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Supporting Information:

5-[(2-Aminoethyl)amino]-2-[2-(dimethylamino)ethyl]indazolo[4,3-gh]isoquinolin-6(2H)-one (12b). (Method A). ^{1}H NMR ($CDCl_3$ + CD_3OD): δ 9.51 (s, 1H); 8.66 (d, 1H); 8.18 (dd, 1H); 7.70 (d, 1H); 7.04 (d, 1H); 4.58 (t, 2H); 3.65 (t, 2H); 3.13 (t, 2H); 2.95 (t, 2H); 2.30 (s, 6H).

2-[2-(Dimethylamino)ethyl]-5-[[2-[N-[(1,1-dimethylethoxy)carbonyl]-N-methylamino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12c). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.67 (s, 1H); 9.31 (br. t, 1H); 8.80 (d, 1H); 8.30 (d, 1H); 7.73 (d, 1H); 7.20-7.00 (m, 1H); 4.64 (t, 2H); 3.55 (t, 2H); 3.00-2.75 (m, 7H); 2.33 (s, 6H); 1.47 (s, 9H).

2-[2-(Dimethylamino)ethyl]-5-[[2-[(2-hydroxyethyl)amino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12d). (Method A). mp 156-157°C; ^{1}H NMR ($CDCl_3$): δ 9.60 (s, 1H); 9.45 (br, 1H); 8.75 (d, 1H); 8.25 (dd, 1H); 7.60 (d, 1H); 6.90 (d, 1H); 4.60 (t, 2H); 3.75 (m, 2H); 3.60 (t, 2H); 3.08 (t, 2H); 2.91 (m, 4H); 2.30 (s, 6H).

[2-(Dimethylamino)ethyl]-5-[[2-(diethylamino)ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12e). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.67 (s, 1H); 9.33 (br., 1H); 8.80 (d, 1H); 8.34 (d, 1H); 7.74 (d, 1H); 7.02 (d, 1H); 4.64 (t, 2H); 3.56 (q, 2H); 2.95 (t, 2H); 2.86 (t, 2H); 2.67 (q, 4H); 2.35 (s, 6H); 1.12 (t, 6H).

2-[2-(Dimethylamino)ethyl]-5-[[2-(4-morpholinyl)ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12f). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.67 (s, 1H); 9.37 (t, 1H); 8.81 (d, 1H); 8.34 (d, 1H); 7.74 (d, 1H); 7.01 (d, 1H); 4.65 (t, 2H); 3.83 (m, 4H); 3.61 (q, 2H); 2.95 (t, 2H); 2.80 (t, 2H); 2.60 (m, 4H); 2.35 (s, 6H).

2-[2-(Dimethylamino)ethyl]-5-[3-(dimethylamino)propyl]indazolo[4,3-gh]isoquinoline-6(2H)-one (12g). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.69 (s, 1H); 9.29 (t, 1H); 8.80 (d, 1H); 8.31 (d, 1H); 7.72 (d, 1H); 7.08 (d, 1H); 4.65 (t, 2H); 3.58 (q, 2H); 2.93 (t, 2H); 2.48 (t, 2H); 2.33 (s, 6H); 2.28 (s, 6H); 1.98 (m, 2H).

5-[(2-Aminopropyl)amino]-2-[2-(dimethylamino)ethyl]indazolo[4,3-gh]isoquinolin-6(2H)-one (12h). (Method A). ^{1}H NMR ($CDCl_3$) :δ 9.69 (s, 1H); 9.34 (t, 1H); 8.81 (d, 1H); 8.31 (d, 1H); 7.74 (d, 1H); 7.05 (d, 1H); 4.65 (t, 2H); 3.61 (q, 2H); 2.96 (m, 4H); 2.34 (s,

6H); 1.86 (m, 2H).

2-[2-(Dimethylamino)ethyl]-5-[2-(1-piperidinyl)ethyl]indazolo[4,3-gh]isoquinoline-6(2H)-one (12i). (Method A). ^{1}H NMR ($CDCl_3$) δ 9.65 (d, J = 0.8 Hz, 1H); 9.29 (br. t, J = 5.4 Hz, 1H); 8.79 (d, J = 5.3 Hz, 1H); 8.30 (dd, J = 5.3, 0.8 Hz, 1H); 7.71 (d, J = 9.1 Hz, 1H); 7.04 (d, J = 9.1 Hz, 1H); 4.63 (t, J = 6.75 Hz, 2H); 3.64 (q, J = 6.0 Hz, 2H); 2.94 (t, J = 6.75 Hz, 2H); 2.77 (t, J = 6.75 Hz, 2H); 2.65-2.49 (m, 4H); 2.33 (s, 6H); 1.79-1.61 (m, 4H); 1.59-1.42 (m, 2H).

2-[2-(Dimethylamino)ethyl]-5-[[2-[4-[(1,1-dimethylethoxy)carbonyl]piperazin-1-yl]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12j). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.66 (s, 1H); 9.36 (br. t, 1H); 8.80 (d, 1H); 8.31 (d, 1H); 7.72 (d, 1H); 6.98 (d, 1H); 4.64 (t, 2H); 3.65-3.45 (m, 6H); 2.94 (t, 2H); 2.79 (t, 2H); 2.57-2.49 (m, 4H); 2.34 (s, 6H); 1.48 (s, 9H)

2-[2-(Dimethylamino)ethyl]-5-[(2-hydroxyethyl)amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12k). (Method A). mp 155-157°C; ^{1}H-NMR (DMSO-d_6): δ 9.51 (s, 1H); 9.35 (br. t, J = 5.5 Hz, 1H); 8.79 (d, J = 5.5 Hz, 1H); 8.21 (d, J = 5.5 Hz, 1H); 8.13 (d, J = 9.2 Hz, 1H); 7.24 (d, J = 9.2 Hz, 1H); 5.04 (t, J = 4.7 Hz, 1H); 4.70 (t, J = 6.3 Hz, 2H); 3.77-3.53 (m, 4H); 2.81 (t, J = 4.7 Hz, 2H); 2.20 (s, 6H).

[2-(Dimethylamino)ethyl]-5-[[2-[bis(2-hydroxyethyl)amino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12l). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.86 (br. t, 1H); 9.68 (s, 1H); 8.79 (d, 1H); 8.34 (d, 1H); 7.76 (d, 1H); 6.95 (d, 1H); 4.65 (t, 2H); 3.76 (t, 4H); 3.56 (q, 2H); 3.03-2.89 (m, 4H); 2.78 (t, 4H); 2.33 (s, 6H).

2-[2-(Dimethylamino)ethyl]-5-[[2-(imidazol-1-yl)ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12m). (Method B). ^{1}H NMR ($CDCl_3$): δ 9.67 (s, 1H); 9.32 (br. t, 1H); 8.82 (d, 1H); 8.28 (d, 1H); 7.67 (d, 1H); 7.56 (sharp m, 1H); 7.08 (sharp m, 1H); 7.02 (sharp m, 1H); 6.71 (d, 1H); 4.63 (t, 2H); 4.33 (t, 2H); 3.87 (q, 2H); 2.94 (t, 2H); 2.28 (s, 6H).

2-[2-(Dimethylamino)ethyl]-5-[[2-[(2-hydroxyethyl)methylamino]ethyl]amino]indazolo[4,3-gh]isoquinolin-6(2H)-one(12n).

(Method A). ^{1}H NMR ($CDCl_3$) δ 9.66 (m, 2H); 8.78 (d, 1H); 8.33 (dd, 1H); 7.71 (d, 1H); 6.94 (d, 1H); 4.63 (t, 2H); 3.75 (m, 3H); 3.56 (q, 2H); 2.93 (t, 2H); 2.86 (t, 2H); 2.72 (br. t, 2H); 2.41 (s, 3H); 2.33 (s, 6H).

2-[2-(Dimethylamino)ethyl]-5-[[2-[[2-(dimethylamino)ethyl]amino]ethyl]-amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12p). (Method A). ^{1}H NMR ($CDCl_3$) δ 9.66 (d, 1H); 9.32 (br. t, 1H); 8.79 (d, 1H); 8.30 (dd, 1H); 7.70 (d, 1H); 7.02 (d, 1H); 4.63 (t, 2H); 3.62 (q, 2H); 3.06 (t, 2H); 2.93 (t, 2H); 2.80 (t, 2H); 2.47 (t, 2H); 2.33 (s, 6H); 2.24 (s, 6H).

2-[2-(Dimethylamino)ethyl]-5-[[2-[[2-(dimethylamino)ethyl]amino]ethyl]-amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12p). (Method A). ^{1}H NMR ($CDCl_3$) δ 9.66 (d, 1H); 9.32 (br. t, 1H); 8.79 (d, 1H); 8.30 (dd, 1H); 7.70 (d, 1H); 7.02 (d, 1H); 4.63 (t, 2H); 3.62 (q, 2H); 3.06 (t, 2H); 2.93 (t, 2H); 2.80 (t, 2H); 2.47 (t, 2H); 2.33 (s, 6H); 2.24 (s, 6H).

2-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]-5-[[2-(dimethylamino)ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12q). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.65 (s, 1H); 9.32 (br. t, 1H); 8.80 (d, 1H); 8.32 (d, 1H); 7.70 (d, 1H); 6.98 (d, 1H); 4.96 (br. t, 1H); 4.67 (t, 2H); 3.75 (q, 2H); 3.57 (q, 2H); 2.72 (t, 2H); 2.39 (s, 6H); 1.44 (s, 9H).

2-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]-5-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12r). (Method A). mp 211-213°C; ^{1}H NMR ($CDCl_3$: DMSO-d_6; 9:1): 9.49 (s, 1H); 9.20 (br, 1H); 8.65 (d, 1H); 8.15 (d, 1H); 7.70 (d, 1H); 7.05 (d, 1H); 6.40 (br, 1H); 6.20 (br, 1H); 4.58 (t, 2H); 3.58 (m, 4H); 3.32 (q, 2H); 1.4 (s, 9H); 1.3 (s, 9H)

2-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]-5-[[2-[N-[(1,1-dimethylethoxy)carbonyl]-N-methylamino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12s). (Method B). ^{1}H NMR ($CDCl_3$): δ 9.60 (s, 1H); 9.25 (t, 1H); 8.75 (d, 1H); 8.22 (d, 1H); 7.68 (d, 1H); 7.05 (m, 1H); 5.19 (br., 1H); 4.64 (t, 2H); 3.68 (m, 6H); 2.97 (s, 3H); 1.49 (s, 9H); 1.45 (s, 9H).

2-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]5-[[2-[(2-hydroxyethyl)amino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12t). (Method A). ^{1}H-NMR ($CDCl_3$): δ 9.52 (s, 1H); 9.42 (br. t, 1H, exchangeable with D2O); 8.65 (d, 1H); 8.15 (dd, 1H); 7.58 (d, 1H); 6.85 (d, 1H); 5.40 (m, 1H, exchangeable with D2O); 4.63 (t, 2H); 3.80 (m, 4H); 3.60 (q, 2H); 3.14 (t, 2H); 2.95 (t, 2H); 1.45 (s, 9H).

2-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]-5-[[2-(diethylamino)ethyl]amino]-indazolo[4,3-gh]isoquinoline-6(2H)-one (12u). (Method A). ^{1}H NMR ($CDCl_3$): δ 9.51 (s, 1H); 9.28 (br. t, 1H); 8.78 (d, 1H); 8.29 (d, 1H); 7.64 (d, 1H); 6.94 (d, 1H); 5.15 (br. t, 1H); 4.66 (t, 2H); 3.76 (q, 2H); 3.53 (q, 2H); 2.84 (t, 2H); 2.69 (q, 4H); 1.43 (s, 9H); 1.12 (t, 6H).

2-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]-5-[[2-(4-morpholinyl)ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12v). (Method A). ^{1}H NMR (DMSO-d_6): δ 9.51 (s, 1H); 9.35 (br. t, 1H); 8.79 (d, 1H); 8.22 (d, 1H); 7.99 (d, 1H); 7.23 (d, 1H); 6.96 (br. t, 1H); 4.62 (t, 2H); 3.70-3.54 (m, 6H); 3.45 (q, 2H); 3.33-3.27 (m, 4H); 2.68 (t, 2H); 1.23 (s, 9H).

2-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]-5-[[2-[bis(2-hydroxyethyl)amino]ethyl]amino] indazolo[4,3-gh]isoquinoline-6(2H)-one (12w). (Method A). ^{1}H NMR (DMSO-d_6): δ 9.52 (s, 1H); 9.35 (br. t, 1H); 8.79 (d, 1H); 8.22 (d, 1H); 7.98 (d, 1H); 7.23 (d, 1H); 6.95 (br. t, 1H); 4.64 (br. t, 2H); 4.37 (t, 2H); 3.64-3.36 (m, 8H); 2.87 (t, 2H); 2.67 (t, 4H); 1.25 (s, 9H).

2-[2-[N-[(1,1-Dimethylethoxy)carbonyl]-N-(2-hydroxyethyl)amino]ethyl]-5-[[2-[(2-hydroxyethyl)amino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12aa). (Method A) . ^{1}H NMR (CD_3OD): δ 9.28 (s, 1H); 8.69-8.61 (m, 1H); 8.20-8.09 (m, 1H); 7.70 (d, 1H); 7.10-6.98 (m, 1H); 4.67 (t, 2H); 3.85-3.58 (m, 8H); 3.50 (t, 0.8H; part of a split methylene signal); 3.25 (t, 1.2H; part of a split methylene signal); 3.03 (t, 2H); 2.86 (t, 2H); 1.29 (s, 4H; part of the Boc signal); 0.92 (s, 5H; part of the Boc signal).

5-[[2-[Bis(2-hydroxyethyl)amino]ethyl]amino]-2-[2-[[(1,1-dimethylethoxy)carbonyl](2-hydroxyethyl)amino]ethyl]indazolo[4,3-gh]isoquinoline-6(2H)-one (12bb). (Method A). ^{1}H NMR (CD_3OD): δ 9.37 (s, 1H); 8.69 (d, 1H); 8.25-8.20 (m, 1H); 7.82-7.72 (m, 1H); 7.11-

7.00 (m, 1H); 4.72 (t, 2H); 3.85-3.40 (m, 10H); 3.25 (t, 1H; part of a split signal); 2.98 (br. t, 3H; part of a split signal); 2.80 (t, 4H); 1.29 (br. s, 4H; part of the Boc signal); 0.92 (br. s, 5H; part of the split signal).

2-[2-[N-[(1,1-Dimethylethoxy)carbonyl]-N-(2-hydroxyethyl)amino]ethyl]-5-[(2-hydroxyethyl)amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12cc) (Method A).

mp 178.6-179.9°C; ^{1}H NMR ($CDCl_3$, 313°K): δ 9.33 (s, 1H); 9.28 (t, 1H); 8.71 (d, 1H); 8.12 (d, 1H); 7.50-7.28 (br. m, 1H); 6.91 (d, 1H); 4.64 (br. t, 2H); 4.05 (br. s, 2H); 3.85-3.55 (m, 8H); 3.23 (br. s, 2H); 1.15 (br. d, 9H).

Anal. ($C_{24}H_{28}N_5O_5$) C, H, N.

2-[3-(Dimethylamino)propyl]-5-[[2-(dimethylamino)ethyl]aminoindazolo[4,3-gh]isoquinoline-6(2H)-one (12dd). (Method A). mp 110-112°C; ^{1}H NMR ($CDCl_3$): δ 9.62 (s, 1H); 9.29 (br t, 1H); 8.74 (d, 1H); 8.28 (d, 1H); 7.71 (d, 1H); 6.94 (d, 1H); 4.57 (t, 2H); 3.52 (q, 2H); 2.67 (t, 2H); 2.33 (s, 6H); 2.30-2.08 (m, 10H).

2-[3-(Dimethylamino)propyl]-5-[[2-[(2-hydroxyethyl)amino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H)-one (12ee). (Method A). mp 110-112°C; ^{1}H NMR ($CDCl_3$) δ 9.62 (s, 1H); 9.49 (br t, 1H); 8.77 (d, 1H); 8.26 (d, 1H); 7.69 (d, 1H); 6.94 (d, 1H); 4.59 (t, 2H); 3.75 (t, 2H); 3.60 (t, 2H); 2.35-2.10 (m, 10H).

2-[2-[N-[(1,1-Dimethylethoxy)carbonyl]-N-methylamino]ethyl]-5-[[2-[(2-hydroxyethyl)amino]ethyl]amino]indazolo[4,3-gh]isoquinoline-6(2H0-one (12gg). (Method A). ^{1}H NMR (DMSO-d_6, 328°): 9.51 (d, J = 0.9 Hz, 1H); 9.32 (t, J = 5.6 Hz, 1H); 8.78 (d, J = 5.3 Hz, 1H); 8.21 (dd, J = 0.9, 5.3 Hz, 1H); 7.98 (d, J = 9.2 Hz, 1H); 7.24 (d, J = 9.2 Hz, 1H); 4.74 (t, J = 5.9 Hz, 2H); 4.28 (br t, 1H); 3.71 (t, J = 5.9 Hz, 2H); 3.65-3.45 (m, 4H); 2.91 (t, J = 6.1 Hz, 2H); 2.72 (s, 3H); 2.70 (t, J = 5.7 Hz, 2H); 1.06 (br s, 9H).

UV spectra for target compounds 13.

Compound	UV spectrum
13a	UV in H_2O: λ_{max} (log ε) 368 (3.973), 469 (4.100), 490 (4.110).
13b	UV in 0.1N HCl : λ_{max} (log ε) 507 (4.044), 381 (3.993), 236 (4.405).
13c	UV in H_2O: λ_{max} (log ε) 491 (4.083), 470 (4.072), 367 (3.952).
13d	UV in H_2O: λ_{max} (log ε) 491 (4.119), 368 (3.993).
13e	UV in H_2O: λ_{max} (log ε) 491 (4.046), 471 (4.031), 368 (3.870).
13f	UV in H_2O: λ_{max} (log ε) 500 (4.053), 477 (4.053), 367 (3.879).
13g	UV in H_2O: λ_{max} (log ε) 499 (4.120), 474 (4.099), 366 (3.957).
13h	UV in H_2O: λ_{max} (log ε) 500 (4.145), 475 (4.120), 368 (3.969).
13i	UV in H_2O: λ_{max} (log ε) 492 (4.081), 470 (4.066), 368 (3.944).
13j	UV in H_2O: λ_{max} (log ε) 502 (4.134), 477 (4.115), 368 (3.972).
13k	UV in H_2O: λ_{max} (log ε) 515 (4.069), 382 (4.018), 237 (4.372).
13l	UV in H_2O: λ_{max} (log ε) 490 (4.060), 470 (4.052), 368 (3.934).
13m	UV in H_2O: λ_{max} (log ε) 494 (4.120), 471 (4.103), 370 (3.963).
13n	UV in H_2O: λ_{max} (log ε) 506 (4.032), 381 (3.983), 236 (4.408).
13o	UV in 0.1N HCl: λ_{max} (log ε) 514 (4.054), 328 (4.014), 286 (3.846), 249 (4.181).
13p	UV in H_2O: λ_{max} (log ε) 505 (3.968), 381 (3.919), 236 (4.347).
13q	UV in 0.1N HCl: λ_{max} (log ε) 507 (4.028), 382 (3.974), 236 (4.348).
13r	UV in H_2O: λ_{max} (log ε) 230 (4.483), 240 (4.414), 370 (4.057), 491 (4.204).
13s	UV in H_2O: λ_{max} (log ε) 491 (4.096), 470 (4.087), 368 (3.946), 240 (4.310), 230 (4.377).
13t	UV in H_2O: λ_{max} (log ε) 507 (4.035), 382 (3.974), 236 (4.363).
13u	UV in H_2O: λ_{max} (log ε) 501 (4.015), 380 (3.958), 236 (4.345).
13v	UV in H_2O: λ_{max} (log ε) 502 (4.002), 381 (3.953), 236 (4.346).
13w	UV in H_2O: λ_{max} (log ε) 490 (4.080), 367 (3.954).
13x	UV in H_2O: λ_{max} (log ε) 507 (4.056), 381 (4.009), 236 (4.425).
13y	UV in 0.1N HCl: λ_{max} (log ε) 508 (4.000), 381 (3.949), 236 (4.332).
13z	UV in 0.01 NHCl: λ_{max} (log ε) 501 (4.038), 381 (3.987), 236 (4.385).
13aa	UV in H_2O: λ_{max} (log ε) 492 (4.128), 470 (4.116), 370 (3.983), 240 (4.343), 230 (4.405).
13bb	UV in H_2O: λ_{max} (log ε) 504 (4.046), 382 (4.002), 236 (4.371).
13cc	UV in H_2O: λ_{max} (log ε) 511 (4.052), 381 (4.007), 236 (4.344).
13dd	UV in H_2O: λ_{max} (log ε) 492 (4.092), 471 (4.077), 368 (3.963).

13ee	UV in H_2O: λ_{max} (log ε) 509 (4.026), 384 (3.984), 237 (4.349).
13ff	UV in H_2O: λ_{max} (log ε) 507 (4.061), 382 (4.009), 236 (4.387).
13gg	UV in 0.1N HCl: λ_{max} (log ε) 508 (4.008), 382 (3.964), 237 (4.335).
13hh	UV in H_2O: λ_{max} (log ε) 494 (3.990), 472 (3.992), 376 (3.871), 230 (4.347).
13ii	UV in H_2O: λ_{max} (log ε) 506 (4.021), 385 (3.971), 237 (4.335).

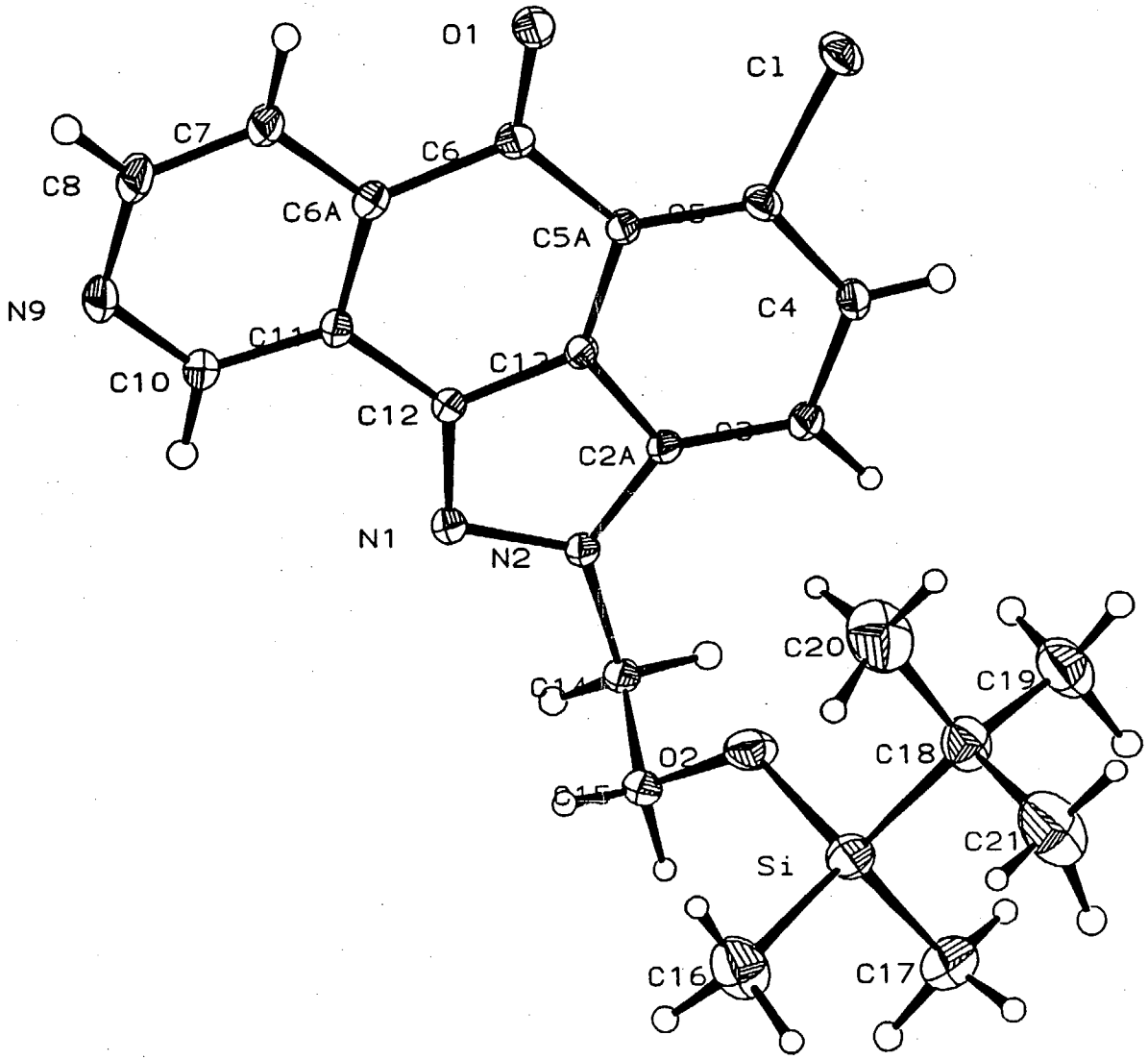
HPLC purities of target compounds 13

Compound	t_R (min)	Purity (% Area)	Method
13a	14.43	96.8%	A
13b	13.4	95%	A
13c	7.25	97%	D
13d	12.58	98%	A
13e	11.06	99.55%	A
13f	7.92	98.1%	B
13g	8.34	98%	B
13h	6.08	99.2%	H
13i	8.78	97.9%	D
13j	9.29	96.7%	D
13k	8.30	98%	C
13l	4.90	99.7%	F
13m	6.78	98.5%	F
13n	10.42	96.8%	E
13o	6.20	98%	E
13p	8.50	96.21%	I
13q	14.01	97%	A
13r	5.95	97%	G
13s	15.12	97.6%	D
13t	6.31	97.5%	D
13u	12.51	97.04 %	C
13v	11.44	96.76%	C
13w	7.24	97.2%	C
13x	19.8	99.06 %	C
13y	9.53	97.44%	A
13z	7.37	97%	D
13aa	14.07	97.2%	D
13bb	9.38	97.8%	E
13cc	6.48	98.7%	D
13dd	9.84	96.53%	C
13ee	15.06	97.68%	E
13ff	9.24	97.5%	J
13gg	8.07	97.65%	D
13hh	6.44	97%	D
13ii	8.65	99.6%	C

Methods

Flow rates were 0.7-1.4 ml/min (1 ml/min in most cases). Detection wavelengths were set at the shortest maximum wavelength in the UV spectrum of the compound.

Method	Column	Mobile phase
A	LiChrospher RP18, 5µm, 150mm	H_2O:CH_3CN:Dioxane 75:20:5, 20 mM n-$C_7H_{15}SO_3Na$, 15 mM KH_2PO_4, pH 2.7 with H_3PO_4
B	LiChrospher RP18, 5µm, 100mm	H_2O:CH_3CN:Dioxane 75:20:5, 20 mM n-$C_7H_{15}SO_3Na$, 15 mM KH_2PO_4, pH 3.0 with H_3PO_4
C	Supelcosil LC-ABZ 5µm150 mm	H_2O:CH_3CN:THF 75:15:10, 25 mM n-$C_8H_{17}SO_3Na$, pH 2.5 with H_3PO_4
D	LiChrospher RP8, 5µm, 250mm	H_2O:CH_3CN:Dioxane 75:20:5, 10 mM n-$C_7H_{15}SO_3Na$, 15 mM KH_2PO_4, pH 2.7 with H_3PO_4
E	TOSOHAAS ODS 5µm, 250 mm	H_2O:CH_3CN:Dioxane 75:20:5, 10 mM n-$C_7H_{15}SO_3Na$, 15 mM KH_2PO_4, pH 2.7 with H_3PO_4
F	LiChrospher RP8, 5µm, 250mm	H_2O:CH_3CN:Dioxane 70:20:10, 10 mM n-$C_7H_{15}SO_3Na$, 15 mM KH_2PO_4, pH 2.7 with H_3PO_4
G	LiChrospher RP18, 5µm, 250mm	H_2O:CH_3CN:Dioxane 70:20:10, 20 mM n-$C_7H_{15}SO_3Na$, pH 2.8 with H_3PO_4
H	LiChrospher RP8, 5µm, 250mm	H_2O:CH_3CN:Dioxane 60:30:10, 10 mM n-$C_7H_{15}SO_3Na$, pH 3 with H_3PO_4
I	LiChrospher RP8, 5µm, 250mm	H_2O:CH_3CN:Dioxane 75:15:10, 10 mM n-$C_7H_{15}SO_3Na$, 15 mM KH_2PO_4, pH 2.7 with H_3PO_4
J	LiChrospher RP8, 5µm, 250mm	H_2O:CH_3CN:Dioxane 77:18:5, 7 mM n-$C_7H_{15}SO_3Na$, 20 mM KH_2PO_4, pH 2.7 with H_3PO_4



X-ray Crystallographic Structure for 15b

Experimental section

A crystal sample of 0.10 X 0.20 X 0.35 mm. was mounted on a glass fiber in air at room temperature on a Siemens SMART CCD area-detector diffractometer. Graphite-monochromatized Mo-Kα radiation was used with the generator working at 50 kV. and 35 mA. Approximate cell parameters and an orientation matrix were obtained from least-squares refinement on 48 reflections misured in three different sets of 15 frames each, in the range $0 < \theta < 23°$.

The intensity data were collected using ω-scan technique within the sphere $2\theta < 53.7°$ in the full sphere. Frame width was set at 0.3° and the detector exposition for each frame was 20 s. The sample-detector distance was fixed at 5.5 cm.

The first 151 frames, containing 1234 reflections were recollected at the end of data collection to have a monitoring of crystal decay, which was not observed, thus no time-decay correction was needed. The 2093 collected frames were then processed by software SAINT; no absorption correction was applied [19199 ($R_\sigma = 0.032$) collected reflections, 4552 of which are unique, with $R_{int} = 0.043$].

The structure was solved by Direct Methods (SIR92) and Difference Fourier methods and refined with full-matrix-block least squares method (SHELX93) on the basis of 3312 independent refiections with $I > 2\sigma(I)$; anisotropic temperature factors were assigned to all non-hydrogen atoms. Hydrogens were refined with isotropic thermal parameters, riding on the carbon atoms to which they are attached. The final conventional agreement indexes R_1 and wR_2 were 0.053 and 0.106 ($F_o > 4\sigma(F_o)$).

Table 1. Crystallographic Data for **15b**

chemical formula	$C_{21}H_{24}ClN_3O_2Si$	μ =	0.25 mm^{-1}
a =	12.8344(4) Å	ρ_{calc} =	1.251 g /cm^3
b =	10.7401(3) Å	T =	295 K
c =	16.8791(5) Å	λ =	0.71073Å
β =	109.162(1)°	scan method	ω
V =	2197.8(2) $Å^3$	frame width	0.3°
Z =	4	time per frame	20 s
formula weight	413.97	n. of frames	2093
crystal system	*monoclinic*	detector-sample distance	
	5.5 cm		
space group	*P2₁/c* (No.14)		

n. of reflections (total; independent)	19199; 4552
R_{int}; R_σ [a]	0.043; 0.032
R indices [$F_o > 4\sigma(F_o)$] (3312 data)	R1[d] 0.053, wR2[c] 0.106

[a] $R_{int} = \Sigma \mid F_o^2 - F^2_{(mean)} \mid / \Sigma F_o^2$;

$$R_\sigma = \Sigma [\sigma(F_o^2)] / \Sigma F_o^2$$

[b] $R1 = \Sigma \mid |F_o| - |F_c| \mid / \Sigma |F_o|$,

[c] $wR2 = [\Sigma (F_o^2 - F_c^2)^2 / \Sigma wF_o^4]^{1/2}$

Weighting: $w = 1/[\sigma^2 (F_o^2)+(0.0309P)^2]$ where $P = (F_o^2 +2 F_c^2)/3$

Tables of revelant crystallographic data for compound 15b

Bond lengths and angles

Cl - C5	Distance 1.737 (0.001)	Angles				
	Cl -					
Si - O2	Distance 1.643 (0.001)	Angles				
C16	1.851 (0.002)	109.76 (0.09)				
C18	1.866 (0.002)	104.24 (0.07)	112.59 (0.09)			
C17	1.870 (0.002)	108.83 (0.09)	109.63 (0.12)	111.61 (0.		
11)						
	Si -	O2	C16	C18		
O1 - C6	Distance 1.220 (0.002)	Angles				
	O1 -					
O2 - C15	Distance 1.418 (0.002)	Angles				
Si	1.643 (0.001)	125.32 (0.10)				
	O2 -	C15				
N1 - C12	Distance 1.335 (0.002)	Angles				
N2	1.365 (0.001)	105.31 (0.10)				
	N1 -	C12				
N2 - N1	Distance 1.365 (0.001)	Angles				
C2A	1.369 (0.002)	112.18 (0.10)				
C14	1.465 (0.002)	120.74 (0.10)	127.01 (0.11)			

	N2 -	N1	C2A
N9 - C10	Distance 1.330 (0.002)	Angles	
C8	1.338 (0.002)	116.09 (0.13)	
	N9 -	C10	
C2A - N2	Distance 1.369 (0.002)	Angles	
C3	1.389 (0.002)	134.85 (0.12)	
C13	1.391 (0.002)	105.38 (0.11)	119.75 (0.12)
	C2A -	N2	C3
C3 - C4	Distance 1.378 (0.002)	Angles	
C2A	1.389 (0.002)	116.69 (0.12)	
	C3 -	C4	
C4 - C3	Distance 1.378 (0.002)	Angles	
C5	1.407 (0.002)	123.10 (0.13)	
	C4 -	C3	
C5 - C5A	Distance 1.390 (0.002)	Angles	
C4	1.407 (0.002)	121.12 (0.12)	
C1	1.737 (0.001)	122.42 (0.10)	116.46 (0.10)
	C5 -	C5A	C4
C5A - C5	Distance 1.390 (0.002)	Angles	
C13	1.398 (0.002)	114.56 (0.11)	
C6	1.479 (0.002)	130.45 (0.12)	114.98 (0.11)
	C5A -	C5	C13
C6 -	Distance	Angles	

O1	1.220 (0.002)		
C5A	1.479 (0.002)	123.83 (0.13)	
C6A	1.518 (0.002)	119.54 (0.12)	116.63 (0.11)
	C6 -	O1	C5A
C6A - C7	Distance 1.392 (0.002)	Angles	
C11	1.411 (0.002)	117.06 (0.13)	
C6	1.518 (0.002)	118.58 (0.12)	124.36 (0.12)
	C6A -	C7	C11
C7 - C8	Distance 1.371 (0.002)	Angles	
C6A	1.392 (0.002)	119.38 (0.14)	
	C7 -	C8	
C8 - N9	Distance 1.338 (0.002)	Angles	
C7	1.371 (0.002)	124.62 (0.14)	
	C8 -	N9	
C10 - N9	Distance 1.330 (0.002)	Angles	
C11	1.389 (0.002)	124.62 (0.14)	
	C10 -	N9	
C11 - C10	Distance 1.389 (0.002)	Angles	
C6A	1.411 (0.002)	118.23 (0.12)	
C12	1.454 (0.002)	125.35 (0.13)	116.41 (0.12)
	C11 -	C10	C6A
C12 - N1	Distance 1.335 (0.002)	Angles	
C13	1.402 (0.002)	110.91 (0.11)	

C11	1.454 (0.002)	130.55 (0.12)	118.52 (0.12)	
	C12 -	N1	C13	
C13 - C2A	Distance 1.391 (0.002)	Angles		
C5A	1.398 (0.002)	124.77 (0.12)		
C12	1.402 (0.002)	106.22 (0.11)	129.00 (0.12)	
	C13 -	C2A	C5A	
C14 - N2	Distance 1.465 (0.002)	Angles		
C15	1.498 (0.002)	112.37 (0.10)		
	C14 -	N2		
C15 - O2	Distance 1.418 (0.002)	Angles		
C14	1.498 (0.002)	108.43 (0.12)		
	C15 -	O2		
C16 - Si	Distance 1.851 (0.002)	Angles		
	C16 -			
C17 - Si	Distance 1.870 (0.002)	Angles		
	C17 -			
C18 - C19	Distance 1.533 (0.003)	Angles		
C21	1.539 (0.003)	107.69 (0.18)		
C20	1.553 (0.003)	107.43 (0.19)	111.29 (0.20)	
Si	1.866 (0.002)	110.24 (0.13)	110.65 (0.16)	109.48 (0.
15)	C18 -	C19	C21	C20
C19 -	Distance	Angles		

C18	1.533 (0.003)	
	C19 -	
C20 -	Distance	Angles
C18	1.553 (0.003)	
	C20 -	
C21 -	Distance	Angles
C18	1.539 (0.003)	
	C21 -	

Final atomic positional and thermal parameters

CELL 12.8344 10.7401 16.8791 90.0000 109.1620 90.0000

(2 rows for each atom. Thermal parameters in the second row)

Atom			x	y	z	
C1			0.38650	0.45070	-0.10480	0
0 0.11070	0.03810	0.04800	-0.00990	0.03240	0.00410	8
Si			0.04440	0.14140	0.15570	0
0 0.05540	0.06470	0.08690	0.00260	0.03270	0.00050	8
O1			0.39670	0.21700	-0.20620	0
0 0.10930	0.04870	0.04340	-0.00360	0.03820	0.00240	8
O2			0.15880	0.09520	0.14100	0
0 0.06030	0.06920	0.08640	0.01570	0.03820	0.02740	8
N1			0.35230	-0.07220	0.04570	0
0 0.04770	0.03420	0.04470	0.00240	0.01940	0.00060	8
N2			0.34830	0.02360	0.09780	0
0 0.05200	0.03590	0.03830	0.00320	0.02200	0.00310	8
N9			0.36580	-0.24710	-0.19010	0
0 0.08050	0.04460	0.05780	-0.00240	0.02820	-0.01410	8
C2A			0.35360	0.13740	0.06280	0
0 0.04190	0.03730	0.03450	0.00180	0.01650	0.00200	8
C3			0.35390	0.26010	0.08890	0
0 0.06140	0.04130	0.03780	0.00050	0.02230	-0.00550	8
C4			0.36350	0.35090	0.03400	0
0 0.06960	0.03120	0.04620	-0.00070	0.02360	-0.00530	8
C5			0.37360	0.32400	-0.04480	0
0 0.05720	0.03500	0.03800	-0.00320	0.01670	0.00450	8

C5A			0.37320	0.20190	-0.07220	0
0	0.04380	0.03600	0.03270	-0.00010	0.01330	0.00010	8
C6				0.38350	0.15210	-0.15100	0
0	0.04970	0.04250	0.03610	-0.00060	0.01560	0.00180	8
C6A				0.37680	0.01170	-0.16170	0
0	0.04100	0.04320	0.03620	0.00170	0.01320	-0.00400	8
C7				0.38150	-0.03890	-0.23640	0
0	0.06690	0.05260	0.04370	0.00150	0.02300	-0.00580	8
C8				0.37520	-0.16550	-0.24730	0
0	0.08850	0.05590	0.05210	0.00150	0.02970	-0.01860	8
C10				0.36260	-0.19900	-0.11840	0
0	0.05480	0.04160	0.05120	-0.00170	0.02240	-0.00580	8
C11				0.36720	-0.07250	-0.10030	0
0	0.03700	0.03620	0.04120	0.00220	0.01240	-0.00450	8
C12				0.36110	-0.01820	-0.02300	0
0	0.03620	0.03420	0.03710	0.00080	0.01450	-0.00040	8
C13				0.36250	0.11190	-0.01560	0
0	0.03550	0.03570	0.03450	0.00170	0.01360	0.00040	8
C14				0.33430	-0.00060	0.17910	0
0	0.05530	0.04010	0.03840	0.00350	0.02110	0.00870	8
C15				0.21570	-0.01710	0.17210	0
0	0.06360	0.04480	0.05440	-0.00030	0.03020	0.00820	8
C16				-0.06390	0.02140	0.11630	0
0	0.06690	0.08560	0.16750	-0.00520	0.03370	-0.00370	8
C17				0.07220	0.16600	0.27050	0
0	0.14360	0.10770	0.10570	0.00340	0.07350	-0.00090	8
C18				0.00940	0.29040	0.09600	0
0	0.06790	0.06840	0.10330	0.00960	0.02520	0.00360	8
C19				0.09450	0.39090	0.13800	0
0	0.09660	0.06620	0.15690	0.00350	0.04410	0.01400	8
C20				0.01350	0.27090	0.00590	0
0	0.17060	0.10810	0.09750	0.03130	0.01740	0.03530	8
C21				-0.10440	0.33780	0.09430	0
0	0.07880	0.09420	0.26600	0.02870	0.04950	0.03360	8
H3				0.35090	0.28300	0.14100	0
0	1.23209	0.00000	0.00000	0.00000	0.00000	0.00000	6
H4				0.36240	0.43030	0.04660	0
0	1.80058	0.00000	0.00000	0.00000	0.00000	0.00000	6
H7				0.39030	0.01690	-0.27850	0
0	1.76899	0.00000	0.00000	0.00000	0.00000	0.00000	6
H8				0.37550	-0.19830	-0.29720	0
0	1.94545	0.00000	0.00000	0.00000	0.00000	0.00000	6
H10				0.35810	-0.25250	-0.07450	0
0	1.95574	0.00000	0.00000	0.00000	0.00000	0.00000	6
H14A				0.37640	-0.07540	0.20340	0
0	1.94784	0.00000	0.00000	0.00000	0.00000	0.00000	6
H15A				0.21360	-0.03610	0.22790	0
0	1.18471	0.00000	0.00000	0.00000	0.00000	0.00000	6
H14B				0.36640	0.07260	0.21510	0
0	1.90047	0.00000	0.00000	0.00000	0.00000	0.00000	6
H15B				0.18370	-0.08310	0.13540	0

0 1.38210	0.00000	0.00000	0.00000	0.00000	0.00000	6
H16A			-0.07750	0.01780	0.05650	0
0 1.18818	0.00000	0.00000	0.00000	0.00000	0.00000	6
H16B			-0.04100	-0.06440	0.14190	0
0 1.64338	0.00000	0.00000	0.00000	0.00000	0.00000	6
H16C			-0.12340	0.03740	0.13540	0
0 1.27504	0.00000	0.00000	0.00000	0.00000	0.00000	6
H17A			0.08500	0.08130	0.30650	0
0 1.95167	0.00000	0.00000	0.00000	0.00000	0.00000	6
H17B			0.11950	0.22680	0.28860	0
0 1.39622	0.00000	0.00000	0.00000	0.00000	0.00000	6
H17C			0.00370	0.20650	0.27060	0
0 1.35674	0.00000	0.00000	0.00000	0.00000	0.00000	6
H19A			0.08270	0.46430	0.10600	0
0 1.62209	0.00000	0.00000	0.00000	0.00000	0.00000	6
H19B			0.16800	0.36320	0.13790	0
0 1.81984	0.00000	0.00000	0.00000	0.00000	0.00000	6
H19C			0.10280	0.40210	0.20910	0
0 1.75153	0.00000	0.00000	0.00000	0.00000	0.00000	6
H20A			-0.06570	0.21340	-0.01670	0
0 1.34885	0.00000	0.00000	0.00000	0.00000	0.00000	6
H20B			-0.00800	0.34330	-0.02750	0
0 1.30662	0.00000	0.00000	0.00000	0.00000	0.00000	6
H20C			0.09300	0.23250	0.01280	0
0 1.14153	0.00000	0.00000	0.00000	0.00000	0.00000	6
H21A			-0.10000	0.32570	0.16570	0
0 1.91459	0.00000	0.00000	0.00000	0.00000	0.00000	6
H21B			-0.11540	0.41550	0.06950	0
0 1.03541	0.00000	0.00000	0.00000	0.00000	0.00000	6
H21C			-0.16130	0.27950	0.06890	0
0 1.20948	0.00000	0.00000	0.00000	0.00000	0.00000	6