Supporting Information

A New One-Pot Synthesis of pyrido[2,3-*b*][1,4]oxazin-2-ones

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General Comments. Melting points were determined with a capillary apparatus and uncorrected. ^1H and ^{13}C NMR spectra were recorded on a 300 MHz spectrometer with chemical shift values reported in units (ppm) relative to an internal standard (TMS). IR spectra were obtained on an IR spectrophotometer. Elemental analyses were performed with a Perkin Elmer 240C. X-Ray analysis was carried out on a imaging Plate diffractometer with graphite monochromated Mo-K α radiation. Open-bed UV-chromatography (using quartz tube, made in korea) was carried out on silica gel F254 (70 ~ 230 mesh, Merck) using gravity flow. The column was packed as slurries with the elution solvent. Mass spectra (MS) were obtained using electrospray ionization.

General Procedure for the Synthesis of *N*-substituted acetamide (1a-1r**):**

To a solution of organic amine (6.11 g, 50.42mmol) and K_2CO_3 (8.0g, 57.98mmol) in dichloromethane (100mL) was slowly added 2-chloroacetylchloride (or 2-chloropropionamide) (6.26g, 55.46mmol) for 30min at room temperature. After 30min, the mixture was refluxed for 4hrs and then stirred for additional 30 min at room temperature. The reaction mixture was poured into cold water (200mL) and extracted with dichloromethane (2 x 100mL). The combined organic extracts were washed water and dried over MgSO_4 . The solution was concentrated under reduced pressure and the residue was purified by column chromatography on silica gel using EtOAc /*n*-hexane (1:1, v/v) as eluent to afford **1a-1r** as white solid.

Method A: General procedure for the Synthesis of 1-Substituted-1*H*-Pyrido[2,3-*b*]-1,4-oxazin-2-ones (4a-4r) via one step.

To a 100mL flask equipped with a magnetic stirrer was added *N*-substituted-2-chloroacetamide **1** (11.5mmol), 2-halo-3-pyridinol **2** (11.5mmol), Cs₂CO₃ (24.2mmol) and acetonitrile (50mL). The mixture was heated to reflux with vigorous stirring for 3 hours, monitored by TLC. The solvent was removed under reduced pressure, and CH₂Cl₂/H₂O was added to the residue. After separating the organic layer, the product was extracted with CH₂Cl₂ from the resulting aqueous layer. The combined methylene chloride solution was dried over anhydrous MgSO₄ and evaporated in vacuo. The crude products were purified by flash column chromatography using EtOAc/*n*-hexane (1:2, v/v) as eluent. Fractions containing the product were combined and the solvent was evaporated under reduced pressure to afford **4a-4r**. The result products were recrystallized from suitable solvent to give analytically pure **4a-4r**.

Method B: General Procedure for the Synthesis of Pyrido[2,3-*b*][1,4]oxazin-2-ones via two step.

Step 1: Synthesis of *N*-substituted 2-(2-halopyridin-3-yloxy)acetamides (3a-3r)

To a 100mL flask equipped with a magnetic stirrer was added *N*-substituted 2-chloroacetamides **1** (11.5mmol), 2-halo-3-pyridinols **2** (11.5mmol), K₂CO₃ (12.1mmol) and acetonitrile (50mL). The mixture was refluxed for 4-6 hours. The solvent was removed under reduced pressure, and CH₂Cl₂/H₂O was added to the residue. After separating the organic layer, aqueous layer was extracted with CH₂Cl₂. The combined organic layer was dried over anhydrous MgSO₄ and evaporated in *vacuo*. The crude products were purified by flash column chromatography using EtOAc/*n*-hexane (1:2, v/v) as eluent. Fractions containing the product were combined and the solvent was evaporated under reduced pressure to give only **3a-3r**. The result products were recrystallized from suitable solvent to give analytically pure **3a-3r**.

Step 2: Synthesis of 1-Substituted-1*H*-Pyrido[2,3-*b*][1,4]oxazin-2-ones (**4a-4r**)

To a 100mL flask equipped with a magnetic stirrer was added **3a-3r** (11.5mmol), Cs₂CO₃ (12.1mmol) and acetonitrile (50mL). The mixture was refluxed for 3 hours. After filtering the mixture, the resulting filtrate was concentrated under reduced pressure. The residue was purified by flash column chromatography using EtOAc/*n*-hexane (1:2, v/v) as eluent. Fractions containing the product were combined and the solvent was evaporated under reduced pressure to afford only **4a-4r**. The result products were recrystallized from suitable solvent to give analytically pure **4a-4r**.

2-(2-Bromopyridin-3-yloxy)-*N*-benzylacetamide (3a): R_f = 0.60 (CH₂Cl₂/EtOAc, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:2, v/v); Yield: 95%; mp. 104-105 °C; IR (KBr) 3272, 3050, 2922, 1652, 1544, 1408, 1296, 1084, 1072, 660 cm⁻¹; ¹H NMR(CDCl₃) δ 8.07-8.09 (dd, *J* = 1.5, 4.2Hz, 1H), 7.29-7.40 (m, NH + Aro-5H, D₂O exch., 6H), 7.26-7.28 (dd, *J* = 3.3, 5.1Hz, 1H), 7.14-7.17 (dd, *J* = 1.5, 8.1Hz, 1H), 4.61 (s, 2H), 4.60 (d, *J* = 5.7Hz, 2H); ¹³C NMR(CDCl₃) δ 43.15, 67.85, 120.29, 123.73, 127.58, 127.75, 128.84, 132.86, 137.31, 142.80, 150.48, 166.50; MS (m/z): 321 (M⁺). Anal. Calcd for C₁₄H₁₃BrN₂O₂: C, 52.36; H, 4.08; N, 8.72. Found: C, 52.28; H, 4.05; N, 8.69.

2-(2-Bromopyridin-3-yloxy)-*N*-benzylpropionamide (3b): R_f = 0.80 (CH₂Cl₂/EtOAc,4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:2, v/v); Yield: 94%; mp 85-86 °C; IR (KBr) 3260, 3078, 2984, 1658, 1556, 1414, 1286, 1050, 782 cm⁻¹; ¹H NMR(CDCl₃) δ 8.03-8.05 (dd, *J* = 1.5, 4.5Hz, 1H), 7.14-7.36 (m, NH+ Aro-5H, D₂O exch., 8H), 4.75-4.82 (q, 1H), 4.50 (d, *J* = 6.0Hz, 2H), 1.67 (d, *J* = 6.6Hz, 3H); ¹³C NMR (CDCl₃) δ 18.30, 43.11, 76.33, 121.32, 123.57, 127.46, 127.59, 128.69, 133.45, 137.41, 142.67, 150.22, 170.44; MS (m/z): 335 (M⁺). Anal. Calcd for C₁₅H₁₅BrN₂O₂: C, 53.75; H, 4.51; N, 8.36. Found: C, 53.78; H, 4.52; N, 8.39.

2-(2-Bromopyridin-3-yloxy)-N-(tetrahydrofuran-2-ylmethyl)acetamide (3c): $R_f = 0.48$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:4, v/v); Yield: 94%; mp 94-95 °C; IR (KBr) 3276, 3106, 2998, 2974, 2882, 1674, 1572, 1428, 1270, 1094, 808 cm^{-1} ; ^1H NMR(CDCl_3) δ 8.07-8.09 (dd, $J = 1.2, 4.5\text{Hz}$, 1H), 7.20 (bs, NH, D_2O exch., 1H), 7.15-7.18 (dd, $J = 1.2, 7.8\text{Hz}$, 1H), 4.57 (s, 2H), 4.02-4.10 (m, 1H), 3.87-3.94 (m, 1H), 3.74-3.81 (m, 1H), 3.57-3.65 (m, 1H), 3.37-3.46 (m, 1H), 1.87-2.04 (m, 3H), 1.55-1.64 (m, 1H); ^{13}C NMR(CDCl_3) δ 25.82, 28.37, 42.44, 67.58, 68.24, 120.03, 123.57, 132.78, 142.53, 150.43, 166.60; MS (m/z): 315 (M^+). Anal. Calcd for $\text{C}_{12}\text{H}_{15}\text{BrN}_2\text{O}_3$: C, 45.73; H, 4.80; N, 8.89. Found: C, 45.76; H, 4.78; N, 8.90.

2-(2-Chloropyridin-3-yloxy)-N-(tetrahydrofuran-2-ylmethyl)propionamide (3d): $R_f = 0.50$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:4, v/v); Yield: 95%; mp 58-59 °C; IR (KBr) 3280, 3100, 2936, 2854, 2660, 1568, 1422, 1290, 1082, 796 cm^{-1} ; ^1H NMR(CDCl_3 , diastereoisomer mixture) δ 8.06-8.08 (m, 1H), 7.23-7.24 (m, 2H), 6.97-7.06 (bs, NH, D_2O exch. 1H), 4.72-4.79 (m, 1H), 3.70-4.10 (m, 3H), 3.28-3.58 (m, 2H), 1.38-1.93 (m, 4H), 1.65 (d, 2H); ^{13}C NMR(CDCl_3) δ 18.68, 26.11, 28.60, 42.68, 68.57, 76.55, 77.49, 122.18, 123.62, 141.78, 142.24, 149.44, 171.08; MS (m/z): 284 (M^+). Anal. Calcd for $\text{C}_{13}\text{H}_{17}\text{ClN}_2\text{O}_3$: C, 54.84; H, 6.02; N, 9.84. Found: C, 54.79 H, 5.98; N, 9.86.

2-(2-Bromopyridin-3-yloxy)-N-cyclohexylacetamide (3e): $R_f = 0.66$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 96%; mp 132-133 °C; IR (KBr) 3212, 3098, 2942, 1656, 1560, 1452, 1302, 1200, 798 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.07-8.09 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.27-7.31 (dd, $J = 4.8, 8.1\text{Hz}$, 1H), 7.13-7.17 (dd, $J = 1.2, 8.1\text{Hz}$, 1H), 6.84 (bs, NH, D_2O exch., 1H),

4.53 (s, 2H), 3.86-3.95 (m, 1H), 1.19-1.97 (m, 10H); ^{13}C NMR (CDCl_3) δ 24.42, 25.33, 32.73, 47.70, 67.75, 120.20, 123.71, 132.81, 142.62, 150.49,

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165.41; MS (m/z): 313 (M^+). Anal. Calcd for $\text{C}_{13}\text{H}_{17}\text{BrN}_2\text{O}_2$: C, 49.86; H, 5.47; N, 8.94. Found: C, 49.87 H, 5.48; N, 8.91.

2-(2-Bromopyridin-3-yloxy)-*N*-cyclohexylpropionamide (3f): $R_f = 0.73$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1/3, v/v); Yield: 97%; mp 143-144 °C; IR (KBr) 3280, 3076, 2934, 2850, 1652, 1554, 1418, 1284, 1050, 784 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.05-8.07 (dd, $J = 1.5$, 4.8Hz, 1H), 7.24-7.28 (dd, $J = 4.2$, 8.1Hz, 1H), 7.15-7.18 (dd, $J = 1.5$, 8.4Hz, 1H), 6.71 (bs, NH, D_2O exch., 1H), 4.68-4.75 (q, $J = 6.6\text{Hz}$, 1H), 3.76-3.85 (m, 1H), 1.65 (d, $J = 6.6\text{Hz}$, 3H), 1.09-1.96 (m, 10H); ^{13}C NMR (CDCl_3) δ 18.30, 24.47, 24.53, 25.31, 32.73, 47.77, 76.29, 121.13, 123.61, 133.42, 142.56, 150.29, 169.36; MS (m/z): 327 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{19}\text{BrN}_2\text{O}_2$: C, 51.39; H, 5.85; N, 8.56. Found: C, 51.36; H, 5.83; N, 8.53.

2-(2-Bromopyridin-3-yloxy)-*N*-cyclohexylmethylacetamide (3g): $R_f = 0.63$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:2, v/v); Yield: 95%; mp 128-129 °C; IR (KBr) 3256, 3092, 2930, 1664, 1568, 1418, 1256, 1054, 798 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.08-8.10 (dd, $J = 1.5$, 4.8Hz, 1H), 7.27-7.31 (dd, $J = 4.8$, 8.1Hz, 1H), 7.14-7.17 (dd, $J = 1.5$, 8.1Hz, 1H), 6.94 (bs, NH, D_2O exch., 1H), 4.55 (s, 2H), 3.22-3.26 (t, 2H), 0.94-1.83 (m, 11H); ^{13}C NMR (CDCl_3) δ 25.70, 26.24, 30.64, 37.77, 45.20, 67.67, 120.14, 123.72, 132.76, 142.65, 150.46, 166.36; MS (m/z): 327 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{19}\text{BrN}_2\text{O}_2$: C, 51.39; H, 5.85; N, 8.56. Found: C, 51.36 H, 5.81; N, 8.51.

2-(2-Bromopyridin-3-yloxy)-N-cyclohexylmethylpropionamide (3h): $R_f = 0.71$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:2, v/v); Yield: 94%; mp 90-91 °C; IR (KBr) 3274, 3100,

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2924, 2850, 1662, 1562, 1442, 1418, 1293, 1048, 790 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.05-8.07 (dd, $J = 1.5$, 4.5Hz, 1H), 7.24-7.28 (dd, $J = 4.2$, 8.1Hz, 1H), 7.15-7.19 (dd, $J = 1.5$, 8.7Hz, 1H), 6.81 (bs, NH, D_2O exch., 1H), 4.72-4.79 (q, 1H), 3.09-3.23 (m, 2H), 1.66 (d, $J = 7.2\text{Hz}$, 3H), 0.86-1.69 (m, 11H); ^{13}C NMR (CDCl_3) δ 18.40, 25.73, 26.27, 30.65, 37.84, 45.29, 76.20, 121.09, 123.65, 133.42, 142.61, 150.28, 170.38; MS (m/z): 341 (M^+). Anal. Calcd for $\text{C}_{15}\text{H}_{21}\text{BrN}_2\text{O}_2$: C, 52.80; H, 6.20; N, 8.21. Found: C, 52.77 H, 6.16; N, 8.27.

2-(2-Bromopyridin-3-yloxy)-N-[2-(3,4-dimethoxyphenyl)ethyl]acetamide (3i): $R_f = 0.37$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 3:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 97%; mp 112-113 °C; IR (KBr) 3300, 3120, 2952, 1670, 1528, 1422, 1240, 938 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.05-8.07 (dd, $J = 1.5$, 4.8Hz, 1H), 7.07-7.10 (dd, $J = 1.5$, 8.1Hz, 1H), 6.85 (bs, NH, D_2O exch., 1H), 6.72-6.82 (m, 3H), 4.51 (s, 2H), 3.87 (d, 2OCH_3 , 6H), 3.64-3.70 (q, $J = 6.6\text{Hz}$, 2H), 2.82-2.87 (t, $J = 6.6\text{Hz}$, 2H); ^{13}C NMR (CDCl_3) δ 34.93, 40.02, 55.78, 55.82, 67.58, 111.20, 111.49, 119.95, 120.65, 123.60, 130.42, 132.71, 142.60, 147.70, 148.99, 150.36, 166.41; MS (m/z): 395 (M^+). Anal. Calcd for $\text{C}_{17}\text{H}_{19}\text{BrN}_2\text{O}_4$: C, 51.66; H, 4.85; N, 7.09. Found: C, 51.59 H, 4.83; N, 7.11.

2-(2-Bromopyridin-3-yloxy)-N-[2-(3,4-dimethoxyphenyl)ethyl]propionamide (3j): $R_f = 0.61$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 3:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 97%; mp 126-127 °C; IR (KBr) 3292, 3090, 2922, 1666, 1518, 1416, 1234, 1140, 670 cm^{-1} ; ^1H MR (CDCl_3) δ 8.04-8.04 (dd, $J = 1.4$, 4.2Hz, 1H), 7.19-7.23 (dd, $J = 4.2$, 8.1Hz, 1H), 7.05-7.08 (dd, $J = 1.2$, 7.8Hz, 1H), 6.61-6.77

(m, NH + Aro-3H, 4H), 4.66-4.72 (q, $J = 6.6\text{Hz}$, 1H), 3.87 (s, OCH₃, 3H), 3.86 (s, OCH₃, 3H), 3.55-3.65 (m, 2H), 2.76-2.80 (t, $J = 6.6\text{Hz}$, 2H), 1.61 (d, $J = 6.6\text{Hz}$, 3H); ¹³C NMR (CDCl₃) δ 18.40,

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35.04, 40.15, 55.80, 55.87, 76.12, 111.19, 111.47, 120.62, 120.93, 123.55, 130.52, 133.42, 142.60, 147.68, 148.98, 150.21, 170.45; MS (m/z): 409 (M⁺). Anal. Calcd for C₁₈H₂₁BrN₂O₄: C, 52.82; H, 5.17; N, 6.84. Found: C, 52.79 H, 5.13; N, 6.89.

2-(2-Bromopyridin-3-yloxy)-N-phenethylacetamide (3k): R_f = 0.56 (CH₂Cl₂/EtOAc, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 95%; mp 114-115 °C; IR (KBr) 3332, 3036, 2934, 1658, 1520, 1412, 1300, 1196, 1072, 694 cm⁻¹; ¹H NMR (CDCl₃) δ 8.04-8.06 (dd, $J = 1.5$, 4.8Hz, 1H), 7.21-7.34 (m, Aro-6H), 7.07-7.10 (dd, $J = 1.5$, 8.1Hz, 1H), 6.85 (bs, NH, D₂O exch., 1H), 4.50 (s, 2H), 3.66-3.72 (q, 2H), 2.87-2.91 (t, 2H); ¹³C NMR (CDCl₃) δ 35.31, 39.70, 67.53, 119.91, 123.56, 126.65, 128.63, 128.72, 132.72, 138.05, 142.52, 150.34, 166.36; MS (m/z): 335 (M⁺). Anal. Calcd for C₁₅H₁₅BrN₂O₂: C, 53.75; H, 4.51; N, 8.36. Found: C, 53.76 H, 4.53; N, 8.33.

2-(4-chloropyridin-2-yloxy)-N-phenethylpropionamide (3l): R_f = 0.75 (CH₂Cl₂/EtOAc, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 96%; mp 97-98 °C; IR (KBr) 3270, 3124, 3062, 2974, 1674, 1582, 1476, 1440, 1306, 1272, 1110, 812, 716 cm⁻¹; ¹H NMR (CDCl₃) δ 8.04-8.06 (dd, $J = 1.5$, 4.5Hz, 1H), 7.10-7.35 (m, Aro-7H), 6.84 (bs, NH, D₂O exch., 1H), 4.64-4.71 (q, $J = 7.2\text{Hz}$, 1H), 3.50-3.69 (m, 2H), 2.74-2.89 (m, 2H), 1.60 (d, $J = 6.9\text{Hz}$, 3H); ¹³C NMR (CDCl₃) δ 18.34, 35.36, 40.05, 76.04, 121.60, 123.25, 126.60, 128.55, 128.63, 138.07, 141.24, 141.80, 148.94, 170.47; MS (m/z): 304 (M⁺). Anal. Calcd for C₁₆H₁₇ClN₂O₂: C, 63.05; H, 5.62; N, 9.19. Found: C, 63.00 H, 5.63; N, 9.15.

(S)-2-(2-Bromopyridin-3-yloxy)-N-(1-phenylethyl)acetamide (3m): $R_f = 0.71$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:5, v/v); Yield: 94%; mp 102-103 °C; IR (KBr) 3372, 3044, 2972, 2926, 1660, 1522, 1424, 1284, 1206, 1082, 1054, 806, 700 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.05-8.07 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.11-7.36 (m, NH + Aro-7H, D_2O exch., 8H), 5.16-5.26 (m, 1H), 4.48-4.60 (dd, $J = 13.8, 21.9\text{Hz}$, 2H), 1.56 (d, $J = 6.6\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 22.25, 48.63, 67.70, 120.24, 123.66, 125.84, 127.47, 128.68, 132.71, 142.50, 142.59, 150.35, 165.47; MS (m/z): 335 (M^+). Anal. Calcd for $\text{C}_{15}\text{H}_{15}\text{BrN}_2\text{O}_2$: C, 53.75; H, 4.51; N, 8.36. Found: C, 53.69 H, 4.89; N, 8.31.

(S)-2-(2-Bromopyridin-3-yloxy)-N-(1-phenylethyl)propionamide (3n): $R_f = 0.80$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:5, v/v); Yield: 93%; mp 99-100 °C; IR (KBr) 3274, 3082, 2998, 2950, 1660, 1561, 1454, 1420, 1382, 1296, 1246, 1142, 1056, 894 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.02-8.04 (dd, $J = 1.2, 4.5\text{Hz}$, 1H), 7.07-7.34 (m, NH + Aro-7H, D_2O exch., 8H), 5.07-5.17 (m, 1H), 4.67-4.74 (q, $J = 6.6\text{Hz}$, 1H), 1.68 (d, $J = 6.6\text{Hz}$, 3H), 1.55 (d, $J = 6.9\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 18.24, 22.15, 48.76, 76.27, 121.27, 123.63, 125.92, 126.26, 127.44, 128.65, 133.42, 142.65, 150.21, 169.53; MS (m/z): 349 (M^+). Anal. Calcd for $\text{C}_{16}\text{H}_{17}\text{BrN}_2\text{O}_2$: C, 55.03; H, 4.91; N, 8.02. Found: C, 55.00 H, 4.92; N, 8.03.

2-(2-Chloropyridin-3-yloxy)-N-(4-phenoxyphenyl)acetamide (3o): $R_f = 0.84$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 96%; mp 150-151 °C; IR (KBr) 3406, 3063, 2938, 1700, 1544, 1426, 1308, 1230, 840 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.55 (bs, NH, D_2O exch.

1H), 8.12-8.13 (dd, $J = 2.7, 4.2\text{Hz}$, 1H), 7.57-7.60 (m, 2H), 7.27-7.36 (m, 4H), 6.98-7.13 (m, 5H), 4.69 (s, 2H); ^{13}C NMR (CDCl_3) δ 67.94, 118.51, 119.65, 121.24, 121.72, 123.24, 123.62, 129.77, 132.01, 140.34,

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142.40, 149.15, 154.08, 157.25, 164.47; MS (m/z): 354 (M^+). Anal. Calcd for $\text{C}_{19}\text{H}_{15}\text{ClN}_2\text{O}_3$: C, 64.32; H, 4.26; N, 7.90. Found: C, 64.35 H, 4.24; N, 7.92.

2-(2-Chloropyridin-3-yloxy)-*N*-(4-phenoxyphenyl)propionamide (3p): $R_f = 0.90$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 3:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 95%; mp 123-124 °C; IR (KBr) 3268, 3100, 1676, 1520, 1438, 1260, 1110, 854, 704 cm^{-1} ; ^1H -NMR (CDCl_3) δ 8.55 (bs, NH, D_2O exch. 1H), 8.11 (d, $J = 3.30\text{Hz}$, 1H), 7.55 (d, $J = 8.70\text{Hz}$, 2H), 7.25-7.35 (m, 4H), 6.97-7.12 (m, 5H), 4.83-4.89 (q, $J = 6.60\text{Hz}$, 1H), 1.75 (d, $J = 6.60\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 18.38, 76.76, 118.47, 119.69, 121.56, 122.50, 123.20, 123.57, 129.76, 132.33, 141.58, 142.53, 148.98, 153.95, 157.37, 168.41; MS (m/z): 368 (M^+). Anal. Calcd for $\text{C}_{20}\text{H}_{17}\text{ClN}_2\text{O}_3$: C, 65.13; H, 4.65; N, 7.60. Found: C, 65.11 H, 4.63; N, 7.58.

2-(2-Chloropyridin-3-yloxy)-*N*-phenylacetamide (3q): $R_f = 0.80$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 96%; mp 152-153 °C; IR (KBr) 3426, 3074, 2952, 1698, 1550, 1427, 1302, 1222, 1000, 820, 774 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.58 (bs, NH, D_2O exch. 1H), 8.10-8.12 (dd, $J = 1.8, 4.5\text{Hz}$, 1H), 7.57-7.61 (m, 2H), 7.24-7.38 (m, 4H), 7.13-7.18 (m, 1H), 4.82-4.89 (q, $J = 7.2\text{Hz}$, 1H), 1.74 (d, $J = 6.9\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 67.93, 119.87, 122.21, 123.53, 125.02, 129.12, 136.58, 140.83, 142.31, 149.12, 164.49; MS (m/z): 262 (M^+). Anal. Calcd for $\text{C}_{13}\text{H}_{11}\text{ClN}_2\text{O}_2$: C, 59.44; H, 4.22; N, 10.66. Found: C, 59.41 H, 4.23; N, 10.65.

2-(2-Chloropyridin-3-yloxy)-*N*-phenylpropionamide (3r): $R_f = 0.85$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 97%; mp 108-110 °C; IR (KBr) 3260, 3202, 3150, 3098, 2996, 1666, 1558, 1422, 1298, 1254, 1096, 798, 757 cm^{-1} ; ^1H NMR (CDCl_3) δ 8.57 (bs, NH, D_2O exch).

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1H), 8.11-8.13 (dd, $J = 1.8, 4.5\text{Hz}$, 1H), 7.59-7.63 (m, 2H), 7.26-7.40 (m, 4H), 7.14-7.20 (m, 1H), 4.67 (s, 2H); ^{13}C NMR (CDCl_3) δ 18.34, 76.72, 119.83, 122.43, 123.56, 124.93, 129.14, 136.85, 141.55, 142.47, 148.96, 168.50; MS (m/z): 276 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{13}\text{ClN}_2\text{O}_2$: C, 60.77; H, 4.74; N, 10.12. Found: C, 60.73 H, 4.73; N, 10.09.

1-Benzyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4a): $R_f = 0.66$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:3, v/v); Yield: 90%; mp 88-89 °C; IR (KBr) 3078, 3024, 2952, 1702, 1586, 1474, 1408, 1340, 1238, 1062, 800, 730 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.88-7.91 (dd, $J = 1.5, 4.5\text{Hz}$, 1H), 7.16-7.37 (m, 6H), 6.89-6.91 (dd, $J = 5.0, 8.0\text{Hz}$, 1H), 5.15 (s, 2H), 4.96 (s, 2H); ^{13}C NMR (CDCl_3) δ 44.72, 57.96, 119.22, 123.76, 127.24, 128.24, 1129.78, 135.30, 142.04, 152.10, 164.00; MS (m/z): 240 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_2$: C, 69.99; H, 5.03; N, 11.66. Found: C, 69.95 H, 5.00; N, 11.64.

1-Benzyl-2-methyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4b): $R_f = 0.73$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:3, v/v); Yield: 87%; mp 112-113 °C; IR (KBr) 3094, 3002, 2958, 1700, 1590, 1468, 1408, 1320, 1118, 812, 738 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.88-7.90 (dd, $J = 1.5, 5.1\text{Hz}$, 1H), 7.21-7.36 (m, 5H), 7.12-7.15 (dd, $J = 1.5, 8.1\text{Hz}$, 1H), 6.87-6.91 (dd, $J = 5.1, 8.1\text{Hz}$, 1H), 5.12 (s, 2H), 4.96-5.03 (q, $J = 6.9\text{Hz}$, 1H), 1.71(d, $J = 6.9\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 17.03, 44.93, 73.75, 118.72, 122.93, 123.67, 126.36, 127.64, 128.92, 135.06, 141.68, 151.27, 166.02; MS (m/z): 254 (M^+). Anal. Calcd for $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2$: C, 70.85; H, 5.55; N, 11.02. Found: C, 70.79 H, 5.51; N, 11.04.

1-(Tetrahydrofuran-2-ylmethyl)-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4c): $R_f = 0.49$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); liquid ; Yield: 90%; IR (KBr) 3100, 2984, 2900, 1708, 1600, 1480, 1418, 1334, 1250, 1100, 1068, 808, 778 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.91-7.93 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.62-7.66 (dd, $J = 1.5, 7.8\text{Hz}$, 1H), 7.00-7.04 (dd, $J = 4.8, 7.8\text{Hz}$, 1H), 4.83 (d, $J = 1.2\text{Hz}$, 2H), 4.16-4.24 (m, 2H), 3.86-3.94 (m, 1H), 3.71-3.81 (m, 2H), 1.60-2.15 (m, 4H); ^{13}C NMR (CDCl_3) δ 25.47, 29.36, 45.93, 67.36, 68.26, 76.90, 118.88, 124.09, 124.17, 141.69, 151.65, 163.49; MS (m/z): 234 (M^+). Anal. Calcd for $\text{C}_{12}\text{H}_{14}\text{N}_2\text{O}_3$: C, 61.53; H, 6.02; N, 11.96. Found: C, 61.58 H, 6.08.; N, 12.01.

2-Methyl-1-(tetrahydrofuran-2-ylmethyl)-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4d): $R_f = 0.53$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); liquid ; Yield: 88%; IR (KBr) 3058, 2928, 1686, 1580, 1458, 1396, 1200, 1060, 788 cm^{-1} ; ^1H NMR (CDCl_3 , diastereoisomer mixture) δ 7.92 (m, 1H), 7.61-7.68 (dd, $J = 7.8\text{Hz}, 12.3\text{Hz}$, 1H), 7.01-7.05 (m, 1H), 4.80-4.94 (m, 1H), 4.07-4.23 (m, 1H), 3.68-3.93 (m, 2H), 1.88-2.15 (m, 3H), 1.59-1.67 (d, 3H); ^{13}C NMR (CDCl_3) δ 16.61, 25.49, 19.15, 29.35, 45.83, 68.20, 73.66, 76.91, 118.84, 123.82, 141.64, 151.05, 166.03; MS (m/z): 248 (M^+). Anal. Calcd for $\text{C}_{13}\text{H}_{16}\text{N}_2\text{O}_3$: C, 62.89; H, 6.50; N, 11.28. Found: C, 62.93 H, 6.53; N, 11.35.

1-Cyclohexyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4e): $R_f = 0.64$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:5, v/v); Yield: 90%; mp 121-122 $^\circ\text{C}$; IR (KBr) 3024, 2968, 2928, 2866, 1686, 1586, 1474, 1364, 1240, 1072, 800 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.91-7.93 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.48-7.51 (dd, $J = 1.5, 8.1\text{Hz}$, 1H), 7.01-7.05 (dd, $J = 4.8, 8.1\text{Hz}$, 1H), 4.69 (s, 2H), 4.14-

4.24 (m, 1H), 1.23-2.36 (m, 9H); ^{13}C NMR (CDCl_3) δ 25.24, 26.23, 29.21, 56.45, 68.18, 118.78, 124.01, 124.23, 141.53, 152.93, 164.93; MS (m/z): 232 (M^+). Anal. Calcd for $\text{C}_{13}\text{H}_{16}\text{N}_2\text{O}_2$: C, 67.22; H, 6.94; N, 12.06. Found: C, 67.23 H, 6.91; N, 12.01.

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1-Cyclohexyl-2-methyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4f): R_f = 0.69 ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); liquid; Yield: 93%; IR (KBr) 3026, 2976, 2874, 1700, 1594, 1478, 1384, 1320, 1120, 1068, 822 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.92-7.94 (dd, J = 1.5, 4.8Hz, 1H), 7.48-7.51 (dd, J = 1.5, 8.1Hz, 1H), 7.00-7.05 (dd, J = 4.8, 8.1Hz, 1H), 4.67-4.74 (q, J = 6.9Hz, 1H), 4.17-4.28 (m, 1H), 1.58 (d, J = 6.6Hz, 3H), 1.22-2.35 (m, 9H); ^{13}C NMR (CDCl_3) δ 20.97, 25.17, 26.11, 28.88, 60.30, 74.21, 118.56, 123.70, 124.25, 141.44, 152.48, 167.13; MS (m/z): 246 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{18}\text{N}_2\text{O}_2$: C, 68.27; H, 7.37; N, 11.37. Found: C, 68.25 H, 7.36; N, 11.38.

1-Cyclohexylmethyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4g): R_f = 0.71 ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:5, v/v); Yield: 93%; mp 104-105 $^\circ\text{C}$; IR (KBr) 3112, 3092, 3044, 2950, 2872, 1698, 1590, 1474, 1410, 1330, 1238, 1062, 820 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.91-7.93 (dd, J = 1.5, 4.2Hz, 1H), 7.27-7.29 (dd, J = 1.5, 7.8Hz, 1H), 7.02-7.06 (m, 1H), 4.82 (d, J = 1.2Hz, 2H), 3.77-3.80 (m, 2H), 1.02-1.78 (m, 11H); ^{13}C NMR (CDCl_3) δ 25.66, 26.12, 30.64, 35.36, 46.59, 67.26, 118.80, 122.88, 123.56, 141.40, 151.78, 163.32; MS (m/z): 246 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{18}\text{N}_2\text{O}_2$: C, 68.27; H, 7.37; N, 11.37. Found: C, 68.22 H, 7.39; N, 11.35.

1-Cyclohexylmethyl-2-methyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4h): R_f = 0.75 ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:6, v/v); Yield: 89%; mp 96-97 $^\circ\text{C}$; IR (KBr) 3082, 3006, 2948, 2862, 1690, 1592, 1462, 1402, 1318, 1108, 802 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.92 (d, J =

4.5Hz, 1H), 7.26-7.29 (dd, $J = 1.5, 7.8\text{Hz}$, 1H), 7.01-7.06 (dd, $J = 4.8, 7.8\text{Hz}$, 1H), 4.83-4.90 (q, $J = 6.6\text{Hz}$, 1H), 3.69-3.85 (m, 2H), 1.62 (d, $J = 7.2\text{Hz}$, 3H), 1.04-1.85 (m, 6H); ^{13}C NMR (CDCl_3) δ 17.11, 25.70, 26.13, 30.62, 30.70, 35.52, 46.96, 73.73, 118.75, 122.60, 123.97, 141.46, 151.47, 165.97; MS (m/z):

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260 (M^+). Anal. Calcd for $\text{C}_{15}\text{H}_{20}\text{N}_2\text{O}_2$: C, 69.20; H, 7.74; N, 10.76. Found: C, 69.22 H, 7.73; N, 10.78.

1-[2-(3,4-Dimethoxyphenyl)ethyl]-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4i): $R_f = 0.54$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:2, v/v); Yield: 93%; mp 139-140°C; IR (KBr) 3002, 2950, 1686, 1518, 1464, 1416, 1228, 1144, 1022 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.92-7.94 (dd, $J = 1.5, 5.1\text{Hz}$, 1H), 7.22-7.25 (dd, $J = 1.5, 8.1\text{Hz}$, 1H), 7.00-7.05 (dd, $J = 5.1, 8.1\text{Hz}$, 1H), 6.72-6.82 (m, 3H), 4.80 (s, 2H), 4.09-4.14 (t, $J = 7.5\text{Hz}$, 2H), 3.87 (s, OCH_3 , 3H), 3.86 (s, OCH_3 , 3H), 2.87-2.92 (t, $J = 8.1\text{Hz}$, 2H); ^{13}C NMR (CDCl_3) δ 32.64, 42.60, 55.88, 67.33, 111.22, 111.75, 118.89, 120.66, 122.41, 123.23, 129.98, 141.60, 147.87, 148.98, 162.99; MS (m/z): 314 (M^+). Anal. Calcd for $\text{C}_{17}\text{H}_{18}\text{N}_2\text{O}_4$: C, 64.96; H, 5.77; N, 8.91. Found: C, 64.92 H, 5.75; N, 8.92.

1-[2-(3,4-Dimethoxyphenyl)ethyl]-2-methyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4j): $R_f = 0.67$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:2, v/v); Yield: 92%; mp 96-98°C; IR (KBr) 3060, 2982, 2938, 2800, 1678, 1508, 1456, 1400, 1252, 1220, 1136, 1020, 798 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.92-7.94 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.19-7.22 (dd, $J = 1.5, 8.1\text{Hz}$, 1H), 6.99-7.03 (m, $J = 4.8, 7.8\text{Hz}$, 1H), 6.72-6.81 (m, 3H), 4.81-4.87 (q, $J = 6.6\text{Hz}$, 1H), 4.01-4.18 (m, 2H), 3.87 (s, OCH_3 , 3H), 3.86 (s, OCH_3 , 3H), 2.86-2.91 (t, $J = 6.6\text{Hz}$, 2H), 1.60 (d, $J = 6.6\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 16.91, 32.75, 42.97, 55.86, 55.89, 73.75, 111.22, 111.80, 118.82, 120.69, 122.16, 123.64, 130.10,

141.67, 147.85, 148.95, 151.52, 165.62; MS (m/z): 328 (M^+). Anal. Calcd for $C_{18}H_{20}N_2O_4$: C, 65.84; H, 6.14; N, 8.53. Found: C, 65.88 H, 6.17; N, 8.52.

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1-Phenethyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4k): $R_f = 0.50$ (CH_2Cl_2 /EtOAc, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:3, v/v); Yield: 92%; mp 97-98 °C; IR (KBr) 3108, 3036, 2958, 1692, 1600, 1480, 1428, 1344, 1260, 1152, 1106, 1072, 816, 774, 716 cm^{-1} ; 1H NMR ($CDCl_3$) δ 7.89-7.91 (dd, $J = 1.5, 4.8Hz$, 1H), 7.21-7.33 (m, 6H), 6.98-7.03 (dd, $J = 5.1, 8.1Hz$, 1H), 4.77 (s, 2H), 4.08-4.13 (t, $J = 7.2Hz$, 2H), 2.91-2.97 (t, $J = 7.2Hz$, 2H); ^{13}C NMR ($CDCl_3$) δ 32.95, 42.47, 67.19, 118.79, 122.26, 123.14, 126.83, 128.66, 137.47, 141.45, 151.62, 162.81; MS (m/z): 254 (M^+). Anal. Calcd for $C_{15}H_{14}N_2O_2$: C, 70.85; H, 5.55; N, 11.02. Found: C, 70.81 H, 5.57; N, 11.03.

2-Methyl-1-phenethyl-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4l): $R_f = 0.67$ (CH_2Cl_2 /EtOAc, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:3, v/v); Yield: 92%; mp 73-74 °C; IR (KBr) 3100, 3036, 2984, 1704, 1602, 1478, 1430, 1330, 1126, 820, 742 cm^{-1} ; 1H NMR ($CDCl_3$) δ 7.88-7.90 (dd, $J = 1.5, 4.8Hz$, 1H), 7.19-7.31 (m, 6H), 6.96-7.00 (dd, $J = 5.1, 8.1Hz$, 1H), 4.76-4.83 (q, $J = 6.6Hz$, 1H), 4.00-4.17 (m, 2H), 2.85-2.94 (m, 2H), 1.57 (d, $J = 6.6Hz$, 3H); ^{13}C NMR ($CDCl_3$) δ 16.55, 32.76, 42.51, 73.31, 118.49, 121.80, 123.29, 126.48, 128.33, 128.42, 137.30, 141.19, 151.09, 165.11; MS (m/z): 268 (M^+). Anal. Calcd for $C_{16}H_{16}N_2O_2$: C, 71.62; H, 6.01; N, 10.44. Found: C, 71.58 H, 5.98; N, 10.43.

(*S*)-1-(1-Phenylethyl)-1*H*-pyrido[2,3-*b*][1,4]oxazin-2-one (4m): $R_f = 0.67$ (CH_2Cl_2 /EtOAc, 3:1, v/v); $[a]_D^{23} -99.5$ (c 1.91, CH_3OH); colorless liquid; Yield: 92%; IR (KBr) 3082, 3012, 2958, 1694, 1592,

1476, 1410, 1360, 1062, 708 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.84-7.86 (dd, $J = 1.2, 4.8\text{Hz}$, 1H), 7.27-7.40 (m, 5H), 6.95-6.98 (dd, $J = 1.5, 8.1\text{Hz}$, 1H), 6.73-6.77 (dd, $J = 4.8, 8.1\text{Hz}$, 1H), 6.37-6.43 (q, $J = 6.9\text{Hz}$, 1H), 4.90 (d, $J = 2.7\text{Hz}$, 2H), 1.79 (d, $J = 7.2\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 15.73, 49.73, 118.40, 125.30, 125.95, 127.51, 128.99, 138.96, 141.61, 152.75, 164.58; MS (m/z): 254 (M^+). Anal. Calcd for $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2$: C, 70.85; H, 5.55; N, 11.02. Found: C, 70.78 H, 5.51; N, 11.00.

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(S)-2-Methyl-1-((S)-1-phenylethyl)-1H-pyrido[2,3-*b*][1,4]oxazin-2-one (4n-a): $R_f = 0.30$ (*n*-Hexane/EtOAc, 3:1, v/v); $[\alpha]_D^{23} -11.6$ (c 1.12, CH_3OH); White solid (Diethyl ether/*n*-Hexane, 1:10, v/v); Yield: 47%; mp 64-66 $^\circ\text{C}$; IR (KBr) 3082, 3016, 2958, 1700, 1596, 1472, 1318, 1120, 798 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.82-7.85 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.25-7.39 (m, 5H), 6.94-6.97 (dd, $J = 1.8, 8.1\text{Hz}$, 1H), 6.73-6.77 (dd, $J = 4.8, 7.5\text{Hz}$, 1H), 6.38-6.45 (q, $J = 7.2\text{Hz}$, 1H), 4.84-4.91 (q, $J = 6.9\text{Hz}$, 1H), 1.73 (t, $J = 7.8\text{Hz}$, 6H); ^{13}C NMR (CDCl_3) δ 15.28, 16.19, 49.29, 73.37, 118.09, 122.02, 124.74, 125.51, 127.08, 128.66, 139.07, 141.24, 152.46, 166.62; MS (m/z): 268 (M^+). Anal. Calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2$: C, 71.62; H, 6.01; N, 10.44. Found: C, 71.59 H, 6.00; N, 10.45.

(S)-2-Methyl-1-((R)-1-phenylethyl)-1H-pyrido[2,3-*b*][1,4]oxazin-2-one (4n-b): $R_f = 0.34$ (*n*-Hexane/EtOAc, 3:1, v/v); $[\alpha]_D^{23} -135.1$ (c 3.07, CH_3OH); liquid; Yield: 45%; IR (KBr) 3082, 3016, 2958, 1700, 1596, 1472, 1318, 1120, 798 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.82-7.84 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.24-7.38 (m, 5H), 6.95-6.98 (dd, $J = 1.8, 8.1\text{Hz}$, 1H), 6.71-6.75 (dd, $J = 4.8, 8.1\text{Hz}$, 1H), 6.33-6.40 (q, $J = 7.5\text{Hz}$, 1H), 4.93-5.00 (q, $J = 6.9\text{Hz}$, 1H), 1.78 (d, $J = 7.5\text{Hz}$, 3H), 1.65 (d, $J = 7.2\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 15.50, 16.75, 49.40, 73.83, 117.93, 121.69, 124.56, 125.54, 127.18, 128.68, 138.85, 141.38, 151.55, 166.61; MS (m/z): 268 (M^+). Anal. Calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2$: C, 71.62; H, 6.01; N, 10.44. Found: C, 71.64 H, 5.99; N, 10.44.

1-(4-Phenoxyphenyl)-1H-pyrido[2,3-*b*][1,4]oxazin-2-one (4o): $R_f = 0.72$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:2, v/v); Yield: 90%; mp 149-150 °C; IR (KBr) 3068, 2896, 1684, 1583, 1460, 1238, 790 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.93-7.95 (dd, $J = 1.8, 4.8\text{Hz}$, 1H), 7.38-7.44 (m, 2H), 7.10-7.27 (m, 7H), 6.88-6.92 (dd, $J = 4.8, 7.8\text{Hz}$, 1H), 6.81-6.84 (dd, $J = 1.8, 8.1\text{Hz}$, 1H), 4.99 (s, 2H); ^{13}C NMR (CDCl_3) δ 67.82, 118.79, 119.31, 119.92, 124.36, 125.40, 128.85, 129.81, 130.00,

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141.97, 151.28, 155.74, 158.31, 163.26; MS (m/z): 318 (M^+). Anal. Calcd for $\text{C}_{19}\text{H}_{14}\text{N}_2\text{O}_3$: C, 71.69; H, 4.43; N, 8.80. Found: C, 71.65 H, 4.39; N, 8.81.

2-Methyl-1-(4-phenoxyphenyl)-1H-pyrido[2,3-*b*][1,4]oxazin-3-one (4p): $R_f = 0.82$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Ethyl acetate/*n*-Hexane, 1:3, v/v); Yield: 91%; mp 152-153 °C; IR (KBr) 3050, 2998, 2942, 1686, 1584, 1450, 1380, 1242, 1106, 786, 690 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.93-7.95 (dd, $J = 1.5, 4.8\text{Hz}$, 1H), 7.37-7.42 (m, 2H), 7.09-7.21 (m, 6H), 6.88-6.92 (dd, $J = 4.8, 7.8\text{Hz}$, 1H), 6.79-6.82 (dd, $J = 1.5, 8.1\text{Hz}$, 1H), 4.99-5.06 (q, $J = 6.9\text{Hz}$, 1H), 1.72 (d, $J = 6.6\text{Hz}$, 3H); ^{13}C NMR (CDCl_3) δ 16.84, 74.21, 118.67, 119.29, 119.73, 124.04, 124.19, 125.71, 129.41, 129.75, 129.91, 141.94, 151.155.80, 158.02, 165.79; MS (m/z): 332 (M^+). Anal. Calcd for $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}_3$: C, 72.28; H, 4.85; N, 8.43. Found: C, 72.25 H, 4.83; N, 8.39.

1-Phenyl-1H-pyrido[2,3-*b*][1,4]oxazin-2-one (4q): $R_f = 0.66$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:3, v/v); Yield: 90%; mp 147-148 °C; IR (KBr) 3100, 3048, 2924, 1720, 1600, 1480, 1396, 1378, 1258, 1100, 1072, 778 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.91-7.94 (dd, $J = 1.8,$

5.1Hz, 1H), 7.47-7.60 (m, 3H), 7.26-7.30 (m, 2H), 6.85-6.89 (dd, $J = 4.5, 8.1$ Hz, 1H), 6.74-6.78 (dd, $J = 1.8, 8.1$ Hz, 1H), 4.98 (s, 2H); ^{13}C NMR (CDCl_3) δ 67.85, 118.80, 124.42, 125.36, 128.50, 129.34, 130.31, 134.76, 141.97, 151.32, 163.05; MS (m/z): 226 (M^+). Anal. Calcd for $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2$: C, 69.02; H, 4.46; N, 12.38. Found: C, 69.00 H, 4.43; N, 12.39.

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2-Methyl-1-phenyl-1H-pyrido[2,3-*b*][1,4]oxazin-2-one (4r): $R_f = 0.67$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 3:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:3, v/v); Yield: 91%; mp 120-121 °C; IR (KBr) 3100, 3022, 2952, 2876, 1700, 1450, 1378, 1320, 1252, 1118, 808, 750, 702 cm^{-1} ; ^1H NMR (CDCl_3) δ 7.93-7.95 (dd, $J = 1.8, 4.5$ Hz, 1H), 7.46-7.59 (m, 3H), 7.24-7.28 (m, 2H), 6.85-6.89 (dd, $J = 4.5, 8.1$ Hz, 1H), 6.73-6.76 (dd, $J = 1.8, 8.1$ Hz, 1H), 5.00-5.07 (q, $J = 6.6$ Hz, 1H), 1.72 (d, $J = 6.6$ Hz, 3H); ^{13}C NMR (CDCl_3) δ 16.94, 74.34, 118.75, 124.18, 125.74, 128.50, 129.18, 130.24, 135.29, 142.04, 151.13, 165.71; MS (m/z): 240 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_2$: C, 69.99; H, 5.03; N, 11.66. Found: C, 70.03 H, 5.01; N, 11.59.

Synthesis of 4-Benzyl-4H-pyrido[3,2-*b*][1,4]oxazin-3-one (5)

To a 100mL flask equipped with a magnetic stirrer was added 4H-pyrido[3,2-*b*][1,4]oxazin-3-one (3g, 19.98mmol), benzyl chloride (2.58g, 20.38mmol), K_2CO_3 (2.90g, 20.98mmol) and DMF (30mL). The mixture was stirred under nitrogen for 6hrs, monitored by TLC. CH_2Cl_2 (100mL) was added to the reaction mixture. After separating the organic layer, aqueous layer was extracted with CH_2Cl_2 . The combined methylene chloride layer was dried over anhydrous MgSO_4 and evaporated in vacuo. The crude products were purified by flash column chromatography using EtOAc/ CH_2Cl_2 as eluent to afford

compound **5** in 93% yield.: $R_f = 0.43$ ($\text{CH}_2\text{Cl}_2/\text{EtOAc}$, 4:1, v/v); White solid (Diethyl ether/*n*-Hexane, 1:4, v/v); mp 53-55°C; IR (KBr) 3022, 2958, 1708 (C=O), 1464, 1410, 1346, 1230, 1064, 730 cm^{-1} ; ^1H NMR (DMSO-d_6) δ 7.98 (dd, $J = 1.0, 4.5\text{Hz}$, 1H), 7.40 (dd, $J = 1.5, 8.0\text{Hz}$, 1H), 7.27~7.31 (m, 4H), 7.21~7.23 (m, 1H), 7.04 (dd, $J = 5.0, 8.0\text{Hz}$, 3H), 5.25 (s, 2H), 4.86 (s, 2H); ^{13}C NMR (CDCl_3) δ 68.3, 120.8, 124.8, 128.6, 129.6, 138.6, 141.8, 142.0, 142.7, 166.1; MS (m/z): 240 (M^+). Anal. Calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_2$: C, 69.99; H, 5.03; N, 11.66. Found: C, 69.94 H, 5.00; N, 11.64.

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ORTEP plot for X-ray crystal structures of **4a**

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X-Ray Analytical Data for 4a;

Experimental

Data Collection

A colorless block crystal of $C_{14}H_{12}N_2O_2$ having approximate dimensions of 0.20 x 0.07 x 0.05 mm was mounted in a loop. All measurements were made on a Rigaku RAXIS-RAPID Imaging Plate diffractometer with graphite monochromated Mo-K α radiation.

Indexing was performed from 3 oscillations which were exposed for 0.6 minutes. The camera radius was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

$$a = 9.421(3) \text{ \AA}$$

$$b = 5.663(2) \text{ \AA} \quad \beta = 89.15(3)^\circ$$

$$c = 21.299(8) \text{ \AA}$$

$$V = 1136.2(7) \text{ \AA}^3$$

For $Z = 4$ and F.W. = 240.26, the calculated density is 1.40 g/cm³. The systematic absences of:

$$h0l: h+l \pm 2n$$

$$0k0: k \pm 2n$$

Uniquely determine the space group to be:

$$P2_1/n \text{ (#14)}$$

$$S20$$

The data were collected at a temperature of $-180 \pm 1^\circ\text{C}$ to a maximum 2θ value of 60.0° . A total of 55 images, corresponding to 220.0° oscillation angles, were collected with 2 different goniometer

settings. Exposure time was 1.00 minutes per degree. The camera radius was 127.40 mm. Readout was performed in the 0.100 mm pixel mode. Data was processed by the PROCESS-AUTO program package.

Data Reduction

Of the 13591 reflections which were collected, 3298 were unique ($R_{\text{int}} = 0.052$); equivalent reflections were merged.

The linear absorption coefficient, μ , for Mo-K α radiation is 1.0 cm^{-1} . A symmetry-related absorption correction using the program ABSCOR¹ was applied which resulted in transmission factors ranging from 0.89 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods² and expanded using Fourier techniques³. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement⁴ was based on 3298 observed reflections ($I > -3.00\sigma(I)$, $2\theta < 60.04$) and 163 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma (F_o^2 - F_c^2) / \Sigma F_o^2 = 0.069$$

$$R_w = [(\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w (F_o^2)^2)]^{1/2} = 0.063$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| = 0.038 \quad \text{for } I > 2.0\sigma(I) \text{ data}$$

The standard deviation of an observation of unit weight⁵ was 0.90. The weighting scheme was based on counting statistics and included a factor ($p = 0.002$) to downweight the intense reflections. Plots of $\Sigma w (F_o^2 - F_c^2)^2$ versus F_o^2 reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.43 and -0.35 e⁻/Å³, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁶. Anomalous dispersion effects were included in Fcalc⁷; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁸. The values for the mass attenuation coefficients are those of Creagh and Hubbel⁹. All calculations were performed using the teXsan¹⁰ crystallographic software package of Molecular Structure Corporation.

References

- (1) ABSCOR: Higashi T. (1995). Program for Absorption Correction, Rigaku Corporation, Tokyo, Japan.
- (2) SIR97: Altomare, A., Burla, M.C., Camalli, M., Cascarano, G.L., Giacovazzo, C., Guagliardi, A., Moliterni, A.G.G., Polidori, G. Spagna, R. (1999). J. Appl. Cryst. 32, 115-119.
- (3) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
- (4) Least-Squares:

Function minimized: $\Sigma w(F_o^2 - F_c^2)^2$ where

$$w = 1/[\sigma^2(F_o^2)] = [\sigma_c^2(F_o^2) + (p (\text{Max}(F_o^2, 0) + 2F_c^2)/3)^2]^{-1}$$

$\sigma_c(F_o^2)$ = e.s.d. based on counting statistics

p = p-factor

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations

N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J. ; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1999).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{14}H_{12}N_2O_2$
Formula Weight	240.26
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.20 X 0.07 X 0.05 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2 θ range)	9510 (7.1 - 60.1 $^\circ$)
Indexing Images	3 oscillations at 0.6 minutes
Camera Radius	127.40 mm
Lattice Parameters	$a = 9.421(3) \text{ \AA}$ $b = 5.663(2) \text{ \AA}$ $c = 21.299(8) \text{ \AA}$ $\beta = 89.15(3)^\circ$ $V = 1136.2(7) \text{ \AA}^3$
Space Group	P2 ₁ /n (#14)
Z value	4
D _{calc}	1.404 g/cm ³
F ₀₀₀	504.00
$\mu(\text{MoK}\alpha)$	0.96 cm ⁻¹

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID Imaging Plate	
Radiation	MoK α ($\lambda = 0.71075 \text{ \AA}$)	
	graphite monochromated	
Temperature	-180.0 °C	
Voltage, Current	60 kV, 90 mA	
Collimator Size	0.5 mm	
Detector Aperture	280.0 mm x 256.0 mm	
Data Images	55 exposures at 1.0 minutes per degree	
Oscillation Range ($\phi=90.0^\circ, \chi=45.0^\circ$)	ω 130.0 - 190.0° with 4.0° step	
Oscillation Range ($\phi=270.0^\circ, \chi=45.0^\circ$)	ω 0.0 - 160.0° with 4.0° step	
Camera Radius	127.40 mm	
Pixel Size	0.100 mm	
$2\theta_{\text{max}}$	60.0°	
No. of Reflections Measured	Total: 13591	
	Unique: 3298 ($R_{\text{int}} = 0.052$)	
Corrections	Lorentz-polarization	
	Absorption	
	(trans. factors: 0.8940 - 0.9950)	

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w (F_o^2 - F_c^2)^2$
Least Squares Weights	$1/\sigma^2(F_o^2)$
p-factor	0.0020
Anomalous Dispersion	All non-hydrogen atoms
No. of Observations ($I > -3.00\sigma(I)$, $2\theta < 60.04^\circ$)	3298
No. Variables	163
Reflection/Parameter Ratio	20.23
Residuals: R; R _w	0.069 ; 0.063
Residuals: R ₁	0.038
No. of Reflections to calc R ₁	1813
Goodness of Fit Indicator	0.90
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.43 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.35 e ⁻ /Å ³

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B _{eq}
O(1)	-0.01206(10)	-0.0671(2)	0.64084(4)	1.50(2)
O(2)	0.1561(1)	0.3702(2)	0.73301(5)	1.82(2)
N(1)	0.0478(1)	-0.2399(2)	0.54792(5)	1.42(2)
N(2)	0.2152(1)	0.2456(2)	0.63418(5)	1.23(2)
C(1)	0.1974(1)	0.0722(2)	0.58690(6)	1.18(3)
C(2)	0.2858(1)	0.0526(3)	0.53475(7)	1.45(3)
C(3)	0.2536(1)	-0.1151(3)	0.48898(7)	1.60(3)
C(4)	0.1346(2)	-0.2545(3)	0.49694(7)	1.58(3)
C(5)	0.0810(1)	-0.0815(3)	0.59090(6)	1.19(3)
C(6)	0.0533(1)	0.0079(3)	0.69797(7)	1.44(3)
C(7)	0.1446(1)	0.2256(3)	0.69060(6)	1.28(3)
C(8)	0.3060(1)	0.4510(2)	0.62252(7)	1.38(3)
C(9)	0.4624(1)	0.4167(3)	0.63441(6)	1.15(3)
C(10)	0.5544(1)	0.5982(3)	0.61595(7)	1.53(3)
C(11)	0.6977(1)	0.5894(3)	0.62993(7)	1.84(3)
C(12)	0.7506(1)	0.3962(3)	0.66246(7)	1.73(3)
C(13)	0.6611(1)	0.2128(3)	0.67968(6)	1.55(3)
C(14)	0.5173(1)	0.2222(3)	0.66569(6)	1.33(3)
H(2)	0.3669	0.1513	0.5301	1.7
H(3)	0.3129	-0.1330	0.4528	1.9
H(4)	0.1126	-0.3659	0.4652	1.9
H(6a)	-0.0194	0.0406	0.7281	1.7
H(6b)	0.1111	-0.1172	0.7127	1.7
H(8a)	0.2959	0.4953	0.5798	1.7
H(8b)	0.2732	0.5756	0.6489	1.7

H(10)	0.5183	0.7297	0.5935	1.8
H(11)	0.7592	0.7143	0.6174	2.2
H(12)	0.8482	0.3901	0.6728	2.1

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(13)	0.6980	0.0798	0.7012	1.9
H(14)	0.4565	0.0954	0.6775	1.6

$$B_{eq} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.0147(5)	0.0245(6)	0.0178(5)	-0.0040(5)	-0.0003(4)	-0.0016(5)
O(2)	0.0215(5)	0.0252(6)	0.0223(6)	0.0000(5)	0.0014(4)	-0.0083(5)
N(1)	0.0167(6)	0.0179(7)	0.0195(6)	0.0008(6)	-0.0033(5)	0.0002(6)
N(2)	0.0126(6)	0.0149(6)	0.0192(6)	-0.0031(5)	0.0002(5)	-0.0009(5)
C(1)	0.0150(7)	0.0141(7)	0.0159(7)	0.0009(6)	-0.0035(5)	0.0013(6)
C(2)	0.0163(7)	0.0197(8)	0.0192(7)	-0.0027(6)	-0.0015(6)	0.0032(6)
C(3)	0.0225(8)	0.0219(8)	0.0165(7)	0.0028(7)	0.0005(6)	-0.0011(7)
C(4)	0.0217(8)	0.0191(8)	0.0192(7)	0.0024(7)	-0.0044(6)	-0.0013(7)
C(5)	0.0123(6)	0.0163(7)	0.0165(7)	0.0022(6)	-0.0014(5)	0.0031(6)
C(6)	0.0158(7)	0.0233(8)	0.0157(7)	-0.0009(6)	0.0000(6)	0.0007(6)
C(7)	0.0110(7)	0.0195(7)	0.0182(7)	0.0032(6)	-0.0022(6)	-0.0008(6)

C(8)	0.0151(7)	0.0143(7)	0.0230(8)	-0.0009(6)	-0.0008(6)	0.0004(6)
C(9)	0.0137(7)	0.0154(7)	0.0145(7)	-0.0004(6)	0.0008(5)	-0.0036(6)
C(10)	0.0191(7)	0.0140(7)	0.0250(8)	-0.0011(7)	-0.0010(6)	0.0015(7)
C(11)	0.0174(7)	0.0196(8)	0.0331(9)	-0.0038(7)	0.0010(6)	-0.0034(7)
C(12)	0.0142(7)	0.0272(9)	0.0243(8)	0.0018(7)	-0.0024(6)	-0.0075(7)
C(13)	0.0206(7)	0.0220(8)	0.0163(7)	0.0056(7)	-0.0014(6)	0.0000(7)
C(14)	0.0184(7)	0.0171(7)	0.0150(7)	-0.0008(6)	0.0027(5)	-0.0016(6)

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
O(1)	C(5)	1.371(2)	O(1)	C(6)	1.436(2)
O(2)	C(7)	1.226(2)	N(1)	C(4)	1.352(2)
N(1)	C(5)	1.323(2)	N(2)	C(1)	1.418(2)
N(2)	C(7)	1.370(2)	N(2)	C(8)	1.463(2)
C(1)	C(2)	1.383(2)	C(1)	C(5)	1.401(2)
C(2)	C(3)	1.398(2)	C(3)	C(4)	1.380(2)
C(6)	C(7)	1.510(2)	C(8)	C(9)	1.511(2)
C(9)	C(10)	1.397(2)	C(9)	C(14)	1.391(2)
C(10)	C(11)	1.388(2)	C(11)	C(12)	1.391(2)
C(12)	C(13)	1.383(2)	C(13)	C(14)	1.393(2)

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(2)	H(2)	0.95	C(3)	H(3)	0.95
C(4)	H(4)	0.95	C(6)	H(6a)	0.95
C(6)	H(6b)	0.95	C(8)	H(8a)	0.95
C(8)	H(8b)	0.95	C(10)	H(10)	0.95
C(11)	H(11)	0.95	C(12)	H(12)	0.95
C(13)	H(13)	0.95	C(14)	H(14)	0.95

Table 5. Bond Angles($^{\circ}$)

Atom	atom	atom	angle	atom	atom	atom	angle
C(5)	O(1)	C(6)	113.4(1)	C(4)	N(1)	C(5)	116.8(1)
C(1)	N(2)	C(7)	120.3(1)	C(1)	N(2)	C(8)	120.3(1)
C(7)	N(2)	C(8)	119.3(1)	N(2)	C(1)	C(2)	123.3(1)
N(2)	C(1)	C(5)	119.2(1)	C(2)	C(1)	C(5)	117.4(1)
C(1)	C(2)	C(3)	118.7(1)	C(2)	C(3)	C(4)	119.2(1)
N(1)	C(4)	C(3)	123.0(1)	O(1)	C(5)	N(1)	114.9(1)
O(1)	C(5)	C(11)	120.1(1)	N(1)	C(5)	C(1)	124.9(1)
O(1)	C(6)	C(7)	113.8(1)	O(2)	C(7)	N(2)	123.0(1)
O(2)	C(7)	C(6)	121.7(1)	N(2)	C(7)	C(6)	115.3(1)
N(2)	C(8)	C(9)	116.0(1)	C(8)	C(9)	C(10)	117.4(1)
C(8)	C(9)	C(14)	123.5(1)	C(10)	C(9)	C(14)	118.9(1)
C(9)	C(10)	C(11)	121.0(1)	C(10)	C(11)	C(12)	119.5(1)
C(11)	C(12)	C(13)	120.1(1)	C(12)	C(13)	C(14)	120.4(1)
C(9)	C(14)	C(13)	120.2(1)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(2)	120.6	C(3)	C(2)	H(2)	120.7
C(2)	C(3)	H(3)	120.4	C(4)	C(3)	H(3)	120.4
N(1)	C(4)	H(4)	118.5	C(3)	C(4)	H(4)	118.5
O(1)	C(6)	H(6a)	108.4	O(1)	C(6)	H(6b)	108.4
C(7)	C(6)	H(6a)	108.4	C(7)	C(6)	H(6b)	108.4
H(6a)	C(6)	H(6b)	109.5	N(2)	C(8)	H(8a)	107.8
N(2)	C(8)	H(8b)	107.8	C(9)	C(8)	H(8a)	107.8
C(9)	C(8)	H(8b)	107.8	H(8a)	C(8)	H(8b)	109.5
C(9)	C(10)	H(10)	119.5	C(11)	C(10)	H(10)	119.5
C(10)	C(11)	H(11)	120.3	C(12)	C(11)	H(11)	120.3
C(11)	C(12)	H(12)	120.0	C(13)	C(12)	H(12)	120.0
C(12)	C(13)	H(13)	119.8	C(14)	C(13)	H(13)	119.8
C(9)	C(14)	H(14)	119.9	C(13)	C(14)	H(14)	119.9

Table 7. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	atom	atom	distance
O(1)	C(11) ¹⁾	3.367(2)	O(1)	C(12) ²⁾	3.474(2)
O(1)	C(13) ²⁾	3.550(2)	O(2)	C(7) ³⁾	3.211(2)
O(2)	C(6) ³⁾	3.222(2)	O(2)	C(14) ³⁾	3.346(2)
O(2)	O(2) ³⁾	3.421(1)	O(2)	O(2) ⁴⁾	3.421(1)

N(1)	C(8) ⁵⁾	3.409(2)	N(1)	C(4) ⁶⁾	3.428(2)
N(1)	C(4) ⁷⁾	3.480(2)	N(1)	N(1) ⁶⁾	3.523(2)
N(1)	C(3) ⁶⁾	3.576(2)	C(3)	C(12) ⁸⁾	3.598(2)
C(4)	C(5) ⁶⁾	3.370(2)	C(4)	C(8) ⁵⁾	3.560(2)
C(5)	C(8) ⁵⁾	3.464(2)	C(6)	C(14) ⁴⁾	3.382(2)

Symmetry operations

(1)	X-1,Y-1,Z	(2)	X-1,Y,Z
(3)	-X+1/2,Y+1/2,-Z+3/2	(4)	-X+1/2,Y-1/2,-Z+3/2
(5)	X,Y-1,Z	(6)	-X,-Y,-Z+1
(7)	-X,-Y-1,-Z+1	(8)	-X+1,-Y,-Z+1

C:\WINNMR95\8DCRO\OXAZINE\OXAZ-

DFILE COMMENT
DATEIN Fri Jan 03 16:46:06 2003
ORNUC 1H
EXMCO NOX
ORFRO 300.40 MHz
ORSET 130.00 MHz
ORFIN 1150.0 Hz
POINT 16384
FREQO 6013.2 Hz
SCANS 16
ACQTM 2.725 sec
PU 1.551 sec
PWL 5.6 us
INNUC 1H
CTEMP 13.9 C
SLVNT CDCL3
EXRBF 0.00 DEM
BF 0.52 Hz
RGAIN 13

C:\WINNER95\SDCHO\OXAZINE\OKA-
 Eri Jan 03 17:36:09 2003
 1H
 NS
 300.40 MHz
 130.00 KHz
 1150.0 Hz
 16384
 6013.2 Hz
 16
 2.725 sec
 1.551 sec
 5.6 us
 1H
 13.5 c
 CDCL3
 0.00 ppm
 0.62 Hz
 13
 1.0000

C:\WINNER95\SDCHO\DATA\TNE\OKA-

DATE: Fri Jan 03 13:25:04 2003
 NAME: TNE
 INSTR: 13C
 EXMOD: BOW
 OBSFQ: 75.45 MHz
 OBSF2: 124.00 KHz
 OBSF3: 1640.0 Hz
 POINT: 32768
 FREQ: 20408.1 Hz
 SCANS: 63
 ACQTM: 1.606 sec
 PD: 3.000 sec
 F41: 4.2 us
 IRMUC: 1h
 CTMP: 14.6 C
 SLVNT: CDCL3
 EXREF: 77.00 ppm
 RF: 0.62 Hz
 RGAIN: 24

C:\WINNR95\SDCHO\OXAZINE\OMA-

DEFILE
 COMMENT
 DATEIN Fri Jan 03 14:55:51 2003
 ORNUC 13C
 EXMOC BCM
 ORFRQ 75.45 MHz
 ORSET 124.00 MHz
 ORPIN 1840.0 Hz
 POINT 32766
 FREQU 20408.1 Hz
 SCANS 151
 ACQTM 1.606 sec
 PD 3.000 sec
 PR1 4.2 us
 IRMOC 1H
 CTMCP 15.3 C
 SLANT CDCL3
 EXREF 77.00 ppm
 BP 0.15 Hz
 RGAIN 24

C:\WINNR95\SDCHO\OXAZINE\OXA-

DFILE
 COMMENT
 DATEM
 OBMUC
 EXMOD
 OBFRO
 OBFST
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTH
 PD
 PM1
 IFMUC
 CTEMP
 SLANT
 EXREF
 RF
 REAIN

Fri Jan 03 14:38:23 2003
 13C
 BCM
 75.45 MHz
 124.00 KHz
 1940.0 Hz
 32768
 20408.1 Hz
 130
 1.606 sec
 3.000 sec
 4.2 us
 1H
 15.6 c
 CDCL3
 77.00 ppm
 0.15 Hz
 24

Variable	Value
DFILE	0.000
COMINT	0.087
DATIN	1.096
CBNUC	1.136
EXMOD	1.171
CBFRQ	1.171
CBSET	1.199
CBFIN	1.211
FOINT	1.222
PRECO	1.222
SCANS	1.264
ACQTH	1.303
PD	1.340
PM1	1.384
IRNUC	1.420
CTEMP	1.430
SLVNT	1.457
EXRET	1.468
BF	1.588
RGRIN	1.600
	1.613
	1.613
	1.646
	1.668
	1.702
	1.716
	1.761
	1.810
	1.851
	1.911
	1.961
	2.054
	3.755
	3.789
	3.803
	3.810
	3.852
	4.683
	4.707
	4.729
	4.751
	6.705
	6.729
	7.150
	7.155
	7.176
	7.183
	7.236
	7.250
	7.263
	7.277
	7.286
	8.053
	8.058
	8.069
	8.074

C:\WINNMR55\SDCHO\OXALINE\OXA-

DRFILE
CONRT
DATIM
DEHUC
EXHOD
OBFRQ
OBSET
OBFIN
POINT
FREQ
SCANS
ACQTM
PD
FWI
IRHUC
CTEMP
SLVNT
EXREF
BF
RGAIN

Exi Jan 03 13:47:55 2003

13C

BCN

75.45 MHz

124.00 kHz

1840.0 Hz

32768

20408.1 Hz

216

1.506 sec

3.000 sec

4.2 us

14.6 C

CDCL3

77.00 ppm

0.15 Hz

24

C:\WINNMR95\SDCHNO\OXAZINE\OXA

DEFILE
CORRECTION
DATE: Jan 03 17:22:39 2003
PULPROG zgpg30
INSTRUM spect
PROBHD 5mm QNP 1H/13
P1 13.5
PC 1.50
PD 0.00
PF 0.62
RG 14

C:\WINNMR95\SDCHO\OXAZINE\OXA-

Fri Jan 03 14:11:39 2003

DATE
 13C
 EXPT
 75.45 MHz
 124.00 KHz
 1840.0 Hz
 32768
 20408.1 Hz
 181
 1.606 sec
 3.000 sec
 4.2 us
 18
 14.5 C
 CDCL3
 77.00 ppm
 0.15 Hz
 24

C:\WINNERS\SDCHO\OXAZINE\OXAZ

DEFILE
COMET
DATEIN
QENOC IN
EXMOD NON
OBFREQ
OBFSET
OBFIN
POINT
FREQ
SCANS
ACQTN
PD
PWI
IRFUC
CTEMP
SLVNT
EXREF
BP
RGAIN

C:\WINNMR95\3DCHEM\OKAZINE\OKA

DFILE
 COMPT
 DATIM
 CERNUC
 EXMDO
 OBPRO
 OBSET
 OBPTM
 POINT
 FREQD
 SCANS
 ACQTM
 PD
 PW1
 TRNUC
 CHMEP
 SLVNT
 EXREF
 BF
 RGAIN

ERI Jan 03 16:21:14 2003
 1H
 NON
 300.40 MHz
 130.00 KHz
 1150.0 Hz
 16384
 6013.2 Hz
 32
 2.725 sec
 1.551 sec
 5.6 us
 1H
 14.3 C
 CDCL3
 0.00 ppm
 0.62 Hz
 14

C:\WINNERS5\SDCHN\OXAZINE\OXA-

DEFILE
COMPT
DATIM
DEMOD
DEPRO
DESET
DEFIN
POINT
FREQ
SCANS
ACQTM
PD
FWI
IRNUC
CTEMP
SLVMT
EXREF
DF
NGAIN

F11 JAN 03 16:14:45 2003
13C
BCN

75.45 MHz
124.00 KHz
1840.0 Hz
32768

20408.1 Hz
94

1.506 sec
3.000 sec
4.2 us

1H
14.9 c

CDCLE
77.00 ppm
0.62 Hz
26

C:\WINNR95\9DCMO\OXAZINE\OXA-

DTITLE
CONRT
DATIN
QENUC
EXNOO
QENFRQ
QENSET
QENFIN
POINT
FREQU
SCANS
AQTN
PD
PMI
IRNUC
CTEMP
SLVNT
EXREF
BY
RGAIN

771 Jan 03 16:00:27 2003

13C
BCW

75.45 MHz

124.00 KHz

1840.0 Hz

32768

20408.1 Hz

228

1.606 sec

3.000 sec

4.2 us

1H

14.9 C

CDCL3

0.00 ppm

0.52 Hz

24

D:\WINNR95\SDCHO\OXAZINE\OXA-
 COMPT
 DATEM Fri Jan 03 14:22:28 2003
 OBRUC 13C
 EXMOD BOM

OBFNQ 75.45 MHz
 OBFSE7 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 51
 ACQTM 1.606 sec
 PD 3.000 sec
 PW1 4.2 us
 IRNUC 1H
 CTUNE 14.9 C
 STUNT CDCL3
 EXREF 77.00 ppm
 BP 0.15 Hz
 RGAIN 24

C:\WINNKS95\COMMON\DEFAULT.A

DFILE
 COMPT
 DATIM Wed Jan 15 11:14:10 2003
 CBRUC 1H
 EXMOD NON
 CBFRC 300.40 MHz
 CBFST 130.00 KHz
 CBFIN 1150.0 Hz
 POINT 16384
 FREQU 6013.2 Hz
 SCANS 8
 ACQTM 2.725 sec
 PD 1.551 sec
 PW1 5.6 us
 IRMDC 1H
 CTEMP 14.3 C
 SLVNT CDCL3
 EXRET 0.00 ppm
 BT 0.62 Hz
 RGAIN 15

```

DEFILE          CCENT          DATIM          CBNUC          EXMOD          CBFRQ          CBSET          CBFIN          POINT          FREQU          SCANS          ACQTH          PD          FMI          INNUC          CTMP          SLVNT          EXREF          BF          RGAIN

```

C:\WINNMR95\COMMON_DEFAULT.A

DFILE COMET
 DATIN Mon Jan 06 14:39:24 2003
 QMDC 1B
 EXMOD ROW
 ORFREQ 300.10 MHz
 ORSET 130.00 KHz
 ORPIN 1150.0 KHz
 POINT 16364
 FREQO 6013.2 KHz
 SCANS 16
 ACQTM 2.725 sec
 PD 1.551 sec
 PW1 5.6 us
 IRMDC 1H
 CTMPC 12.9 C
 SLVTC CDCl3
 EXREF 0.00 ppm
 BF 0.62 Hz
 RGAIN 13

C:\WINNMR95\COMMON\DEFAULT.AJ

DFILE COMET
 DATIM Mon Jan 06 14:28:43 2003
 ORNOC 13C
 EXMOD BOM
 OBTRQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQO 20408.1 Hz
 SCANS 53
 ACQTM 1.606 sec
 PD 3.000 sec
 PW1 4.2 us
 INNUC 1H
 CTMP 13.0 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.62 Hz
 RGAIN 26

D:\WINNMR95\COMMON\DEFAULT.AJ
 Mon Jan 06 15:15:39 2003

NAME: 13C
 EXPNO: 20408.1 Hz
 FREQ: 124.00 MHz
 PROC: 1.606 sec
 PD: 3.000 sec
 PULP: 4.2 us
 FWH: 1H
 T1RHO: 13.6 s
 CTDCP: CDCL3
 SLEWT: 0.00 ppm
 EXREF: 0.62 Hz
 RF: 24
 RGAIN:

75.45 MHz
 124.00 MHz
 1640.0 Hz
 32768
 20408.1 Hz
 245
 1.606 sec
 3.000 sec
 4.2 us
 1H
 13.6 s
 CDCL3
 0.00 ppm
 0.62 Hz
 24

C:\WINNR95\COMMON\DEFAULT.A

Tue Jan 28 19:10:06 2003

DETLE
 COMET
 DATIN
 CENUC 1H
 EXMOD NON
 OBSFQ 300.40 MHz
 OBSFET 130.00 kHz
 OBSFIN 1150.0 Hz
 POINT 16384
 PRGCU 6013.2 Hz
 SCANS 16
 ACQTM 2.725 sec
 PD 1.551 sec
 PW1 5.6 us
 TRNUC 1H
 CTMP 11.3 C
 SLANT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 16

C:\WINNERS5\COMMON\DEFAULT.AJ
 Tue Jan 28 19:07:06 2003
 DATE
 13C
 BOM

75.45 MHz
 124.00 KHz
 1840.0 Hz
 32768
 20408.1 Hz
 101
 1.506 sec
 3.000 sec
 4.2 us
 1H
 11.7 c
 CDCL3
 0.00 ppm
 0.12 Hz
 24

FILE C:\WINNR95\SDCE0\34.A18
 COUNT
 DATE Tue Jan 28 18:30:50 2003
 CERNUC 1H
 EXNO2 NON
 OBSFQ 300.40 MHz
 OBSFQ 130.00 MHz
 OBSFQ 1150.0 Hz
 POINT 16384
 FREQ 6013.2 Hz
 SCANS 16
 ACQTN 2.725 sec
 PD 1.551 sec
 PW 5.6 us
 CERNUC 1H
 CTMP 11.3 c
 SLVT CDCl3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 14

C:\WINNMR95\COMMON\DEFAULT.A

DFILE COMPT
 DATEM Tue Jan 28 18:22:20 2003
 CDETC 13C
 EXPROD BCU
 CDETC 75.45 MHz
 CDETC 124.00 KHz
 CDETC 1840.0 Hz
 CDETC 32766
 POINT 20408.1 Hz
 SCANS 64
 ACQTM 1.606 sec
 PD 3.000 sec
 PW 4.2 us
 TRNUC 1H
 CDETC 12.1 c
 SLEWT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 24

C:\WINNERS5\COMMON\DEFAULT.A

DFILE COMPT
 DATIM Thu Feb 13 05:24:44 2003
 QENDC 1H
 EXMOD NCV
 QBFREQ 300.10 MHz
 QBSSET 130.00 MHz
 QBPIN 1150.0 Hz
 POINT 16384
 FREQ 6013.2 Hz
 SCANS 16
 ACQTM 2.725 sec
 PD 1.561 sec
 PW1 5.6 us
 IRNDC 1H
 CTEND 16.7 c
 SLANT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 14

C:\WINNERS\COMMON\DEFAULT.A1

DFILE
 COMET
 DATIN
 OBNOC
 EXHOD
 BOM

Thu Feb 13 05:21:39 2003

75.45 MHz
 124.00 KHz
 1640.0 Hz
 32768
 20408.1 Hz
 218
 1.605 sec
 3.000 sec
 4.2 us
 1H
 17.2 C
 CDCL3
 77.00 ppm
 0.12 Hz
 26

C:\WINNERS5\COMMON\DEFAULT.AI

OFILE
 COMPT
 DATIN
 QNUC
 EXMOD
 QBFQ
 QBSY
 QBSY
 POINT
 FREQ
 SCANS
 ACQTH
 PD
 PUL
 IRNUC
 CTMP
 SLVNT
 EXREF
 RF
 RGAIN

Thu Feb 13 04:47:04 2003
 1H
 BOC
 300.40 MHz
 130.00 KHz
 1150.0 Hz
 16384
 6013.2 Hz
 10
 2.725 sec
 1.551 sec
 5.6 us
 1H
 16.6 c
 CDCl3
 0.00 ppm
 0.12 Hz
 17

C:\WINNMR95\호수봉\COCAINE\OXA-

DFILE
 CONNT
 DATA
 CHNUC
 EXMOD
 QBFREQ
 QMSEF
 QBFIN
 POINT
 FREQ
 SCANS
 ACQTS
 PD
 PW1
 IRNUC
 CTMP
 SLVNT
 EXREF
 BF
 RGAIN

Thu Feb 13 04:59:33 2003
 13C
 BOM
 75.45 MHz
 124.00 KHz
 1849.0 Hz
 32768
 20406.1 Hz
 129
 1.606 sec
 3.000 sec
 4.2 us
 1H
 17.4 C
 CDCL3
 0.00 ppm
 0.12 Hz
 26

000111-1A-Chol. in CDCl₃ 25degC
Pulse Sequence: zgpg30

in CDCl₃

840-3-013
 Pulse Sequence: zgpg30
 Solvent: CDCl3
 Temp: 25.0 C / 298.1 K
 User: j-14-47
 File: 840-3-013
 INOVA-600 1H-13C-500
 Relax: 40102 1.000 sec
 Pulse 50.3 degrees
 Acq. time 1.340 sec
 Width 23499.9 Hz
 F2: 234.999 MHz
 F1: 125.761 MHz
 DECOUPLE: 13C, 125.761 MHz
 Power 12.00
 Continuously on
 13C: 125.761 MHz
 1H: 400.146 MHz
 F1: 400.146 MHz
 F2: 125.761 MHz
 Total time 6 hr, 14 min, 50 sec

```

DEFILE
COUNT
DATIM
OEMOC
EXMOO
OEFRO
OEBET
OEBIN
POINT
FREQU
SCANS
ACQTN
PD
PW1
LINUC
CTEMP
SLVHT
ECREF
BT
RGAIN

```

Chemical shift (ppm)	Integration	Assignment
300.40 MHz	16	CDLH3
130.00 MHz	2.725 sec	
1150.0 Hz	1.551 sec	1H
16384	5.6 us	
6013.2 Kz	13.3 c	
	0.00 ppm	
	0.62 Hz	
	19

C:\WINNER95\SDCHO\VOXAZINE\VOXA-

DETAILS
 COMMENT
 DATE
 QNAME
 QINSTR
 QPROG
 QP1
 QP2
 QP3
 QP4
 QP5
 QP6
 QP7
 QP8
 QP9
 QP10
 QP11
 QP12
 QP13
 QP14
 QP15
 QP16
 QP17
 QP18
 QP19
 QP20
 QP21
 QP22
 QP23
 QP24
 QP25
 QP26
 QP27
 QP28
 QP29
 QP30
 QP31
 QP32
 QP33
 QP34
 QP35
 QP36
 QP37
 QP38
 QP39
 QP40
 QP41
 QP42
 QP43
 QP44
 QP45
 QP46
 QP47
 QP48
 QP49
 QP50
 QP51
 QP52
 QP53
 QP54
 QP55
 QP56
 QP57
 QP58
 QP59
 QP60
 QP61
 QP62
 QP63
 QP64
 QP65
 QP66
 QP67
 QP68
 QP69
 QP70
 QP71
 QP72
 QP73
 QP74
 QP75
 QP76
 QP77
 QP78
 QP79
 QP80
 QP81
 QP82
 QP83
 QP84
 QP85
 QP86
 QP87
 QP88
 QP89
 QP90
 QP91
 QP92
 QP93
 QP94
 QP95
 QP96
 QP97
 QP98
 QP99
 QP100
 QP101
 QP102
 QP103
 QP104
 QP105
 QP106
 QP107
 QP108
 QP109
 QP110
 QP111
 QP112
 QP113
 QP114
 QP115
 QP116
 QP117
 QP118
 QP119
 QP120
 QP121
 QP122
 QP123
 QP124
 QP125
 QP126
 QP127
 QP128
 QP129
 QP130
 QP131
 QP132
 QP133
 QP134
 QP135
 QP136
 QP137
 QP138
 QP139
 QP140
 QP141
 QP142
 QP143
 QP144
 QP145
 QP146
 QP147
 QP148
 QP149
 QP150
 QP151
 QP152
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C:\winmr95\spchov\oxazine\oxa-

Thu Jan 02 20:02:50 2003

1H

EXMOD

NOE

300.40 MHz

130.00 MHz

1150.0 Hz

16384

6013.2 Hz

16

2.725 sec

1.551 sec

5.6 us

1H

IRNUC

CTEMP

13.2 C

CDCL3

0.00 ppm

0.62 Hz

19

RGAIN

in CDCl₃

DFILE

COMPT

DATIN

OBNUC

EXMOD

NOE

OBPRQ

OBSET

OBFIN

POINT

FREQD

SCANS

ACQTM

PD

FM1

IRNUC

CTEMP

SLVNT

EXREF

RF

RGAIN

D:\WINMR95\SDCHO\OXAZINE\OKA-
 CONFT
 DATIM
 Thu Jan 02 20:28:53 2003
 L3C
 ORNUC
 EXPROD BOM

75.45 MHz
 124.00 KHz
 1840.0 Hz
 32768
 20408.1 Hz
 256
 1.606 sec
 3.000 sec
 4.2 us
 1H
 13.7 C
 CUXL3
 77.00 ppm
 0.62 Hz
 24

in CDCl₃

C:\WINNIE95\SDCINO\OXAZINE\OXAZ-

DFILE
COMMT
DATEM
OBNUC
EXMOD
OBTRO
OBSST
OBSIN
POINT
FREQ
SCANS
ACQTH
PD
PWL
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

Fri Jan 03 17:48:44 2003
1H
NM

300.40 MHz
130.00 MHz
1150.0 Hz
16384
6013.2 Hz
16
2.725 sec
1.551 sec
5.6 us
1H
13.5 c
CDCL3
0.00 ppm
0.62 Hz
10

in CDCl₃

C:\WINNR95\COMMON\DEFAULT.AJ

Wed Jan 15 11:49:02 2003

1H

MON

300.40 MHz

130.00 KHz

1150.0 Hz

16384

6013.2 Hz

16

2.725 sec

1.551 sec

5.6 us

1H

IRNOC

13.4 C

CDCL3

0.00 ppm

0.62 Hz

15

in CDCl₃

DFILE

CONDT

DATIN

OBNUC

EXMOC

CEFTQ

OBSET

OBFIN

POINT

FREQD

SCANS

ACQTH

PD

FW1

IRNOC

CTEMP

SLVNT

EXREF

RF

RGAIN

C:\WINNR95\COMMON\DEFAULT.AI

DFILE
 COMPT
 DATIM Wed Jan 15 11:58:02 2003
 CBNUC 13C
 EXMOD BCP
 OBSFQ 75.45 MHz
 OBSFQ 124.00 MHz
 OBSFQ 1640.0 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 40
 ACQTM 1.606 sec
 PD 3.000 sec
 PW 4.2 us
 IRNUC 1H
 CTMPC 13.6 C
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.52 Hz
 RGAIN 24

in CDCl₃

D:\WINNMR95\COMMON\DEFAULT.AL
 Wed Jan 15 12:10:22 2003
 QMNOG 13C
 EXMOD BCM

QMFRQ 75.45 MHz
 QMSET 124.00 MHz
 QMFIN 1840.0 Hz
 POINT 32768
 FREQ0 20408.1 Hz
 SCANS 56
 ACQTN 1.606 sec
 PD 3.000 sec
 PUL 4.2 us
 IRMOC 1H
 CTMP 13.9 C
 CDCL3
 SMT 77.00 ppm
 EXREF 0.62 Hz
 RF 24
 RGAIN

C:\WINNMR55\8DCHO\OXA2\FINE\OXA-

Thu Jan 02 10:33:13 2003

1H

NON

300.40 MHz

130.00 KHz

1150.0 Kz

16384

6013.2 Kz

16

2.725 sec

1.551 sec

5.6 us

13.3 c

0.00 ppm

0.62 Hz

13

in CDCl₃

DEFILE
COMMIT
DATE
GEMUC
EXMDO
OBSFNG
OBSST
OBSFIN
POINT
FREQ
SCANS
ACQTM
PD
PM1
IRADC
CTEMP
SLVNT
EXREF
BF
RGAIN

0.006
0.000
0.129
1.042
1.080
1.144
1.170
1.334
1.651
1.689
1.843
2.074

3.969
3.796
3.772
4.940
4.824
4.817
4.797

7.928
7.914
7.425
7.291
7.265
7.149
7.056
7.051
7.040
7.034
7.031
7.015

DFILE COMINT DATIM CBNUC ECHOD OBERQ OBSET OBFIN POINT FREQU SCANS ACQTM PD PW1 IRRUC CTEMP SLVNT EXREF BY RGAIN

in CDCl_3

D:\WINNMR95\90CHO\OXA2INE\OXA-
 F11 Jan 03 12:21:01 2003
 13C
 EXM00 BCM

OBFTQ 75.45 MHz
 OBSET 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 FREQ0 20408.1 Hz
 SCANS 100
 ACQTM 1.606 sec
 PD 3.000 sec
 PUL 4.2 us
 1H
 INNUC 14.5 C
 CDCL3
 SLWT 0.00 ppm
 EXREF 0.62 Hz
 RF 26
 RGAIN

in CDCl₃

C:\WINNER55\SDCHO\OXAZINE\OXA-

DFILE
 COMPT
 DATIN
 CBNOC
 EXMOD
 OBFTQ
 OBSET
 OBFTN
 POINT
 FREQ
 SCANS
 ACQTM
 PD
 PM1
 TRMUC
 CTZMF
 BLVNT
 EXREF
 BF
 NGRIN

300.40 MHz
 130.00 MHz
 1150.0 Hz
 32768
 6013.2 Hz
 32
 5.449 sec
 1.500 sec
 5.6 us
 1H
 19.3 C
 CDCL3
 0.00 ppm
 0.62 Hz
 17

in CDCl₃

D:\WINNERS\SDCHO\OXAZINE\OXA-
 COUNT
 DATEM Jan 02 19:22:39 2003
 QMNO 13C
 EXMO BOM

75.45 MHz
 124.00 MHz
 1840.0 Hz
 32768
 20408.1 Hz
 256
 1.606 sec
 3.000 sec
 4.2 us
 13.7 °
 CDCL3
 0.00 ppm
 0.62 Hz
 24

in CDCl₃

C:\WINNER95\9DCHO\OXAZINE\OXA-

DFILE
COMET
DATEIN
OBNUC
OBNUC
EXMOD
OBFREQ
OBSSET
OBSSET
OBSSET
POINT
FREQU
SCANS
ACQTM
ED
PWL
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

Pr1 Jan 03 10:12:22 2003
1R
NON
300.40 MHz
130.00 kHz
1150.0 Hz
16384
6013.2 Hz
16
2.725 sec
1.551 sec
5.6 us
1R
13.2 c
CDCL3
0.00 ppm
0.62 Hz
16

C:\WINNER95\SDCHO\0323\NEWONA-

DFILE
COMET
DATEM
GBMUC
EXMOD
OBPFO
OBSET
OBFIN
POINT
FREQ
SCANS
ACQTM
PD
FWI
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

75.45 MHz
124.00 KHz
1840.0 Hz
32768
20408.1 Hz
213
1.606 sec
3.000 sec
4.2 us
18
14.6 c
CDCl3
0.00 ppm
0.62 Hz
26

in CDCl₃

D:\WINNMR95\COMMON\DEFAULT.AL

COMPT Thu Jan 02 16:55:59 2003

QBRUC 1B

EXMOD MON

OBFRQ 300.40 MHz

OBSET 130.00 KHz

OBFIN 1150.0 Hz

POINT 32768

FREQ2 6013.2 Hz

SCANS 16

ACQTM 5.449 sec

PD 1.551 sec

FW1 5.6 us

IRRUC 1H

CTEMP 13.2 C

SLVNT CDCL3

EXREF 0.00 ppm

RF 0.62 Hz

RGAIN 12

in CDCl₃

C:\WINNMR95\SPCH0\OXAZINE\OXA-

Thu Jan 02 17:26:29 2003

13C
BCR

QBPFRQ 75.45 MHz

QBPFRQ 124.00 KHz

QBPFRQ 1840.0 Hz

POINT 32768

FREQD 20408.1 Hz

SCANS 211

ACQTM 1.506 sec

PD 3.000 sec

PM1 4.2 us

IRNUC 1H

CTEMP 13.9 c

SLVNT CDCL3

EXREF 77.00 ppm

RF 0.62 Hz

RGAIN 24

in CDCl₃

DFILE
COUNT
DATIM
ORNUC
EXMOD
OBFRO
OBSBY
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PWL
IRNUC
CTENE
SLVNT
EXREF
BT
RGAIN

000'0—

1.584
1.563

2.943
2.918
2.893
2.870
2.845

ZARDO	300.40 MHz
OBFRQ	130.00 KHz
OBSET	1150.0 Hz
OBFIN	16384
POINT	5013.2 Hz
FREQO	16
SCANS	2.725 sec
ACQTM	1.551 sec
FW	5.6 us
PD1	
IRNUC	1R
GRNPE	
SLVNT	CDCL3
EXREF	13.2 C
BF	0.00 ppm
RGAIN	0.62 Hz
	8

C:\WINNMR55\SDCHO\OXA2INE\OXA-
 FILE
 COMPT
 DATIN
 QMNUC
 EXMOD
 CBPRQ
 CBSET
 QBFIN
 POINT
 FREQ
 SCANS
 ACQTM
 PD
 PWL
 IRNUC
 CTMRP
 BLVRT
 XREF
 RF
 RGMN

Fri Jan 03 12:49:35 2003
 13C
 BCM
 75.45 MHz
 124.00 KHz
 1840.0 Hz
 32768
 20409.1 Hz
 53
 1.606 sec
 3.000 sec
 4.2 us
 1H
 14.7 C
 CDCL3
 77.00 ppm
 0.62 Hz
 25

C:\WINNER95\SDCHO\OXAZINE\OXA-

DEFILE
 COMMT
 DATIM
 OBNUC
 EXMOD
 OBSFRQ
 OBSSET
 OBSFIN
 POINT
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 SCANS
 ACQTM
 PD
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 IRNUC
 CTMP
 SLVNT
 EXREF
 RF
 RGAIN

Thu Jan 02 19:52:06 2003

1H

NON

300.40 MHz
 130.00 KHz
 1150.0 Hz
 16384
 6013.2 Hz
 16
 2.725 sec
 1.551 sec
 5.6 us
 1H
 13.3 C
 CDCL3
 0.00 ppm
 0.62 Hz
 19

in CDCl₃

C:\WINNERS\COMMON\DEFAULT.AL

DFILE
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2003
 13C
 BOM
 75.45 MHz
 124.00 KHz
 1840.0 Hz
 32768
 20408.1 Hz
 128
 1.606 sec
 3.000 sec
 4.2 us
 1H
 14.6 c
 CDCL3
 77.00 ppm
 0.62 Hz
 24

in CDCl₃

FILE C:\WINNMR55\SPCH04\19.ATL
 COMMENT
 DATEIN Tue Jan 20 19:55:08 2003
 CHNAC 1H
 EXPOD 1H
 EXPOD 1H

300.40 MHz
 130.00 MHz
 1150.0 Hz
 16384
 6013.2 Hz
 2.725 sec
 1.551 sec
 5.6 us
 1H
 10.9 C
 CDCL3
 0.00 ppm
 0.12 Hz
 9

in CDCl₃

C:\WINNER95\COMMON\DEFAULT.AL

Tue Jan 20 19:51:23 2003

13C

EXPOD BCU

75.45 MHz

124.00 KHz

1840.0 Hz

32768

20408.1 Hz

21

1.606 sec

3.000 sec

4.2 us

1H

12.1 c

CDCL3

77.00 ppm

0.12 Hz

25

DEFILE
COUNT
DATEIN
QENDC
EXPOD
QBFREQ
QBFREQ
QBFREQ
POINT
FREQO
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

in CDCl₃

C:\WINNER95\COMMON\DEFAULT.A

Thu Feb 13 02:29:56 2003

DETAIL
 COUNT
 DATEIN
 CHNUC 1H
 EXMOD NMR
 OBSFQ 300.40 MHz
 OBSFQ 130.00 KHz
 OBSFQ 1150.0 KHz
 POINT 16384
 FREQ0 6013.2 Hz
 SCANS 16
 ACQTM 2.725 sec
 PD 1.551 sec
 PUL 5.6 us
 1H
 TENDC 17.5 c
 CTENDP CDCL3
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 9

in CDCl₃

DF112 C:\WINNMR95\COMMON\DEFAULT.AL

COMET Thu Feb 13 02:26:34 2003

QBMUC 13C
BON

QBFREQ 75.45 MHz
QBSZT 124.00 kHz
QBFIN 1840.0 Hz

POINT 32768
FREQI 20408.1 Hz
SCANS 38

ACQTN 1.606 sec
PD 3.000 sec
PM1 4.2 us

IRNUC 1H
CTEMP 17.9 C
SLVNT CDCL3

EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24

in CDCl₃

C:\MINI695\COMMON\DEFAULT.AL

DFILE
 COMPT
 DATIN
 OBSID
 EXMOD
 OBPRO
 OBRET
 OBFIN
 POINT
 FREQ
 SCANS
 ACQTS
 PD
 PML
 IRMOC
 CTMPC
 SLVNT
 EXREF
 BE
 REACH

Tue Jan 28 18:53:45 2003
 13C
 BCM

75.45 MHz
 124.00 KHz
 1840.0 Hz
 32768
 20408.1 Hz
 81
 1.606 sec
 3.000 sec
 4.2 us

1H
 12.3 C
 CDCL3
 77.00 ppm
 0.12 Hz
 25

in CDCl₃

C:\WINNERS95\SDCHQ\33.ALS
 DFILF
 COMPT
 DATIM
 CBRUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQ
 SCANS
 ACQTN
 PD
 PM1
 IRRUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

Tue Jan 28 17:50:34 2003
 1R
 NON
 300.40 MHz
 130.00 KHz
 1150.0 Hz
 16384
 6019.2 Hz
 16
 2.725 sec
 1.551 sec
 5.6 us
 1R
 12.2 C
 CDCL3
 0.00 ppm
 0.12 Hz
 12

DFILE C:\WINNERS5\COMMON\DEFAULT.A1

COMNT Tue Jan 28 17:43:28 2003

CHRG 13C

EXMOD BOM

OBFRQ 75.45 MHz

OBSET 124.00 KHz

OBFTN 1840.0 Hz

POINT 32768

FREQ 20408.1 Hz

SCANS 42

ACQTH 1.606 sec

PD 3.000 sec

PM 4.2 us

IRNUC 1H

CTMP 12.2 c

SLUNT CDCL3

EXREF 77.00 ppm

BF 0.12 Hz

RGAIN 25

C:\WINNMR95\COMMON\DEFAULT.AL

Thu Feb 13 01:46:41 2003

NAME 1K
 EXMOD NON
 QBFREQ 300.40 MHz
 QBSFREQ 130.00 MHz
 QBSFREQ 1150.0 Hz
 POINT 16384
 FREQ 6013.2 Hz
 SCANS 11
 ACQTIME 2.725 sec
 PD 1.551 sec
 PW 5.6 us
 IRFREQ 1H
 CTBPF 16.9 C
 SLVNT CDCL3
 EXREF 0.00 ppm
 RF 0.12 Hz
 RGAIN 14

in CDCl₃

C:\WINNER95\COMMON\DEFAULT.AL

DFILE
 COUNT
 DATE
 TIME
 OBNO
 EXNO
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 INRUC
 CTENP
 BLUNT
 EXDEF
 BF
 REBIN

0.008
 67.853
 76.672
 77.092
 77.521
 118.803
 124.416
 125.363
 126.504
 129.344
 130.308
 134.759
 141.970
 151.316
 163.052

in CDCl₃

C:\WINNMR95\COMMON_DEFAULT.AI

Thu Feb 13 01:58:25 2003

IN 300.40 MHz
 QMDC 130.00 MHz
 QMDC 1150.0 Hz
 POINT 16384
 FREQ 6013.2 Hz
 SCANS 16
 ACQTM 2.725 sec
 PD 1.551 sec
 PW1 5.6 us
 INDC 1H
 CTMP 16.3 C
 CLV1 CDCL3
 EXRF 0.00 ppm
 BF 0.12 Hz
 RGAIN 1.4

in CDCl₃

DFILE
 COMET
 DATIN
 QMDC
 QMDC
 EXDC
 QMDC
 QMDC
 POINT
 FREQ
 SCANS
 ACQTM
 PD
 PW1
 INDC
 CTMP
 CLV1
 EXRF
 BF
 RGAIN

C:\WINNERS5\COMMON\DEFAULT.AL

DFTILE
 COMPT
 DATIN
 OBNDIC
 EXMOD
 OBSFQ
 OBSRT
 OBSFIN
 POINT
 FREQ
 SCANS
 ACQTH
 PD
 BW
 IRFUC
 CTBPF
 SLVNT
 EXREF
 RF
 NGAIN

0.000
 16.937
 74.340
 76.639
 77.059
 77.480
 118.754
 124.177
 125.743
 128.504
 129.479
 130.243
 135.286
 142.036
 151.127
 165.706

Thu Feb 13 02:16:08 2003
 13C
 BCM

75.45 MHz
 128.00 MHz
 1840.0 Hz
 32768
 20406.1 Hz
 128
 1.606 sec
 3.000 sec
 4.2 us
 17.3 C
 CDCL3
 0.00 ppm
 0.12 Hz
 25

in CDCl₃

NOE(2D NMR) for 1-Benzyl-1H-pyrido[2,3-b][1.4]oxazin-2-one (4a)

020911-NOESY-Cho1 mix=100ms in cdc13 25degC
Pulse Sequence: noesy