HPLC (Whelk-01, 3% *i*-PrOH/hexanes, 1.0 mL/min) R) = 46.1 min, (S) = 28.8 min.



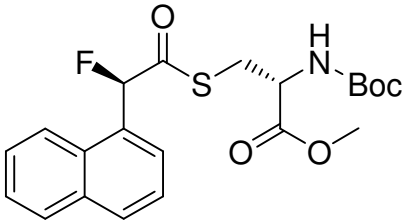
(R)-methyl 2-fluoro-2-phenylacetate (2e): colorless oil: % yield = 61, %ee = 99; $[\bullet]_D$ = -118º (c = 0.47, $CHCl_3$), lit.[3] $[\bullet]_D$ = -116º (c = 1.0, $CHCl_3$).



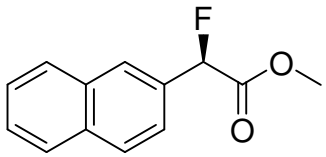
(R)-2-fluoro-2-phenylacetic acid (2f): white solid: % yield = 60, % ee = 99; $[\bullet]_D$ = -154º (c = 0.92, $CHCl_3$), mp = 101-102 ºC; lit.[4] $[\bullet]_D$ = -153º (c = 1.25, $CHCl_3$), mp = 103 ºC.



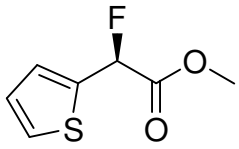
(R)-methyl 2-fluoro-2-(naphthalen-1-yl)acetate (2g): white solid: % yield = 68; % ee = 98; mp = 52-53 ºC (CH_2Cl_2); $[\bullet]_D$ = -70.9º (c = 0.30, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 8.19 (d, 1H), 7.92 (t, 2H), 7.49-7.65 (m, 4H), 6.37 (d, 1H, J = 47.2 Hz), 3.78 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 169.5, 169.2, 130.6, 128.8, 127.1, 126.9, 126.8, 126.2, 125.0, 123.6, 89.8, 87.4, 52.7; ^{19}F NMR ($CDCl_3$) δ -178.4 (d, J = 47.2 Hz); IR (CH_2Cl_2) 1763 cm^{-1}; HRMS (ESI+) calc for $C_{13}H_{11}FO_2Na^+$: 241.063529, found: 241.063164; HPLC (Whelk-01, 1% *i*-PrOH/hexanes, 1.0 mL/min) (R) =21.7 min, (S) = 13.4 min.



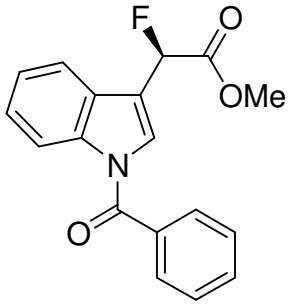
(R)-methyl 2-(tert-butoxycarbonyl)-3-((R)-2-fluoro-2-(naphthalen-1-yl)acetylthio)propanoate (2h): viscous yellow oil: % yield = 80, % de = 99; $[\bullet]_D$ = -26.9° (c = 0.40, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 °C) δ 8.12 (d, 1H), 7.89 (m, 2H), 7.65-7.45 (m, 4H), 6.45 (d, 1H, J = 46.8 Hz), 5.19 (m, 1H), 4.55 (m, 1H), 3.68 (s, 3H), 3.51 (m, 1H), 3.35 (m, 1H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$) δ 197.2, 196.8, 170.7, 133.9, 130.80, 130.77, 130.6, 128.9, 127.1, 126.7, 126.6, 126.3, 125.0, 123.7, 95.6, 93.1, 52.8, 52.7, 30.5, 28.2; ^{19}F NMR ($CDCl_3$) δ -176.5 (d, J = 46.8 Hz); IR (CH_2Cl_2) 1745, 1716, 1714 cm^{-1}; HRMS (ESI+) calc for $C_{21}H_{24}FNO_5Na^+$: 444.125142, found: 444.124568; HPLC (Whelk-01, 5% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 36.26 min, (S) = 20.26 min.



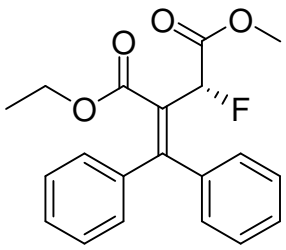
(R)-methyl 2-fluoro-2-(napthalen-2-yl)acetate (2i): white solid: % yield = 63; % ee = >99; mp = 55 °C ; $[\bullet]_D$ = -137° (c = 0.35, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 °C) δ 7.97 (s, 1H), 7.88 (m, 3H), 7.55 (m, 3H), 5.99 (d, 1H, J = 47.6 Hz), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 169.2, 133.7, 132.9, 128.8, 128.3, 127.8, 127.0, 126.7, 126.6, 123.5, 123.4, 90.8, 88.3, 52.7; ^{19}F NMR ($CDCl_3$) δ -180.1 (d, J = 47.5 Hz); IR (CH_2Cl_2) 1760 cm^{-1}; HRMS (ESI+) calc for $C_{13}H_{11}FO_2Na^+$: 241.069529, found: 241.063167; HPLC (Whelk-01, 1% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 16.8 min, (S) = 11.1 min.



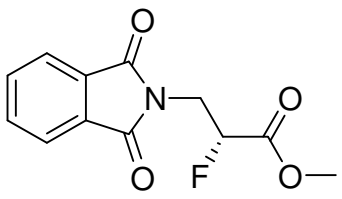
(S)-methyl 2-fluoro-2-(thiophen-2-yl)acetate (2j): colorless oil: % yield = 69, % ee = 99; $[\bullet]_D$ = -112° (c = 0.35, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 °C) δ 7.42 (d, 1H), 7.23 (t, 1H), 7.04 (t, 1H), 6.01 (d, 1H, J = 48.5 Hz), 3.78 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 168.3, 167.9, 135.4, 135.1, 128.7, 128.6, 128.3, 128.2, 127.1, 127.1, 86.0, 83.5, 52.9, 31.6; ^{19}F NMR ($CDCl_3$) δ -164.6 (d, J = 48.5 Hz); IR (CH_2Cl_2) 1764, cm^{-1}; HRMS (ESI+) calc for $C_7H_7FO_2SNa^+$: 197.004304, found: 197.003985; HPLC (Whelk-01, 0.5% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 11.4 min, (S) = 9.8 min.



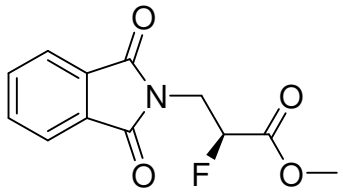
***(R)*-methyl 2-(1-benzoyl-1H-indol-3-yl)-2-fluoroacetateacetate (2k):** viscous yellow oil: % yield = 58, %ee = 94; $[\bullet]_D$ = -68.34° (c = 0.250, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 °C) δ 8.40-8.35 (d, 1H), 7.77-7.34 (m, 9H), 6.01 (d, 1H, J = 47.6 Hz), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 168.7, 168.6, 168.5, 136.6, 134.1, 132.5, 129.4, 129.0, 127.9, 127.6, 127.5, 126.0, 124.6, 120.0, 116.7, 115.6, 115.3, 84.8, 83.0, 52.9; ^{19}F NMR ($CDCl_3$) δ -180.6 (dd, J = 47.3, 3.8 Hz); IR (CH_2Cl_2) 1760, 1694 cm^{-1}; HRMS (ESI+) calc for $C_{18}H_{14}FNO_3Na^+$: 334.084990, found: 334.084355; HPLC (Whelk-01, 15% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 24.3 min, (S) = 18.7 min.



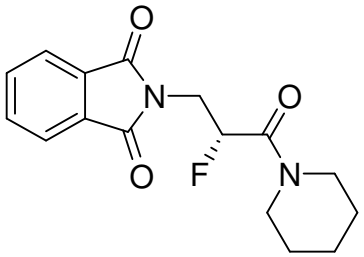
(R)-1-ethyl 4-methyl 2-(diphenylmethylene)-3-fluorosuccinate (2l): yellow oil: % yield = 71, % ee = 99; $[\bullet]_D$ = -151° (c = 0.35, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 °C) δ 7.40-7.31 (m, 8H), 7.18 (d, 2H), 5.51 (d, 1H, J = 46.4 Hz), 3.97 (q, 2H), 3.83 (s, 3H), 0.88 (t, 2H); ^{13}C NMR ($CDCl_3$) δ 168.8, 168.4, 158.2, 158.1, 141.1, 139.3, 129.4, 129.4, 129.3, 128.8, 128.7, 128.7, 128.6, 128.0, 125.7, 125.4, 88.4, 85.9, 61.1, 52.6, 13.4; ^{19}F NMR ($CDCl_3$) δ -180.2 (d, J = 46.9 Hz); IR (CH_2Cl_2) 1770, 1710 cm^{-1}; HRMS (ESI+) calc for $C_{20}H_{19}FO_4Na^+$: 365.115958, found: 365.115422; HPLC (Whelk-01, 5% CH_2Cl_2/hexanes, 1.0 mL/min) (R) = 74 min, (S) = 69 min.



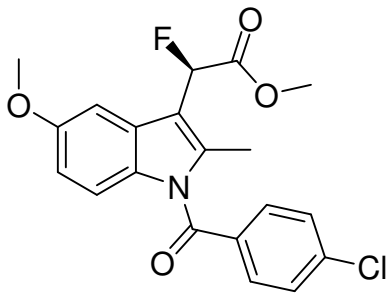
(R)-methyl 2-(1,3-dioxoisoindolin-2-yl)-2-fluoroacetate (2m). white solid: % yield = 60, % ee = >99; mp = 114-117 ºC; Lit.[5] value mp = 116-118 ºC; $[\bullet]_D$ = +18.0º (c = 0.30, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.88 (m, 2H), 7.75 (m, 2H), 5.21 (dt, 1H, major J = 48.0 Hz), 4.21 (dd, 2H, major J = 19.5 Hz), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 167.6, 134.3, 131.8, 123.6, 86.5, 84.0, 52.9, 39.1, 38.8; ^{19}F NMR ($CDCl_3$) δ -179.4 (dt, J = 48.3, 19.6 Hz); IR (CH_2Cl_2) 1772, 1725 cm^{-1}; HRMS (ESI+) calc for $C_{12}H_{10}FNO_4Na^+$: 274.048607, found: 274.048297; HPLC (OD, 10% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 23 min, (S) = 27.1 min.



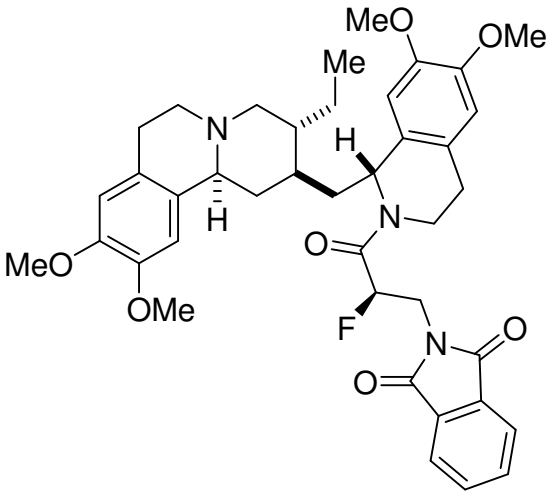
(S)-methyl 2-(1,3-dioxoisoindolin-2-yl)-2-fluoroacetate (2n): white solid: % yield = 74; % ee = 99; $[\bullet]_D$ = -19.3º (c =0.35, CH_2Cl_2); Characterization data: See Above (**2m**)



(R)-2-(2-fluoro-3-oxo-3-(piperidin-1-yl)propyl)isoindoline-1,3-dione (2o): white solid: % yield = 79, % ee = >99; mp = 125-126 ºC; $[\bullet]_D$ = +36.9º (c = 0.35, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.85 (m, 2H), 7.74 (m, 2H), 5.48 (ddd, 1H, major J = 49.6 Hz), 4.39 (m, 1H), 3.99 (m, 1H), 3.35-4.92 (m, 4H), 1.61 (m, 6H); ^{13}C NMR ($CDCl_3$) δ 167.9, 164.3, 164.1, 134.2, 131.9, 129.0, 126.4, 123.4, 86.7, 84.3, 46.5, 46.4, 43.3, 39.4, 39.1, 26.4, 25.4, 24.4; ^{19}F NMR ($CDCl_3$) δ -191.3 (ddd, J = 48.3, 33.0, 13.8); IR (CH_2Cl_2) 1775, 1720 cm^{-1}; HRMS (ESI+) calc for $C_{16}H_{17}FN_2O_3Na^+$: 327.111542, found: 327.111021; HPLC (Whelk-01, 50% CH_2Cl_2/hexanes, 1.0 mL/min) (R) = 18.7 min, (S) = 16.1 min.



(R)-methyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)-2-fluoroacetate (4): pale yellow solid: % yield = 84, % ee = 95; mp = 102-104 ºC; $[\bullet]_D$ = -54.6º (c = 0.35, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.68 (d, 2H), 7.49 (d, 2H), 7.12 (s, 1H), 6.79 (d, 1H), 6.67 (d, 1H), 6.06 (d, 1H, J = 46.7 Hz), 3.52 (s, 3H), 3.49 (s, 3H), 2.50 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 168.3, 156.2, 140.0, 133.1, 131.4, 130.7, 129.3, 127.9, 114.8, 112.7, 101.6, 84.3, 81.9, 55.7, 52.8, 13.1; ^{19}F NMR ($CDCl_3$) δ -181.4 (d, J = 46.7 Hz); IR (CH_2Cl_2) 1762, 1748, 1689 cm^{-1}; HRMS (ESI+) calc for $C_{20}H_{17}ClFNO_4Na^+$: 412.072235, found: 412.073118; HPLC (Whelk-01, 5% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 34.8 min, (S) = 29.3 min.



2-((R)-3-((R)-3-(((2R,3R)-3-ethyl-9,10-dimethoxy-2,3,4,6,7,11b-hexahydro-1H-pyrido[2,1-a]isoquinolin-2-yl)methyl)-6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)-2-fluoro-3-oxopropyl)isoindoline-1,3-dione (7): pale yellow solid: % yield = 91, % de = >99; mp = 55 ºC (decomp); $[\bullet]_D$ = +2.02º (c = 0.40, CH_2Cl_2); ^{1}H NMR ($CDCl_3$) (@ 25 ºC) δ 7.51 (d, 2H), 7.38 (d, 2H), 6.80 (s, 1H), 6.56 (s, 2H), 6.50 (s, 1H), 6.35 (d, 1H, J = 48.4 Hz), 4.18-4.07 (m, 1H), 4.05-3.90 (m, 2H), 3.80 (m, 12H), 3.29 (m, 1H), 3.09 (m, 4H), 2.95 (m, 1H), 2.78 (m, 2H), 2.63 (m, 2H), 2.40 (m, 1H), 2.10 (m, 2H), 1.80 (m, 1H), 1.75-1.60 (m, 2H), 1.45 (m, 2H), 1.13 (m, 1H), 0.89 (t, 3H); ^{13}C NMR ($CDCl_3$) δ 167.8, 167.5, 147.5, 147.2, 147.1, 134.6, 134.2, 131.6, 131.4, 129.7, 129.3, 128.9, 127.7, 126.1, 125.0, 124.6, 123.3, 122.9, 112.0, 111.8, 110.5, 86.8, 84.9, 55.6, 55.4, 55.3, 55.2, 49.0, 28.2, 14.1; ^{19}F

NMR ($CDCl_3$) δ -190.2, -190.6, rotameric mixture; IR (CH_2Cl_2) 1775, 1718 cm^{-1}; HRMS (ESI+) calc for $C_{40}H_{46}FN_3O_7Na^+$: 722.321201, found: 722.321822; proton-decoupled ^{19}F NMR ($CDCl_3$): (R) = δ -183.1, -187.6 (mixture of rotamers); (S) = δ -190.2, -190.6 (mixture of rotamers), (stereochemistry refers to fluorine center).

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