Synthesis of 3,4-Benzo-7-hydroxy-2,9-diazabicyclo[3.3.1]non-7-enes by Cyclization of 1,3-Bis(Silyl Enol Ethers) with Quinazolines

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Supporting Information

Contents:

Experimental Section

Computational details: All structures were optimized at the B3LYP/6-31G(d)[16] level of density functional theory. All optimized structures were characterized by frequency calculation as energy minimums without imaginary frequencies (NImag = 0) or transition states with only one imaginary frequency (NImag = 1) at the same level of theory.[17] The thermal corrections to Gibbs free energies at 298 K at B3LYP/6–31G* from the frequency calculations have been added to the total electronic energies for analyzing the selectivity, which has been estimated on the basis of the relationship of $\Delta\Delta G = -RT\ln K$, in which $\Delta\Delta G$ is the difference of the Gibbs free energy, and K presents the considered equilibrium constant of the two competing reactions. All calculations have been carried out by using the Gaussian 03 program package.[18]

General. Chemical shifts of the ^{1}H and ^{13}C NMR are reported in parts per million using the solvent internal standard (chloroform, 7.26 and 77.0 ppm, respectively). Infrared spectra were recorded on a FTIR spectrometer. Mass spectrometric data (MS) were obtained by electron ionization (EI, 70 eV),

chemical ionization (CI, isobutane) or electrospray ionization (ESI). Melting points are uncorrected. Analytical thin layer chromatography was performed on 0.20 mm 60 A silica gel plates. Column chromatography was performed using 60 A silica gel (60 – 200 mesh). All cyclization reactions were carried out in Schlenk tubes under an argon atmosphere. The bis(silyl enol ethers) were prepared as described in the literature. Crystallographic data were collected on a Bruker X8Apex with $Mo_{K\alpha}$ radiation (λ = 0.71073 Å). The structures were solved by direct methods using SHELXS-97 and refined against F^2 on all data by fullmatrix least-squares with SHELXL-97. All non-hydrogen atoms were refined anisotropically, all hydrogen atoms were refined in the model at geometrically calculated positions and refined using a riding model.

General procedure for the synthesis of substituted quinazolines 3. To a solution of aniline **1** (10.0 mmol) in THF (100 mL) were added triethylamine (20.0 mmol) and ethyl chloroformate (20.0 mmol). The solution was stirred for 1 h at 20 °C, filtered and concentrated in vacuo. To the residue was added ethyl acetate (100 mL) and the solution was washed with water (2 x 100 mL). The combined organic layers were dried (Na_2SO_4), filtered and concentrated in vacuo. To the residue was added TFA (70 mL). Hexamethylenetetramine (HMTA) (9.800 g, 70.0 mmol) was added and the solution was heated under reflux for 1 h. To the solution was added hydrochloric acid (4 M, 400 mL) and the solution was filtered and concentrated in vacuo. To the residue was added a 1:1-mixture of water and ethanol (600 mL). To the solution was added KOH (66.60 g) and $K_3Fe(CN)_6$ (25.00 g) and the solution was heated under reflux for 4 h. Water (600 mL) was added and the solution was extracted with toluene (5 x 100 mL). The combined organic layers were dried (Na_2SO_4), filtered and concentrated in vacuo. The residue was purified by column chromatography (silica gel, heptane → heptane-EtOAc = 2:1).

6-Ethylquinazoline (3d). Starting with 4-ethylaniline (1.212 g, 10.0 mmol), triethylamine (2.020 g, 20.0 mmol) and ethyl chloroformate (2.170 g, 20.0 mmol) in THF (100 mL) and with hexamethylenetetramine (9.800 g, 70.0 mmol) in TFA (70 mL), **3d** was obtained as a slightly brownish oil (0.255 g, 21%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.30 (t, ^3J = 7.5 Hz, 3H, CH_3), 2.82 (q, ^3J = 7.5 Hz, 2H, CH_2), 7.64 (d, ^4J = 1.0 Hz, 1H, Hetar), 7.73 (dd, ^3J = 8.8 Hz, ^4J = 1.9 Hz, 1H, Hetar), 7.92 (d, ^3J = 8.8 Hz, 1H, Hetar), 9.22 (s, 1H, NCH), 9.28 (s, 1H, NCH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 15.0 (CH_3), 28.8 (CH_2), 124.3, 128.0, 135.4 (CH_{Hetar}), 125.1, 144.2, 148.7 (C_{Hetar}), 154.5, 159.5 (NCH_{Hetar}). IR (neat, cm^{-1}): $\tilde{\nu}$ = 3430 (br, w), 2967 (m), 2932 (m), 2873 (w), 1662 (w), 1626 (w), 1573 (s), 1495 (m), 1457 (m), 1410 (w), 1380 (m), 1309 (w), 1148 (m), 1075 (w), 842 (m), 644 (m). MS

(EI, 70 eV): *m/z* (%) = 158 (M^+, 68), 143 (100), 130 (6), 116 (11), 103 (8), 89 (12), 77 (6), 63 (7). HRMS (EI): Calcd for $C_{10}H_{10}N_2$ (M^+) 158.08385, found 158.084054.

6-Isopropylquinazoline (3e). Starting with 4-isopropylaniline (1.352 g, 10.0 mmol), triethylamine (2.020 g, 20.0 mmol) and ethyl chloroformate (2.170 g, 20.0 mmol) in THF (100 mL) and with hexamethylenetetramine (9.800 g, 70.0 mmol) in TFA (70 mL), **3e** was obtained as brownish oil (0.380 g, 35%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.33 (d, ^3J = 6.9 Hz, 6H, $CH(CH_3)_2$), 3.11 (sept, ^3J = 6.9 Hz, 1H, $CH(CH_3)_2$), 7.69 (d, ^4J = 1.9 Hz, 1H, Hetar), 7.82 (dd, ^3J = 8.8 Hz, ^4J = 2.1 Hz, 1H, Hetar), 7.96 (d, ^3J = 8.8 Hz, 1H, Hetar), 9.25 (s, 1H, NCH), 9.33 (s, 1H, NCH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 23.6 ($CH(CH_3)_2$), 34.1 ($CH(CH_3)_2$), 123.0, 128.2, 134.2 (CH_{Hetar}), 125.2, 148.8, 148.9 (C_{Hetar}), 154.7, 159.7 (NCH_{Hetar}). IR (neat, cm^{-1}): $\tilde{\nu}$ = 3439 (br, w), 3039 (w), 3017 (w), 2962 (s), 2929 (m), 2871 (m), 1683 (w), 1663 (w), 1626 (m), 1575 (s), 1495 (s), 1460 (m), 1411 (w), 1379 (s), 1318 (w), 1311 (w), 1184 (m), 1150 (m), 1070 (m), 1043 (w), 930 (m), 842 (s), 644 (m), 560 (m). MS (EI, 70 eV): *m/z* (%) = 172 (M^+, 46), 157 (100), 130 (33), 103 (17), 77 (11). HRMS (EI): Calcd for $C_{11}H_{12}N_2$ (M^+) 172.09950, found 172.099493.

6-*tert*-Butylquinazoline (3f). Starting with 4-*tert*-butylaniline (1.500 g, 10.0 mmol), triethylamine (2.020 g, 20.0 mmol) and ethyl chloroformate (2.170 g, 20.0 mmol) in THF (100 mL) and with hexamethylenetetramine (9.800 g, 70.0 mmol) in TFA (70 mL), **3f** was obtained as a red oil (0.540 g, 30%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.41 (s, 9H, $C(CH_3)_3$), 7.81 (d, ^3J = 2.1 Hz, 1H, Hetar), 7.98 (s, 1H, Hetar), 8.00 (d, ^3J = 2.1 Hz, 1H, Hetar), 9.26 (s, 1H, NCH), 9.34 (s, 1H, NCH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 31.0 ($C(CH_3)_3$), 35.1 ($C(CH_3)_3$), 121.9, 127.9, 133.2 (CH_{Hetar}), 124.9, 148.6, 151.1 (C_{Hetar}), (154.8, 160.0 NCH_{Hetar}). IR (neat, cm^{-1}): $\tilde{\nu}$ = 3432 (br, w), 3040 (w), 2964 (s), 2910 (m), 2871 (m), 1663 (w), 1625 (m), 1576 (s), 1496 (s), 1465 (m), 1396 (m), 1378 (s), 1370 (s), 1314 (m), 1256 (w), 1213 (m), 1183 (m), 1154 (m), 1074 (m), 931 (m), 891 (m), 843 (s), 644 (m), 561 (s). MS (EI, 70 eV): *m/z* (%) = 186 (M^+, 31), 171 (100), 143 (27), 131 (8), 115 (11). HRMS (EI): Calcd for $C_{12}H_{14}N_2$ (M^+) 186.11515, found 186.115190.

6-Hexylquinazoline (3g). Starting with 4-hexylaniline (1.773 g, 10.0 mmol), triethylamine (2.020 g, 20.0 mmol) and ethyl chloroformate (2.170 g, 20.0 mmol) in THF (100 mL) and with hexamethylenetetramine (9.800 g, 70.00 mmol) in TFA (70 mL) **3g** was obtained as red oil (0.718 g, 30%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.85 (t, ^3J = 7.0 Hz, 3H, CH_3), 1.27 – 1.34 (m, 6H, $(CH_2)_3CH_3$), 1.68 (m, 2H, CCH_2CH_2), 2.79 (t, ^3J = 7.6 Hz, 2H, CCH_2), 7.65 (d, ^4J = 1.0 Hz, 1H,

Hetar), 7.74 (dd, ^3J = 8.7 Hz, ^4J = 1.8 Hz, 1H, Hetar), 7.94 (d, ^3J = 8.7 Hz, 1H, Hetar), 9.25 (s, 1H, NCH), 9.31 (s, 1H, NCH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 14.0 (CH_3), 22.5, 28.8, 31.0, 31.6, 35.9 (CH_2), 125.1, 128.1, 135.8 (CH_{Hetar}), 135.8, 143.1, 148.8 (C_{Hetar}), 154.6, 159.6 (NCH_{Hetar}). IR (neat, cm^{-1}): $\tilde{\nu}$ = 3038 (w), 3016 (w), 2956 (s), 2928 (s), 2857 (s), 1668 (w), 1625 (m), 1573 (s), 1495 (s), 1465 (m), 1379 (s), 1312 (m), 1147 (m), 1075 (m), 929 (m), 839 (s), 644 (m), 565 (m). MS (EI, 70 eV): *m/z* (%) = 214 (M^+, 32), 144 (100), 116 (11), 89 (11). HRMS (EI): Calcd for $C_{14}H_{18}N_2$ (M^+) 214.14645, found 214.146250.

7,8-Dihydro-6*H*-cyclopenta[*g*]quinazoline (3h). Starting with 5-aminoindane (1.330 g, 10.0 mmol), triethylamine (2.020 g, 20.0 mmol) and ethyl chloroformate (2.170 g, 20.0 mmol) in THF (100 mL) and with hexamethylenetetramine (9.800 g, 70.0 mmol) in TFA (70 mL), **3h** was obtained as a slightly yellow solid (0.910 g, 54%); mp 97 – 98 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.15 (m, 2H, $CH_2CH_2CH_2$), 3.08 (m, 4H, $CH_2CH_2CH_2$), 7.65, 7.79 (2s, 2H, Hetar), 9.18 (s, 1H, NCH), 9.23 (s, 1H, NCH). ^{13}C NMR (250 MHz, $CDCl_3$): δ = 25.9 ($CH_2CH_2CH_2$), 32.4, 33.2 ($CH_2CH_2CH_2$), 121.0, 122.5 (CH_{Hetar}) 124.4, 145.7, 153.0, 149.8 (C_{Hetar}), 154.4, 159.1 (NCH_{Hetar}). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3018 (w), 2976 (w), 2954 (m), 2910 (m), 2873 (w), 1653 (w), 1626 (m), 1570 (m), 1467 (m), 1421 (m), 1374 (m), 1357 (m), 1314 (w), 1281 (w), 1203 (w), 1155 (w), 1087 (w), 1064 (w), 1039 (w), 937 (m), 871 (m). MS (EI, 70 eV): *m/z* (%) = 170 (M^+, 100), 142 (17), 115 (46), 89 (8). HRMS (EI): Calcd for $C_{11}H_{10}N_2$ (M^+) 170.08385, found 170.083376.

6,7-Dimethylquinazoline (3i). Starting with 3,4-dimethylaniline (1.210 g, 10.0 mmol), triethylamine (2.020 g, 20.0 mmol) and ethyl chloroformate (2.170 g, 20.0 mmol) in THF (100 mL) and with hexamethylenetetramine (9.800 g, 70.0 mmol) in TFA (70 mL) **3i** was obtained as a red oil (0.550 g, 35%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.45 (s, 3H, CH_3), 2.48 (s, 3H, CH_3), 7.62, 7.77 (2s, 2H, Hetar), 9.20 (s, 1H, NCH), 9.23 (s, 1H, NCH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 20.1, 20.9 (CH_3), 123.9, 126.1(d) (CH_{Hetar}), 127.5, 138.2, 145.4, 149.2 (C_{Hetar}), 154.6, 158.8 (NCH_{Hetar}). IR (neat, cm^{-1}): $\tilde{\nu}$ = 3253 (w), 3015 (w), 2974 (m), 2944 (m), 2923 (m), 2872 (w), 1671 (s), 1627 (m), 1576 (s), 1489 (s), 1455 (m), 1406 (w), 1370 (m), 1352 (w), 1320 (w), 1261 (w), 1215 (w), 1178 (w), 1112 (w), 1077 (w), 1025 (m), 1003 (w). MS (EI, 70 eV): *m/z* (%) = 158 (M^+, 100), 143 (25), 131 (14), 104 (31). HRMS (EI): Calcd for $C_{10}H_{10}N_2$ (M^+) 158.08385, found 158.083300.

General procedure for the reaction of 1,3-bis(silyl enol ethers) with quinazolines. To a solution of quinazoline **20** (4.0 mmol) in CH_2Cl_2 (40 mL) were added at 0 °C the 1,3-bis(silyl enol ether)

(5.6 mmol) and the chloroformate (16.0 mmol). The solution was stirred for 2 h at 0 °C and for 12 h at 20 °C. The solvent was removed in vacuo. The residue was purified by column chromatography (silica gel, heptane → heptane-EtOAc = 2:1).

11-Hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5a). Starting with quinazoline **3a** (0.521 g, 4.0 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (1.460 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 mL), **5a** was obtained as a colourless solid (0.750 g, 52%); mp. 133 – 135 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.41 (dd, ^2J = 17.5 Hz, ^3J = 1.5 Hz, 1H, CH_2), 2.99 (br dd, 1H, CH_2), 3.76, 3.80 (2s, 6H, OCH_3), 3.87 (s, 3H, OCH_3), 5.40 (br, 1H, NC*H*CH_2), 7.03 – 7.13 (m, 2H, Ar), 7.20 – 7.26 (m, 1H, Ar), 7.38 (br, 1H, NCHN), 7.75 (br, 1H, Ar), 12.26 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 38.0 (CH_2), 48.7 (br, N*C*HCH_2), 52.0, 53.2, 53.3 (OCH_3), 58.9 (NCH), 98.0 (*C*CO_2CH_3), 124.2, 124.4, 126.8, 127.6 (CH_{Ar}), 126.3, 134.4 (br) (C_{Ar}), 153.4, 154.0 (NCOO), 170.6 (COO), 173.2 (br, COH). IR (Nujol, cm^{-1}): $\tilde{\nu}$ = 3080 (w), 1707 (s), 1652 (m), 1613 (m), 1494 (m), 1335 (m), 1287 (s), 1263 (m), 1230 (s), 1196 (m), 1142 (m), 1111 (m), 1064 (m), 1039 (m), 1008 (m), 778 (m). MS (EI, 70 eV): *m/z* (%) = 362 (M^+, 10), 303 (100), 271 (36), 212 (23), 180 (21), 239 (13). Anal. Calcd for $C_{17}H_{18}N_2O_7$ (362.33): C, 56.35; H, 5.01; N, 7.73. Found: C, 56.35; H, 5.13; N, 7.46.

11-Hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid-10-ethyl ester-8,13-dimethyl ester (5b). Starting with quinazoline **3a** (0.521 g, 4.0 mmol), 1-ethoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4b** (1.540 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 mL), **5b** was obtained as a colourless solid (0.698 g, 46%); mp. 122 – 123 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 1.33 (t, ^3J = 7.2 Hz, 3H, CH_2CH_3), 2.40 (dd, ^2J = 17.7 Hz, ^3J = 1.5 Hz, 1H, NCHCH_2), 2.97 (br d, 1H, NCHCH_2), 3.75, 3.86 (2s, 6H, OCH_3), 4.23 (m, 2H, CH_2CH_3), 5.39 (br, 1H, NC*H*CH_2), 7.06 – 7.12 (m, 2H, Ar), 7.19 – 7.26 (m, 1H, Ar), 7.37 (br, 1H, NCHN), 7.78 (br, 1H, Ar), 12.34 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 14.0 (CH_2CH_3), 38.2 (NCH*C*H_2), 48.9 (br, N*C*HCH_2), 53.2, 53.2 (OCH_3), 58.8 (NCHN), 61.0 (OCH_2), 98.2 (*C*COO), 124.2, 124.3, 126.3, 127.7 (CH_{Ar}), 126.8, 134.6 (C_{Ar}), 153.5, 154.0 (NCOO), 170.2 (COO), 172.7 (COH). IR (cm^{-1}, Nujol): $\tilde{\nu}$ = 3077 (w), 1719 (s), 1708 (s), 1646 (m), 1615 (m), 1495 (m), 1334 (s), 1285 (s), 1263 (s), 1230 (s), 1194 (m), 1140 (m), 1116 (m), 1064 (m), 1038 (m), 1008 (m), 775 (m), 767 (m), 750 (m). MS (CI pos.): *m/z* (%) = 377 ($[M+H]^+$). HRMS (CI neg., Isobutane): Calcd for $C_{18}H_{20}N_2O_7$ ($[M-H]^-$) 375.1198, found 375.1181.

11-Hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid-10-(2-methoxyethyl)ester-8,13-dimethyl ester (5c). Starting with quinazoline **3a** (0.521 g, 4.0 mmol), 1-(2-methoxyethoxy)-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4c** (1.705 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 mL), **5c** was obtained as a colourless solid (0.859 g, 53%); mp. 116 – 118 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.40 (dd, ^2J = 17.7 Hz, ^3J = 1.3 Hz, 1H, NCHC*H*$_2$), 2.97 (br d, ^2J = 17.7 Hz, 1H, NCHC*H*$_2$), 3.38 (s, 3H, CH_2OCH_3), 3.62 (m, 2H, CH_2OCH_3), 3.74, 3.86 (2s, 6H, OCH_3), 4.23 – 4.42 (m, 2H, OCH_2), 5.39 (br, 1H, NC*H*CH$_2$), 7.03 – 7.08 (m, 2H, Ar), 7.10 – 7.24 (m, 1H, Ar), 7.39 (br, 1H, NCHN), 7.74 (br, 1H, Ar), 12.21 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 38.1 (br, NCH*C*H$_2$), 48.9 (br, N*C*HCH$_2$), 53.1, 53.1 (COO*C*H$_3$), 58.9 (CH_2OCH_3), 63.7 (*C*H$_2$OCH$_3$), 70.0 (OCH_2), 98.0 (*C*COO), 124.2 (br), 124.4, 126.3 (br), 127.6 (CH_{Ar}), 126.7, 134.5 (br) (C_{Ar}), 153.4, 153.9 (br) (NCOO), 170.0 (C*C*OO), 173.4 (br, COH). IR (Nujol, cm^{-1}): $\tilde{\nu}$ = 3079 (w), 1723 (s), 1708 (s), 1656 (m), 1618 (m), 1337 (m), 1289 (s), 1223 (s), 1180 (w), 1132 (m), 1067 (m), 1037 (w), 1010 (m), 767 (m). MS (EI, 70 eV): *m/z* (%) = 406 (M^+, 8), 347 (100), 299 (7), 271 (30), 256 (15), 180 (13), 128 (9). Anal. Calcd for $C_{19}H_{22}N_2O_8$ (406.39): C, 56.15; H, 5.46; N, 6.89. Found: C, 56.48; H, 5.57; N, 6.50.

10-Acetyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2,4,6,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5d). Starting with quinazoline **3a** (0.521 g, 4.0 mmol), 2,4-bis(trimethylsilyloxy)-penta-1,3-diene **4d** (1.464 g, 6.0 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 mL), **5d** was obtained as a yellow solid (0.867 g, 63%); mp. 49 – 50 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.35 (s, 3H, $COCH_3$), 2.50 (dd, ^2J = 17.8 Hz, ^3J = 1.5 Hz, 1H, CH_2), 3.01 (dd, ^2J = 17.8 Hz, ^3J = 5.4 Hz, 1H, CH_2), 3.78 (s, 3H, CO_2CH_3), 3.88 (s, 3H, CO_2CH_3), 5.42 (br s, 1H, NC*H*CH$_2$), 7.06–7.27 (m, 3H, Ar), 7.42 (s, 1H, NCHN), 7.49–7.53 (m, 1H, Ar), 15.28 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 24.4 (CO*C*H$_3$), 40.6 (CH_2), 48.6 (N*C*HCH$_2$), 53.3, 53.6 (CO_2CH_3), 60.3 (NCHN), 107.2 (*C*COCH$_3$), 125.0, 125.5, 126.4, 127.6 (CH_{Ar}), 127.2, 133.8 (C_{Ar}), 153.4, 154.5 (NCOO), 181.6 (COH), 196.5 (*C*OCH$_3$). IR (Nujol, cm^{-1}): $\tilde{\nu}$ = 1717 (s), 1608 (m), 1583 (m), 1492 (m) 1338 (m), 1283 (s), 1268 (s), 1233 (m), 1193 (m), 1132 (m), 1102 (m), 1017 (m), 968 (m), 765 (m), 735 (m). MS (EI, 70 eV): *m/z* (%) = 346 (M^+, 14), 287 (100), 255 (41), 237 (55), 207 (50). HRMS (CI pos., Isobutane): Calcd for $C_{17}H_{18}N_2O_6$ (M^+): 346.11594, found 346.11550.

10-Acetyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dibenzyl ester (5d′). Starting with quinazoline **3a** (0.521 g, 4.00 mmol), 2,4-bis(trimethylsilyloxy)penta-1,3-diene **4d** (1.174 g, 4.80 mmol) and benzyl chloroformate (2.050 g,

12.00 mmol) in CH_2Cl_2 (40 ml), **5d′** was obtained as yellowish, highly viscous oil (0.755 g, 38%). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.23 (s, 3H, $COCH_3$), 2.49, 2.50 (d, ^2J = 17.7 Hz, 1H, NCHCH_2, rotamers), 2.99 (br d, ^2J = 17.7 Hz, 1H, NCHCH_2), 5.10 – 5.29 (m, 4H, OCH_2), 5.45 (br, 1H, NCHCH$_2$), 7.05 – 7.24 (m, 4H, Ar), 7.35 (m, 9H, Ar, NCHN), 7.53 (t, ^3J = 8.4 Hz, 2H, Ar). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 24.5 (COCH$_3$), 40.7 (NCHCH$_2$), 48.6 (br), 48.8 (br) (NCHCH$_2$, rotamers), 60.4 (br, NCHN), 67.9, 68.5 (OCH_2), 107.2 (NCHCCO), 125.1, 125.5, 126.4, 127.7, 128.2 (br), 128.2 (br), 128.4, 128.6 (CH_{Ar}), 127.2, 133.8 (br), 135.5, 135.8 (C_{Ar}), 152.8, 153.6 (NCOO), 184.7 (br, COH), 196.4 (br, COCH$_3$). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3064 (w), 3032 (w), 2952 (w), 2899 (w), 1700 (s), 1606 (m), 1583 (m), 1490 (m), 1454 (m), 1417 (m), 1382 (m), 1363 (m), 1327 (m), 1301 (m), 1262 (s), 1214 (s), 1176 (m), 1129 (m), 1098 (m), 1050 (m), 1017 (m), 1001 (m), 733 (s). MS (EI, 70 eV): *m/z* (%) = 498 (M^+, 3), 390 (3), 363 (36), 319 (15), 228 (4), 91 (100), 57 (17). HRMS (EI): Calcd for $C_{29}H_{26}N_2O_8$ (M^+) 498.17854, found 498.179402.

10-(2,2-Dimethyl-propionyl)-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5e). Starting with quinazoline **3a** (0.261 g, 2.0 mmol), 5,5-dimethyl-2,4-bis(trimethylsilyloxy)-hexa-1,3-diene **4e** (0.802 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol) in CH_2Cl_2 (20 mL), **5e** was obtained after HPLC (heptane/EtOAc = 2:1) as a colourless solid (0.092 g, 12%); mp. 126 – 127 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.21 (s, 9H, C_4H_9), 2.54 (m, ^2J = 14.3 Hz, 1H, CH_2, rotamers), 3.27 (br d, ^2J = 14.3 Hz, 1H, CH_2, rotamers), 3.78, 3.81 (s, 3H, $COOCH_3$, rotamers), 3.86 (s, 3H, $COOCH_3$), 4.18, 4.21 (br, 1H, COCHCO, rotamers), 5.59, 5.69 (br, 1H, NCHCH$_2$, rotamers), 6.81, 6.92 (br, 1H, Ar, rotamers), 7.04 – 7.24 (m, 3H, Ar), 7.91, 8.04 (br, 1H, NCHN, rotamers). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 25.6 (C(CH$_3$)$_3$), 27.0, 27.1 (COCHCO, rotamers), 46.6 (C(CH$_3$)$_3$), 47.8, 48.0 (CH_2, rotamers), 51.1, 51.5 (NCHCH$_2$, rotamers), 53.5 (OCH_3), 62.1 (OCH_3), 64.1, 64.5 (NCHN, rotamers), 122.0, 124.3, 124.6, 126.3, 126.6, 128.4, 128.5 (CH_{Ar}, rotamers), 125.2, 125.5, 132.8, 133.2 (C_{Ar}, rotamers), 153.1, 153.4, 153.7, 154.0 (NCOO, rotamers), 201.7, 206.9. 207.3 (CO, rotamers). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2968 (m), 2933 (w), 1719 (s), 1693 (s), 1488 (m), 1453 (s), 1422 (m), 1377 (m), 1345 (m), 1309 (s), 1277 (m), 1251 (m), 1231 (m), 1215 (m), 1195 (m), 1130 (m), 1060 (m), 1040 (m), 1026 (m), 766 (m). MS (EI, 70 eV): *m/z* (%) = 388 (M^+, 5), 331 (100), 299 (29), 245 (9), 213 (10), 189 (32), 145 (16), 128 (17). Anal. Calcd for $C_{20}H_{24}N_2O_6$ (388.41): C, 61.84; H, 6.23; N, 7.21. Found: C, 62.04; H, 6.48; N, 6.98.

5-Bromo-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid-10-(2-methoxy-ethyl)ester-8,13-dimethyl ester (5g). Starting with 7-

bromoquinazoline **3b** (0.418 g, 2.0 mmol), 1-(2-methoxy-ethoxy)-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4c** (0.853 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol) in CH_2Cl_2 (20 mL), **5g** was obtained as a colourless solid (0.220 g, 23%); mp. 114 – 117 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.40 (dd, ^2J = 17.7 Hz, ^3J = 1.5 Hz, 1H NCHC*H*$_2$), 2.98 (dd, ^2J = 17.7 Hz, ^3J = 5.0 Hz, 1H, NCHC*H*$_2$), 3.38 (s, 3H, CH_2OCH_3), 3.62 (m, 2H, CH_2OCH_3), 3.75, 3.87 (2s, 6H, $COOCH_3$), 4.33 (m, 2H, $COOCH_2$), 5.36 (br, 1H, NC*H*CH$_2$), 7.20 (d, ^3J = 2.1 Hz, 1H, Ar), 7.30 – 7.37 (m, 2H, Ar), 7.67 (br, 1H, NCHN), 12.23 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 38.0 (NCH*C*H$_2$), 48.6 (br, N*C*HCH$_2$), 53.3 (2 COO*C*H$_3$), 58.8 (br, NCHN), 58.9 CH_2OCH_3), 63.8 (CH_2OCH_3), 70.1 ($COOCH_2$), 97.9 (*C*COO), 117.0 (C_{Ar}Br), 126.1, 129.0, 130.8 (CH_{Ar}), 128.7, 133.9 (C_{Ar}), 153.4, 153.7 (NCOO), 169.9 (C*C*OO), 173.1 (br, COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2997 (w), 2954 (w), 2909 (w), 1725 (s), 1705 (s), 1652 (m), 1610 (m), 1484 (m), 1456 (s), 1418 (m), 1378 (m), 1328 (m), 1287 (s), 1230 (m), 1178 (m), 1119 (m), 1067 (m), 1014 (m), 845 (m), 830 (m), 769 (m). MS (EI, 70 eV): *m/z* (%) = 486 (M^+, ^{81}Br, 4), 484 (M^+, ^{79}Br, 4), 427 (^{81}Br, 40), 425 (^{79}Br, 41), 351 (^{81}Br, 15), 349 (^{79}Br, 15), 256 (18), 180 (19), 149 (24). HRMS (EI): Calcd for $C_{19}H_{21}BrN_2O_8$ (M^+, ^{79}Br) 484.04758, found 484.047931.

10-Acetyl-5-bromo-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2,4,6,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5h). Starting with 7-bromo-quinazoline **3b** (0.418 g, 2.0 mmol), 2,4-bis(trimethylsilyloxy)penta-1,3-diene **4d** (0.685 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol) in CH_2Cl_2 (20 mL), **5h** was obtained as a colourless solid (0.314 g, 37%); mp. 168 – 171 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.35 (s, 3H, $COCH_3$), 2.50 (dd, ^2J = 17.8 Hz, ^3J = 1.4 Hz, 1H, CH_2), 3.01 (dd, ^2J = 17.8 Hz, ^3J = 5.3 Hz, 1H, CH_2), 3.78 (s, 3H, CO_2CH_3), 3.88 (s, 3H, CO_2CH_3), 5.39 (br s, 1H, NC*H*CH$_2$), 7.22 (d, ^3J = 2.1 Hz, 1H, Ar), 7.39 (br s, 1H, NCHN), 7.29–7.47 (m, 2H, Ar), 15.28 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 24.5 ($CO*C*H_3$), 40.4 (CH_2), 48.4 (N*C*HCH$_2$), 53.4, 53.8 (CO_2*C*H_3), 60.4 (NCHN), 107.0 (*C*COCH$_3$), 118.0 (CBr), 127.1, 129.1, 130.8 (CH_{Ar}), 129.2, 133.1 (C_{Ar}), 153.3, 154.1 (NCOO), 184.2 (COH), 196.5 (*C*OCH$_3$). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2954 (w), 1723 (s), 1701 (s), 1616 (m), 1490 (m), 1455 (s), 1418 (m), 1370 (s), 1280 (s), 1230 (m), 1193 (w), 1139 (m), 1109 (m), 1044 (m), 1005 (m), 769 (m). MS (EI, 70 eV): *m/z* (%) = 426 (M^+, ^{81}Br, 17), 424 (M^+, ^{79}Br, 17), 367 (99), 365 (100), 335 (20), 333 (20), 196 (54). Anal. Calcd for $C_{17}H_{17}BrN_2O_7$ (425.23): C, 48.02; H, 4.03; N, 6.59. Found: C, 47.67; H, 4.11; N, 6.24.

11-Hydroxy-4-methyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5i). Starting with 6-methylquinazoline **3c** (0.462 g, 3.2 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (1.170 g, 4.5 mmol) and methyl chloroformate

(1.210 g, 12.8 mmol) in CH_2Cl_2 (32 mL), **5i** was obtained as a yellow solid (0.522 g, 43%); mp. 155 – 156 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.28 (s, 3H, CCH_3), 2.40 (dd, ^2J = 17.6 Hz, ^3J = 1.3 Hz, 1H, CH_2), 2.96 (dd, ^2J = 17.6 Hz, ^3J = 4.6 Hz, 1H, CH_2), 3.75 (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 5.34 (br, 1H, NC*H*CH_2), 6.85 (s, 1H, Ar), 7.03 (dd, ^3J = 8.5 Hz, ^4J = 1.4 Hz, 1H, Ar), 7.35 (br, 1H, NCHN), 7.61 (br, 1H, Ar), 12.26 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 20.7 (C*C*H_3), 38.1 (CH_2), 48.6, 48.9 (N*C*HCH_2, rotamers), 52.0, 53.1, 53.2 (OCH_3), 58.8 (NCHN), 98.0 (NCH*C*CO), 124.3, 126.6 (br), 128.5 (CH_{Ar}), 126.6 (br), 131.8, 133.9 (C_{Ar}), 153.5, 154.1 (NCOO), 170.6 (*C*OOCH_3), 173.2 (br, COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3068 (w), 3000 (w), 2954 (w), 2918 (w), 2860 (w), 1702 (s), 1650 (s), 1613 (m), 1505 (m), 1456 (s), 1441 (s), 1408 (m), 1376 (s), 1362 (m), 1331 (s), 1284 (s), 1243 (s), 1224 (m), 1193 (m), 1137 (m), 1108 (m), 1070 (m), 1045 (m), 1012 (w), 775 (m). MS (EI, 70 eV): *m/z* (%) = 376 (M^+, 13), 317 (100), 285 (63), 253 (22), 212 (37), 180 (31), 84 (59), 49 (54). HRMS (EI): Calcd for $C_{18}H_{20}N_2O_7$ (M^+) 376.12650, found 376.125661.

10-Acetyl-11-hydroxy-4-methyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5j). Starting with 6-methylquinazoline **3c** (0.160 g, 1.1 mmol), 2,4-bis(trimethylsilyloxy)penta-1,3-diene **4d** (0.377 g, 1.5 mmol) and methyl chloroformate (0.416 g, 4.4 mmol) in CH_2Cl_2 (11 mL), **5j** was obtained as a colourless solid (0.121 g, 31%); mp. 136 – 138 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.29, 2.33 (CCH_3, $COCH_3$), 2.49 (dd, ^2J = 17.7 Hz, ^3J = 1.3 Hz, 1H, CH_2), 2.98 (br dd, ^2J = 17.7 Hz, ^3J = 5.1 Hz, 1H, CH_2), 3.76 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 5.35 (br, 1H, NC*H*CH_2), 6.86 (s, 1H, Ar), 7.02 (d, ^3J = 8.6 Hz, 1H, Ar), 7.38 (br, 2H, Ar, NCHN), 16.34 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 20.8, 24.4 ($C_{Ar}CH_3$, CO*C*H_3), 40.7 (CH_2), 48.6 (br, N*C*HCH_2), 53.3, 53.5 (OCH_3), 60.4 (br, NCHN), 107.3 (*C*CO), 125.2, 126.7, 126.7, 128.5 (CH_{Ar}, rotamers), 127.0, 131.2, 134.8 (C_{Ar}), 153.5, 154.5 (NCOO), 184.7 (br, COH), 196.4 (C*C*O). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3059 (w), 3000 (w), 2955 (w), 2918 (w), 2858 (w), 1726 (s), 1703 (s), 1617 (m), 1505 (m), 1455 (s), 1411 (s), 1371 (s), 1323 (m), 1301 (m), 1279 (s), 1232 (m), 1192 (m), 1158 (w), 1138 (m), 1110 (m), 1047 (m), 1008 (w), 824 (m), 771 (m), 735 (m). MS (EI, 70 eV): *m/z* (%) = 360 (M^+, 12), 328 (5), 313 (5), 301 (100), 283 (6), 269 (37), 251 (6), 196 (26), 130 (9). HRMS (EI): Calcd for $C_{18}H_{20}N_2O_6$ (M^+) 360.13159, found 360.130603.

4-Ethyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5k). Starting with 6-ethylquinazoline **3d** (0.316 g, 2.0 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (0.728 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol), **5k** was obtained as a slightly yellow solid (0.330 g, 43%); mp. 137 – 139 °C. ^{1}H

NMR (300 MHz, $CDCl_3$): δ = 1.20 (t ^3J = 7.6 Hz, 3H, CH_2CH_3), 2.40 (dd, ^2J = 17.6 Hz, ^3J = 1.7 Hz, 1H NCHCH_2), 2.58 (q, ^3J = 7.6 Hz, 2H, CH_2CH_3), 2.97 (dd, ^2J = 17.6 Hz, ^3J = 4.7 Hz, 1H, NCHCH_2), 3.75, 3.79, 3.86 (3s, 9H, OCH_3), 5.36 (br, 1H, NCHCH$_2$), 6.87 (s, 1H, Ar), 7.06 (dd, ^3J = 8.5 Hz, ^4J = 1.7 Hz, 1H, Ar), 7.36 (br, 1H, NCHN), 7.64 (br, 1H, Ar), 12.27 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 15.4 (CH_2CH_3), 28.1 (CH_2CH_3), 38.1 (br, NCHCH_2), 48.8 (br, N$CHCH_2$), 52.0, 53.1, 53.2 (3 OCH_3), 58.9 (br, NCHN), 98.0 (NCHCCO), 124.3, 125.5, 126.6 (CH_{Ar}), 127.3, 132.0 (br), 140.2 (C_{Ar}), 153.5, 154.1 (NCOO), 170.6 (CCOO), 173.3 (br, COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3073 (w), 2962 (m), 2930 (w), 2873 (w), 2856 (w), 1721 (s), 1700 (s), 1659 (s), 1619 (m), 1500 (m), 1460 (s), 1446 (s), 1412 (s), 1379 (s), 1328 (m), 1286 (s), 1236 (s), 1196 (m), 1164 (m), 1136 (m), 1069 (m), 1047 (m), 1009 (m), 842 (m), 769 (m), 753 (m). MS (EI, 70eV): *m/z* (%) = 391 (M^+, 100), 371 (63), 341 (20), 177 (25), 113 (17). Anal. Calcd for $C_{19}H_{22}N_2O_7$ (390.39): C, 58.46; H, 5.68; N, 7.18. Found: C, 58.71; H, 5.87; N, 6.64.

4-Ethyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid 10-ethyl ester 8,13-dimethyl ester (5l). Starting with 6-ethyl-quinazoline **3d** (0.400 g, 2.5 mmol), 1-ethoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4b** (0.971 g, 3.5 mmol) and methyl chloroformate (0.945 g, 10.0 mmol), **5l** was obtained as a yellowish solid (0.379 g, 37%); mp. 127 – 130 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.20 (t, ^3J = 7.6 Hz, 3H, CH_2CH_3), δ = 1.33 (t, ^3J = 7.2 Hz, 3H, CH_2CH_3), 2.40 (dd, ^2J = 17.6 Hz, ^3J = 1.4 Hz, 1H, NCHCH_2), 2.58 (q, ^3J = 7.6 Hz, 2H, CH_3CH_2), 2.97 (dd, ^2J = 17.6 Hz, ^3J = 4.9 Hz, 1H, NCHCH_2), 3.75, 3.85 (2s, 6H, OCH_3), 4.23 (q, ^3J = 7.2 Hz, 2H, CH_3CH_2O), 5.36 (br, 1H, NCHCH$_2$), 6.87 (br s, 1H, Ar), 7.06 (dd, ^3J = 8.5 Hz, ^2J = 1.7 Hz, 1H, Ar), 7.36 (br, 1H, NCHN), 7.68 (br, 1H, Ar), 12.34 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 14.03, 15.38 (CH_2CH_3), 28.1 (CH_3CH_2Ar), 38.2 (br, NCHCH_2), 49.0 (br, N$CHCH_2$), 53.0, 53.1 (OCH_3), 58.9 (br, NCHN), 61.0 (CH_3CH_2O), 98.2 (NCHCCO), 124.2, 125.4, 126.6 (CH_{Ar}), 127.3, 132.1 (br), 140.1 (C_{Ar}), 153.6, 154.1 (NCOO), 170.3 (CCOO), 173.0 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3069 (w), 2993 (w), 2962 (m), 2930 (w), 2874 (w), 1708 (s), 1655 (s), 1618 (m), 1503 (m), 1455 (s), 1413 (m), 1381 (s), 1327 (m), 1286 (s), 1262 (m), 1236 (s), 1220 (m), 1193 (m), 1171 (m), 1151 (m), 1136 (m), 1105 (m), 1068 (m), 1044 (m), 1006 (m), 837 (m), 773 (m). MS (EI, 70 eV): *m/z* (%) = 404 (M^+, 11), 345 (100), 299 (45), 267 (15), 226 (41), 180 (27). HRMS (EI): Calcd for $C_{20}H_{24}N_2O_7$ (M^+) 404.15780, found 404.157772.

10-Acetyl-4-ethyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5m). Starting with 6-ethylquinazoline **3d** (0.255 g, 1.6 mmol), 2,4-

bis(trimethylsilyloxy)penta-1,3-diene **4d** (0.549 g, 2.2 mmol) and methyl chloroformate (0.605 g, 6.4 mmol) in CH_2Cl_2 (16 mL), **5m** was obtained as a yellow, highly viscous oil (0.154 g, 26%). NMR (300 MHz, $CDCl_3$): $\delta = 1.20$ (t, $^3J = 7.6$ Hz, 3H, CH_2CH_3), 2.33 (s, 3H, $COCH_3$), 2.50 (dd, $^2J = 17.7$ Hz, $^3J = 1.2$ Hz, 1H, $NCHCH_2$), 2.59 (q, $^3J = 7.6$ Hz, 2H, CH_2CH_3), 2.99 (dd, $^2J = 17.7$ Hz, $^3J = 5.1$ Hz, 1H, CH_2CH_3), 3.76 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 6.88 (s, 1H, Ar), 7.06 (dd, $^3J = 8.4$ Hz, $^4J = 1.7$ Hz, 1H, Ar), 7.40 (br, 2H, NCHN, Ar), 16.36 (s, 1H, OH). ^{13}C NMR (300 MHz, $CDCl_3$): $\delta = 15.3$ (CH_2CH_3), 24.4 ($COCH_3$), 28.1 (CH_2CH_3), 40.7 ($NCHCH_2$), 48.7 (br, $NCHCH_2$), 53.3, 53.5 (OCH_3), 60.4 (br, NCHN), 107.3 ($NCHCCO$), 125.3, 125.5, 127.3 (CH_{Ar}), 127.0, 131.4 (C_{Ar}), 141.1 ($C_{Ar}CH_2$), 153.5, 154.5 (NCOO), 184.7 (br, COH), 196.4 ($COCH_3$). IR (KBr, cm^{-1}): $\tilde{\nu} = 3005$ (w), 2962 (m), 2932 (w), 2872 (w), 1723 (s), 1702 (s), 1602 (m), 1504 (m), 1452 (s), 1411 (m), 1371 (m), 1340 (m), 1307 (s), 1285 (s), 1234 (m), 1190 (m), 1137 (m), 1108 (m), 1048 (m), 994 (m), 969 (m), 829 (m), 776 (m), 734 (m). MS (CI pos., Isobutane): *m/z* (%) = 375 ($[M+H]^+$). HRMS (CI pos., Isobutane): Calcd for $C_{19}H_{23}N_2O_6$ ($[M+1]^+$) 375.15506, found 375.155416.

11-Hydroxy-4-isopropyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5n). Starting with 6-isopropyl-quinazoline **3e** (0.626 g, 3.5 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (1.275 g, 4.9 mmol) and methyl chloroformate (1.323 g, 14.0 mmol), **5n** was obtained as light yellow solid (0.620 g, 44%); mp. 151 °C. ^{1}H NMR (300 MHz, $CDCl_3$): $\delta = 1.20$ (d, $^3J = 7.0$ Hz, 3H, $CHCH_3$), 1.21 (d, $^3J = 6.9$ Hz, 3H, $CHCH_3$), 2.40 (dd, $^2J = 17.7$ Hz, $^3J = 1.1$ Hz, 1H, $NCHCH_2$), 2.84 (m, 1H, $CH(CH_3)_2$), 2.97 (dd, $^2J = 17.7$ Hz, $^3J = 4.4$ Hz, 1H, $NCHCH_2$), 3.74, 3.79, 3.85 (3s, 9H, OCH_3), 5.37 (br, 1H, $NCHCH_2$), 6.88 (s, 1H, Ar), 7.09 (dd, $^3J = 8.6$ Hz, $^4J = 1.8$ Hz, 1H, Ar), 7.36 (br, 1H, NCHN), 7.65 (br, 1H, Ar), 12.27 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): $\delta = 21.8$, 22.0 ($CH(CH_3)_2$), 31.4 ($CH(CH_3)_2$), 36.2 (br, $NCHCH_2$), 46.9 (br, $NCHCH_2$), 50.0, 51.1, 51.2 (OCH_3), 56.9 (br, NCHN), 96.1 ($NCHCCO$), 122.0, 122.3, 123.9 (CH_{Ar}), 124.5, 130.1 (br), 142.8 (C_{Ar}), 151.5, 152.1 ($NCOO$), 168.6 ($CCOO$), 171.2 (COH). IR (KBr, cm^{-1}): $\tilde{\nu} = 2958$ (m), 2931 (w), 2870 (w), 1723 (s), 1658 (s), 1618 (m), 1502 (m), 1445 (s), 1412 (m), 1378 (s), 1330 (m), 1287 (s), 1264 (s), 1240 (s), 1225 (s), 1195 (m), 1170 (m), 1135 (m), 1114 (m), 1066 (m), 1044 (m), 1009 (m), 835 (m), 768 (m). MS (EI, 70 eV): *m/z* (%) = 404 (M^+, 12), 345 (100), 313 (44), 281 (16), 212 (50), 180 (25). HRMS (EI): Calcd for $C_{20}H_{24}N_2O_7$ (M^+) 404.15780, found 404.158017.

11-Hydroxy-4-isopropyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid 10-ethyl ester 8,13-dimethyl ester (5o). Starting with 6-isopropylquinazoline **3e**

(0.344 g, 2.0 mmol), 1-ethoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4b** (0.768 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol), **5o** was obtained as a slightly yellow solid (0.368 g, 44%); mp. 134–136 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.20 (d, ^3J = 1.4 Hz, 3H, CH(CH_3)$_2$), 1.22 (d, ^3J = 1.4 Hz, 3H, CH(CH_3)$_2$), 1.33 (t, ^3J = 7.1 Hz, 3H, CH_3CH$_2$), 2.40 (dd, ^2J = 17.6 Hz, ^3J = 1.3 Hz, 1H, NCHCH_2), 2.84 (m, 1H, CH(CH$_3$)$_2$), 2.97 (br dd, ^2J = 17.6 Hz, ^3J = 4.8 Hz, 1H, NCHCH_2), 3.74, 3.85 (2s, 6H, OCH$_3$), 4.22 (q, ^3J = 7.1 Hz, 2H, OCH_2CH$_3$), 5.37 (br, 1H, NCHCH$_2$), 6.88 (br s, 1H, Ar), 7.01 (dd, ^3J = 8.6 Hz, ^2J = 1.8 Hz, 1H, Ar), 7.35 (br, 1H, NCHN), 7.69 (br, 1H, Ar), 12.35 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 14.0 (*C*H$_3$CH$_2$), 23.8, 24.0 (CH(*C*H$_3$)$_2$), 33.4 (*C*H(CH$_3$)$_2$), 38.2 (br, NCH*C*H$_2$), 49.0 (br, N*C*HCH$_2$), 53.0, 53.1 (OCH$_3$), 58.9 (br, NCHN), 61.0 (O*C*H$_2$CH$_3$), 98.2 (NCH*C*CO), 124.1, 125.8 (CH$_{Ar}$), 126.5, 132.1, 144.8, (C$_{Ar}$), 153.6, 154.1 (NCOO), 170.3 (C*C*OO), 173.0 (br, COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3048 (w), 2957 (m), 2912 (w), 2871 (w), 1706 (s), 1658 (s), 1618 (m), 1502 (m), 1453 (s), 1402 (s), 1377 (s), 1328 (s), 1296 (s), 1260 (s), 1236 (m), 1217 (s), 1192 (m), 1181 (m), 1139 (m), 1120 (m), 1080 (m), 1062 (m), 1044 (m), 1003 (m), 834 (m), 771 (m). MS (EI, 70 eV): *m/z* (%) = 418 (M$^+$, 9), 359 (100), 313 (30), 281 (10), 226 (29), 180 (17). HRMS (EI): Calcd for $C_{21}H_{26}N_2O_7$ (M$^+$) 418.17345, found 418.173096.

10-Acetyl-11-hydroxy-4-isopropyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5p). Starting with 6-isopropylquinazoline **3e** (0.314 g, 1.8 mmol), 2,4-bis(trimethylsilyloxy)-penta-1,3-diene **4d** (0.624 g, 2.6 mmol) and methyl chloroformate (0.688 g, 7.3 mmol) in CH_2Cl_2 (18 mL), **5p** was obtained as a yellow solid (0.269 g, 38%); mp. 115 – 118 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.21 (d, ^3J = 6.9 Hz, 3H, CH(CH_3)$_2$), 1.21 (d, ^3J = 6.9 Hz, 3H, CH(CH_3)$_2$), 2.33 (s, 3H, COCH$_3$), 2.50 (dd, ^2J = 17.7 Hz, ^3J = 1.3 Hz, 1H, CH$_2$), 2.84 (sept, ^3J = 6.9 Hz, 1H, CH(CH$_3$)$_2$), 2.99 (dd, ^2J = 17.7 Hz, ^3J = 5.3 Hz, 1H, CH$_2$), 3.76 (s, 3H, OCH$_3$), 3.86 (s, 3H, OCH$_3$), 5.38 (br, 1H, NCHCH$_2$), 6.89 (d, ^4J = 1.5 Hz, 1H, Ar), 7.09 (dd, ^3J = 8.6 Hz, ^4J = 1.9 Hz, 1H, Ar), 7.40 (br, 2H, NCHN, Ar), 16.37 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 23.7, 23.9 (CH(*C*H$_3$)$_2$), 24.3 (*C*H(CH$_3$)$_2$), 33.5 (CO*C*H$_3$), 40.7 (br, CH$_2$), 48.7 (br, N*C*HCH$_2$), 53.2, 53.5 (OCH$_3$), 60.4 (br, NCHN), 107.3 (*C*CO), 124.0, 125.2, 125.9 (CH$_{Ar}$), 127.0, 131.4 (C$_{Ar}$), 145.7 (*C*$_{Ar}$CH(CH$_3$)$_2$), 153.5, 154.5 (NCOO), 184.8 (br, COH), 196.4 (C*C*O). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2958 (m), 2929 (m), 2872 (w), 1727 (s), 1701 (s), 1601 (m), 1503 (m), 1451 (s), 1405 (s), 1373 (s), 1281 (s), 1227 (m), 1193 (m), 1167 (m), 1135 (m), 1110 (m), 1057 (m), 1042 (m), 1004 (m), 968 (m), 832 (m), 775 (m), 731 (m). MS (EI, 70 eV): *m/z* (%) = 388 (M$^+$, 13), 340 (11), 329 (100), 297 (28), 196 (29), 177 (26), 97 (19), 71 (25), 57 (40). HRMS (EI): Calcd for $C_{20}H_{24}N_2O_6$ (M$^+$) 388.16289, found 388.162516.

4-*tert*-Butyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5q). Starting with 6-*tert*-butylquinazoline **3f** (0.372 g, 2.0 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (0.728 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol), **5q** was obtained as a slightly yellow solid (0.422 g, 50%); mp. 150 – 151 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.28 (s, 9H, C(CH_3)$_3$), 2.41 (dd, ^2J = 17.6 Hz, ^3J = 1.1 Hz, 1H, NCHCH_2) 3.0 (dd, ^2J = 17.6 Hz, ^3J = 4.7 Hz, 1H, NCHCH_2), 3.75, 3.79, 3.86 (3s, 9H, OCH_3), 5.39 (br, 1H, NCHCH_2), 7.03 (br, 1H, Ar), 7.25 (dd, ^3J = 8.6 Hz, ^4J = 2.0 Hz, 1H, Ar), 7.37 (br, 1H, NCHN), 7.67 (br, 1H, Ar), 12.28 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 31.2 (C(*C*H$_3$)$_3$), 34.3 (*C*(CH$_3$)$_3$), 38.2 (br, NCH*C*H$_2$), 49.0 (br, N*C*HCH$_2$), 52.0, 53.1, 53.2 (OCH_3), 58.9 (br, NCHN), 98.1 (NCH*C*CO), 122.9 (br), 124.0, 125.0 (CH_{Ar}), 126.2, 131.8 (br), 147.2 (C_{Ar}), 153.5, 154.1 (NCOO), 170.7 (C*C*OO), 173.2 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2957 (m), 2907 (w), 2869 (w), 1716 (s), 1659 (s), 1620 (m), 1502 (m), 1444 (s), 1380 (m), 1333 (s), 1295 (s), 1267 (s), 1232 (s), 1195 (m), 1146 (m), 1117 (m), 1067 (m), 1049 (m), 1010 (m), 835 (m), 767 (m), 747 (m). MS (EI, 70 eV): *m/z* (%) = 418 (M$^+$, 10), 359 (100), 327 (38), 295 (13), 212 (43), 180 (21). HRMS (EI): Calcd for $C_{21}H_{26}N_2O_7$ ([M]$^+$) 418.17345, found 418.173725.

4-*tert*-Butyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid-10-(2-methoxy-ethyl)ester-8,13-dimethyl ester (5r). Starting with 6-*tert*-butylquinazoline **3f** (0.372 g, 2.0 mmol), 1-(2-methoxy-ethoxy)-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4c** (0.856 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol) in CH_2Cl_2 (20 mL), **5r** was obtained as a yellow solid (0.349 g, 38%); mp. 91 – 95 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.27 (s, 9H, C(CH$_3$)$_3$), 2.40 (d, ^2J = 17.6 Hz, 1H, NCHCH_2), 2.98 (br dd, ^2J = 17.6 Hz ,^3J = 4.8 Hz, NCHCH_2) 3.39 (s, 3H, CH_2OCH_3), 3.63 (t, ^3J = 5.0 Hz, 2H, CH_2OCH$_3$), 3.74 (s, 3H, $COOCH_3$), 3.85 (s, 3H, $COOCH_3$), 4.33 (m, 2H, $COOCH_2$), 5.38 (br, 1H, NCHCH_2), 7.02 (s, 1H, Ar), 7.25 (dd, ^3J = 8.8 Hz, ^4J = 2.1 Hz, 1H, Ar), 7.38 (br, 1H, NCHN), 7.66 (br, 1H, Ar), 12.24 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 31.2 (C(*C*H$_3$)$_3$), 34.2 (*C*(CH$_3$)$_3$), 38.2 (NCH*C*H$_2$), 48.9 (br, N*C*HCH$_2$), 53.1 (2 COO*C*H$_3$), 58.9 (CH_2OCH_3, NCHN), 63.7 (*C*H$_2$OCH$_3$), 70.1 (COO*C*H$_2$), 98.1 (NCH*C*CO), 122.8, 123.8, 124.9 (CH_{Ar}), 126.1, 131.8 (C_{Ar}), 147.1 (*C*$_{Ar}$C(CH$_3$)$_3$), 153.5, 154.0 (NCOO), 170.1 (C*C*OO), 173.2 (br, COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2958 (m), 2905 (m), 2874 (m), 1717 (s), 1654 (s), 1620 (m), 1503 (m), 1454 (s), 1416 (s), 1380 (s), 1332 (s), 1294 (s), 1264 (s), 1231 (s), 1182 (m), 1118 (m), 1067 (m), 1049 (m), 1012 (m), 833 (m), 770 (m). MS (EI, 70 eV): *m/z* (%) = 462 (M$^+$, 9), 403 (100), 386 (12), 327 (27), 302 (20), 256 (20), 180 (10). HRMS (EI): Calcd for $C_{23}H_{30}N_2O_8$ (M$^+$) $C_{23}H_{30}N_2O_8$ 462.19967, found 462.198773.

4-*tert*-Butyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid 10-isobutyl ester 8,13-dimethyl ester (5s). Starting with 6-*tert*-butylquinazoline **3f** (0.372 g, 2.0 mmol), 1-isobutyl-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4g** (0.847 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol), **5s** was obtained as a slightly yellow solid (0.500 g, 54%); mp. 104-106 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.96 (t, ^3J = 6.5 Hz, 6H, CH(CH_3)$_2$), 1.28 (s, 9H, C(CH_3)$_3$), 2.00 (m, 1H, CH(CH_3)$_2$), 2.40 (dd, ^2J = 17.6 Hz, ^3J = 1.3 Hz, 1H, NCHCH_2), 2.97 (br dd, ^2J = 17.6 Hz, ^3J = 4.8 Hz, 1H, NCHCH_2), 3.75, 3.83 (2s, 6H, OCH_3), 3.89 (m, 1H, OCH_2), 4.05 (m, 1H, OCH_2), 5.38 (br, 1H, NCHCH_2), 7.03 (m, 1H, Ar), 7.25 (m, 1H, Ar), 7.37 (br, 1H, NCHN), 7.62 (br, 1H, Ar), 12.44 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 18.9, 18.9 (CH(*C*H_3)$_2$), 27.6 (*C*H(CH_3)$_2$), 31.2 (C(*C*H_3)$_3$), 34.3 (*C*(CH_3)$_3$), 38.3 (br, NCH*C*H_2), 49.0 (br, N*C*HCH_2), 53.1 (2 OCH_3), 58.9 (br, NCHN), 71.1 (OCH_2), 98.2 (NCH*C*CO), 122.8 (br), 124.1, 124.9 (CH_{Ar}), 126.3, 131.9, 147.2 (C_{Ar}), 153.5, 154.2 (NCOO), 170.5 (C*C*OO), 173.0 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2960 (m), 2907 (w), 2874 (w), 1709 (s), 1653 (s), 1622 (m), 1503 (m), 1455 (s), 1414 (s), 1380 (m), 1330 (s), 1287(s), 1263(s), 1231 (s), 1182 (m), 1144 (m), 1118 (m), 1064 (m), 1048 (m), 1012 (m), 834 (m). MS (EI): *m/z* (%) = 460 (M$^+$, 9), 401 (100), 327 (37), 302 (15), 254 (23), 198 (23). HRMS (EI): Calcd for $C_{24}H_{32}N_2O_7$ (M$^+$) 460.22040, found 460.220738.

10-Acetyl-4-*tert*-butyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5t). Starting with 6-*tert*-butylquinazoline **3f** (0.234 g, 1.3 mmol), 2,4-bis(trimethylsilyloxy)penta-1,3-diene **4d** (0.430 g, 1.8 mmol) and methyl chloroformate (0.476 g, 5.0 mmol) in CH_2Cl_2 (15 mL), **5t** was obtained as a yellowish solid (0.223 g, 44%); mp. 143 – 145 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.28 (s, 9H, C(CH_3)$_3$), 2.34 (s, 3H, $COCH_3$), 2.50 (d, ^2J = 17.9 Hz, 1H, CH_2), 3.00 (br dd, ^2J = 17.9 Hz, ^3J = 5.1 Hz, 1H, CH_2), 3.76 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 5.40 (br, 1H, NCHCH_2), 7.04 (d, ^4J = 2.0 Hz, 1H, Ar), 7.25 (dd, ^3J = 8.7 Hz, ^4J = 2.0 Hz, 1H, Ar), 7.41 (br, 2H, Ar, NCHN), 16.39 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 24.4 (CO*C*H_3), 31.2 (C(*C*H_3)$_3$), 34.3 (*C*(CH_3)$_3$), 40.8 (CH_2), 48.9 (br, N*C*HCH_2), 53.3, 53.5 (OCH_3), 60.4 (br, NCHN), 107.3 (NCH*C*CO), 122.9, 124.9, 125.0 (CH_{Ar}), 126.6, 131.2 (C_{Ar}), 148.0 (*C*$_{Ar}$C(CH_3)$_3$), 153.5, 154.5 (NCOO), 184.8 (br, COH), 196.4 (*C*OCH_3). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3036 (w), 2959 (m), 2907 (w), 2870 (w), 1722 (s), 1702 (s), 1616 (m), 1505 (m), 1452 (s), 1409 (m), 1376 (m), 1339 (m), 1306 (s), 1286 (s), 1236 (m), 1186 (m), 1146 (m), 1109 (m), 1041 (m), 1001 (m), 973 (m), 774 (m). MS (EI, 70 eV): *m/z* (%) = 402 (M$^+$, 13), 343 (100), 311 (17), 269 (4), 240 (9), 196 (24). HRMS (EI): Calcd for $C_{21}H_{26}N_2O_6$ (M$^+$) 402.17854, found 402.177942.

4-Hexyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5u). Starting with 6-hexylquinazoline **3g** (0.419 g, 2.0 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (0.714 g, 2.7 mmol) and methyl chloroformate (0.749 g, 7.8 mmol), **5u** was obtained as a yellowish solid (0.322 g, 37%); mp. 118-120 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.87 (m, 3H, $CH_2CH_2CH_3$), 1.28 (m, 6H, $CH_3CH_2CH_2CH_2CH_2CH_2$), 1.56 (m, 2H, $CH_3CH_2CH_2CH_2CH_2CH_2$), 2.40 (dd, ^2J = 17.6 Hz, ^3J = 1.4 Hz, 1H, NCHCH_2), 2.53 (t, ^3J = 7.8 Hz, 2H, $CH_3CH_2CH_2CH_2CH_2CH_2$), 3.0, (dd, ^2J = 17.6 Hz, ^3J = 4.6 Hz, 1H, NCHCH_2), 3.75, 3.79, 3.85 (3s, 9H, OCH_3), 5.36 (br, 1H, NCHCH$_2$), 6.84 (br, 1H, Ar), 7.04 (dd, ^3J = 8.5 Hz, ^4J = 1.8 Hz, 1H, Ar), 7.36 (br, 1H, NCHN), 7.63 (br, 1H, Ar), 12.26 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 14.0 ($CH_3CH_2CH_2$), 22.5, 28.9, 31.3, 31.6, 35.2 ($CH_3CH_2CH_2CH_2CH_2CH_2$), 38.1 (br, NCHCH_2), 48.9 (br, N$CHCH_2$), 52.0, 53.1, 53.2 (OCH_3), 58.9 (br, NCHN), 98.0 (NCHCCO), 124.2, 126.0, 126.5 (CH_{Ar}), 127.8, 132.0 (br), 139.0 (C_{Ar}), 153.5, 154.1 (NCOO), 170.6 ($CCOCH_3$), 173.0 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2956 (m), 2929 (m), 2856 (w), 1716 (s), 1656 (m), 1618 (m), 1501 (m), 1444 (m), 1412 (w), 1379 (m), 1332 (m), 1289 (m), 1264 (m), 1237 (m), 1194 (w), 1172 (w), 1137 (w), 1067 (w), 1050 (w), 1011 (w). MS (EI, 70 eV): *m/z* (%) = 446 (M^+, 10), 387 (100), 355 (40), 330 (28), 212 (44), 180 (20). HRMS (EI): Calcd for $C_{23}H_{30}N_2O_7$ ($[M]^+$) 446.20475, found 446.205676.

10-Acetyl-4-hexyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5v). Starting with 6-hexylquinazoline **3g** (0.647 g, 3.0 mmol), 2,4-bis(trimethylsilyloxy)-penta-1,3-diene **4d** (1.026 g, 4.2 mmol) and methyl chloroformate (1.134 g, 12.0 mmol), **5v** was obtained as a yellowish, highly viscous oil (0.684 g, 53%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.86 (br t, ^3J = 6.6 Hz, 3H, $CH_2CH_2CH_3$), 1.27 (br m, 6H, $CH_3CH_2CH_2CH_2CH_2CH_2$), 1.56 (br m, 2H, $CH_3CH_2CH_2CH_2CH_2CH_2$), 2.33 (s, 3H, CCH_3O), 2.51 (m, 3H, (2H, $C_{Ar}CH_2$ and 1H, NCHCH_2)), 3.00 (dd, ^2J = 22.9 Hz, ^3J = 5.2 Hz, 1H, NCHCH_2), 3.76, 3.85 (2s, 6H, OCH_3), 5.37 (br, 1H, NCHCH$_2$), 6.86 (m, 1H, Ar), 7.03 (m, 1H, Ar), 7.39 (br, 2H, (1H, Ar and 1H, NCHN), 16.35 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 14.0 ($CH_3CH_2CH_2$), 22.5, 28.9, 31.2, 31.6, 35.2 (5 CH_2), 24.3 (CH_3CO), 40.7 (br, NCHCH_2), 48.6 (br, N$CHCH_2$), 53.2, 53.5 (OCH_3), 60.3 (br, NCHN), 107.2 (NCHCCO), 125.2, 126.0, 127.8 (CH_{Ar}), 126.9, 131.3, 139.8 (C_{Ar}), 153.4, 154.5 (NCOO), 184.8 (br $CCOCH_3$), 196.3 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2956 (m), 2927 (s), 2856 (m), 1715 (s), 1605 (m), 1501 (s), 1452 (s), 1410 (s), 1372 (s), 1337 (s), 1286 (s), 1193(m), 1136(m), 1110 (m), 1048 (m), 1016 (m), 970 (m), 941 (m), 830 (m), 774 (m), 733 (m). MS (EI, 70 eV): *m/z* (%) = 430 (M^+, 19), 371 (100), 339 (38), 329 (16), 196 (57), 43 (23). HRMS (EI): Calcd for $C_{23}H_{30}N_2O_6$ ($[M]^+$) 430.20984, found 430.210108.

11-Hydroxy-4,5(1´,3´)-propylene-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5w). Starting with 7,8-dihydro-6*H*-cyclopenta[g]quinazoline **3h** (0.400 g, 2.3 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (0.838 g, 3.22 mmol) and methyl chloroformate (0.870 g, 9.2 mmol), **5w** was obtained as a slightly yellow solid. (0.415 g, 51%); mp. 159 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.03 (m, 2H, $CH_2CH_2CH_2$), 2.39 (dd, ^2J = 17.6 Hz, ^3J = 1.2 Hz, 1H, NCHCH_2), 2.88 (m, 5H, (4H, $CH_2CH_2CH_2$ and 1H, NCHCH_2), 3.74, 3.79, 3.86 (3s, 9H, OCH_3), 5.34 (br, 1H, NCHCH$_2$), 6.89 (s, 1H, Ar), 7.35 (br, 1H, NCHN), 7.57 (br, 1H, Ar), 12.26 (s, 1H, OH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 25.6, 32.3, 32.9 ($CH_2CH_2CH_2$), 38.3 (br, NCHCH_2), 49.0 (br, N$CHCH_2$), 51.2, 53.1, 53.2 (OCH_3), 58.9 (br, NCHN), 98.0 (NCHCCO), 120.3, 121.8 (CH_{Ar}), 124.6, 132.4 (br), 140.4, 144.0 (C_{Ar}), 153.5, 154.3 (NCOO), 170.6 (CCOO), 173.2 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3081 (w), 2998 (w), 2956 (m), 2921 (w), 2848 (w), 1722 (s), 1707 (s), 1654 (s), 1613 (m), 1487 (m), 1455 (s), 1445 (s), 1412 (m), 1390 (m), 1360 (m), 1333 (s), 1295 (s), 1283 (s), 1264 (s), 1241 (s), 1221 (s), 1195 (m), 1177 (m), 1143 (m), 1119 (m), 1089 (m), 1065 (m), 1023 (m), 1011 (m), 787 (m), 774 (m). MS (EI, 70 eV): *m/z* (%) = 402 (M$^+$, 20), 343 (100), 311 (64), 279 (24), 212 (46), 180 (32). HRMS (EI): Calcd for $C_{20}H_{22}N_2O_7$ ([M]$^+$) 402.14215, found 402.141755.

10-Acetyl-11-hydroxy-4,5(1´,3´)-propylene-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5x). Starting with 7,8-dihydro-6*H*-cyclopenta[g]quinazoline **3h** (0.340 g, 2.0 mmol), 2,4-bis(trimethylsilyloxy)-penta-1,3-diene **4d** (0.684 g, 2.8 mmol) and methyl chloroformate (0.756 g, 8.0 mmol), **5x** was obtained as a slightly yellow solid (0.415 g, 53%); mp. 98–99 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.04 (m, 2H, $CH_2CH_2CH_2$), 2.33 (s, 3H, CCH_3O), 2.48 (dd, ^2J = 17.7 Hz, ^3J = 1.2 Hz, 1H, NCHCH_2), 2.83 (m, 4H, $CH_2CH_2CH_2$), 2.97 (dd, ^2J = 17.7 Hz, ^3J = 5.0 Hz, 1H, NCHCH_2), 3.76, 3.86 (2s, 6H, OCH_3), 5.35 (br, 1H, NCHCH$_2$), 6.90 (s, 1H, Ar), 7.31 (br, 1H, NCHN), 7.37 (br, 1H, Ar), 16.34 (s, 1H, OH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 24.3 (COCH_3), 25.6, 32.3, 32.8 ($CH_2CH_2CH_2$), 40.9 (br, NCHCH_2), 48.8 (br, N$CHCH_2$), 53.2, 53.5 (OCH_3), 60.4 (br, NCHN), 107.3 (NCHCCO), 121.1, 121.2 (CH_{Ar}, rotamers), 121.8 (CH_{Ar}), 125.0, 131.7 (br), 141.4, 144.1 (C_{Ar}), 153.5, 154.7 (NCOO), 185.0 (CCOO), 196.2 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2955 (m), 2845 (w), 1716 (s), 1605 (m), 1576 (m), 1489 (m), 1440 (s), 1410 (m), 1377 (m), 1339 (m), 1289 (s), 1252 (m), 1196 (m), 1154 (w), 1112 (m), 1089 (m), 1039 (w). MS (EI, 70 eV): *m/z* (%) = 386 (M$^+$, 12), 327 (100), 295 (27), 196 (21), 156 (5). HRMS (EI): Calcd for $C_{20}H_{22}N_2O_6$ (M$^+$) 386.14724, found 386.147092.

11-Hydroxy-4,5-dimethyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-tricarboxylic acid trimethyl ester (5y). Starting with 6,7-dimethylquinazoline **3i** (0.237 g, 1.5 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-buta-1,3-diene **4a** (0.546 g, 2.1 mmol) and methyl chloroformate (0.567 g, 6.0 mmol), **5y** was obtained as a yellowish solid (0.270 g, 46%); mp. 173–175 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.19, 2.21, 2.22 (3s, 6H, $C_{Ar}CH_3$, rotamers), 2.38 (dd, ^2J = 17.6 Hz, ^3J = 1.3 Hz, 1H, NCHC*H*$_2$), 2.95 (br dd, ^2J = 17.6 Hz, ^3J = 4.3 Hz, 1H, NCHC*H*$_2$), 3.74-3.86 (m, 9H, OCH_3), 5.32, 5.59 (br, 1H, NC*H*CH$_2$, rotamers), 6.80, 7.03, 7.05 (s, 1H, Ar), 7.35 (br, 1H, NCHN), 7.52 (br, 1H, Ar), 12.23, 12.26 (s, 1H, OH, rotamers). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 19.1, 19.8, 20.1 (2 CH_3), 35.9, 38.2 (br, NCH*C*H$_2$, rotamers), 47.0, 48.5 (br, N*C*HCH$_2$, rotamers), 51.9, 52.0, 53.1, 53.2 (3 OCH_3, rotamers), 58.3, 58.9 (br, NCHN, rotamers), 97.7, 98.0 (br, NCH*C*CO, rotamers), 122.4, 124.1, 125.0, 127.1 (2 CH_{Ar}, rotamers), 128.7, 132.0 (br), 132.8, 136.2, (C_{Ar}), 153.5, 154.2 (NCOO), 170.6 (C*C*OO), 173.3 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2998 (w), 2955 (m), 2923 (w), 2859 (s), 1716 (s), 1658 (s), 1618 (m), 1506 (m), 1445 (s), 1414 (m), 1380 (m), 1332 (s), 1296 (s), 1252 (s), 1223 (m), 1197 (m), 1172 (m), 1119 (m), 1068 (m), 1017 (m), 786 (m), 773 (m). MS (EI, 70 eV): *m/z* (%) = 390 (M^+, 18), 331 (100), 299 (56), 267 (19), 212 (62), 180 (33). HRMS (EI): Calcd for $C_{19}H_{22}N_2O_7$ (M^+) 390.14215, found 390.141802.

10-Acetyl-11-hydroxy-4,5-dimethyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5z). Starting with 6,7-dimethylquinazoline **3i** (0.237 g, 1.5 mmol), 2,4-bis(trimethylsilyloxy)penta-1,3-diene **4d** (0.513 g, 2.1 mmol) and methyl chloroformate (0.567 g, 6.0 mmol), **5z** was obtained as a yellowish solid (0.268 g, 48 mp. 87–89 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.18-2.23 (m, 6H, 2 CH_3), 2.33, 2.35 (2s, 3H, $COCH_3$, rotamers), 2.47 (dd, ^2J = 17.8 Hz, ^3J = 1.5 Hz, 1H, NCHC*H*$_2$), 2.97 (br dd, ^2J = 17.8 Hz, ^3J = 4.9 Hz, 1H, NCHC*H*$_2$), 3.76, 3.77, 3.83, 3.86 (4s, 6H, OCH_3, rotamers), 5.33, 5.58 (br, 1H, NC*H*CH$_2$, rotamers), 6.81, 7.03, 7.05, 7.36 (br, 3H, 2H, Ar and 1H, NCHN) 16.28, 16.35 (2s, 1H, OH, rotamers). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 19.2, 19.8, 20.1 (2C, CH_3, rotamers), 24.3, 24.4 (CO*C*H$_3$, rotamers), 38.4, 40.75 (br, NCH*C*H$_2$, rotamers), 46.9, 48.4 (br, N*C*HCH$_2$, rotamers), 53.2, 53.3, 53.5 (2 OCH_3, rotamers), 59.9, 60.4 (br, NCHN, rotamers), 106.9, 107.3 (NCH*C*CO, rotamers), 124.6, 131.3 (br), 133.7, 136.2 (C_{Ar}), 126.1 (d), 127.1 (CH_{Ar}), 153.5, 154.6, 154.8 (2 NCOO, rotamers), 184.9 (C*C*OO), 196.3 (COH). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2956 (m), 2922 (w), 2858 (w), 1716 (s), 1605 (m), 1505 (m), 1450 (s), 1412 (m), 1376 (m), 1337 (m), 1297 (s), 1195 (m), 1115 (m), 1019 (m). MS (EI, 70 eV): *m/z* (%) = 374 (M^+, 22), 315 (100), 340 (11), 283 (35), 196 (42), 177 (19). HRMS (EI): Calcd for $C_{19}H_{22}N_2O_6$ (M^+) 374.14724, found 374.146557.

12-Ethyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid trimethyl ester (5aa). Starting with quinazoline **3a** (0.521 g, 4.0 mmol), 1-methoxy-1,3-bis(trimethylsilyloxy)-hexa-1,3-diene **4h** (1.613 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 mL), **5aa** was obtained as a colourless, highly viscous oil (0.665 g, 43%); dr = 7:3. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 1.16 – 1.27 (m, 3H, CH_2CH_3), 1.33 – 1.62 (m, 1H, CH_2), 1.73 –1.89 (m, 1H, CH_2), 1.99 – 2.09 (m, 1H, NCHC*H*, diastereomers), 2.31 (ddd, ^3J = 10.1 Hz, ^3J = 4.2 Hz, ^3J = 1.4 Hz, 1H, NCHC*H*, diastereomers), 3.74, 3.75 (s, 3H, OCH_3, diastereomers), 3.79 (s, 3H, OCH_3), 3.85, 3.87, 3.87 (s, 3H, OCH_3, diastereomers, rotamers), 5.21, 5.31 (br, 1H, NC*H*CH, diastereomers), 7.03 – 7.11 (m, 2H, Ar), 7.17 – 7.24 (m, 1H, Ar), 7.33 (br, 1H, NCHN), 7.78 (br, 1H, Ar), 12.29, 12.68 (s, 1H, OH, diastereomers); dr = 7 : 3. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 12.3, 12.6 (CH_2CH_3, diastereomers), 18.5, 23.1 (CH_2, diastereomers), 51.0, 51.5, 53.6, 53.7 (br, N*C*HCH, diastereomers, rotamers), 51.2 (NCH*C*H), 52.0, 53.1 (br) (OCH_3), 58.7, 58.8 (br, NCHN, diastereomers), 96.7, 96.7 (*C*COO, diastereomers), 124.1, 124.2, 126.4, 126.4, 127.3, 127.5 (CH_{Ar}, diastereomers), 126.9, 134.6 (C_{Ar}), 154.0, 154.2 (NCOO), 170.7 (C*C*OO), 175.9, 176.6 (br, COH, diastereomers). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 2957 (m), 1717 (s), 1654 (m), 1617 (m), 1491 (m), 1445 (s), 1382 (m), 1337 (m), 1300 (s), 1261 (s), 1226 (s), 1204 (m), 1137 (m), 1058 (m), 1039 (m), 767 (m). MS (CI pos., Isobutane): *m/z* = 391 ([M+H]$^+$). HRMS (EI): Calcd for $C_{19}H_{22}N_2O_7$ (M^+) 390.14215, found 390.141115.

12-Ethyl-11-hydroxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,10,13-tricarboxylic acid-10-ethyl ester-8,13-dimethyl ester (5ab). Starting with quinazoline **3a** (0.521 g, 4.0 mmol), 1-ethoxy-1,3-bis(trimethylsilyloxy)-hexa-1,3-diene **4i** (1.700 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 mL), **5ab** was obtained as a colourless, highly viscous oil (0.808 g, 50%); dr = 2:1. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 1.16 – 1.28 (m, 3H, $CHCH_2CH_3$), 1.30 – 1.36 (m, 3H, OCH_2CH_3), 1.54 (m, 1H, CHCH_2, diastereomers), 1.80 (m, 1H, CHCH_2), 2.03 (m, 1H, CHCH_2, diastereomers), 2.31 (dd, ^3J = 10.1 Hz, ^3J = 2.8 Hz, 1H, C*H*CH_2, diastereomers), 2.80 (m, 1H, C*H*CH_2, diastereomers), 3.74, 3.75 (s, 3H, OMe, diastereomers), 3.84, 3.86 (s, 3H, OCH_3, diastereomers), 4.22 (q, ^3J = 7.0 Hz, 2H, OCH_2), 5.21, 5.30 (br, 1H, NC*H*CH, diastereomers), 7.00 – 7.11 (m, 2H, Ar), 7.17 – 7.25 (m, 1H, Ar), 7.34 (br, 1H, NCHN), 7.80 (br, 1H, Ar), 12.38, 12.77 (s, 1H, OH, diastereomers). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 12.3, 12.5 ($CHCH_2CH_3$, diastereomers), 14.0 (OCH_2CH_3), 18.5, 23.1 (CH*C*H_2, diastereomers), 47.7 (br, N*C*HCH, diastereomers), 51.0, 51.5 (br, N*C*HCH, diastereomers, rotamers), 51.2 (NCH*C*H), 53.0, 53.1 (OCH_3), 58.8, 59.4 (br, NCHN, diastereomers), 60.9, 60.9 (O*C*H_2, diastereomers), 96.5, 96.9

(NCH*C*CO, diastereomers), 123.0, 123.0, 124.0, 124.1, 124.2, 126.4 (br), 127.4, 127.7 (CH_{Ar}, diastereomers), 127.0, 134.6, 134.9 (C_{Ar}, diastereomers), 153.4, 153.9, 154.2 (NCOO, diastereomers), 170.4, 170.7 (C*C*OO, diastereomers), 176.0, 176.2 (br, COH, diastereomers). IR (Nujol, cm^{-1}): $\tilde{\nu}$ = 1721 (s), 1708 (s), 1646 (m), 1618 (m), 1300 (s), 1227 (m), 1139 (m), 1104 (m), 1064 (w), 1036 (m), 768 (m), 744 (m). MS (CI neg., Isobutane): *m/z* (%) = 404 (M^-). Anal. Calcd for $C_{20}H_{24}N_2O_7$ (404.41): C, 59.40; H, 5.98; N, 6.93. Found: C, 59.37; H, 6.06; N, 6.72.

11-Hydroxy-12-methyl-10-propionyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (5ac). Starting with quinazoline **3a** (0.521 g, 4.0 mmol), 3,5-bis(trimethylsilyloxy)-hepta-2,4-diene **4j** (1.526 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 mL), **5ac** was obtained as a colourless, highly viscous oil (1.128 g, 75%); dr = 6:1. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 0.95 (br m, 3H, CH_2CH_3, diastereomers, rotamers), 1.09 – 1.16 (m, 6H, CH_2CH_3, $CHCH_3$, diastereomers, rotamers), 1.22 (d, ^3J = 7.3 Hz, 3H, $CHCH_3$, diastereomers, rotamers), 1.32 (d, ^3J = 7.0 Hz, 3H, $CHCH_3$, diastereomers, rotamers), 2.22 (br m, 1H, $CHCH_3$), 2.81 (br m, 2H, CH_2CH_3), 3.71, 3.74, 3.75, 3.77 (s, 3H, OCH_3, diastereomers, rotamers), 3.81, 3.84, 3.86 (s, 3H, OCH_3, diastereomers, rotamers), 4.84 (m, 1H, NC*H*CH, diastereomers, rotamers), 5.27 (m, 1H, NC*H*CH, diastereomers, rotamers), 7.03 – 7.26 (m, 3H, Ar), 7.42 – 7.48 (m, 2H, Ar, NCHN), 14.79, 15.28 (s, 1H, OH, diastereomers). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 8.4 (CH_2CH_3), 16.4 ($CHCH_3$), 30.3, 31.6 (br) (CH_2, diastereomers, rotamers), 45.7 ($CHCH_3$), 52.8, 52.9, 53.3, 53.6 (N*C*HCH, OCH_3, diastereomers, rotamers), 59.9 (br), 60.0 (br) (NCHN, diastereomers, rotamers), 105.3 (NCH*C*CO), 124.9, 125.3, 125.3, 126.5, 126.5, 127.5 (CH_{Ar}, diastereomers, rotamers), 127.6, 133.7, 133.7 (C_{Ar}, diastereomers, rotamers), 154.3, 154.4 (NCOO), 185.9 (br, COH), 201.6 (br, C*C*O). IR ((KBr, cm^{-1}): $\tilde{\nu}$ = 2988 (w), 2957 (w), 2879 (w), 1717 (s), 1608 (m), 1493 (m), 1448 (s), 1374 (m), 1266 (s), 1219 (m), 1134 (w), 1104 (w), 1056 (w), 766 (m). MS (EI, 70 eV): *m/z* (%) = 374 (M^+, 14), 359 (13), 342 (32), 315 (100), 313 (52), 283 (53), 224 (53), 159 (20), 130 (20), 84 (47). HRMS (EI): Calcd for $C_{19}H_{22}N_2O_6$ (M^+) 374.14724, found 374.147003.

Preparation of 10-acetyl-11-trifluormethanesulfonyloxy-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraen-8,13-dicarboxylic acid dimethyl ester (6). To a CH_2Cl_2 solution (21 mL) of **5f** (0.723 g, 2.1 mmol) and pyridine (0.331 g, 4.2 mmol) was dropwise added trifluoromethanesulfonic acid anhydride (0.708 g, 2.5 mmol) at −78 °C. The solution was allowed to warm up to 20 °C within 4 h and was then concentrated *in vacuo*. The residue was purified by column chromatography (silica gel, heptane → heptane-ethyl acetate = 2:1) to give **6** as a yellowish oil (0.570 g, 57%). ^{1}H NMR

(250 MHz, $CDCl_3$): δ = 2.36 (s, 3H, $COCH_3$), 2.36 (s, 3H, $COCH_3$), 2.53 (dd, ^2J = 17.7 Hz, ^3J = 1.53 Hz, 1H, CH_2), 3.21 (br dd, ^2J = 17.7 Hz, ^3J = 5.2 Hz, 1H, CH_2), 3.78 (s, 3H, $COOCH_3$), 3.87 (s, 3H, $COOCH_3$), 5.46 (br, 1H, NC*H*CH_2), 7.08–7.19 (m, 2H, Ar), 7.28 (m, 1H, Ar), 7.52 (br, 1H, NCHN), 7.70 (br m, 1H, Ar). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 30.7 ($CO\mathit{C}H_3$), 37.5 (CH_2), 49.4 (br, N*C*HCH_2), 53.6, 53.9 ($COO\mathit{C}H_3$), 60.4 (NCHN), 118.1 (q, ^1J = 320.4 Hz, CF_3), 124.2, 125.0, 126.4, 128.5 (CH_{Ar}), 125.6, 128.8, 134.0 (C_{Ar}, *C*CO), 150.8 (br, COS), 153.3, 153.8 (NCOO), 194.8 ($C\mathit{C}OCH_3$). ^{19}F NMR (235 MHz, $CDCl_3$): δ = –117.6 (CF_3). MS (EI, 70 eV): *m/z* (%) = 478 (M^+, 34), 345 (22), 269 (100), 251 (17), 211 (8), 117 (5), 63 (23). HRMS (EI): Calcd for $C_{18}H_{17}F_3N_2O_8S$ (M^+) 478.06522, found 478.064923.

General procedure for the synthesis of 7a,b. To a solution of triflate **6** (1.00 mmol) in 1,4-dioxane (2.5 ml) were added at 20 °C boronic acid (1.30 mmol), potassium phosphate (1.60 mmol) and tetrakis(triphenyl phosphine)palladium(0) (0.03 mmol). The solution was refluxed for 20 h. After cooling to 20 °C a saturated aqueous solution of ammonium chloride (3 ml) was added. The solution was diluted with CH_2Cl_2 (15 ml). The phases were separated and the aqueous phase was extracted with CH_2Cl_2 (20 ml). The collected organic phases were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by column chromatography (silica gel, heptane → heptane-ethyl acetate = 2:1).

10-Acetyl-11-phenyl-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (7a). Starting with **6** (0.546 g, 1.14 mmol), phenyl boronic acid (0.181 g, 1.48 mmol), potassium phosphate (0.387 g, 1.82 mmol and tetrakis(triphenyl phosphine)palladium(0) (0.040 g, 0.03 mmol) in 1,4-dioxane (3 ml), **7a** was obtained as a yellow solid (0.303 g, 65%); mp. 130 – 131 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 1.51 (s, 3H, $COCH_3$), 2.66 (dd, ^2J = 18.3 Hz, ^3J = 1.5 Hz, 1H, CH_2), 2.97 (dd, ^2J = 18.3 Hz, ^3J = 1.2 Hz, 1H, CH_2, rotamers), 2.99 (dd, ^2J = 18.3 Hz, ^3J = 1.2 Hz, 1H, CH_2, rotamers), 3.77 (s, 3H, OCH_3), 3.85 (s, 3H, OCH_3), 5.48 (br, 1H, NC*H*CH_2), 6.96 – 7.00 (m, 2H, Ar), 7.14 – 7.32 (m, 6H, Ar), 7.49 (br, 1H, Ar), 7.76 (br, 1H, NCHN). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 30.8 ($CO\mathit{C}H_3$), 40.4 (CH_2), 49.1 (N*C*HCH_2), 53.1, 53.5 ($NCOO\mathit{C}H_3$), 60.4 (NCHN), 123.7, 124.3, 124.3, 126.1, 127.3, 127.6, 127.8, 128.7, 129.1 (CH_{Ar}, rotamers), 134.9, 134.9, 135.1, 138.9 (C_{Ar}, NCH*C*CO), 143.5 (br, $CH_2\mathit{C}C$), 153.7, 154.0 (NCOO), 201.9 ($C\mathit{C}O$). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3027 (w), 2955 (w), 2927 (w), 2853 (w), 1717 (s), 1491 (m), 1448 (s), 1413 (m), 1374 (m), 1332 (m), 1273 (s), 1222 (m), 1134 (m), 1059 (m), 1024 (m). MS (EI, 70 eV): *m/z* (%) = 406 (M^+, 58), 347

(100), 315 (62), 256 (22), 212 (7), 180 (8), 128 (5). HRMS (EI): Calcd for $C_{23}H_{22}N_2O_5$ (M^+) 406.15232, found 406.152301.

10-Acetyl-11-(3,5-dimethyl-phenyl)-8,13-diaza-tricyclo[7.3.1.0^{2,7}]trideca-2(7),3,5,10-tetraene-8,13-dicarboxylic acid dimethyl ester (7b). Starting with **6** (0.577 g, 1.20 mmol), 3,5-(dimethyl-phenyl)boronic acid (0.234 g, 1.56 mmol), potassium phosphate (0.408 g, 1.92 mmol and tetrakis(triphenyl phosphine)palladium(0) (0.042 g, 0.04 mmol) in 1,4-dioxane (3 ml), **7b** was obtained as a yellow, highly viscous oil (0.209 g, 40%). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 1.54 (s, 3H, $COCH_3$), 2.23 (s, 6H, $C_{Ar}CH_3$), 2.64 (dd, ^2J = 18.2 Hz, ^3J = 1.3 Hz, 1H, CH_2), 2.94, 2.94 (dd, ^2J = 18.2 Hz, ^3J = 4.9 Hz, 1H, CH_2, rotamers), 3.77 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 5.47 (br, 1H, NCHC*H*$_2$), 6.58 (s, 2H, Ar), 6.94 (s, 1H, Ar), 7.15–7.29 (m, 3H, Ar), 7.50 (m, 1H, Ar), 7.72 (br, 1H, NCHN). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 21.1 ($C_{Ar}CH_3$), 30.8 ($COCH_3$), 40.5 (CH_2), 49.2 (br, N*C*HCH$_2$), 53.1, 53.5 (OCH_3), 60.5 (br, NCHN), 123.4, 123.8, 124.3, 125.6, 126.2, 127.6, 130.8 (CH_{Ar}), 127.5, 134.7, 135.0, 138.4, 138.9 (C_{Ar}), 153.8, 154.1 (NCOO), 201.8 (CH_3CO). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3034 (w), 2954 (w), 2919 (w), 2893 (w), 2855 (w), 1709 (s), 1681 (m), 1599 (w), 1490 (w), 1435 (m), 1368 (m), 1329 (m), 1283 (s), 1266 (m), 1240 (s), 1217 (s), 1191 (m), 1132 (m), 1098 (m), 1055 (m), 1031 (m). MS (EI, 70 eV): *m/z* (%) = 434 (M^+, 75), 419 (7), 375 (100), 343 (61), 284 (27), 240 (7), 208 (7), 97 (12), 71 (18), 57 (29), 44 (37). HRMS (EI): Calcd for $C_{25}H_{26}N_2O_5$ (M^+) 434.18362, found 434.183655.

1-[3-(2-Methoxyethoxycarbonyl)-2-oxo-propyl]-1*H*-phthalazine-2-carboxylic acid methyl ester (9a). Starting with phthalazine (0.521 g, 4.0 mmol), **4c** (1.705 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 ml), **9a** was isolated as a yellow, viscous oil (0.775 g, 56%). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.31 (br m, 1H, NCHC*H*$_2$, enol), 2.59 (br m, 1H, NCHC*H*$_2$, enol), 2.82 (dd, ^2J = 16.3 Hz, ^3J = 4.4 Hz, 1H, NCHC*H*$_2$, keto), 3.03 (dd, ^2J = 16.3 Hz, ^3J = 8.7 Hz, 1H, NCHC*H*$_2$, keto), 3.32 (d, ^2J = 15.7 Hz, 1H, $COCH_2CO$), 3.33 (s, 3H, CH_2OCH_3), 3.45 (d, ^2J = 15.7 Hz, 1H, $COCH_2CO$), 3.55 (m, 2H, CH_2OCH_3), 3.89 (s, 3H, $COOCH_3$), 4.21 (m, 2H, $COOCH_2$), 4.83 (s, 1H, COC*H*COH, enol), 6.00 (dd, ^2J = 8.4 Hz, ^3J = 4.4 Hz, 1H, NC*H*CH$_2$), 7.14–7.46 (m, 4H, Ar), 7.70 (s, 1H, NCONCH). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 39.7 (NCH*C*H$_2$), 47.3 ($COCH_2CO$, rotamers), 49.2 (CH_2OCH_3), 49.5 ($COCH_2CO$, rotamers), 54.0 (N*C*HCH$_2$), 58.9, 59.0 ($COOCH_3$), 63.1 (CH_2OCH_3, enol), 64.3 (CH_2OCH_3, Keto), 70.1, 70.3 ($COOCH_2$, rotamers), 92.0 (CO*C*HCOH, enol), 123.3, 123.4 (C_{Ar}, rotamers), 125.9, 126.0, 126.2, 126.9, 128.1, 128.7, 129.0, 131.8, 132.0, 132.3 (CH_{Ar}, keto, enol, rotamers), 132.7 (C_{Ar}), 143.2 (NCON*C*H), 154.3 (NCOO), 166.6 ($COOCH_2$), 172.0, 173.0 (COH, enol, rotamers), 199.0 CH_2COCH_2). IR (neat, cm^{-1}): $\tilde{\nu}$ = 2955 (m), 2932 (m), 2894 (m), 2821 (w),

1742 (s), 1711 (s), 1655 (m), 1566 (m), 1445 (s), 1379 (s), 1321 (s), 1197 (s), 1157 (s), 1128 (s), 1099 (m), 1040 (m), 983 (w), 924 (m), 847 (w), 766 (m), 551 (m), 531 (m). MS (EI, 70 eV): *m/z* (%) = 348 (M^+, 3), 289 (9), 203 (20), 189 (100), 145 (84), 130 (26), 117 (13), 76 (8). Anal. Calcd. for $C_{17}H_{20}N_2O_6$ (348.35): C, 58.61; H, 5.79; N, 8.04. Found: C, 58.42; H, 5.93; N, 7.84.

1-(2,4-Dioxopentyl)-1*H*-phthalazine-2-carboxylic acid methyl ester (9b). Starting with phthalazine (0.521 g, 4.0 mmol), **4f** (1.366 g, 5.6 mmol) and methyl chloroformate (1.512 g, 16.0 mmol) in CH_2Cl_2 (40 ml), **9b** was isolated as a slightly yellow solid (0.653 g, 57%); mp. = 93–94 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.98 (s, 3H, $COCH_3$, enol), 2.13 (s, 3H, $COCH_3$, keto), 2.45 (br m, 1H, NCHCH_2, enol), 2.64 (dd, ^2J = 13.4 Hz, ^3J = 6.0 Hz, 1H, NCHCH_2, enol), 2.76 (dd, ^2J = 16.1 Hz, ^3J = 5.1 Hz, 1H, NCHCH_2, keto), 2.94 (dd, ^2J = 16.1 Hz, ^3J = 8.1 Hz, 1H, NCHCH_2, keto), 3.87 (s, 3H, OCH_3), 5.32 (s, 1H, COC*H*COH, enol), 5.90 (m, 1H, NC*H*CH_2), 7.16 (m, 1H, Ar), 7.26 – 7.43 (m, 3H, Ar), 7.71 (br, 1H, NCONCH), 15.22 (br, 1H, OH, enol). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 25.1 (CO*C*H_3), 42.6 (NCH*C*H_2, enol), 48.1 (NCH*C*H_2, keto), 49.3, 51.2 (br), 53.8, 53.9 (NC*H*CH_2, OCH_3, keto, enol), 58.1 (CO*C*H_2CO, keto), 101.4 (CO*C*HCOH, enol), 123.2, 123.3 (C_{Ar}, keto, enol), 125.9, 126.2, 126.3, 128.6, 131.8, 131.9 (CH_{Ar}, keto, enol), 132.6, 132.7 (C_{Ar}, keto, enol), 143.1 (br), 143.2 (br) (NCON*C*H, keto, enol), 154.3 (NCOO), 187.6 (br, COH), 192.4 (br), 192.5 (br) (CH*C*O, keto, enol). IR (KBr, cm^{-1}): $\tilde{\nu}$ = 3046 (w), 3023 (w), 2965 (w), 1705 (s), 1606 (m), 1562 (m), 1457 (s), 1390 (s), 1314 (m), 1253 (m), 1223 (m), 1159 (m), 1125 (m), 1013 (w), 974 (w), 949 (w), 929 (w), 911 (w), 819 (w), 777 (m), 757 (m), 637 (w), 549 (w), 530 (w), 455 (w). MS (CI pos., isobutane): *m/z* = 289 ($[M+H]^+$). Anal. Calcd. for $C_{15}H_{16}N_2O_4$ (288.30): C, 62.49; H, 5.59; N, 9.72. Found: C, 62.77; H, 5.84; N, 9.44.

Electronic Supplementary Materials

Table S1. The B3LYP/6-31G* computed sum of electronic and thermal Free Energies (in au, at 298 K) and the number of imaginary frequencies (NImag)

	E(sum)	NImag
Me3SiCl	-869.440860	0
Me3Si(+)	-408.904349	0
ClCOOMe	-688.640021	0
(+)COOMe	-228.104004	0
3a	-417.876859	0
4a-trans	-1238.111010	0
4a-cis	-1238.113477	0
3a+R3	-646.070945	0
3a+R1	-646.061887	0
Allyl-cis-endo	-1884.222150	0
Allyo-cis-exo	-1884.220173	0
Allyl-trans-endo	-1884.227038	0
Allyl-trans-exo	-1884.224976	0
A-cis-endo	-1475.236189	0
A-cis-exo	-1475.233648	0
B-cis-endo	-1703.440801	0
B-cis-exo	-1703.439122	0
A-trans-endo	-1475.232661	0
A-trans-exo	-1475.227363	0
B-trans-endo	-1703.436523	0
B-trans-exo	-1703.434801	0
5a-endo-keton	-1294.461970	0
5a-pyran-trans	-1294.453209	0
5a-exo-keton	-1294.465091	0
5a-pyran-cis	-1294.448222	0
5a-enol	-1294.466623	0

The B3LYP/6-31G* Cartesian Coordinates

Me3SiCl

Cl	0.0000000	0.0000000	-1.7731823
Si	0.0000000	0.0000000	0.3377837
C	1.7968162	0.0000000	0.8958566
C	-0.8984081	1.5560885	0.8958566
C	-0.8984081	-1.5560885	0.8958566
H	-0.9297673	-1.6104043	1.9916226
H	-1.9302361	-1.5720805	0.5283020
H	-0.3963436	-2.4576738	0.5283020
H	-0.3963436	2.4576738	0.5283020
H	-1.9302361	1.5720805	0.5283020
H	-0.9297673	1.6104043	1.9916226
H	1.8595347	0.0000000	1.9916226
H	2.3265798	-0.8855933	0.5283020
H	2.3265798	0.8855933	0.5283020

Me3Si(+)

Si	0.0000000	0.0000000	1.0000000
C	1.8435426	-0.0001050	1.0000000
C	-0.9216804	1.5966072	1.0000000
C	-0.9218622	-1.5965023	1.0000000
H	2.2184238	0.5463060	0.1219399
H	-1.5823268	1.6480584	0.1219399
H	-0.6360970	-2.1943644	0.1219399
H	2.2184238	0.5463060	1.8780601
H	-1.5823268	1.6480584	1.8780601
H	-0.6360970	-2.1943644	1.8780601
H	2.2691562	-1.0074604	1.0000000
H	-0.2620918	2.4688771	1.0000000
H	-2.0070644	-1.4614167	1.0000000

ClCOOMe

O	-0.0310376	0.0001630	-0.0000000
C	1.1640964	-0.0065447	-0.0000000
O	1.9889750	1.0361504	-0.0000000
Cl	2.1349295	-1.4977984	-0.0000000
C	1.3250979	2.3230481	-0.0000000
H	2.1318778	3.0546711	-0.0000000
H	0.7049447	2.4263286	0.8931601
H	0.7049447	2.4263286	-0.8931602

(+)COOMe

O	0.2107325	-0.8474997	0.0000000
C	0.8678174	0.0850413	0.0000000
O	1.6381870	1.0154783	0.0000000
C	1.3391551	2.5547560	0.0000000
H	2.3467236	2.9607247	0.0000000
H	0.7874101	2.7376358	0.9194768
H	0.7874101	2.7376358	-0.9194768

3a

C	0.7026469	0.0000000	-0.0044934
C	-0.7236747	0.0000000	0.0112917
C	1.4055870	0.0000000	1.2276398
C	-1.4191692	0.0000000	1.2469192
N	1.3927557	0.0000000	-1.1831130
C	-1.3536270	0.0000000	-1.2601153
C	0.6741894	0.0000000	-2.2835068
N	-0.6852799	0.0000000	-2.3944907
C	-0.7126457	0.0000000	2.4288194
C	0.7065868	0.0000000	2.4150504
H	2.4906119	0.0000000	1.1985700
H	-2.5067918	0.0000000	1.2452567
H	1.2173574	0.0000000	-3.2267369
H	-1.2379158	0.0000000	3.3797786
H	1.2452917	0.0000000	3.3589168
H	-2.4433217	0.0000000	-1.3249847

4a-trans

C	2.4212125	-2.9162037	1.6244251
H	3.2510534	-2.6708924	2.2766133
H	2.3005350	-3.9518070	1.3256712
C	1.5432564	-1.9744962	1.2229223
C	0.3712195	-2.3093127	0.4186988
H	0.2148036	-3.3710228	0.2653344
C	-0.5221534	-1.4856170	-0.1781909
O	-0.3496722	-0.1462620	-0.2460042
C	-1.5157559	0.6762488	-0.3307163
H	-2.1753975	0.5160050	0.5305094
H	-2.0700372	0.4935241	-1.2548557
H	-1.1453179	1.7026910	-0.3162174
O	1.6734103	-0.6671376	1.6222525
Si	2.8387291	0.4399996	1.1117581
C	2.1327654	2.1132290	1.6050759
H	1.1925816	2.3092327	1.0780762
H	2.8291899	2.9278502	1.3714288
H	1.9260054	2.1482414	2.6810308
C	4.4739006	0.1449369	2.0100460

H	5.2043665	0.9242032	1.7566610
H	4.9146813	-0.8210711	1.7387552
H	4.3375902	0.1577701	3.0979336
C	3.0901330	0.3031115	-0.7503787
H	2.1467908	0.4744870	-1.2794204
H	3.4521260	-0.6942772	-1.0256885
H	3.8257441	1.0349064	-1.1068346
O	-1.6261330	-1.9133665	-0.8365707
Si	-2.6352212	-3.2634395	-0.5792669
C	-4.1534045	-2.8576907	-1.6097025
H	-3.8923364	-2.7312668	-2.6665937
H	-4.6290589	-1.9308957	-1.2695105
H	-4.8990788	-3.6593276	-1.5438993
C	-3.0472466	-3.3937533	1.2521329
H	-2.1425221	-3.4677504	1.8645040
H	-3.6610534	-4.2814983	1.4485167
H	-3.6106102	-2.5177208	1.5940844
C	-1.8175224	-4.8336606	-1.2241938
H	-1.4428405	-4.6904926	-2.2443348
H	-2.5473576	-5.6528954	-1.2515949
H	-0.9781951	-5.1639435	-0.6028118

4a-cis

C	-0.2849534	0.6262372	-1.5075775
H	-0.3645362	0.7706551	-2.5783295
H	-0.7138898	1.3804684	-0.8650531
C	0.3256808	-0.4537386	-0.9823077
C	0.5097281	-0.7861442	0.4295649
H	1.0385047	-1.7150888	0.5977385
C	0.1107348	-0.0929457	1.5218409
O	0.8923504	-1.4496094	-1.7556467
Si	1.0176294	-1.6459449	-3.4249958
C	1.9431849	-3.2748450	-3.6082021
H	1.3894544	-4.0987715	-3.1436722
H	2.9290911	-3.2252633	-3.1319780
H	2.0943457	-3.5271523	-4.6650969
C	-0.6892522	-1.7825682	-4.2194629
H	-1.2902950	-0.8790687	-4.0744886
H	-1.2488119	-2.6223638	-3.7907860
H	-0.6011710	-1.9583508	-5.2991154
C	2.0199213	-0.2447979	-4.1965378
H	1.5520557	0.7335779	-4.0467632
H	2.1362336	-0.4003988	-5.2766017
H	3.0235323	-0.2003497	-3.7573250
O	-0.5538229	1.0789009	1.4064327
O	0.3176871	-0.4665912	2.8027719
Si	1.0769968	-1.8311751	3.4911615

C	0.1652237	-3.3952103	2.9765891
H	-0.8869817	-3.3506438	3.2808354
H	0.6129455	-4.2739595	3.4575243
H	0.1908272	-3.5569108	1.8942532
C	2.8924961	-1.8683236	2.9960389
H	3.4040462	-2.7075891	3.4838127
H	3.3991079	-0.9465329	3.3048039
H	3.0295228	-1.9758577	1.9153262
C	0.8915562	-1.5221210	5.3350280
H	1.3822501	-0.5887053	5.6332258
H	1.3426402	-2.3360085	5.9157476
H	-0.1636774	-1.4531067	5.6225664
C	-0.9592593	1.7666047	2.5899210
H	-1.6489156	1.1634312	3.1885258
H	-1.4671255	2.6647687	2.2343071
H	-0.0993158	2.0464853	3.2061976

3a+R3

C	-0.0029792	0.5977644	-0.2771332
C	0.1099613	-0.7957612	0.0690704
C	1.1432731	1.4111621	-0.2409325
C	1.3687704	-1.3427998	0.4437035
N	-1.2086921	1.1365364	-0.6394041
C	-1.0556677	-1.5541651	0.0162651
C	-2.2544706	0.3781298	-0.6686355
N	-2.2171472	-0.9782346	-0.3459449
C	2.4709223	-0.5207859	0.4692274
C	2.3549467	0.8527650	0.1270723
H	1.0477896	2.4589843	-0.5033249
H	1.4433009	-2.3946886	0.7029218
H	-3.2234394	0.7697006	-0.9501606
H	3.4400031	-0.9184581	0.7521786
H	3.2427968	1.4773198	0.1563784
H	-1.1077481	-2.6122643	0.2520359
C	-3.4190646	-1.8449908	-0.3807056
O	-3.3342820	-3.0054363	-0.0946261
O	-4.4591614	-1.1377613	-0.7499193
C	-5.7288162	-1.8642781	-0.8311397
H	-6.4525459	-1.1164323	-1.1466974
H	-5.6366761	-2.6658300	-1.5648811
H	-5.9741192	-2.2680935	0.1517657

3a+R1

C	0.2465435	0.7431984	0.0535040
C	0.0586937	-0.6771859	0.0129547
C	1.5370260	1.2781940	-0.0969417

C	1.1706635	-1.5320791	-0.1982553
N	-0.9107792	1.5025159	0.2817597
C	-1.2413339	-1.1823689	0.2008206
C	-2.1092731	0.8921473	0.4527541
N	-2.3055849	-0.4137566	0.4187841
C	2.4270594	-0.9939120	-0.3526516
C	2.5980828	0.4074181	-0.2952438
H	1.7065991	2.3437154	-0.0767636
H	1.0079487	-2.6052019	-0.2279993
H	-2.9566167	1.5441206	0.6223825
H	3.2864079	-1.6362971	-0.5132340
H	3.5939056	0.8244486	-0.4107867
H	-1.4178508	-2.2563540	0.1746889
C	-0.8761780	2.9883414	0.2734465
O	-0.0477969	3.5995526	-0.3380030
O	-1.8685782	3.4438553	1.0063140
C	-2.0096353	4.9007382	1.0518350
H	-2.8688477	5.0718856	1.6962777
H	-1.1025359	5.3348628	1.4734926
H	-2.1835190	5.2791603	0.0437090

Allyl-cis-endo

H	-2.6996849	2.9314153	-2.6793631
C	-2.6269371	3.3685124	-1.6855917
C	-2.4409214	4.4955976	0.8670349
C	-2.1396037	2.6051687	-0.6248712
C	-3.0192099	4.6915966	-1.4744750
C	-2.9194172	5.2544090	-0.1984538
C	-2.0541083	3.1652689	0.6629292
H	-3.3992870	5.2813546	-2.3031156
H	-3.2230226	6.2840461	-0.0344909
H	-2.3748327	4.9042064	1.8703562
C	-1.6074585	1.2039253	-0.8218109
H	-2.1541769	0.6840229	-1.6077152
N	-1.7774998	0.4487474	0.4315034
C	-1.5913699	1.1340644	1.6412051
H	-1.4175789	0.4888032	2.4967279
N	-1.6487423	2.4048291	1.7786218
C	-1.9846068	-0.9263777	0.4803825
O	-1.9228552	-1.5881785	1.5000163
O	-2.2668098	-1.4254369	-0.7381176
C	-2.6284013	-2.8215072	-0.7544821
H	-3.4632722	-3.0048378	-0.0756115
H	-1.7783382	-3.4410654	-0.4579709
H	-2.9172476	-3.0299750	-1.7841892
C	-0.0876145	1.2970530	-1.2339520

H	0.4432055	1.8522692	-0.4634116
H	-0.0522466	1.8687214	-2.1651124
C	0.5655391	-0.0296518	-1.4948676
O	0.3761272	-0.4458839	-2.7259086
Si	1.0622093	-1.6251217	-3.8237175
C	0.3079114	-1.1163512	-5.4547536
H	0.5845664	-0.0903446	-5.7204950
H	-0.7857490	-1.1746521	-5.4261841
H	0.6540838	-1.7732152	-6.2616833
C	0.5086997	-3.3405211	-3.2979947
H	0.7819026	-4.0616378	-4.0785534
H	-0.5791780	-3.3894985	-3.1785660
H	0.9726072	-3.6832265	-2.3672015
C	2.9255286	-1.4080889	-3.7778441
H	3.3915899	-2.0832099	-4.5061804
H	3.3627418	-1.6322662	-2.7989735
H	3.2136462	-0.3865971	-4.0502170
C	1.2539767	-0.8081267	-0.5712082
H	1.5731257	-1.7944403	-0.8795958
C	1.6132183	-0.4651700	0.7562902
O	1.4325834	0.7594898	1.1899912
C	1.7890135	1.1183366	2.5540335
H	1.3505776	0.4096203	3.2569613
H	1.3630371	2.1100967	2.6910601
H	2.8758927	1.1337116	2.6518067
O	2.1774541	-1.2928263	1.5712558
Si	2.2033705	-3.0044140	2.0393830
C	2.0341999	-4.0825193	0.5141162
H	2.1630860	-5.1303796	0.8141986
H	2.8012223	-3.8707014	-0.2394578
H	1.0453069	-4.0020722	0.0503045
C	0.7637030	-3.1794525	3.2149493
H	0.6563283	-4.2280627	3.5195922
H	-0.1806335	-2.8652904	2.7554439
H	0.9152189	-2.5893104	4.1257711
C	3.8878353	-3.1472273	2.8316134
H	4.0381937	-4.1625809	3.2180375
H	3.9964117	-2.4551727	3.6735822
H	4.6927913	-2.9431517	2.1169787

Allyl-cis-exo

H	0.7307401	2.8572209	1.7917279
C	-0.1658650	3.3541249	1.4264645
C	-2.4560819	4.6404828	0.4752751
C	-0.8033044	2.8741502	0.2821244
C	-0.6693298	4.4693347	2.0975760

C	-1.8206327	5.1060187	1.6234681
C	-1.9476759	3.5280399	-0.2080498
H	-0.1671443	4.8404739	2.9859912
H	-2.2155799	5.9722699	2.1457849
H	-3.3368430	5.1316764	0.0743395
C	-0.3467505	1.6155000	-0.4230490
H	0.7352152	1.5096182	-0.3618954
N	-0.7194388	1.7037255	-1.8423987
C	-1.9281916	2.3354855	-2.1742525
H	-2.2928910	2.1059040	-3.1705915
N	-2.5670979	3.1406123	-1.4112946
C	0.0054263	1.1008062	-2.8710748
O	-0.3512896	1.0810302	-4.0304054
O	1.1427290	0.5452502	-2.4062660
C	1.9729955	-0.0575027	-3.4215551
H	2.2806264	0.6924721	-4.1528763
H	1.4308824	-0.8578500	-3.9295705
H	2.8373424	-0.4507032	-2.8868167
C	-1.0182905	0.3690820	0.2782909
H	-2.0998140	0.4640829	0.1621385
H	-0.7786041	0.4435401	1.3389658
C	-0.5809571	-0.9639607	-0.2540918
O	-1.2547254	-1.4973239	-1.2395482
Si	-2.8688023	-1.8051651	-1.8633171
C	-2.6299695	-1.6945767	-3.7125456
H	-1.9796530	-2.4987861	-4.0745999
H	-2.1859744	-0.7417899	-4.0201956
H	-3.5952381	-1.7966335	-4.2232455
C	-4.1225692	-0.5852007	-1.1863202
H	-5.0989050	-0.8351876	-1.6224139
H	-3.9150133	0.4582364	-1.4437919
H	-4.2367028	-0.6586166	-0.0986372
C	-3.2368755	-3.5454833	-1.2696476
H	-4.2082231	-3.8761702	-1.6578179
H	-3.2863174	-3.6048884	-0.1762680
H	-2.4826649	-4.2591261	-1.6187480
C	0.5197988	-1.6993494	0.1837952
H	0.6690745	-2.6527110	-0.3057193
C	1.4462067	-1.3716826	1.1882581
O	1.4017731	-0.1913065	1.7760487
C	2.3323864	0.1019199	2.8526933
H	2.2062814	-0.6153779	3.6650947
H	2.0648397	1.1050344	3.1794556
H	3.3566955	0.0756493	2.4780729
O	2.3828316	-2.1729346	1.5924293
Si	2.8573732	-3.8573449	1.2873352
C	3.4375359	-3.9465846	-0.4917877
H	3.8592656	-4.9408622	-0.6851334

H	4.2288756	-3.2149310	-0.6898762
H	2.6350070	-3.7884433	-1.2200387
C	1.3653787	-4.9263197	1.6630553
H	1.6548044	-5.9829923	1.6038832
H	0.5364730	-4.7766037	0.9637904
H	0.9918588	-4.7494205	2.6779334
C	4.2425505	-4.0703484	2.5198136
H	4.6616142	-5.0813377	2.4501231
H	3.8923909	-3.9297112	3.5482165
H	5.0583458	-3.3624706	2.3369932

Allyl-trans-endo

H	-3.7487289	2.8294833	1.3683395
C	-3.9940471	2.9555039	0.3155615
C	-4.6305498	3.2944963	-2.3842099
C	-3.0655094	2.5999138	-0.6629751
C	-5.2369797	3.4757777	-0.0496387
C	-5.5551374	3.6385719	-1.4011962
C	-3.3788340	2.7800493	-2.0230432
H	-5.9539955	3.7519241	0.7175633
H	-6.5223956	4.0413395	-1.6864307
H	-4.8460173	3.4304923	-3.4391571
C	-1.7447862	1.9478645	-0.3160783
H	-1.3357439	2.3571381	0.6064105
N	-0.7721003	2.2354491	-1.3788168
C	-1.2272474	2.3281690	-2.7039967
H	-0.4555376	2.2363725	-3.4611040
N	-2.4461639	2.5143308	-3.0443572
C	0.5649316	2.3610333	-1.0156668
O	0.9643462	2.2037299	0.1241209
O	1.3406080	2.6714665	-2.0667002
C	2.7334456	2.8914911	-1.7593071
H	3.1765968	1.9913437	-1.3271517
H	2.8377919	3.7204824	-1.0565071
H	3.1997314	3.1356821	-2.7130775
C	-1.9752017	0.4011883	-0.1256060
H	-2.4951515	0.0337431	-1.0150601
H	-2.6578974	0.2813398	0.7213584
C	-0.7392462	-0.4342690	0.0970102
O	-0.2494219	-0.5984278	1.2891705
Si	-0.5771492	-0.2464422	2.9716280
C	-2.1125242	-1.2248679	3.4284400
H	-2.3041833	-1.1272488	4.5043401
H	-1.9888726	-2.2921336	3.2136065
H	-3.0121059	-0.8760285	2.9086569
C	-0.7758038	1.6015894	3.2133613
H	-1.7632358	1.9688071	2.9129377

H	-0.0121739	2.1562084	2.6579113
H	-0.6552759	1.8388996	4.2778258
C	0.9693890	-0.9012416	3.7922219
H	0.9064888	-0.7923848	4.8814225
H	1.8558439	-0.3538627	3.4534941
H	1.1180778	-1.9638300	3.5713716
C	-0.1445759	-1.0355557	-1.0074755
H	-0.6171875	-0.8746062	-1.9657800
C	1.0210573	-1.8314868	-1.0166592
O	1.6633585	-2.0619216	0.1015742
C	2.8577033	-2.8849142	0.0809801
H	2.6169421	-3.8884628	-0.2742707
H	3.1883348	-2.9100687	1.1175394
H	3.6171720	-2.4304225	-0.5574181
O	1.5179745	-2.3632328	-2.0924413
Si	1.0409135	-2.5002236	-3.7955218
C	0.8143399	-0.7655028	-4.4733850
H	0.8638432	-0.8020552	-5.5688294
H	1.6071744	-0.0885340	-4.1351411
H	-0.1509482	-0.3197000	-4.2115368
C	-0.5209376	-3.5323871	-3.8217510
H	-0.8484351	-3.6806049	-4.8582445
H	-1.3497246	-3.0599593	-3.2834493
H	-0.3537192	-4.5236930	-3.3862651
C	2.5267156	-3.3694345	-4.5169591
H	2.3779221	-3.5509082	-5.5881694
H	2.6977567	-4.3400253	-4.0388741
H	3.4376281	-2.7706013	-4.4077951

Allyl-trans-exo

H	-0.6552623	-3.6981171	2.9292309
C	0.2858381	-4.0573284	2.5169903
C	2.6993967	-4.9905627	1.4604589
C	0.8375802	-3.4341726	1.3974771
C	0.9361365	-5.1410193	3.1099299
C	2.1462943	-5.6020663	2.5827999
C	2.0463541	-3.9084771	0.8568710
H	0.5008291	-5.6225122	3.9803621
H	2.6538337	-6.4436285	3.0446553
H	3.6274138	-5.3421046	1.0211548
C	0.2168119	-2.2020376	0.7766451
H	-0.8726069	-2.2482048	0.8184372
N	0.5866590	-2.1395053	-0.6457997
C	1.8616050	-2.5950876	-1.0254767
H	2.2042728	-2.2492485	-1.9948116
N	2.5993346	-3.3651479	-0.3188890
C	-0.3435897	-1.6338587	-1.5499315

O	-1.4414200	-1.2201582	-1.2233132
O	0.1260144	-1.6594763	-2.8070122
C	-0.7892439	-1.1936211	-3.8213811
H	-1.0431580	-0.1450124	-3.6511582
H	-1.6984622	-1.7978749	-3.8139289
H	-0.2542651	-1.3139964	-4.7624686
C	0.6954503	-0.9294841	1.5655396
H	1.7860336	-0.9001458	1.5459121
H	0.3866511	-1.0759913	2.6055239
C	0.1336023	0.3783436	1.0642573
O	0.8483509	1.1277685	0.2753765
Si	2.4590199	1.5665546	-0.2357932
C	2.3438730	1.4818979	-2.1027850
H	1.6183374	2.2066717	-2.4880665
H	2.0436573	0.4869486	-2.4496120
H	3.3159490	1.7120837	-2.5550717
C	3.7722374	0.4260225	0.4677385
H	4.7501353	0.7931733	0.1287554
H	3.6860379	-0.6122388	0.1307141
H	3.7955181	0.4367220	1.5634459
C	2.6573105	3.3141238	0.4081856
H	3.6101309	3.7387491	0.0692344
H	2.6550138	3.3458602	1.5036215
H	1.8538587	3.9657135	0.0489795
C	-1.1625613	0.7287447	1.4109805
H	-1.7127157	0.0258321	2.0204620
C	-1.8771364	1.8696862	0.9914744
O	-1.2566167	2.8301357	0.3474231
C	-2.0102305	3.9909869	-0.0868914
H	-2.7984167	3.6906409	-0.7796325
H	-1.2771963	4.6214694	-0.5867298
H	-2.4399361	4.5047916	0.7745671
O	-3.1384832	2.0527871	1.2342078
Si	-4.5074997	1.0059810	1.6664214
C	-4.1733727	0.2652304	3.3583052
H	-5.1107621	-0.1487702	3.7510953
H	-3.8328325	1.0242497	4.0716915
H	-3.4434865	-0.5510921	3.3506258
C	-4.6412360	-0.2478073	0.2842465
H	-5.3637984	-1.0278500	0.5542927
H	-3.6872363	-0.7364751	0.0569277
H	-4.9993533	0.2248180	-0.6372810
C	-5.9045122	2.2440784	1.7149870
H	-6.0237171	2.7568927	0.7544122
H	-5.7461134	3.0026409	2.4894485
H	-6.8515407	1.7378805	1.9379073

A-cis-endo

H	-1.3729977	3.4026120	-3.0386269
C	-1.7688512	3.7772684	-2.0968214
C	-2.7783030	4.7365867	0.3230164
C	-1.9678593	2.8951653	-1.0349648
C	-2.0676679	5.1337739	-1.9539862
C	-2.5687788	5.6120132	-0.7398839
C	-2.4859876	3.3734136	0.1831623
H	-1.9063991	5.8141547	-2.7854581
H	-2.7998399	6.6675120	-0.6247312
H	-3.1798053	5.0805605	1.2712905
C	-1.5689926	1.4376751	-1.1115801
H	-1.7279359	1.0366274	-2.1135517
N	-2.4428561	0.6716291	-0.1996015
C	-2.7858544	1.2543411	1.0247800
H	-3.0943140	0.5591322	1.7973597
N	-2.7677593	2.5136831	1.2629638
C	-2.8305714	-0.6090363	-0.5637855
O	-2.5583315	-1.1252377	-1.6318975
O	-3.5645937	-1.1983416	0.4023609
C	-3.9900475	-2.5395742	0.1096304
H	-3.1258871	-3.1985990	-0.0056845
H	-4.5872553	-2.5612106	-0.8048971
H	-4.5896351	-2.8427273	0.9680817
C	-0.0664800	1.2744642	-0.7310931
H	0.0882928	1.6355566	0.2838544
H	0.5003658	1.9129432	-1.4186492
C	0.4598685	-0.1281629	-0.8868360
O	0.6158122	-0.4325543	-2.1915789
Si	0.9923045	-1.8682850	-3.0437148
C	0.5612470	-1.4141176	-4.8141718
H	0.8122082	-2.2297948	-5.5032356
H	1.1076985	-0.5215974	-5.1393484
H	-0.5103466	-1.2082951	-4.9137601
C	-0.0535505	-3.3123746	-2.4440632
H	-0.0391625	-4.1144965	-3.1929490
H	-1.0907794	-2.9901553	-2.3055238
H	0.3016167	-3.7362555	-1.4988402
C	2.8368960	-2.2073492	-2.8617944
H	3.1228838	-3.0918128	-3.4449271
H	3.1241637	-2.3917446	-1.8206721
H	3.4317495	-1.3622082	-3.2269902
C	0.7743958	-1.0016534	0.1040387
H	1.1892528	-1.9654548	-0.1685171
C	0.6825383	-0.8632986	1.5612048
O	0.0691474	0.2704968	2.0041497
C	0.0001020	0.4152650	3.4304090

H	-0.5215132	-0.4340001	3.8795450
H	-0.5519226	1.3407242	3.5980801
H	1.0031502	0.4791278	3.8614156
O	1.1074559	-1.7086925	2.3297232

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H	0.5104978	2.9163230	1.7922590
C	-0.2593642	3.5105003	1.3052518
C	-2.2476379	5.0183084	0.0512671
C	-0.8372506	3.0439807	0.1248195
C	-0.6711547	4.7233241	1.8611227
C	-1.6699598	5.4738609	1.2338580
C	-1.8317194	3.8060318	-0.5151031
H	-0.2177070	5.0787038	2.7822602
H	-1.9948923	6.4162106	1.6664243
H	-3.0153990	5.5886037	-0.4625466
C	-0.4870548	1.6934628	-0.4638368
H	0.5649430	1.4556659	-0.3019230
N	-0.6937140	1.7666225	-1.9256039
C	-1.7989790	2.4848722	-2.3961325
H	-2.1384526	2.2159040	-3.3906037
N	-2.3978143	3.4108410	-1.7429711
C	0.1716095	1.0779573	-2.7605296
O	1.1302729	0.4381635	-2.3730340
O	-0.1718390	1.2254858	-4.0606970
C	0.7246960	0.6074953	-4.9991415
H	0.7108927	-0.4796972	-4.8894835
H	1.7437690	0.9717808	-4.8510378
H	0.3516645	0.8957591	-5.9822220
C	-1.3588222	0.5827597	0.1949302
H	-2.4031291	0.7416401	-0.0956079
H	-1.2754858	0.7141996	1.2727345
C	-0.9804295	-0.8278961	-0.1758216
O	-1.5767995	-1.2068205	-1.3287978
Si	-1.4962434	-2.6280424	-2.2783162
C	-2.4303283	-2.1119958	-3.8259037
H	-1.9676096	-1.2341253	-4.2915518
H	-3.4680926	-1.8512668	-3.5891013
H	-2.4491298	-2.9186138	-4.5687375
C	-2.3880777	-4.0236528	-1.3827926
H	-2.3903171	-4.9327898	-1.9972776
H	-3.4315777	-3.7576252	-1.1788147
H	-1.9136982	-4.2721076	-0.4272044
C	0.2929578	-3.0643154	-2.6742906
H	0.3385465	-3.6584545	-3.5958430
H	0.7740881	-3.6477532	-1.8822415
H	0.8870417	-2.1552681	-2.8210319

C	-0.1739962	-1.6612397	0.5278106
H	-0.0240305	-2.6722085	0.1672449
C	0.5739667	-1.4276310	1.7642751
O	0.5775042	-0.1365818	2.2141940
C	1.3014141	0.0665960	3.4367732
H	0.8885590	-0.5494398	4.2399638
H	1.1877080	1.1260196	3.6719178
H	2.3570155	-0.1863336	3.3068503
O	1.1716201	-2.3118601	2.3522362

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H	-2.6629920	-3.2261444	-0.0792934
C	-3.3368796	-2.3889168	-0.2389955
C	-5.0685971	-0.2231806	-0.6297386
C	-2.8556191	-1.0883722	-0.0883445
C	-4.6646037	-2.6136360	-0.5991790
C	-5.5226778	-1.5307396	-0.7932438
C	-3.7289263	-0.0108372	-0.2907066
H	-5.0278729	-3.6287857	-0.7227693
H	-6.5599775	-1.6972333	-1.0651333
H	-5.7470945	0.6054608	-0.7720865
C	-1.4052355	-0.8261477	0.2295583
H	-0.9880507	-1.6145729	0.8557864
N	-1.3319343	0.4254274	1.0416763
C	-2.1175203	1.4486555	0.7541116
H	-1.8820366	2.4231966	1.1543189
N	-3.2148830	1.3114062	0.0072249
C	-0.2913016	0.5346961	2.0415048
O	0.3351310	-0.4292402	2.3913377
O	-0.1977247	1.7800690	2.4822448
C	0.8224945	2.0145629	3.4955514
H	1.8054351	1.7943769	3.0769345
H	0.6280021	1.3839148	4.3641577
H	0.7300904	3.0696320	3.7449283
C	-0.5529641	-0.6695440	-1.0594441
H	-0.9716442	0.1172431	-1.6848537
H	-0.6296444	-1.6210246	-1.5959692
C	0.9071190	-0.4116431	-0.7692477
O	1.5171895	-1.5406089	-0.3937810
Si	3.1609607	-1.9643943	-0.0363834
C	3.0062009	-3.7740855	0.4189590
H	3.9895646	-4.2007673	0.6497279
H	2.5760428	-4.3588270	-0.4016371
H	2.3711173	-3.9094549	1.3015630
C	3.7785628	-0.9429061	1.4182773
H	4.7090368	-1.3804339	1.8010786

H	3.0494559	-0.9465658	2.2360656
H	3.9960765	0.0979421	1.1547847
C	4.1811762	-1.6973146	-1.5901931
H	5.2210621	-1.9981697	-1.4128600
H	4.1936245	-0.6504342	-1.9121823
H	3.8018256	-2.3005673	-2.4226532
C	1.5335293	0.7941862	-0.8290301
H	2.5892609	0.8350313	-0.5873624
C	1.0479476	2.1099781	-1.2569702
O	-0.2985955	2.1996195	-1.5323626
C	-0.6921921	3.4495492	-2.1349691
H	-0.5999665	4.2713103	-1.4196447
H	-1.7300441	3.3115681	-2.4440194
H	-0.0676273	3.6697645	-3.0026522
O	1.7775611	3.0746157	-1.3625428
C	-3.8812600	2.5139456	-0.4773547
O	-4.6462714	2.4938275	-1.4007818
O	-3.5012654	3.5659925	0.2355845
C	-4.0826565	4.8398838	-0.1698584
H	-3.6629720	5.5686067	0.5205743
H	-3.7999329	5.0616184	-1.1999155
H	-5.1684117	4.7894616	-0.0791897

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H	0.5797308	3.0997892	1.8915546
C	-0.2294869	3.6699702	1.4444227
C	-2.3123144	5.1272648	0.2675532
C	-0.8302341	3.1931984	0.2794705
C	-0.6710868	4.8541517	2.0321148
C	-1.7086323	5.5758094	1.4411920
C	-1.8755755	3.9254129	-0.2986178
H	-0.2044980	5.2139657	2.9435446
H	-2.0518226	6.5038705	1.8868666
H	-3.1065359	5.7018790	-0.1855142
C	-0.4056002	1.8799130	-0.3304529
H	0.6534103	1.6907889	-0.1579683
N	-0.5725896	1.9970608	-1.8118175
C	-1.6188592	2.6280113	-2.3138538
H	-1.8720150	2.4865380	-3.3541969
N	-2.3731696	3.4496544	-1.5767442
C	0.3698202	1.3070357	-2.6670271
O	1.3342289	0.7570558	-2.2112182
O	0.0160382	1.4255789	-3.9403705
C	0.9277329	0.8231334	-4.9038028
H	0.9376413	-0.2594203	-4.7702220
H	1.9297586	1.2307377	-4.7639533

H	0.5237486	1.0943138	-5.8772088
C	-1.2362586	0.6955638	0.2275378
H	-2.2939727	0.8499818	-0.0145778
H	-1.1211559	0.7331467	1.3101559
C	-0.8227774	-0.6606172	-0.2900121
O	-1.4101980	-0.9170597	-1.4859233
Si	-1.5958833	-2.3869655	-2.3765070
C	-2.5734357	-1.8005698	-3.8701206
H	-2.0335077	-1.0286016	-4.4315640
H	-3.5439774	-1.3867553	-3.5737840
H	-2.7664327	-2.6324031	-4.5577081
C	-2.5663346	-3.6091024	-1.3353522
H	-2.7110377	-4.5449555	-1.8890884
H	-3.5583234	-3.2188716	-1.0813757
H	-2.0537450	-3.8586964	-0.4002590
C	0.0901708	-3.0506804	-2.8916346
H	-0.0144659	-3.6878718	-3.7785307
H	0.5654288	-3.6570603	-2.1133937
H	0.7857239	-2.2407836	-3.1419840
C	0.0193259	-1.5206160	0.3235287
H	0.2165181	-2.4817883	-0.1358629
C	0.7637911	-1.3725845	1.5848453
O	0.7463035	-0.1198081	2.1303419
C	1.4686781	-0.0049584	3.3742315
H	1.0648901	-0.6955540	4.1176298
H	1.3325460	1.0279234	3.6973236
H	2.5275564	-0.2251918	3.2211476
O	1.3719775	-2.2921388	2.0920608
C	-3.6639182	3.8787271	-2.1031985
O	-4.4822657	4.4312981	-1.4233147
O	-3.7663621	3.5505177	-3.3845896
C	-5.0313357	3.9027247	-4.0188711
H	-4.9362059	3.5477710	-5.0429925
H	-5.8515689	3.4040685	-3.5007294
H	-5.1657757	4.9846872	-3.9865676

A-trans-endo

H	0.1230730	-4.1425854	-1.1160430
C	1.2092225	-4.0749148	-1.1183692
C	3.9956006	-3.8984701	-1.1198274
C	1.8211624	-2.8271564	-0.9983993
C	1.9815908	-5.2323711	-1.2344858
C	3.3765323	-5.1412668	-1.2298682
C	3.2252855	-2.7329649	-1.0105167
H	1.4965225	-6.2002732	-1.3246412
H	3.9805624	-6.0403088	-1.3168394

H	5.0767331	-3.7997331	-1.1288562
C	1.0289002	-1.5581381	-0.7731611
H	0.0759986	-1.5843127	-1.3041102
N	1.7981367	-0.4249410	-1.3226702
N	3.8898558	-1.4923618	-0.9647986
C	3.1873394	-0.4389355	-1.1712640
H	3.6715846	0.5285938	-1.2509433
C	1.1024799	0.6300601	-1.9089427
O	-0.0997056	0.6388680	-2.0726553
O	1.9379355	1.6213488	-2.2819446
C	1.2907064	2.7677937	-2.8601139
H	0.6031674	3.2198945	-2.1412540
H	0.7393624	2.4824510	-3.7591302
H	2.0979627	3.4579511	-3.1057633
C	0.7572476	-1.3532037	0.7490443
H	1.7156335	-1.2136776	1.2589345
H	0.3200466	-2.2872181	1.1226162
C	-0.1805551	-0.2113732	1.0619845
C	0.2812990	0.9492602	1.5827232
O	-1.4589022	-0.4293243	0.7014273
Si	-2.7959503	-1.1138547	1.4895862
C	-2.8419636	-2.9537532	1.0677963
H	-3.7350819	-3.4293056	1.4928116
H	-1.9693690	-3.4888014	1.4615721
H	-2.8706064	-3.1094194	-0.0172562
C	-2.6323832	-0.8750796	3.3486752
H	-3.5026146	-1.2928531	3.8699025
H	-2.5585597	0.1873510	3.5995519
H	-1.7407130	-1.3762040	3.7438011
C	-4.2944181	-0.2490241	0.7646623
H	-5.2272473	-0.6721103	1.1568453
H	-4.3107663	-0.3525799	-0.3262488
H	-4.2765905	0.8203746	0.9968987
H	1.3465265	1.0263893	1.7688272
C	-0.4288379	2.2005320	1.8783349
O	0.1501458	3.2380494	2.1498698
O	-1.7864850	2.1181830	1.8384695
C	-2.4656888	3.3552368	2.0987239
H	-2.2135848	3.7357239	3.0922885
H	-3.5299568	3.1241179	2.0355087
H	-2.1944812	4.1091291	1.3547087

A-trans-exo

H	-1.1745085	-4.2644241	2.1873206
C	-0.2179926	-4.7438969	1.9898056
C	2.2433189	-5.9696608	1.4873572
C	0.6449010	-4.1971618	1.0411895

C	0.1451760	-5.8969881	2.6893154
C	1.3789803	-6.5048645	2.4397954
C	1.8800466	-4.8188985	0.7756860
H	-0.5303297	-6.3153790	3.4301397
H	1.6640721	-7.3998251	2.9859827
H	3.1991171	-6.4332828	1.2634308
C	0.3621500	-2.8949468	0.3185852
H	-0.7090366	-2.7563729	0.1660316
N	0.9752836	-2.9855702	-1.0242154
C	2.2594881	-3.5427233	-1.1000346
H	2.8455993	-3.2546426	-1.9669667
N	2.7476983	-4.3519171	-0.2327687
C	0.2191967	-2.6730661	-2.1484855
O	-0.9474357	-2.3360913	-2.1145214
O	0.9455938	-2.8026307	-3.2771367
C	0.2361036	-2.4859324	-4.4886946
H	-0.1116179	-1.4504263	-4.4691207
H	-0.6210333	-3.1517343	-4.6131346
H	0.9595995	-2.6360433	-5.2901365
C	0.9644732	-1.7298210	1.1381604
H	2.0420974	-1.9053079	1.2377632
H	0.5705824	-1.8092911	2.1612082
C	0.7717215	-0.2904355	0.6944042
O	1.6210209	0.5437981	1.3367176
Si	3.1814784	1.0963268	0.9589044
C	4.4411628	-0.1464425	1.6149590
H	5.4617838	0.2366225	1.4868715
H	4.3874032	-1.1084575	1.0912648
H	4.2927475	-0.3390869	2.6838998
C	3.3405154	2.7302519	1.8688589
H	4.3387340	3.1646545	1.7357095
H	3.1750684	2.5964994	2.9440528
H	2.6009722	3.4504602	1.5042680
C	3.3726311	1.2756669	-0.9055612
H	4.3930499	1.5890070	-1.1588337
H	2.6746340	2.0175599	-1.3042750
H	3.1826784	0.3269206	-1.4216148
C	-0.2087793	0.1300300	-0.1334969
H	-0.8751307	-0.6062972	-0.5642209
C	-0.5706420	1.4970375	-0.5377688
O	0.2703072	2.4786940	-0.1072414
C	-0.1276029	3.8057319	-0.4798600
H	-0.1789469	3.9073250	-1.5674509
H	0.6370801	4.4668422	-0.0691670
H	-1.1075130	4.0480741	-0.0596197
O	-1.5558390	1.7435287	-1.2106286

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H	0.0782438	-4.1818963	-1.2774120
C	1.1644966	-4.1554875	-1.2859485
C	3.9619487	-4.0686410	-1.3280622
C	1.8171536	-2.9387098	-1.0848575
C	1.8944110	-5.3253833	-1.4876782
C	3.2883270	-5.2756493	-1.5073003
C	3.2184884	-2.9057610	-1.1025325
H	1.3775184	-6.2681840	-1.6350827
H	3.8654127	-6.1794698	-1.6739169
H	5.0409614	-4.0431084	-1.3580728
C	1.0309556	-1.6823302	-0.8060557
H	0.0797256	-1.6872667	-1.3394086
N	1.8004808	-0.5218321	-1.3428008
N	3.8410609	-1.5974355	-1.0180101
C	3.1172512	-0.5021051	-1.2766197
H	3.6347554	0.4315657	-1.4433987
C	1.0519055	0.6415149	-1.8170794
O	-0.1153959	0.5474905	-2.0750693
O	1.8531615	1.6856027	-1.9128092
C	1.2191006	2.9604797	-2.2526094
H	0.7206227	3.3365096	-1.3578123
H	0.5169093	2.8119351	-3.0729513
H	2.0423169	3.6085496	-2.5471547
C	0.7677546	-1.4683995	0.7142485
H	1.7237782	-1.3379375	1.2325512
H	0.3146366	-2.3939564	1.0852483
C	-0.1614312	-0.2996208	0.9766883
C	0.3390382	0.9101020	1.3136643
O	-1.4423772	-0.5399637	0.6683882
Si	-2.7827711	-1.1215857	1.5776753
C	-2.8658711	-2.9828830	1.2934062
H	-3.7455994	-3.4076874	1.7925620
H	-1.9879027	-3.5054537	1.6929661
H	-2.9507534	-3.2222785	0.2266908
C	-2.5134871	-0.7287768	3.3933120
H	-3.3811746	-1.0531130	3.9807730
H	-2.3797365	0.3457981	3.5494720
H	-1.6350986	-1.2429004	3.8012915
C	-4.2710705	-0.2661347	0.8311893
H	-5.1999059	-0.6225001	1.2924010
H	-4.3388995	-0.4608846	-0.2451316
H	-4.2164492	0.8178874	0.9725366
H	1.4122979	1.0051952	1.4406210
C	-0.3607355	2.2100687	1.3262130
O	0.2009317	3.2431852	0.9977939
O	-1.6470069	2.1595817	1.7143845
C	-2.3460907	3.4227597	1.6978955

H	-1.8460891	4.1415975	2.3505421
H	-3.3488925	3.2030101	2.0627596
H	-2.3843627	3.8233173	0.6821488
C	5.2545076	-1.4385654	-0.6924095
O	5.9103209	-2.3288489	-0.2286558
O	5.6493991	-0.2025691	-0.9666561
C	7.0411341	0.0951415	-0.6478406
H	7.1690979	1.1413773	-0.9176719
H	7.2142611	-0.0638730	0.4173496
H	7.6948957	-0.5482457	-1.2380543

B-trans-exo

H	-2.4748881	-3.1558984	-2.5023630
C	-2.7147699	-2.1272252	-2.2464252
C	-3.3597804	0.5006794	-1.5544481
C	-1.9892218	-1.4892096	-1.2381419
C	-3.7372592	-1.4624893	-2.9202453
C	-4.0576811	-0.1509670	-2.5691306
C	-2.3172528	-0.1694000	-0.9059423
H	-4.2879589	-1.9703200	-3.7054893
H	-4.8622478	0.3715264	-3.0763212
H	-3.6224147	1.5132734	-1.2845295
C	-0.8870875	-2.2433923	-0.5304667
H	-1.2237178	-3.2619605	-0.3320419
N	-0.6654469	-1.6248514	0.8077779
C	-0.9017004	-0.3440216	1.0320987
H	-0.4977252	0.1013861	1.9292533
N	-1.6163659	0.4216434	0.2106361
C	0.0905847	-2.4168093	1.7632388
O	0.3321266	-3.5709820	1.5287177
O	0.4207659	-1.6935354	2.8165660
C	1.3744491	-2.3014486	3.7465193
H	2.3718585	-2.2000411	3.3140269
H	1.1107908	-3.3457773	3.9108307
H	1.2805205	-1.7192403	4.6611368
C	0.4733334	-2.3462227	-1.3198073
H	0.2311340	-2.3052198	-2.3870847
H	0.9140911	-3.3214756	-1.1073619
C	1.4582107	-1.2559895	-0.9571092
O	1.1035657	-0.0131700	-1.3506880
Si	1.5256969	0.8525809	-2.7906261
C	1.5571260	2.6472211	-2.2506739
H	1.8043468	3.3006116	-3.0958040
H	2.3068882	2.8095649	-1.4693511
H	0.5810069	2.9646811	-1.8660775
C	0.1585706	0.5548186	-4.0499252
H	0.3343366	1.1649267	-4.9448627

H	-0.8257588	0.8293639	-3.6543297
H	0.1134149	-0.4904101	-4.3783185
C	3.1750892	0.2264333	-3.4271354
H	3.4550004	0.7737692	-4.3356447
H	3.1381173	-0.8374696	-3.6891845
H	3.9687244	0.3644830	-2.6873832
C	2.4919444	-1.5351990	-0.1324889
H	2.6096387	-2.5621669	0.1946116
C	3.4024693	-0.6124983	0.5742676
O	3.6642752	0.5447594	-0.0651205
C	4.5674250	1.4350248	0.6250621
H	4.1459470	1.7389413	1.5863492
H	4.6869920	2.2943473	-0.0342101
H	5.5275180	0.9434426	0.7960863
O	3.8679464	-0.8905682	1.6668895
C	-1.5723020	1.8649206	0.4056326
O	-1.8207870	2.6387574	-0.4775636
O	-1.2202242	2.1460475	1.6519246
C	-1.0869385	3.5644112	1.9600892
H	-0.8025609	3.5946138	3.0098944
H	-0.3156262	4.0057474	1.3270940
H	-2.0426064	4.0636244	1.7956116

5a-endo-keton

H	1.3119169	-4.0104518	1.7802359
C	0.5198097	-3.3883384	1.3685486
C	-1.4799023	-1.7749619	0.3062128
C	0.8749885	-2.2400503	0.6550262
C	-0.8116831	-3.7393081	1.5617777
C	-1.8054260	-2.9259354	1.0173582
C	-0.1346896	-1.4078013	0.1247975
H	-1.0688767	-4.6314298	2.1251418
H	-2.8532049	-3.1847812	1.1425501
H	-2.2595899	-1.1511916	-0.1013993
N	2.5281015	-0.5469951	0.0617371
N	0.2512229	-0.2308460	-0.5879541
C	3.1589411	0.3044642	0.9419010
O	3.7499834	-0.0563626	1.9425744
O	3.0757686	1.5938687	0.5321620
C	3.7447919	2.5364542	1.3845451
H	3.3305127	2.5022400	2.3950055
H	3.5671928	3.5114032	0.9295684
H	4.8157117	2.3226161	1.4295551
C	-0.6341123	0.7939290	-0.8834902
O	-1.7904414	0.8750709	-0.5201593
O	-0.0369513	1.7502089	-1.6449919
C	-0.8971520	2.8393724	-2.0084755

H	-1.7452736	2.4760199	-2.5935366
H	-0.2756770	3.5077703	-2.6057522
H	-1.2687389	3.3530957	-1.1184392
C	2.3479469	-1.9522713	0.4160616
H	2.9256851	-2.1353937	1.3228126
C	2.8953390	-2.8131002	-0.7451733
H	2.7479685	-3.8808362	-0.5641339
H	3.9727118	-2.6237111	-0.8529508
C	1.0823834	-0.7177074	-3.4738732
O	-0.1248463	-0.7762445	-3.4374595
O	1.7928570	-0.4735511	-4.5933318
C	1.0141343	-0.3501792	-5.7968178
H	1.7363537	-0.1738136	-6.5941039
H	0.3152196	0.4864826	-5.7164188
H	0.4526268	-1.2695628	-5.9796306
C	1.6569860	-0.1156550	-1.0121526
H	1.8456810	0.9305827	-1.2108291
C	2.2058324	-2.4473581	-2.0504024
O	1.8770891	-3.2683188	-2.8792692
C	2.0203500	-0.9344108	-2.2931328
H	3.0165896	-0.5746741	-2.5823864

5a-pyran-trans

H	-0.5218450	-4.3817697	0.1727200
C	-1.0833924	-3.4517046	0.1208319
C	-2.4821491	-1.0497488	0.0141344
C	-0.3763902	-2.2503862	0.0459358
C	-2.4744375	-3.4738155	0.1357783
C	-3.1627752	-2.2634733	0.0851030
C	-1.0773326	-1.0266294	-0.0165106
H	-3.0088831	-4.4172562	0.1950559
H	-4.2491306	-2.2508423	0.1031691
H	-3.0321425	-0.1233254	-0.0231978
N	1.6124781	-1.0147202	0.5763765
N	-0.3169684	0.1889723	-0.0921650
C	2.7207191	-0.9810122	1.3950528
O	3.2672298	-1.9722605	1.8389467
O	3.1010284	0.2899317	1.6647612
C	4.2348354	0.4032317	2.5401779
H	4.0170701	-0.0510389	3.5097859
H	4.4079844	1.4742706	2.6479543
H	5.1086899	-0.0858201	2.1027612
C	-0.8937735	1.4470761	-0.2396738
O	-2.0818839	1.7002942	-0.2504886
O	0.0592240	2.4050599	-0.3598106
C	-0.4483880	3.7404353	-0.5053731
H	-1.0702537	3.8184353	-1.4002587

H	0.4356384	4.3721384	-0.5955560
H	-1.0393130	4.0255257	0.3685171
C	1.1365615	-2.2830940	0.0254624
H	1.5106174	-3.0828160	0.6648150
C	1.1428502	0.0949566	-0.1839410
H	1.5805098	1.0146527	0.1727771
C	1.7261139	-2.4350522	-1.3926082
H	1.3257333	-3.3030383	-1.9161119
H	2.8104575	-2.5886444	-1.2943882
C	1.3166897	-2.2999388	-4.4478184
O	1.4902071	-3.4719122	-4.1514461
O	1.0808643	-1.9013160	-5.7264331
C	1.0461227	-2.9552430	-6.6966099
H	0.8578416	-2.4661373	-7.6532527
H	0.2482392	-3.6673787	-6.4673838
H	1.9989078	-3.4917773	-6.7213420
C	1.3183421	-1.1367465	-3.5563911
H	1.1764564	-0.1648393	-4.0152005
C	1.4911977	-1.1954539	-2.2190537
O	1.5448702	0.0105888	-1.5682946

5a-exo-keton

H	-0.8526306	-4.1758946	0.1555005
C	-1.3398122	-3.2031910	0.1492726
C	-2.5460420	-0.6996957	0.1526551
C	-0.5444720	-2.0620998	0.0218879
C	-2.7223271	-3.1161773	0.2743225
C	-3.3145205	-1.8546837	0.2735949
C	-1.1478712	-0.7851387	0.0237761
H	-3.3234789	-4.0147153	0.3768013
H	-4.3921901	-1.7557400	0.3708331
H	-3.0222819	0.2675533	0.1652858
N	1.5961823	-0.9970533	0.3058673
N	-0.3125510	0.3718096	-0.1180529
C	2.6990911	-1.0488434	1.1255760
O	3.1568279	-2.0760158	1.5891243
O	3.1987381	0.1874740	1.3684551
C	4.3731227	0.2018244	2.1940823
H	4.1628024	-0.2397250	3.1712055
H	4.6384825	1.2545441	2.2986007
H	5.1833433	-0.3532798	1.7150198
C	-0.7919852	1.6704321	-0.0491267
O	-1.9167397	2.0209357	0.2510894
O	0.1848429	2.5591135	-0.3822581
C	-0.2116477	3.9375696	-0.3101531
H	-1.0483437	4.1316938	-0.9852048
H	0.6689705	4.5034383	-0.6154443

H	-0.5051926	4.2014045	0.7089047
C	0.9533803	-2.2253715	-0.1402486
H	1.3199936	-3.0326978	0.4944704
C	1.1343581	0.1758101	-0.3840633
H	1.6535719	1.0392312	0.0112458
C	1.3534336	-2.5058982	-1.6136008
H	0.8455032	-3.3894556	-2.0085800
H	2.4386765	-2.6662341	-1.6482932
C	1.4088261	0.0654976	-1.9243852
H	0.8328826	0.8258290	-2.4525055
C	1.0230113	-1.3168527	-2.4945631
O	0.5062432	-1.4095140	-3.5875978
C	2.8914673	0.3025671	-2.1861397
O	3.7860882	-0.4401916	-1.8363619
O	3.0892429	1.4535179	-2.8529059
C	4.4633093	1.7628918	-3.1553774
H	4.4337457	2.7053077	-3.7020090
H	4.9045945	0.9735250	-3.7687186
H	5.0427293	1.8670979	-2.2345548

5a-pyran-cis

H	-2.1324212	3.7687279	-0.0503224
C	-1.7597477	3.1241595	0.7428931
C	-0.8644677	1.4244425	2.7589715
C	-1.3915075	1.8157797	0.4259474
C	-1.6694562	3.6009504	2.0477185
C	-1.2266173	2.7378651	3.0496261
C	-0.9222611	0.9536329	1.4375741
H	-1.9559412	4.6222218	2.2806602
H	-1.1645628	3.0819600	4.0783851
H	-0.5162865	0.7734341	3.5462504
C	-1.5408526	1.2984323	-0.9863627
H	-2.3722869	1.7921089	-1.4894499
N	-0.5744840	-0.3891108	1.0905143
C	-0.8131447	-0.8680696	-0.2732164
H	-1.0365100	-1.9248373	-0.2612598
N	-1.8689181	-0.1265483	-0.8825980
C	-0.2621215	1.4267857	-1.8537433
H	0.0976255	2.4589827	-1.8654808
H	-0.5347545	1.1476330	-2.8812587
O	0.4119565	-0.7643229	-1.0396493
C	0.8222891	0.4954920	-1.3637131
C	2.1258063	0.8316743	-1.3093638
H	2.4172736	1.8141262	-1.6626753
C	0.3033101	-1.1540250	1.8719060
O	0.8721500	-0.7743765	2.8734307
O	0.4120757	-2.3982261	1.3664361

C	1.4749995	-3.1904091	1.9255452
H	2.4359465	-2.7467925	1.6581273
H	1.3672848	-4.1734712	1.4664246
H	1.3737588	-3.2559311	3.0108478
C	-2.8094350	-0.6805550	-1.7267410
O	-3.5166940	-0.0309265	-2.4732464
O	-2.8660743	-2.0247805	-1.5938629
C	-3.8487125	-2.6702379	-2.4198992
H	-4.8513063	-2.3132580	-2.1721354
H	-3.7542183	-3.7337030	-2.1993375
H	-3.6492641	-2.4769606	-3.4767635
C	3.2082010	-0.0230610	-0.7944343
O	3.1146372	-1.1101226	-0.2556609
O	4.4042170	0.6009144	-0.9855219
C	5.5462095	-0.1096864	-0.4925663
H	6.4057675	0.5221662	-0.7202438
H	5.6428894	-1.0801500	-0.9879017
H	5.4656479	-0.2719283	0.5861495

5a-endol

H	-1.9450627	-3.9215472	0.3879120
C	-0.9435906	-3.5315378	0.5587538
C	1.6133124	-2.5224540	0.9770291
C	-0.6586495	-2.2185630	0.1706783
C	0.0251751	-4.3435793	1.1398561
C	1.3045361	-3.8275119	1.3490537
C	0.6416744	-1.7083295	0.3732164
H	-0.2146557	-5.3639753	1.4243819
H	2.0736604	-4.4412773	1.8097892
H	2.6078883	-2.1317364	1.1335916
C	-1.7765675	-1.3712569	-0.4255009
H	-2.3134033	-1.9326663	-1.1914049
N	-1.2090153	-0.1892368	-1.0598806
C	-1.5327916	0.1490972	-2.3454156
O	-2.3049855	-0.4785871	-3.0497188
O	-0.8957289	1.2814836	-2.7378070
C	-1.1884507	1.6952224	-4.0797487
H	-0.6044176	2.6032312	-4.2347348
H	-2.2554641	1.9012897	-4.1974993
H	-0.8938833	0.9233455	-4.7952563
C	-2.7565513	-0.8831936	0.6599486
H	-3.0891336	-1.7055742	1.3020483
H	-3.6529444	-0.4533846	0.1921505
C	-2.1056614	0.1654988	1.5178787
C	-0.9508836	0.8055578	1.1427459
O	-2.7564623	0.4130792	2.6494840
C	-0.3857887	1.7940309	2.0469540

O	-0.8877470	2.1153381	3.1338036
O	0.7510363	2.3562043	1.6027683
C	1.3451386	3.3418545	2.4643086
H	0.6591272	4.1779471	2.6212956
H	2.2436184	3.6733354	1.9437482
H	1.5998128	2.9014362	3.4313641
N	0.9164246	-0.3613341	-0.0151405
C	2.1620695	0.0211636	-0.4840568
O	3.1714978	-0.6578935	-0.4556310
O	2.1397377	1.2825266	-0.9847574
C	3.4040281	1.7525033	-1.4690694
H	3.2195840	2.7727793	-1.8078772
H	3.7565713	1.1320507	-2.2970375
H	4.1530441	1.7404052	-0.6731184
H	-2.2379927	1.1230116	3.1279503
C	-0.2783960	0.5036781	-0.1895381
H	0.0502935	1.4175685	-0.6675175