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Supporting Information

69451 Weinheim, Germany

Synthesis of Highly Substituted Pyridazines via Alkynylboronic Ester Cycloaddition Reactions**

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General Procedures.

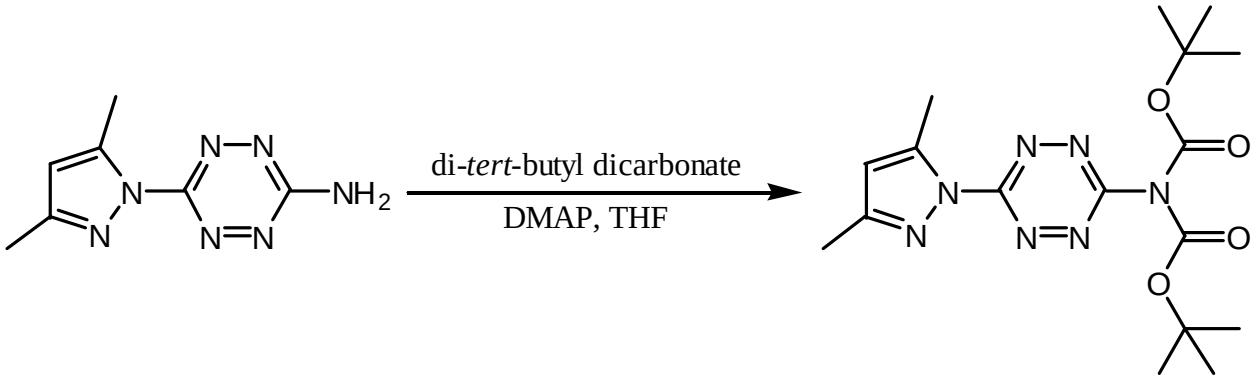
All reactions were conducted in oven or flame-dried glassware under an inert atmosphere of dry nitrogen. Flash chromatography was performed on silica gel (BDH Silica Gel 60 43-60, or Fluorochem Davisil silica gel 43-60), or on florisil (BDH Florisil 60-100 mesh). The solvent system used was a gradient of petroleum ether (40-60), increasing in polarity to ethyl acetate. Very polar compounds required DCM:MeOH:NH_3 mixes in the ratio 10:0.5:0.5 – 10:4:0.5. Thin layer chromatography (TLC) was performed on aluminium backed plates pre-coated with silica (0.2 mm, Merck DC-alufolien Kieselgel 60 F_{254}), or on aluminium backed plates pre-coated with alumina (Merck DC-Alufolien Auminiumoxid 60 F_{254} neutral (Typ E))which were developed using standard visualizing agents: Ultraviolet light or potassium permanganate.

^{1}H NMR spectra were recorded on a Bruker AC-250 (250 MHz) or AMX-400 (400 MHz) supported by an Aspect 3000 data system, unless otherwise stated. Chemical shifts are reported in ppm with the solvent resonance as the internal standard ($CHCl_3$:δ7.27 ppm). Data are reported as follows: chemical shift, integration, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet, br=broad, m=multiplet), coupling constants (*J*) in Hz, and assignment. ^{13}C NMR spectra were recorded on a Bruker AC-250 (62.9 MHz) or AMX-400 (100.6 MHz) with complete proton decoupling. Chemical shifts are reported in ppm with the solvent resonance as the internal standard ($CDCl_3$: δ77.0 ppm). Infrared (FTIR) spectra were recorded on a Perkin Elmer Paragon 100 FTIR spectrophotometer, ν_{max} in cm^{-1}. Bands are characterized as broad (br), strong (s), medium (m) and weak (w).

Samples were recorded as thin films using sodium chloride plates, as a DCM solution or as a KBr disc. Low resolution mass spectra were recorded on Micromass Autospec, operating in E.I., C.I. or FAB mode; or a Perkin-Elmer Turbomass Benchtop GC-MS operating in either E.I. or C.I mode. High-resolution mass spectra (HRMS) recorded for accurate mass analysis, were performed on either a MicroMass LCT operating in Electrospray mode (TOF ES^+) or a MicroMass Prospec operating in either FAB (FAB^+), EI (EI^+) or CI (CI^+) mode. Elemental microanalysis performed using a Perkin-Elmer 2400 CHNS / O Series II Elemental Analyser. Melting points were performed on recrystallised solids and recorded on a Gallenkamp melting point apparatus and are uncorrected. All solvents and reagents were purified using standard, laboratory techniques according to methods published in "Purification of Laboratory Chemicals" by Perrin, Armarego, and Perrin (Pergamon Press, 1966). Microwave mediated coupling reactions were carried out on an Emrys(TM) creator with 'fixed hold time' set to 'off' and 'absorption level' set to 'high'.

Functionalisation of Tetrazine Ring Systems to Form Unsymmetrical 3,6-Disubstituted Tetrazines.

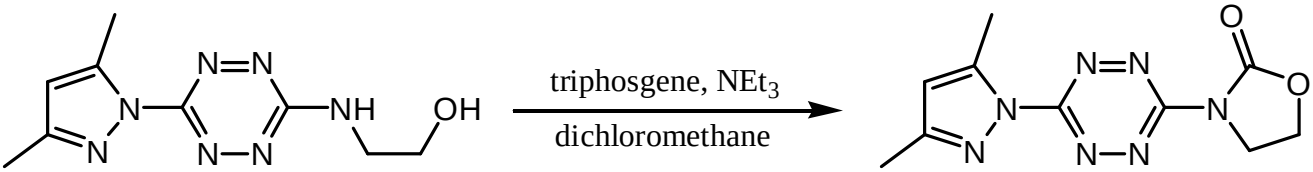
Formation of [6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-dicarbamic acid tert-butyl ester 18.



To a stirred solution of 6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-ylamine (2 g, 10.5 mmol) and 4-dimethylaminopyridine (128 mg, 1.05 mmol) in 70 ml of dry tetrahydrofuran was added dropwise di-*tert*-butyl dicarbonate (5.3 ml, 23.0 mmol). The reaction was stirred at room temperature for 1 hour before all solvents were removed in vacuo and the crude products purified using column chromatography on silica gel to

provide [6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-dicarbamic acid tert-butyl ester (2.87 g, 70 %) as a pink solid m.p. 130.9-131.7 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.42 (18H, s, CH_3), 2.39 (3H, s, CH_3), 2.72 (3H, s, CH_3), 6.21 (1H, s, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 13.9, 15.1, 27.8, 85.3, 112.6, 144.4, 149.1, 155.2, 158.9, 161.7. FTIR: 2981 (s), 2930 (s), 1810 (s), 1775 (s), 1740 (s), 1585 (s), 1495 (s), 1429 (s) cm^{-1}. HRMS calcd for $C_{17}H_{26}N_7O_4$: 392.2046. Found: 392.2063. Anal. Calcd for $C_{17}H_{25}N_7O_4$: C 52.16, H 6.44, N 25.05. Found C 52.34, H 6.26, N 25.18.

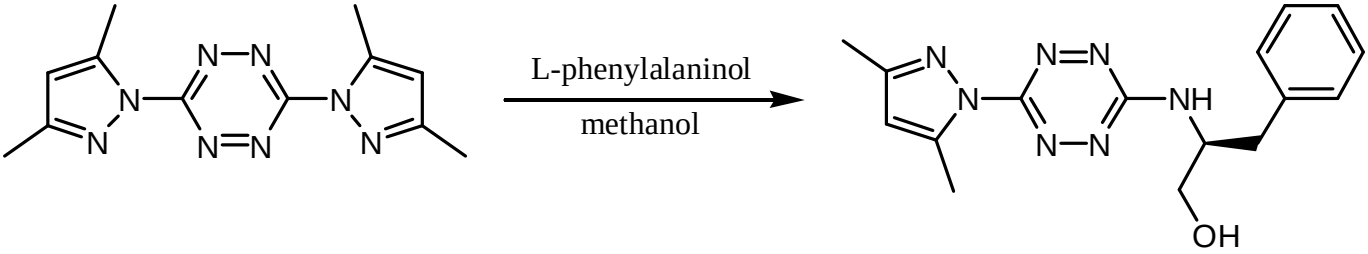
Formation of 3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one 19.



To a stirred solution of 2-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-ylamino]-ethanol[1] (289 mg, 1.2 mmol) and triphosgene (437 mg, 1.5 mmol) in 10 ml of dry dichloromethane at -78^{o}C was added dropwise distilled triethylamine (0.34 ml, 2.5 mmol). Following addition of the triethylamine the temperature was allowed to rise to room temperature and the reaction was stirred for a further 4 hours. The volatiles were removed in vacuo and then the crude materials dissolved in dichloromethane and washed with saturated sodium hydrogen carbonate, dilute hydrochloric acid, water and brine. Finally, the organic fractions were then dried over magnesium sulphate. The solvent was removed in vacuo and the crude materials purified on silica gel to give 3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one (249 mg, 79 %) as a red solid m.p. 183.9-184.9 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 2.30 (3H, s, CH_3), 2.61 (3H, s, CH_3), 4.42 (2H, t, *J* = 8.0 Hz, CH_2), 4.62 (2H, t, *J* = 8.0 Hz, CH_2), 6.10 (3H, s, CH_3). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 13.9, 14.6, 44.2, 62.7, 111.7, 143.6, 152.1, 154.2, 158.4, 158.8. FTIR: 2921 (w), 2845 (w), 1777 (s), 1579 (m), 1472 (s), 1451 (s), 1429 (s), 1380 (m), 1276 (w), 1195 (m), 1078 (s), 1044 (m) cm^{-1}. HRMS calcd for $C_{10}H_{12}N_7O_2$: 262.1052. Found: 262.1041.

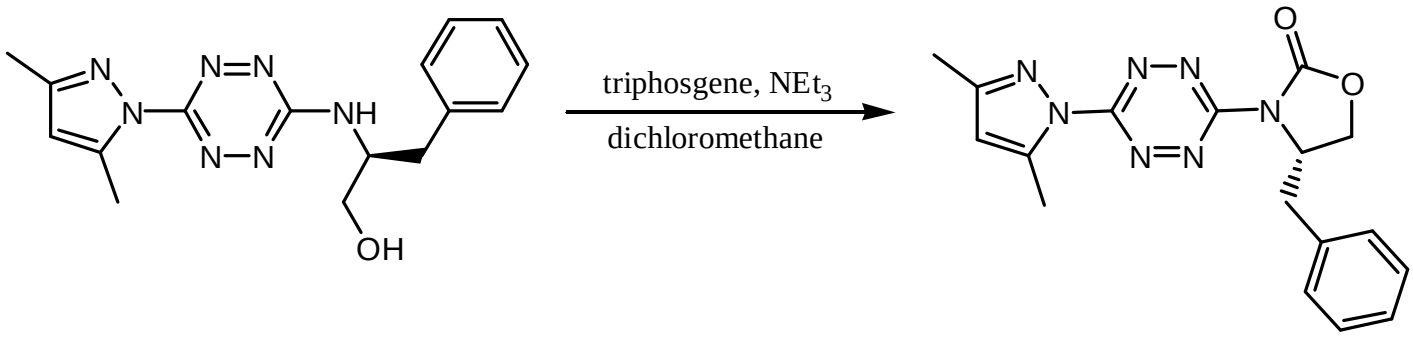
[1] Latosh, N. I.; Rusinov, G. L.; Ganebnykh, I. N.; Chupakhin, O. N. *Russian Journal of Organic Chemistry* **1999**, *35*, 1363.

Formation of (S)-2-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-ylamino]-3-phenyl-propan-1-ol.



3,6-Bis-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazine (1.50 g, 5.5 mmol) and L-phenylalaninol were dissolved in 40 ml of methanol and stirred for 15 minutes. The solvent was removed in vacuo and the products purified on silica gel. Washing with petroleum ether 40-60 removed any residual 3,5-dimethylpyrazole to give (S)-2-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-ylamino]-3-phenyl-propan-1-ol (1.53 g, 85 %) as a bright orange crystalline solid m.p. 150.9-153.7 ^{o}C. $[\alpha]_D^{22}$ = -105 (c = 1, CH_2Cl_2). ^{1}H NMR (250 MHz, $CDCl_3$): δ 2.31 (3H, s, CH_3), 2.51 (3H, s, CH_3), 2.81 (1H, br, OH), 3.03 (2H, dd, *J* = 7.0 Hz, *J* = 3.0 Hz, CH_2), 3.74 (1H, dd, *J* = 11.5 Hz, *J* = 4.5 Hz, CH_2), 3.85 (1H, dd, *J* = 11.5 Hz, *J* = 3.5 Hz, CH_2), 4.41-4.56 (1H, m, CH), 6.07 (1H, s, CH), 6.75 (1H, d, *J* = 8.5 Hz, NH), 7.13-7.30 (5H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 12.2, 13.5, 37.1, 54.7, 62.3, 104.2, 126.6, 128.5, 129.4, 137.6, 142.0, 144.5, 157.2, 161.3. FTIR: 3320 (br), 2926 (m), 2858 (w), 1568 (s), 1484 (s), 1454 (w), 1416 (m), 1364 (w), 1287 (w), 1076 (m), 1038 (m) cm^{-1}. HRMS calcd for $C_{16}H_{20}N_7O$: 326.1729. Found: 326.1729.

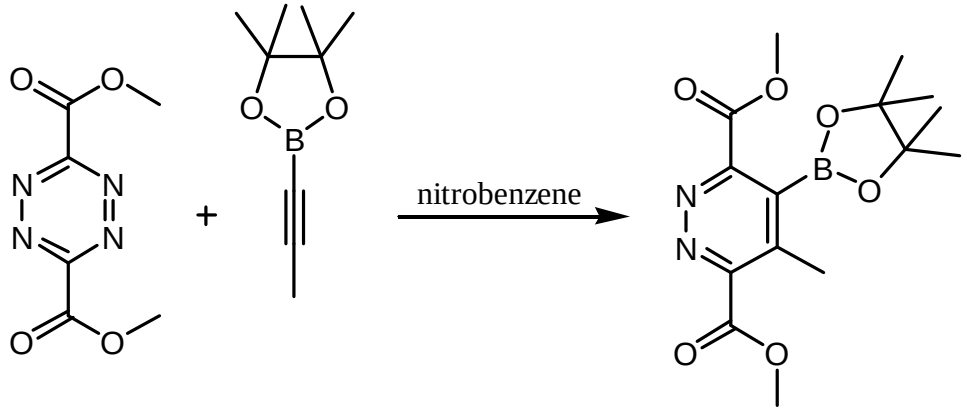
Formation of (S)-4-benzyl-3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one 20.



To a stirred solution of (S)-2-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-ylamino]-3-phenyl-propan-1-ol (1.16 g, 3.6 mmol) and triphosgene (1.27 g, 4.3 mmol) in 40 ml of dry dichloromethane at -78^{o}C was added dropwise distilled triethylamine (0.99 ml, 7.1 mmol). Following addition of the triethylamine the temperature was allowed to rise to room temperature and then the reaction was stirred for a further 4 hours. The reaction mixture was diluted with 150 ml of dichloromethane and then washed with saturated sodium hydrogen carbonate, dilute hydrochloric acid, water and brine. The organic fractions were then dried over magnesium sulphate, the solvent removed in vacuo and the crude materials purified on silica gel to give (S)-4-benzyl-3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one (0.93 g, 74 %) as a bright pink foam m.p. 63.1-64.6 ^{o}C. $[\alpha]_D^{22}$ = -151 (c = 1, CH_2Cl_2). ^{1}H NMR (250 MHz, $CDCl_3$): δ 2.38 (3H, s, CH_3), 2.71 (3H, s, CH_3), 2.90 (1H, dd, *J* = 13.0 Hz and *J* = 3.5 Hz, CH_2), 3.50 (1H, dd, *J* = 13.0 Hz and *J* = 9.5 Hz, CH_2), 4.37-4.53 (2H, m, CH_2), 5.07-5.19 (1H, m, CH), 6.18 (1H, s, CH), 7.21-7.38 (5H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): 13.8, 14.6, 37.6, 56.7, 67.1, 111.7, 127.4, 129.0, 129.4 134.8, 143.6, 151.9, 154.2, 158.4, 158.5. FTIR: 3032 (w), 2973 (w), 2927 (w), 1783 (s), 1579 (m), 1451 (s), 1432 (s), 1285 (w), 1186 (m), 1079 (s) cm^{-1}. HRMS calcd for $C_{17}H_{18}N_7O_2$: 352.1522. Found: 352.1514.

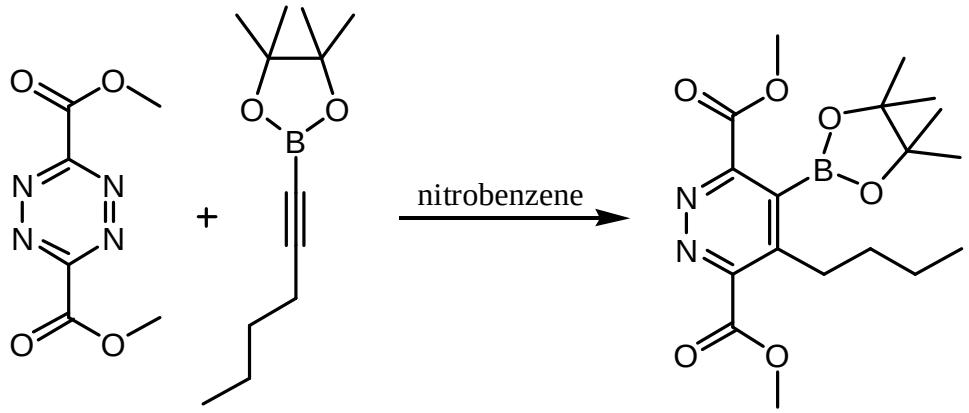
Inverse Electron Demand Cycloaddition Reactions Between Symmetrical 3,6-Disubstituted Tetrazines and Alkynylboronates.

Formation of 4-methyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester 9.



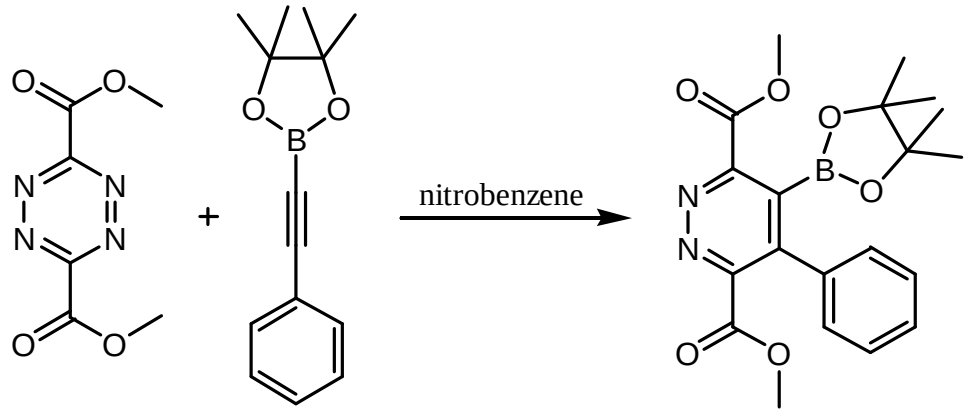
4,4,5,5-Tetramethyl-2-prop-1-ynyl-[1,3,2]dioxaborolane (92 mg, 0.555 mmol) and [1,2,4,5]tetrazine-3,6-dicarboxylic acid dimethyl ester (100 mg, 0.505 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 3 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 4-methyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester (75 mg, 44 %) as a yellow solid m.p. 136.5-138.9 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.45 (12H, s, CH_3), 2.59 (3H, s, CH_3), 4.04 (3H, s, CH_3), 4.08 (3H, s, CH_3). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 18.3, 25.1, 53.2, 53.8, 85.3, 142.2, 152.9, 153.3, 165.4, 166.3. FTIR: 2982 (m), 2956 (w), 1732 (s), 1444 (m), 1374 (m), 1340 (s), 1281 (m), 1242 (s) cm^{-1}. HRMS calcd for $C_{15}H_{22}BN_2O_6$: 337.1571. Found: 337.1570.

Formation of 4-butyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester 10.



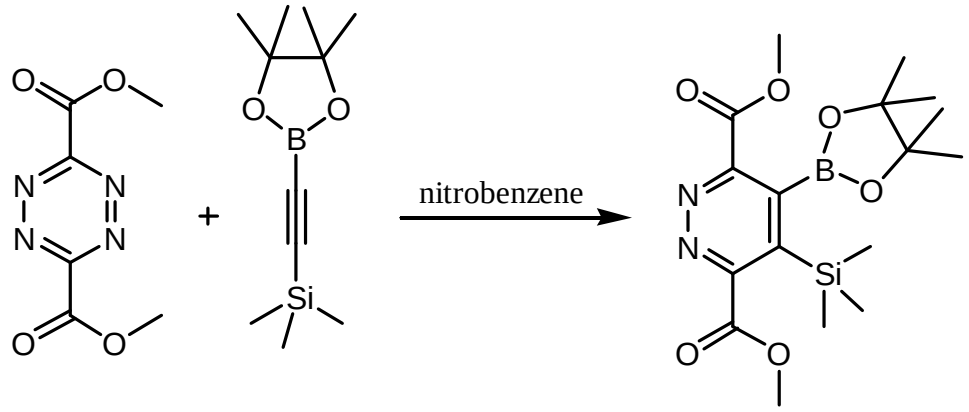
2-Hex-1-ynyl-4,4,5,5-tetramethyl-[1,3,2]dioxaborolane (116 mg, 0.555 mmol) and [1,2,4,5]tetrazine-3,6-dicarboxylic acid dimethyl ester (100 mg, 0.505 mmol) were dissolved in 2 ml of distilled dry nitrobenzene and heated at 140 ^{o}C for 6 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 4-butyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester (144 mg, 75 %) as a yellow/brown oil. ^{1}H NMR (250 MHz, $CDCl_3$): δ 0.87 (3H, t, *J* = 7.5 Hz, CH_3), 1.39 (12H, s, CH_3), 1.46-1.63 (4H, m, CH_2), 2.80 (2H, t, *J* = 8.0 Hz, CH_2), 3.98 (3H, s, CH_3), 4.01 (3H, s, CH_3). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 13.7, 23.0, 25.2, 32.3, 33.4, 53.1, 53.7, 85.3, 146.4, 153.2, 153.4, 165.5, 166.3. FTIR: 2959 (m), 2930 (m), 2874 (w), 1738 (s), 1549 (w), 1443 (m) 1374 (m), 1335 (s), 1278 (m), 1244 (s), 1204 (m), 1168 (w), 1144 (s) cm^{-1}. HRMS calcd for $C_{18}H_{28}BN_2O_6$: 379.2040. Found: 379.2032.

Formation of 4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester 11.



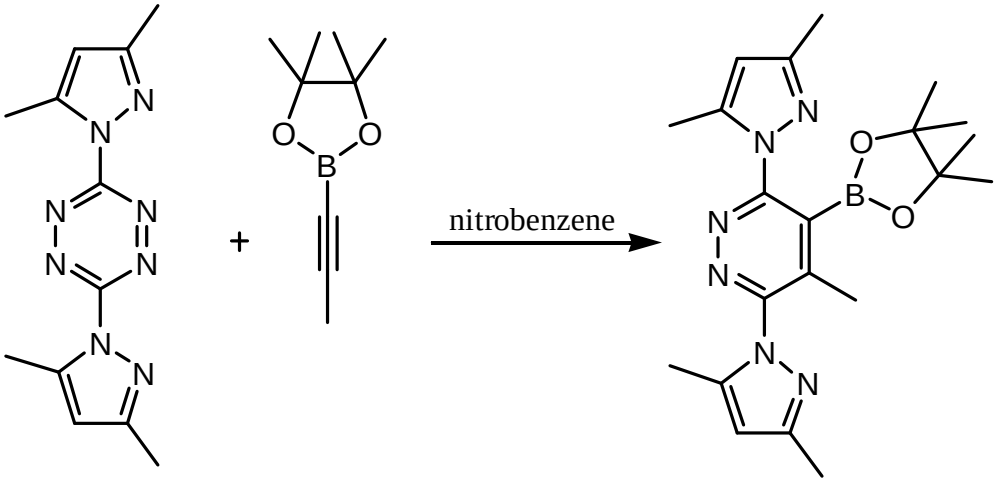
4,4,5,5-Tetramethyl-2-phenylethynyl-[1,3,2]dioxaborolane (127 mg, 0.555 mmol) and [1,2,4,5]tetrazine-3,6-dicarboxylic acid dimethyl ester (100 mg, 0.505 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 4 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester (151 mg, 75 %) as a yellow solid m.p. 138.8-140.9 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.02 (12H, s, CH_3), 3.69 (3H, s, CH_3), 4.04 (3H, s, CH_3), 7.22-7.42 (5H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 24.8, 53.0, 53.8, 85.2, 128.2, 128.9, 129.3, 134.5, 144.0, 152.9, 153.5, 165.3, 166.1. FTIR: 2980 (w), 2956 (w), 1745 (s), 1724 (s), 1540 (m), 1493 (w), 1445 (m), 1374 (m), 1341 (s), 1284 (m), 1244 (w), 1219 (s), 1180 (w), 1144 (m) cm^{-1}. HRMS calcd for $C_{20}H_{24}BN_2O_6$: 399.1727. Found: 399.1725.

Formation of 4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-5-trimethylsilanyl-pyridazine-3,6-dicarboxylic acid dimethyl ester 12.



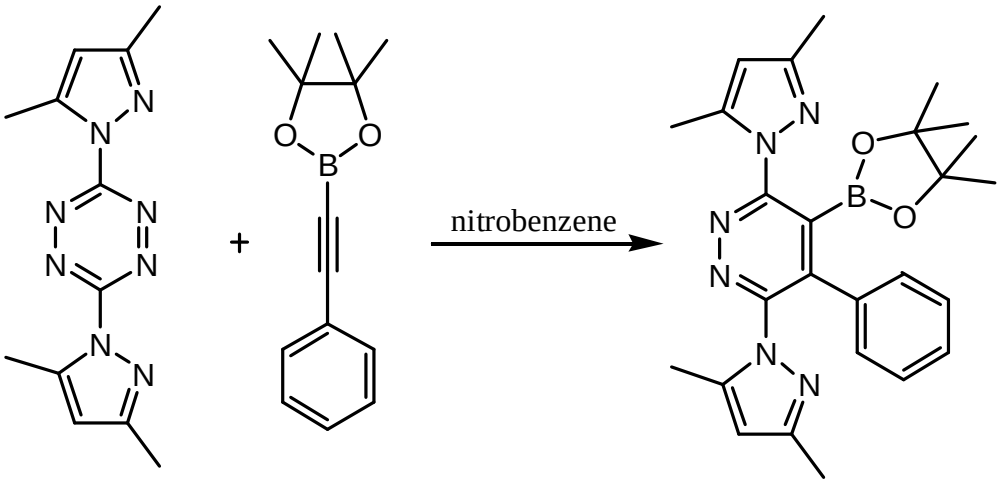
4,4,5,5-Tetramethyl-2-trimethylsilanylethynyl-[1,3,2]dioxaborolane (124 mg, 0.555 mmol) and [1,2,4,5]tetrazine-3,6-dicarboxylic acid dimethyl ester (100 mg, 0.505 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 5 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-5-trimethylsilanyl-pyridazine-3,6-dicarboxylic acid dimethyl ester (178 mg, 89 %) as a yellow/brown wax. ^{1}H NMR (250 MHz, $CDCl_3$): δ 0.35 (9H, s, CH_3), 1.40 (12H, s, CH_3), 3.95 (3H, s, CH_3), 3.99 (3H, s, CH_3). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 0.3, 26.0, 53.2, 53.5, 85.5, 143.9, 153.6, 158.6, 167.0, 167.6. FTIR: 2998 (w), 2981 (m), 2956 (m), 1733 (s), 1441 (m), 1382 (w), 1349 (m), 1301 (m), 1256 (m), 1210 (s), 1177 (m), 1140 (m), 1113 (m) cm^{-1}. HRMS calcd for $C_{17}H_{27}BN_2O_6Si$: 394.1731. Found: 394.1744.

Formation of 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-methyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine 13.



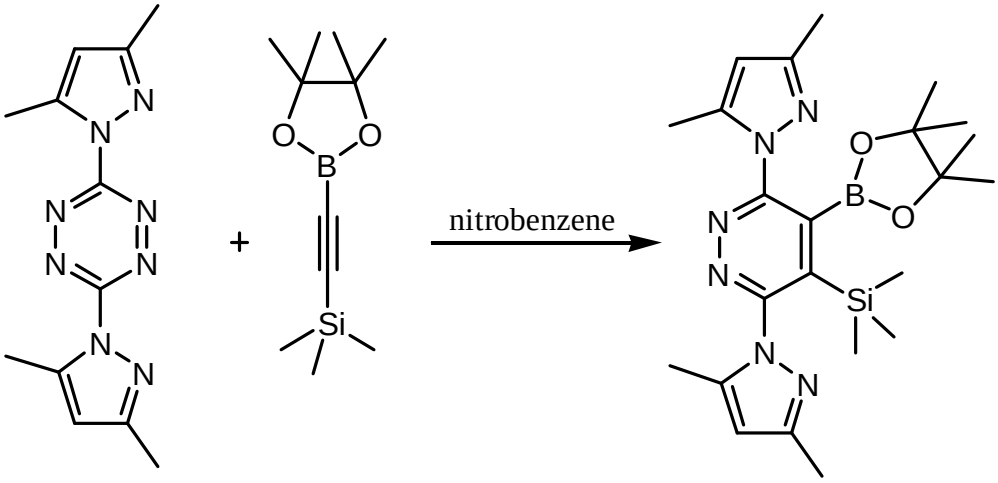
4,4,5,5-Tetramethyl-2-prop-1-ynyl-[1,3,2]dioxaborolane (68 mg, 0.41 mmol) and 3,6-bis(3,5-dimethyl-pyrazol-1-yl)-1,2,4,5-tetrazine (100 mg, 0.37 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 7 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-methyl-5-(4,4,5,5-tetramethyl[1,3,2]dioxa-borolan-2-yl)-pyridazine (122 mg, 81 %) as a light yellow solid m.p. 144.8-147.5 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.34 (12H, s, CH_3), 2.16 (3H, s, CH_3), 2.23 (3H, s, CH_3), 2.28 (3H, s, CH_3), 2.30 (3H, s, CH_3), 2.65 (3H, s, CH_3), 5.95 (1H, s, CH), 5.99 (1H, s, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 11.6, 13.6, 13.8, 14.6, 16.5, 25.7, 84.2, 106.6, 111.0, 141.6, 142.1, 142.6, 150.0, 150.1, 153.8, 157.3. FTIR: 2978 (m), 2930 (w), 1574 (w), 1538 (m), 1470 (s), 1454 (s), 1422 (s), 1404 (s), 1358 (m), 1319 (w), 1139 (s) cm^{-1}. HRMS calcd for $C_{21}H_{30}BN_6O_2$: 409.2523. Found: 409.2504.

Formation of 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine 14.



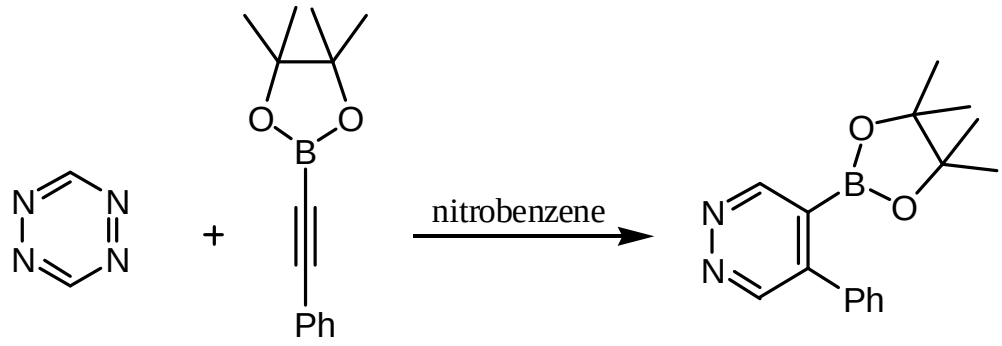
4,4,5,5-Tetramethyl-2-phenylethynyl-[1,3,2]dioxaborolane (92 mg, 0.41 mmol) and 3,6-bis(3,5-dimethyl-pyrazol-1-yl)-1,2,4,5-tetrazine (100 mg, 0.37 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 6 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine (146 mg, 84 %) as a yellow solid m.p. 181.6-184.5 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.02 (12H, s, CH_3), 2.01 (3H, s, CH_3), 2.06 (3H, s, CH_3), 2.32 (3H, s, CH_3), 2.76 (3H, s, CH_3), 5.73 (1H, s, CH), 6.07 (1H, s, CH), 7.15-7.36 (5H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 11.2, 13.3, 13.9, 14.9, 25.2, 84.3, 106.0, 111.1, 127.5, 128.5, 129.3, 133.7, 141.1, 142.4, 145.7, 149.5, 150.4, 152.3, 157.6. FTIR: 2980 (m), 2927 (m), 1579 (m), 1529 (m), 1495 (w), 1476 (m), 1446 (m), 1422 (s), 1371 (w), 1342 (m), 1244 (w), 1208 (w), 1142 (m), 1124 (m) cm^{-1}. HRMS calcd for $C_{26}H_{32}BN_6O_2$: 471.2680. Found: 471.2680.

Formation of 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-5-trimethylsilanyl-pyridazine 15.



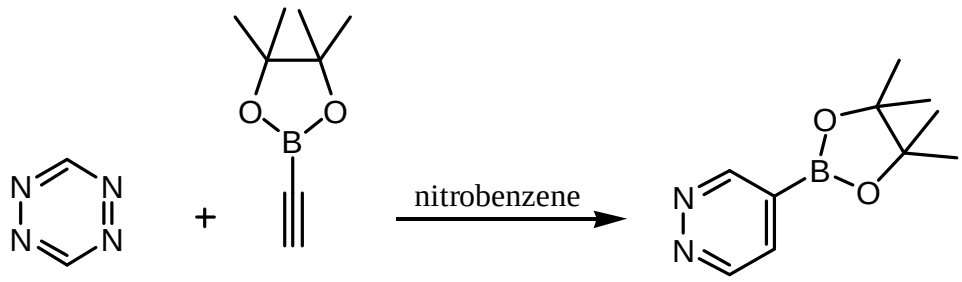
4,4,5,5-Tetramethyl-2-trimethylsilanylethynyl-[1,3,2]dioxaborolane (92 mg, 0.41 mmol) and 3,6-bis(3,5-dimethyl-pyrazol-1-yl)-1,2,4,5-tetrazine (100 mg, 0.37 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 8 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 3,6-bis(3,5-dimethyl-pyrazol-1-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5-(trimethylsilyl)pyridazine (119 mg, 69 %) as an orange oil. ^{1}H NMR (250 MHz, $CDCl_3$): δ 0.00 (9H, s, CH_3), 1.16 (12H, s, CH_3), 2.10 (3H, s, CH_3), 2.14 (3H, s, CH_3), 2.29 (3H, s, CH_3), 2.34 (3H, s, CH_3), 5.88 (2H, br, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 0.4, 12.2, 12.7, 13.4, 13.8, 25.9, 85.0, 108.0, 108.2, 141.3, 141.9, 145.1, 149.7, 149.9, 156.7, 157.8. FTIR: 3083 (w), 2926 (m), 2854 (w), 1579 (m), 1483 (s), 1448 (s), 1425 (s), 1276 (m), 1162 (w), 1079 (s) cm^{-1}. HRMS calcd for $C_{23}H_{36}BN_6O_2Si$: 467.2762. Found: 467.2743.

Formation of 4-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine 16.



4,4,5,5-Tetramethyl-2-phenylethynyl-[1,3,2]dioxaborolane (306 mg, 1.34 mmol) and 1,2,4,5-tetrazine (100 mg, 1.22 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 6 hours. The nitrobenzene was then removed by vacuum distillation and the products recrystallised from ethyl acetate to give 4-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine (206 mg, 60%) as a light yellow solid m.p. 130.5-132.7 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.25 (12H, s, CH_3), 7.40-7.50 (5H, m, CH), 9.22 (1H, d, *J* = 1.0 Hz, CH), 9.31 (1H, d, *J* = 1.0 Hz, CH). ^{13}C NMR (62.9 MHz, d_6-DMSO): δ 24.4, 84.8, 128.7, 129.0, 129.4, 136.0, 143.3, 150.8, 153.6. FTIR: 3063 (w), 2978 (m), 2916 (w), 1573 (w), 1535 (w), 1494 (w), 1444 (w), 1384 (m), 1374 (m), 1362 (m), 1342 (m), 1288 (w), 1250 (w), 1214 (m), 1180 (m), 1148 (s), 1076 (m), 1058 (m), 1043 (m), 1008 (m). HRMS calcd for $C_{16}H_{19}N_2O_2B$: 282.1540. Found: 282.1550.

Formation of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine 17.

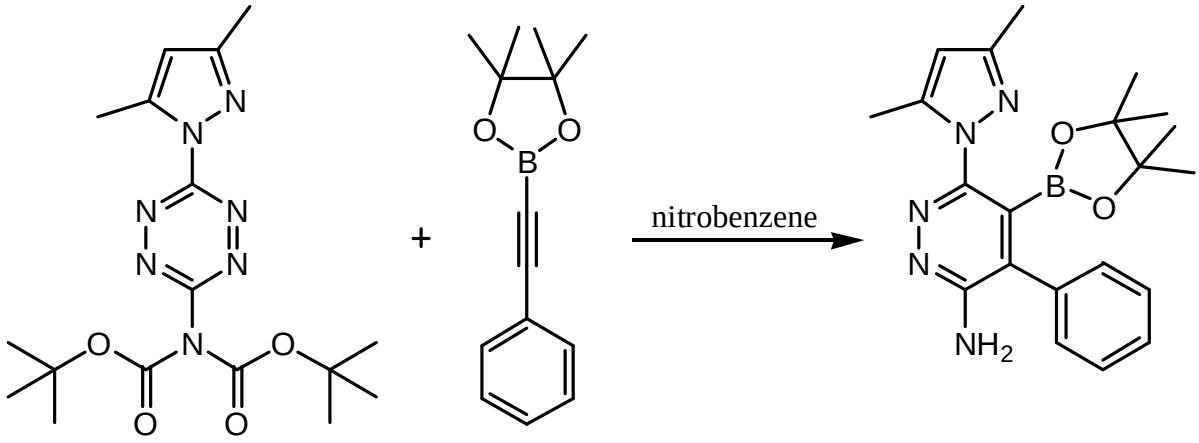


2-Ethynyl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (204 mg, 1.34 mmol) and 1,2,4,5-tetrazine (100 mg, 1.22 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 6 hours. The nitrobenzene was then removed by vacuum distillation and the products purified by sublimation (0.2 mmHg, 120 ^{o}C) to give 4-(4,4,5,5-

tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine (158 mg, 64%) as a colourless solid m.p. 132 ^{o}C (dec.). ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.13 (12H, s, CH_3), 7.98 (1H, d, *J* = 4.5 Hz, CH), 9.05 (1H, d, *J* = 4.5 Hz, CH), 9.42 (1H, s, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 24.9, 84.3, 132.5, 150.5, 154.3. FTIR: 3099 (w), 3064 (w), 2973 (s), 2926 (s), 2856 (m), 1718 (w), 1586 (m), 1540 (w), 1462 m), 1446 (m), 1203 (s), 1183 (s), 1160 (s), 1113 (m), 1089 (s), 1060 (s), 1012 (s). HRMS calcd for $C_{10}H_{16}N_2O_2B$: 207.1305. Found: 207.1296.

Inverse Electron Demand Cycloaddition Reactions Between Unsymmetrical 3,6-Disubstituted Tetrazines and Alkynylboronates.

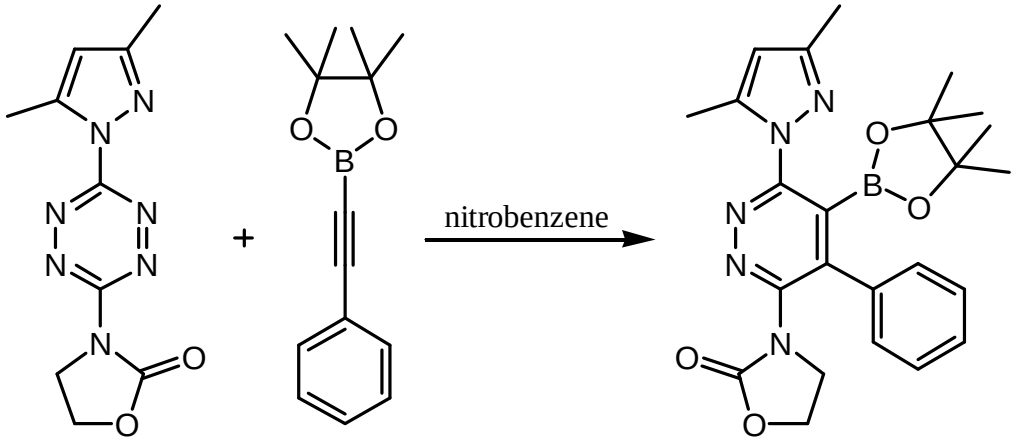
Formation of 6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-ylamine 21.



4,4,5,5-Tetramethyl-2-phenylethynyl-[1,3,2]dioxaborolane (117 mg, 0.51 mmol) and [6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-dicarbamic acid tert-butyl ester (100 mg, 0.26 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 16 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-ylamine (62 mg, 61 %) as a yellow/brown wax. ^{1}H NMR (250 MHz, $CDCl_3$): δ 0.91 (12H, s, CH_3), 2.21 (3H, s, CH_3), 2.58 (3H, s, CH_3), 4.51 (2H, br, NH_2), 5.91 (1H, s, CH), 7.27-7.47 (5H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 13.8, 14.0, 25.1, 84.0, 109.3, 129.0, 129.1, 129.3, 134.2, 134.4, 140.9, 148.6, 152.5, 156.0. FTIR: 3329 (br), 3193 (br), 3066 (w), 2973,

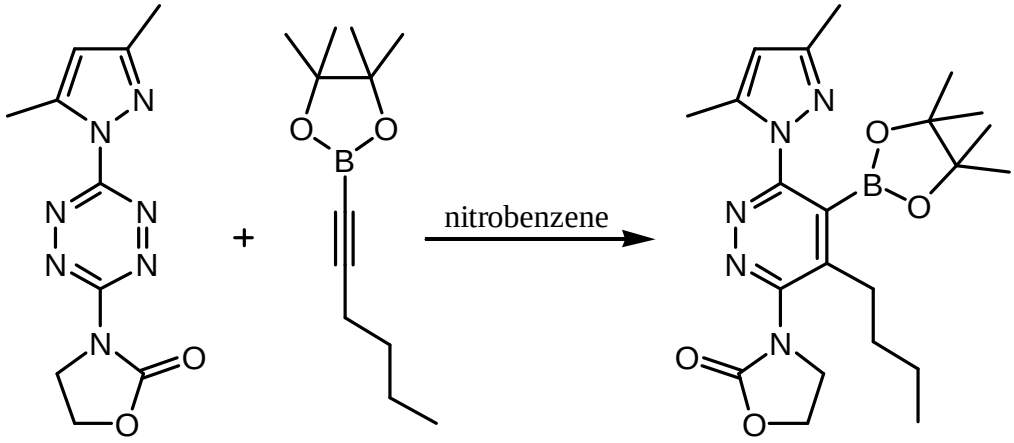
(m), 2926 (m), 2854 (m), 1702 (m), 1560 (m), 1472 (s), 1438 (s), 1421 (s), 1369 (s), 1251 (m), 1141 (s), 1123 (s) cm^{-1}. HRMS calcd for $C_{21}H_{27}BN_5O_2$: 392.2258. Found: 392.2255.

Formation of 3-[6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one 22.



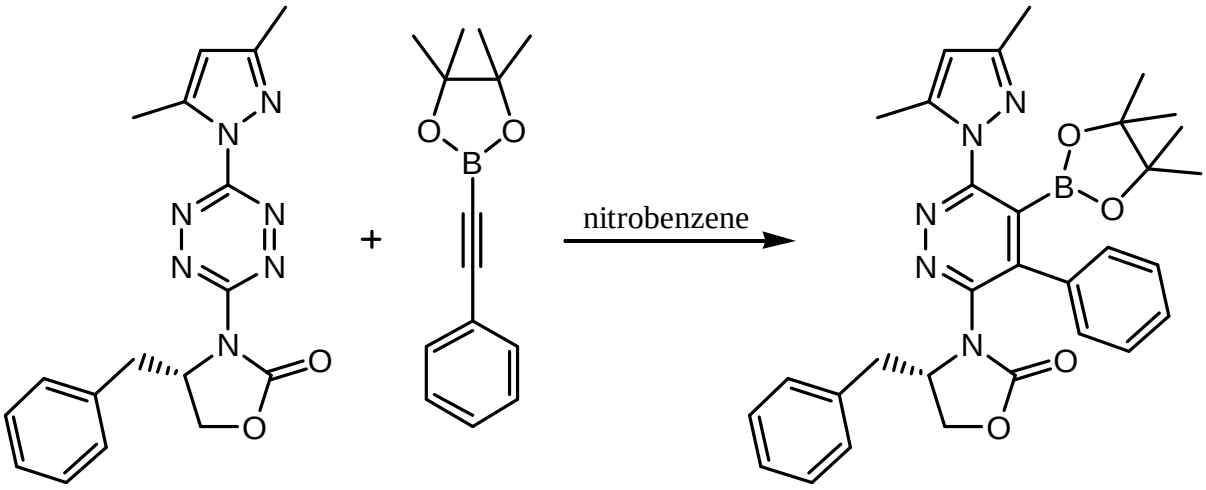
4,4,5,5-Tetramethyl-2-phenylethynyl-[1,3,2]dioxaborolane (96 mg, 0.42 mmol) and 3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one (100 mg, 0.38 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^oC for 6 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 3-[6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one (134 mg, 76 %) as a colourless solid m.p. 207.5-210.3 ^oC. ^1H NMR (250 MHz, $CDCl_3$): δ 1.00 (12H, s, CH_3), 2.30 (3H, s, CH_3), 2.74 (3H, s, CH_3), 3.96 (2H, m, CH_2), 4.30 (2H, m, CH_2), 6.05 (1H, s, CH), 7.40 (5H, br, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 13.9, 14.9, 25.2, 46.6, 62.8, 84.3, 111.1, 127.9, 128.9, 129.3, 134.2, 142.2, 145.6, 150.3, 151.0, 155.6, 157.2. FTIR: 2978 (m), 2928 (m), 1764 (s), 1575 (m), 1529 (m), 1494 (m), 1468 (m), 1419 (s), 1367 (m), 1216 (m), 1140 (m), 1110 (s) cm^{-1}. HRMS calcd for $C_{24}H_{29}BN_5O_4$: 462.2313. Found: 462.2295.

Formation of 3-[4-Butyl-6-(3,5-dimethyl-pyrazol-1-yl)-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one 23.



2-Hex-1-ynyl-4,4,5,5-tetramethyl-[1,3,2]dioxaborolane (88 mg, 0.42 mmol) and 3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one (100 mg, 0.38 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 6 hours. The nitrobenzene was then removed by vacuum distillation and the products purified on florisil gel to give 3-[4-butyl-6-(3,5-dimethyl-pyrazol-1-yl)-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one (111 mg, 70 %) as a orange oil. ^{1}H NMR (250 MHz, $CDCl_3$): δ 0.91 (3H, t, *J* = 7.0 Hz, CH_3), 1.39 (12H, s, CH_3), 1.72-1.40 (4H, m, CH_2), 2.30 (3H, s, CH_3), 2.66 (3H, s, CH_3), 2.84 (2H, t, *J* = 8.0 Hz, CH_2), 4.30 (2H, t, *J* = 8.0 Hz, CH_2), 4.56 (2H, t, *J* = 8.0 Hz, CH_2), 6.01 (1H, s, CH). ^{13}C NMR (92.9 MHz, $CDCl_3$): δ 13.9, 14.5, 22.9, 24.8, 25.7, 30.8, 32.7, 46.9, 63.2, 84.4, 110.6, 141.9, 146.8, 150.0, 152.3, 156.2, 157.4. FTIR: 2961 (m), 2928 (m), 2872 (w), 1761 (s), 1577 (m), 1529 (m), 1468 (m), 1404 (s), 1370 (w), 1350 (w), 1214 (m), 1125 (m), 1090 (m), 1037 (m) cm^{-1}. HRMS calcd for $C_{22}H_{33}BN_5O_4$: 442.2626. Found: 442.2632.

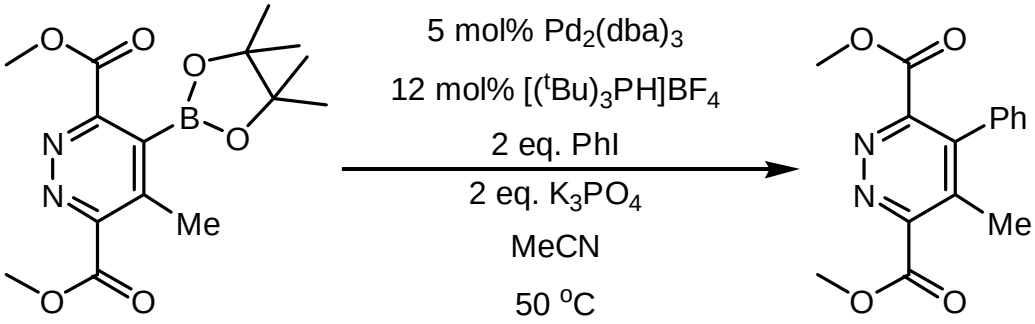
Formation of (S)-4-benzyl-3-[6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one 24.



4,4,5,5-Tetramethyl-2-phenylethynyl-[1,3,2]dioxaborolane (71 mg, 0.31 mmol) and (S)-3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one (100 mg, 0.28 mmol) were dissolved in 2 ml of distilled nitrobenzene and heated at 140 ^{o}C for 16 hours. The nitrobenzene was removed by vacuum distillation and the products purified on florisil gel to give (S)-4-benzyl-3-[6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one (145 mg, 92 %) as cream foam m.p. 69.7-72.0 ^{o}C. $[\alpha]_D^{22}$ = -12 (c = 1, CH_2Cl_2). ^{1}H NMR (250 MHz, $CDCl_3$): δ 0.90 (6H, s, CH_3), 0.98 (6H, s, CH_3), 2.25 (3H, s, CH_3), 2.48 (1H, dd, *J* = 13.0 Hz, *J* = 10.5 Hz, CH_2), 2.72 (3H, s, CH_3), 2.96 (1H, dd, *J* =13.0 Hz, *J* = 4.0 Hz, CH_2), 3.89 (1H, t, *J* = 8.5 Hz, CH_2), 3.99 (1H, t, *J* = 8.5 Hz, CH_2), 4.34-4.50 (1H, m, CH), 6.00 (1H, s, CH), 6.94-7.54 (10H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 13.9, 14.9, 25.2, 25.3, 38.8, 58.5, 68.2, 84.3, 111.2, 127.2, 127.8, 127.9, 128.9, 129.0, 134.1, 135.1, 142.3, 146.5, 150.2, 150.4, 156.0, 157.3. FTIR: 3062 (w), 3028 (w), 2878 (m), 2929 (m), 1766 (s), 1604 (w), 1575 (m), 1530 (m), 1495 (m), 1470 (m), 1418 (s), 1370 (m), 1351 (m), 1217 (m), 1182 (w), 1140 (m), 1112 (s) cm^{-1}. HRMS Calcd for $C_{31}H_{35}BN_5O_4$: 552.2782. Found: 552.2797.

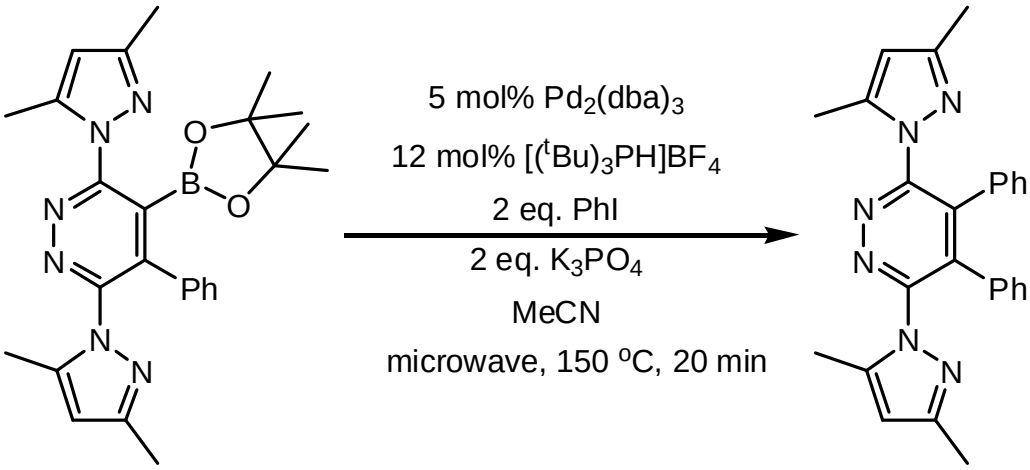
Functionalisation of boronic ester.

Suzuki coupling of Iodobenzene with 4-Methyl-5-(4,4,5,5tetramethyl[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester to give 27



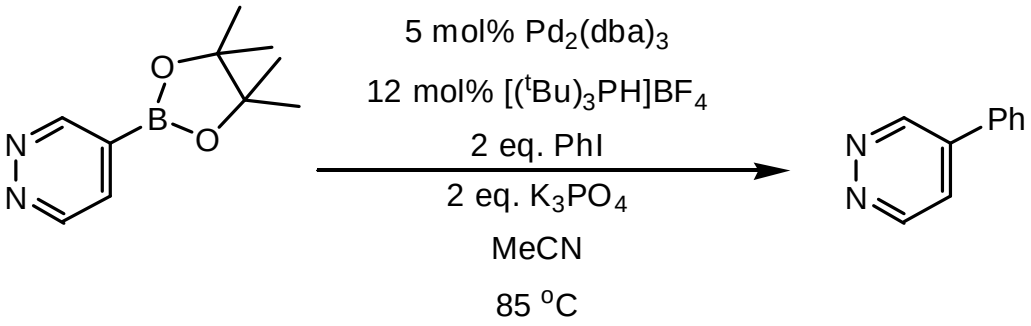
4-Methyl-5-(4,4,5,5tetramethyl[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester (50 mg, 0.17 mmol), tripotassium phosphate (72 mg, 0.34 mmol), tris(dibenzylideneacetone)dipalladium (7 mg, 7.4 μmol) and tri-*tert*-butylphosphonium tetrafluoroborate (5 mg, 17.8 μmol) were dissolved in 1 ml of acetonitrile and iodobenzene (38 μL, 0.34 mmol) added. The suspension was then stirred at room temperature for one hour and then for one and half hours at 50 ^{o}C. The reaction was then quenched with water and extracted three times with dichloromethane, the combined organic extracts were combined and dried over magnesium sulphate. The volitiles were removed under reduced pressure and the products purified on silica gel to give dimethyl 4-methyl-5-phenylpyridazine-3,6-dicarboxylate (28 mg, 57%) as a yellow crystalline solid m.p. 108.9-110.4 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 2.27 (3H, s, CH_3), 3.65 (3H, s, CH_3), 4.01 (3H, s, CH_3), 7.09-7.19 (2H, m, CH), 7.37-7.47 (3H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 15.9, 52.9, 53.3, 128.2, 128.8, 129.2, 133.0, 137.1, 140.3, 153.7, 154.1, 165.2, 165.4. FTIR: 3004 (w), 2955 (w), 2850 (w), 1742 (s), 1529 (w), 1496 (w), 1440 (m), 1401 (w), 1372 (m), 1283 (m), 1226 (m), 1201 (m), 1108 (m), 1088 (m) cm^{-1}. HRMS calc. for $C_{15}H_{15}N_2O_4$: 287.1032. Found: 287.1033. Anal Calcd for $C_{15}H_{14}N_2O_4$: C 62.93, H 4.93, N 9.79. Found C 62.62, H 4.99, N 9.76.

Suzuki coupling of iodobenzene with 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine to give 28



3,6-Bis-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl [1,3,2]dioxaborolane-2-yl)-pyridazine (50 mg, 0.11 mmol), tripotassium phosphate (45 mg, 0.21 mmol), tris(dibenzylideneacetone)dipalladium (5 mg, 5.3 μmol) and tri-*tert*-butylphosphonium tetrafluoroborate (4 mg, 12.8 μmol) were dissolved in 2 ml of acetonitrile inside a microwave reactor vessel and iodobenzene (24 μL, 0.21 mmol) added. The sealed microwave vessel was then stirred for 20 minutes at room temperature then heated to 150 ^{o}C for 20 min using microwave irradiation. The reaction was then quenched with water and extracted three times with dichloromethane, the combined organic extracts were combined and dried over magnesium sulphate. The volatiles were removed under reduced pressure and the products purified on silica gel to give dimethyl 3,6-bis(3,5-dimethyl-1H-pyrazol-1-yl)-4,5-diphenylpyridazine (23 mg, 51%) as a yellow crystalline solid m.p. 151.2-153.2 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.93-1.96 (6H, s, CH_3), 2.08-2.10 (6H, s, CH_3), 5.73-5.77 (2H, s, CH), 6.75-6.83 (4H, m, CH), 6.96-7.13 (6H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 11.3, 13.4, 106.6, 127.9, 128.4, 129.4, 131.9, 139.9, 141.5, 150.2, 155.0. FTIR: 3049 (w), 2924 (m), 2845 (w), 1726 (w), 1676 (w), 1562 (m), 1534 (m), 1493 (m), 1466 (s), 1444 (s), 1422 (s), 1401 (s), 1289 (w), 1221 (w), 1175 (w), 1153 (w), 1117 (m), 1077 (w), 1046 (W), 1018 (w). HRMS calcd for $C_{26}H_{25}N_6$: 421.2141. Found 421.2137.

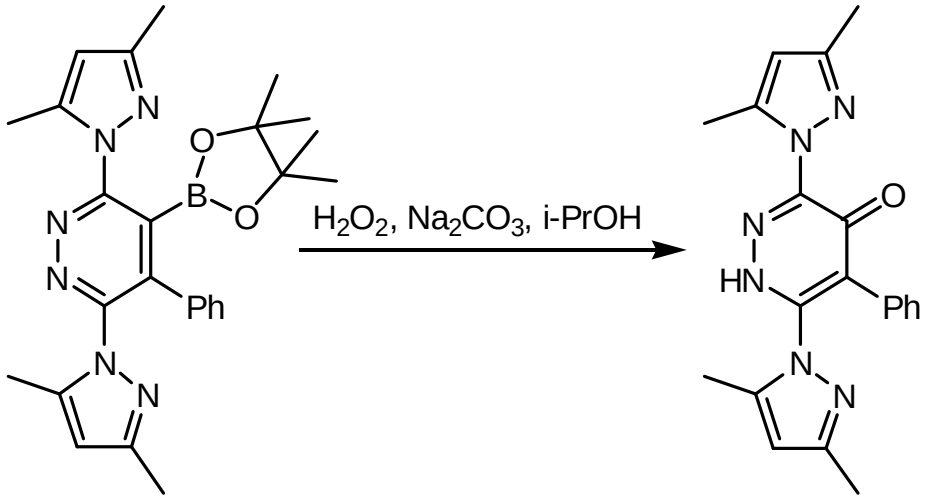
Suzuki coupling of iodobenzene and 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine to give 26



4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine (50 mg, 0.24 mmol), tripotassium phosphate (103 mg, 0.49 mmol), tris(dibenzylideneacetone)dipalladium (11 mg, 12 μmol) and tri-*tert*-butylphosphonium tetrafluoroborate (8 mg, 29 μmol) were dissolved in 2 ml of acetonitrile and iodobenzene (54 μL, 0.49 mmol) added. The suspension was then stirred at room temperature for one hour and then for one hour at 85 °C. The reaction was then quenched with water and extracted three times with dichloromethane, the combined organic extracts were combined and dried over magnesium sulphate. The volitiles were removed under reduced pressure and the products purified on silica gel to give 4-phenylpyridazine (27 mg, 72%) as a colourless solid. This compound showed satisfactory spectroscopic data.[2]

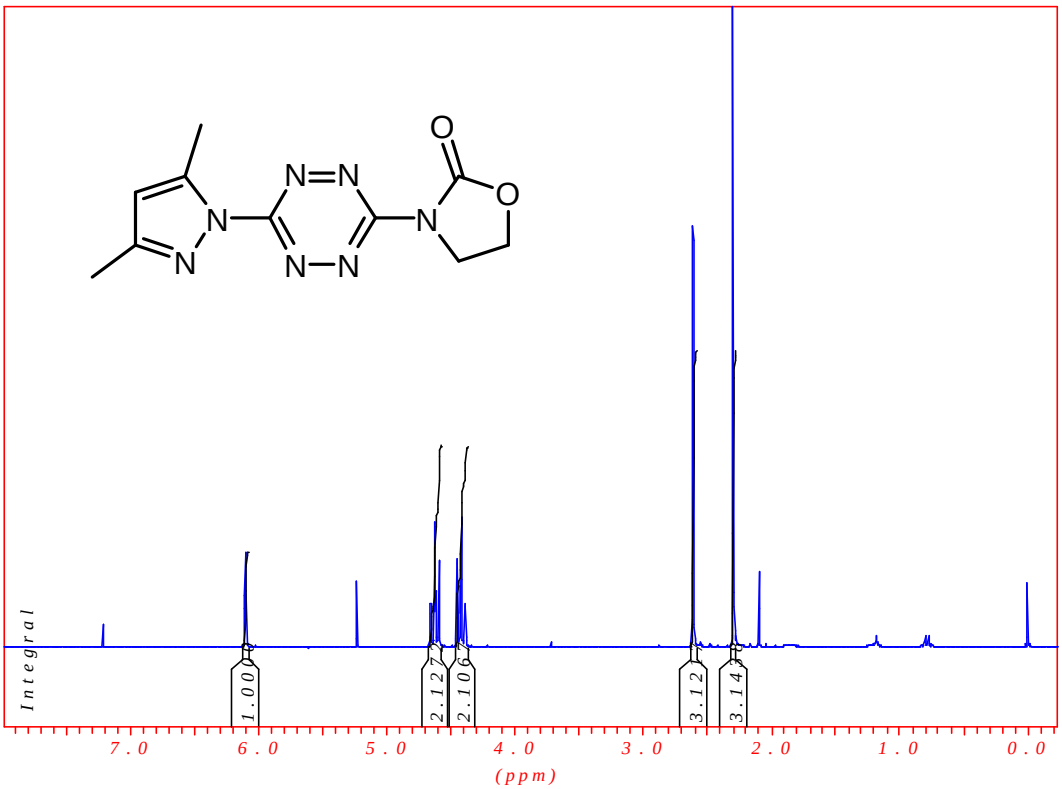
[2] Compared to that reported by Boger, D. L.; Coleman, R. S.; Panek, J. S.; Yohannes, D. *J. Org. Chem.* **1984**, *49*, 4405.

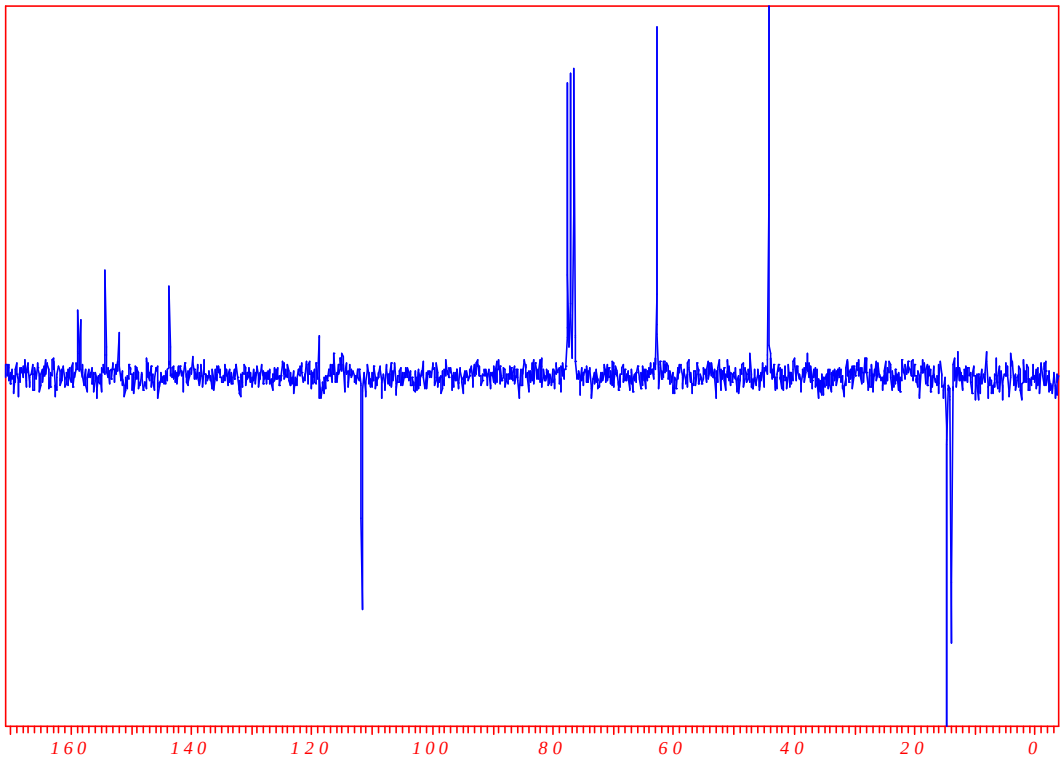
Oxidation of 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine to give 29



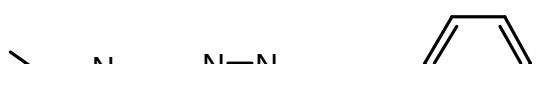
To a refluxing solution of 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine (200 mg, 0.43mmol) in isopropanol was added a solution of sodium carbonate (0.43 mmol, 45 mg) in aqueous hydrogen peroxide (5 ml). After 30 minutes the reaction was allowed to cool to room temperature, quenched with brine and extracted three times with dichloromethane. The combined organic extracts were combined, dried over magnesium sulphate and the volatiles removed in vacuo. The products were then purified on silica gel to give 3,6-bis(3,5-dimethyl-1H-pyrazol-1-yl)-5-phenylpyridazin-4(1H)-one (148 mg, 96%) as yellow solid m.p. 187.0-188.5 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$): δ 1.93 (3H, s, CH_3), 2.17 (3H, s, CH_3), 2.30 (3H, s, CH_3), 2.84 (3H, s, CH_3), 5.79 (1H, s, CH), 6.1 (1H, s, CH), 7.19-7.34 (5H, m, CH). ^{13}C NMR (62.9 MHz, $CDCl_3$): δ 11.2, 13.2, 13.5, 15.6, 106.4, 109.4, 125.9, 128.0, 128.6, 129.5, 129.8, 141.0, 144.4, 145.6, 148.6, 148.9, 149.9, 152.7. FTIR: 2973 (w), 2928 (w), 2854 (w), 1616 (w), 1561 (m), 1527 (s), 1446 (s), 1423 (s), 1370 (m), 1315 (m), 1238 (w), 1183 (w), 1116 (m), 1051 (w), 1018 (w). HMRS calc for $C_{20}H_{21}N_6O$: 361.1777. Found: 361.1769. Anal Calcd for $C_{20}H_{20}N_6O$: C 66.65, H 5.59, N 23.32. Found C 66.45, H 5.24, N 23.09.

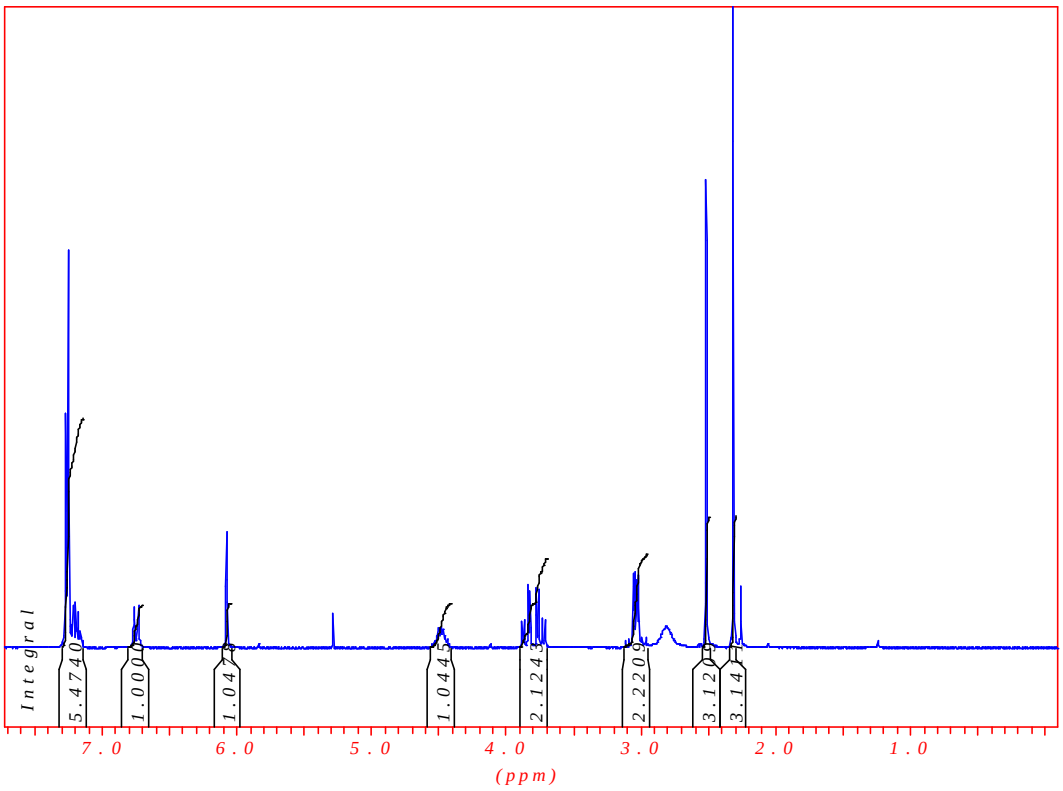
3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one





(S)-2-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-ylamino]-3-phenyl-propan-1-ol




Integral
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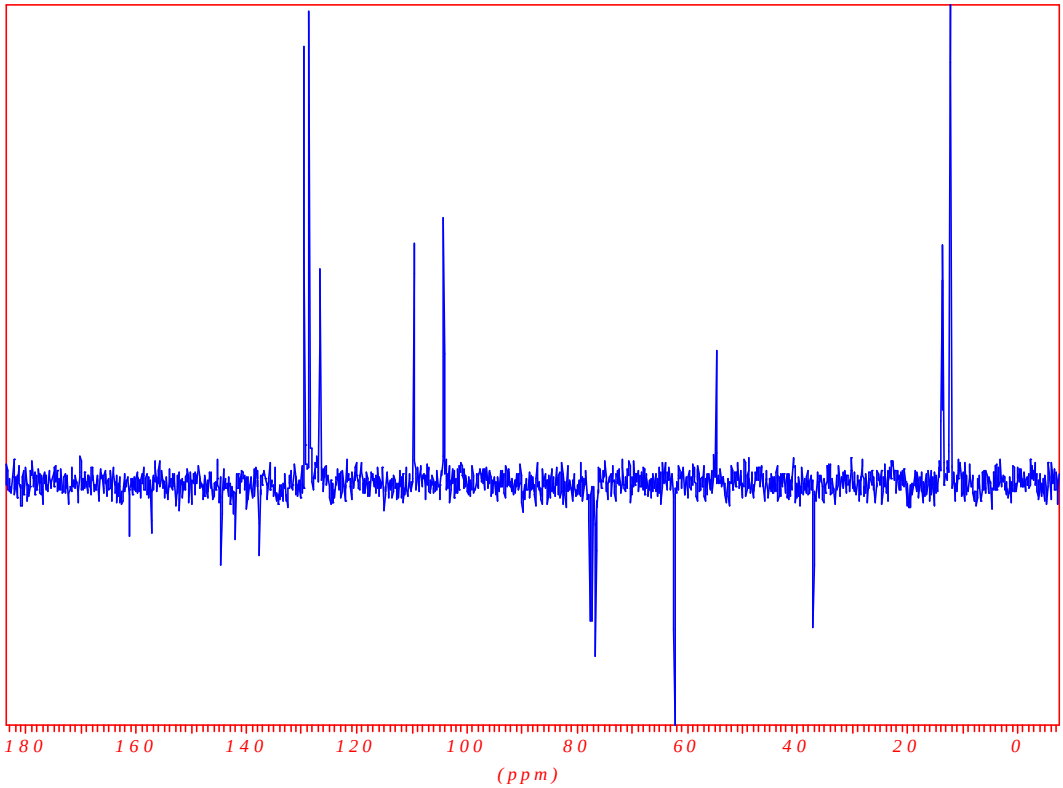
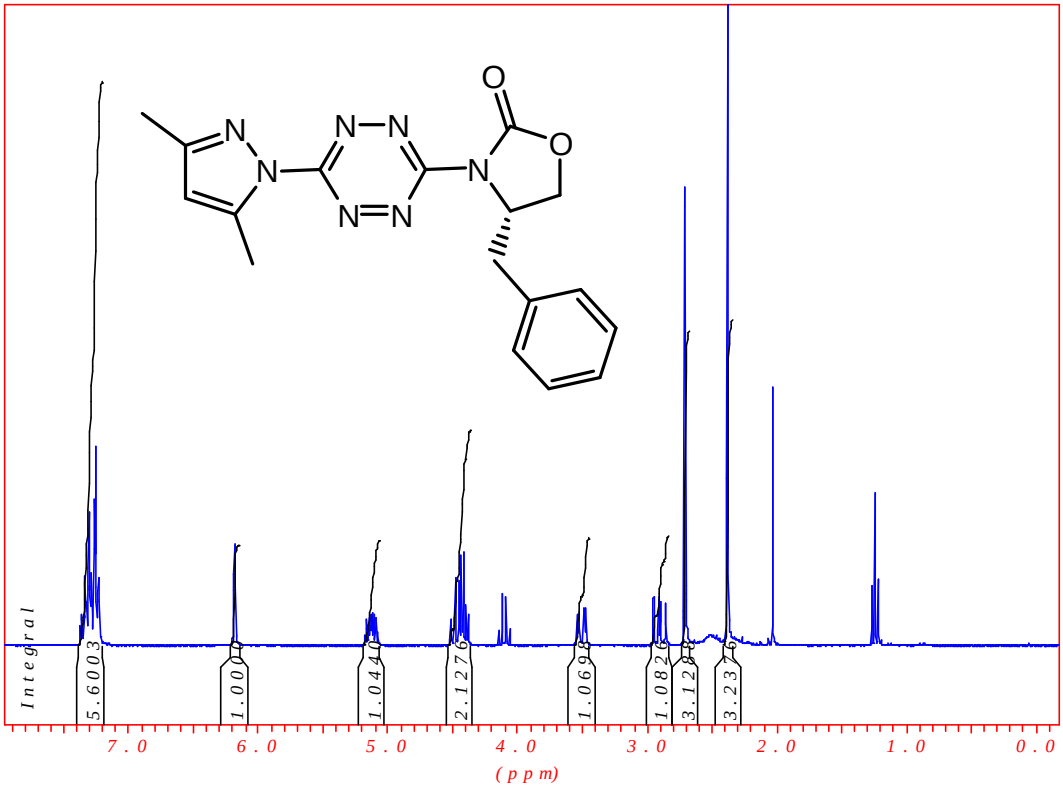
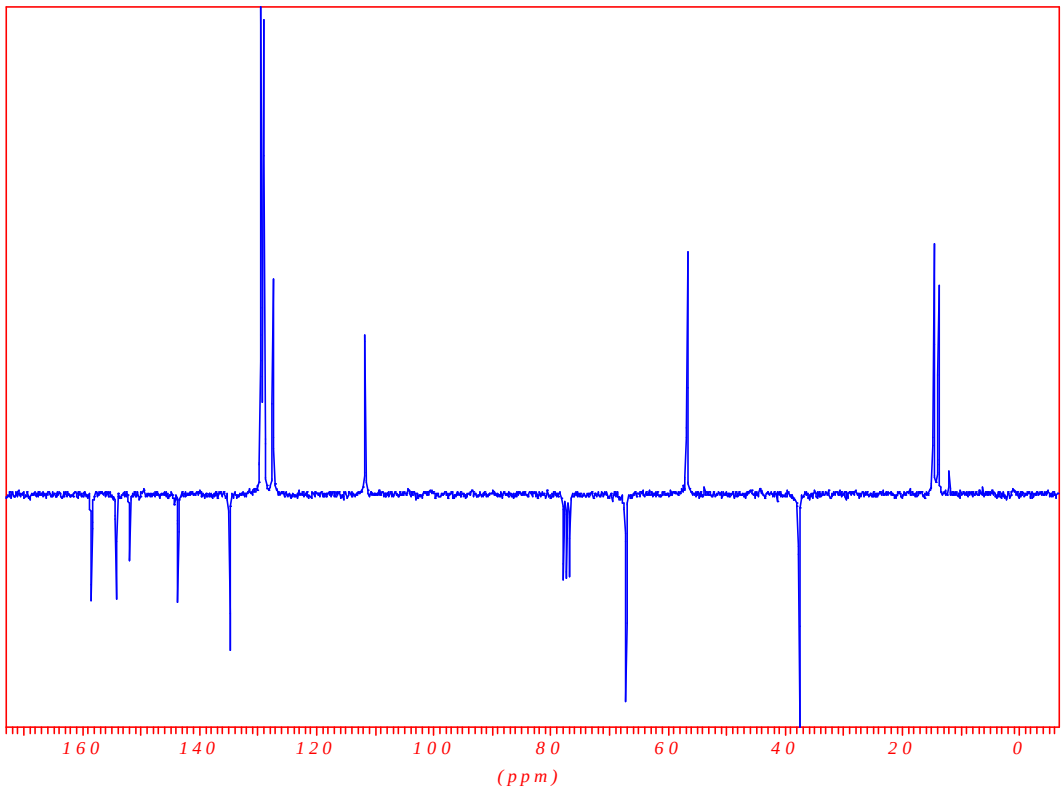
1.000
1.047
1.044
2.1243
2.2209
3.121
3.14
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)

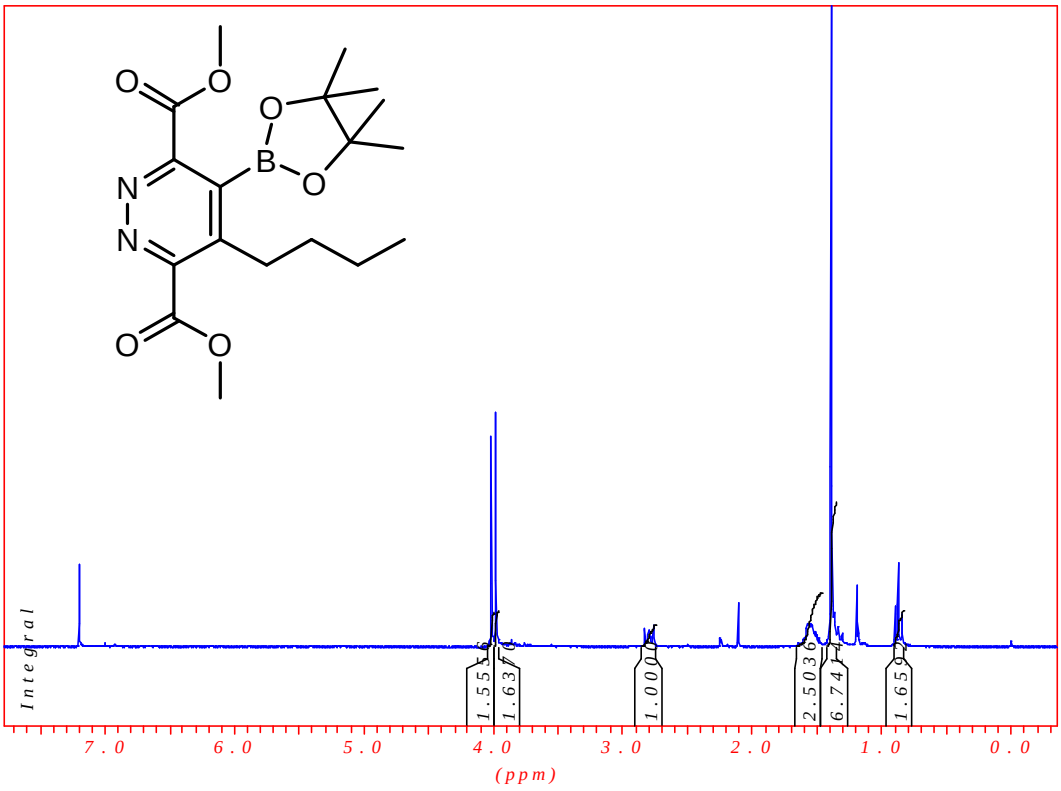

180
160
140
120
100
80
60
40
20
0
(ppm)

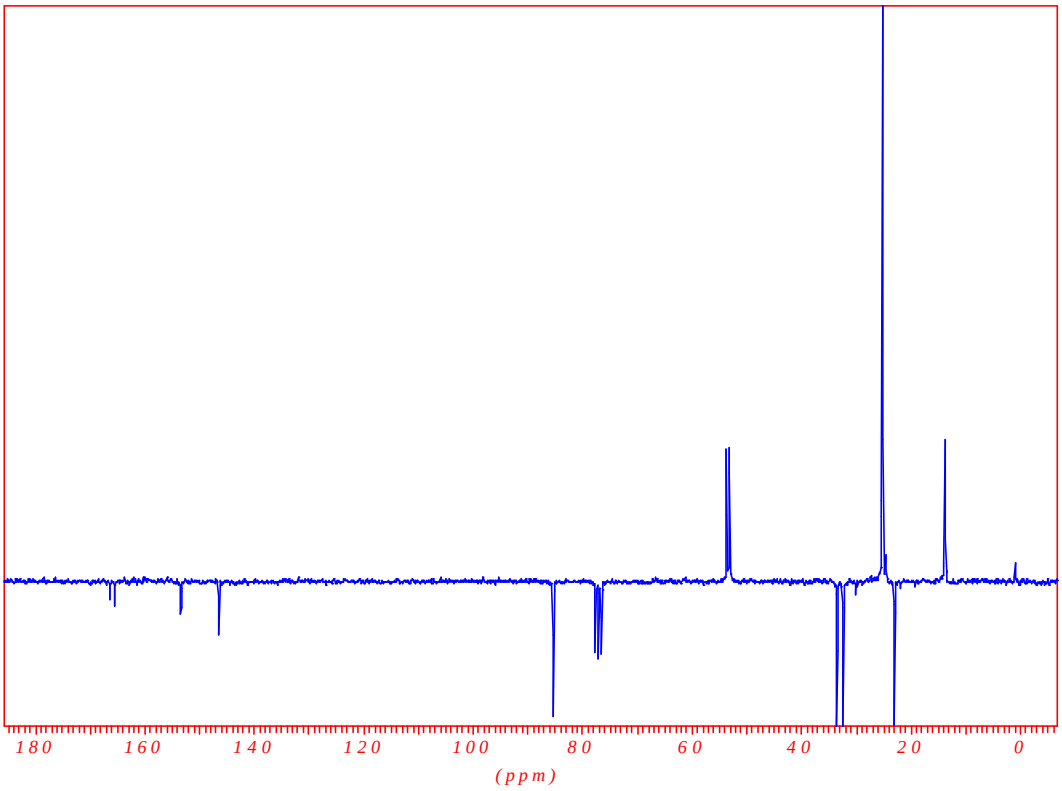
(S)-4-benzyl-3-[6-(3,5-dimethyl-pyrazol-1-yl)-[1,2,4,5]tetrazin-3-yl]-oxazolidin-2-one



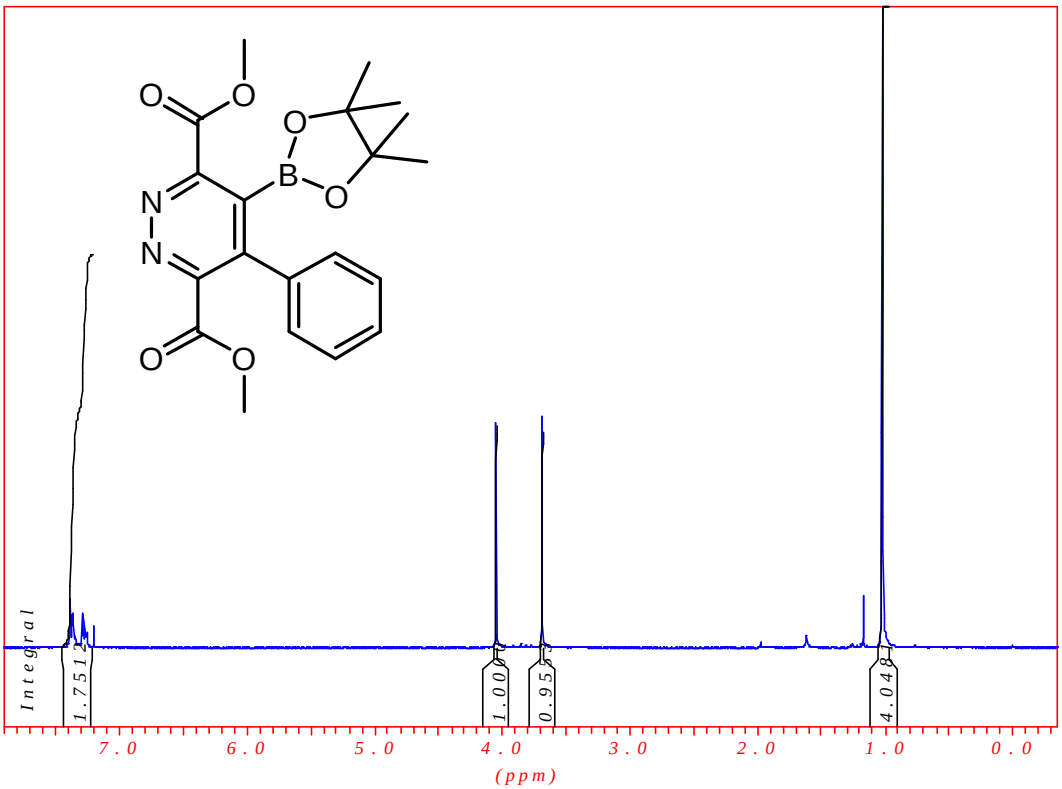


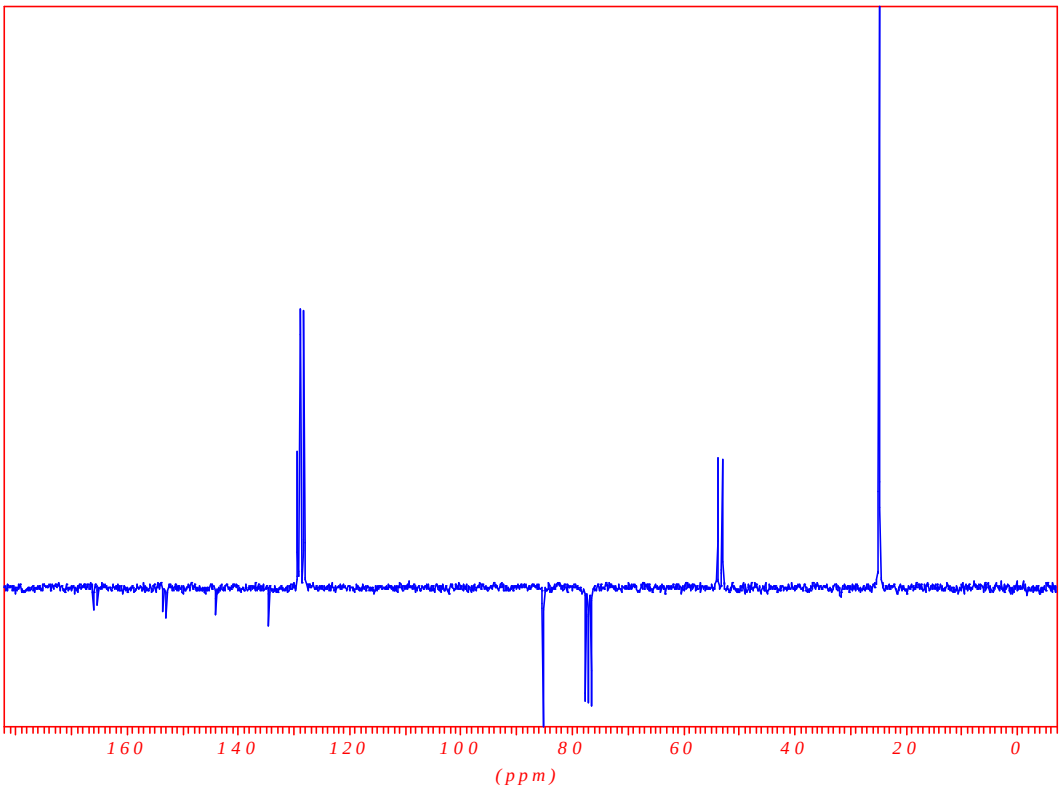
4-butyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester



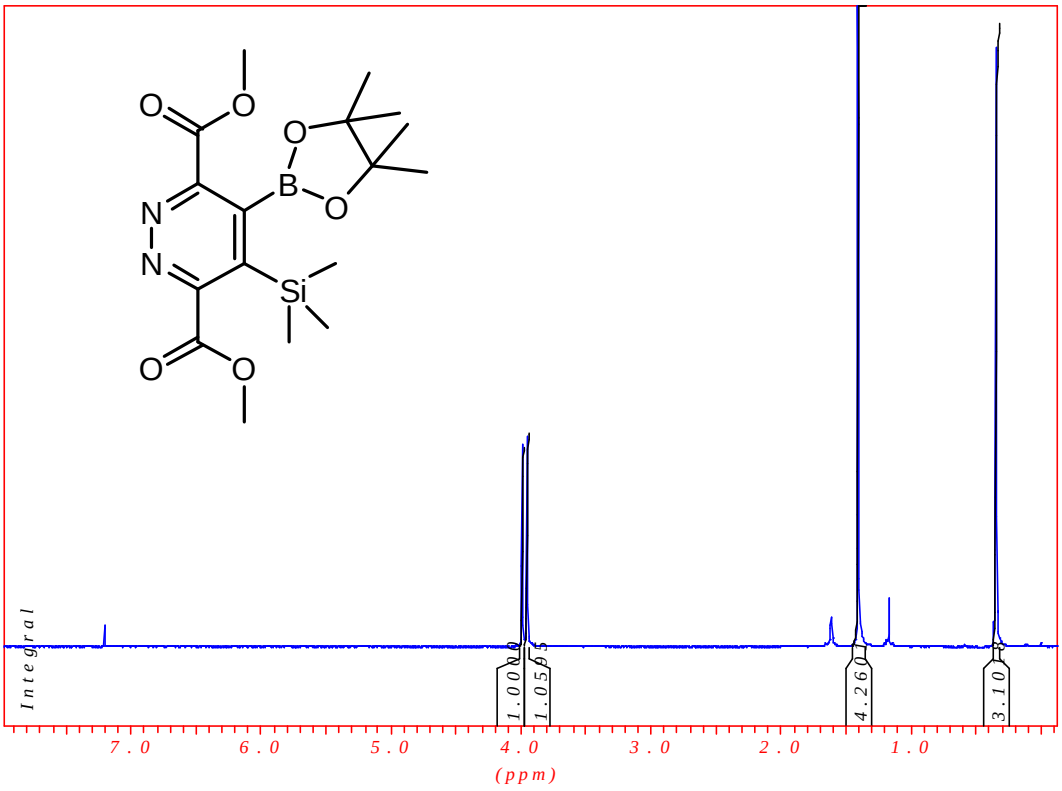


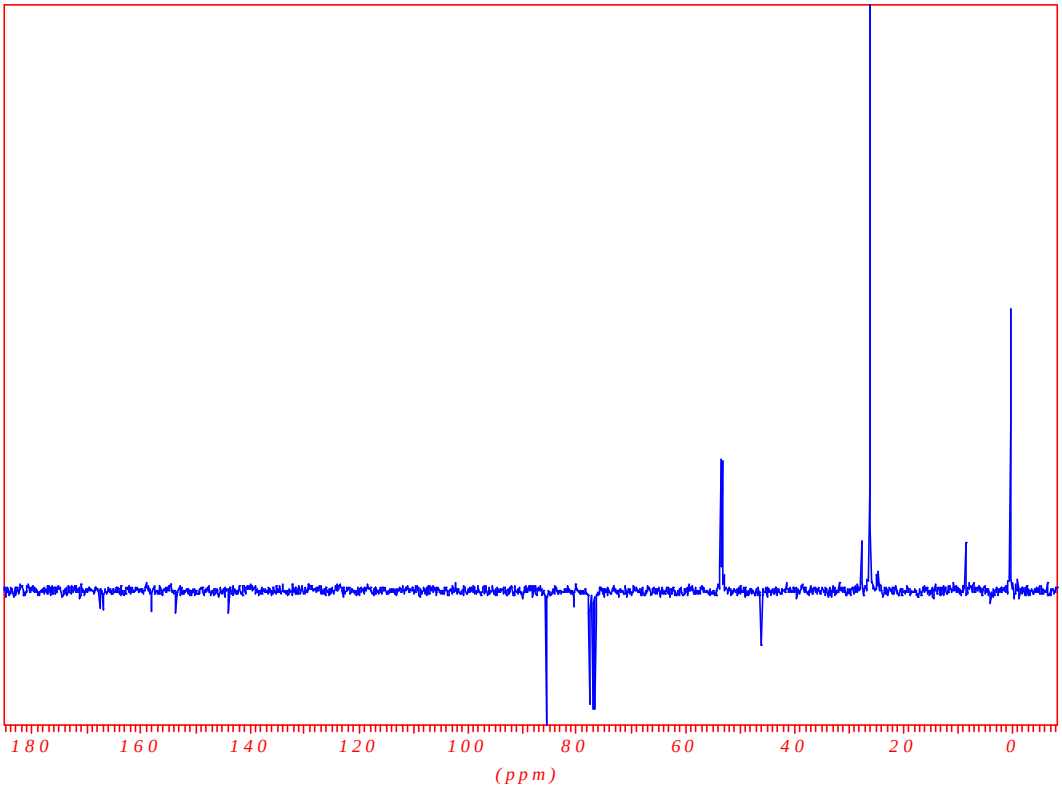
4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester



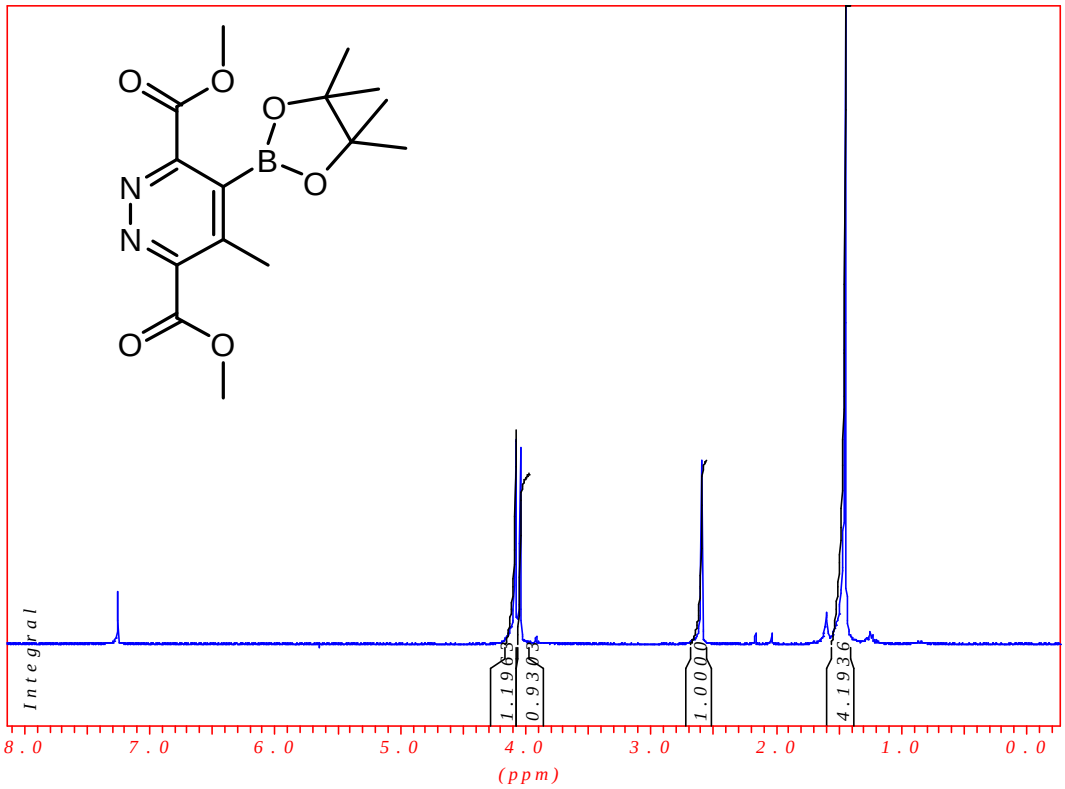


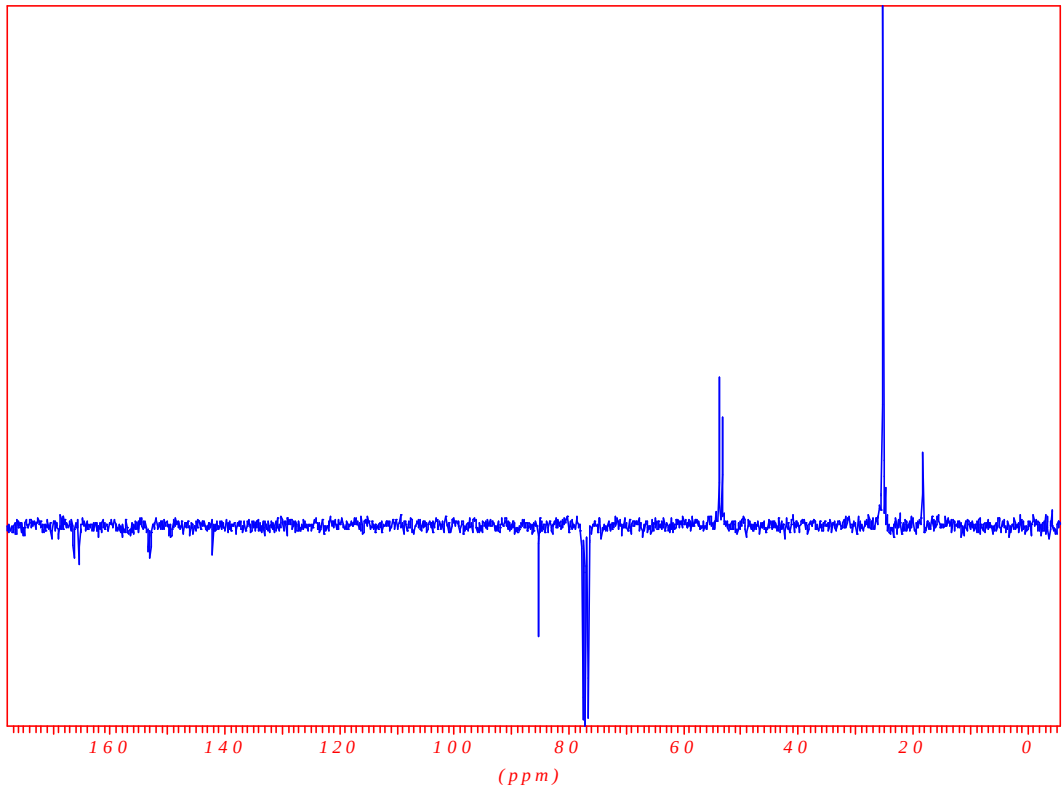
4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-5-trimethylsilanyl-pyridazine-3,6-dicarboxylic acid dimethyl ester



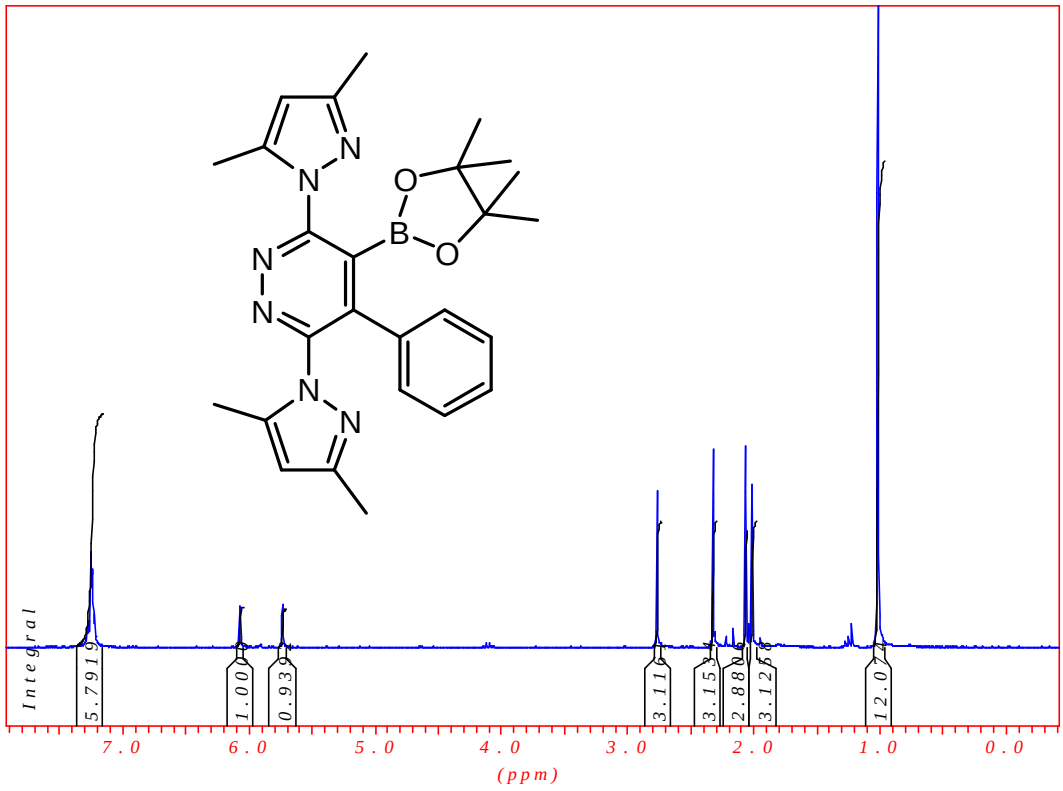


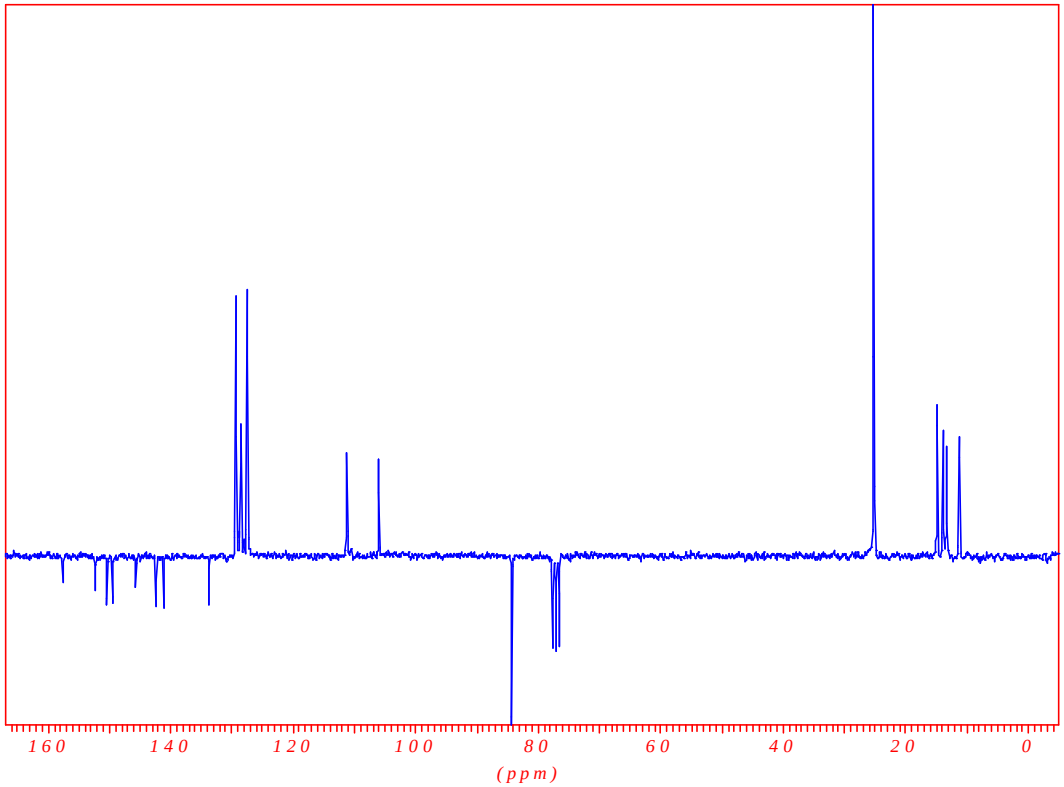
4-methyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine-3,6-dicarboxylic acid dimethyl ester.



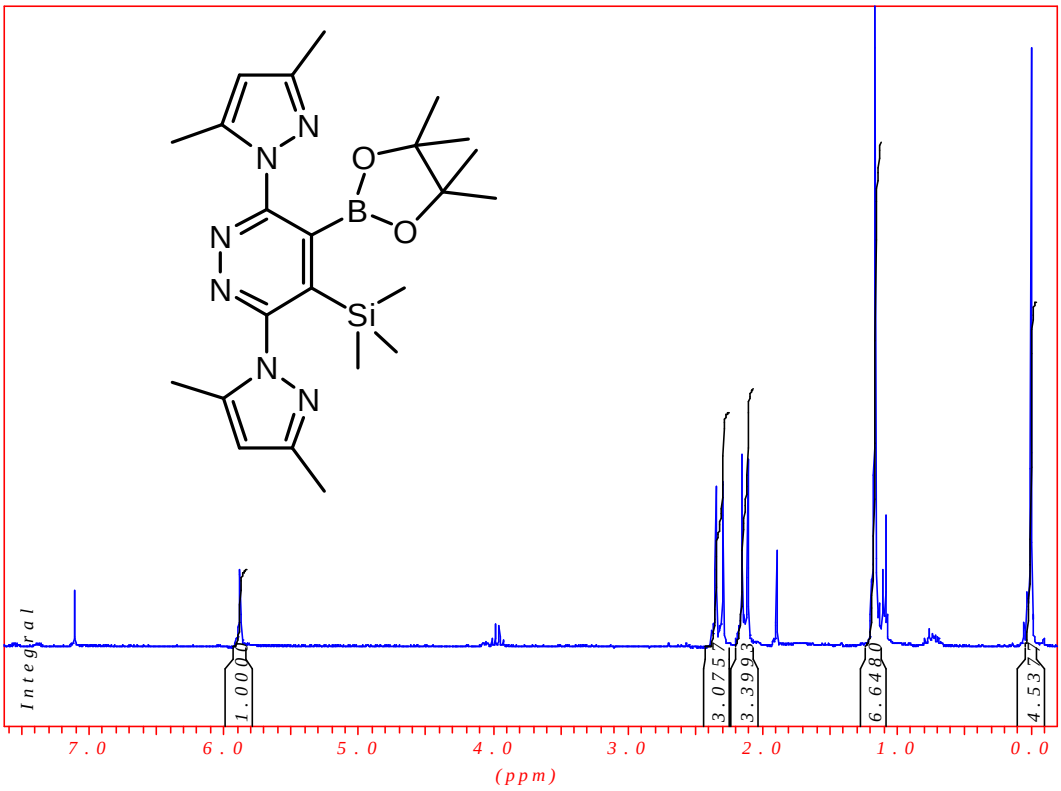


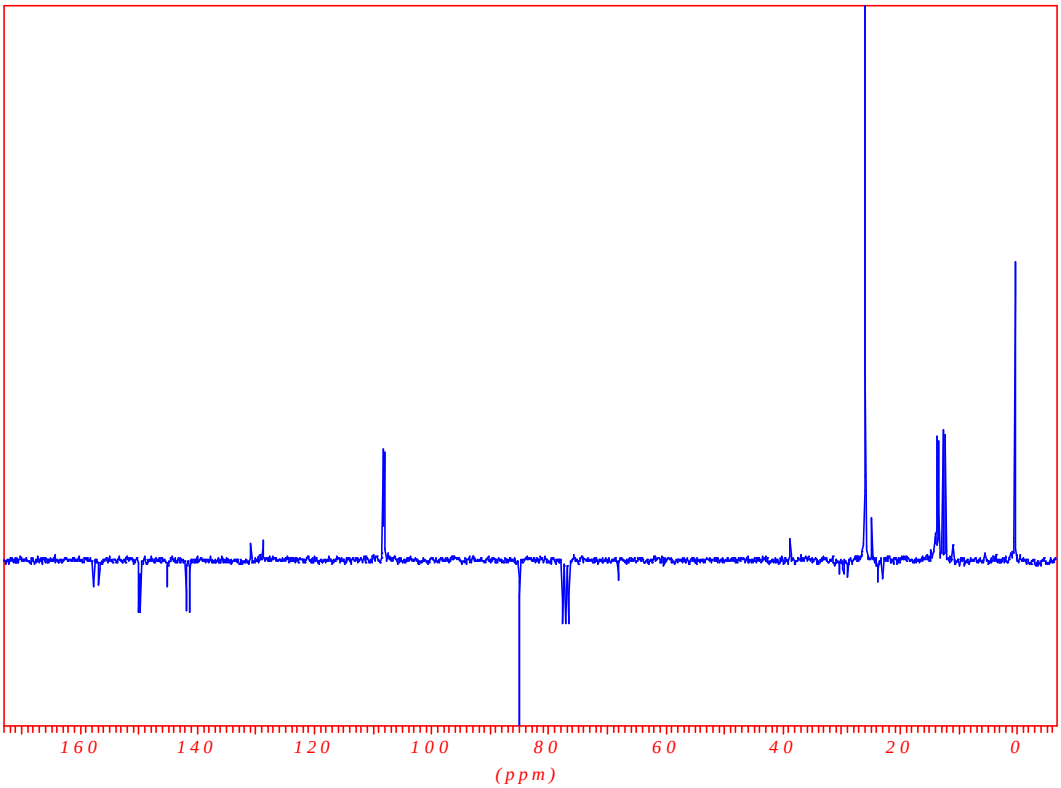
3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine.



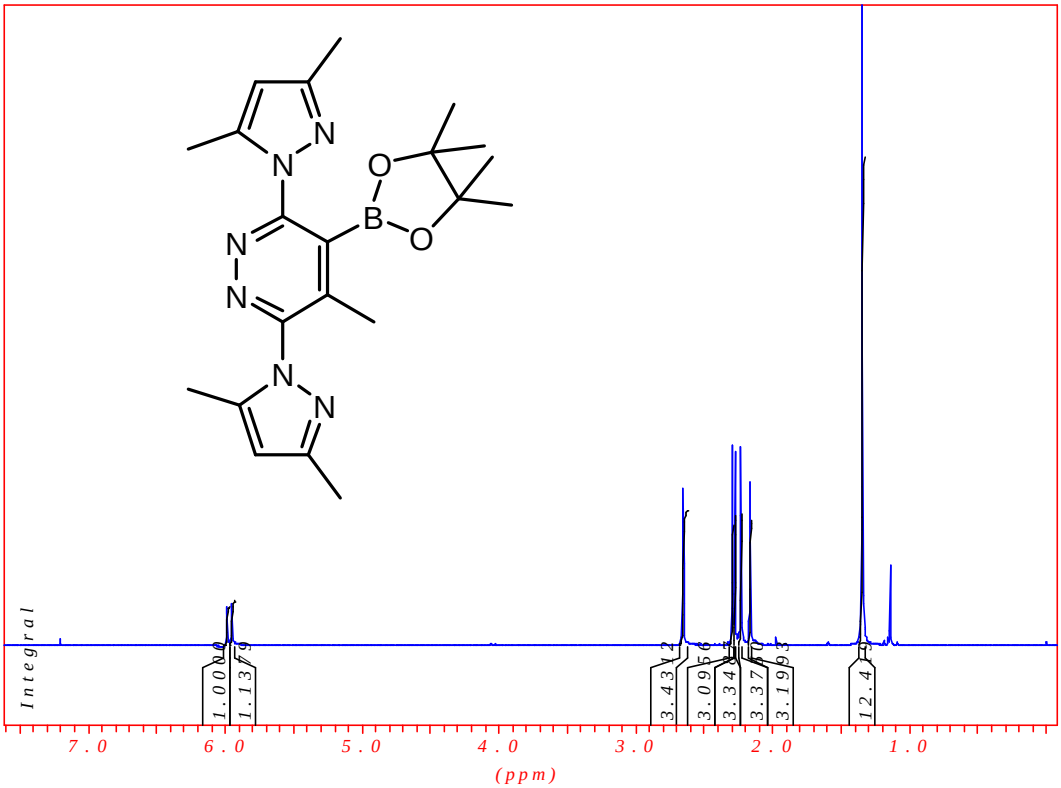


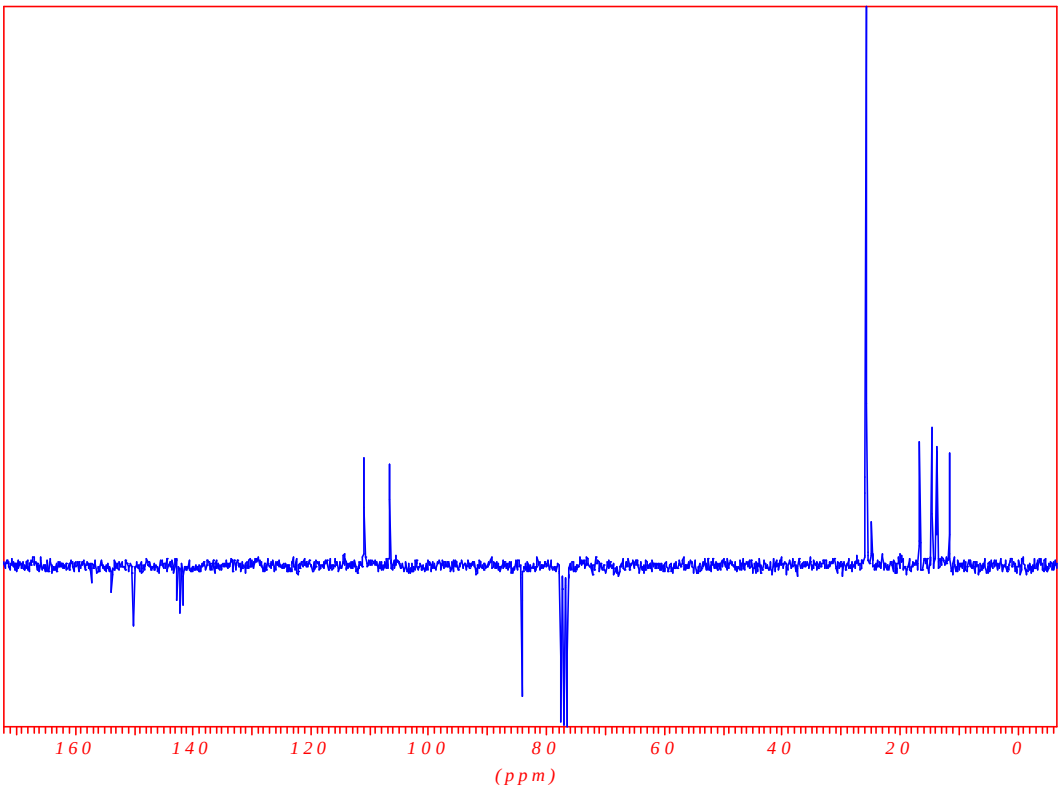
3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-5-trimethylsilanyl-pyridazine.



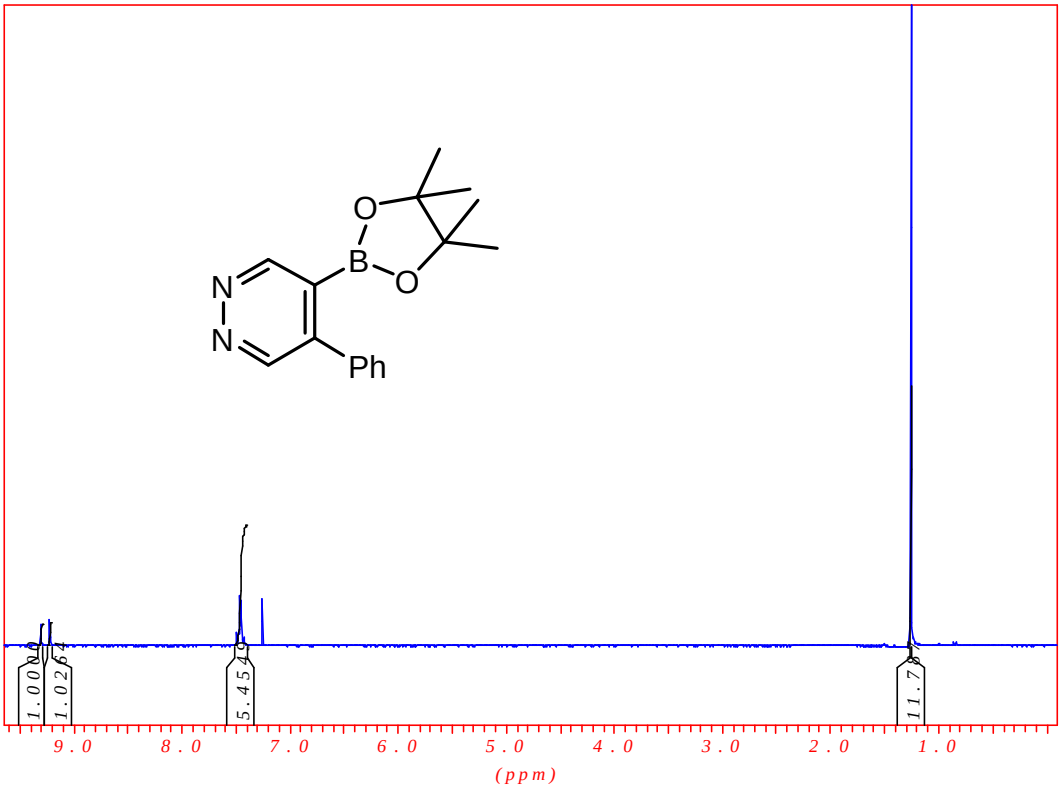


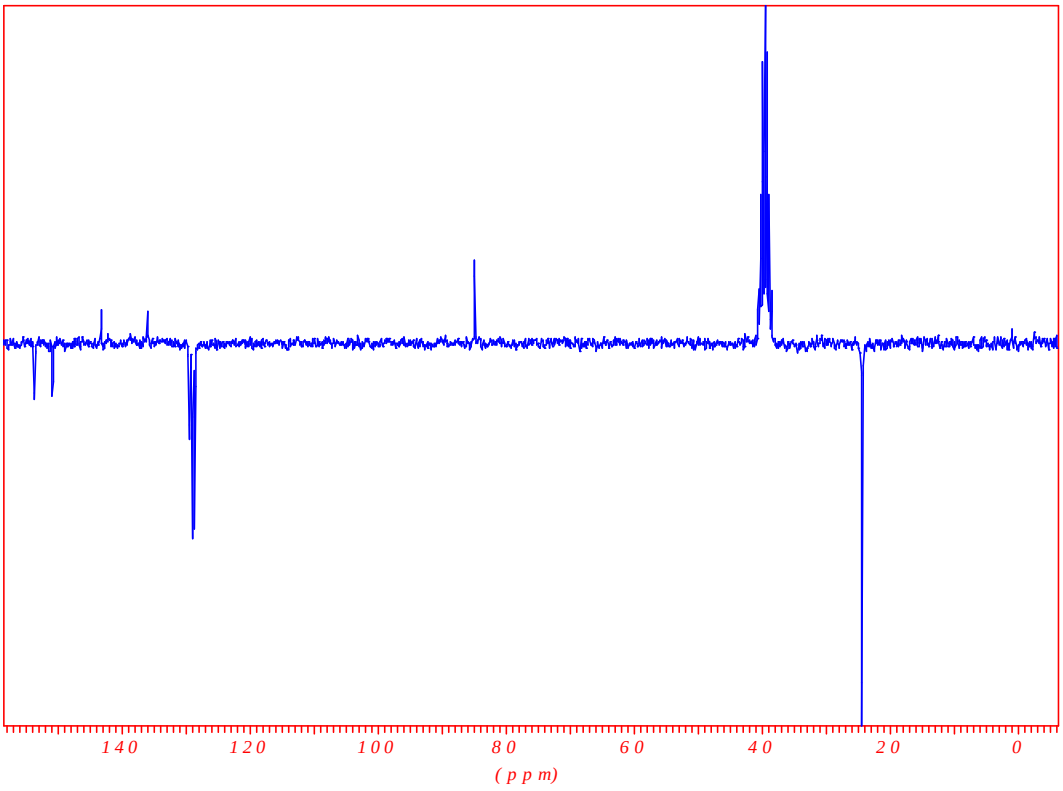
Formation of 3,6-bis-(3,5-dimethyl-pyrazol-1-yl)-4-methyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazine



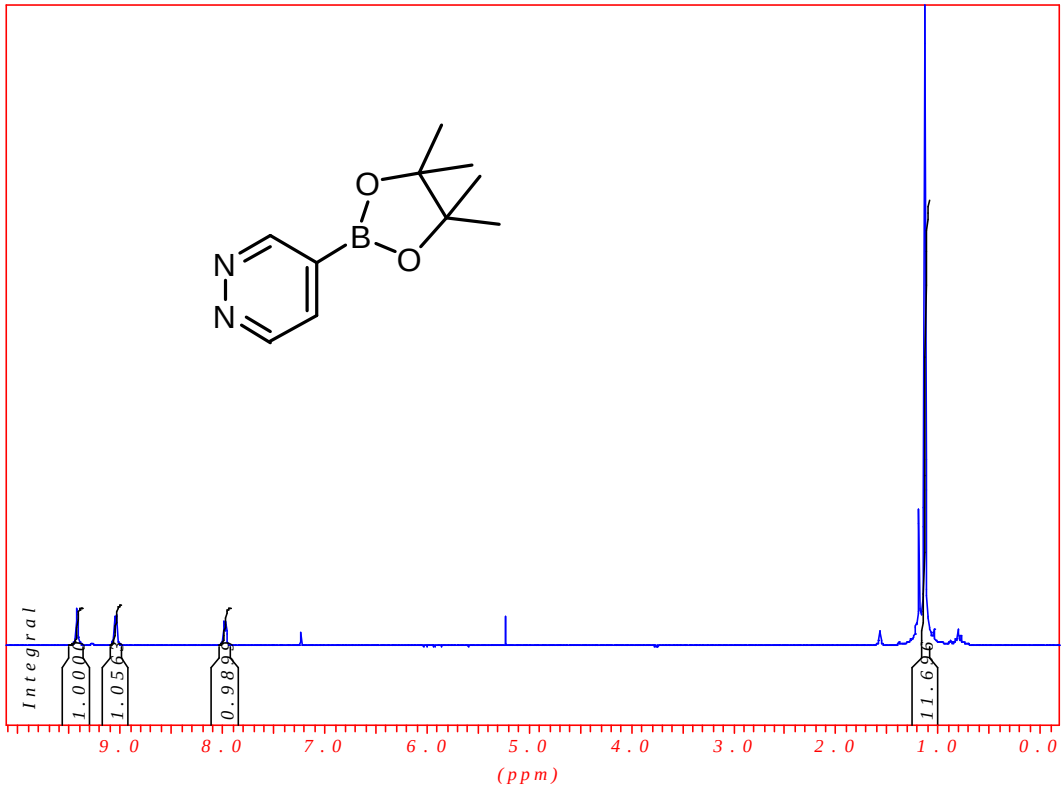


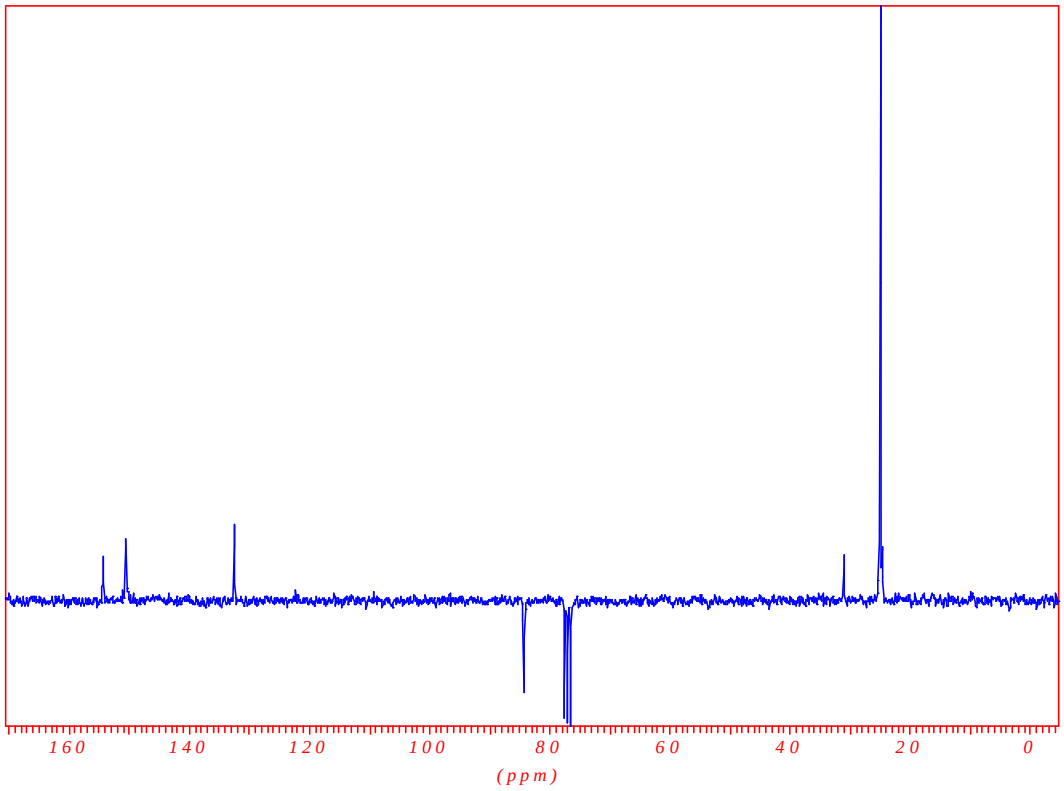
4-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine



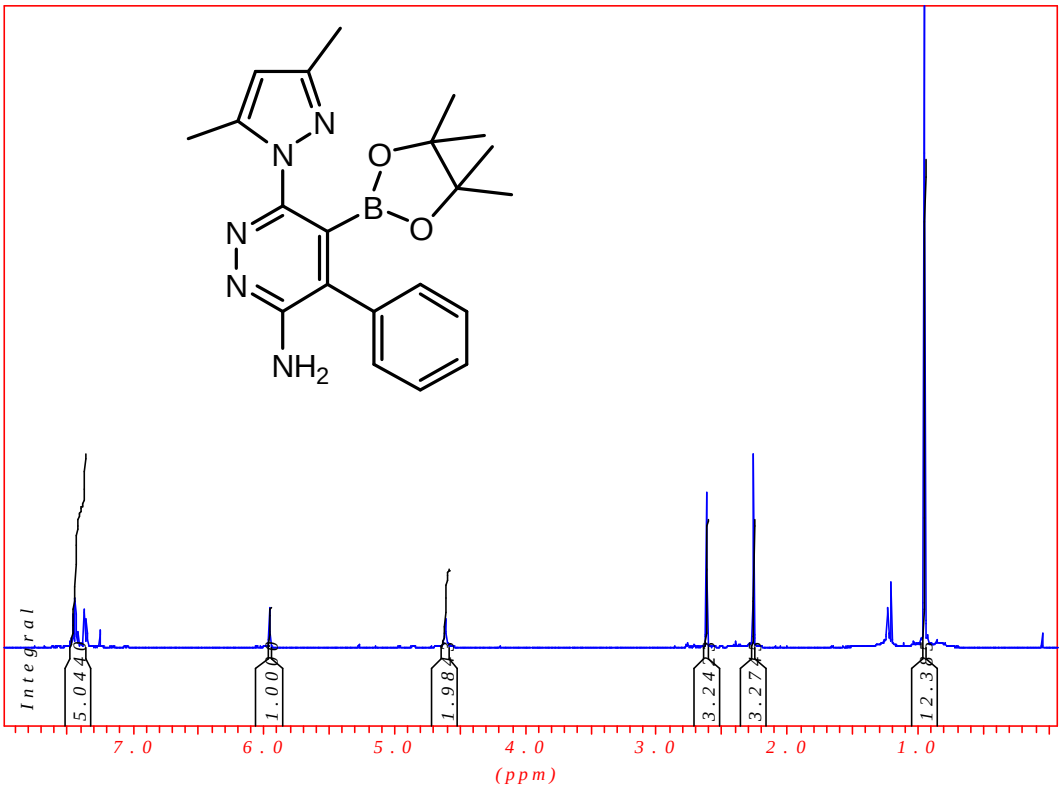


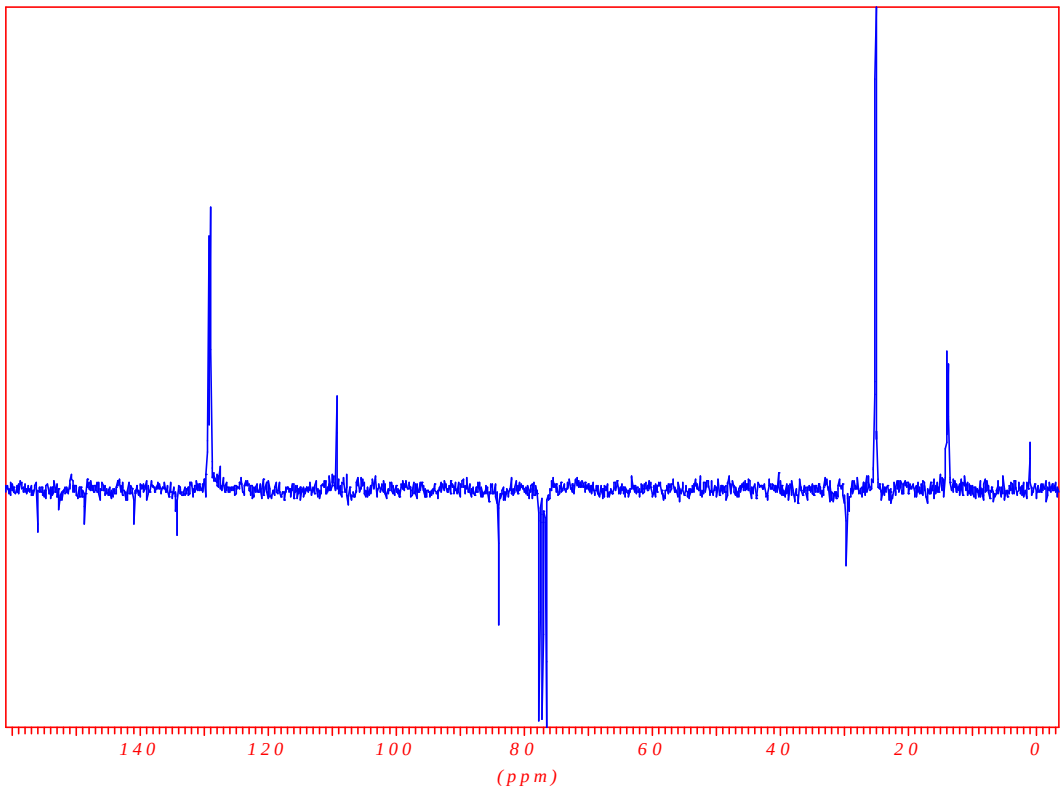
4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine



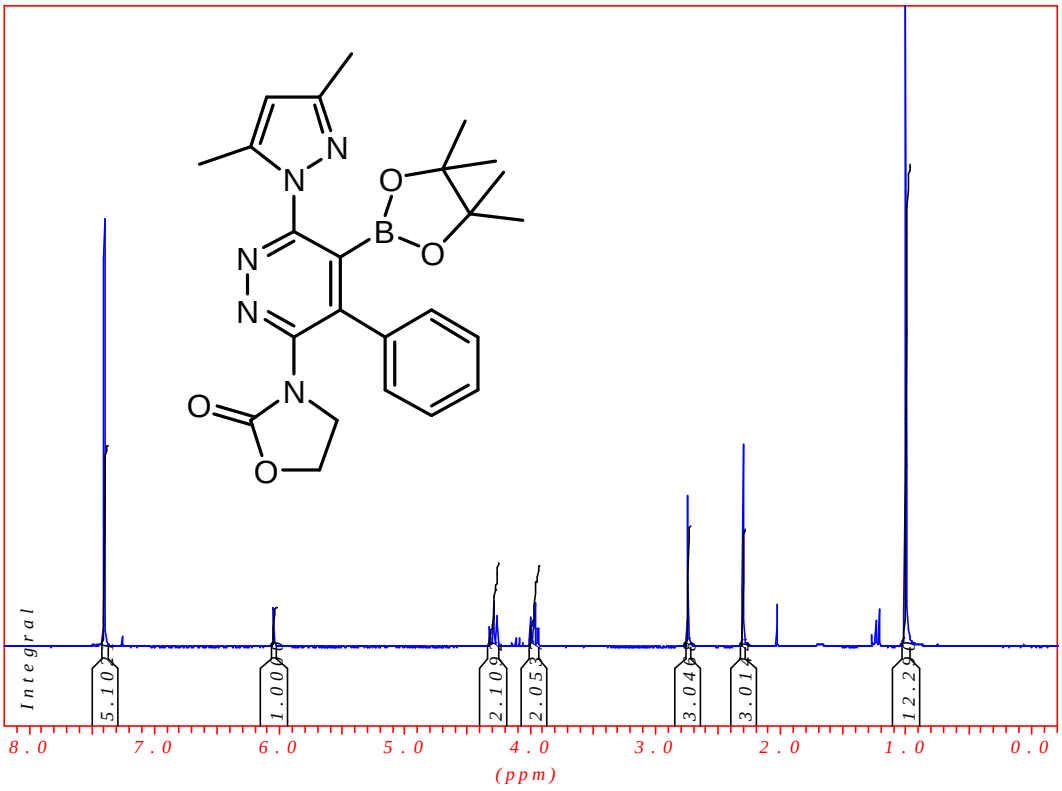


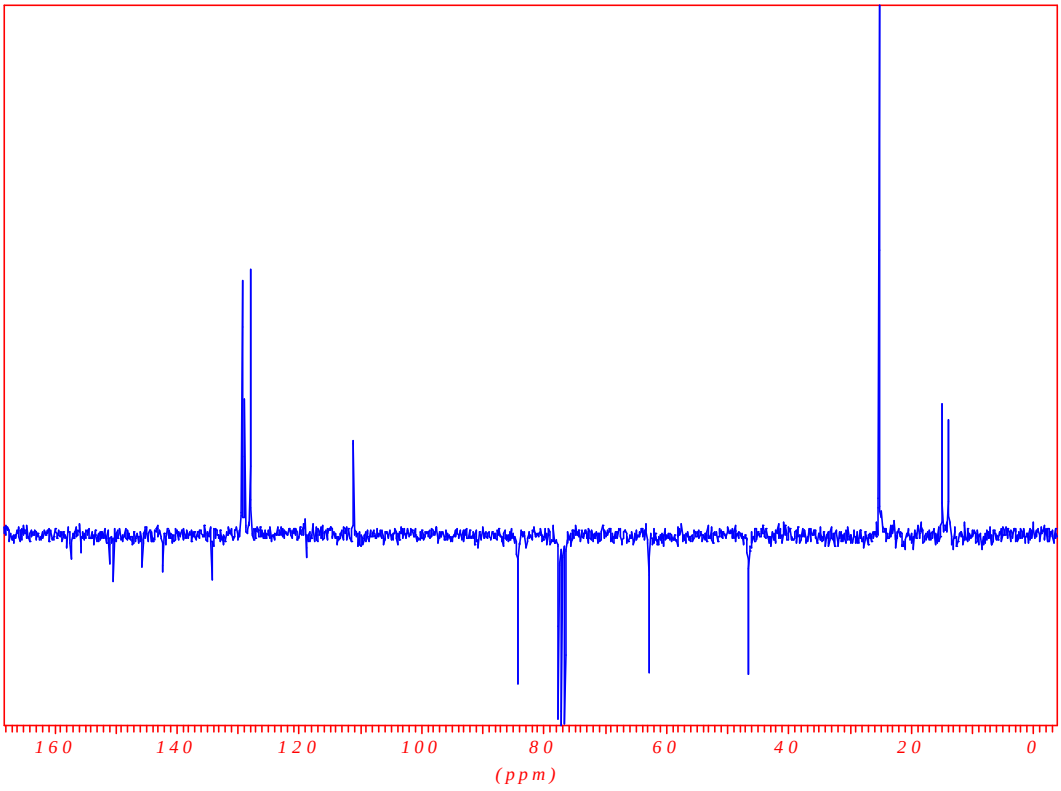
6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-ylamine



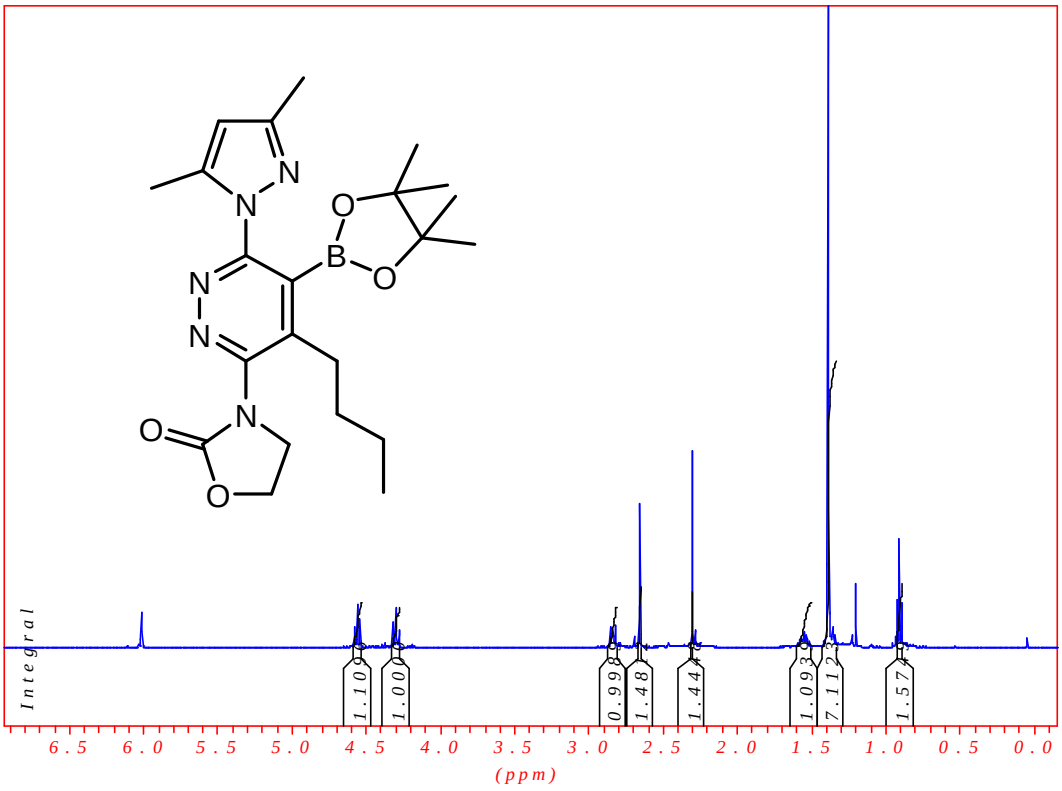


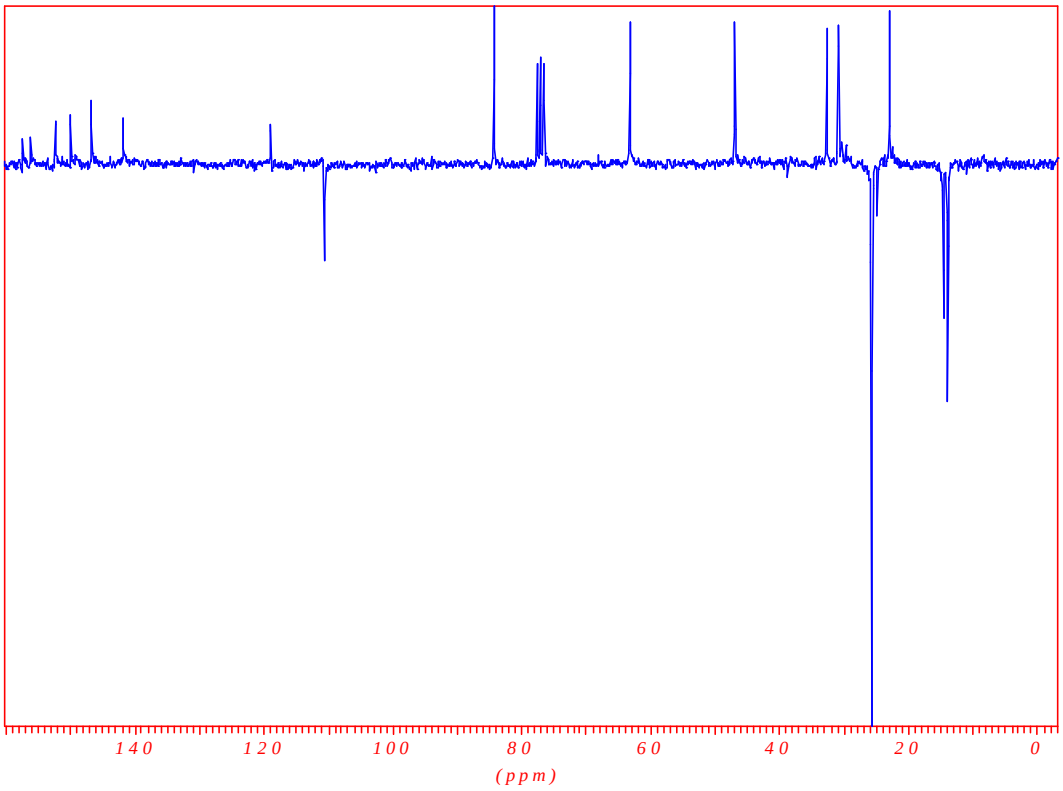
3-[6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one



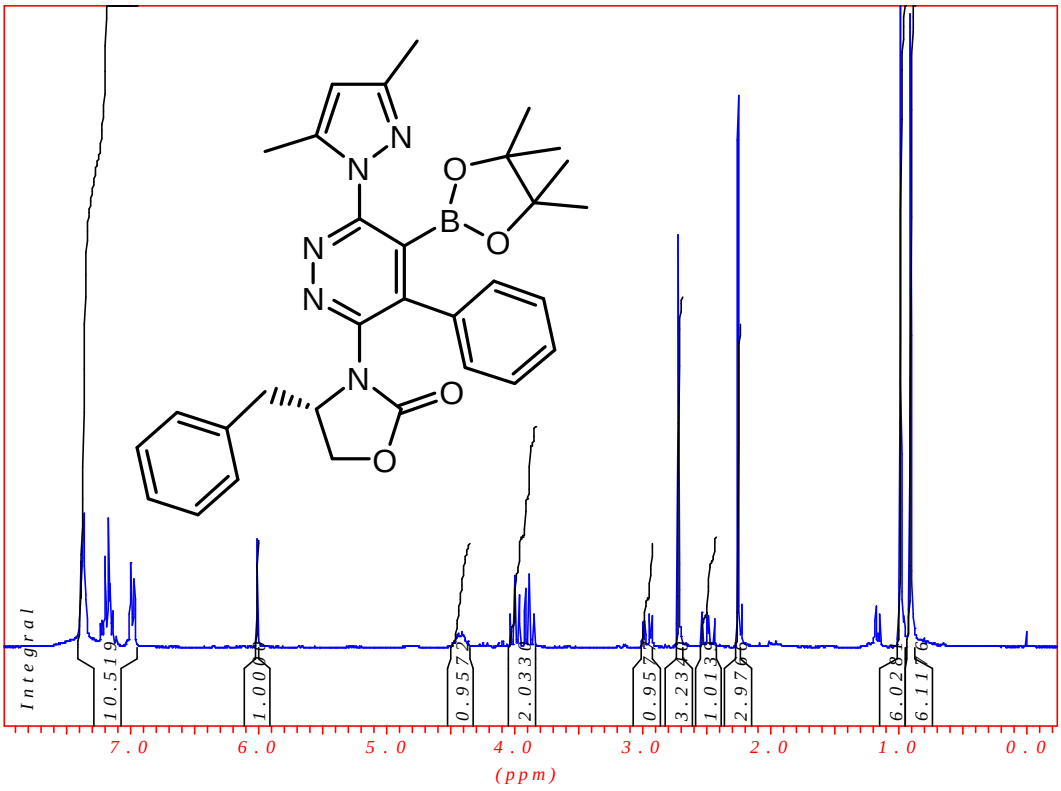


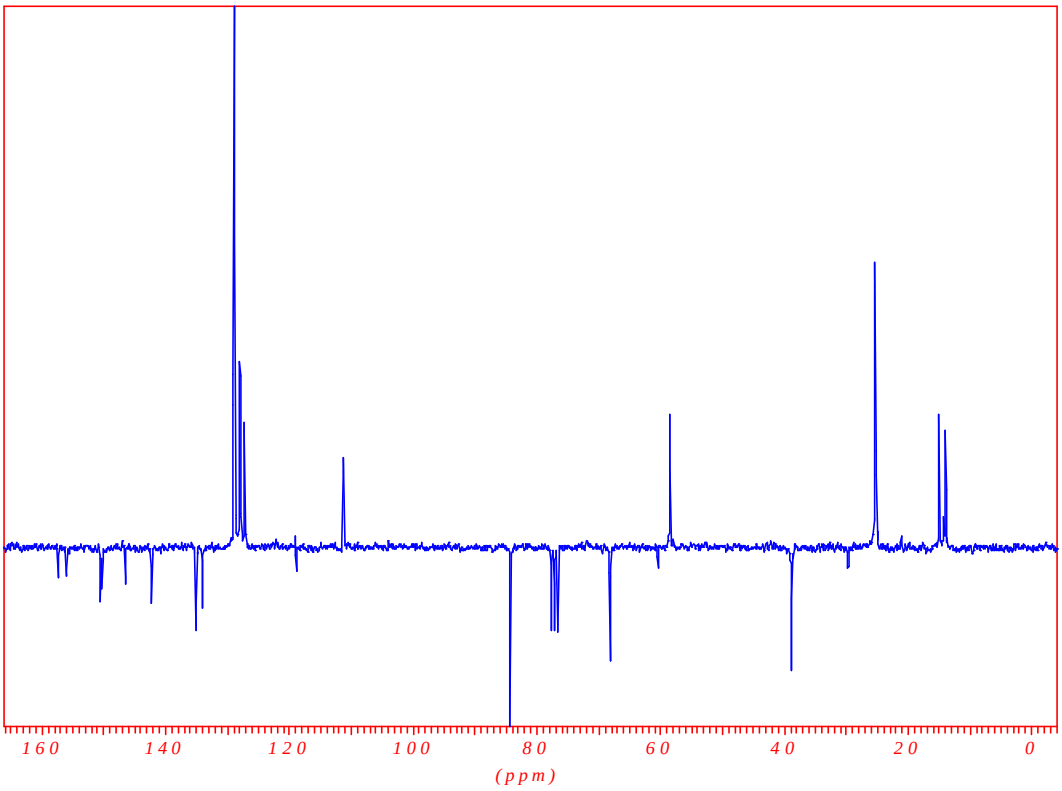
3-[4-Butyl-6-(3,5-dimethyl-pyrazol-1-yl)-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one



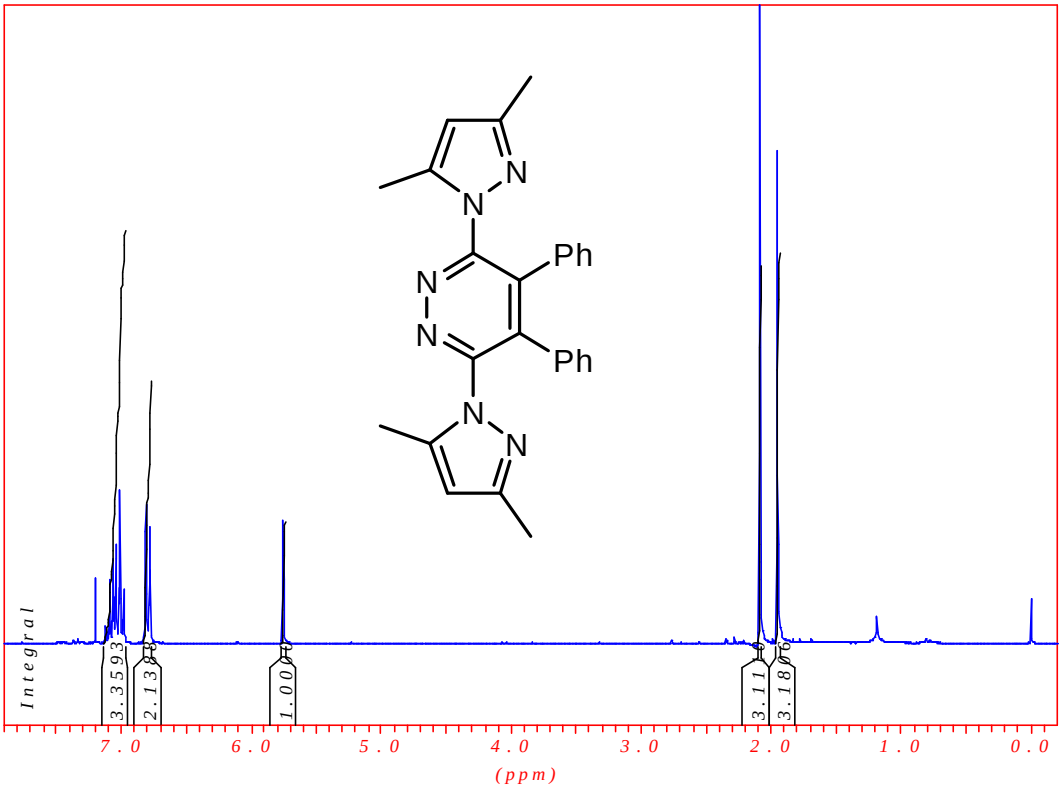


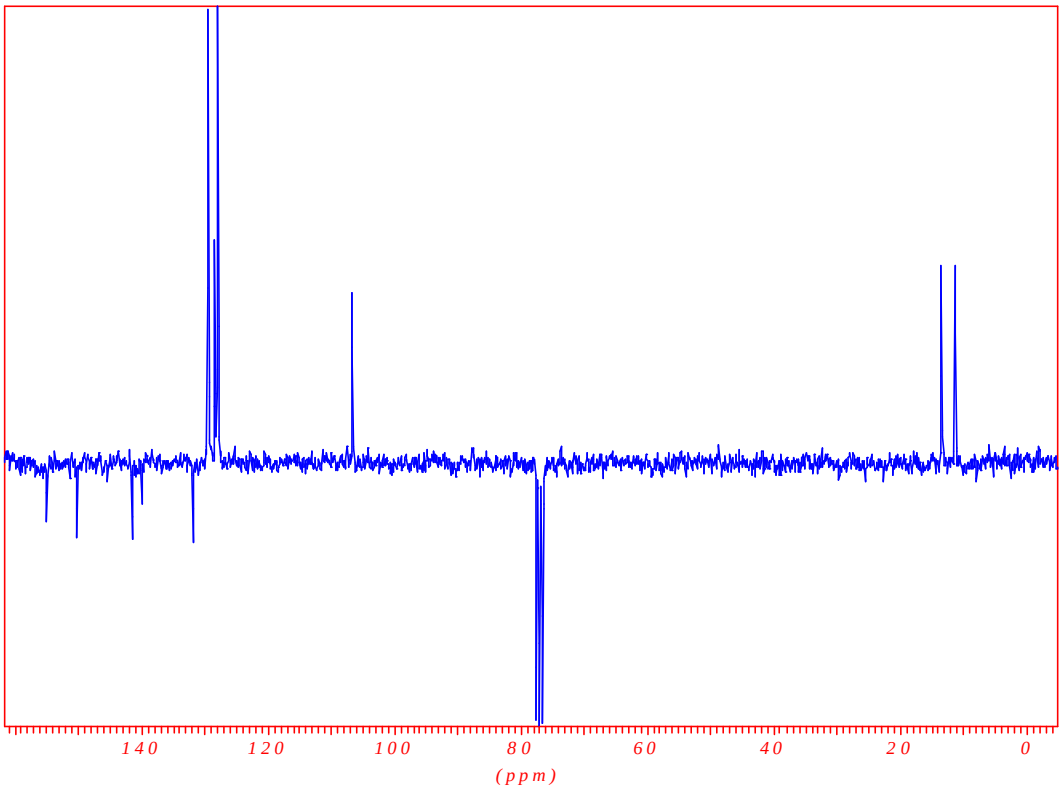
(S)-4-benzyl-3-[6-(3,5-dimethyl-pyrazol-1-yl)-4-phenyl-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-pyridazin-3-yl]-oxazolidin-2-one

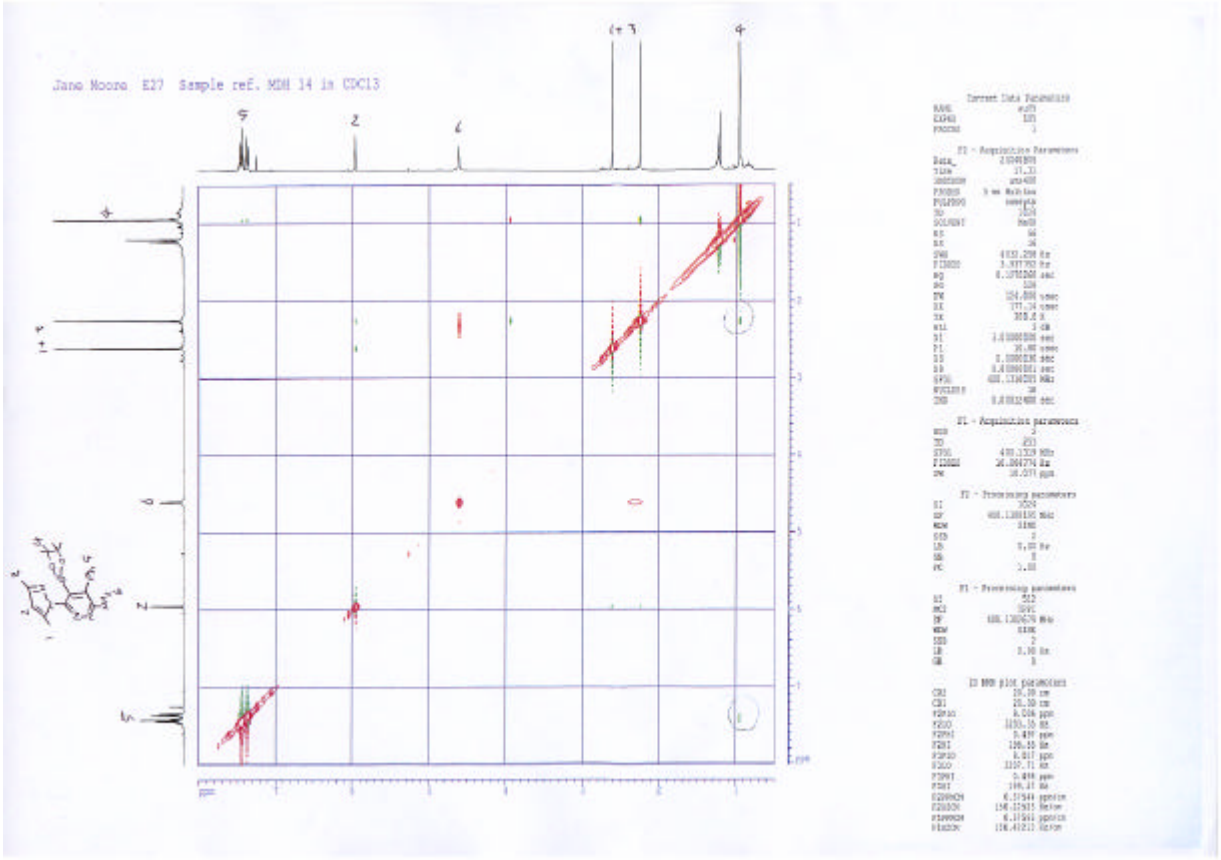


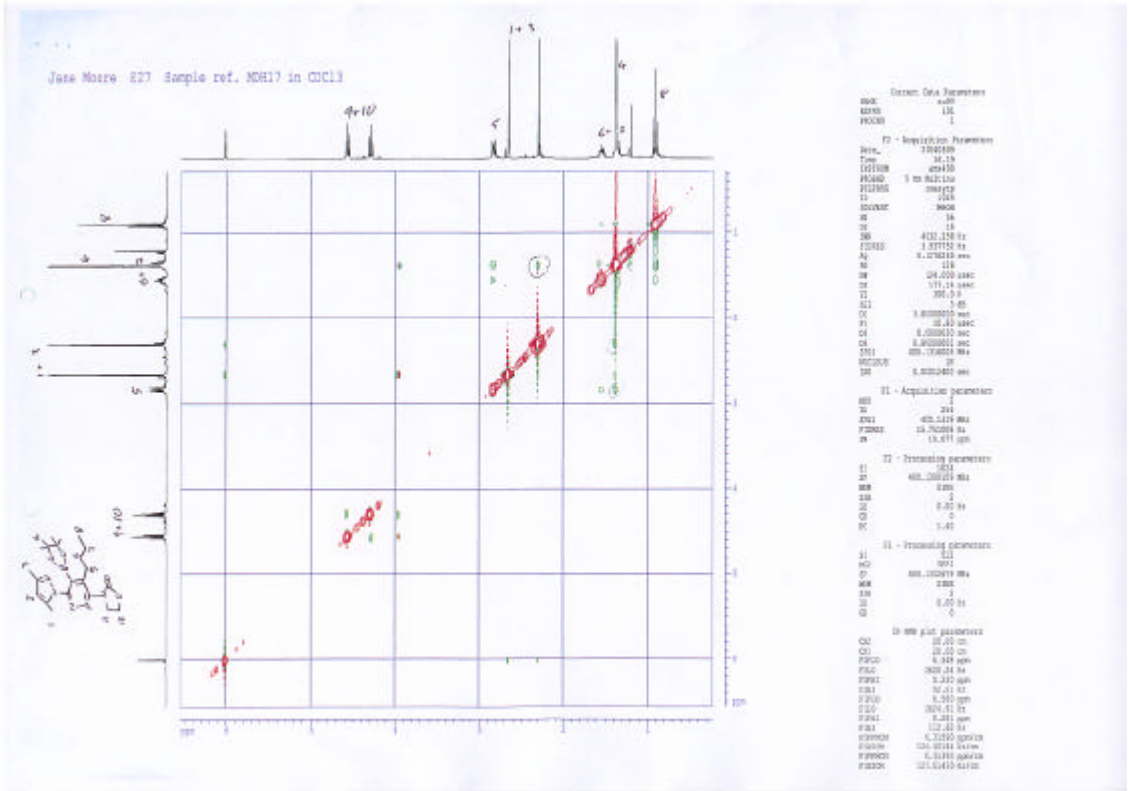


3,6-bis(3,5-dimethyl-1H-pyrazol-1-yl)-4,5-diphenylpyridazine






Jane Moore E27 Sample ref. MDH 14 in CDCl3


Jane Moore E27 Sample ref. MDH17 in CDCl3

Difference spectra plotted with a Y-gain of 16