

Supporting Information

Synthesis of highly substituted 4*H*-pyrido[1,2-*a*]pyrimidines via a one-pot three-component condensation reaction

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Table of Contents

General Consideration	S1
Experimental Procedures and Compound Characterization	S1
Figure Legends	S7
Spectra	S12

General Consideration

Toluene and ethanol (EtOH) were dried with Na and distilled. Acetonitrile (CH₃CN) and *N,N*-dimethylformamide (DMF) was dried with CaH₂ and distilled. All other commercial reagents were used as received without additional purification. Melting point was uncorrected. Mass spectra and HPLC data was recorded on a LC/MS system with ELSD. The ¹H and ¹³C NMR data were obtained on a 300 MHz NMR spectrometer with TMS as the internal standard and CDCl₃ as solvent unless otherwise stated. Multiplicities are indicated as the following: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doubled doublet; br, broad. Coupling constants (*J* values) where noted are quoted in Hertz.

Experimental Procedures and Compound Characterization

General procedure for the synthesis of 4*H*-pyrido[1,2-*a*]pyrimidine **4.** To a stirred mixture of 2-aminopyridine **1** (1.0 mmol), aldehyde **2** (1.1 or 2.0 mmol) and ketone **3** (3.0 mol) or aldehyde **3** (1.1 mmol) in toluene (0.5 mL) was added CF₃SO₃H (44 μL, 0.5 mmol) under N₂. The resulting solution was stirred for the corresponding time under reflux. The reaction mixture was then diluted with CH₂Cl₂ (20 mL), washed with concentrated ammonia solution (20 mL). The water layer was extracted with CH₂Cl₂ (3 x 10 mL). The combined organic layers were washed with brine (30 mL), dried over Na₂SO₄, and concentrated *in vacuo*. Purification by flash column chromatography (CH₂Cl₂/EtOAc/MeOH/ concentrated ammonia solution 100:50:1.5:1.5, v/v) afforded the desired product **4**.

11-(4-Chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline **4{*1,1,1*}.** 69%; yellow solid, mp: 85–87 °C; ¹H NMR: δ 7.51–7.23 (m, 7H), 6.67 (t, 1H, *J* = 6.0), 5.67 (s, 1H), 2.49–2.39 (m, 2H), 1.89–1.62 (m, 6H); ¹³C NMR: δ 148.8, 140.9, 136.5, 135.2, 134.5, 134.0, 129.2, 128.3, 123.2, 109.3, 106.6, 67.9, 29.8, 26.6, 23.0, 22.6; MS (ESI): *m/z* 297.0 [M + H⁺].

11-Phenyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline **4{*1,2,1*}.**

67%; yellow solid, mp: 154–156 °C; ¹H NMR: δ 7.36–7.28 (m, 5H), 6.89 (t, 1H, *J* = 7.8), 6.73–6.69 (m, 2H), 5.98 (t, 1H, *J* = 6.6), 5.37 (s, 1H), 2.38–2.24 (m, 2H),

1.74–1.59 (m, 6H); ^{13}C NMR: δ 148.7, 142.6, 136.8, 135.3, 133.1, 128.7, 128.2, 126.8, 123.6, 108.1, 106.6, 68.3, 30.3, 26.6, 23.1, 22.6; MS (ESI): m/z 263.0 $[\text{M} + \text{H}^+]$.

11-(4-Nitrophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{*I*,3,*I*}.

53%; yellow solid, mp: 150–152 °C; ^1H NMR: δ 8.25–8.22 (m, 2H), 7.54–7.45 (m, 3H), 7.34–7.29 (m, 1H), 7.07 (d, 1H, $J = 6.3$), 6.46 (t, 1H, $J = 6.3$), 5.72 (s, 1H), 2.53–2.37 (m, 2H), 1.91–1.61 (m, 6H); MS (ESI): m/z 308.0 $[\text{M} + \text{H}^+]$.

11-(4-Methoxyphenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{*I*,4,*I*}.

75%; yellow solid, mp: 88–90 °C; ^1H NMR: δ 7.27–7.21 (m, 2H), 6.88–6.84 (m, 3H), 6.76–6.68 (m, 2H), 5.99 (t, 1H, $J = 6.6$), 5.32 (s, 1H), 3.79 (s, 3H), 2.39–2.29 (m, 2H), 1.77–1.57 (m, 6H); ^{13}C NMR: δ 159.7, 148.9, 136.6, 135.4, 135.1, 133.4, 128.3, 123.5, 114.2, 108.6, 107.0, 67.9, 55.3, 30.2, 26.7, 23.2, 22.8; MS (ESI): m/z 293.0 $[\text{M} + \text{H}^+]$.

11-(*p*-Tolyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{*I*,5,*I*}.

65%; yellow solid, mp: 126–127 °C; ^1H NMR: δ 7.24–7.11 (m, 4H), 6.87 (t, 1H, $J = 7.8$), 6.73–6.65 (m, 2H), 5.96 (t, 1H, $J = 6.6$), 5.32 (s, 1H), 2.32–2.30 (m, 5H), 1.79–1.58 (m, 6H); ^{13}C NMR: δ 148.9, 139.8, 138.2, 136.5, 135.4, 133.4, 129.6, 126.9, 123.5, 108.5, 106.9, 66.2, 30.2, 26.7, 23.2, 22.7, 21.2; MS (ESI): m/z 276.9 $[\text{M} + \text{H}^+]$.

11-(*o*-Tolyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{*I*,6,*I*}.

55%; yellow solid, mp: 95–96 °C; ^1H NMR: δ 7.32–7.11 (m, 4H), 6.90–6.85 (m, 1H), 6.66 (d, 1H, $J = 9.3$), 6.55 (d, 1H, $J = 6.6$), 5.93 (t, 1H, $J = 6.6$), 5.82 (s, 1H), 2.37–2.26 (m, 5H), 1.72–1.56 (m, 6H); ^{13}C NMR: δ 149.2, 140.6, 135.9, 135.4, 133.9, 131.1, 129.5, 128.3, 126.8, 123.2, 108.9, 106.5, 66.2, 29.9, 26.4, 23.1, 22.6, 19.2; MS (ESI): m/z 276.9 $[\text{M} + \text{H}^+]$.

11-(*m*-Tolyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{*I*,7,*I*}.

68%; yellow solid, mp: 110–112 °C; ^1H NMR: δ 7.24–7.09 (m, 4H), 6.92–6.87 (m, 1H), 6.73–6.69 (m, 2H), 6.99 (t, 1H, $J = 6.6$), 5.33 (s, 1H), 2.33–2.29 (m, 5H), 1.72–1.59 (m, 6H); ^{13}C NMR: δ 148.9, 142.5, 138.7, 136.1, 135.5, 133.8, 129.3, 128.7, 127.6, 124.2, 123.2, 108.9, 106.9, 68.6, 30.0, 26.6, 23.1, 22.7, 21.5; MS (ESI): m/z 276.9 $[\text{M} + \text{H}^+]$.

11-(Naphthalen-1-yl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{*I*,8,*I*}.

53%; yellow solid, mp: 138–140 °C; ¹H NMR: δ 8.25 (d, 1H, *J* = 8.1), 7.90–7.82 (m, 2H), 7.59–7.42 (m, 4H), 6.92–6.78 (m, 2H), 6.68 (d, 1H, *J* = 6.6), 6.25 (s, 1H), 5.89 (t, 1H, *J* = 6.0), 2.40–2.26 (m, 2H), 1.76–1.44 (m, 6H); ¹³C NMR: δ 149.1, 136.1, 135.0, 134.1, 133.9, 130.6, 129.5, 129.1, 127.7, 127.0, 126.0, 125.3, 123.3, 122.9, 108.6, 107.2, 77.4, 30.1, 26.6, 23.0, 22.6; MS (ESI): *m/z* 313.1 [M + H⁺].

11-(Thiophen-2-yl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{1,9,1}.

38%; yellow solid, mp: 119–120 °C; ¹H NMR: δ 7.28–7.25 (m, 1H), 7.00–6.98 (m, 1H), 6.95–6.86 (m, 3H), 6.66 (d, 1H, *J* = 9.3), 6.08–6.03 (m, 1H), 5.63 (s, 1H), 2.41–2.23 (m, 2H), 2.00–1.59 (m, 6H); ¹³C NMR: δ 148.2, 146.0, 137.3, 135.1, 133.7, 126.8, 126.6, 125.3, 123.2, 109.2, 106.5, 62.7, 29.9, 26.7, 23.1, 22.7; MS (ESI): *m/z* 269.0 [M + H⁺].

11-(Pyridin-4-yl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{1,10,1}.

50%; yellow solid, mp: 140–141 °C; ¹H NMR: δ 8.59 (dd, 2H, *J* = 4.5, 1.5), 7.19 (dd, 2H, *J* = 4.5, 1.5), 6.95 (dd, 1H, *J* = 15.0, 7.8), 6.78 (d, 1H, *J* = 7.8), 6.66 (d, 1H, *J* = 6.9), 6.07 (t, 1H, *J* = 6.6), 5.36 (s, 1H), 2.38–2.23 (m, 2H), 1.85–1.55 (m, 6H); MS (ESI): *m/z* 264.1 [M + H⁺].

11-Butyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{1,11,1}.

48%; yellow oil; ¹H NMR: δ 6.94 (ddd, 1H, *J* = 9.0, 6.3, 1.5), 6.80 (dd, 1H, *J* = 6.9, 1.2), 6.68 (d, 1H, *J* = 9.0), 6.09 (td, 1H, *J* = 6.6, 1.5), 4.34 (t, 1H, *J* = 4.8), 2.33–2.11 (m, 3H), 1.84–1.52 (m, 7H), 1.37–1.12 (m, 4H), 0.85 (t, 3H, *J* = 6.9); ¹³C NMR: δ 149.6, 137.1, 135.2, 134.0, 122.0, 108.7, 105.8, 64.4, 34.5, 29.4, 27.1, 26.6, 23.1, 22.9, 22.7, 14.0; MS (ESI): *m/z* 243.1 [M + H⁺].

11-Propyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{1,12,1}.

46%; yellow oil; ¹H NMR: δ 6.99–6.86 (m, 1H), 6.81–6.77 (m, 1H), 6.65–6.56 (m, 1H), 6.08 (td, 1H, *J* = 6.6, 1.5), 4.34 (t, 1H, *J* = 4.8), 2.31–2.09 (m, 3H), 1.84–1.50 (m, 7H), 1.43–1.21 (m, 2H), 0.87 (t, 3H, *J* = 7.2); MS (ESI): *m/z* 229.2 [M + H⁺].

11-Cyclopentyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{1,13,1}.

85%; yellow solid, mp: 94–96 °C; ¹H NMR: δ 6.94–6.89 (m, 1H), 6.80 (d, 1H, *J* = 5.7), 6.66 (d, 1H, *J* = 9.0), 6.05 (t, 1H, *J* = 6.0), 3.98 (d, 1H, *J* = 6.9), 2.37–2.08 (m, 4H), 1.92–1.47 (m, 11H), 1.30–1.13 (m, 2H); ¹³C NMR: δ 149.7, 138.6, 136.0, 132.9, 122.3,

107.2, 106.6, 67.9, 47.2, 30.2, 30.1, 29.3, 29.0, 24.7, 24.1, 23.4, 23.3; MS (ESI): m/z 255.0 $[M + H^+]$.

11-Cyclohexyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{1,14,1}.

87%; yellow solid, mp: 138–140 °C; 1H NMR: δ 6.93 (t, 1H, $J = 7.2$), 6.74 (d, 1H, $J = 6.6$), 6.65 (d, 1H, $J = 9.0$), 6.04 (t, 1H, $J = 6.6$), 3.98 (d, 1H, $J = 3.9$), 2.37–2.23 (m, 3H), 2.05–1.52 (m, 11H), 1.25–0.8 (m, 5H); ^{13}C NMR: δ 150.1, 138.8, 136.1, 132.9, 122.3, 106.9, 105.1, 69.4, 44.8, 30.7, 30.1, 28.7, 28.1, 26.4, 26.3, 26.2, 23.3, 23.1; MS (ESI): m/z 269.0 $[M + H^+]$.

11-(4-Chlorophenyl)-8-(piperidin-1-yl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{2,1,1}.

62%; yellow solid, mp: 165–167 °C; 1H NMR: δ 7.32–7.21 (m, 4H), 7.00 (s, 2H), 6.09 (s, 1H), 5.34 (s, 1H), 2.81–2.67 (m, 4H), 2.42–2.26 (m, 2H), 1.72–1.49 (m, 12H); ^{13}C NMR: δ 145.5, 140.3, 139.1, 134.6, 132.3, 129.2, 128.3, 122.0, 119.1, 105.3, 68.5, 51.0, 28.5, 26.3, 25.6, 23.7, 22.7, 22.5; MS (ESI): m/z 380.1 $[M + H^+]$.

8-Chloro-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 4{3,1,1}.

68%; yellow solid, mp: 130–132 °C; 1H NMR: δ 7.35–7.32 (m, 2H), 7.27–7.22 (m, 2H), 6.89–6.85 (m, 1H), 6.78 (s, 1H), 6.75 (d, 1H, $J = 2.1$), 5.32 (s, 1H), 2.34–2.23 (m, 2H), 1.77–1.59 (m, 6H); ^{13}C NMR: δ 146.8, 140.4, 136.6, 134.9, 134.8, 132.5, 129.4, 128.3, 124.6, 115.3, 107.4, 68.0, 29.9, 26.6, 22.9, 22.5; MS (ESI): m/z 330.8 $[M + H^+]$.

Ethyl 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline-8-carboxylate 4{4,1,1}.

65%; yellow solid, mp: 123–125 °C; 1H NMR: δ 7.62 (d, 1H, $J = 1.8$), 7.37–7.31 (m, 3H), 7.29–7.24 (m, 2H), 6.64 (d, 1H, $J = 9.6$), 5.34 (s, 1H), 4.30–4.18 (m, 2H), 2.39–2.23 (m, 2H), 1.77–1.58 (m, 6H), 1.30 (t, 3H, $J = 7.2$); ^{13}C NMR: δ 164.0, 147.5, 141.1, 140.2, 136.4, 134.9, 132.2, 129.5, 128.3, 122.3, 112.8, 109.0, 67.9, 61.0, 29.8, 26.5, 22.9, 22.4, 14.4; MS (ESI): m/z 368.9 $[M + H^+]$.

4-(4-Chlorophenyl)-2-ethyl-3-methyl-4H-pyrido[1,2-*a*]pyrimidine 4{1,1,2}.

47%; yellow solid, mp: 103–104 °C; 1H NMR: δ 7.32–7.24 (m, 4H), 6.92–6.87 (m,

1H), 6.77–6.70 (m, 2H), 6.01 (t, 1H, $J = 6.3$), 5.34 (s, 1H), 2.30 (dt, 2H, $J = 13.5, 6.6$), 1.54 (s, 3H), 1.15 (t, 3H, $J = 7.5$); ^{13}C NMR: δ 148.9, 140.9, 140.7, 134.9, 134.5, 133.7, 129.2, 128.3, 123.3, 109.1, 103.0, 68.3, 26.2, 15.6, 13.0; MS (ESI): m/z 285.1 $[\text{M} + \text{H}^+]$.

4-(4-Chlorophenyl)-3-methyl-2-phenyl-4H-pyrido[1,2-*a*]pyrimidine 4{1,1,4}.

41%; yellow solid, mp: 165–166 °C; ^1H NMR: δ 7.44–7.25 (m, 9H), 6.98–6.80 (m, 3H), 6.09 (t, 1H, $J = 6.6$), 5.50 (s, 1H), 1.58 (s, 3H); ^{13}C NMR: δ 148.7, 140.7, 140.0, 139.8, 134.9, 134.5, 133.7, 129.2, 129.0, 128.2, 128.0, 127.2, 123.8, 109.2, 105.4, 68.5, 17.3; MS (ESI): m/z 333.0 $[\text{M} + \text{H}^+]$.

4-(4-Chlorophenyl)-2,3-diphenyl-4H-pyrido[1,2-*a*]pyrimidine 4{1,1,5}.

26%; yellow solid, mp: 179–180 °C; ^1H NMR: δ 7.42–7.39 (m, 4H), 7.34–7.31 (m, 2H), 7.21–7.16 (m, 3H), 7.06–7.01 (m, 5H), 6.95–6.87 (m, 3H), 6.22 (t, 1H, $J = 6.6$), 5.81 (s, 1H); ^{13}C NMR: δ 149.2, 143.4, 140.4, 140.2, 139.4, 135.0, 134.8, 134.3, 130.0, 129.5, 129.4, 128.5, 128.1, 127.9, 127.5, 126.2, 123.9, 110.4, 107.6, 67.8; MS (ESI): m/z 394.8 $[\text{M} + \text{H}^+]$.

4-(4-Chlorophenyl)-3-phenyl-4H-pyrido[1,2-*a*]pyrimidine 4{1,1,6}.

62%; yellow solid, mp: 148–150 °C; ^1H NMR: δ 7.43 (s, 1H), 7.40–7.36 (m, 2H), 7.32–7.22 (m, 6H), 7.15–6.97 (m, 3H), 6.75 (d, 1H, $J = 9.0$), 6.21 (td, 1H, $J = 6.6, J = 1.5$), 6.00 (s, 1H); ^{13}C NMR: δ 149.8, 139.5, 136.6, 135.6, 134.8, 134.5, 133.3, 129.5, 128.6, 128.4, 126.2, 124.1, 123.7, 111.0, 110.8, 65.1; MS (ESI): m/z 319.1 $[\text{M} + \text{H}^+]$.

4-(4-Chlorophenyl)-3-propyl-4H-pyrido[1,2-*a*]pyrimidine 4{1,1,7}.

43%; yellow solid, mp: 75–76 °C; ^1H NMR: δ 7.34–7.29 (m, 4H), 6.92–6.86 (m, 1H), 6.73–6.65 (m, 2H), 6.5 (s, 1H), 6.05–6.00 (m, 1H), 5.51 (s, 1H), 1.82–1.76 (m, 2H), 1.51–1.29 (m, 2H), 0.87 (t, 3H, $J = 7.2$); ^{13}C NMR: δ 149.3, 140.6, 135.4, 134.5, 133.6, 129.7, 129.2, 128.3, 123.6, 113.7, 109.3, 66.5, 33.4, 19.8, 13.8; MS (ESI): m/z 285.1 $[\text{M} + \text{H}^+]$.

4-Cyclohexyl-3-phenyl-4H-pyrido[1,2-*a*]pyrimidine 4{1,14,6}.

65%; yellow solid, mp: 146–148 °C; ^1H NMR: δ 7.44–7.41 (m, 2H), 7.34–7.29 (m, 2H), 7.24 (s, 1H), 7.16 (t, 1H, $J = 7.2$), 7.09–7.05 (m, 1H), 6.96 (d, 1H, $J = 6.6$), 6.77 (d, 1H, $J = 9.0$), 6.24 (t, 1H, $J = 6.6$), 4.87 (d, 1H, $J = 4.2$), 1.75–1.55 (m, 6H),

1.07–0.71 (m, 5H); ^{13}C NMR: δ 151.6, 138.5, 136.8, 134.2, 134.0, 128.8, 125.7, 123.8, 122.9, 111.4, 108.8, 66.8, 45.4, 30.8, 28.4, 26.4, 26.2; MS (ESI): m/z 291.0 $[\text{M} + \text{H}^+]$.

4-Benzyl-3-phenyl-4H-pyrido[1,2-*a*]pyrimidine 4{1,15,6}.

62%; yellow solid, mp: 122–123 °C; ^1H NMR: δ 7.50–7.47 (m, 2H), 7.41–7.35 (m, 2H), 7.25–7.12 (m, 5H), 7.03–6.98 (m, 3H), 6.79 (d, 1H, $J = 8.7$), 6.32 (d, 1H, $J = 6.9$), 5.87 (d, 1H, $J = 6.6$), 5.13 (dd, 1H, $J = 9.4$, $J = 3.2$), 3.08–2.88 (m, 2H); ^{13}C NMR: δ 150.6, 137.1, 136.7, 136.4, 134.6, 133.6, 129.4, 129.0, 128.7, 127.0, 125.9, 123.4, 122.4, 111.1, 108.6, 64.4, 40.4; MS (ESI): m/z 298.9 $[\text{M} + \text{H}^+]$.

11-(4-Chlorophenyl)-6,7,8,9,10,11-hexahydrocyclohepta[*d*]pyrido[1,2-*a*]pyrimidine 4{1,1,9}.

73%; yellow solid, mp: 85–87 °C; ^1H NMR: δ 7.33–7.27 (m, 4H), 6.92–6.72 (m, 3H), 6.05 (d, 1H, $J = 6.0$), 5.42 (s, 1H), 2.53–2.50 (m, 2H), 2.09–2.01 (m, 1H), 1.86–1.78 (m, 1H), 1.68–1.58 (m, 4H), 1.49–1.40 (m, 1H), 1.19–1.08 (m, 1H); MS (ESI): m/z 311.0 $[\text{M} + \text{H}^+]$.

(*E*)-4-(4-Chlorobenzylidene)-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 5{1,1,1}.

8%; yellow solid, mp: 105–106 °C; ^1H NMR: δ 7.54 (s, 1H), 7.34–7.24 (m, 9H), 6.95 (s, 1H), 6.74 (d, 1H, $J = 6.3$), 6.04 (s, 1H), 5.44 (s, 1H), 2.77–2.69 (m, 1H), 2.56–2.47 (m, 1H), 1.96–1.91 (m, 2H), 1.72–1.64 (m, 2H); ^{13}C NMR: δ 149.1, 140.6, 137.1, 135.2, 135.0, 134.7, 134.1, 131.7, 130.8, 129.3, 128.3, 128.1, 124.1, 123.3, 111.2, 109.2, 90.5, 67.8, 27.6, 27.3, 22.7; MS (ESI): m/z 418.9 $[\text{M} + \text{H}^+]$.

Figure Legends:

Fig. S-1: LC-MS-ELSD of 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,1,1}.

Fig. S-2: ¹H Spectra of 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,1,1}.

Fig. S-3: ¹³C Spectra of 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,1,1}.

Fig. S-4: LC-MS-ELSD of 11-phenyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,2,1}.

Fig. S-5: ¹H Spectra of 11-phenyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,2,1}.

Fig. S-6: ¹³C Spectra of 11-phenyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,2,1}.

Fig. S-7: LC-MS-ELSD of 11-(4-nitrophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,3,1}.

Fig. S-8: ¹H Spectra of 11-(4-nitrophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,3,1}.

Fig. S-9: LC-MS-ELSD of 11-(4-methoxyphenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,4,1}.

Fig. S-10: ¹H Spectra of 11-(4-methoxyphenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,4,1}.

Fig. S-11: ¹³C Spectra of 11-(4-methoxyphenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,4,1}.

Fig. S-12: LC-MS-ELSD of 11-(*p*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,5,1}.

Fig. S-13: ¹H Spectra of 11-(*p*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,5,1}.

Fig. S-14: ¹³C Spectra of 11-(*p*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,5,1}.

Fig. S-15: LC-MS-ELSD of 11-(*o*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,6,1}.

Fig. S-16: ¹H Spectra of 11-(*o*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,6,1}.

Fig. S-17: ¹³C Spectra of 11-(*o*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,6,1}.

Fig. S-18: LC-MS-ELSD of 11-(*m*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]
quinazoline 4{1,7,1}.

Fig. S-19: ¹H Spectra of 11-(*m*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]
quinazoline 4{1,7,1}.

Fig. S-20: ¹³C Spectra of 11-(*m*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]
quinazoline 4{1,7,1}.

Fig. S-21: LC-MS-ELSD of 11-(naphthalen-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,8,1}.

Fig. S-22: ¹H Spectra of 11-(naphthalen-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,8,1}.

Fig. S-23: ¹³C Spectra of 11-(naphthalen-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,8,1}.

Fig. S-24: LC-MS-ELSD of 11-(thiophen-2-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,9,1}.

Fig. S-25: ¹H Spectra of 11-(thiophen-2-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,9,1}.

Fig. S-26: ¹³C Spectra of 11-(thiophen-2-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,9,1}.

Fig. S-27: LC-MS-ELSD of 11-(pyridin-4-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,10,1}.

Fig. S-28: ¹H Spectra of 11-(pyridin-4-yl)-2,3,4,11-tetrahydro-1*H*-pyrido
[2,1-*b*]quinazoline 4{1,10,1}.

Fig. S-29: LC-MS-ELSD of 11-butyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]
quinazoline 4{1,11,1}.

Fig. S-30: ^1H Spectra of 11-butyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,11,1}.

Fig. S-31: ^{13}C Spectra of 11-butyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,11,1}.

Fig. S-32: LC-MS-ELSD of 11-propyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,12,1}.

Fig. S-33: ^1H Spectra of 11-propyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,12,1}.

Fig. S-34: LC-MS-ELSD of 11-cyclopentyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,13,1}.

Fig. S-35: ^1H Spectra of 11-cyclopentyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,13,1}.

Fig. S-36: ^{13}C Spectra of 11-cyclopentyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,13,1}.

Fig. S-37: LC-MS-ELSD of 11-cyclohexyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,14,1}.

Fig. S-38: ^1H Spectra of 11-cyclohexyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,14,1}.

Fig. S-39: ^{13}C Spectra of 11-cyclohexyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,14,1}.

Fig. S-40: LC-MS-ELSD of 11-(4-chlorophenyl)-8-(piperidin-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{2,1,1}.

Fig. S-41: ^1H Spectra of 11-(4-chlorophenyl)-8-(piperidin-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{2,1,1}.

Fig. S-42: ^{13}C Spectra of 11-(4-chlorophenyl)-8-(piperidin-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{2,1,1}.

Fig. S-43: LC-MS-ELSD of 8-chloro-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{3,1,1}.

Fig. S-44: ^1H Spectra of 8-chloro-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{3,1,1}.

Fig. S-45: ^{13}C Spectra of 8-chloro-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{3,1,1}.

Fig. S-46: LC-MS-ELSD of ethyl 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline-8-carboxylate 4{4,1,1}.

Fig. S-47: ^1H Spectra of ethyl 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline-8-carboxylate 4{4,1,1}.

Fig. S-48: ^{13}C Spectra of ethyl 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline-8-carboxylate 4{4,1,1}.

Fig. S-49: LC-MS-ELSD of 4-(4-chlorophenyl)-2-ethyl-3-methyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,2}.

Fig. S-50: ^1H Spectra of 4-(4-chlorophenyl)-2-ethyl-3-methyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,2}.

Fig. S-51: ^{13}C Spectra of 4-(4-chlorophenyl)-2-ethyl-3-methyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,2}.

Fig. S-52: LC-MS-ELSD of 4-(4-chlorophenyl)-3-methyl-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,4}.

Fig. S-53: ^1H Spectra of 4-(4-chlorophenyl)-3-methyl-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,4}.

Fig. S-54: ^{13}C Spectra of 4-(4-chlorophenyl)-3-methyl-2-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,4}.

Fig. S-55: LC-MS-ELSD of 4-(4-chlorophenyl)-2,3-diphenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,5}.

Fig. S-56: ^1H Spectra of 4-(4-chlorophenyl)-2,3-diphenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,5}.

Fig. S-57: ^{13}C Spectra of 4-(4-chlorophenyl)-2,3-diphenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,5}.

Fig. S-58: LC-MS-ELSD of 4-(4-chlorophenyl)-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,6}.

Fig. S-59: ^1H Spectra of 4-(4-chlorophenyl)-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,6}.

Fig. S-60: ^{13}C Spectra of 4-(4-chlorophenyl)-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,6}.

Fig. S-61: LC-MS-ELSD of 4-(4-chlorophenyl)-3-propyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,7}.

Fig. S-62: ^1H Spectra of 4-(4-chlorophenyl)-3-propyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,7}.

Fig. S-63: ^{13}C Spectra of 4-(4-chlorophenyl)-3-propyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,7}.

Fig. S-64: LC-MS-ELSD of 4-cyclohexyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,14,6}.

Fig. S-65: ^1H Spectra of 4-cyclohexyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,14,6}.

Fig. S-66: ^{13}C Spectra of 4-cyclohexyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,14,6}.

Fig. S-67: LC-MS-ELSD of 4-benzyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,15,6}.

Fig. S-68: ^1H Spectra of 4-benzyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,15,6}.

Fig. S-69: ^{13}C Spectra of 4-benzyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,15,6}.

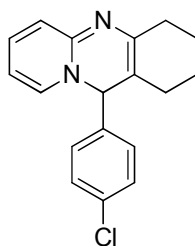
Fig. S-70: LC-MS-ELSD of 11-(4-chlorophenyl)-6,7,8,9,10,11-hexahydrocyclohepta[*d*]pyrido[1,2-*a*]pyrimidine 4{1,1,9}.

Fig. S-71: ^1H Spectra of 11-(4-chlorophenyl)-6,7,8,9,10,11-hexahydrocyclohepta[*d*]pyrido[1,2-*a*]pyrimidine 4{1,1,9}.

Fig. S-72: LC-MS-ELSD of (*E*)-4-(4-chlorobenzylidene)-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 5{1,1,1}.

Fig. S-73: ^1H Spectra of (*E*)-4-(4-chlorobenzylidene)-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 5{1,1,1}.

Fig. S-74: ^{13}C Spectra of (*E*)-4-(4-chlorobenzylidene)-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 5{1,1,1}.



Chemical Formula: C₁₈H₁₇ClN₂

Exact Mass: 296.1

Molecular Weight: 296.8

4{1,1,1}

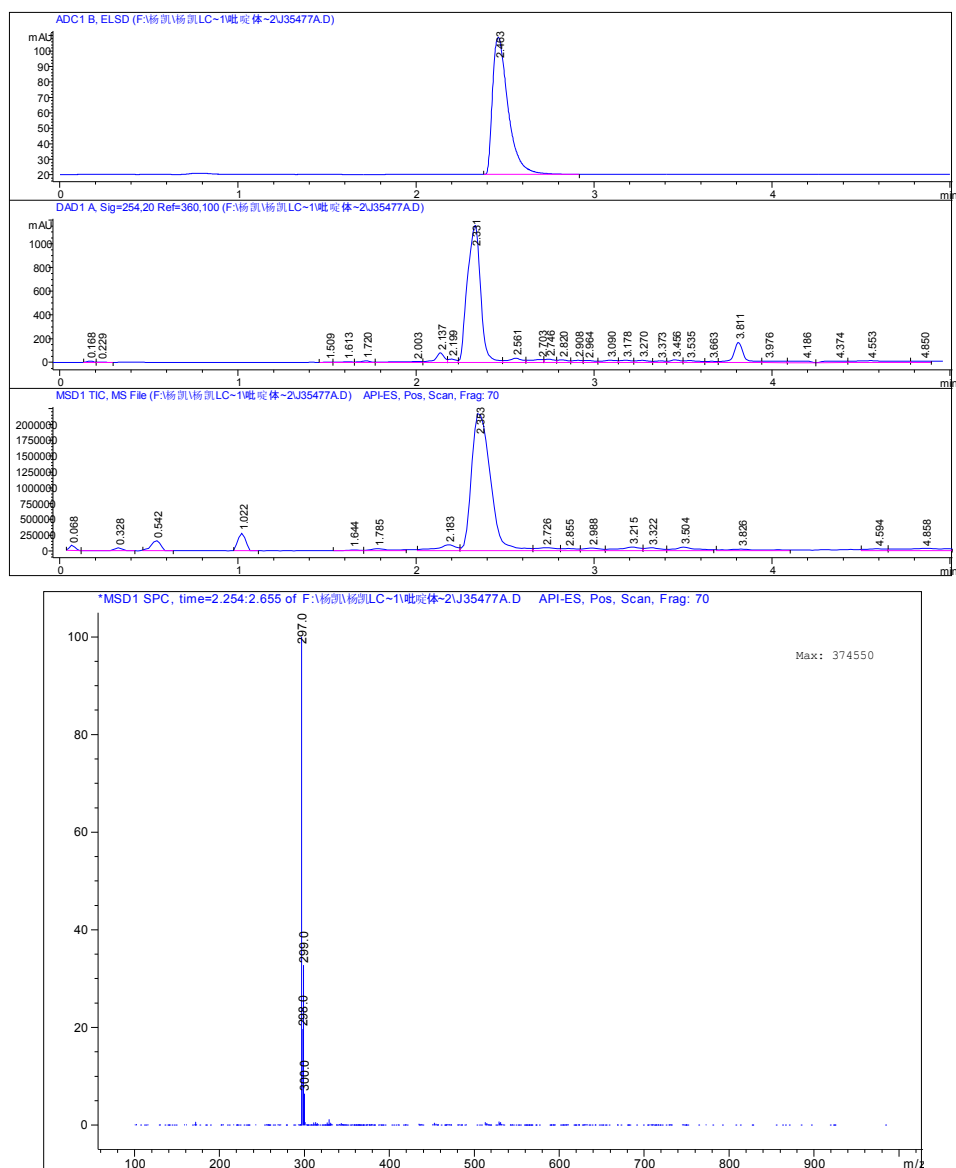


Fig. S-1: LC-MS-ELSD of 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,1,1}.

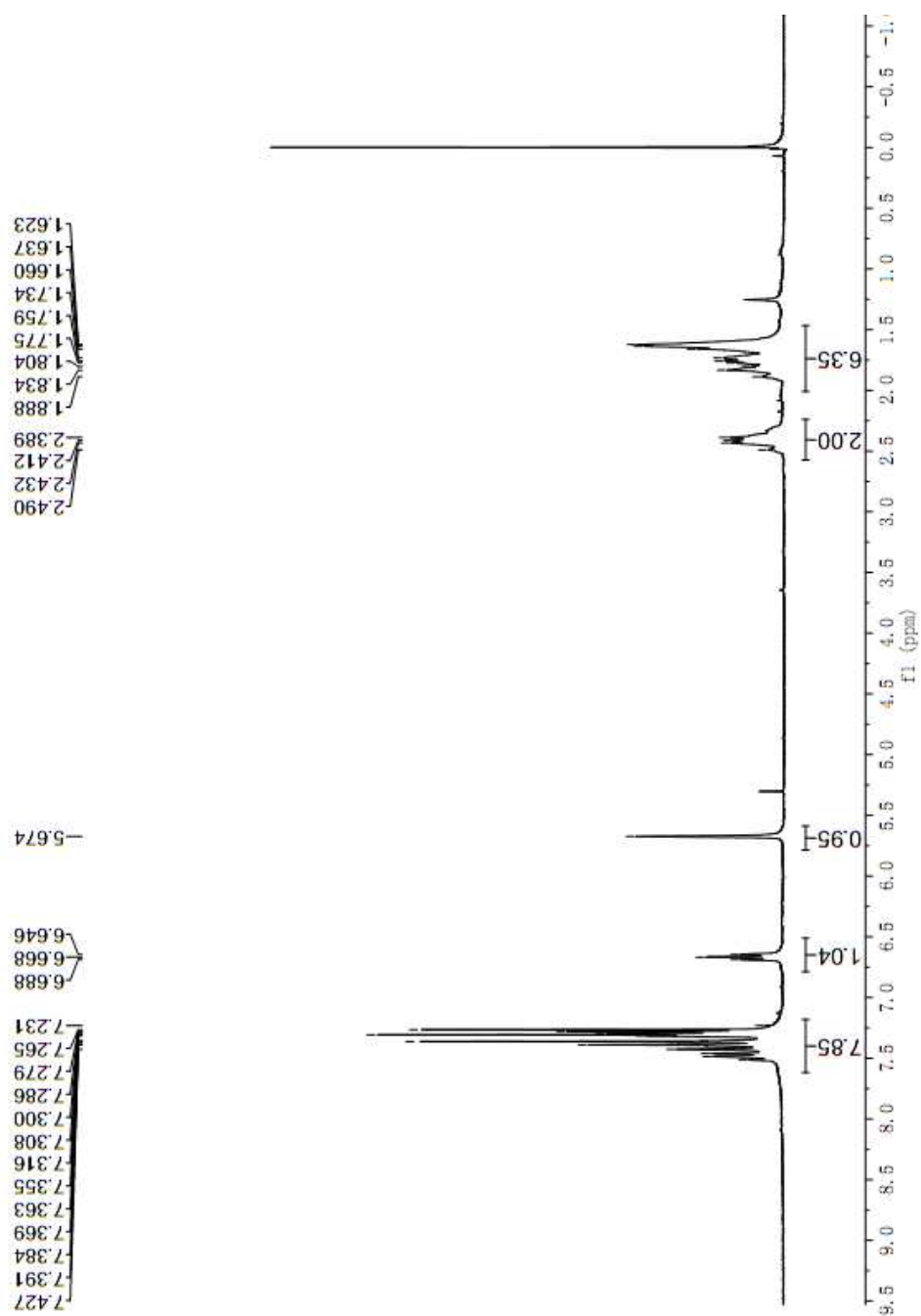


Fig. S-2: ¹H Spectra of 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,1,1}.

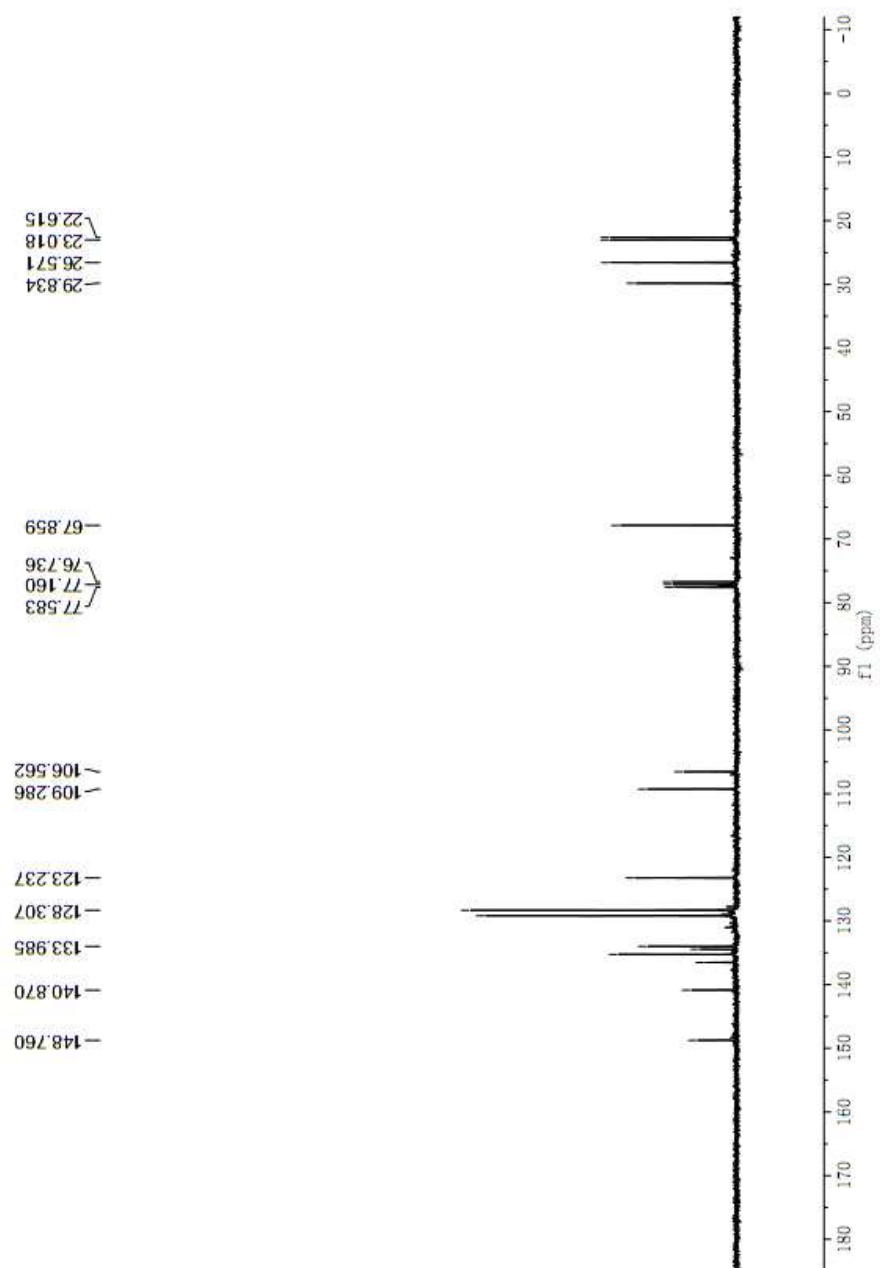
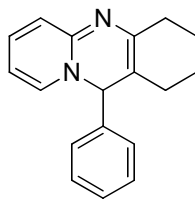


Fig. S-3: ^{13}C Spectra of 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-b]quinazolin 4{1,1,1}.



Chemical Formula: $C_{18}H_{18}N_2$

Exact Mass: 262.1

Molecular Weight: 262.3

4{1,2,1}

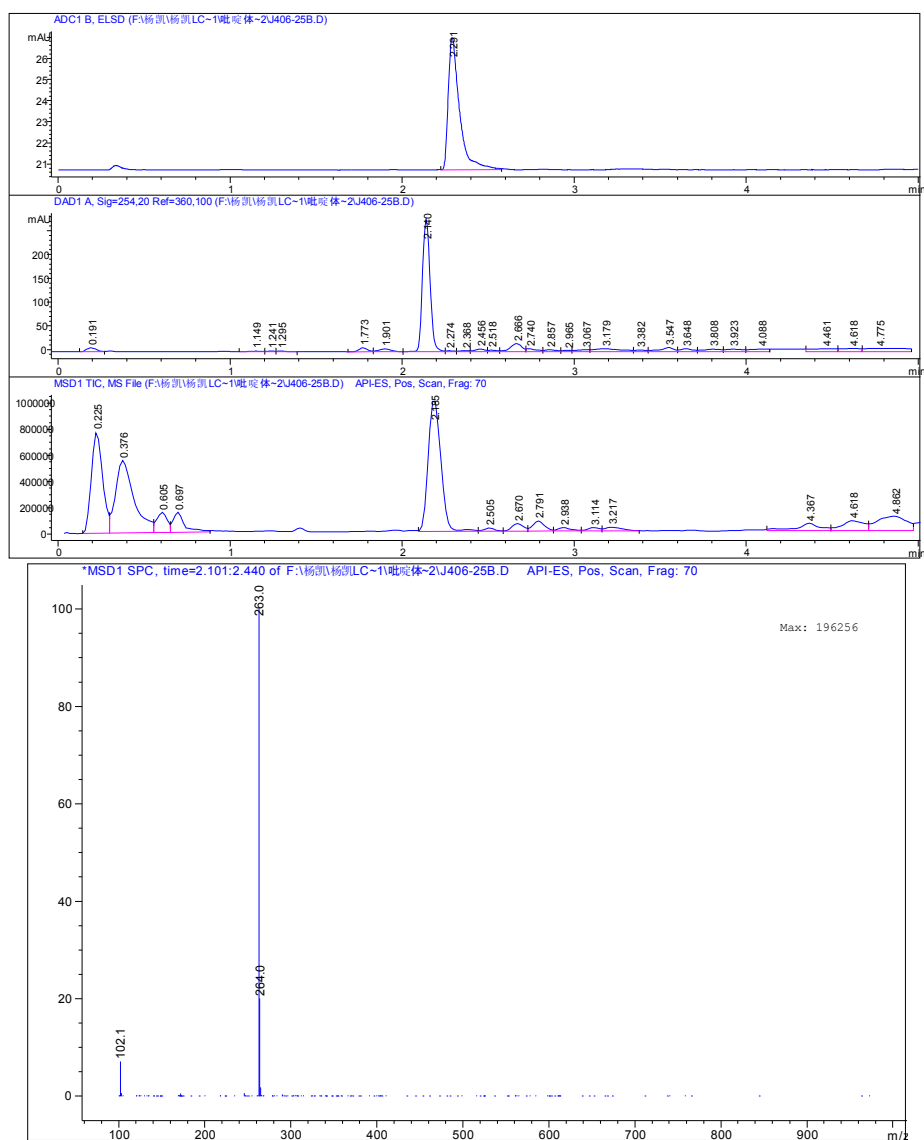


Fig. S-4: LC-MS-ELSD of 11-phenyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,2,1}.

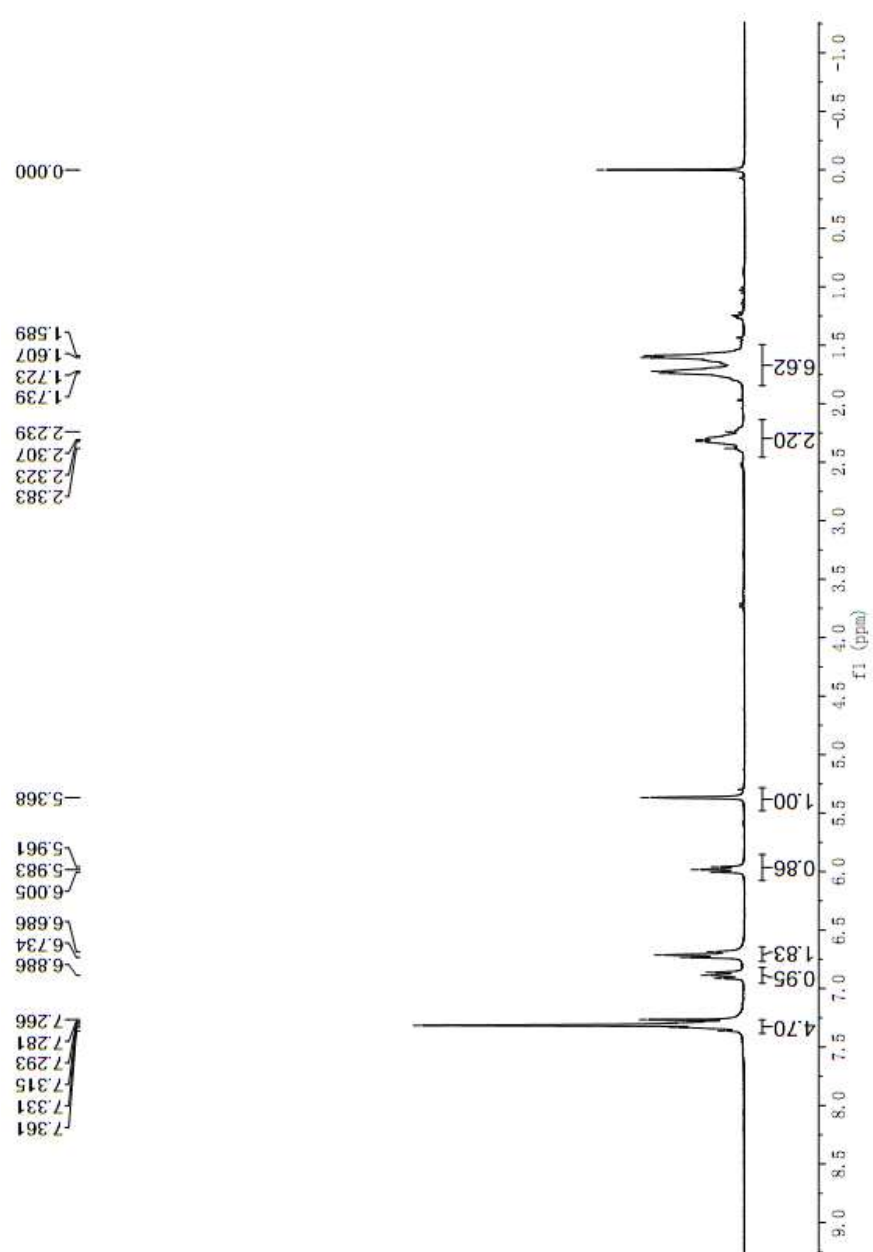


Fig. S-5: ^1H Spectra of 11-phenyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,2,*I*}.

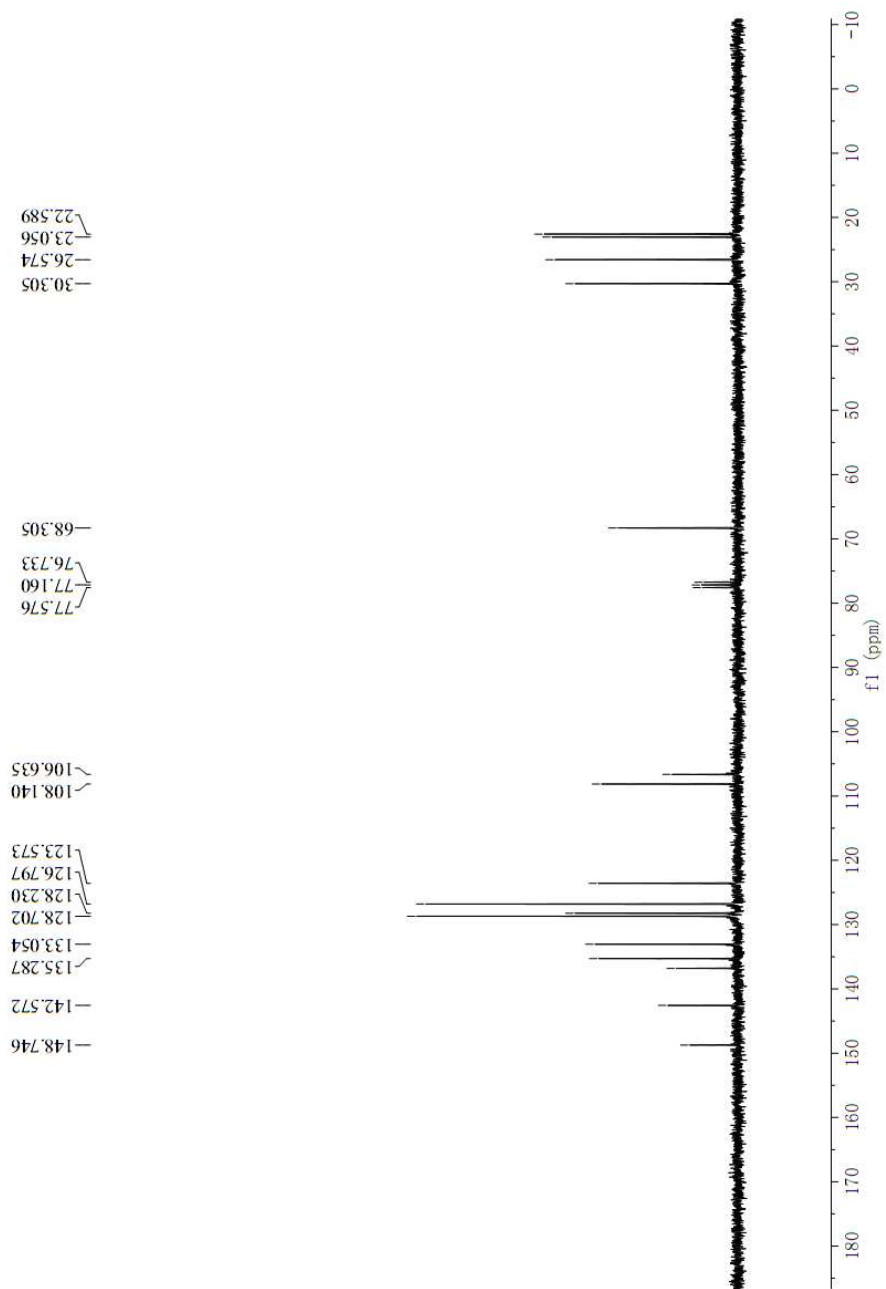
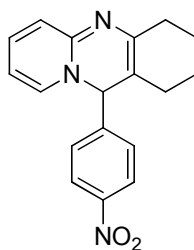


Fig. S-6: ^{13}C Spectra of 11-phenyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,2,1}.



Chemical Formula: C₁₈H₁₇N₃O₂

Exact Mass: 307.1

Molecular Weight: 307.3

4{1,3,I}

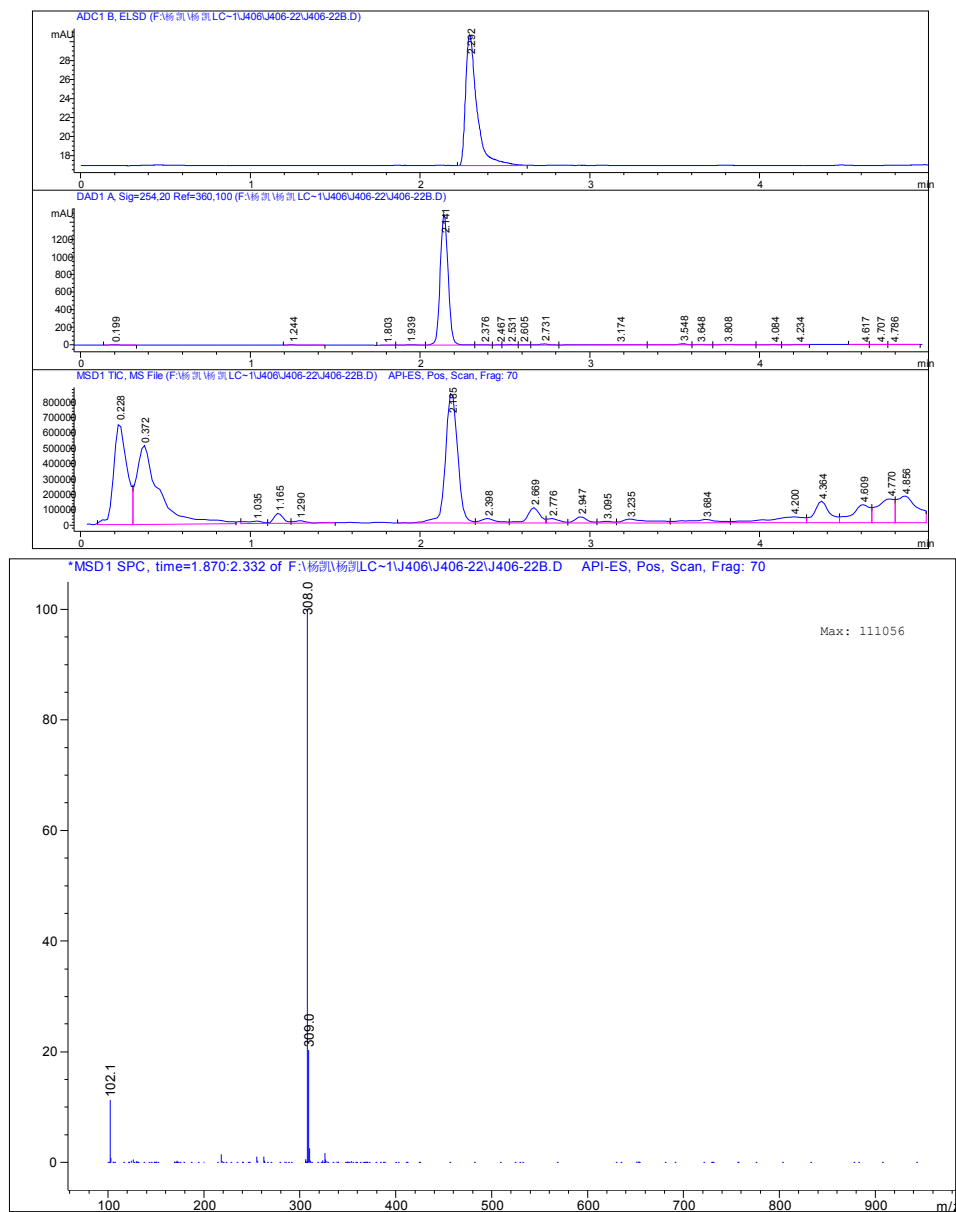


Fig. S-7: LC-MS-ELSD of 11-(4-nitrophenyl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-*b*]quinazoline 4{1,3,I}.

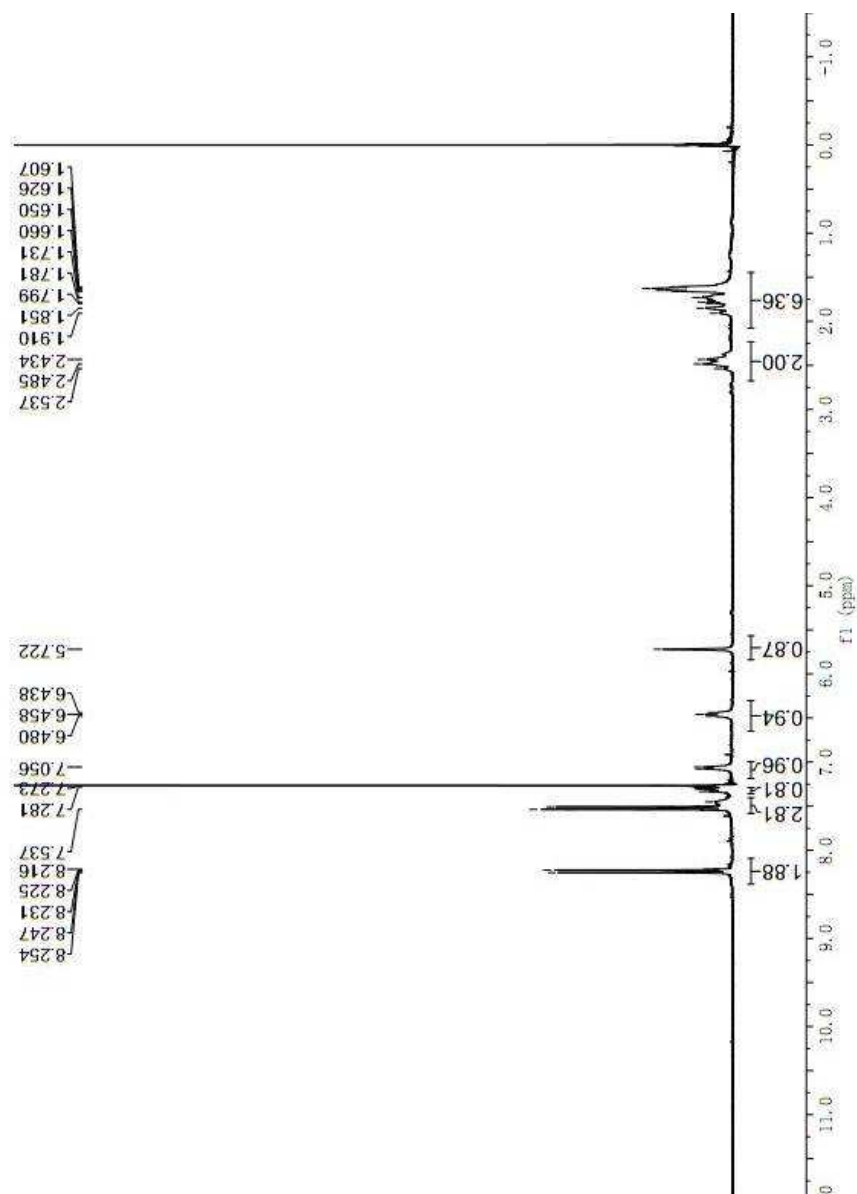
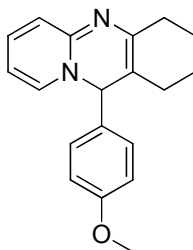


Fig. S-8: ^1H Spectra of 11-(4-nitrophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,3,1}.



Chemical Formula: C₁₉H₂₀N₂O

Exact Mass: 292.2

Molecular Weight: 292.4

4{1,4,I}

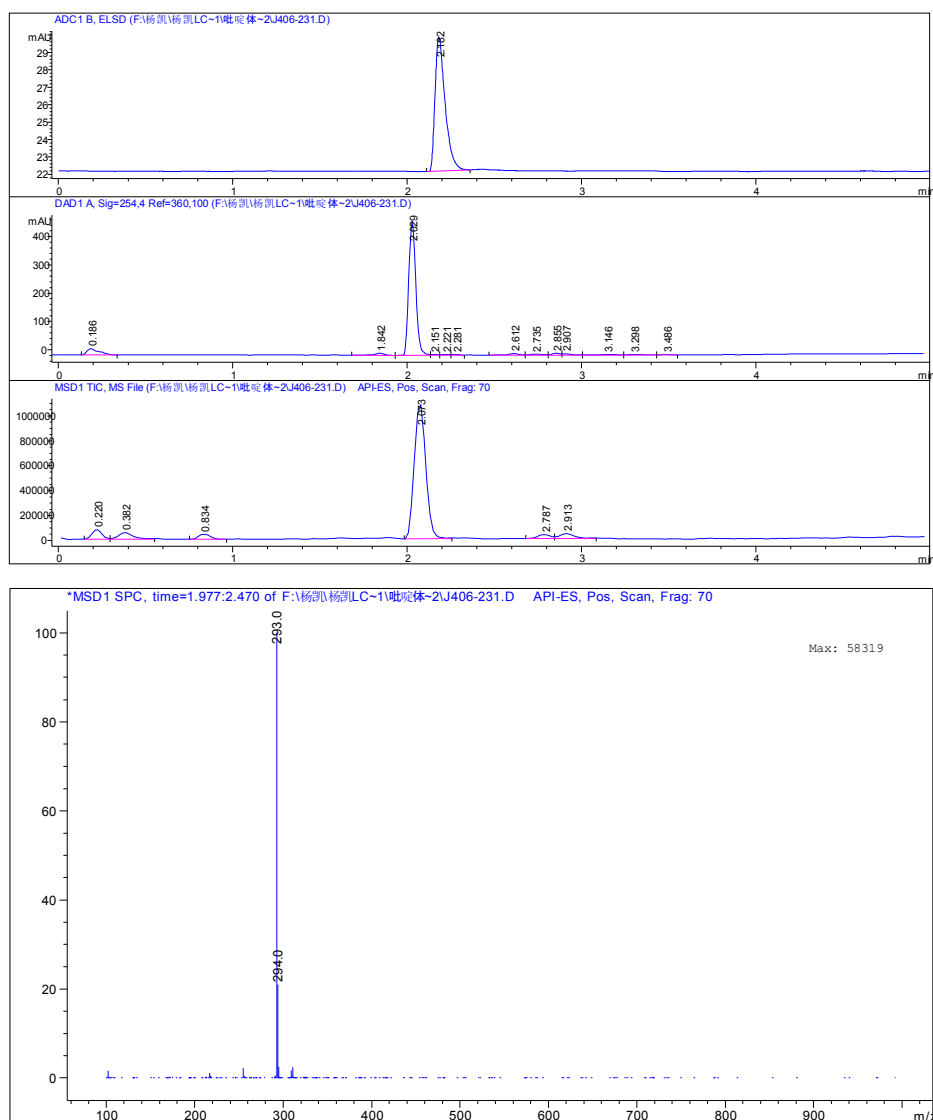


Fig. S-9: LC-MS-ELSD of 11-(4-methoxyphenyl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-*b*]quinazoline 4{1,4,I}.

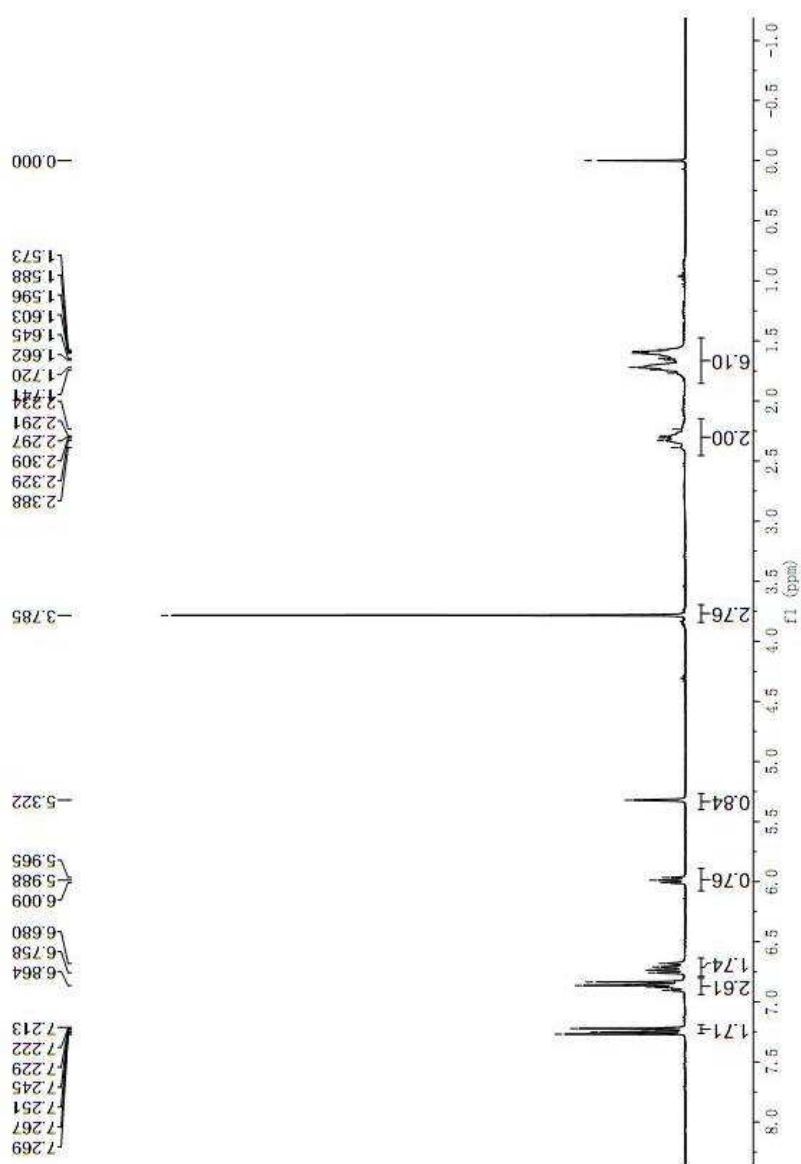


Fig. S-10: ^1H Spectra of 11-(4-methoxyphenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,4,1}.

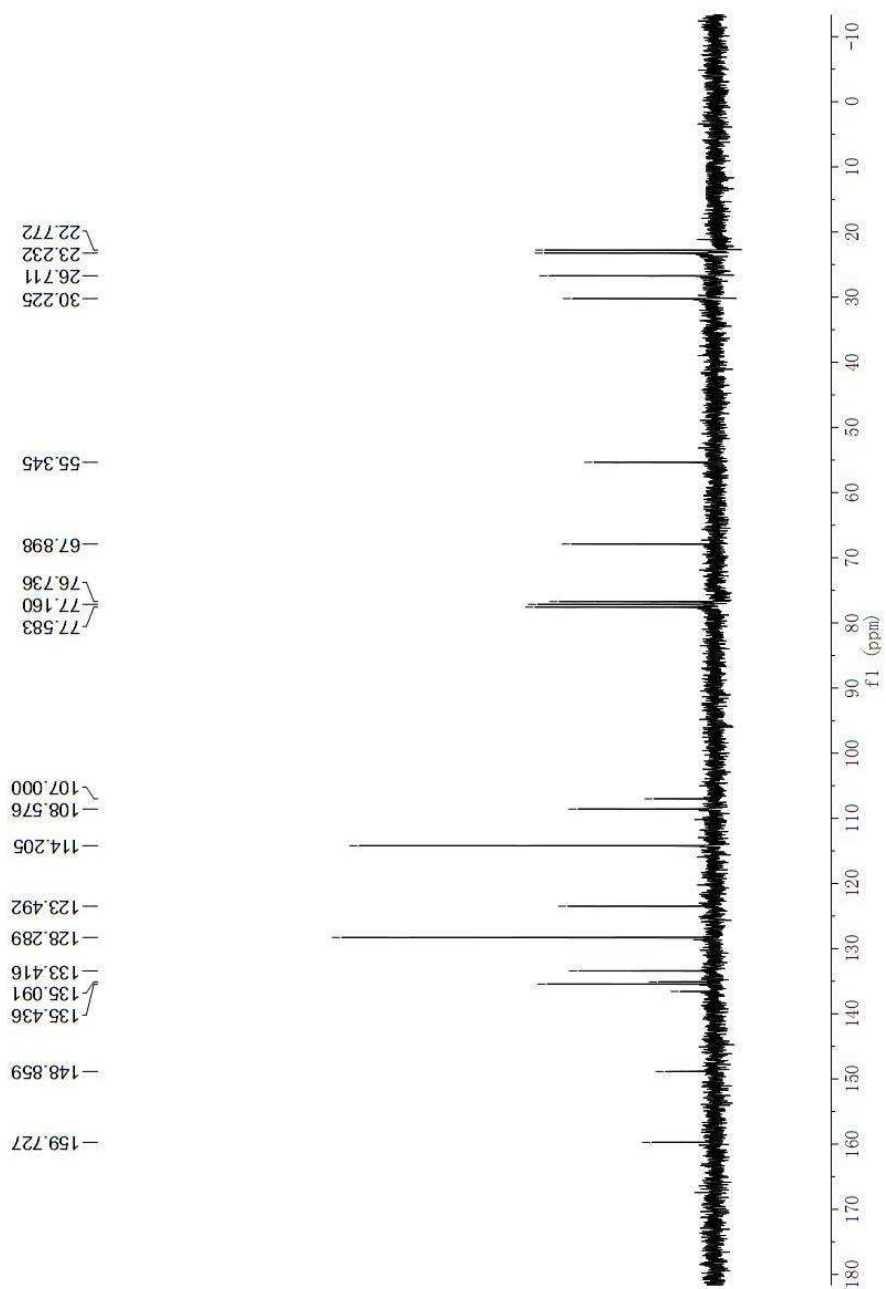
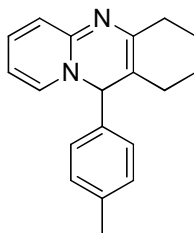


Fig. S-11: ^{13}C Spectra of 11-(4-methoxyphenyl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-b]quinazoline 4{1,4,1}.



Chemical Formula: C₁₉H₂₀N₂

Exact Mass: 276.2

Molecular Weight: 276.4

4{1,5,I}

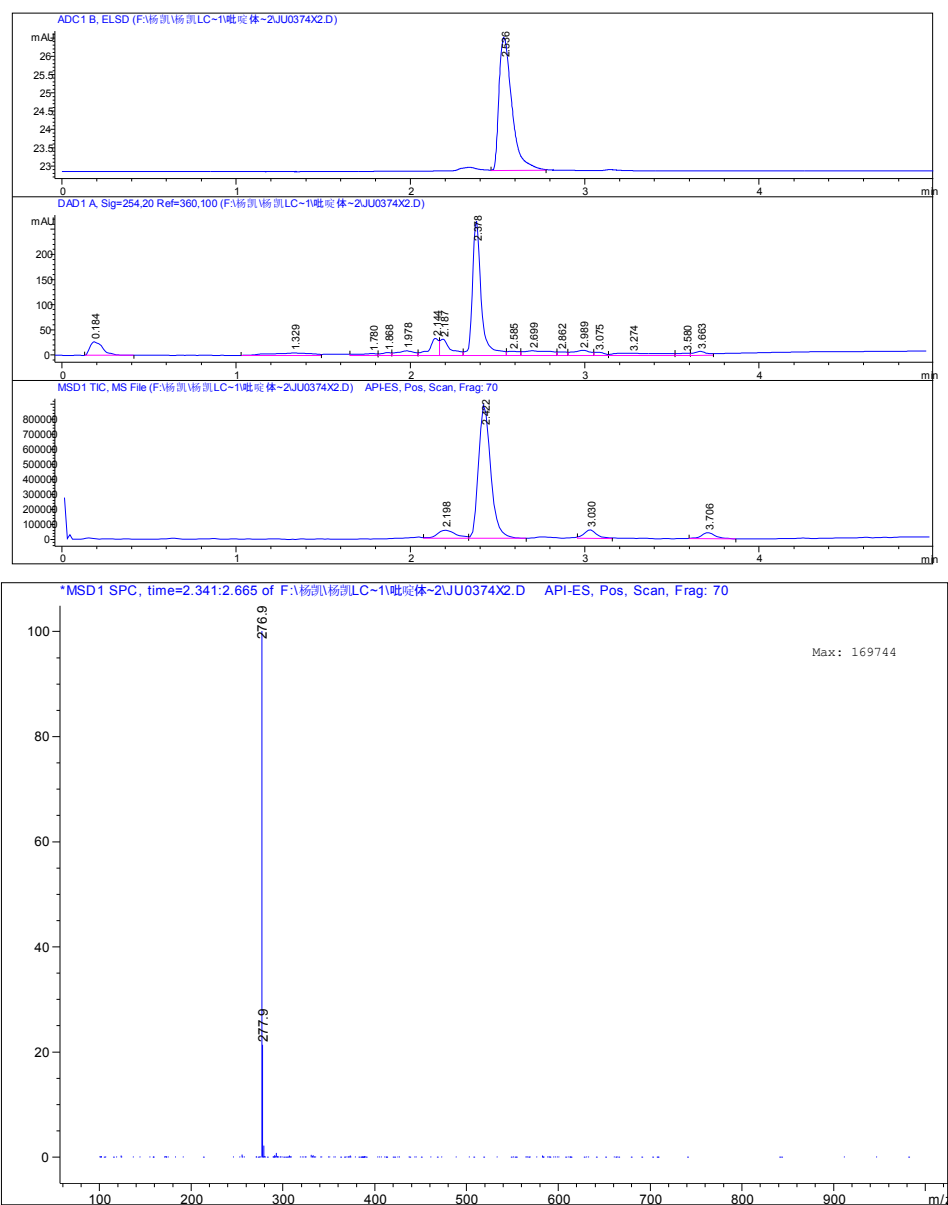


Fig. S-12: LC-MS-ELSD of 11-(*p*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,5,I}.

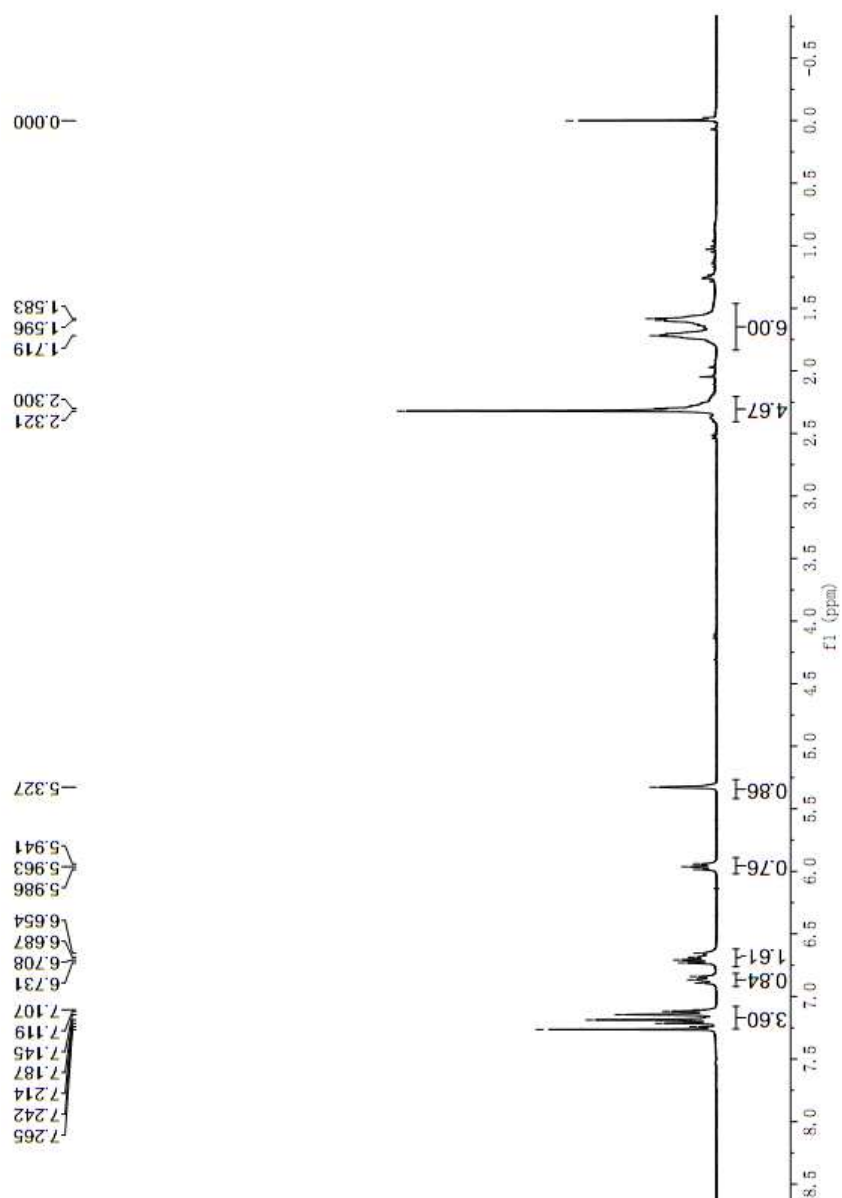


Fig. S-13: ^1H Spectra of 11-(*p*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,5,1}.

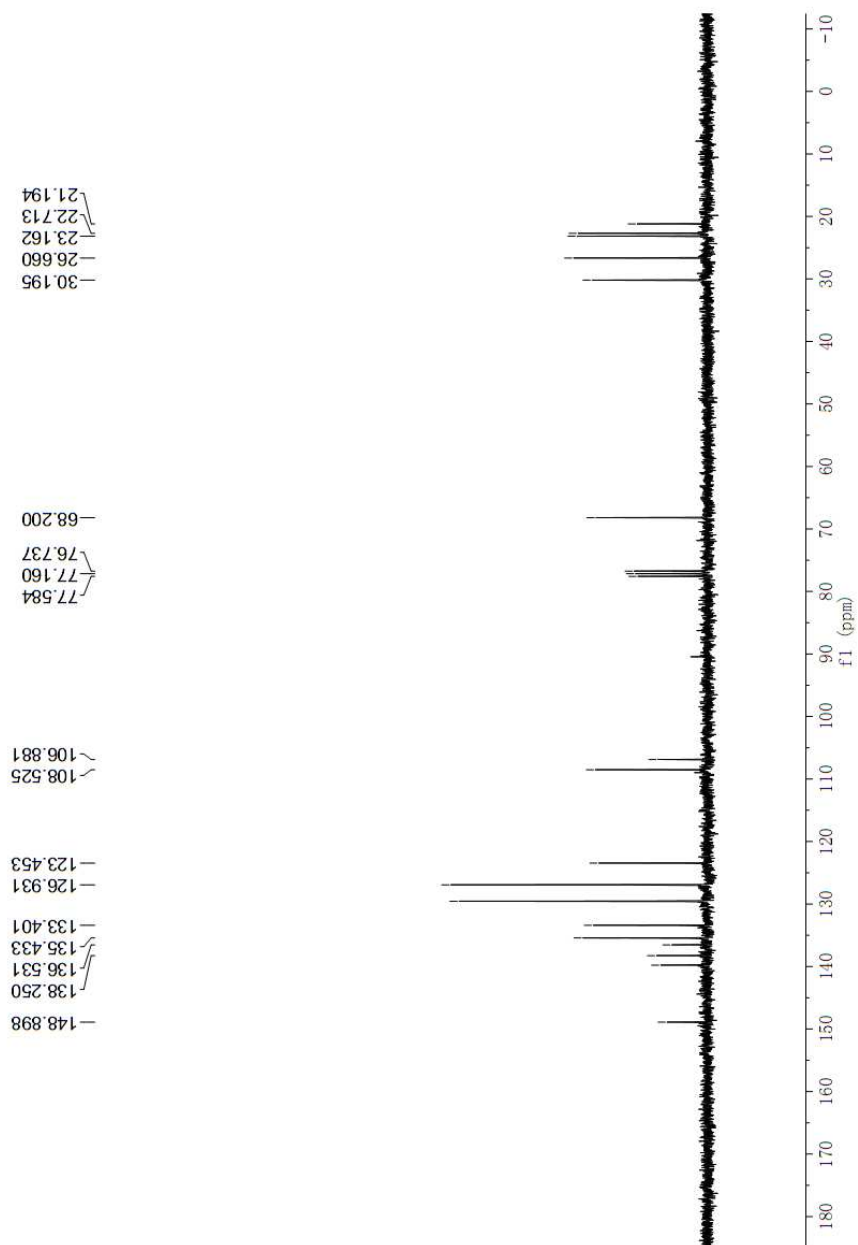
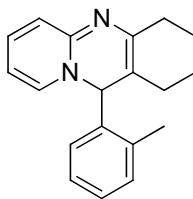


Fig. S-14: ^{13}C Spectra of 11-(*p*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,5,1}.



Chemical Formula: C₁₉H₂₀N₂

Exact Mass: 276.2

Molecular Weight: 276.4

4{1,6,1}

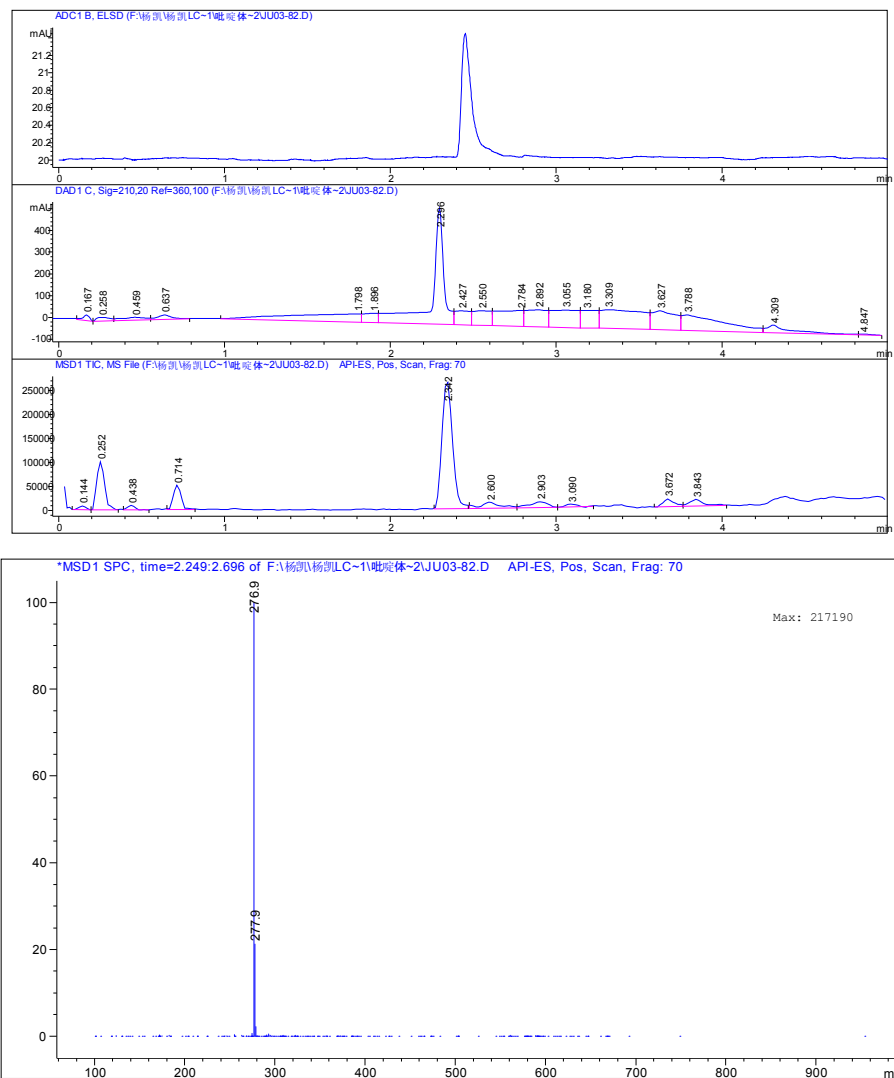


Fig. S-15: LC-MS-ELSD of 11-(*o*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,6,1}.

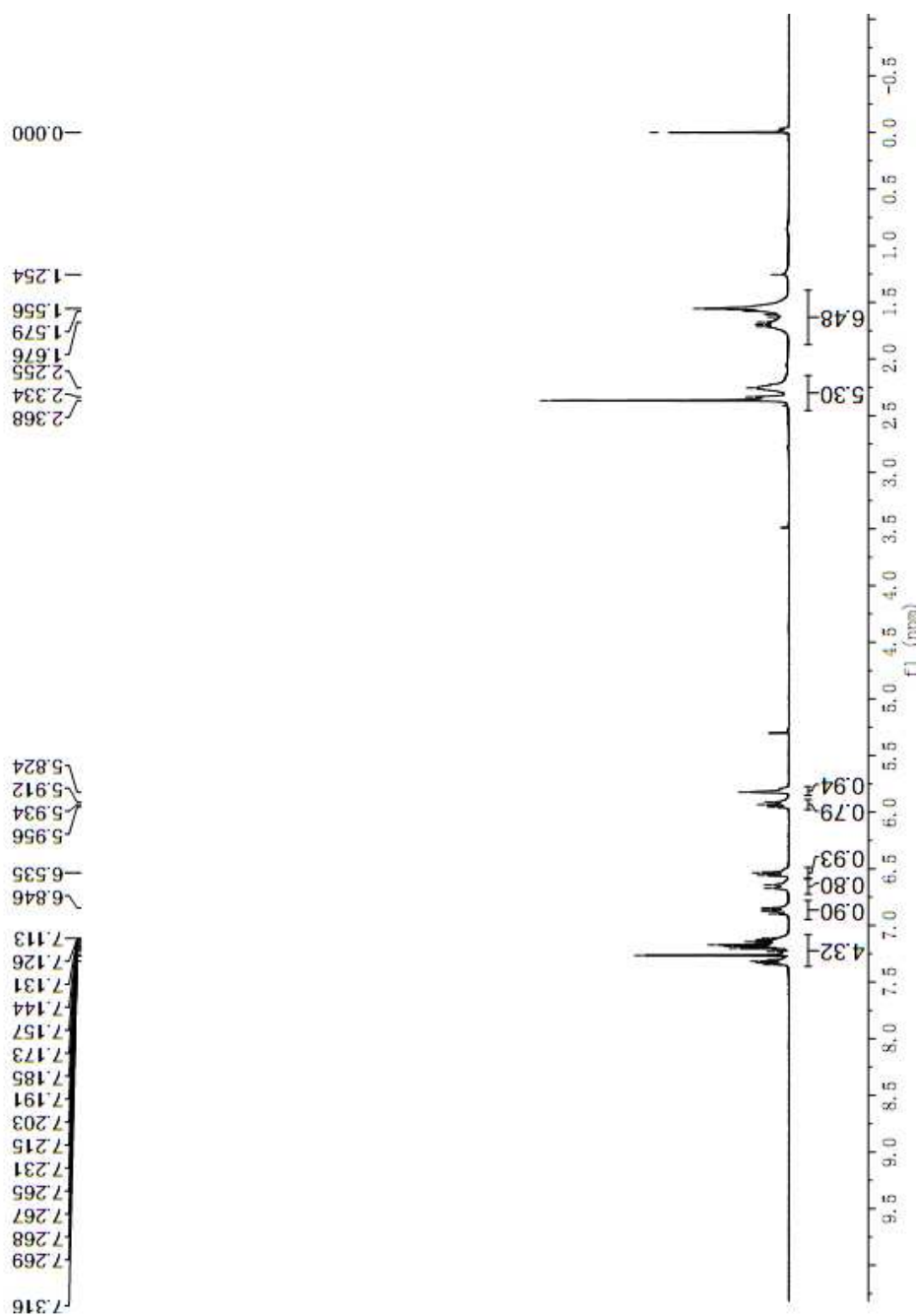


Fig. S-16: ^1H Spectra of 11-(*o*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,6,1}.

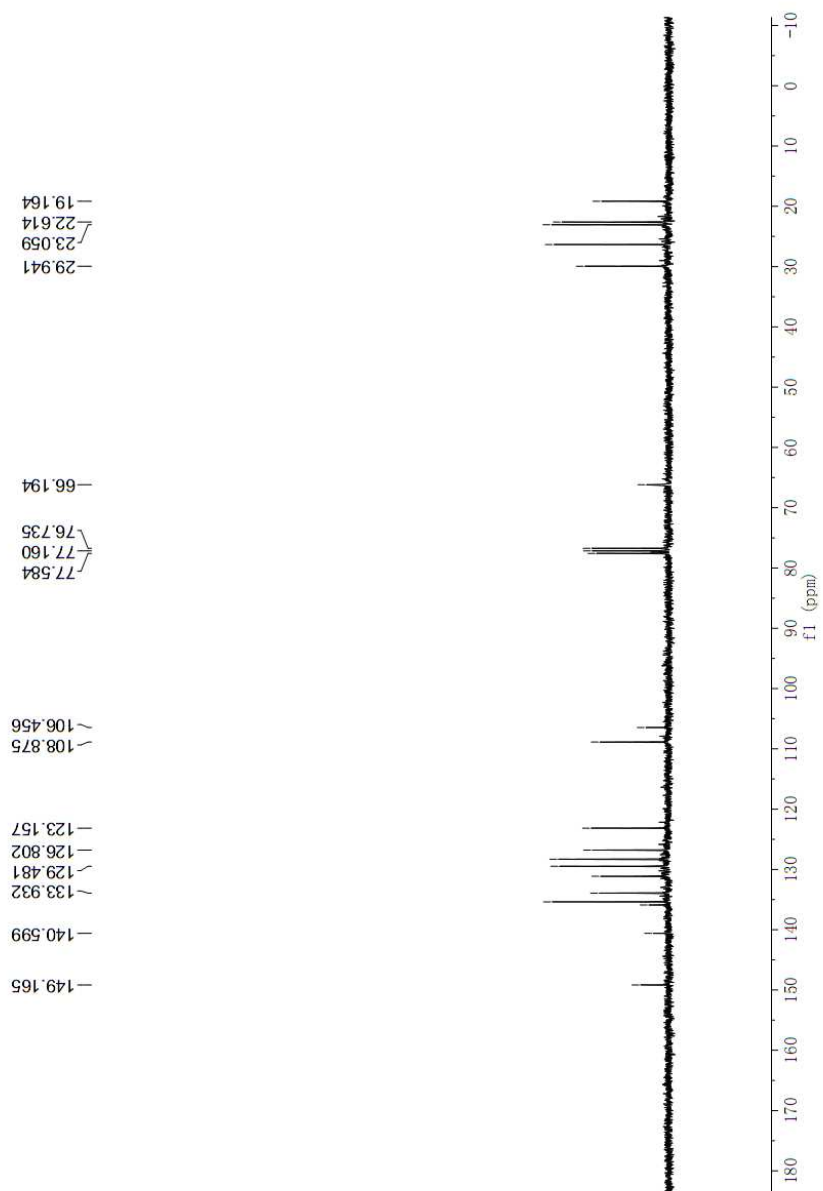
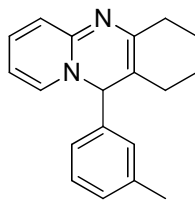


Fig. S-17: ^{13}C Spectra of 11-(*o*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,6,1}.



Chemical Formula: C₁₉H₂₀N₂

Exact Mass: 276.2

Molecular Weight: 276.4

4{I,7,I}

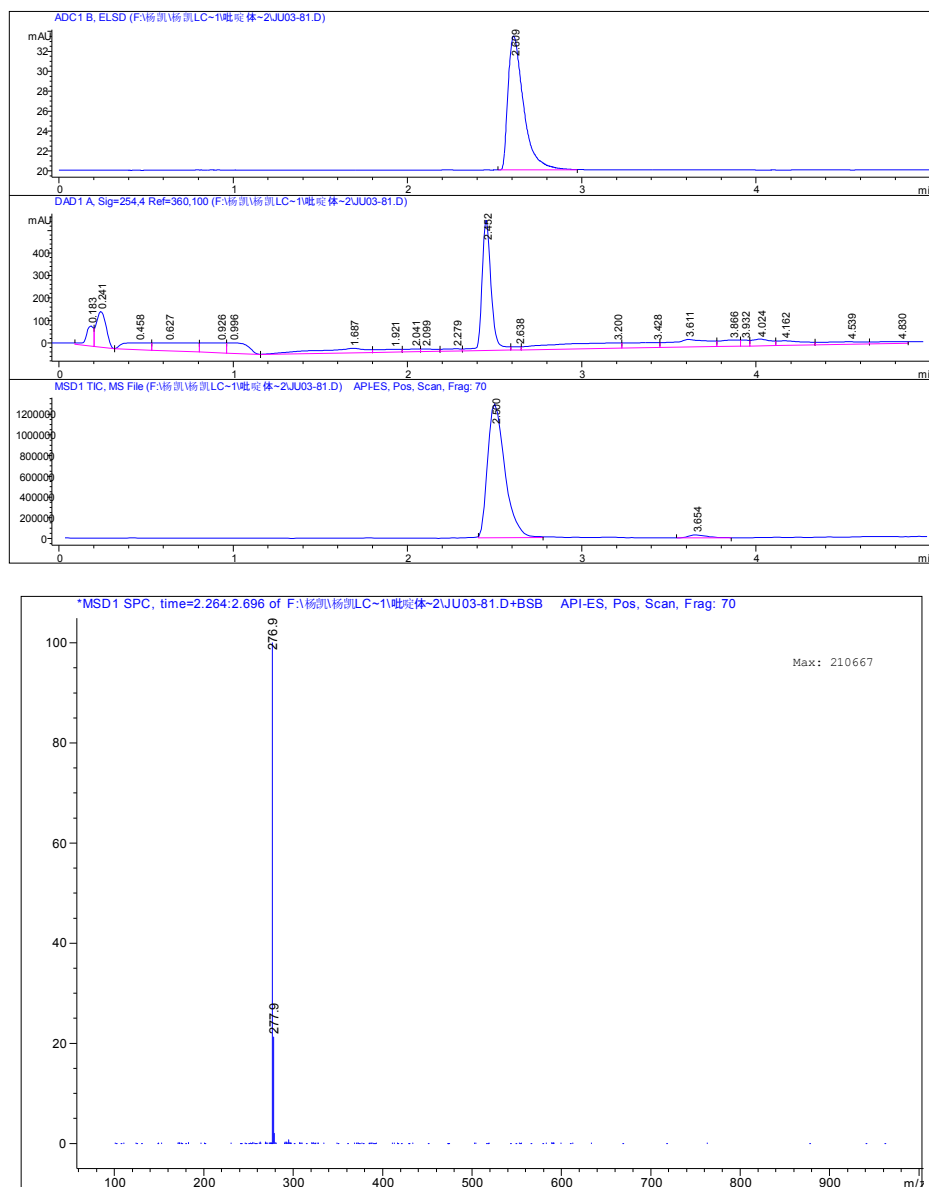


Fig. S-18: LC-MS-ELSD of 11-(*m*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{I,7,I}.

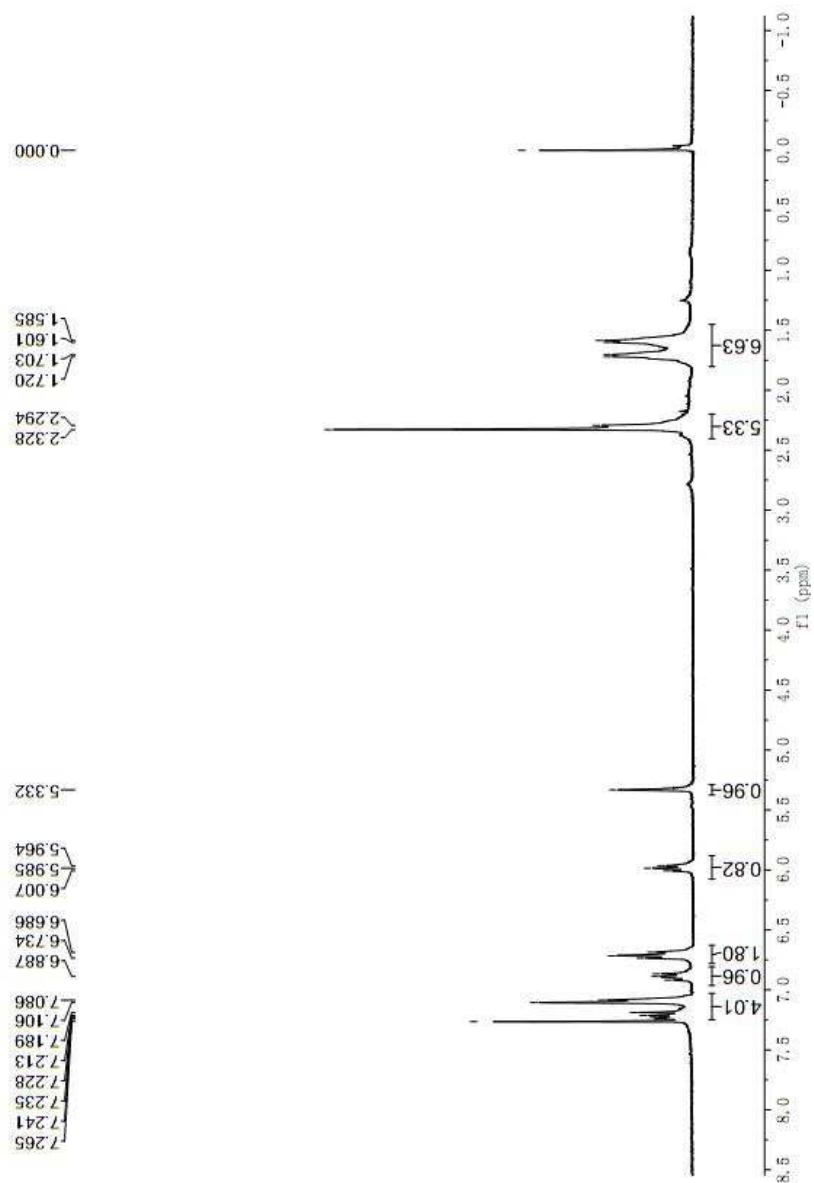


Fig. S-19: ^1H Spectra of 11-(*m*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,7,1}.

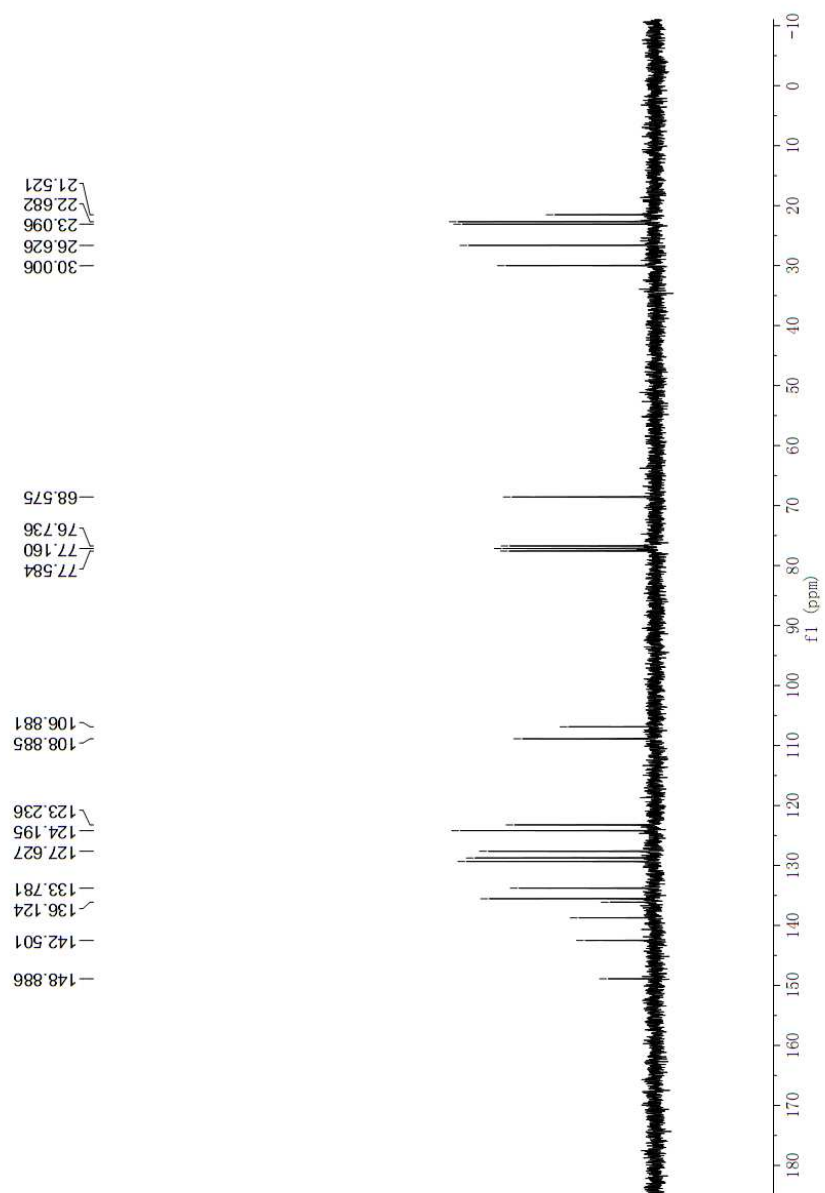
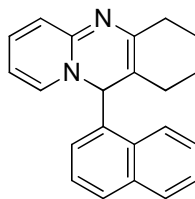


Fig. S-20: ^{13}C Spectra of 11-(*m*-tolyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,7,*I*}.



Chemical Formula: $C_{22}H_{20}N_2$

Exact Mass: 312.2

Molecular Weight: 312.4

4{1,8,I}

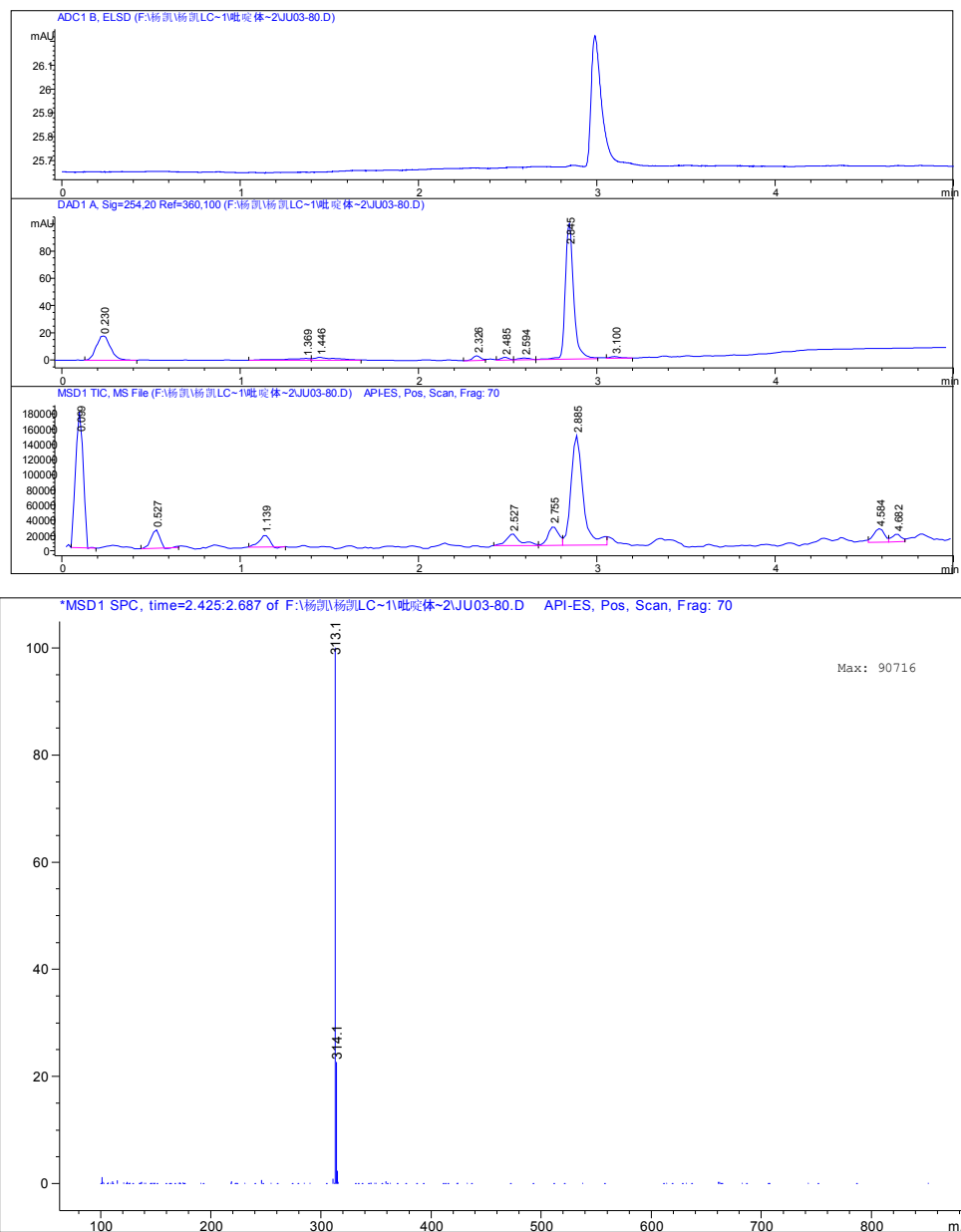


Fig. S-21: LC-MS-ELSD of 11-(naphthalen-1-yl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-b]quinazoline 4{1,8,I}.

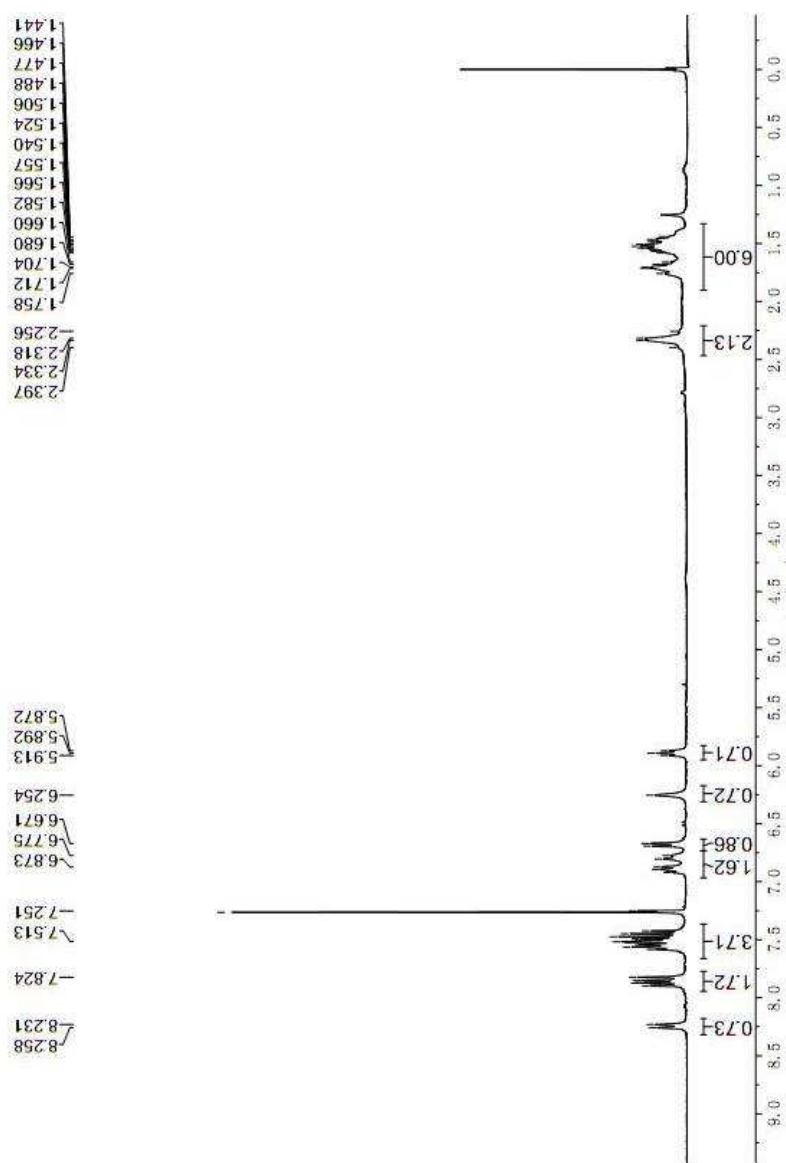


Fig. S-22: ¹H Spectra of 11-(naphthalen-1-yl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-b]quinazoline 4{1,8,1}.

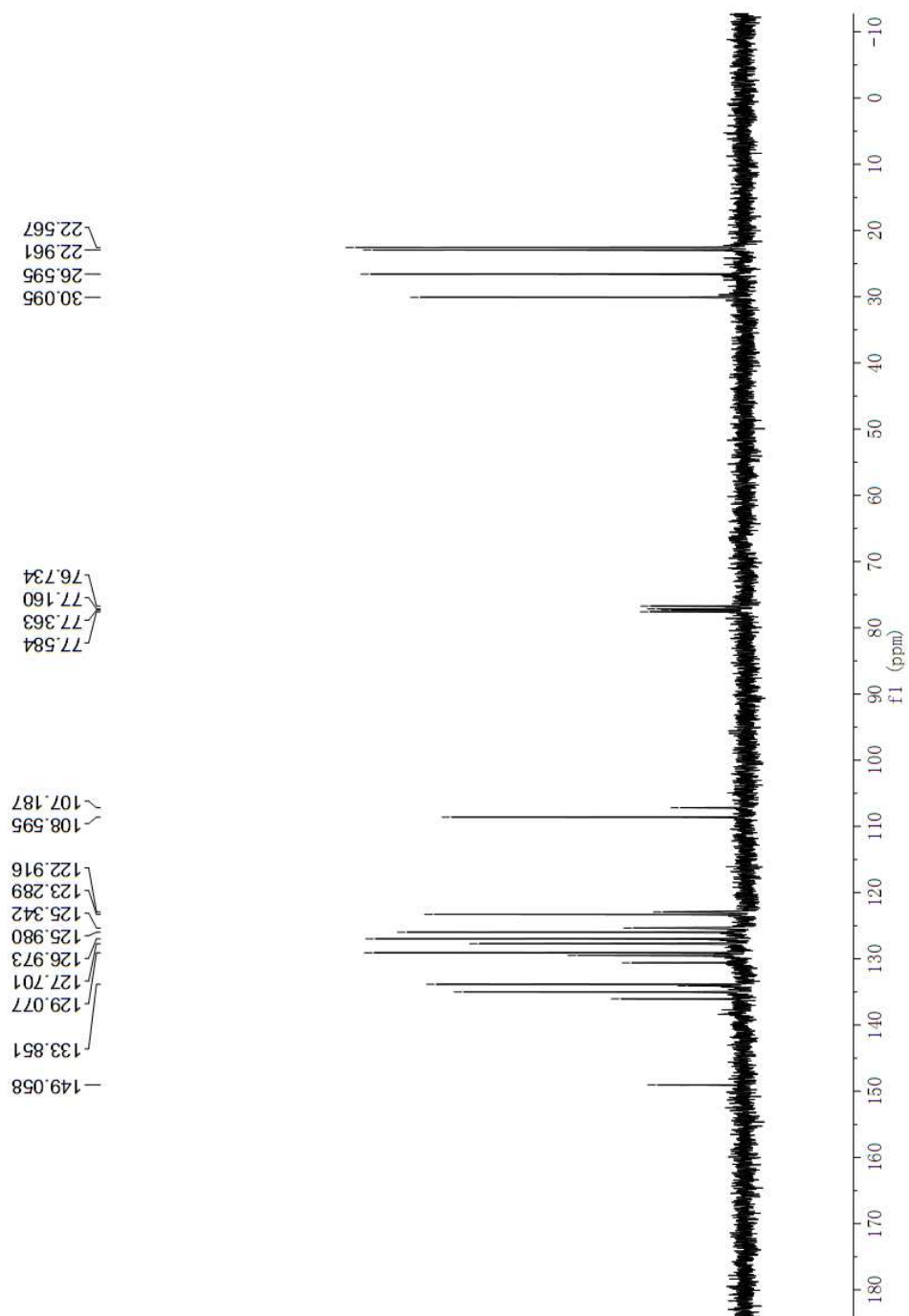
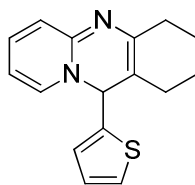


Fig. S-23: ^{13}C Spectra of 11-(naphthalen-1-yl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,8,1}.



Chemical Formula: C₁₆H₁₆N₂S

Exact Mass: 268.1

Molecular Weight: 268.4

4{1,9,1}

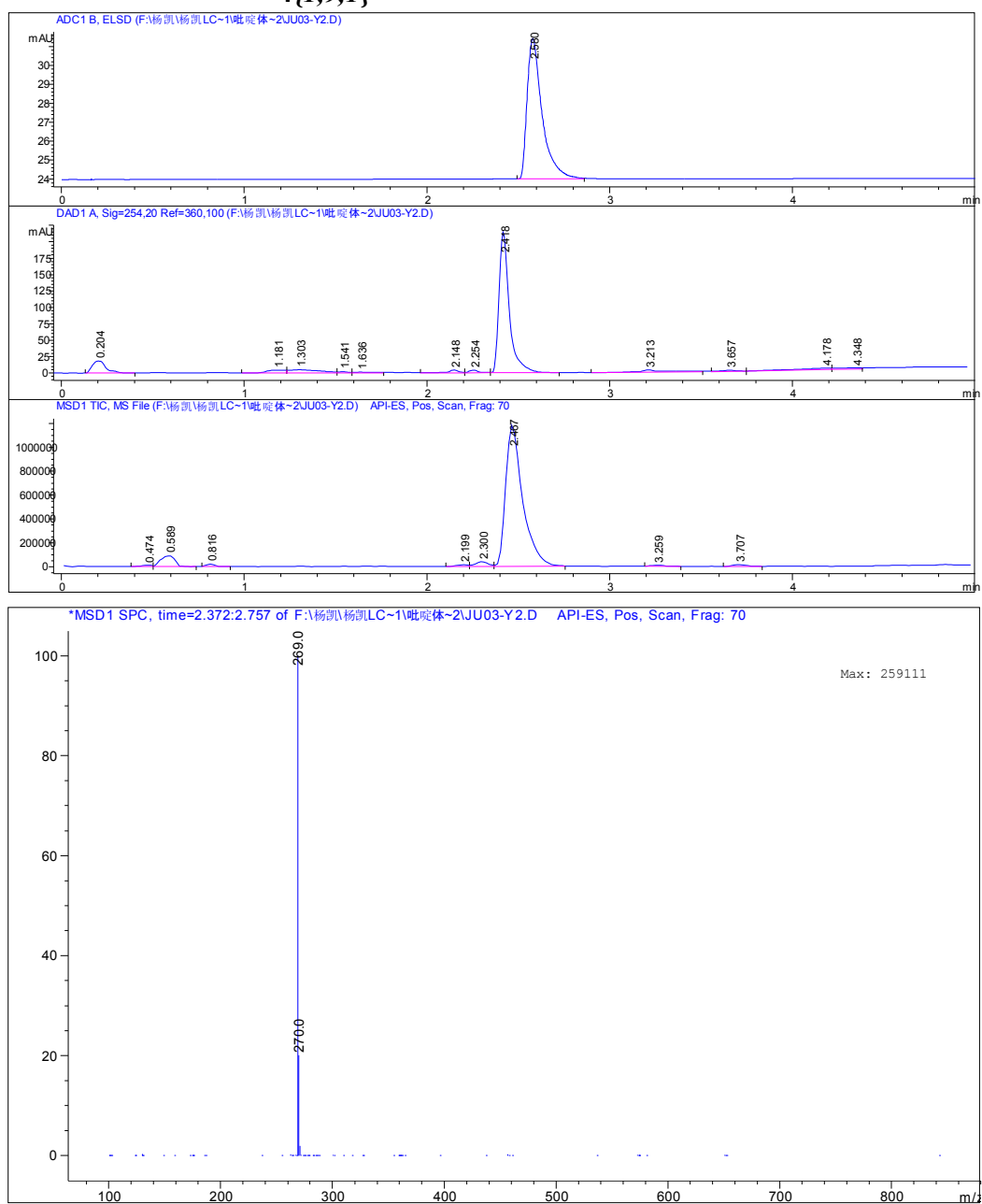


Fig. S-24: LC-MS-ELSD of 11-(thiophen-2-yl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,9,1}.

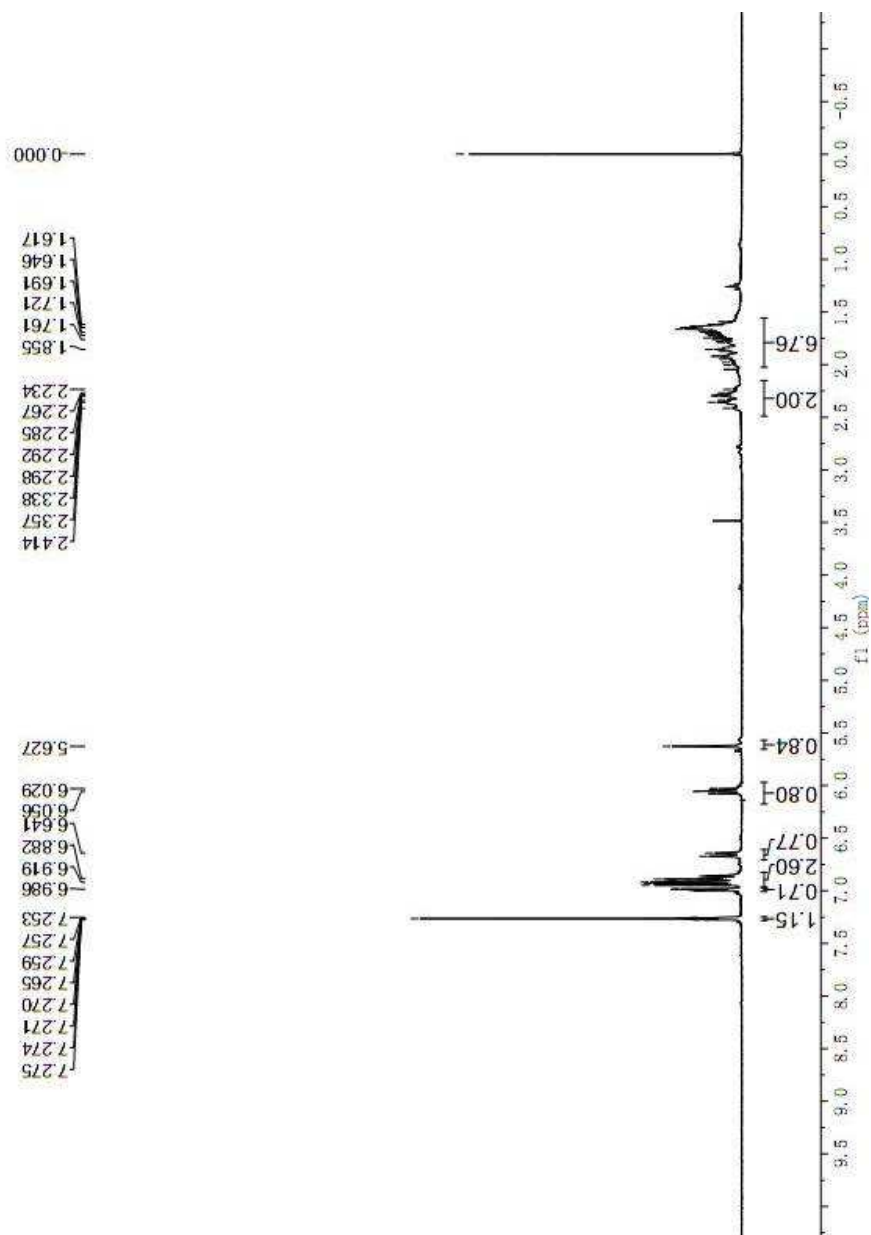


Fig. S-25: ^1H Spectra of 11-(thiophen-2-yl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,9,1}.

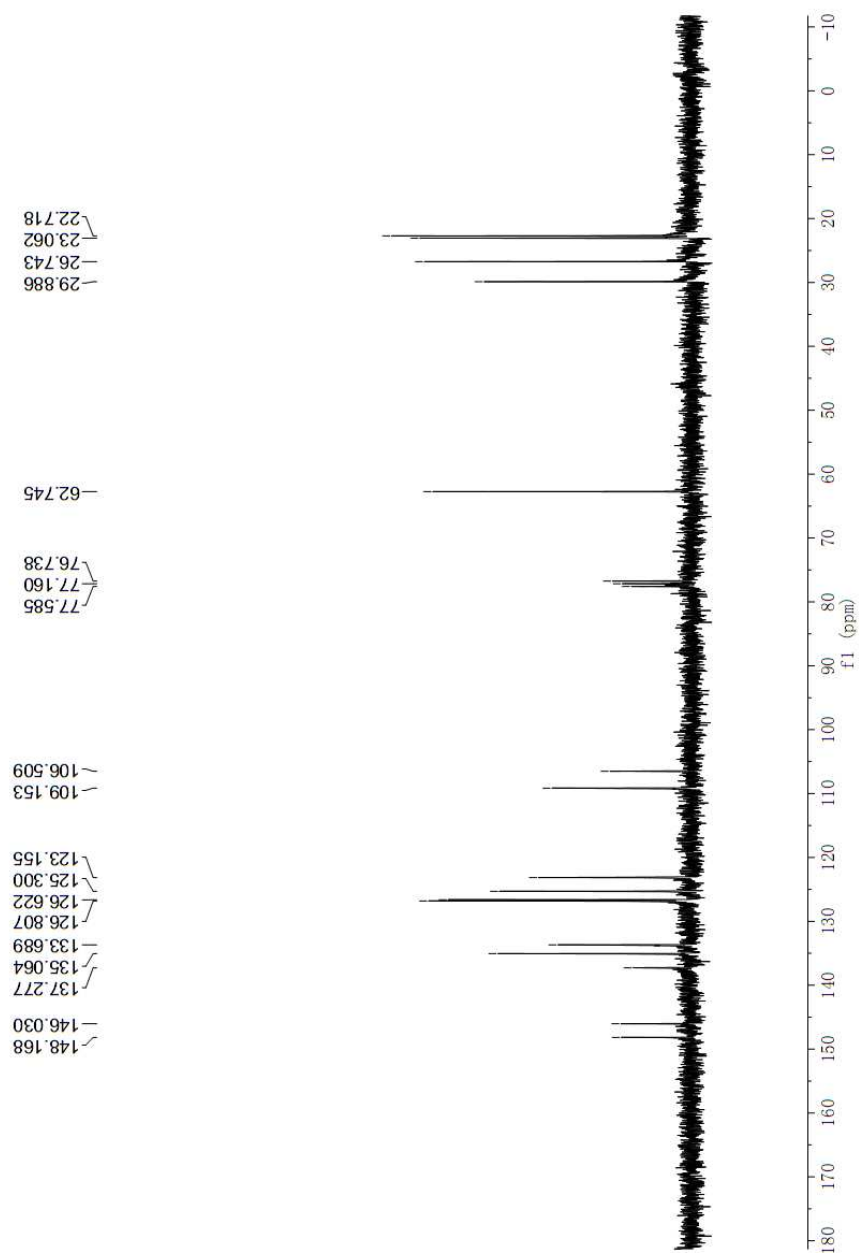
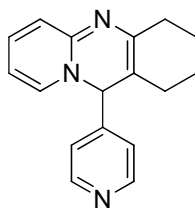


Fig. S-26: ^{13}C Spectra of 11-(thiophen-2-yl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,9,1}.



Chemical Formula: C₁₇H₁₇N₃

Exact Mass: 263.1

Molecular Weight: 263.3

4{1,10,1}

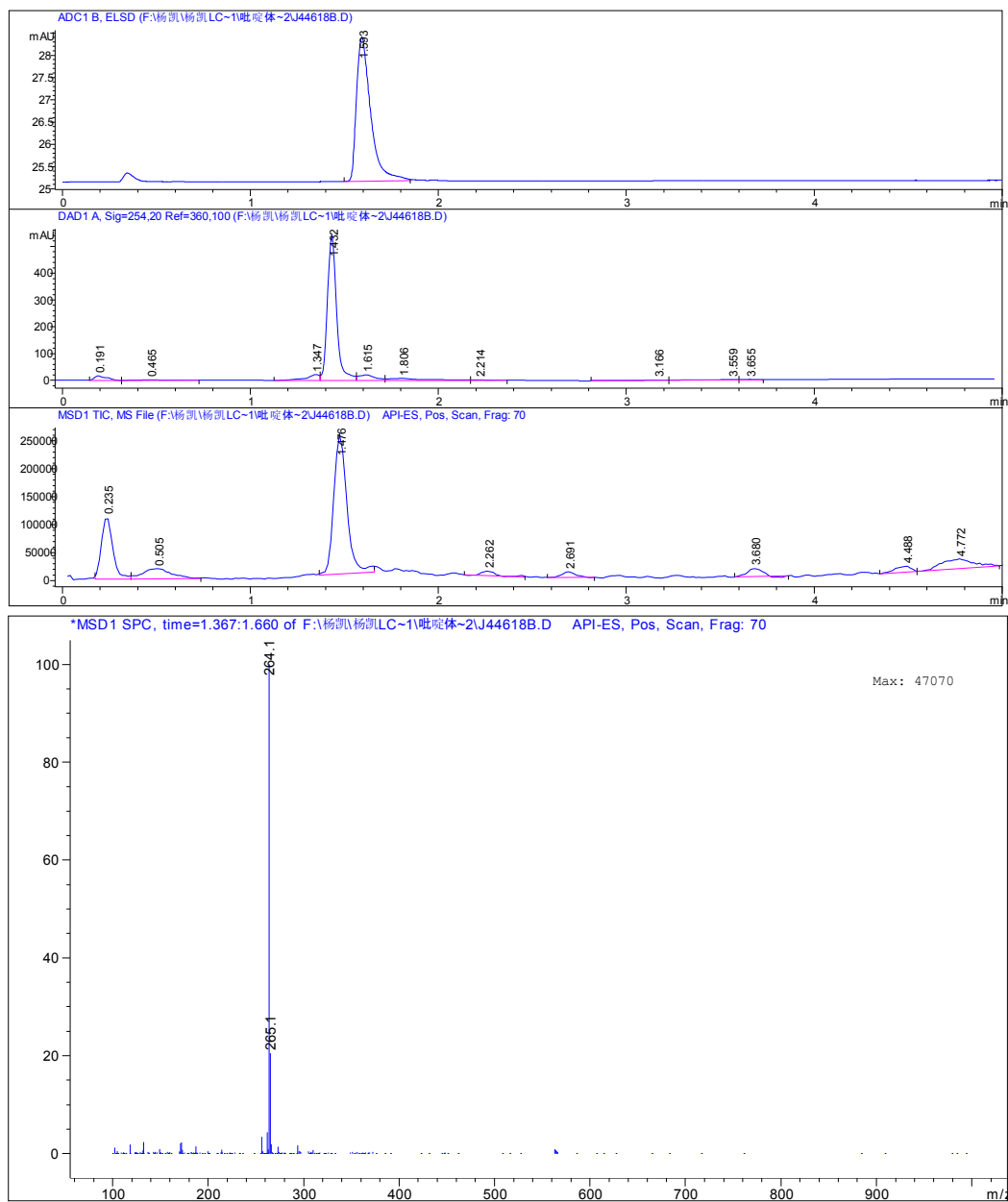


Fig. S-27: LC-MS-ELSD of 11-(pyridin-4-yl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-*b*]quinazoline 4{1,10,1}.

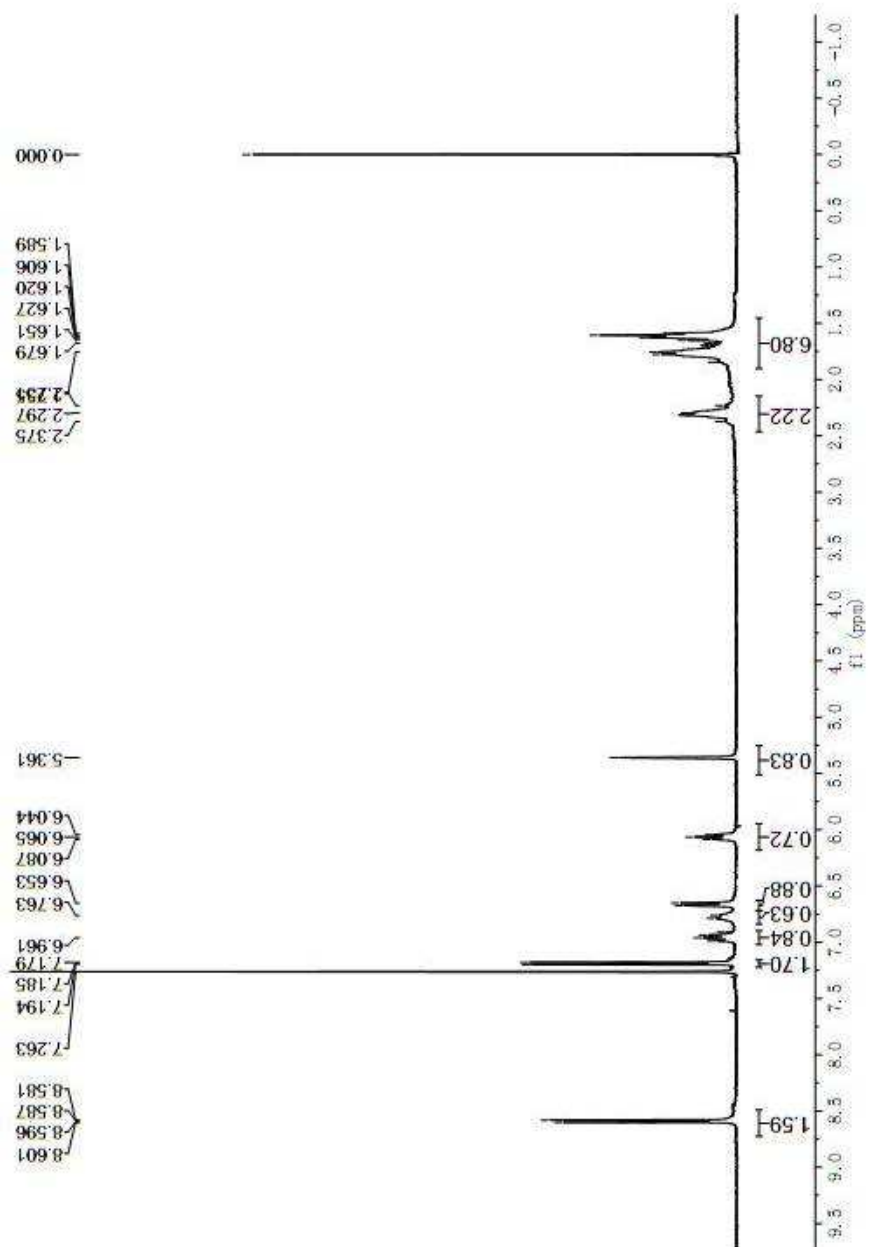
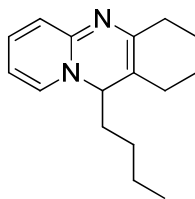


Fig. S-28: ^1H Spectra of 11-(pyridin-4-yl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline 4{1,10,1}.



Chemical Formula: $C_{16}H_{22}N_2$

Exact Mass: 242.2

Molecular Weight: 242.4

4{1,11,I}

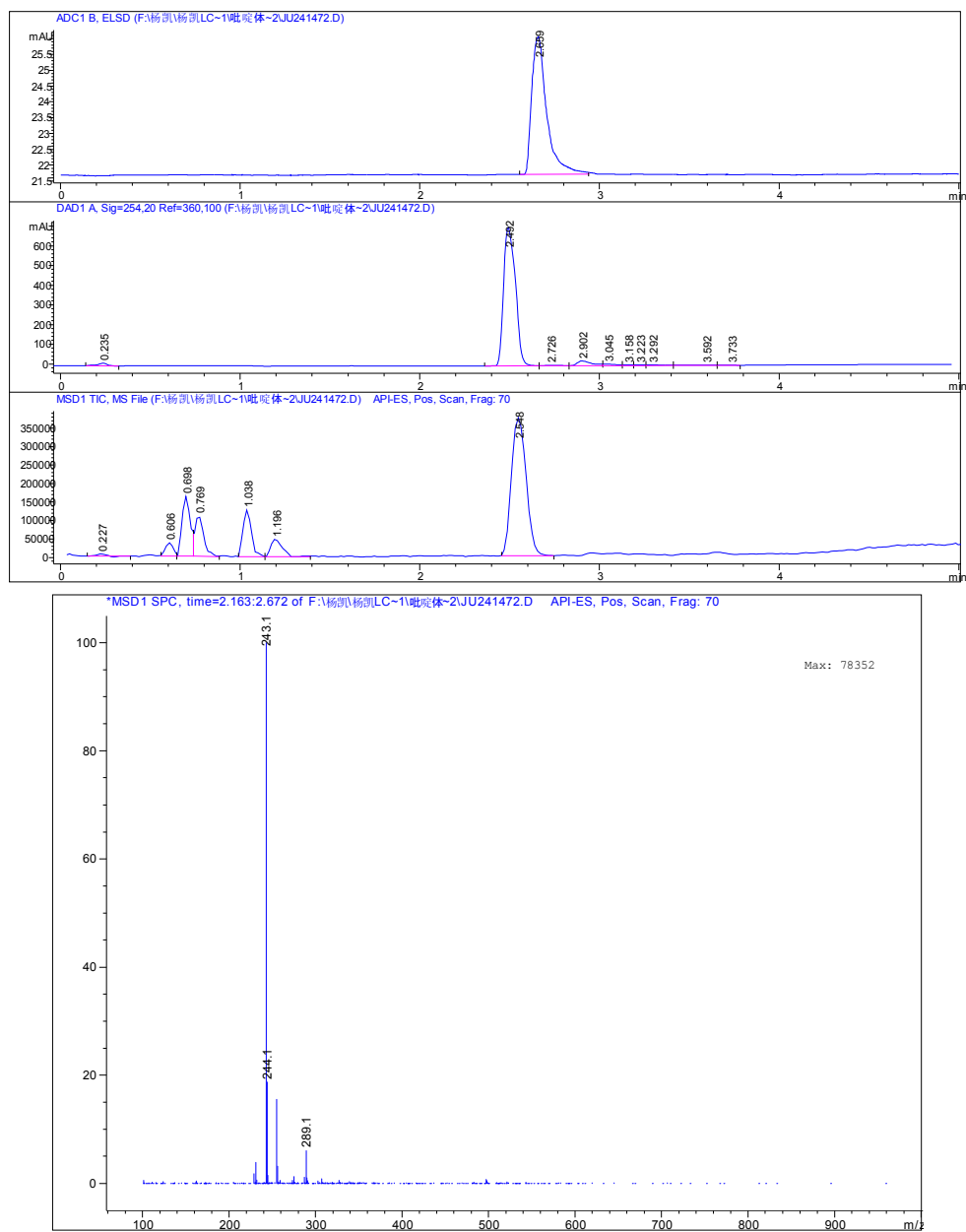


Fig. S-29: LC-MS-ELSD of 11-butyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,11,I}.

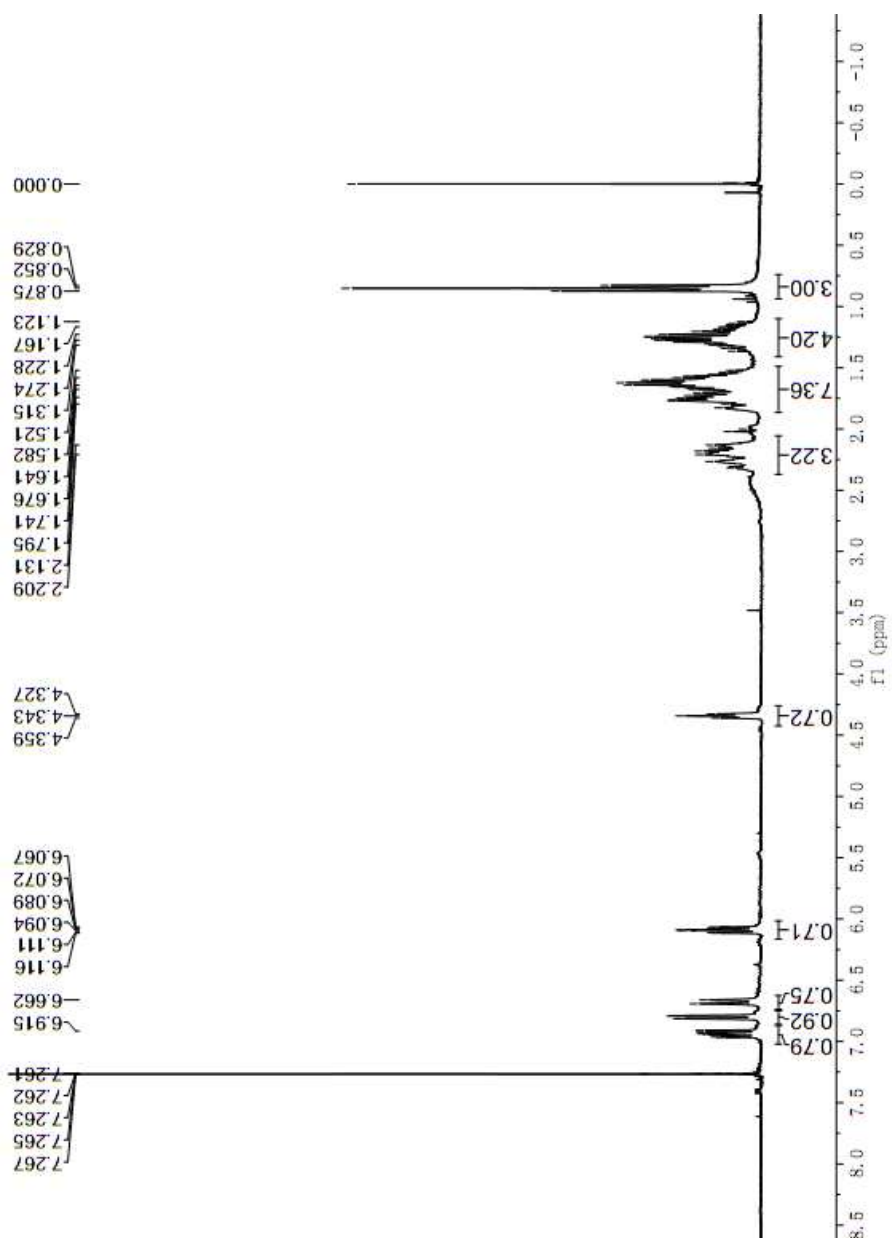


Fig. S-30: ¹H Spectra of 11-butyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,11,1}.

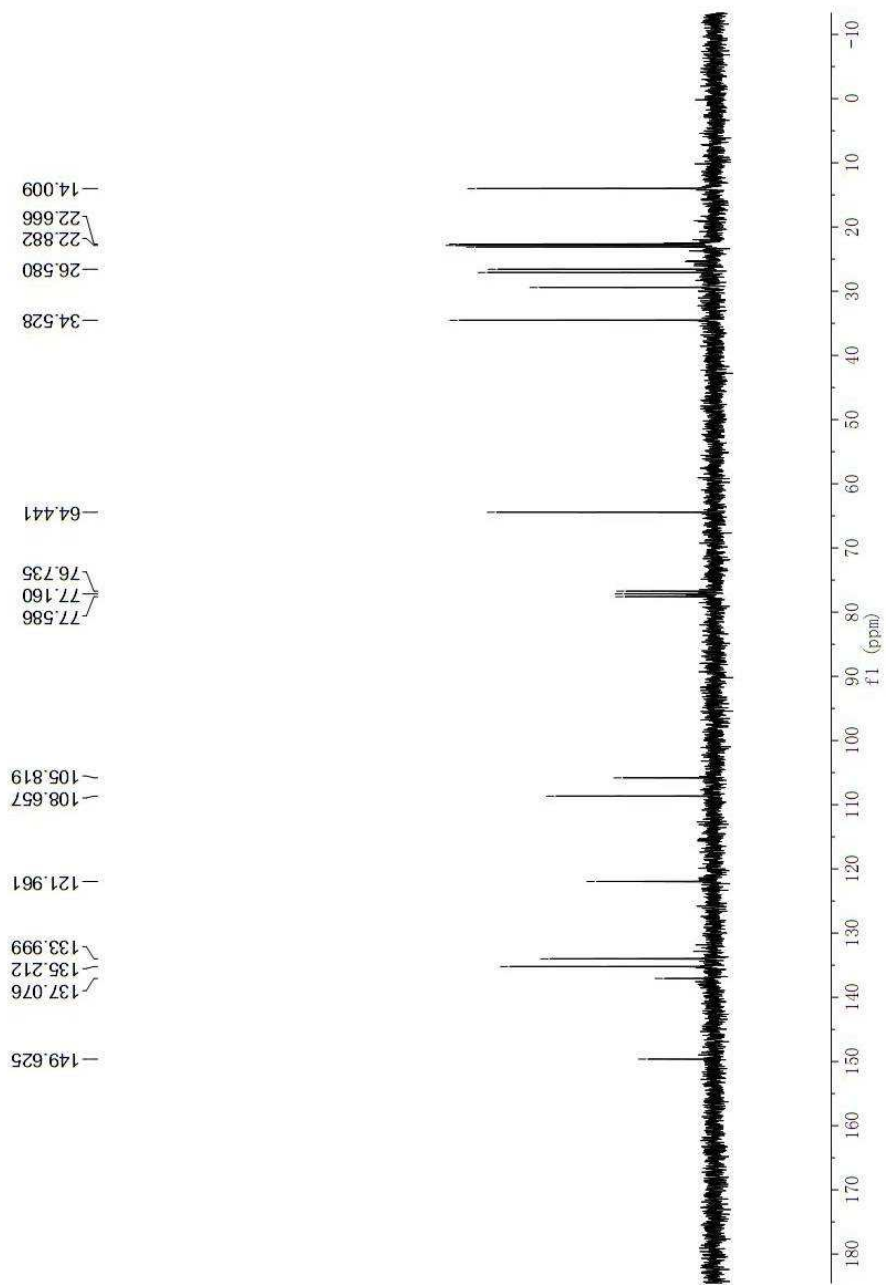
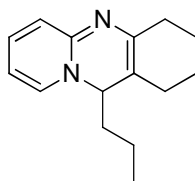


Fig. S-31: ^{13}C Spectra of 11-butyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,11,1}.



Chemical Formula: $C_{15}H_{20}N_2$

Exact Mass: 228.2

Molecular Weight: 228.3

4{1,12,1}

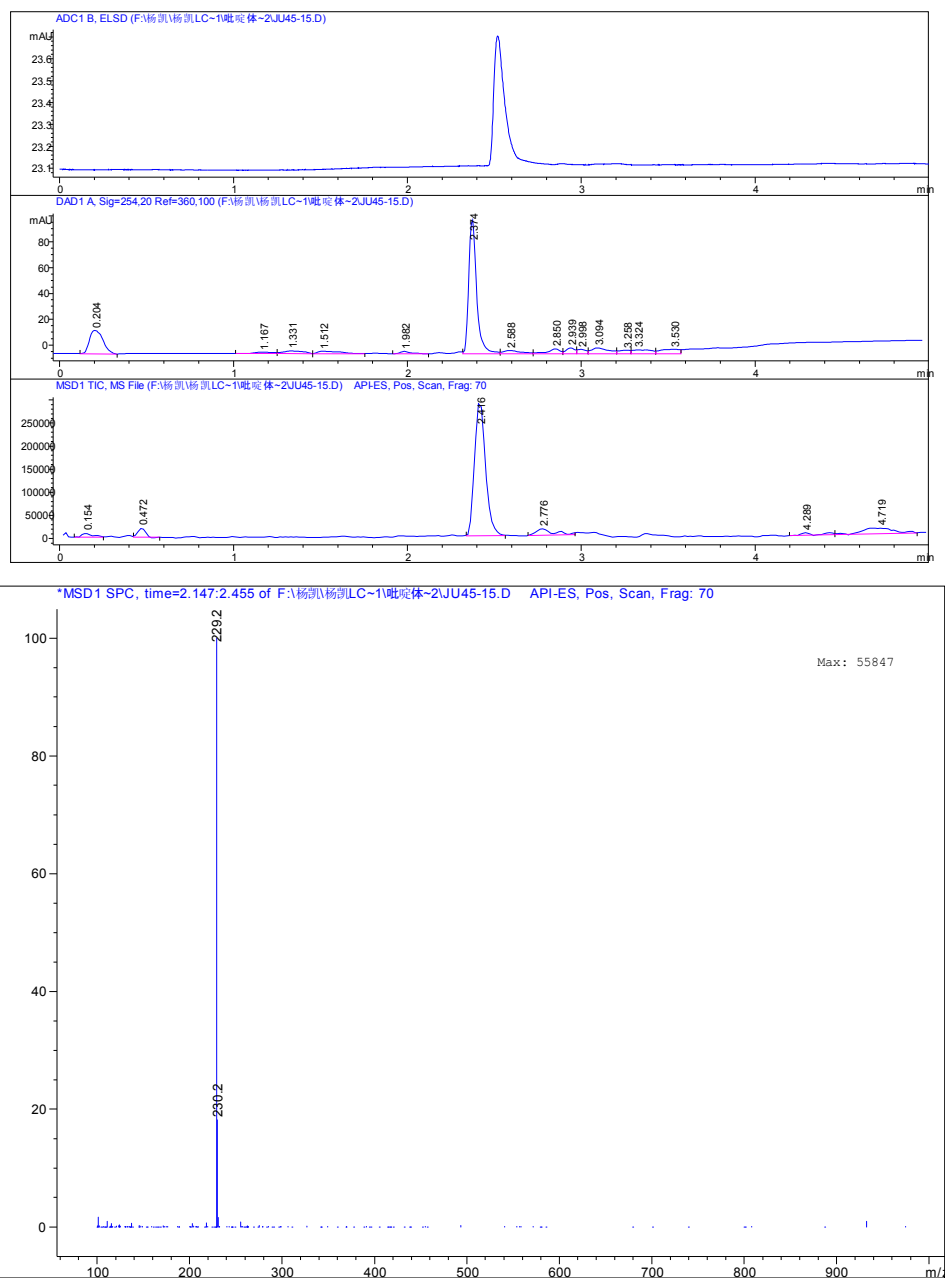


Fig. S-32: LC-MS-ELSD of 11-propyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,12,1}.

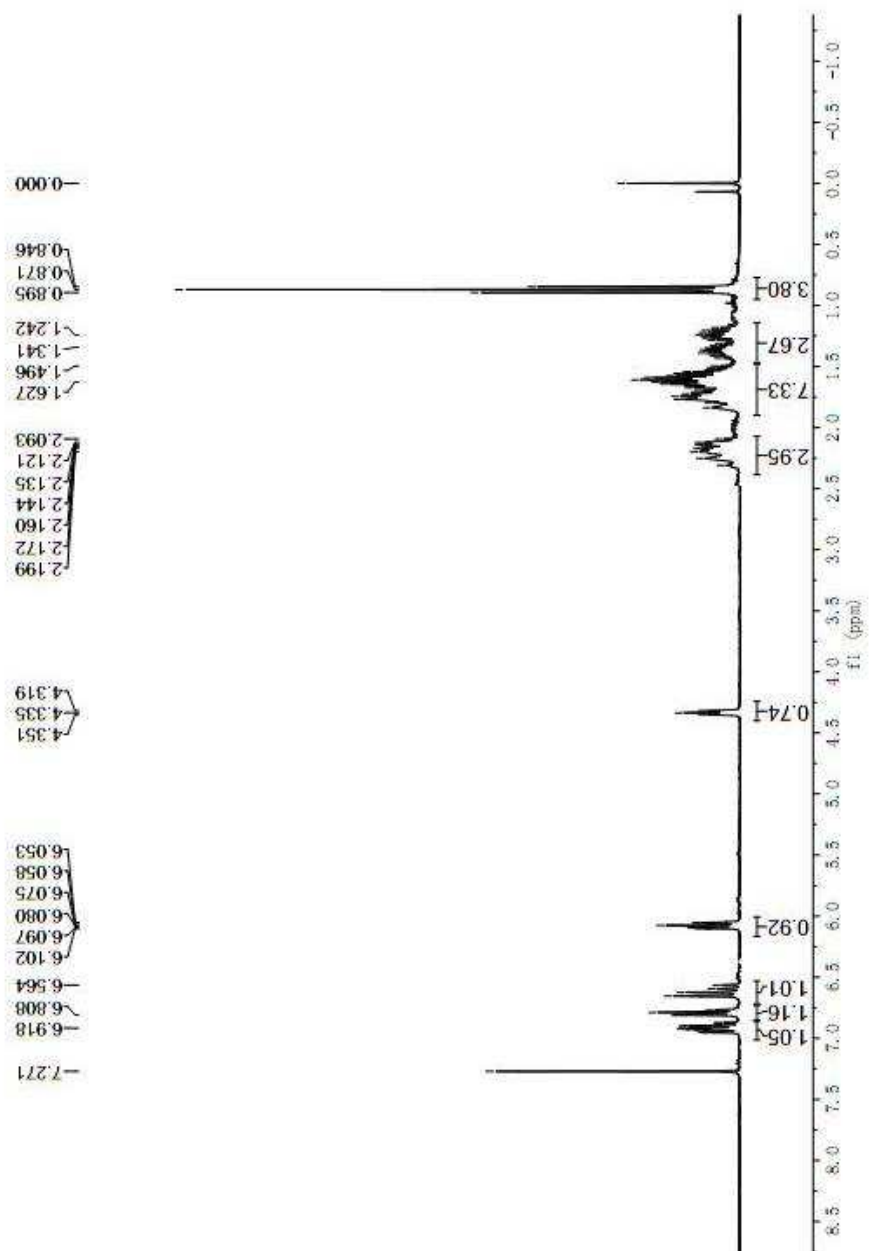
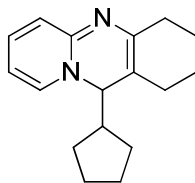


Fig. S-33: ^1H Spectra of 11-propyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,12,*I*}.



Chemical Formula: C₁₇H₂₂N₂

Exact Mass: 254.2

Molecular Weight: 254.4

4{1,13,1}

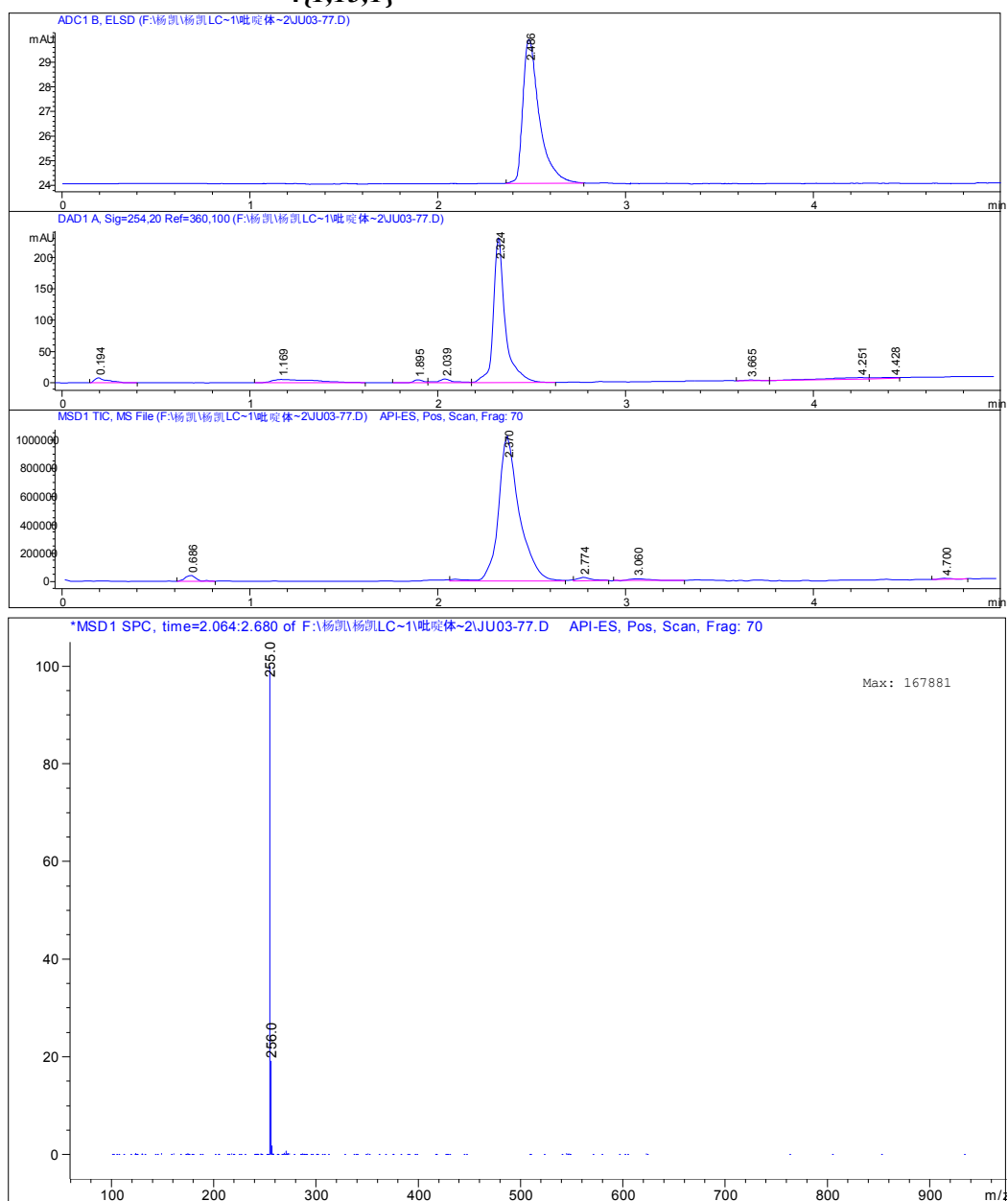


Fig. S-34: LC-MS-ELSD of 11-cyclopentyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,13,1}.

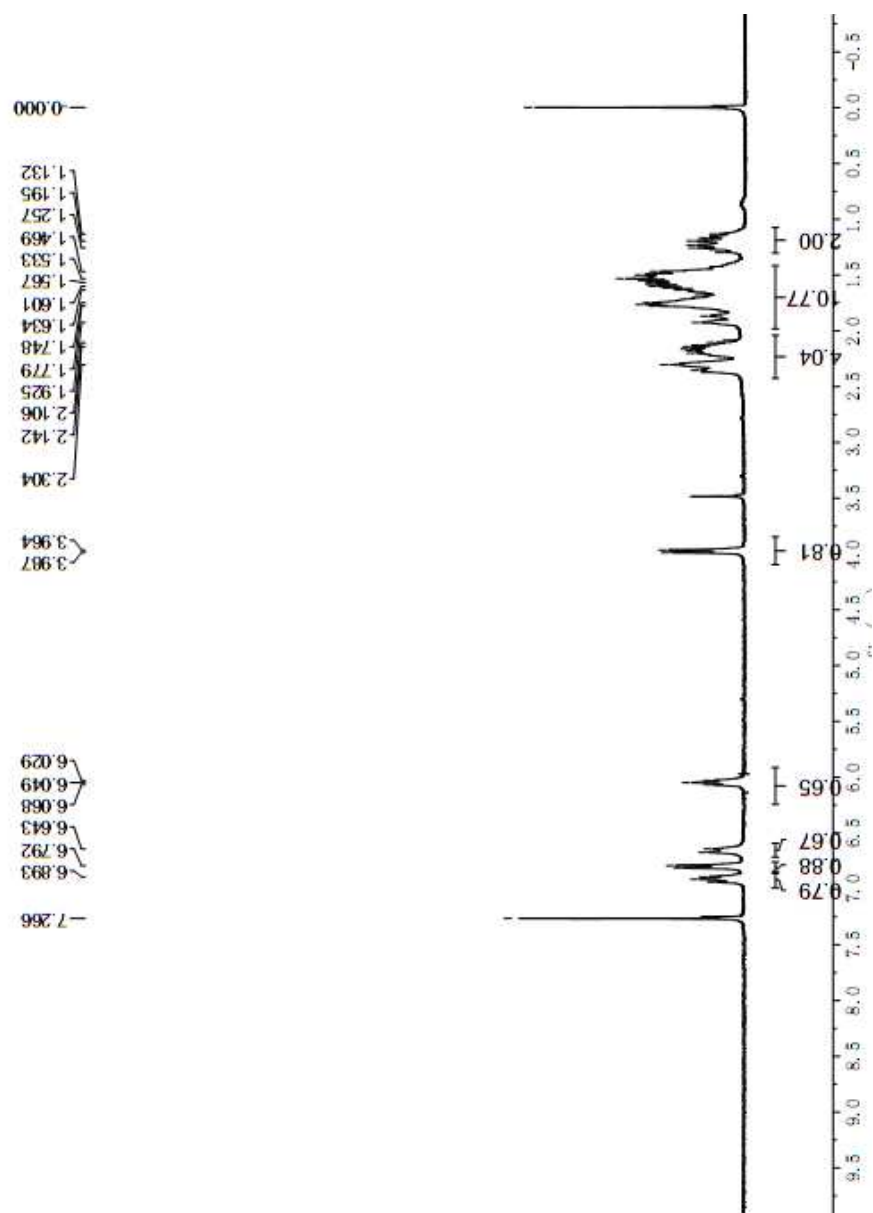


Fig. S-35: ^1H Spectra of 11-cyclopentyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,13,1}.

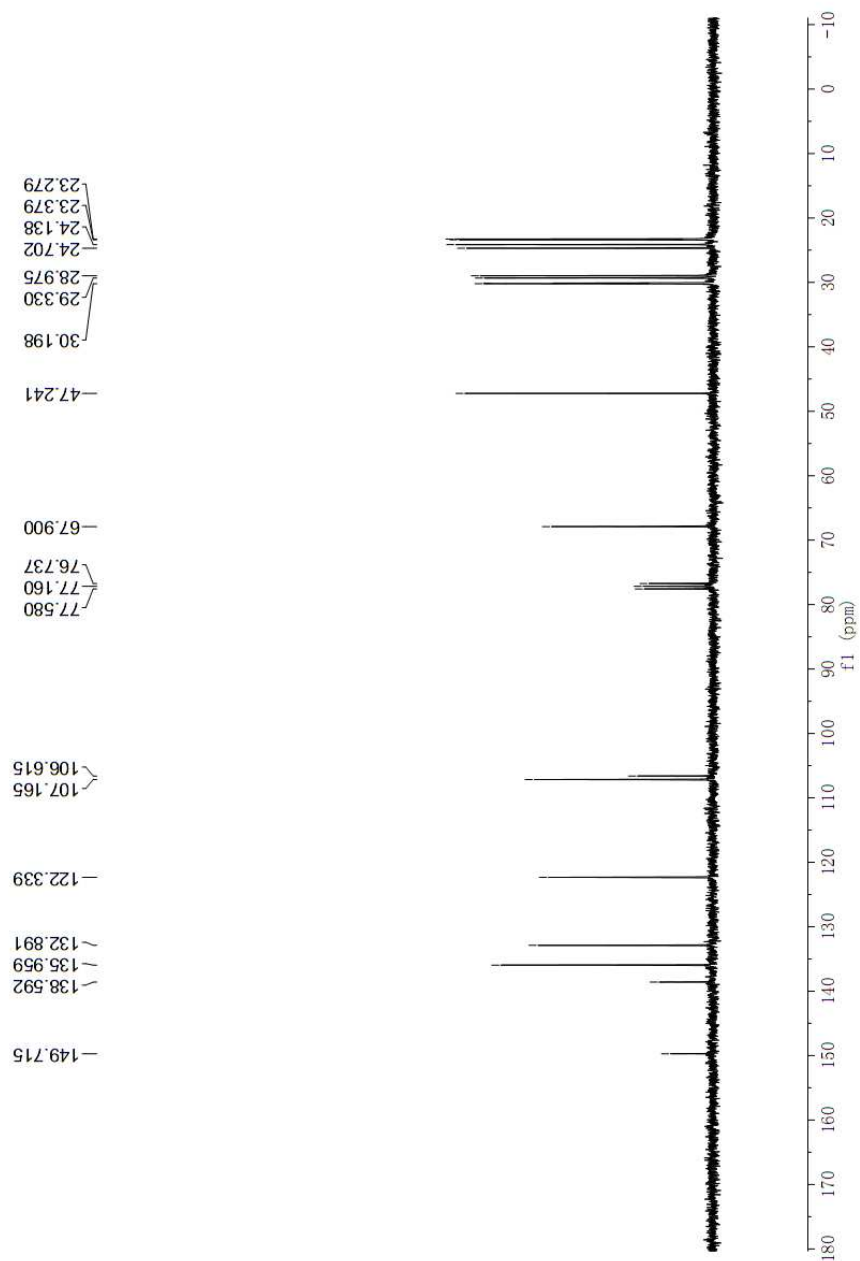
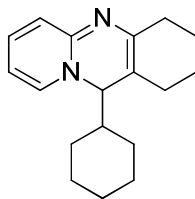


Fig. S-36: ^{13}C Spectra of 11-cyclopentyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,13,*I*}.



Chemical Formula: $C_{18}H_{24}N_2$

Exact Mass: 268.2

Molecular Weight: 268.4

4{1,14,1}

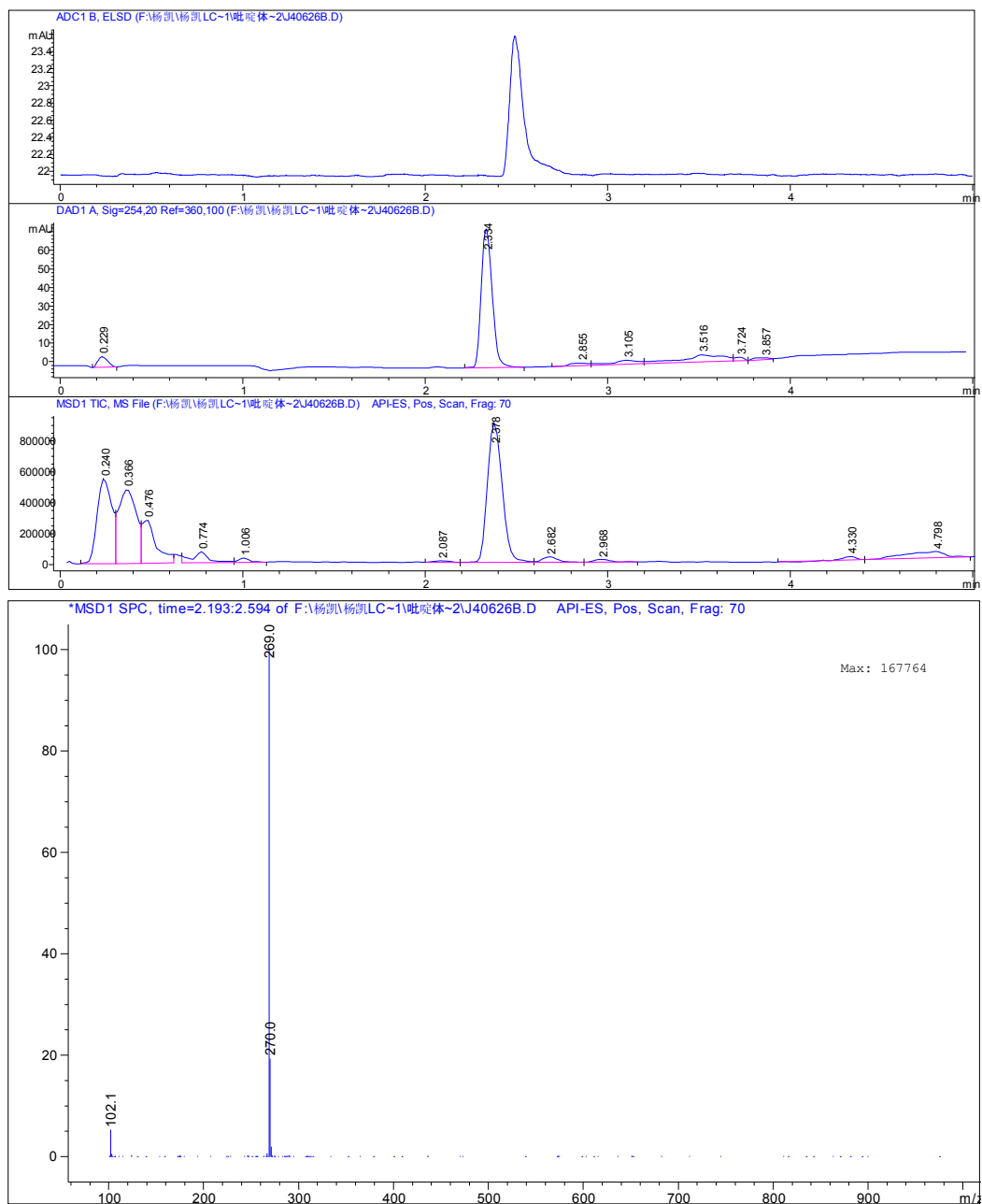


Fig. S-37: LC-MS-ELSD of 11-cyclohexyl-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{1,14,1}.

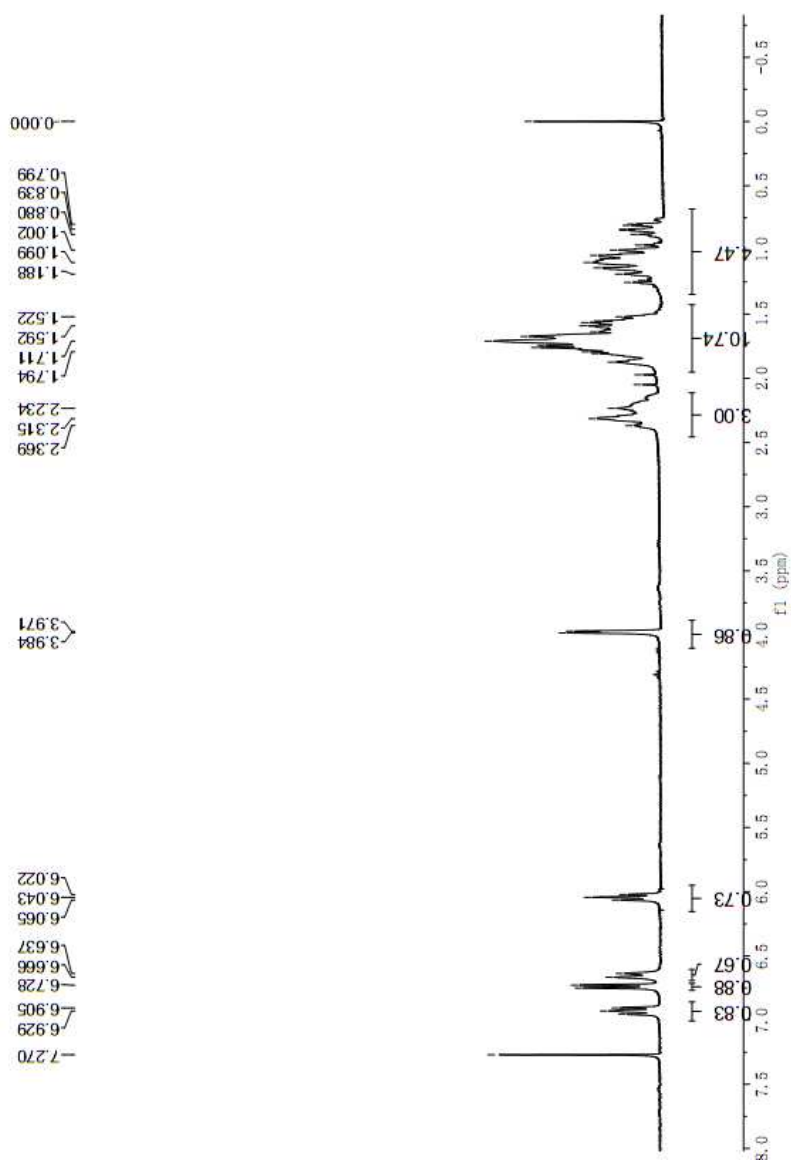


Fig. S-38: ^1H Spectra of 11-cyclohexyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,14,*I*}.

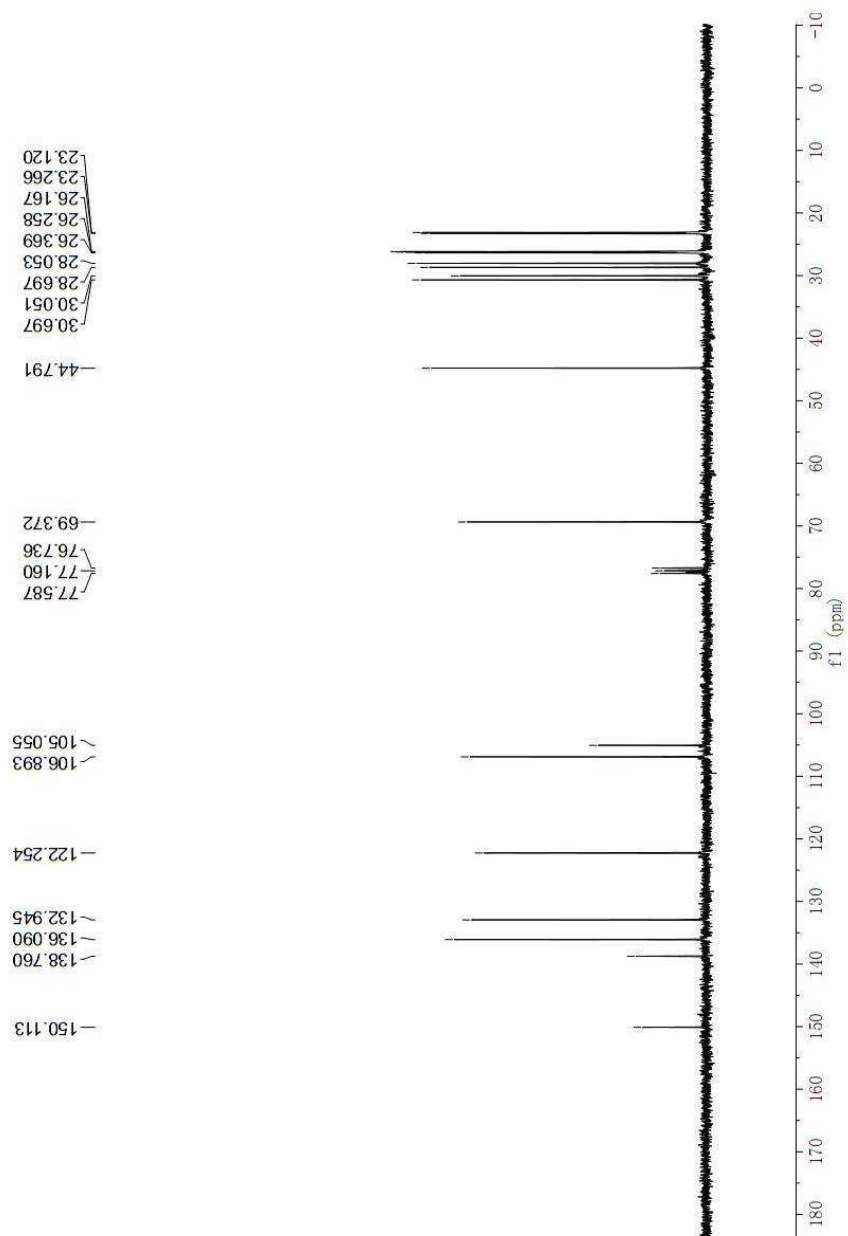
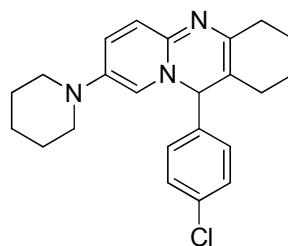


Fig. S-39: ^{13}C Spectra of 11-cyclohexyl-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{1,14,1}.



Chemical Formula: $C_{23}H_{26}ClN_3$

Exact Mass: 379.2

Molecular Weight: 379.9

4{2,I,I}

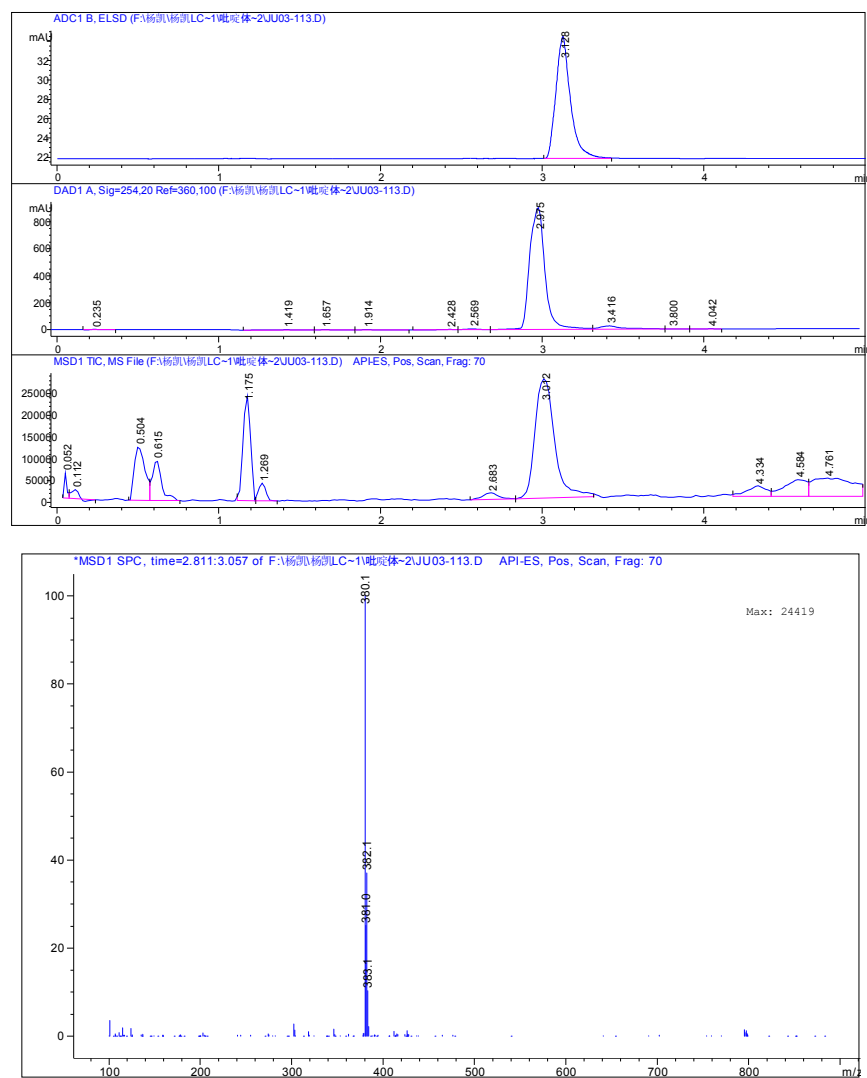


Fig. S-40: LC-MS-ELSD of 11-(4-chlorophenyl)-8-(piperidin-1-yl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{2,I,I}.

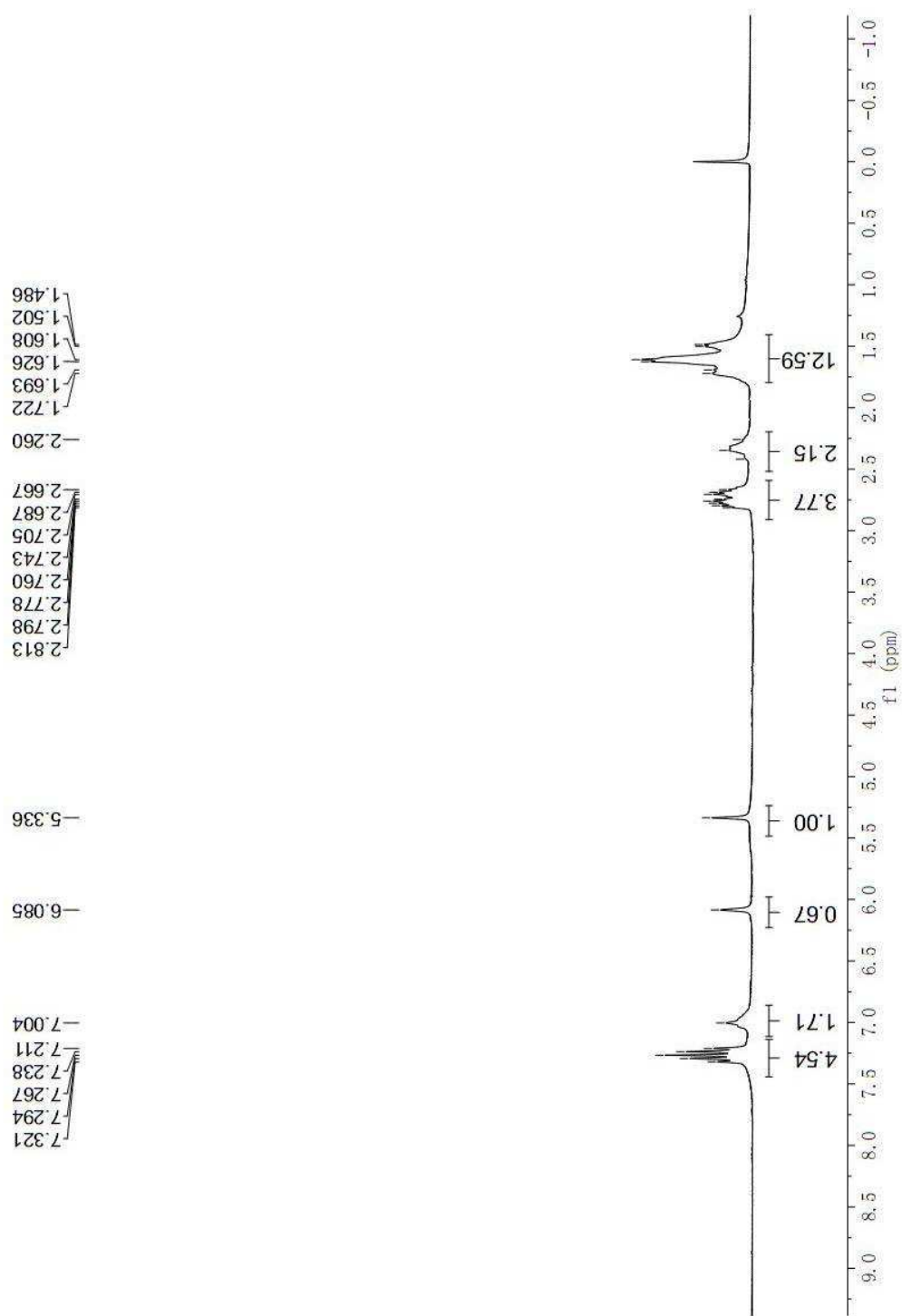


Fig. S-41: ^1H Spectra of 11-(4-chlorophenyl)-8-(piperidin-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{2,1,*I*}.

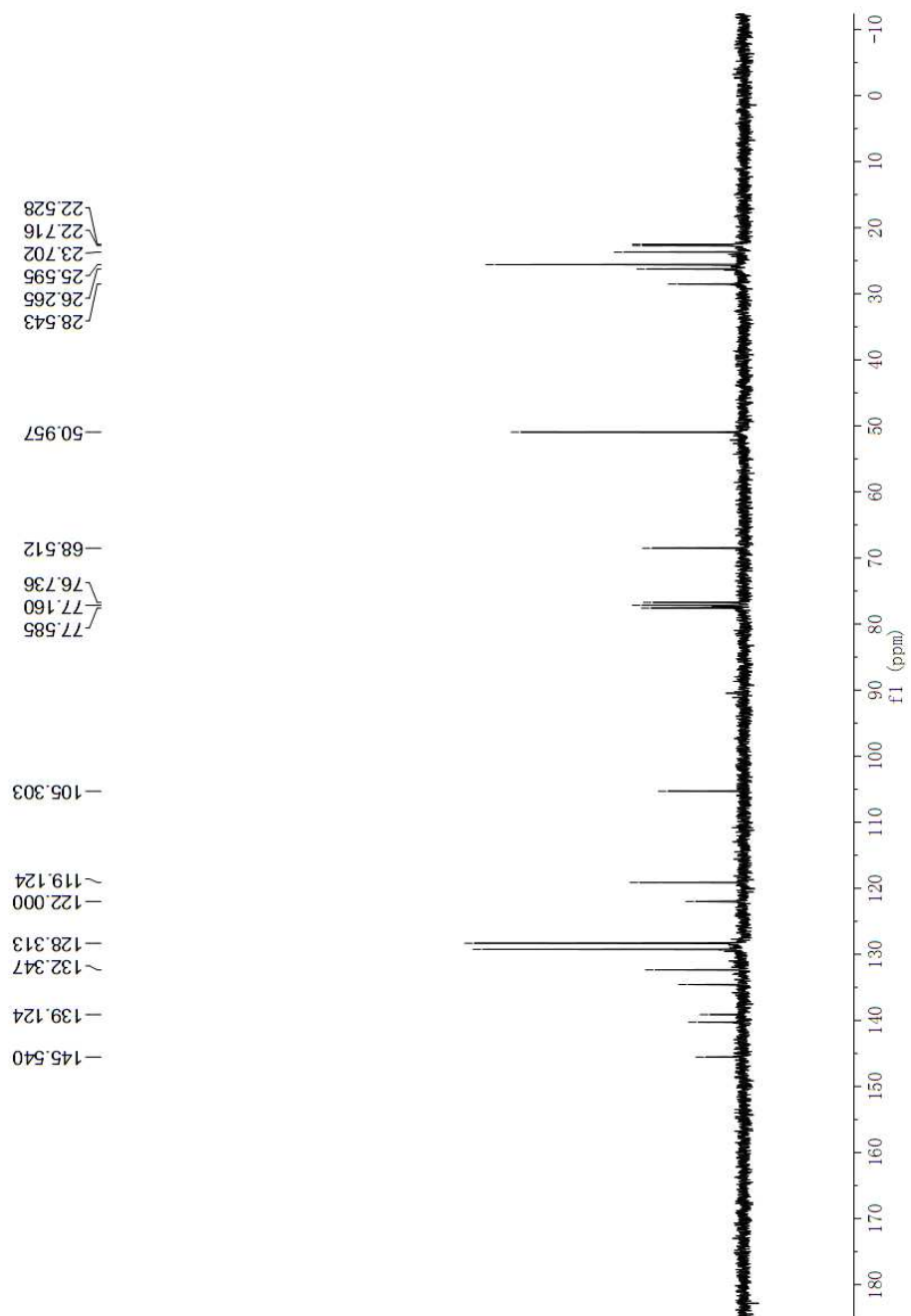
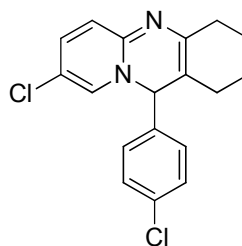


Fig. S-42: ^{13}C Spectra of 11-(4-chlorophenyl)-8-(piperidin-1-yl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{2,1,*I*}.



Chemical Formula: $C_{18}H_{16}Cl_2N_2$

Exact Mass: 330.1

Molecular Weight: 331.2

4{3,1,I}

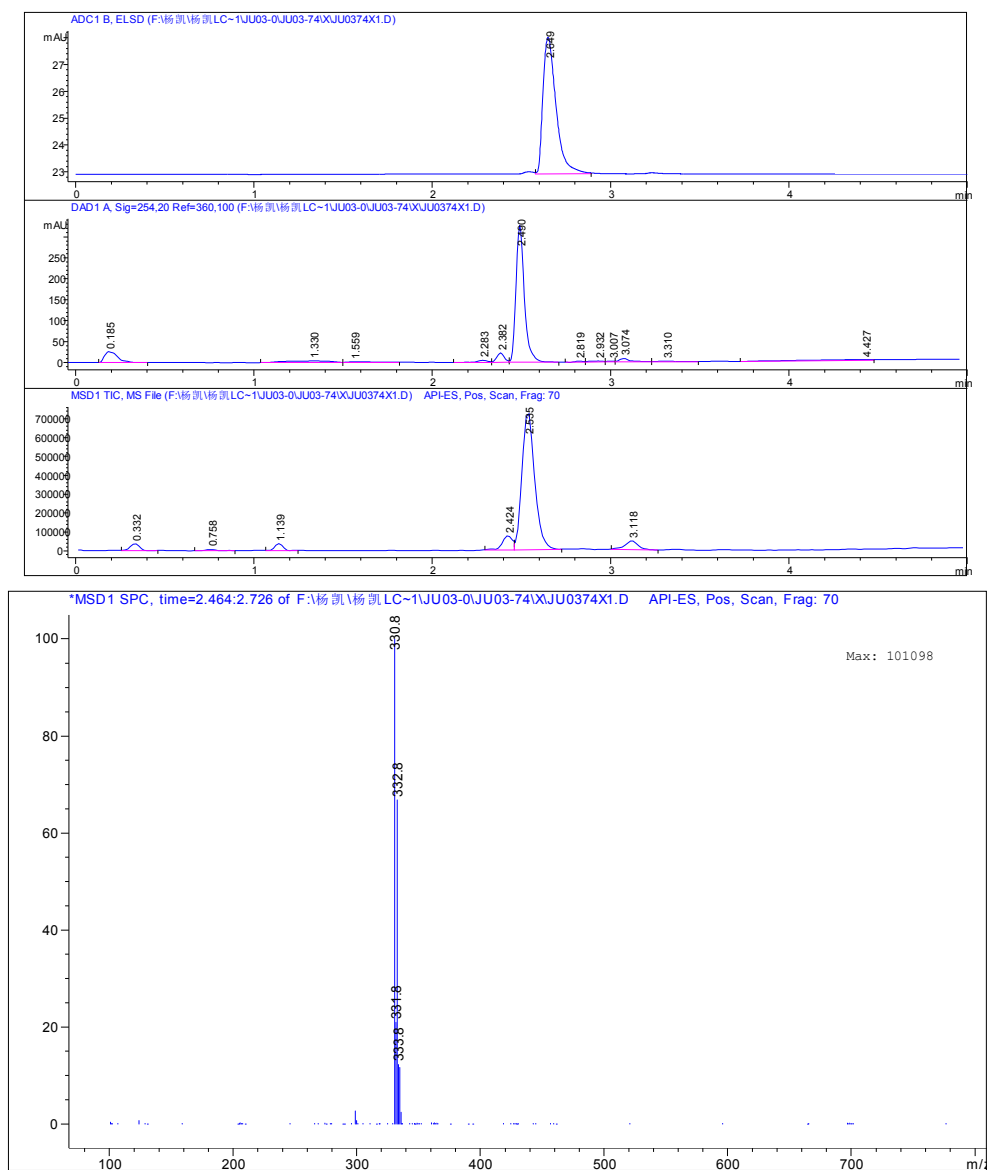


Fig. S-43: LC-MS-ELSD of 8-chloro-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{3,1,I}.

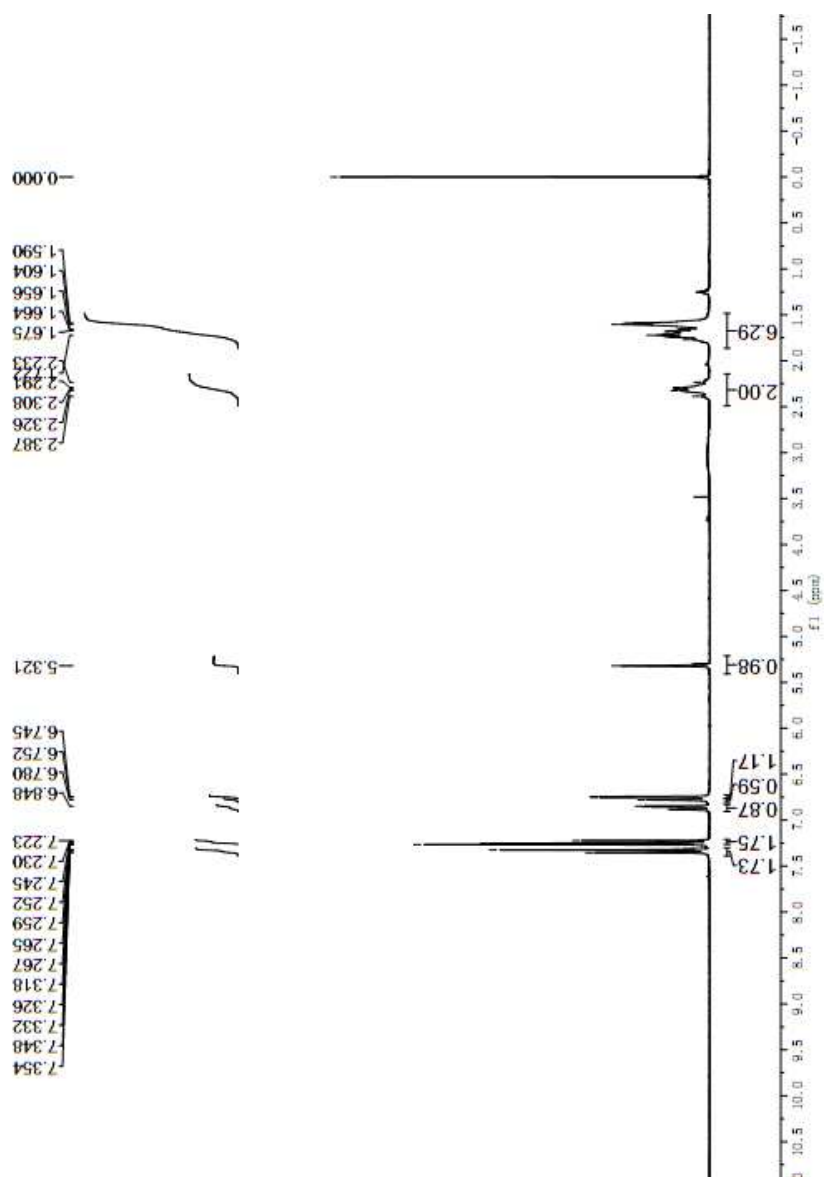


Fig. S-44: ^1H Spectra of 8-chloro-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 4{3,1,*I*}.

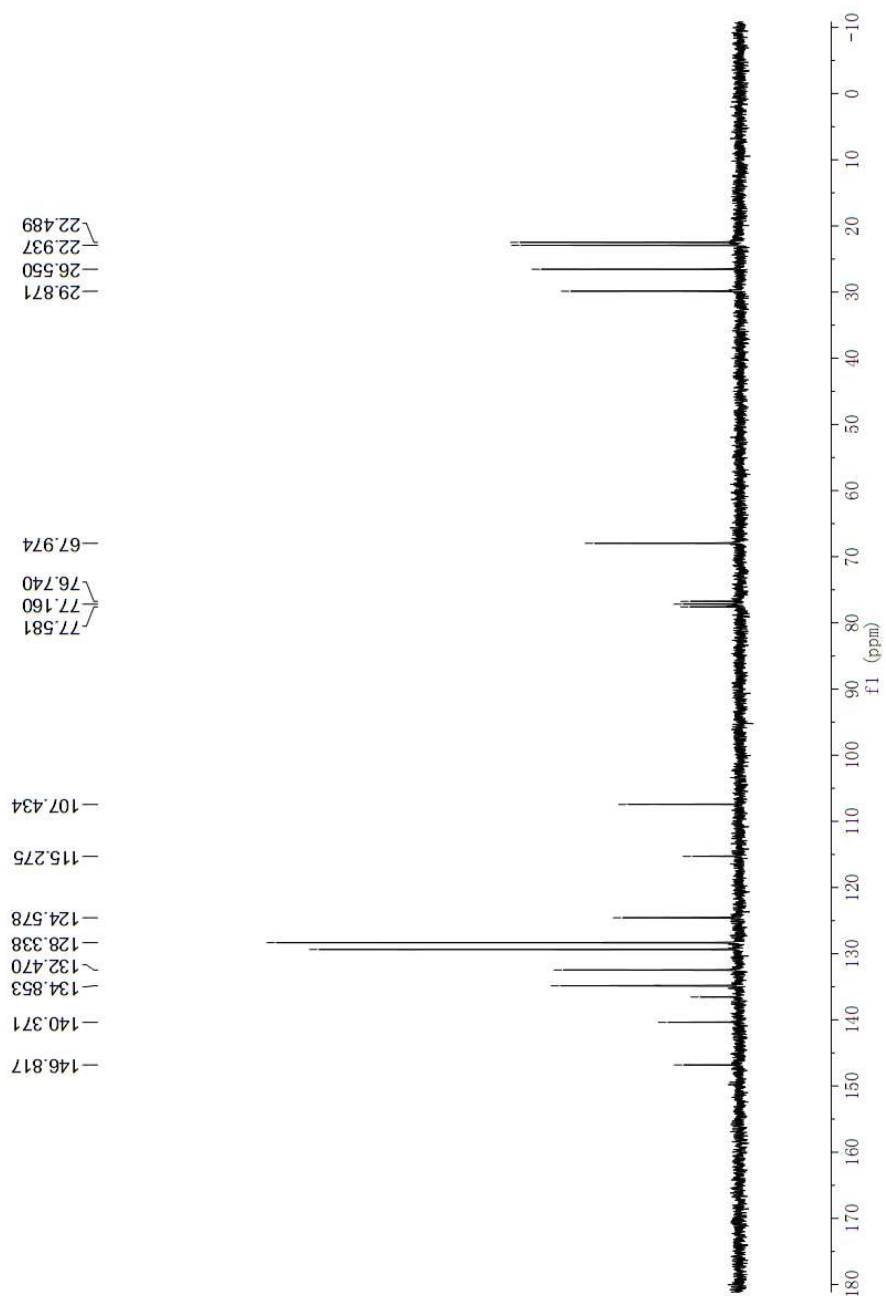
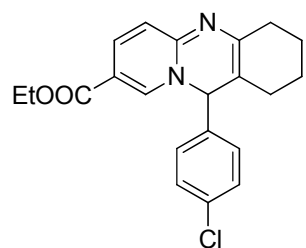


Fig. S-45: ^{13}C Spectra of 8-chloro-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline 4{3,l,l}.



Chemical Formula: $C_{21}H_{21}ClN_2O_2$

Exact Mass: 368.1

Molecular Weight: 368.9

4{4,1,1}

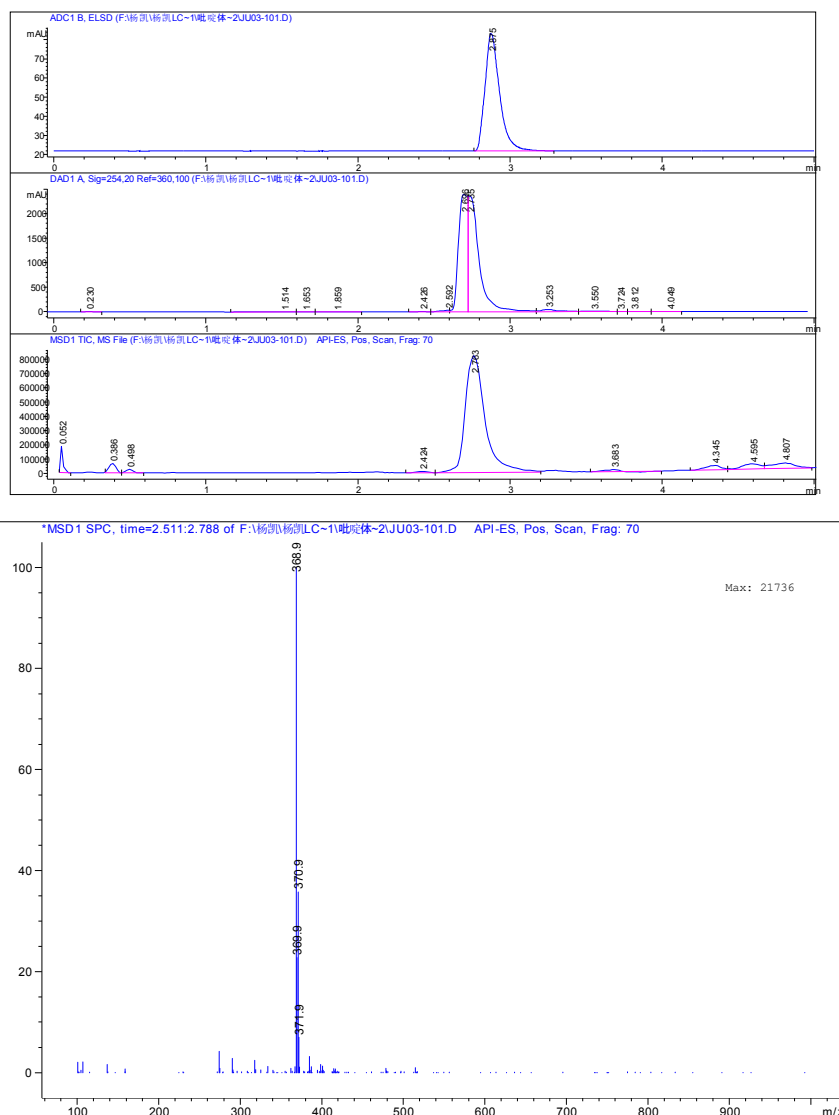


Fig. S-46: LC-MS-ELSD of ethyl 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-b]quinazoline-8-carboxylate 4{4,1,1}.

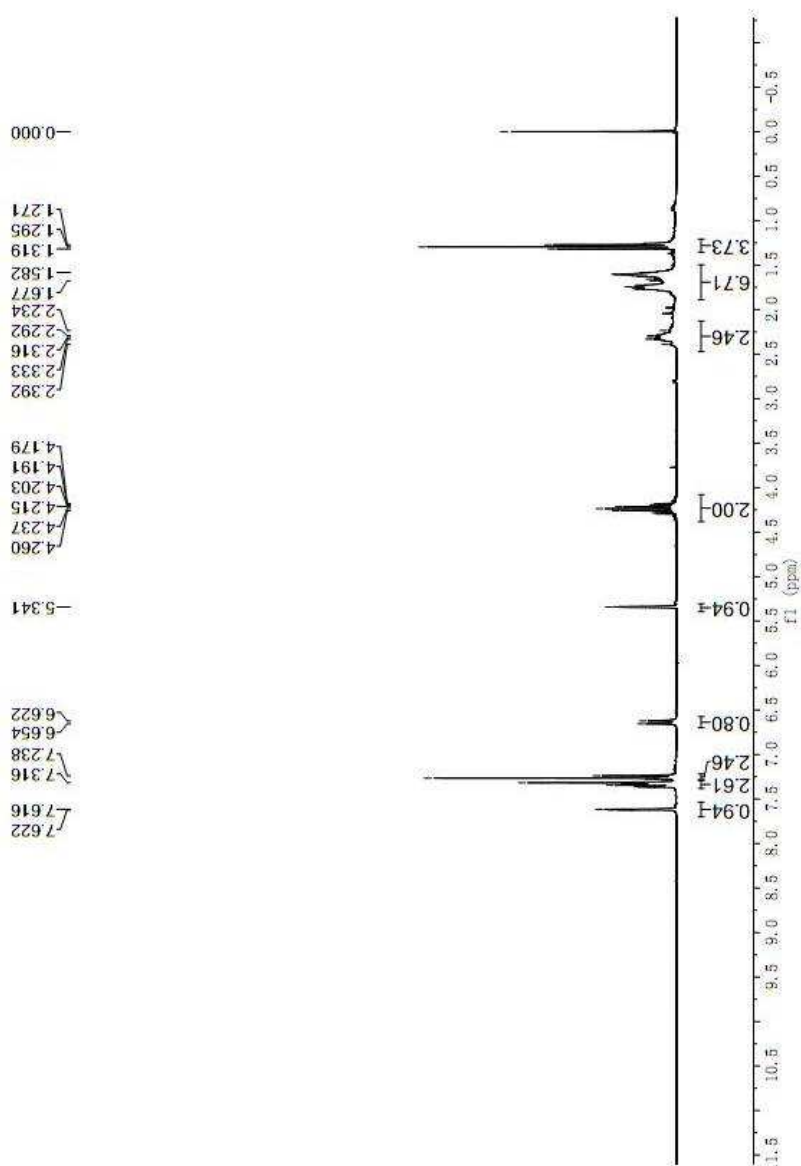


Fig. S-47: ¹H Spectra of ethyl 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido [2,1-b]quinazoline-8-carboxylate 4{4,1,1}.

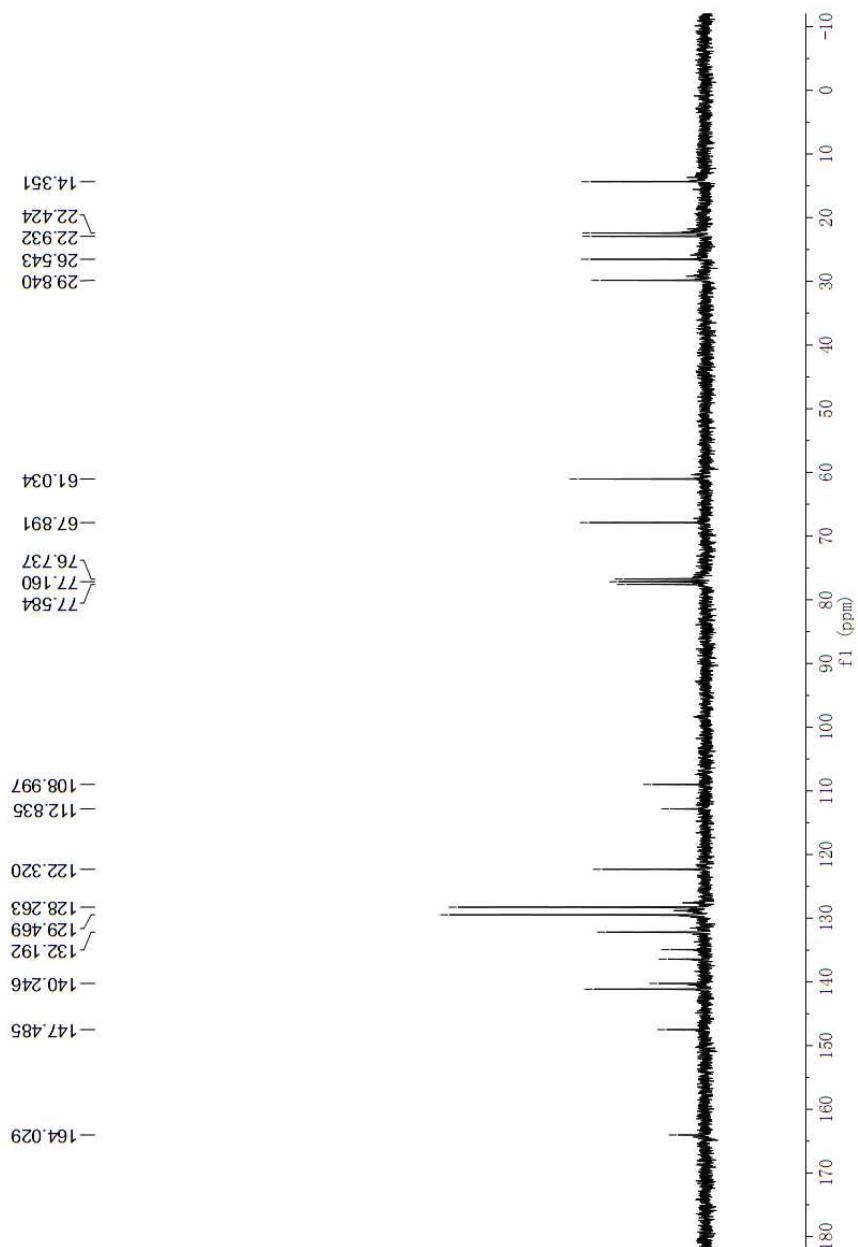
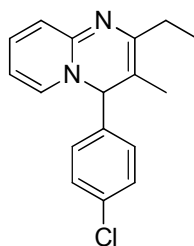


Fig. S-48: ^{13}C Spectra of ethyl 11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido [2,1-*b*]quinazoline-8-carboxylate 4{4,1,1}.



Chemical Formula: C₁₇H₁₇ClN₂

Exact Mass: 284.1

Molecular Weight: 284.8

4{1,1,2}

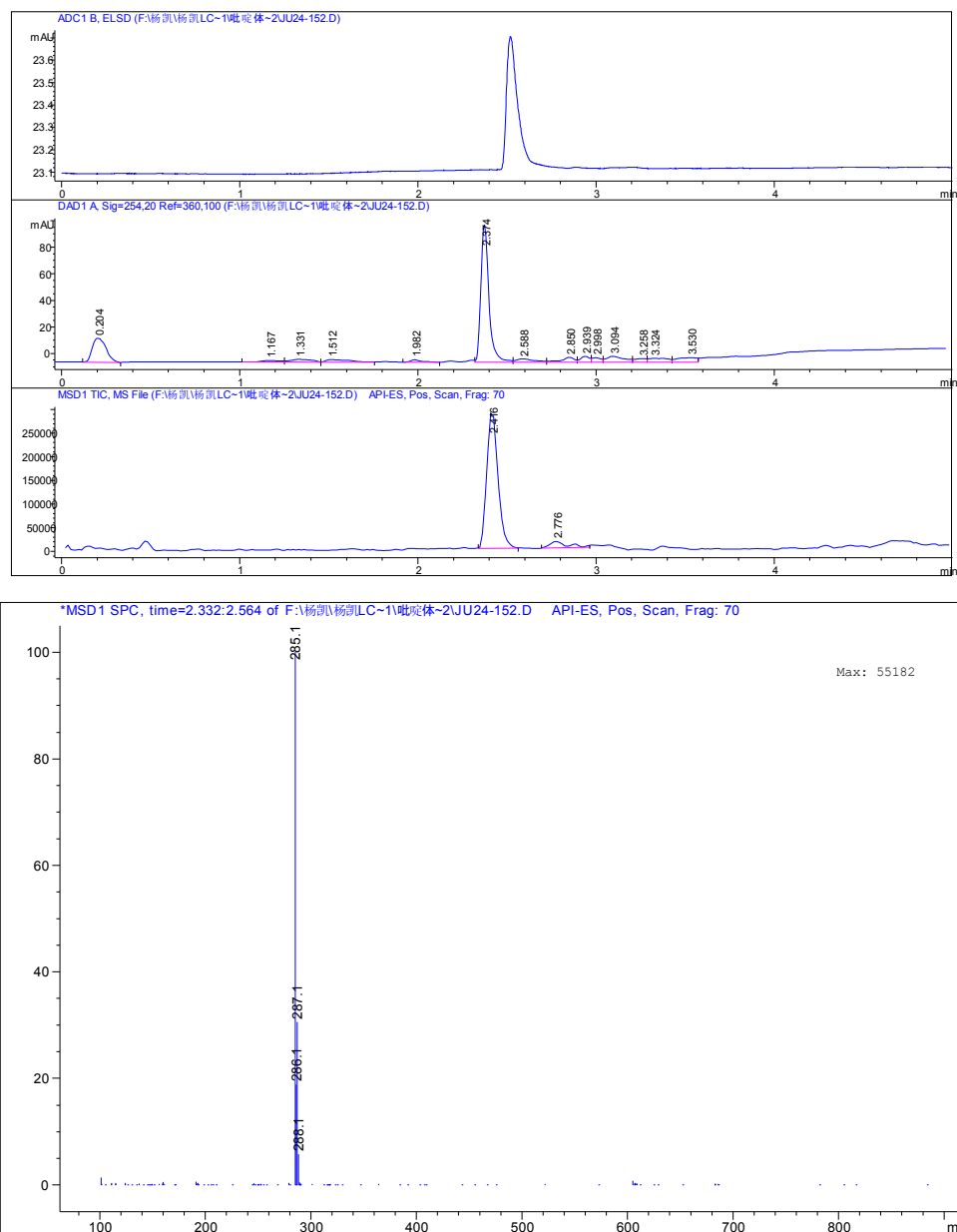


Fig. S-49: LC-MS-ELSD of 4-(4-chlorophenyl)-2-ethyl-3-methyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,2}.

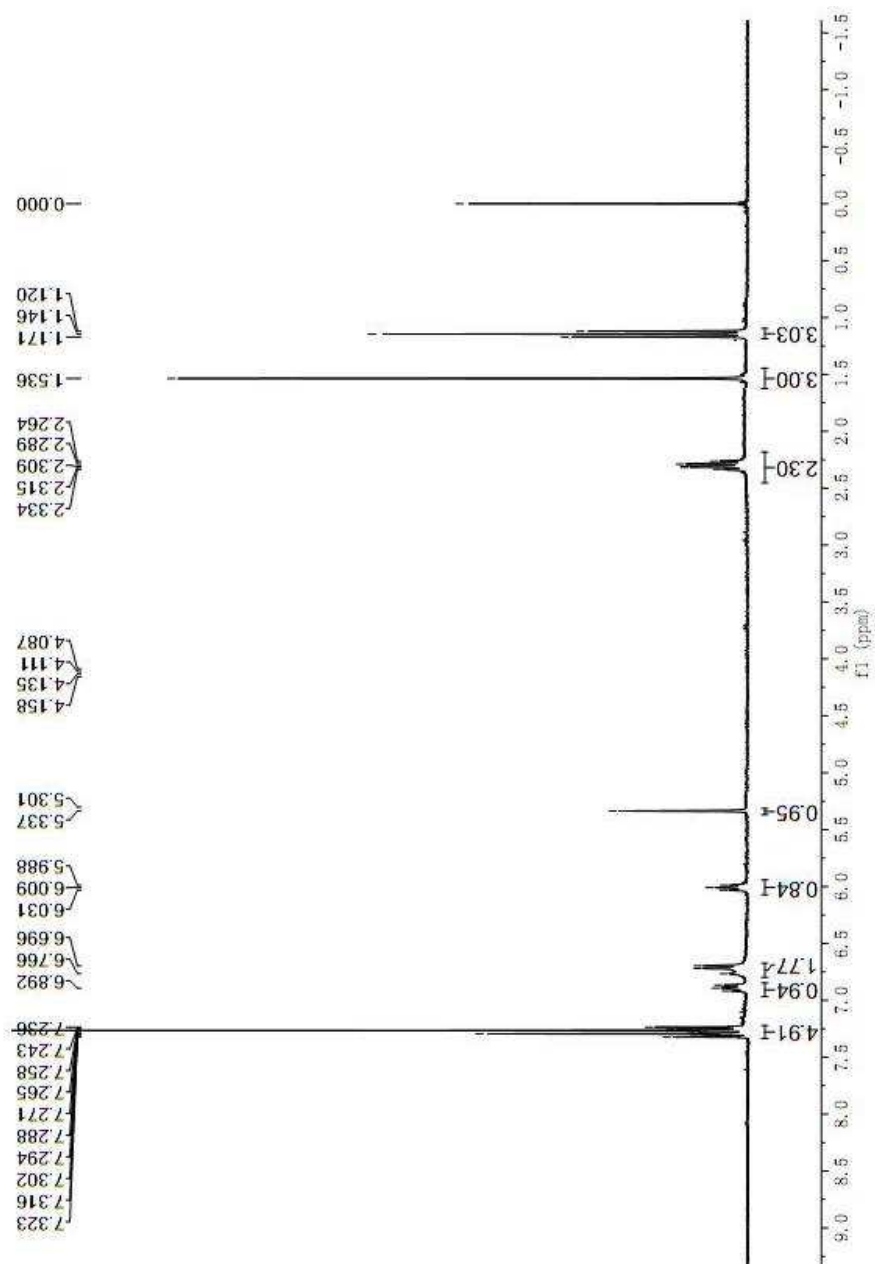


Fig. S-50: ¹H Spectra of 4-(4-chlorophenyl)-2-ethyl-3-methyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,2}.

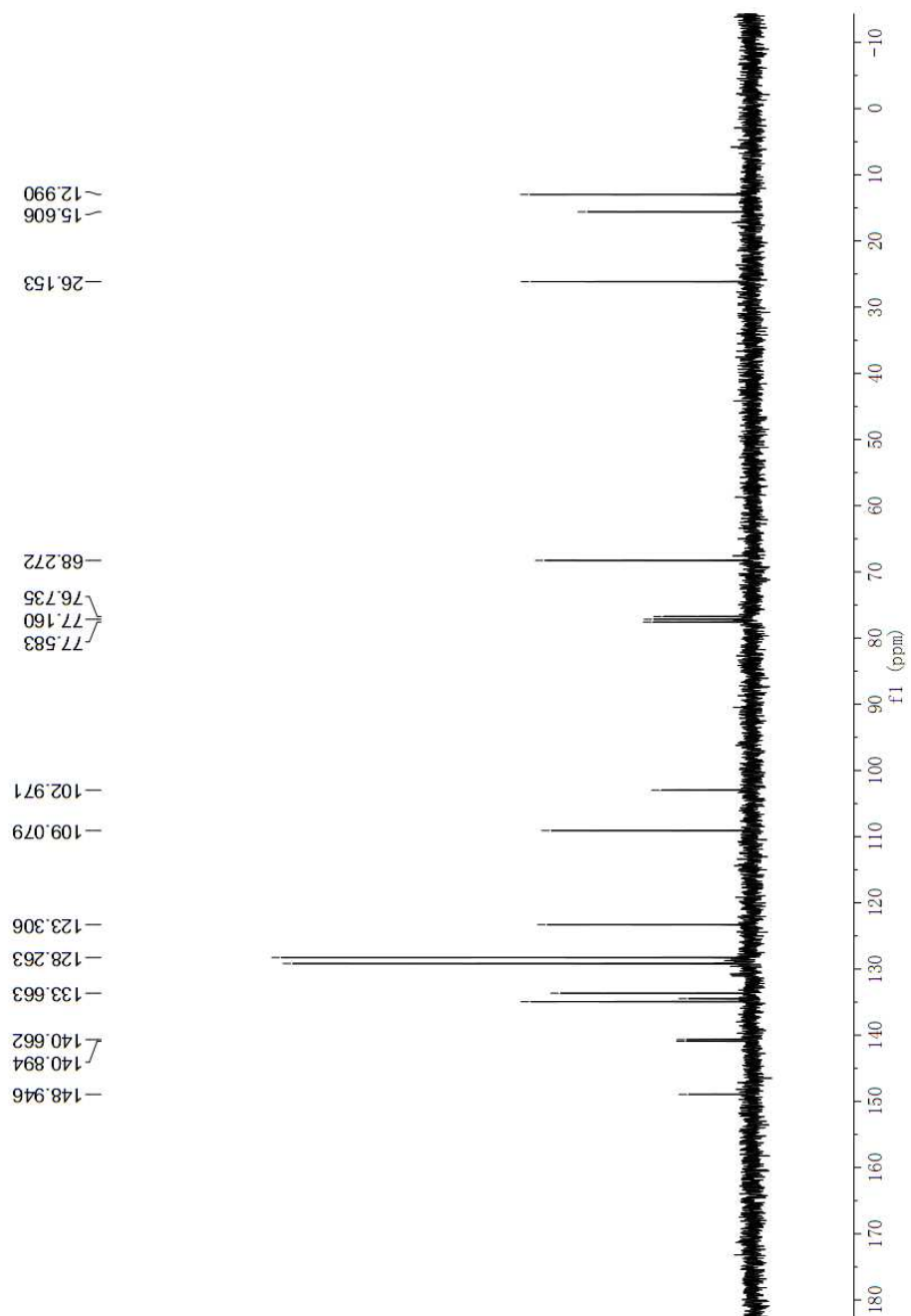
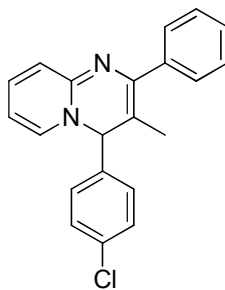


Fig. S-51: ¹³C Spectra of 4-(4-chlorophenyl)-2-ethyl-3-methyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,2}.



Chemical Formula: C₂₁H₁₇ClN₂

Exact Mass: 332.1

Molecular Weight: 332.8

4{1,1,4}

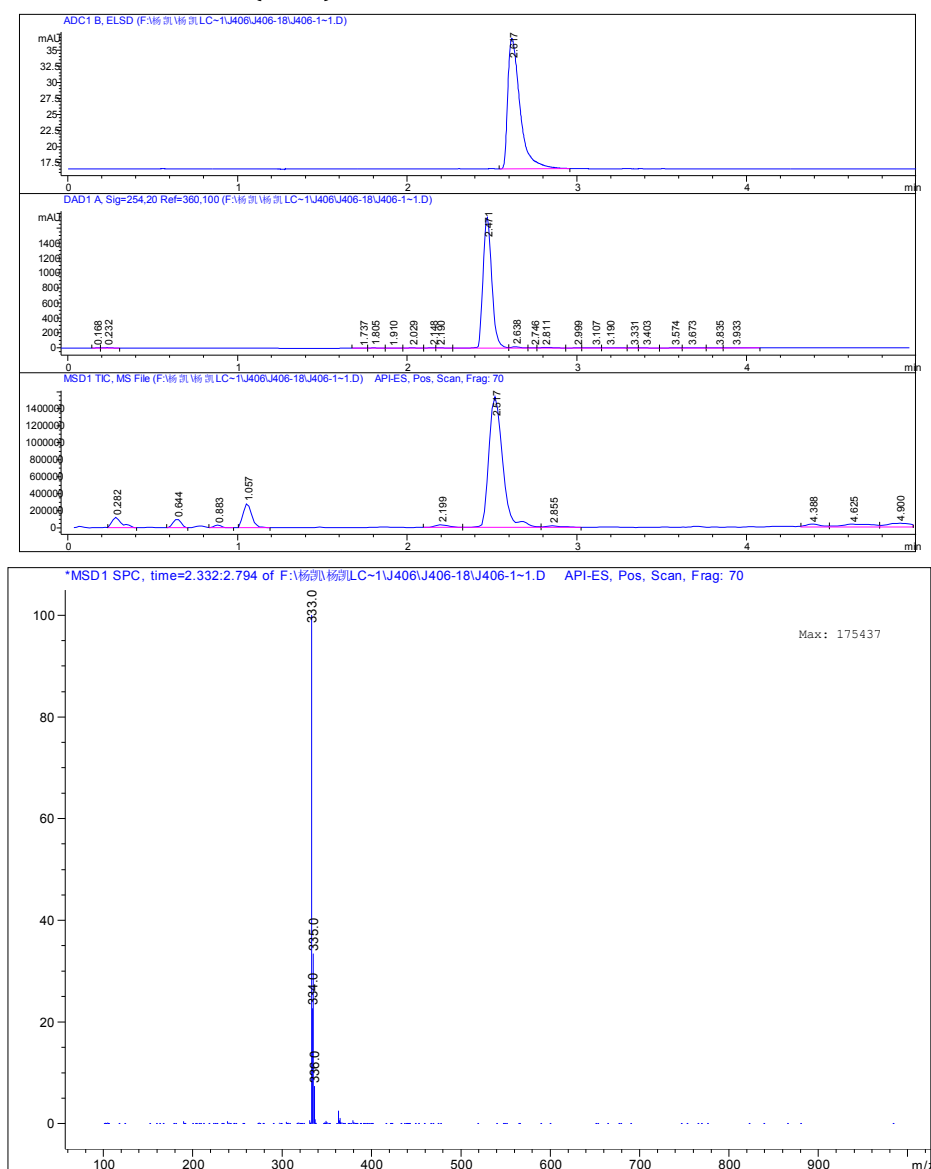


Fig. S-52: LC-MS-ELSD of 4-(4-chlorophenyl)-3-methyl-2-phenyl-4*H*-pyrido [1,2-*a*]pyrimidine 4{1,1,4}.

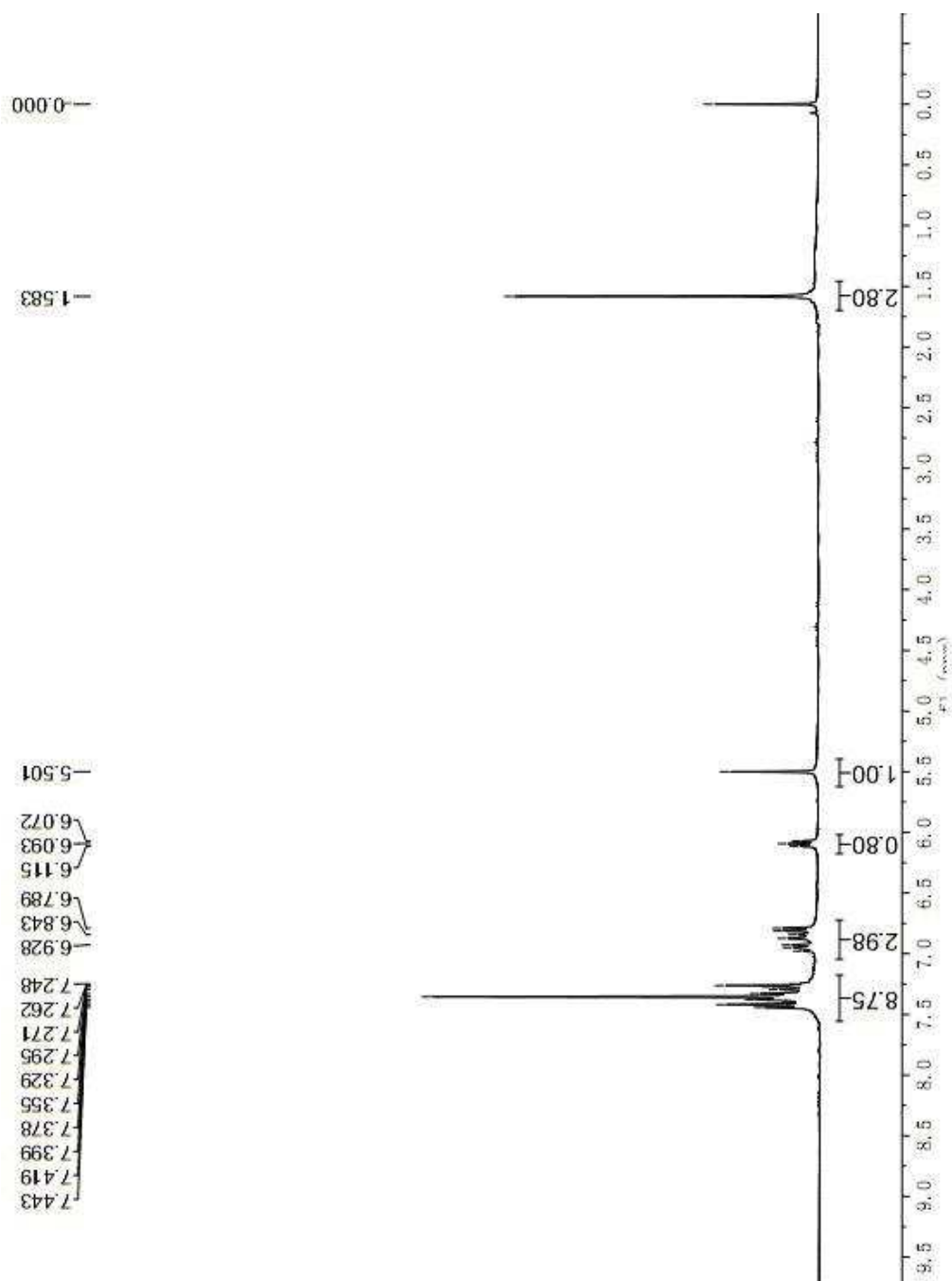


Fig. S-53: ¹H Spectra of 4-(4-chlorophenyl)-3-methyl-2-phenyl-4*H*-pyrido [1,2-*a*]pyrimidine 4{1,1,4}.

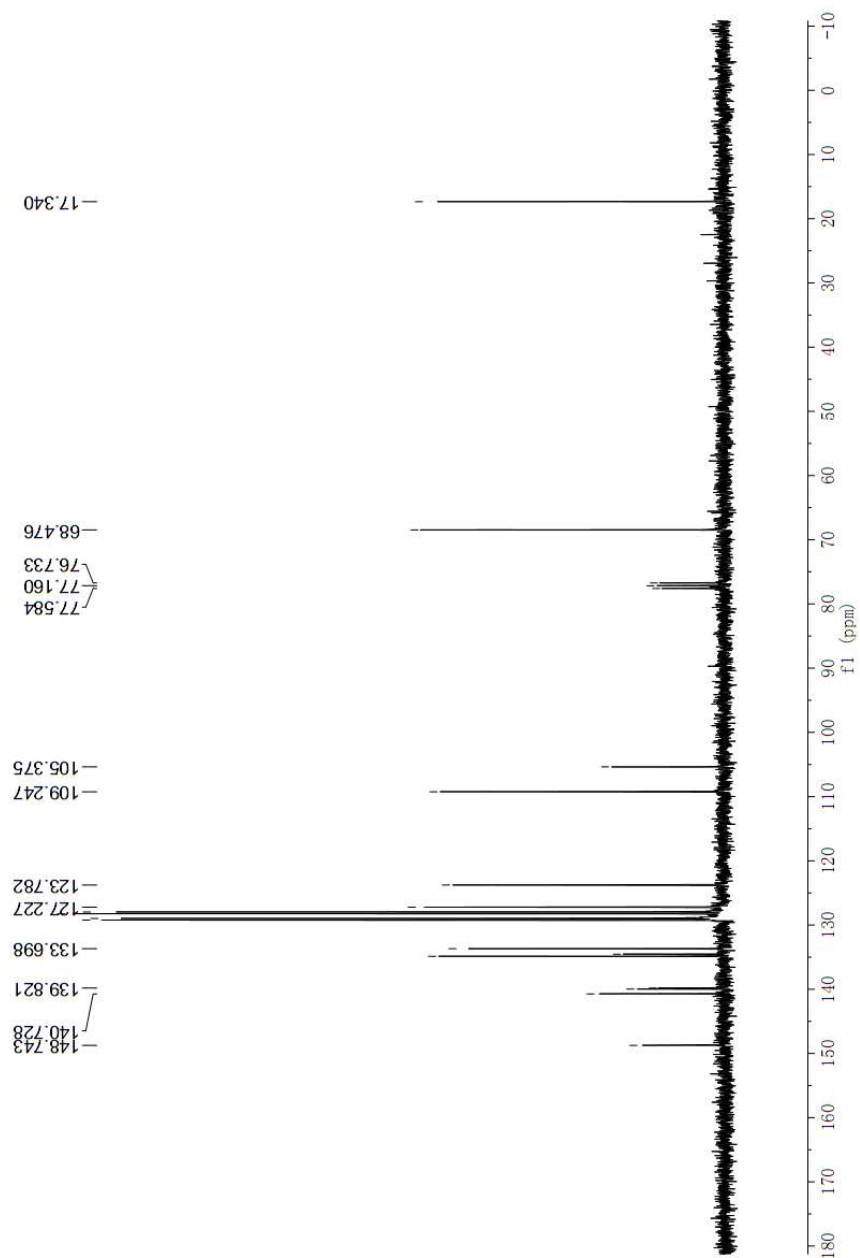
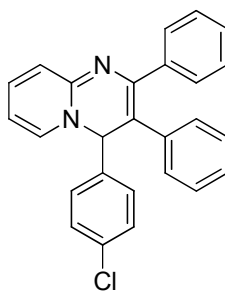


Fig. S-54: ^{13}C Spectra of 4-(4-chlorophenyl)-3-methyl-2-phenyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,4}.



Chemical Formula: $C_{26}H_{19}ClN_2$

Exact Mass: 394.1

Molecular Weight: 394.9

4{1,1,5}

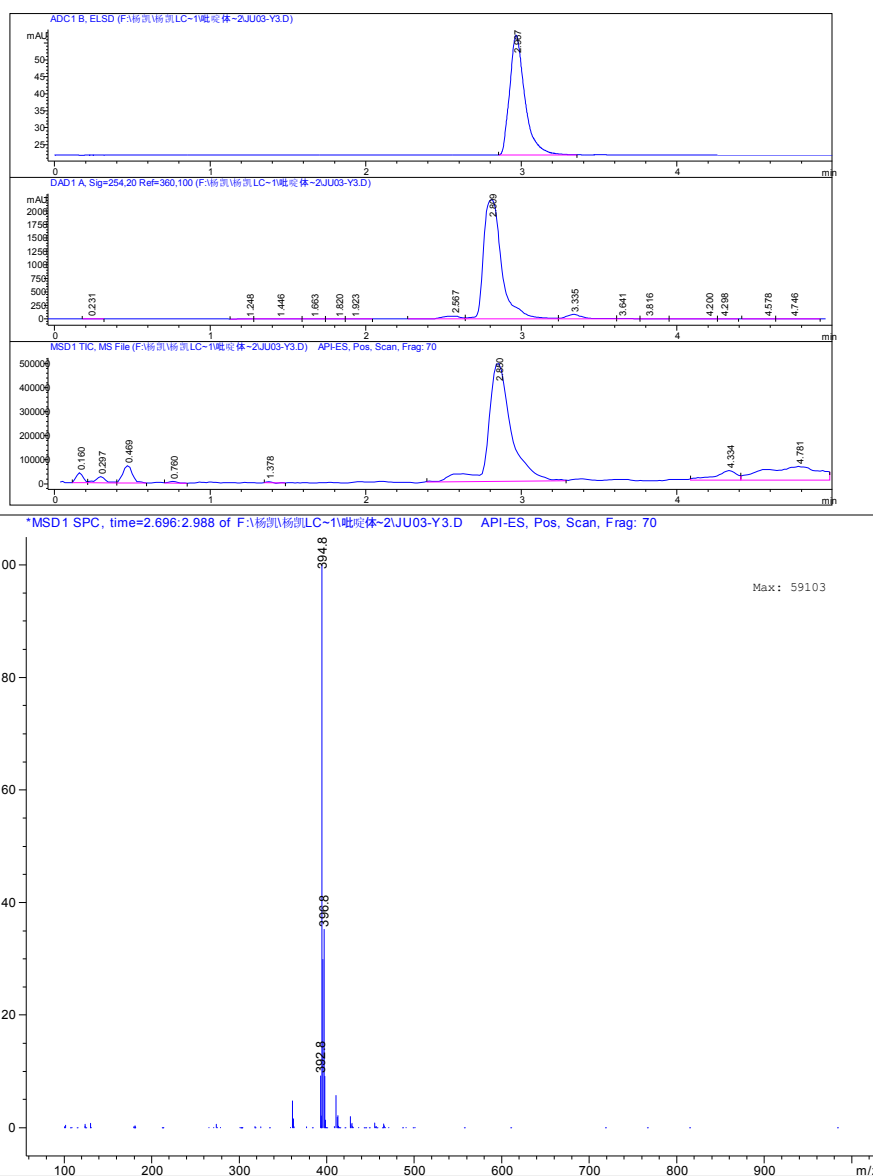


Fig. S-55: LC-MS-ELSD of 4-(4-chlorophenyl)-2,3-diphenyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,5}.

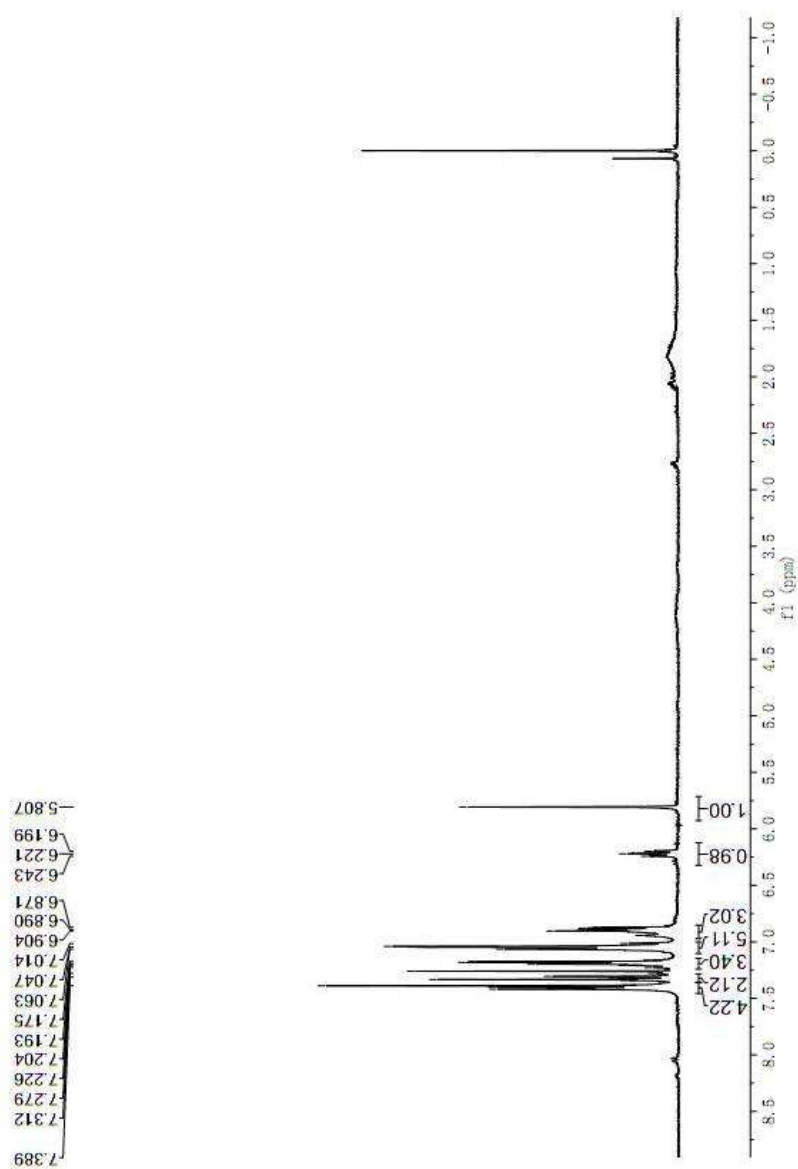


Fig. S-56: ^1H Spectra of 4-(4-chlorophenyl)-2,3-diphenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,5}.

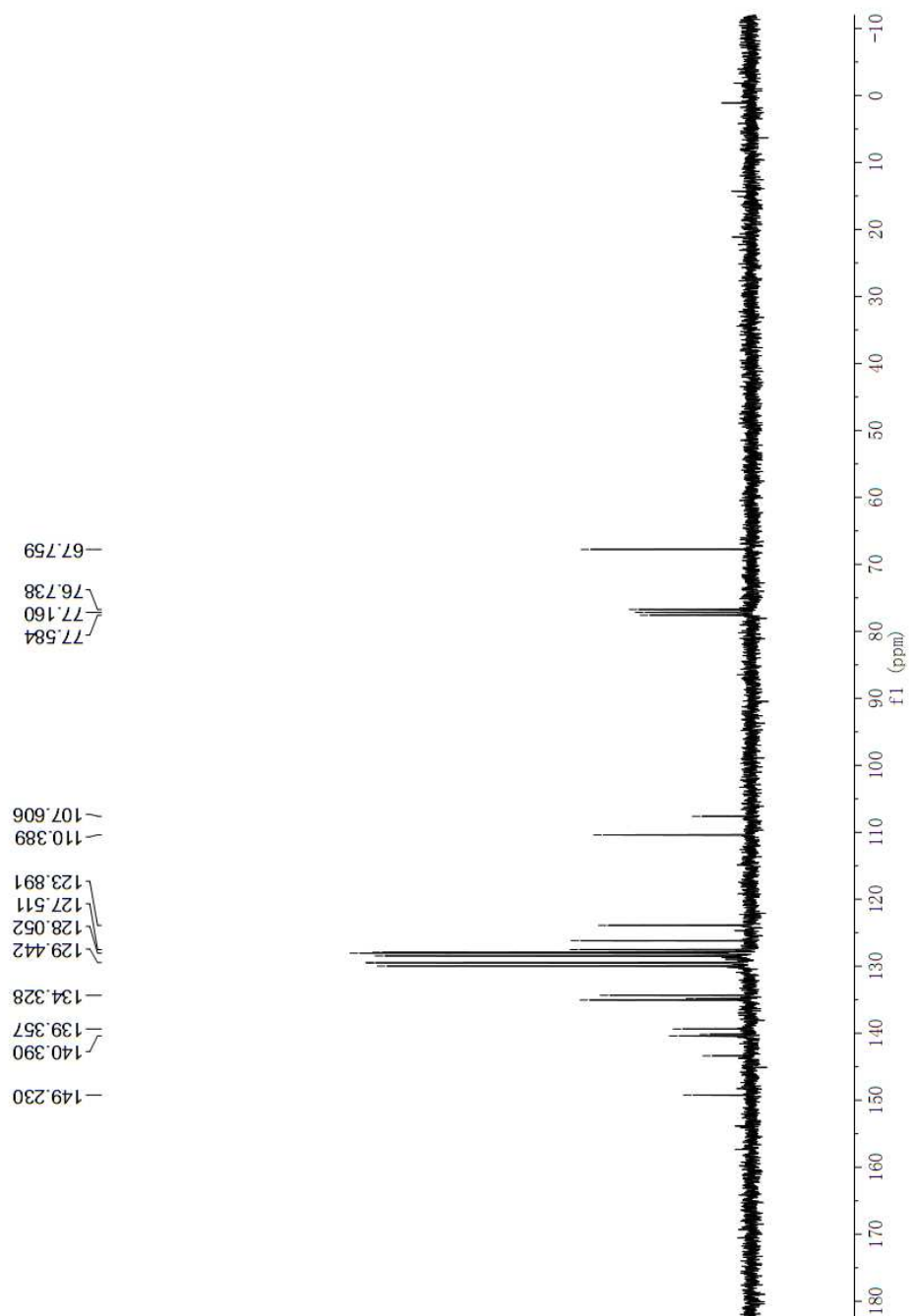
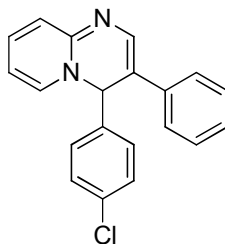


Fig. S-57: ^{13}C Spectra of 4-(4-chlorophenyl)-2,3-diphenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,5}.



Chemical Formula: $C_{20}H_{15}ClN_2$

Exact Mass: 318.1

Molecular Weight: 318.8

4{1,1,6}

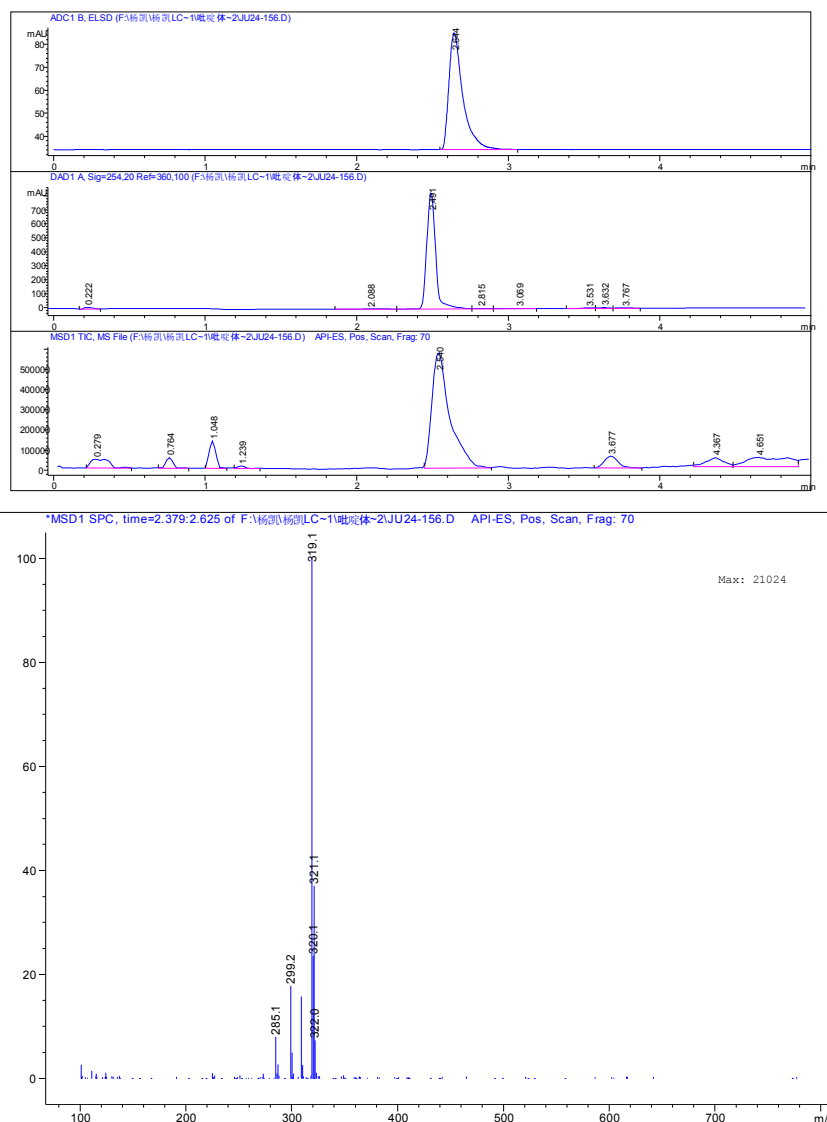


Fig. S-58: LC-MS-ELSD of 4-(4-chlorophenyl)-3-phenyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,6}.

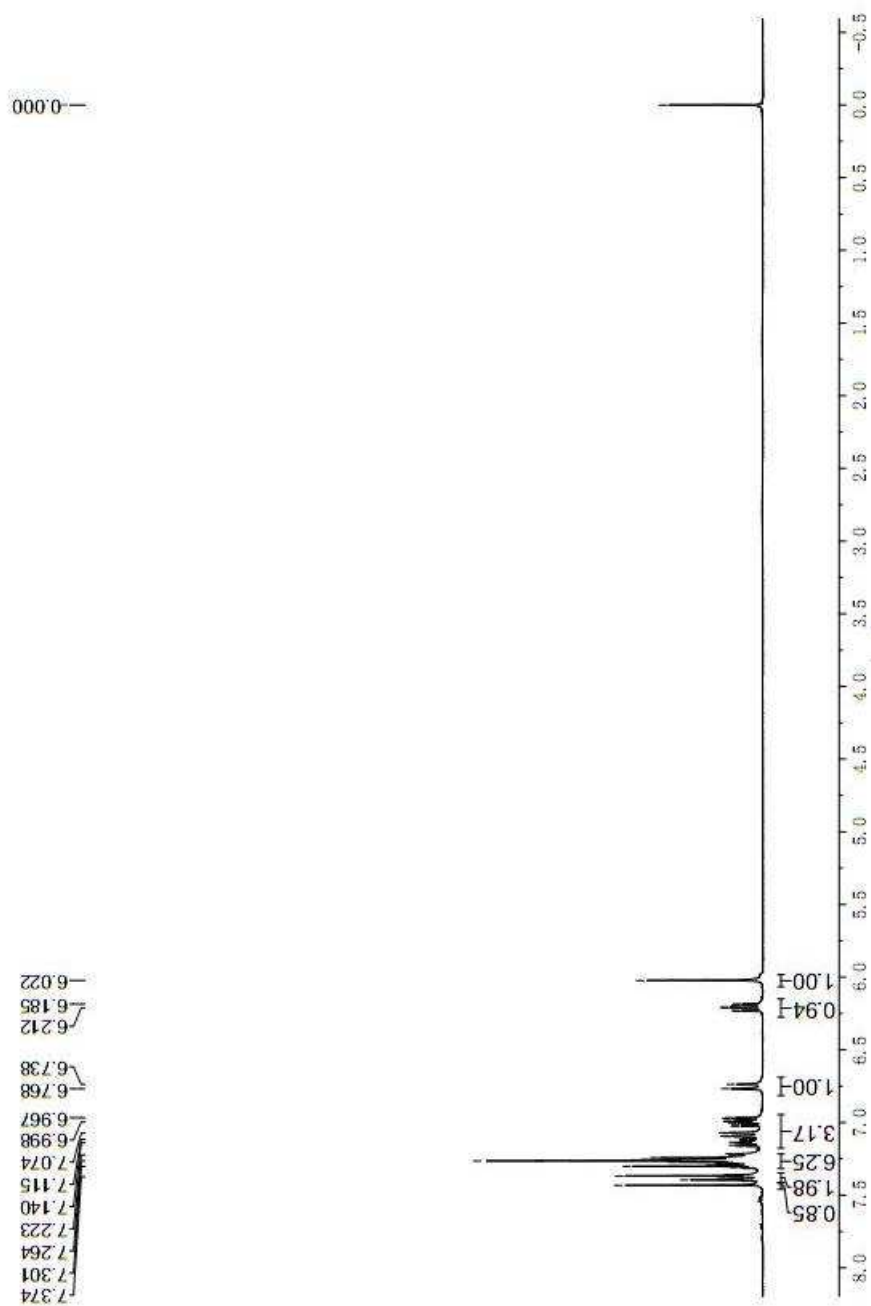


Fig. S-59: ¹H Spectra of 4-(4-chlorophenyl)-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,6}.

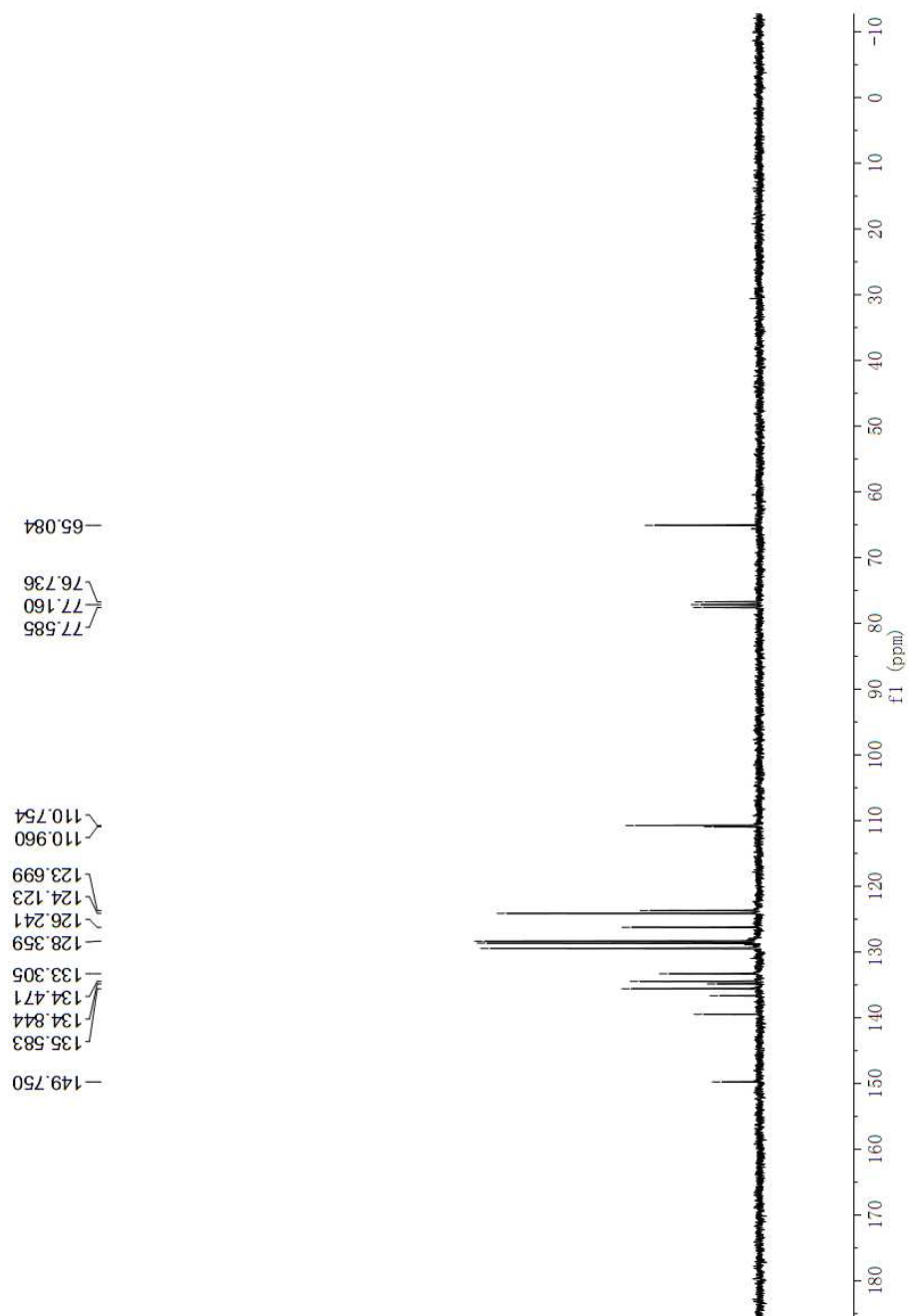
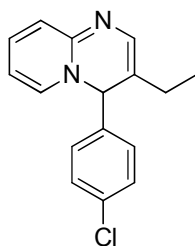


Fig. S-60: ^{13}C Spectra of 4-(4-chlorophenyl)-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,6}.



Chemical Formula: C₁₇H₁₇ClN₂

Exact Mass: 284.1

Molecular Weight: 284.8

4{1,1,7}

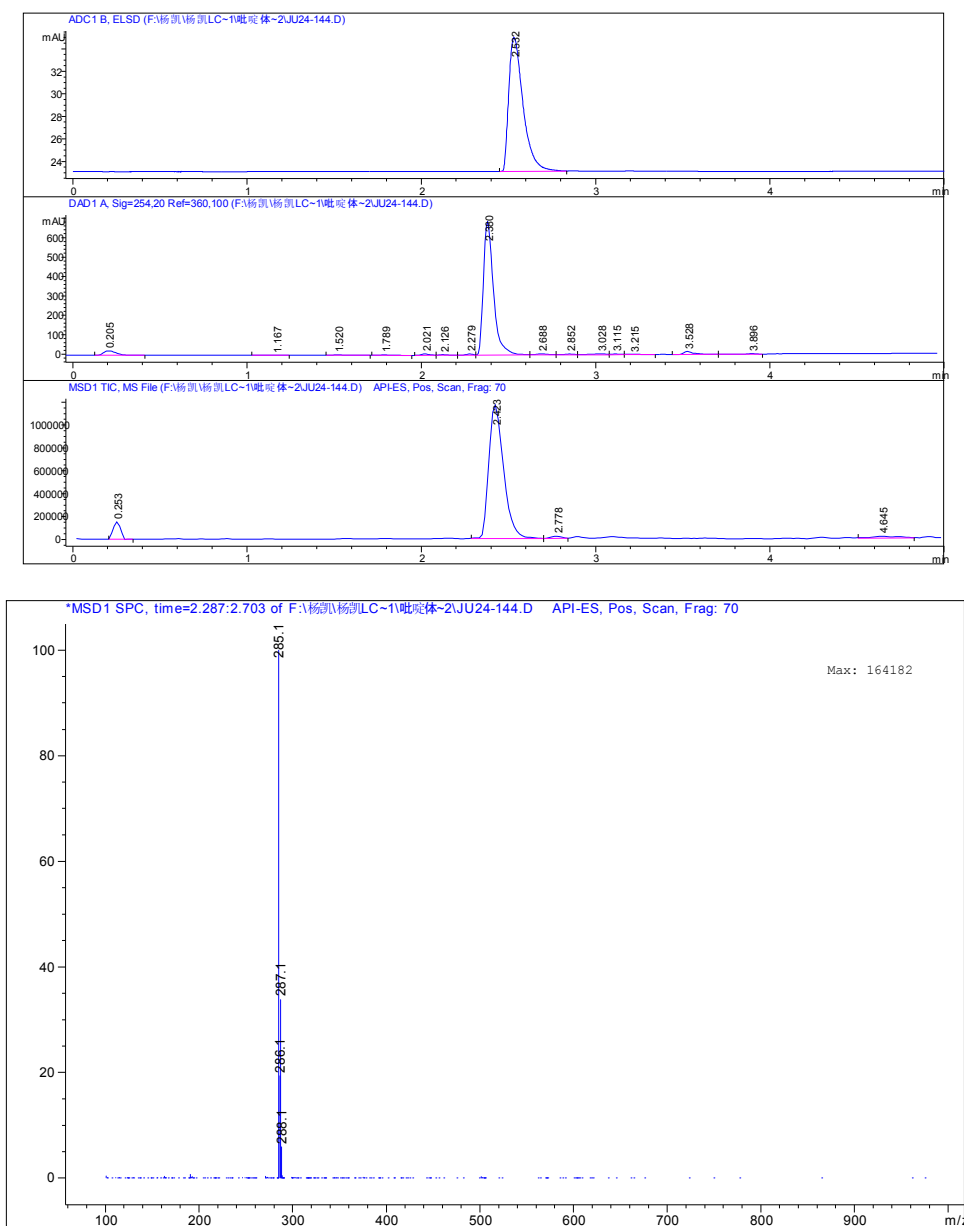


Fig. S-61: LC-MS-ELSD of 4-(4-chlorophenyl)-3-propyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,1,7}.

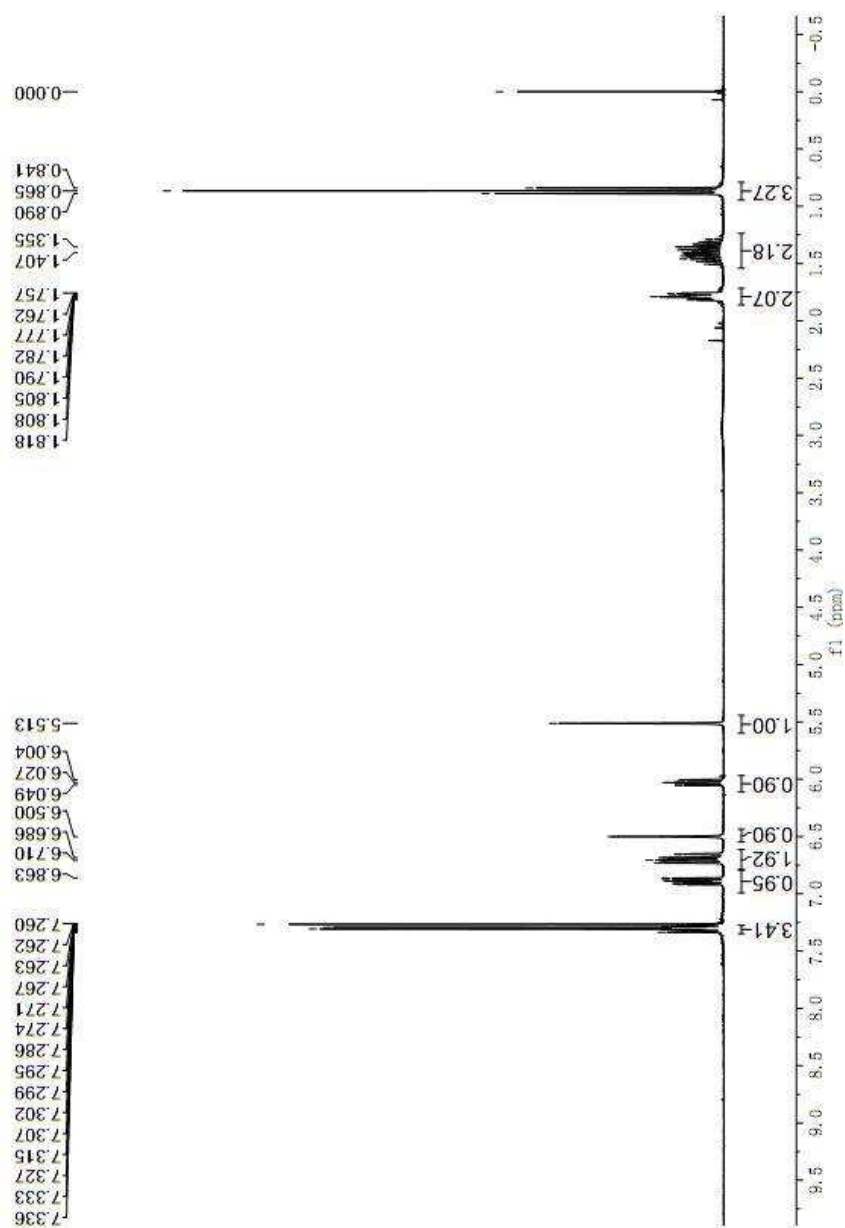


Fig. S-62: ¹H Spectra of 4-(4-chlorophenyl)-3-propyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,7}.

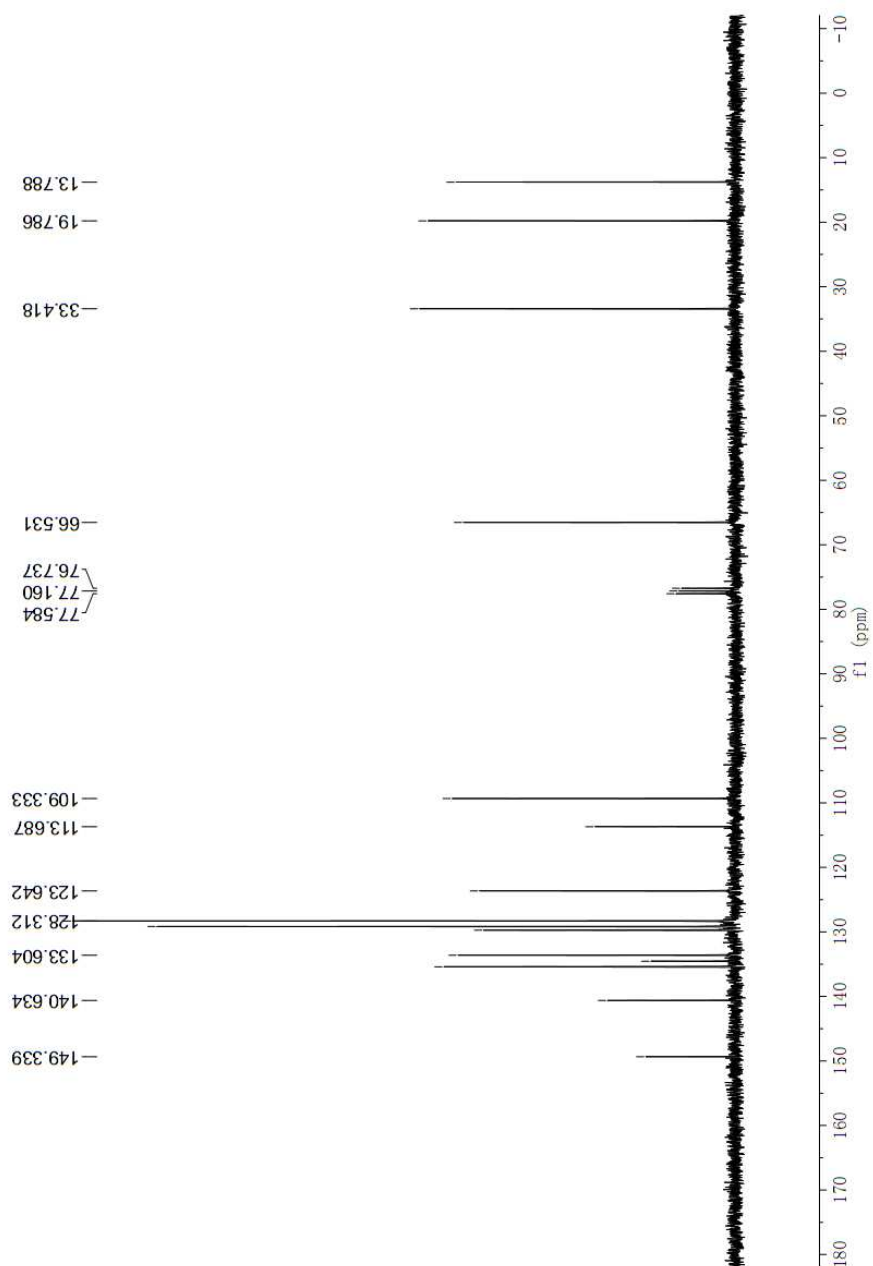
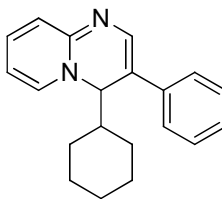


Fig. S-63: ^{13}C Spectra of 4-(4-chlorophenyl)-3-propyl-4H-pyrido[1,2-a]pyrimidine 4{1,1,7}.



Chemical Formula: $C_{20}H_{22}N_2$

Exact Mass: 290.2

Molecular Weight: 290.4

4{1,14,6}

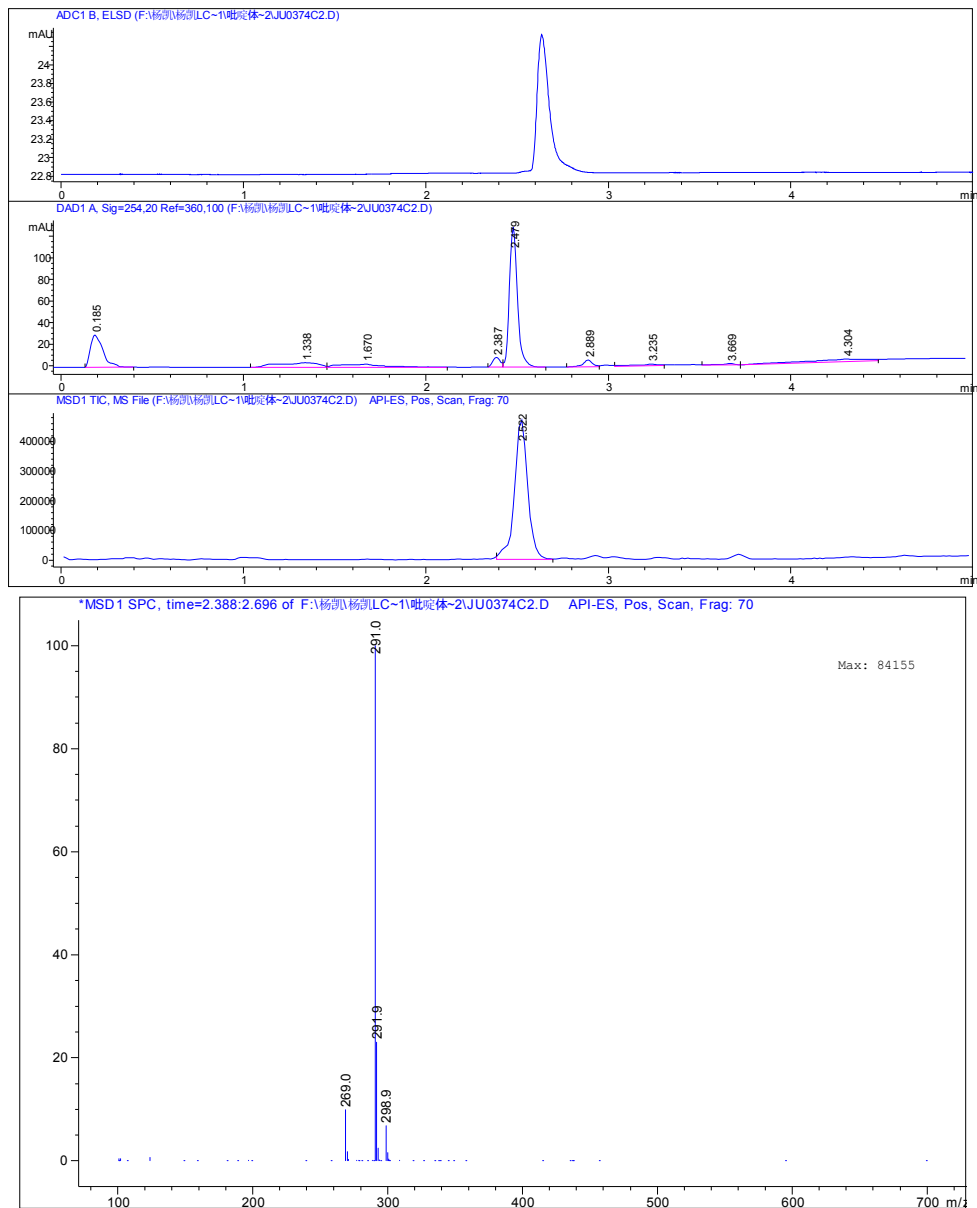


Fig. S-64: LC-MS-ELSD of 4-cyclohexyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,14,6}.

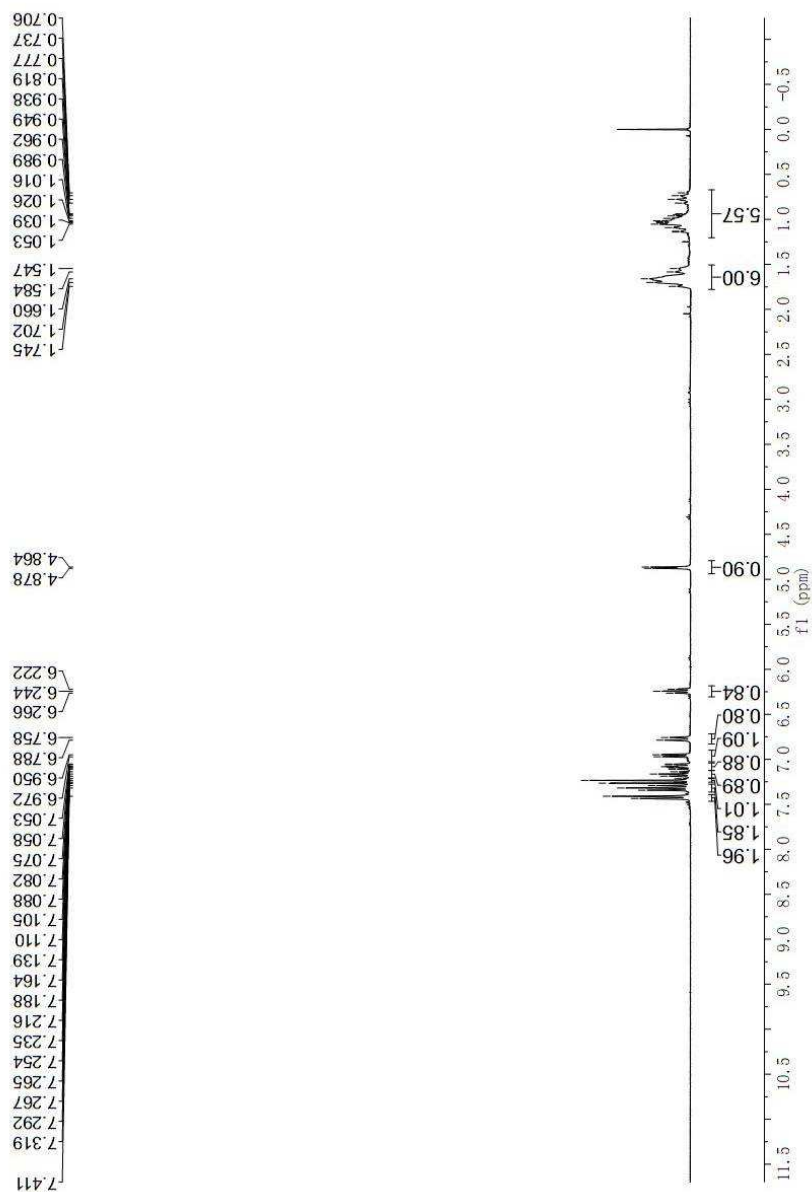


Fig. S-65: ^1H Spectra of 4-cyclohexyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,14,6}.

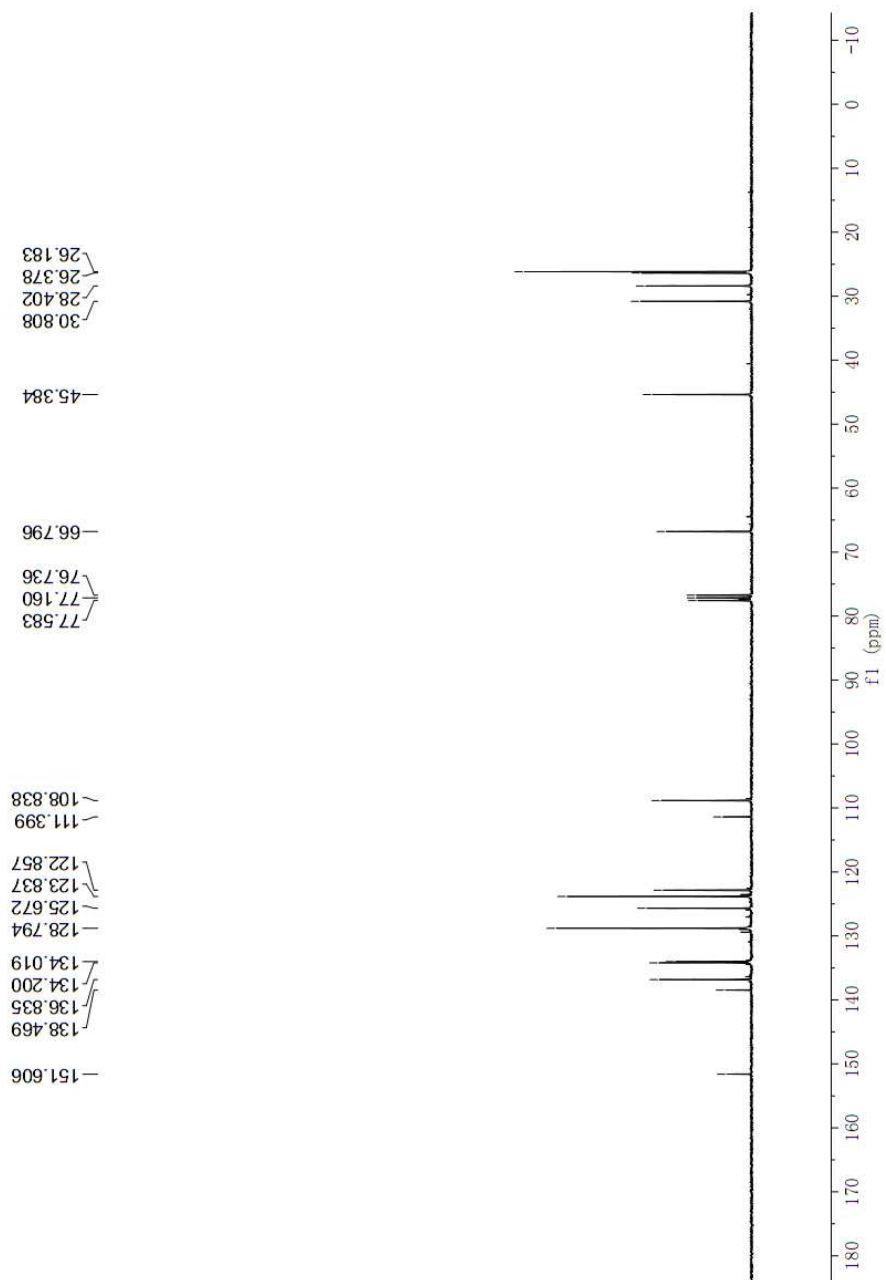
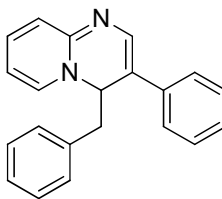


Fig. S-66: ¹³C Spectra of 4-cyclohexyl-3-phenyl-4H-pyrido[1,2-a]pyrimidine 4{1,14,6}.



Chemical Formula: $C_{21}H_{18}N_2$

Exact Mass: 298.1

Molecular Weight: 298.4

4{1,15,6}

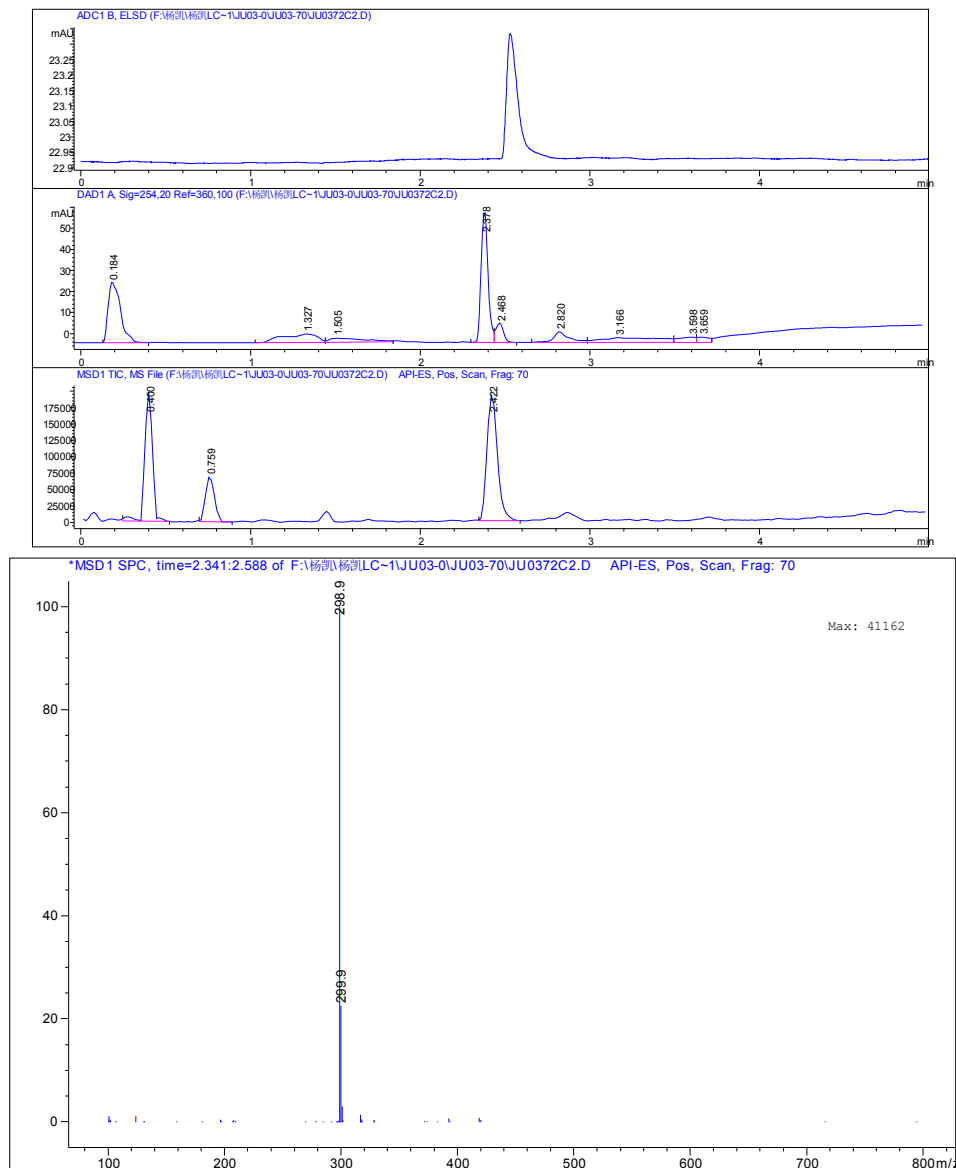


Fig. S-67: LC-MS-ELSD of 4-benzyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,15,6}.

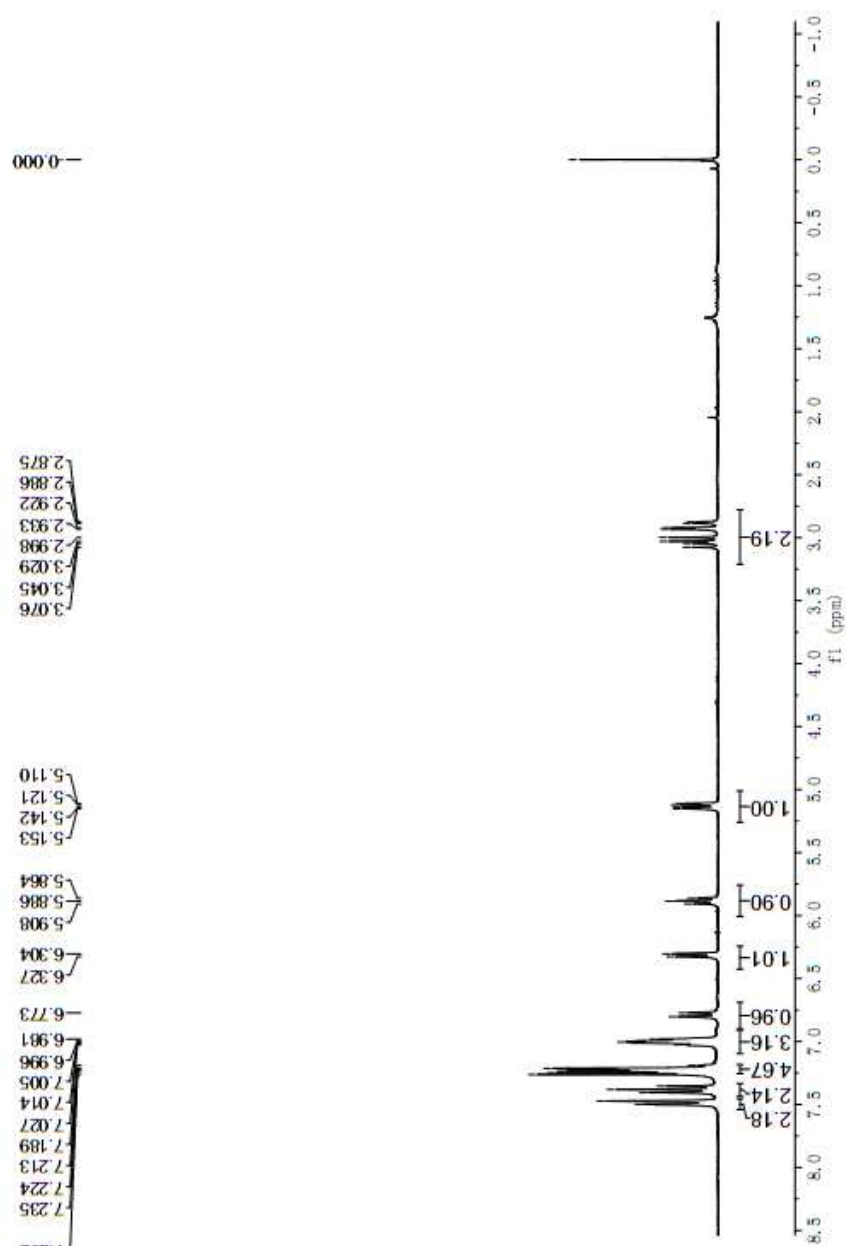


Fig. S-68: ^1H Spectra of 4-benzyl-3-phenyl-4*H*-pyrido[1,2-*a*]pyrimidine 4{1,15,6}.

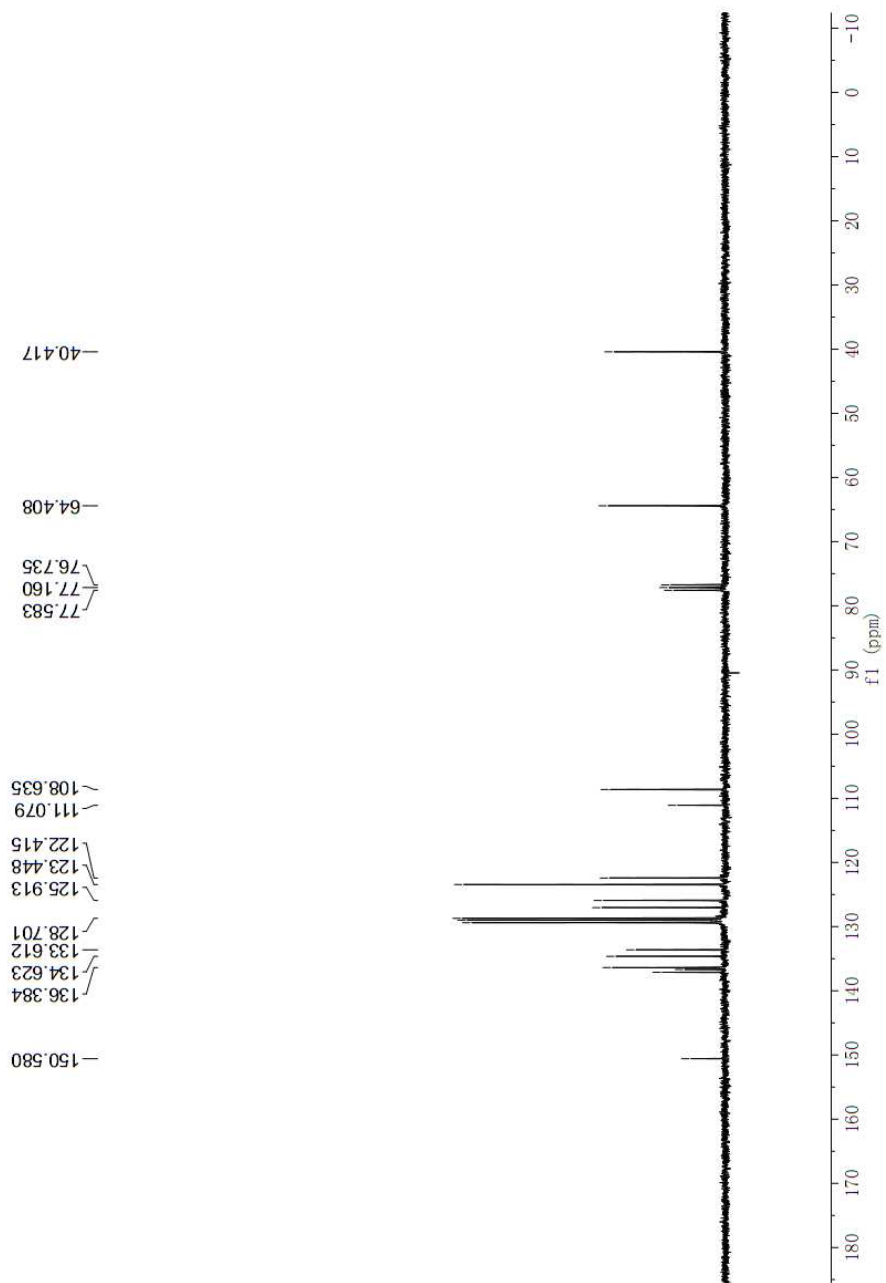
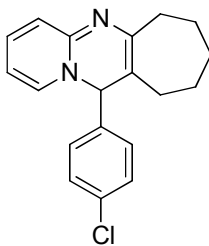


Fig. S-69: ^{13}C Spectra of 4-benzyl-3-phenyl-4H-pyrido[1,2-a]pyrimidine 4{1,15,6}.



Chemical Formula: C₁₉H₁₉ClN₂

Exact Mass: 310.1

Molecular Weight: 310.8

4{1,1,9}

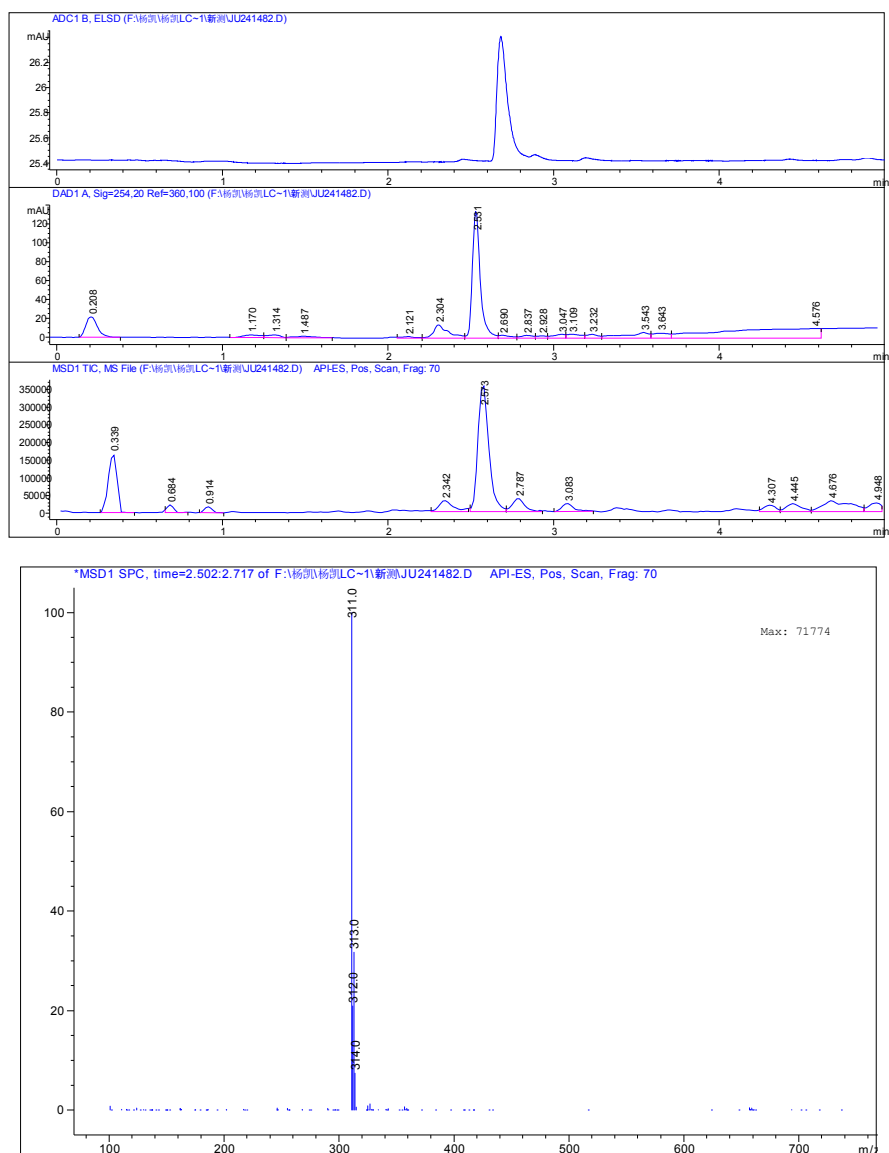


Fig. S-70: LC-MS-ELSD of 11-(4-chlorophenyl)-6,7,8,9,10,11-hexahydrocyclohepta[d]pyrido[1,2-a]pyrimidine 4{1,1,9}.

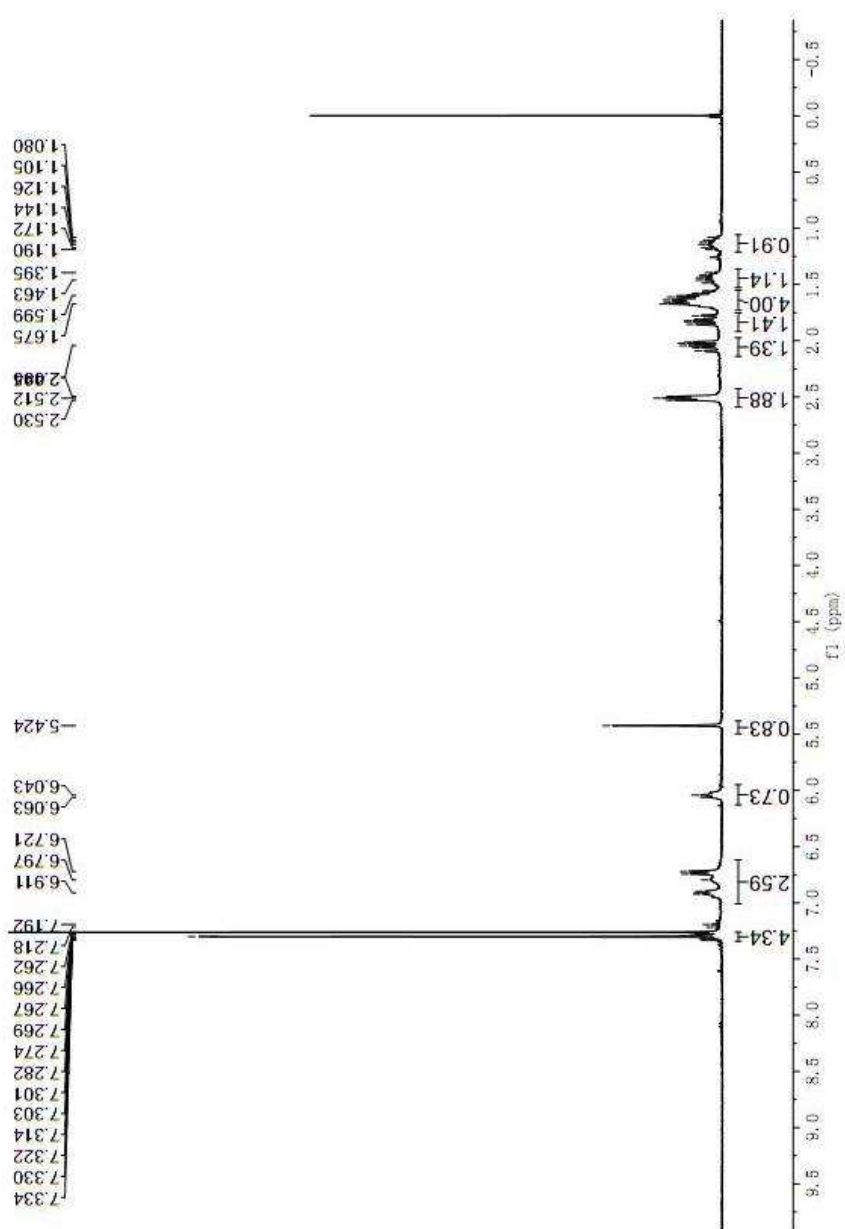
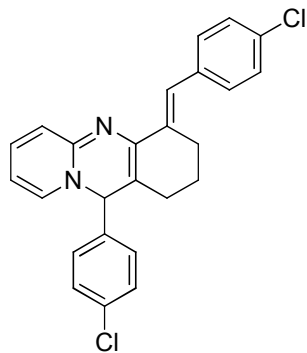


Fig. S-71: ^1H Spectra of 11-(4-chlorophenyl)-6,7,8,9,10,11-hexahydrocyclohepta[*d*]pyrido[1,2-*a*]pyrimidine 4{1,1'6}.



Chemical Formula: $C_{25}H_{20}Cl_2N_2$

Exact Mass: 418.1

Molecular Weight: 419.3

5{1,1,1}

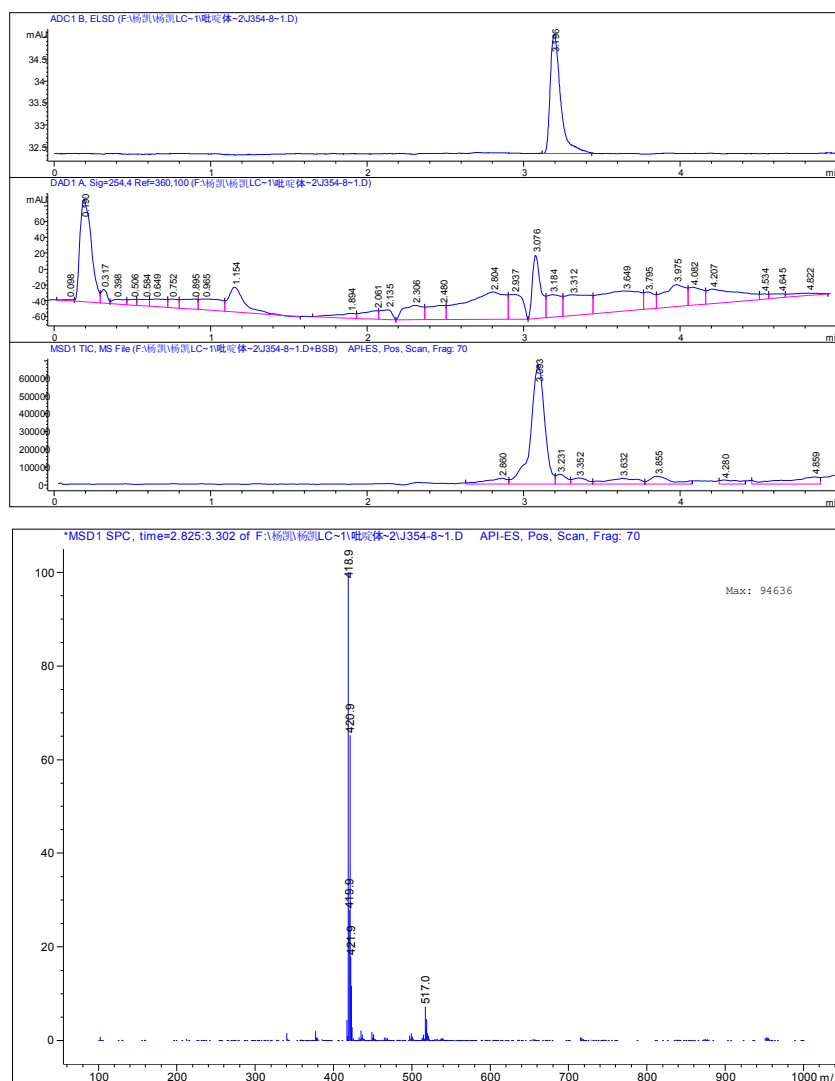


Fig. S-72: LC-MS-ELSD of (*E*)-4-(4-chlorobenzylidene)-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 5{1,1,1}.

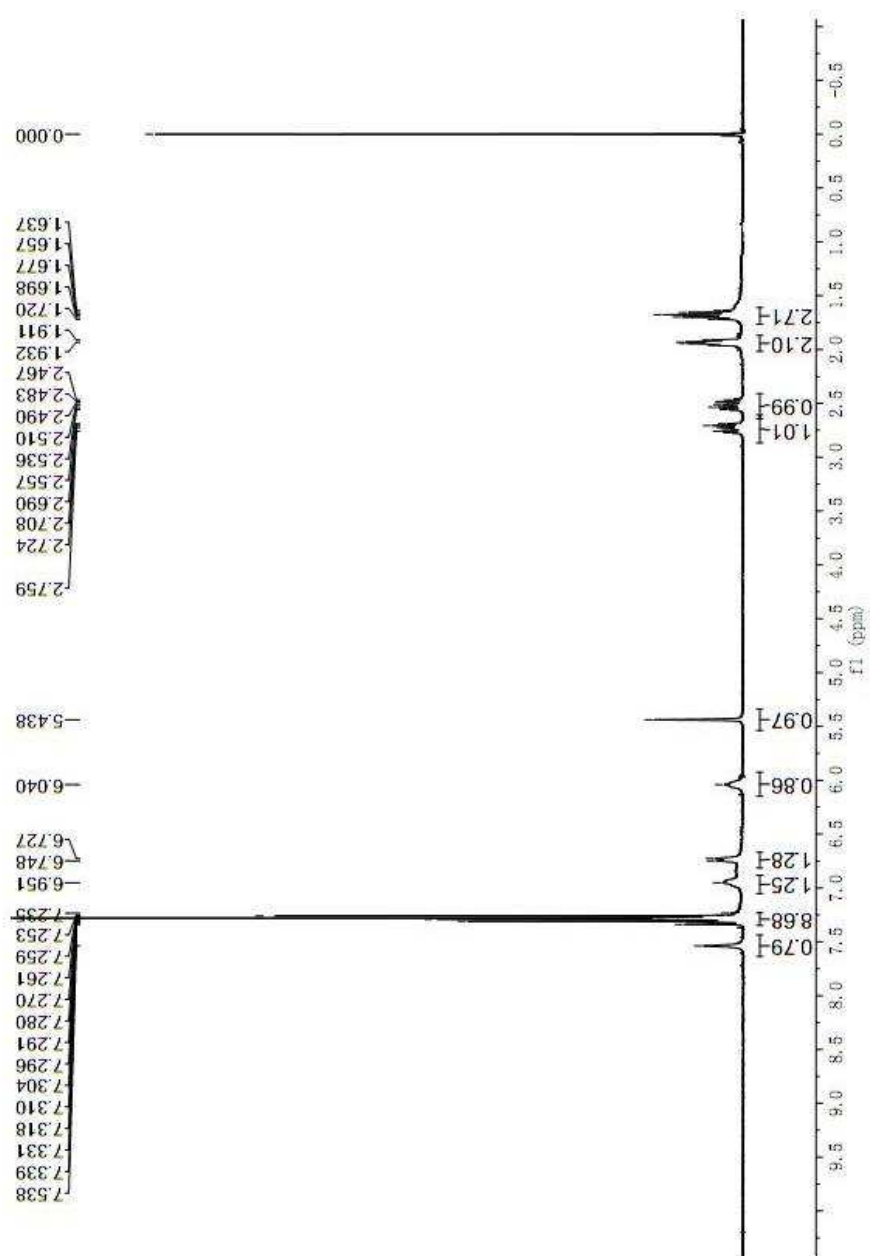


Fig. S-73: ^1H Spectra of (E) -4-(4-chlorobenzylidene)-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1H-pyrido[2,1-*b*]quinazoline 5{1,1,1}.

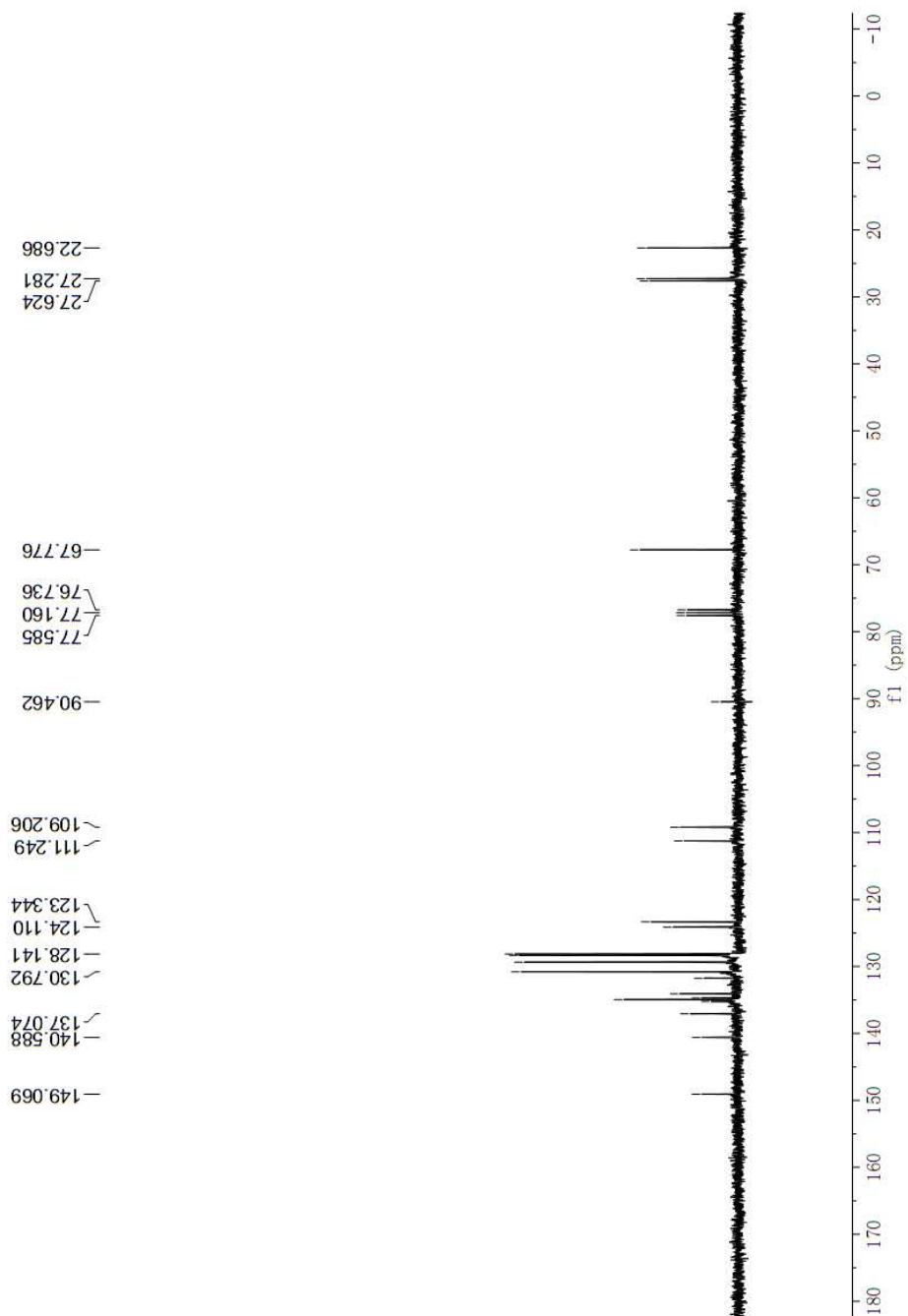


Fig. S-74: ^{13}C Spectra of (*E*)-4-(4-chlorobenzylidene)-11-(4-chlorophenyl)-2,3,4,11-tetrahydro-1*H*-pyrido[2,1-*b*]quinazoline 5{1,1,1}.