

Supporting Information

Assembly of Iodinated Indolo[1,2-*c*]quinazoline Amines *via* I₂/CHP-Promoted Cascade Annulation of Isocyanides and Diarylalkynes

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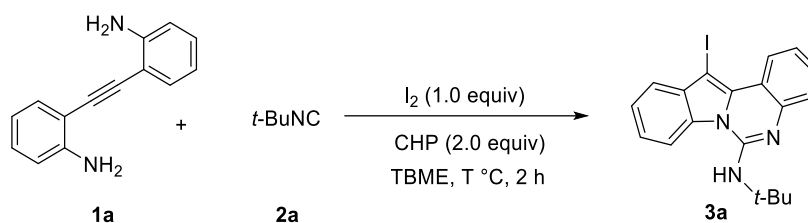
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A. General Information

All purchased reagents and solvents were used without further purification unless otherwise noted. Analytical thin layer chromatography was performed by using commercially prepared 100-400 mesh silica gel plates (GF₂₅₄) and visualization was effected at 254 nm. All the 2,2'-(ethyne-1,2-diyl)dianilines were prepared according to known procedures. ¹H and ¹³C NMR spectra were recorded using a Bruker DRX-400 spectrometer using CDCl₃ as solvent. The chemical shifts are referenced to signals at 7.26 and 77.0 ppm, respectively. Mass spectra were recorded on a Thermo Scientific ISQ gas chromatograph-mass spectrometer. The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). IR spectra were obtained either as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Bruker TENSOR 27 spectrometer. Melting points were determined with a Büchi Melting Point B-545 instrument.

B. Optimization of Reaction Conditions

(a) Optimization for Reaction Temperature^a



Entry	T (°C)	Yield of 3a ^b (%)
1	95	17
2	85	18
3	75	10
4	70	37
5	65	36
6	45	30
7	40	44
8	25	33
9	-5	29

^aReaction Conditions: Unless otherwise noted, all reactions were performed with **1a** (0.1 mmol, 1 equiv), **2a** (0.15mmol, 1.5 equiv), CHP (0.2 mmol, 2.0 equiv), I₂ (1.0 mmol, 1.0 equiv) in TBME under air at T °C for 2 h. ^bDetermined by ¹H NMR using CH₂Br₂ as the internal standard. CHP = Cumene hydroperoxide. TBME = *tert*-Butyl hydroperoxide.

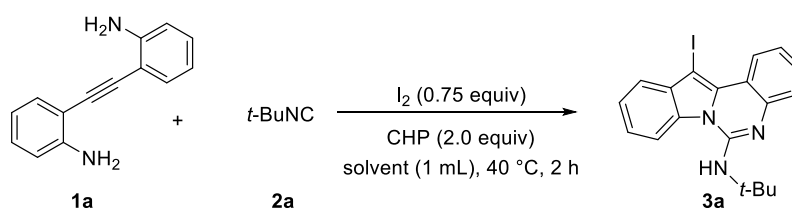
(b) Screening of Iodine Amounts^a



Entry	I_2 (x equiv)	Yield of 3a ^b (%)
1	I_2 (0.5)	38
2	I_2 (0.75)	46
3	I_2 (1.0)	38
4	I_2 (1.5)	25
5	I_2 (2.0)	trace

^aReaction condition: **1a** (0.1 mmol), **2a** (0.15 mmol), I_2 (x equiv), solvent (1 mL), oxidant (0.2 mmol, 2 equiv), 40 °C, 2 h. ^bDetermined by ¹H NMR using CH₂Br₂ as an internal standard. CHP = Cumene hydroperoxide. TBME = *tert*-Butyl hydroperoxide.

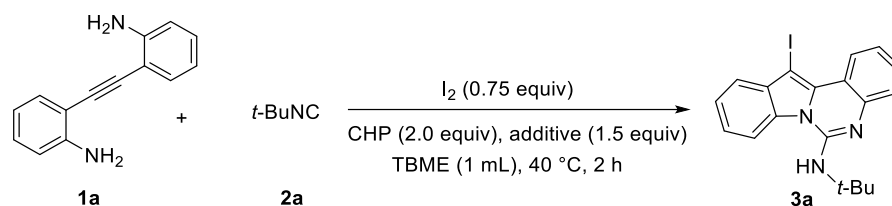
(c) Screening of Solvent^a



Entry	Solvent	Yield of 3a ^b (%)
1	THF	n.d.
2	1,4-Dioxane	45
3	DECS	40
4	Toluene	28
5	DMSO	24
6	CPME	48
7	TBME	52

^aReaction condition: **1a** (0.1 mmol), **2a** (0.15 mmol), oxidant (0.2 mmol, 2.0 equiv), I₂ (0.075 mmol, 0.75 equiv) in solvent (1 mL) under air at 40 °C for 2 h. ^bDetermined by ¹H NMR using CH₂Br₂ as an internal standard. CHP = Cumene hydroperoxide. DECS = 2-(2-Ethoxyethoxy)ethanol. CPME = Cyclopentyl methyl ether. TBME = *tert*-Butyl hydroperoxide. n.d. = not detected.

(d) Screening of Additive^a

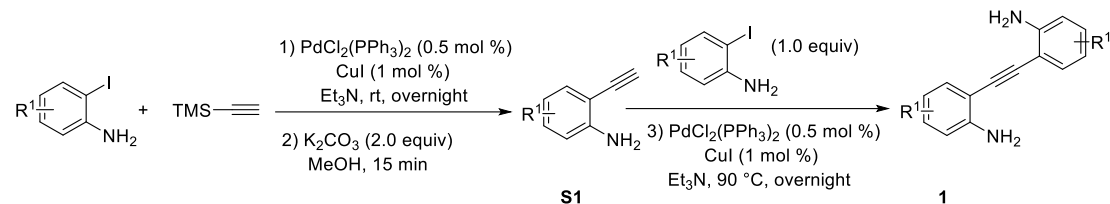


Entry	Additive	Yield of 3a ^b (%)
1	Ca(OH) ₂	16
2	NaNO ₂	49
3	KHCO ₃	53
4	Na ₂ HPO ₄	38
5	Na ₂ SO ₃	48
6	NaHSO ₃	54
7	NaOOCPh	55
8	Malonic acid	2
9	NH ₄ Cl	32
10	CaCO ₃	40
11	NaH	13
12	KBF ₄	62
13	KBr	39
14	Zn(OAc)₂	76 (70)

^aReaction Conditions: Unless otherwise noted, all reactions were performed with **1a** (0.1 mmol, 1.0 equiv), **2a** (0.15 mmol, 1.5 equiv), additive (0.15 mmol, 1.5 equiv), CHP (0.2 mmol, 2.0 equiv), I₂ (0.075 mmol, 0.75 equiv) in TBME under air at 40 °C for 2 h. ^bDetermined by ¹H NMR using CH₂Br₂ as the internal standard. TBME = *tert*-Butyl hydroperoxide. CHP = Cumene hydroperoxide. Data in the parentheses was referred to isolated yield.

C. General Procedure for the Synthesis of Starting Materials

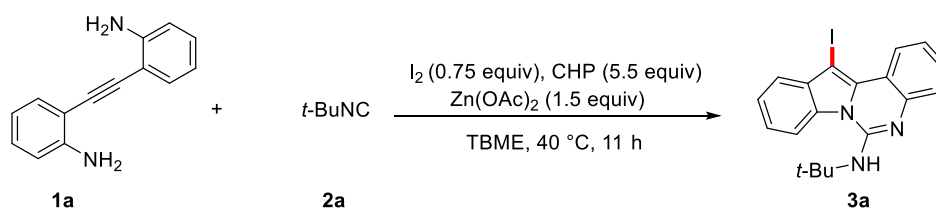
Unless otherwise specified, functionalized alkynes were synthesized *via* the following steps:



Step 1: To an oven-dried round bottom flask containing a magnetic stir bar was added aryl halide (1.0 equiv), Pd(PPh₃)₂Cl₂ (0.5 mol %), and CuI (1 mol %). The vessel was then sealed with a rubber septum, evacuated, and backfilled with argon three times. Et₃N (solvent, *c* = 0.5 M) and trimethylsilylacetylene (1.5 equiv) were added in sequence. After the reaction was completed at room temperature (monitored by TLC), solvent was removed under reduced pressure and the resulting residue was directly purified by flash column chromatography (eluent: hexanes/EtOAc) on silica gel. To the crude product (1.0 equiv) in MeOH (solvent, *c* = 0.2 M) was added K₂CO₃ (2.0 equiv) in one portion. After the reaction was completed at room temperature (monitored by TLC), the resulting mixture was filtered through a short pad of silica gel and washed with petroleum ether. The filtrate was concentrated under reduced pressure to afford product **S1** which was directly used for next step without further purification.

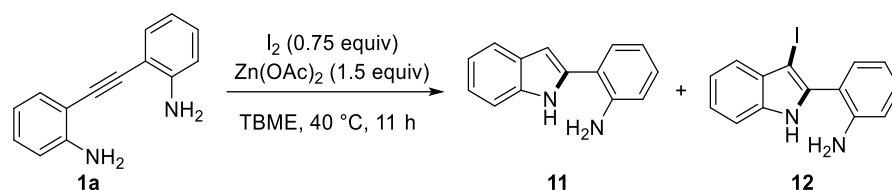
Step 2: To an oven-dried round bottom flask containing a magnetic stir bar was added the aryl halide (1.0 equiv), Pd(PPh₃)₂Cl₂ (0.5 mol %), and CuI (1 mol %). The vessel was then sealed with a rubber septum, evacuated, and backfilled with argon three times. Et₃N (solvent, *c* = 0.5 M) and **S1** (1.2 equiv) were added in sequence. After the reaction was completed at 90 °C overnight, solvent was removed under reduced pressure and the resulting residue was directly purified by flash column chromatography (eluent: hexanes/EtOAc = 5:1-10:1) on silica gel to give the final product **1** (yields: 25-80%)

D. General Procedure for the Synthesis of 3a

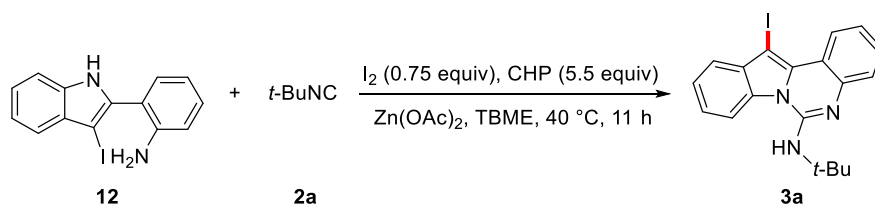


A mixture of diarylalkynes (**1a**, 0.10 mmol, 20.8 mg), *tert*-butyl isocyanide (**2a**, 0.15 mmol, 12.5 mg), I₂ (0.75 equiv, 19.0 mg), CHP (5.5 equiv, 104.6 mg), Zn(OAc)₂ (1.5 equiv, 27.5 mg) and 1.0 mL of TBME was added to a test tube equipped with a magnetic stirring bar. The mixture was then stirred at 40 °C under air for 11 h. Then the reaction was quenched by H₂O and extracted with ethyl acetate, dried over anhydrous Na₂SO₄, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on neutral alumina with light petroleum ether/ethyl acetate as eluent to afford the desired product **3a** (33.8 mg, 81%).

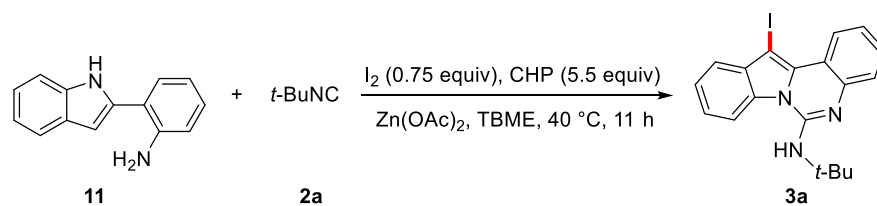
E. Mechanistic Studies



(a) A mixture of 2,2'-(ethyne-1,2-diyl)dianiline (**1a**, 0.10 mmol, 20.8 mg), I_2 (0.75 equiv, 19.0 mg), $Zn(OAc)_2$ (1.5 equiv, 27.5 mg) and 1.0 mL of TBME was added to a test tube equipped with a magnetic stirring bar. The mixture was then stirred at 40 °C under air for 11 h. Then the reaction was quenched by H_2O and extracted with ethyl acetate, dried over anhydrous Na_2SO_4 , filtered, and evaporated under vacuum. The crude product was purified by column chromatography on neutral alumina with light petroleum ether/ethyl acetate as eluent to afford product **11** (2.0 mg, 10%) and product **12** (20.7 mg, 62%).

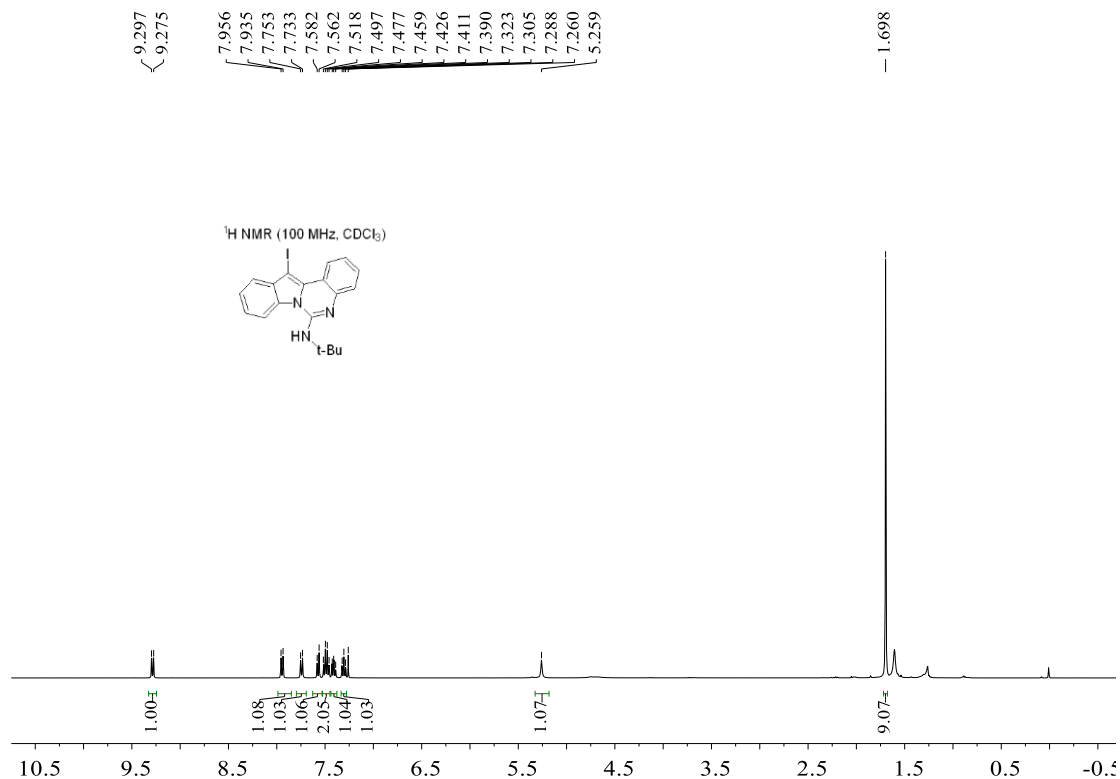


(b) 2-(3-iodo-1*H*-indol-2-yl)aniline (**12**, 0.1 mmol, 33.4 mg), *tert*-butyl isocyanide (**2a**, 0.15 mmol, 12.5 mg), I_2 (0.75 equiv, 19.0 mg), CHP (5.5 equiv, 104.6 mg), $Zn(OAc)_2$ (1.5 equiv, 27.5 mg), and 1.0 mL of TBME were added to a tube equipped with a stir bar and stirred at 40 °C for 11 h. Then the reaction was quenched by H_2O and extracted with ethyl acetate, dried over anhydrous Na_2SO_4 , filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with light petroleum ether as eluent to afford the desired product **3a** (29.9 mg, 72%).

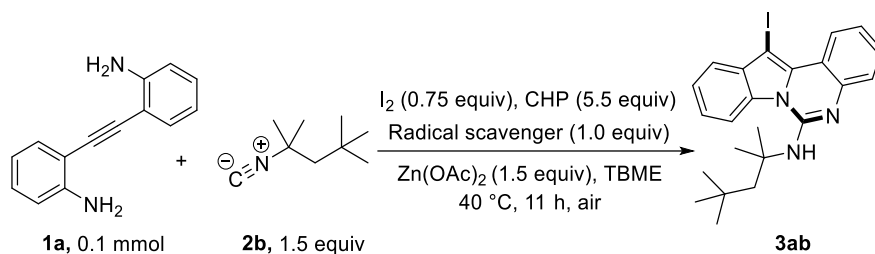


(c) 2-(1*H*-indol-2-yl)aniline (**11**, 0.1 mmol, 20.8 mg), *tert*-butyl isocyanide (**2a**, 0.15 mmol, 12.5 mg), I_2 (0.75 equiv, 19.0 mg), CHP (5.5 equiv, 104.6 mg), $Zn(OAc)_2$ (1.5 equiv, 27.5 mg), and 1.0 mL of TBME were added to a tube equipped with a stir bar and stirred at 40 °C for 11 h. Then the reaction was quenched by H_2O and extracted with ethyl acetate, dried over anhydrous Na_2SO_4 , filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with light petroleum ether as eluent to afford the desired product **3a** (26.1 mg, 63%).

***N*-(*tert*-Butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3a) (400MHz, CDCl₃)**



(d) A mixture of 2,2'-(ethyne-1,2-diyl)dianiline (**1a**, 0.10 mmol, 20.8 mg), *tert*-butyl isocyanide (**2a**, 0.15 mmol, 12.5 mg), I₂ (0.75 equiv, 19.0 mg), CHP (5.5 equiv, 104.6 mg), Radical scavenger (1.0 equiv), Zn(OAc)₂ (1.5 equiv, 27.5 mg) and 1.0 mL of TBME was added to a test tube equipped with a magnetic stirring bar. The mixture was then stirred at 40 °C under air for 11 h. Then the reaction was quenched by H₂O and extracted with ethyl acetate, dried over anhydrous Na₂SO₄, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on neutral alumina with light petroleum ether/ethyl acetate as eluent. Through adding different radical scavengers to the standard condition, product **3ab** was provided with the following yield.

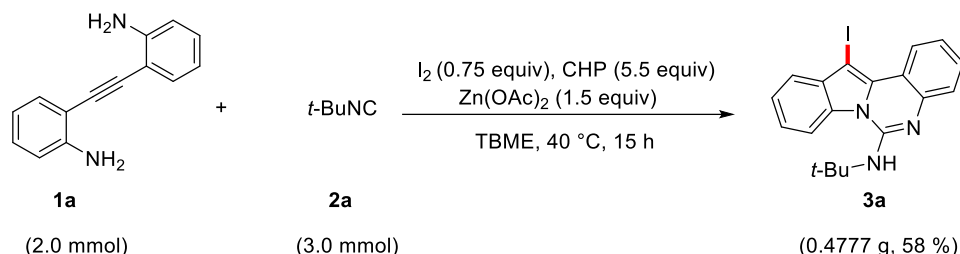


Entry ^a	Radical scavenger (1.0 equiv)	Yield of 3ab (%) ^b
1	TEMPO	n.d.
2	BHT	n.d.
3	1,1-diphenylethylene	70%

^aReaction conditions: **1a** (0.1 mmol), **2b** (0.15 mmol, 1.5 equiv), I₂ (0.075 mmol, 0.75 equiv), CHP (0.55 mmol, 5.5 equiv), Zn(OAc)₂ (0.15 mmol, 1.5 equiv) and TBME were added to a test tube at 40 °C under air for 11 h. TEMPO = 2,2,6,6-Tetramethylpiperidine 1-oxyl, BHT = Butylated hydroxytoluene. CHP = Cumene hydroperoxide. TBME = *tert*-Butyl hydroperoxide. ^bIsolated yield. n.d. = not detected

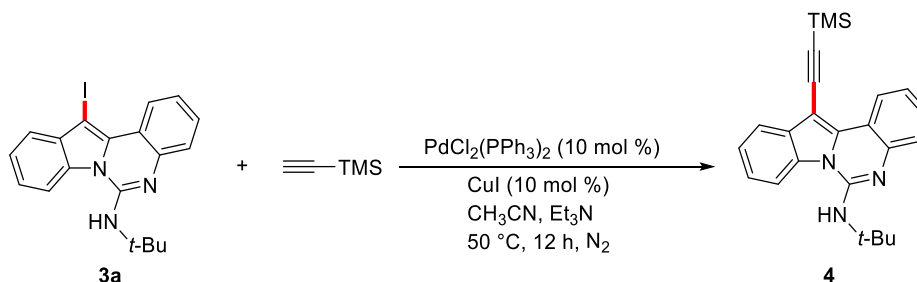
F. General Procedures for the Synthetic Applications

(i) 2.0 mmol Experiment



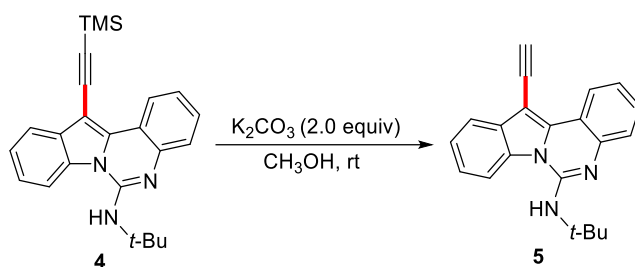
A mixture of 2,2'-(ethyne-1,2-diyl)dianiline (**1a**, 2.00 mmol, 0.416 g), *tert*-butyl isocyanide (**2a**, 3.00 mmol, 0.249 g), I₂ (0.75 equiv, 380 mg), CHP (5.5 equiv, 2.093 g), Zn(OAc)₂ (1.5 equiv, 0.550 g), and 10.0 mL of TBME were added to a tube equipped with a stir bar and stirred at 40 °C for 15 h. Then the reaction was quenched by H₂O and extracted with ethyl acetate, dried over anhydrous Na₂SO₄, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on neutral alumina with light petroleum ether as eluent to afford the desired product **3a** (0.4777 g, 58%).

(ii) Synthetic Procedure for 4



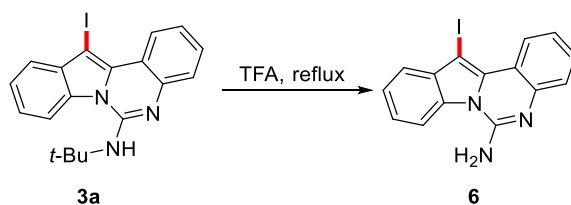
N-(*tert*-butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3a**, 0.1 mmol, 41.5 mg), ethynyltrimethylsilane (0.2 mmol, 19.6 mg), PdCl₂(PPh₃)₂ (10 mol %, 7.0 mg), CuI (10 mol %, 2.0 mg), CH₃CN (1.0 mL) and Et₃N (1.0 mL) were added to a test tube under nitrogen atmosphere. Then the mixture was stirred at 50 °C for 12 h. After the reaction was completed (monitored by TLC), the resulting mixture was extracted with ethyl acetate. The combined organic layers were evaporated under vacuum, and then washed with brine and dried over anhydrous Na₂SO₄. Filtration, evaporation, and chromatography on silica gel with light petroleum as eluent afforded the desired product **4** (35.4 mg, 92%).

(iii) Deprotection of 4



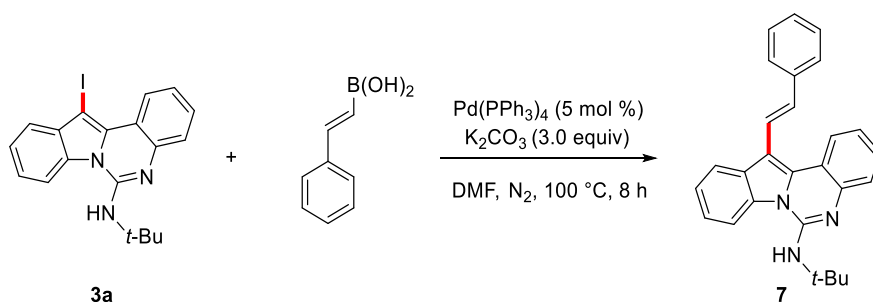
To a side-necked sealable tube equipped with stir bar was added **4** (38.5 mg, 0.1 mmol), K_2CO_3 (2.0 equiv, 27.6 mg) and CH_3OH (1.0 mL). The reaction was sealed and stirred at room temperature for 15 min. The product was then extracted with dichloromethane. The combined organics were dried with anhydrous Na_2SO_4 , filtered, and concentrated under reduced pressure. The resulting residue was purified by column chromatography on silica gel with light petroleum ether/ethyl acetate as eluent to afford the desired product **5** (30.6 mg, 98%).

(iv) Deprotection of **3a**



To a side-necked sealable tube equipped with stir bar was added **3a** (41.5 mg, 0.1 mmol) and TFA (1.0 mL). The reaction was sealed and heated at reflux for 3 h. The reaction tube was allowed to cool to room temperature. The mixture was dropped slowly into saturated aqueous NaHCO_3 . The product was then extracted with diethyl ether. The combined organics were dried with anhydrous Na_2SO_4 , filtered, and concentrated under reduced pressure. The resulting residue was purified by column chromatography on silica gel with light petroleum ether/ethyl acetate as eluent to afford the desired product **6** (26.5 mg, 41%).

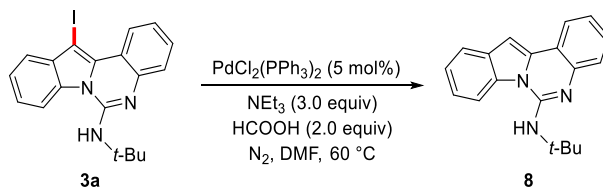
(v) Synthetic Procedure for **7**



N-(*tert*-butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3a**, 0.1 mmol, 41.5 mg), (*E*)-styrylboronic acid (0.2 mmol, 29.6 mg), $\text{Pd}(\text{PPh}_3)_4$ (5 mol %, 5.8 mg), K_2CO_3 (3.0 equiv, 41.5 mg) and DMF (1.0 mL) were added to a test tube under nitrogen atmosphere. Then the mixture was stirred at 100 °C for 8 h. After the reaction was completed (monitored by TLC), the resulting mixture was extracted with ethyl acetate. The combined organic layers were evaporated under vacuum and then washed

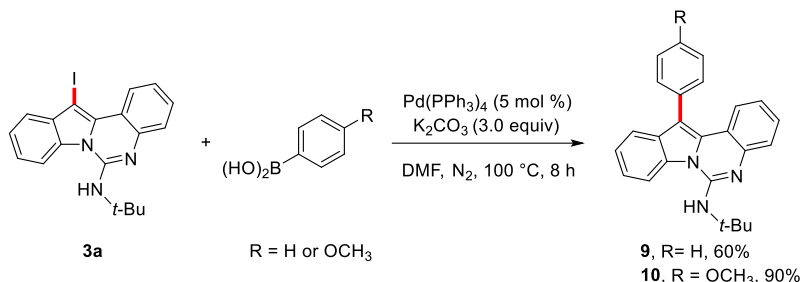
with brine and dried over anhydrous Na₂SO₄. Filtration, evaporation, and chromatography on silica gel with light petroleum as eluent afforded the desired product **7** (34.3 mg, 88%).

(vi) Synthetic Procedure for **8**



N-(*tert*-butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3a**, 0.1 mmol, 41.5 mg), PdCl₂(PPh₃)₂ (5 mol %, 3.5 mg), NEt₃ (3.0 equiv, 42 μL), HCOOH (2.0 equiv, 9.2 mg) and DMF (1.0 mL) were added to a test tube under nitrogen atmosphere. After the reaction was completed (monitored by TLC), the resulting mixture was extracted with ethyl acetate. The combined organic layers were evaporated under vacuum and then washed with brine and dried over anhydrous Na₂SO₄. Filtration, evaporation, and chromatography on silica gel with light petroleum as eluent afforded the desired product **8** (25.1 mg, 87%).

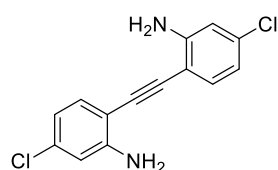
(vii) Synthetic Procedure for **9** or **10**



N-(*tert*-butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3a**, 0.1 mmol, 41.5 mg), phenylboronic acid (0.2 mmol, 24.4 mg) or (4-methoxyphenyl)boronic acid (0.2 mmol, 30.4 mg), Pd(PPh₃)₄ (5 mol %, 5.8 mg), K₂CO₃ (3.0 equiv, 41.5 mg) and DMF (1.0 mL) were added to a test tube under nitrogen atmosphere. Then the mixture was stirred at 100 °C for 8 h. After the reaction was completed (monitored by TLC), the resulting mixture was extracted with ethyl acetate. The combined organic layers were evaporated under vacuum and then washed with brine and dried over anhydrous Na₂SO₄. Filtration, evaporation, and chromatography on silica gel with light petroleum as eluent afforded the desired product **9** (21.9 mg, 60 %) or **10** (35.4 mg, 90%).

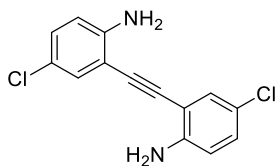
G. Characterization Data for Starting Materials

6,6'-(Ethyne-1,2-diyl)bis(3-chloroaniline) (**1k**)



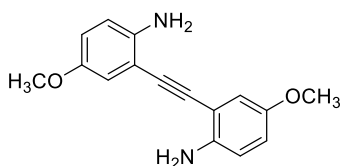
Yellow solid (25%, 138.0 mg); mp: 157.2-157.5 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 10/1); ¹H NMR (400 MHz, CDCl₃) δ 7.25 (d, *J* = 8.3 Hz, 1H), 6.91 – 6.56 (m, 2H), 4.33 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 146.3, 131.2, 129.9, 122.3, 115.5, 108.8, 90.7. IR: ν_{max}(KBr) = 3459, 3365, 3217, 2360, 1613, 1613, 1551, 1490, 1422, 1248, 1092, 914, 852, 802, 741 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₁₄H₁₀Cl₂N₂ [M-H]⁻: 275.0150 (100%), 277.0119 (63.9%), found 275.0148 (100%), 277.0119 (63.9%).

2,2'-(Ethyne-1,2-diyl)bis(4-chloroaniline) (1c)



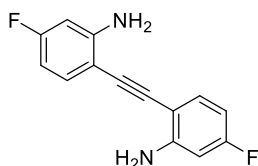
Yellow solid (60%, 331.2 mg); mp: 168.9-169.9 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 10/1); ¹H NMR (400 MHz, CDCl₃) δ 7.31 (s, 1H), 7.10 (dd, *J* = 8.6, 2.4 Hz, 2H), 6.66 (d, *J* = 8.7 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 146.3, 131.2, 129.9, 122.3, 115.5, 108.8, 90.7, 77.3, 77.0, 76.6; IR: ν_{max}(KBr) = 3447, 3358, 3053, 2922, 2854, 2356, 1710, 1613, 1486, 1414, 1306, 1243, 1147, 1088, 884, 812, 755, 650 cm⁻¹; HRMS (ESI) m/z: calcd for C₁₄H₁₀Cl₂N₂ [M+H]⁺: 277.0290 (100 %), 279.0260 (63.9 %), found 277.0294 (100 %), 279.0264 (63.9 %).

2,2'-(Ethyne-1,2-diyl)bis(4-methoxyaniline) (1g)



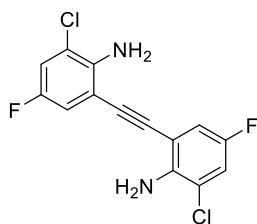
Yellow solid (30%, 160.8 mg); mp: 180.3-181.3 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 6/1); ¹H NMR (400 MHz, CDCl₃) δ 6.91 (d, *J* = 2.9 Hz, 1H), 6.79 (dd, *J* = 8.8, 2.9 Hz, 1H), 6.69 (d, *J* = 8.8 Hz, 1H), 3.75 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 151.9, 141.8, 117.4, 116.0, 115.7, 108.6, 91.1, 77.3, 77.0, 76.6, 55.8. IR: ν_{max}(KBr) = 3424, 3346, 3202, 2966, 2928, 2358, 1714, 1606, 1495, 1456, 1316, 1277, 1244, 1208, 1172, 1139, 1032, 959, 849, 809, 755, 666 cm⁻¹; HRMS (ESI) m/z: calcd for C₁₆H₁₆N₂O₂ [M+H]⁺: 269.1285, found 269.1279.

6,6'-(Ethyne-1,2-diyl)bis(3-fluoroaniline) (1i)



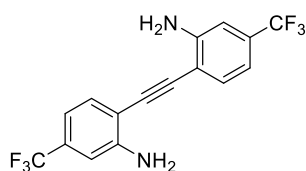
Yellow solid (40%, 195.2 mg); mp: 133.5-134.5 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 10/1); ¹H NMR (400 MHz, CDCl₃) δ 7.29 (dd, *J* = 9.2, 6.3 Hz, 1H), 6.50 – 6.32 (m, 2H), 4.42 (d, *J* = 22.3 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 163.7 (d, *J* = 245.8 Hz), 149.4 (d, *J* = 11.7 Hz), 133.6 (d, *J* = 10.4 Hz), 105.3 (d, *J* = 22.5 Hz), 103.9 (d, *J* = 2.4 Hz), 101.1 (d, *J* = 25.3 Hz), 89.6; ¹⁹F NMR (376 MHz, CDCl₃) δ -109.6; IR: ν_{max}(KBr) = 3449, 3361, 2358, 1615, 1503, 1436, 1253, 1169, 970, 845, 805, 677, 509, 463 cm⁻¹; HRMS (ESI) m/z: calcd for C₁₄H₁₀F₂N₂ [M+H]⁺: 245.0885, found 245.0881.

6,6'-(Ethyne-1,2-diyl)bis(2-chloro-4-fluoroaniline) (1o)



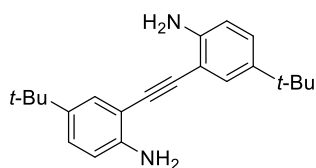
Yellow solid (60%, 374.4 mg); mp: 154.5-155.5 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 10/1); ¹H NMR (400 MHz, CDCl₃) δ 7.19 – 7.10 (m, 1H), 7.03 (dd, *J* = 10.5, 2.3 Hz, 1H), 4.29 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 150.7 (d, *J* = 241.4 Hz), 135.4 (d, *J* = 13.6 Hz), 126.8 (d, *J* = 3.3 Hz), 121.5 (d, *J* = 10.6 Hz), 116.7 (d, *J* = 21.8 Hz), 109.7 (d, *J* = 6.0 Hz), 90.4 (d, *J* = 5.0 Hz); ¹⁹F NMR (376 MHz, CDCl₃) δ -131.4; IR: ν_{max}(KBr) = 2360, 1701, 1622, 1567, 1524, 1483, 1430, 1300, 1218, 1171, 1085, 987, 906, 852, 739, 674 cm⁻¹; HRMS (ESI) m/z: calcd for C₁₄H₈Cl₂F₂N₂ [M+H]⁺: 313.0101 (100%), 315.0070 (63.9%), found 313.0105 (100%), 315.0076 (63.9%).

6,6'-(Ethyne-1,2-diyl)bis(3-(trifluoromethyl)aniline) (1j)



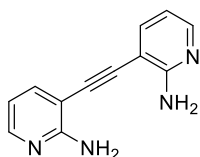
Yellow solid (30%, 206.4 mg); mp: 85.5-86.5 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 8/1); ^1H NMR (400 MHz, CDCl_3) δ 7.44 (t, $J = 7.4$ Hz, 1H), 7.07 – 6.84 (m, 2H), 4.49 (d, $J = 19.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 147.8, 133.6, 132.5, 131.9 (q, $J = 32.3$ Hz), 123.8 (q, $J = 270.7$ Hz), ;114.4 (q, $J = 3.5$ Hz), 110.9 (q, $J = 3.9$ Hz), 91.6; ^{19}F NMR (376 MHz, CDCl_3) δ -63.1; IR: $\nu_{\text{max}}(\text{KBr}) = 1616, 1504, 1437, 1336, 1244, 1165, 1119, 925, 865, 811, 751$ cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{16}\text{H}_{10}\text{F}_6\text{N}_2$ $[\text{M}-\text{H}]^-$: 343.0675, found 343.0675.

2,2'-(Ethyne-1,2-diyl)bis(4-(tert-Butyl)aniline) (1h)



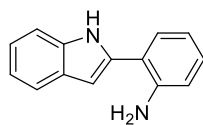
Yellow solid (44%, 281.8 mg); mp: 150.4-151.4 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 10/1); ^1H NMR (400 MHz, CDCl_3) δ 7.39 (d, $J = 2.1$ Hz, 1H), 7.20 (dd, $J = 8.4, 2.2$ Hz, 1H), 6.70 (d, $J = 8.5$ Hz, 1H), 4.19 (s, 2H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.2, 140.91, 128.6, 126.9, 114.3, 107.7, 91.0, 33.8, 31.3; IR $\nu_{\text{max}}(\text{KBr}) = 3489, 3401, 3316, 3265, 3185, 2956, 2860, 2361, 1715, 1623, 1504, 1464, 1416, 1361, 1322, 1258, 1207, 1161, 1104, 1023, 884, 821, 744, 693, 627$ cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{22}\text{H}_{28}\text{N}_2$ $[\text{M}+\text{H}]^+$: 321.2325, found 321.2318.

3,3'-(Ethyne-1,2-diyl)bis(pyridin-2-amine) (1p)



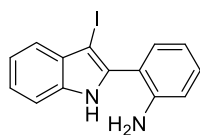
Yellow solid (40%, 168.1 mg); mp: 244.5-245.5 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 6/1); ^1H NMR (400 MHz, CDCl_3) δ 8.05 (dd, $J = 5.0, 1.8$ Hz, 1H), 7.60 (dt, $J = 7.5, 1.8$ Hz, 1H), 6.65 (ddd, $J = 12.8, 7.6, 5.0$ Hz, 1H), 5.17 (d, $J = 18.6$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.6, 148.2, 140.1, 113.6, 102.6, 90.4; IR: $\nu_{\text{max}}(\text{KBr}) = 3455, 3379, 3303, 2924, 2854, 2358, 2216, 1718, 1615, 1563, 1494, 1452, 1319, 1272, 1163, 1027, 819, 755, 693$ cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{12}\text{H}_{10}\text{N}_4$ $[\text{M}+\text{H}]^+$: 211.0978, found 211.0975.

2-(1H-Indol-2-yl)aniline (11)^[1]



Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.47 (s, 1H), 7.66 (d, $J = 7.8$ Hz, 1H), 7.47 – 7.35 (m, 2H), 7.25 – 7.10 (m, 3H), 6.94 – 6.78 (m, 2H), 6.73 (d, $J = 2.1$ Hz, 1H), 4.10 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 144.0, 136.1, 135.8, 129.2, 129.0, 128.8, 122.1, 120.3, 120.1, 119.0, 118.7, 116.5, 110.8, 101.5.

2-(3-iodo-1H-indol-2-yl)aniline (12)^[2]

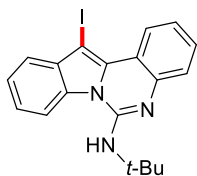


Brown solid. ^1H NMR (400 MHz, CDCl_3) δ 8.65 (s, 1H), 7.51 (d, $J = 7.2$ Hz, 1H), 7.37 – 7.31 (m, 2H), 7.28 (d, $J = 5.5$ Hz, 1H), 7.23 (d, $J = 7.0$ Hz, 1H), 6.88 (t, $J = 7.8$ Hz, 1H), 6.81 (d, $J = 8.1$ Hz, 1H), 3.84 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 144.7, 136.9, 136.2, 131.5, 131.1, 130.4, 123.4, 121.2, 120.9, 118.5, 117.7, 116.1,

111.1, 60.5.

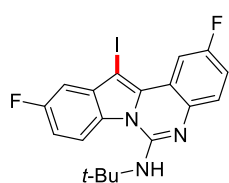
H. Characterization Data for All Products

N-(tert-Butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3a)



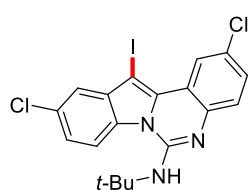
Yellow solid (81%, 33.6 mg); mp: 173.1-174.1 °C; Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 9.29 (d, *J* = 9.0 Hz, 1H), 7.95 (d, *J* = 8.3 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.49 (q, *J* = 7.8, 7.3 Hz, 2H), 7.44 – 7.38 (m, 1H), 7.31 (t, *J* = 6.9 Hz, 1H), 5.26 (s, 1H), 1.70 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 143.7, 141.9, 133.3, 133.2, 130.0, 129.6, 125.4, 123.6, 123.3, 122.9, 122.3, 117.3, 112.8, 52.9, 29.2. IR: ν_{\max} (KBr) = 1611, 1528, 1448, 1347, 1267, 1204, 753 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₁₉H₁₈IN₃ [M+H]⁺: 416.0618, found 416.0616.

***N*-(*tert*-Butyl)-2,10-difluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3b)**



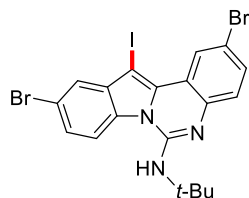
White solid (72%, 32.5 mg); mp: 209.8-210.7 °C; Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.91 (d, *J* = 10.4 Hz, 1H), 7.89 (dd, *J* = 9.0, 3.9 Hz, 1H), 7.52 (dd, *J* = 8.8, 5.5 Hz, 1H), 7.34 (d, *J* = 8.9 Hz, 1H), 7.27 – 7.17 (m, 1H), 7.12 (t, *J* = 8.8 Hz, 1H), 5.00 (s, 1H), 1.68 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 159.7 (d, *J* = 240.7 Hz), 158.0 (d, *J* = 238.9 Hz), 142.9, 138.3, 134.5 (d, *J* = 10.4 Hz), 133.9 (d, *J* = 4.1 Hz), 127.1 (d, *J* = 8.4 Hz), 126.5, 117.7 (d, *J* = 23.4 Hz), 114.2 (d, *J* = 9.6 Hz), 111.5 (d, *J* = 26 Hz), 108.7 (d, *J* = 25.9 Hz), 107.5 (d, *J* = 24.5 Hz), 53.1, 29.2; ¹⁹F NMR (376 MHz, CDCl₃) δ -117.7, -117.8; IR: ν_{\max} (KBr) = 2831, 1619, 1540, 1470, 1364, 1319, 1267, 1197, 1091, 1025, 967, 847, 809, 757 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₁₉H₁₆F₂IN₃ [M+H]⁺: 452.0430, found 452.0421.

***N*-(*tert*-Butyl)-2,10-dichloro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3c)**



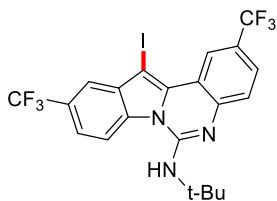
White solid (63%, 30.4 mg); mp: 256.4-257.4 °C; Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 9.20 (s, 1H), 7.84 (d, *J* = 8.9 Hz, 1H), 7.69 (s, 1H), 7.48 (d, *J* = 8.6 Hz, 1H), 7.42 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.35 (dd, *J* = 8.9, 2.1 Hz, 1H), 5.09 (s, 1H), 1.68 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 143.4, 140.4, 134.4, 130.1, 128.4, 127.6, 126.9, 125.5, 123.5, 122.6, 121.9, 113.9, 53.2, 29.2; IR: ν_{\max} (KBr) = 1615, 1441, 1342, 1267, 816, 755 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₁₉H₁₆Cl₂IN₃ [M-H]⁻: 481.9691 (100%), 483.9660 (63.9%), found 481.9693 (100%), 483.9664 (63.9%).

2,10-Dibromo-*N*-(*tert*-Butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3d)



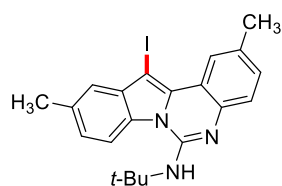
White solid (61%, 34.8 mg); mp: 198.4-199.4 °C; Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 9.34 (s, 1H), 7.84 (s, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 9.8 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.41 (d, *J* = 8.6 Hz, 1H), 5.09 (s, 1H), 1.67 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 143.5, 140.8, 134.8, 132.9, 128.7, 127.2, 126.1, 125.6, 125.0, 118.4, 117.4, 115.2, 114.2, 53.3, 29.2; IR: ν_{\max} (KBr) = 2962, 2855, 2813, 1621, 1547, 1387, 1346, 1267, 1204, 1033, 856, 803, 758 cm⁻¹; HRMS (ESI) Calcd for C₁₉H₁₆Br₂IN₃ [M-H]⁻: 569.8682 (51.4%), 571.8661 (100%), found 569.8683 (51.4%), 571.8662 (100%).

***N*-(*tert*-Butyl)-12-iodo-2,10-bis(trifluoromethyl)indolo[1,2-*c*]quinazolin-6-amine (3e)**



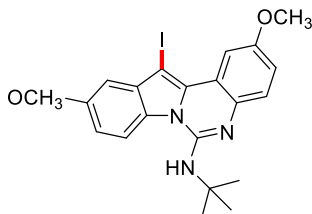
White solid (48%, 26.4 mg); mp: 225.5-226.4 °C; Isolation by column chromatography (petroleum ether); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.56 (d, $J = 2.0$ Hz, 1H), 8.06 – 7.99 (m, 2H), 7.69 (ddd, $J = 14.5, 8.6, 1.9$ Hz, 2H), 7.63 (d, $J = 8.5$ Hz, 1H), 5.34 (s, 1H), 1.71 (s, 9H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.4, 144.3 (d, $J = 0.7$ Hz), 134.0, 133.0, 131.3, 126.6 (q, $J = 3.7$ Hz), 126.1, 124.6 (q, $J = 270$ Hz), 124.3 (q, $J = 270.5$ Hz), 124.1 (q, $J = 32.4$ Hz), 120.9 (q, $J = 4.1$ Hz), 120.3 (q, $J = 4.0$ Hz), 120.1 (q, $J = 3.4$ Hz), 116.7, 113.3, 54.4, 53.6, 29.1; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -61.1, -61.7; IR: ν_{max} (KBr) = 2853, 1661, 1555, 1331, 1111, 878, 832, 797, 754 cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{21}\text{H}_{16}\text{F}_6\text{IN}_3$ $[\text{M}+\text{H}]^+$: 552.0290, found 552.0295.

N-(*tert*-Butyl)-12-iodo-2,10-dimethylindolo[1,2-*c*]quinazolin-6-amine (3f)



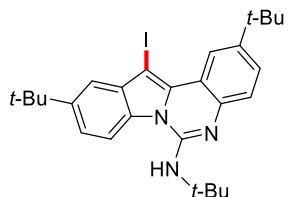
White solid (54%, 23.9 mg); mp: 167.1-168.1 °C; Isolation by column chromatography (petroleum ether); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.12 (d, $J = 8.2$ Hz, 1H), 7.71 (s, 1H), 7.58 (d, $J = 8.1$ Hz, 1H), 7.38 (s, 1H), 7.30 – 7.23 (m, 1H), 7.11 (d, $J = 8.2$ Hz, 1H), 5.23 (s, 1H), 2.59 (s, 3H), 2.46 (s, 3H), 1.69 (s, 9H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 143.9, 141.8, 139.6, 133.0, 132.6, 131.2, 130.2, 125.4, 125.0, 123.6, 123.0, 121.7, 114.9, 113.0, 52.8, 52.2, 29.2, 22.3, 21.5; IR: ν_{max} (KBr) = 3308, 2963, 1707, 1635, 1542, 1372, 1326, 1212, 794, 752 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{21}\text{H}_{22}\text{IN}_3$ $[\text{M}+\text{H}]^+$: 444.0931, found 444.0929.

N-(*tert*-Butyl)-12-iodo-2,10-dimethoxyindolo[1,2-*c*]quinazolin-6-amine (3g)



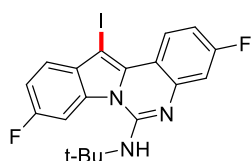
White solid (35%, 16.6 mg); mp: 147.2-148.2 °C; Isolation by column chromatography (petroleum ether); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.81 (d, $J = 2.7$ Hz, 1H), 7.87 (d, $J = 9.1$ Hz, 1H), 7.53 (d, $J = 8.9$ Hz, 1H), 7.17 – 7.08 (m, 2H), 7.01 (dd, $J = 9.1, 2.5$ Hz, 1H), 4.99 (s, 1H), 3.97 (s, 6H), 1.67 (s, 9H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 156.6, 154.9, 142.6, 136.1, 134.2, 133.6, 126.7, 124.9, 118.2, 117.5, 114.1, 112.9, 105.5, 103.2, 55.7, 55.7, 52.8, 52.3, 29.3; IR: ν_{max} (KBr) = 3315, 2829, 1717, 1624, 1547, 1366, 1323, 1205, 774 cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{21}\text{H}_{20}\text{IN}_3$ $[\text{M}+\text{H}]^+$: 476.0829, found 476.0822.

N,2,10-Tri-*tert*-Butyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3h)



White solid (81%, 42.7 mg); mp: 143.9-144.6 °C; Isolation by column chromatography (petroleum ether); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.35 (s, 1H), 7.89 (d, $J = 8.8$ Hz, 1H), 7.72 (s, 1H), 7.60 – 7.45 (m, 3H), 5.21 (s, 1H), 1.68 (s, 9H), 1.48 (d, $J = 5.4$ Hz, 18H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 146.8, 145.3, 143.6, 139.6, 133.7, 132.9, 128.1, 127.3, 124.9, 121.1, 119.8, 118.2, 116.6, 112.6, 52.8, 35.0, 34.8, 31.7, 31.6, 29.2; IR: ν_{max} (KBr) = 2848, 2385, 2343, 1710, 1663, 1588, 1526, 1480, 1378, 780 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{27}\text{H}_{34}\text{IN}_3$ $[\text{M}+\text{H}]^+$: 528.1870, found 528.1871.

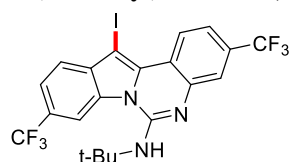
N-(*tert*-Butyl)-3,9-difluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3i)



White solid (33%, 14.9 mg); mp: 200.4-201.4 °C; Isolation by column chromatography (petroleum ether); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.17 (dd, $J = 8.9, 6.1$ Hz, 1H), 7.71 – 7.57 (m, 2H), 7.25 – 7.18 (m, 2H), 7.05 – 6.98 (m, 1H), 5.05 (s, 1H), 1.68 (s, 9H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 163.5 (d, $J =$

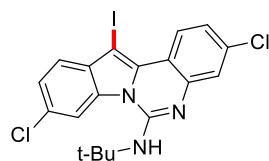
246.7 Hz), 159.5 (d, $J = 239.4$ Hz), 143.9, 143.7 (d, $J = 12.4$ Hz), 133.4 (d, $J = 4.2$ Hz), 129.5, 129.0 (d, $J = 11.5$ Hz), 124.7 (d, $J = 9.6$ Hz), 123.1 (d, $J = 9.7$ Hz), 113.9, 112.3 (d, $J = 24$ Hz), 111.0 (d, $J = 21.6$ Hz), 110.4 (d, $J = 22.6$ Hz), 105.1 (d, $J = 28.9$ Hz), 53.2, 52.0, 29.1; ^{19}F NMR (376 MHz, CDCl_3) δ -110.9, -117.0; IR: $\nu_{\text{max}}(\text{KBr}) = 3314, 2960, 1706, 1639, 1598, 1535, 1471, 1365, 1323, 1274, 1208, 1148, 1104, 978, 929, 844, 805, 739, 695$ cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{19}\text{H}_{16}\text{F}_2\text{IN}_3$ $[\text{M}+\text{H}]^+$: 452.0430, found, 452.0420.

***N*-(*tert*-Butyl)-12-iodo-3,9-bis(trifluoromethyl)indolo[1,2-*c*]quinazolin-6-amine (3j)**



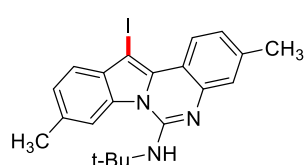
White solid (55%, 30.3 mg); mp: 238.5-239.5 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 9.32 (d, $J = 8.4$ Hz, 1H), 8.26 (s, 1H), 7.86 – 7.77 (m, 2H), 7.71 (d, $J = 8.5$ Hz, 1H), 7.51 (d, $J = 8.4$ Hz, 1H), 5.16 (s, 1H), 1.72 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.9, 141.9, 135.3, 134.5, 131.8 (q, $J = 30.9$ Hz), 124.5 (q, $J = 270.4$ Hz), 129.0, 125.3 (q, $J = 32.5$ Hz), 123.9 (q, $J = 271.0$ Hz), 124.0, 123.1, 122.7 (q, $J = 4$ Hz), 120.6 (q, $J = 3$ Hz), 119.3, 118.7 (q, $J = 3.6$ Hz), 110.4 (q, $J = 4.8$ Hz), 54.4, 53.6, 29.0; ^{19}F NMR (376 MHz, CDCl_3) δ -60.8, -62.7; IR: $\nu_{\text{max}}(\text{KBr}) = 2830, 1625, 1537, 1366, 1329, 1267, 1203, 1162, 1111, 893, 809, 757, 701$ cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{21}\text{H}_{16}\text{F}_6\text{IN}_3$ $[\text{M}+\text{H}]^+$: 552.0290, found 552.0295.

***N*-(*tert*-Butyl)-3,9-dichloro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3k)**



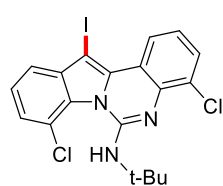
White solid (47%, 22.7 mg); mp: 201.2-202.2 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 9.11 (d, $J = 8.7$ Hz, 1H), 7.91 (s, 1H), 7.60 (d, $J = 8.6$ Hz, 1H), 7.55 (s, 1H), 7.43 (d, $J = 8.5$ Hz, 1H), 7.23 (d, $J = 6.9$ Hz, 1H), 5.07 (s, 1H), 1.69 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.9, 142.8, 135.3, 133.2, 131.6, 129.9, 128.8, 124.9, 124.4, 124.1, 123.0, 122.7, 115.6, 113.0, 53.4, 53.0, 29.1; IR: $\nu_{\text{max}}(\text{KBr}) = 2963, 2357, 1623, 1593, 1541, 1452, 1330, 1266, 1198, 1085, 1028, 943, 870, 802, 754, 677$; HRMS (ESI) m/z : calcd for $\text{C}_{19}\text{H}_{16}\text{Cl}_2\text{IN}_3$ $[\text{M}-\text{H}]^-$: 481.9694 (100%), 483.9662 (63.9%), found 481.9693 (100%), 483.9664 (63.9%).

***N*-(*tert*-Butyl)-12-iodo-3,9-dimethylindolo[1,2-*c*]quinazolin-6-amine (3l)**



White solid (50%, 22.2 mg); mp: 170.0-170.6 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 9.12 (d, $J = 8.2$ Hz, 1H), 7.71 (s, 1H), 7.57 (d, $J = 8.1$ Hz, 1H), 7.38 (s, 1H), 7.27 (d, $J = 8.4$ Hz, 1H), 7.12 (d, $J = 8.2$ Hz, 1H), 5.23 (s, 1H), 2.58 (s, 3H), 2.46 (s, 3H), 1.70 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.9, 141.8, 139.6, 133.0, 132.6, 131.2, 130.3, 125.4, 125.1, 123.7, 123.0, 121.7, 115.0, 113.0, 52.9, 52.0, 29.3, 22.3, 21.5; IR: $\nu_{\text{max}}(\text{KBr}) = 3300, 2961, 1714, 1600, 1539, 1458, 1369, 1322, 1212, 1166, 1030, 873, 796, 754, 703$ cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{21}\text{H}_{22}\text{IN}_3$ $[\text{M}+\text{H}]^+$: 444.0931, found 444.0928.

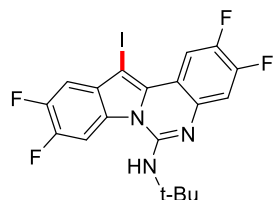
***N*-(*tert*-Butyl)-4,8-dichloro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3m)**



Yellow solid (60%,), mp: 183.5-184.4 °C, Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 8.92 (d, $J = 8.1$ Hz, 1H), 7.61 (d, $J = 7.5$ Hz, 1H), 7.56 (d, $J = 7.8$ Hz, 1H), 7.47 – 7.36 (m, 2H), 7.10 (t, $J = 7.9$ Hz, 1H), 5.71 (s, 1H), 1.68 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.3, 140.1, 137.1, 136.6, 130.4, 128.9, 127.8, 126.2, 125.3, 122.1, 121.4, 121.1, 118.7, 118.4,

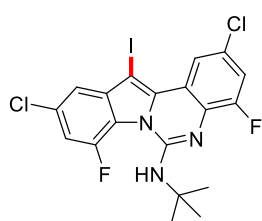
55.9, 53.7, 28.6; IR: ν_{\max} (KBr) = 3447, 2968, 2923, 2308, 1837, 1744, 1688, 1620, 1524, 1462, 1402, 1327, 1272, 1200, 1124, 925, 752 cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{19}\text{H}_{16}\text{Cl}_2\text{IN}_3$ [$\text{M}-\text{H}$] $^-$: 481.9692 (100%), 483.9661 (63.9%) found 481.9693 (100%), 483.9664 (63.9%).

***N*-(*tert*-Butyl)-2,3,9,10-tetrafluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3n)**



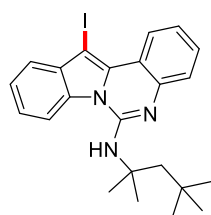
Brown solid (36%, 17.5 mg); mp: 216.5-217.5 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 9.06 – 8.92 (m, 1H), 7.81 (dd, J = 11.0, 6.4 Hz, 1H), 7.46 (dd, J = 10.1, 7.9 Hz, 1H), 7.32 (dd, J = 11.4, 7.8 Hz, 1H), 4.86 (s, 1H), 1.67 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 151.4 (dd, J = 14.3, 250.6 Hz), 148.7 (dd, J = 223.5, 14.2 Hz), 147.7 (dd, J = 242.5, 14.5 Hz), 146.3 (dd, J = 13.5, 221.6 Hz), 143.4, 139.1 (dd, J = 1.5, 10.2 Hz), 133.5 (dd, J = 2.5, 5.2 Hz), 130.8, 129.5 (d, J = 8.1 Hz), 128.8, 124.3 (d, J = 9.3 Hz), 113.3 (d, J = 17.4 Hz), 110.6 (d, J = 21.5 Hz), 109.2 (d, J = 0.3 Hz), 102.2 (d, J = 24.5 Hz), 53.4, 52.0, 29.2; ^{19}F NMR (376 MHz, CDCl_3) δ -133.7, -139.2, -139.8, -141.4; IR: ν_{\max} (KBr) = 1711, 1533, 1477, 1376, 1328, 863, 751 cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{19}\text{H}_{14}\text{F}_4\text{IN}_3$ [$\text{M}+\text{H}$] $^+$: 488.0241, found 488.0235.

***N*-(*tert*-Butyl)-2,10-dichloro-4,8-difluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3o)**



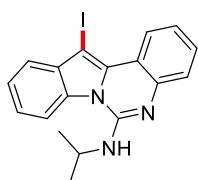
White solid (31%, 16.1 mg); mp: 240.6-240.8 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 8.93 (s, 1H), 7.51 (s, 1H), 7.24 – 7.17 (m, 2H), 6.63 (d, J = 29.4 Hz, 1H), 1.65 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 155.8 (d, J = 252.2 Hz), 147.8 (d, J = 242.4 Hz), 141.9, 137.1 (d, J = 4.2 Hz), 134.5 (d, J = 3.2 Hz), 130.7 (d, J = 11.9 Hz), 129.7 (d, J = 11.8 Hz), 125.9 (d, J = 9.9 Hz), 118.8 (d, J = 3.2 Hz), 118.7 (d, J = 4.1 Hz), 118.1 (d, J = 3.6 Hz), 116.7 (d, J = 22.1 Hz), 116.0 (d, J = 7.5 Hz), 111.5 (d, J = 30.8 Hz), 55.1, 53.4, 28.6; ^{19}F NMR (376 MHz, CDCl_3) δ -110.4, -124.6; IR: ν_{\max} (KBr) = 3341, 2961, 1616, 1536, 1473, 1386, 1349, 1265, 1207, 912, 837, 756 cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{19}\text{H}_{14}\text{Cl}_2\text{F}_2\text{IN}_3$ [$\text{M}-\text{H}$] $^-$: 517.9500 (100%), 519.9470 (63.9%), found, 517.9505 (100%), 519.9475 (63.9 %).

12-Iodo-*N*-(2,4,4-trimethylpentan-2-yl)indolo[1,2-*c*]quinazolin-6-amine (3aa)



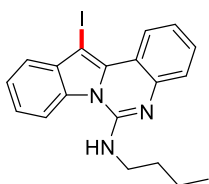
White solid (76%, 35.8 mg); mp: 153.4-154.4 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 9.30 (d, J = 9.2 Hz, 1H), 7.96 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 8.5 Hz, 1H), 7.58 (d, J = 9.0 Hz, 1H), 7.50 (q, J = 7.4 Hz, 2H), 7.44 (d, J = 8.4 Hz, 1H), 7.31 (d, J = 15.2 Hz, 1H), 5.33 (s, 1H), 2.24 (s, 2H), 1.74 (s, 6H), 1.04 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.5, 141.9, 133.4, 133.2, 129.9, 129.6, 125.4, 123.6, 123.3, 123.0, 122.4, 122.2, 117.2, 112.6, 56.8, 53.0, 50.4, 31.8, 31.6, 30.2; IR: ν_{\max} (KBr) = 3389, 3320, 3257, 3049, 2954, 2832, 1715, 1629, 1563, 1368, 1317, 1211, 757 cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{23}\text{H}_{26}\text{IN}_3$ [$\text{M}+\text{H}$] $^+$: 472.1244, found 472.1239.

12-Iodo-*N*-isopropylindolo[1,2-*c*]quinazolin-6-amine (3ab)



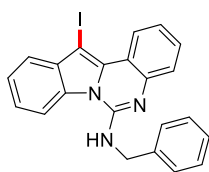
White solid (85%, 34.1 mg); mp: 166.6-167.6 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 30/1); ¹H NMR (400 MHz, CDCl₃) δ 9.27 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.44 – 7.38 (m, 1H), 7.31 (t, *J* = 7.0 Hz, 1H), 5.17 (d, *J* = 6.2 Hz, 1H), 4.56 (dq, *J* = 13.0, 6.5 Hz, 1H), 1.46 (d, *J* = 6.5 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 144.8, 142.2, 133.2, 133.1, 129.9, 129.7, 125.2, 123.7, 123.4, 123.0, 122.4, 122.3, 117.4, 112.9, 53.2, 43.8, 23.0; IR: ν_{\max} (KBr) = 1676, 1535, 1376, 1324, 1217, 742 cm⁻¹; HRMS (ESI) Calcd for C₁₈H₁₆IN₃ [M+H]⁺: 402.0462, found 402.0461.

***N*-Butyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3ac)**



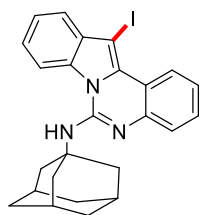
White solid (67%, 27.8 mg); mp: 160.1-160.7 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 30/1); ¹H NMR (400 MHz, CDCl₃) δ 9.24 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.47 (dt, *J* = 15.4, 7.5 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 5.23 (s, 1H), 3.70 (s, 2H), 1.91 – 1.71 (m, 2H), 1.56 (q, *J* = 7.4 Hz, 2H), 1.05 (t, *J* = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 145.6, 142.0, 133.2, 132.9, 129.9, 129.7, 125.1, 123.7, 123.4, 123.1, 122.5, 122.3, 117.4, 112.8, 53.4, 42.0, 31.5, 20.4, 13.9; IR: ν_{\max} (KBr) = 1628, 1533, 1373, 1323, 743 cm⁻¹; HRMS (ESI) Calcd for C₁₉H₁₈IN₃ [M+H]⁺: 416.0618, found 416.0615.

***N*-Benzyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3ad)**



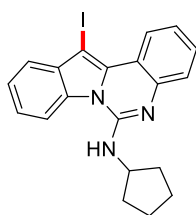
White solid (50%, 22.5 mg); mp: 162.5-163.2 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 30/1); ¹H NMR (400 MHz, CDCl₃) δ 9.28 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.9 Hz, 3H), 7.47 – 7.39 (m, 3H), 7.38 – 7.30 (m, 3H), 5.56 (s, 1H), 4.93 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 145.3, 141.7, 138.2, 133.2, 132.9, 129.9, 129.8, 128.8, 128.1, 127.7, 125.2, 123.8, 123.4, 123.3, 122.8, 122.3, 117.7, 112.9, 46.5; IR: ν_{\max} (KBr) = 1667, 1537, 1324, 746 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₂₁H₂₀IN₃ [M+H]⁺: 450.0462, found 450.0454.

***N*-((3*s*,5*s*,7*s*)-Adamantan-1-yl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3ae)**



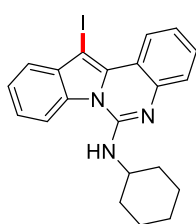
White solid (81%, 39.9 mg); mp: 228.5-229.5 °C; Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 9.28 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.47 (dt, *J* = 14.6, 7.5 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.28 (dd, *J* = 13.6, 6.3 Hz, 1H), 5.19 (s, 1H), 2.40 (s, 6H), 2.22 (s, 3H), 1.81 (s, 5H); ¹³C NMR (100 MHz, CDCl₃) δ 143.3, 141.9, 133.3, 133.2, 130.0, 129.6, 125.3, 123.5, 123.3, 122.8, 122.3, 122.2, 117.3, 112.9, 53.6, 52.9, 42.2, 36.6, 29.7; IR: ν_{\max} (KBr) = 2901, 2834, 1710, 1621, 1537, 1364, 1313, 1210, 727 cm⁻¹; HRMS (ESI) Calcd for C₂₅H₂₄IN₃ [M+H]⁺: 494.1088, found 494.1083.

***N*-Cyclopentyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3af)**



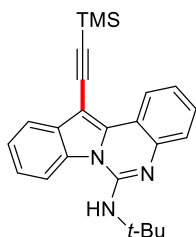
White solid (69%, 29.5 mg); mp: 149.7-150.7 °C; Isolation by column chromatography (petroleum ether/ethyl acetate: 30/1); ^1H NMR (400 MHz, CDCl_3) δ 9.27 (d, $J = 8.1$ Hz, 1H), 7.93 (d, $J = 8.2$ Hz, 1H), 7.73 (d, $J = 8.0$ Hz, 1H), 7.58 (d, $J = 8.0$ Hz, 1H), 7.49 (q, $J = 8.0, 7.5$ Hz, 2H), 7.41 (t, $J = 8.3$ Hz, 1H), 7.31 (t, $J = 7.6$ Hz, 1H), 5.31 (s, 1H), 4.64 (s, 1H), 2.29 (dd, $J = 11.7, 5.8$ Hz, 2H), 1.92 – 1.59 (m, 7H); ^{13}C NMR (100 MHz, CDCl_3) δ 133.3, 133.0, 130.0, 129.7, 125.2, 123.7, 123.4, 123.1, 122.5, 122.3, 117.4, 112.8, 53.8, 33.5, 23.9; IR: $\nu_{\text{max}}(\text{KBr}) = 2856, 2809, 1652, 1525, 1389, 1340, 801, 756$ cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{20}\text{H}_{18}\text{IN}_3$ $[\text{M}+\text{H}]^+$: 428.0618, found 428.0617.

***N*-Cyclohexyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3ag)**



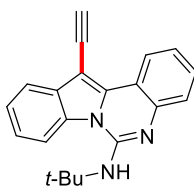
White solid (74%, 32.6 mg); mp: 177.6-178.6 °C, Isolation by column chromatography (petroleum ether/ethyl acetate: 30/1); ^1H NMR (400 MHz, CDCl_3) δ 9.27 (d, $J = 8.1$ Hz, 1H), 7.94 (d, $J = 8.2$ Hz, 1H), 7.73 (d, $J = 7.8$ Hz, 1H), 7.57 (d, $J = 7.9$ Hz, 1H), 7.48 (q, $J = 7.6$ Hz, 2H), 7.41 (t, $J = 7.2$ Hz, 1H), 7.30 (t, $J = 7.5$ Hz, 1H), 5.28 (s, 1H), 4.30 (s, 1H), 2.27 (d, $J = 7.6$ Hz, 2H), 1.84 (d, $J = 13.4$ Hz, 2H), 1.73 (d, $J = 9.0$ Hz, 1H), 1.57 (q, $J = 11.3$ Hz, 2H), 1.44 (q, $J = 9.7$ Hz, 2H), 1.34 (d, $J = 9.3$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 144.7, 133.3, 130.0, 129.7, 125.1, 123.7, 123.4, 123.1, 122.3, 117.4, 112.9, 50.2, 33.2, 25.8, 24.8; IR: $\nu_{\text{max}}(\text{KBr}) = 2924, 2853, 1605, 1525, 1451, 1341, 1214, 1083, 746$ cm^{-1} ; HRMS (ESI) Calcd for $\text{C}_{21}\text{H}_{20}\text{IN}_3$ $[\text{M}+\text{H}]^+$: 442.0775, found 442.0775.

***N*-(*tert*-Butyl)-12-((trimethylsilyl)ethynyl)indolo[1,2-*c*]quinazolin-6-amine (4)**



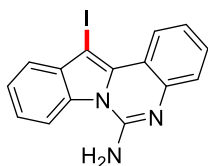
Brown solid (92%, 35.4 mg); mp: 221.2-222.2 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 9.09 (d, $J = 7.5$ Hz, 1H), 7.94 (dd, $J = 16.8, 8.1$ Hz, 2H), 7.58 (d, $J = 7.8$ Hz, 1H), 7.49 (dt, $J = 14.4, 7.8$ Hz, 2H), 7.39 (t, $J = 7.6$ Hz, 1H), 7.29 (dd, $J = 15.4, 8.4$ Hz, 1H), 5.28 (s, 1H), 1.71 (s, 9H), 0.41 (s, 7H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.8, 141.7, 138.1, 131.6, 129.8, 129.1, 125.1, 124.0, 123.5, 122.8, 122.7, 120.4, 117.9, 112.8, 101.7, 99.5, 92.0, 52.9, 29.2, 1.0; IR: $\nu_{\text{max}}(\text{KBr}) = 2961, 2139, 1609, 1554, 1452, 1391, 1335, 1261, 1207, 848, 753$ cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{24}\text{H}_{28}\text{N}_3\text{Si}$ $[\text{M}+\text{H}]^+$: 386.2044, found 386.2039.

***N*-(*tert*-Butyl)-12-ethynylindolo[1,2-*c*]quinazolin-6-amine (5)**



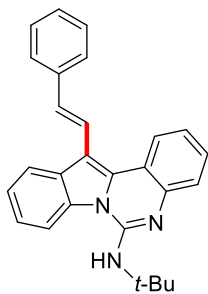
Yellow solid (98%, 30.6 mg); mp: 163.7-164.2 °C; Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 9.04 (d, $J = 9.1$ Hz, 1H), 7.95 (t, $J = 8.3$ Hz, 2H), 7.57 (d, $J = 8.1$ Hz, 1H), 7.53 – 7.43 (m, 2H), 7.39 (t, $J = 8.4$ Hz, 1H), 7.28 (d, $J = 6.9$ Hz, 1H), 5.29 (s, 1H), 3.75 (s, 1H), 1.71 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.8, 141.7, 138.3, 131.8, 129.9, 129.1, 125.2, 123.9, 123.5, 123.0, 122.8, 120.1, 117.6, 112.8, 90.6, 84.3, 78.2, 77.3, 77.0, 76.6, 53.0, 29.2; IR: $\nu_{\text{max}}(\text{KBr}) = 3930, 3814, 3771, 3713, 3442, 3360, 3255, 3182, 2957, 2921, 2850, 2781, 2712, 2666, 2604, 2432, 2089, 1654, 1608, 1556, 1461, 1391, 1323, 1248, 1200, 1122, 1078, 1025, 965, 804, 735, 606$ cm^{-1} ; HRMS (ESI) m/z : calcd for $\text{C}_{21}\text{H}_{19}\text{N}_3$ $[\text{M}+\text{H}]^+$: 314.1652, found 314.1643.

12-Iodoindolo[1,2-*c*]quinazolin-6-amine (6)



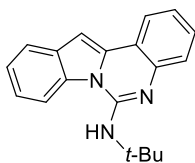
White solid (40%, 14.3 mg); mp: 234.8-235.8 °C, Isolation by column chromatography (petroleum ether/ethyl acetate: 5/1); ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.37 (d, *J* = 8.1 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.31 (m, 5H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.12 (s, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 146.5, 135.1, 129.4, 128.6, 122.5, 122.5, 122.2, 121.0, 119.5, 114.4, 94.8; IR: ν_{\max} (KBr) = 2830, 1628, 1548, 1367, 1319, 755 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₁₅H₁₁IN₃ [M+H]⁺: 359.9992, found 359.9992.

(*E*)-*N*-(*tert*-Butyl)-12-styrylindolo[1,2-*c*]quinazolin-6-amine (7)



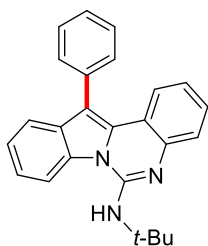
Brown solid (88%, 34.4 mg); mp : 151.5-152.5 °C, Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.27 (d, *J* = 7.8 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 8.07 (d, *J* = 8.3 Hz, 1H), 7.80 – 7.68 (m, 3H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.49 (dt, *J* = 19.5, 7.2 Hz, 5H), 7.39 (t, *J* = 7.4 Hz, 1H), 7.34 – 7.25 (m, 2H), 5.36 (s, 1H), 1.79 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 144.1, 142.1, 138.0, 132.8, 131.9, 129.9, 129.5, 128.8, 128.7, 127.3, 126.1, 125.3, 124.6, 123.1, 123.0, 122.2, 121.4, 120.2, 118.6, 112.9, 109.3, 52.8, 29.2; IR: ν_{\max} (KBr) = 2829, 1697, 1625, 1547, 1368, 1324, 1268, 755 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₂₇H₂₅N₃ [M+H]⁺: 392.2043, found 392.2042.

***N*-(*tert*-Butyl)indolo[1,2-*c*]quinazolin-6-amine (8)**



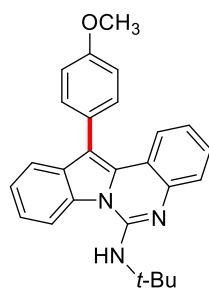
White solid (87%, 25.1 mg); mp: 126.9-127.3 °C, Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 7.96 (dd, *J* = 13.2, 8.0 Hz, 2H), 7.83 (d, *J* = 7.4 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.47 – 7.31 (m, 3H), 7.28 – 7.20 (m, 1H), 7.15 (s, 1H), 5.32 (s, 1H), 1.72 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 144.1, 141.0, 136.8, 130.8, 130.2, 128.9, 125.3, 122.9, 122.8, 122.6, 121.3, 120.9, 117.4, 112.8, 94.6, 52.7, 29.3; IR: ν_{\max} (KBr) = 3428, 3057, 2960, 2922, 2364, 1619, 1556, 1513, 1473, 1447, 1390, 1361, 1331, 1272, 1240, 1198, 1118, 1023, 941, 914, 837, 786, 731, 646 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₁₉H₂₀N₃ [M+H]⁺: 290.1652, found 290.1648.

***N*-(*tert*-Butyl)-12-phenylindolo[1,2-*c*]quinazolin-6-amine (9)**



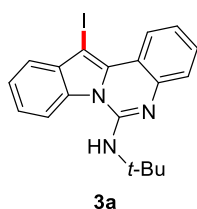
Brown solid (60%, 21.9 mg); mp : 208.1-208.9 °C, Isolation by column chromatography (petroleum ether); ¹H NMR (400 MHz, CDCl₃) δ 8.02 (d, *J* = 7.0 Hz, 1H), 7.62 – 7.46 (m, 8H), 7.42 – 7.31 (m, 3H), 6.92 (t, *J* = 7.6 Hz, 1H), 5.34 (s, 1H), 1.73 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 144.2, 141.7, 135.0, 131.5, 130.9, 129.2, 128.9, 128.7, 127.5, 125.3, 123.5, 122.8, 122.4, 122.0, 119.7, 117.9, 112.7, 112.2, 52.8, 29.3; IR: ν_{\max} (KBr) = 2831, 1609, 1360, 1268, 756 cm⁻¹; HRMS (ESI) *m/z*: calcd for C₂₅H₂₄N₃ [M+H]⁺: 366.1965, found 366.1960.

***N*-(*tert*-Butyl)-12-(4-methoxyphenyl)indolo[1,2-*c*]quinazolin-6-amine (10)**

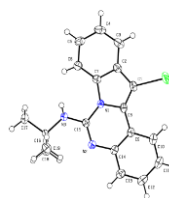


Brown solid (90%, 35.6 mg); mp: 159.8-160.7 °C, Isolation by column chromatography (petroleum ether); ^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, $J = 8.5$ Hz, 1H), 7.63 (dd, $J = 14.1, 8.5$ Hz, 2H), 7.56 (d, $J = 8.0$ Hz, 1H), 7.50 (d, $J = 8.6$ Hz, 2H), 7.38 (q, $J = 9.1, 7.9$ Hz, 3H), 7.13 (d, $J = 8.6$ Hz, 2H), 6.97 (t, $J = 7.6$ Hz, 1H), 5.36 (s, 1H), 3.96 (s, 3H), 1.76 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.0, 144.2, 141.6, 131.9, 131.7, 131.5, 129.1, 128.5, 127.6, 126.9, 125.2, 123.4, 122.7, 122.4, 121.9, 119.6, 118.1, 114.4, 114.1, 112.7, 111.9, 55.3, 52.8, 29.3; IR: $\nu_{\text{max}}(\text{KBr}) = 3299, 2960, 2830, 1566, 1509, 1455, 1362, 1241, 1110, 1032, 932, 830, 752, 607 \text{ cm}^{-1}$; HRMS (ESI) m/z : calcd for $\text{C}_{26}\text{H}_{26}\text{N}_3$ $[\text{M}+\text{H}]^+$: 396.2070, found 396.2062.

I. X-ray Crystallographic Analysis for Product 3a



≡



CCDC: 2205149

Empirical formula	$\text{C}_{19}\text{H}_{18}\text{IN}_3$
Formula weight	415.26
Temperature	150.0 K
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	$a = 21.6151 (11) \text{ \AA}$ $\alpha = 90 \text{ deg.}$ $b = 10.3343 (4) \text{ \AA}$ $\beta = 125.115 (3) \text{ deg}$ $c = 18.5855 (9) \text{ \AA}$ $\gamma = 90 \text{ deg.}$
Volume	$3396.0 (3) \text{ \AA}^3$
Z, Calculated density	8, 1.624 g/cm^3
F(000)	1648.0
Crystal size	$0.15 \times 0.08 \times 0.07 \text{ mm}^3$
Theta range for data collection	4.566 to 52.86 deg
Limiting indices	$-26 \leq h \leq 26, -12 \leq k \leq 12, -23 \leq l \leq 23$
Reflections collected / unique	19018 / 3460 [R(int) = 0.0366, R(sigma) = 0.0267]
Completeness to theta = 26.430	99.3%
Data / restraints / parameters	3460/2/219
Goodness-of-fit on F^2	1.022

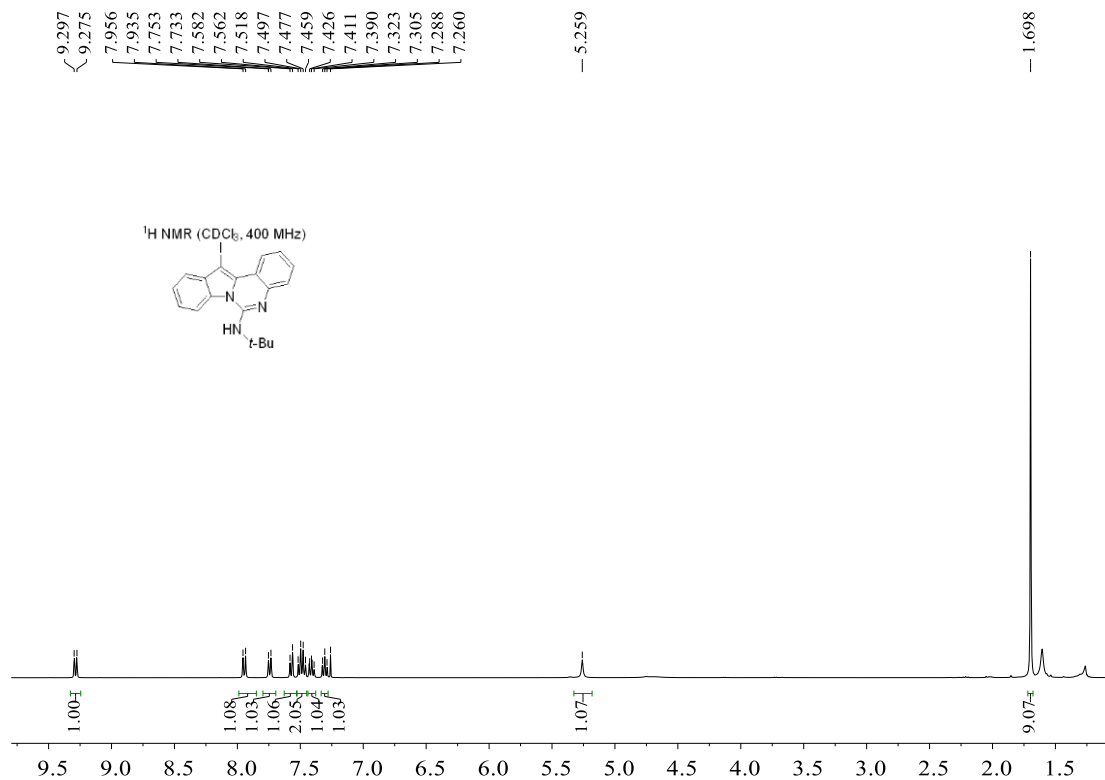
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0316, wR2 = 0.0644
R indices (all data)	R1 = 0.0397, wR2 = 0.0700

J. References

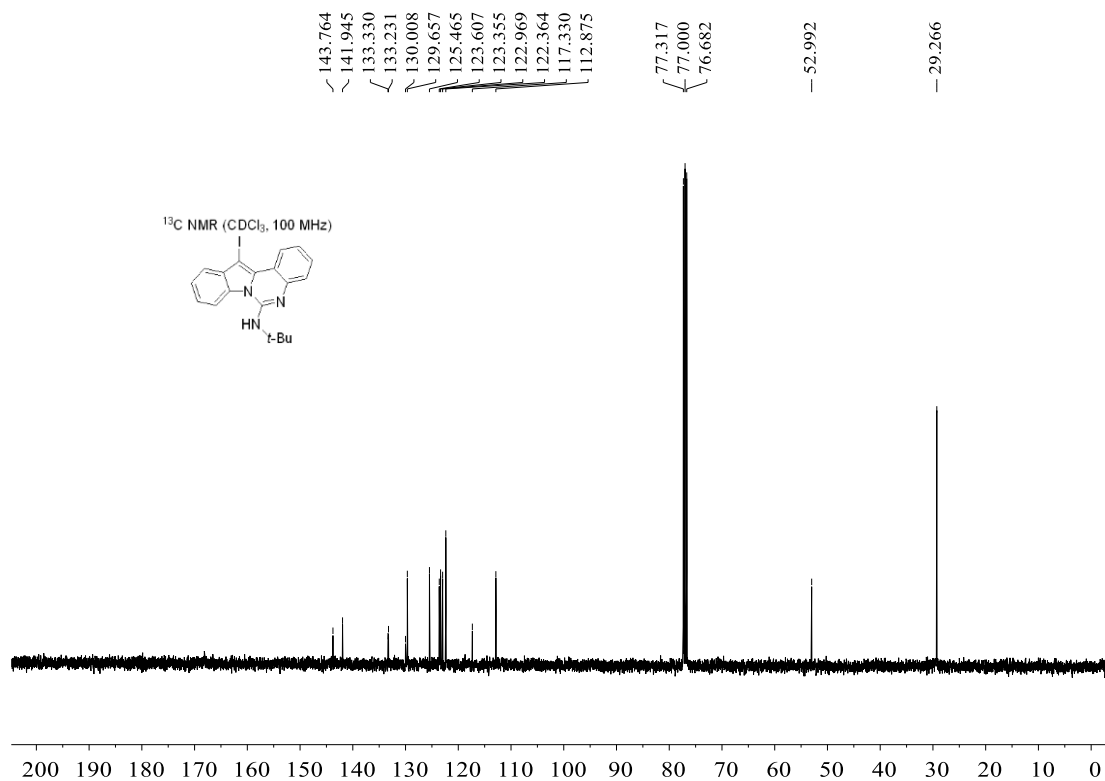
- [1] Kumar, K. S.; Ramulu, M. S.; Rajesham, B.; Kumar, N. P.; Voorab, V.; Kanchab, R. K. *Org. Biomol. Chem.* **2017**, *15*, 4468.
- [2] Reddy, B. V.; Swain, M.; Reddy, S. M.; Yadav, J. S.; Sridhar, B. *Eur. J. Org. Chem.*, **2014**, 3313-3318.

K. Copies of ^1H , ^{13}C and ^{19}F NMR Spectra
***N*-(*tert*-Butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3a)**

^1H NMR (400MHz, CDCl_3) of compound 3a

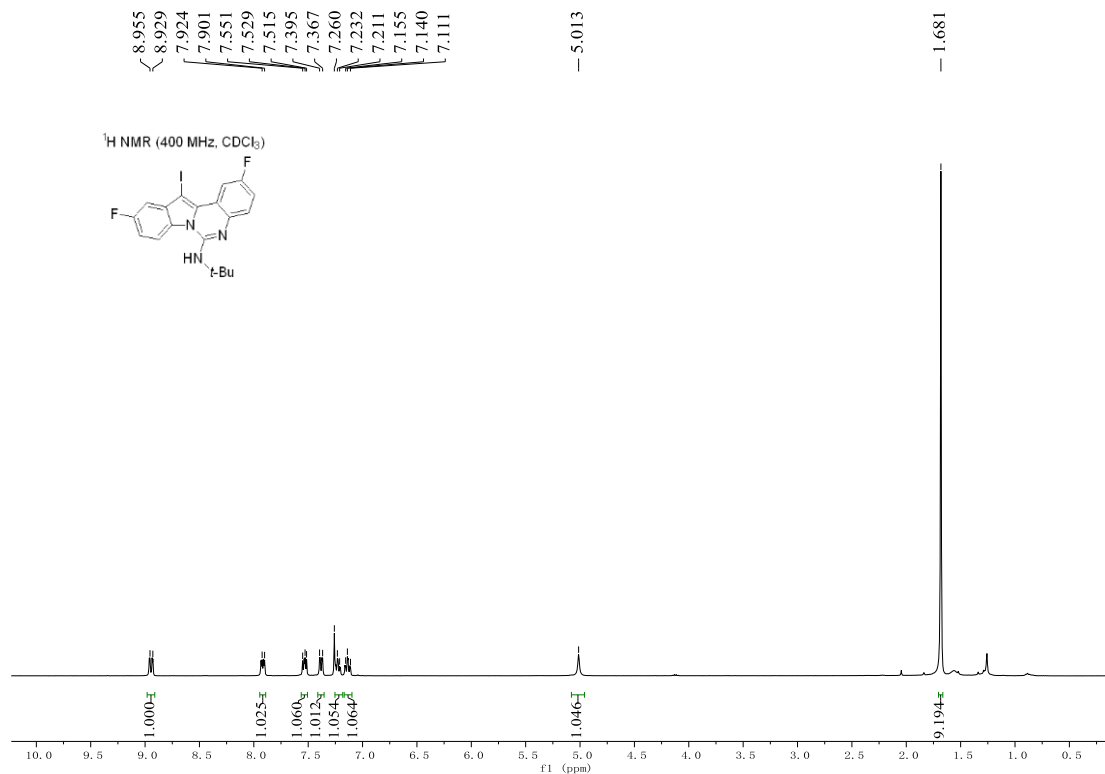


^{13}C NMR (100 Mz, CDCl_3) of compound 3a

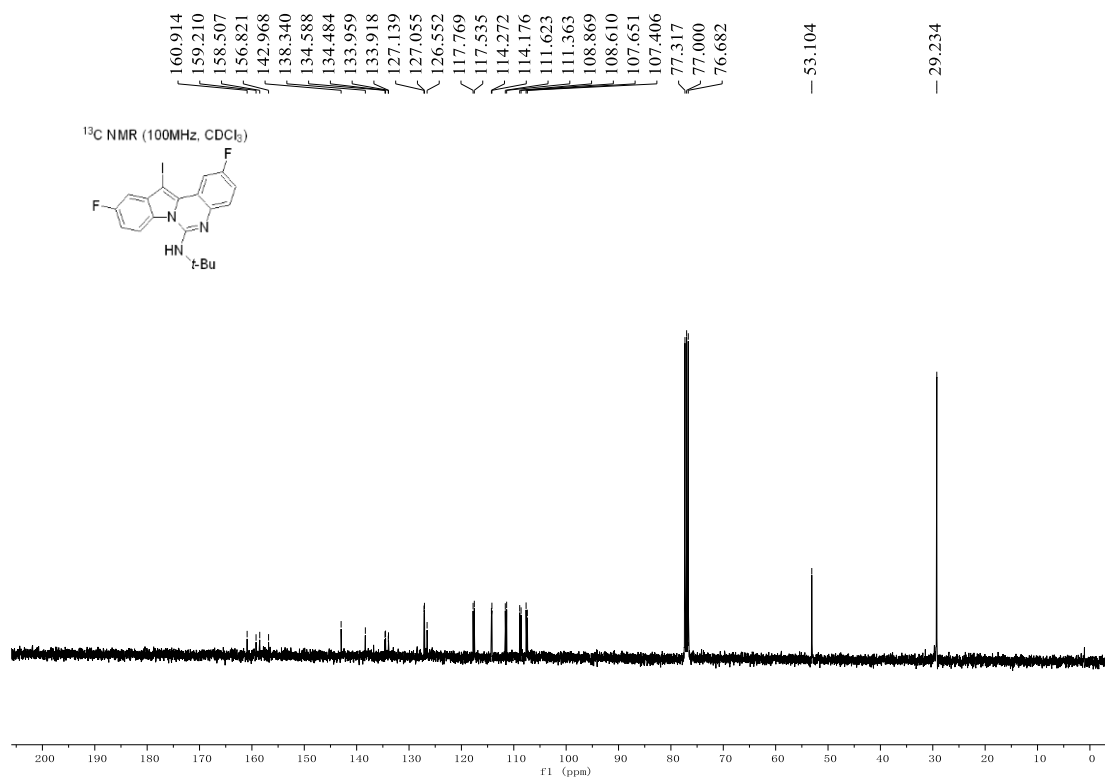


***N*-(*tert*-Butyl)-2,10-difluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3b)**

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



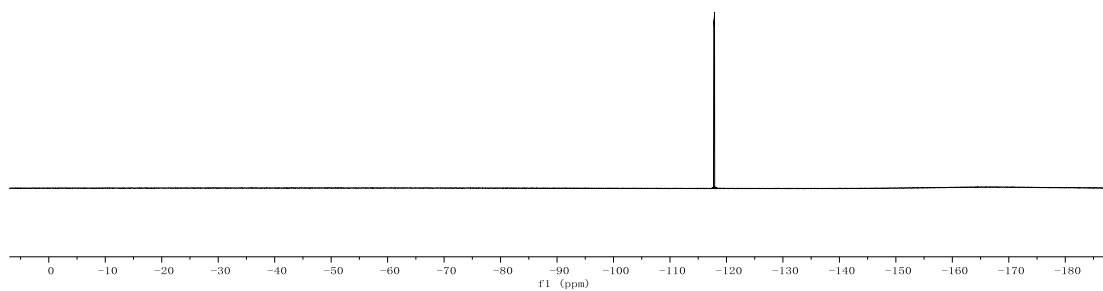
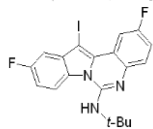
¹³C NMR (100 Mz, CDCl₃) of compound **3b**



^{19}F NMR (376 Mz, CDCl_3) of compound **3b**

$\left\{ \begin{array}{l} -117.759 \\ -117.884 \end{array} \right.$

^{19}F NMR (376 MHz, CDCl_3)

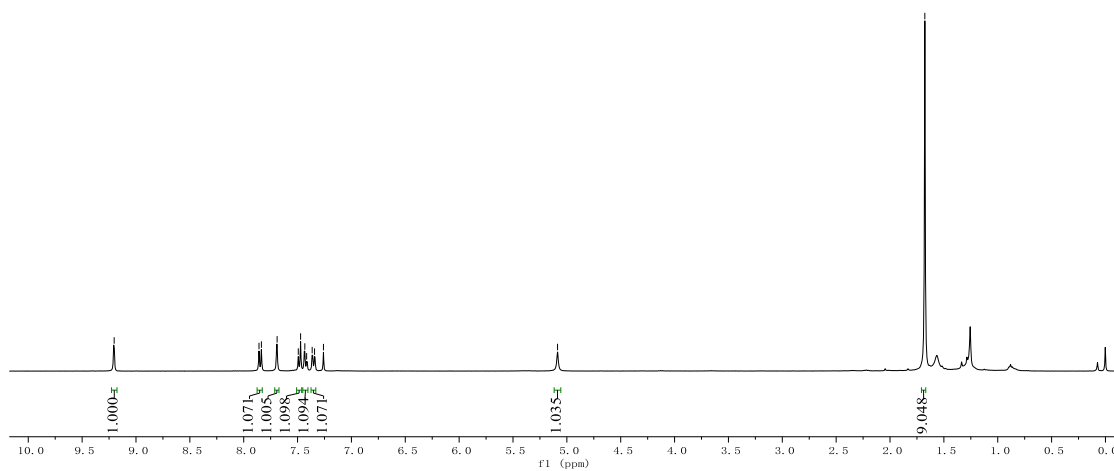
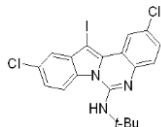


N-(*tert*-Butyl)-2,10-dichloro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3c**)

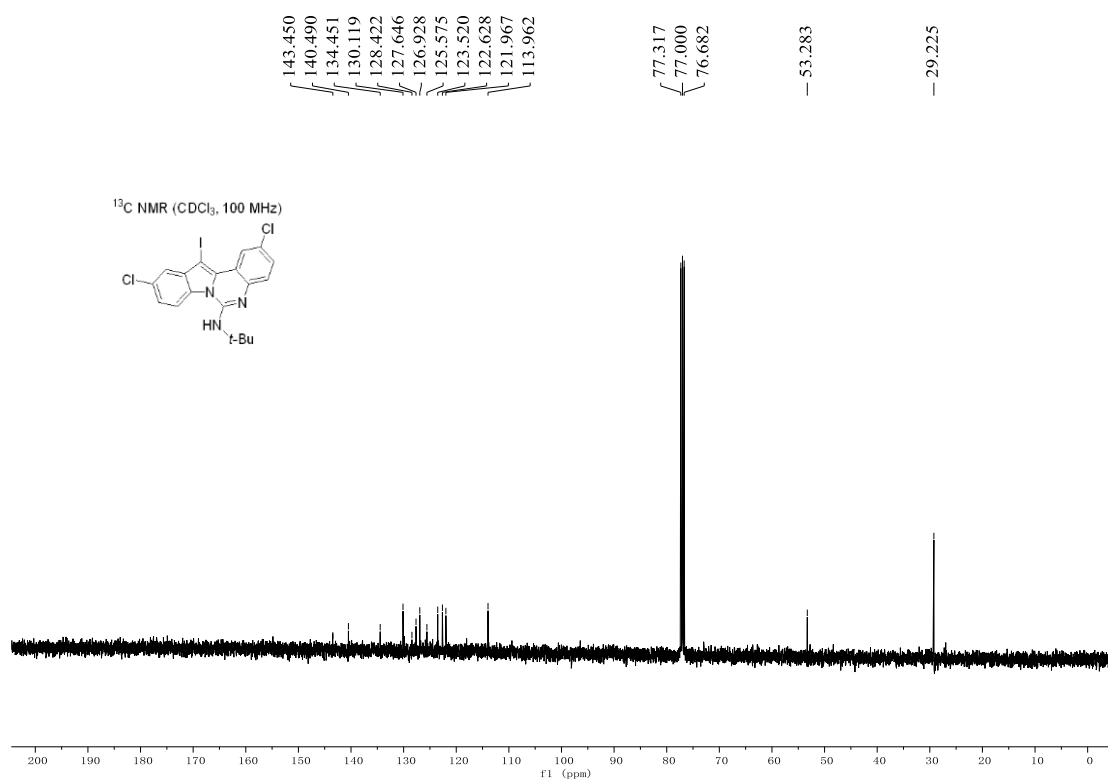
^1H NMR (400 MHz, CDCl_3) of compound of **3c**

9.203
7.858
7.836
7.690
7.493
7.472
7.433
7.416
7.364
7.342
7.260
5.086
1.677

^1H NMR (400 MHz, CDCl_3)

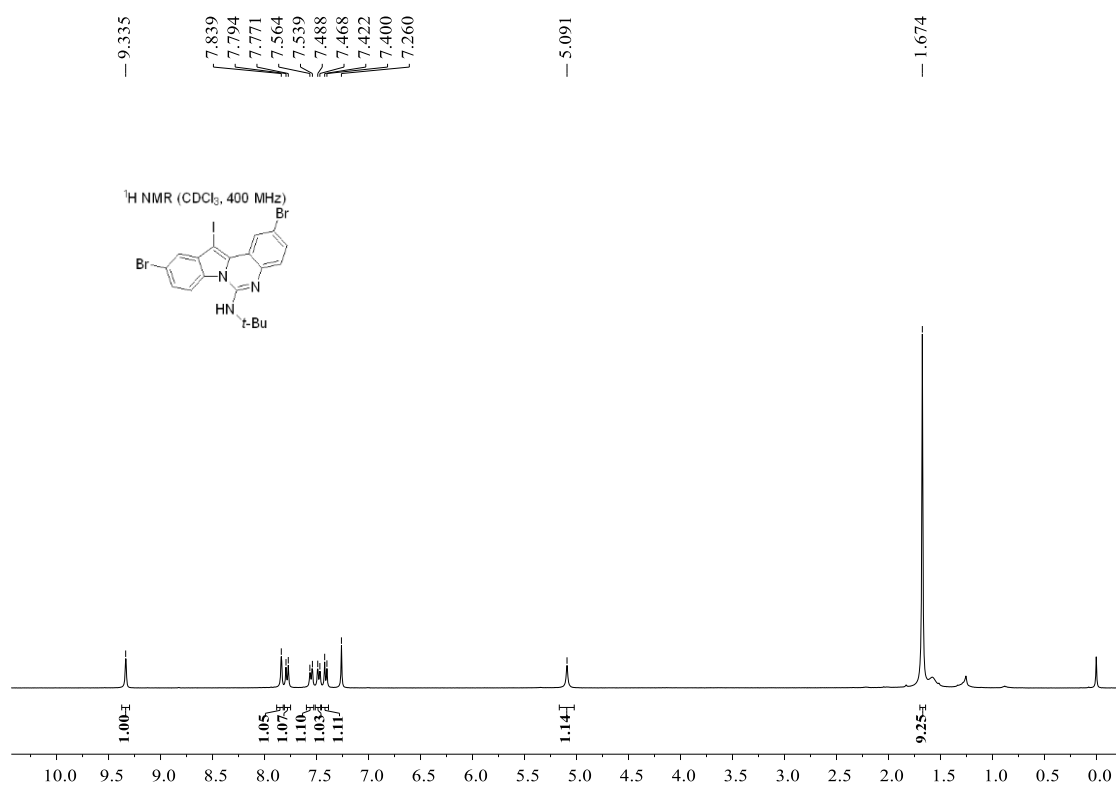


^{13}C NMR (100 Mz, CDCl_3) of compound **3c**

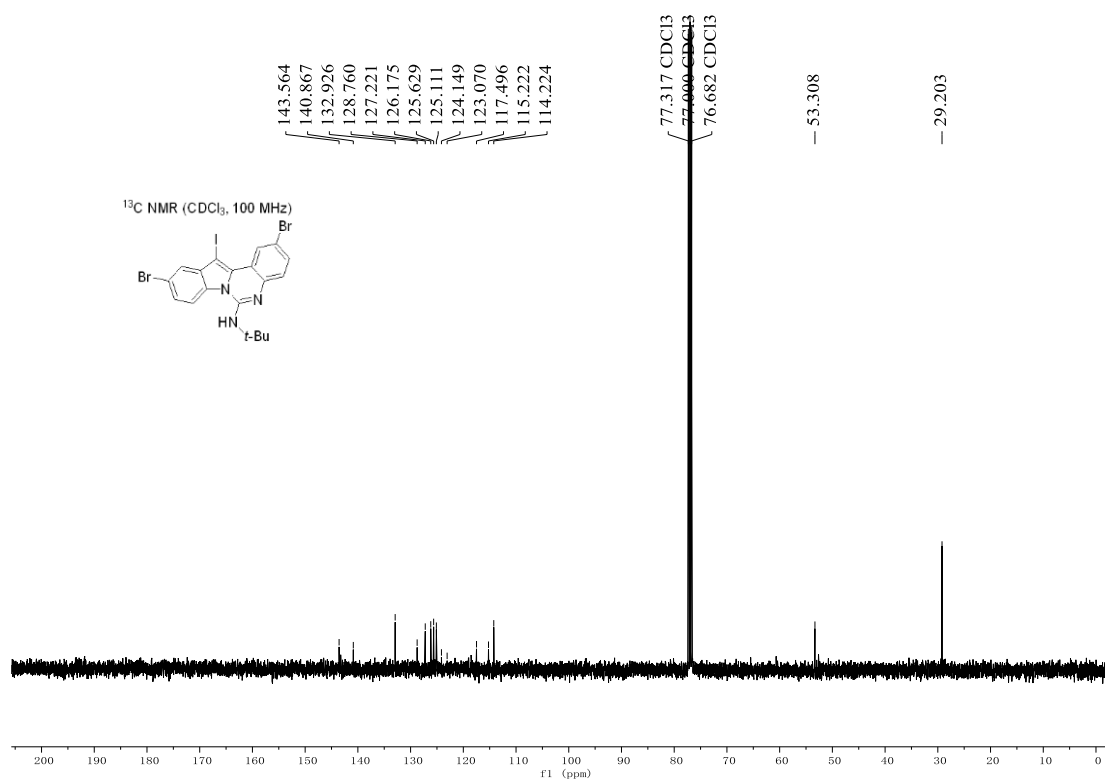


2,10-Dibromo-*N*-(*tert*-butyl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3d**)**

^1H NMR (400 MHz, CDCl_3) of compound of **3d**

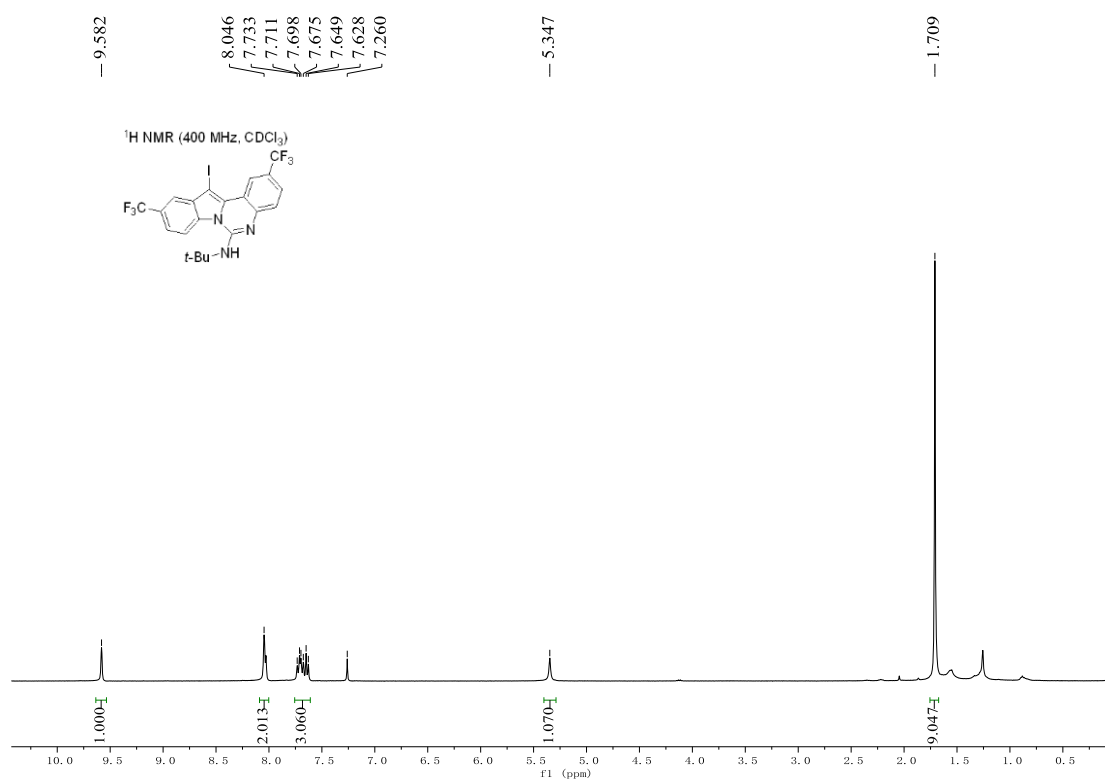


^{13}C NMR (100 Mz, CDCl_3) of compound **3d**

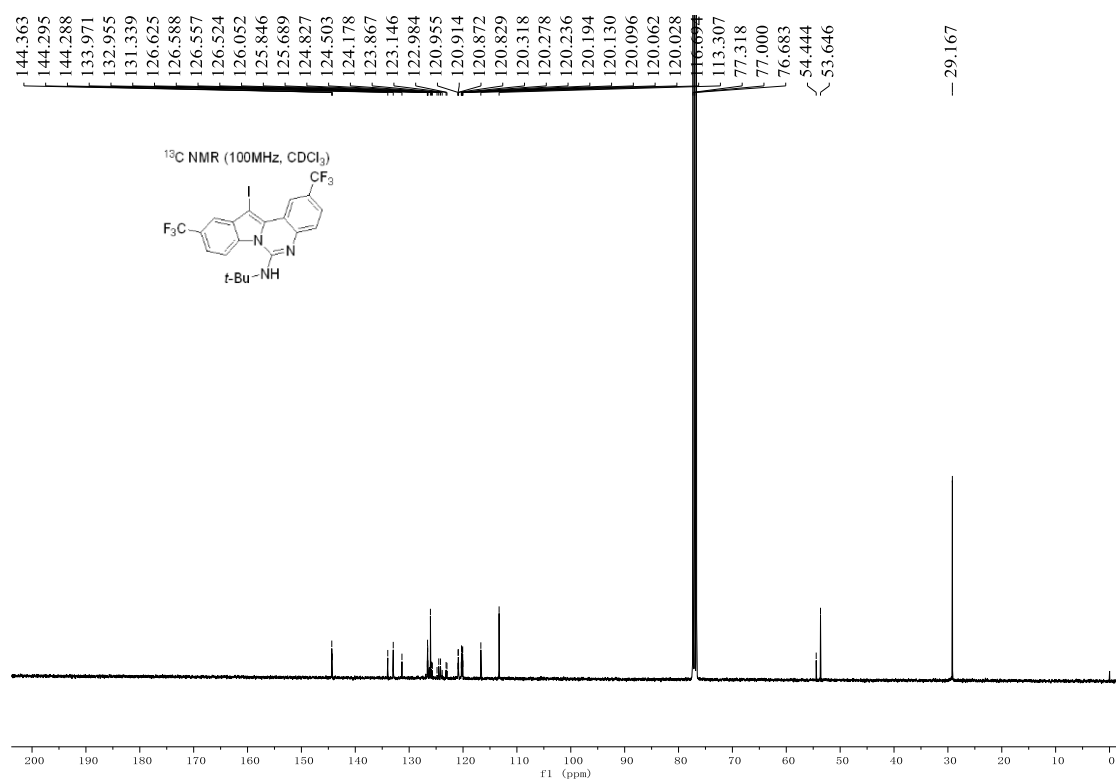


N-(*tert*-Butyl)-12-iodo-2,10-bis(trifluoromethyl)indolo[1,2-*c*]quinazolin-6-amine (**3e**)

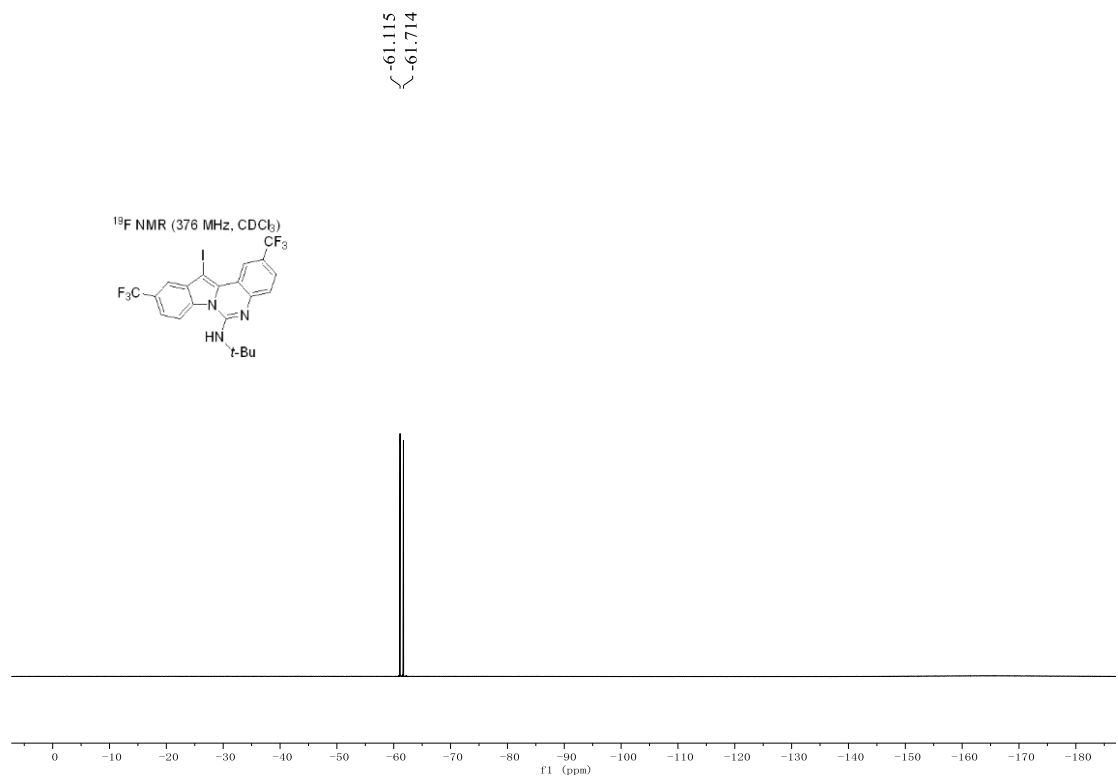
^1H NMR (400 MHz, CDCl_3) of compound of **3e**



¹³C NMR (100 Mz, CDCl₃) of compound **3e**

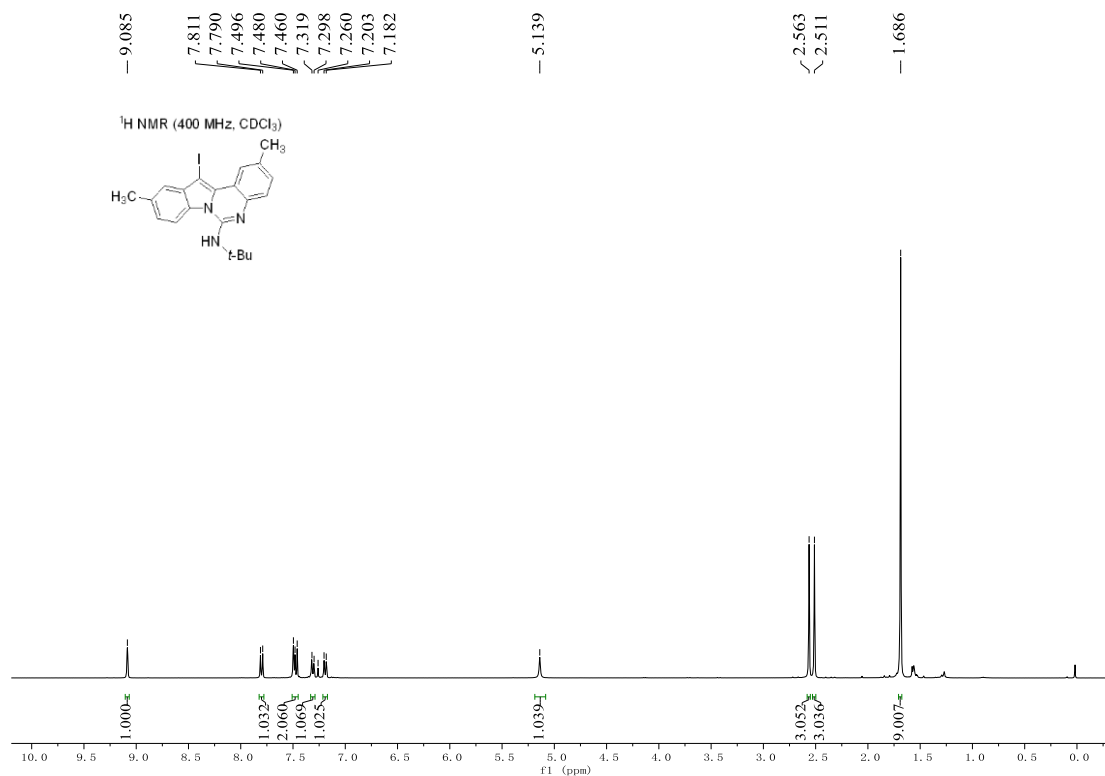


¹⁹F NMR (376 Mz, CDCl₃) of compound **3e**

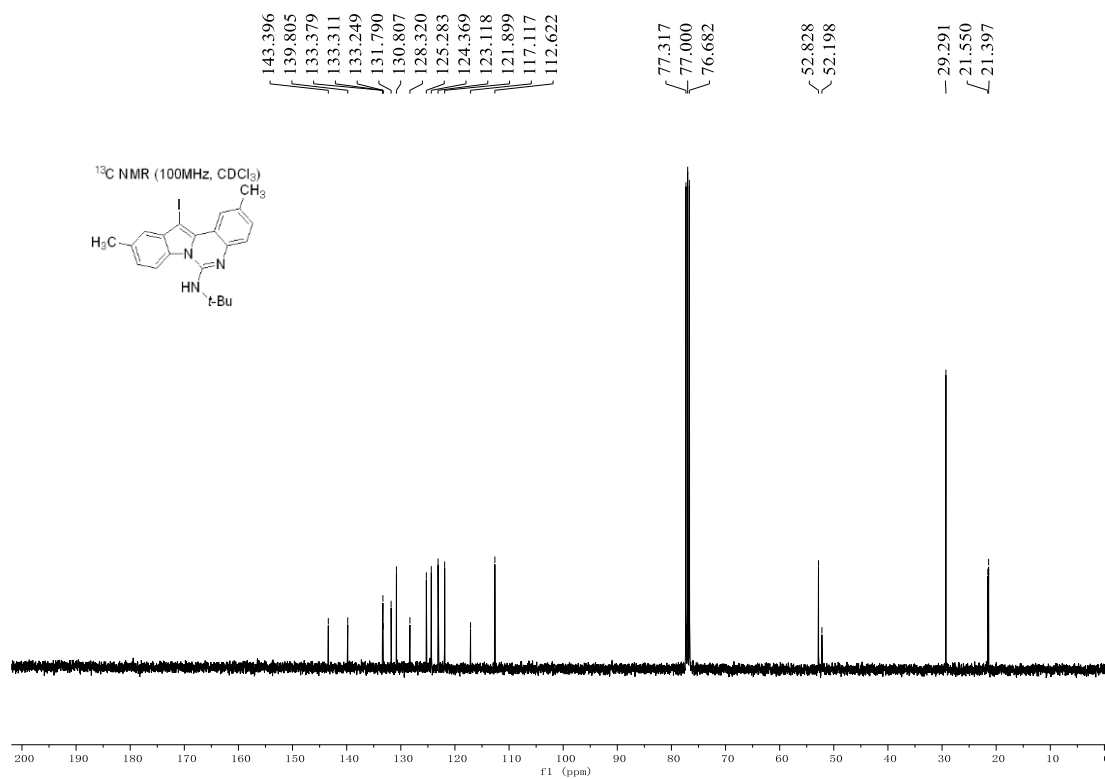


***N*-(*tert*-Butyl)-12-iodo-2,10-dimethylindolo[1,2-*c*]quinazolin-6-amine (3f)**

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

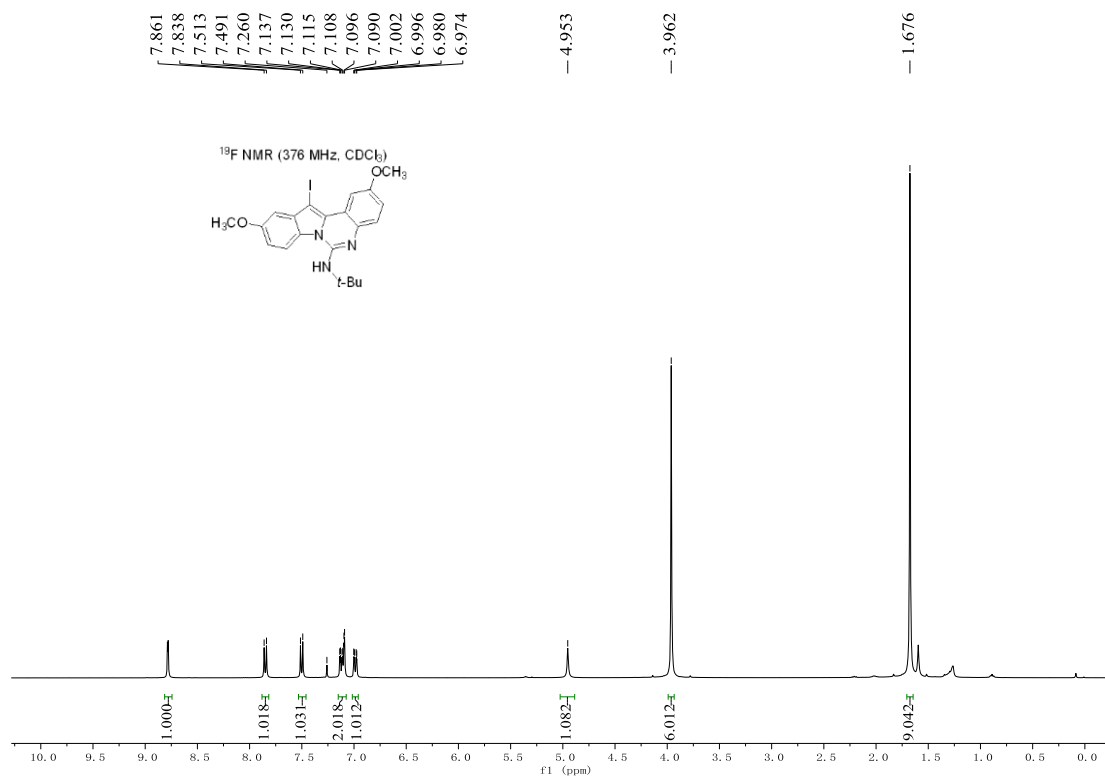


¹³C NMR (100 MHz, CDCl₃) of compound **3f**

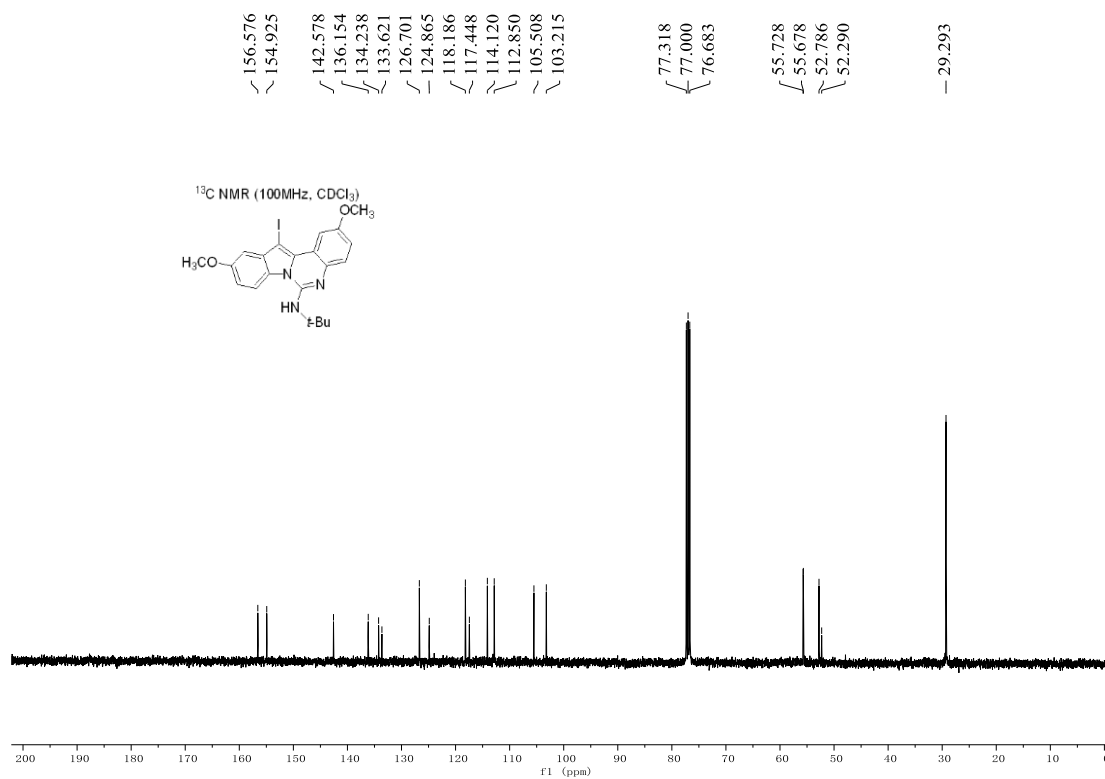


***N*-(*tert*-Butyl)-12-iodo-2,10-dimethoxyindolo[1,2-*c*]quinazolin-6-amine (3g)**

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

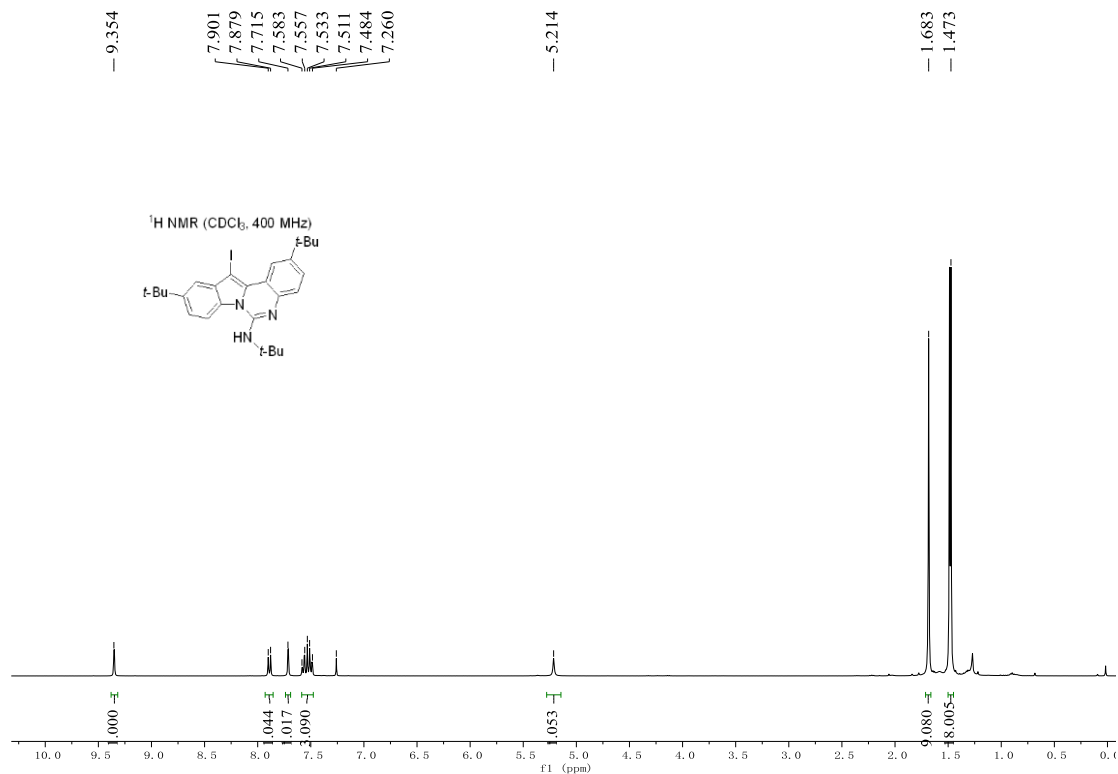


¹³C NMR (100 Mz, CDCl₃) of compound **3g**

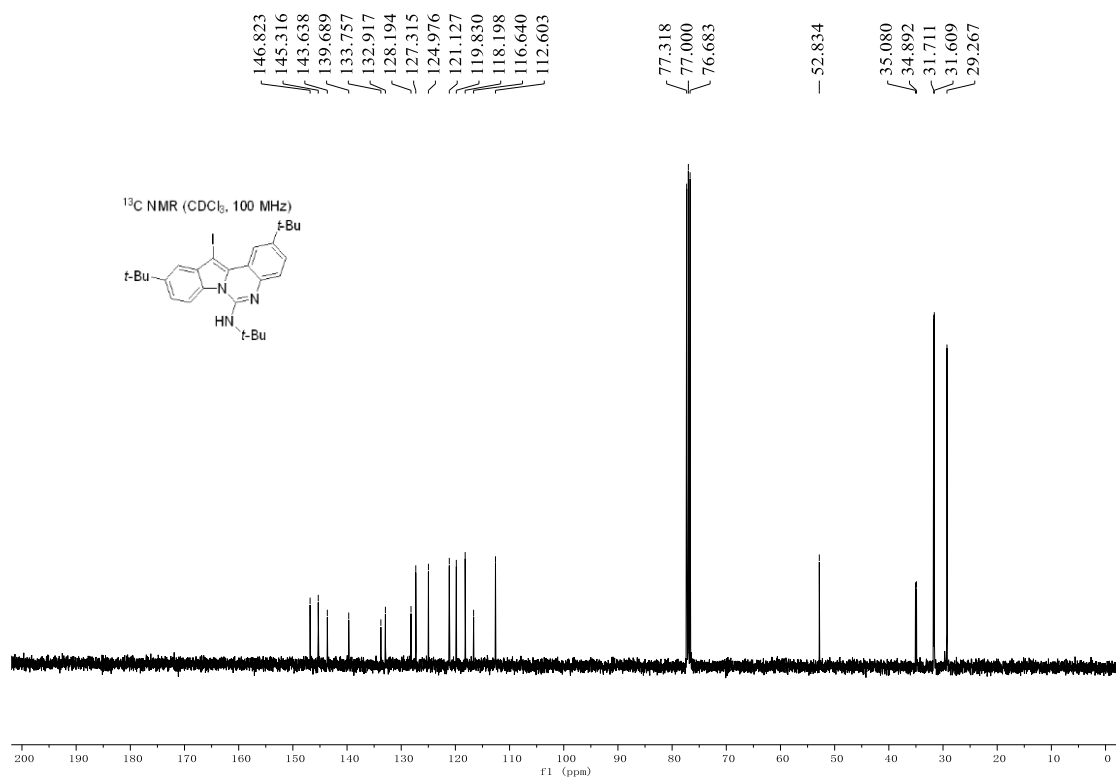


***N*,2,10-Tri-*tert*-butyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3h)**

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

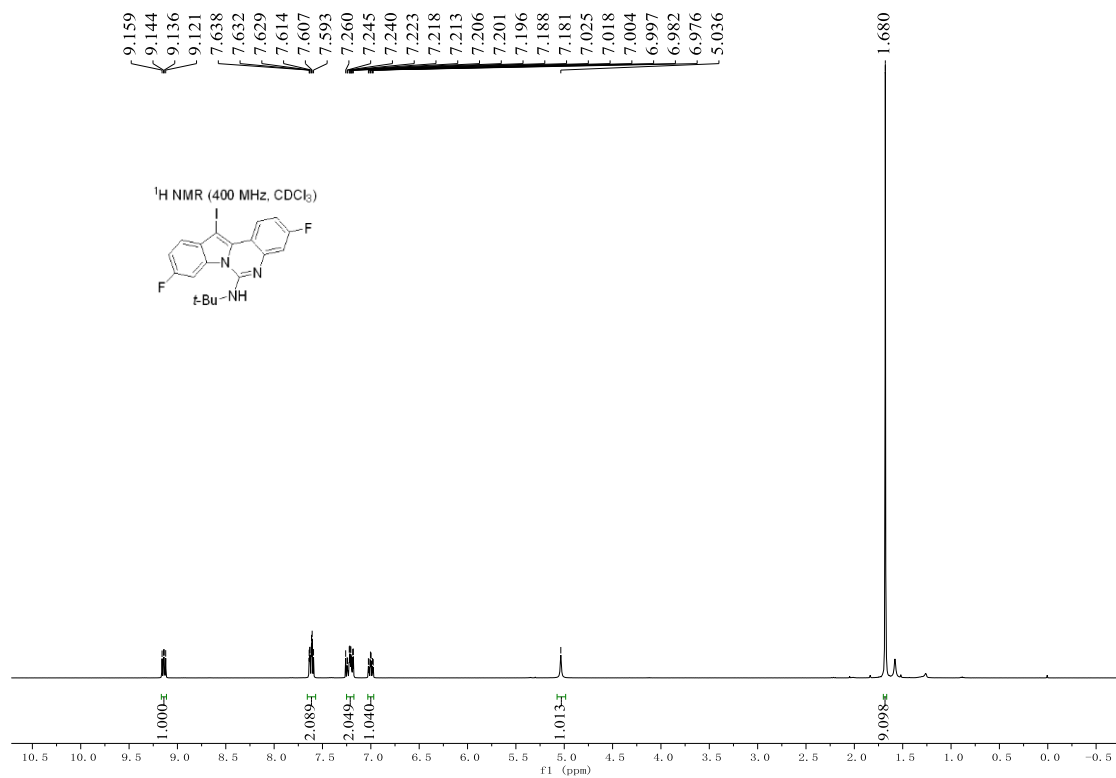


¹³C NMR (100 Mz, CDCl₃) of compound **3h**

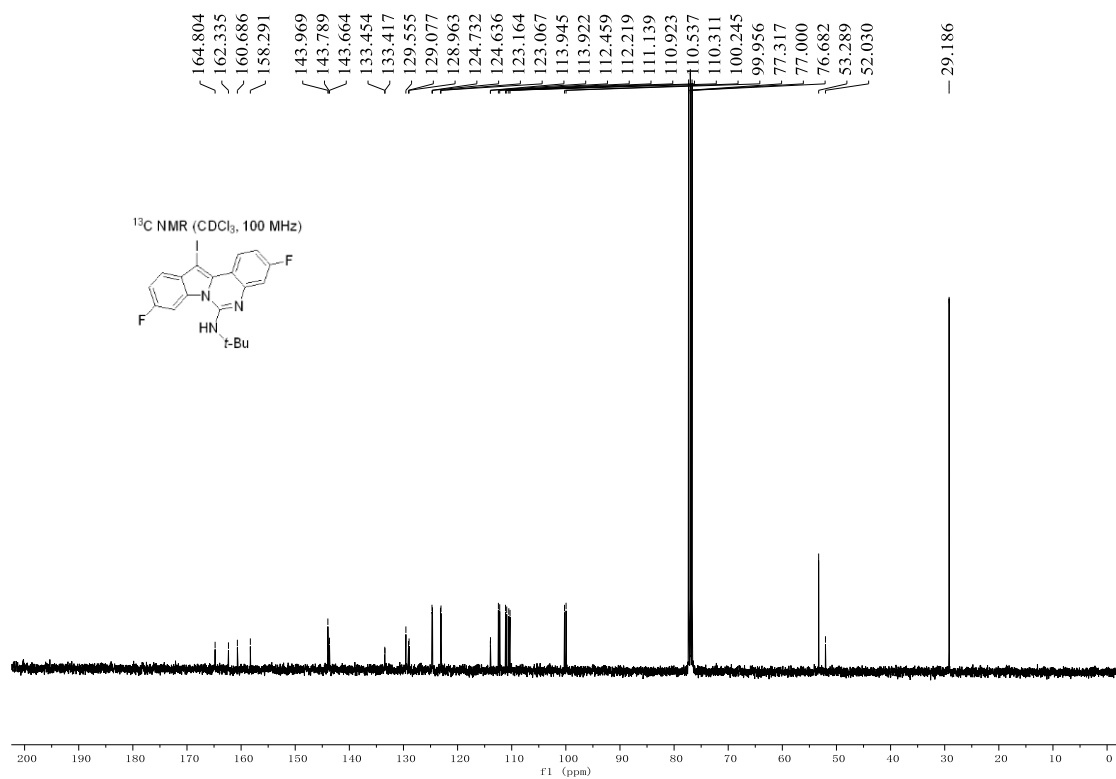


***N*-(*tert*-Butyl)-3,9-difluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3i)**

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

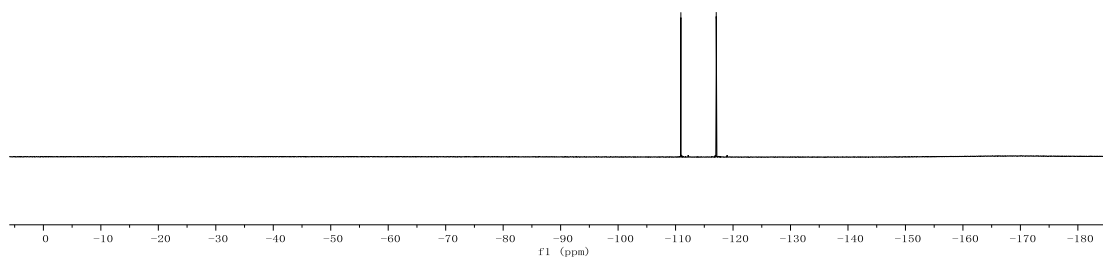


¹³C NMR (100 Mz, CDCl₃) of compound **3i**



^{19}F NMR (376 Mz, CDCl_3) of compound **3i**

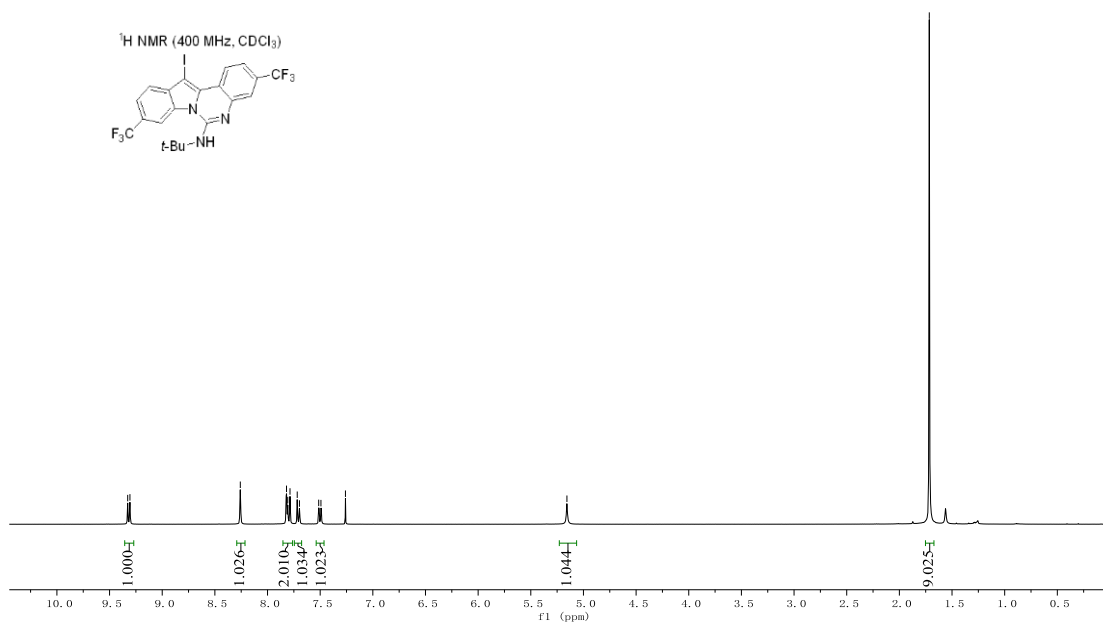
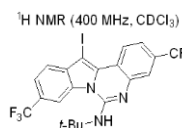
— -110.923
— -117.075



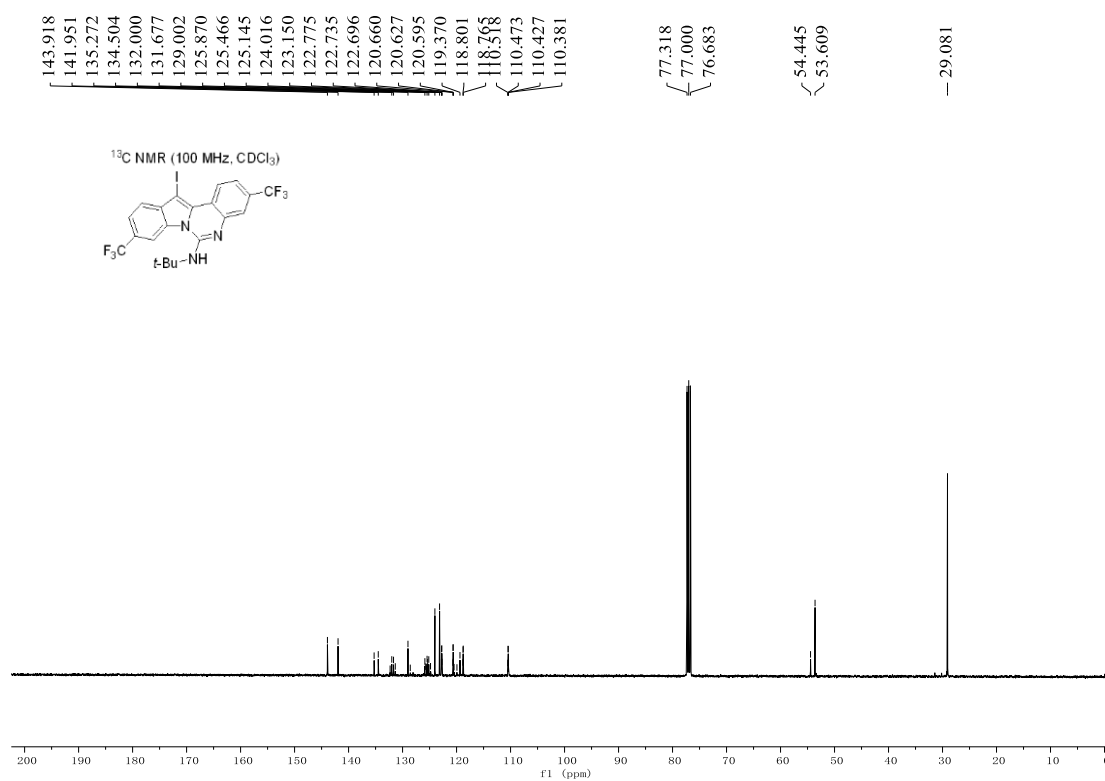
***N*-(*tert*-Butyl)-12-iodo-3,9-bis(trifluoromethyl)indolo[1,2-*c*]quinazolin-6-amine (**3j**)**

^1H NMR (400 MHz, CDCl_3) of compound of **3j**

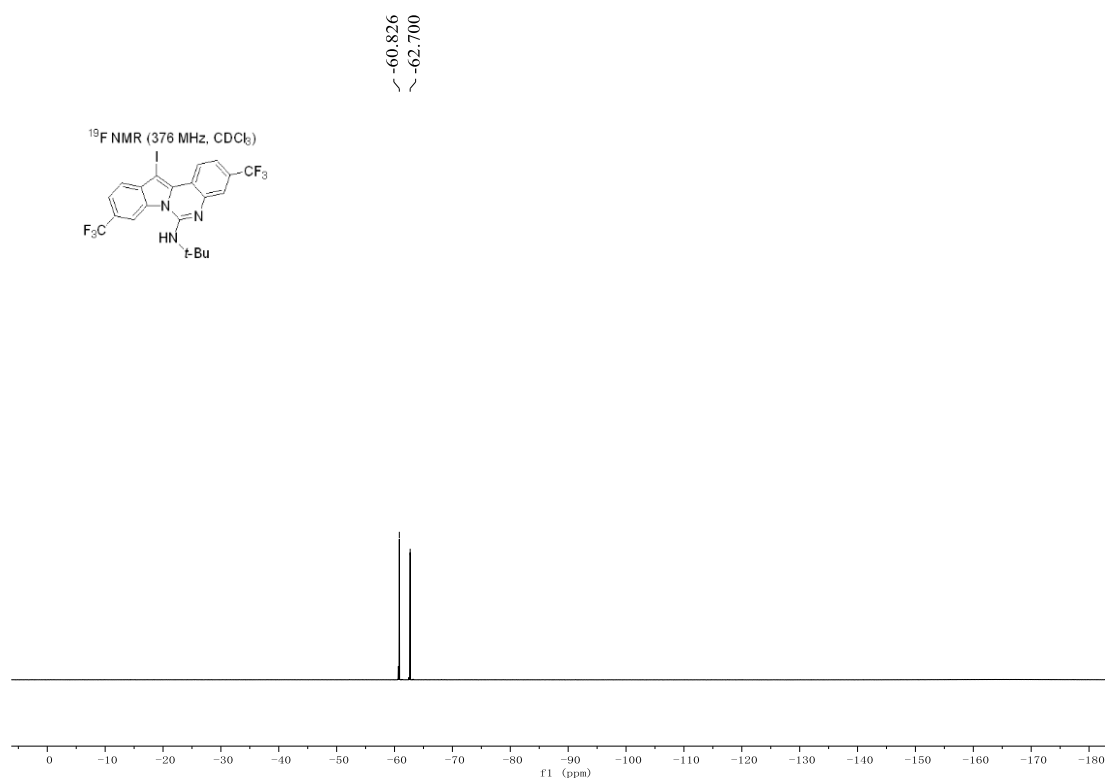
9.328, 9.307, 8.258, 7.820, 7.808, 7.787, 7.718, 7.697, 7.514, 7.493, 7.260, 5.157, 1.716



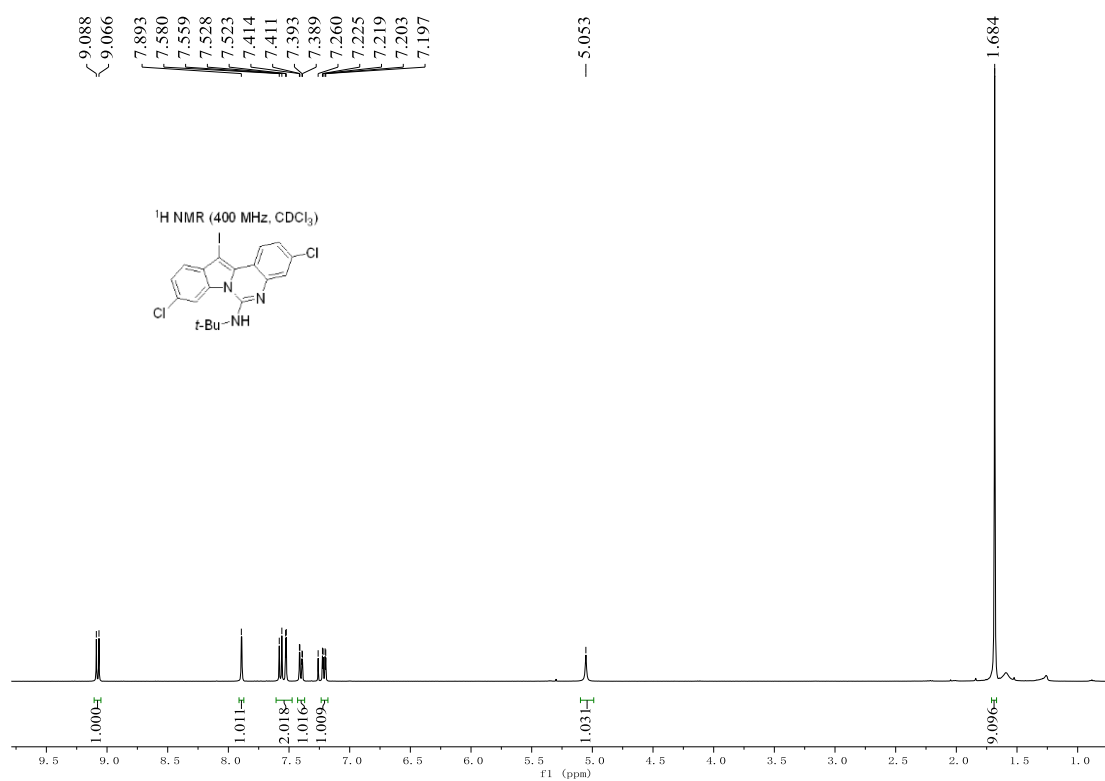
¹³C NMR (100 Mz, CDCl₃) of compound **3j**



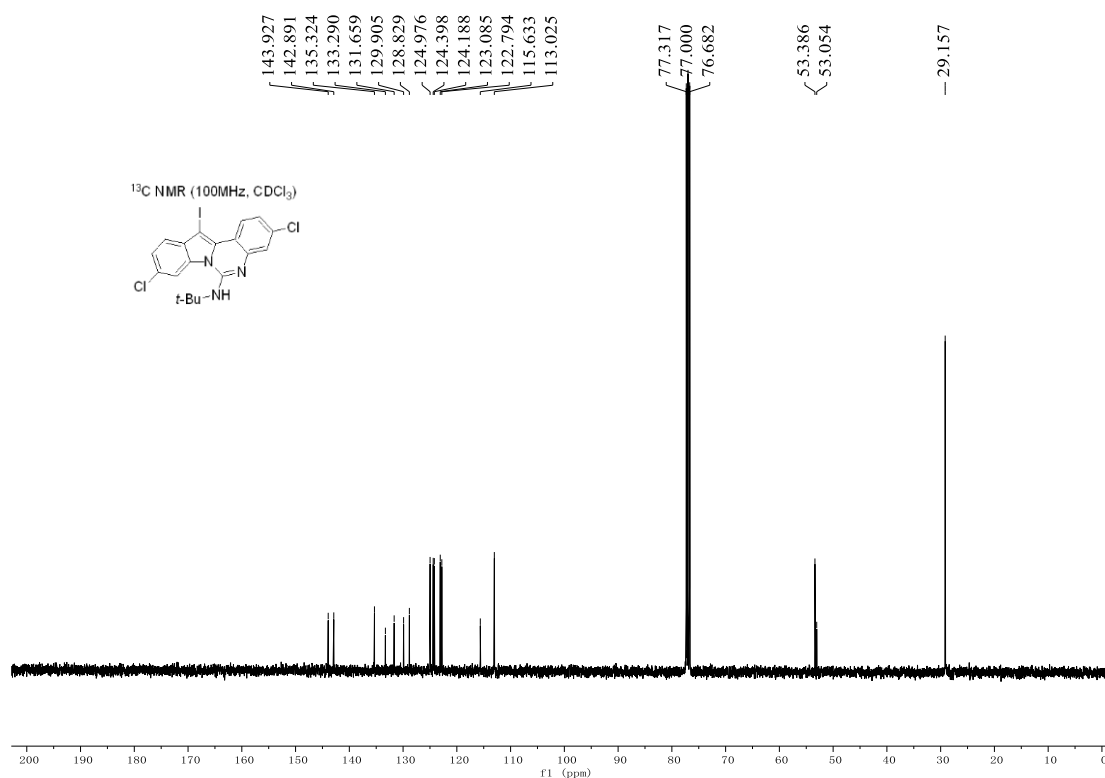
¹⁹F NMR (376 Mz, CDCl₃) of compound **3j**



***N*-(*tert*-Butyl)-3,9-dichloro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3k)**

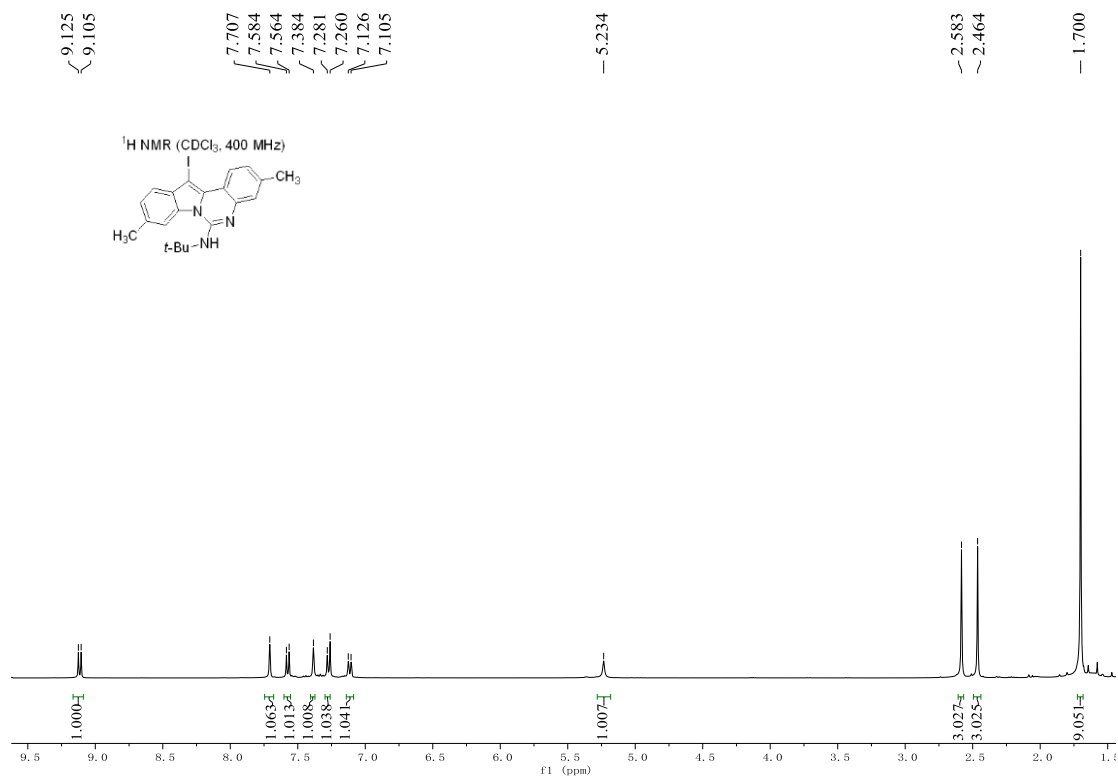


¹³C NMR (100 Mz, CDCl₃) of compound **3k**

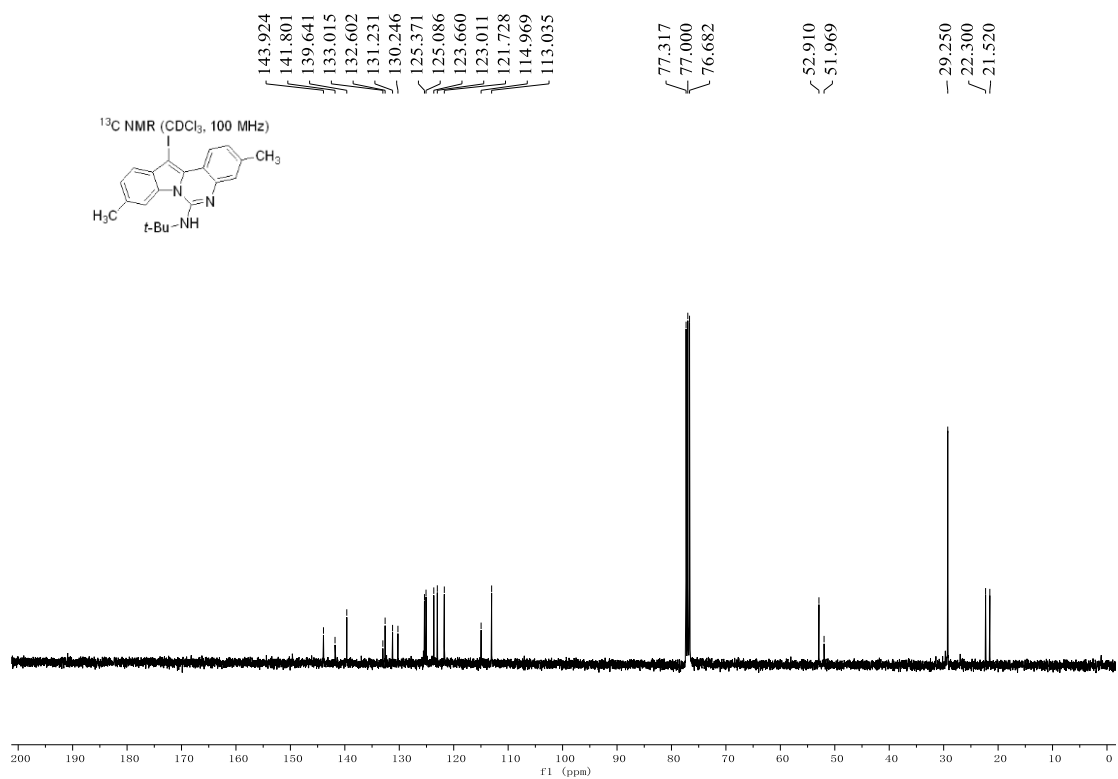


***N*-(*tert*-Butyl)-12-iodo-3,9-dimethylindolo[1,2-*c*]quinazolin-6-amine (31)**

¹H NMR (400 MHz, CDCl₃) of compound of **31**

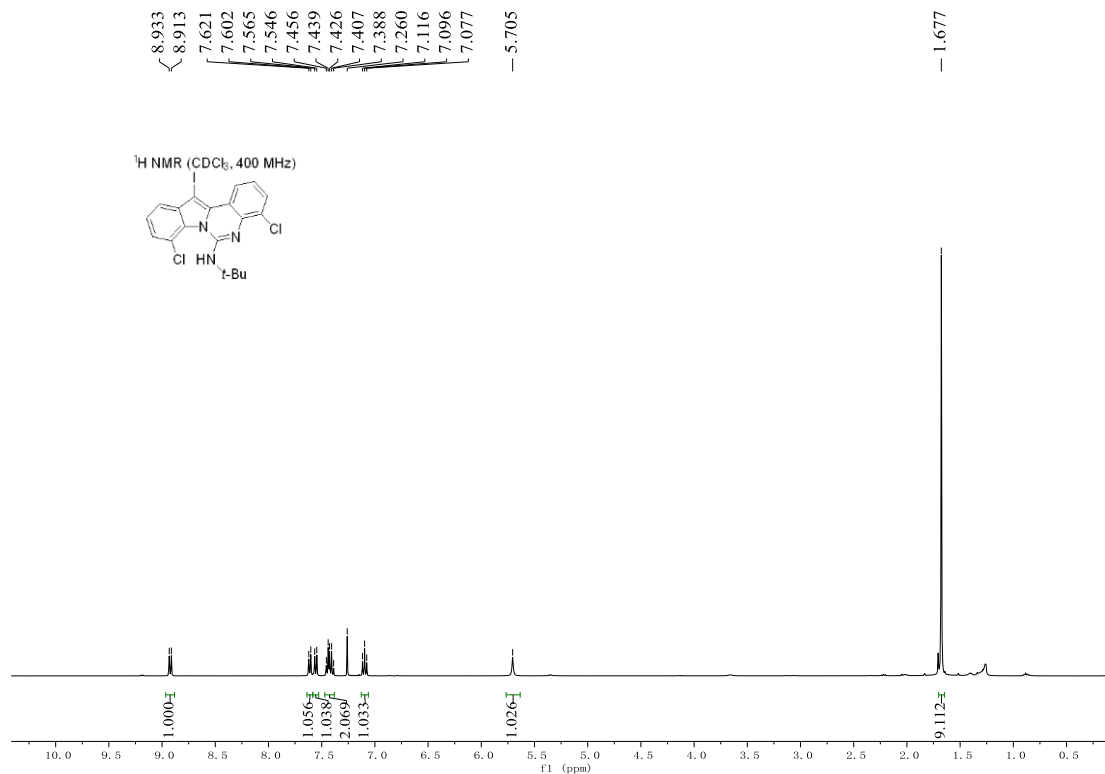


¹³C NMR (100 Mz, CDCl₃) of compound **31**

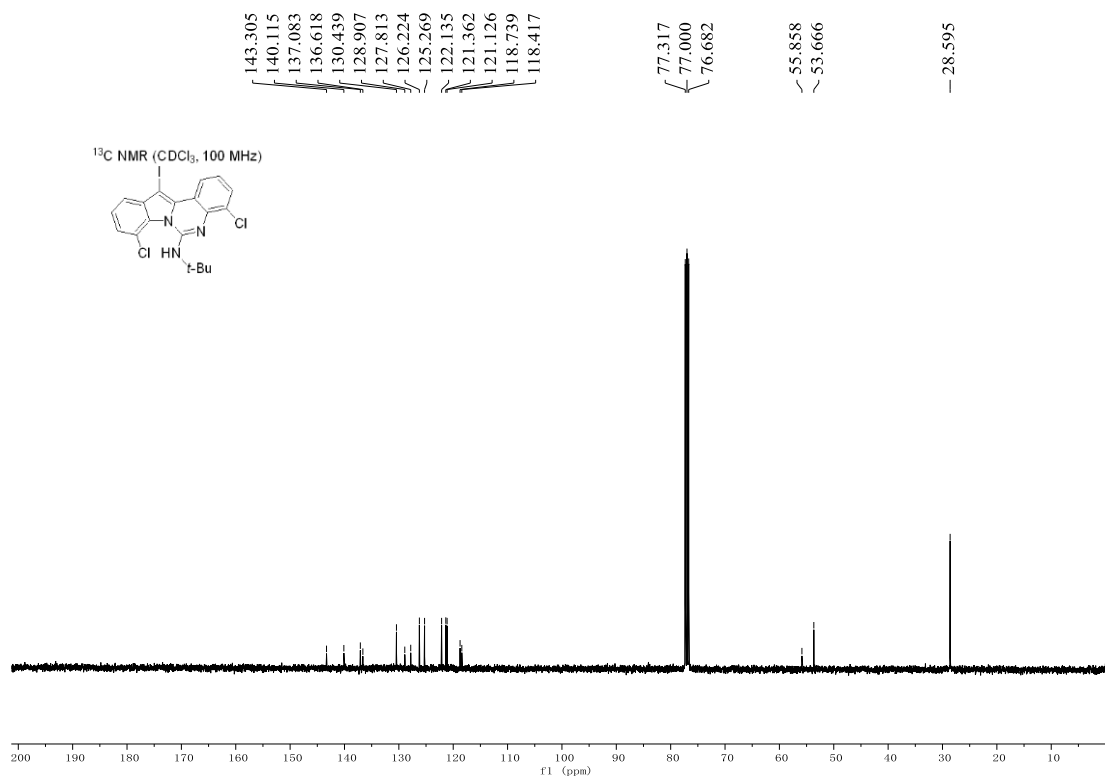


***N*-(*tert*-Butyl)-4,8-dichloro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3m**)**

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

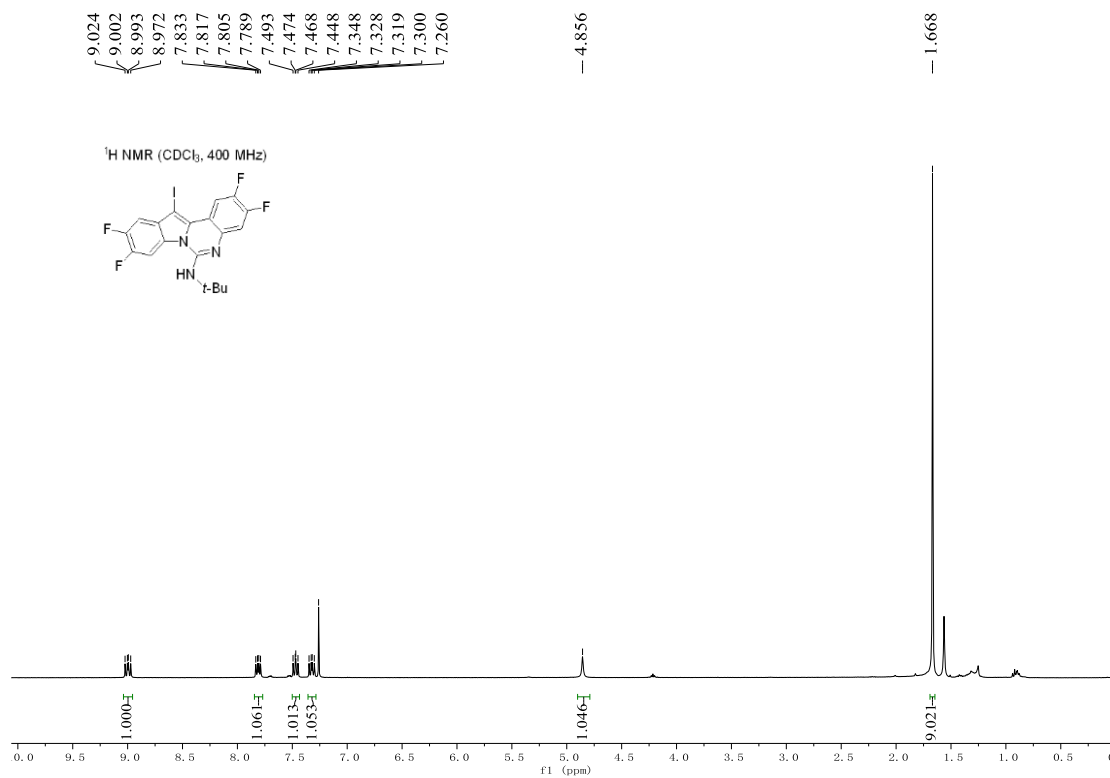


¹³C NMR (100 Mz, CDCl₃) of compound **3m**

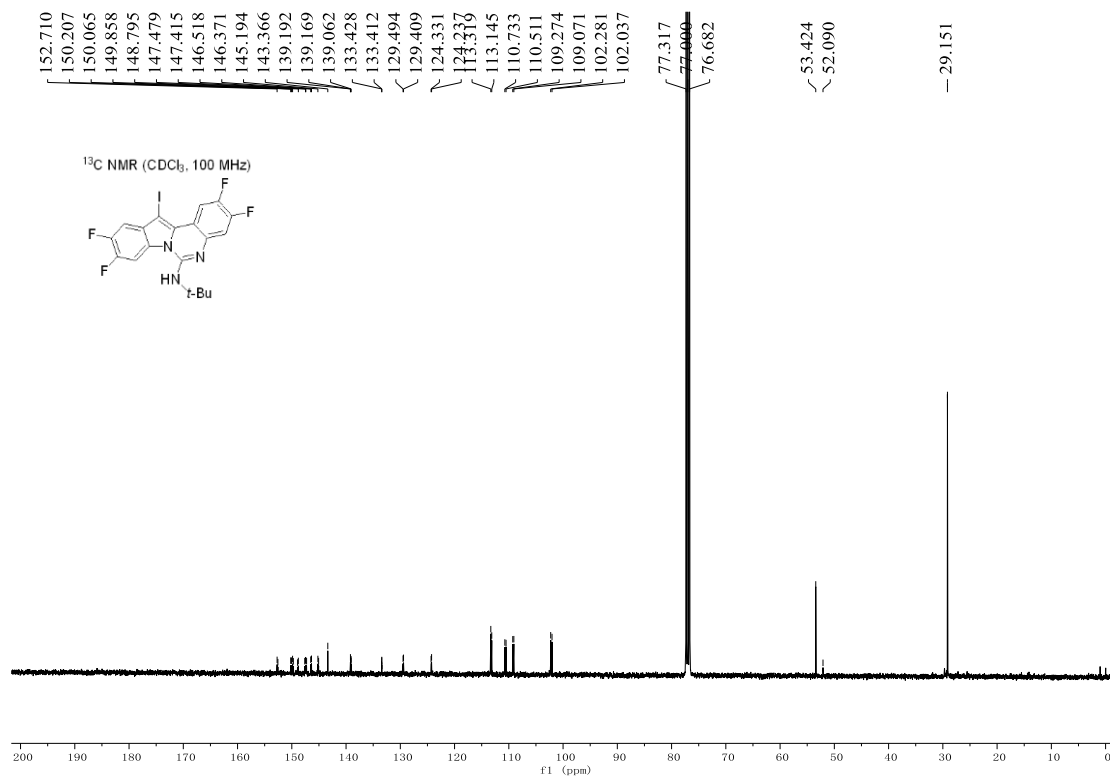


***N*-(*tert*-Butyl)-2,3,9,10-tetrafluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3n)**

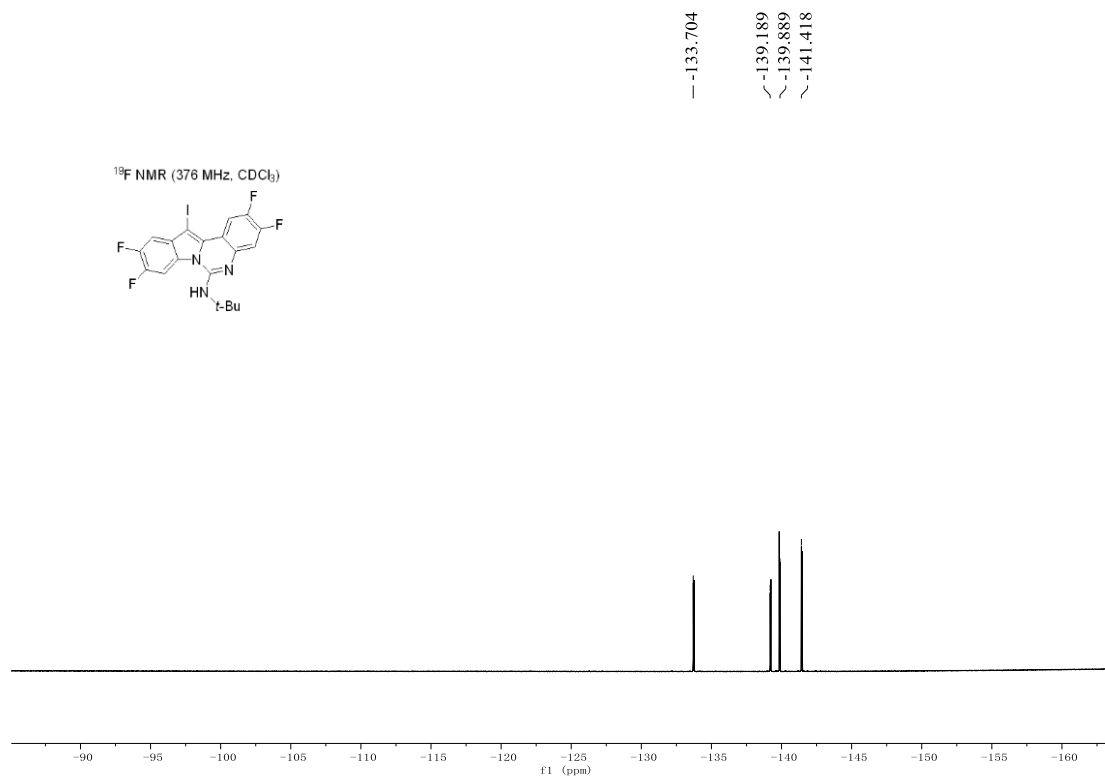
¹H NMR (400 MHz, CDCl₃) of compound of **3n**



¹³C NMR (100 Mz, CDCl₃) of compound **3n**

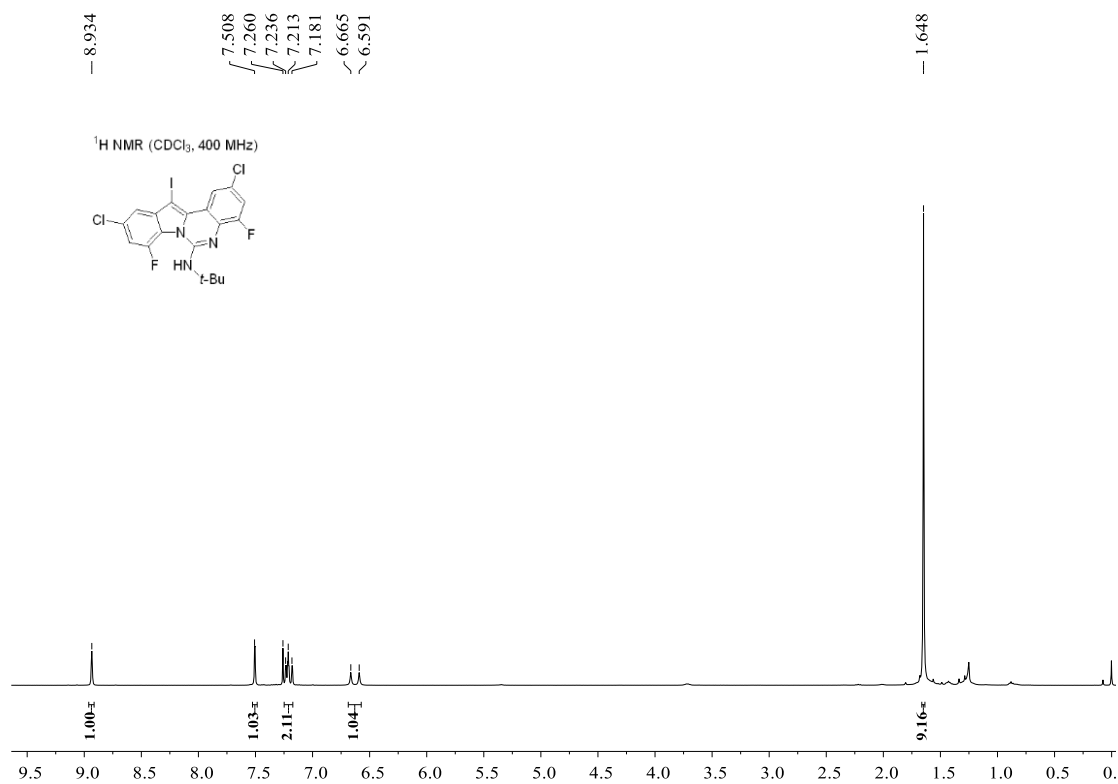


^{19}F NMR (376 Mz, CDCl_3) of compound **3n**

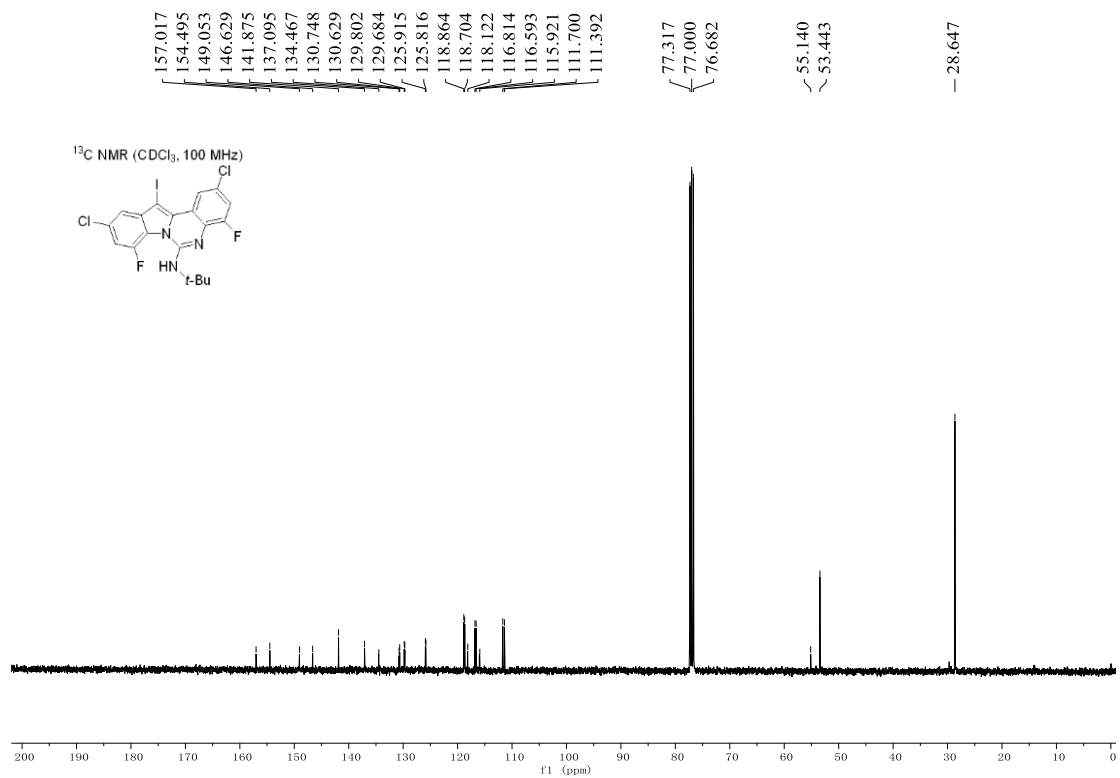


***N*-(*tert*-Butyl)-2,10-dichloro-4,8-difluoro-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3o)**

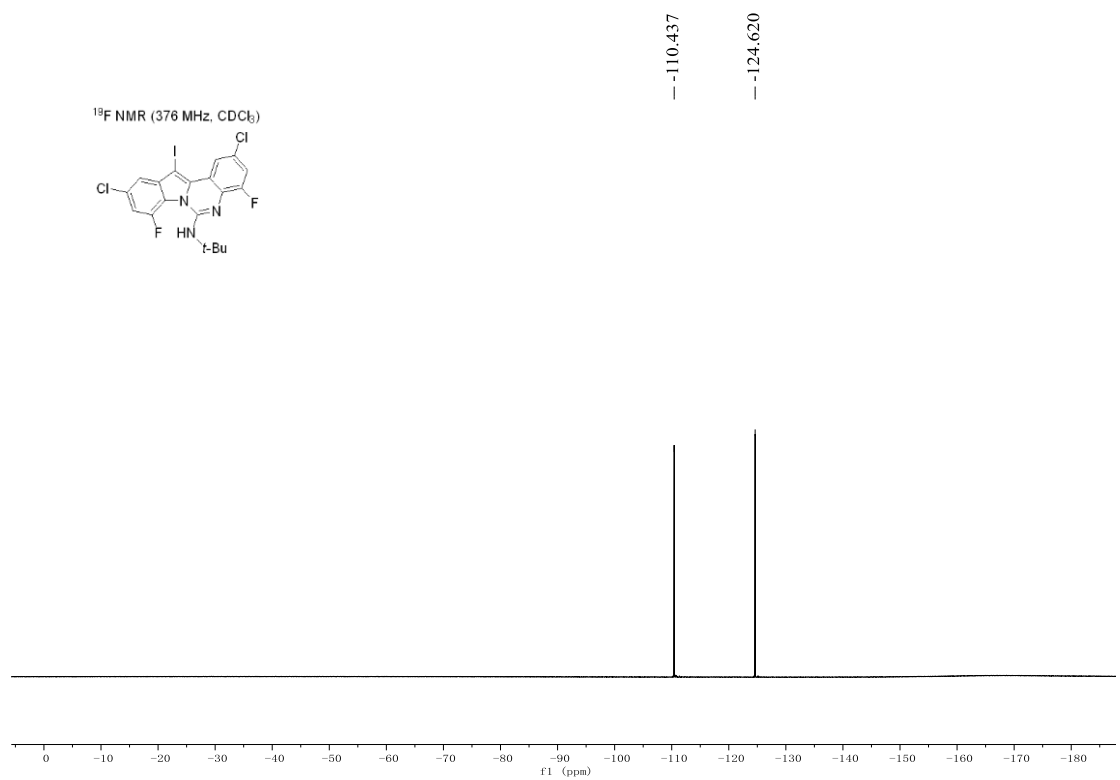
^1H NMR (400 MHz, CDCl_3) of compound of **3o**:



^{13}C NMR (100 Mz, CDCl_3) of compound **3o**:

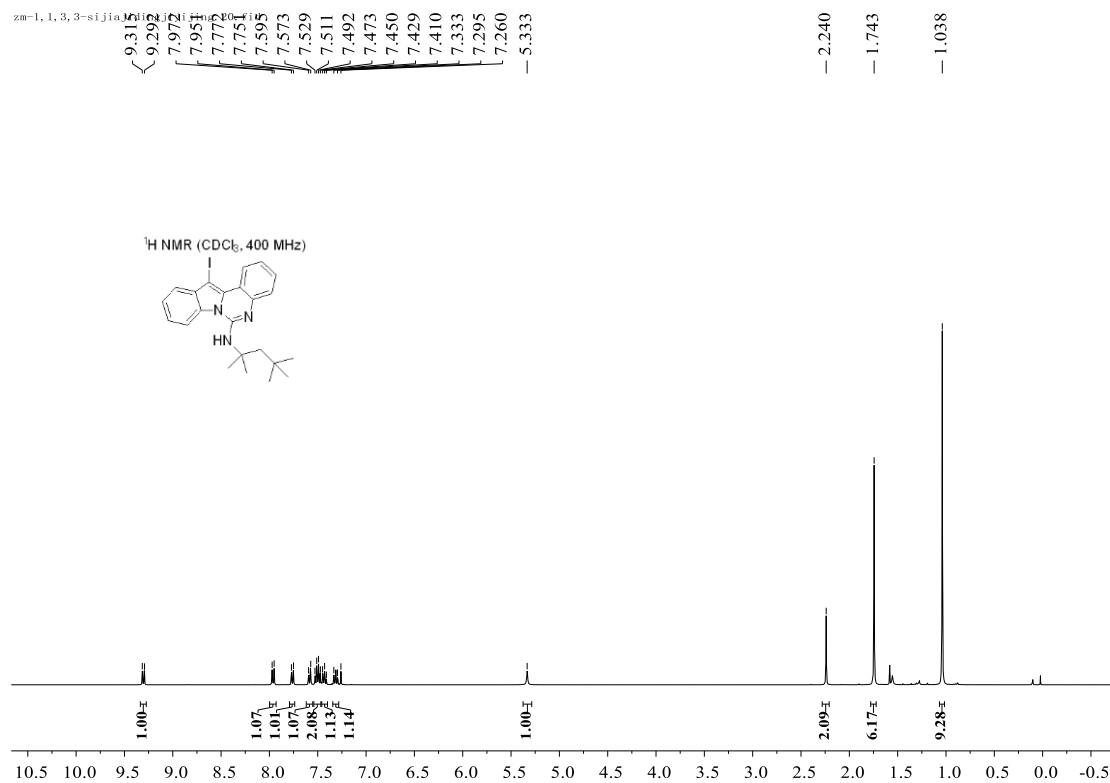


¹⁹F NMR (376 Mz, CDCl₃) of compound **3o**:

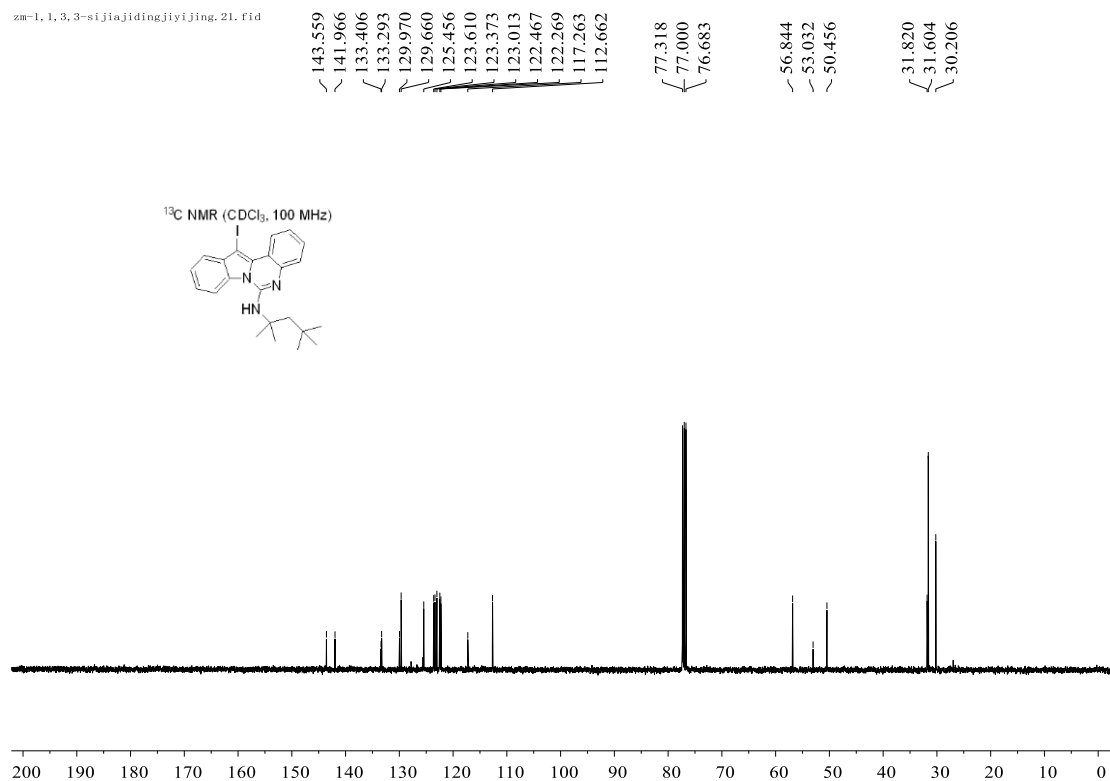


12-Iodo-N-(2,4,4-trimethylpentan-2-yl)indolo[1,2-c]quinazolin-6-amine (3aa)

¹H NMR (400 MHz, CDCl₃) of compound of 3aa

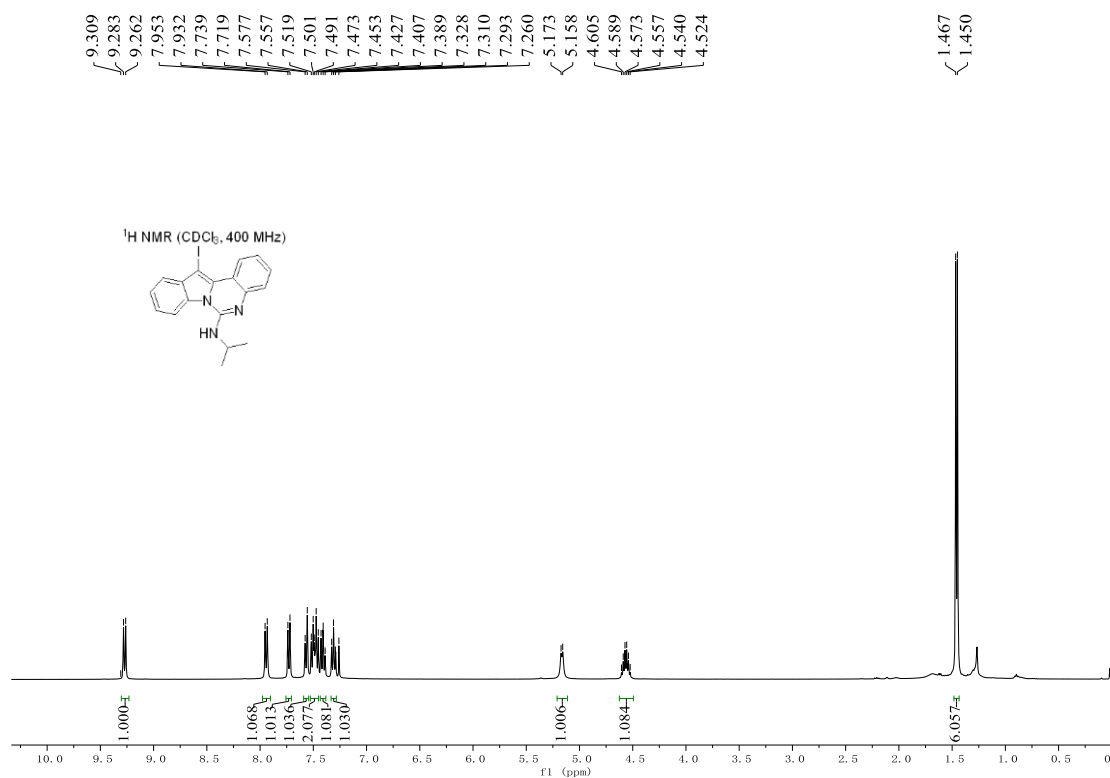


¹³C NMR (100 Mz, CDCl₃) of compound 3aa

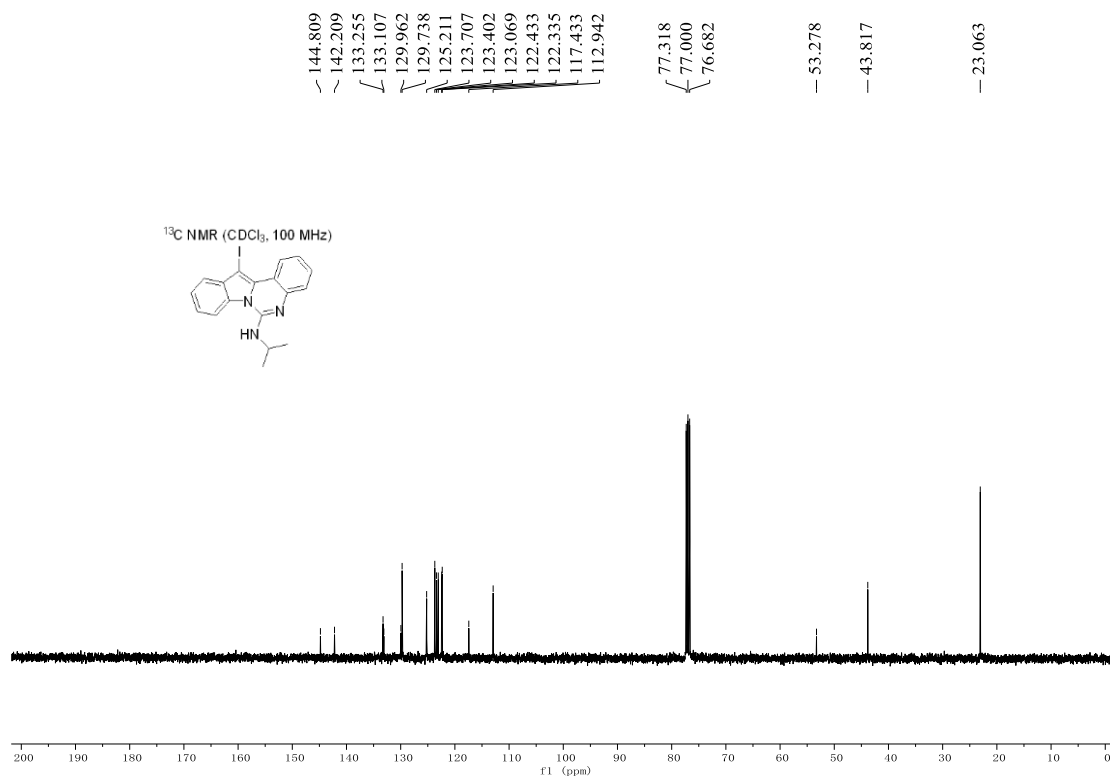


12-Iodo-*N*-isopropylindolo[1,2-*c*]quinazolin-6-amine (3ab)

^1H NMR (400 MHz, CDCl_3) of compound of **3ab**

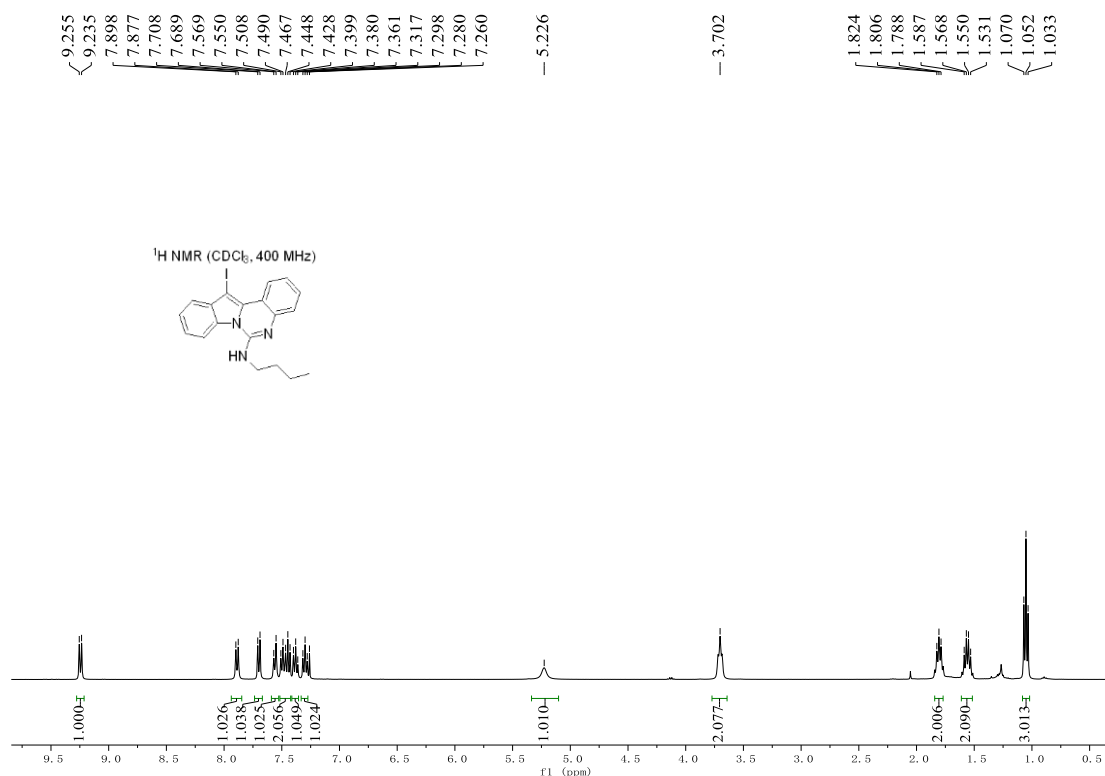


^{13}C NMR (100 Mz, CDCl_3) of compound **3ab**

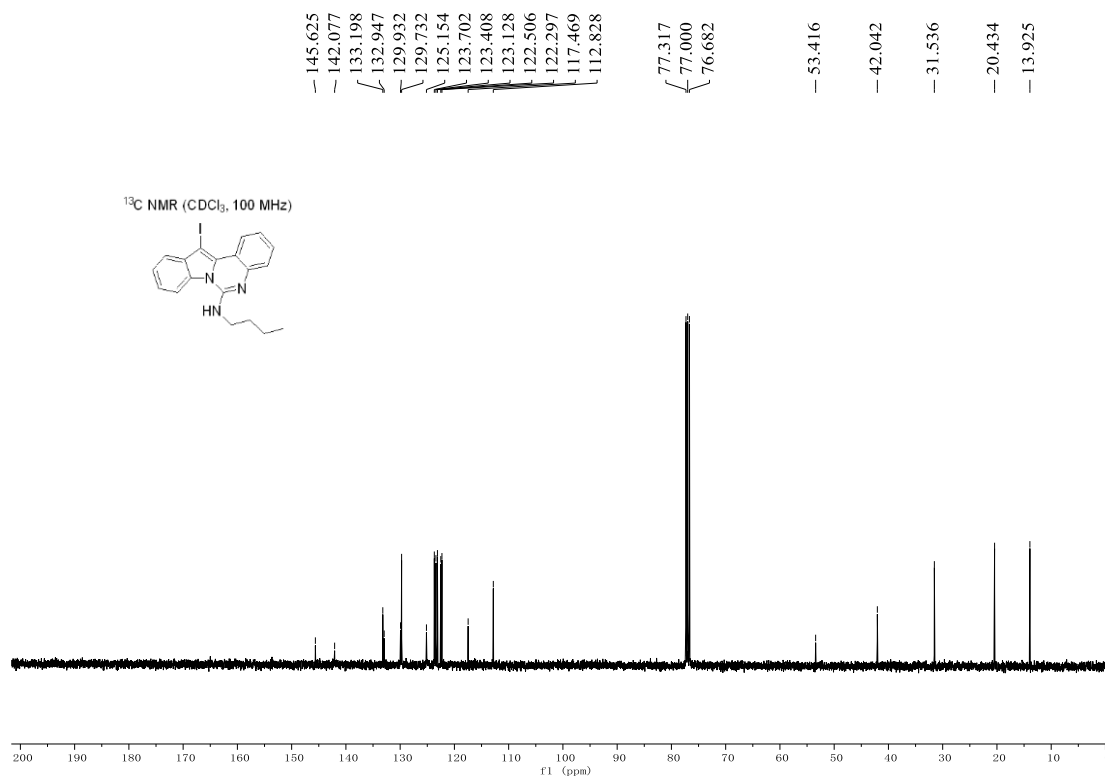


N-Butyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3ac**)

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

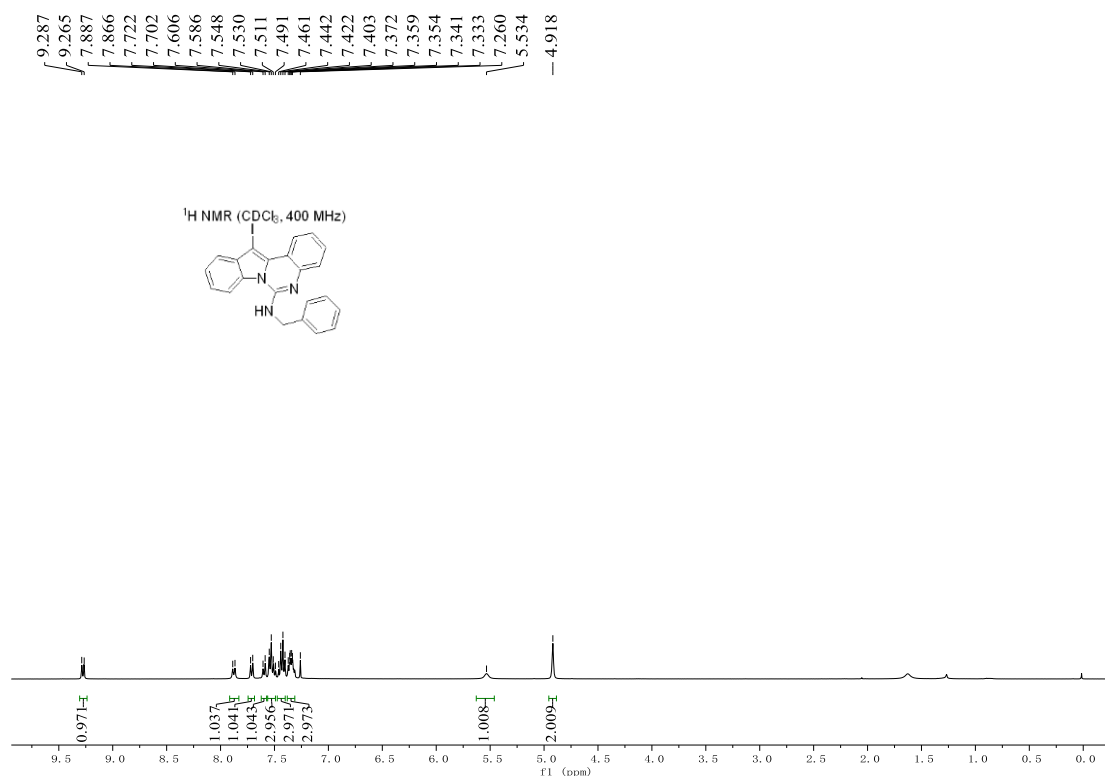


¹³C NMR (100 Mz, CDCl₃) of compound **3ac**

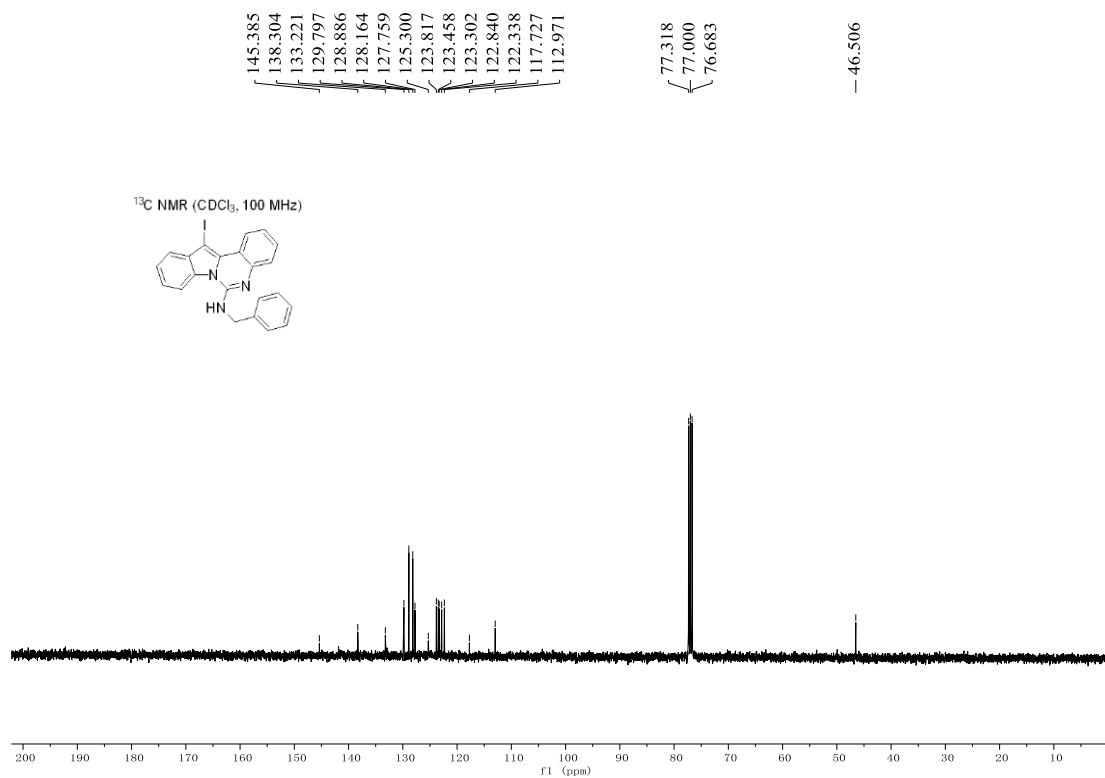


N-Benzyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3ad**)

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

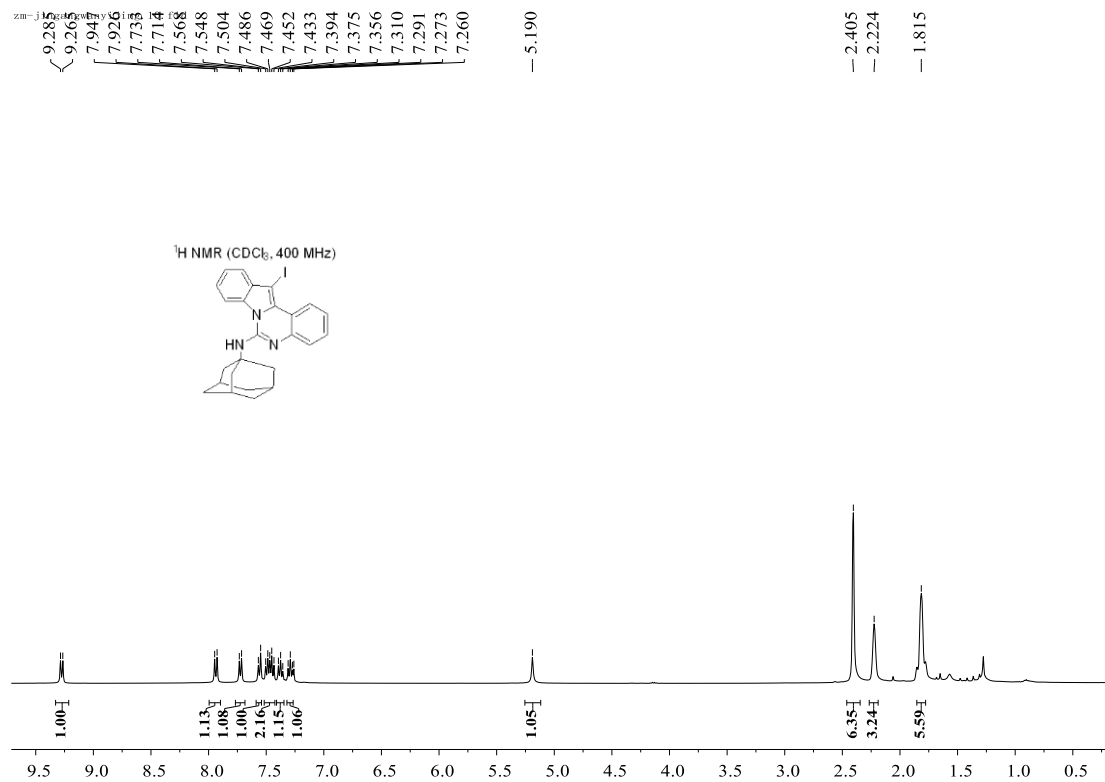


¹³C NMR (100 Mz, CDCl₃) of compound **3ad**

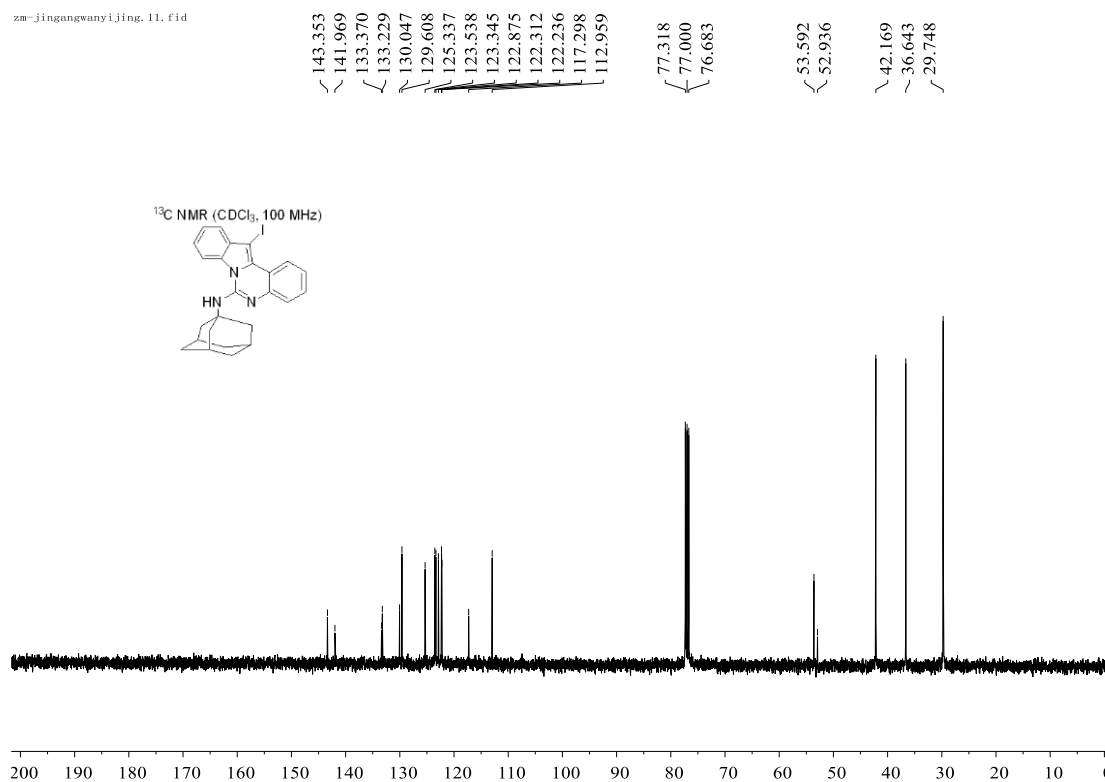


***N*-((3*s*,5*s*,7*s*)-Adamantan-1-yl)-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3ae)**

¹H NMR (400 MHz, CDCl₃) of compound of 3ae

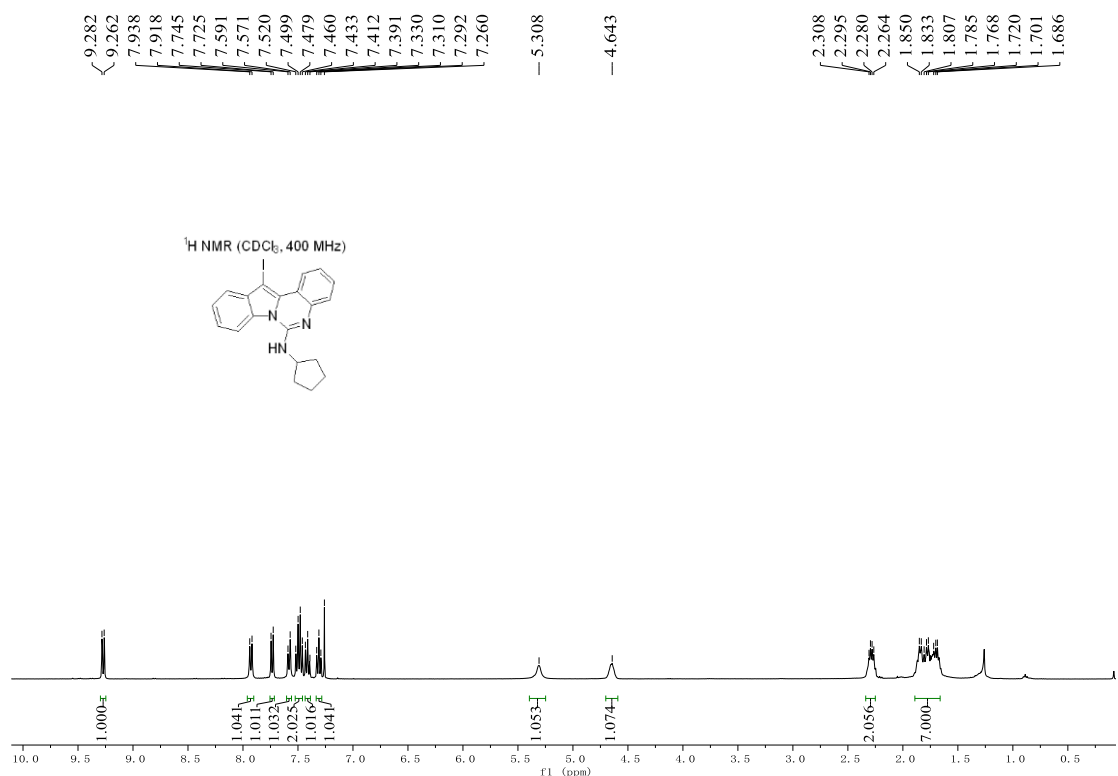


¹³C NMR (100 Mz, CDCl₃) of compound 3ae

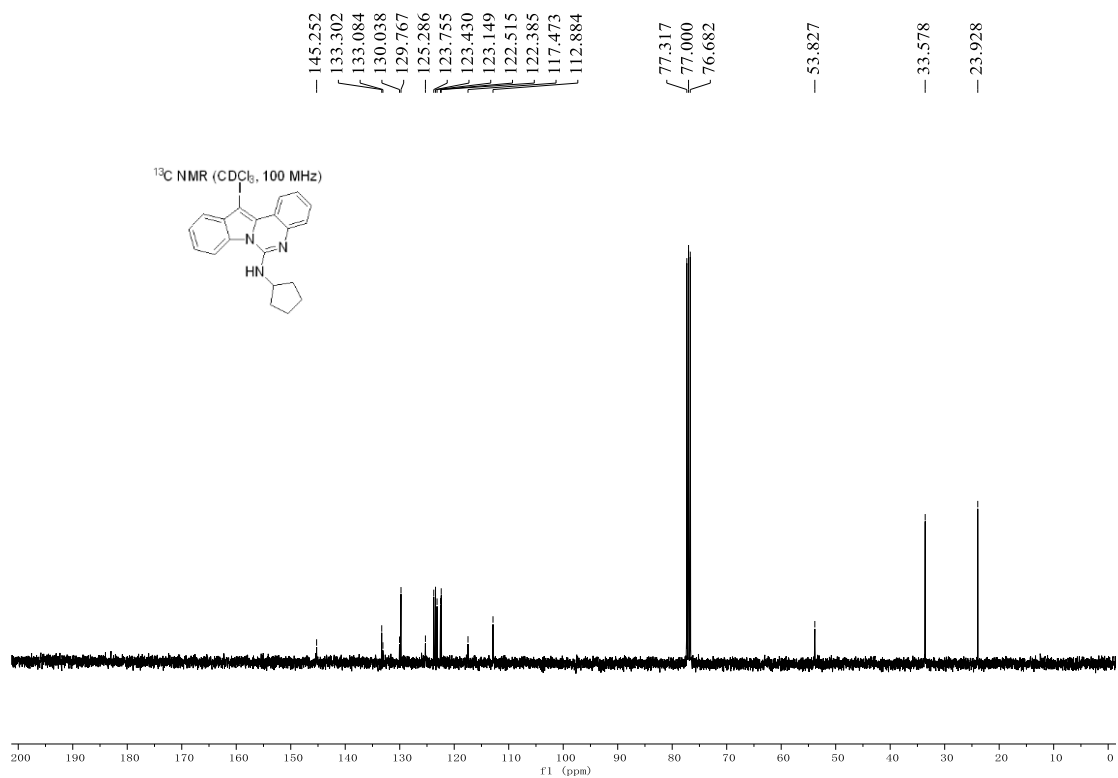


N-Cyclopentyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (3af)

¹H NMR (400 MHz, CDCl₃) of compound of 3af

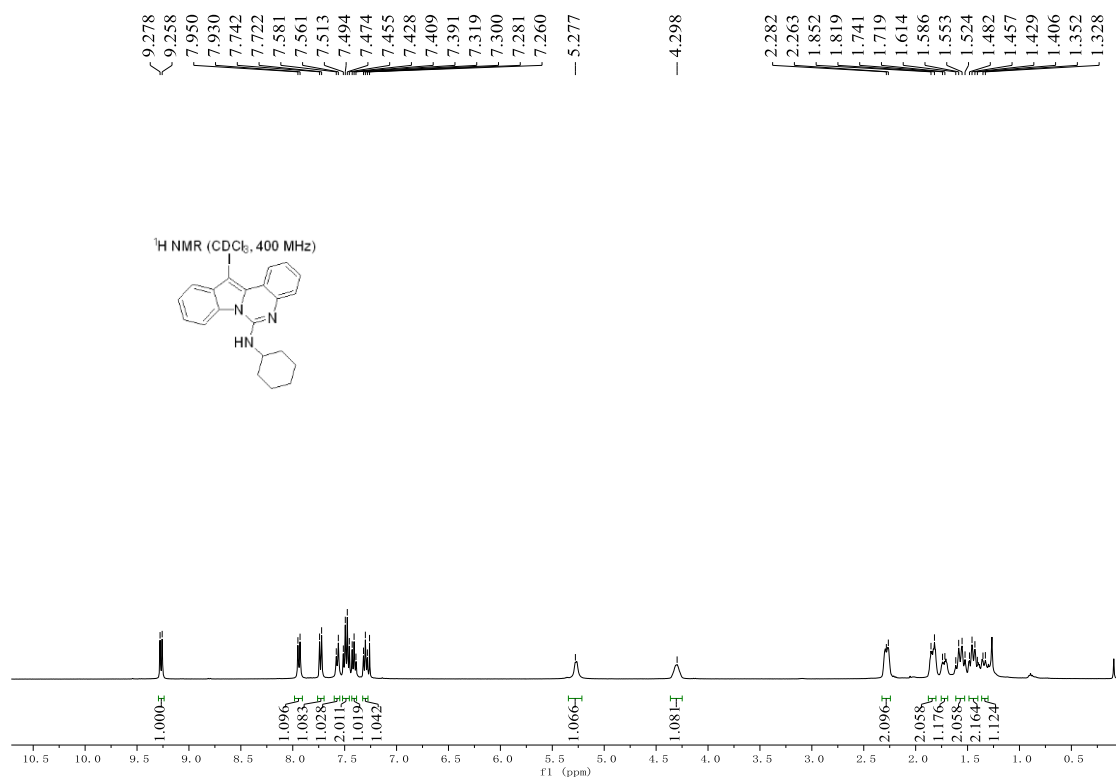


¹³C NMR (100 Mz, CDCl₃) of compound 3af

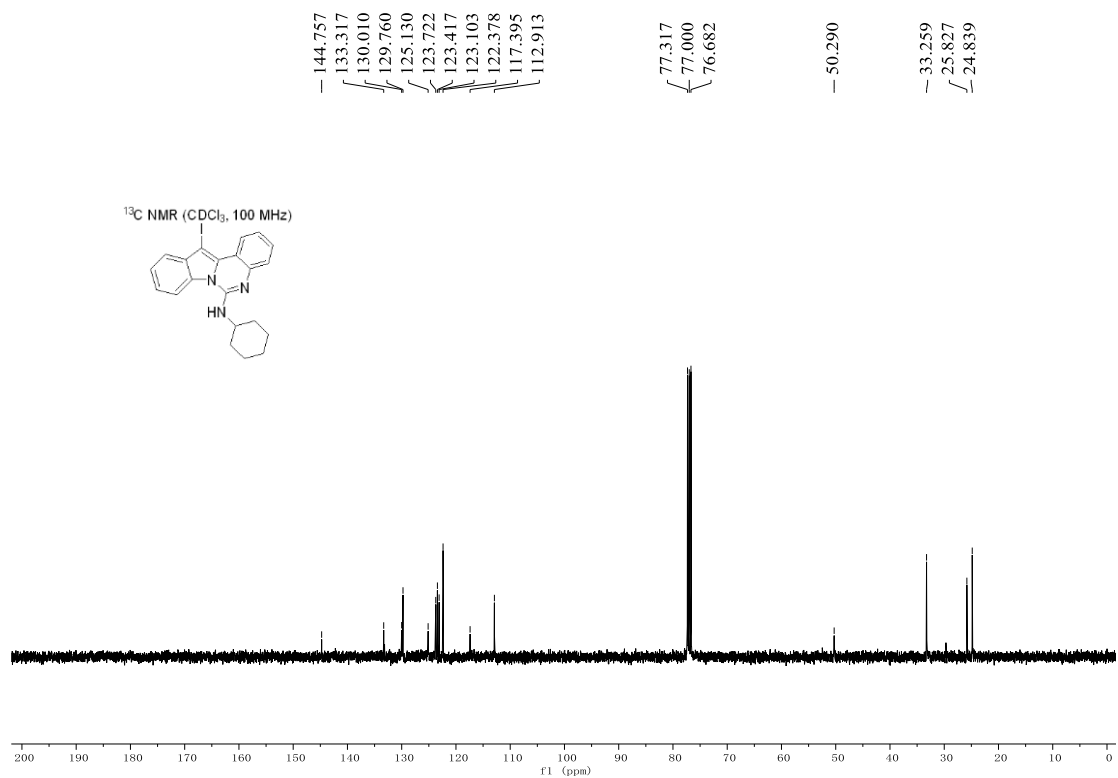


N-Cyclohexyl-12-iodoindolo[1,2-*c*]quinazolin-6-amine (**3ag**)

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

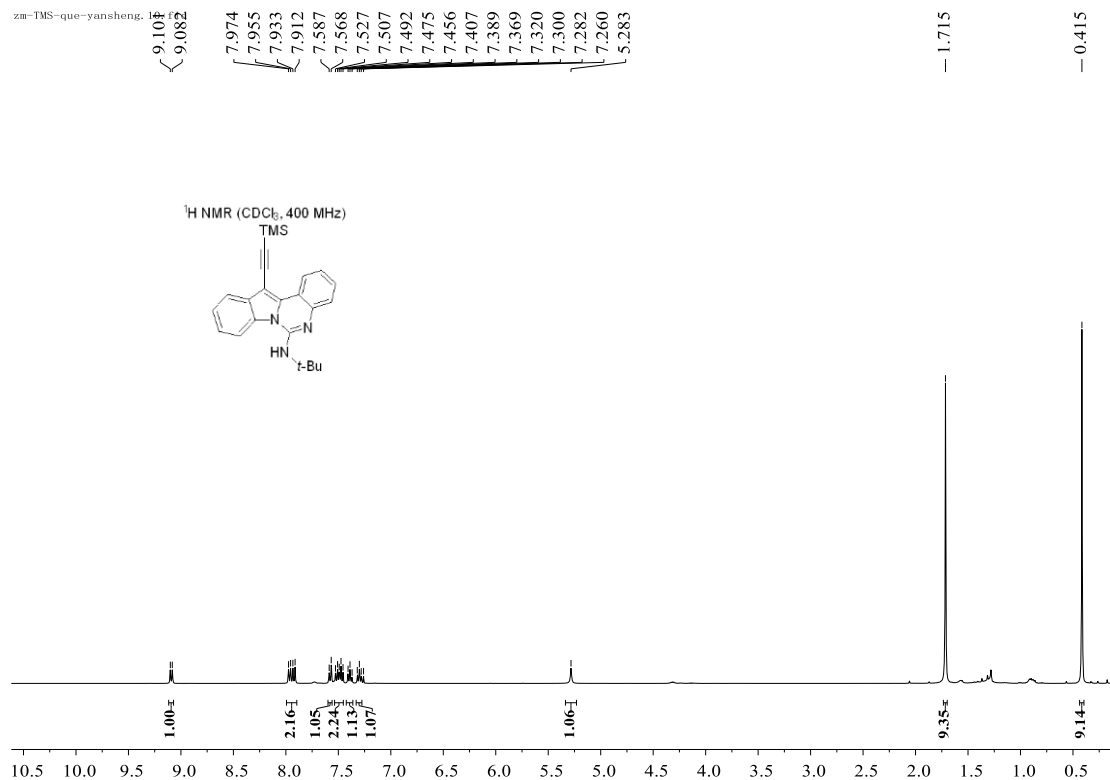


¹³C NMR (100 Mz, CDCl₃) of compound **3ag**

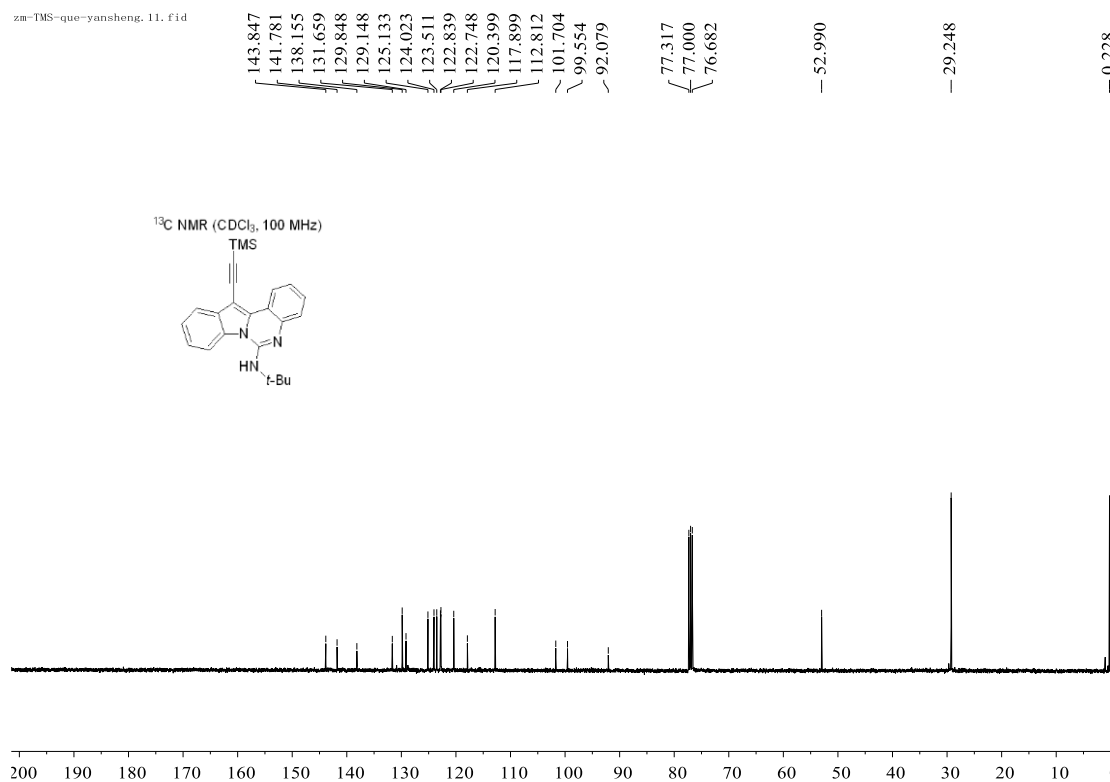


***N*-(*tert*-Butyl)-12-((trimethylsilyl)ethynyl)indolo[1,2-*c*]quinazolin-6-amine (4)**

¹H NMR (400 MHz, CDCl₃) of compound of 4

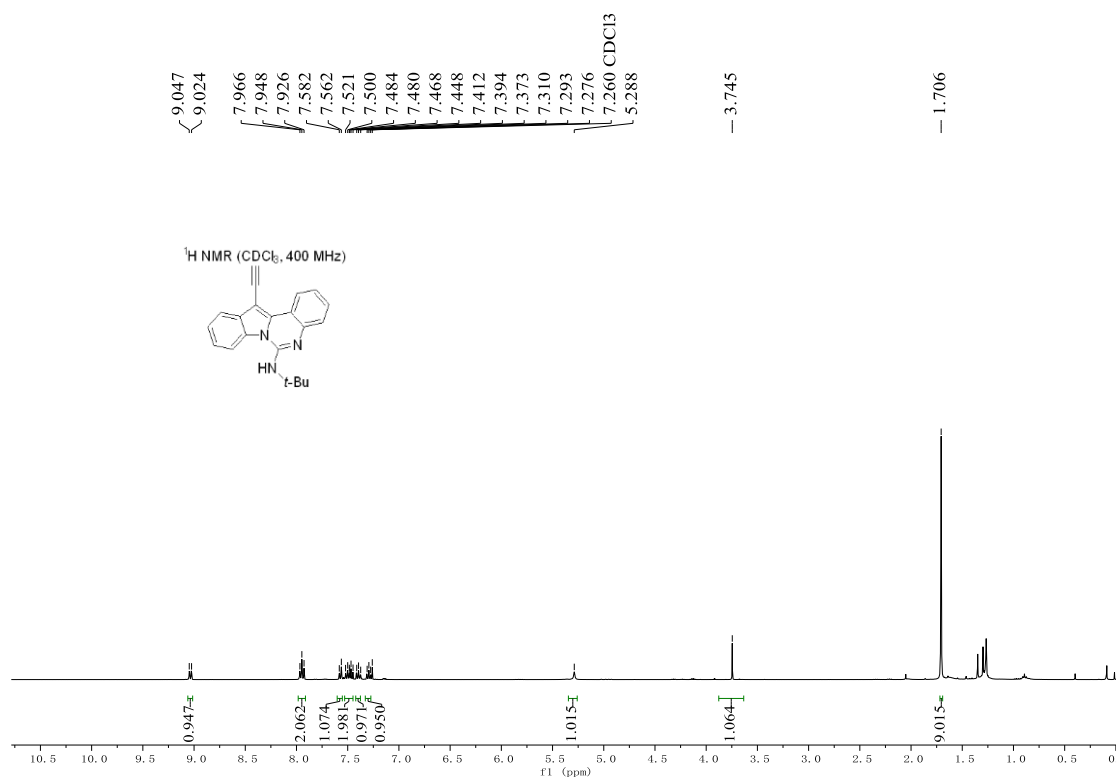


¹³C NMR (100 Mz, CDCl₃) of compound 4

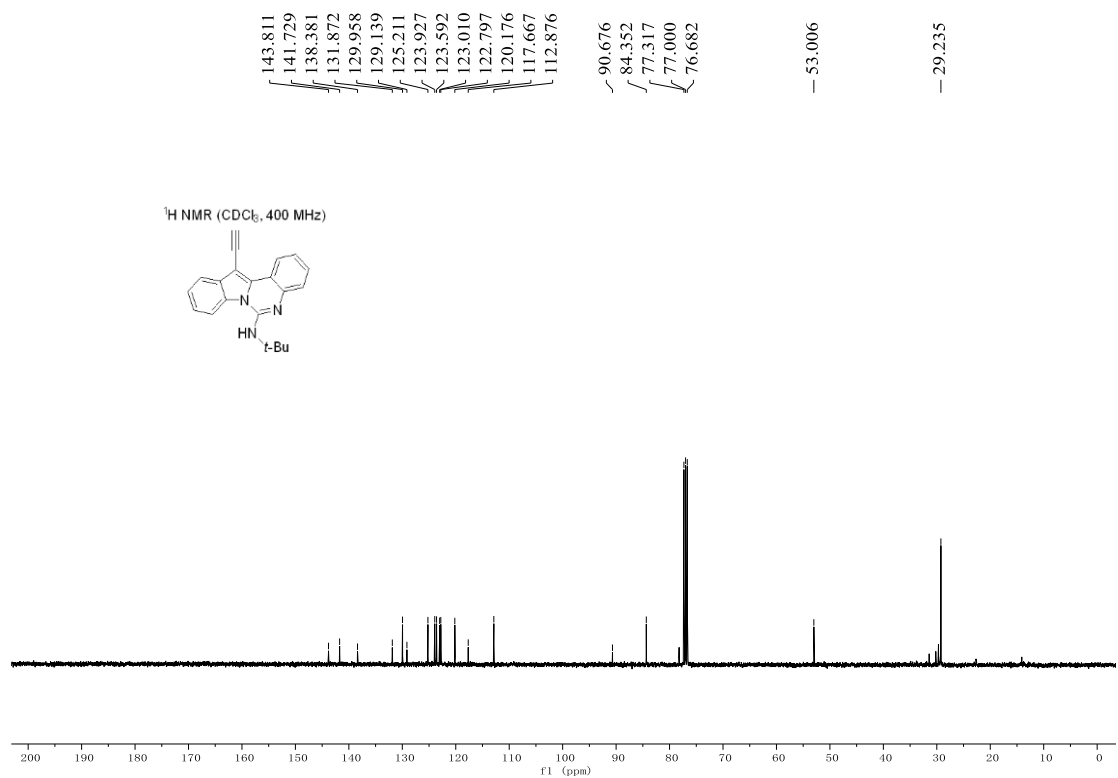


***N*-(*tert*-Butyl)-12-ethynylindolo[1,2-*c*]quinazolin-6-amine (5)**

¹H NMR (400 MHz, CDCl₃) of compound of 5



¹³C NMR (100 Mz, CDCl₃) of compound 5



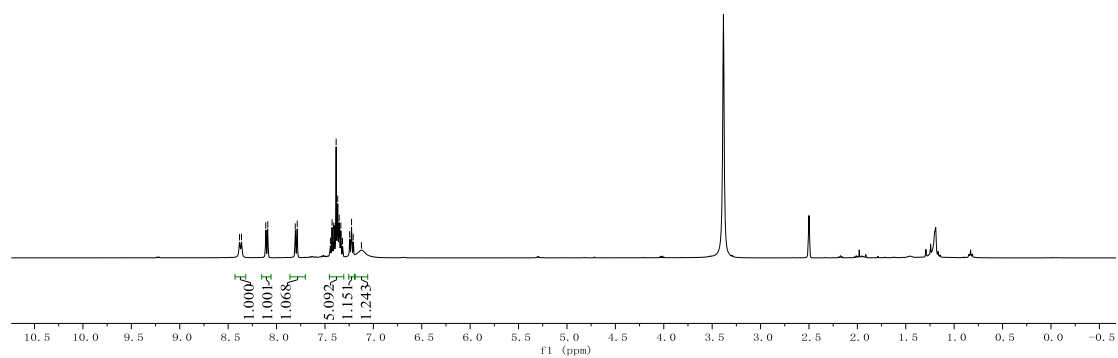
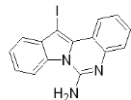
12-Iodoindolo[1,2-c]quinazolin-6-amine (6)

$^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) of compound of 6

8.382
8.362
8.111
8.090
7.807
7.787
7.443
7.426
7.409
7.384
7.368
7.353
7.336
7.318
7.245
7.225
7.208
7.123

— 2.495

$^1\text{H NMR}$ (CDCl_3 , 400 MHz)



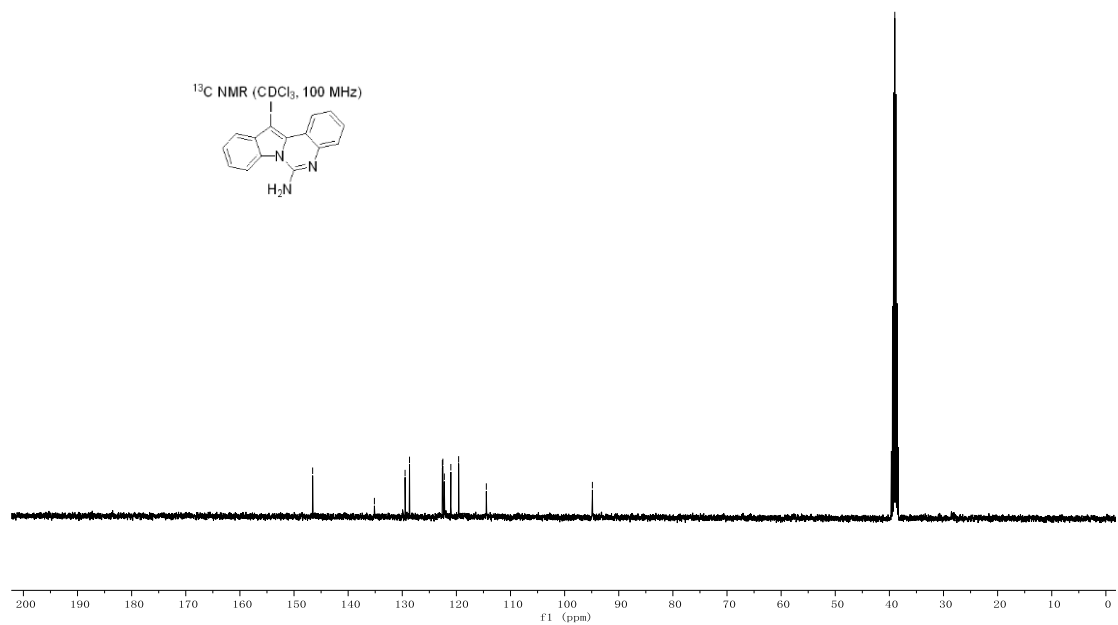
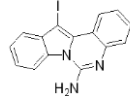
$^{13}\text{C NMR}$ (100 Mz, $\text{DMSO-}d_6$) of compound 6

146.559
135.147
129.481
128.660
122.594
122.498
122.228
121.025
119.585
114.467

— 94.869

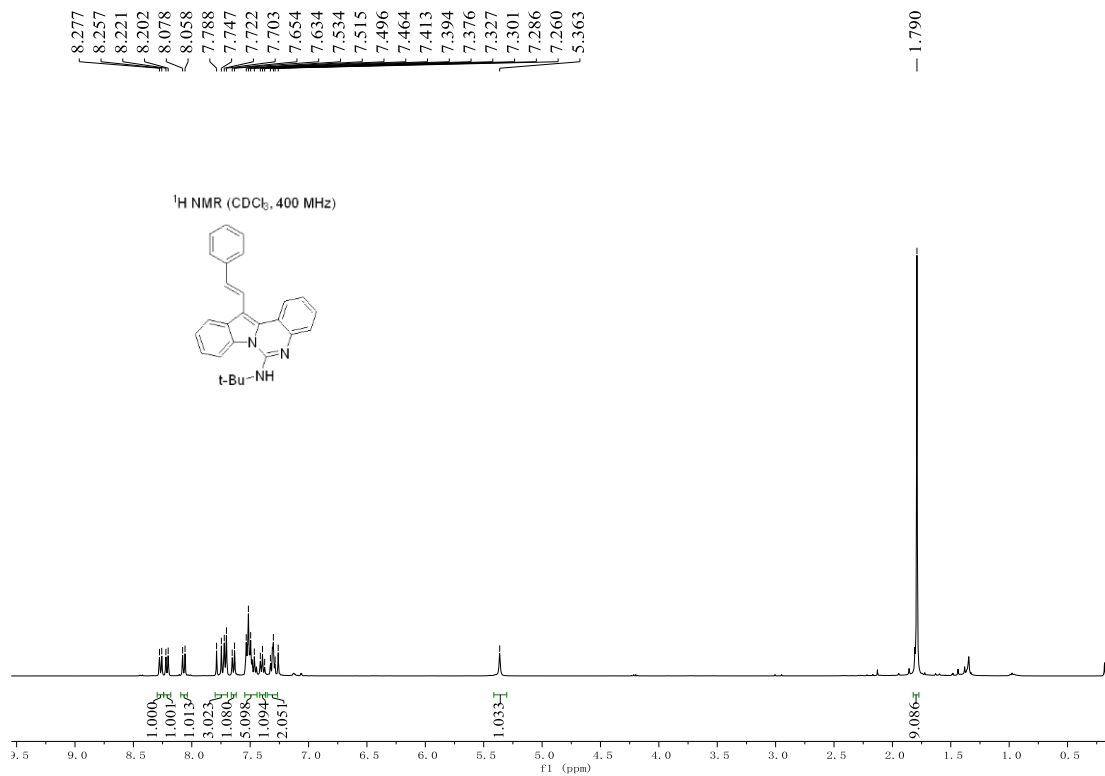
— 39.000

$^{13}\text{C NMR}$ (CDCl_3 , 100 MHz)

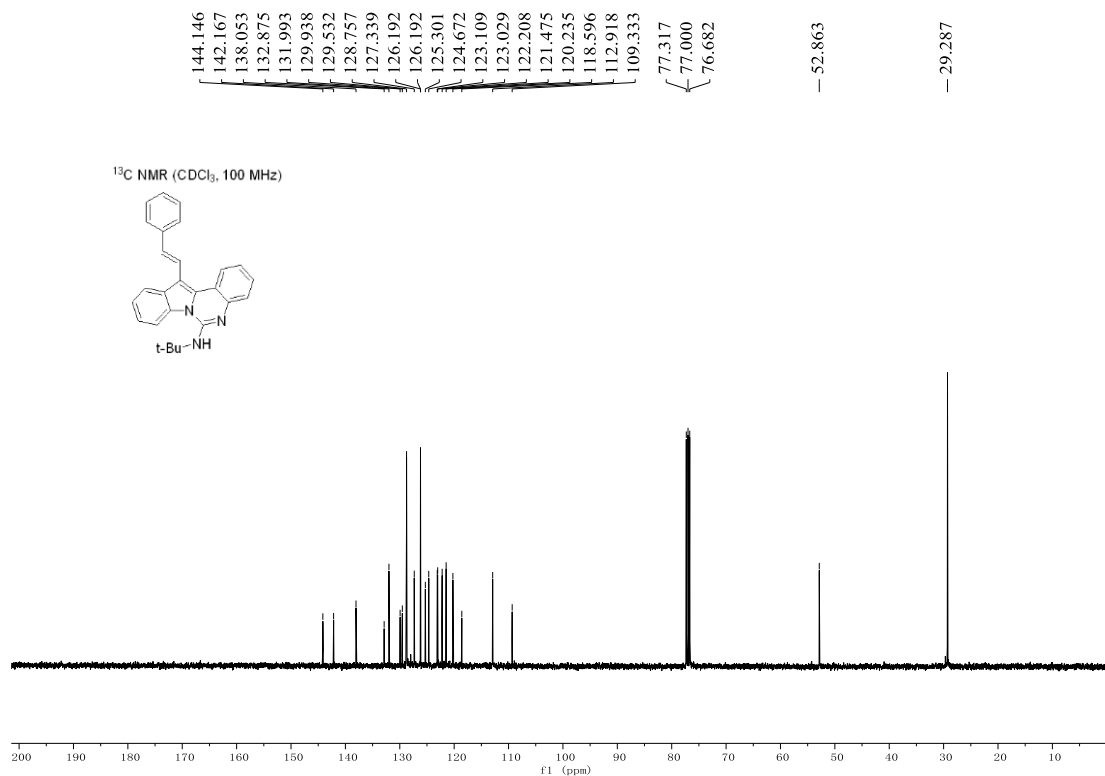


(E)-N-(tert-Butyl)-12-styrylindolo[1,2-c]quinazolin-6-amine (7)

¹H NMR (400 MHz, CDCl₃) of compound of 7

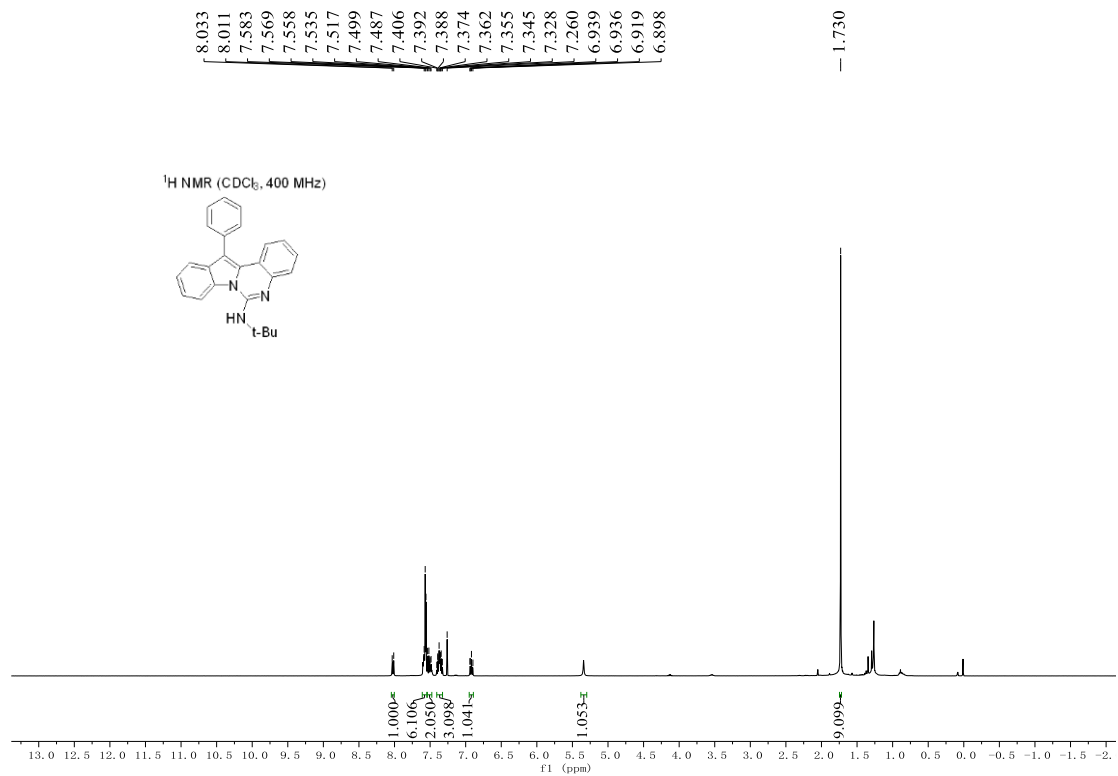


¹³C NMR (100 Mz, CDCl₃) of compound 7

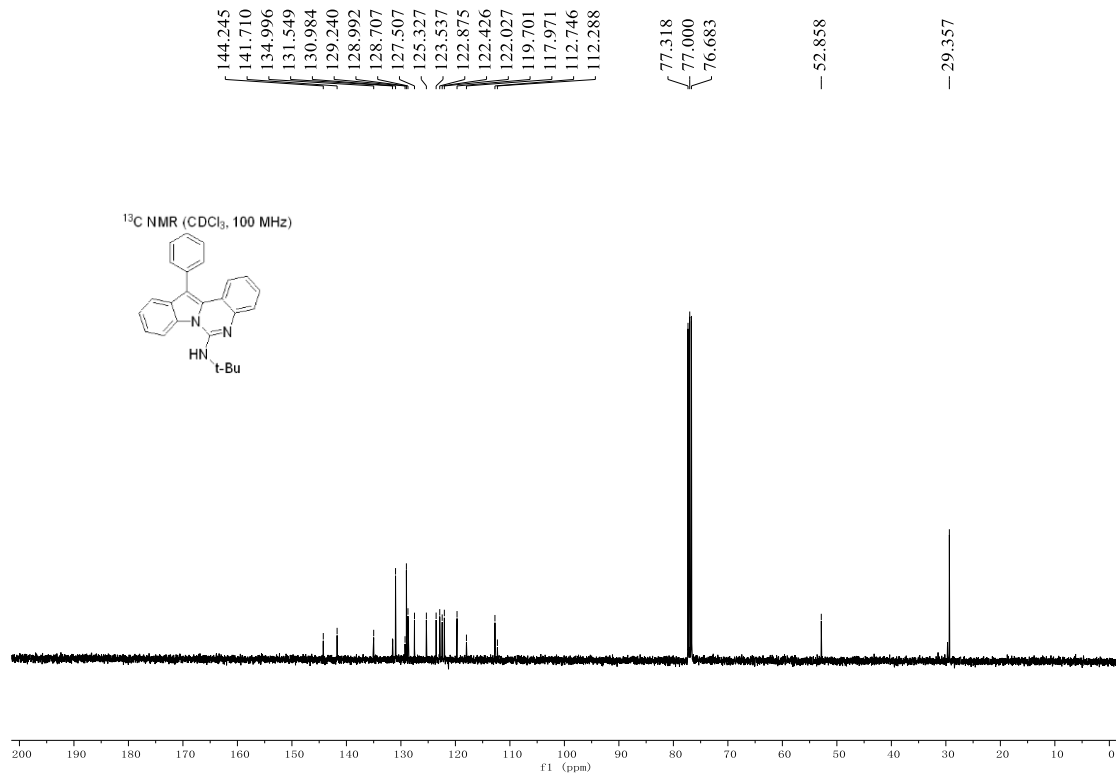


***N*-(*tert*-Butyl)-12-phenylindolo[1,2-*c*]quinazolin-6-amine (8)**

¹H NMR (400 MHz, CDCl₃) of compound **8**

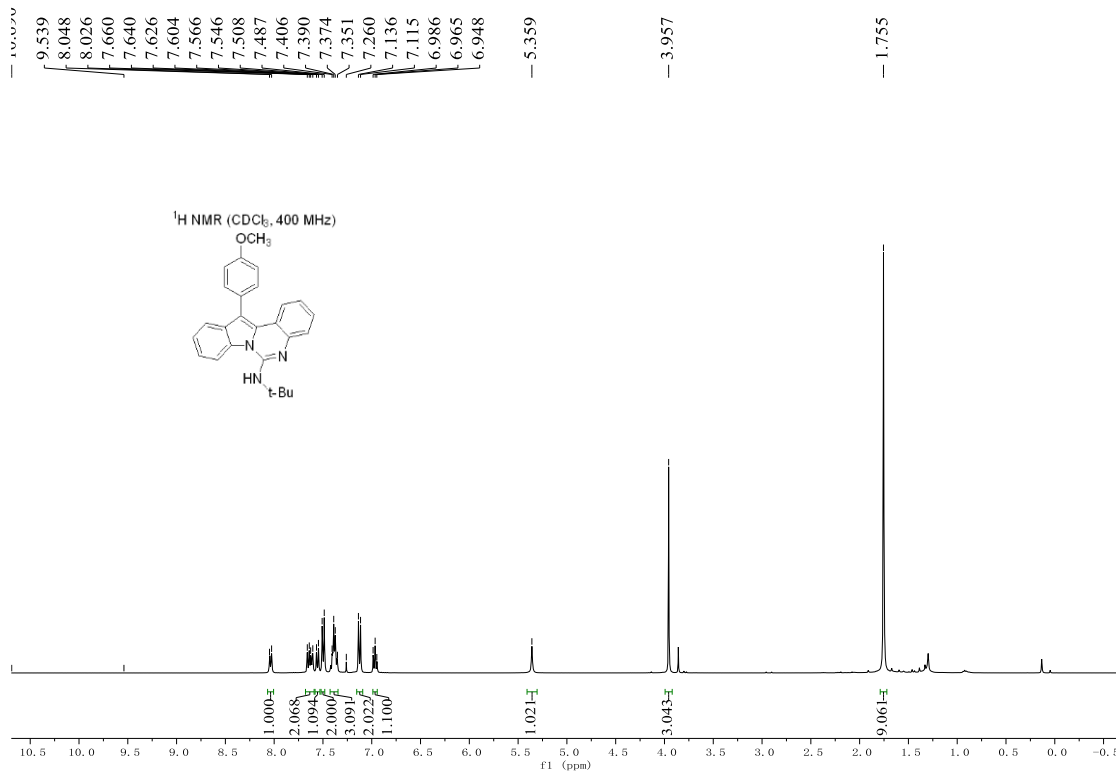


¹³C NMR (100 Mz, CDCl₃) of compound **8**

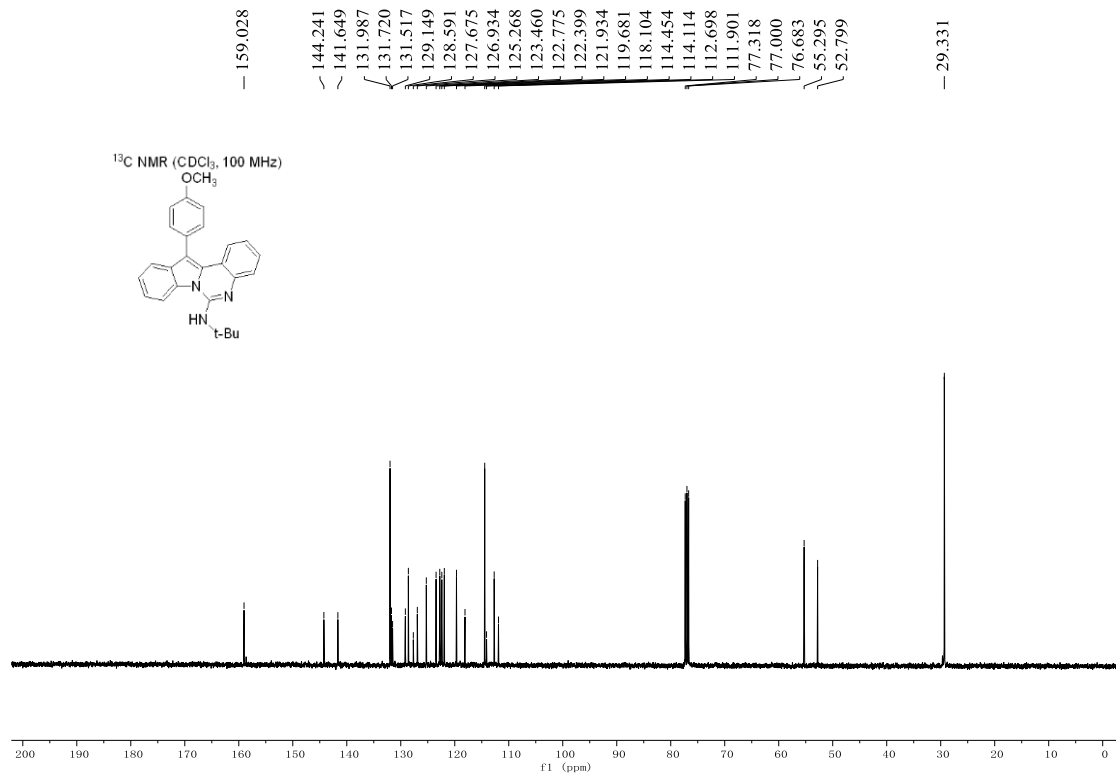


***N*-(*tert*-Butyl)-12-(4-methoxyphenyl)indolo[1,2-*c*]quinazolin-6-amine (9)**

¹H NMR (400 MHz, CDCl₃) of compound of 9

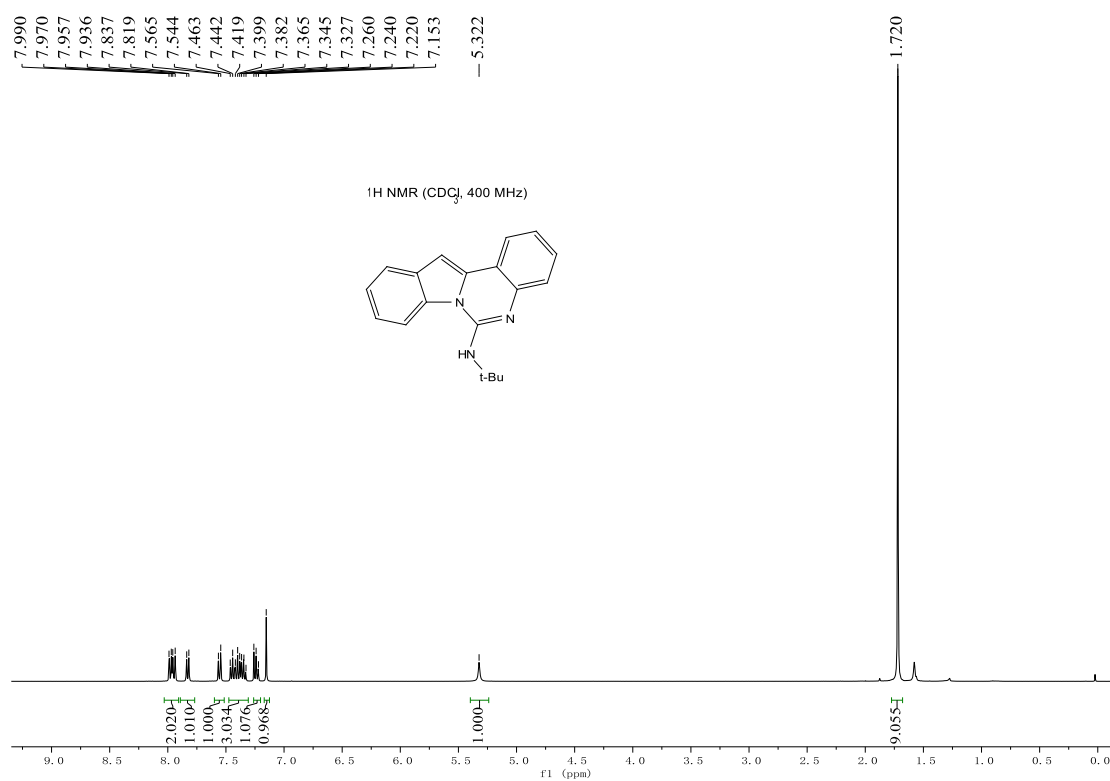


¹³C NMR (100 Mz, CDCl₃) of compound 9



***N*-(*tert*-Butyl)indolo[1,2-*c*]quinazolin-6-amine (10)**

¹H NMR (400 MHz, CDCl₃) of compound **10**



¹³C NMR (100 Mz, CDCl₃) of compound **10**

