

Oxidative coupling of 1-(2-methyl-4-phenylquinolin-3-yl)ethanone with ethanol and unexpected deacetylative synthesis of 3-hydroxy quinoline

Parul Chauhan,^a Makthala Ravi,^a Ruchir Kant,^b Prem. P. Yadav^{*a}

^a*Divisions of Medicinal and Process Chemistry, CSIR-Central Drug Research Institute, Lucknow- 226001, India.*

^b*Division of Molecular and Structural Biology, CSIR-Central Drug Research Institute, Lucknow-226031, India.*

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General Experimental Details:

^1H NMR and ^{13}C NMR spectra were recorded on Bruker Avance-400 using CDCl_3 and DMSO- d_6 as solvent and tetramethylsilane as internal reference. Splitting patterns are described as singlet (s), doublet (d), triplet (t), multiplet (m) and broad (br). IR spectra were recorded on a FT-IR spectrophotometer and melting points were determined on melting point apparatus and are uncorrected.. Electrospray ionization mass spectrometry (ESI-MS) was obtained on Thermo LCQ Advantage Max Spectrometer and HRMS was recorded on Agilent 6520 Q-TOF. Reactions were monitored on silica gel TLC plates (coated with TLC grade silica gel, obtained from Merck). All glass apparatus were oven dried prior to use. Column chromatography was performed over silica gel (230-400 Mesh) by using Smart flash EPCLC AI-700X YAMAZEN with minimal amount of solvent. All chemicals and reagents were obtained from Aldrich (USA) and Alfa Aesar (England) and were used without further purification.

General procedure for the synthesis of product 2:

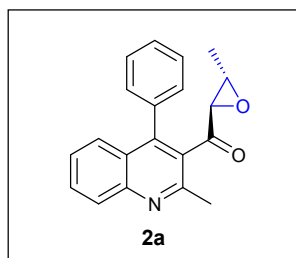
Take solution of 1-(2-methyl-4-phenylquinolin-3-yl)ethanone **1** (1.0 mmol), N-bromosuccinimide (1.5 mmol), tert-butyl hydroperoxide (5 mmol) and potassium carbonate (3.0 mmol) in ethanol (20 mL) was stirred at room temperature for 24 hours. Next, the ethanol was removed under reduced pressure and the crude of reaction was diluted with water (80 mL). The aqueous layer was extracted with ethylacetate (3×20 mL) three times. The organic layer was further dried over sodium sulphate (anhydrous) and removed under reduced pressure to give crude product, which further purified by column chromatography over silica gel afforded the desired product **2a-2r**.

General procedure for the synthesis of product 5:

Take solution of 1-(2-methyl-4-phenylquinolin-3-yl)ethanone **1** (1.0 mmol), N-bromosuccinimide (1.5 mmol) and potassium carbonate (3.0 mmol) in methanol (20 mL) was stirred at room temperature for 6 hours. Next, the methanol was removed under reduced pressure and the crude of reaction was diluted with water (80 mL). The aqueous layer was extracted with ethylacetate (3×20 mL) three times. The organic layer was further dried over sodium sulphate (anhydrous) and removed under reduced pressure to give crude product, which further purified by column chromatography over silica gel afforded the desired product **5a-5h**.

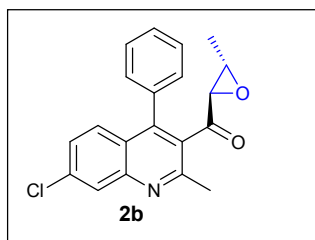
Compound Characterization Data:

(2-methyl-4-phenylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2a):



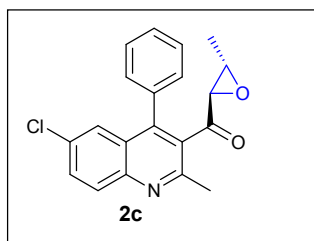
Yield 78% as white solid: mp 100-102°C; FT-IR (KBr, cm^{-1}) 3019, 1635, 1215, 1069; ^1H NMR (400 MHz, CDCl_3) δ 1.06 (d, $J = 5.12$ Hz, 3H), 2.70-2.77 (m, 4H), 3.07 (d, $J = 1.80$ Hz, 1H), 7.32-7.34 (m, 1H), 7.47-7.52 (m, 2H), 7.53-7.59 (m, 3H), 7.65-7.68 (dd, $J = 8.4, 0.8$ Hz, 1H), 7.75-7.79 (m, 1H), 8.12 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.57 (CH_3), 23.98 (CH_3), 56.89 (CH), 60.21 (CH), 124.81 (C), 126.19 (CH), 127.49 (CH), 128.99 (CH), 129.12 (CH), 129.17 (CH), 129.57 (CH), 130.46 (CH), 130.69 (CH), 131.15 (CH), 131.72 (C), 134.74 (C), 145.69 (C), 147.70 (C), 154.16 (C) 203.26 (C); ESI-MS (m/z) 304 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{18}\text{NO}_2$ ($\text{M} + \text{H}$) $^+$ 304.1338, found 304.1330.

(7-chloro-2-methyl-4-phenylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2b):



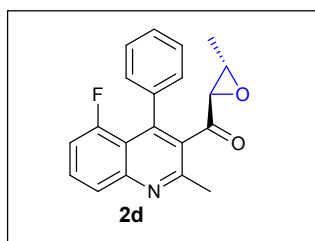
Yield 63% as white solid: mp 114-116°C; FT-IR (KBr, cm^{-1}) 3019, 1644, 1215, 1069; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 0.97 (d, $J = 5.04$ Hz, 3H), 2.60-2.65 (m, 4H), 3.41 (d, $J = 1.80$ Hz, 1H), 7.29-7.32 (m, 1H), 7.42-7.44 (m, 1H), 7.51-7.62 (m, 5H), 8.10 (d, $J = 2.04$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.55 (CH_3), 24.02 (CH_3), 56.94 (CH), 60.15 (CH), 123.59 (C), 127.72 (CH), 128.09 (CH), 128.31 (CH), 129.09 (CH), 129.26 (CH), 129.78 (CH), 130.42 (CH), 130.64 (CH), 131.97 (C), 134.24 (C), 135.86 (C), 145.85 (C), 148.08 (C), 155.87 (C) 202.96 (C); ESI-MS (m/z) 338 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{17}\text{ClNO}_2$ ($\text{M} + \text{H}$) $^+$ 338.0948, found 338.0933.

(6-chloro-2-methyl-4-phenylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2c):



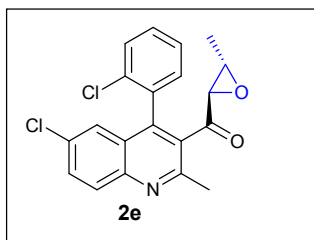
Yield 72% as white solid: mp 142-143°C; FT-IR (KBr, cm^{-1}) 3019, 1636, 1215, 1068; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 0.99 (d, $J = 5.04$ Hz, 3H), 2.60 (s, 3H), 2.63-2.66 (m, 1H), 3.43 (d, $J = 1.84$ Hz, 1H), 7.31-7.33 (m, 1H), 7.42-7.46 (m, 2H), 7.56-7.64 (m, 3H), 7.84-7.87 (dd, $J = 8.96, 2.4$ Hz, 1H), 8.08 (d, $J = 8.96$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 17.57 (CH_3), 23.97 (CH_3), 56.97 (CH), 60.12 (CH), 124.72 (CH), 125.79 (C), 129.20 (CH), 129.36 (CH), 129.89 (CH), 130.42 (CH), 130.62 (CH), 131.41 (CH), 131.66 (CH), 131.97 (C), 132.49 (C), 134.01 (C), 144.98 (C), 146.14 (C), 154.98 (C), 203.01 (C); ESI-MS (m/z) 338 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{17}\text{ClNO}_2$ ($\text{M} + \text{H}$) $^+$ 338.0948, found 338.0947.

(5-fluoro-2-methyl-4-phenylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2d):



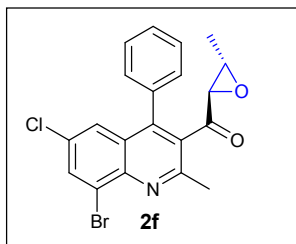
Yield 70% as white solid: mp 75-78°C; FT-IR (KBr, cm^{-1}) 3019, 1637, 1215, 1069; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 1.02 (d, $J = 5.04$ Hz, 3H), 2.54-2.56 (m, 1H), 2.58 (s, 3H), 3.44 (d, $J = 1.64$ Hz, 1H), 7.28-7.34 (m, 2H), 7.40 (brd, 1H), 7.43-7.49 (m, 3H), 7.79-7.84 (m, 1H), 7.92 (d, $J = 8.36$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 17.59 (CH_3), 23.83 (CH_3), 56.91 (CH), 60.07 (CH), 112.85 (d, $J = 21.32$ Hz, CH), 115.30 (C), 125.67 (CH), 128.19 (2 \times CH), 128.98 (CH), 129.43 (CH), 129.68 (CH), 131.32 (d, $J = 9.62$ Hz, CH), 133.79 (C), 136.85 (C), 142.70 (C), 148.97 (C), 154.85 (C), 159.76 (d, $J = 256.54$ Hz, C-F), 203.07 (C); ESI-MS (m/z) 322 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{17}\text{FNO}_2$ ($\text{M}+\text{H}$) $^+$ 322.1243, found 322.1239.

(6-chloro-4-(2-chlorophenyl)-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2e):



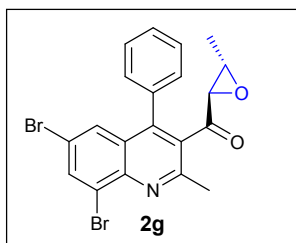
Yield 66% as white solid: mp 162-164°C; FT-IR (KBr, cm^{-1}) 3019, 1637, 1215, 1071; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 1.12 (d, $J = 5.04$ Hz, 3H), 2.66 (s, 3H), 2.73-2.77 (m, 1H), 3.62 (d, $J = 1.72$ Hz, 1H), 7.16 (d, $J = 2.28$ Hz, 1H), 7.49-7.52 (dd, $J = 7.52, 1.80$ Hz, 1H), 7.57-7.66 (m, 2H), 7.71-7.73 (dd, $J = 7.8, 1.08$ Hz, 1H), 7.87-7.89 (dd, $J = 8.96, 2.32$ Hz, 1H), 8.12 (d, $J = 8.96$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.59 (CH_3), 24.06 (CH_3), 57.21 (CH), 59.80 (CH), 124.30 (CH), 125.46 (C), 128.05 (CH), 130.35 (CH), 131.54 (CH), 131.95 (CH), 132.06 (CH), 132.33 (C), 132.54 (CH), 132.68 (C), 132.83 (C), 133.21 (C), 142.10 (C), 146.03 (C), 155.25 (C) 201.76 (C); ESI-MS (m/z) 372 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{16}\text{Cl}_2\text{NO}_2$ ($\text{M}+\text{H}$) $^+$ 372.0558, found 372.0551..

(8-bromo-6-chloro-2-methyl-4-phenylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2f):



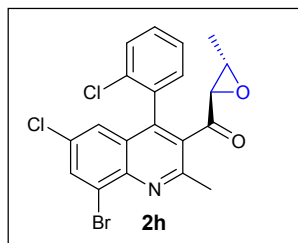
Yield 64% as light yellow solid: mp 142-144°C; FT-IR (KBr, cm^{-1}) 3019, 1637, 1215, 1069; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 1.00 (d, $J = 5.04$ Hz, 3H), 2.63-2.65 (m, 4H), 3.44 (d, $J = 1.8$ Hz, 1H), 7.31-7.33 (m, 1H), 7.41-7.45 (m, 2H), 7.56-7.64 (m, 3H), 8.33 (d, $J = 2.24$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.55 (CH_3), 24.25 (CH_3), 56.99 (CH), 60.07 (CH), 124.91 (CH), 125.91 (C), 126.77 (C), 129.20 (CH), 129.35 (CH), 130.04 (CH), 130.43 (CH), 130.67 (CH), 131.68 (C), 133.26 (C), 133.69 (C), 134.32 (CH), 143.08 (C), 145.74 (C), 156.00 (C) 202.66 (C); ESI-MS (m/z) 416 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{16}\text{BrClINO}_2$ ($\text{M}+\text{H}$) $^+$ 416.0053, found 416.0057.

(6,8-dibromo-2-methyl-4-phenylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2g):



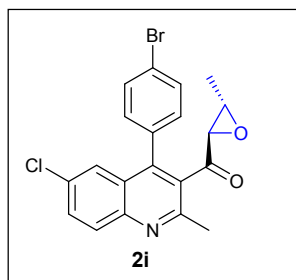
Yield 69% as light yellow solid: mp 141-143°C; FT-IR (KBr, cm^{-1}) 3019, 1637, 1210, 1069; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 1.01 (d, $J = 4.88$ Hz, 3H), 2.66 (m, 4H), 3.46 (s, 1H), 7.34 (d, $J = 5.44$ Hz, 1H), 7.46 (d, $J = 6.68$ Hz, 1H), 7.58-7.62 (m, 4H), 8.42 (d, $J = 1.64$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.52 (CH_3), 24.26 (CH_3), 57.04 (CH), 60.06 (CH), 119.93 (C), 125.92 (C), 127.32 (C), 128.14 (CH), 129.20 (CH), 129.35 (CH), 130.06 (CH), 130.40 (CH), 130.64 (CH), 133.23 (C), 133.65 (C), 136.62 (CH), 143.24 (C), 145.61 (C), 156.08 (C) 202.66 (C); ESI-MS (m/z) 462 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{16}\text{Br}_2\text{NO}_2$ ($\text{M}+\text{H}$) $^+$ 461.9527, found 461.9526.

(8-bromo-6-chloro-4-(2-chlorophenyl)-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2h):



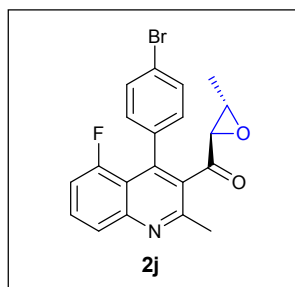
Yield 65% as light yellow solid: mp 138-140°C; FT-IR (KBr, cm^{-1}) 3019, 1635, 1215, 1068; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 1.12 (d, $J = 5.04$ Hz, 3H), 2.69 (m, 3H), 2.73-2.77 (m, 1H), 3.63 (d, $J = 1.6$ Hz, 1H), 7.17 (d, $J = 2.16$ Hz, 1H), 7.49-7.51 (dd, $J = 7.48, 1.64$ Hz, 1H), 7.57-7.66 (m, 2H), 7.70-7.72 (dd, $J = 7.84, 0.92$ Hz, 1H), 8.35 (d, $J = 2.16$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.57 (CH_3), 24.35 (CH_3), 57.25 (CH), 59.75 (CH), 124.42 (CH), 126.05 (C), 126.39 (C), 128.07 (CH), 130.37 (CH), 132.16 (C), 132.23 (CH), 132.34 (C), 132.55 (CH), 132.80 (C), 134.03 (C), 134.66 (CH), 142.83 (C), 143.01 (C), 156.32 (C) 201.45 (C); ESI-MS (m/z) 450 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{15}\text{BrCl}_2\text{NO}_2$ ($\text{M}+\text{H}$) $^+$ 449.9663, found 449.9650.

(4-(4-bromophenyl)-6-chloro-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2i):



Yield 71% as light yellow solid: mp 140-142°C; FT-IR (KBr, cm^{-1}) 3019, 1700, 1215, 1070; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 1.06 (d, $J = 5.04$ Hz, 3H), 2.61 (s, 3H), 2.75-2.79 (m, 1H), 3.47 (d, $J = 1.84$ Hz, 1H), 7.28-7.31 (dd, $J = 8.12, 2.16$ Hz, 1H), 7.40-7.44 (m, 2H), 7.78-7.89 (m, 3H), 8.09 (d, $J = 8.92$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.44 (CH_3), 23.96 (CH_3), 56.98 (CH), 60.13 (CH), 123.60 (C), 124.60 (CH), 125.51 (C), 131.41 (CH), 131.80 (CH), 132.20 (C), 132.26 (C & CH), 132.35 (CH), 132.49 (CH), 132.82 (CH), 132.21 (C), 143.94 (C), 146.13 (C), 154.99 (C), 203.00 (C); ESI-MS (m/z) 416 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{16}\text{BrClNO}_2$ ($\text{M}+\text{H}$) $^+$ 416.0053, found 416.0055.

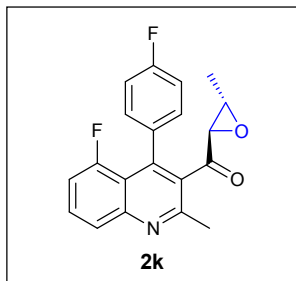
(4-(4-bromophenyl)-5-fluoro-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2j):



Yield 63% as light yellow solid: mp 102-104°C; FT-IR (KBr, cm^{-1}) 3019, 1619, 1215, 1069; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 1.09 (d, $J = 5.04$ Hz, 3H), 2.59 (s, 3H), 2.69-2.73 (m, 1H), 3.48 (d, $J = 1.76$ Hz, 1H), 7.27-7.29 (dd, $J = 8.04, 2.08$ Hz, 1H), 7.32-7.38 (m, 2H), 7.66-7.72 (m, 2H), 7.81-7.86 (m, 1H), 7.93 (d, $J = 7.84$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 17.47 (CH_3), 23.85 (CH_3), 57.02 (CH), 60.08 (CH), 112.96 (d, $J = 21.27$ Hz, CH), 115.11 (d, $J = 8.96$ Hz, C), 122.64 (CH), 125.76 (CH), 131.19 (2 \times CH), 131.37 (C), 131.49 (CH), 131.95 (CH), 133.49 (C), 136.07 (C), 141.59 (C), 148.93 (CH), 154.94 (C), 159.65 (d, $J = 255.95$).

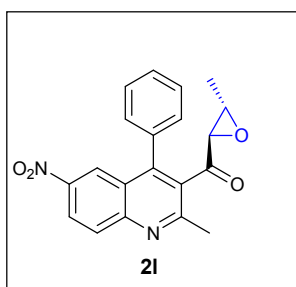
Hz, C-F), 203.09 (C); ESI-MS (m/z) 400 ($M+H$)⁺; HRMS (ESI) calculated for $C_{20}H_{16}BrFNO_2$ ($M + H$)⁺ 400.0348, found 400.0341.

(5-fluoro-4-(4-fluorophenyl)-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2k):



Yield 67% as white solid: mp 108-110°C; FT-IR (KBr, cm^{-1}) 3019, 1637, 1216, 1069; ¹H NMR (400 MHz, CD_3OD) δ 1.14 (d, J = 5.08 Hz, 3H), 2.67 (s, 3H), 2.72-2.74 (m, 1H), 3.35 (d, J = 1.6 Hz, 1H), 7.21-7.29 (m, 3H), 7.32-7.36 (m, 1H), 7.47-7.51 (m, 1H), 7.79-7.84 (m, 1H), 7.94 (d, J = 8.48 Hz, 1H); ¹³C NMR (100 MHz, CD_3OD) δ 16.11 (CH_3), 22.10 (CH_3), 56.61 (CH), 59.97 (CH), 112.23 (d, J = 21.85 Hz, CH), 114.55 (d, J = 21.87 Hz, CH), 114.69 (d, J = 21.95 Hz, CH), 115.38 (d, J = 9.3 Hz, C), 124.42 (d, J = 3.89 Hz, CH), 130.78 (d, J = 9.68 Hz, CH), 131.13-131.22 (m, CH), 131.57-131.66 (m, CH), 132.59 (C), 133.51 (C), 142.60 (C), 148.65 (C), 155.02 (C), 159.88 (d, J = 257.23 Hz, C-F), 164.28 (d, J = 245.89 Hz, C-F), 202.97 (C); ESI-MS (m/z) 334 ($M+H$)⁺; HRMS (ESI) calculated for $C_{20}H_{16}F_2NO_2$ ($M + H$)⁺ 340.1149, found 340.1140.

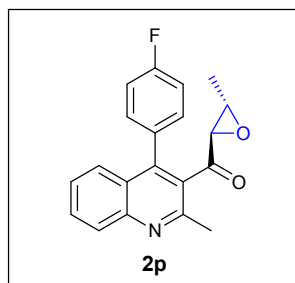
(2-methyl-6-nitro-4-phenylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2l):



Yield 52% as white solid: mp 153-155°C; FT-IR (KBr, cm^{-1}) 3019, 1626, 1216, 1069; ¹H NMR (400 MHz, $DMSO-d_6$) δ 1.00 (d, J = 5.04 Hz, 3H), 2.68-2.71 (m, 4H), 3.46 (d, J = 1.80 Hz, 1H), 7.38-7.39 (m, 1H), 7.51-7.53 (m, 1H), 7.61-7.69 (m, 3H), 8.27 (d, J = 9.2 Hz, 1H), 8.36 (d, J = 2.44 Hz, 1H), 8.52-8.55 (dd, J = 9.16, 2.56 Hz, 1H); ¹³C NMR (100 MHz, $DMSO-d_6$) δ 17.55 (CH_3), 23.39 (CH_3), 57.05 (CH), 60.12 (CH), 123.02 (CH), 124.17 (C), 124.47 (CH), 129.32 (CH), 129.47 (CH), 130.30 (CH), 130.57 (CH), 130.79 (CH), 131.17

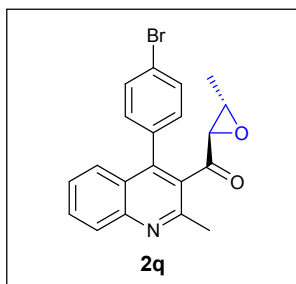
(CH), 133.08 (C), 133.49 (C), 145.72 (C), 147.48 (C), 149.67 (C), 158.74 (C) 202.66 (C); ESI-MS (m/z) 349 ($M+H$)⁺; HRMS (ESI) calculated for C₂₀H₁₇N₂O₄ ($M+H$)⁺ 349.1188, found 349.1190.

(4-(4-fluorophenyl)-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2p):



Yield 64% as white solid: mp 118-120°C; FT-IR (KBr, cm⁻¹) 3019, 1619, 1215, 1076; ¹H NMR (400 MHz, CD₃OD) δ 1.08 (d, J = 5.08 Hz, 3H), 2.66 (s, 3H), 2.73-2.77 (m, 1H), 3.25 (d, J = 1.76 Hz, 1H), 7.30-7.37 (m, 3H), 7.49-7.63 (m, 3H), 7.79-7.84 (m, 1H), 8.05 (d, J = 8.44 Hz, 1H); ¹³C NMR (100 MHz, CD₃OD) δ 16.08 (CH₃), 22.09 (CH₃), 56.55 (CH), 60.09 (CH), 115.49 (d, J = 21.89 Hz, CH), 115.53 (d, J = 21.86 Hz, CH), 124.95 (C), 125.68 (CH), 126.97 (CH), 127.71 (CH), 130.59 (d, J = 3.51 Hz, C), 130.81 (CH), 131.49 (C), 132.29 (d, J = 8.45 Hz, CH), 132.65 (d, J = 8.26 Hz, CH), 145.69 (C), 147.29 (C), 154.36 (C), 164.56 (d, J = 246.78 Hz, C-F), 203.11 (C); ESI-MS (m/z) 322 ($M+H$)⁺; HRMS (ESI) calculated for C₂₀H₁₇FNO₂ ($M+H$)⁺ 322.1243, found 322.1243.

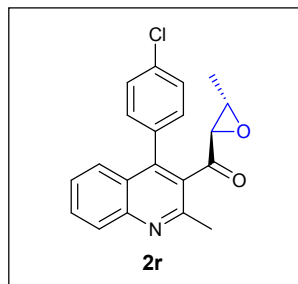
(4-(4-bromophenyl)-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2q):



Yield 71% as yellow solid: mp 124-126°C; FT-IR (KBr, cm⁻¹) 3019, 1637, 1215, 1069; ¹H NMR (400 MHz, DMSO-*d*₆) δ 1.05 (d, J = 5.08 Hz, 3H), 2.52 (s, 3H), 2.74-2.78 (m, 1H), 3.46 (d, J = 1.84 Hz, 1H), 7.27-7.29 (dd, J = 8.08, 2.16 Hz, 1H), 7.39-7.42 (dd, J = 8.2, 2.2 Hz, 1H), 7.50-7.53 (dd, J = 8.36, 0.88 Hz, 1H), 7.57-7.61 (m, 1H), 7.77-7.87 (m, 3H), 8.06 (d, J = 7.96 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 17.45 (CH₃), 23.98 (CH₃), 56.93 (CH), 60.20 (CH), 123.27 (C), 124.55 (C), 126.08 (CH), 127.68 (CH), 129.15 (CH), 131.31 (CH), 131.46 (C), 132.00 (CH), 132.17 (CH), 132.53 (CH), 132.89 (CH), 133.94 (C), 144.65

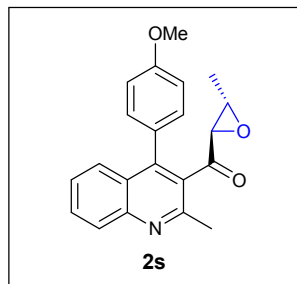
(C), 147.67 (C), 154.21 (C), 203.27 (C); ESI-MS (m/z) 382 ($M+H$)⁺; HRMS (ESI) calculated for C₂₀H₁₇BrNO₂ ($M + H$)⁺ 382.0443, found 382.0442.

(4-(4-chlorophenyl)-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2r):



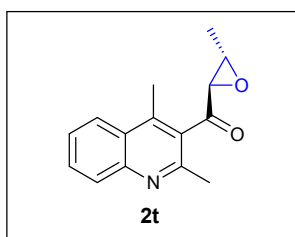
Yield 72% as white solid: mp 105-107°C; FT-IR (KBr, cm⁻¹) 3019, 1643, 1215, 1069; ¹H NMR (400 MHz, DMSO-*d*₆) δ 1.04 (d, J = 5.04 Hz, 3H), 2.61 (s, 3H), 2.74-2.76 (m, 1H), 3.45 (d, J = 1.84 Hz, 1H), 7.33-7.36 (dd, J = 8.12, 2.12 Hz, 1H), 7.45-7.51 (m, 2H), 7.56-7.69 (m, 3H), 7.82-7.86 (m, 1H), 8.06 (dd, J = 8.04 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 17.44 (CH₃), 23.96 (CH₃), 56.88 (CH), 60.20 (CH), 124.63 (C), 126.06 (CH), 127.66 (CH), 129.08 (CH), 129.14 (CH), 129.23 (CH), 131.29 (CH), 131.54 (C), 132.28 (CH), 132.64 (CH), 133.56 (C), 134.55 (C), 144.61 (C), 147.67 (C), 154.19 (C), 203.27 (C); ESI-MS (m/z) 338 ($M+H$)⁺; HRMS (ESI) calculated for C₂₀H₁₇ClNO₂ ($M + H$)⁺ 338.0948, found 338.0944.

(4-(4-methoxyphenyl)-2-methylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2s):



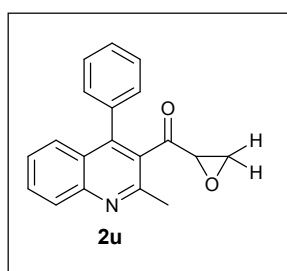
Yield 67% as white solid: mp 112-114°C; FT-IR (KBr, cm⁻¹) 3019, 1637, 1215, 1069; ¹H NMR (400 MHz, DMSO-*d*₆) δ 1.00 (d, J = 5.04 Hz, 3H), 2.59 (s, 3H), 3.36 (d, J = 1.84 Hz, 1H), 3.85 (s, 3H), 7.10-7.17 (m, 2H), 7.22-7.25 (dd, J = 8.24, 2.0 Hz, 1H), 7.35-7.37 (dd, J = 8.44, 2.2 Hz, 1H), 7.54-7.61 (m, 2H), 7.79-7.84 (m, 1H), 8.03 (d, J = 8.32 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 17.58 (CH₃), 23.95 (CH₃), 55.79 (CH₃), 56.75 (CH), 60.23 (CH), 114.58 (CH), 114.63 (CH), 125.13 (C), 126.23 (CH), 123.63 (C), 127.37 (CH), 129.10 (CH), 131.08 (CH), 131.72 (C), 131.98 (CH), 132.16 (CH), 145.70 (C), 147.75 (C), 154.21 (C), 160.27 (C), 203.42 (C); ESI-MS (m/z) 334 ($M+H$)⁺; HRMS (ESI) calculated for C₂₁H₂₀NO₃ ($M + H$)⁺ 334.1443, found 334.1430.

(2,4-dimethylquinolin-3-yl)(3-methyloxiran-2-yl)methanone (2t):



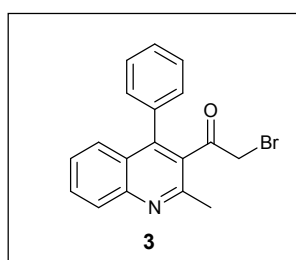
Yield 62% as white solid: mp 120-122°C; FT-IR (KBr, cm^{-1}) 3021, 1636, 1216, 1069; ^1H NMR (300 MHz, CDCl_3) δ 1.43 (d, $J = 5.13$ Hz, 3H), 2.60 (s, 3H), 2.64 (s, 3H), 3.04-3.09 (m, 1H), 3.56 (d, $J = 1.83$ Hz, 1H), 7.53-7.59 (m, 1H), 7.70-7.76 (m, 1H), 7.97-8.04 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 15.79 (CH_3), 17.42 (CH_3), 23.73 (CH_3), 55.67 (CH), 61.45 (CH), 123.73 (CH), 125.71 (C), 126.47 (CH), 129.33 (CH), 130.27 (CH), 130.55 (C), 141.66 (C), 147.31 (C), 153.89 (C), 205.13 (C); ESI-MS (m/z) 242 ($\text{M}+\text{H}$) $^+$ for $\text{C}_{15}\text{H}_{16}\text{NO}_3$.

(2-methyl-4-phenylquinolin-3-yl)(oxiran-2-yl)methanone (2u):



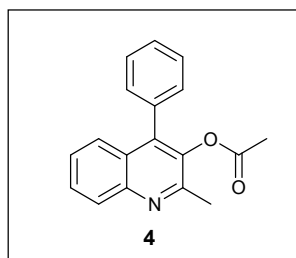
Yield 20% as white solid: mp 133-135°C; FT-IR (KBr, cm^{-1}) 3019, 1651, 1215, 1069; ^1H NMR (400 MHz, CDCl_3) δ 2.45-2.47 (dd, $J = 6.44, 2.36$ Hz, 1H), 2.59-2.62 (q, $J = 4.48$ Hz, 1H), 2.72 (s, 3H), 3.26-3.27 (q, $J = 2.36$ Hz, 1H), 7.31-7.33 (m, 1H), 7.45-7.56 (m, 5H), 7.65-7.67 (m, 1H), 7.74-7.78 (m, 1H), 8.10 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.95 (CH_3), 47.54 (CH_2), 53.55 (CH), 124.80 (C), 126.20 (CH), 126.75 (CH), 128.52 (CH), 128.70 (CH), 129.01 (CH), 129.22 (CH), 130.35 (CH), 130.70 (C&CH), 130.76 (CH), 134.84 (C), 146.35 (C), 148.04 (C), 154.40 (C), 203.13 (C); ESI-MS (m/z) 290 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{19}\text{H}_{16}\text{NO}_2$ ($\text{M} + \text{H}$) $^+$ 290.1181, found 290.1179.

2-bromo-1-(2-methyl-4-phenylquinolin-3-yl)ethanone (3):



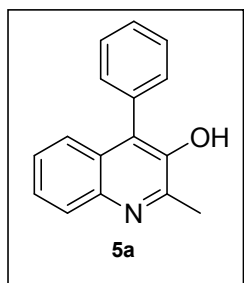
Yield 90% as white solid: mp 175-177°C; FT-IR (KBr, cm^{-1}) 3021, 1621, 1215, 1069; ^1H NMR (400 MHz, CDCl_3) δ 2.75 (s, 3H), 3.51 (s, 2H), 7.37-7.39 (m, 2H), 7.45-7.49 (m, 1H), 7.53-7.57 (m, 3H), 7.64-7.66 (dd, $J = 8.4, 0.8$ Hz, 1H), 7.73-7.78 (m, 1H), 8.10 (d, $J = 8.44$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 24.01 (CH_3), 35.21 (CH_2), 124.61 (C), 126.25 (CH), 126.79 (CH), 129.05 (CH), 129.15 (2 \times CH), 129.47 (CH), 129.92 (2 \times CH), 130.70 (CH), 131.36 (C), 134.96 (C), 144.77 (C), 147.96 (C), 154.93 (C), 198.35 (C); ESI-MS (m/z) 340 ($\text{M}+\text{H}$) $^+$ for $\text{C}_{18}\text{H}_{15}\text{BrNO}$.

2-methyl-4-phenylquinolin-3-yl acetate (4):



Yield 50% as light yellow solid: mp 97-99°C; FT-IR (KBr, cm^{-1}) 3019, 1626, 1216, 1069; ^1H NMR (400 MHz, CDCl_3) δ 2.78 (s, 3H), 3.58 (s, 2H), 7.34-7.37 (m, 2H), 7.41-7.51 (m, 4H), 7.57-7.59 (dd, $J = 8.4, 0.84$ Hz, 1H), 7.69-7.74 (m, 1H), 8.08 (d, $J = 8.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.80 (CH_3), 52.15 (CH_3), 125.09 (C), 126.46 (CH), 126.54 (CH), 127.28 (CH), 128.28 (2 \times CH), 128.50 (CH), 128.88 (CH), 129.25 (2 \times CH), 130.32 (CH), 135.69 (C), 146.41 (C), 147.78 (C), 154.56 (C), 169.01 (C); ESI-MS (m/z) 278 ($\text{M}+\text{H}$) $^+$ for $\text{C}_{18}\text{H}_{16}\text{NO}_2$.

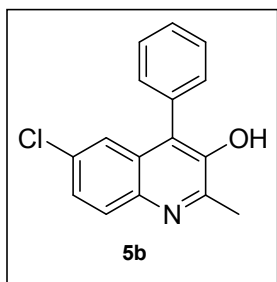
2-methyl-4-phenylquinolin-3-ol (5a):



Yield 62% as light yellow solid: mp 239-241°C; FT-IR (KBr, cm^{-1}) 3400, 3019, 1638, 1215, 1068; ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 2.64 (s, 3H), 7.24-7.26 (dd, $J = 8.35, 0.8$ Hz, 1H), 7.33-7.37 (m, 3H), 7.47-7.51 (m, 2H), 7.54-7.57 (m, 2H), 7.87-7.89 (m, 3H), 8.90 (s, 1H);

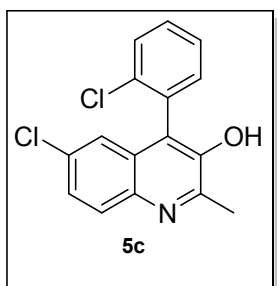
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 21.72 (CH_3), 124.63 (CH), 126.24 (CH), 126.30 (CH), 128.01 (C), 128.35 (CH), 128.70 (CH), 128.99 ($2\times\text{CH}$), 129.23 (C), 130.84 ($2\times\text{CH}$), 134.29 (C), 142.58 (C), 145.92 (C), 153.02 (C); ESI-MS (m/z) 236 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{14}\text{NO}$ ($\text{M} + \text{H}$) $^+$: 236.1075, found 236.1075.

6-chloro-2-methyl-4-phenylquinolin-3-ol (5b):



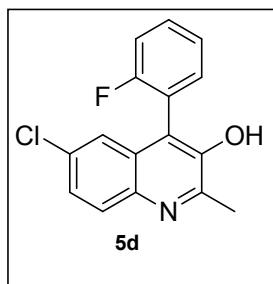
Yield 61% as light brown solid: mp 235-237°C; FT-IR (KBr, cm^{-1}) 3399, 3019, 1603, 1216, 1071; ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 2.63 (s, 3H), 7.15 (d, $J = 2.2$ Hz, 1H), 7.35-7.37 (m, 2H), 7.48-7.53 (m, 2H), 7.56-7.59 (m, 2H), 7.90 (d, $J = 8.9$ Hz, 1H), 9.19 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 21.73 (CH_3), 123.09 (CH), 126.66 (CH), 128.24 (C), 128.70 (CH), 129.11 (C), 129.22 ($2\times\text{CH}$), 130.78 ($2\times\text{CH}$), 130.83 (C), 130.92 (CH), 133.59 (C), 140.89 (C), 146.86 (C), 153.83 (C); ESI-MS (m/z) 270 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{13}\text{ClNO}$ ($\text{M} + \text{H}$) $^+$: 270.0686, found 270.0676.

6-chloro-4-(2-chlorophenyl)-2-methylquinolin-3-ol (5c):



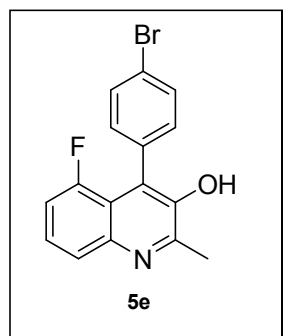
Yield 58% as white solid: mp 221-223°C; FT-IR (KBr, cm^{-1}) 3400, 3019, 1638, 1215, 1068; ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 2.64 (s, 3H), 6.90 (d, $J = 2.25$ Hz, 1H), 7.37-7.39 (dd, $J = 7.5, 1.8$ Hz, 1H), 7.49-7.58 (m, 3H), 7.68-7.69 (dd, $J = 7.8, 1.15$ Hz, 1H), 7.92 (d, $J = 8.9$ Hz, 1H), 9.51 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 21.65 (CH_3), 122.54 (CH), 125.07 (C), 126.73 (CH), 128.12 (CH), 128.71 (C), 130.19 (CH), 130.92 (CH), 130.98 (CH), 131.12 (C), 132.59 (C), 132.85 (CH), 134.04 (C), 140.66 (C), 147.40 (C), 153.86 (C); ESI-MS (m/z) 304 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{12}\text{Cl}_2\text{NO}$ ($\text{M} + \text{H}$) $^+$: 304.0296, found 304.0286.

6-chloro-4-(2-fluorophenyl)-2-methylquinolin-3-ol (5d):



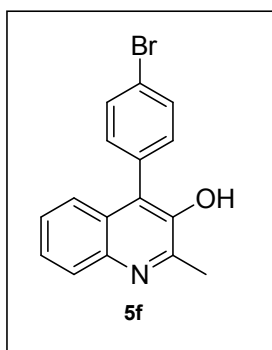
Yield 63% as light yellow solid: mp 237-239°C; FT-IR (KBr, cm^{-1}) 3399, 3019, 1619, 1215; ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 2.64 (s, 3H), 7.07 (s, 1H), 7.38-7.44 (m, 3H), 7.51-7.53 (dd, $J = 8.85, 2.3$ Hz, 1H), 7.57-7.62 (m, 1H), 7.92 (d, $J = 8.85$ Hz, 1H), 9.54 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 21.68 (CH_3), 116.60 (d, $J = 21.6$ Hz, CH), 121.04 (d, $J = 16.82$ Hz, C), 121.96 (C), 122.61 (CH), 125.33 (CH), 126.83 (CH), 128.88 (C), 131.02 (CH), 131.20 (C), 131.48 (d, $J = 8.1$ Hz, CH), 133.0 (CH), 140.73 (C), 147.77 (C), 153.83 (C), 161.56 (d, $J = 243.59$ Hz, C-F); ESI-MS (m/z) 288 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{12}\text{ClFNO}$ ($\text{M} + \text{H}$) $^+$: 288.0591, found 288.0581.

6-chloro-4-(2-fluorophenyl)-2-methylquinolin-3-ol (5e):



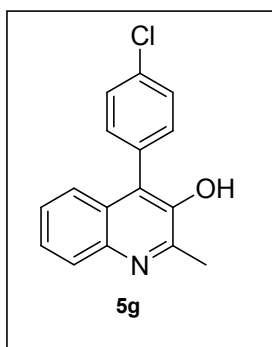
Yield 56% as white yellow solid: mp 277-279°C; FT-IR (KBr, cm^{-1}) 3400, 3019, 1609, 1215, 1069; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 2.62 (s, 3H), 7.09-7.15 (m, 1H), 7.27 (d, $J = 8.24$ Hz, 2H), 7.44-7.49 (m, 1H), 7.61-7.65 (m, 2H), 7.74 (d, $J = 7.92$ Hz, 1H), 9.07 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 21.62 (CH_3), 111.80 (d, $J = 21.22$ Hz, CH), 117.82 (d, $J = 8.74$ Hz, C), 121.36 (C), 124.80 (C), 125.29 (CH), 126.19 (d, $J = 9.46$ Hz, CH), 131.26 (2 \times CH), 132.14 (2 \times CH), 135.64 (C), 143.88 (C), 147.25 (C), 153.96 (C), 158.57 (d, $J = 251.96$ Hz, C-F); ESI-MS (m/z) 332 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{12}\text{BrFNO}$ ($\text{M}+\text{H}$) $^+$: 332.0086, found 332.0088.

4-(4-bromophenyl)-2-methylquinolin-3-ol (5f):



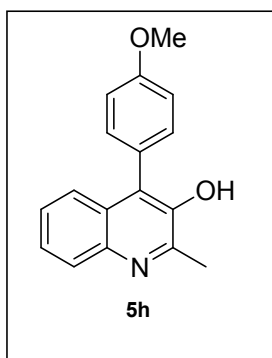
Yield 52% as white solid: mp 288-290°C; FT-IR (KBr, cm^{-1}) 3399, 3019, 1618, 1215; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 2.63 (s, 3H), 7.24 (d, $J = 8.16$ Hz, 1H), 7.31-7.38 (m, 3H), 7.48-7.52 (m, 1H), 7.74 (d, $J = 8.32$ Hz, 2H), 7.88 (d, $J = 8.16$ Hz, 2H), 9.03 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 21.69 (CH_3), 121.87 (C), 124.38 (CH), 126.40 (CH), 126.45 (CH), 127.66 (C), 127.78 (C), 128.76 (CH), 132.04 ($2\times\text{CH}$), 133.13 ($2\times\text{CH}$), 133.55 (C), 142.51 (C), 145.95 (C), 153.02 (C); ESI-MS (m/z) 314 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{13}\text{BrNO}$ ($\text{M} + \text{H}$) $^+$: 314.0181, found 314.0184.

4-(4-chlorophenyl)-2-methylquinolin-3-ol (5g):



Yield 55% as white solid: mp 270-273°C; FT-IR (KBr, cm^{-1}) 3399, 3019, 1602, 1215, 1070; ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 2.64 (s, 3H), 7.25 (d, $J = 8.95$ Hz, 1H), 7.34-7.40 (m, 3H), 7.48-7.57 (m, 3H), 7.91 (d, $J = 1.9$ Hz, 2H), 9.03 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 21.79 (CH_3), 126.66 (CH), 126.77 (C & CH), 127.29 (CH), 128.58 (CH), 129.11 ($2\times\text{CH}$), 129.27 (C), 130.80 (C & $2\times\text{CH}$), 133.77 (C), 142.83 (C), 146.37 (C), 154.68 (C); ESI-MS (m/z) 270 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{13}\text{ClNO}$ ($\text{M} + \text{H}$) $^+$: 270.0686, found 270.0677.

4-(4-methoxyphenyl)-2-methylquinolin-3-ol (5h):



Yield 64% as light yellow solid: mp 221-222°C; FT-IR (KBr, cm^{-1}) 3399, 3019, 1643, 1215, 1068; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 2.63 (s, 3H), 3.86 (s, 3H), 7.10-7.14 (m, 2H), 7.27-7.38 (m, 4H), 7.46-7.51 (m, 1H), 7.87-7.89 (m, 1H), 8.82 (s, 1H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 21.69 (CH_3), 55.61 (CH_3), 114.54 ($2\times\text{CH}$), 124.73 (CH), 126.00 (C), 126.13 (CH), 126.21 (CH), 128.31 (C), 128.67 (CH), 128.84 (C), 132.09 ($2\times\text{CH}$), 142.62 (C), 146.14 (C), 152.88 (C), 159.41 (C); ESI-MS (m/z) 266 ($\text{M}+\text{H}$) $^+$; HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{16}\text{NO}_2$ ($\text{M} + \text{H}$) $^+$: 266.1181, found 266.1174.

X-Ray Data Collection and Structure Refinement Details:

A good quality single crystal of size 0.20 x 0.20 x 0.20 mm, was selected under a polarizing microscope and was mounted on a glass fiber for data collection. Single crystal X-ray data for compound **2b** were collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC12 goniometer and enhanced sensitivity (HG) Saturn724+ CCD detector in the 4x4 bin mode using the monochromated Mo-K α radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using ω -scans of 0.5 $^\circ$ steps at 293(2) K. Cell determination, data collection and data reduction was performed using the Rigaku CrystalClear-SM Expert 2.1 b24¹ software. Structure solution and refinement were performed by using SHELX-97². Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model.

ORTEP diagram of compound **2b** (CCDC 1492781)

1. CrystalClear 2.1, Rigaku Corporation, Tokyo, Japan.
2. Sheldrick, G. M. Acta Crystallogr., Sect. A 2008, 64, 112–122.

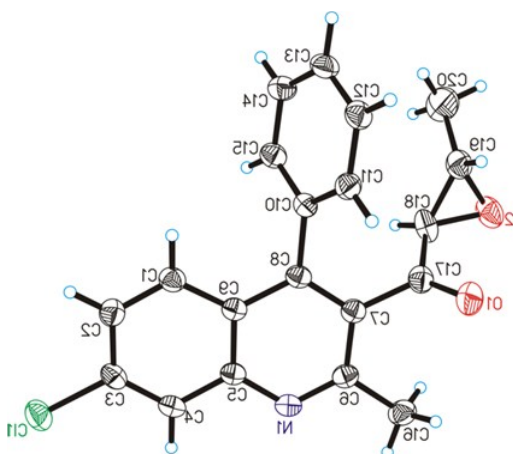
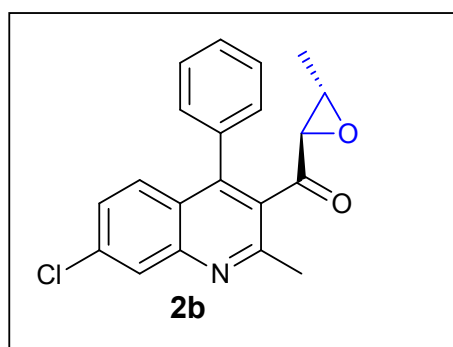
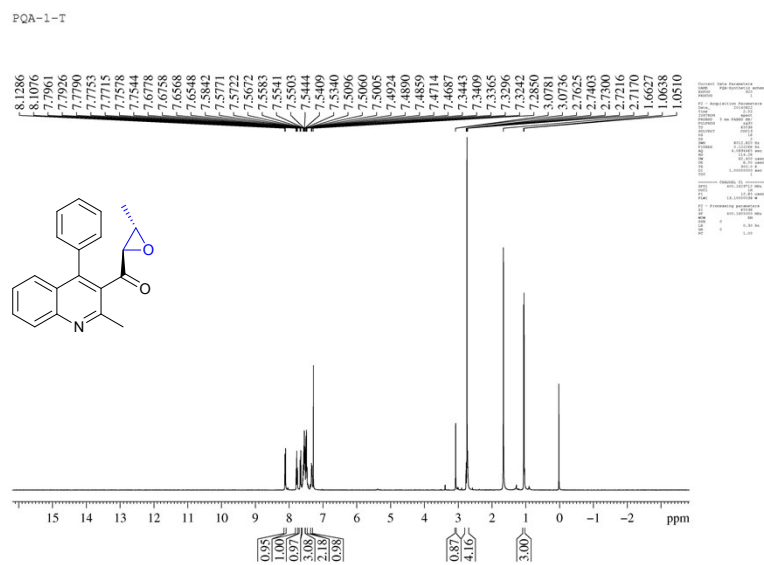


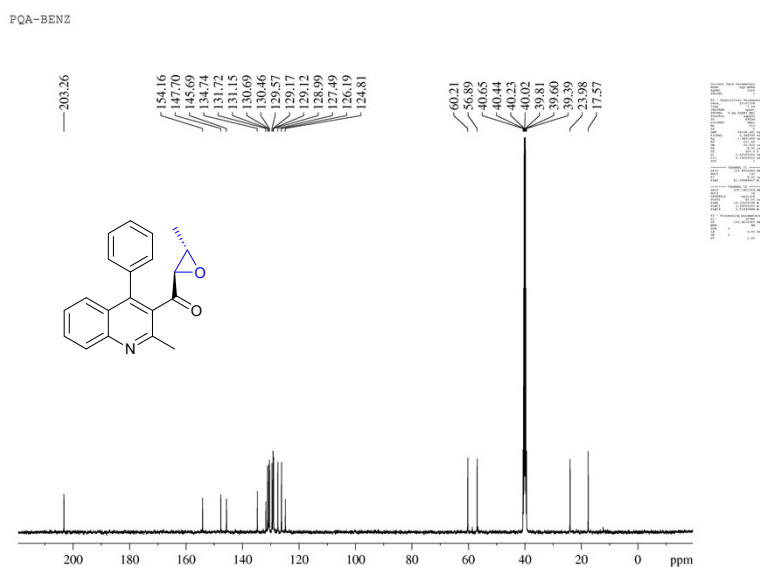
Figure 1 ORTEP diagram drawn with 30% ellipsoid probability for non-H atoms of the asymmetric unit of the crystal structure of compound **2b** determined at 293 K.

Table 1 Crystal data and structure refinement details for **2b**

Compound	2b
Empirical formula	C ₂₀ H ₁₆ Cl N O ₂
Formula weight	337.79
Crystal System	Orthorhombic
Space group	Pbca
a (Å)	7.8745(17)
b (Å)	19.699(4)
c (Å)	21.755(5)
α (°)	90.00
β (°)	90.00
γ (°)	90.00
V (Å ³)	3374.6(13)
Z	8
D _c (g/cm ³)	1.330
F ₀₀₀	1408
μ (mm ⁻¹)	0.238
θ_{\max} (°)	25.25
Total reflections	19869
Unique reflections	3017
Reflections [I 2 σ (I)]	1861
Parameters	225
R _{int}	0.1129
Goodness-of-fit	0.879
R [F ² > 2 σ (F ²)]	0.0469
wR (F ² , all data)	0.1126
CCDC No.	1492781

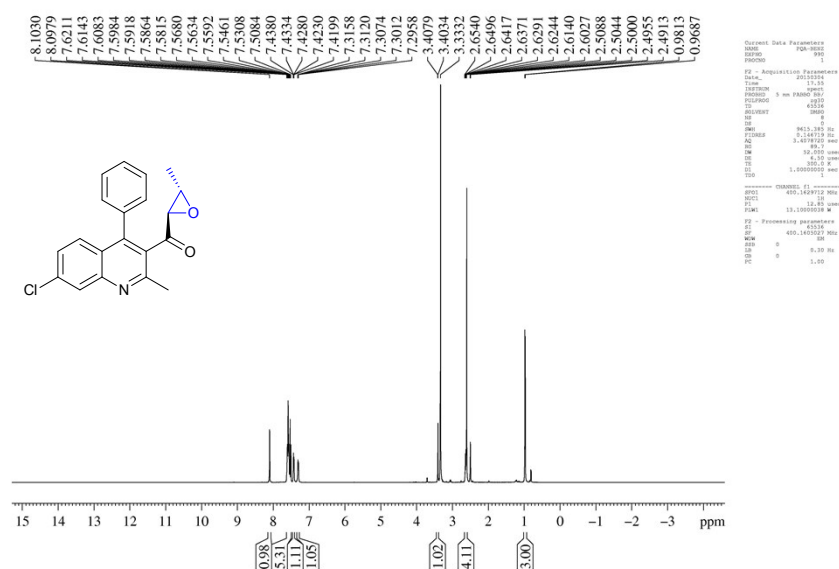


¹H NMR Spectra of **2a** (400 MHz, CDCl₃)



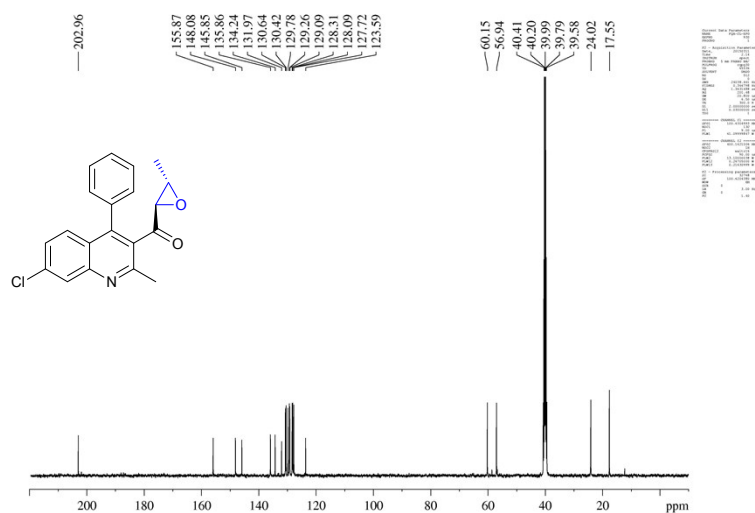
¹³C NMR Spectra of **2a** (100 MHz, DMSO-*d*₆)

PQA-4CL-E



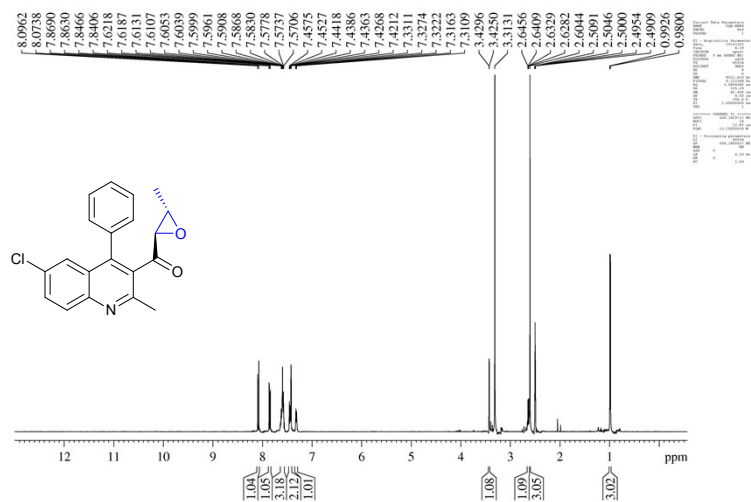
¹H NMR Spectra of **2b** (400 MHz, DMSO-*d*₆)

PQA-4CL-E



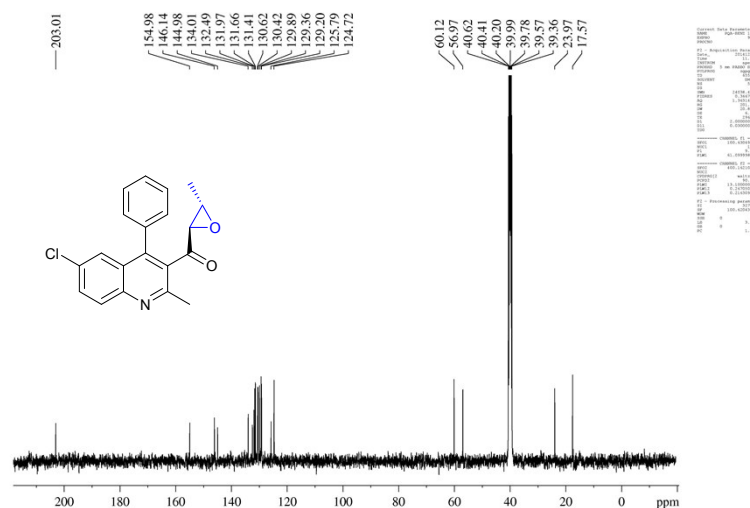
¹³C NMR Spectra of **2b** (100 MHz, DMSO-*d*₆)

CL-E

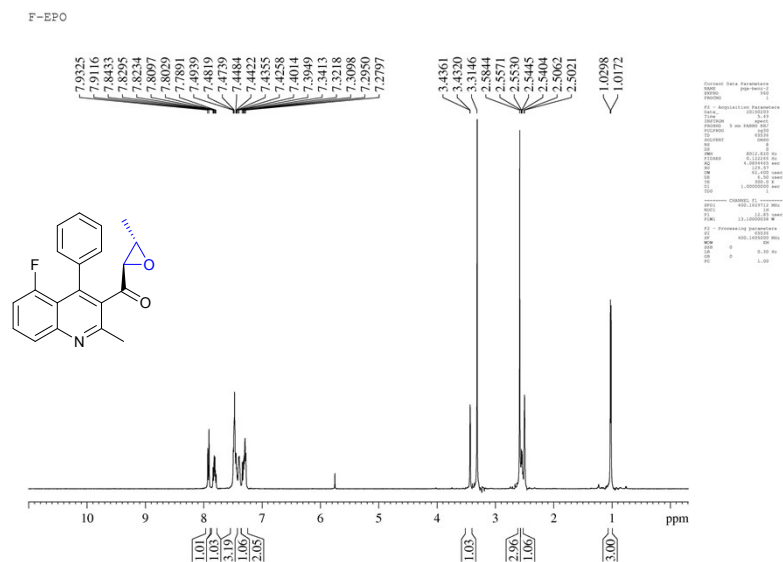


¹H NMR Spectra of **2c** (400 MHz, DMSO-*d*₆)

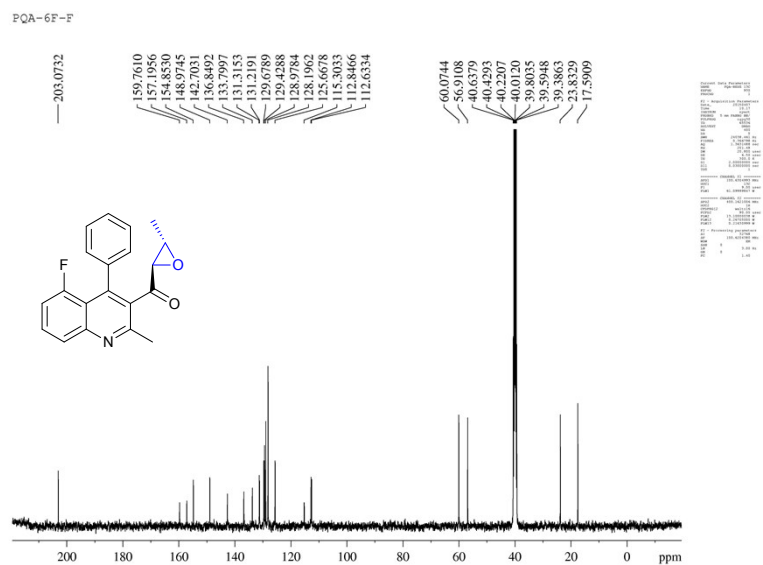
CL-E



¹³C NMR Spectra of **2c** (100 MHz, DMSO-*d*₆)

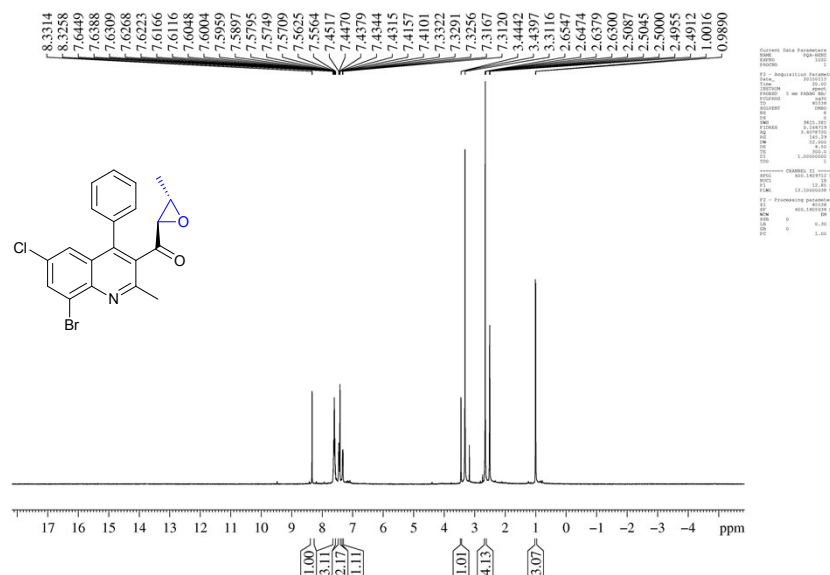


¹H NMR Spectra of **2d** (400 MHz, DMSO-*d*₆)



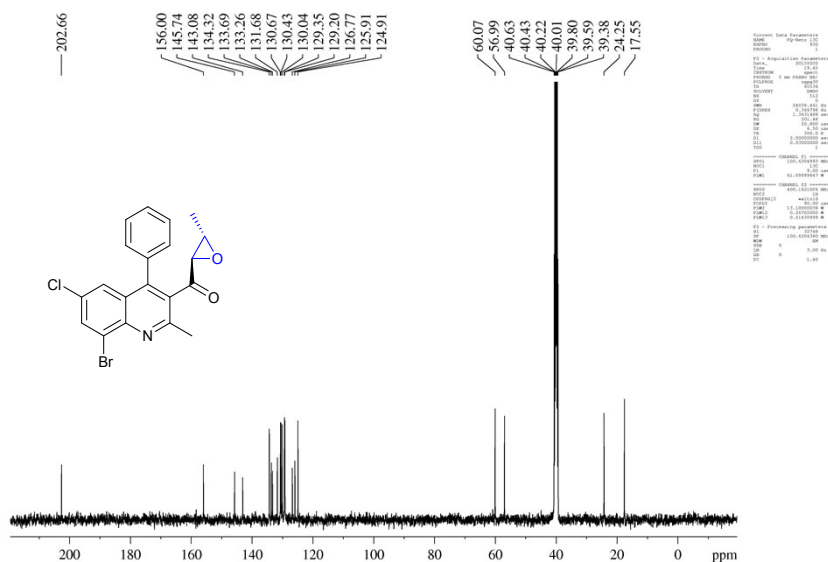
¹³C NMR Spectra of **2d** (100 MHz, DMSO-*d*₆)

CLBR-E



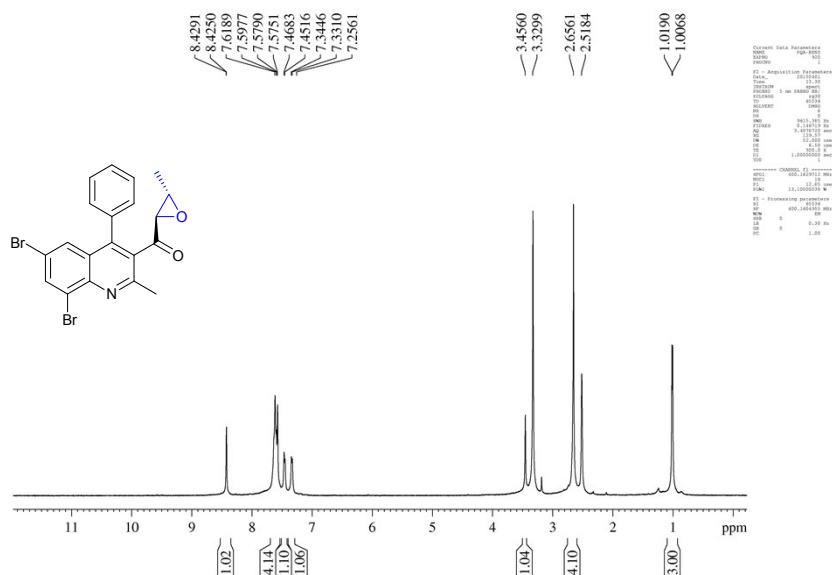
¹H NMR Spectra of **2f** (400 MHz, DMSO-*d*₆)

CLBR-E



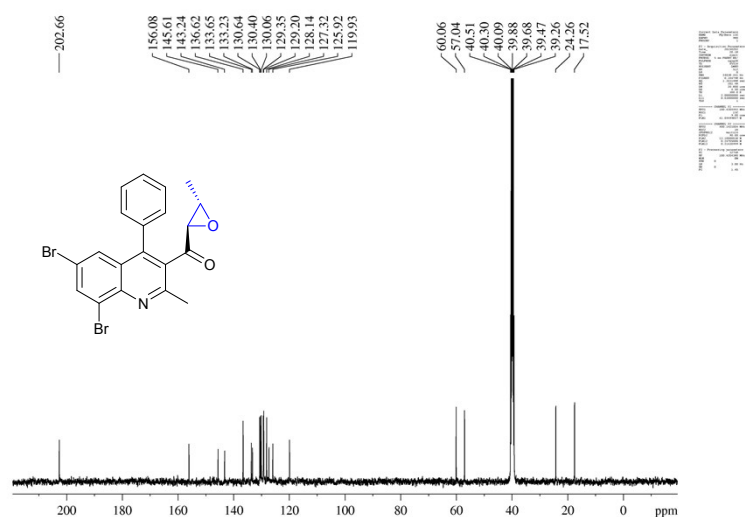
¹³C NMR Spectra of **2f** (100 MHz, DMSO-*d*₆)

PQA-DIBR-E



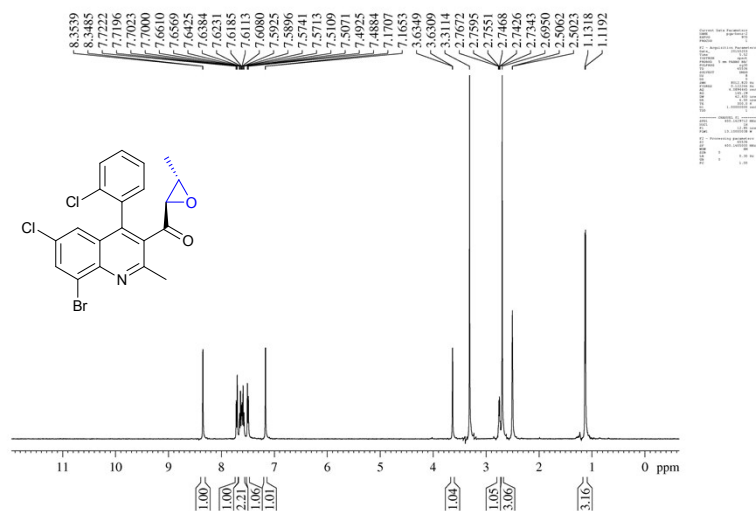
¹H NMR Spectra of **2g (400 MHz, DMSO-*d*₆)**

dibr-e



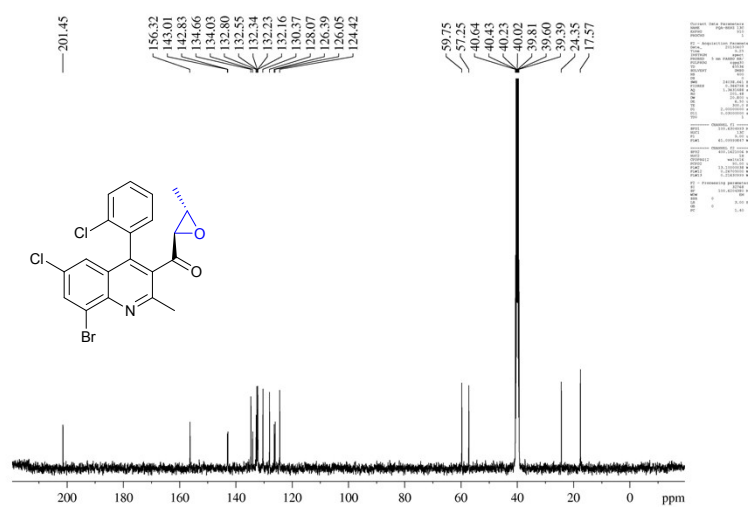
¹³C NMR Spectra of **2g (100 MHz, DMSO-*d*₆)**

DICL BR-EPO



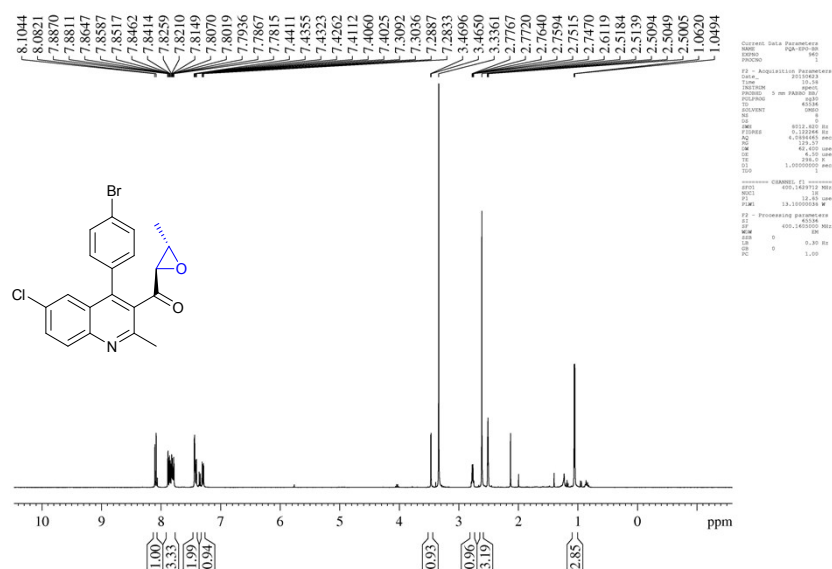
¹H NMR Spectra of **2h** (400 MHz, DMSO-*d*₆)

DICLBR-F



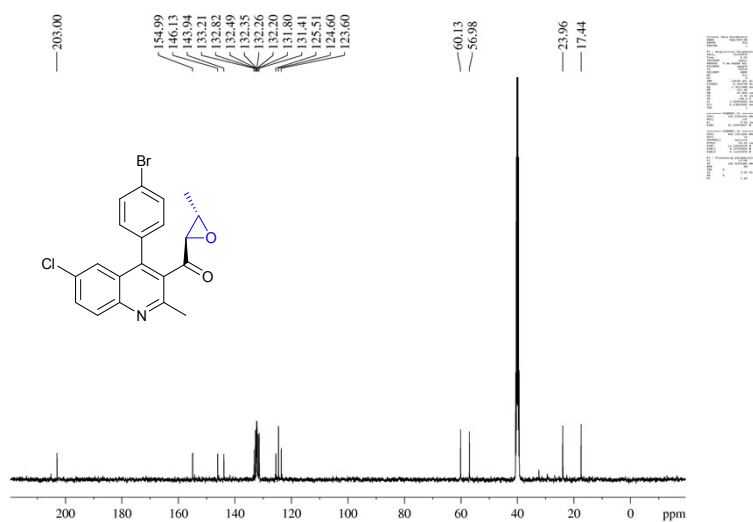
¹³C NMR Spectra of **2h** (100 MHz, DMSO-*d*₆)

5Cl-4Br



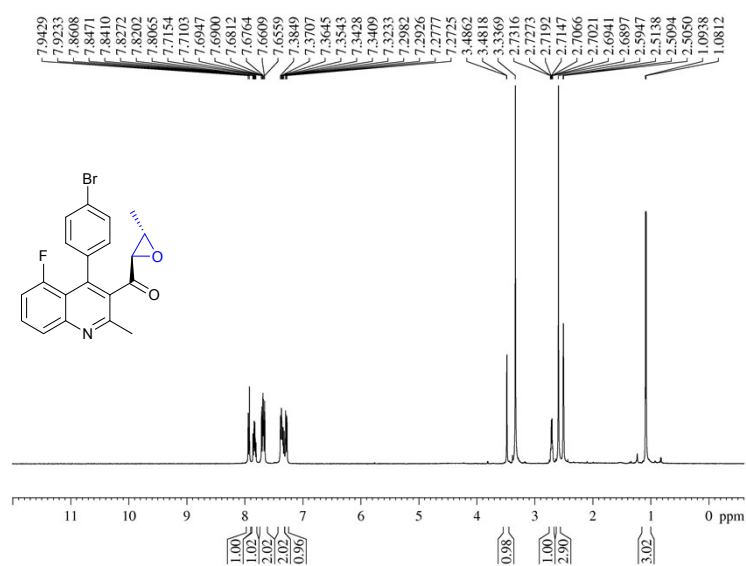
¹H NMR Spectra of **2i** (400 MHz, DMSO-*d*₆)

5U-4BR



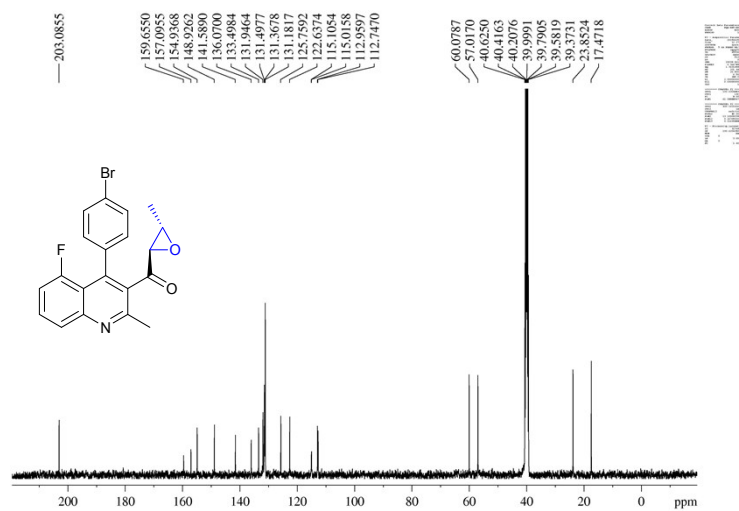
¹³C NMR Spectra of **2i** (100 MHz, DMSO-*d*₆)

6F-4Br

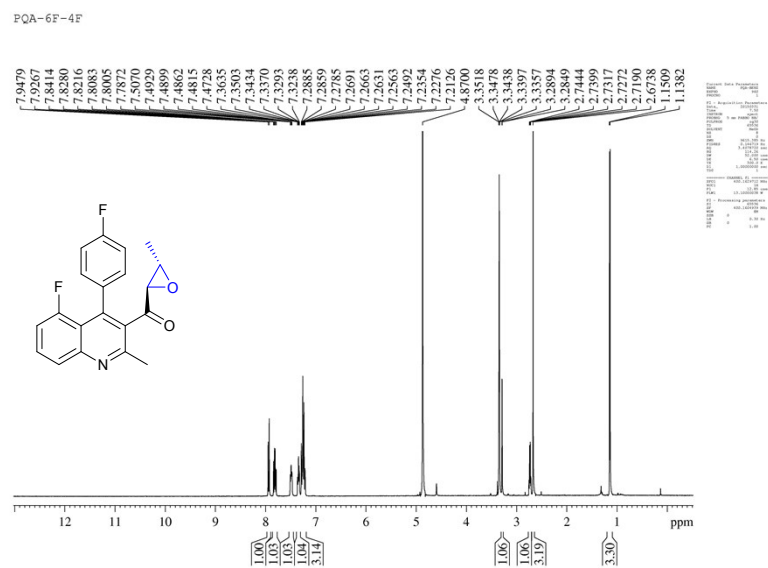


¹H NMR Spectra of **2j** (400 MHz, DMSO-*d*₆)

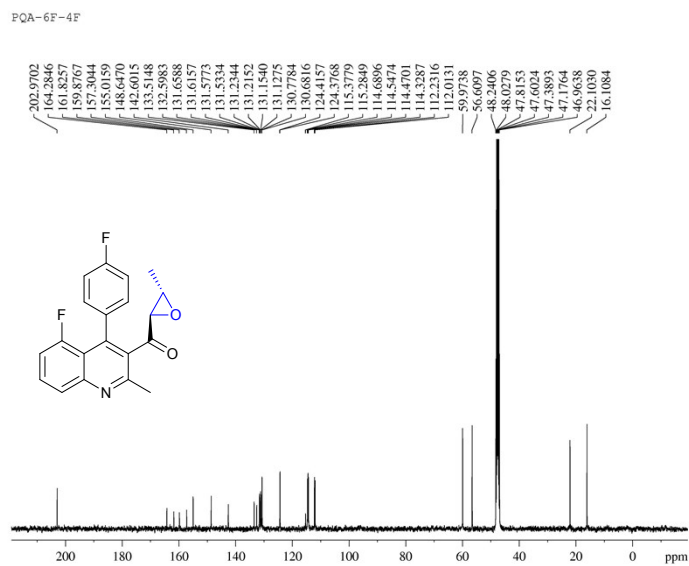
6F-4Br



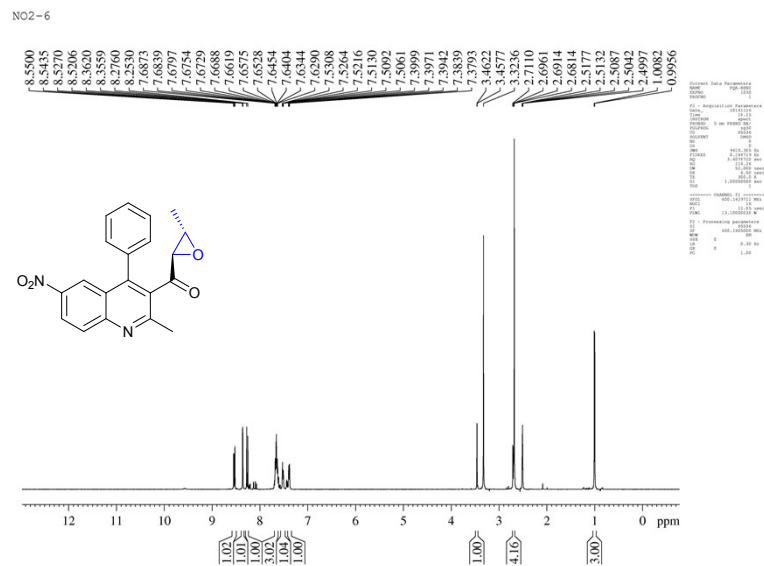
¹³C NMR Spectra of **2j** (100 MHz, DMSO-*d*₆)



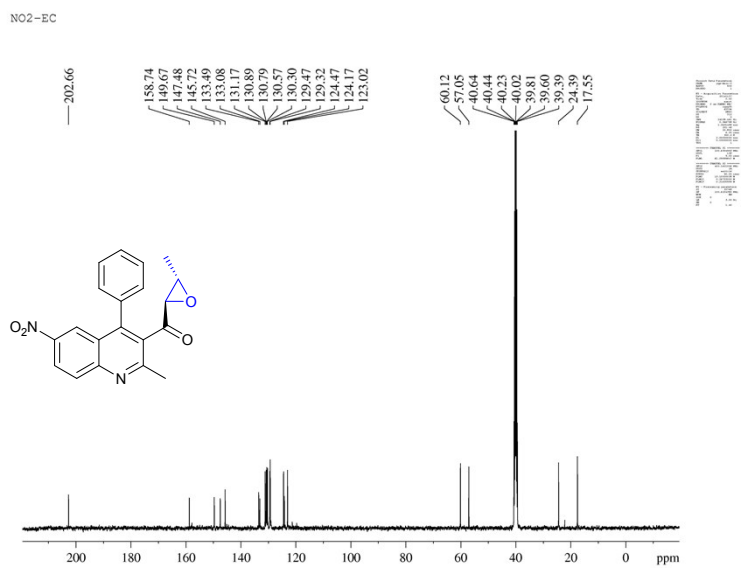
¹H NMR Spectra of **2k** (400 MHz, CD₃OD)



¹³C NMR Spectra of **2k** (100 MHz, CD₃OD)

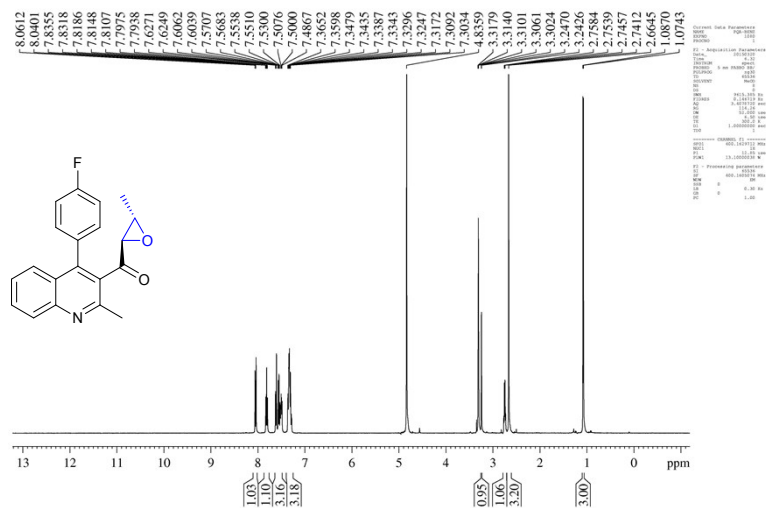


¹H NMR Spectra of **21** (400 MHz, DMSO-*d*₆)



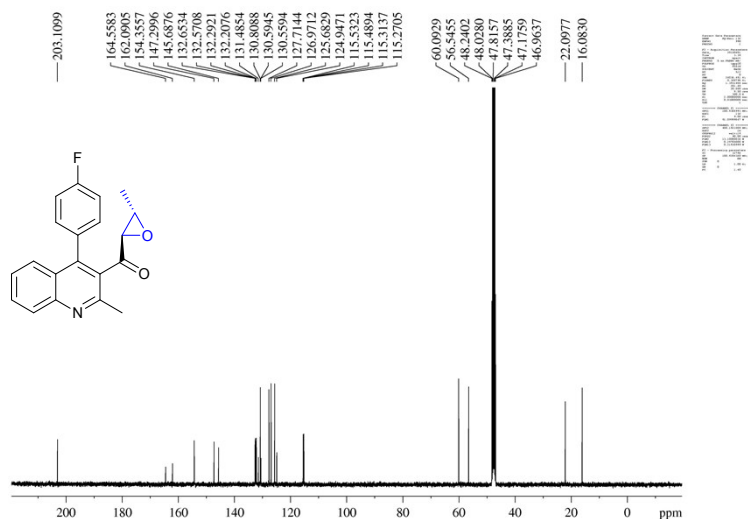
¹³C NMR Spectra of **2l** (100 MHz, DMSO-*d*₆)

PQA-4F-E



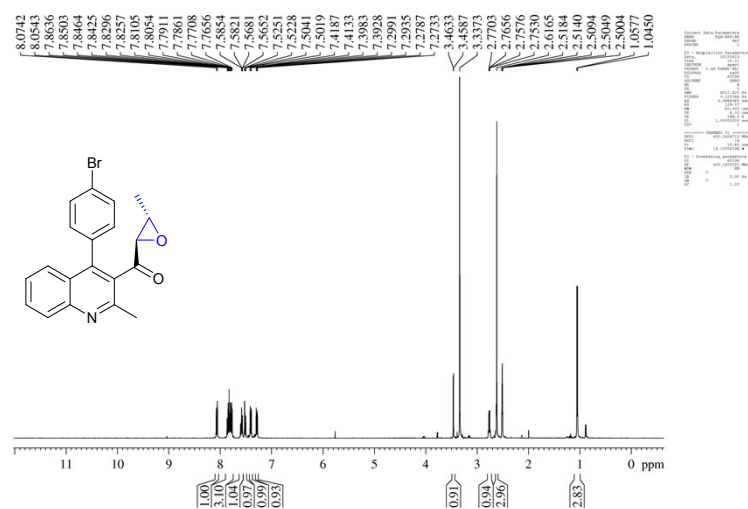
¹H NMR Spectra of **2p** (400 MHz, CD₃OD)

PQA-4F-E



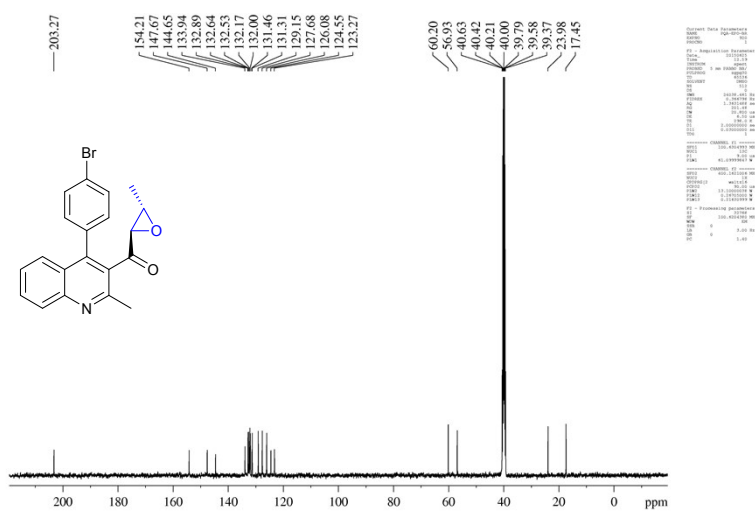
¹³C NMR Spectra of **2p** (100 MHz, CD₃OD)

PQA-4Br



¹H NMR Spectra of 2q (400 MHz, DMSO-*d*₆)

PQA-4BR



¹³C NMR Spectra of 2q (100 MHz, DMSO-*d*₆)

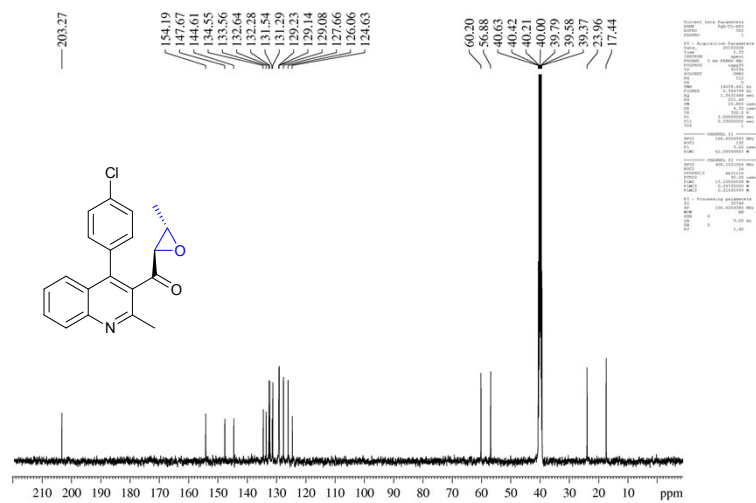
Chemical structure of 2-(4-chlorophenyl)-2-methyl-1,2,3,4-tetrahydroquinolin-3-one:

Cc1c2ccccc2n(c1C(=O)OC3CC3)c4ccc(Cl)cc4

¹H NMR spectrum (CDCl₃) showing peaks from 0 to 8 ppm. The spectrum includes a multiplet for aromatic protons (7.2-7.7 ppm), a doublet for the methine proton (3.4 ppm), and a singlet for the methyl group (1.0 ppm). Integration values are provided below the baseline.

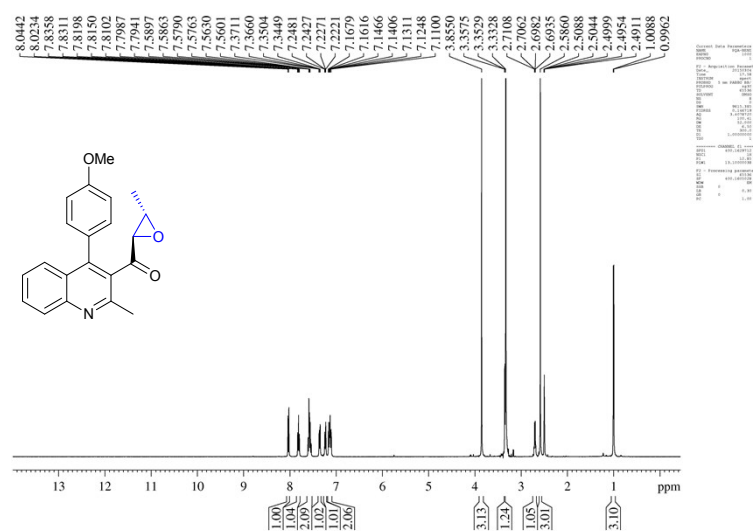
Chemical Shift (ppm)	Integration
7.2-7.7 (multiplet)	1.06, 1.05, 1.05, 2.11, 1.00
3.4 (doublet)	1.13
1.0 (singlet)	1.06, 3.16, 3.07

PQA-4CL-E



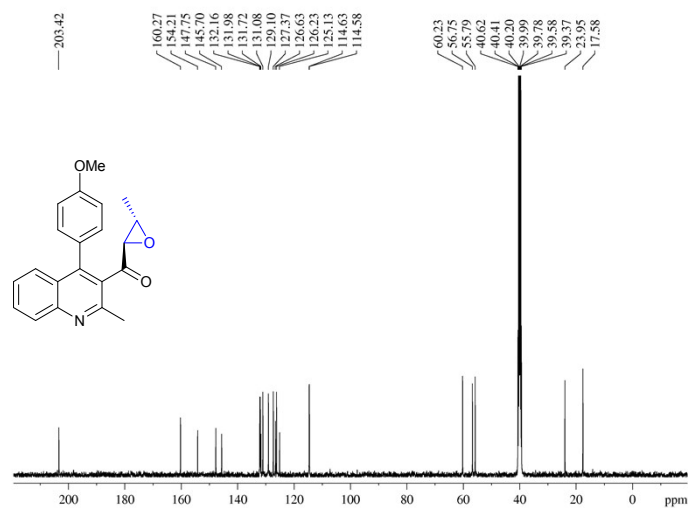
33

PQA-4OMe-E

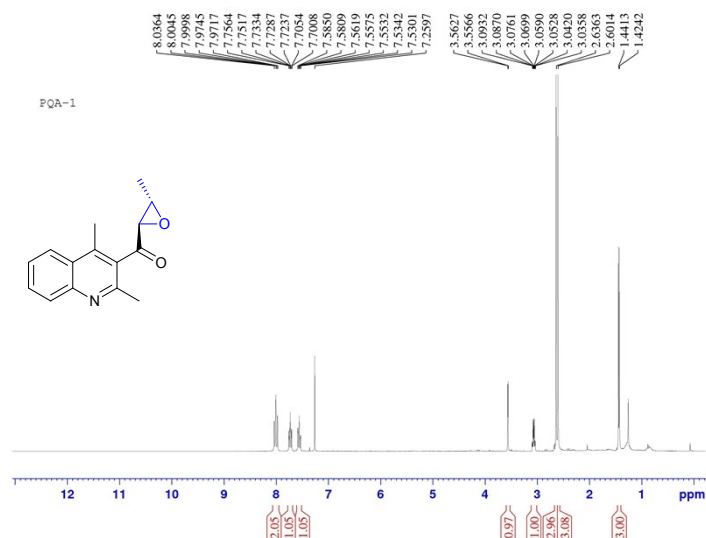


¹H NMR Spectra of **2s** (400 MHz, DMSO-*d*₆)

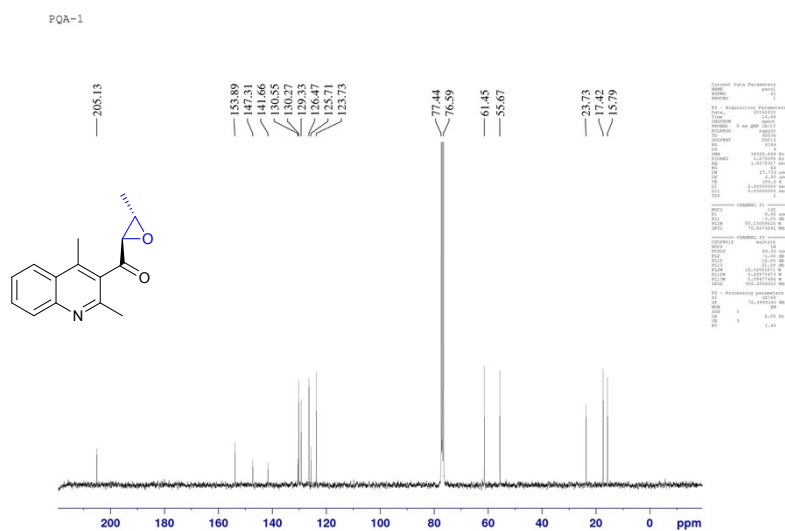
PQA-4OMe-E



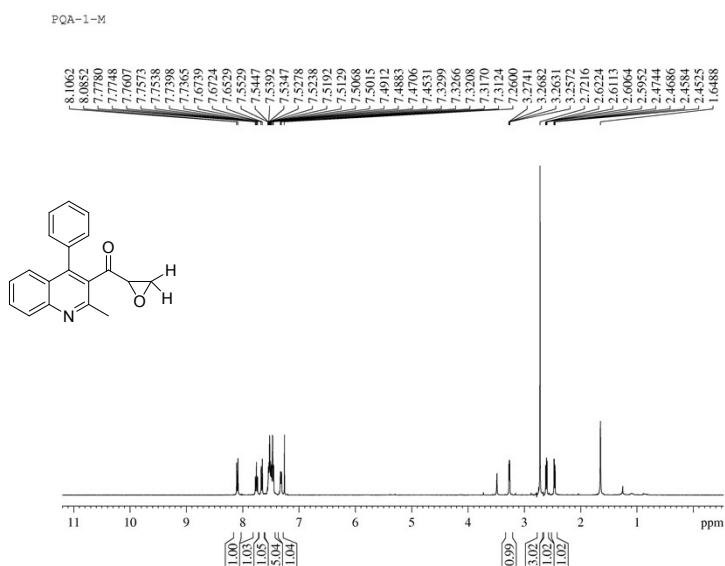
¹³C NMR Spectra of **2s** (100 MHz, DMSO-*d*₆)



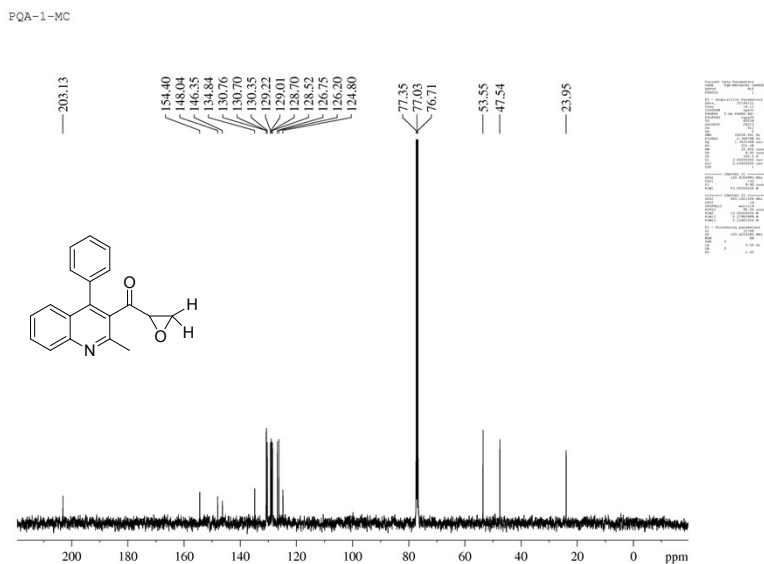
^1H NMR Spectra of **2t** (300 MHz, CDCl_3)



^{13}C NMR Spectra of **2t** (75 MHz, CDCl_3)

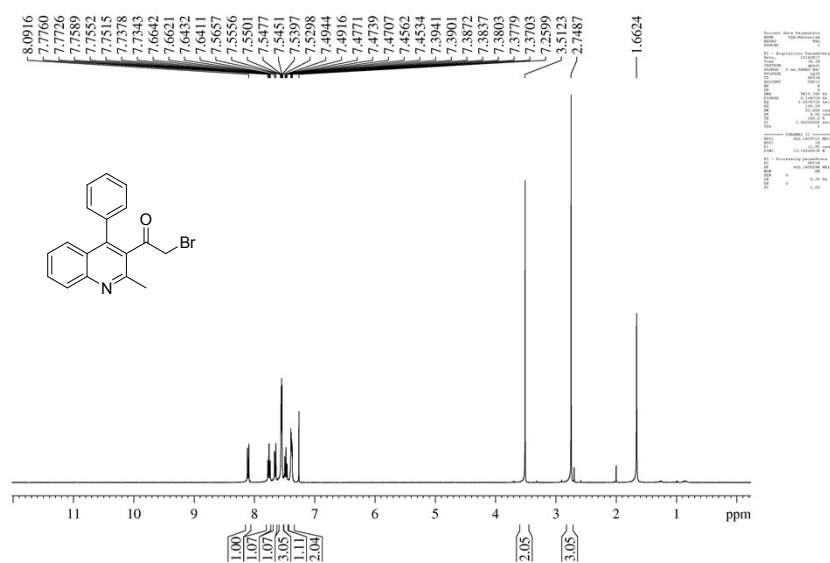


¹H NMR Spectra of **2u** (400 MHz, CDCl₃)



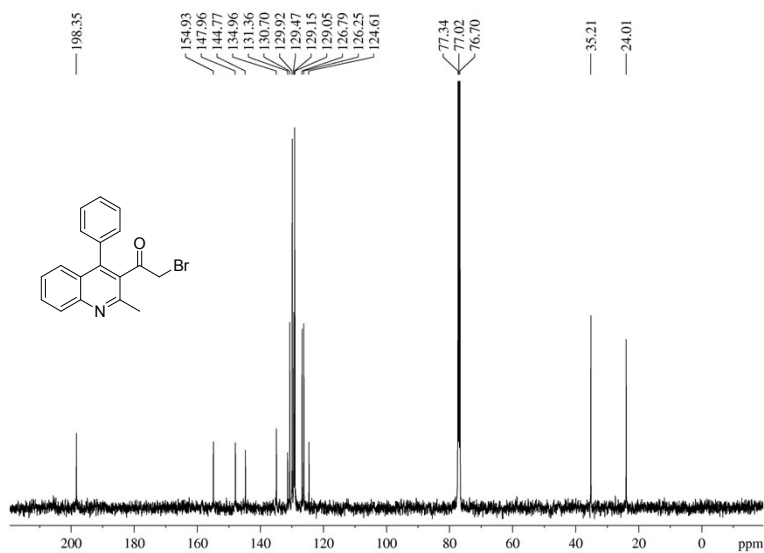
¹³C NMR Spectra of **2u** (100 MHz, CDCl₃)

PQA 1 B



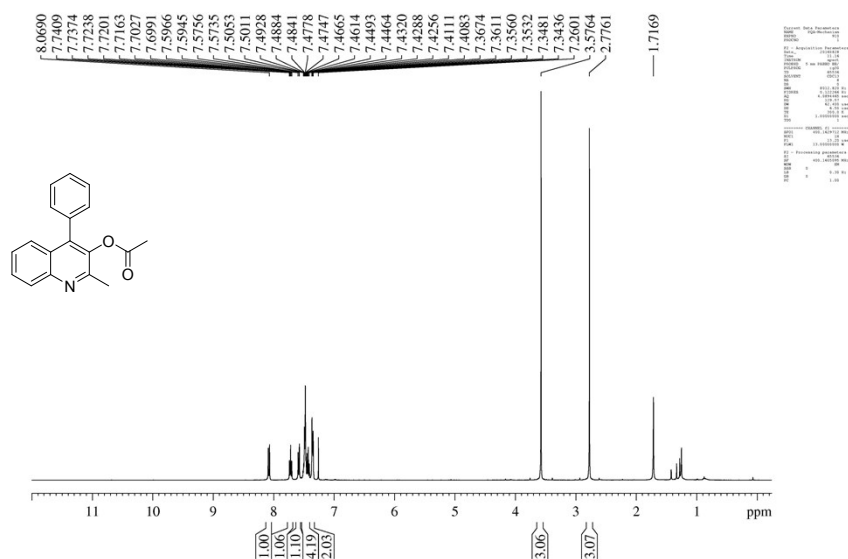
¹H NMR Spectra of **3** (400 MHz, CDCl₃)

PQA 1 BC



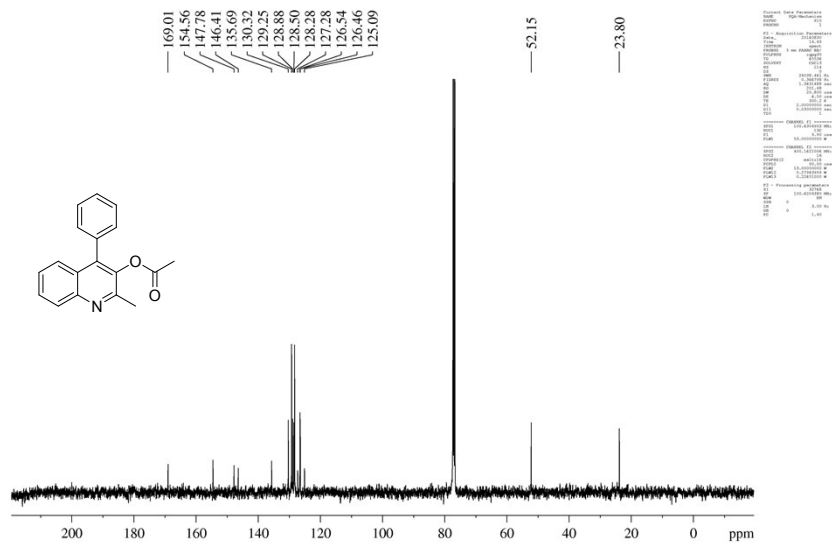
¹³C NMR Spectra of **3** (100 MHz, CDCl₃)

PQA-1-CON

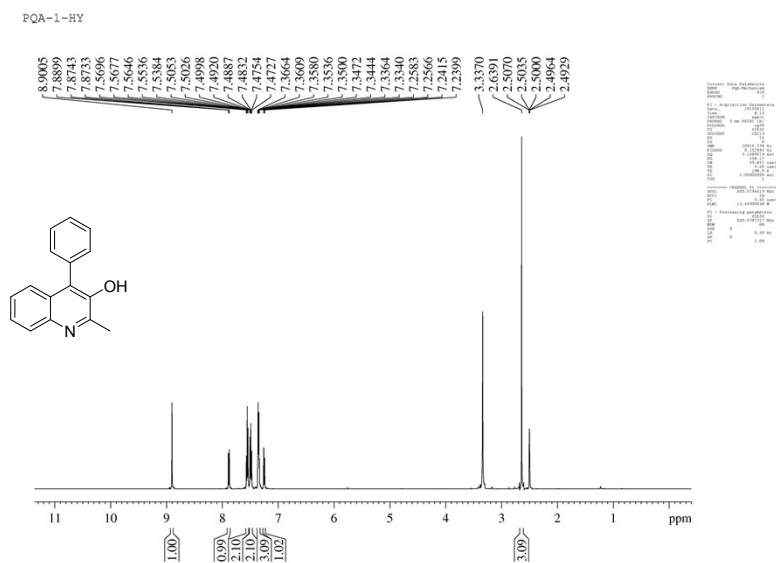


¹H NMR Spectra of **4** (400 MHz, CDCl₃)

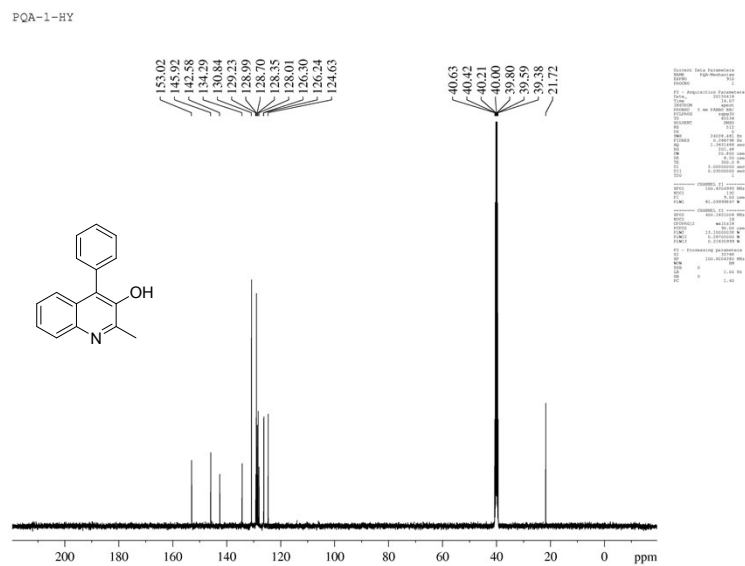
PQA-1-CON



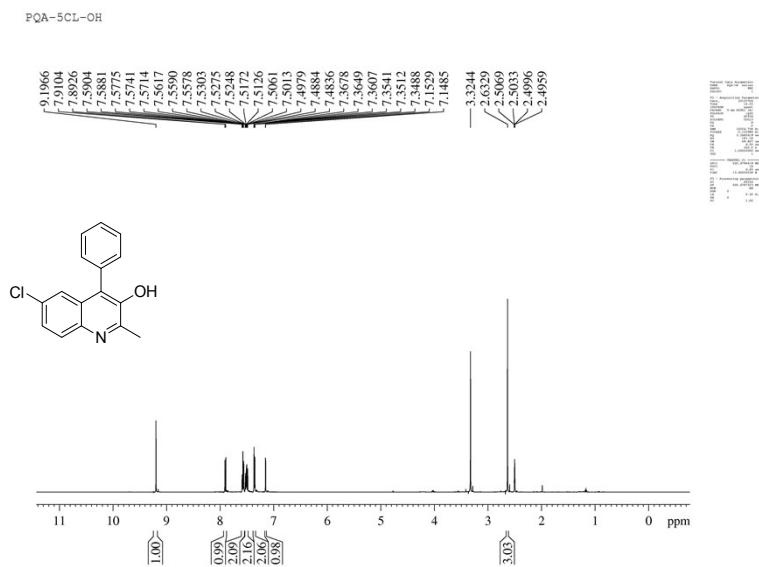
¹³C NMR Spectra of **4** (100 MHz, CDCl₃)



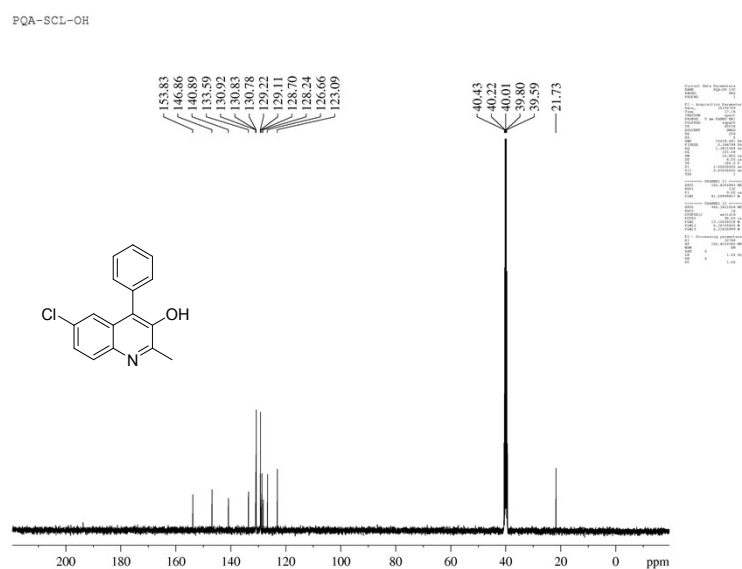
¹H NMR Spectra of **5a** (500 MHz, DMSO-*d*₆)



¹³C NMR Spectra of **5a** (100 MHz, DMSO-*d*₆)

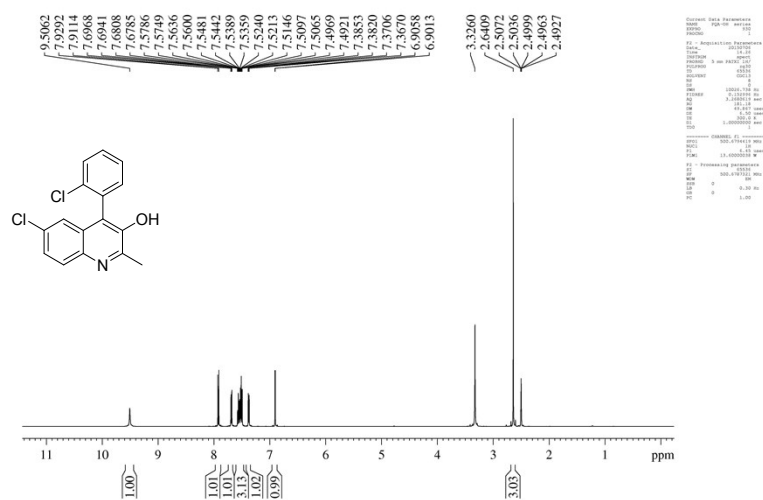


¹H NMR Spectra of **5b** (500 MHz, DMSO-*d*₆)

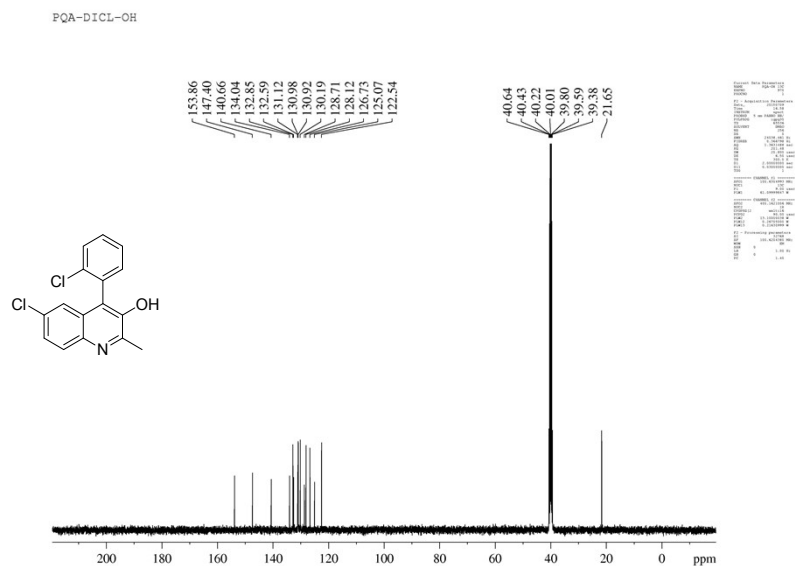


¹³C NMR Spectra of **5b** (100 MHz, DMSO-*d*₆)

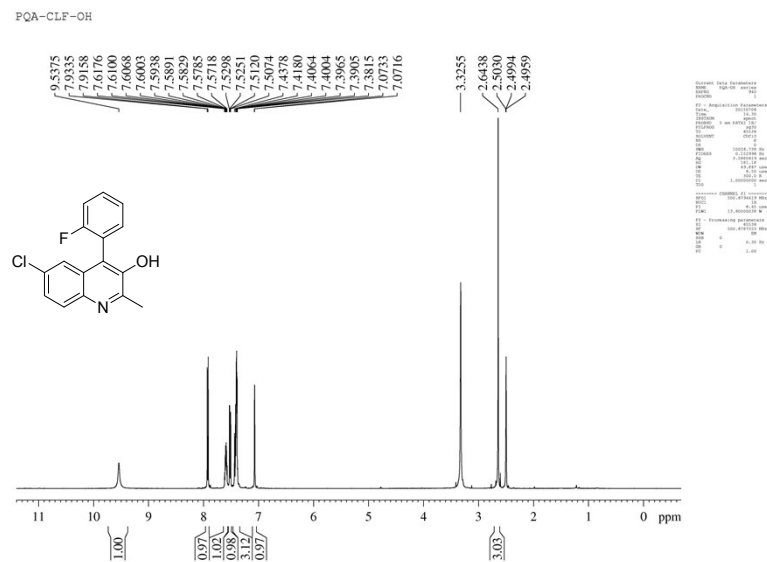
PQA-DICL-OH



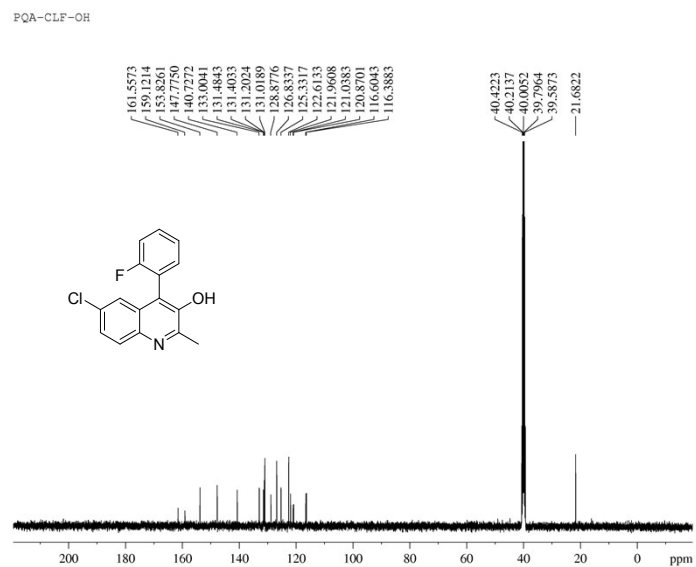
¹H NMR Spectra of **5c** (500 MHz, DMSO-*d*₆)



¹³C NMR Spectra of **5c** (100 MHz, DMSO-*d*₆)



¹H NMR Spectra of **5d** (500 MHz, DMSO-*d*₆)



¹³C NMR Spectra of **5d** (100 MHz, DMSO-*d*₆)

Chemical structure of 2-fluoro-4-(4-bromophenyl)-6-methyl-1H-benzimidazole-3-ol:

Cc1nc2cc(F)ccc2n1C3=CC=C(C=C3)Br

¹H NMR spectrum (CDCl₃) showing peaks (ppm) and integration values:

- 9.0686, 7.7516, 7.7318, 7.6472, 7.6412, 7.6366, 7.6349, 7.6201, 7.6140, 7.4907, 7.4771, 7.4708, 7.4571, 7.4502, 7.4367, 7.2842, 7.2565, 7.1597, 7.1484, 7.1313, 7.1289, 7.1189, 7.1166, 7.0995, 7.0971
- 3.3336, 2.6201, 2.5083, 2.5038, 2.4993, 2.4948

Integration values (from left to right): 1.00, 1.04, 2.11, 1.10, 2.15, 1.04, 3.10.

¹H NMR Spectra of **5e** (400 MHz, DMSO-*d*₆)

Chemical structure of 2-methyl-6-fluoro-4-(4-bromophenyl)-1H-benzimidazole-3-carboxamide:

Cc1nc2cc(F)ccc2n1-c3ccc(Br)cc3C(=O)N

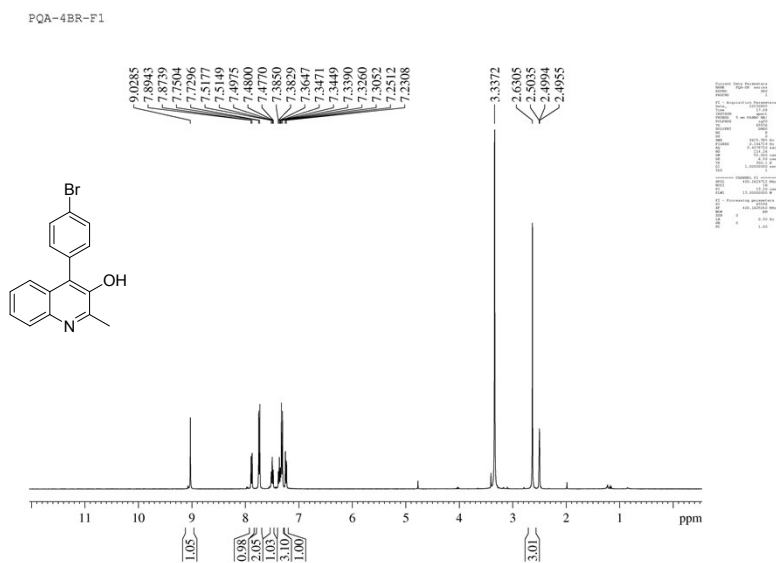
¹³C NMR spectrum (CDCl₃) showing peaks (ppm):

Peak (ppm)
158.5707
156.0511
153.9588
147.2496
143.8786
133.6433
132.1367
131.2563
128.1840
126.9975
125.2975
124.8026
121.3636
117.8208
117.7334
111.8032
111.5910
40.5649
40.3562
40.1472
39.9384
39.7297
39.5210
39.3118
39.1026
21.6179

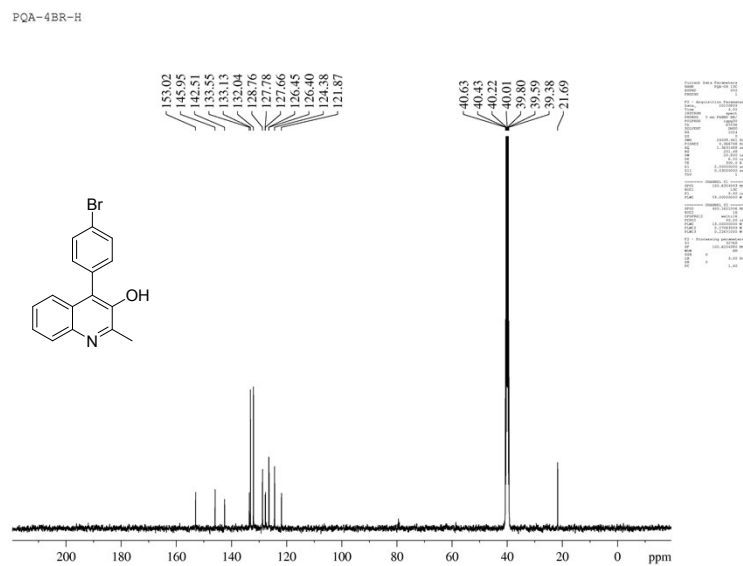
Table of peak data:

Peak (ppm)	Integration	Area (a.u.)	Area (%)
158.5707	0.00	0.00	0.00
156.0511	0.00	0.00	0.00
153.9588	0.00	0.00	0.00
147.2496	0.00	0.00	0.00
143.8786	0.00	0.00	0.00
133.6433	0.00	0.00	0.00
132.1367	0.00	0.00	0.00
131.2563	0.00	0.00	0.00
128.1840	0.00	0.00	0.00
126.9975	0.00	0.00	0.00
125.2975	0.00	0.00	0.00
124.8026	0.00	0.00	0.00
121.3636	0.00	0.00	0.00
117.8208	0.00	0.00	0.00
117.7334	0.00	0.00	0.00
111.8032	0.00	0.00	0.00
111.5910	0.00	0.00	0.00
40.5649	0.00	0.00	0.00
40.3562	0.00	0.00	0.00
40.1472	0.00	0.00	0.00
39.9384	0.00	0.00	0.00
39.7297	0.00	0.00	0.00
39.5210	0.00	0.00	0.00
39.3118	0.00	0.00	0.00
39.1026	0.00	0.00	0.00
21.6179	0.00	0.00	0.00

¹³C NMR Spectra of **5e** (100 MHz, DMSO-*d*₆)

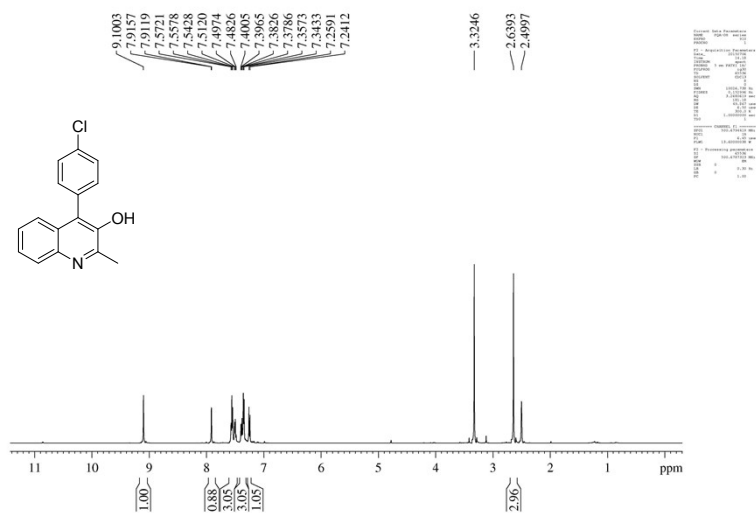


¹H NMR Spectra of **5f** (400 MHz, DMSO-*d*₆)



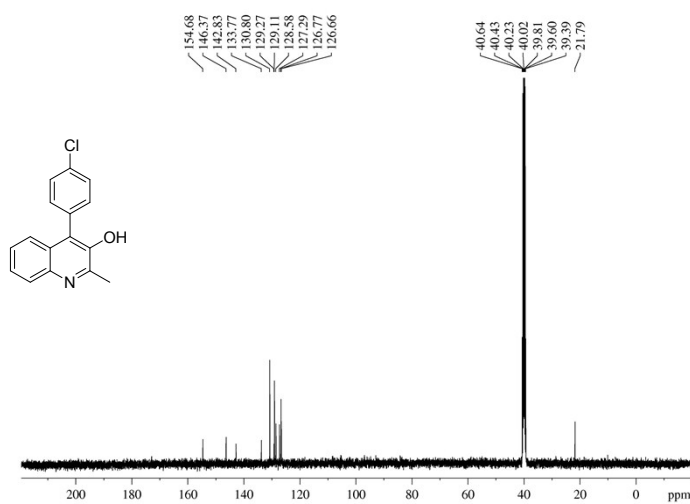
¹³C NMR Spectra of **5f** (100 MHz, DMSO-*d*₆)

PQA-4CL-OH

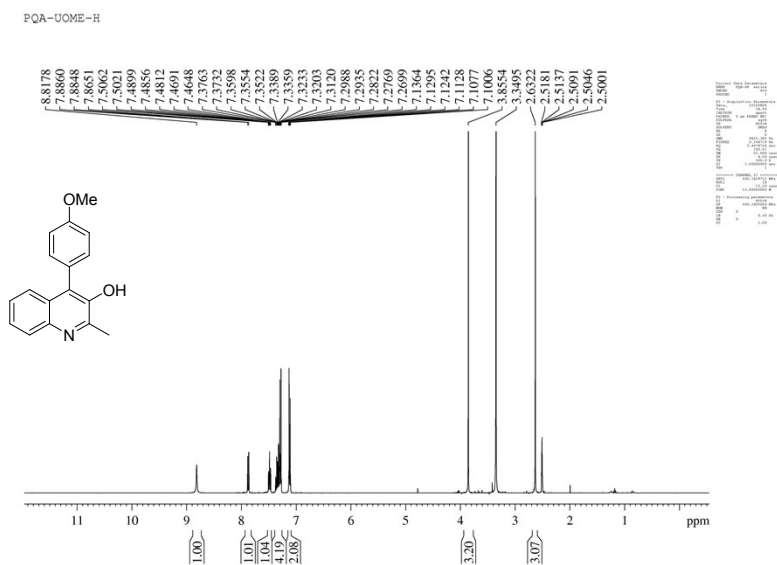


¹H NMR Spectra of **5g** (500 MHz, DMSO-*d*₆)

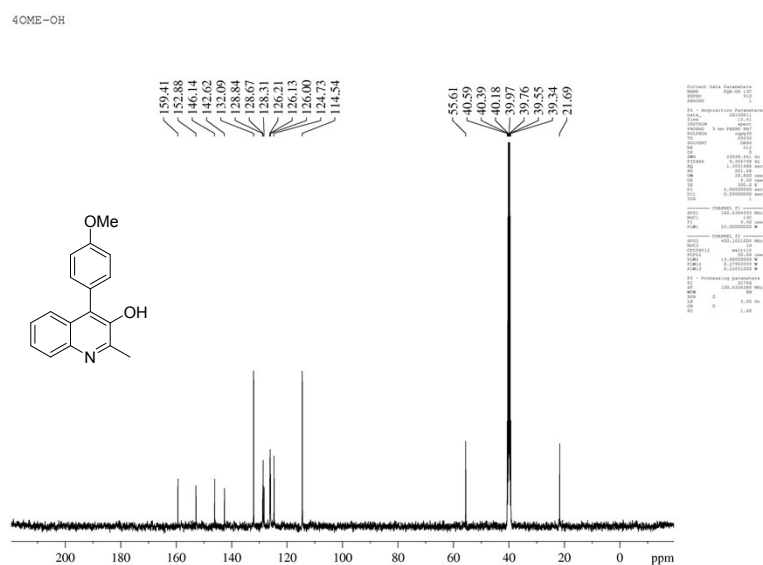
PQA-4CL-O-1



¹³C NMR Spectra of **5g** (100 MHz, DMSO-*d*₆)



¹H NMR Spectra of **5h** (400 MHz, DMSO-*d*₆)



¹³C NMR Spectra of **5h** (100 MHz, DMSO-*d*₆)