

Supporting Information

Organocatalytic One-pot Asymmetric Synthesis of

2-Aryl-2,3-dihydro-4-quinolones

Gao-Fei Pan, Li Su, Yan-Lei Zhang, Shi-Huan Guo, and Yong-Qiang Wang*

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education,
Department of Chemistry & Materials Science, Northwest University, Xi'an 710069, P. R. China
<mailto:wangyq@nwu.edu.cn>

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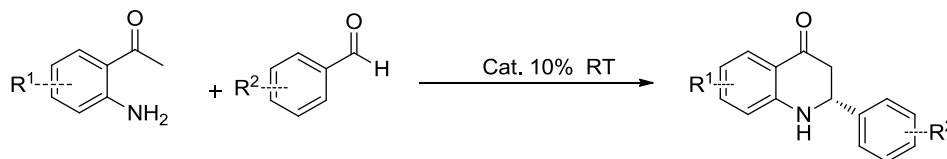
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1 General information

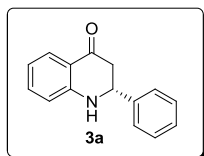
All commercial reagents and solvents were used as received without further purification. Reactions were followed with TLC (0.254 mm silica gel 60-F plates). Visualization was accomplished with UV light. Flash chromatographies were carried out on silica gel 200-300 mesh. Optical rotations were reported as follows: $[\alpha]_D^{27}$ (c g/100 mL, in solvent). Melting points (m. p.) were measured on electrothermal digital melting point apparatus and were uncorrected. ^1H NMR and ^{13}C NMR spectra were recorded at 400 MHz using CDCl_3 or $(\text{CD}_3)_2\text{SO}$ as solvent. Spectra were referenced internally to the residual proton resonance in CDCl_3 (δ 7.26 ppm), $(\text{CD}_3)_2\text{SO}$ (δ 2.50 ppm) or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br. s = broad singlet. Infrared (IR) data were recorded as films on potassium bromide plates on a Bruker Tensor 27 FT-IR spectrometer. Absorbance frequencies are reported in reciprocal centimeters (cm^{-1}). High resolution mass spectra were acquired on a Bruker Daltonics MicroTof-QII mass spectrometer. X-ray crystal structure analyses were measured on Bruker Smart APEXIICCD instrument using Mo-K α radiation. The structures were solved and refined using the SHELXTL software package. High performance liquid chromatography (HPLC) analysis was performed on a SHIMADZU LC-2010AHT instrument equipped with a quaternary pump, using a Daicel Chiralcel AD column (250 \times 4.6 mm). UV absorption was monitored at 214 nm.

2. Experimental procedures and characterization data

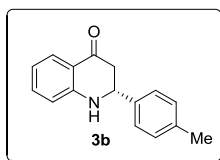
General procedure for 2-Aryl-2,3-dihydro-4-quinolones synthesis:



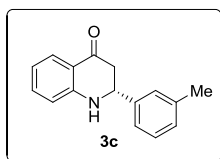
To a 1.5 mL test tube were added 0.01mmol (10 mmol%) of organocatalyst **4a**, 0.1 mmol of 2'-hydroxyacetophenones and 0.1 mmol of benzaldehydes. Then the reaction mixture was left at room temperature for sufficient time (based on monitoring by thin-layer chromatography), and finally purified by column chromatography with 10% EtOAc/hexanes as eluent to give the products (**3**).



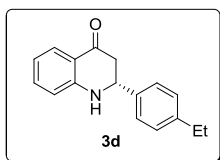
(R)-2-phenyl-2,3-dihydroquinolin-4(1H)-one (3a)^[1,2,3] Prepared according to general procedure to afford as yellow solid (72% yield). $R_f = 0.42$ (EtOAc/hexanes 1:10); m. p. = 144–145 °C. $[\alpha]_D^{23.2} = -21.5$ ($c = 0.5$, CHCl₃). ¹H NMR (400MHz, CDCl₃): $\delta = 7.88$ (d, $J = 8.0$ Hz, 1H, H-Ar), 7.47–7.33 (m, 6H, H-Ar), 6.80 (t, $J = 8.0$ Hz, 1H, H-Ar), 6.72 (d, $J = 8.0$ Hz, 1H, H-Ar), 4.76 (dd, $J = 4.0$ Hz, 16.0Hz, 1H, CH), 4.52 (s, 1H, NH), 2.93–2.76 (m, 2H, CH₂). ¹³C NMR (100MHz, CDCl₃): $\delta = 193.4, 151.7, 141.1, 135.6, 129.1, 128.6, 127.8, 126.8, 119.2, 118.6, 116.1, 58.7, 46.59$. HRMS (ESI) m/z calcd for C₁₅H₁₃NONa 246.0889 [M+Na⁺]; found 246.0879. IR (KBr): 3338, 3127, 1658, 1351, 1351, 1330, 1108, 792, 765, 717 cm⁻¹. [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 28.4 min, minor enantiomer t_R , 32.0 min; 98% ee]. Absolute configuration was determined as *R* by comparison of optical rotation to literature values, [lit., $[\alpha]_D^{20} = +27.1$ ($c = 0.42$, CHCl₃) for 98% ee of the (*S*)-enantiomer], and the configurations of other products were assigned by analogy.^[2,3] Analytical data match those reported in the literature.^[2] CCDC1418014 contains the crystallographic data for **3a** that can be obtained free of charge from the CCDC via www.ccdc.cam.ac.uk/data_request/cif.



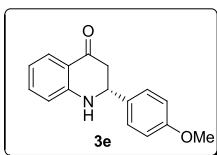
(R)-2-(p-tolyl)-2,3-dihydroquinolin-4(1H)-one (3b)^[1,2,8] Prepared according to general procedure to afford as yellow solid (63% yield). $R_f = 0.40$ (EtOAc/hexanes 1:10); m. p. = 149–150 °C. $[\alpha]^{23.0}_D = -24.6$ ($c = 0.3$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 7.85$ (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 7.33–7.32 (m, 3H, H-Ar), 7.20–7.18 (m, 2H, H-Ar), 6.77–6.69 (m, 2H, H-Ar), 4.68 (d, $J = 16.0\text{Hz}$, 1H, CH), 4.54 (s, 1H, NH), 2.88–2.70 (m, 2H, CH_2), 2.36 (s, 3H, CH_3). $^{13}\text{C NMR}$ (100MHz, CDCl_3): $\delta = 193.6$, 151.8, 138.4, 138.1, 135.5, 129.7, 127.7, 126.6, 119.1, 118.4, 116.0, 58.3, 46.6, 21.3. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{15}\text{ONNa}$ 260.1046 [$\text{M}+\text{Na}^+$]; found 260.1035. IR (KBr): 3374, 2295, 1650, 1508, 1328, 1147, 763, 646, 495 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 28.0 min, minor enantiomer t_R , 35.5 min; 98% ee].



(R)-2-(m-tolyl)-2,3-dihydroquinolin-4(1H)-one (3c)^[1] Prepared according to general procedure to afford as yellow solid (70% yield). $R_f = 0.41$ (EtOAc/hexanes 1:10); m. p. = 104–105 °C. $[\alpha]^{23.0}_D = -11.4$ ($c = 0.3$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 7.76$ (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 7.26–7.13 (m, 4H, H-Ar), 7.06 (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 6.70–6.62 (m, 2H, H-Ar), 4.60 (dd, $J = 4.0\text{Hz}$, 16.0Hz, 1H, CH), 4.52 (s, 1H, NH), 2.78–2.60 (m, 2H, CH_2), 2.28 (s, 3H, CH_3). $^{13}\text{C NMR}$ (100MHz, CDCl_3): $\delta = 193.5$, 151.8, 141.0, 138.8, 135.5, 129.2, 128.9, 127.6, 127.4, 123.8, 119.0, 118.4, 116.0, 58.5, 46.5, 21.6. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{15}\text{ONNa}$ 260.1046; found 260.1035 [$\text{M}+\text{Na}^+$]. IR (KBr): 3334, 2289, 1656, 1479, 1330, 1119, 1114, 1002, 865, 763, 701, 620 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 24.9 min, minor enantiomer t_R , 29.7 min; 98% ee].

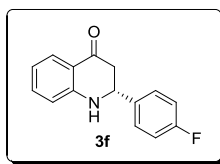


(R)-2-(4-ethylphenyl)-2,3-dihydroquinolin-4(1H)-one (3d) Prepared according to general procedure to afford as yellow solid (53% yield). $R_f = 0.39$ (EtOAc/hexanes 1:10); m. p. = 110–111 °C. $[\alpha]^{23.0}_D = +15.4$ ($c = 0.3$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 7.79$ (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 7.38–7.22 (m, 5H, H-Ar), 6.70 (t, $J = 8.0\text{Hz}$, 1H, H-Ar), 6.62 (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 4.64 (dd, $J = 8.0\text{Hz}$, 8.0Hz, 1H, CH), 4.53 (s 1H, NH), 2.91–2.72 (m, 2H, CH_2), 2.59 (q, 2H, $J = 8.0\text{Hz}$, CH_2), 1.1 (t, $J = 8.0\text{Hz}$, 3H, CH_3). $^{13}\text{C NMR}$ (100MHz, CDCl_3): $\delta = 193.7$, 151.8, 144.8, 138.3, 135.5, 128.6, 127.7, 126.8, 119.1, 118.4, 116.0, 58.3, 46.6, 28.7, 15.7. HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{17}\text{NONa}$ 274.1202 $[\text{M}+\text{Na}^+]$; found 274.1202. IR (KBr): 3301, 2976, 1611, 1511, 1476, 1333, 1259, 1219, 1213, 1120, 1035, 1069, 826, 749, 641 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 25.4 min, minor enantiomer t_R , 30.0 min; 96% ee].

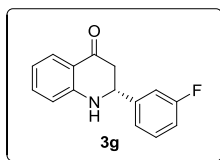


(R)-2-(4-methoxyphenyl)-2,3-dihydroquinolin-4(1H)-one (3e)^[1,3] Prepared according to general procedure to afford as yellow solid (85% yield). $R_f = 0.36$ (EtOAc/hexanes 1:10); m. p. = 132–133°C. $[\alpha]^{23.0}_D = -35.7$ ($c = 0.4$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 7.74$ (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 7.26–7.16 (m, 3H, H-Ar), 6.82–6.80 (m, 2H, H-Ar), 6.68–6.61 (m, 2H, H-Ar), 4.56–4.54 (m, 2H, CH, NH), 3.71 (s, 3H, OCH_3), 2.75–2.57 (m, 2H, CH_2). $^{13}\text{C NMR}$ (100MHz, CDCl_3): $\delta = 193.69$, 159.58, 151.77, 135.44, 133.08, 127.88, 127.56, 118.91, 118.28, 116.02, 114.26, 57.86, 55.38, 46.54. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{15}\text{NNaO}_2\text{Na}$ 276.0995 $[\text{M}+\text{Na}^+]$; found 276.0990. IR (KBr): 3289, 2924, 1649, 1605, 1507, 1475, 1434, 1302, 1248, 1212, 1152, 1036, 910, 825, 753, 635, 442 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214nm; major enantiomer t_R , 47.7 min,

minor enantiomer t_R , 55.0 min; 85% ee].

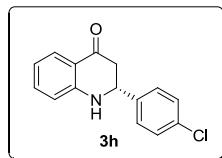


(R)-2-(4-fluorophenyl)-2,3-dihydroquinolin-4(1H)-one (3f)^[1,6,7] Prepared according to general procedure to afford as yellow solid (80% yield). $R_f = 0.35$ (EtOAc/hexanes 1:10); m. p. = 134–135 °C. $[\alpha]^{23.0}_D = +9.3$ ($c = 0.2$, CHCl₃). ¹H NMR (400MHz, CDCl₃): $\delta = 7.86$ (d, $J = 8.0$ Hz, 1H, H-Ar), 7.53–7.51 (m, 2H, H-Ar), 7.35–7.33 (m, 3H, H-Ar), 6.83–6.72 (m, 2H, H-Ar), 4.72 (dd, $J = 4.0$ Hz, 16.0Hz, 1H, CH), 4.42 (s, 1H, NH), 2.86–2.73 (m, 2H, CH₂). ¹³C NMR (100MHz, CDCl₃): $\delta = 193.2$, 162.7 (d, $J_{F-C} = 246.0$ Hz), 151.5, 136.9, 135.6, 128.5 (d, $J_{F-C} = 8.0$ Hz), 127.8, 119.2, 118.8, 116.1 (d, $J_{F-C} = 8.0$ Hz), 115.9, 58.0, 46.7. HRMS (ESI) m/z calcd for C₁₅H₁₂FONNa 264.0795; found 264.0781 [M+Na⁺]. IR (KBr): 3299, 2974, 1645, 1506, 1326, 1216, 1118, 1002, 835, 759, 649, 509 cm⁻¹. [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 27.9 min, minor enantiomer t_R , 35.7 min; 99% ee].

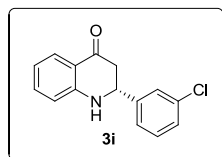


(R)-2-(3-fluorophenyl)-2,3-dihydroquinolin-4(1H)-one (3g)^[1,2,8] Prepared according to general procedure to afford as yellow solid (80% yield). $R_f = 0.36$ (EtOAc/hexanes 1:10); m. p. = 138–139 °C. $[\alpha]^{23.0}_D = +5.2$ ($c = 0.3$, CHCl₃). ¹H NMR (400MHz, (CD₃)₂SO): $\delta = 7.62$ (d, $J = 8.0$ Hz, 1H, H-Ar), 7.44–7.33 (m, 4H, H-Ar), 7.18–7.13 (m, 2H, H-Ar), 6.92 (d, $J = 8.0$ Hz, 1H, H-Ar), 6.66 (t, $J = 8.0$ Hz, 1H, H-Ar), 4.81 (d, $J = 8.0$ Hz, 1H, CH), 2.88–2.69 (m, 2H, CH₂). ¹³C NMR (100MHz, (CD₃)₂SO): $\delta = 192.2$, 162.2 (d, $J_{F-C} = 242.0$ Hz), 152.3, 144.7 (d, $J_{F-C} = 7.0$ Hz), 135.2, 130.6 (d, $J_{F-C} = 8.0$ Hz), 126.4, 123.0, 117.8, 116.7, 116.3, 114.5 (d, $J_{F-C} = 21.0$ Hz), 113.7 (d, $J_{F-C} = 21.0$ Hz), 55.7, 45.0. HRMS (ESI) m/z calcd for C₁₅H₁₂FONNa 264.0795 [M+Na⁺]; found 264.0781. IR (KBr): 3332, 2947, 1608, 1479, 1330, 1145,

875, 763, 640 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_{R} , 23.9 min, minor enantiomer t_{R} , 25.8 min; 84% ee].

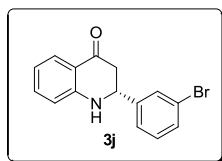


(R)-2-(4-chlorophenyl)-2,3-dihydroquinolin-4(1H)-one (3h)^[2] Prepared according to general procedure to afford as yellow solid (78% yield). $R_{\text{f}} = 0.33$ (EtOAc/hexanes 1:10); m. p. = 173–174 °C. $[\alpha]_{\text{D}}^{23.0} = -12.4$ ($c = 0.4$, CHCl_3). ^1H NMR (400MHz, CDCl_3): $\delta = 7.79$ (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 7.34–7.26 (m, 5H, H-Ar), 6.73 (t, $J = 8.0\text{Hz}$, 1H, H-Ar), 6.66 (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 4.66 (dd, $J = 4.0\text{Hz}$, 16.0Hz, 1H, CH), 4.51 (s, 1H, NH), 2.86–2.71 (m, 2H, CH_2). ^{13}C NMR (100MHz, CDCl_3): $\delta = 192.0$, 150.5, 138.7, 134.7, 133.3, 128.3, 127.1, 126.7, 118.2, 117.8, 115.1, 57.03, 45.6. HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{12}\text{NOCINa}$ 280.0500 [$\text{M}+\text{Na}^+$]; found 280.0498. IR (KBr): 3305, 2906, 1650, 1481, 1328, 1147, 765, 644, 495 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_{R} , 27.7 min, minor enantiomer t_{R} , 33.6 min; 82% ee].

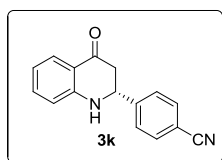


(R)-2-(3-chlorophenyl)-2,3-dihydroquinolin-4(1H)-one (3i)^[2] Prepared according to general procedure to afford as yellow solid (84% yield). $R_{\text{f}} = 0.33$ (EtOAc/hexanes 1:10); m. p. = 130–131 °C. $[\alpha]_{\text{D}}^{23.0} = +65.3$ ($c = 0.3$, CHCl_3). ^1H NMR (400MHz, CDCl_3): $\delta = 7.85$ (d, 1H, H-Ar), 7.47 (s, 1H, H-Ar), 7.37–7.32 (m, 4H, H-Ar), 6.82–6.73 (m, 2H, H-Ar), 4.71 (dd, $J = 4.0\text{Hz}$, 16.0Hz, 1H, CH), 4.62 (s, 1H, NH), 2.85–2.71 (m, 2H, CH_2). ^{13}C NMR (100MHz, CDCl_3): $\delta = 193.0$, 151.5, 143.2, 135.7, 134.9, 130.4, 128.7, 127.7, 126.9, 125.0, 119.1, 118.8, 116.1, 58.1, 46.4. HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{12}\text{NOCINa}$ 280.0500 [$\text{M}+\text{Na}^+$]; found 280.0498. IR (KBr): 3328, 2937, 1660, 1477, 1330, 1155, 997, 761, 638 cm^{-1} . [Daicel chiralpak AD column,

eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 24.1 min, minor enantiomer t_R , 26.1 min; 87% ee].

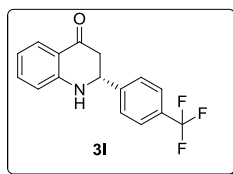


(R)-2-(3-bromophenyl)-2,3-dihydroquinolin-4(1H)-one (3j)^[1] Prepared according to general procedure to afford as yellow solid (72% yield). R_f = 0.36 (EtOAc/hexanes 1:10); m. p. = 118–119 °C. $[\alpha]^{23.0}_D = +12.0$ ($c = 0.3$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 7.86$ (dd, $J = 4.0\text{Hz}$, 16.0Hz , 1H, H-Ar), 7.64 (s, 1H, H-Ar), 7.49–7.46 (m, 1H, H-Ar), 7.38–7.33 (m, 2H, H-Ar), 7.28–7.24 (m, 1H, H-Ar), 6.83–6.73 (m, 2H, H-Ar), 4.71 (dd, $J = 4.0\text{Hz}$, 16.0Hz , 1H, CH), 4.56 (s, 1H, NH), 2.87–2.72 (m, 2H, CH_2). $^{13}\text{C NMR}$ (100MHz, CDCl_3): $\delta = 193.0$, 151.5, 143.4, 135.7, 131.6, 130.6, 129.8, 127.6, 125.4, 123.0, 119.0, 118.7, 116.2, 58.0, 46.3. HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{12}\text{ONBrNa}$ 323.9994 $[\text{M}+\text{Na}^+]$; found 323.9998. IR (KBr): 3328, 2938, 1658, 1475, 1330, 1285, 1114, 763, 642 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 23.1 min, minor enantiomer t_R , 26.1 min; 83 % ee].

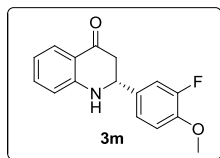


(R)-4-(4-oxo-1,2,3,4-tetrahydroquinolin-2-yl)benzonitrile (3k) Prepared according to general procedure to afford as yellow solid (70% yield). R_f = 0.35 (EtOAc/hexanes 1:10); m. p. = 145–146 °C. $[\alpha]^{23.0}_D = +19.5$ ($c = 0.4$, CHCl_3). $^1\text{H NMR}$ (400MHz, $(\text{CD}_3)_2\text{SO}$): $\delta = 7.86$ (d, $J = 8.0\text{Hz}$, 2H, H-Ar), 7.69 (d, $J = 8.0\text{Hz}$, 2H, H-Ar), 7.36–7.24 (m, 2H, H-Ar), 6.90 (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 6.66 (t, $J = 8.0\text{Hz}$, 1H, H-Ar), 4.89 (dd, $J = 4.0\text{Hz}$, 16.0 Hz , 1H, CH), 2.86–2.71 (m, 2H, CH_2). $^{13}\text{C NMR}$ (100MHz, $(\text{CD}_3)_2\text{SO}$): $\delta = 191.9$, 152.2, 147.4, 135.3, 132.6, 127.9, 126.4, 118.8, 117.8, 116.9, 116.3, 110.5, 55.8, 44.7. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{12}\text{N}_2\text{ONa}$ 271.0842 $[\text{M}+\text{Na}^+]$; found 271.0853. IR (KBr): 3338, 2956, 1693, 1607, 1472, 1364, 1305, 1226, 1150,

1116, 962, 765, 656 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 254 nm; major enantiomer t_R , 39.5 min, minor enantiomer t_R , 45.9 min; 96% ee].

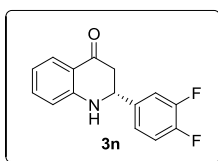


(R)-2-(4-(trifluoromethyl)phenyl)-2,3-dihydroquinolin-4(1H)-one (3l)^[7] Prepared according to general procedure to afford as yellow solid (75% yield). R_f = 0.40 (EtOAc/hexanes 1:10); m. p. = 160–161 °C. $[\alpha]^{23.0}_D = -29.5$ ($c = 0.45$, CHCl_3). ^1H NMR (400MHz, CDCl_3): $\delta = 7.86$ (d, $J = 4.0\text{Hz}$, 1H), 7.67–7.57 (m, 4H, H-Ar), 7.39–7.34 (m, 1H, H-Ar), 7.26 (s, 1H, H-Ar), 4.82 (dd, $J = 4.0\text{Hz}$, 12.0Hz, 1H, CH), 4.62 (s, 1H, NH), 2.87–2.74 (m, 2H, CH_2). ^{13}C NMR (100MHz, CDCl_3): $\delta = 191.67$, 150.39, 144.15, 134.74, 129.80 (q, $J_{F-C} = 32.0\text{Hz}$), 126.72, 126.14, 125.18, 125.14, 125.10, 125.07, 123.03 (q, $J_{F-C} = 271.0\text{Hz}$), 118.19, 117.97, 57.19, 45.37. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{12}\text{F}_3\text{NONa}$ 314.0763 [$\text{M}+\text{Na}^+$]; found 314.0771. IR (KBr): 3368, 2971, 1657, 1612, 1508, 1478, 1328, 1155, 1278, 1120, 1062, 766, 690, 639, 574 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214nm; major enantiomer t_R , 30.1 min, minor enantiomer t_R , 34.7 min; 86% ee].

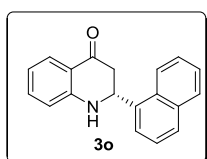


(R)-2-(3-fluoro-4-methoxyphenyl)-2,3-dihydroquinolin-4(1H)-one (3m) Prepared according to general procedure to afford as yellow solid (75% yield). R_f = 0.39 (EtOAc/hexanes 1:10); m. p. = 123–124 °C. $[\alpha]^{23.0}_D = -10.7$ ($c = 0.3$, CHCl_3). ^1H NMR (400MHz, CDCl_3): $\delta = 7.85$ (d, $J = 4.0\text{Hz}$, 1H), 7.36–7.33 (m, 1H, H-Ar), 7.19–7.13 (m, 2H, H-Ar), 6.95 (t, $J = 8.0\text{Hz}$, 1H, H-Ar), 6.81–6.72 (m, 2H, H-Ar),

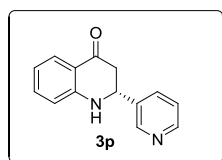
4.66 (dd, $J = 4.0\text{Hz}$, 12.0 Hz , 1H, CH), 4.57 (s, 1H, NH), 3.89 (s, 3H, OCH₃), 2.84–2.70 (m, 2H, CH₂). ¹³C NMR (100MHz, CDCl₃): $\delta = 193.2$, 152.4 (d, $J_{F-C} = 225.0\text{Hz}$), 151.5 , 147.7 (d, $J_{F-C} = 10.0\text{Hz}$), 135.6 , 134.1 (d, $J_{F-C} = 5.0\text{Hz}$), 127.6 , 122.6 (d, $J_{F-C} = 3.0\text{Hz}$), 119.1 , 118.7 , 116.1 , 114.5 (d, $J_{F-C} = 19.0\text{Hz}$), 113.6 , 57.7 , 56.4 , 46.6 . HRMS (ESI) m/z calcd for C₁₆H₁₄O₂NFNa 294.0901 [M+Na⁺]; found 294.0884. IR (KBr): 3322, 2836, 1656, 1612, 1504, 1278, 1130, 767, 630, 576 cm⁻¹. [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 43.1 min, minor enantiomer t_R , 48.7 min; 80% ee].



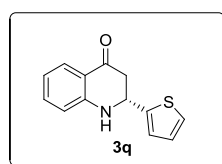
(R)-2-(3,4-difluorophenyl)-2,3-dihydroquinolin-4(1H)-one (3n) Prepared according to general procedure to afford as yellow solid (82% yield). $R_f = 0.34$ (EtOAc/hexanes 1:10); m. p. = 141–142 °C. $[\alpha]^{23.0}_D = +34.5$ ($c = 0.3$, CHCl₃). ¹H NMR (400MHz, CDCl₃): $\delta = 7.82$ (d, $J = 8.0\text{Hz}$, 1H, H-Ar), 7.37 – 7.27 (m, 2H, H-Ar), 7.20 – 7.14 (m, 2H, H-Ar), 6.81 – 6.75 (m, 2H, H-Ar), 4.71 – 4.67 (m, 2H, CH, NH), 2.80 – 2.68 (m, 2H, CH₂). ¹³C NMR (100MHz, CDCl₃): $\delta = 192.8$, 150.5 (dd, $J_{F-C} = 248.0\text{Hz}$, 13.0Hz), 151.4 , 150.1 (dd, $J_{F-C} = 248.0\text{Hz}$, 13.0Hz), 138.2 , 135.7 , 127.5 , 122.7 , 118.9 , 118.8 , 117.8 (d, $J_{F-C} = 18.0\text{Hz}$), 116.2 , 115.7 (d, $J_{F-C} = 18.0\text{Hz}$), 57.5 , 46.4 . HRMS (ESI) m/z calcd for C₁₅H₁₁ONF₂Na 282.0701 [M+Na⁺]; found 282.0715. IR (KBr): 3316, 2923, 1656, 1608, 1403, 1151, 763, 667 cm⁻¹. [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 24.5 min, minor enantiomer t_R , 27.1 min; 92% ee]. CCDC1418015 contains the crystallographic data for **3l** that can be obtained free of charge from the CCDC via www.ccdc.cam.ac.uk/data_request/cif.



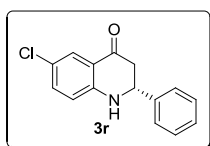
(R)-2-(naphthalen-1-yl)-2,3-dihydroquinolin-4(1H)-one (3o)^[7] Prepared according to general procedure to afford as yellow solid (67% yield). $R_f = 0.45$ (EtOAc/hexanes 1:10); m. p. = 166–167 °C. $[\alpha]^{23.0}_D = -31.6$ ($c = 0.5$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 7.90\text{--}7.83$ (m, 5H, H-Ar), 7.57–7.50 (m, 3H, H-Ar), 7.34–7.38 (m, 1H, H-Ar), 6.82–6.74 (m, 2H, H-Ar), 4.88 (dd, $J = 4.0\text{Hz}$, 16.0Hz, 1H, CH), 4.64 (s, 1H, NH), 2.99–2.80 (m, 2H, CH_2). $^{13}\text{C NMR}$ (100MHz, CDCl_3): δ 193.4, 151.7, 138.5, 135.6, 133.4, 133.4, 129.0, 128.0, 127.9, 127.7, 126.7, 126.5, 125.7, 124.4, 119.2, 118.6, 116.1, 58.7, 46.5. HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{15}\text{ONNa}$ 296.1046 $[\text{M}+\text{Na}^+]$; found 296.1058. IR (KBr): 3320, 3054, 2978, 1656, 1605, 1508, 1326, 1149, 750, 576, 442 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 38.6 min , minor enantiomer t_R , 42.0 min; 99% ee].



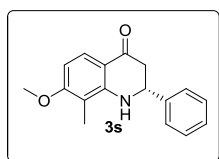
(R)-2-(pyridin-3-yl)-2,3-dihydroquinolin-4(1H)-one (3p)^[7] Prepared according to general procedure to afford as yellow solid (78% yield). $R_f = 0.21$ (EtOAc/hexanes 1:10); m. p. = 152–153 °C. $[\alpha]^{23.0}_D = +16.0$ ($c = 0.4$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 8.64$ (s, 1H, H-Ar), 8.57–8.55 (m, 1H, H-Ar), 7.85–7.80 (m, 2H, H-Ar), 7.37–7.29 (m, 2H, H-Ar), 6.82–6.77 (m, 2H, H-Ar), 4.95 (s, 1H, NH), 4.76 (dd, $J = 8.0\text{ Hz}$, 8.0 Hz, 1H, CH), 2.88–2.71 (m, 2H, CH_2). $^{13}\text{C NMR}$ (100MHz, CDCl_3): $\delta = 192.6$, 151.5, 149.9, 148.5, 136.6, 135.7, 134.4, 127.6, 123.9, 119.0, 118.8, 116.2, 56.1, 46.0. HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{ONa}$ 247.0836 $[\text{M}+\text{Na}^+]$; found 247.0836. IR (KBr): 3218, 2929, 1666, 1475, 1303, 1145, 1024, 771, 710 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 254 nm; major enantiomer t_R , 27.9 min, minor enantiomer t_R , 32.7 min; 98% ee].



(R)-2-(thiophen-2-yl)-2,3-dihydroquinolin-4(1H)-one (3q)^[1,3] Prepared according to general procedure to afford as yellow solid (71% yield). $R_f = 0.30$ (EtOAc/hexanes 1:10); m. p. = 140–141°C. $[\alpha]^{23.0}_D = -30.7$ ($c = 0.4$, CHCl_3). $^1\text{H NMR}$ (400MHz, CDCl_3): $\delta = 7.76$ (d, $J = 4.0\text{Hz}$, 1H), 7.26–7.17 (m, 2H, H-Ar), 6.96–6.87 (m, 2H, H-Ar), 6.72–6.63 (m, 2H, H-Ar), 4.92 (dd, $J = 4.0\text{Hz}$, 12.0 Hz, 1H,CH), 4.71 (s, 1H, NH), 2.82–2.79 (m, 2H, CH_2). $^{13}\text{C NMR}$ (100MHz, CDCl_3) : $\delta = 192.80$, 150.94, 144.55, 135.56, 127.54, 126.93, 125.18, 125.07, 119.21, 118.77, 116.11, 53.72, 47.04. HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{11}\text{NOSNa}$ 252.0454 [$\text{M}+\text{Na}^+$]; found 252.0462. IR (KBr): 3320, 2919, 1656, 1478, 1335, 1144, 1015, 778, 710, 678 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.4 mL/min, 214 nm; major enantiomer t_R , 24.3 min, minor enantiomer t_R , 27.3 min; 80% ee].

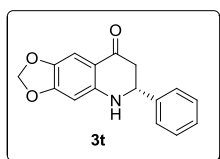


(R)-6-chloro-2-phenyl-2,3-dihydroquinolin-4(1H)-one (3r) Prepared according to general procedure to afford as yellow solid (67% yield). $R_f = 0.42$ (EtOAc/hexanes 1:10); m. p. = 162–163 °C. $[\alpha]^{23.0}_D = -29.5$ ($c = 0.50$, CHCl_3). $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.77$ (d, $J = 4.0\text{Hz}$, 1H), 7.37–7.29 (m, 5H, H-Ar), 7.22–7.19 (m, 1H, H-Ar), 4.67 (dd, $J = 4.0\text{Hz}$, 12.0Hz, 1H,CH), 4.48 (s, 1H, NH), 2.84–2.68 (m, 2H, CH_2). $^{13}\text{C NMR}$ (100MHz, CDCl_3) : $\delta = 192.28$, 192.28, 150.03, 140.66, 135.43, 129.22, 128.80, 127.02, 126.74, 123.95, 119.83, 117.62, 58.54, 46.18. HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{12}\text{ONClNa}$ 280.0500 [$\text{M}+\text{Na}^+$]; found 280.0508. IR (KBr): 3439, 3338, 2923, 1657, 1615, 1497, 1402, 1198, 855, 761, 701, 494 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 26.5 min, minor enantiomer t_R , 30.3 min; 89% ee].



(R)-7-methoxy-6-methyl-2-phenyl-2,3-dihydroquinolin-4(1H)-one (3s) Prepared

according to general procedure to afford as yellow solid (62% yield). $R_f = 0.41$ (EtOAc/hexanes 1:10); m.p. = 132–133 °C. $[\alpha]^{23.0}_D = -40.7$ ($c = 0.5$, CHCl_3). ^1H NMR (400 MHz, CDCl_3): $\delta = 7.77$ (d, $J = 4.0$ Hz, 1H, H-Ar), 7.43–7.41 (m, 2H, H-Ar), 7.37–7.30 (m, 3H, H-Ar), 6.39 (d, $J = 4.0$ Hz, 1H, H-Ar), 4.66 (dd, $J = 4.0$ Hz, 12.0 Hz, 1H, CH), 4.33 (s, 1H, NH), 3.81 (s, 3H, OCH_3), 2.83–2.65 (m, 2H, CH_2), 1.94 (s, 3H, CH_3). ^{13}C NMR (100 MHz, CDCl_3): $\delta = 192.80, 162.45, 151.03, 141.58, 129.16, 128.56, 127.21, 126.82, 113.87, 108.81, 102.35, 77.48, 77.16, 76.84, 58.58, 55.89, 46.22, 8.66$. HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{17}\text{O}_2\text{NNa}$ 290.1151 $[\text{M}+\text{Na}^+]$; found 290.1160. IR (KBr): 3340, 3073, 3011, 1655, 1601, 1461, 1265, 1096, 1024, 758, 695, 564, 487 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 29.6 min, minor enantiomer t_R , 35.2 min; 84% ee].

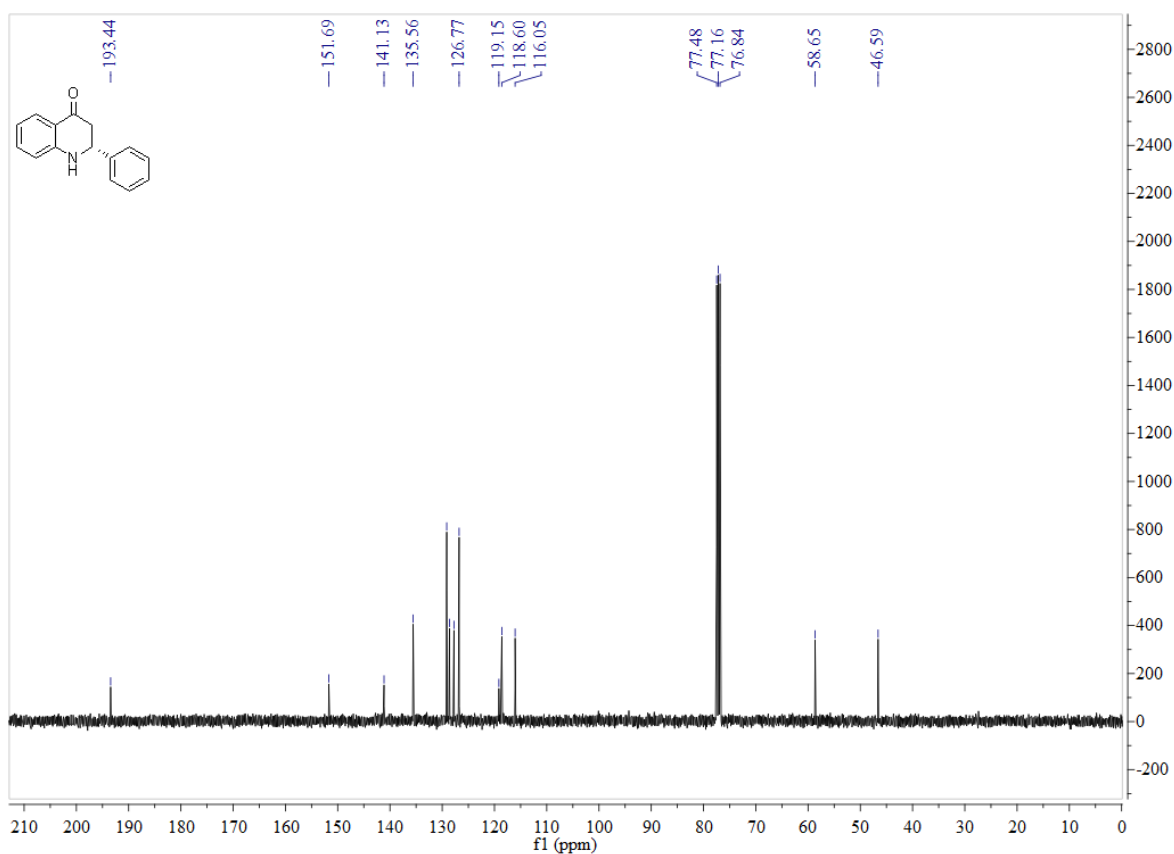
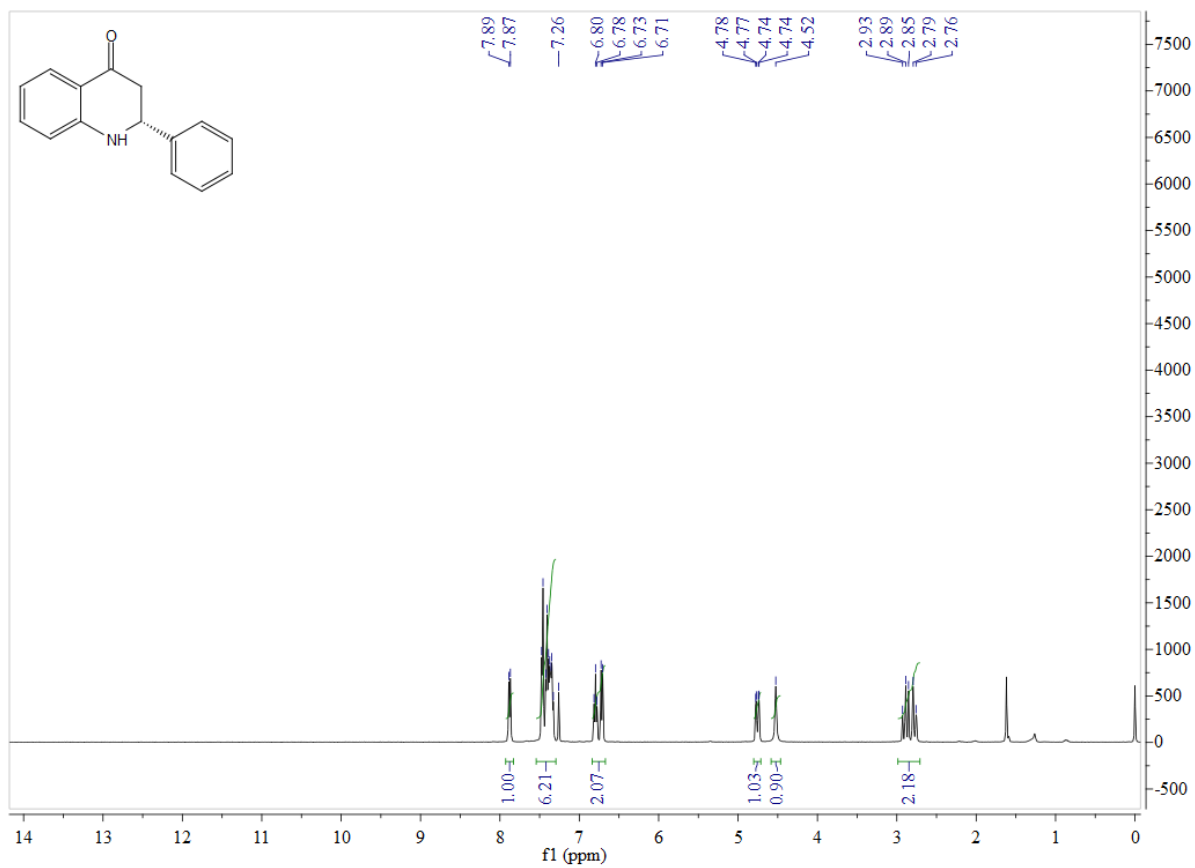


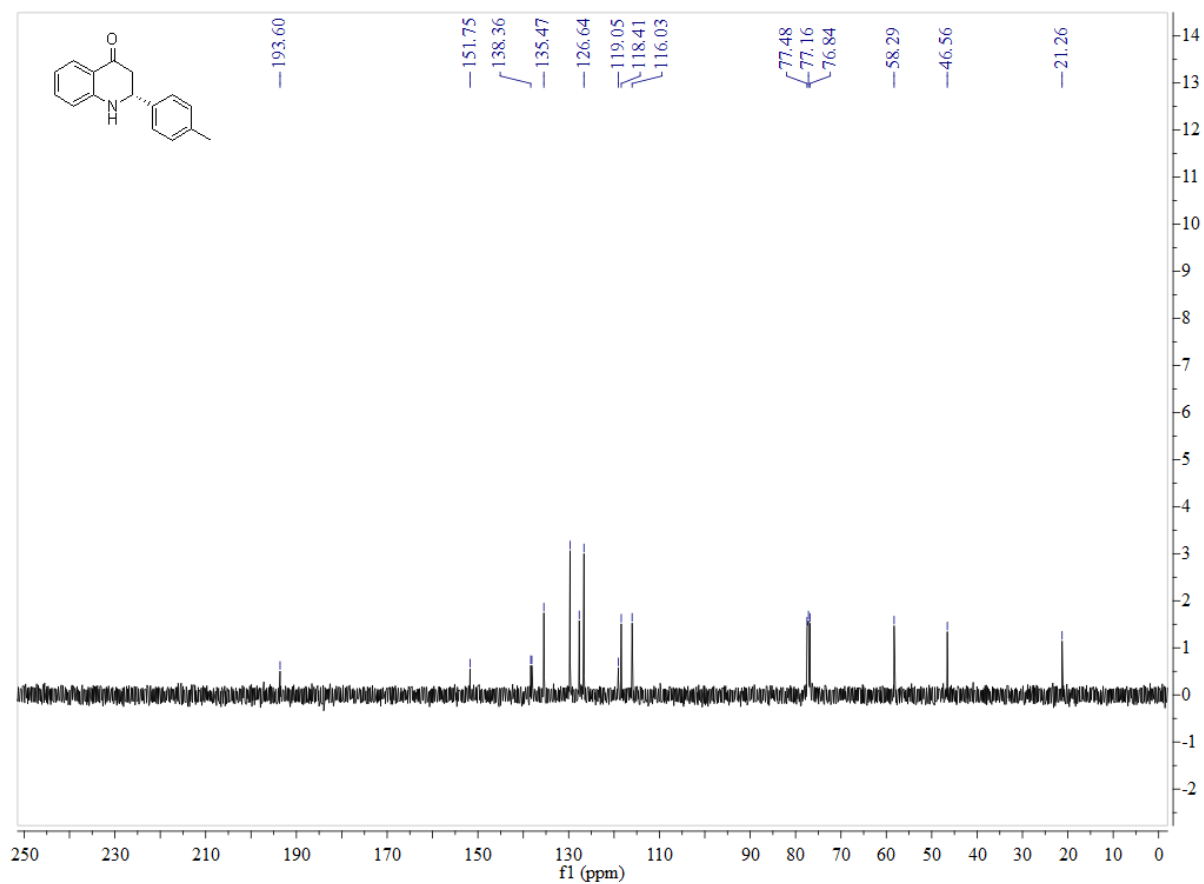
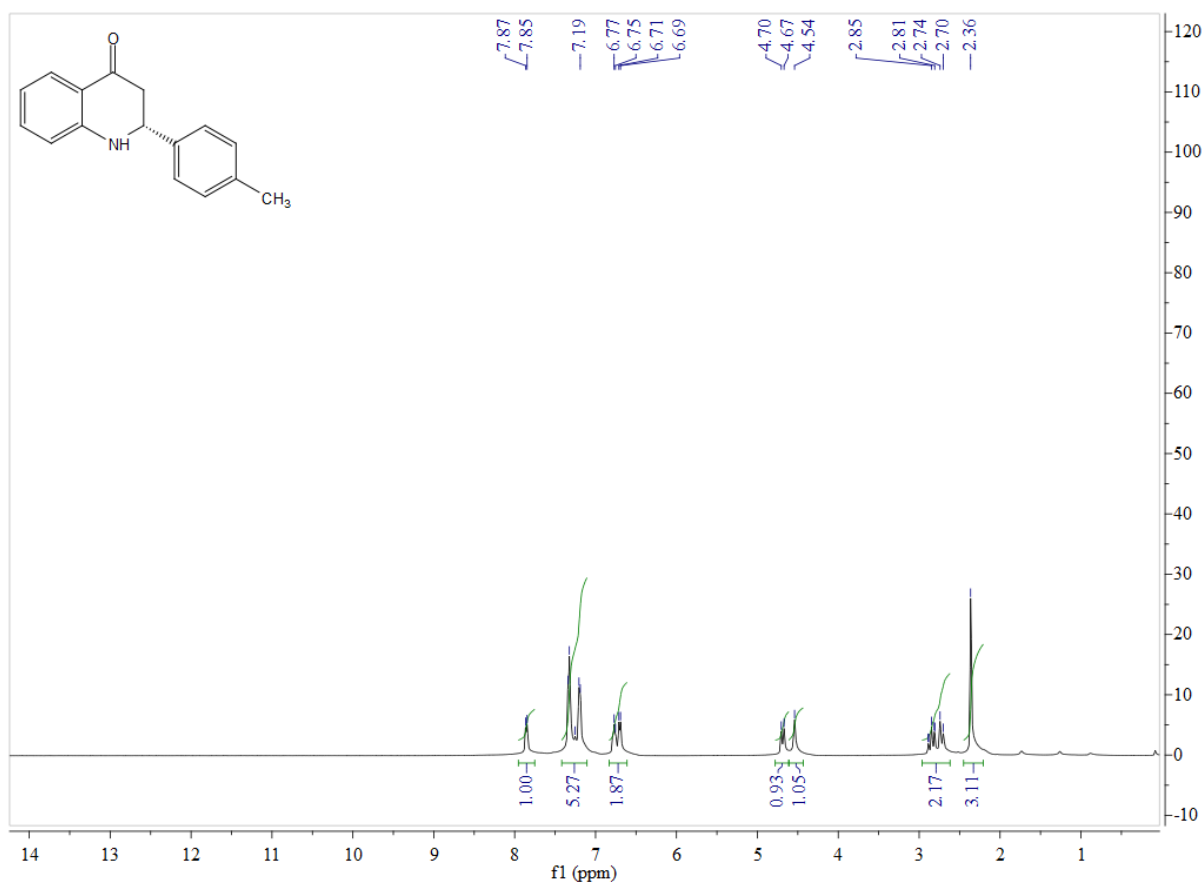
(R)-6-phenyl-6,7-dihydro-[1,3]dioxolo[4,5-g]quinolin-8(5H)-one (3t) Prepared according to general procedure to afford as yellow solid (55% yield). $R_f = 0.29$ (EtOAc/hexanes 1:10); m. p. = 241–242 °C. $[\alpha]^{23.0}_D = +20.4$ ($c = 0.5$, CHCl_3). ^1H NMR (400 MHz, CDCl_3): $\delta = 7.49$ –7.33 (m, 6H, H-Ar), 7.29 (s, 1H, H-Ar), 6.18 (s, 1H, H-N), 5.94 (dd, $J = 2.5$ Hz, 5.5 Hz, 2H, OCH_2O), 4.70 (dd, $J = 4.0$ Hz, 16.0 Hz, 1H, CH), 2.86–2.69 (m, 2H, CH_2). ^{13}C NMR (100 MHz, CDCl_3) $\delta = 191.5, 154.4, 150.1, 141.7, 141.1, 129.1, 128.6, 126.8, 112.8, 105.1, 101.6, 95.9, 59.2, 46.0$. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{NO}_3\text{Na}$ 290.0787 $[\text{M}+\text{Na}^+]$; found 290.0787. IR (KBr): 3276, 2919, 1608, 1475, 1243, 1364, 1305, 1226, 1150, 1116, 1069, 1035, 962, 889, 855, 819, 694, 654 cm^{-1} . [Daicel chiralpak AD column, eluting with hexane/isopropanol = 80 : 20, 0.3 mL/min, 214 nm; major enantiomer t_R , 38.0 min, minor enantiomer t_R , 46.5 min; 99% ee].

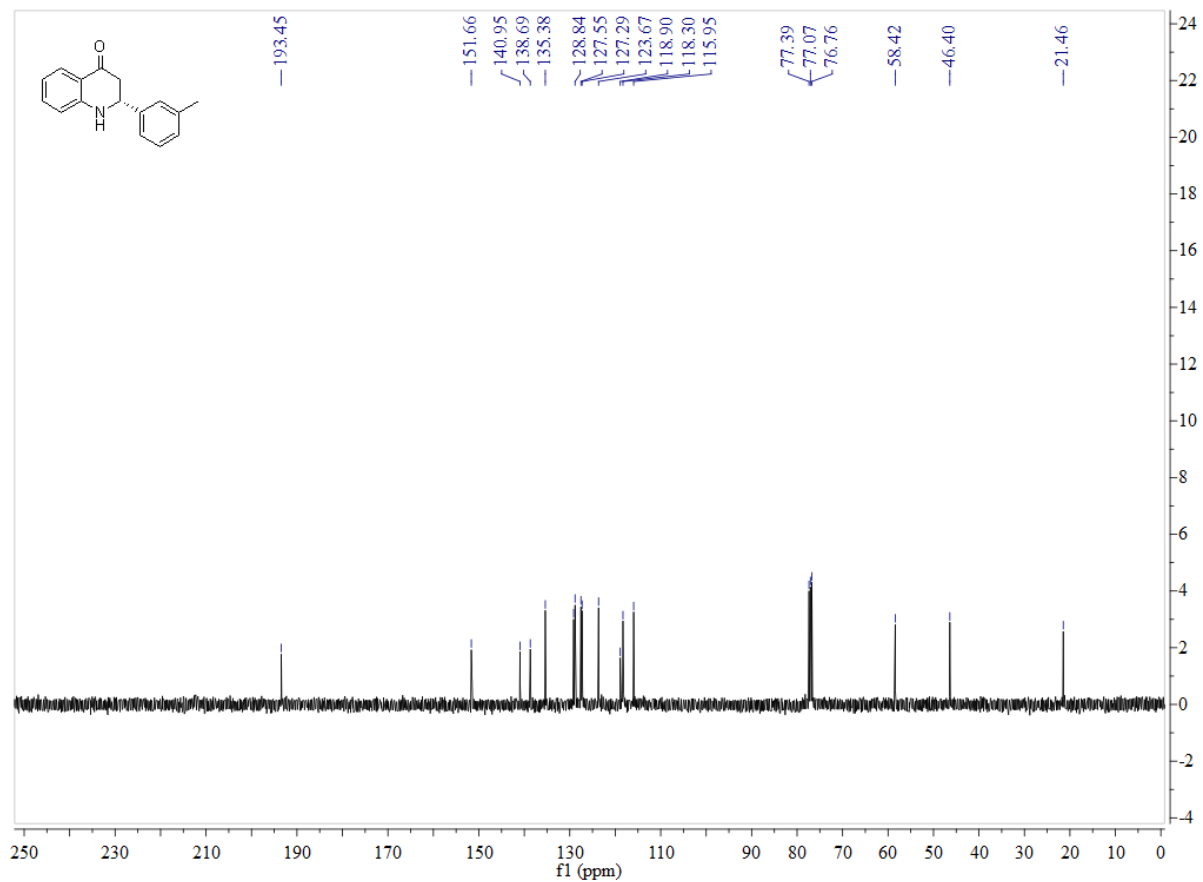
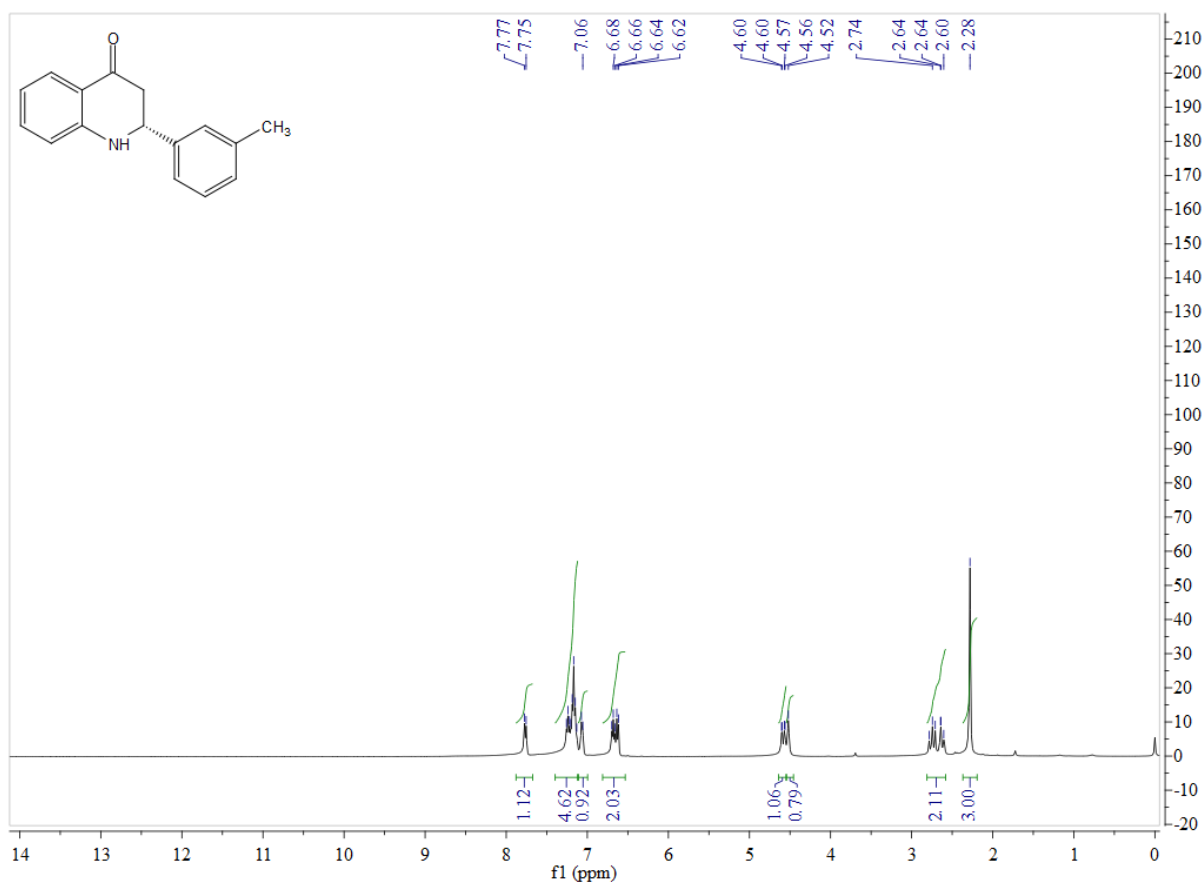
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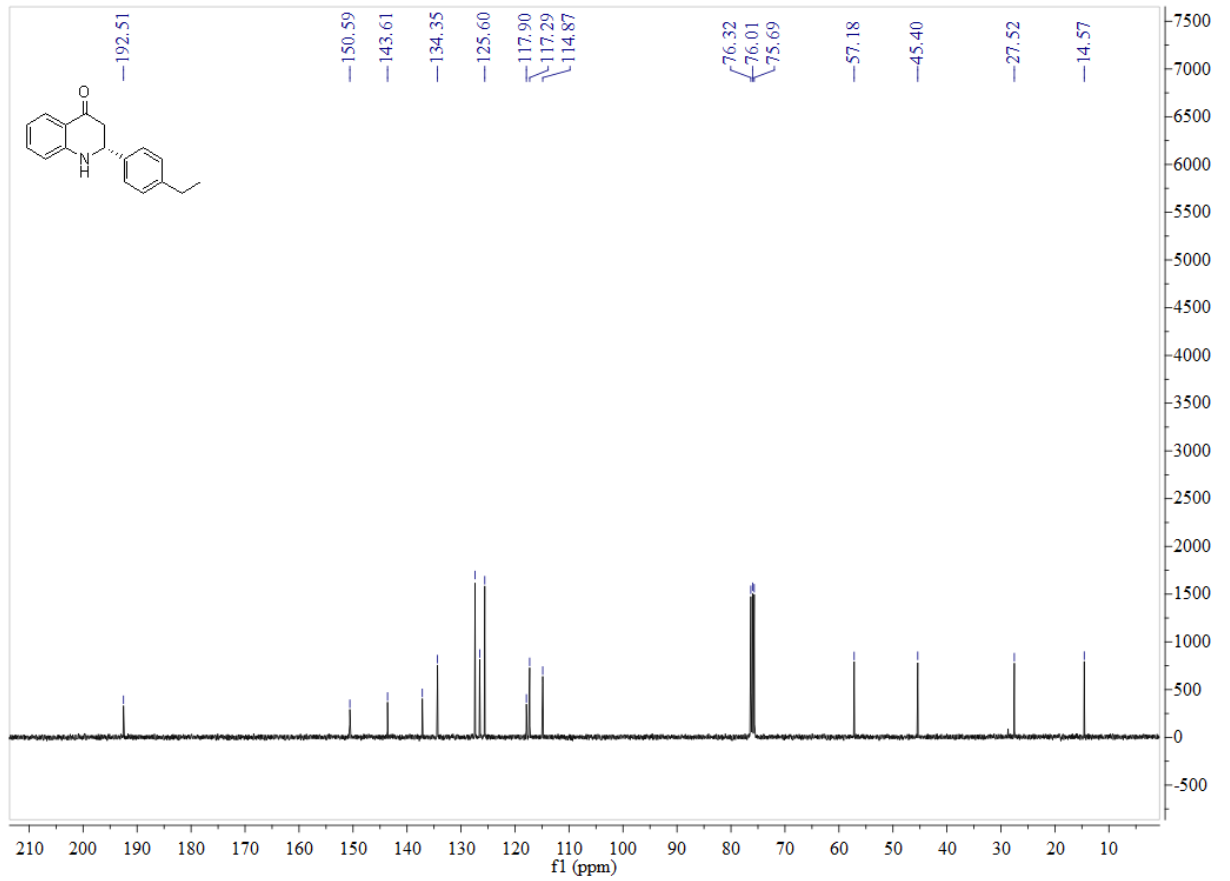
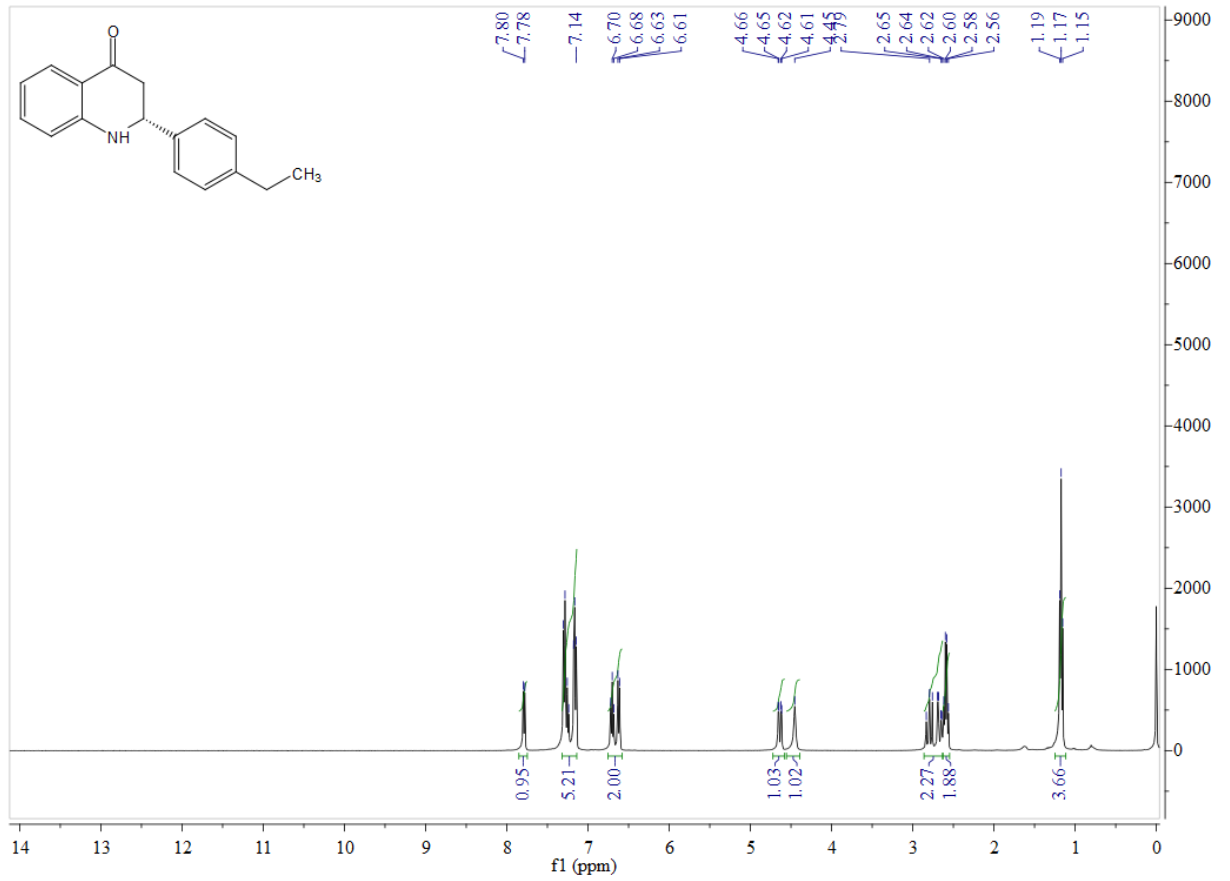
- (1) Saito, K.; Moriya, Y.; Akiyama, T. *Org. Lett.* **2015**, *17*, 3202.
- (2) Kanagaraj, K.; Pichumani, K. *J. Org. Chem.* **2013**, *78*, 744.
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- (7) Sharma, S.; Thakur, V.; Budhiraja, A.; Mohinder, P.; *Letters in Drug Design & Discovery*, **2013**, *10*, 327.
- (8) Bhattacharya, R.; Kundu, P.; Maiti, G. *Synth. Commun.* **2010**, *40*, 476.
- (9) Chelghouma, M.; Bahnous, M.; Bouraiou, A.; Bouacida, S. ;Belfaitaha, A. *Tetrahedron lett.*, **2012**, *53*, 4059.
- (10) Zheng, H.; Liu, Q.; Wen, S.; Yang, H.; Luo, Y. *Tetrahedron: Asymmetry*, **2013**, *24*, 875.

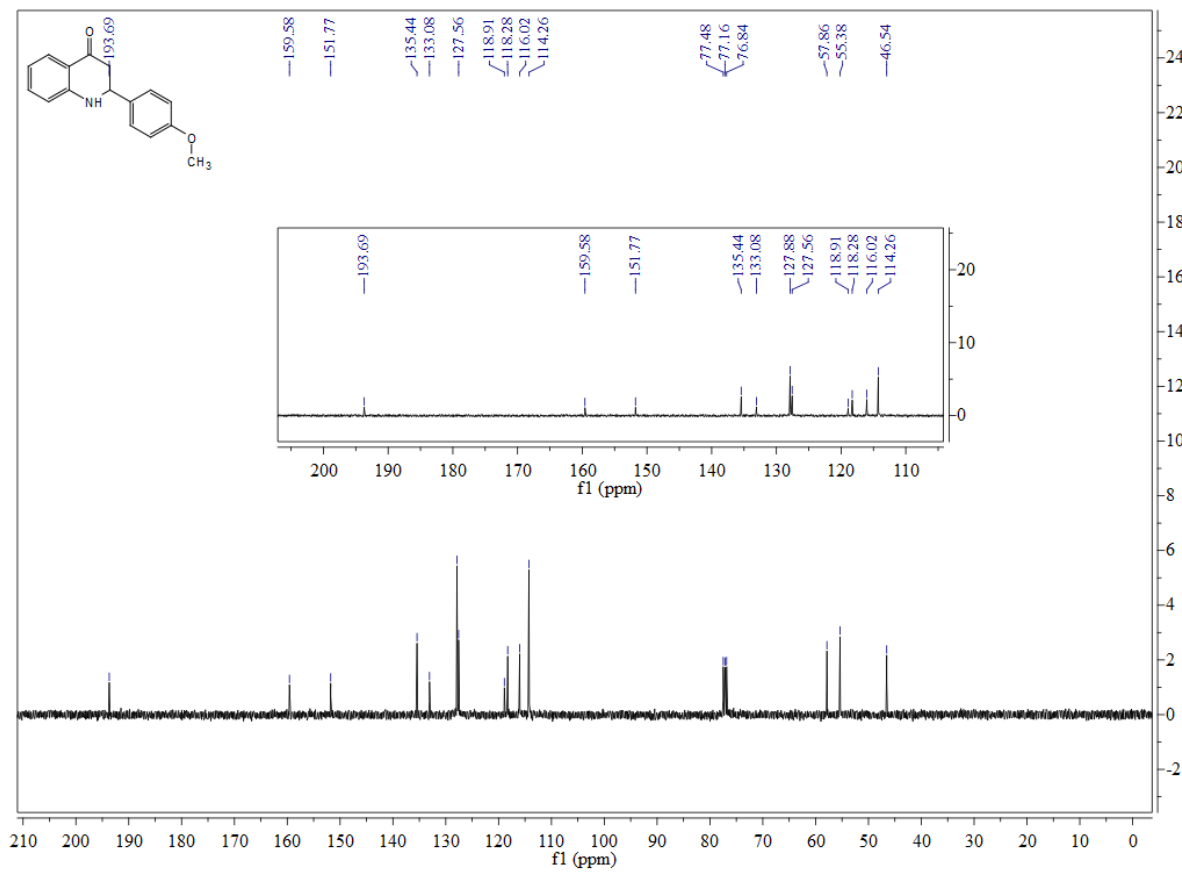
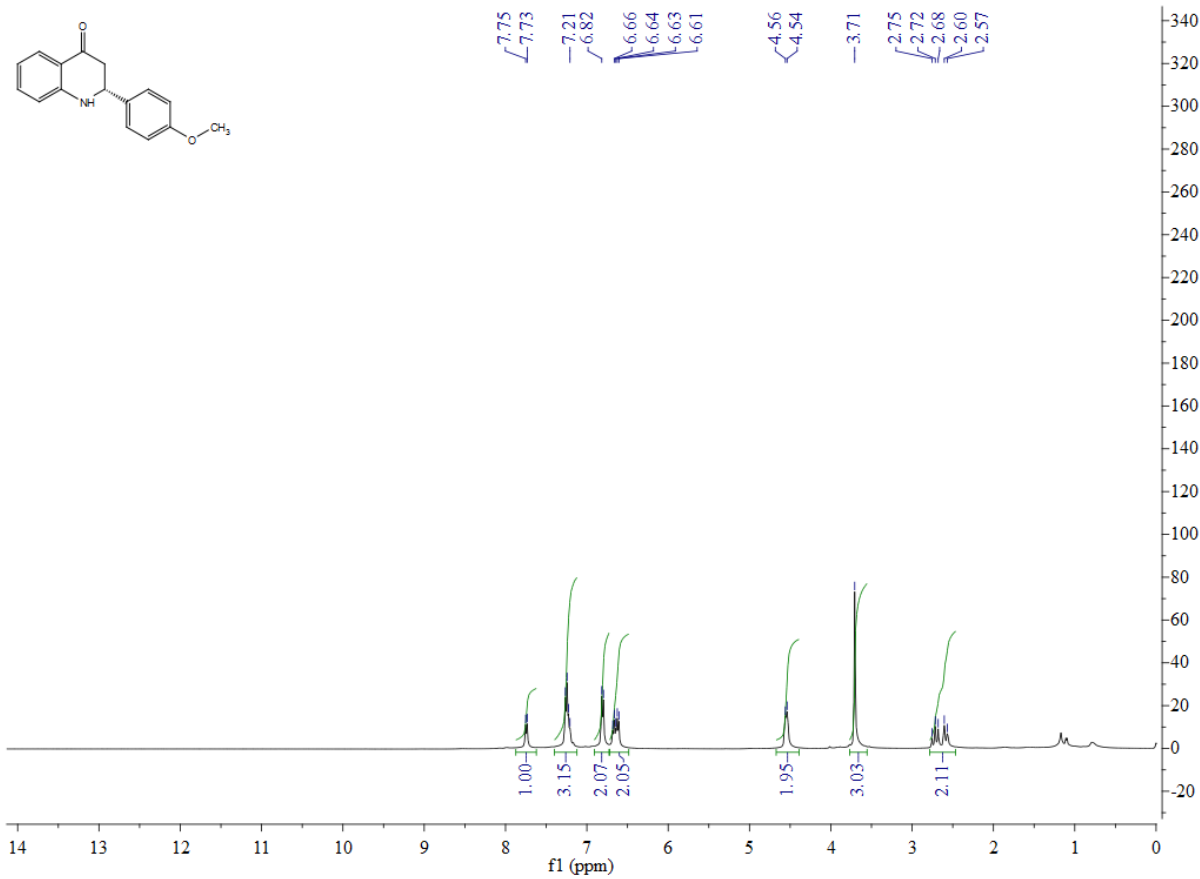
4. NMR Spectra

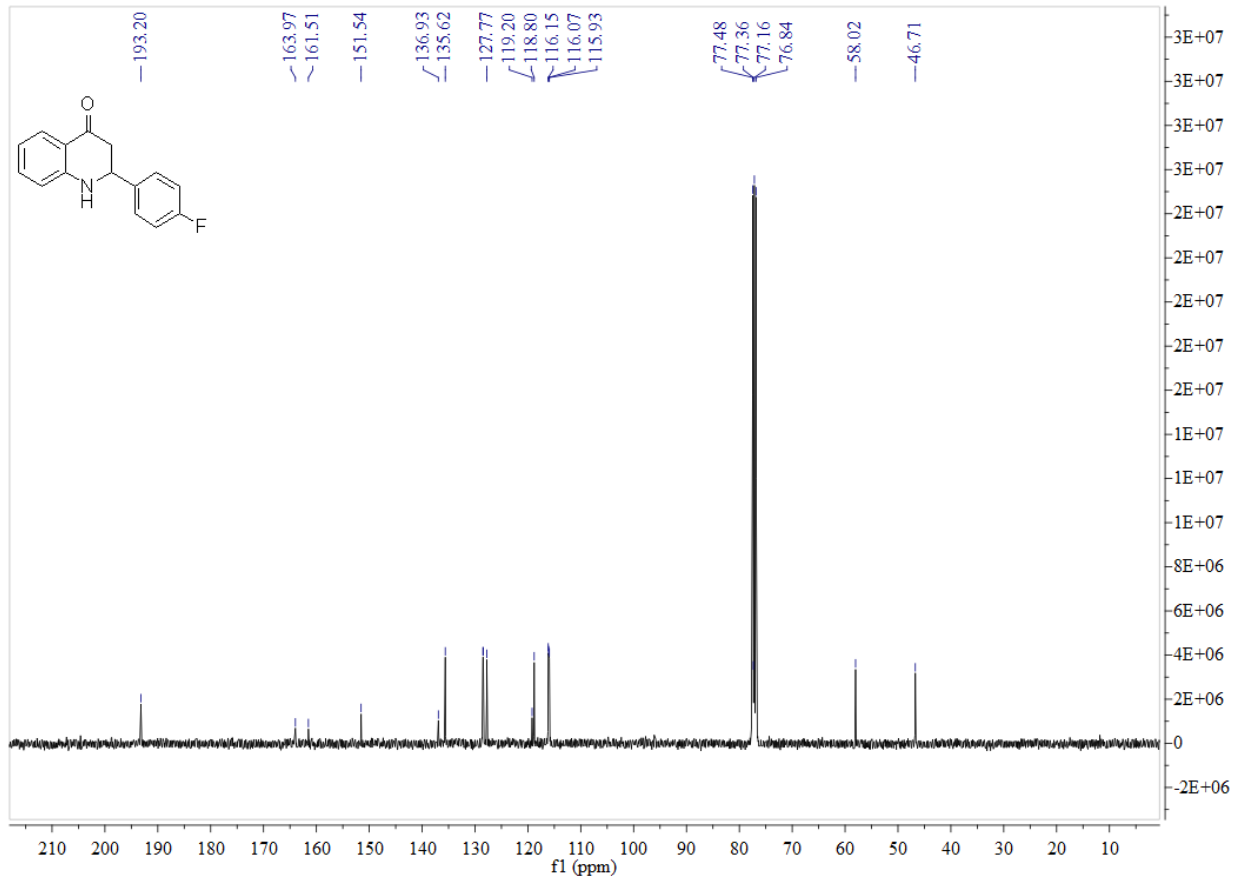
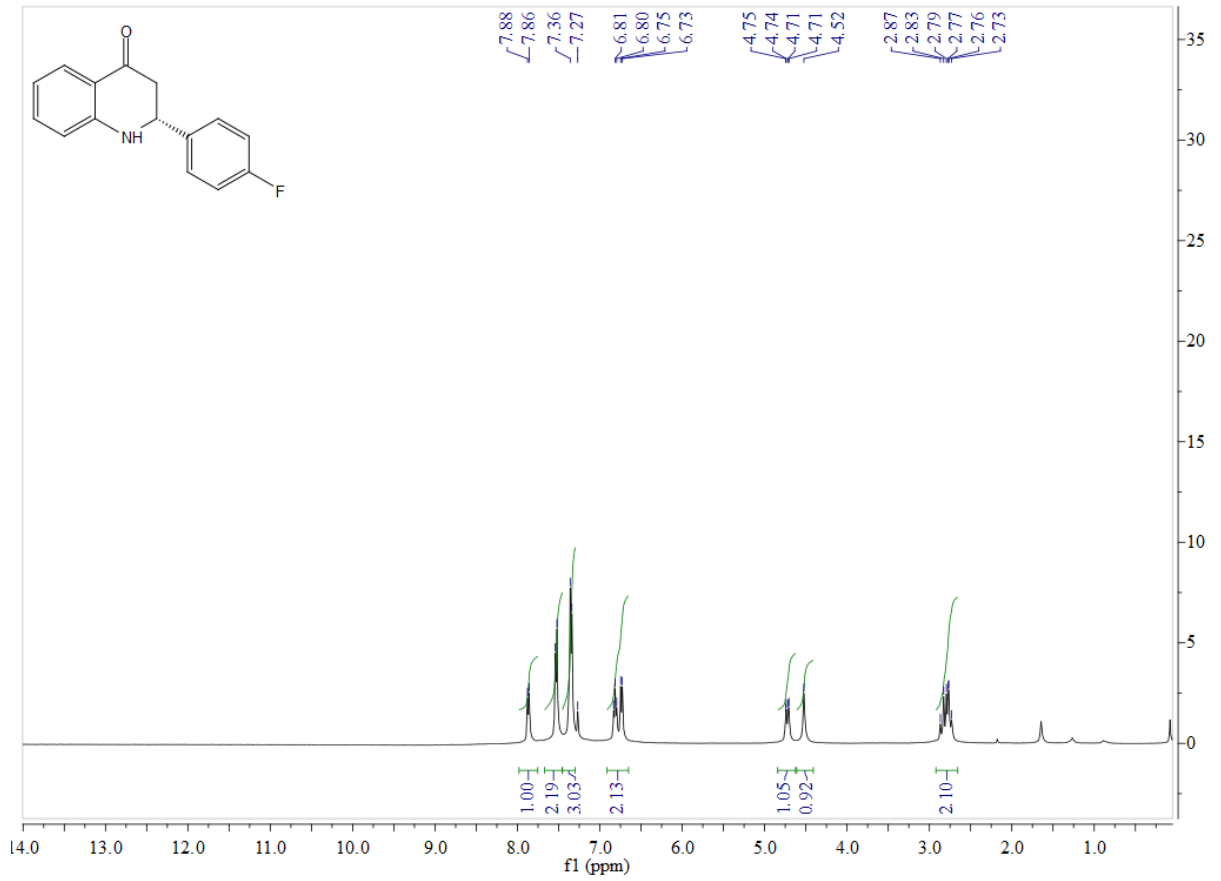


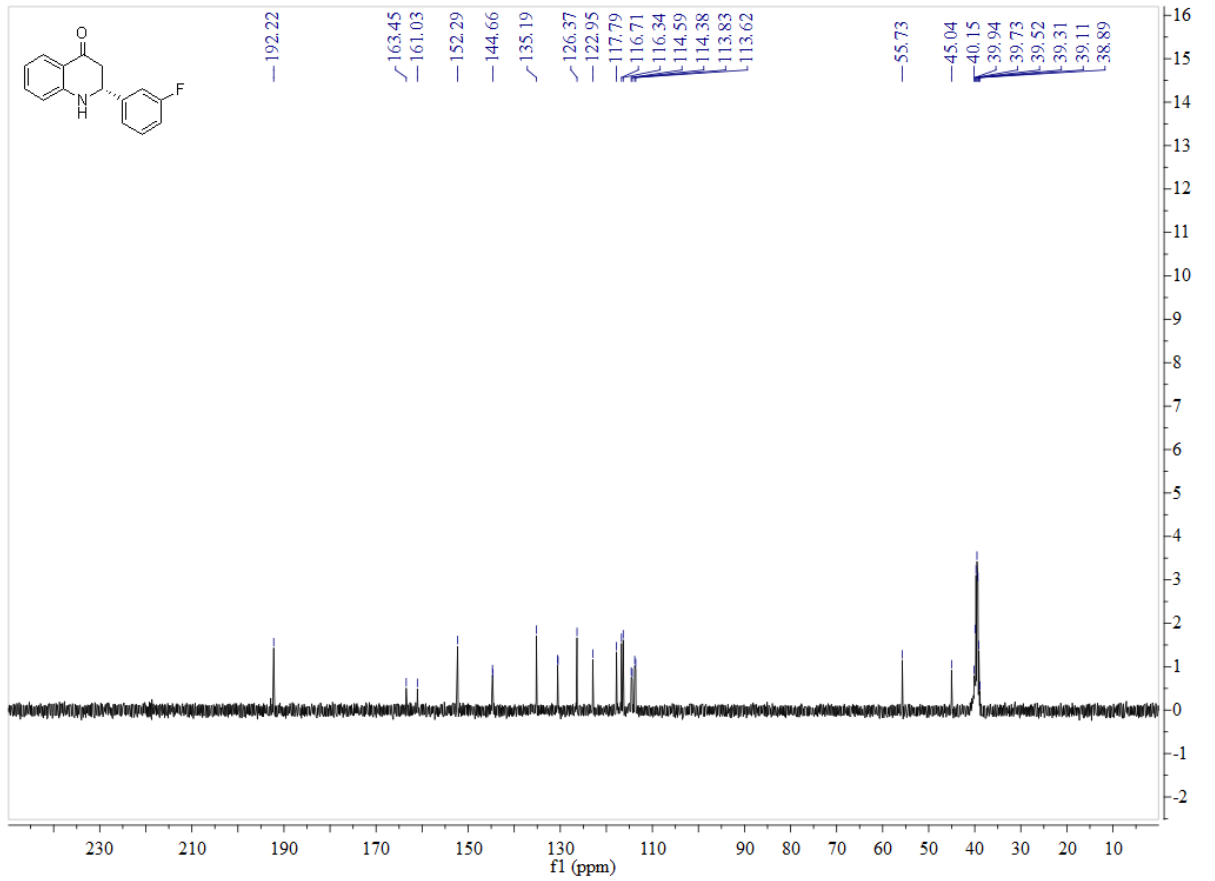
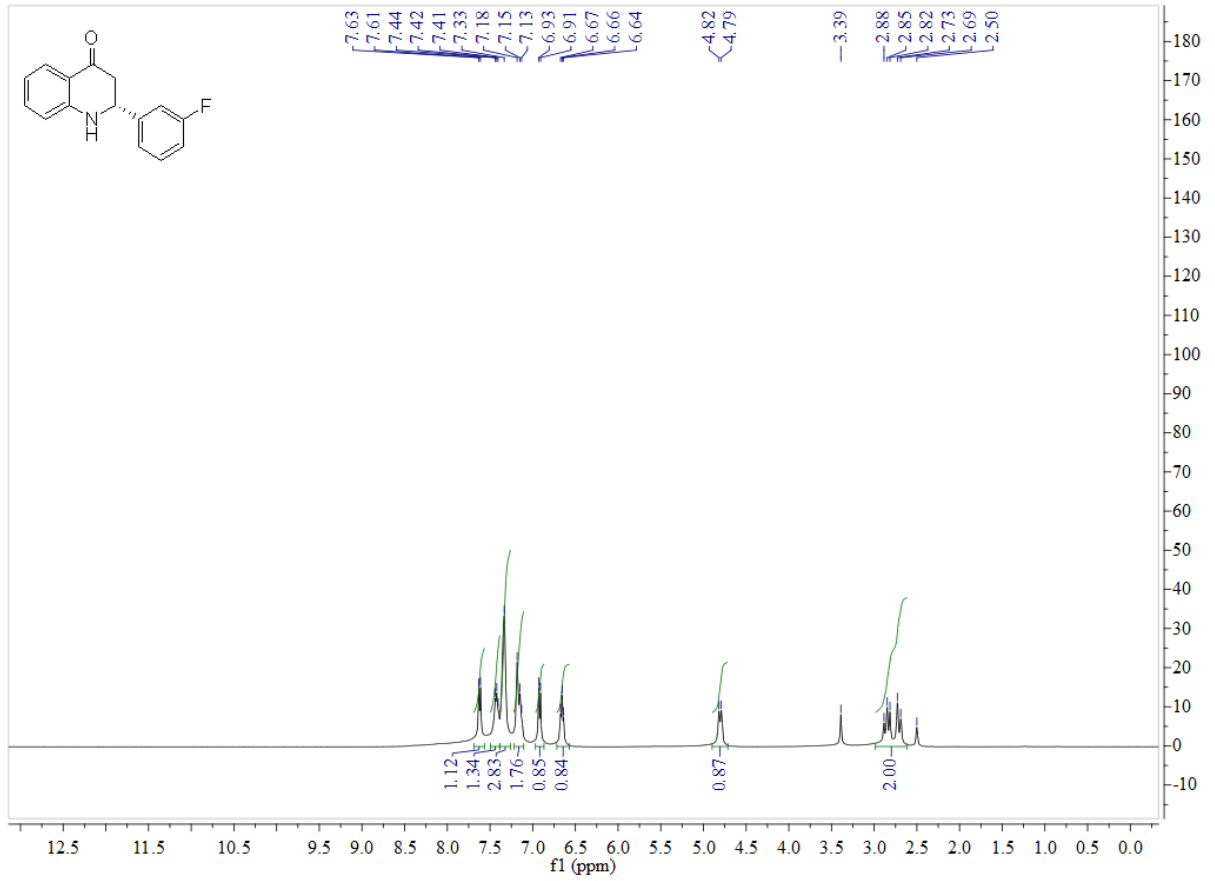


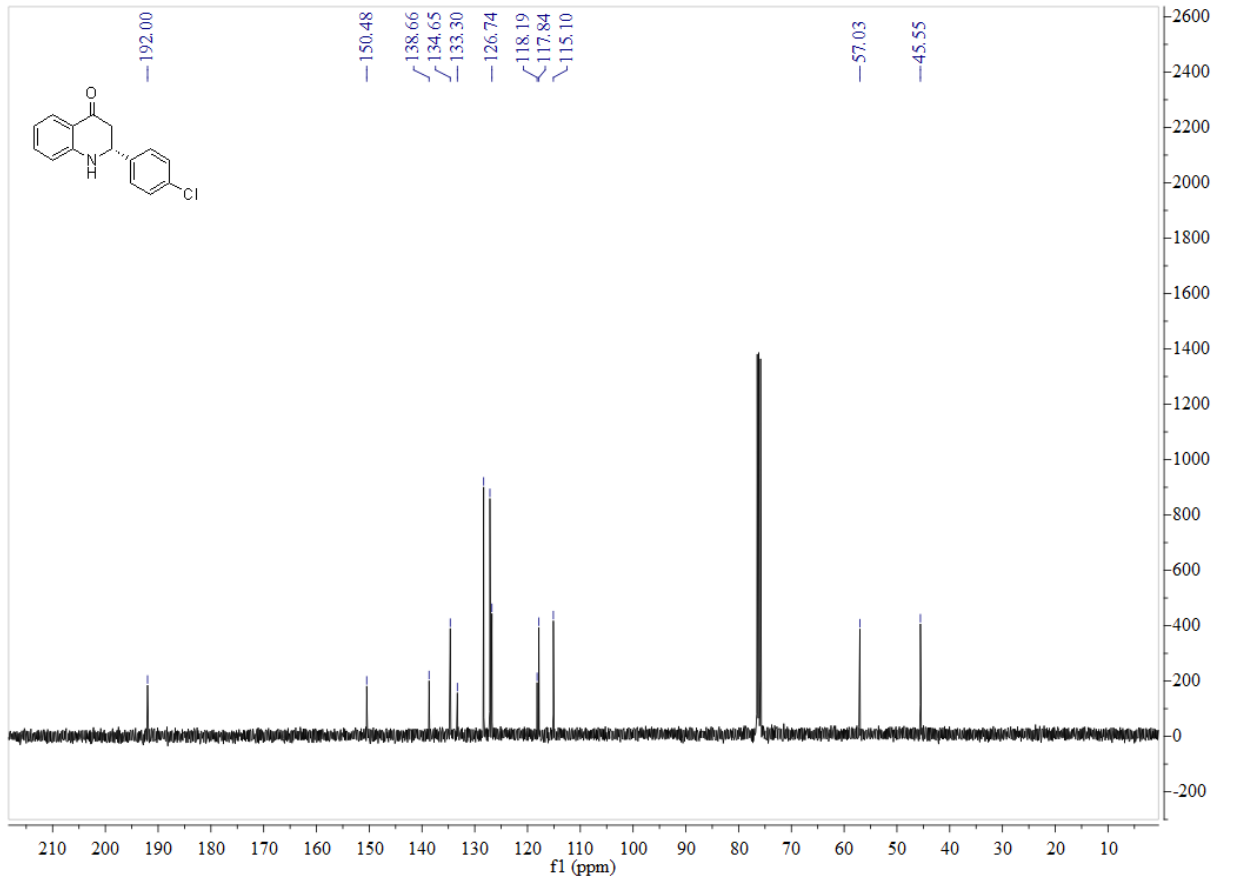
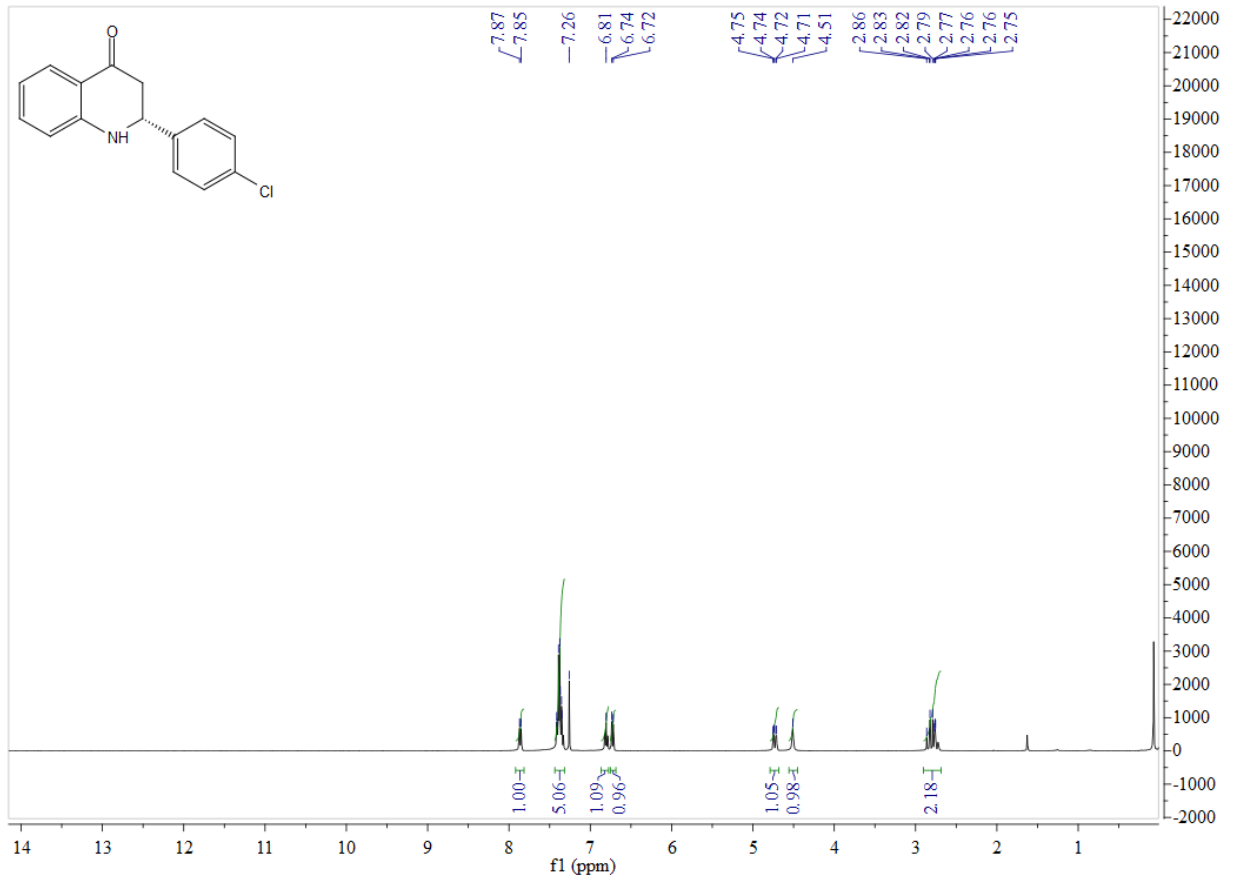


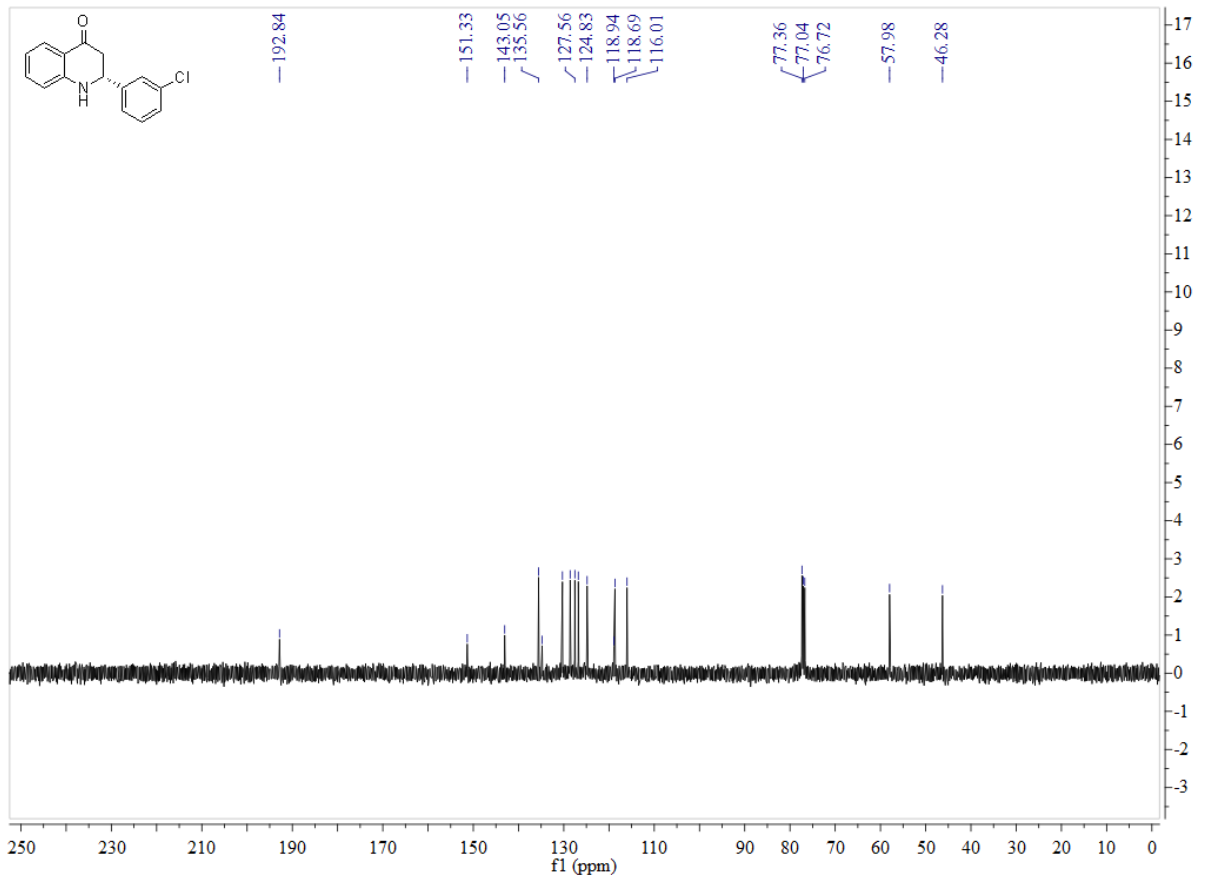
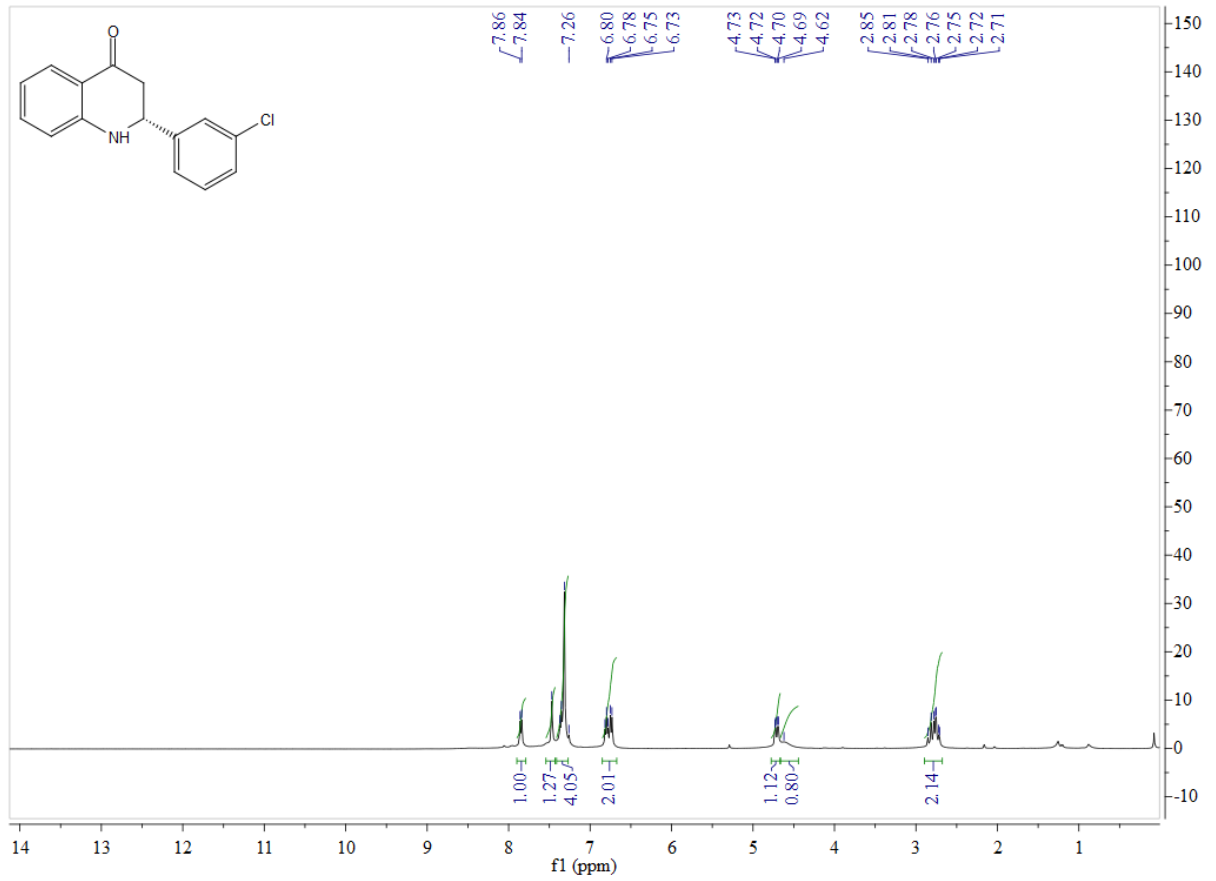


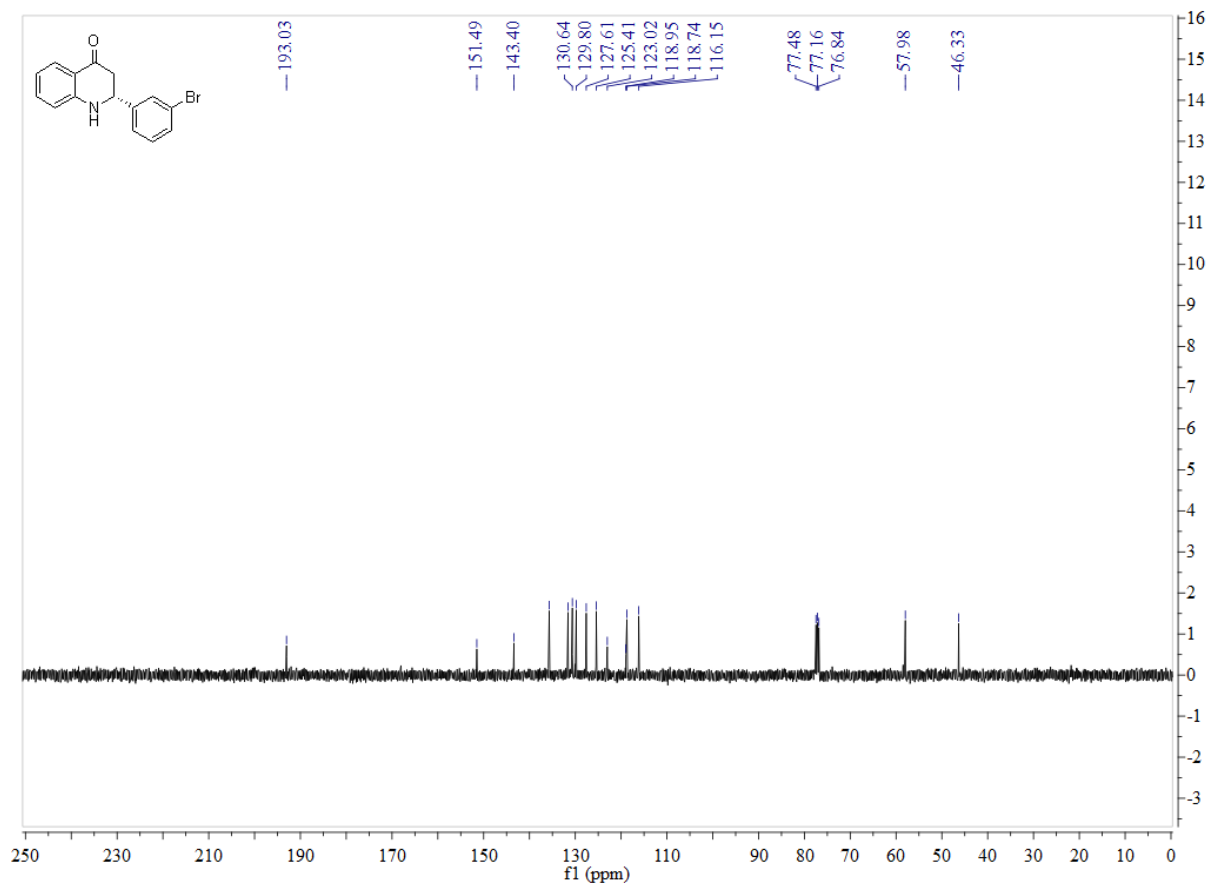
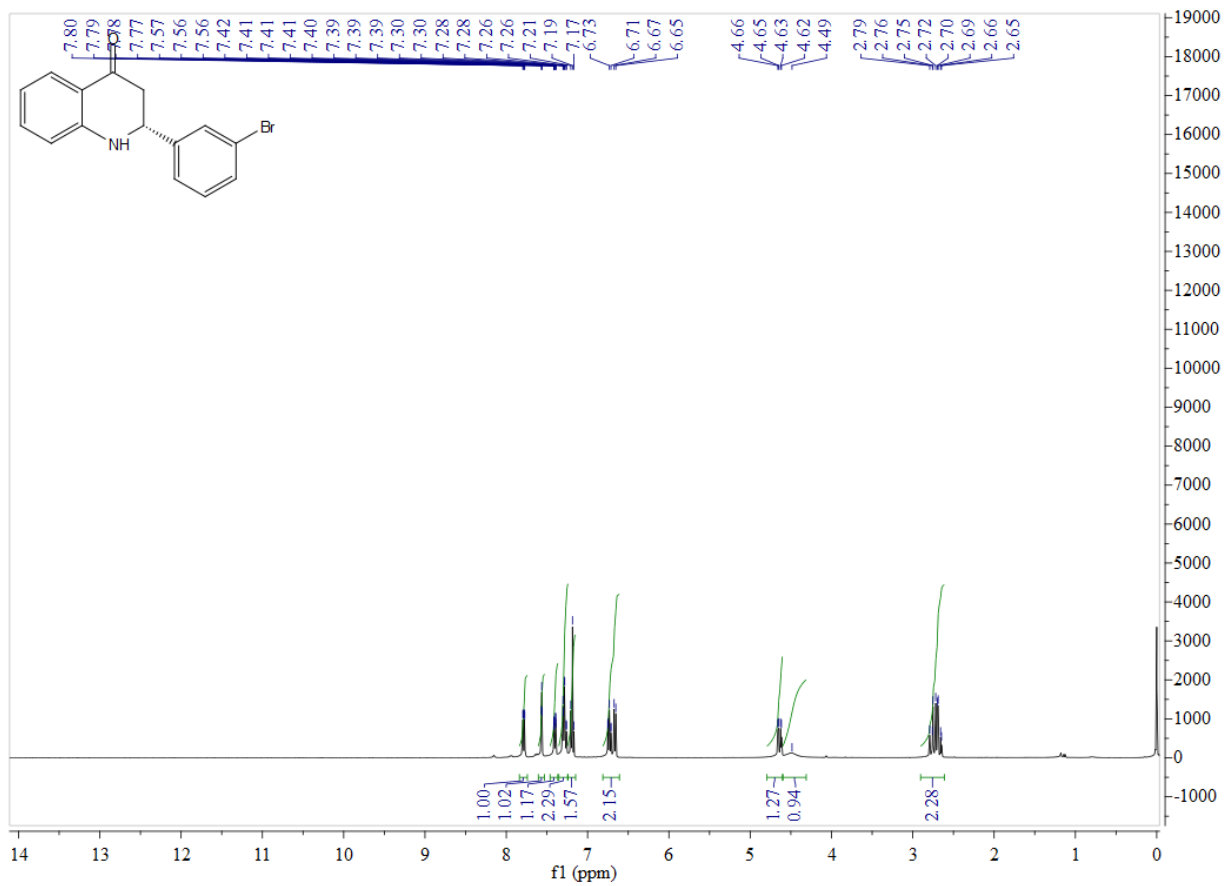


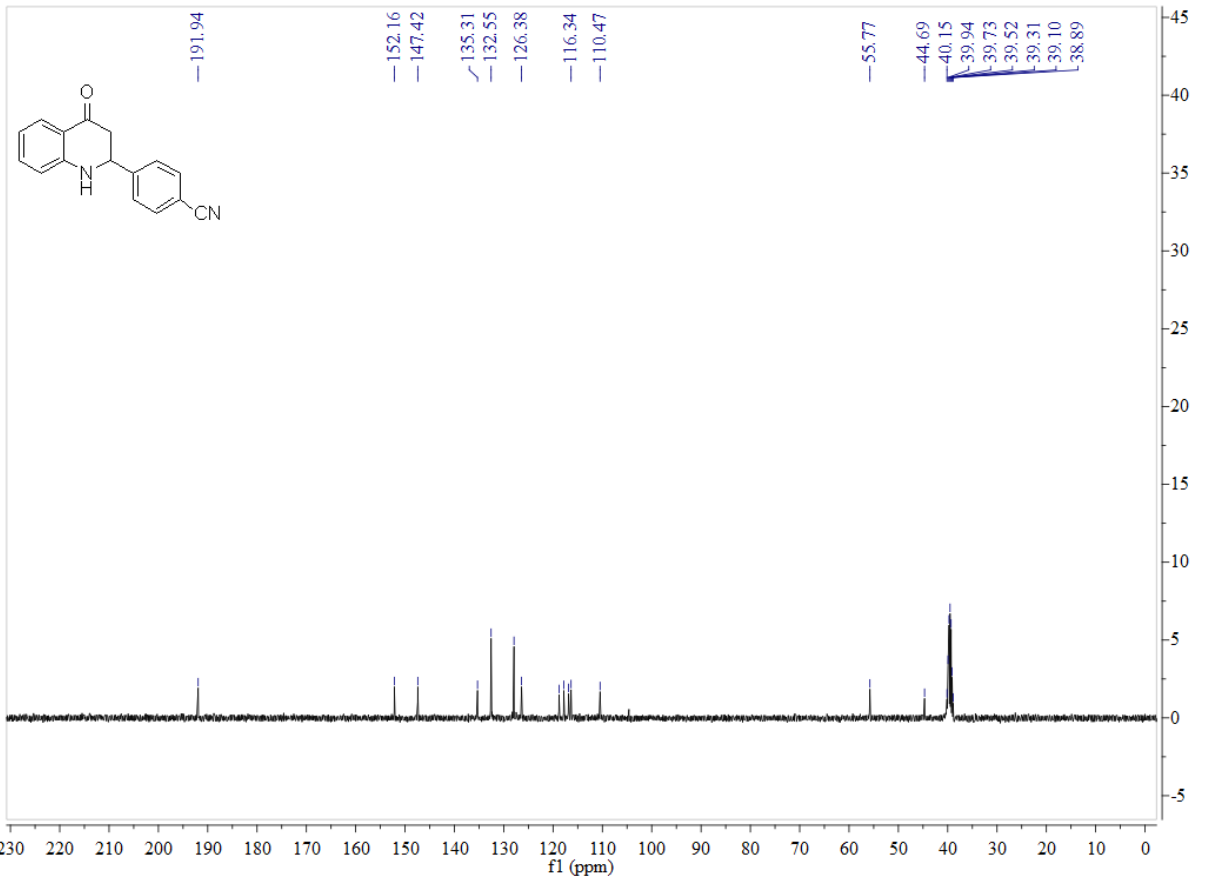
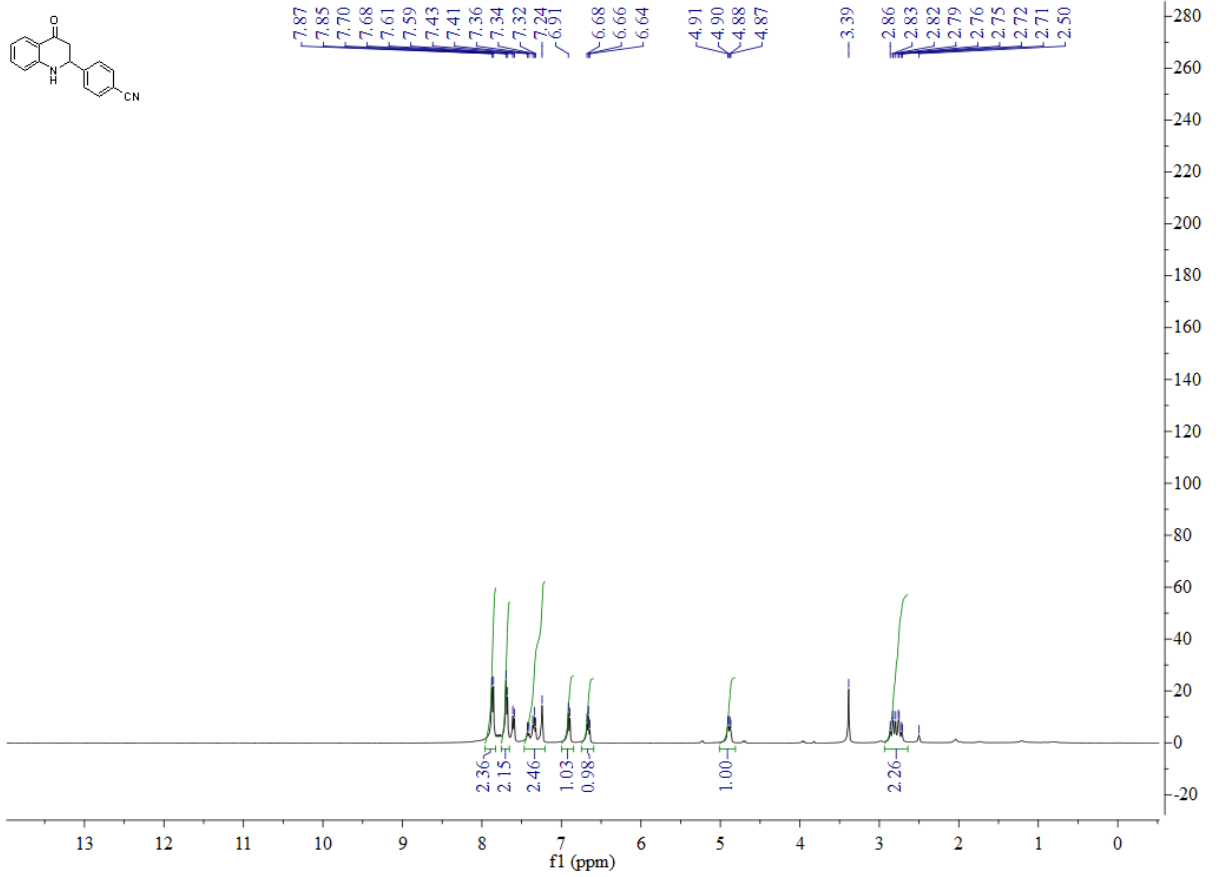
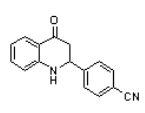


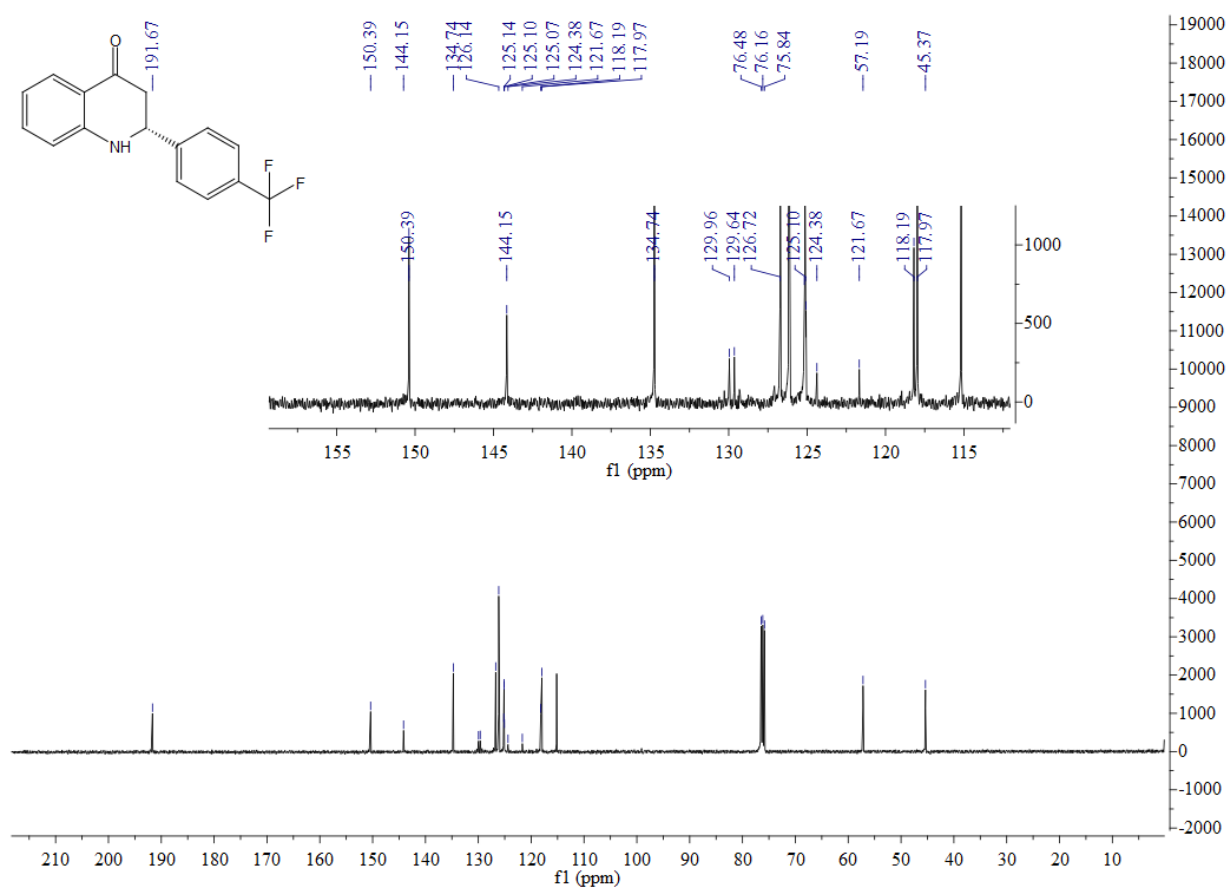
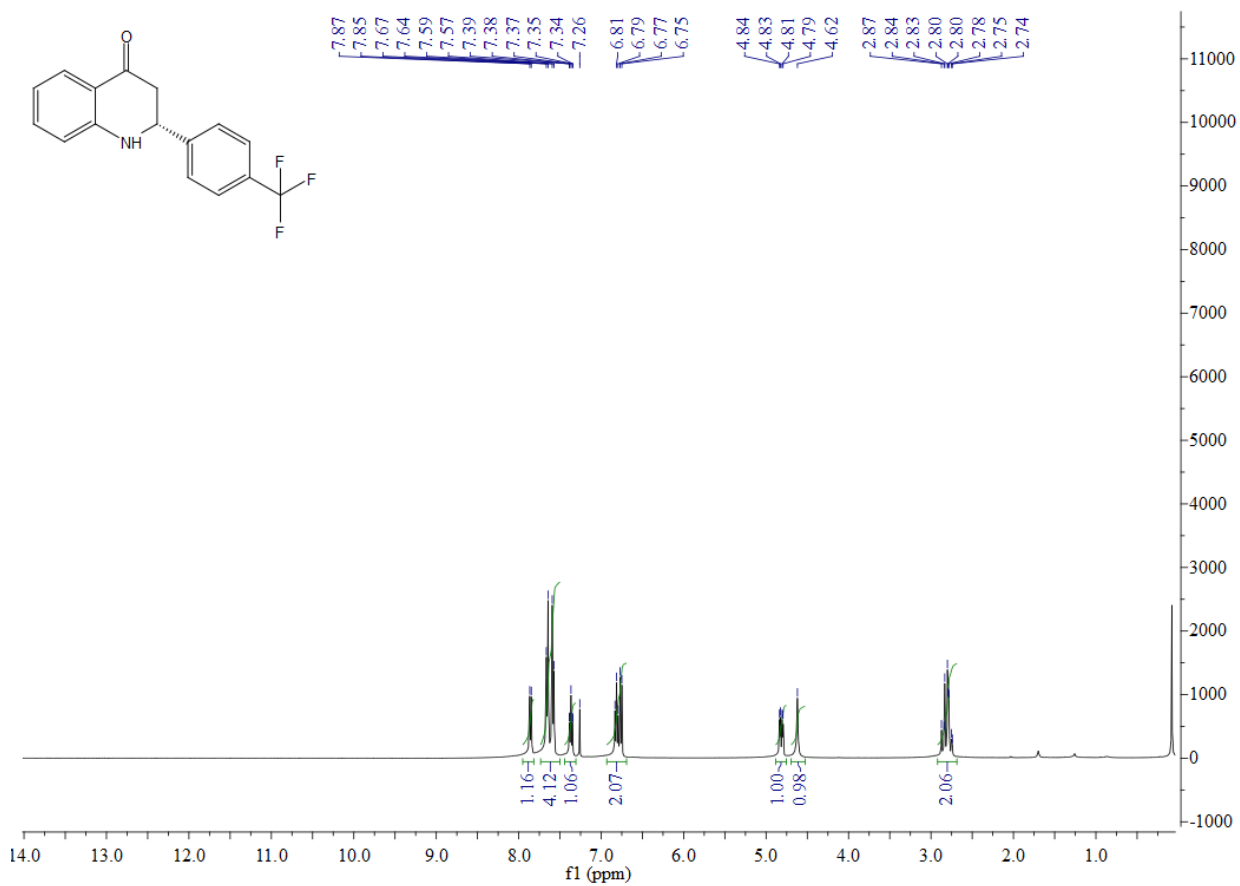


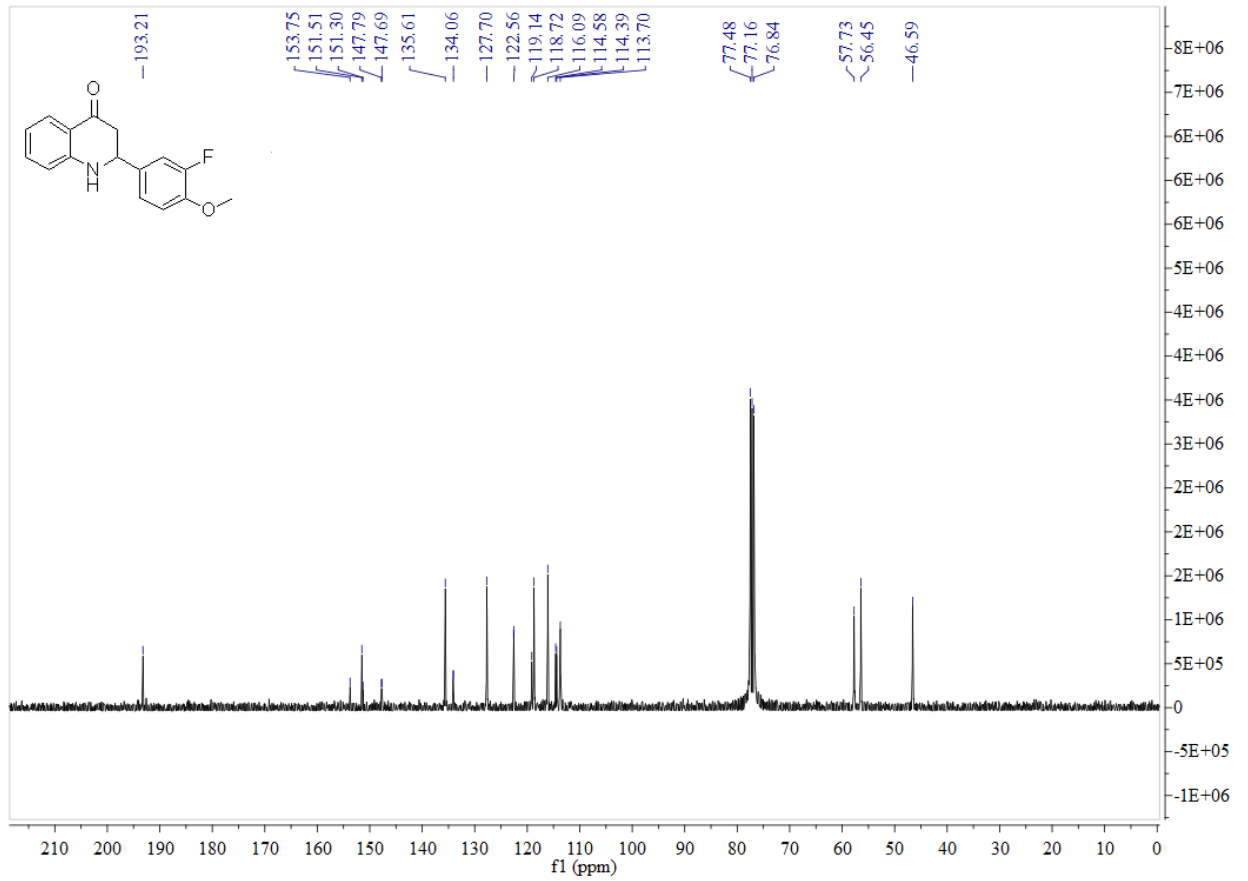
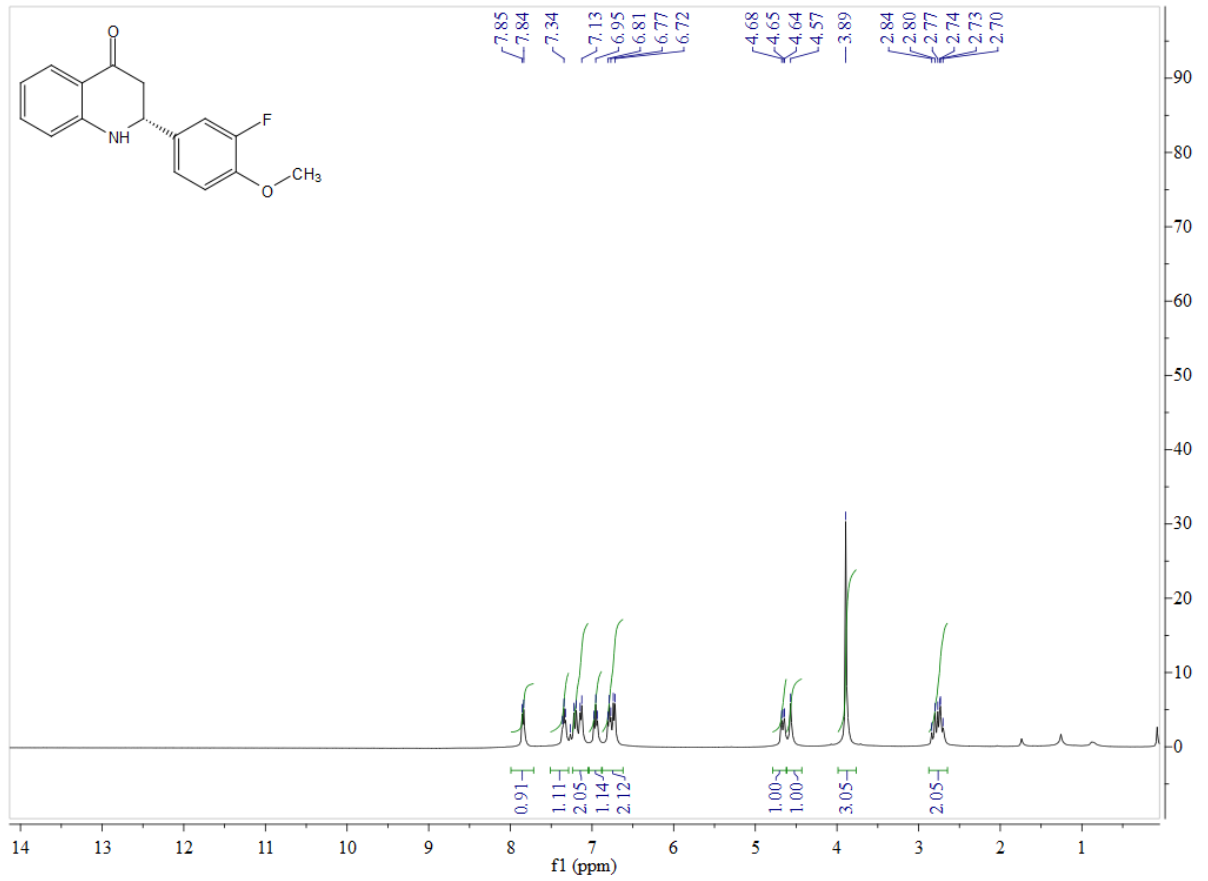


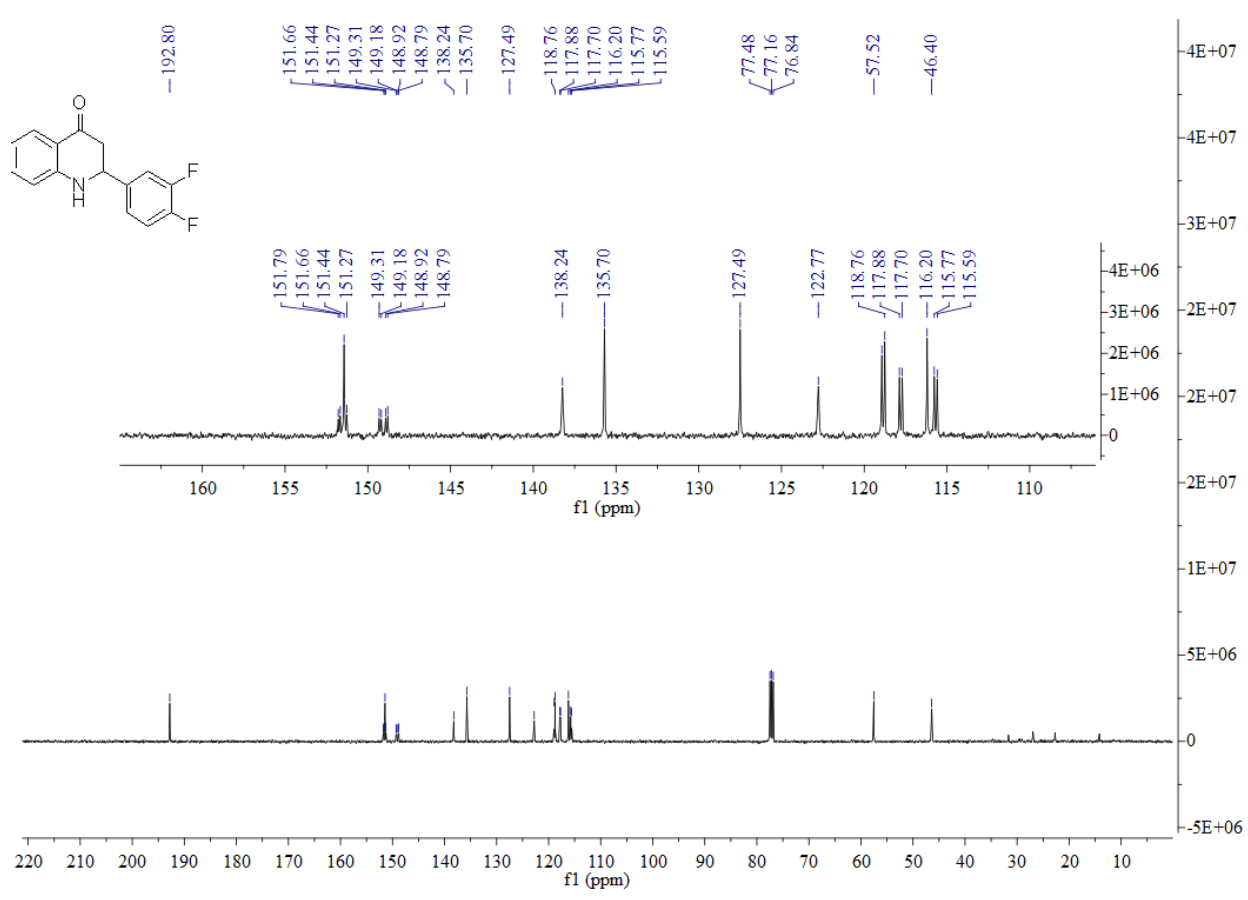
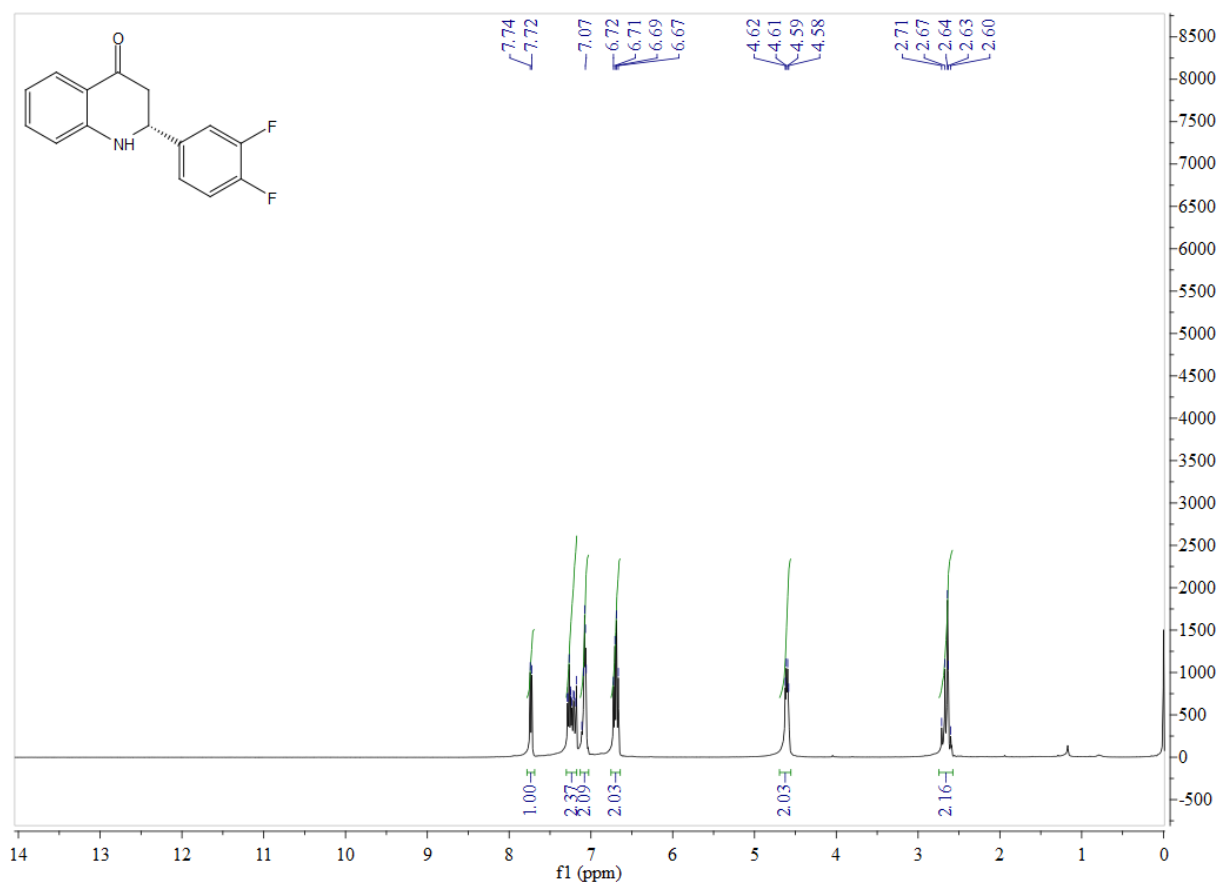


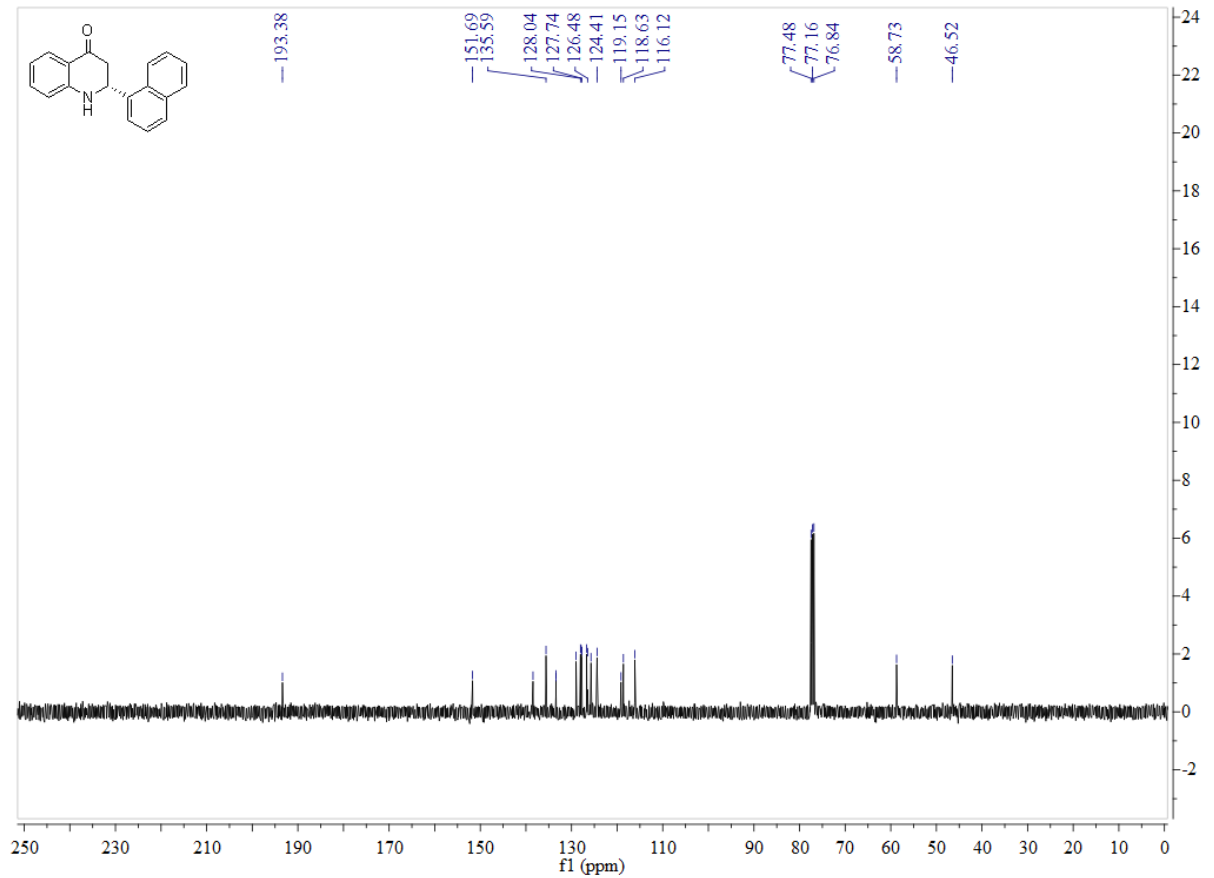
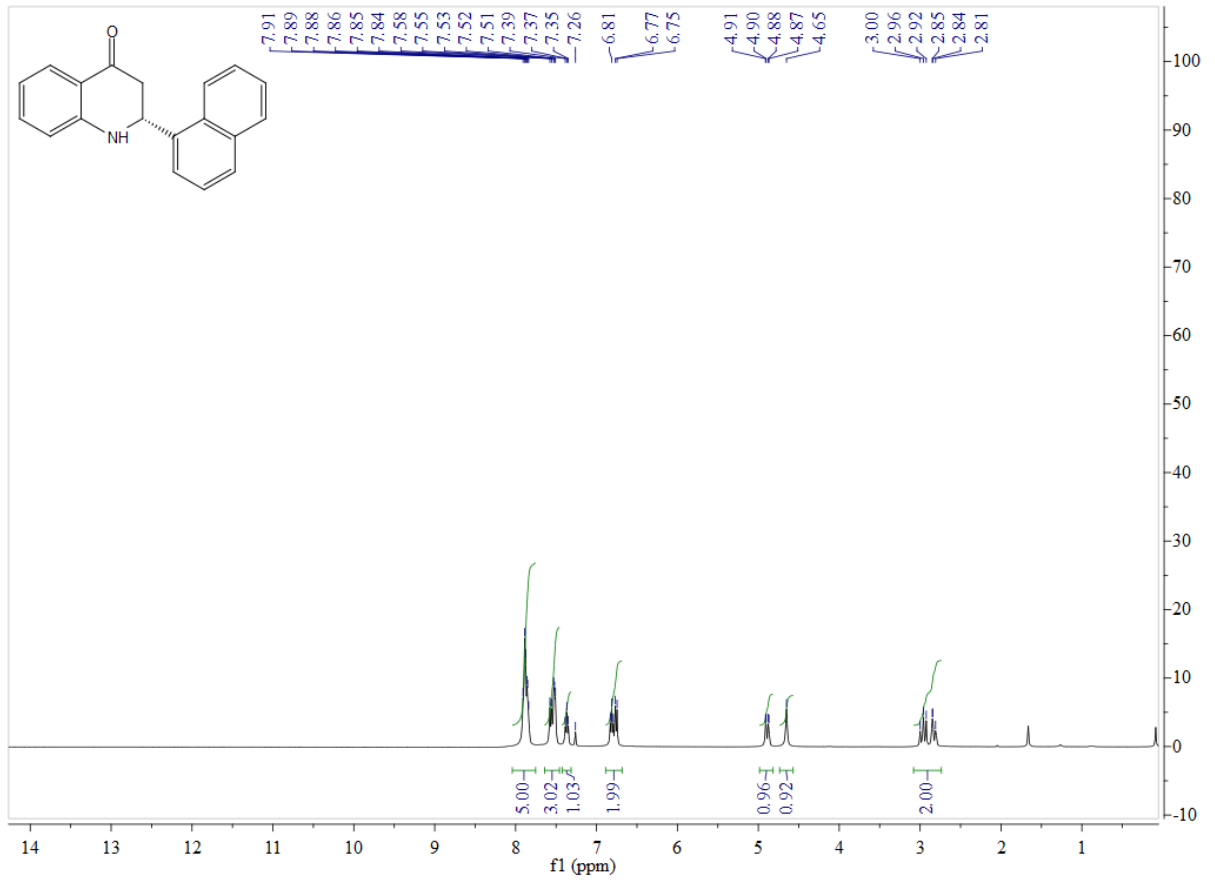


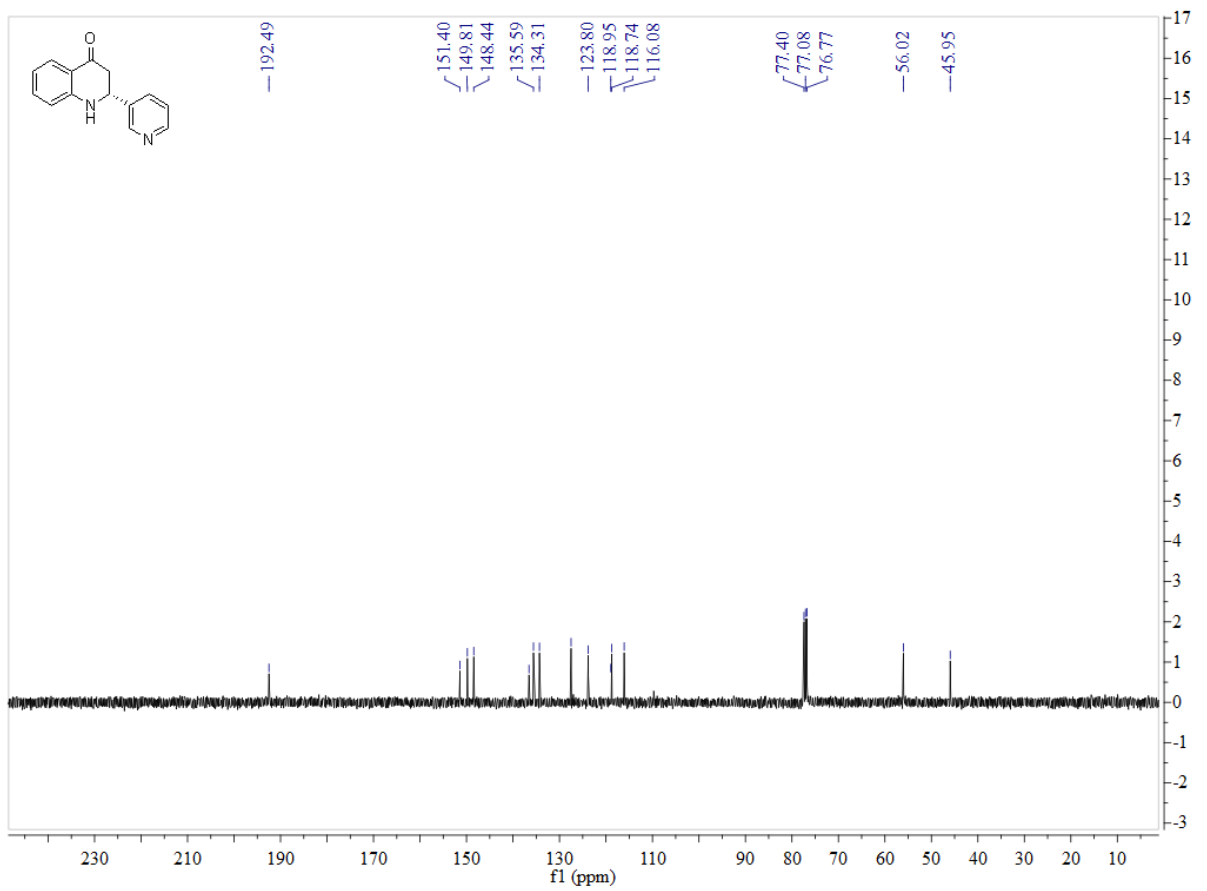
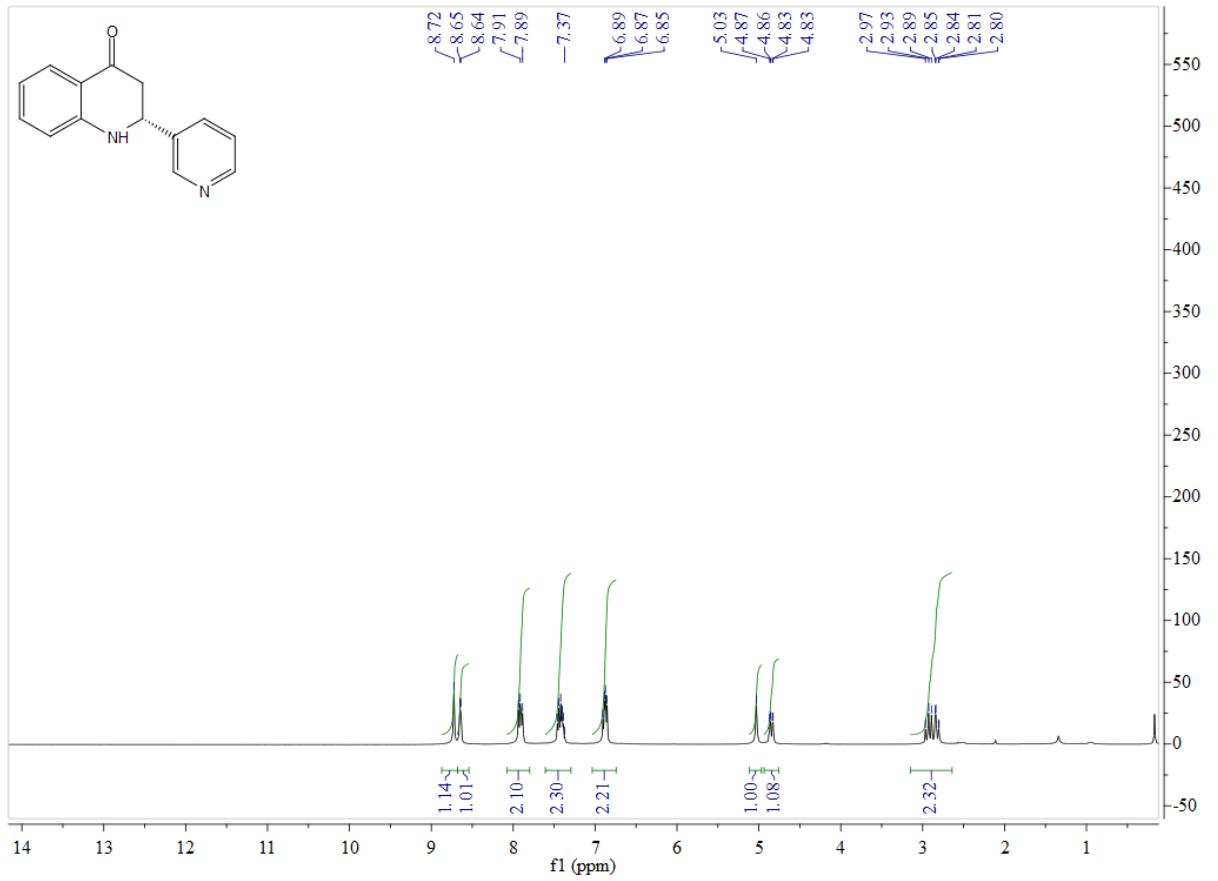


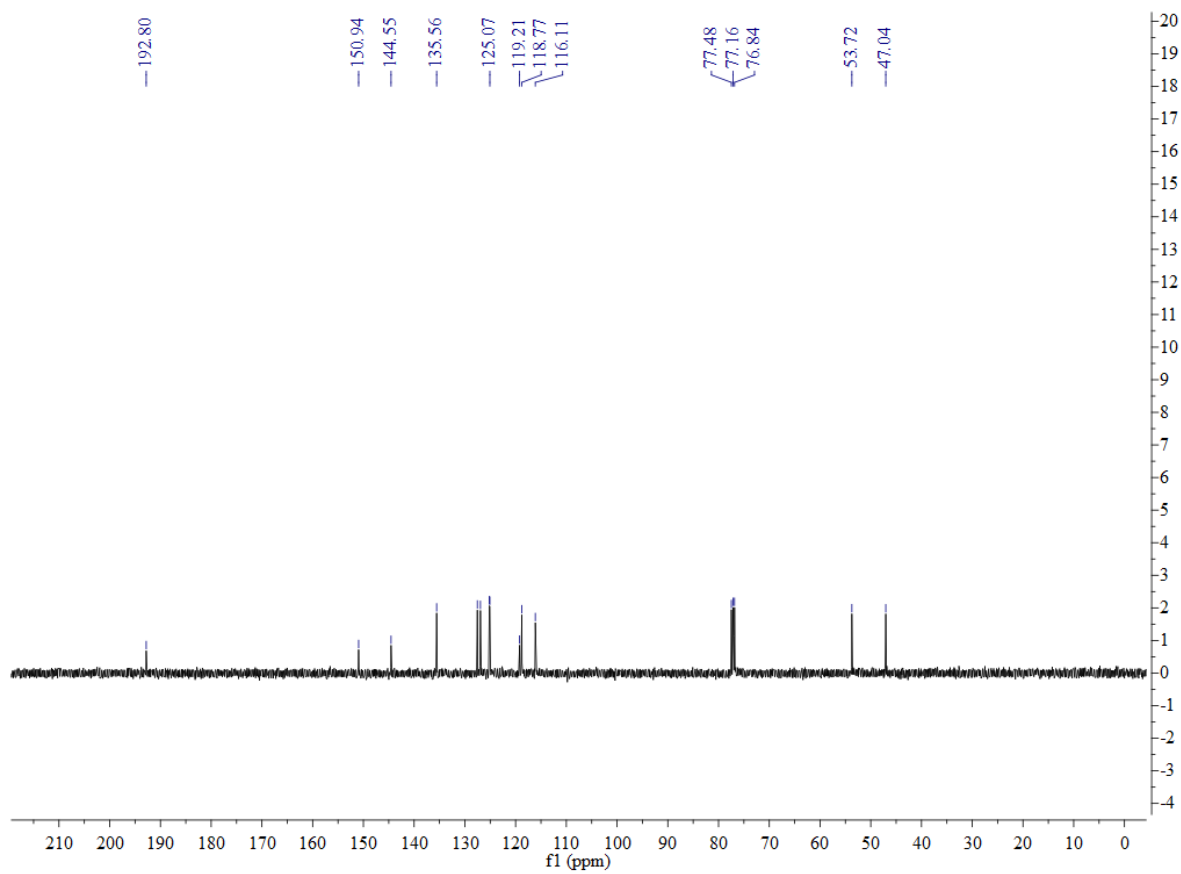
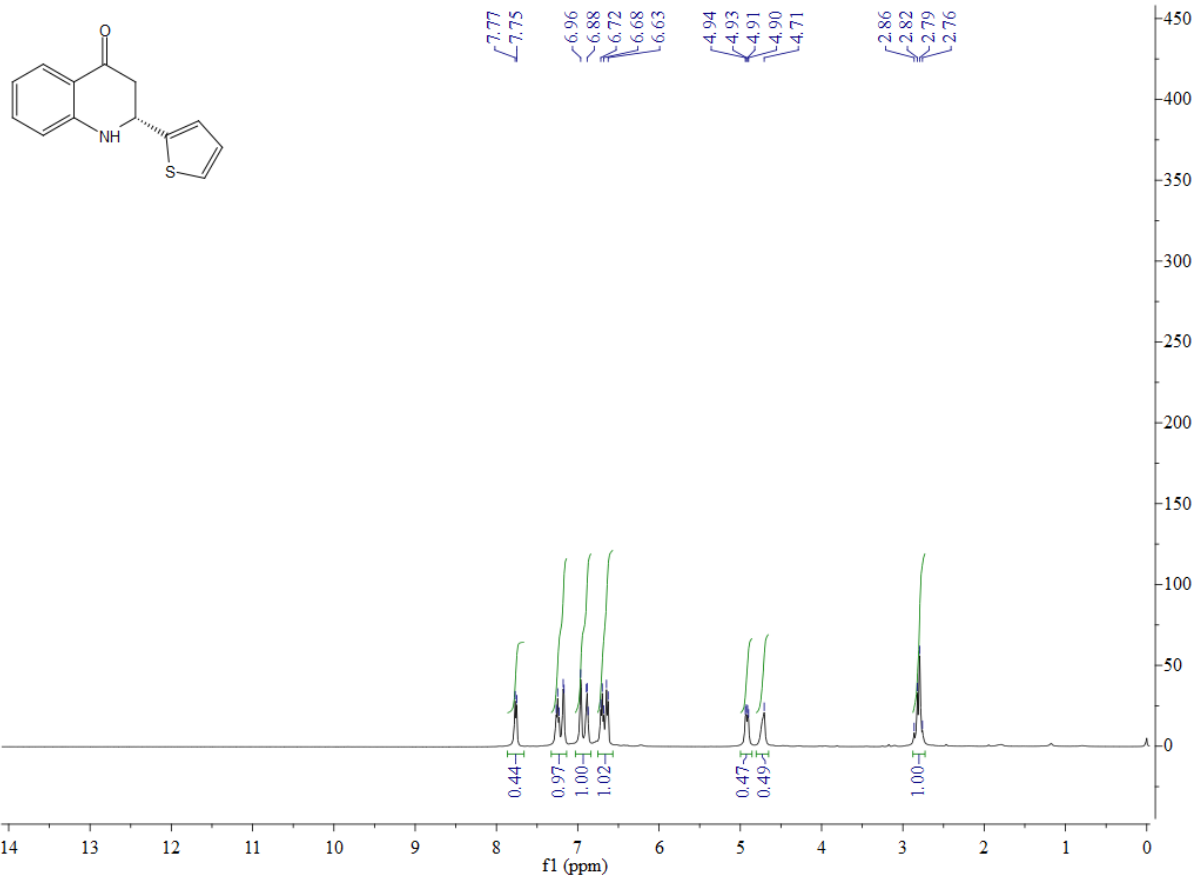


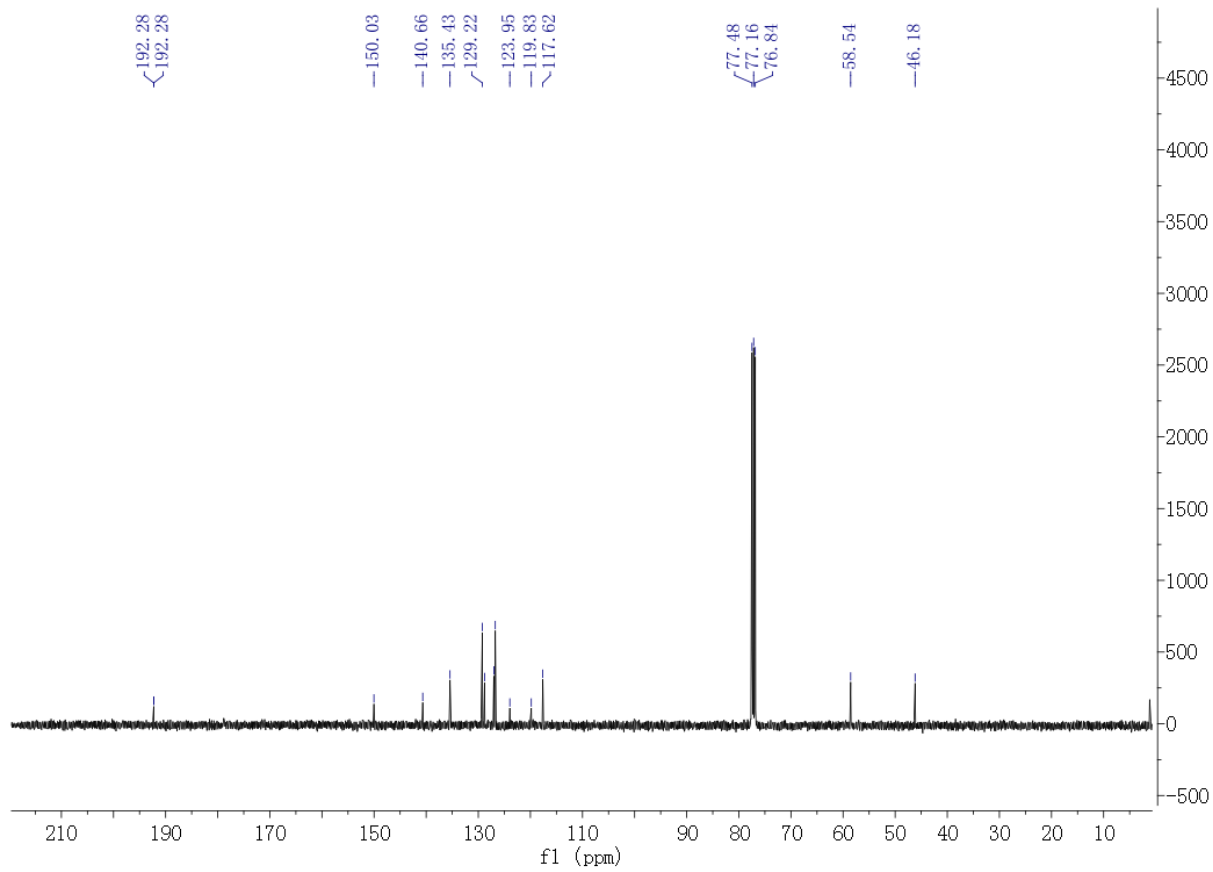
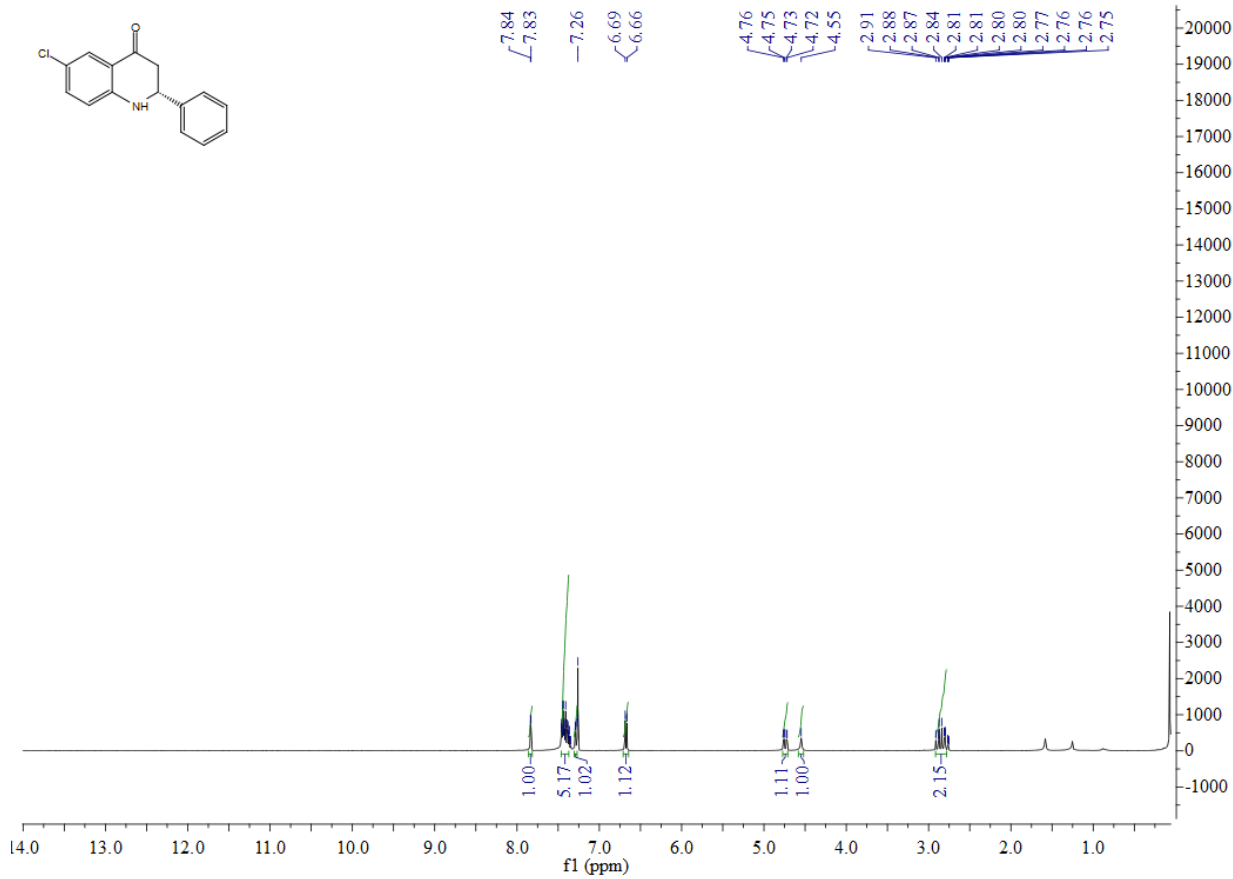


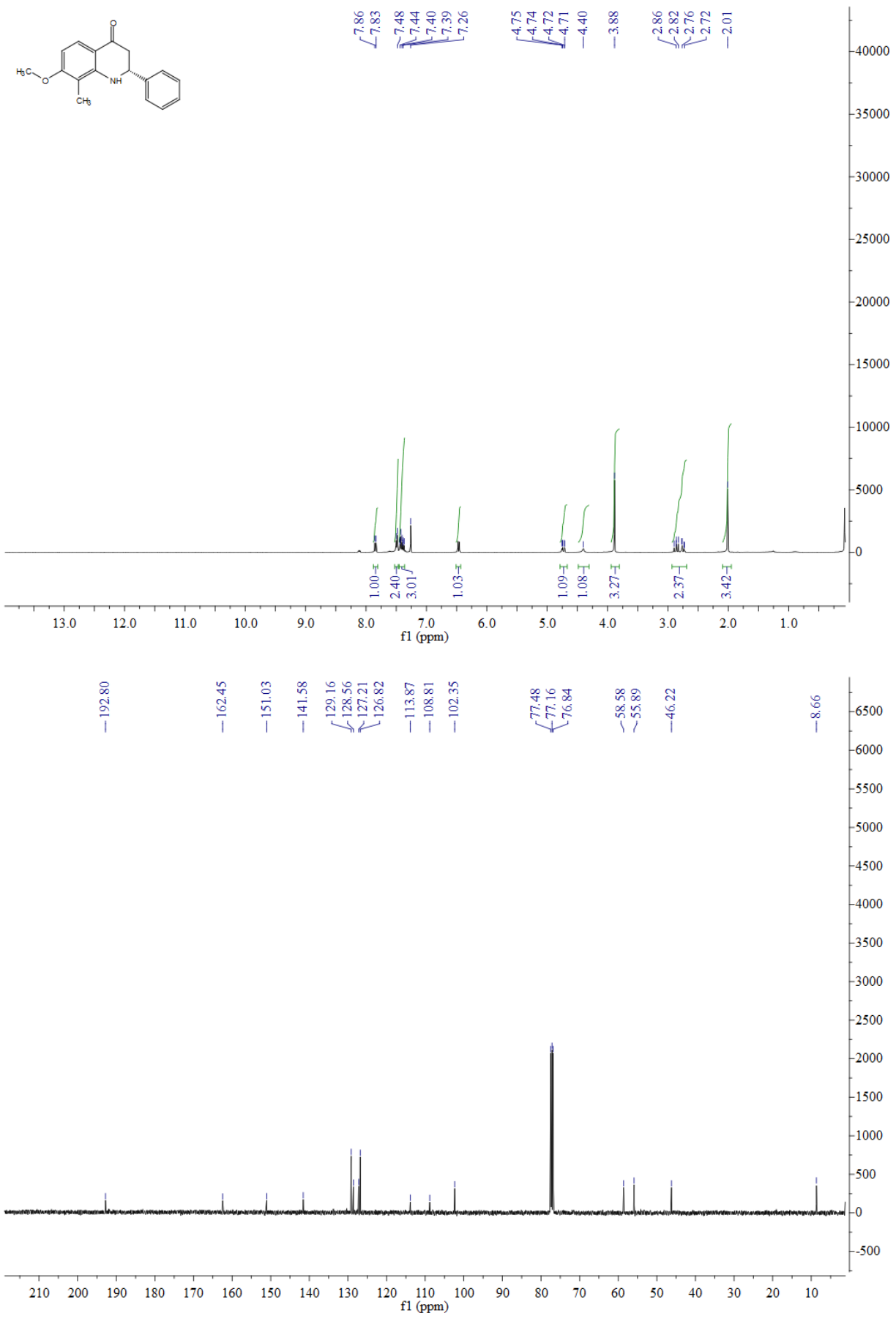


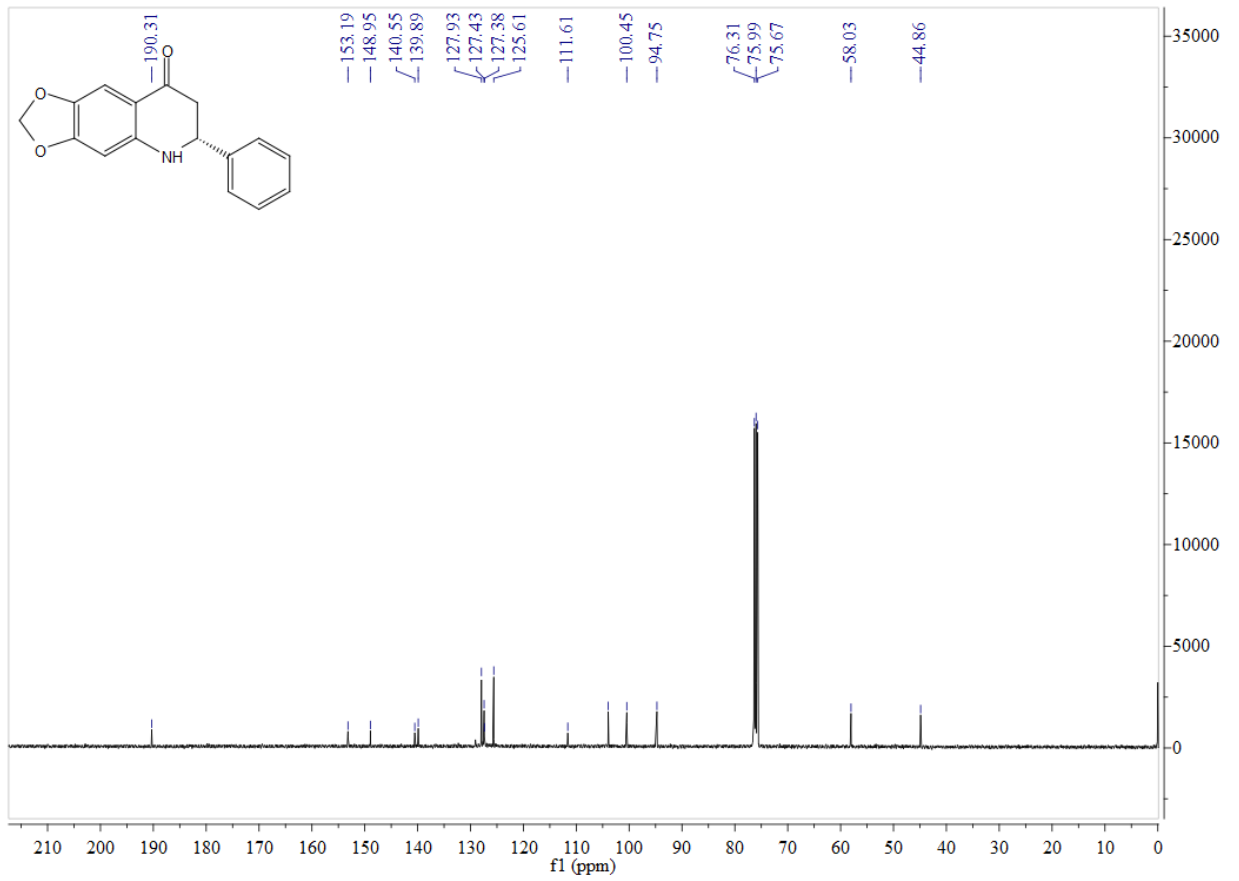
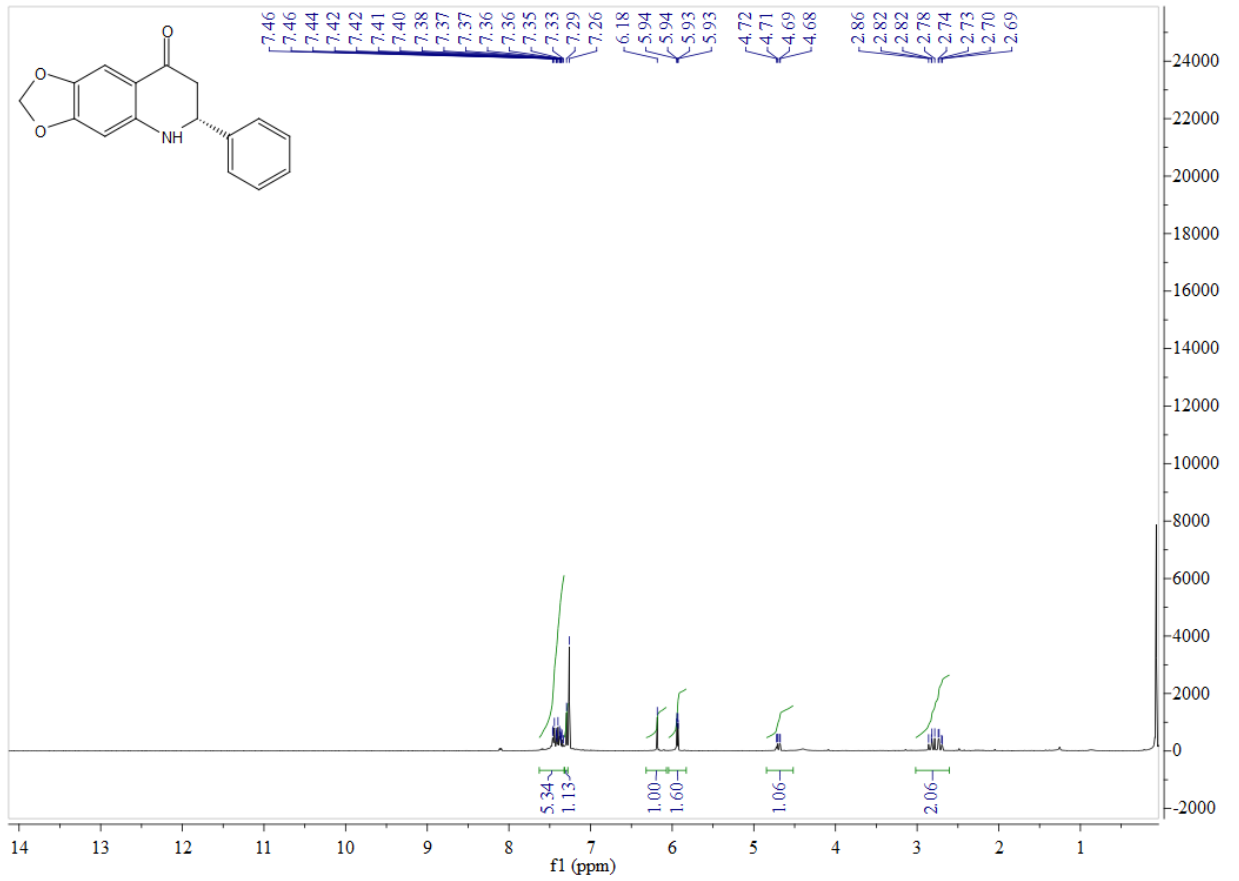




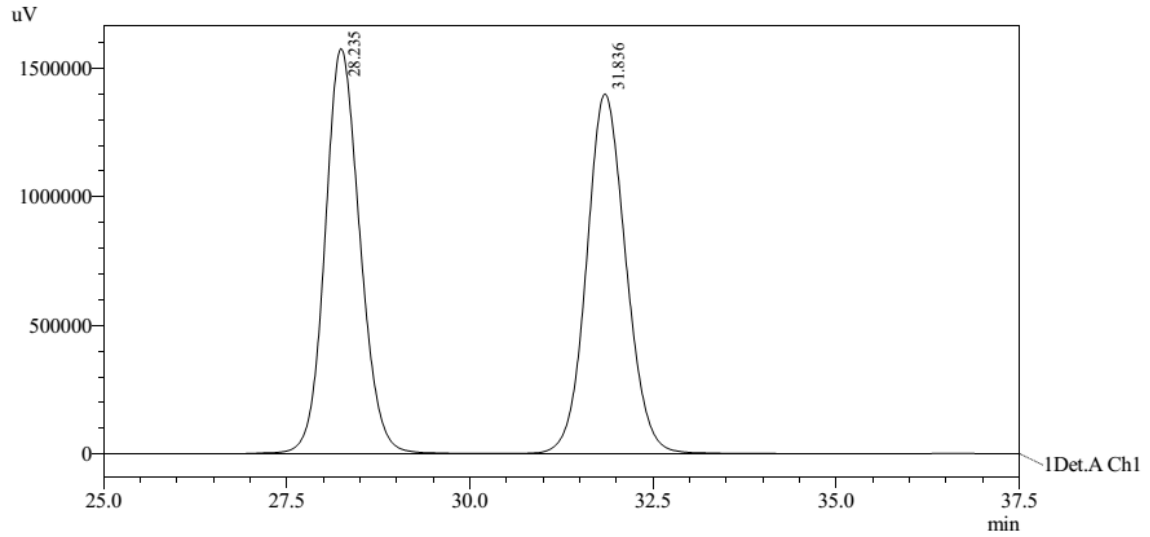
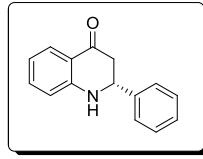








5. HPLC spectra:

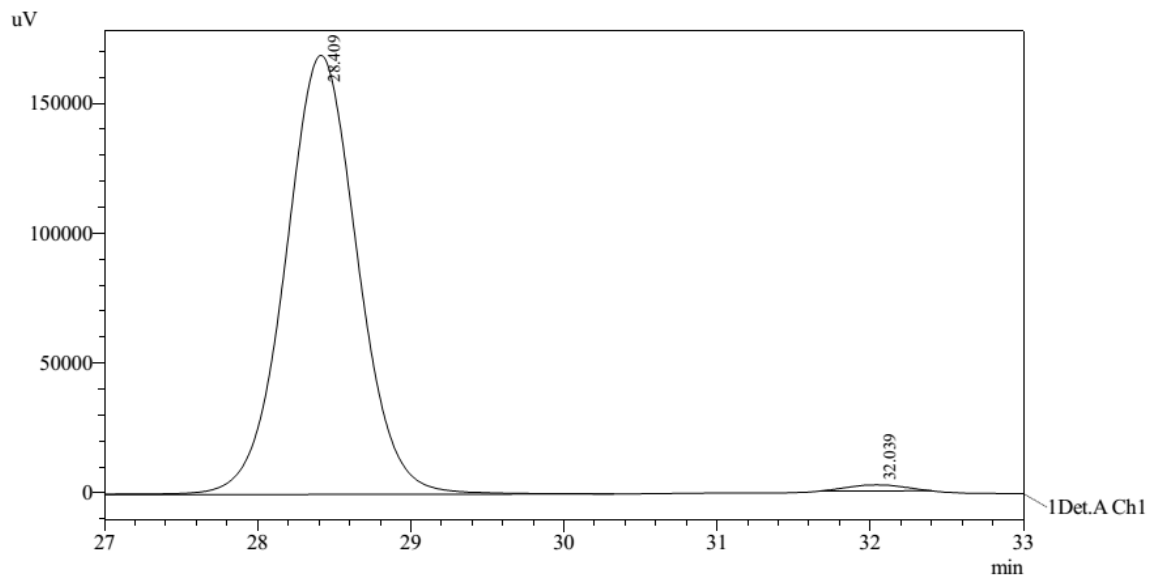


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.235	52261773	1574924	49.937	52.952
2	31.836	52392719	1399301	50.063	47.048
Total		104654493	2974225	100.000	100.000

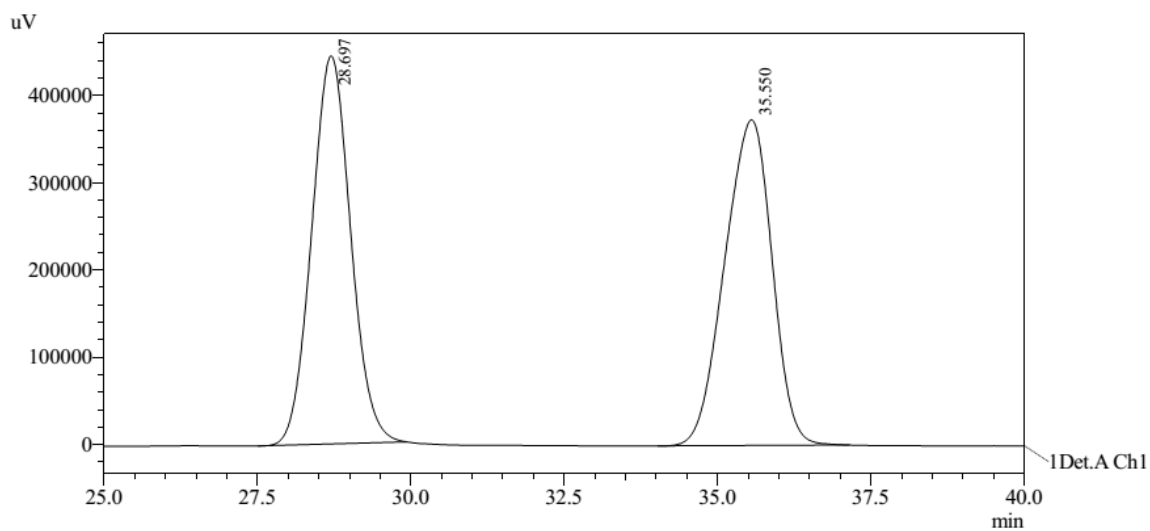
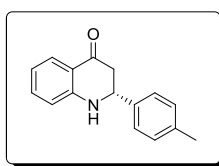


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

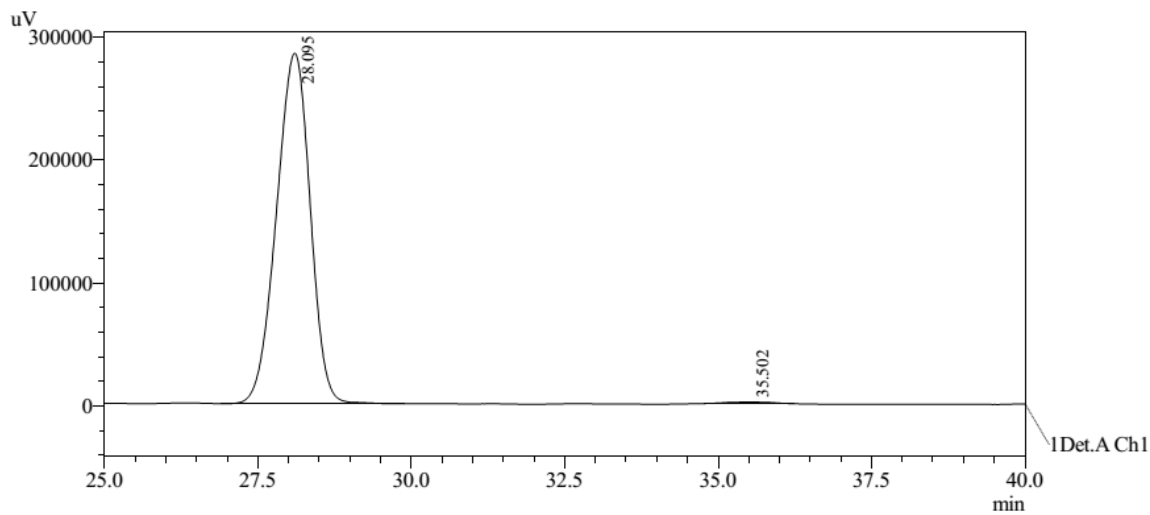
Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.409	5548010	168979	98.948	98.639
2	32.039	58982	2332	1.052	1.361
Total		5606992	171311	100.000	100.000



1 Det.A Ch1 / 214nm

PeakTable

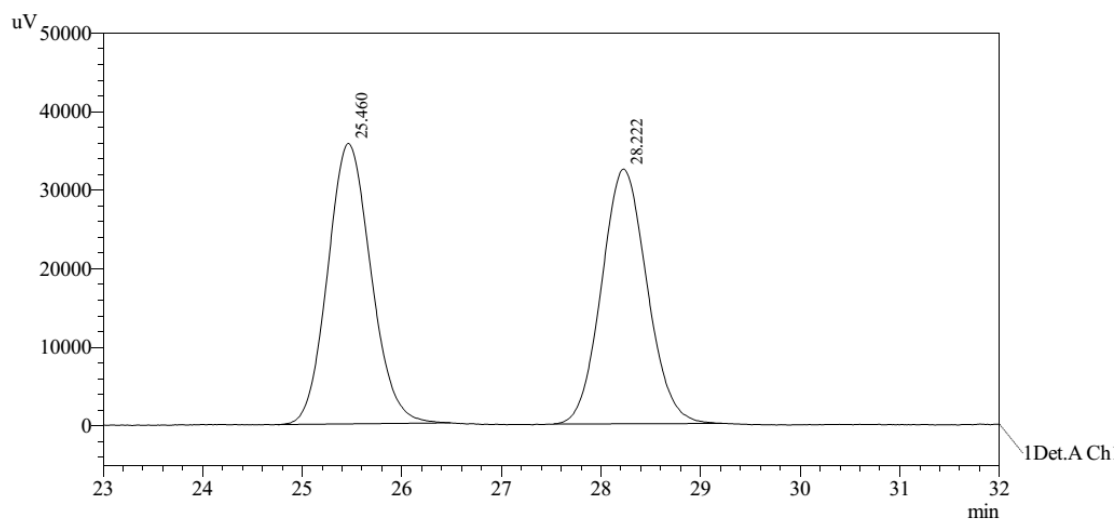
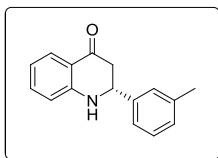
Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.697	19671765	444649	49.531	54.374
2	35.550	20044505	373108	50.469	45.626
Total		39716270	817757	100.000	100.000



1 Det.A Ch1 / 214nm

PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.095	10910780	285351	99.382	99.490
2	35.502	67871	1461	0.618	0.510
Total		10978651	286812	100.000	100.000

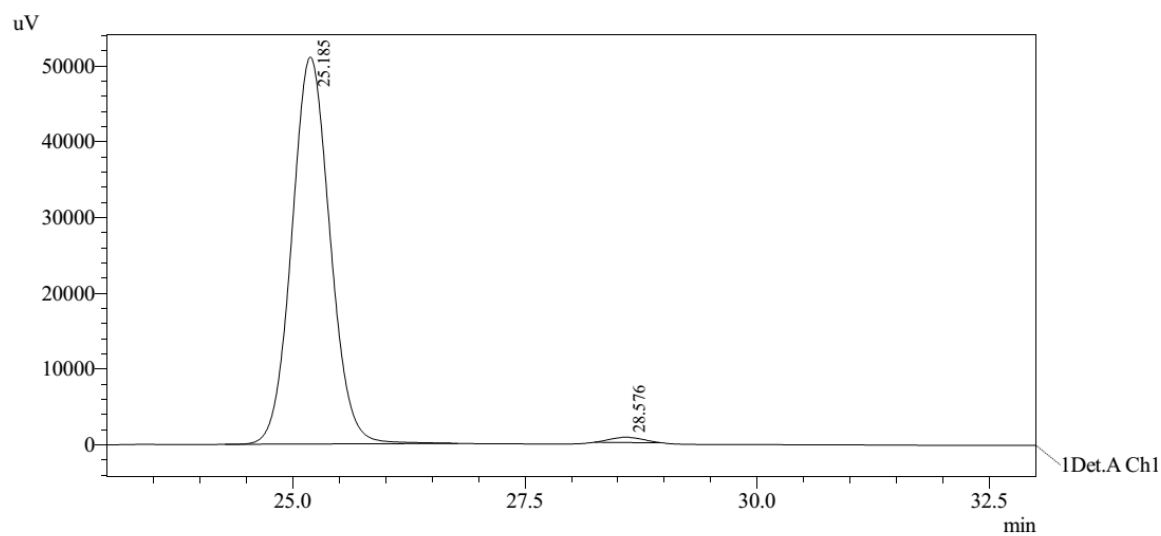


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.460	1079151	35701	51.192	52.409
2	28.222	1028912	32418	48.808	47.591
Total		2108064	68119	100.000	100.000

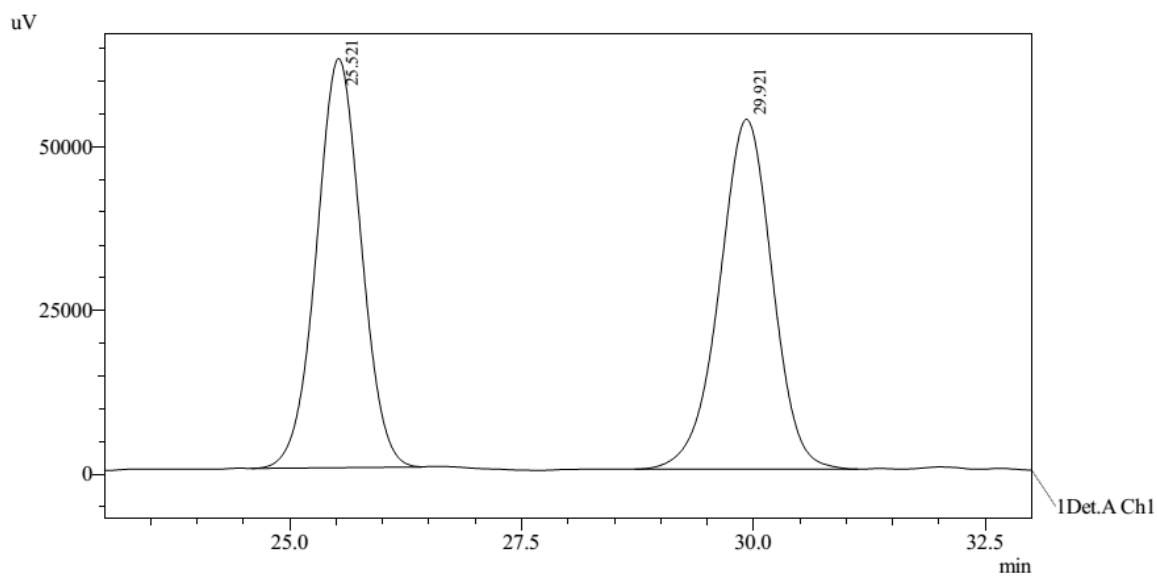
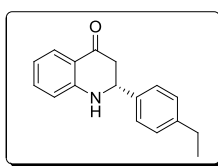


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.185	1457941	51031	98.853	98.662
2	28.576	16922	692	1.147	1.338
Total		1474864	51723	100.000	100.000

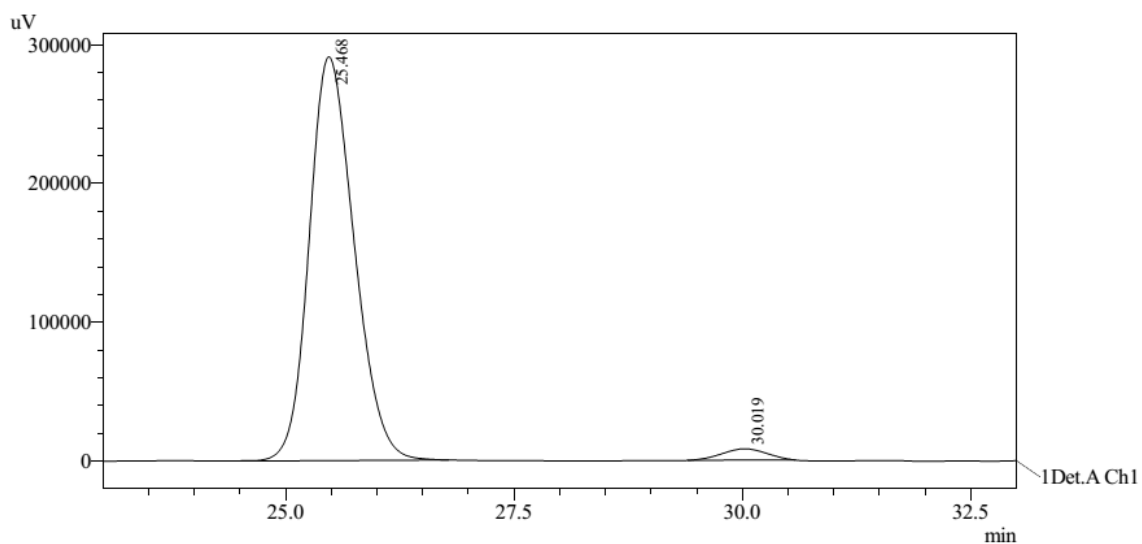


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.521	2094913	62420	49.643	53.895
2	29.921	2125063	53398	50.357	46.105
Total		4219976	115819	100.000	100.000

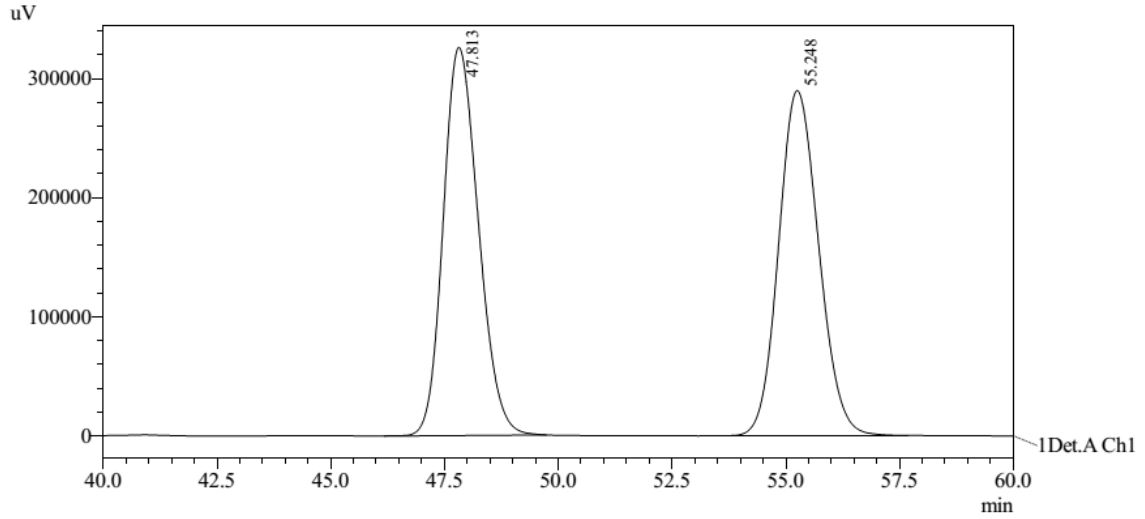
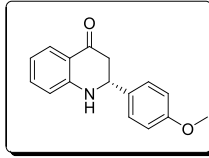


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.468	9951347	290912	97.258	97.282
2	30.019	280589	8127	2.742	2.718
Total		10231936	299040	100.000	100.000

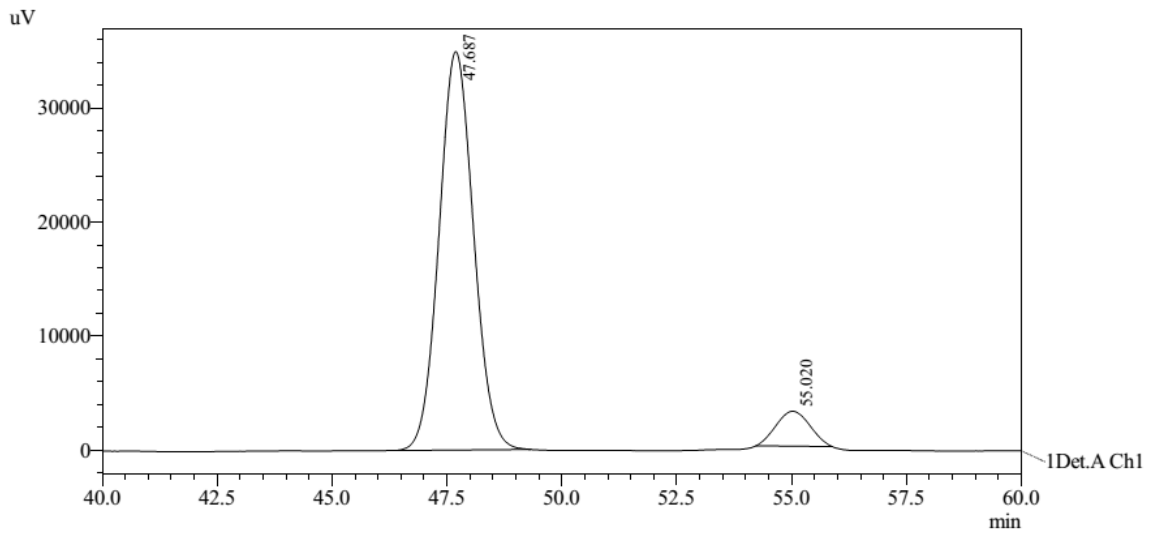


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	47.813	17558918	325965	49.697	52.922
2	55.248	17772686	289964	50.303	47.078
Total		35331605	615930	100.000	100.000

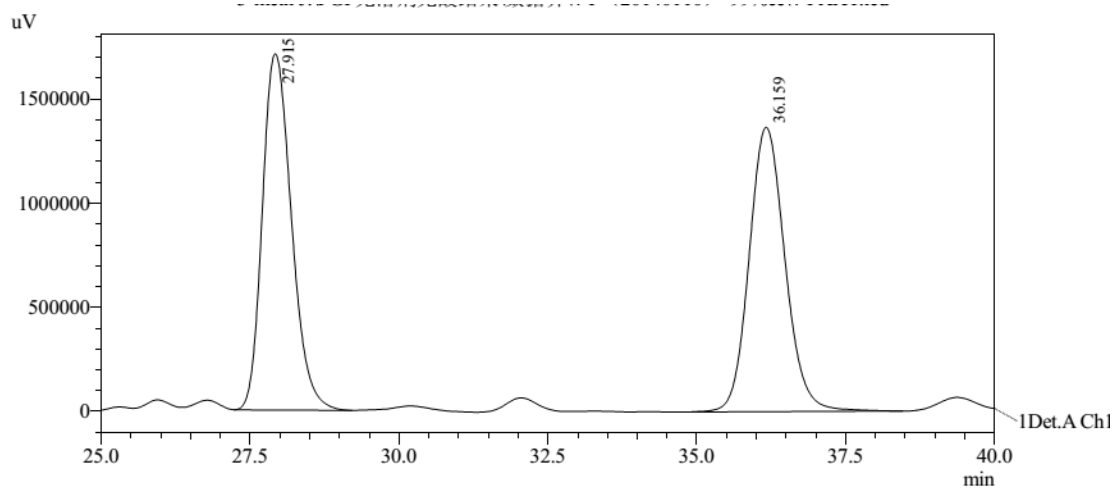
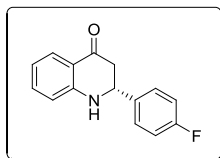


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	47.687	1827722	34934	92.091	91.956
2	55.020	156958	3056	7.909	8.044
Total		1984680	37989	100.000	100.000

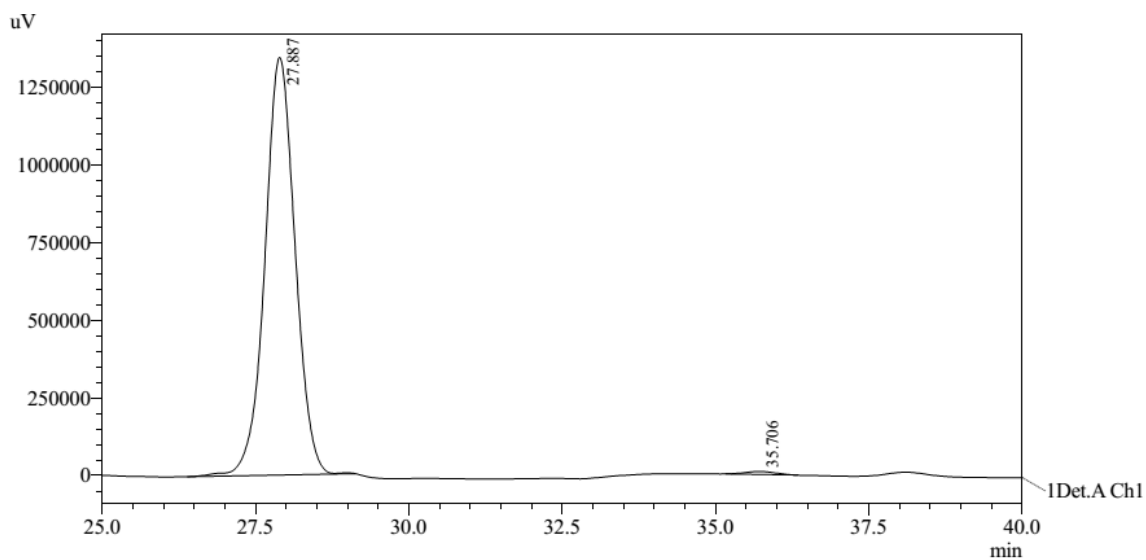


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.915	58185368	1709696	50.321	55.597
2	36.159	57442042	1365468	49.679	44.403
Total		115627410	3075164	100.000	100.000

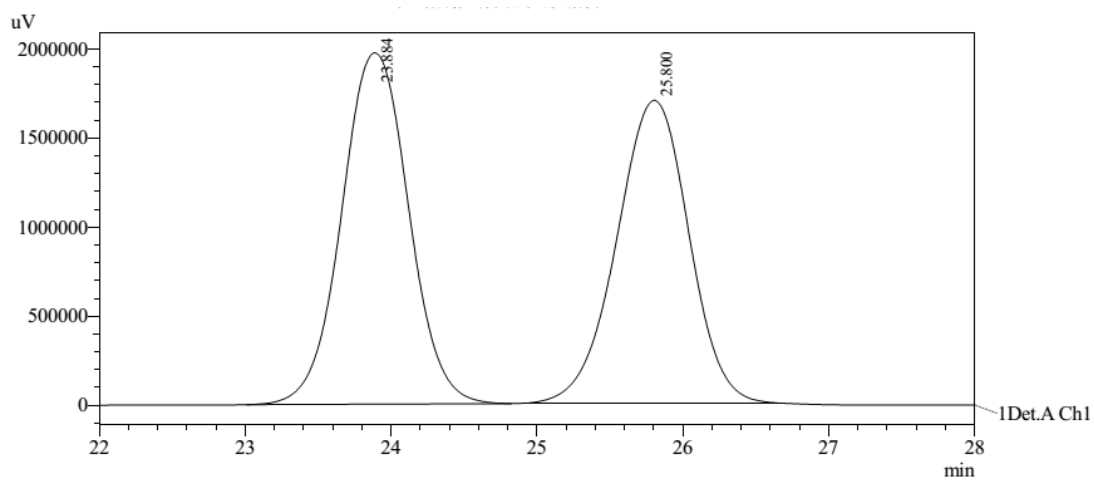
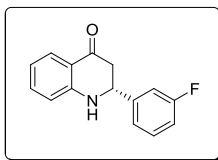


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.887	46201997	1345823	99.282	99.293
2	35.706	333904	9584	0.718	0.707
Total		46535901	1355407	100.000	100.000

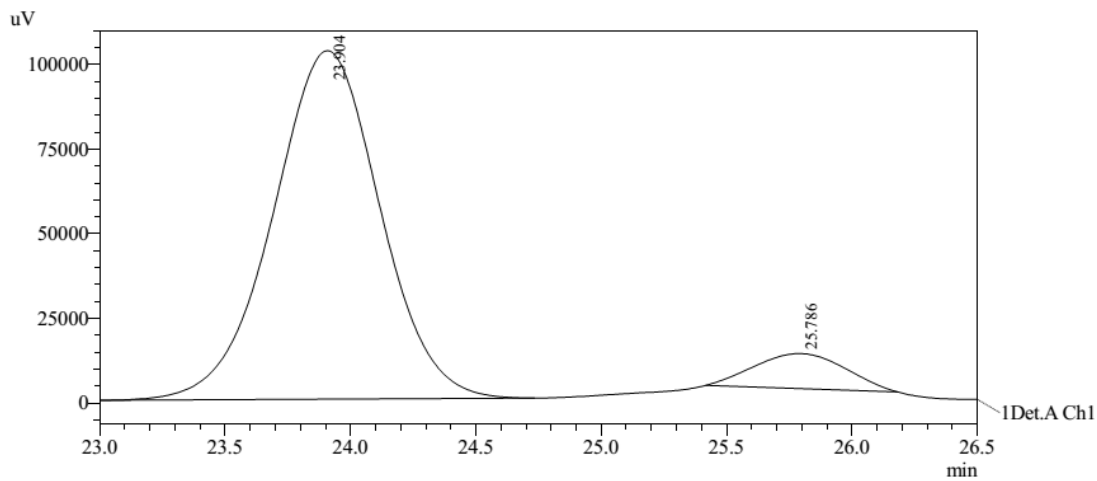


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.884	63047094	1971333	51.832	53.699
2	25.800	58589477	1699739	48.168	46.301
Total		121636571	3671072	100.000	100.000

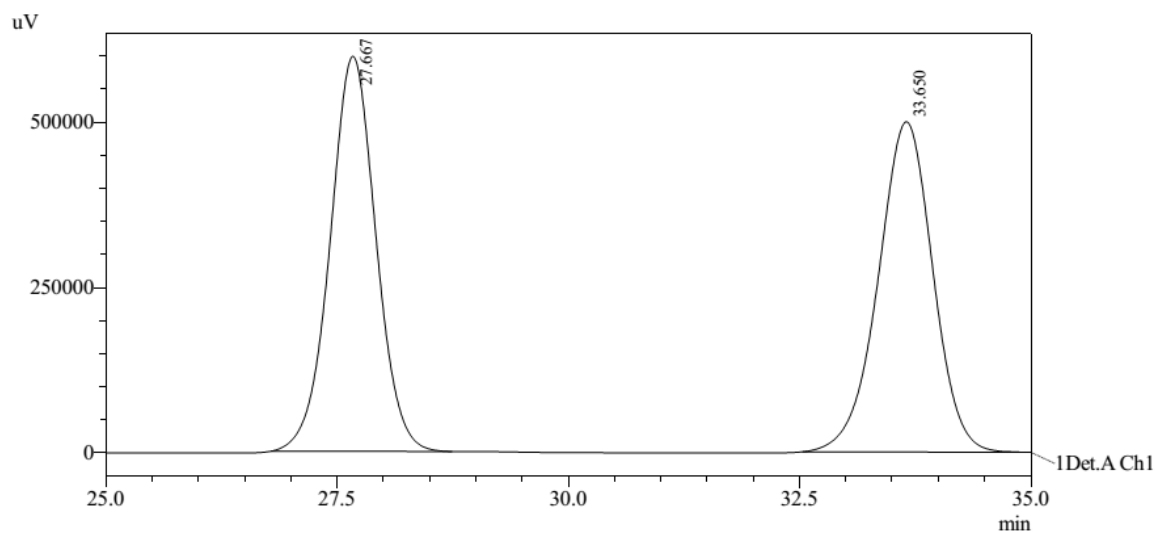
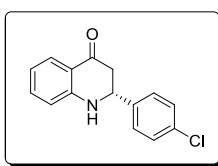


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.904	3054508	102987	92.127	90.880
2	25.786	261038	10335	7.873	9.120
Total		3315545	113323	100.000	100.000

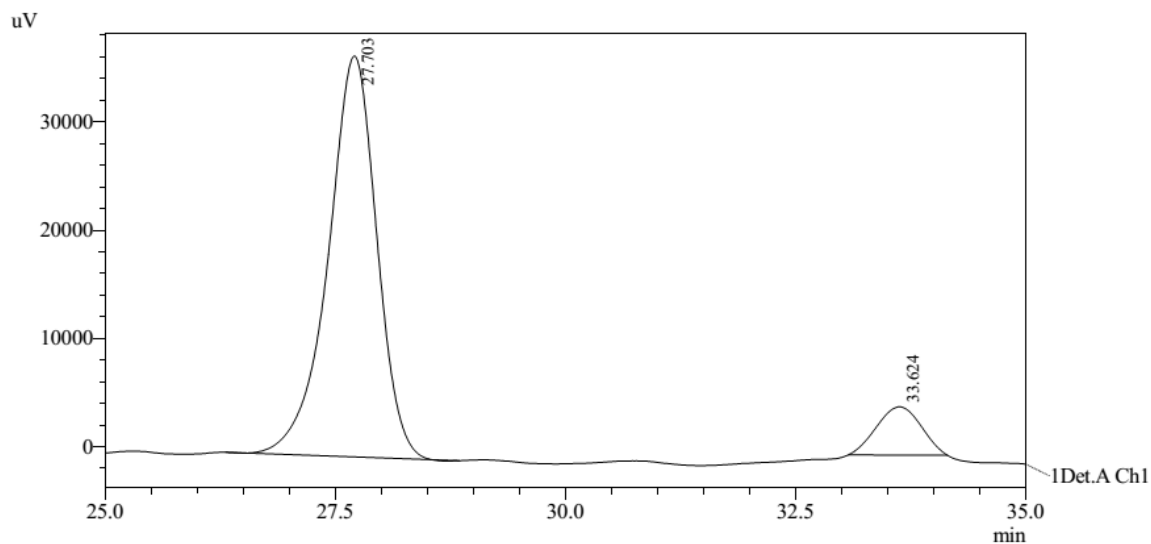


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.667	20635220	597089	50.126	54.463
2	33.650	20531680	499240	49.874	45.537
Total		41166900	1096329	100.000	100.000

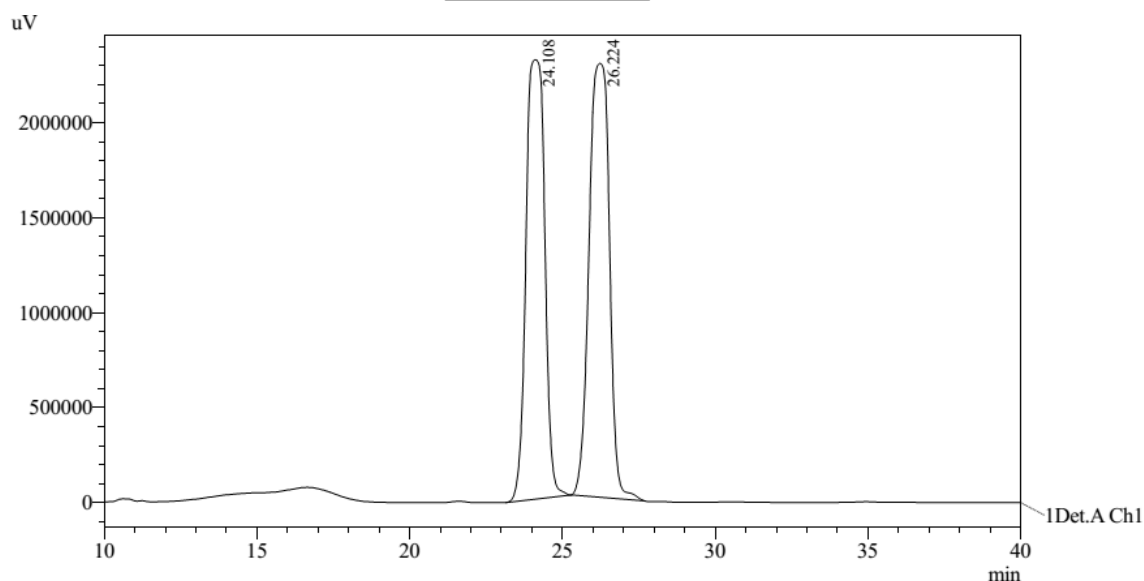
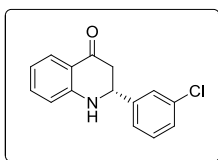


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.703	1359347	37005	90.066	89.264
2	33.624	149930	4451	9.934	10.736
Total		1509277	41456	100.000	100.000

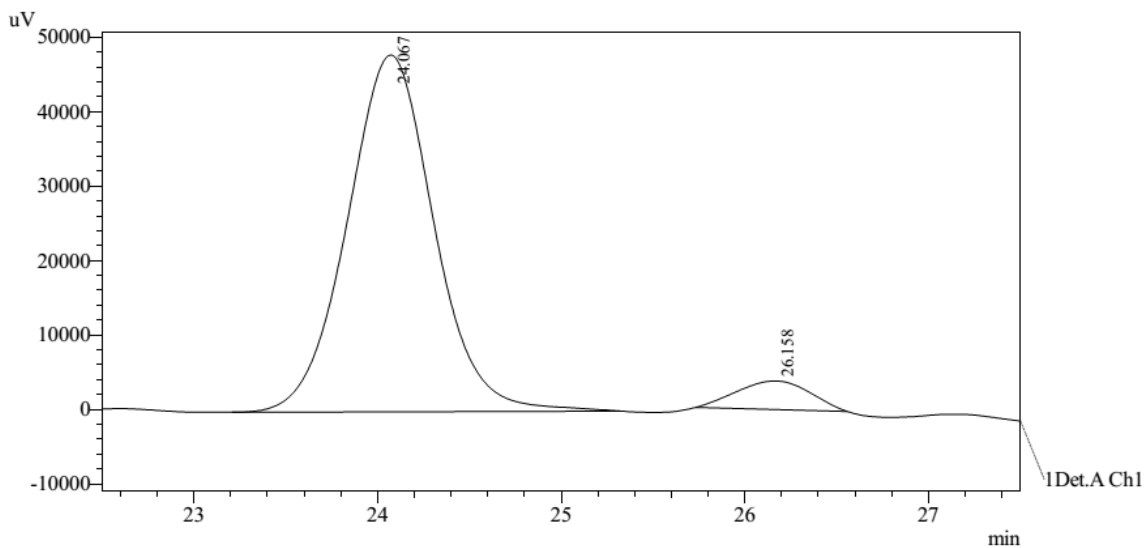


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.108	98878474	2312920	48.254	50.317
2	26.224	106035082	2283801	51.746	49.683
Total		204913556	4596720	100.000	100.000

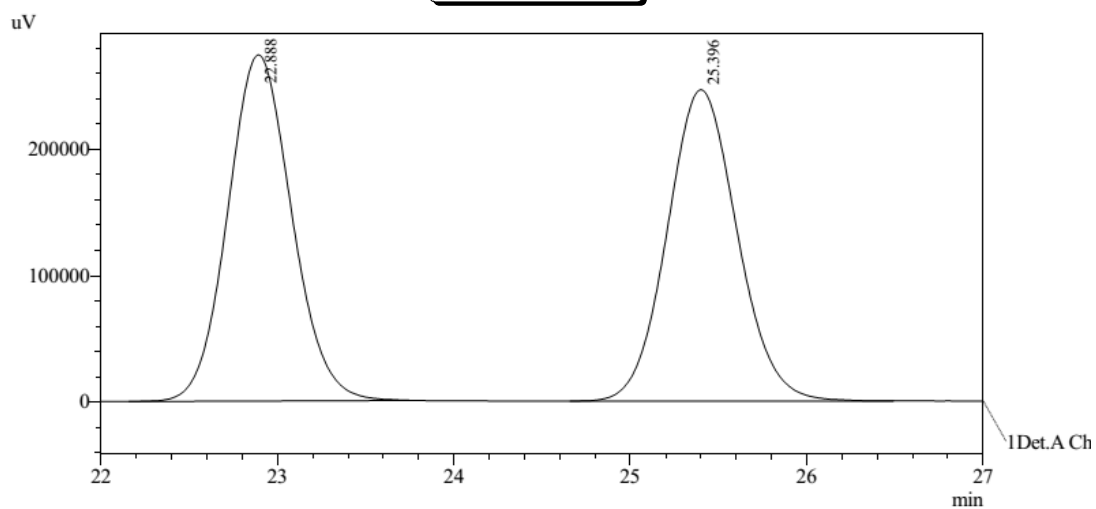
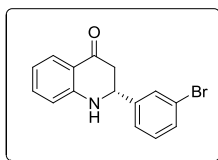


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.067	1568865	47905	93.672	92.591
2	26.158	105993	3833	6.328	7.409
Total		1674858	51738	100.000	100.000

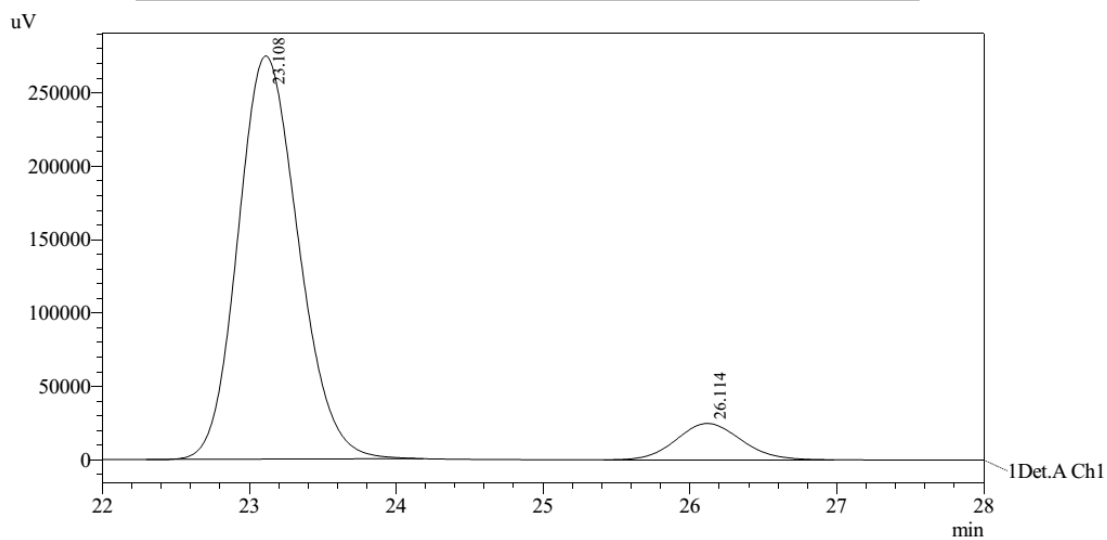


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.888	6911281	274085	50.370	52.637
2	25.396	6809734	246627	49.630	47.363
Total		13721016	520712	100.000	100.000

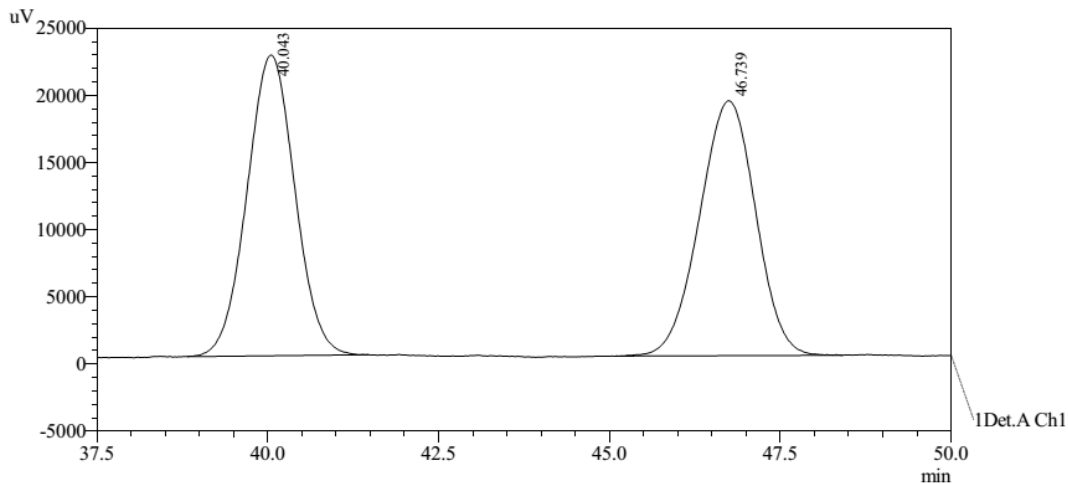
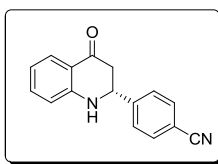


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.108	7845742	274510	91.195	91.751
2	26.114	757489	24681	8.805	8.249
Total		8603230	299191	100.000	100.000

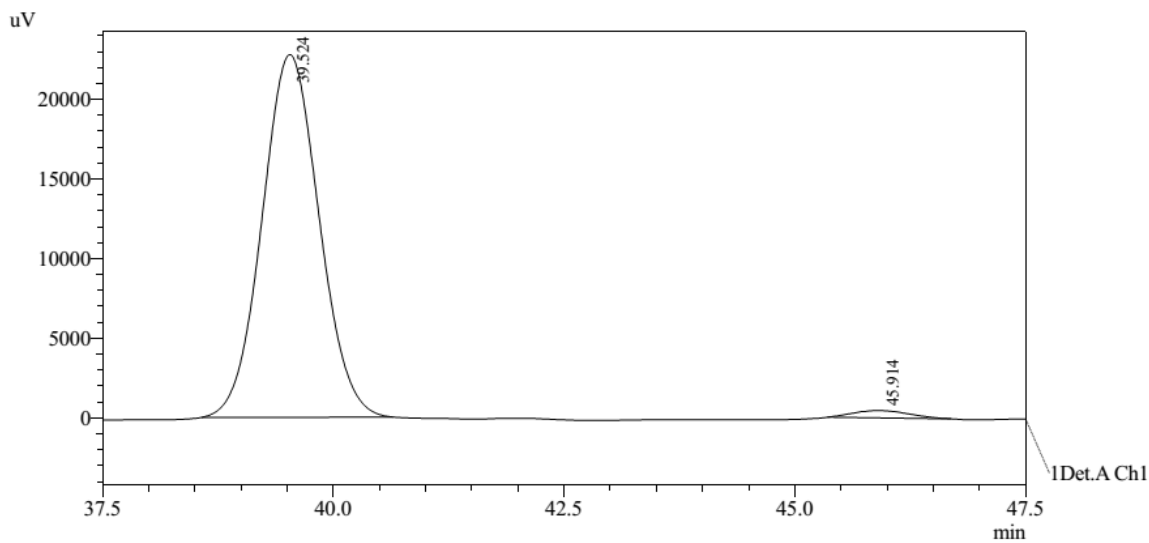


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	40.043	1093378	22390	50.184	54.128
2	46.739	1085357	18975	49.816	45.872
Total		2178735	41365	100.000	100.000

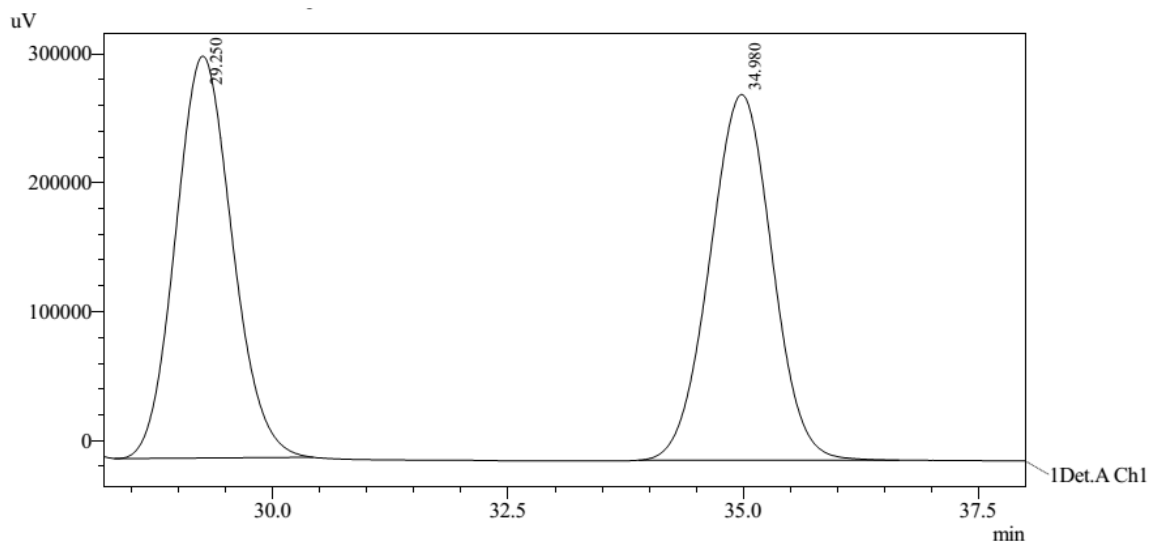
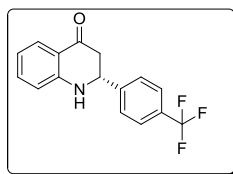


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	39.524	979196	22774	98.033	97.982
2	45.914	19642	469	1.967	2.018
Total		998839	23243	100.000	100.000

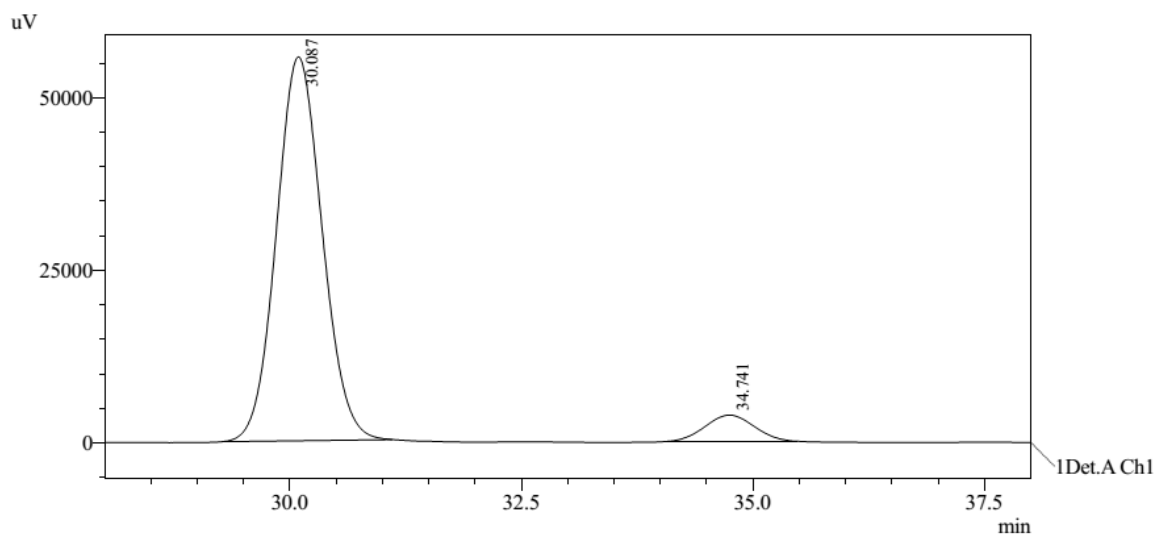


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	29.250	13083240	311709	49.954	52.354
2	34.980	13107368	283681	50.046	47.646
Total		26190608	595390	100.000	100.000

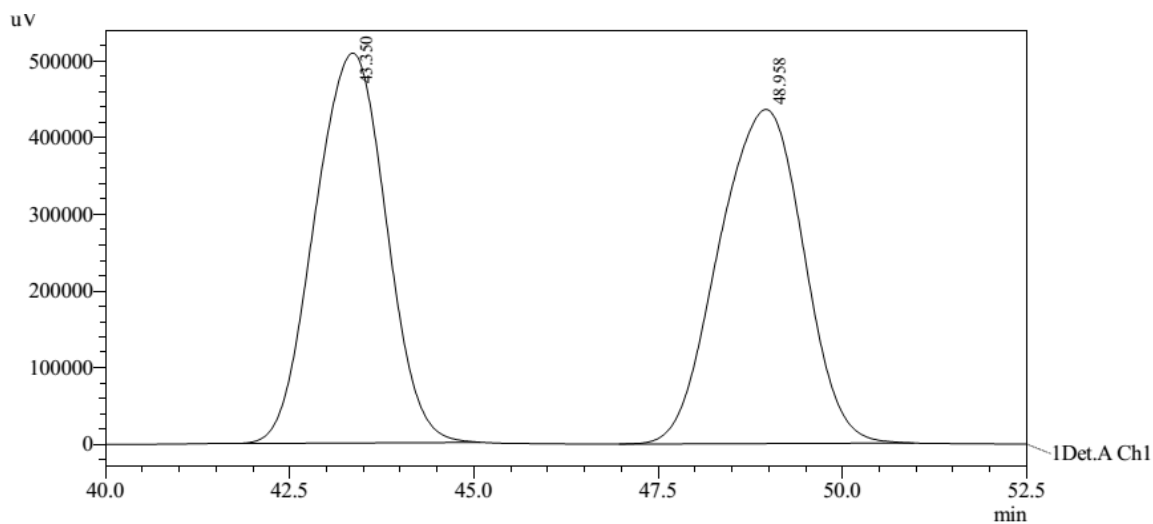
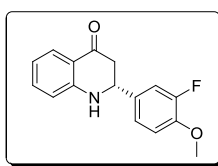


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	30.087	1915886	55658	93.148	93.603
2	34.741	140926	3804	6.852	6.397
Total		2056812	59462	100.000	100.000

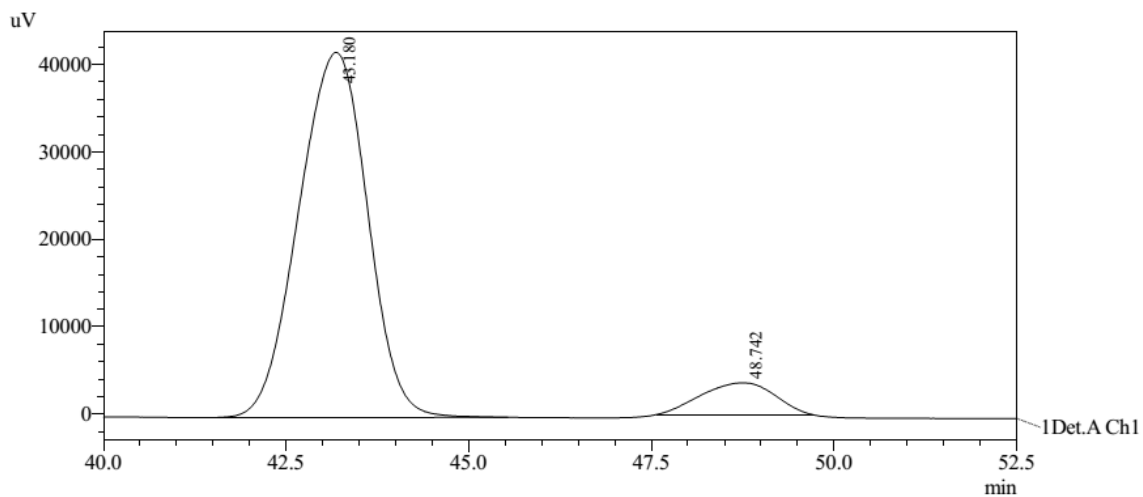


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	43.350	34261232	508640	49.521	53.848
2	48.958	34924369	435939	50.479	46.152
Total		69185601	944579	100.000	100.000

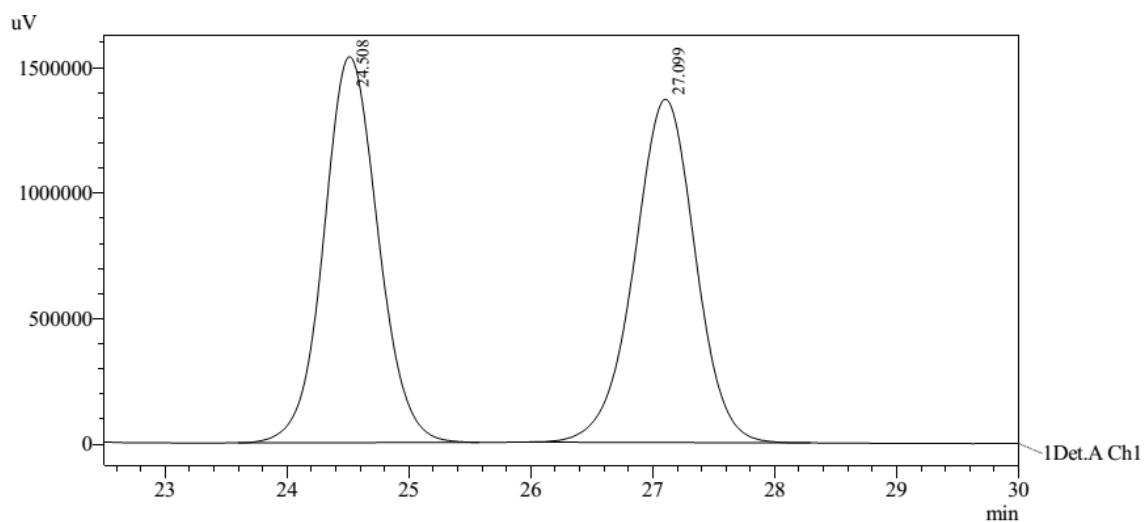
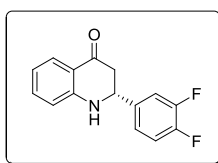


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	43.180	2736125	41746	91.470	91.969
2	48.742	255167	3646	8.530	8.031
Total		2991292	45391	100.000	100.000

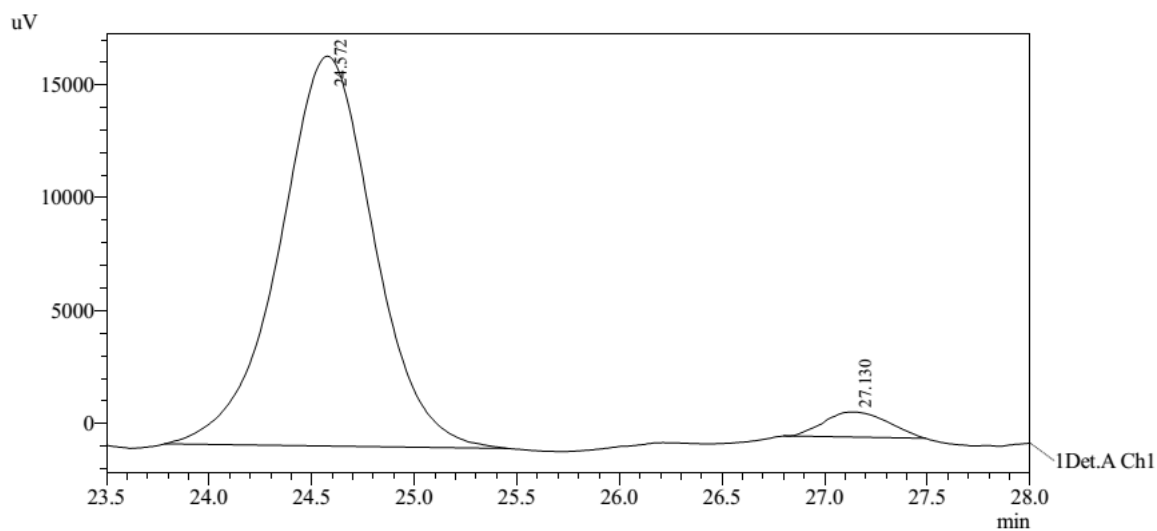


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.508	47771466	1537486	49.969	52.933
2	27.099	47831470	1367097	50.031	47.067
Total		95602936	2904582	100.000	100.000

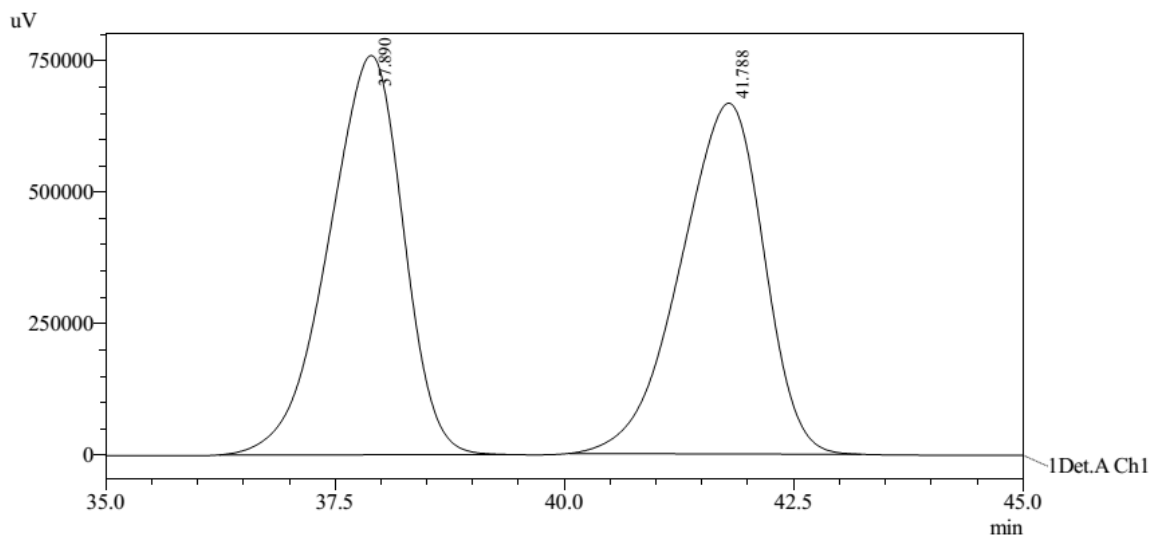
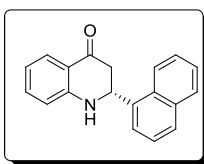


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.572	551622	17274	95.813	93.967
2	27.130	24103	1109	4.187	6.033
Total		575725	18383	100.000	100.000

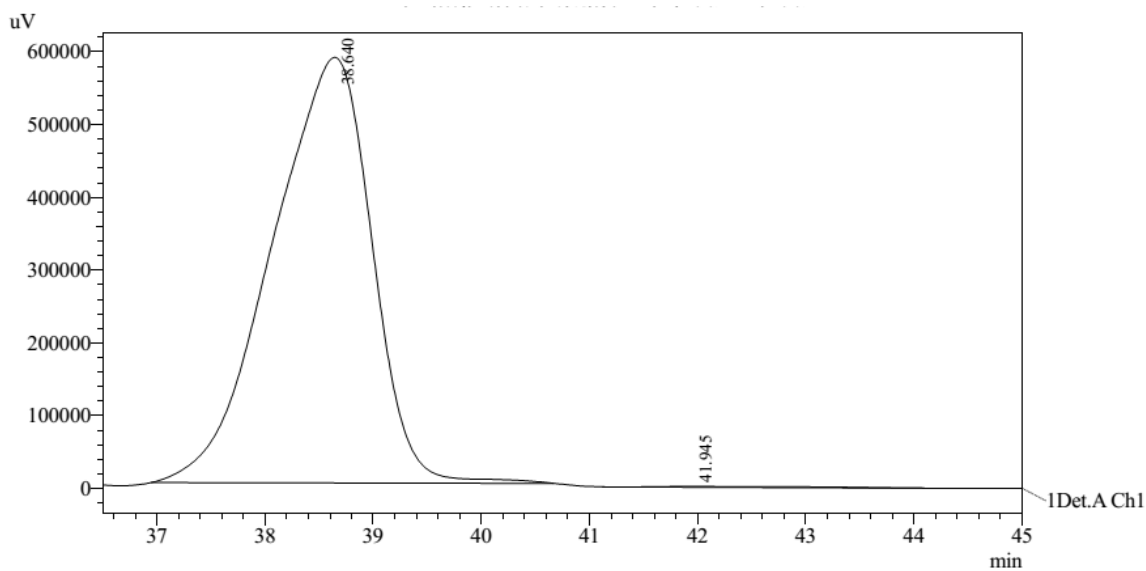


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	37.890	43129737	759112	50.540	53.227
2	41.788	42207700	667065	49.460	46.773
Total		85337437	1426177	100.000	100.000

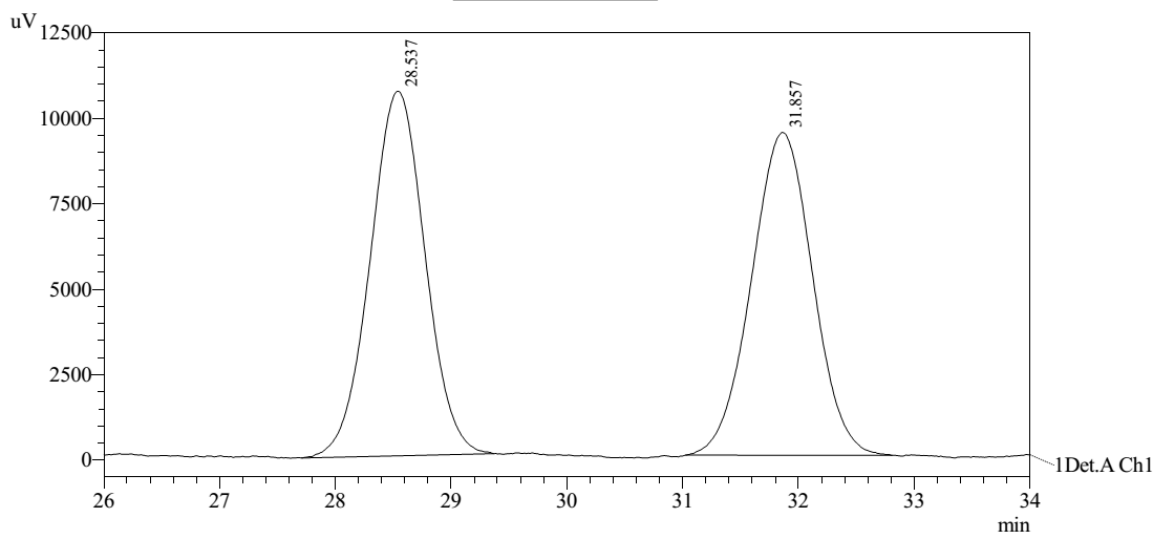
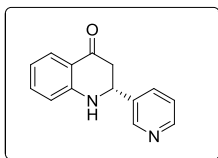


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.640	37473410	584542	99.710	99.843
2	41.945	109009	917	0.290	0.157
Total		37582419	585459	100.000	100.000

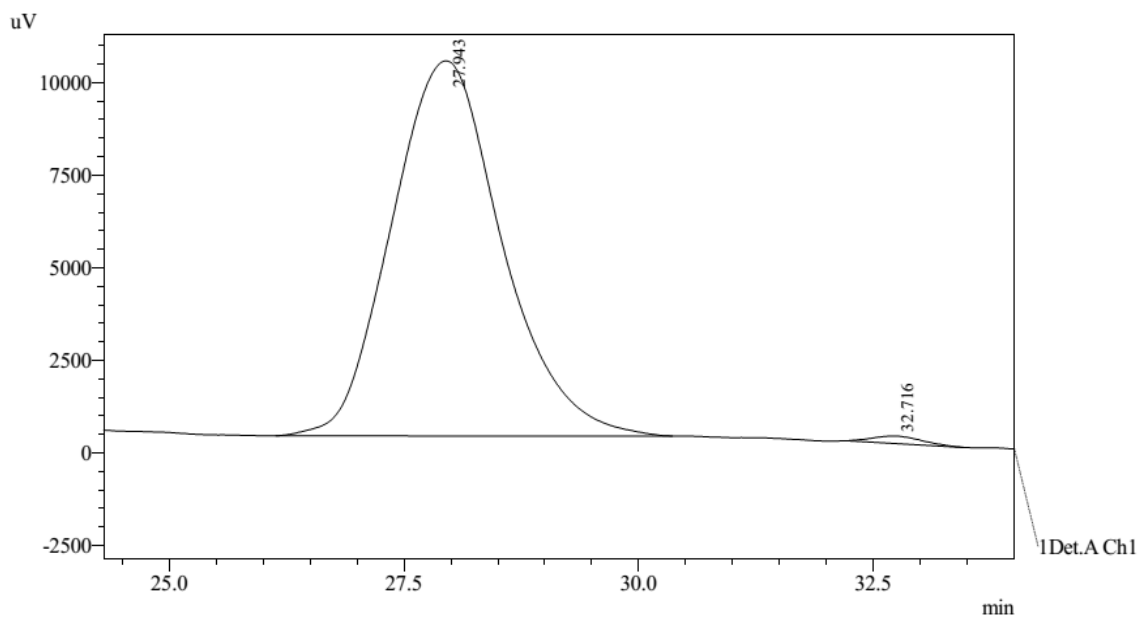


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.537	351505	10666	50.331	53.043
2	31.857	346878	9442	49.669	46.957
Total		698383	20108	100.000	100.000

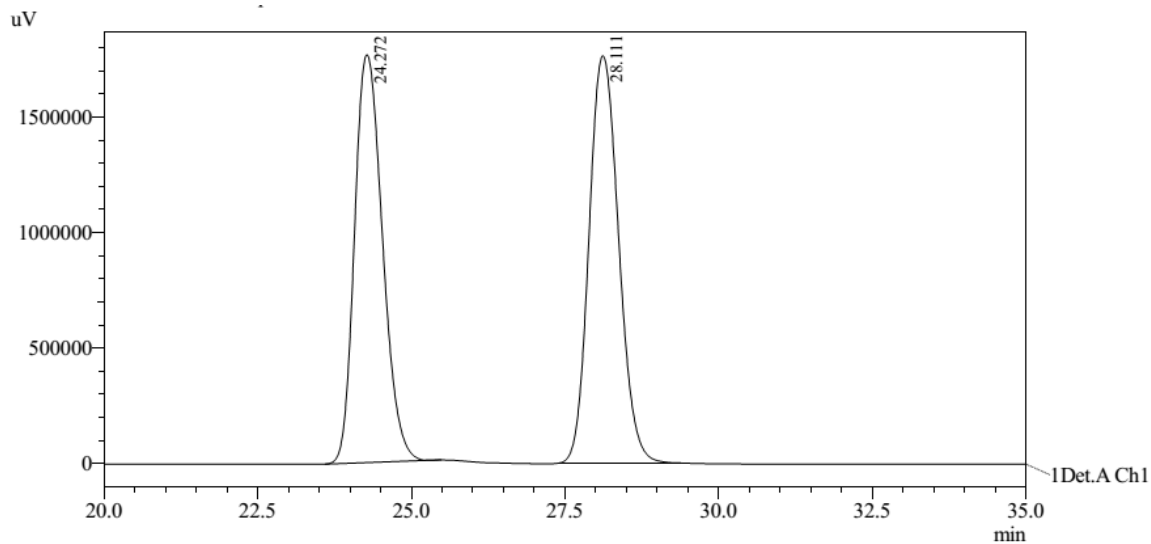
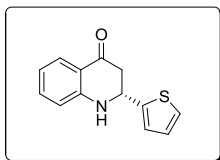


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

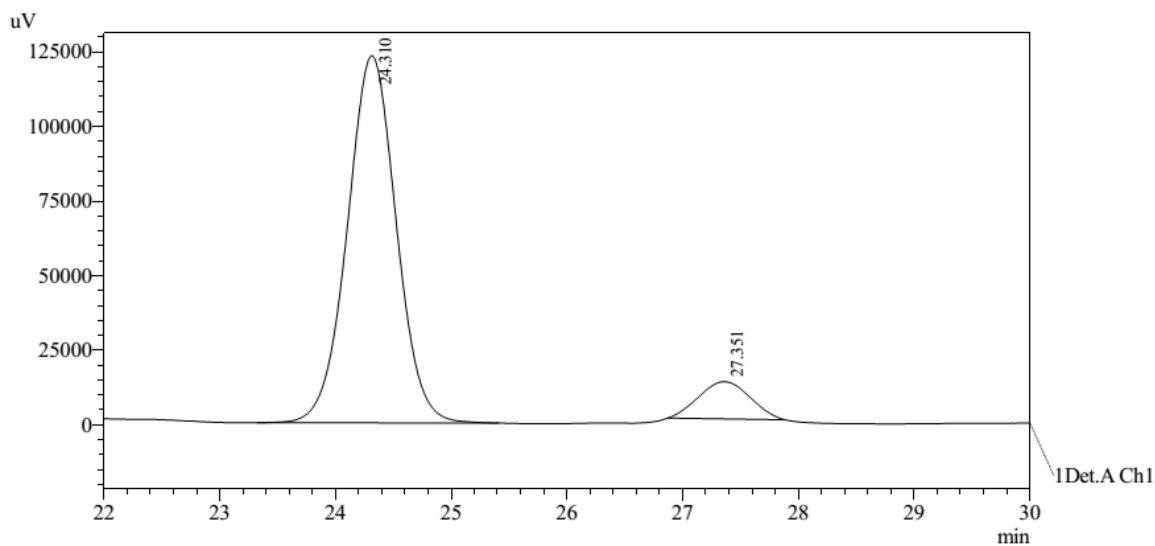
Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.943	828580	10135	99.125	98.062
2	32.716	7318	200	0.875	1.938
Total		835898	10335	100.000	100.000



1 Det.A Ch1 / 254nm

PeakTable

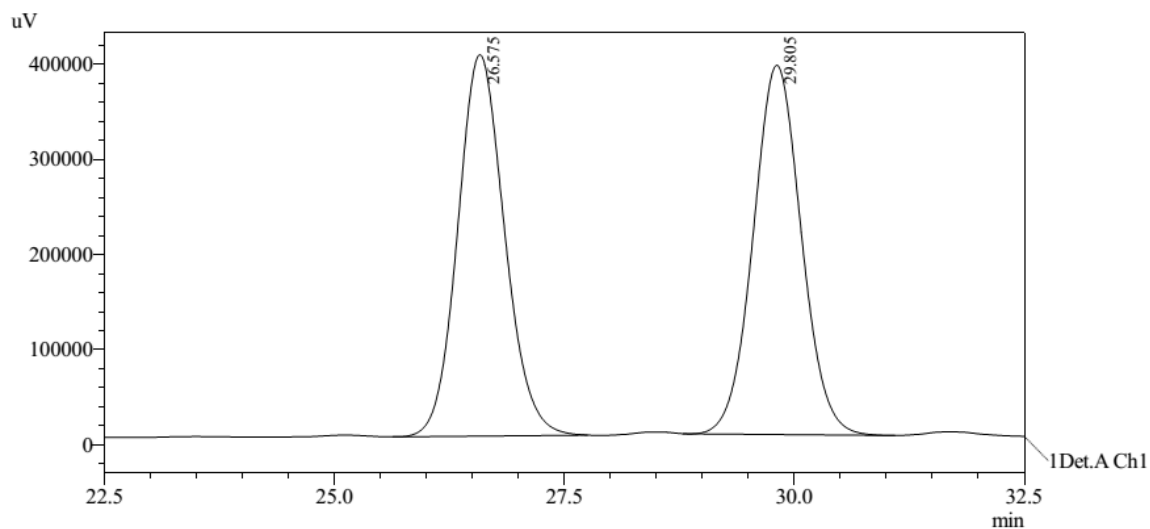
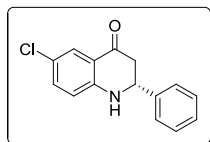
Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.272	55785385	1764938	48.572	50.049
2	28.111	59065021	1761490	51.428	49.951
Total		114850406	3526428	100.000	100.000



1 Det.A Ch1 / 214nm

PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	24.310	3617303	123018	90.422	90.823
2	27.351	383160	12430	9.578	9.177
Total		4000463	135448	100.000	100.000

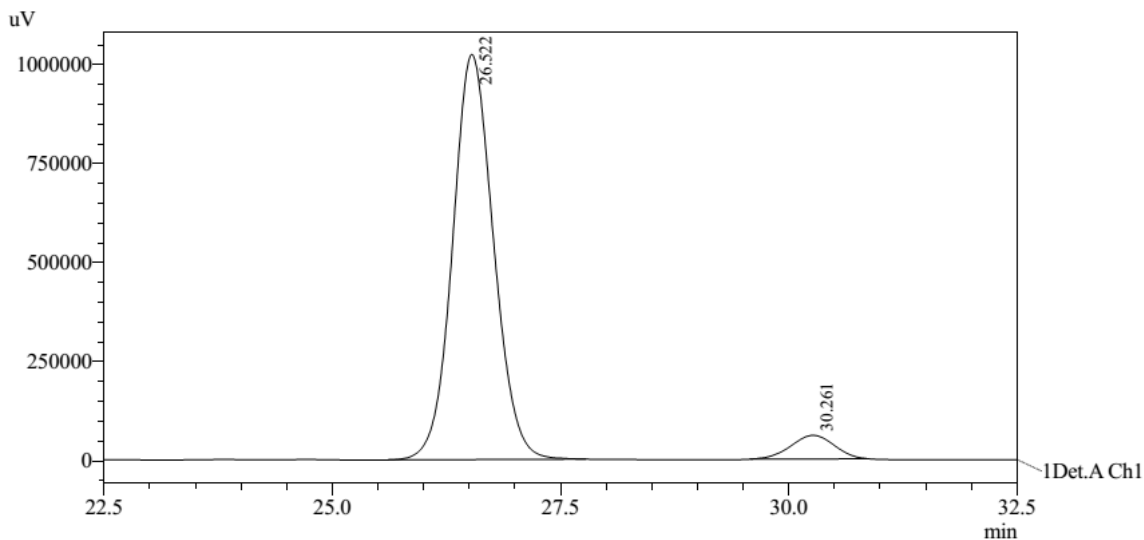


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.575	14226420	401140	50.112	50.809
2	29.805	14162847	388365	49.888	49.191
Total		28389267	789505	100.000	100.000

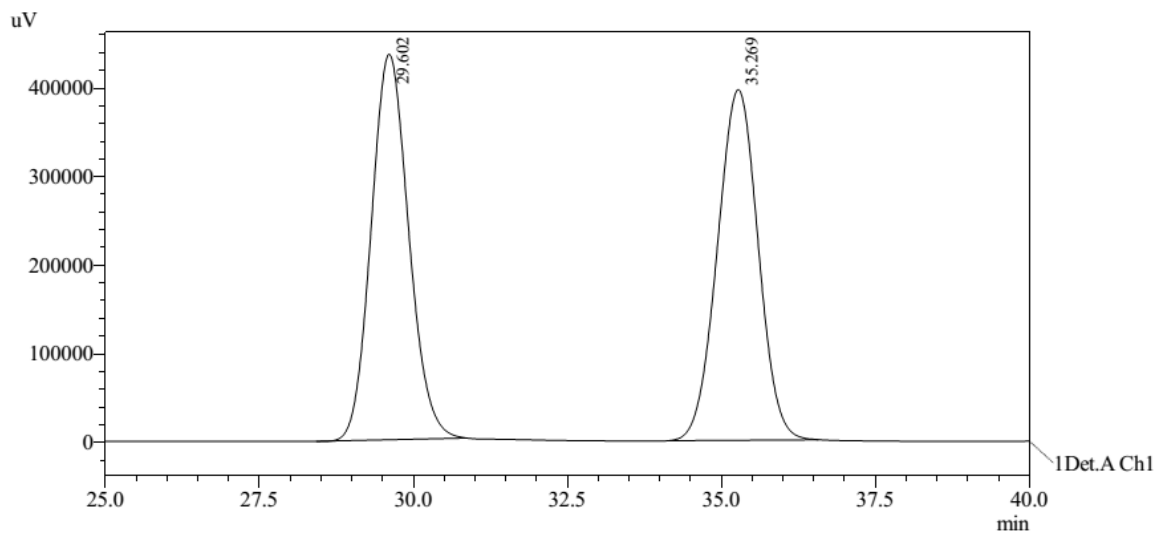
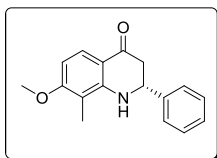


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.522	31898220	1022741	94.154	94.480
2	30.261	1980459	59753	5.846	5.520
Total		33878679	1082495	100.000	100.000

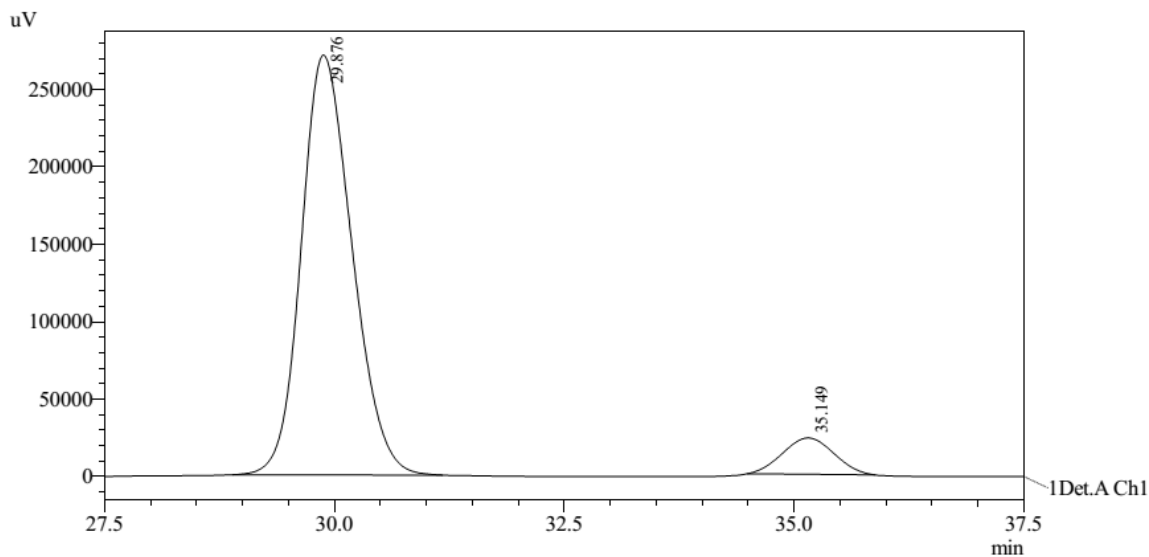


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	29.602	18417001	435114	50.225	52.363
2	35.269	18251708	395843	49.775	47.637
Total		36668709	830957	100.000	100.000

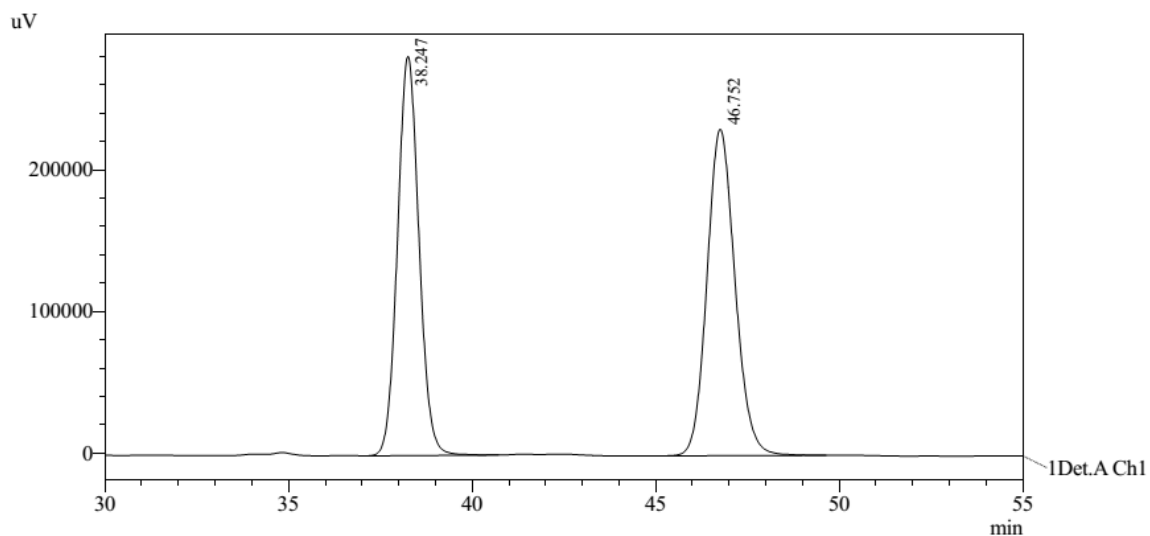
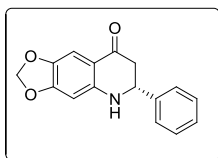


1 Det.A Ch1 / 254nm

PeakTable

检测器 A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	29.876	10423856	271112	91.930	92.035
2	35.149	915021	23462	8.070	7.965
Total		11338877	294574	100.000	100.000

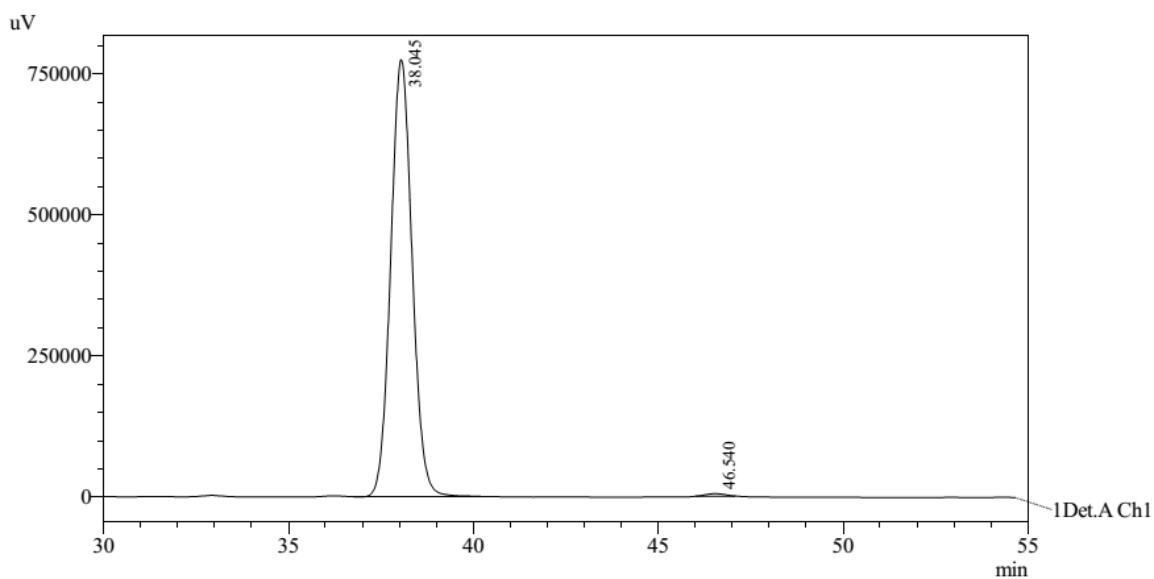


1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.247	11485643	281760	48.398	55.023
2	46.752	12246194	230318	51.602	44.977
Total		23731838	512078	100.000	100.000



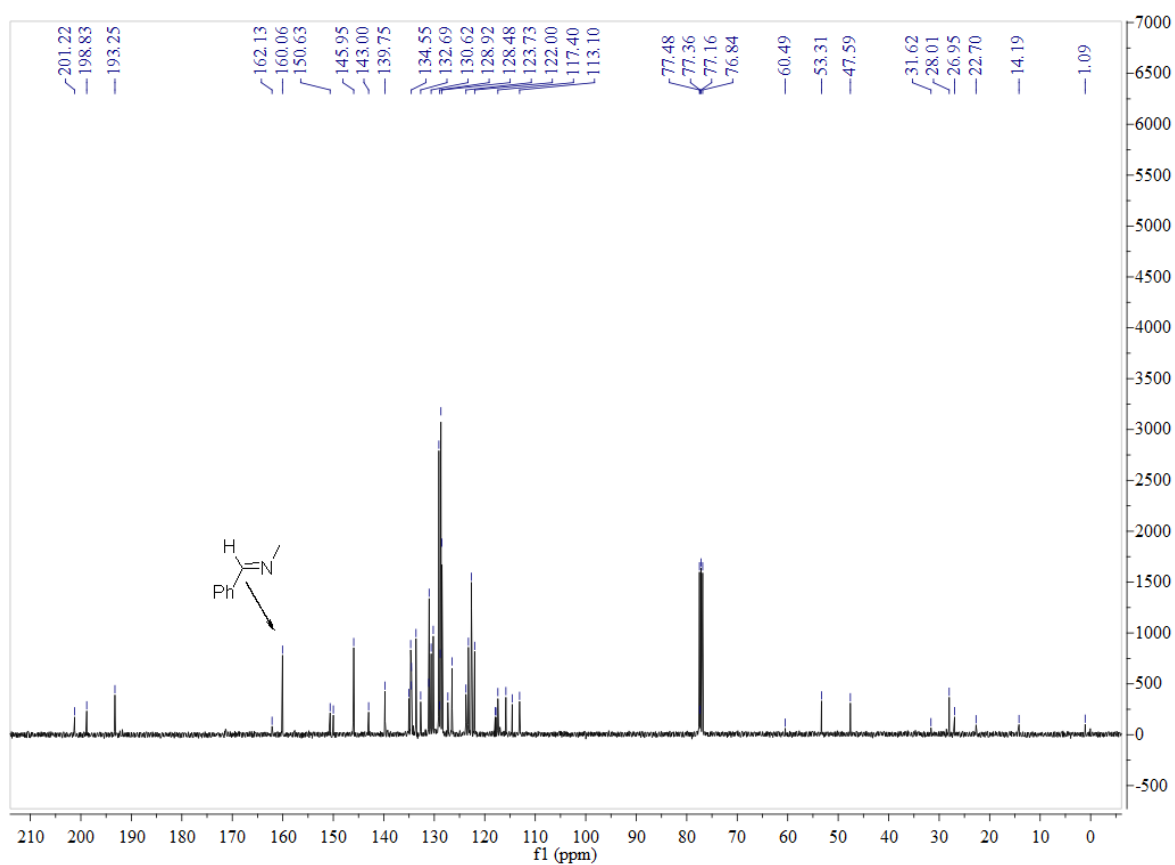
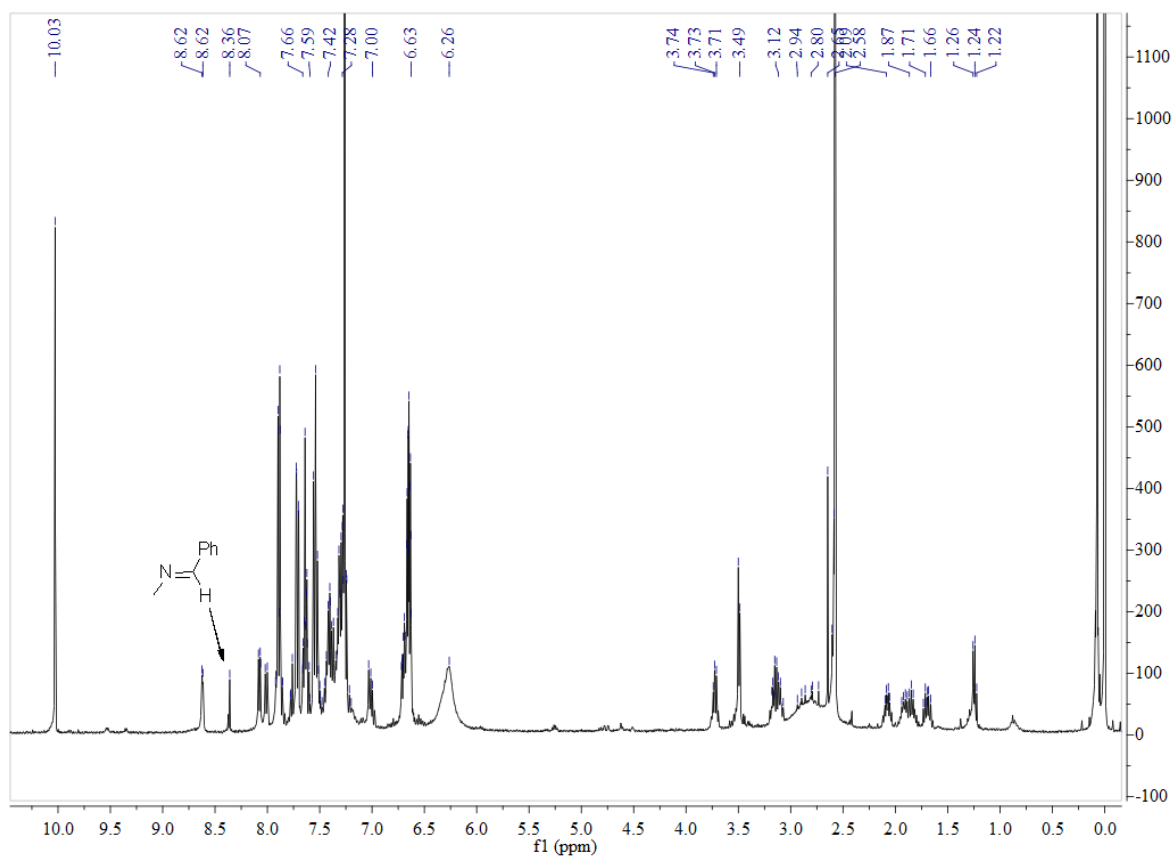
1 Det.A Ch1 / 214nm

PeakTable

检测器 A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.045	31238175	775189	99.498	99.453
2	46.540	157472	4263	0.502	0.547
Total		31395647	779452	100.000	100.000

6. ¹HNMR, ¹³CNMR and HRMS for the mechanism



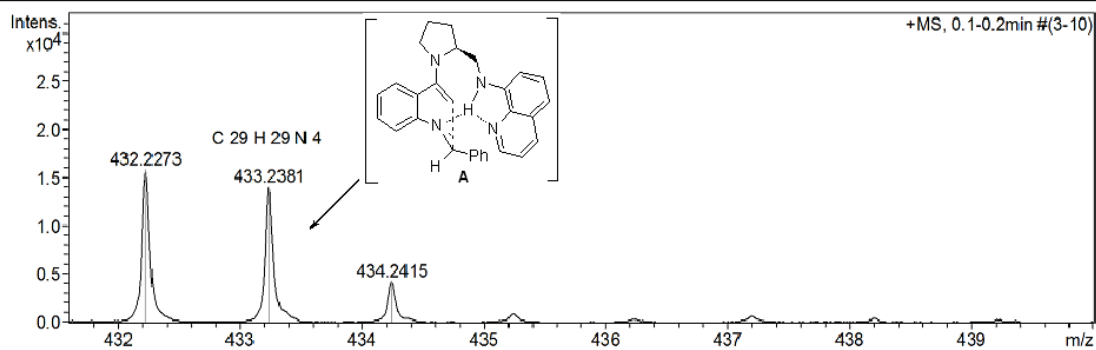
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	G:\±»ú»Ælé[ª]»úÁiÑD¾¿¿\β·Ö±æ\wangyongqiang-20150618-pgf-0112.d	Acquisition Date	2015/6/18 15:09:10
Method	tune_low 50-500.m	Operator	NWU
Sample Name		Instrument / Ser#	microTOF-Q II 10280
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	110.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e;¶ Conf	mSig ma	Std I	Std Mean m/z	Std I VarN orm	Std m/z Diff	Std Com b Dev
433.2381	1	C 29 H 29 N 4	433.2387	1.3	1.2	17.5	ok	even	29.21	0.0447	0.0005	0.0229	0.0001	0.8427

7. X-Ray structure of 3a, 3l

