Supporting information

For

Highly Enantioselective Synthesis of Dihydroquinazolinones Catalyzed by SPINOL-Phosphoric Acids

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CONTENTS

1. General Information

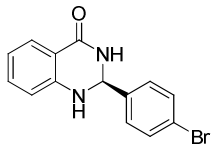
All reactions were carried out in oven-dried glassware with magnetic stirring under dry nitrogen atmosphere unless otherwise mentioned. All aldehydes were freshly distilled or dissolved in ethyl acetate, washed with saturated aqueous $NaHCO_3$ for three times, dried over Na_2SO_4, filtered through a pad of silica, concentrated, and subjected to high vacuum (<0.2 Torr) before use. Solvents were purified and dried according to standard methods prior to use. Powdered 3Å molecular sieves were activated at 200 °C for 2 h under vacuum (<0.2 Torr). Catalysts **1a-1j** were prepared according to the methods reported in the literature[1,2] and washed with 4 *N* HCl before use.[3]

^{1}H NMR spectra were recorded on 400 MHz spectrometer. The chemical shifts were reported relative to internal standard 2.5 in DMSO-d_6. The following abbreviations were used to describe peak patterns where appropriate: br=broad, s=singlet, d=doublet, t=triplet, q=quartet, m=multiplet. Coupling constants were reported in Hertz (Hz). ^{13}C NMR spectra were recorded on 100 MHz spectrometer, referred to the internal solvent signals (40.0 for DMSO-d_6). Infrared spectra were recorded on IR spectrometer. Optical rotations were determined using a Perkin Elmer Model 341 polarimeter at 20 °C. The enantiomeric excesses (ee) were determined by chiral HPLC analysis on Daicel Chiralpak AD-H, AS-H and Daicel Chiralcel OD-H. HRMS were obtained using EI ionization.

2. General Procedure for the Catalytic Asymmetric Synthesis of Dihydroquinazolinones

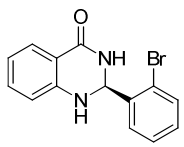
A mixture of 2-aminobenzamide **2** (0.05 mmol), aldehyde **3** (0.055 mmol), catalyst **1j** (0.005 mmol), 3Å molecular sieves (75 mg, powdered) in 1.0 mL $CHCl_3$ was stirred for 24 h at room temperature under a nitrogen atmosphere. After the reaction was completed, the mixture was directly purified by flash column chromatography (ethyl acetate / petroleum ether = 1/2) to afford the desired product **4**.

(*S*)-2-(4-bromophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4a)



White solid; m.p. 199-200°C; 98% yield; 88% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.2 mL/min, λ = 254 nm, t (major) = 12.541 min, t (minor) = 20.257 min]. $[\alpha]_D^{20}$ = +127.0° (c = 1.0, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.76 (s, 1 H), 6.66-6.70 (m, 1 H), 6.75 (d, *J* = 8.0 Hz, 1 H), 7.15 (s, 1 H), 7.23-7.27 (m, 1 H), 7.43-7.46 (m, 2 H), 7.58-7.62 (m, 3 H), 8.34 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 67.0, 114.9, 115.4, 117.6, 127.3, 127.8, 128.8, 128.9, 133.8, 142.1, 148.3, 164.1; IR (KBr, cm^{-1}) 3309, 3191, 3065, 2931, 1654, 1609, 1484, 1384, 1149, 1006, 789, 753, 664; HRMS (EI-TOF): calcd for $C_{14}H_{11}BrN_2O$ 302.0055, found 302.0046.

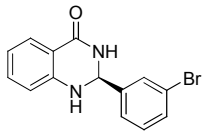
(*S*)-2-(2-bromophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4b)



White solid; m.p. 176-178°C; 99% yield; 98% ee, determined by HPLC [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm, t (major) = 15.479 min, t (minor) = 23.275 min]. $[\alpha]_D^{20}$ = +151.2° (c = 1.0, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.11 (s, 1 H), 6.71-6.75 (m, 1 H), 6.78 (d, *J* = 8.0 Hz, 1 H), 6.99 (s, 1 H), 7.25-7.30 (m, 1 H), 7.32-7.36 (m, 1 H), 7.43-7.47 (m, 1 H), 7.65-7.70 (m, 3 H), 8.20 (s, 1 H); ^{13}C NMR (100

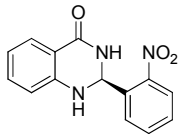
MHz, DMSO-d_6) δ 66.9, 115.1, 115.2, 118.0, 122.7, 127.8, 128.5, 129.6, 131.2, 133.3, 133.9, 139.6, 148.2, 164.1; IR (KBr, cm^{-1}) 3365, 3190, 3062, 2923, 1651, 1613, 1503, 1394, 1253, 1182, 1120, 746, 545; HRMS (EI-TOF): calcd for $C_{14}H_{11}BrN_2O$ 302.0055, found 302.0062.

(*S*)-2-(3-bromophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4c)



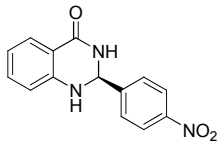
White solid; m.p. 183-184°C; 98% yield; 87% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 85 / 15, 1.0 mL/min, λ = 254 nm, t (major) = 25.098 min, t (minor) = 30.998 min]. $[\alpha]_D^{20}$ = +127.0° (c = 0.77, THF); **This sample showed identical optical rotation to that of the previously reported synthesis, allowing us to assign the absolute stereochemistry as *S*.**[4] ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.77 (s, 1 H), 6.67-6.71 (m, 1 H), 6.75-6.78 (m, 1 H), 7.22-7.28 (m, 2 H), 7.35 (t, *J* = 8.0 Hz, 1 H), 7.49 (d, *J* = 8.0 Hz, 1 H), 7.54 (d, *J* = 8.0 Hz, 1 H), 7.60-7.63 (m, 1 H), 7.67 (s, 1 H), 8.41 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 65.9, 115.0, 115.4, 117.9, 122.1, 126.3, 127.9, 130.2, 131.1, 131.7, 134.0, 145.1, 147.9, 163.9; IR (KBr, cm^{-1}) 3289, 3196, 3065, 1647, 1614, 1514, 1442, 1386, 1299, 1156, 819, 757, 698; HRMS (EI-TOF): calcd for $C_{14}H_{11}BrN_2O$ 302.0055, found 302.0060.

(*S*)-2-(2-nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4d)



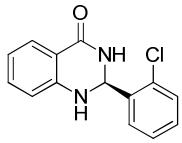
Yellow solid; m.p. 192-193°C; 99% yield; 95% ee, determined by HPLC [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.7 mL/min, λ = 254 nm, t (minor) = 26.489 min, t (major) = 40.962 min]. $[\alpha]_D^{20}$ = +195.2° (c = 0.75, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.34 (s, 1H), 6.72 (t, *J* = 8.0 Hz, 1 H), 6.77 (d, *J* = 8.0 Hz, 1 H), 7.01 (s, 1 H), 7.24-7.28 (m, 1 H), 7.61-7.67 (m, 2 H), 7.77-7.81 (m, 1 H), 7.86 (dd, J_1 =8.0 Hz, J_2 = 1.2 Hz, 1 H), 8.07 (dd, J_1 =8.4 Hz, J_2 = 1.2 Hz, 1 H), 8.22 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 62.6, 115.0, 115.4, 118.1, 125.2, 127.8, 129.4, 130.3, 134.0, 134.4, 136.4, 147.6, 148.1, 163.8; IR (KBr, cm^{-1}) 3422, 3188, 3061, 2934, 1670, 1612, 1514, 1342, 1152, 855, 742, 697; HRMS (EI-TOF): calcd for $C_{14}H_{11}N_3O_3$ 269.0800, found 269.0802.

(*S*)-2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4e)



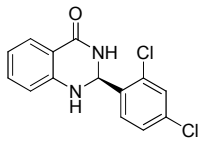
Yellow solid; m.p. 199-200°C; 97% yield; 80% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.2 mL/min, λ = 254 nm, t (major) = 18.716 min, t (minor) = 35.274 min]. $[\alpha]_D^{20}$ = +123.5° (c = 0.72, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.92 (s, 1 H), 6.69 (t, *J* = 7.2 Hz, 1 H), 6.77 (d, *J* = 8.0 Hz, 1 H), 7.26 (t, *J* = 7.6 Hz, 1 H), 7.34 (s, 1 H), 7.61 (d, *J* = 7.6 Hz, 1 H), 7.75 (d, *J* = 7.6 Hz, 2 H), 8.26 (d, *J* = 8.0 Hz, 2 H), 8.54 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 65.8, 115.0, 115.4, 117.9, 124.1, 127.9, 128.5, 134.0, 147.7, 147.9, 149.8, 163.8; IR (KBr, cm^{-1}) 3283, 3156, 3037, 2924, 1646, 1610, 1520, 1485, 1389, 1348, 1157, 855, 750, 694; HRMS (EI-TOF): calcd for $C_{14}H_{11}N_3O_3$ 269.0800, found 269.0799.

(*S*)-2-(2-chlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4f)



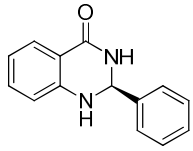
White solid; m.p. 208-210°C; 99% yield; 98% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm, t (major) = 13.066 min, t (minor) = 16.992 min]. $[\alpha]_D^{20}$ = +172.6° (c = 0.82, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.15 (s, 1 H), 6.67-6.74 (m, 1 H), 6.77 (d, *J* = 8.0 Hz, 1 H),7.02 (s, 1 H), 7.24-7.28 (m, 1 H), 7.38-7.42 (m, 2 H), 7.48-7.51 (m, 1 H), 7.66-7.69 (m, 2 H), 8.22 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 64.2, 115.0, 115.2, 117.9, 127.8, 127.9, 129.2, 130.1, 130.8, 132.3, 133.9, 138.4, 148.1, 164.1; IR (KBr, cm^{-1}) 3361, 3197, 3065, 1647, 1614, 1502, 1390, 1256, 1188, 1051, 739, 539; HRMS (EI-TOF): calcd for $C_{14}H_{11}ClN_2O$ 258.0560, found 258.0567.

(*S*)-2-(2,4-dichlorophenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4g)



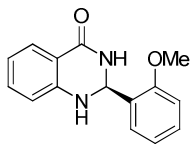
White solid; m.p. 162-164°C; 98% yield; 96% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm, t (major) = 12.169 min, t (minor) = 18.463 min]. $[\alpha]_D^{20}$ = +157.1° (c = 0.68, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.12 (s, 1 H), 6.71-6.77 (m, 2 H), 7.03 (s, 1 H), 7.25-7.29 (m, 1 H), 7.50 (dd, J_1 =8.4 Hz, J_2 = 2.0 Hz, 1 H), 7.64-7.67 (m, 3 H), 8.23 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 63.8, 115.07, 115.12, 118.1, 127.9, 128.1, 129.4, 130.6, 133.4, 134.0, 134.4, 137.4, 148.0, 164.0; IR (KBr, cm^{-1}) 3339, 3189, 1660, 1611, 1484, 1377, 1292, 1099, 1051, 776, 758; HRMS (EI-TOF): calcd for $C_{14}H_{10}Cl_2N_2O$ 292.0170, found 292.0163.

(*S*)-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (4h)



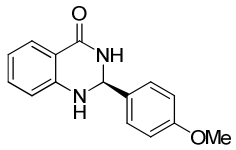
White solid; m.p. 227-229°C; 99% yield; 90% ee, determined by HPLC [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm, t (major) = 11.697 min, t (minor) = 14.652 min]. $[\alpha]_D^{20}$ = +181.5° (c = 0.72, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.76 (s, 1H), 6.68 (t, *J* = 7.6 Hz, 1 H), 6.76 (d, *J* = 8.4 Hz, 1 H), 7.11 (s, 1 H), 7.25 (t, *J* = 7.6 Hz, 1 H), 7.33-7.41 (m, 3 H), 7.49-7.51 (m, 2 H), 7.62 (d, *J* = 7.6 Hz, 1 H), 8.29 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 67.0, 114.9, 115.4, 117.6, 127.3, 127.8, 128.8, 128.9, 133.8, 142.1, 148.3, 164.1; IR (KBr, cm^{-1}) 3303, 3187, 3064, 1654, 1615, 1511, 1391, 1300, 1149, 813, 748, 699; HRMS (EI-TOF): calcd for $C_{14}H_{12}N_2O$ 224.0950, found 224.0948.

(*S*)-2-(2-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4i)



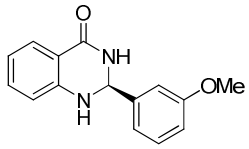
White solid; m.p. 152-154°C; 99% yield; 94% ee, determined by HPLC [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.7 mL/min, λ = 254 nm, t (minor) = 17.423 min, t (major) = 35.927 min]. $[\alpha]_D^{20}$ = +127.9° (c = 0.72, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.83 (s, 3 H), 6.02 (s, 1 H), 6.64-6.68 (m, 1 H), 6.75-6.78 (m, 2 H), 6.95 (t, *J* = 7.6 Hz, 1 H), 7.05 (d, *J* = 7.6 Hz, 1 H), 7.20-7.24 (m, 1 H), 7.30-7.34 (m, 1 H), 7.40 (dd, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1 H), 7.62 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1 H), 8.00 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 56.0, 61.4, 111.6, 114.9, 115.2, 117.5, 120.6, 127.3, 127.8, 129.4, 130.1, 133.7, 148.4, 156.8, 164.3; IR (KBr, cm^{-1}) 3389, 3317, 3191, 3050, 2933, 1662, 1610, 1487, 1387, 1240, 1111, 1026, 752, 649; HRMS (EI-TOF): calcd for $C_{15}H_{14}N_2O_2$ 254.1055, found 254.1051.

(*S*)-2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4j)



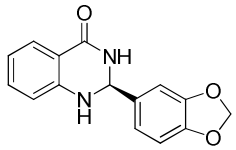
White solid; m.p. 190-192°C; 89% yield; 89% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.2 mL/min, λ = 254 nm, t (major) = 17.657 min, t (minor) = 23.454 min]. $[\alpha]_D^{20}$ = +157.9° (c = 0.70, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.75 (s, 3 H), 5.71 (s, 1 H), 6.67 (t, *J* = 7.2 Hz, 1 H), 6.74 (d, *J* = 8.0 Hz, 1 H), 6.95 (d, *J* = 7.6 Hz, 2 H), 7.02 (s, 1 H), 7.24 (t, *J* = 7.6 Hz, 1 H), 7.42 (d, *J* = 7.6 Hz, 2 H), 7.62 (d, *J* = 7.6 Hz, 1 H), 8.20 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.7, 66.8, 114.1, 114.9, 115.5, 117.6, 127.8, 128.7, 133.7, 133.9, 148.5, 159.9, 164.2; IR (KBr, cm^{-1}) 3298, 3184, 2833, 1653, 1612, 1508, 1389, 1305, 1255, 1174, 1032, 804, 758; HRMS (EI-TOF): calcd for $C_{15}H_{14}N_2O_2$ 254.1055, found 254.1054.

(*S*)-2-(3-methoxyphenyl)-2,3-dihydroquinazolin-4(1*H*)-one (4k)



White solid; m.p. 145-147°C; 95% yield; 93% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm, t (major) = 21.969 min, t (minor) = 28.897 min]. $[\alpha]_D^{20}$ = +169.7° (c = 0.68, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.74 (s, 3 H), 5.72 (s, 1 H), 6.67 (t, *J* = 7.2 Hz, 1 H), 6.76 (d, *J* = 8.0 Hz, 1 H), 6.91 (dd, J_1 = 8.0 Hz, J_2 = 2.4 Hz, 1 H), 7.05-7.06 (m, 2 H), 7.12 (s, 1 H), 7.22-7.32 (m, 2 H), 7.61 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1 H), 8.29 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.6, 66.7, 113.0, 114.1, 114.9, 115.4, 117.6, 119.4, 127.8, 129.9, 133.8, 143.8, 148.3, 159.7, 164.0; IR (KBr, cm^{-1}) 3293, 3184, 2830, 1651, 1615, 1486, 1389, 1259, 1154, 1033, 887, 757, 700; HRMS (EI-TOF): calcd for $C_{15}H_{14}N_2O_2$ 254.1055, found 254.1050.

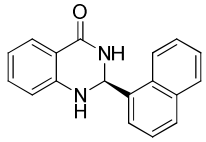
(*S*)-2-(benzo[*d*][1,3]dioxol-5-yl)-2,3-dihydroquinazolin-4(1*H*)-one (4l)



White solid; m.p. 200-201°C; 95% yield; 87% ee, determined by HPLC [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.7 mL/min, λ = 254 nm, t (minor) = 33.820 min, t (major) = 43.737 min]. $[\alpha]_D^{20}$ = +159.6° (c = 0.75, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.68 (s, 1 H), 6.01 (s, 2 H), 6.67 (t, *J* = 6.8 Hz, 1 H), 6.75 (d, *J* =

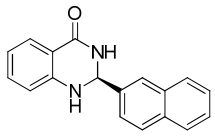
8.0 Hz, 1 H), 6.90 (d, *J* = 6.8 Hz, 1 H), 6.95 (d, *J* = 7.6 Hz, 1 H), 7.04 (s, 2 H), 7.24 (t, *J* = 7.2 Hz, 1 H), 7.61 (d, *J* = 7.2 Hz, 1 H), 8.22 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 66.8, 101.6, 107.6, 108.3, 114.9, 115.4, 117.6, 120.9, 127.8, 133.8, 136.0, 147.7, 147.8, 148.3, 164.1; IR (KBr, cm^{-1}) 3283, 3187, 3052, 2903, 1654, 1611, 1485, 1446, 1382, 1248, 1036, 930, 755, 679; HRMS (EI-TOF): calcd for $C_{15}H_{12}N_2O_3$ 268.0848, found 268.0847.

(*S*)-2-(naphthalen-1-yl)-2,3-dihydroquinazolin-4(1*H*)-one (4m)



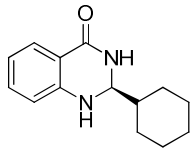
White solid; m.p. 169-171°C; 99% yield; 97% ee, determined by HPLC [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 60 / 40, 0.7 mL/min, λ = 254 nm, t (minor) = 26.200 min, t (major) = 35.487 min]. $[\alpha]_D^{20}$ = +198.8° (c = 0.52, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.51 (s, 1 H), 6.72-6.79 (m, 2 H), 7.10 (s, 1 H), 7.25-7.30 (m, 1 H), 7.52-7.61 (m, 3 H), 7.71-7.74 (m, 2 H), 7.97-8.01 (m, 2 H), 8.29 (s, 1 H), 8.56-8.58 (m, 1 H)**;** ^{13}C NMR (100 MHz, DMSO-d_6) δ 66.4, 115.0, 115.5, 117.7, 125.0, 125.7, 126.3, 126.5, 128.0, 129.1, 129.8, 131.0, 133.7, 134.2, 135.7, 148.9, 164.5; IR (KBr, cm^{-1}) 3384, 3310, 3060, 1655, 1611, 1501, 1484, 1374, 1158, 779, 757, 640; HRMS (EI-TOF): calcd for $C_{18}H_{14}N_2O$ 274.1106, found 274.1110.

(*S*)-2-(naphthalen-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one (4n)



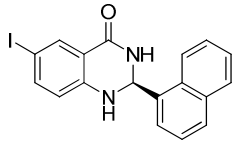
White solid; m.p. 220-222°C; 89% yield; 89% ee, determined by HPLC [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 80 / 20, 0.7 mL/min, λ = 254 nm, t (major) = 28.714 min, t (minor) = 33.105 min]. $[\alpha]_D^{20}$ = +139.5° (c = 0.61, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 5.96 (s, 1 H), 6.68-6.72 (m, 1 H), 6.79 (d, *J* = 7.6 Hz, 1 H), 7.26 (ddd, *J* = 8.6, 7.4, 1.6 Hz, 1 H), 7.20 (s, 1 H), 7.52-7.55 (m, 2 H), 7.66 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1 H), 7.71 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1 H), 7.91-7.97 (m, 4 H), 8.40 (s, 1 H)**;** ^{13}C NMR (100 MHz, DMSO-d_6) δ 67.3, 114.9, 115.4, 117.7, 125.3, 126.3, 126.85, 126.90, 127.9, 128.1, 128.4, 128.6, 130.0, 133.5, 133.8, 139.3, 148.4, 164.1; IR (KBr, cm^{-1}) 3282, 3188, 3053, 1649, 1611, 1513, 1388, 1298, 1158, 825, 745, 688; HRMS (EI-TOF): calcd for $C_{18}H_{14}N_2O$ 274.1106, found 274.1105.

(*S*)-2-cyclohexyl-2,3-dihydroquinazolin-4(1*H*)-one (4o)



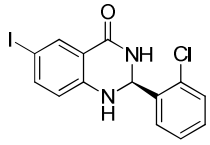
White solid; m.p. 177-179°C; 98% yield; 84% ee, determined by HPLC [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.6 mL/min, λ = 254 nm, t (major) = 11.475 min, t (minor) = 17.255 min]. $[\alpha]_D^{20}$ = +85.8° (c = 0.72, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ 1.12 (s, 5 H), 1.54-1.70 (m, 6 H), 4.44 (s, 1 H), 6.57 (s, 1 H), 6.62 (t, *J* = 7.3 Hz, 1 H), 6.74 (d, *J* = 8.0 Hz, 1 H), 7.17-7.21 (m, 1 H), 7.55 (d, *J* = 7.6 Hz, 1 H), 7.89 (s, 1 H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 26.0, 26.1, 26.4, 27.2, 27.5, 43.3, 69.0, 114.6, 115.3, 116.9, 127.7, 133.5, 148.8, 164.2; IR (KBr, cm^{-1}) 3366, 3173, 3056, 2923, 2851, 1644, 1611, 1505, 1485, 1390, 1313, 1146, 1030, 810, 752; HRMS (EI-TOF): calcd for $C_{14}H_{18}N_2O$ 230.1419, found 230.1425.

(*S*)-6-iodo-2-(naphthalen-1-yl)-2,3-dihydroquinazolin-4(1*H*)-one (4p)



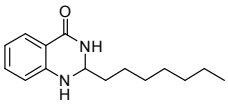
White solid; m.p. 203-206°C; 88% yield; 93% ee, determined by HPLC [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 70 / 30, 0.8 mL/min, λ = 254 nm, t (minor) = 9.232 min, t (major) = 13.246 min]. $[\alpha]_D^{20}$ = +87.9° (c = 1.5, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 8.50 (d, *J* = 8.7 Hz, 1 H), 8.43 (s, 1 H), 7.99 (t, *J* = 7.8 Hz, 2 H), 7.92 (s, 1 H), 7.69 (d, *J* = 7.0 Hz, 1 H), 7.56 (ddd, *J* = 16.9, 10.6, 5.2 Hz, 4 H), 7.33 (s, 1 H), 6.61 (d, *J* = 8.5 Hz, 1 H), 6.52 (s, 1 H). ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 163.11, 148.21, 141.64, 135.99, 135.37, 134.23, 130.88, 129.95, 12 9.10, 126.87, 126.22, 125.69, 124.90, 117.61, 78.53, 66.04; IR (KBr, cm^{-1}) 3421, 3172, 3047, 1673, 1598, 1509, 1435, 1307, 1158, 777; HRMS (EI-TOF): calcd for $C_{18}H_{13}IN_2O$ 400.0073, found 400.0073.

(*S*)-2-(2-chlorophenyl)-6-iodo-2,3-dihydroquinazolin-4(1*H*)-one (4q)



White solid; m.p. 164-166°C; 88% yield; 94% ee, determined by HPLC [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 70 / 30, 0.8 mL/min, λ = 254 nm, t (major) = 8.705 min, t (minor) = 11.937 min]. $[\alpha]_D^{20}$ = +150.0° (c = 1.5, THF); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 8.35 (s, 1H), 7.87 (d, *J* = 2.0 Hz, 1 H), 7.62 (dd, *J* = 5.8, 3.6 Hz, 1 H), 7.51 (ddd, *J* = 6.3, 5.8, 2.5 Hz, 2 H), 7.41 (dd, *J* = 5.9, 3.5 Hz, 2 H), 7.26 (s, 1 H), 6.61 (d, *J* = 8.6 Hz, 1 H), 6.16 (s, 1 H). ^{13}C NMR (100 MHz, DMSO) δ (ppm) 162.66, 147.44, 141.82, 138.14, 135.83, 132.24, 130.90, 130.14, 129.16, 128.05, 117.69, 117.18, 78.77, 64.04.; ^{13}C NMR (100 MHz, DMSO-d_6) δ 64.2, 78.9, 117.3, 117.9, 128.2, 129.2, 130.4, 131.1, 132.4, 136.0, 138.3, 142.1, 147.5, 163.0; IR (KBr, cm^{-1}) 3277, 3039, 2920, 1652, 1604, 1474, 1313, 1164, 1051, 813, 748; HRMS (EI-TOF): calcd for $C_{14}H_{10}ClIN_2O$ 383.9526, found 383.9513.

(*S*)-2-heptyl-2,3-dihydroquinazolin-4(1H)-one (4r)



Yellow solid; m.p. 153-155°C; 89% yield; 59% *ee*, determined by HPLC [Daicel Chiralcel AS-H, *n*-hexane / *i*-propanol = 70 / 30, 0.8 mL/min, λ = 254 nm, t (major) = 6.99min, t (minor) = 8.41 min]. $[\alpha]_D^{20}$ = -28.0° (c = 0.92, $CHCl_3$); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 8.03-7.80 (s, 1 H), 7.68-7.46 (s, 1 H), 7.31-7.00 (s, 1 H), 6.88-6.57 (m, 2 H), 4.90-4.50 (t, 1 H), 1.81-1.52 (m, 2 H), 1.49-1.34 (m, 2 H), 1.26 (m, 8 H), 0.86 (t, 3 H);^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 164.40, 148.99, 133.48, 127.81, 117.32, 115.50, 114.83, 64.91,, 35.50, 31.67, 29.39, 29.14, 23.71, 22.57, 14.43; IR (KBr) γ, 3323, 2949, 12924, 2852, 1645, 1611, 772, 748 cm^{-1}; HRMS (EI-TOF): calcd for $C_{15}H_{22}N_2O$ 246.1732, found 3246.1738.

3. References

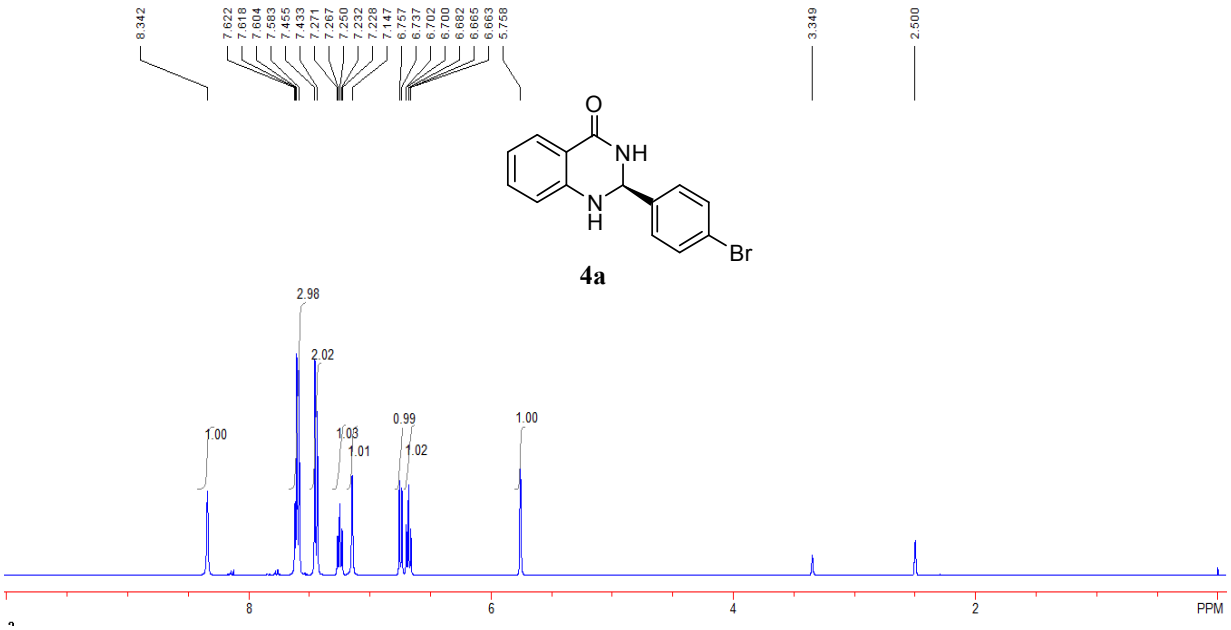
(1) Xu, F. X.; Huang, D.; Han, C.; Shen, W.; Lin, X. F.; Wang, Y. G. *J. Org. Chem.* **2010**, *75*, 8677-8680.

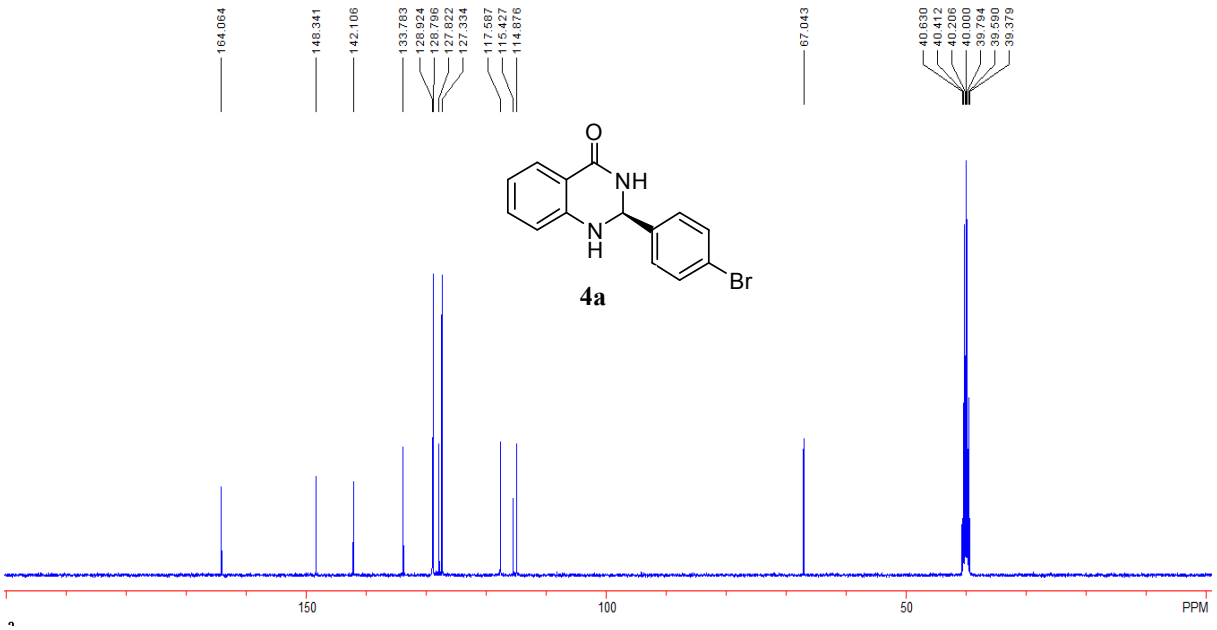
(2) Müller, S.; Webber, M. J.; List. B. *J. Am. Chem. Soc.* **2011**, *133*, 18534-18537.

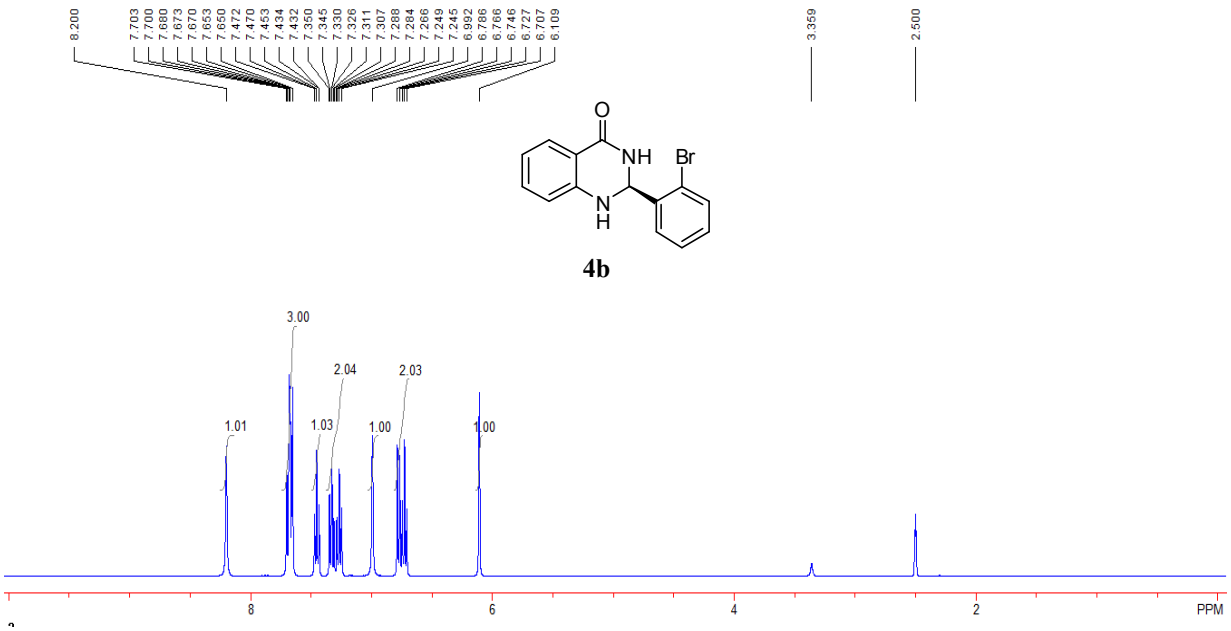
(3) Čorić, I.; Müller, S.; List, B. *J. Am. Chem. Soc.* **2010**, *132*, 17370-17373.

(4) Rueping, M.; Antonchick, A. P.; Sugiono, E.; Grenader, K. *Angew. Chem.*, *Int. Ed.* **2009**, *48*, 908-910.

5. NMR spectra for all compounds



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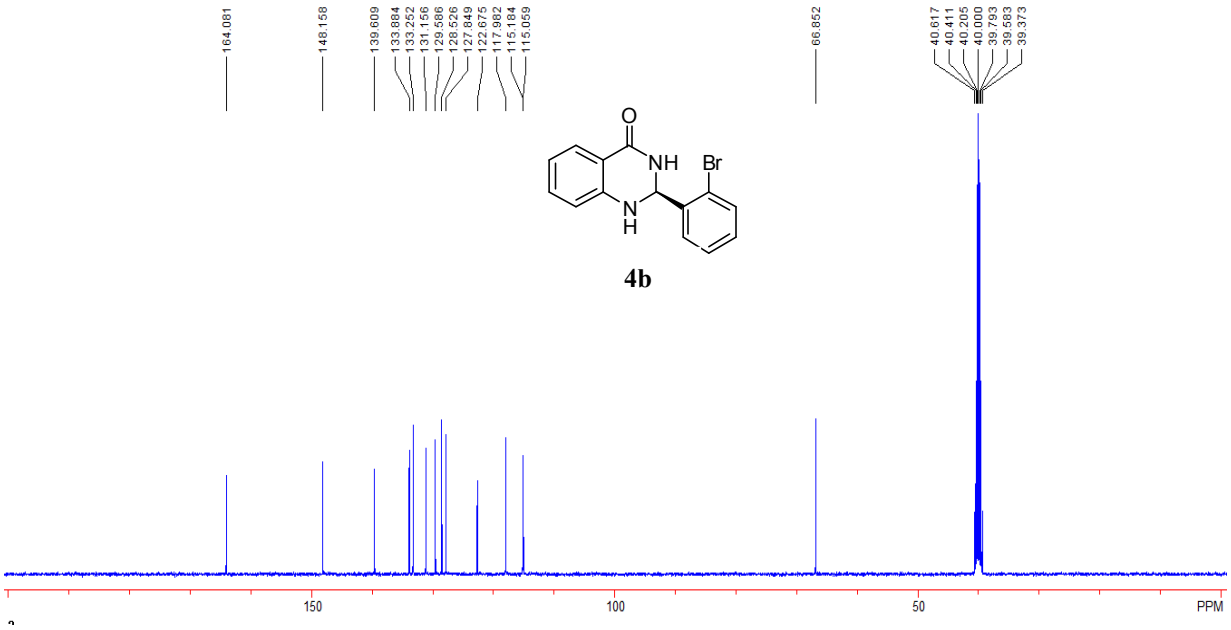
4b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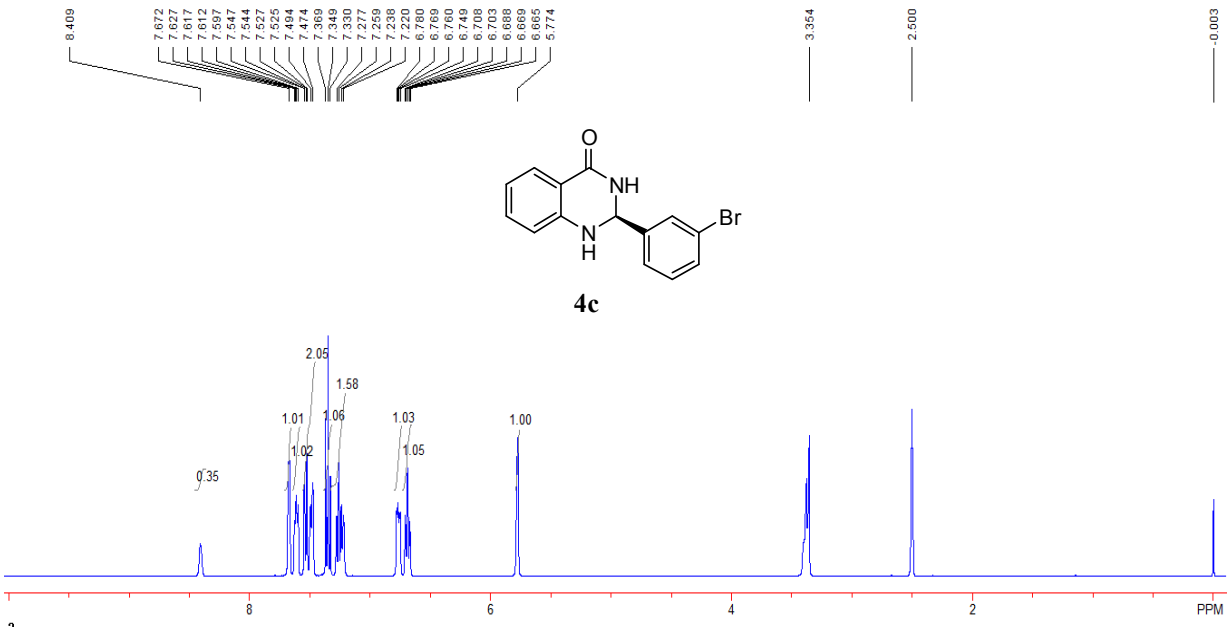
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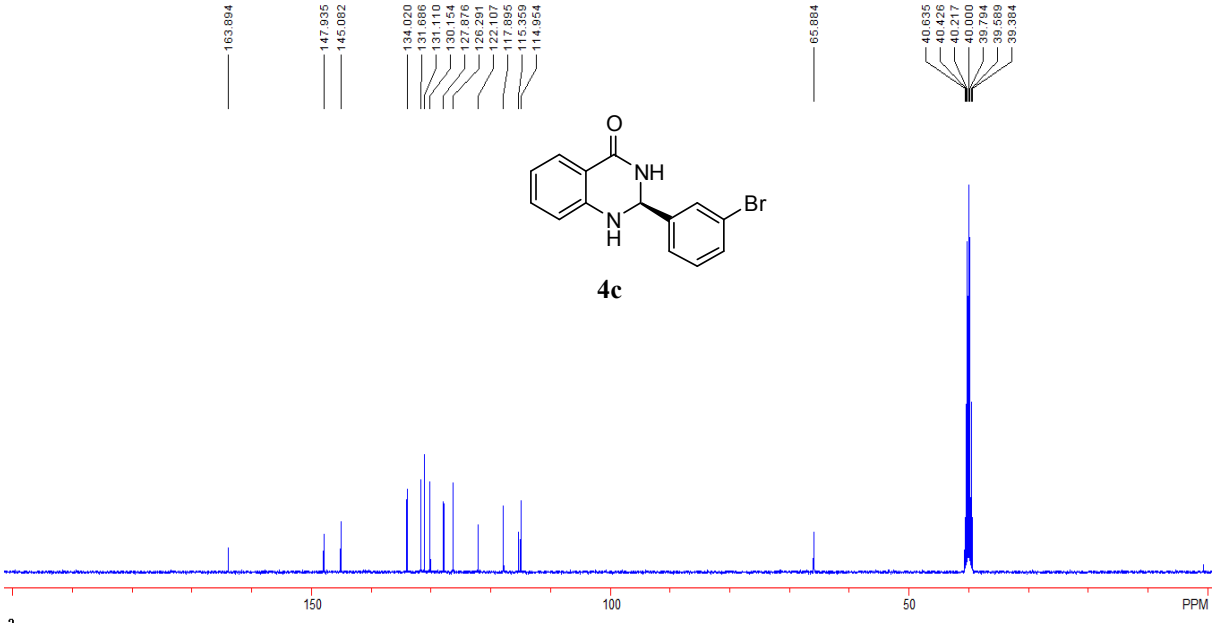
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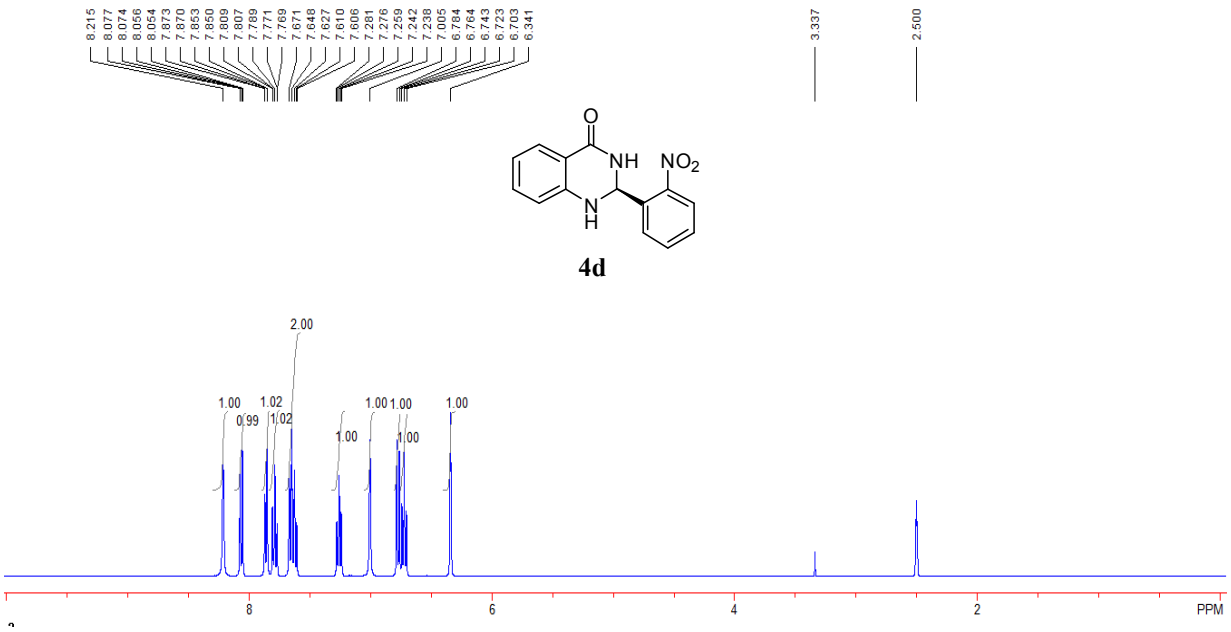
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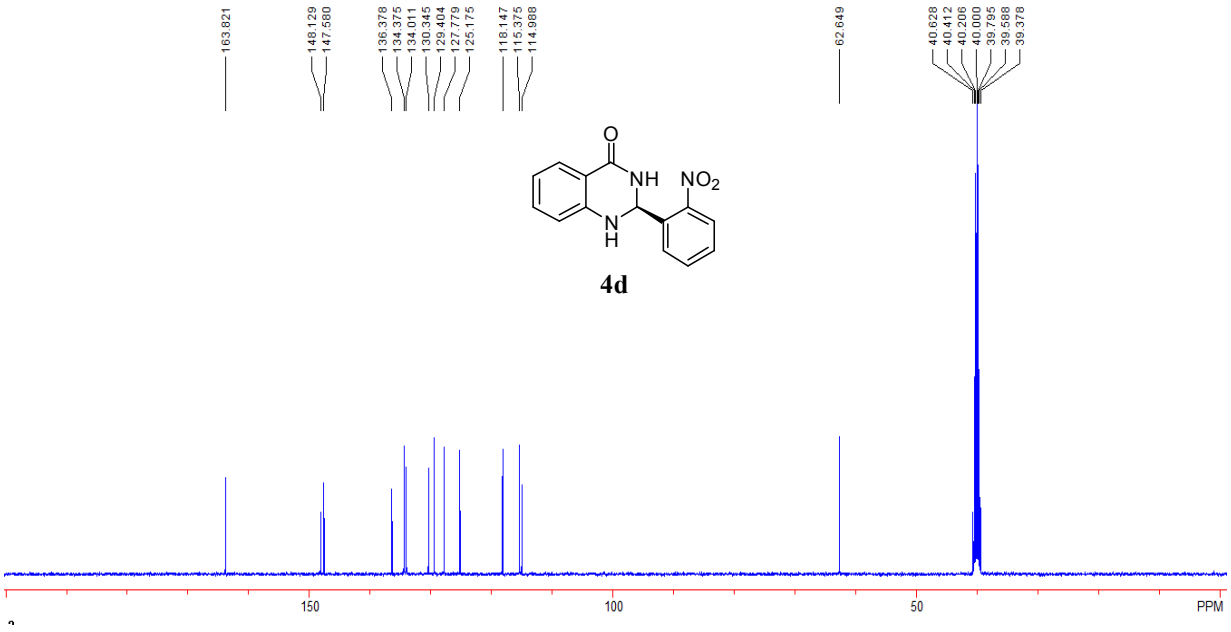
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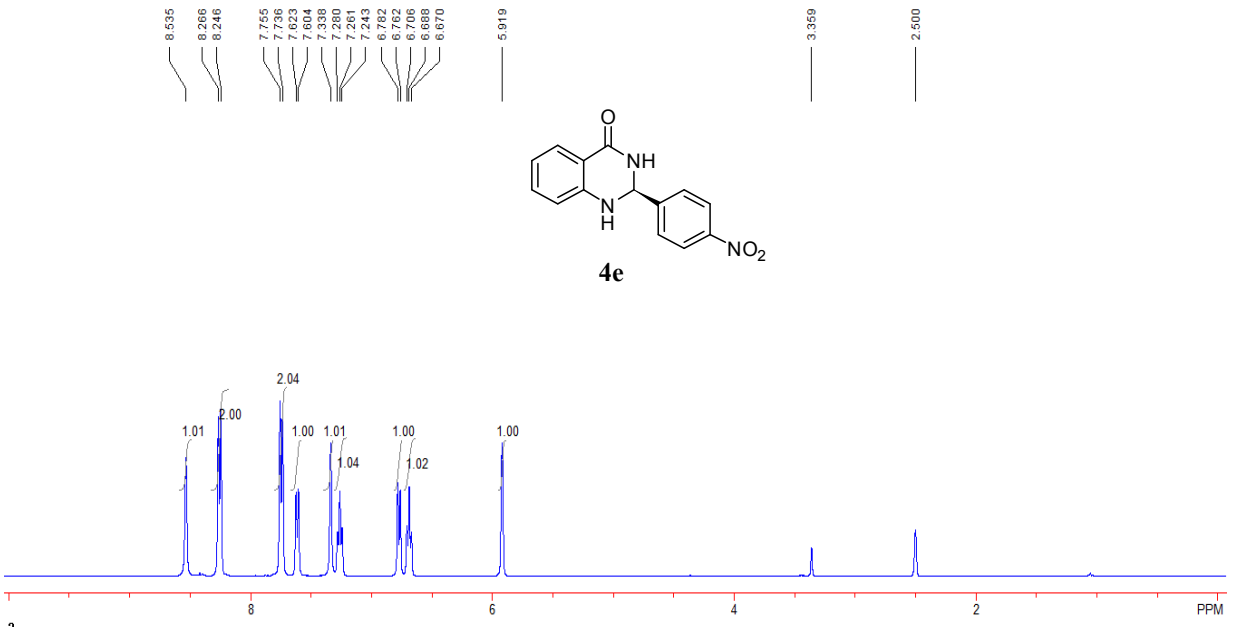
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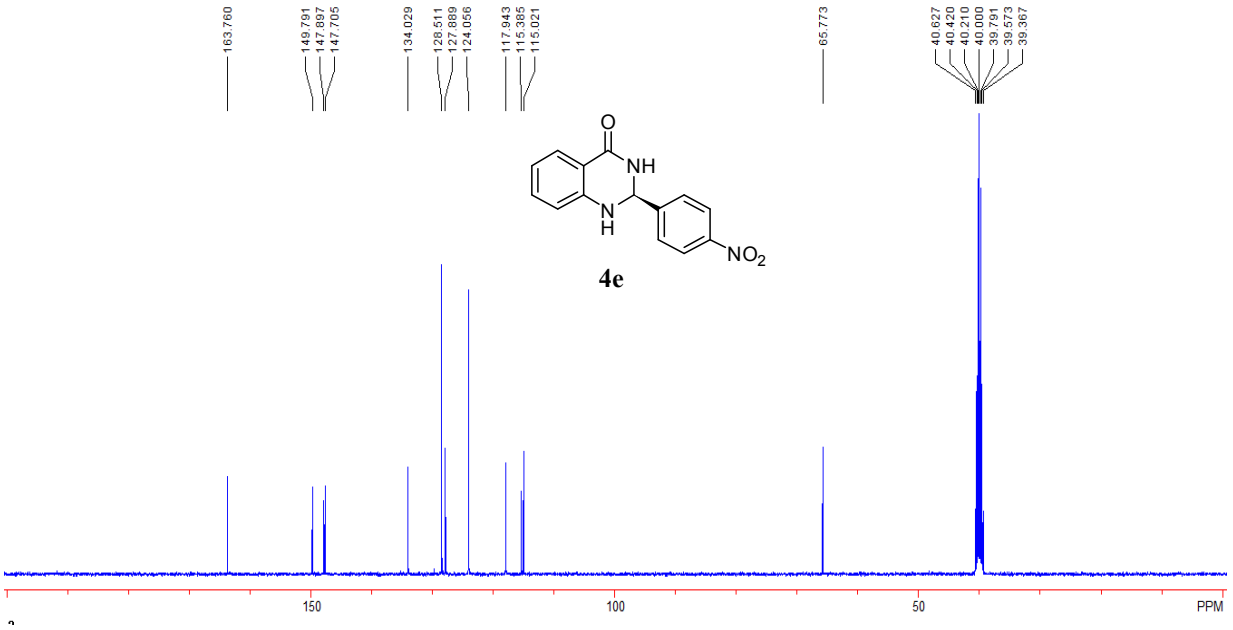
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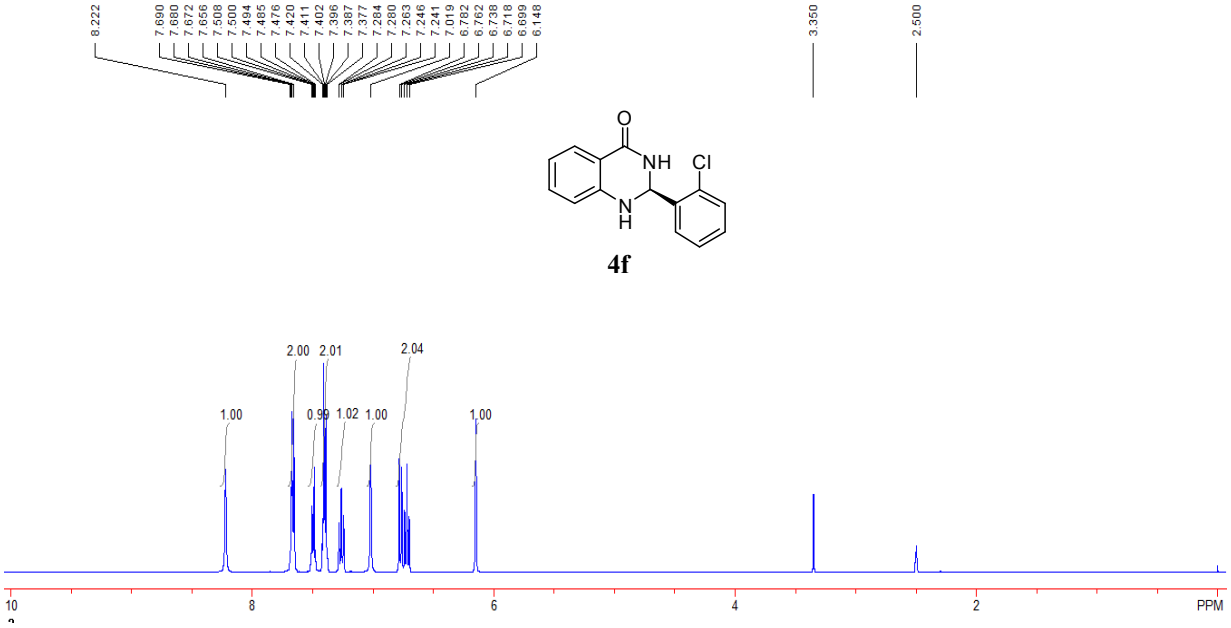
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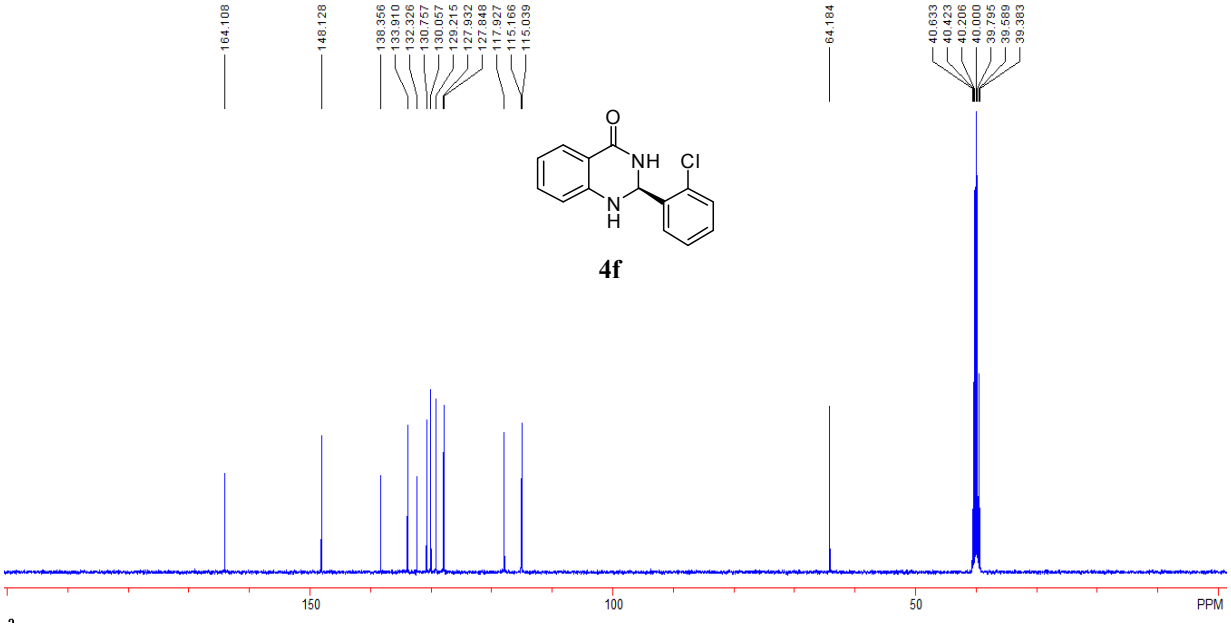
4f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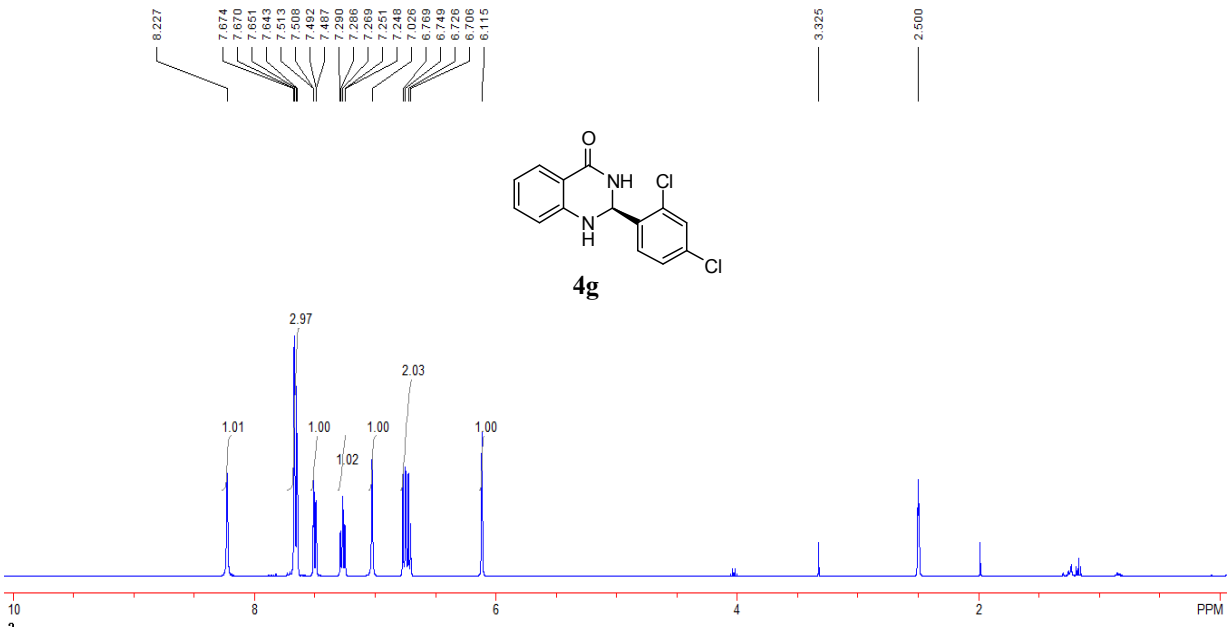
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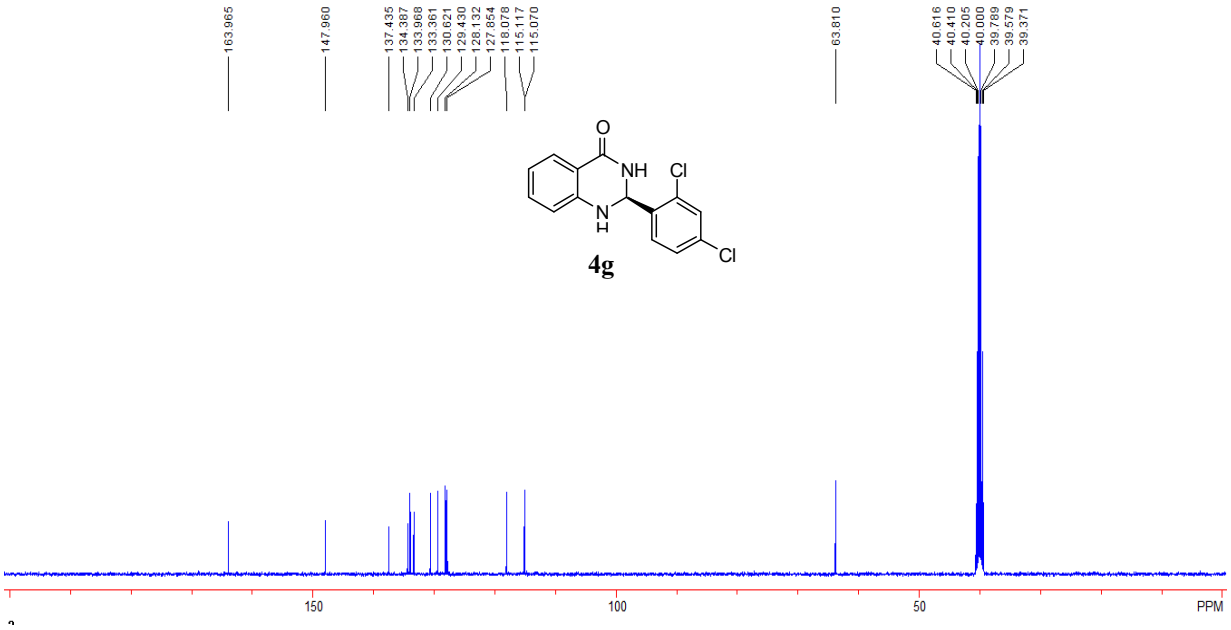
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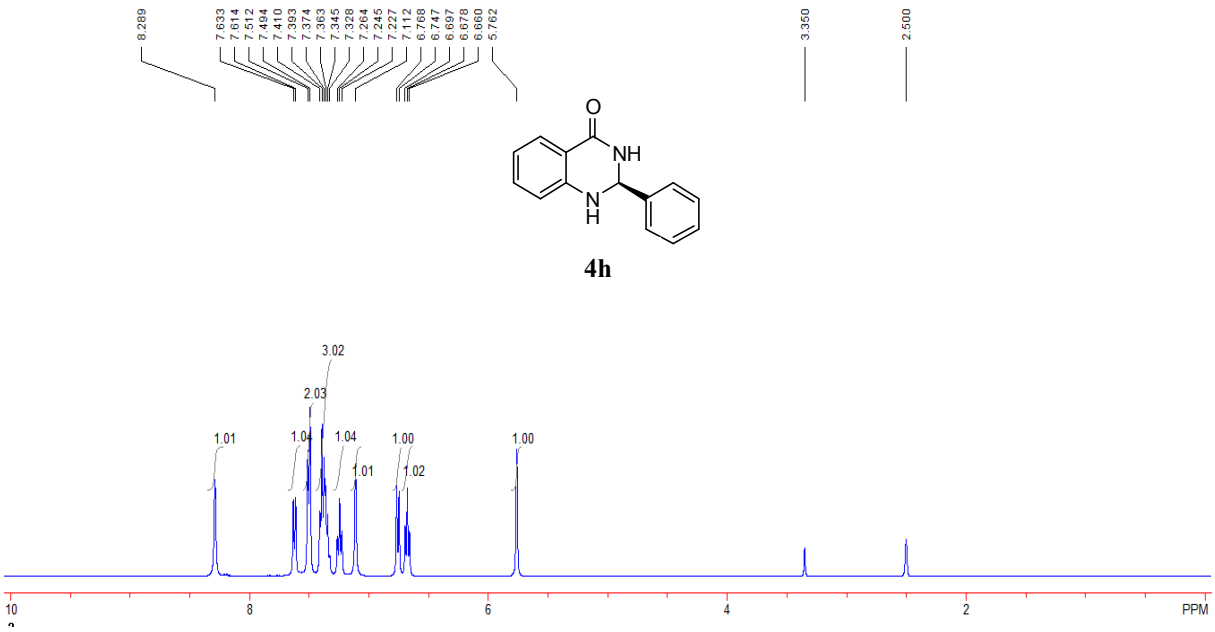
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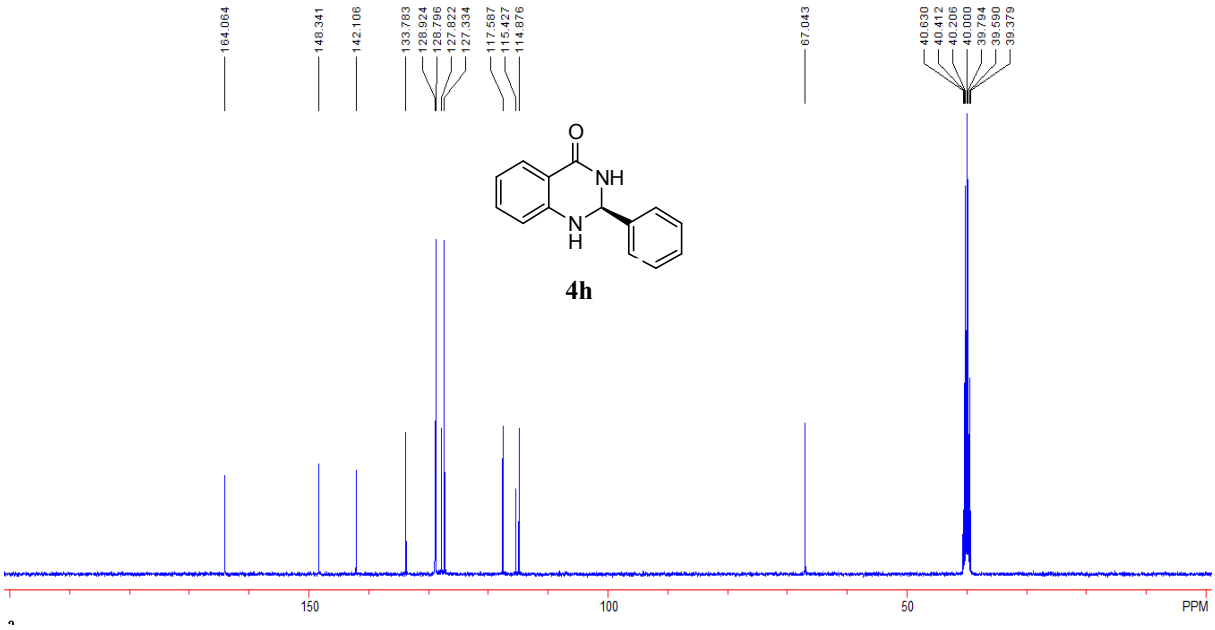
4h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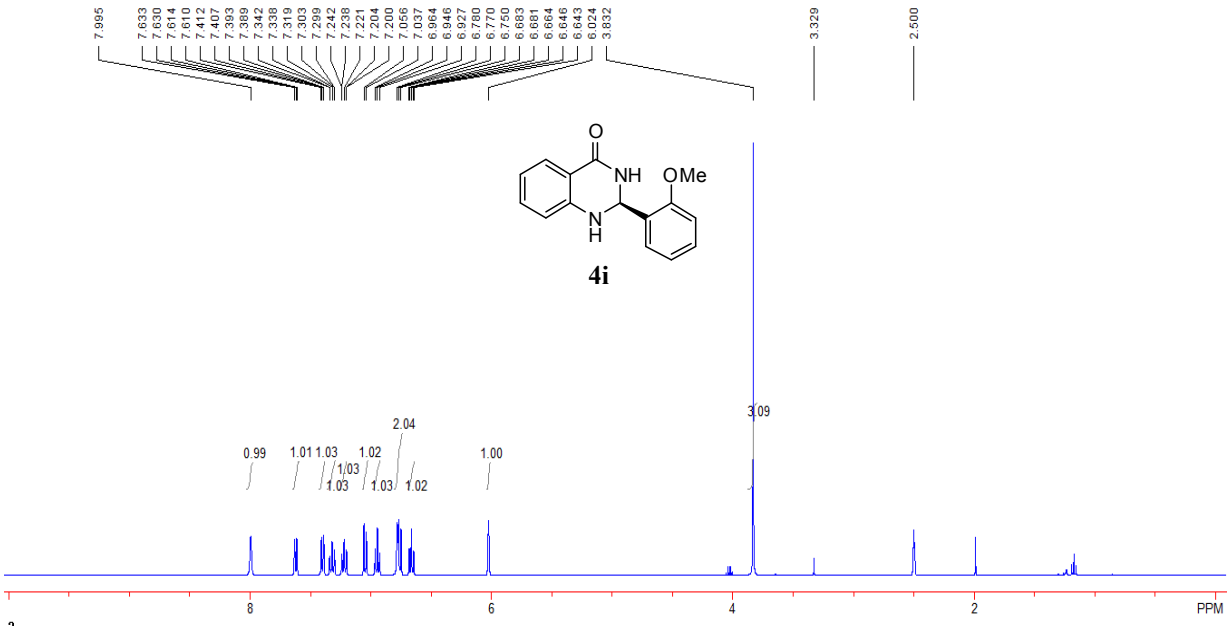
PPM

4h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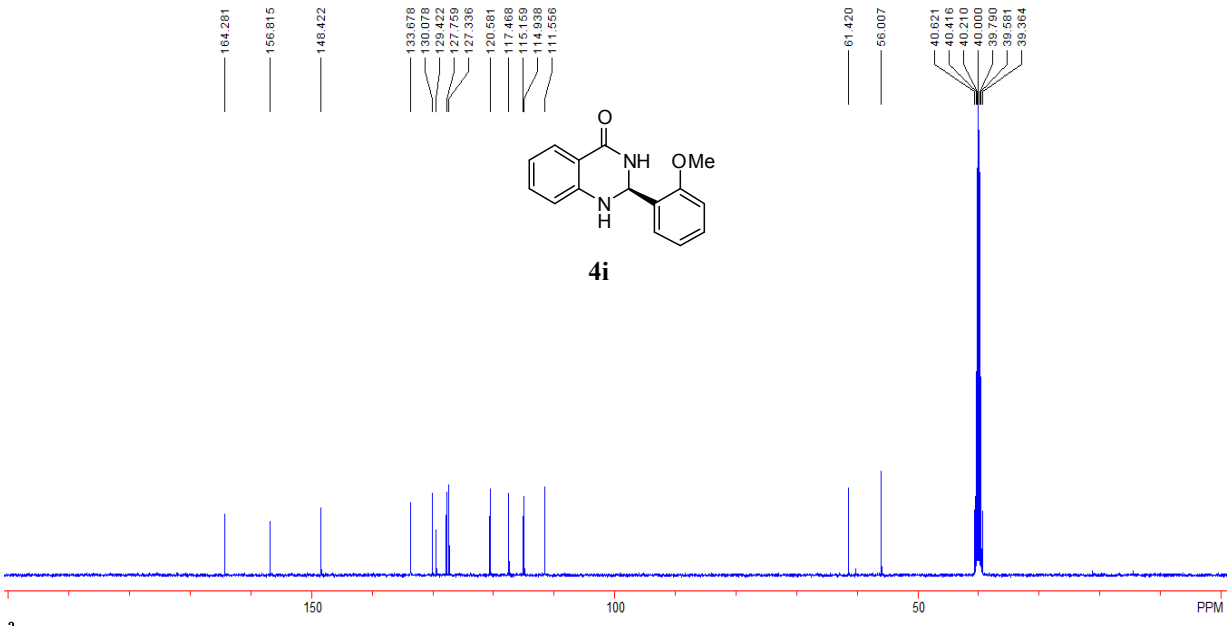
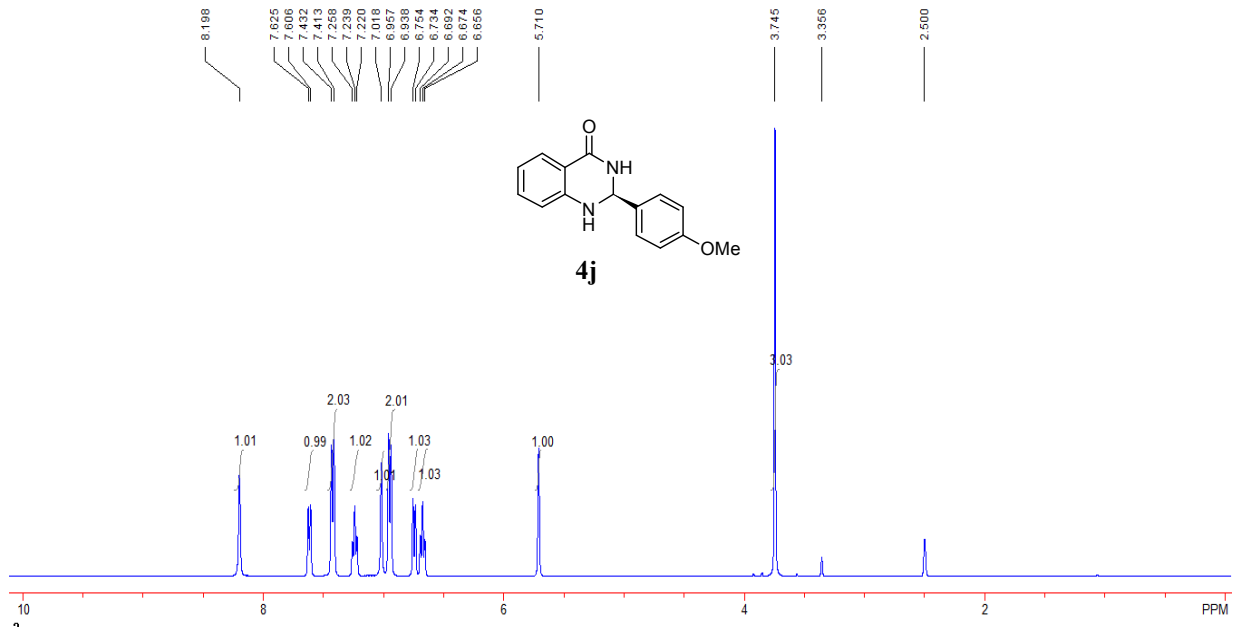
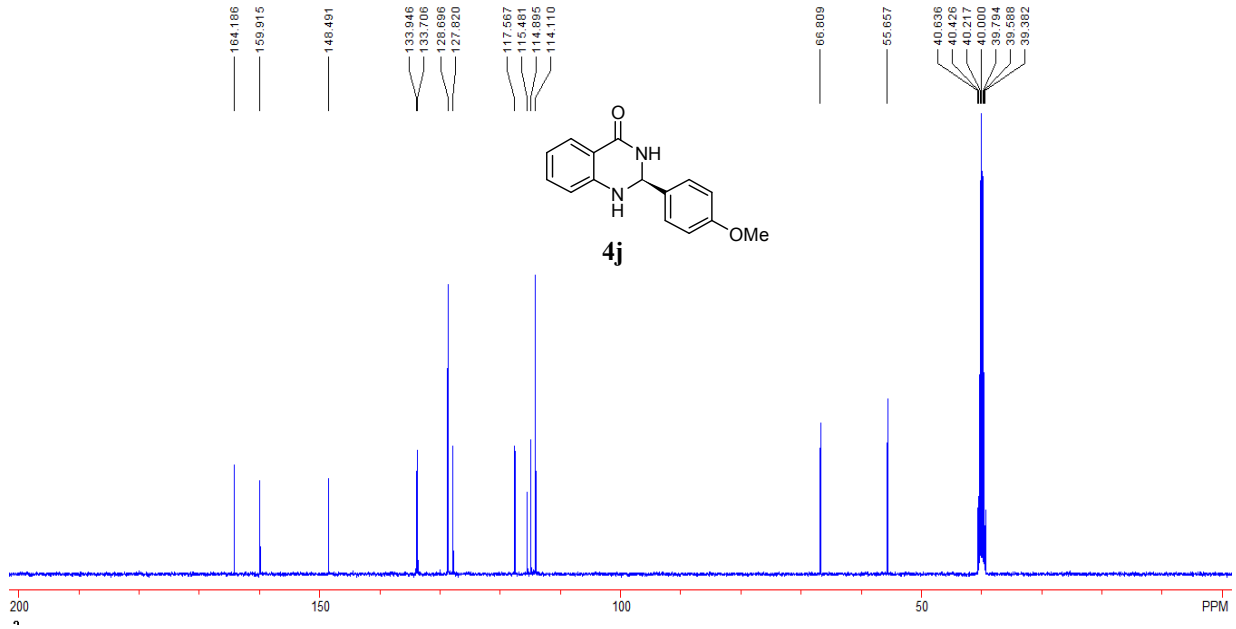
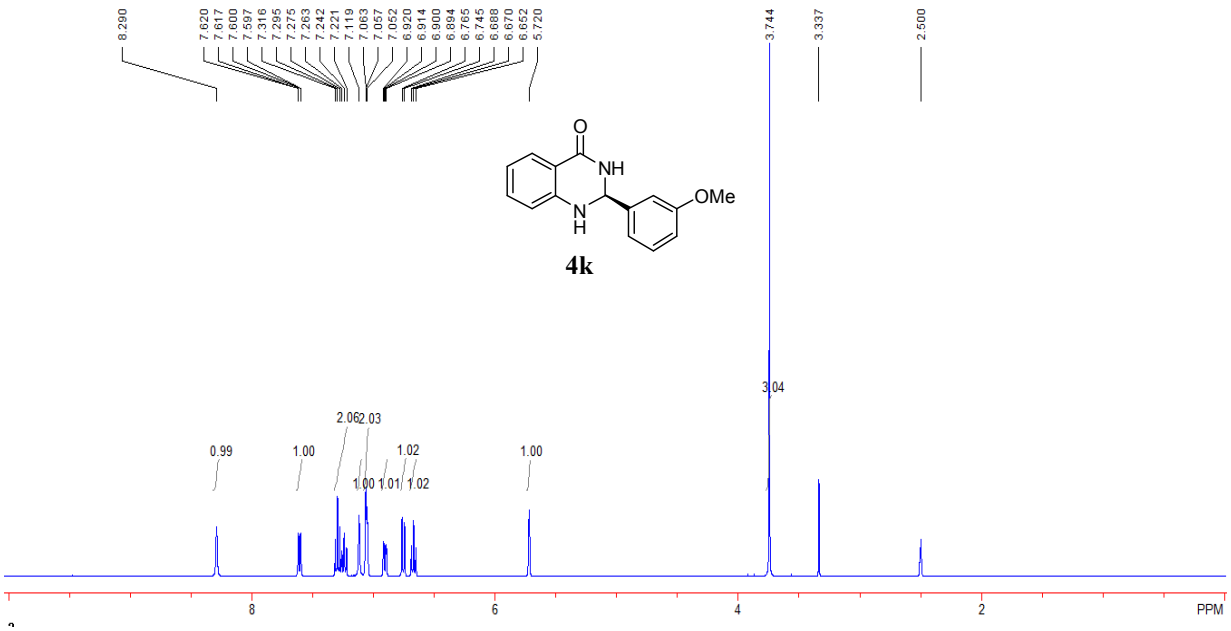
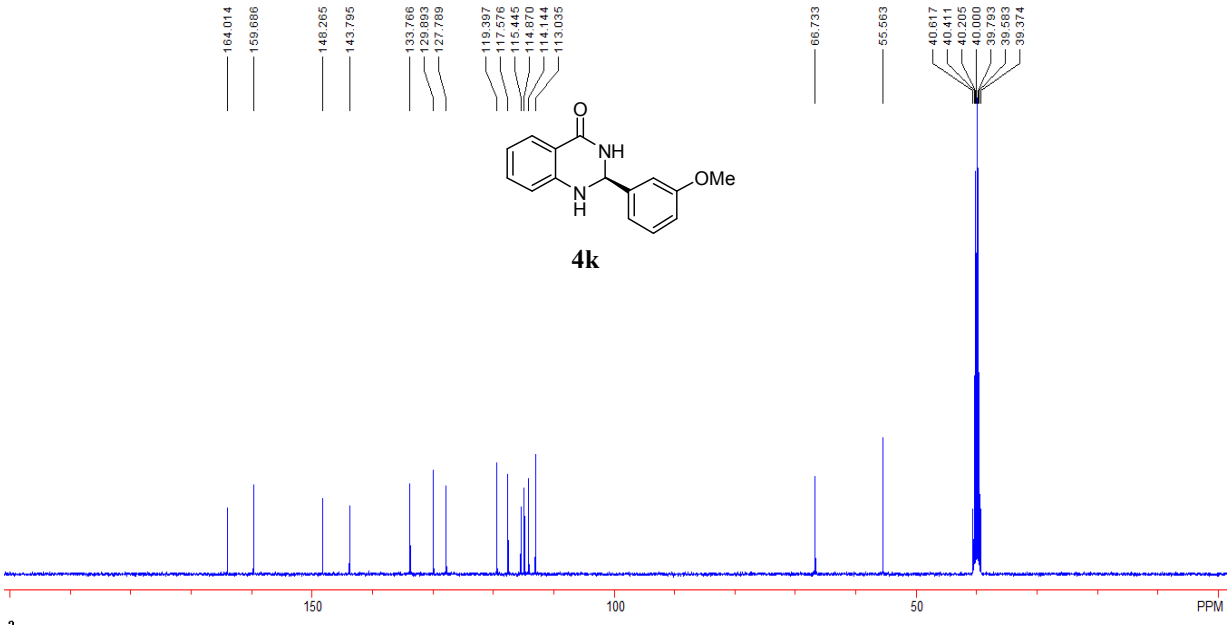
7.633
7.630
7.614
7.610
7.412
7.407
7.393
7.389
7.342
7.338
7.319
7.303
7.299
7.242
7.238
7.221
7.204
7.200
7.056
7.037
6.964
6.946
6.927
6.780
6.770
6.750
6.683
6.681
6.664
6.646
6.643
6.024
3.832
3.329
2.500
O
NH
OMe
N
H
4i
3.09
2.04
0.99
1.01
1.03
1.02
1.03
1.03
1.03
1.02
1.00
8
6
4
2
PPM


164.281
156.815
148.422
133.678
130.078
129.422
127.759
127.336
120.581
117.468
115.159
114.938
111.556
61.420
56.007
40.621
40.416
40.210
40.000
39.790
39.581
39.364
O
NH
OMe
N
H
4i
150
100
50
PPM


8.198
7.625
7.606
7.432
7.413
7.258
7.239
7.220
7.018
6.957
6.938
6.754
6.734
6.692
6.674
6.656
5.710
3.745
3.356
2.500
O
NH
N
H
OMe
4j
3.03
2.03
2.01
1.01
0.99
1.02
1.03
1.01
1.03
1.00
10
8
6
4
2
PPM


164.186
159.915
148.491
133.946
133.706
128.696
127.820
117.567
115.481
114.895
114.110
66.809
55.657
40.636
40.426
40.217
40.000
39.794
39.588
39.382
O
NH
N
H
OMe
4j
200
150
100
50
PPM


8.290
7.620
7.617
7.600
7.597
7.316
7.295
7.275
7.263
7.242
7.221
7.119
7.063
7.057
7.052
6.920
6.914
6.900
6.894
6.765
6.745
6.688
6.670
6.652
5.720
3.744
3.337
2.500
O
NH
N
H
OMe
4k
3.04
2.06
2.03
0.99
1.00
1.02
1.00
1.00
1.01
1.02
1.00
8
6
4
2
PPM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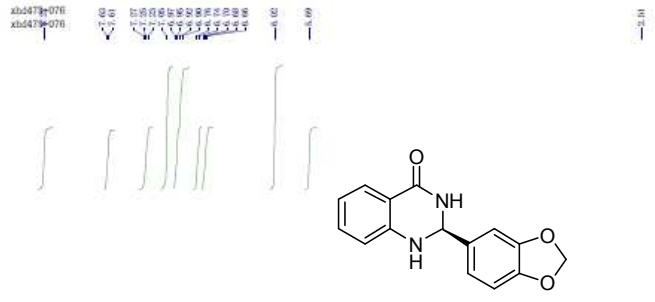
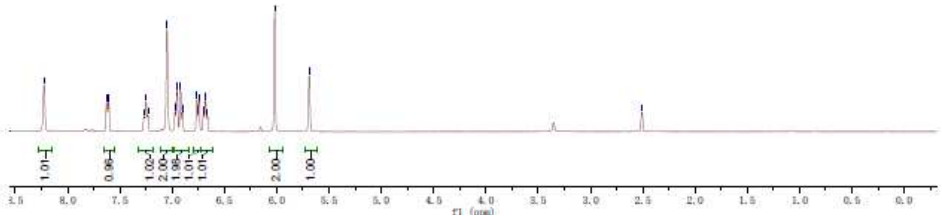
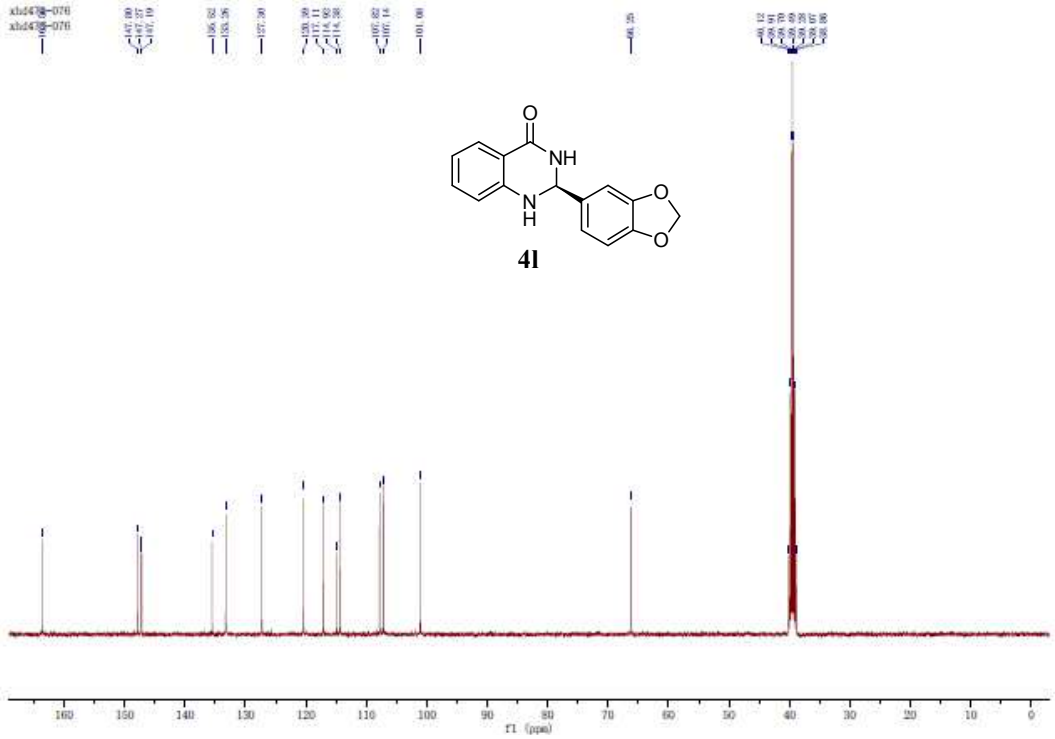
159.686
148.265
143.795
133.766
129.893
127.789
119.397
117.576
115.445
114.870
114.144
113.035
66.733
55.563
40.617
40.411
40.205
40.000
39.793
39.583
39.374
O
NH
N
H
OMe
4k
150
100
50
PPM

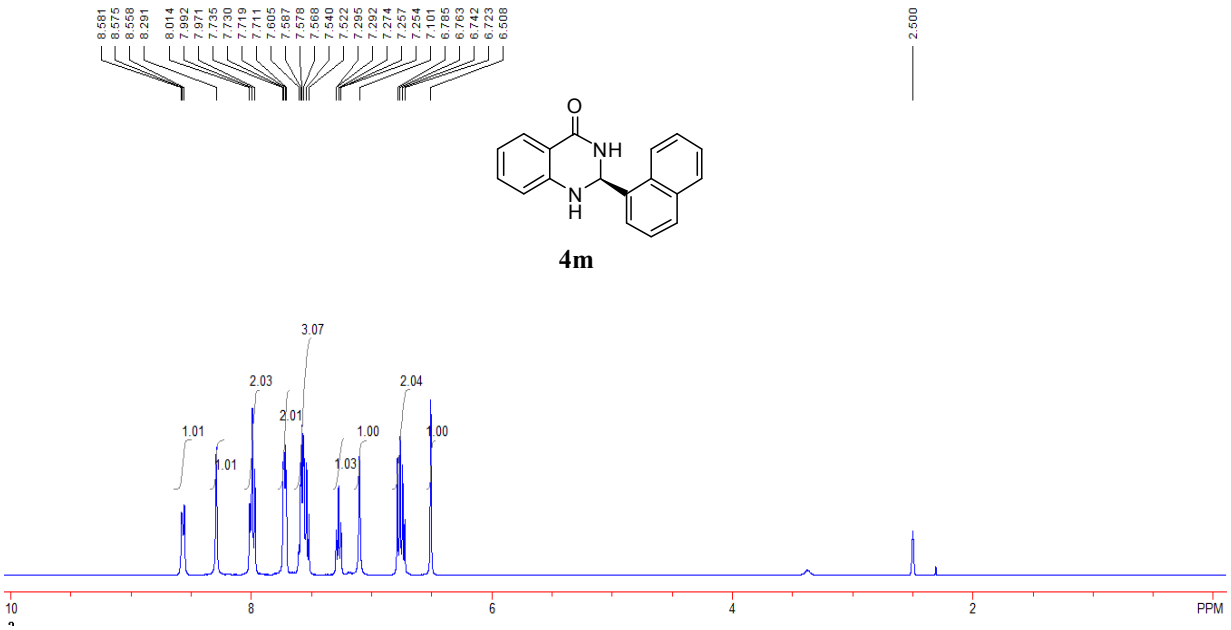

O
NH
N
H
O
O

4l

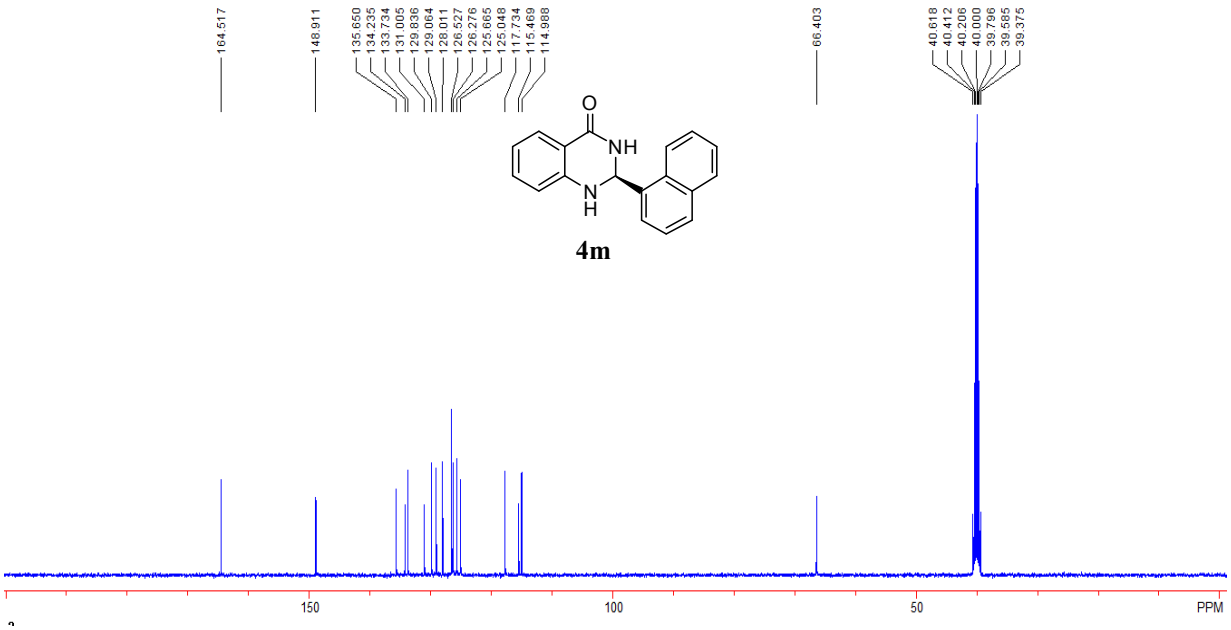

1.01
0.96
1.02
2.00
1.96
1.01
1.01
2.00
1.00
f1 (ppm)


O
NH
N
H
O
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

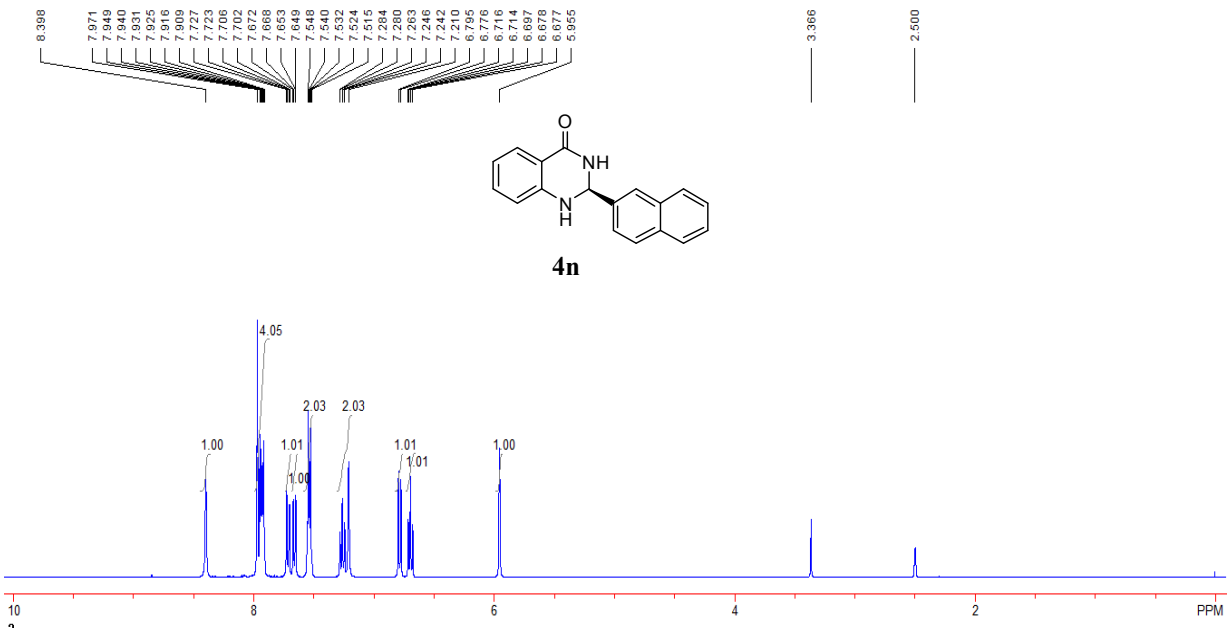
4l


8.581
8.575
8.558
8.291
8.014
7.992
7.971
7.735
7.730
7.719
7.711
7.605
7.587
7.578
7.568
7.540
7.522
7.295
7.292
7.274
7.257
7.254
7.101
6.785
6.763
6.742
6.723
6.508
2.500
O
NH
N
H
3.07
2.03
2.04
2.01
1.01
1.01
1.00
1.03
1.00
10
8
6
4
2
PPM

4m


164.517
148.911
135.650
134.235
133.734
131.005
129.836
129.064
128.011
126.527
126.276
125.665
125.048
117.734
115.469
114.988
66.403
40.618
40.412
40.206
40.000
39.796
39.585
39.375
O
NH
N
H
150
100
50
PPM

4m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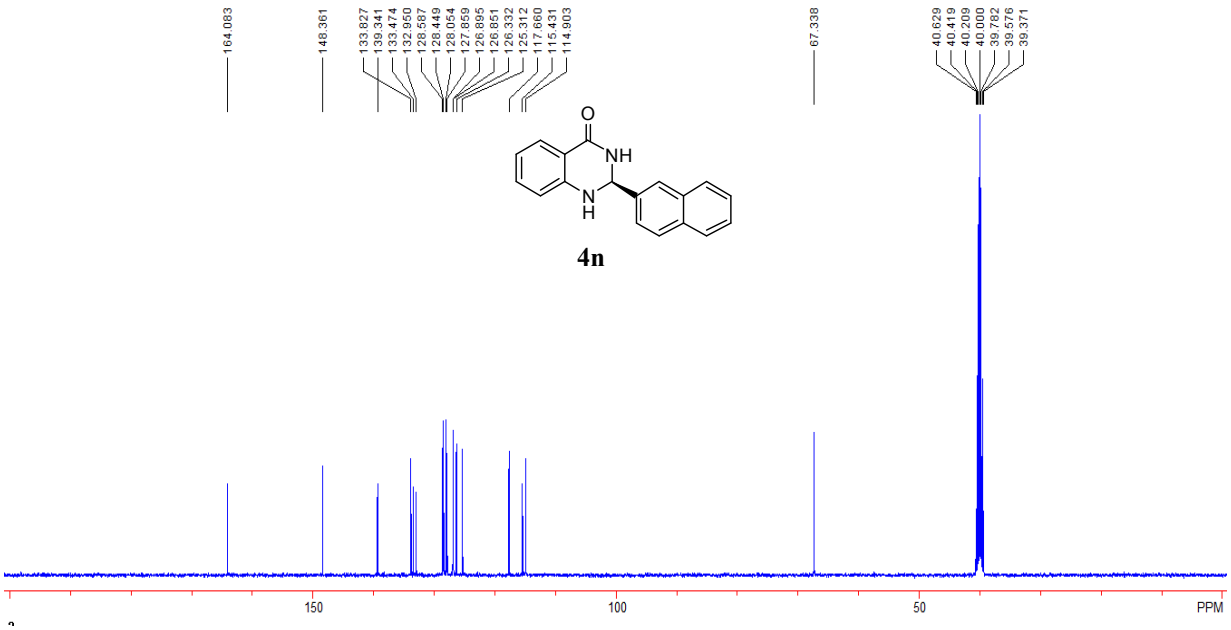
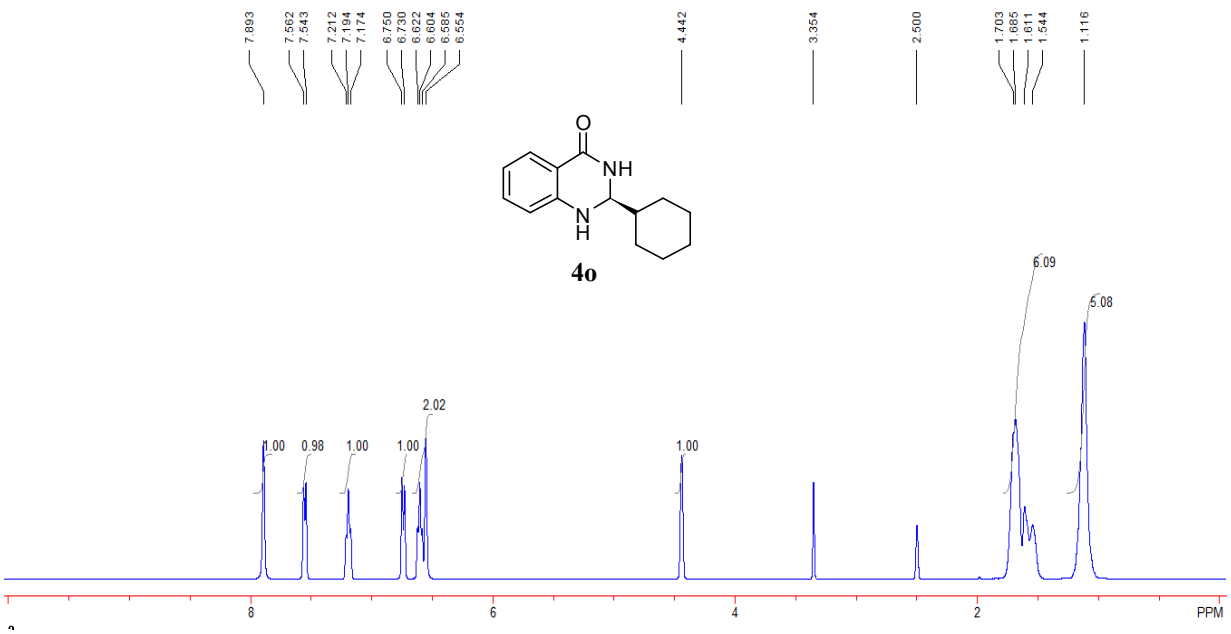
7.971
7.949
7.940
7.931
7.925
7.916
7.909
7.727
7.723
7.706
7.702
7.672
7.668
7.653
7.649
7.548
7.540
7.532
7.524
7.515
7.284
7.280
7.263
7.246
7.242
7.210
6.795
6.776
6.716
6.714
6.697
6.678
6.677
5.955
3.366
2.500
O
NH
N
H
4.05
2.03
2.03
1.00
1.01
1.00
1.01
1.01
1.00
10
8
6
4
2
PPM

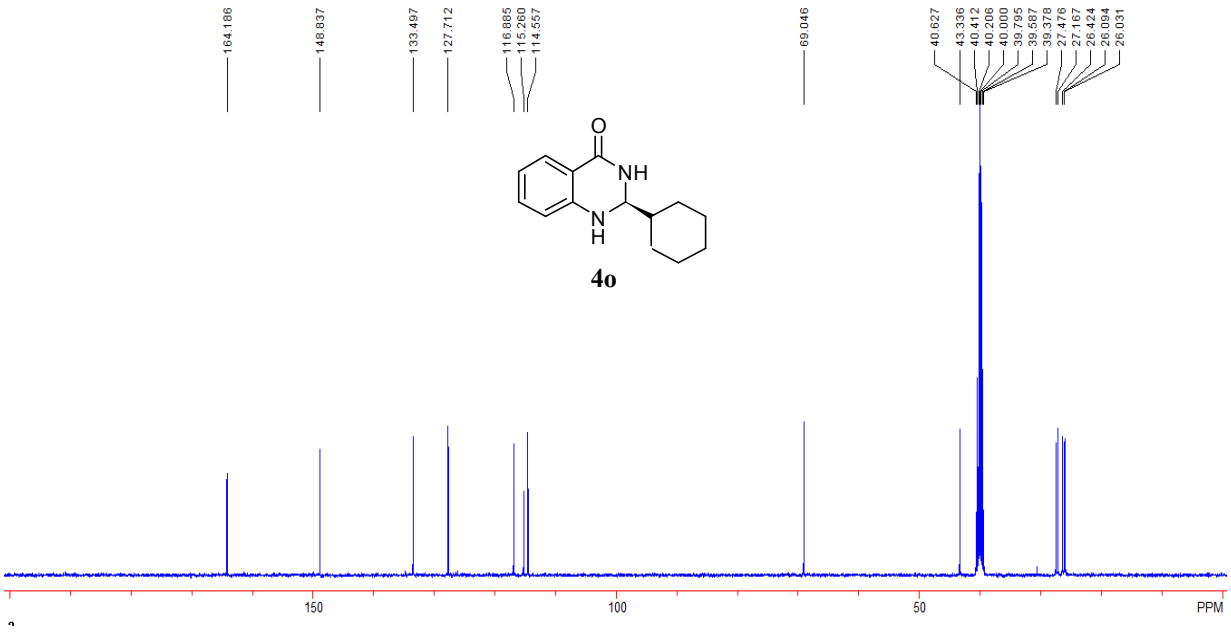
4n


164.083
148.361
133.827
139.341
133.474
132.950
128.587
128.449
128.054
127.859
126.895
126.851
126.332
125.312
117.660
115.431
114.903
67.338
40.629
40.419
40.209
40.000
39.782
39.576
39.371
O
NH
N
H
150
100
50
PPM

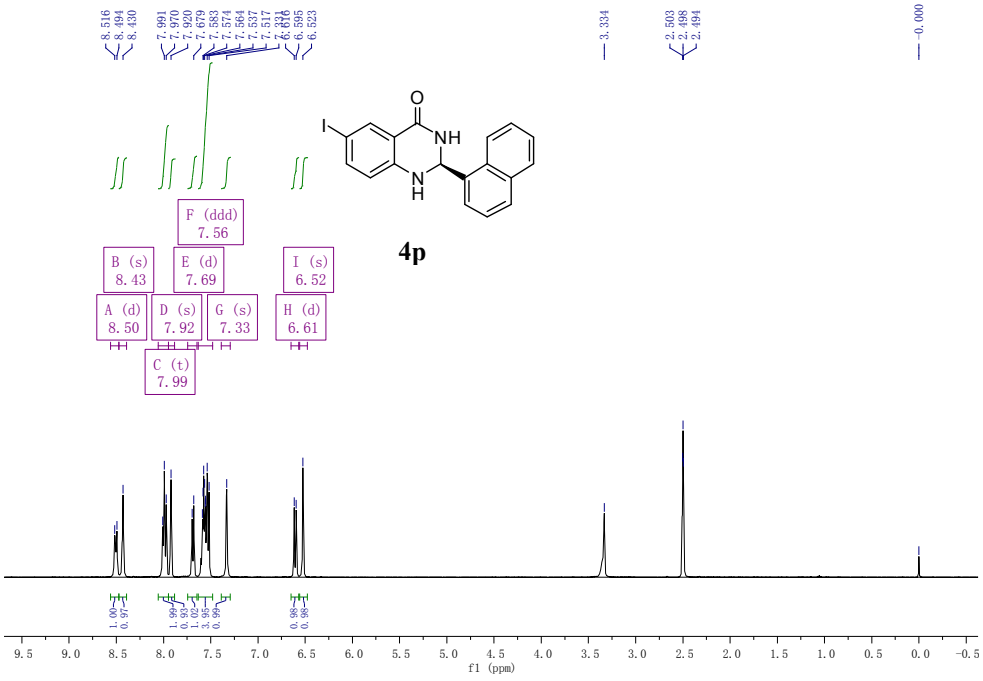
4n


7.893
7.562
7.543
7.212
7.194
7.174
6.750
6.730
6.622
6.604
6.585
6.554
4.442
3.354
2.500
1.703
1.685
1.611
1.544
1.116
O
NH
N
H
6.09
5.08
2.02
1.00
0.98
1.00
1.00
1.00
8
6
4
2
PPM

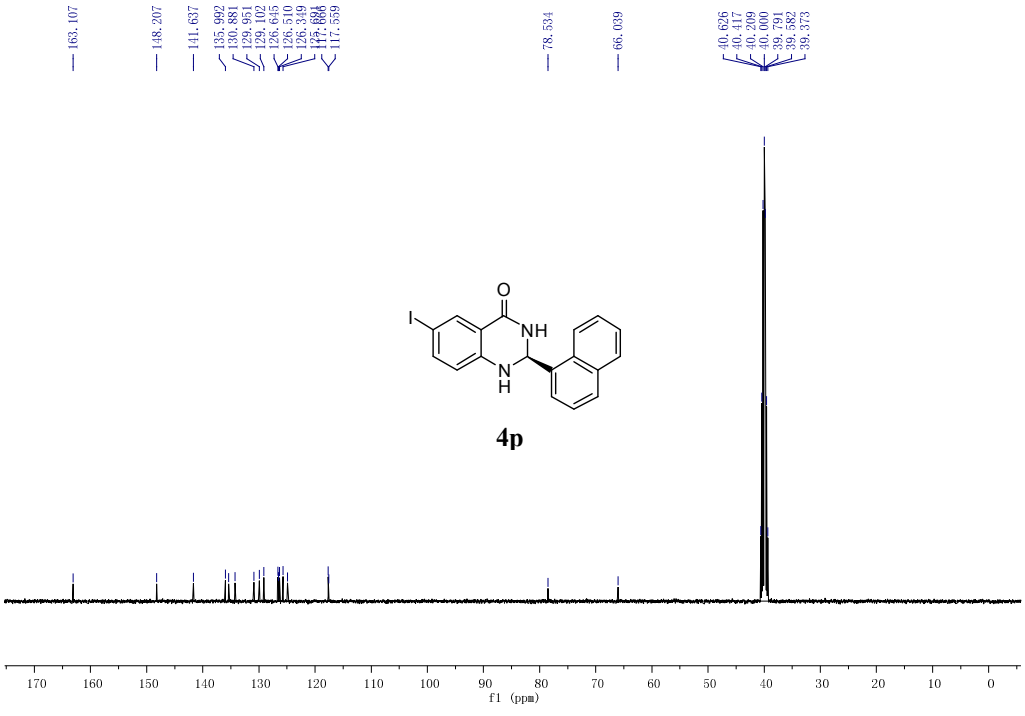
4o


164.186
148.837
133.497
127.712
116.885
115.260
114.557
69.046
40.627
43.336
40.412
40.206
40.000
39.795
39.587
39.378
27.476
27.167
26.424
26.094
26.031
O
NH
N
H
150
100
50
PPM

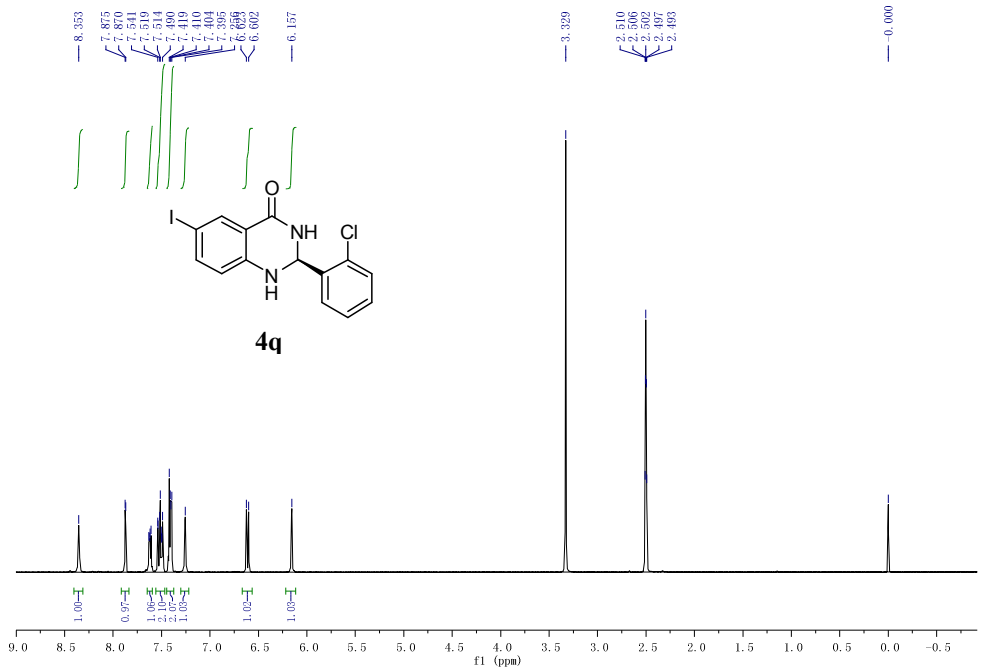
4o


8.516
8.494
8.430
7.991
7.970
7.920
7.679
7.583
7.574
7.564
7.537
7.517
6.611
6.595
6.523
3.334
2.503
2.498
2.494
-0.000
O
I
NH
N
H
F (ddd)
7.56
B (s)
8.43
E (d)
7.69
I (s)
6.52
A (d)
8.50
D (s)
7.92
G (s)
7.33
H (d)
6.61
C (t)
7.99
1.00
0.97
1.99
0.93
1.05
3.00
0.99
0.98
0.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

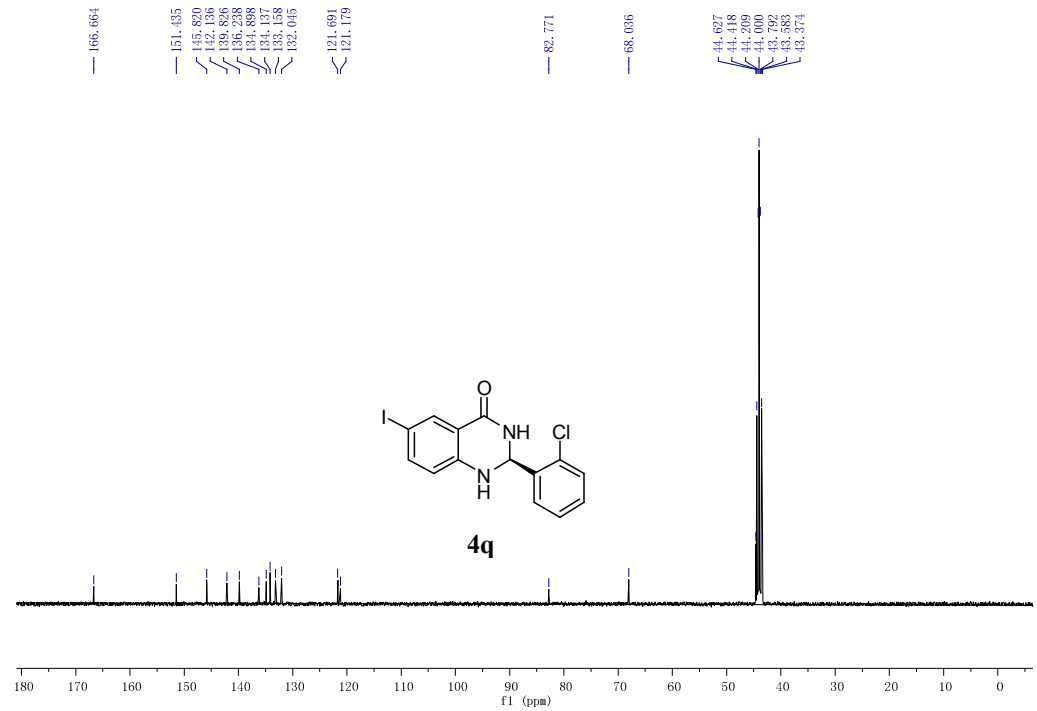
4p


163.107
148.207
141.637
135.992
130.881
129.951
129.102
126.645
126.510
126.349
125.686
125.684
117.559
78.534
66.039
40.626
40.417
40.209
40.000
39.791
39.582
39.373
O
I
NH
N
H
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

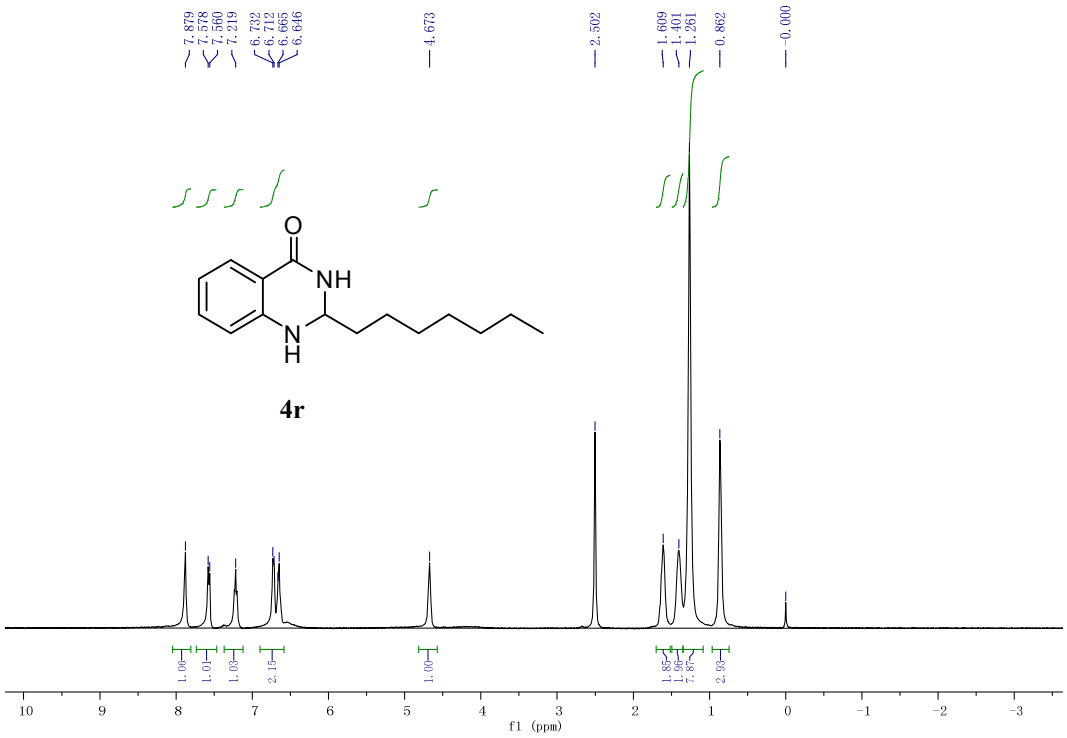
4p

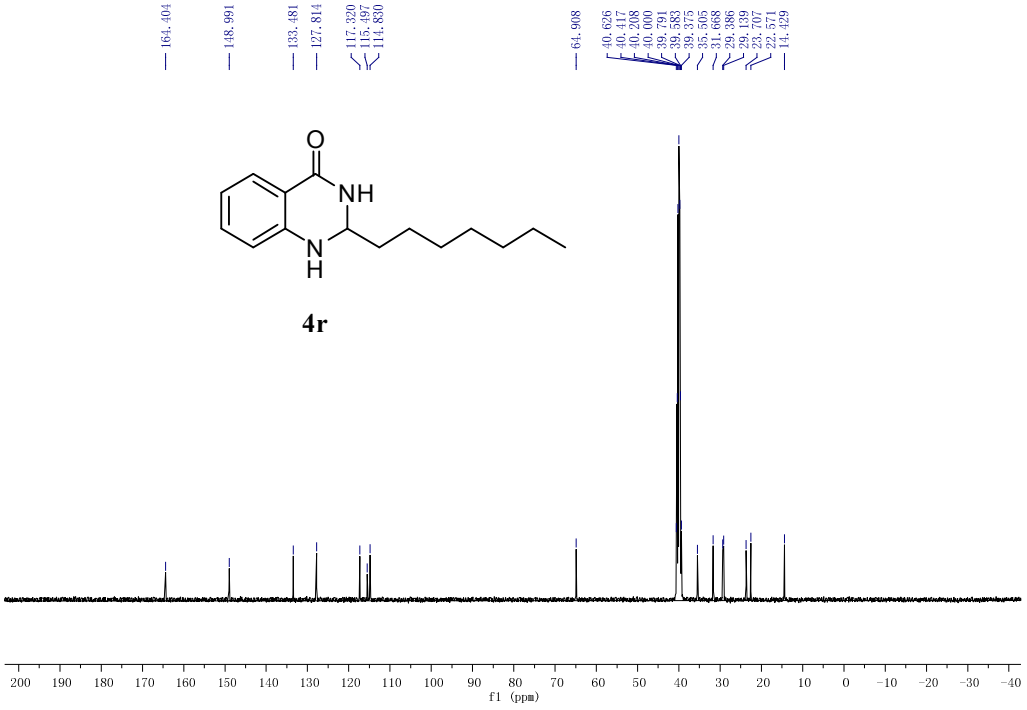

8.353
7.875
7.870
7.541
7.519
7.514
7.490
7.419
7.410
7.404
7.395
6.624
6.602
6.157
3.329
2.510
2.506
2.502
2.497
2.493
0.000
O
I
NH
Cl
N
H
1.00
0.97
1.06
1.07
2.07
1.03
1.02
1.03
f1 (ppm)

4q

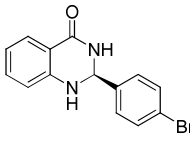

166.664
151.435
145.820
142.136
139.826
136.238
134.898
134.137
133.158
132.045
121.691
121.179
82.771
68.036
44.627
44.418
44.209
44.000
43.792
43.583
43.374
O
I
NH
Cl
N
H
f1 (ppm)

4q


7.879
7.578
7.560
7.219
6.732
6.712
6.665
6.646
4.673
2.502
1.609
1.401
1.261
0.862
-0.000
O
NH
N
H
4r
1.06
1.01
1.03
2.15
1.00
1.85
1.96
7.87
2.99
f1 (ppm)

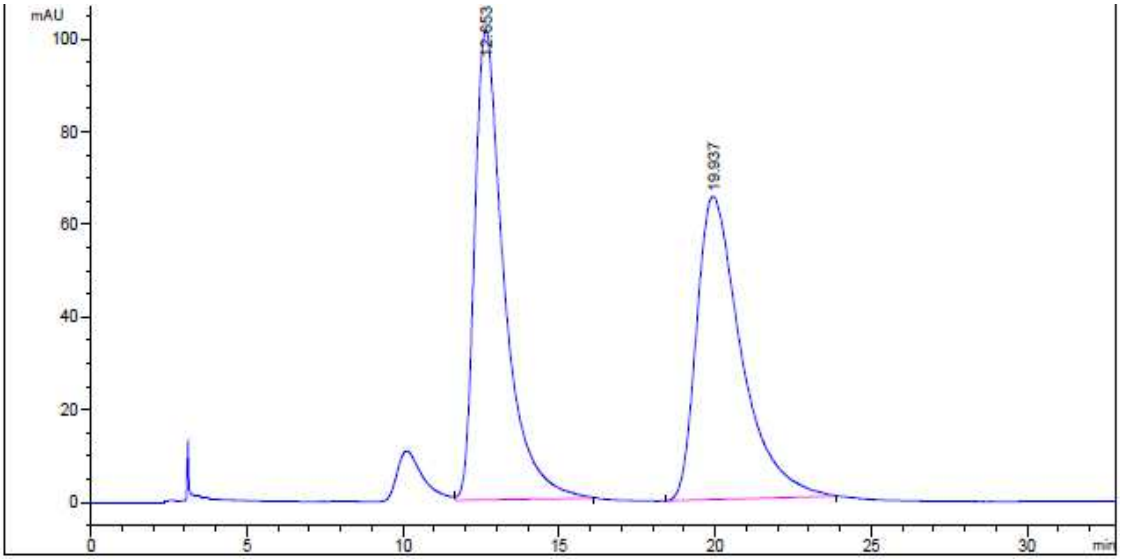

164.404
148.991
133.481
127.814
117.320
115.497
114.830
64.908
40.626
40.417
40.208
40.000
39.791
39.583
39.375
35.505
31.668
29.386
29.139
23.707
22.571
14.429
O
NH
N
H
4r
f1 (ppm)

5. HPLC spectra for all compounds

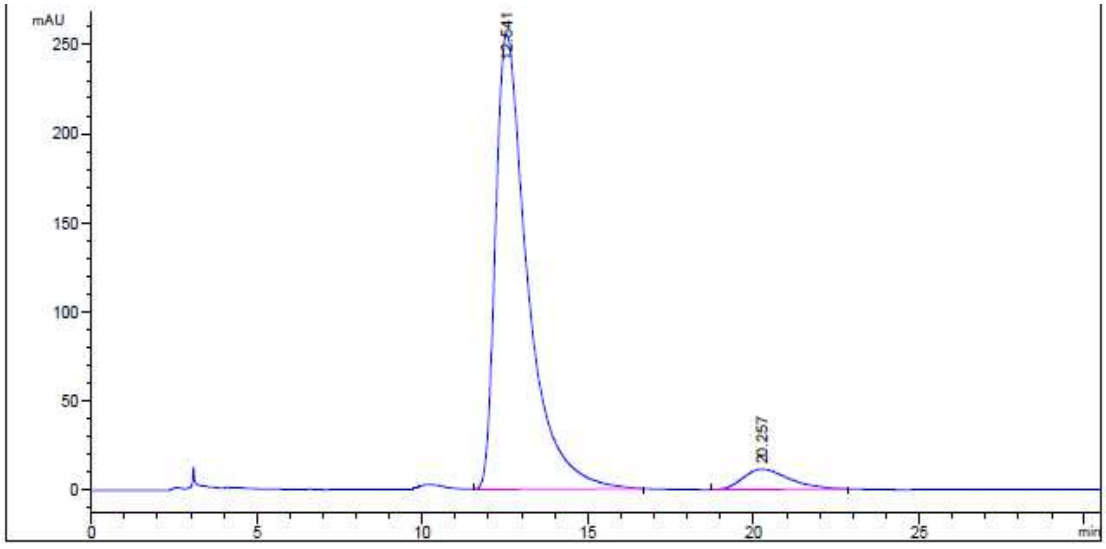


4a

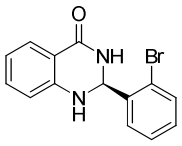
88% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.2 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	12.653	BB	0.9819	6682.49512	101.53258	50.6959
2	19.937	BB	1.3608	6499.04102	65.45489	49.3041
总量 :				1.31815e4	166.98746	

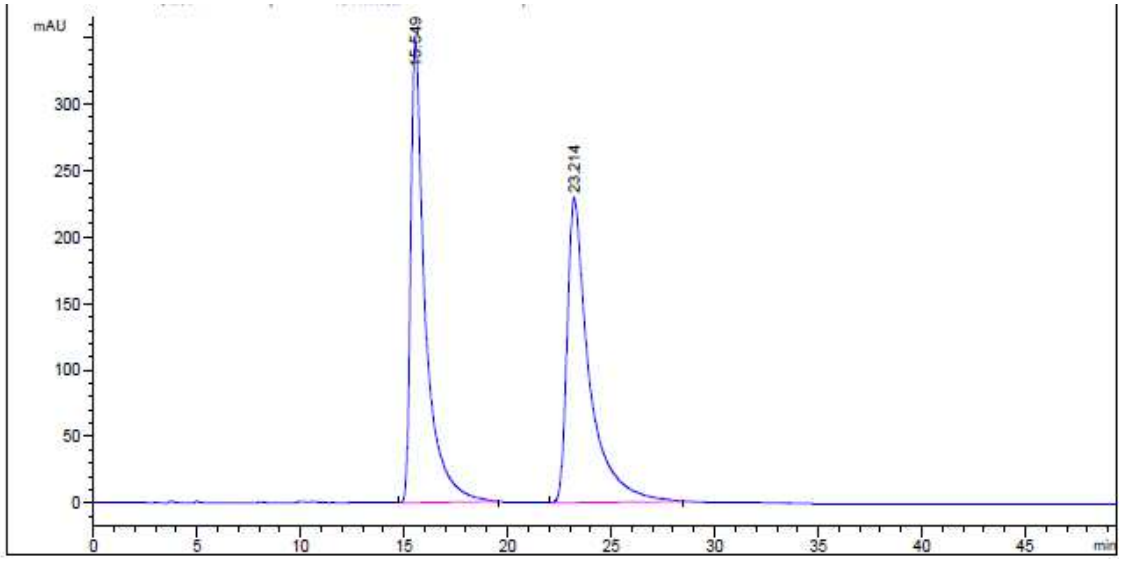


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	12.541	BB	0.9955	1.71812e4	255.54759	93.9421
2	20.257	BB	1.2059	1107.94336	11.36352	6.0579
总量 :				1.82892e4	266.91111	

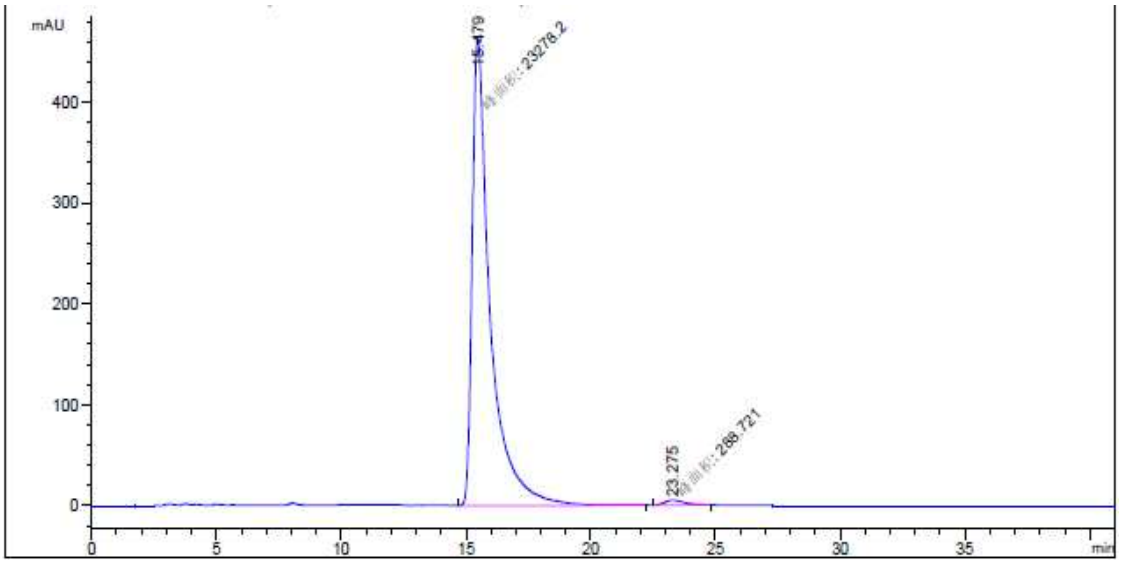


4b

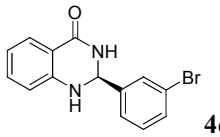
98% ee. [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	15.549	BB	0.6955	1.70947e4	347.94348	50.2332
2	23.214	BB	1.0513	1.69360e4	229.20905	49.7668
总量 :				3.40307e4	577.15253	

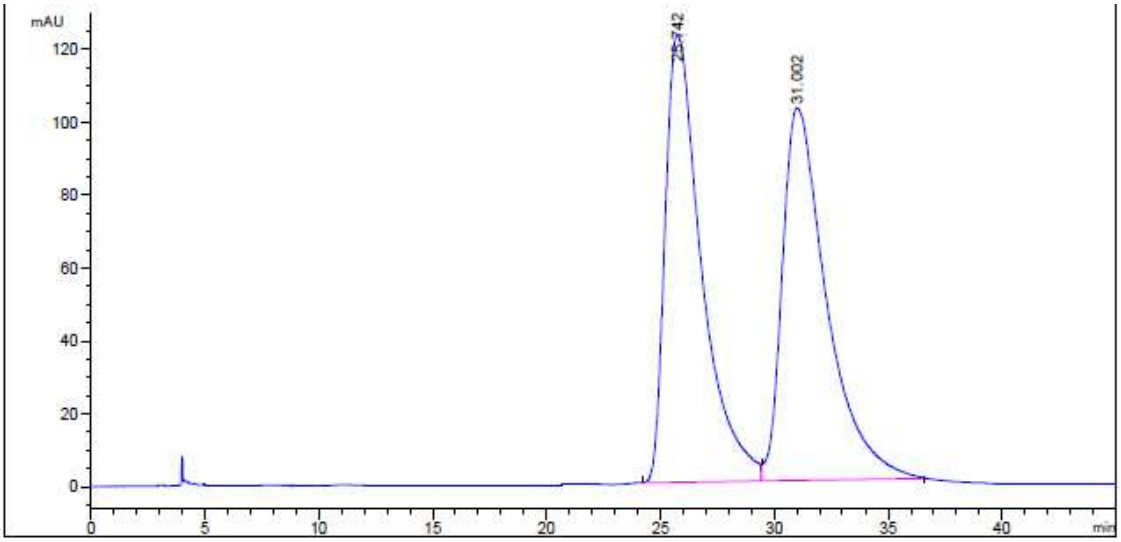


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	15.479	MM	0.8391	2.32782e4	462.33936	98.7749
2	23.275	MM	0.9807	288.72089	4.90692	1.2251
总量 :				2.35669e4	467.24627	

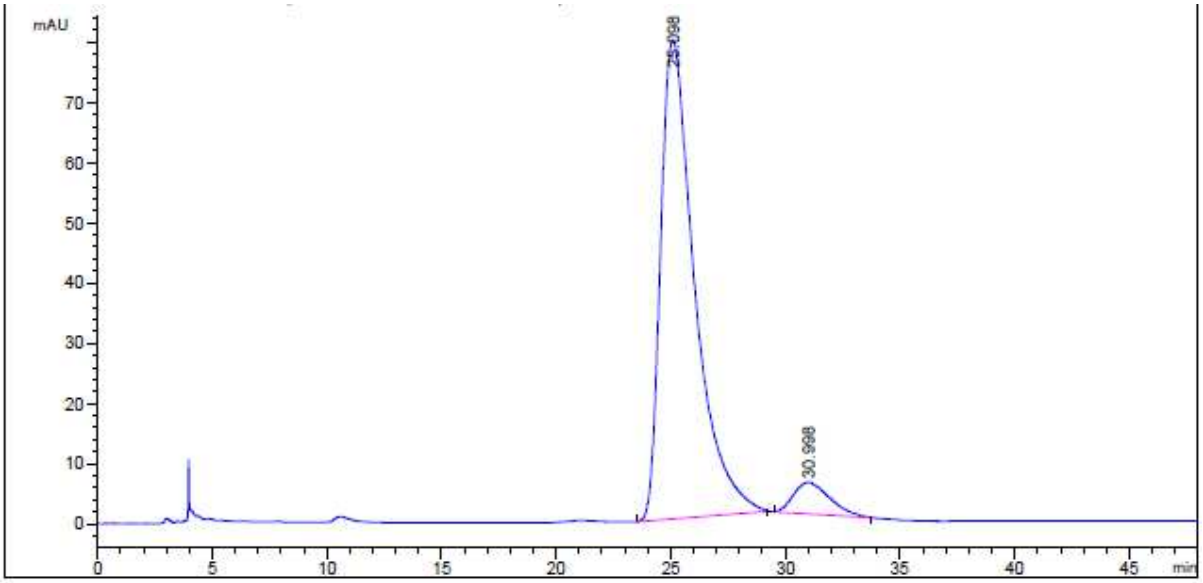


4c

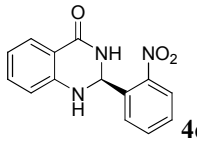
87% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 85 / 15, 1.0 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	25.742	BB	1.6112	1.36377e4	122.56718	49.6801
2	31.002	BB	1.9182	1.38133e4	102.15989	50.3199
总量 :				2.74511e4	224.72707	

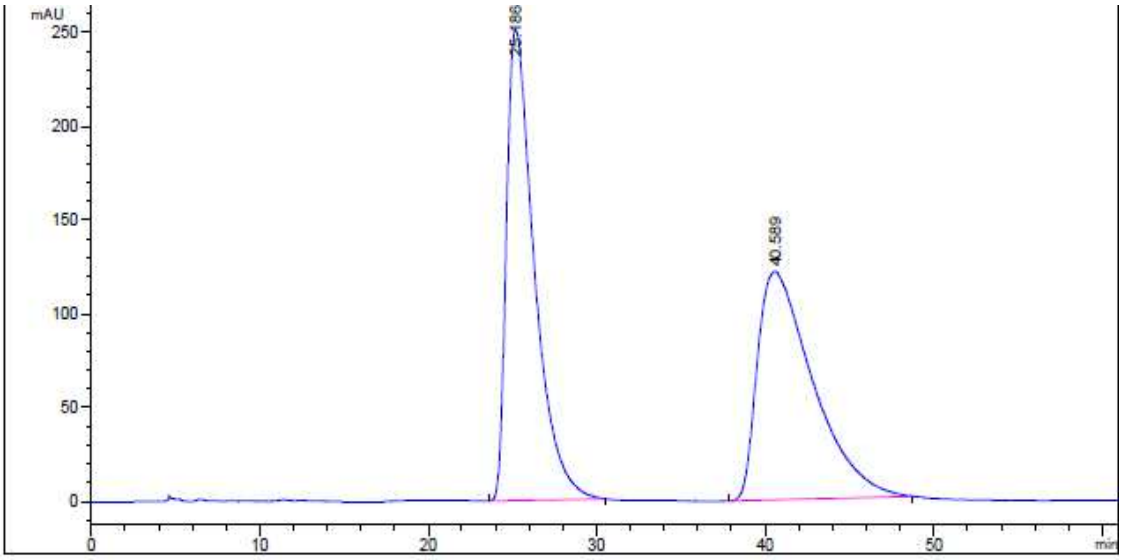


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	25.098	BB	1.4866	8202.57031	79.56847	93.4725
2	30.998	BB	1.2939	572.80896	5.21776	6.5275
总量 :				8775.37927	84.78622	

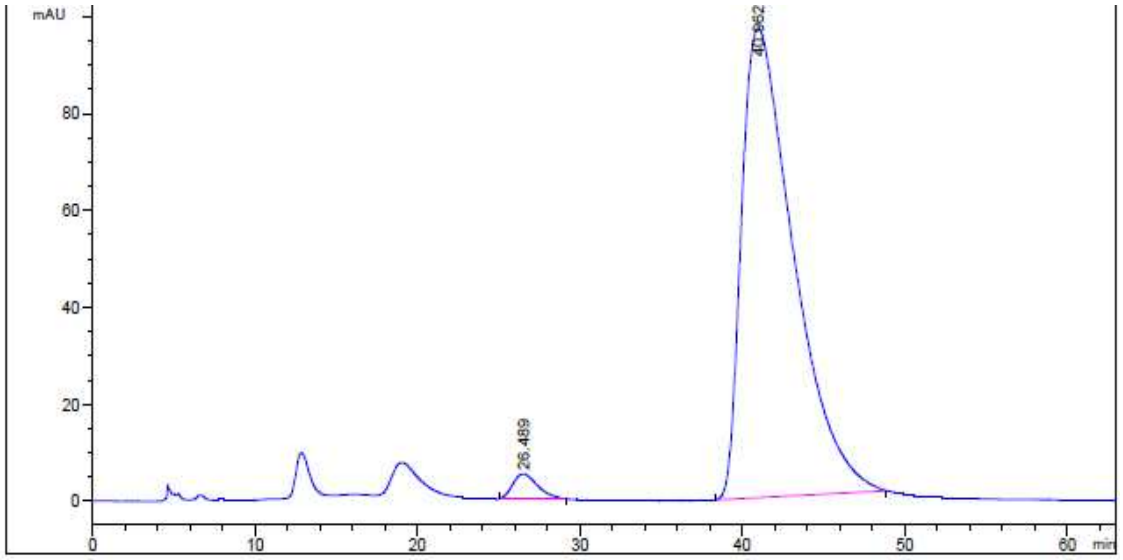


4d

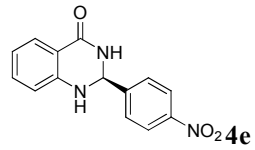
95% ee. [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.7 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	25.186	BB	1.6839	2.89022e4	251.58864	50.8324
2	40.589	BB	2.7710	2.79557e4	121.92812	49.1676
总量 :				5.68579e4	373.51675	

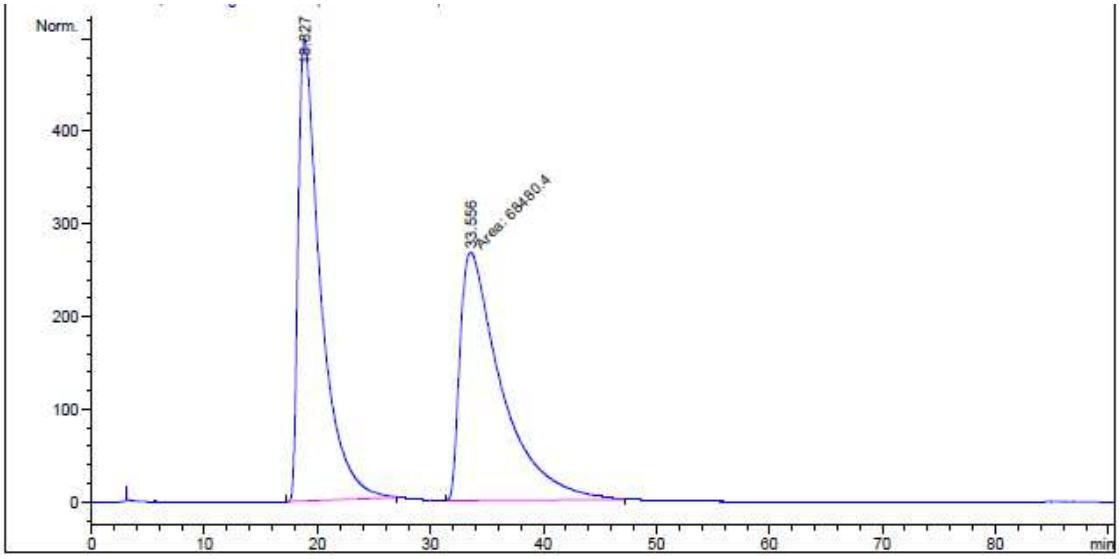


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	26.489	BB	1.2470	546.81573	5.15797	2.4711
2	40.962	BB	2.9390	2.15817e4	96.79398	97.5289
总量 :				2.21285e4	101.95195	

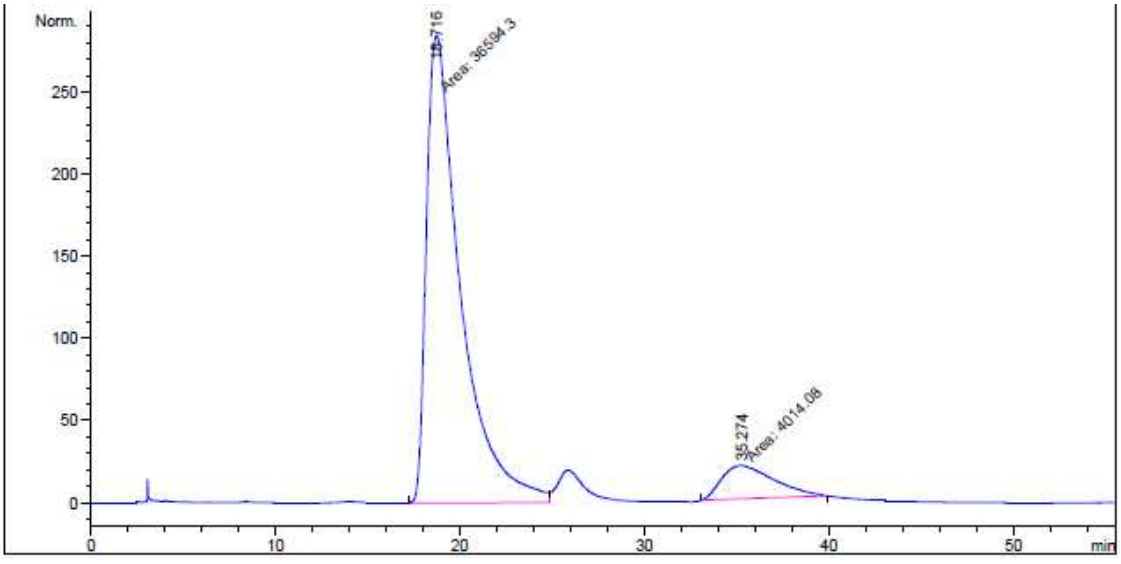


4e

80% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.2 mL/min, λ = 254 nm]

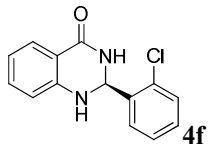


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.827	PB	1.9346	6.86698e4	498.07175	50.0691
2	33.556	MM	4.2552	6.84804e4	268.22528	49.9309
Totals :				1.37150e5	766.29703	



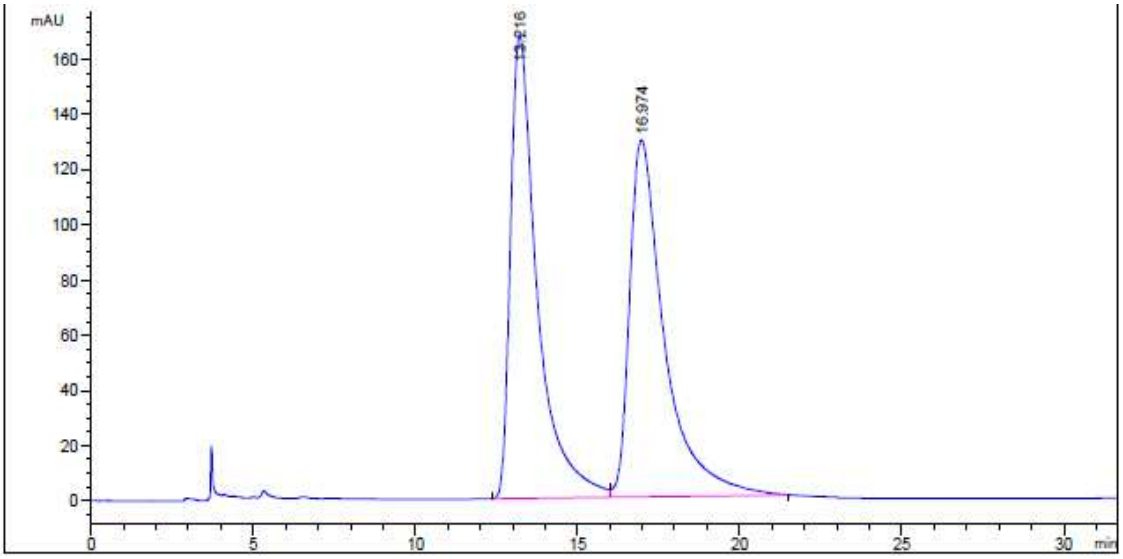
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.716	MF	2.1414	3.65943e4	284.82028	90.1151
2	35.274	MM	3.3111	4014.08472	20.20523	9.8849
Totals :				4.06084e4	305.02551	

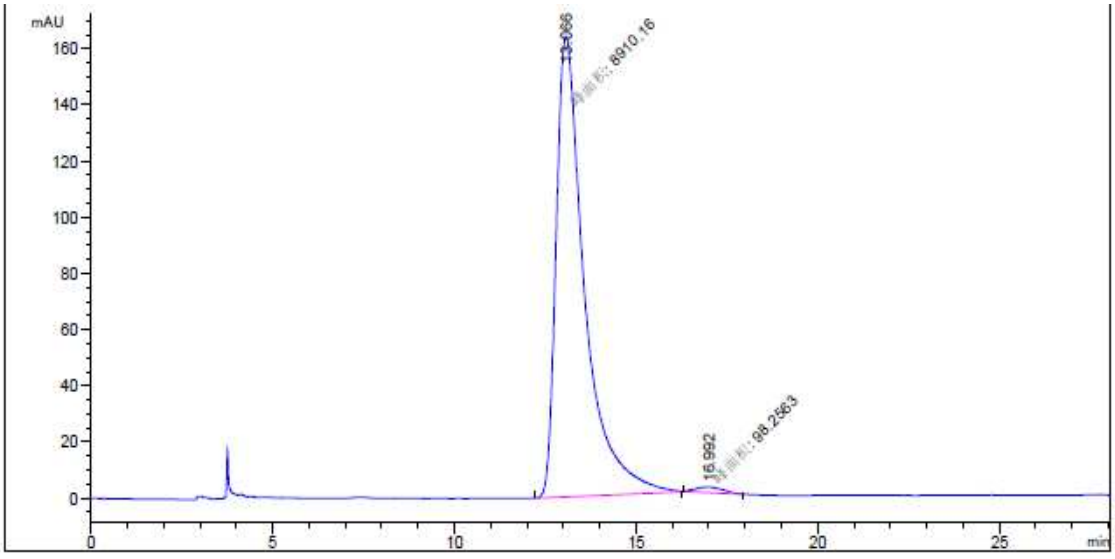


4f

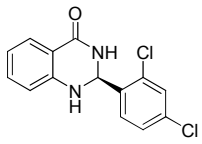
98% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	13.216	BV	0.8508	9649.69922	167.95702	49.9396
2	16.974	VB	1.0935	9673.05078	129.39204	50.0604
总量 :				1.93228e4	297.34906	

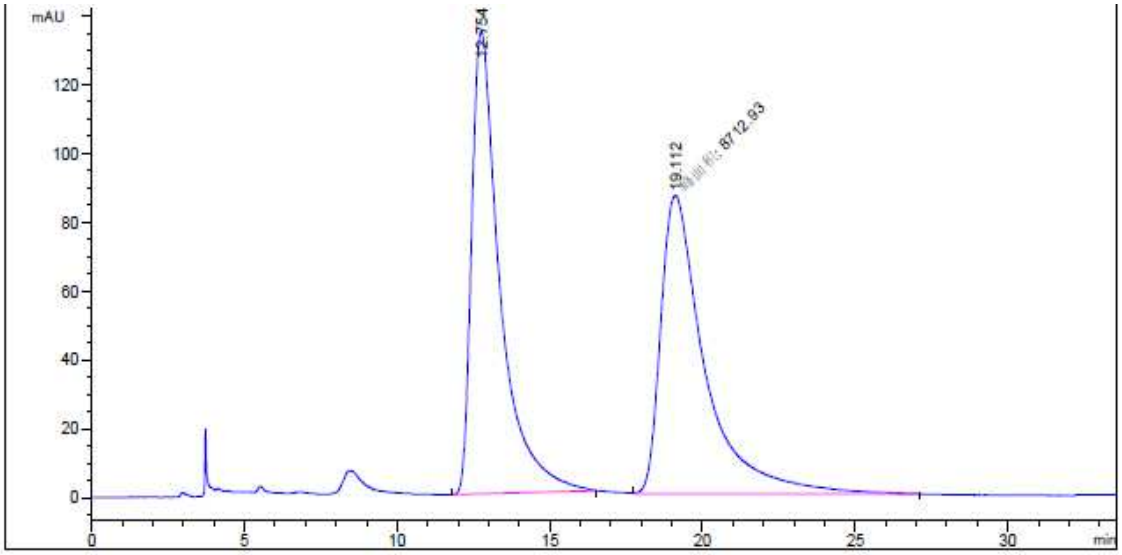


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	13.066	MM	0.9065	8910.15527	163.81483	98.9093
2	16.992	MM	0.8194	98.25626	1.99848	1.0907
总量 :				9008.41154	165.81331	

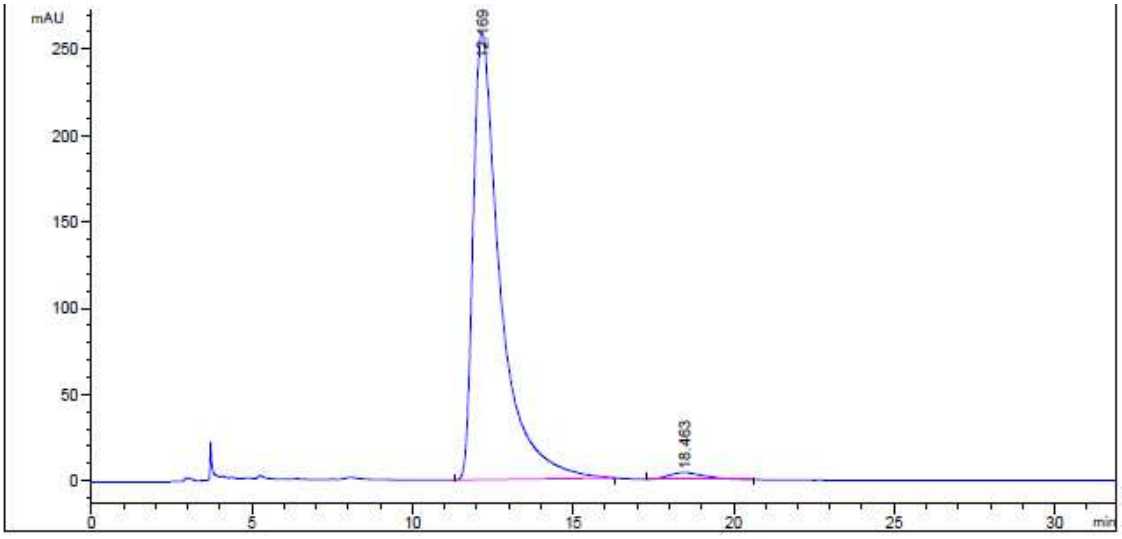


4g

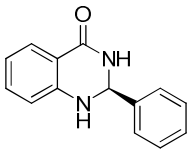
96% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	12.754	BB	0.9549	8703.74707	134.41751	49.9736
2	19.112	MM	1.6761	8712.92871	86.63719	50.0264
总量 :				1.74167e4	221.05470	

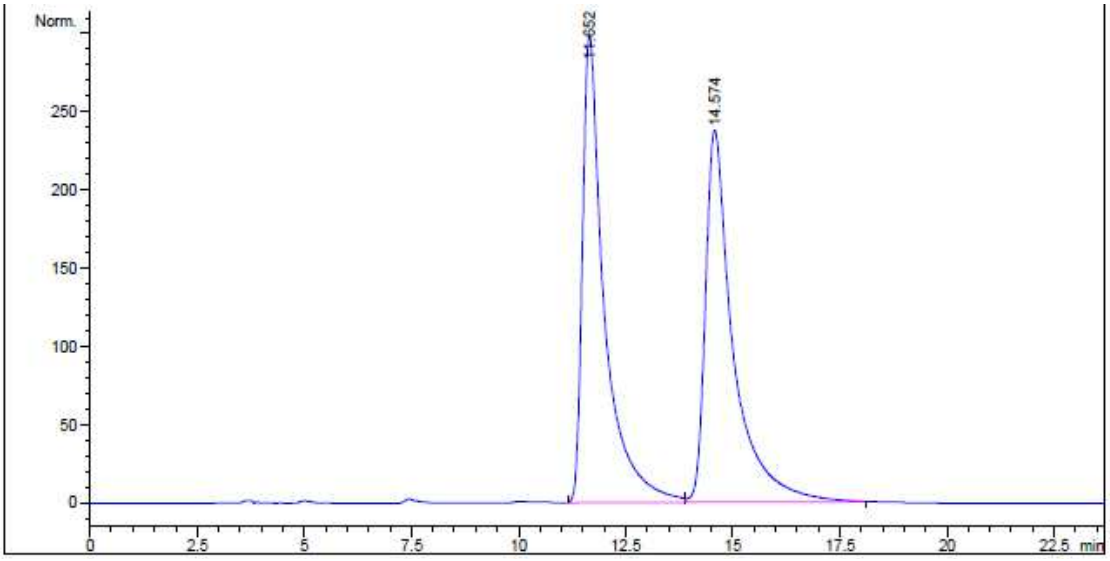


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	12.169	BB	0.8562	1.51698e4	259.15967	98.0073
2	18.463	BB	0.9399	308.42896	3.90707	1.9927
总量 :				1.54782e4	263.06674	

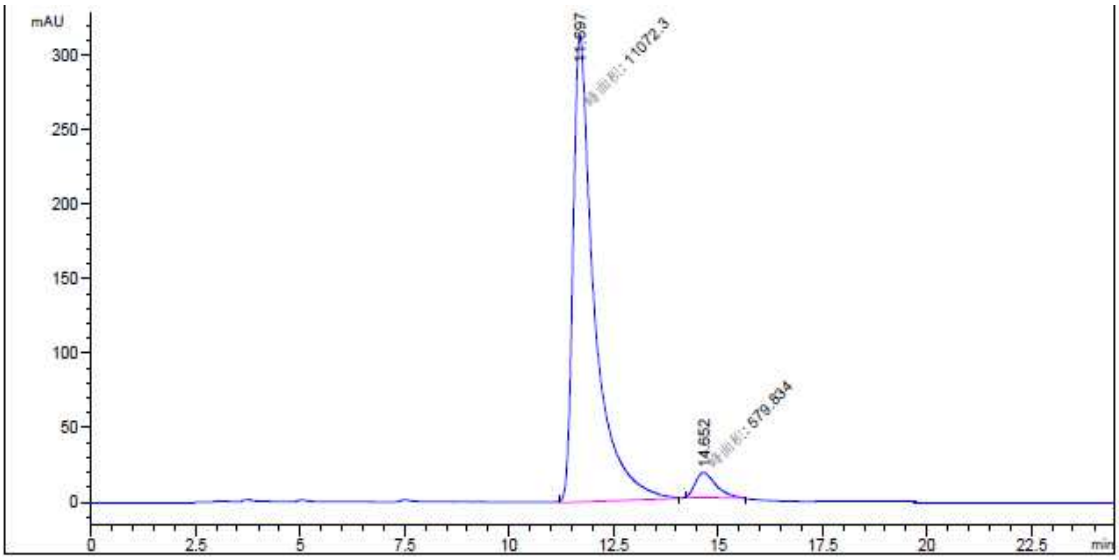


4h

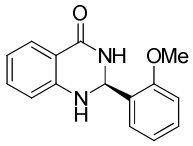
90% ee. [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm]



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.652	BV	0.5091	1.06540e4	298.83023	49.7322
2	14.574	VB	0.6501	1.07687e4	238.01666	50.2678
Totals :				2.14227e4	536.84689	

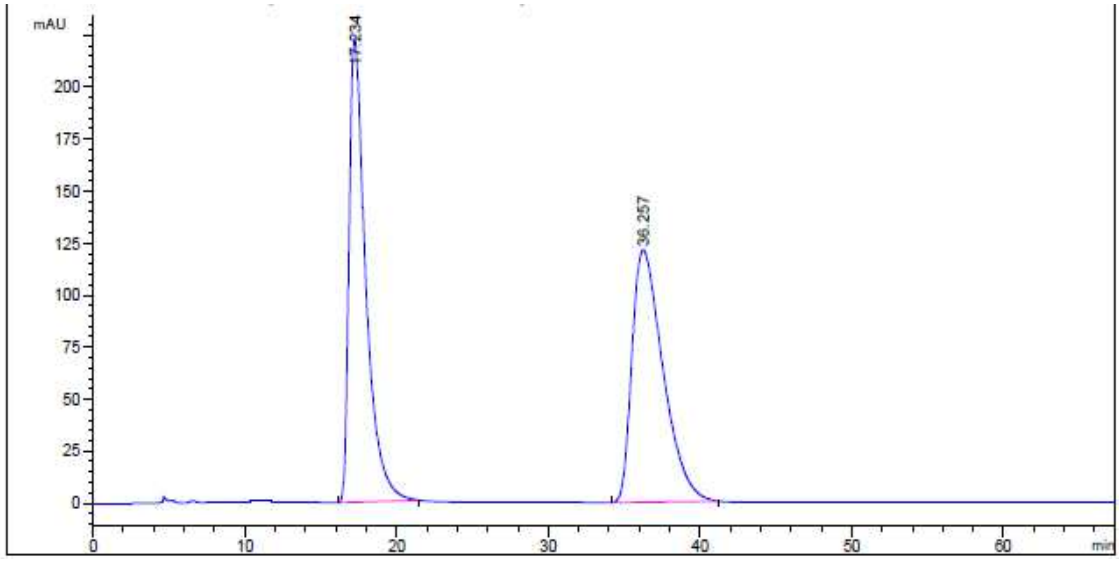


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	11.697	MM	0.5900	1.10723e4	312.78958	95.0238
2	14.652	MM	0.5808	579.83405	16.63978	4.9762
总量 :				1.16521e4	329.42936	

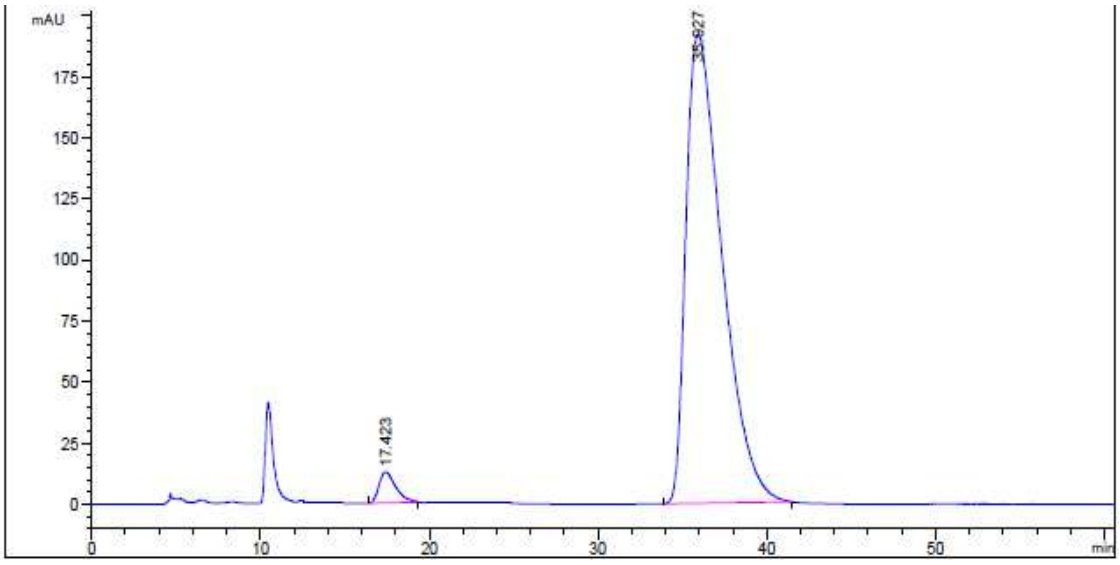


4i

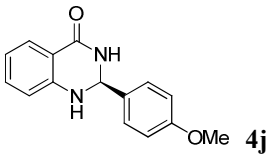
94% ee. [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.7 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	17.234	BB	1.1329	1.70977e4	223.08710	49.7588
2	36.257	BB	2.0906	1.72635e4	121.25342	50.2412
总量：				3.43612e4	344.34052	

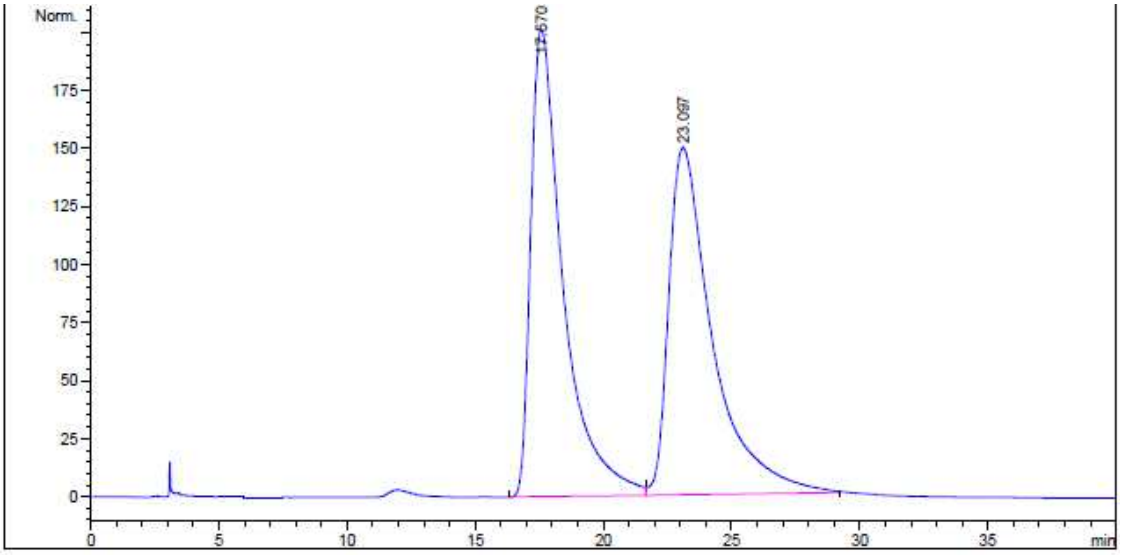


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	17.423	BB	0.9312	880.31952	12.67384	2.9956
2	35.927	BB	2.1583	2.85067e4	192.05519	97.0044
总量：				2.93871e4	204.72903	

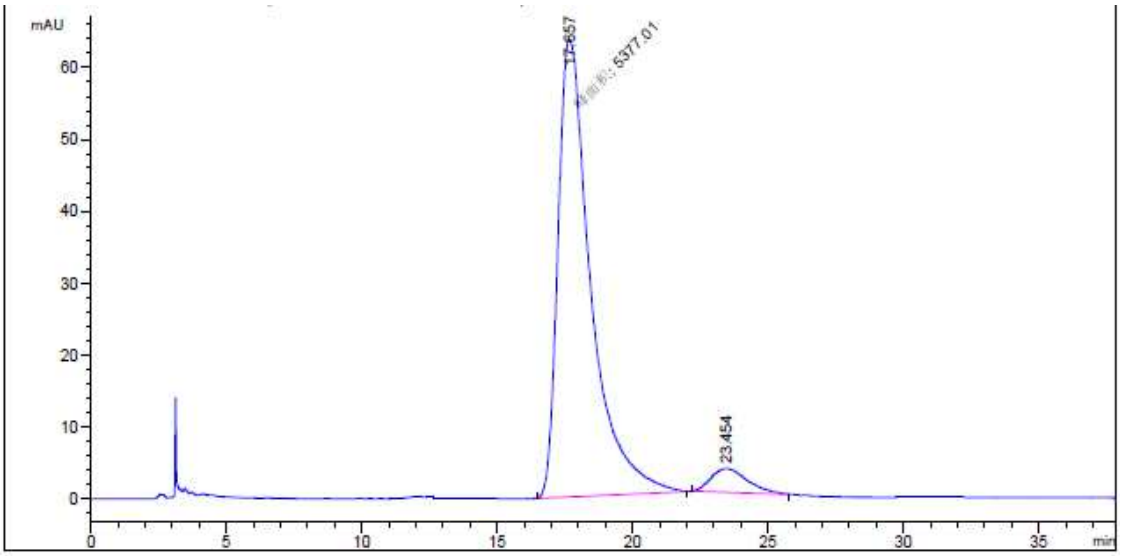


4j

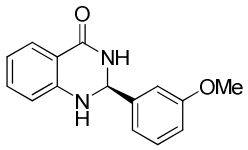
89% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.2 mL/min, λ = 254 nm]



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	17.570	PV	1.3102	1.77749e4	201.20497	50.0229
2	23.097	VB	1.6904	1.77586e4	149.63054	49.9771
Totals :				3.55335e4	350.83551	

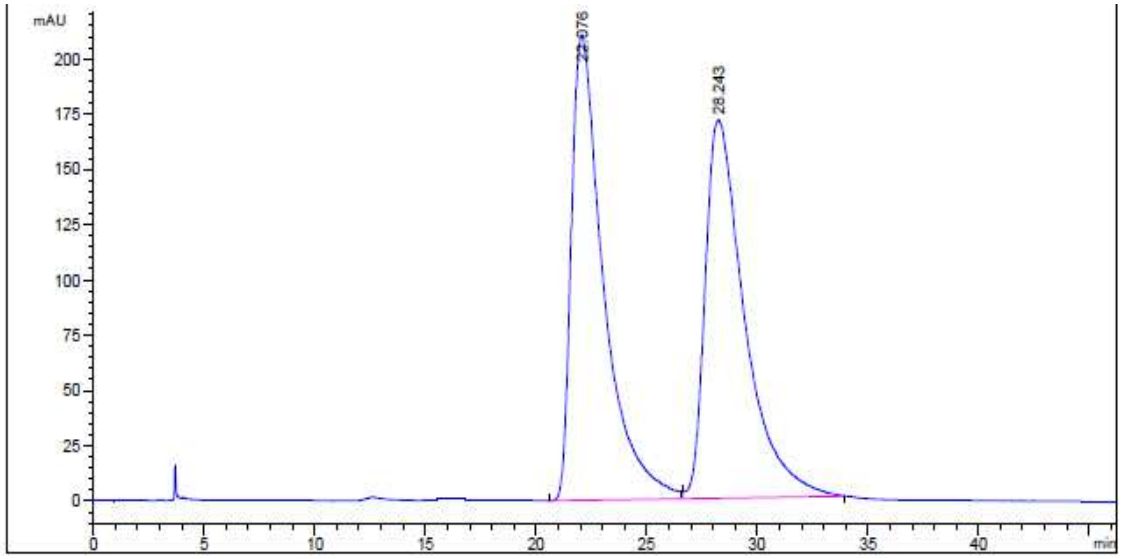


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	17.657	MM	1.4057	5377.01123	63.75361	94.5705
2	23.454	BB	1.1055	308.70575	3.29257	5.4295
总量 :				5685.71698	67.04618	

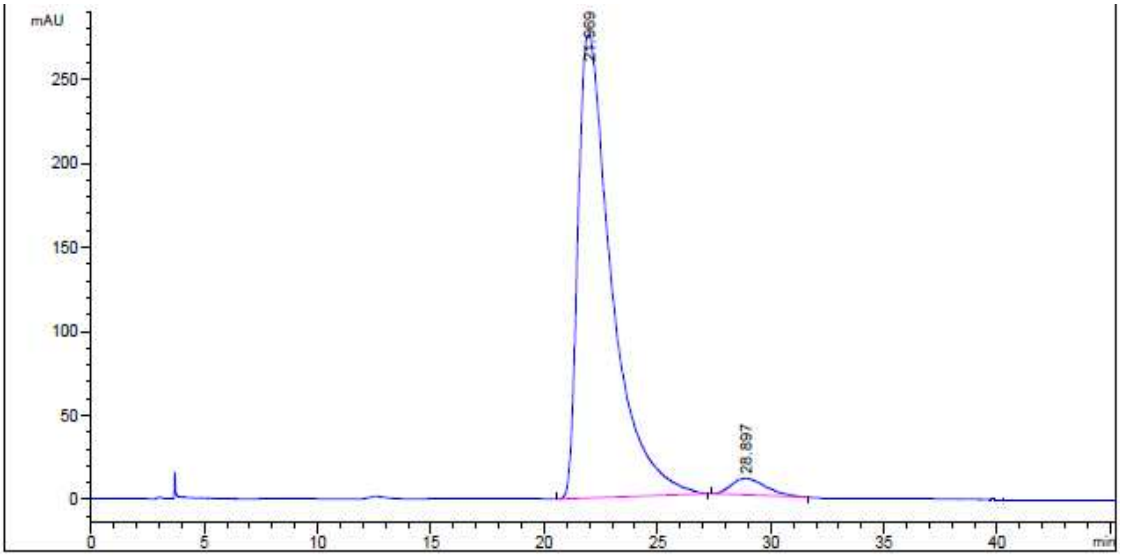


4k

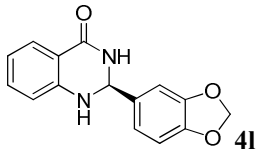
93% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 80 / 20, 1.0 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	22.076	BB	1.4988	2.13883e4	210.70053	50.2139
2	28.243	BB	1.7144	2.12061e4	171.37779	49.7861
总量：				4.25944e4	382.07832	

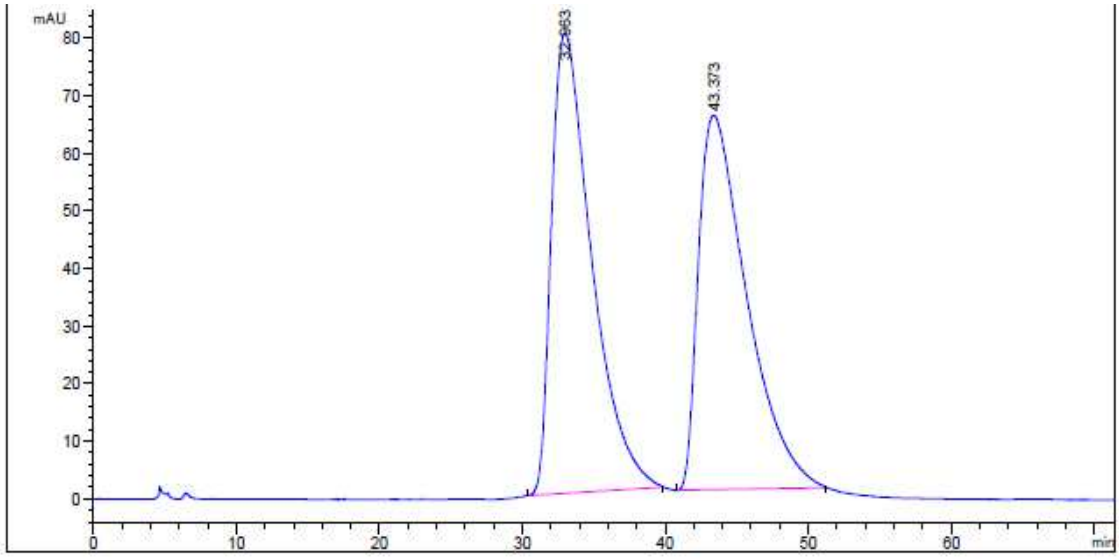


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	21.969	BB	1.4550	2.84514e4	275.90280	96.4441
2	28.897	BB	1.2564	1049.00342	9.99539	3.5559
总量：				2.95004e4	285.89819	

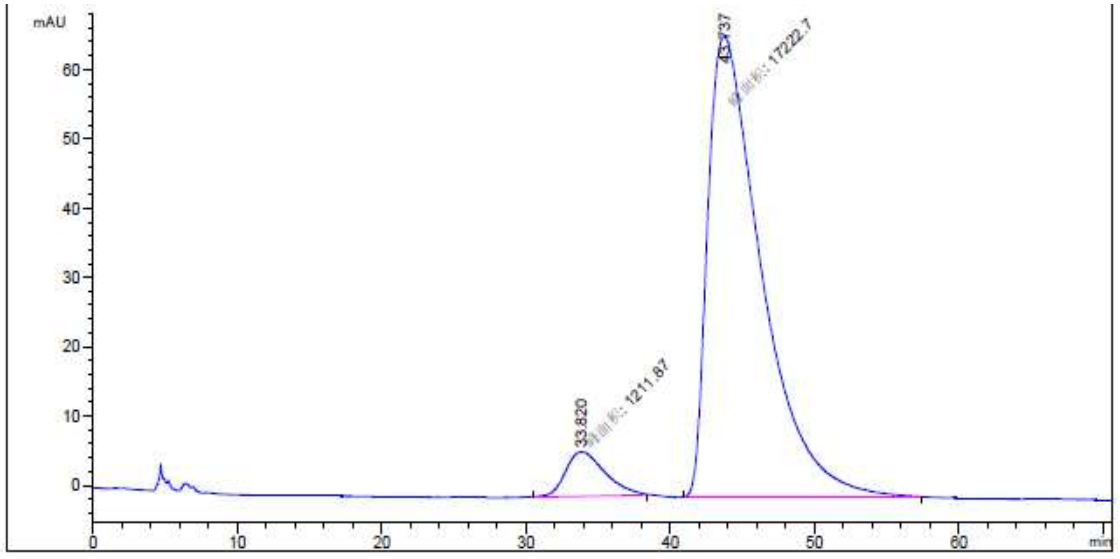


4l

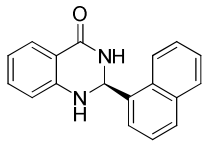
87% ee. [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.7 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	32.963	BB	2.3592	1.56092e4	79.95190	50.5478
2	43.373	BB	2.8125	1.52709e4	65.03032	49.4522
总量 :				3.08801e4	144.98222	

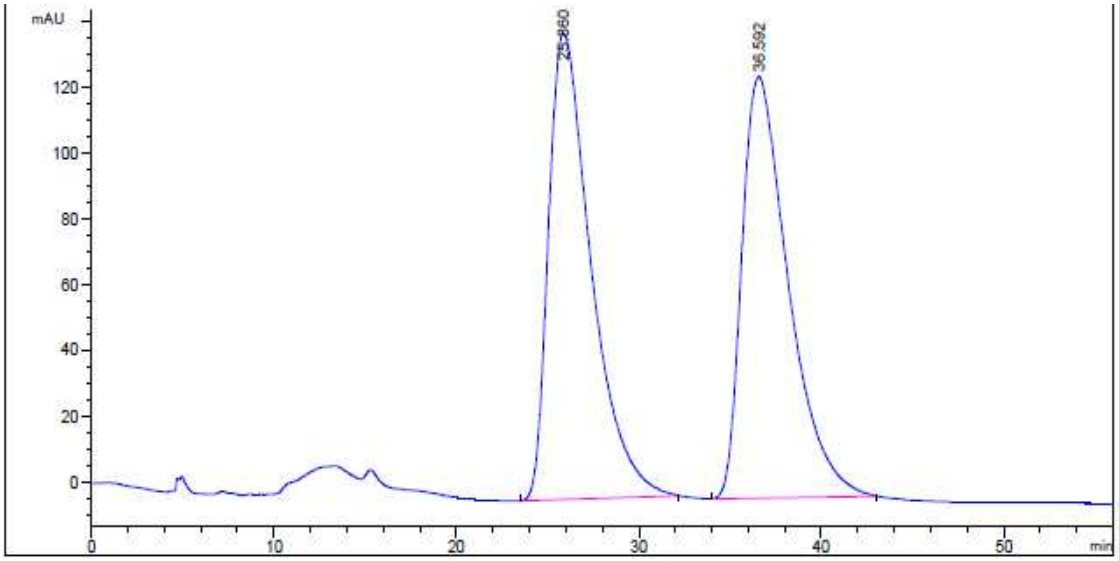


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	33.820	MM	3.1458	1211.86511	6.42054	6.5739
2	43.737	MM	4.3159	1.72227e4	66.50784	93.4261
总量 :				1.84345e4	72.92838	

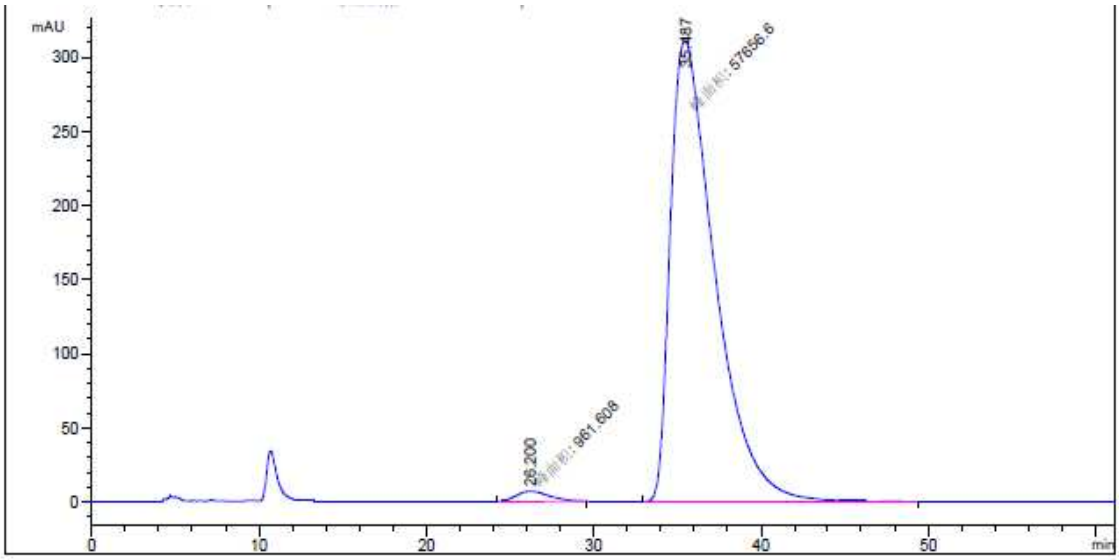


4m

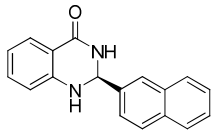
97% ee. [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 60 / 40, 0.7 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	25.860	BB	2.3521	2.30509e4	141.92198	50.3951
2	36.592	BB	2.5173	2.26895e4	128.31454	49.6049
总量 :				4.57404e4	270.23653	

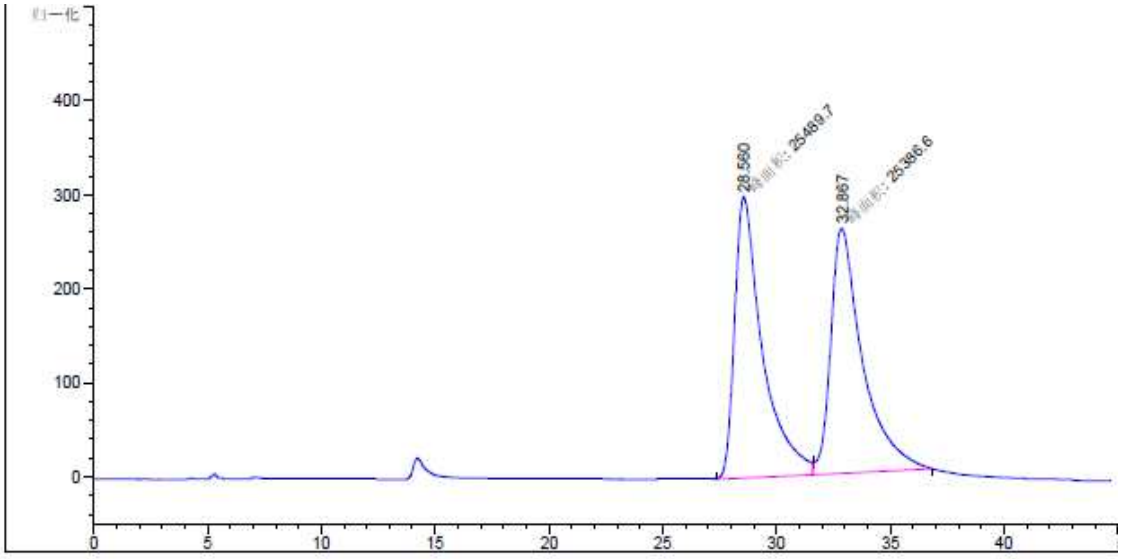


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	26.200	MM	2.3160	961.60840	6.92013	1.6405
2	35.487	MM	3.0890	5.76566e4	311.08728	98.3595
总量 :				5.86182e4	318.00741	

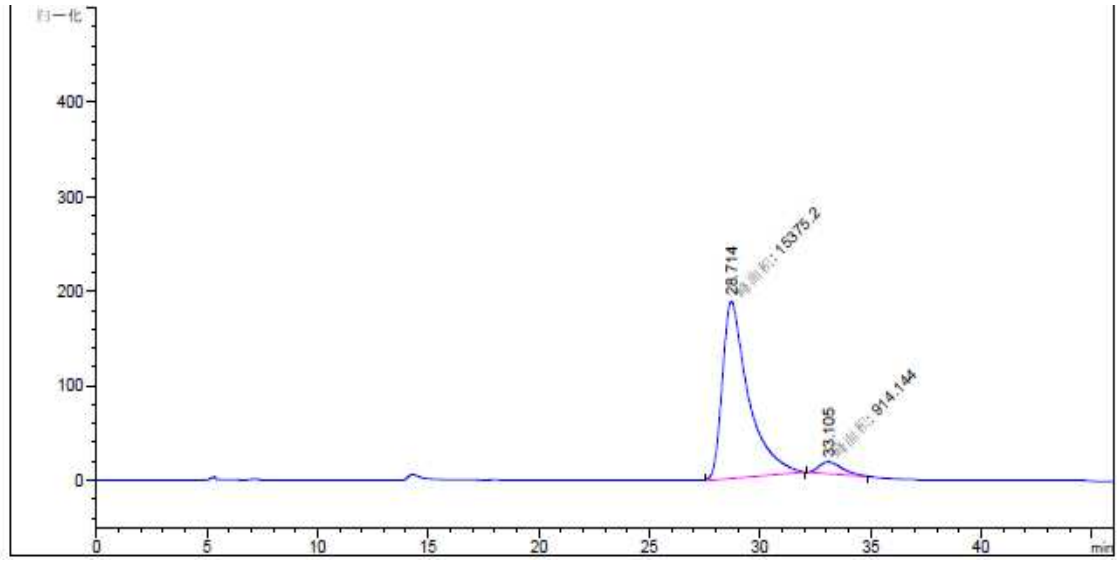


4n

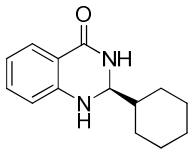
89% ee. [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 80 / 20, 0.7 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	28.560	MF	1.4181	2.54897e4	299.58112	50.1013
2	32.867	FM	1.6228	2.53866e4	260.73431	49.8987
总量 :				5.08763e4	560.31543	

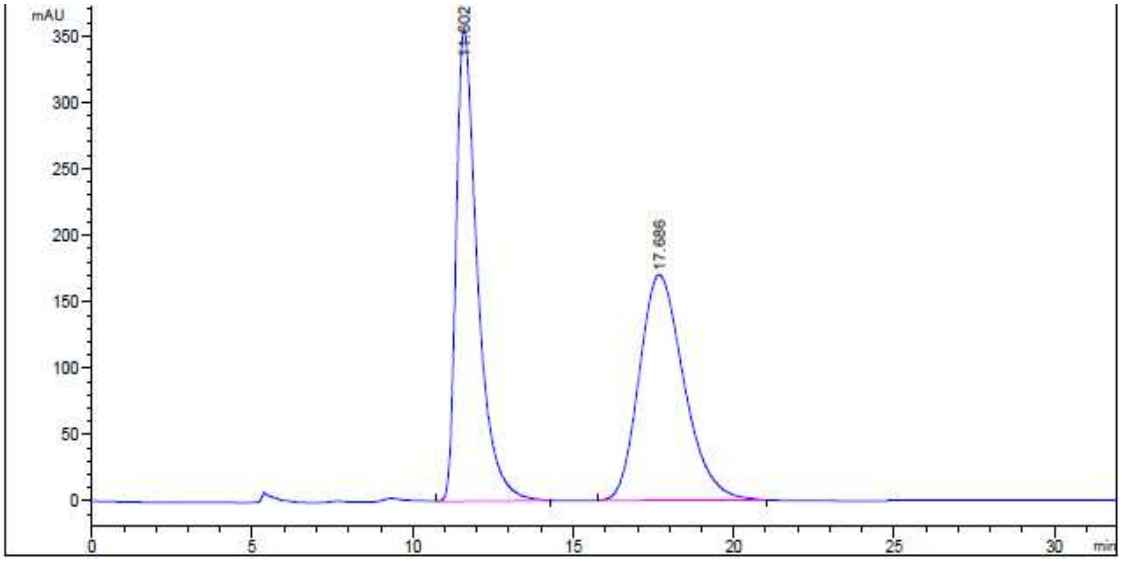


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	28.714	MM	1.3657	1.53752e4	187.63676	94.3881
2	33.105	MM	1.1949	914.14404	12.75068	5.6119
总量 :				1.62893e4	200.38744	

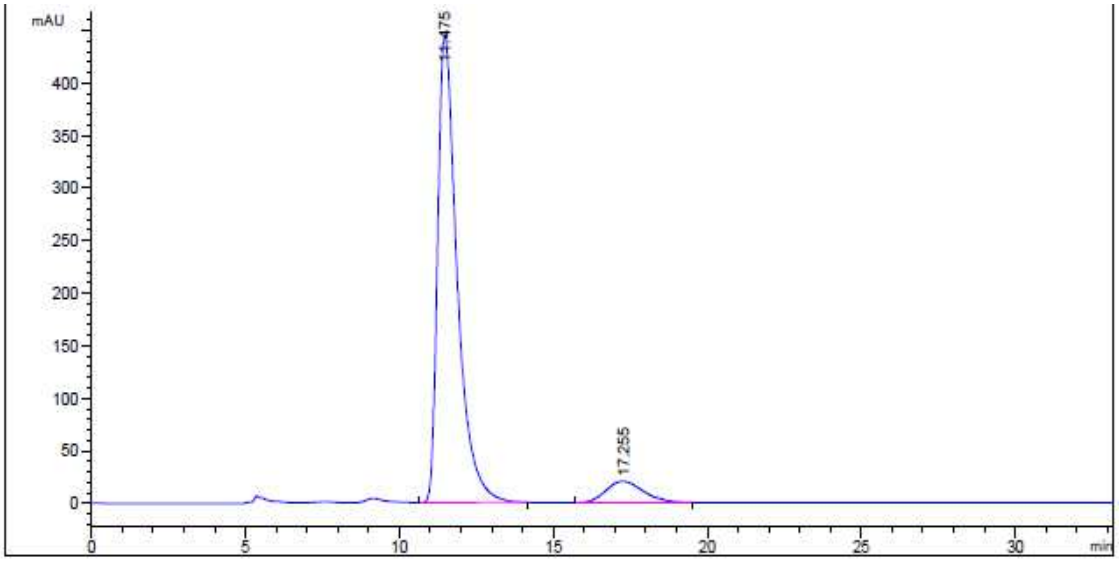


4o

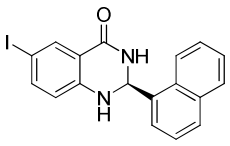
84% ee. [Daicel Chiralpak AS-H, *n*-hexane / *i*-propanol = 50 / 50, 0.6 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	11.602	VB	0.6973	1.64647e4	354.74652	50.0702
2	17.686	BB	1.4720	1.64185e4	169.53250	49.9298
总量：				3.28831e4	524.27902	

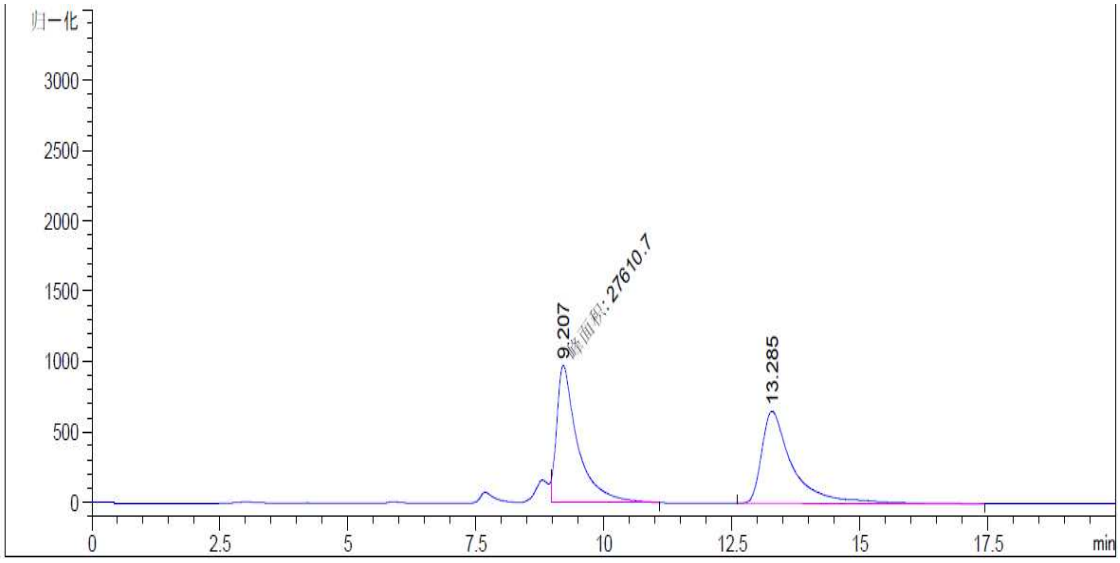


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	11.475	VB	0.6624	1.95932e4	444.79687	91.8766
2	17.255	BB	1.1027	1732.35510	20.40336	8.1234
总量：				2.13255e4	465.20024	

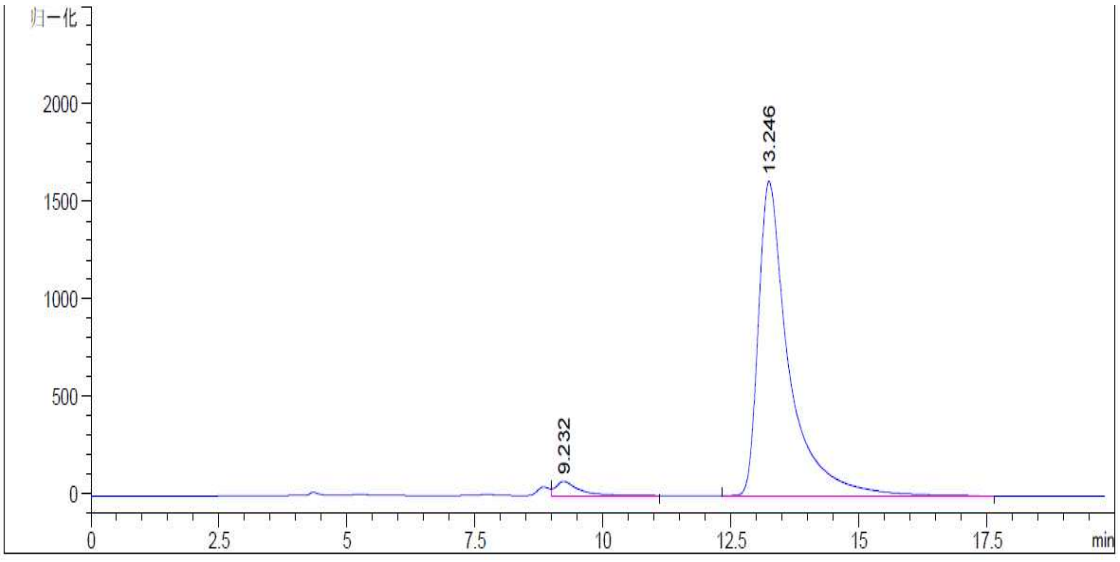


4p

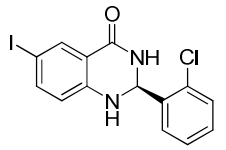
93% ee. [Daicel Chiralpak AD-H, *n*-hexane / *i*-propanol = 70 / 30, 0.8mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	9.207	MM	0.4735	2.76107e4	971.88367	49.9969
2	13.285	VB	0.6071	2.76140e4	654.72113	50.0031
总量 :				5.52247e4	1626.60480	

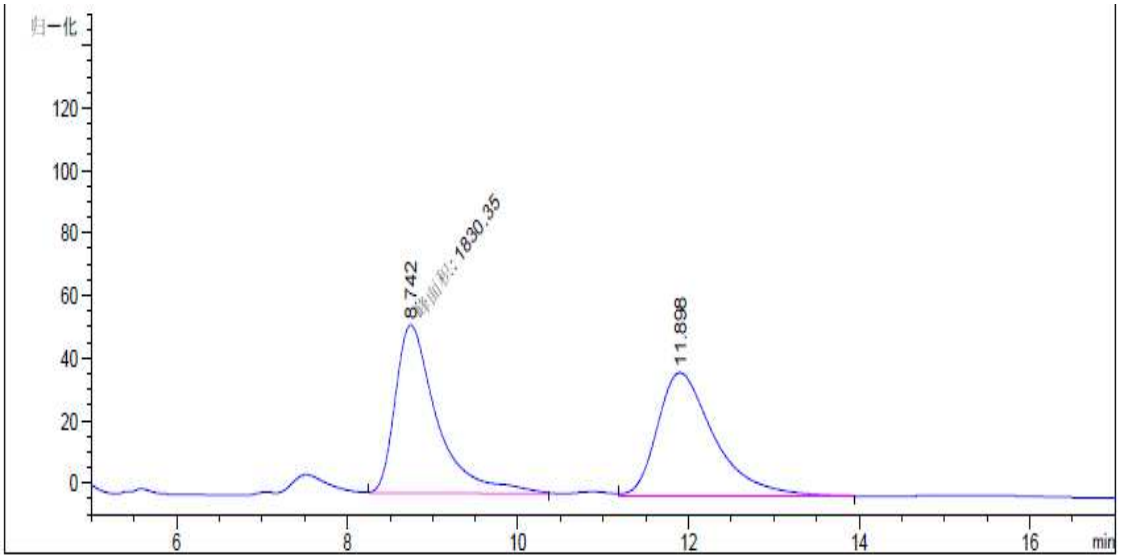


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	9.232	VB	0.4382	2276.00879	72.95386	3.2977
2	13.246	BB	0.5998	6.67424e4	1611.19604	96.7023
总量 :				6.90184e4	1684.14990	

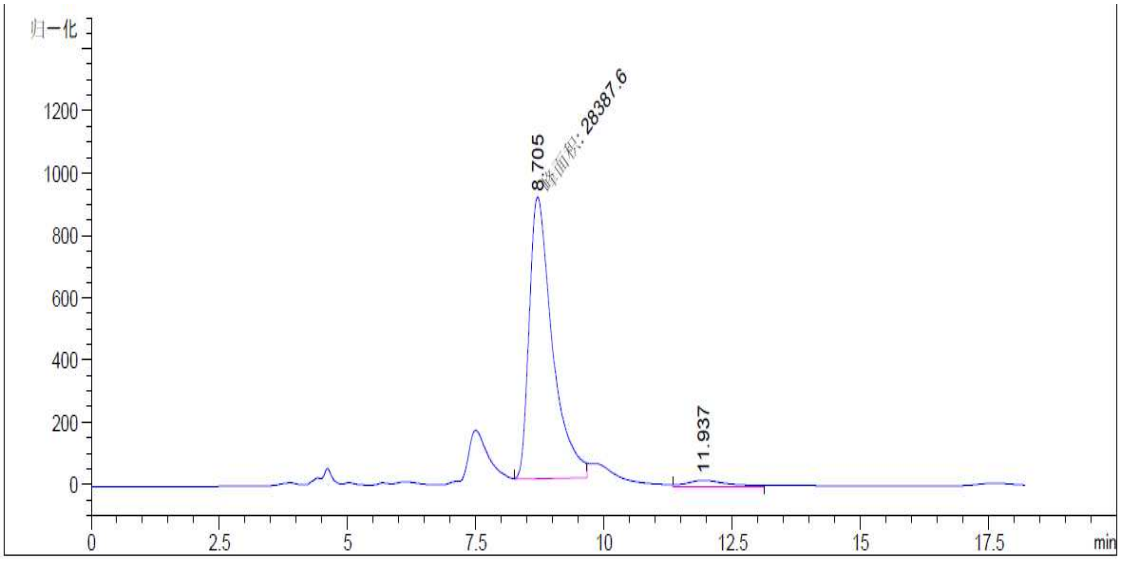


4q

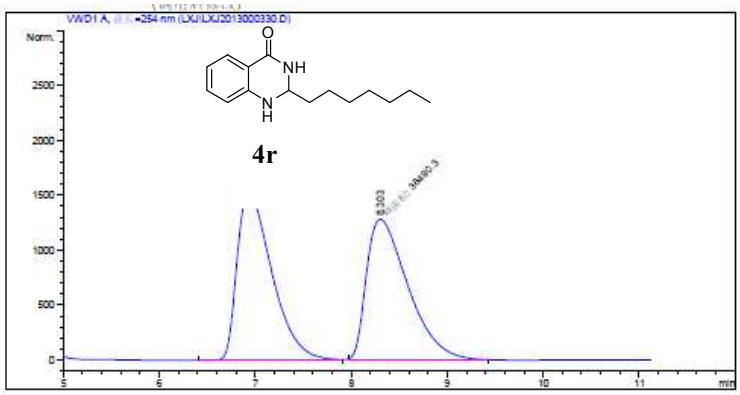
94% ee. [Daicel Chiralcel OD-H, *n*-hexane / *i*-propanol = 70 / 30, 0.8 mL/min, λ = 254 nm]



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	8.742	MM	0.5669	1830.35168	53.80982	49.8578
2	11.898	VB	0.6966	1840.78943	39.49788	50.1422
总量 :				3671.14111	93.30770	



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	8.705	MM	0.5231	2.83876e4	904.50183	96.9519
2	11.937	BB	0.7167	892.47412	18.27933	3.0481
总量 :				2.92801e4	922.78116	



4r

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面积百分比报告
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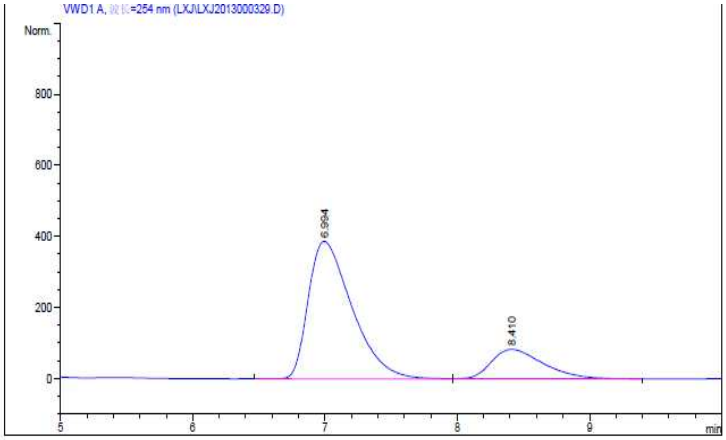
排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	6.937	BV	0.3890	3.86153e4	1522.74060	50.0810
2	8.303	MM	0.5017	3.84903e4	1278.63196	49.9190



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面积百分比报告
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排序 : 信号
乘积因子 : 1.0000
稀释因子 : 1.0000
内标使用乘积因子和稀释因子

信号 1: VWD1 A, 波长=254 nm

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	6.994	BV	0.3541	8904.45117	387.31531	79.5750
2	8.410	VB	0.4197	2285.56421	83.15965	20.4250