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# Supporting Information

## An efficient Selectfluor-mediated condensation of indoles and anthranilates for synthesis of indoloquinazolinones

Xinzhe Wang, Zhipeng Wu, Guogang Tu, Yuanyue Zhao, Xiaodong Xiong*

School of Pharmacy, Nanchang University, Nanchang, Jiangxi 330006, China
E-mail: xiongxd@ncu.edu.cn

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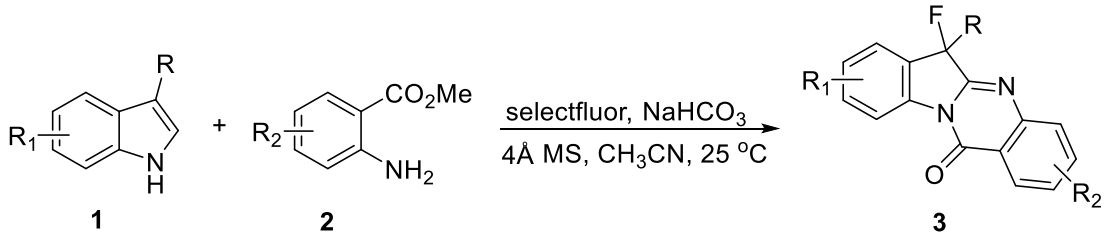
## (A) General information

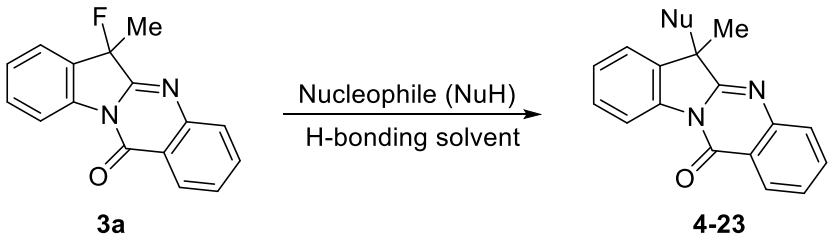
Commercially available reagents were used directly without further purification. For others, we prepared them in suitable reaction conditions. NMR spectra were recorded on a Brucker ADVANCE III 400MHz spectrometer ($^{1}$H NMR: 400 MHz, $^{13}$C NMR: 100 MHz). Chemical shifts (δ) were reported in ppm relative to $CDCl_3$ (δ 7.26) for the $^{1}$H NMR and to $CDCl_3$ (δ 77.16) for the $^{13}$C NMR measurements. Mass spectra were recorded on Therno Finnigan MAT 95 XL spectrometer and Bruker solariX 9.4 Tesla FTICR spectrometer. GC/MS analysis was conducted on a Shimadzu GCMSQP2010 instrument equipped with a Restec-5HT column (30 m × 0.25 mm, Hewlett-Packard). IR spectra were recorded on a PerkinElmer FT-IR spectrophotometer and reported in terms of wavenumber of absorption ($cm^{-1}$). Flash column chromatography was performed on 300-400 mesh silica gel from Qingdao Haiyang Chemical Co., Ltd. Reactions were monitored by thin-layer chromatography (TLC) using 254 nm UV light to visualize the progress of the reactions.

**(B) General Procedure for the Preparation of Indoloquinazolinone 3**



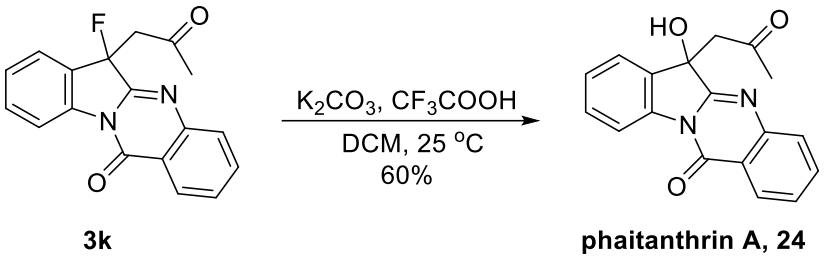

To a stirred solution of indole **1** (0.25 mmol, 1.0 eq), aniline **2** (0.5 mmol, 2.0 eq), $NaHCO_3$ (0.75 mmol, 3.0 eq) and 4Å MS (100 mg) in $CH_3CN$ (1 mL) were added selectfluor (0.38 mmol, 1.5 eq). The reaction mixture was stirred at room temperature for 5 h. Upon completion, the reaction was quenched with saturated aqueous $Na_2SO_3$ (30 mL). The organic layer was separated, and the aqueous layer was extracted with dichloromethane (3×15 mL). The combined organic layers were dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (hexane/EtOAc = 10:1) to yield **3**.

**(C) General Procedure for the Intermolecular Solvolytic Coupling of Indoloquinazolinone 3a with Various Nucleophiles**




To a stirred solution of indoloquinazolinone **3a** (0.1 mmol, 1.0 eq) in the indicated solvent (2 mL) were added nucleophile (0.2 mmol, 2.0 eq). The reaction mixture was stirred at indicated temperature. Upon completion, the reaction mixture was diluted with dichloromethane (20 mL), and washed with brine (10 mL). The organic layer was dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (hexane/EtOAc = 10:1) to yield the corresponding products **4-23**.

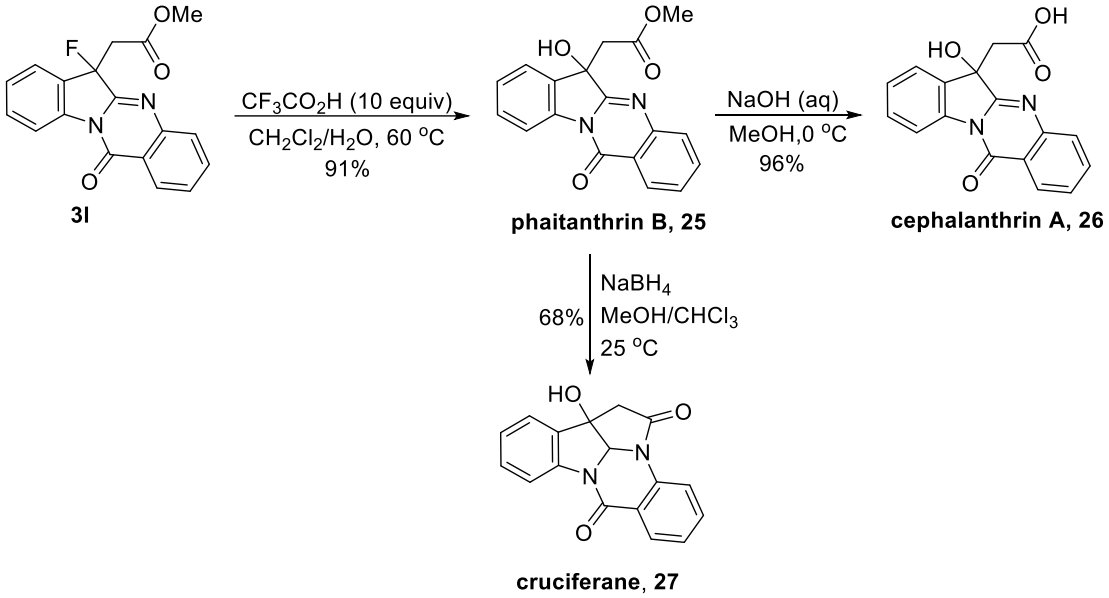
**(D) General Procedure for Synthesis of Phaitanthrin A**




**3k** **phaitanthrin A, 24**

To a stirred solution of indoloquinazolinone **3k** (0.1 mmol, 1.0 eq) and $K_2CO_3$ (0.15 mmol, 1.5 eq) in DCM (2 mL) were added $CF_3COOH$ (1.0 mmol, 1.0 eq). The reaction mixture was stirred at 25 °C for 24 h. Upon completion, the reaction mixture was diluted with dichloromethane (20 mL), and washed with brine (10 mL). The organic layer was dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (hexane/EtOAc = 2:1) to provide phaitanthrin A **24** (18.4 mg, 60%).

## (E) General Procedure for Synthesis of Phaitanthrin B, Cephalanthrin A and Cruciferane




**3l** **phaitanthrin B, 25** **cephalanthrin A, 26**

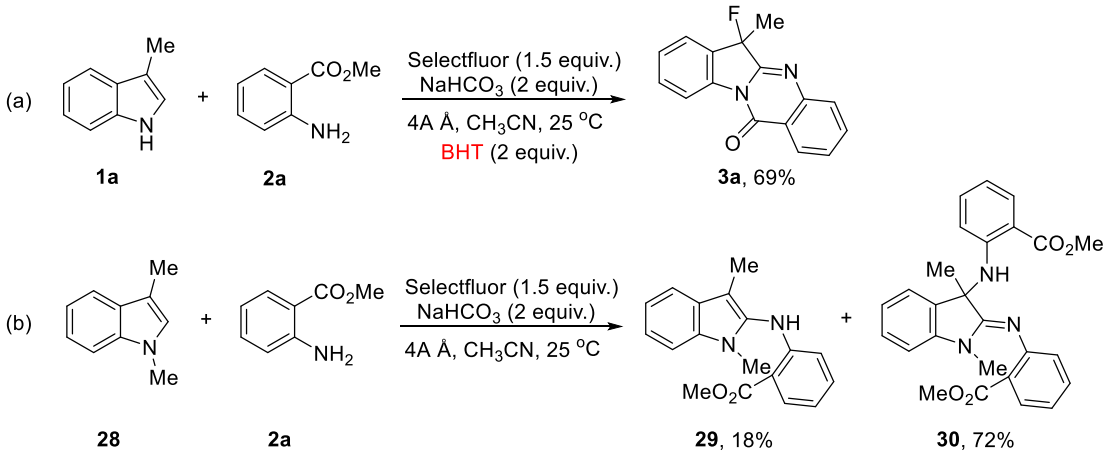
**cruciferane, 27**

1) To a stirred solution of indoloquinazolinone **3l** (0.3 mmol, 1.0 eq) in DCM/$H_2O$ (10 mL, v/v 10/1) were added $CF_3COOH$ (3.0 mmol, 10.0 eq). The reaction mixture was stirred at 60 °C for 12 h. Upon completion, the reaction mixture was diluted with ethyl acetate (30 mL), and washed with brine (10 mL). The organic layer was dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (hexane/EtOAc = 1:1) to provide phaitanthrin B **25** (87.9 mg, 91%).
2) To a stirred solution of phaitanthrin B (0.1 mmol, 1.0 eq) in MeOH (4 mL) were added 20% NaOH aqueous (0.15 mmol, 1.5 eq). The reaction mixture was stirred at 0 °C for 1 h. Upon completion, the reaction was quenched with 2N HCl (4 mL),

and the mixture was extracted with ethyl acetate (3 x 10mL), washed with brine (10 mL). The organic layer was dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (hexane/EtOAc = 2:1) to provide cephalanthrin A **26** (29.6 mg, 96%).

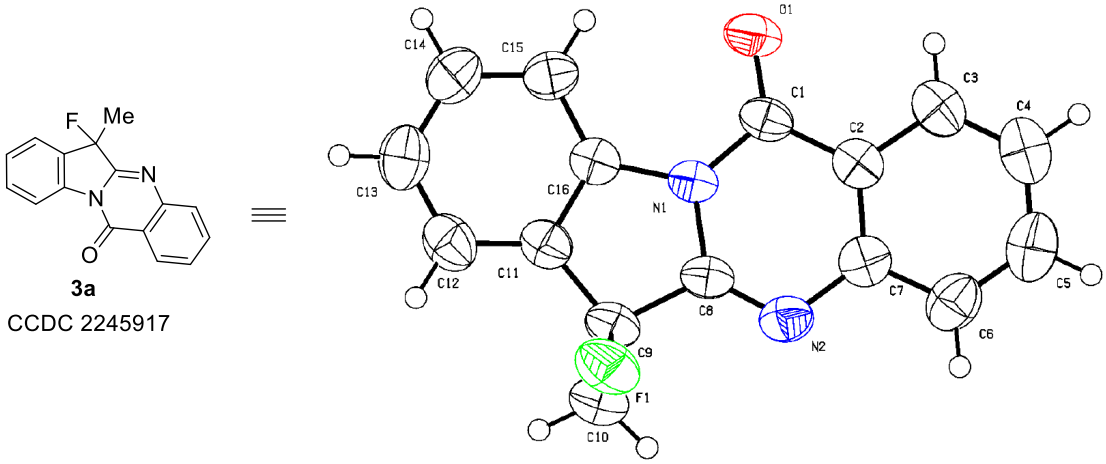
3) To a stirred solution of phaitanthrin B (0.1 mmol, 1.0 eq) in MeOH/$CHCl_3$ (2 mL, v/v 1/1) was added $NaBH_4$ (0.2 mmol, 2.0 eq) in small portions at 25 °C. The reaction mixture was stirred at 25 °C for 6 h. Upon completion, the reaction mixture was quenched with 2N HCl (1 mL). The reaction mixture was concentrated in vacuo and the obtained residue was dissolved in ethyl acetate (20 mL), and washed with brine (10 mL). The organic layer was dried over anhydrous $Na_2SO_4$, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (hexane/EtOAc = 1:1) to provide cruciferane **27** (19.9 mg, 68%).

**(F) Preliminary mechanistic study**

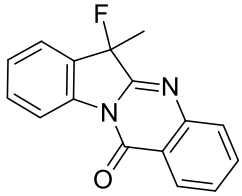



To gain a clearer picture on the mechanism, radical capture experiment was conducted. Introducing the radical scavenger butylated hydroxytoluene (BHT) into this Selectfluor mediate fluorocyclization of **1a** with **2a** under standard conditions provided **3a** in 69% yield. This result suggests the involvement of radical pathway was impossible. The indole **28**, which protected by methyl group, was examined. It was found that the intermolecular fluorination gave compound **29** in 18% yield and compound **30** in 72% yield, suggesting that fluorinated intermediate was unstable which subsequently underwent the defluorination, oxidation and nucleophilic substitution.

## (G) X-ray diffraction data of 3a (CCDC 2245917)

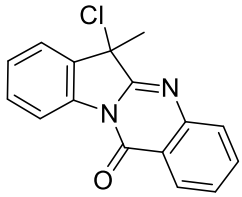



## (H) Analytical Data



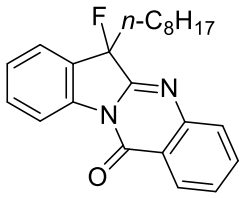

**6-fluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3a)**

White solid. $R_f$ = 0.50 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.07 (d, $J$ = 20.8 Hz, 3H), 7.39 (t, $J$ = 7.6 Hz, 1H), 7.54-7.60 (m, 2H), 7.64-7.67 (m, 1H), 7.81 (dt, $J$ = 1.6, 7.6 Hz, 1H), 7.87 (dd, $J$ = 1.2, 8.4 Hz, 1H), 8.41 (dd, $J$ = 1.6, 8.0 Hz, 1H), 8.55 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.4, 156.3, 156.1, 147.1 (2), 139.4 (2), 134.8, 132.0 (2), 129.4, 129.2, 128.5 (2), 128.3, 127.2 (2), 127.1, 124.3 (2), 122.6 (2), 117.5 (2), 94.5, 92.7, 23.1, 22.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.2 (q, $J$= 20.8 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{12}FN_2O$ *m/z* $[M+H]^+$: 267.0928, found: 267.0932.



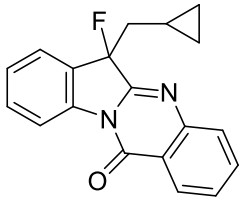

**6-chloro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (4)**

White solid. $R_f$ = 0.50 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.23 (s, 3H), 7.41 (dt, $J$ = 1.2, 7.6 Hz, 1H), 7.52 (dt, $J$ = 1.6, 8.0 Hz, 1H), 7.58 (dt, $J$ = 1.6, 7.2 Hz, 1H), 7.66 (dd, $J$ = 1.2, 7.6 Hz, 1H), 7.82 (dt, $J$ = 1.2, 6.8 Hz, 1H), 7.88 (dd, $J$ = 1.2, 8.0 Hz, 1H), 8.43 (dd, $J$ = 1.6, 8.0 Hz, 1H), 8.57 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.6, 159.0, 147.3, 138.0, 134.8, 133.1, 131.0, 128.3, 128.0, 127.3, 127.2, 123.9, 122.1, 117.5, 64.7, 28.2. HRMS (ESI) calcd for $C_{16}H_{12}ClN_2O$ *m/z* $[M+H]^+$: 283.0633, found: 283.0635.



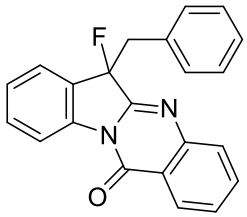

**6-fluoro-6-octylindolo[2,1-b]quinazolin-12(6H)-one (3b)**

Pale yellow oil. $R_f$ = 0.40 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.83 (t, *J* = 6.8 Hz, 3H), 1.12-1.28 (m, 12H), 2.37-2.58 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.54-7.63 (m, 3H), 7.81 (dt, *J* = 1.6, 8.4 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 8.42 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.56 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.4, 156.1, 155.9, 147.2, 147.1, 140.1, 140.0, 134.7, 131.9 (2), 128.6, 128.5, 128.3 (2), 128.2, 127.2, 127.1, 127.0, 124.6, 122.6, 117.5, 97.2, 95.3, 36.5, 36.2, 31.8, 29.5, 29.2, 29.1, 23.1 (2), 22.7, 14.1. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –141.0 (t, *J*= 12.2 Hz, 1F). HRMS (ESI) calcd for $C_{23}H_{26}N_2OF$ *m/z* $[M+H]^+$: 365.2024, found: 365.2028.




**6-(cyclopropylmethyl)-6-fluoroindolo[2,1-b]quinazolin-12(6H)-one (3c)**

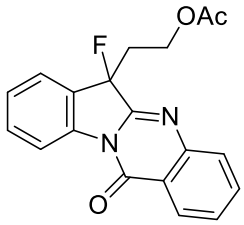
White solid. $R_f$ = 0.30 (PE:DCM = 1:1); $^1$H NMR (400 MHz, $CDCl_3$) δ -0.04-0.08 (m, 2H), 0.17-0.42 (m, 3H), 2.25-2.33 (m, 1H), 2.56-2.63 (m, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.55-7.60 (m, 2H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.81 (dt, *J* = 1.6, 7.2 Hz, 1H), 7.87 (dd, *J* = 1.2, 8.0 Hz, 1H), 8.43 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.57 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.5, 156.5, 156.3, 147.1 (2), 140.2, 140.1, 134.7, 131.9 (2), 128.6, 128.5, 128.4, 128.2, 127.2, 126.9 (2), 125.0, 122.5, 117.4, 97.3, 95.4, 41.1, 40.8, 5.0, 4.9, 4.4, 4.0. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –141.2 (t, *J*= 10.5 Hz, 1F). HRMS (ESI) calcd for $C_{19}H_{16}N_2OF$ *m/z* $[M+H]^+$: 307.1241, found: 307.1245.



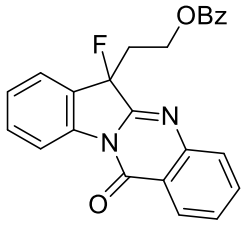

**6-benzyl-6-fluoroindolo[2,1-b]quinazolin-12(6H)-one (3d)**

Yellow solid. $R_f$ = 0.30 (PE:DCM = 1:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.54 (dd, *J* = 6.8, 13.6 Hz, 1H), 3.92 (dd, *J* = 4.0, 9.6 Hz, 1H), 7.03 (d, *J* = 6.8 Hz, 2H), 7.10-7.17 (m, 3H), 7.21-7.24 (m, 1H), 7.28 (t, *J* = 8.0 Hz, 1H), 7.47-7.51 (m, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.84 (dt, *J* = 1.6, 7.6 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 8.39 (dd, *J* = 1.2, 7.6 Hz, 1H), 8.42 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.2, 155.9, 155.7, 147.0 (2), 139.9 (2), 134.8, 132.6 (2), 131.9 (2), 130.8, 128.5, 128.4, 128.3,

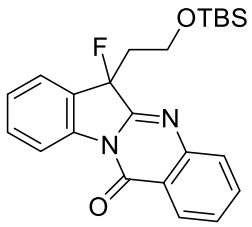
127.6, 127.5, 127.4, 127.2, 126.6 (2), 125.6, 122.5, 117.3, 96.6, 94.7, 43.0, 42.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –142.3 (q, *J*= 9.9 Hz, 1F). HRMS (ESI) calcd for $C_{22}H_{16}N_2OF$ *m/z* $[M+H]^+$: 343.1241, found: 343.1236.




**2-(6-fluoro-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl)ethyl acetate (3e)**
Pale yellow solid. $R_f$ = 0.30 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.59 (s, 3H), 2.74-2.83 (m, 1H), 2.95-3.05 (m, 1H), 3.92-3.98 (m, 1H), 4.22-4.29 (m, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.56-7.64 (m, 3H), 7.81 (dt, *J* = 1.6, 6.8 Hz, 1H), 7.87 (dd, *J* = 1.2, 8.4 Hz, 1H), 8.42 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.57 (dd, *J* = 0.8, 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.3, 159.3, 155.5, 155.3, 147.0 (2), 140.1 (2), 134.9, 132.4 (2), 128.6, 128.5 (2), 127.4, 127.2, 127.1 (2), 124.8 (2), 122.5 (2), 117.6 (2), 95.7, 93.8, 77.5, 77.2, 76.8, 59.2, 59.1, 35.3, 35.0, 20.4. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –140.2 (t, *J*= 11.3 Hz, 1F). HRMS (ESI) calcd for $C_{19}H_{16}N_2O_3F$ *m/z* $[M+H]^+$: 339.1139, found: 339.1137.

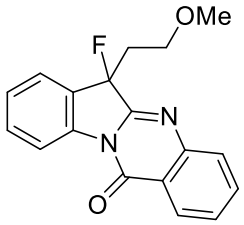



**2-(6-fluoro-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl)ethyl benzoate (3f)**
Brown solid. $R_f$ = 0.20 (PE:DCM = 1:2); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.85-2.94 (m, 1H), 3.19-3.29 (m, 1H), 4.14-4.21 (m, 1H), 4.48-4.54 (m, 1H), 7.08 (t, *J* = 7.8 Hz, 1H), 7.32-7.39 (m, 2H), 7.48-7.57 (m, 4H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.72-7.79 (m, 2H), 8.31 (dd, *J* = 1.6, 7.8 Hz, 1H), 8.53 (d, *J* = 7.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.9, 159.22, 155.6, 155.4, 147.0 (2), 140.2 (2), 134.7, 133.0, 132.4 (2), 129.3, 129.1, 128.5 (2), 128.2, 128.1, 127.2 (2), 127.1 (2), 127.0, 124.8 (2), 122.5 (2), 117.7 (2), 95.9, 94.1, 77.5, 77.2, 76.8, 59.9, 59.8, 35.2, 34.9. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.0 (t, *J*= 10.5 Hz, 1F). HRMS (ESI) calcd for $C_{24}H_{18}N_2O_3F$ *m/z* $[M+H]^+$: 401.1296, found: 401.1299.



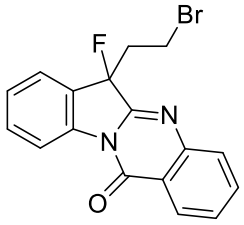
**6-(2-((tert-butyldimethylsilyl)oxy)ethyl)-6-fluoroindolo[2,1-b]quinazolin-12(6H)-one (3g)**

Brown oil. $R_f$ = 0.30 (PE:DCM = 1:1); $^1$H NMR (400 MHz, $CDCl_3$) δ -0.38 (s, 3H), -0.35 (s, 3H), 0.54 (s, 9H), 2.56-2.65 (m, 1H), 3.02-3.11 (m, 1H), 3.39-3.46 (m, 1H), 3.67-3.73 (m, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.54-7.62 (m, 3H), 7.80 (dt, *J* = 1.6, 6.8 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 8.42 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.57 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.5, 156.5, 156.3, 147.2 (2), 140.4 (2), 134.6, 132.0 (2), 128.5, 128.4, 128.0, 127.6, 127.4, 127.0, 126.8 (2), 124.9 (2), 122.6 (2), 117.6 (2), 96.7, 94.9, 58.8, 58.7, 38.8, 38.5, 25.7, 18.1, -5.9 (2). $^{19}$F NMR (376 MHz, $CDCl_3$) δ –139.0 (q, *J*= 6.8 Hz, 1F). HRMS (ESI) calcd for $C_{23}H_{28}FN_2O_2Si$ *m/z* $[M+H]^+$: 411.1899, found: 411.1896.



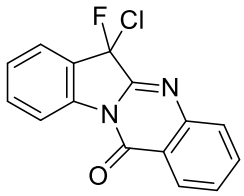

**6-fluoro-6-(2-methoxyethyl)indolo[2,1-b]quinazolin-12(6H)-one (3h)**

White solid. $R_f$ = 0.20 (PE:DCM = 1:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.58 (s, 3H), 2.74-2.83 (m, 1H), 2.96-3.05 (m, 1H), 3.90-3.96 (m, 1H), 4.22-4.28 (m, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.57-7.65 (m, 3H), 7.21 (dt, *J* = 1.6, 7.6 Hz, 1H), 7.87 (dd, *J* = 1.2, 8.0 Hz, 1H), 8.42 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.56 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 170.4, 159.3, 155.5, 155.3, 147.0, 146.9, 140.1, 140.0, 134.9, 132.4 (2), 128.5 (3), 127.3, 127.2 (2), 127.1 (2), 124.8 (2), 122.5, 117.6 (2), 95.7, 93.8, 59.2 (2), 35.3, 35.0, 20.4. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –140.2 (t, *J*= 10.9 Hz, 1F). HRMS (ESI) calcd for $C_{18}H_{16}FN_2O_2$ *m/z* $[M+H]^+$: 311.1190, found: 311.1194.



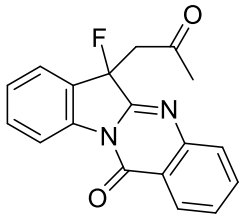

**6-(2-bromoethyl)-6-fluoroindolo[2,1-b]quinazolin-12(6H)-one (3i)**

Brown solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.84-2.96 (m, 1H), 3.08-3.19 (m, 1H), 3.41-3.48 (m, 1H), 3.63-3.69 (m, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.58-7.64 (m, 3H), 7.81-7.88 (m, 2H), 8.42 (d, *J* = 8.0 Hz, 1H), 8.57 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.3, 154.8, 154.7, 146.9, 146.8, 140.0 (2), 134.9, 132.6 (2), 128.7, 128.6, 127.2 (2), 127.0, 124.7, 122.6, 117.7, 95.8, 93.9, 40.1, 39.7, 24.6, 24.5. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –143.2 (q, *J*= 9.0 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{13}N_2OBrF$ *m/z* $[M+H]^+$: 359.0190, found: 359.0193.



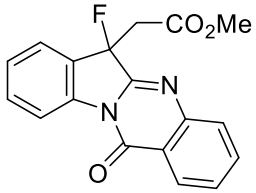
**6-chloro-6-fluoroindolo[2,1-b]quinazolin-12(6H)-one (3j)**

Purple solid. $R_f$ = 0.40 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 7.45 (t, *J* = 7.6 Hz, 1H), 7.62-7.70 (m, 2H), 7.78 (d, *J* = 7.2 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.57 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 158.7, 149.1, 146.5, 139.7, 139.6, 135.2, 134.4, 129.3, 129.2, 127.5, 127.4, 124.7, 123.1, 122.8, 122.5, 122.3, 117.7, 115.3, 112.8. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –102.3 (s, 1F). HRMS (ESI) calcd for $C_{15}H_9N_2OClF$ *m/z* $[M+H]^+$: 287.0382, found: 287.0384.



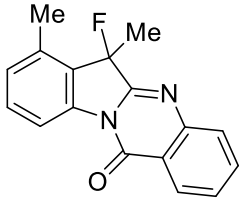
**6-fluoro-6-(2-oxopropyl)indolo[2,1-b]quinazolin-12(6H)-one (3k)**

Yellow solid. $R_f$ = 0.20 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.13 (s, 3H), 3.79-3.99 (m, 2H), 7.35 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.53-7.60 (m, 3H), 7.76-7.81 (m, 2H), 8.43 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.59 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 203.0, 202.9, 159.4, 155.6, 155.5, 147.0 (2), 140.9, 140.8, 134.6, 132.3 (2), 128.3 (2), 128.2, 127.5, 127.4, 127.3, 126.8 (2), 123.9, 122.7, 117.6 (2), 94.0, 92.2, 49.7, 49.4, 30.5, 30.4. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –141.8 (t, *J*= 8.3 Hz, 1F). HRMS (ESI) calcd for $C_{18}H_{14}FN_2O_2$ *m/z* $[M+H]^+$: 309.1034, found: 309.1035.



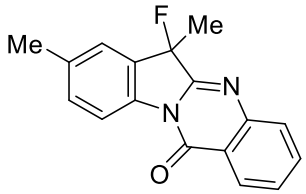
**methyl 2-(6-fluoro-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl)acetate (3l)**

Yellow solid. $R_f$ = 0.30 (PE:EtOAc = 4:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 3.46 (s, 3H), 3.61 (dd, *J* = 6.8, 16.4 Hz, 1H), 3.83 (dd, *J* = 9.2, 16.4 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.55-7.59 (m, 2H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.79 (dt, *J* = 1.6, 7.2 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 8.42 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.57 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.2, 168.0, 159.3, 155.4, 155.2, 147.1, 147.0, 140.8 (2), 134.6, 132.5 (2), 128.5, 128.4, 128.3, 127.3, 127.2, 127.0, 126.9 (2), 124.3 (2), 122.8, 117.5 (2), 93.6, 91.8, 77.5, 77.2 (2), 76.8, 52.1, 40.7, 40.3. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –140.1 (t, *J*= 10.2 Hz, 1F). HRMS (ESI) calcd for $C_{18}H_{14}FN_2O_3$ *m/z* $[M+H]^+$: 325.0983, found: 325.0986.



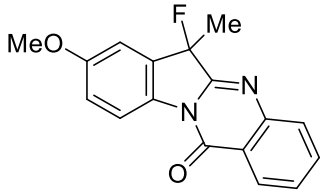

**6-fluoro-6,7-dimethylindolo[2,1-b]quinazolin-12(6H)-one (3m)**

White solid. $R_f$ = 0.30 (PE:DCM = 1:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.14 (d, *J* = 20.4 Hz, 3H), 2.60 (s, 3H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.42 (dt, *J* = 1.6, 8.0 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.81 (dt, *J* = 1.6, 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 8.39-8.42 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.4, 156.8, 156.6, 147.1 (2), 139.5, 139.4, 136.6, 134.7, 131.5 (2), 129.4, 129.3, 128.4, 128.1, 127.2, 127.0, 126.9, 122.6, 114.9, 95.5, 93.6, 22.7, 22.4, 18.0. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –148.1 (q, *J*= 20.2 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{14}N_2OF$ *m/z* $[M+H]^+$: 281.1085, found: 281.1089.



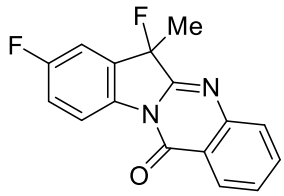

**6-fluoro-6,8-dimethylindolo[2,1-b]quinazolin-12(6H)-one (3n)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.05 (d, *J* = 20.8 Hz, 3H), 2.44 (s, 3H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.44 (s, 1H), 7.56 (t, *J* = 6.8 Hz, 1H), 7.79 (dt, *J* = 1.6, 7.2 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 8.40 (dd, *J* = 1.6, 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.2, 156.5, 156.3, 147.2 (2), 137.3, 137.2 (2), 137.1, 134.6, 132.5, 132.4, 129.5, 129.3, 128.5, 128.2, 127.1, 124.8, 122.7, 117.2, 94.6, 92.8, 23.0, 22.7, 21.4. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.2 (q, *J*= 20.7 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{14}N_2OF$ *m/z* $[M+H]^+$: 281.1085, found: 281.1088.



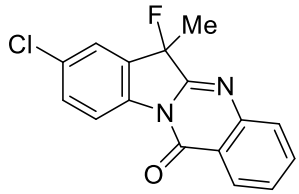

**6-fluoro-8-methoxy-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3o)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.05 (d, *J* = 20.8 Hz, 3H), 3.88 (s, 3H), 7.04 (d, *J* = 8.8 Hz, 1H), 7.16 (s, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.78 (dt, *J* = 1.6, 7.2 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 8.39 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.43 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.0 (2), 158.9, 156.5, 156.3, 147.1 (2), 134.5, 132.8, 132.7, 131.0, 130.8, 128.5, 128.2, 127.0, 122.7, 118.5, 116.7 (2), 110.3, 94.6, 92.7, 56.0, 23.1, 22.8. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.9 (q, *J*= 20.7 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{14}N_2O_2F$ *m/z* $[M+H]^+$: 297.1034, found: 297.1037.



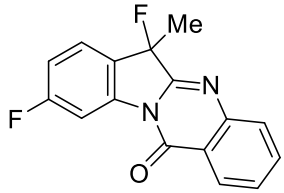
**6,8-difluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3p)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 15:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.8 Hz, 3H), 7.22-7.27 (m, 1H), 7.33-7.36 (m, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.82 (dt, *J* = 1.6, 7.2 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 8.39 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.51-8.54 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.6 (2), 160.2, 160.1, 159.2, 156.0, 155.8, 147.0, 146.9, 135.4 (3), 135.3, 134.9, 131.4, 131.3, 131.2, 131.1, 128.5, 128.4, 127.1, 122.5, 119.0, 118.9, 118.8, 118.7, 118.5 (2), 112.2, 111.9, 94.1 (2), 92.3 (2), 23.0, 22.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –113.14- –113.08 (m, 1F), –146.4 (q, *J*= 20.7 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{11}N_2OF_2$ *m/z* $[M+H]^+$: 285.0834, found: 285.0839.



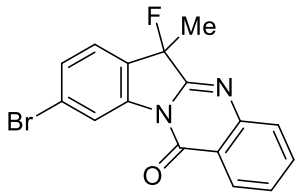
**8-chloro-6-fluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3q)**

White solid. $R_f$ = 0.30 (PE:DCM = 1:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.8 Hz, 3H), 7.52 (dd, *J* = 2.0, 8.8 Hz, 1H), 7.56-7.61 (m, 2H), 7.81 (t, *J* = 7.4 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 8.47 (d, *J* = 8.8 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.2, 155.8, 155.6, 147.1 (2), 137.9, 137.8, 134.9, 132.8, 132.7, 132.0 (2), 131.2, 131.0, 128.6, 128.5, 127.2, 124.8, 122.5, 118.6, 94.1, 92.2, 22.9, 22.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.7 (q, *J*= 20.3 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{10}N_2OFClNa$ *m/z* $[M+Na]^+$: 323.0358, found: 323.0362.



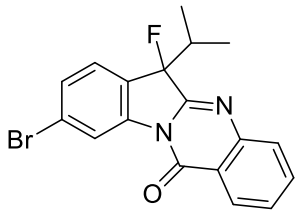
**6,9-difluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3r)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.4 Hz, 3H), 7.08 (dt, *J* = 1.6, 8.4 Hz, 1H), 7.57-7.63 (m, 2H), 7.82 (dt, *J* = 1.6, 6.8 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 8.30 (dd, *J* = 2.4, 9.2 Hz, 1H), 8.39 (dd, *J* = 1.6, 7.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.9 (2), 163.4 (2), 159.2, 156.3, 156.1, 140.7 (2), 140.6, 135.0, 128.6, 128.5, 127.3, 125.7, 125.6, 125.3, 125.2, 125.1, 125.0, 122.4, 114.1, 114.0, 113.8 (2), 106.3, 106.0, 94.0, 92.2, 23.0, 22.6. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –105.66- –105.58 (m, 1F), –136.5 (dq, *J* = 5.6, 21.1 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{11}N_2OF_2$ *m/z* $[M+H]^+$: 285.0834, found: 285.0838.



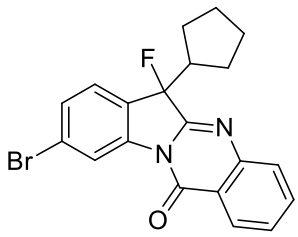

**9-bromo-6-fluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3s)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.05 (d, $J$ = 20.4 Hz, 3H), 7.49-7.55 (m, 2H), 7.59 (t, $J$ = 7.6 Hz, 1H), 7.80-7.88 (m, 2H), 8.40 (d, $J$ = 8.0 Hz, 1H), 8.77 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.2, 155.9, 155.7, 147.0 (2), 140.3 (2), 135.1, 130.2 (2), 128.6, 128.5, 128.4, 128.2, 127.3, 125.9, 125.8, 125.5, 122.4, 120.9, 94.1, 92.3, 22.9, 22.6. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.0 (q, $J$ = 20.6 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{11}N_2OFBr$ *m/z* $[M+H]^+$: 345.0033, found: 345.0037.



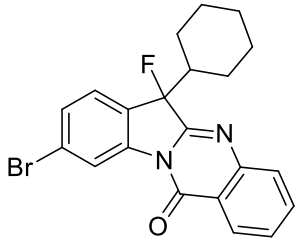

**9-bromo-6-fluoro-6-isopropylindolo[2,1-b]quinazolin-12(6H)-one (3t)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 12:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.05 (d, $J$ = 20.4 Hz, 3H), 7.49-7.55 (m, 2H), 7.59 (t, $J$ = 7.6 Hz, 1H), 7.82 (t, $J$ = 8.0 Hz, 1H), 7.87 (d, $J$ = 8.0 Hz, 1H), 8.40 (d, $J$ = 8.0 Hz, 1H), 8.77 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.2, 155.9, 155.7, 146.9 (2), 141.1, 141.0, 135.1, 129.9, 128.7, 128.5, 127.2, 126.5, 126.3, 126.1, 125.6 (2), 122.2, 120.7, 99.0, 97.1, 35.8, 35.5, 16.2 (2), 15.9 (2). $^{19}$F NMR (376 MHz, $CDCl_3$) δ –150.2 (d, $J$ = 7.1 Hz, 1F). HRMS (ESI) calcd for $C_{18}H_{15}N_2OFBr$ *m/z* $[M+H]^+$: 373.0346, found: 373.0348.



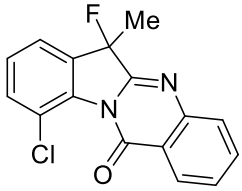

**9-bromo-6-cyclopentyl-6-fluoroindolo[2,1-b]quinazolin-12(6H)-one (3u)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 15:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.49-1.59 (m, 6H), 1.63-1.72 (m, 1H), 1.83-1.89 (m, 1H), 3.00-3.10 (m, 1H), 7.50-7.60 (m, 2H), 7.59 (t, $J$ = 7.6 Hz, 1H), 7.80-7.87 (m, 2H), 8.40 (d, $J$ = 8.0 Hz, 1H), 8.80 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.3, 155.9, 155.7, 147.0 (2), 140.9 (2), 135.0, 130.0 (2), 128.7, 128.4, 127.3, 127.2 (2), 126.3, 125.6, 125.5, 122.2, 120.7, 98.0, 96.1, 46.8, 46.6, 27.0 (2), 26.6 (2), 25.8, 25.6. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –146.4 (d, $J$= 10.5 Hz, 1F). HRMS (ESI) calcd for $C_{20}H_{16}N_2OFBrNa$ *m/z* $[M+Na]^+$: 421.0322, found: 421.0327.



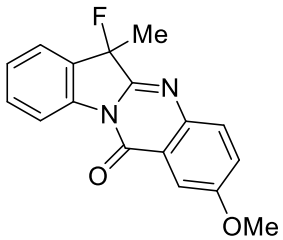

**9-bromo-6-cyclohexyl-6-fluoroindolo[2,1-b]quinazolin-12(6H)-one (3v)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 15:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.94-1.13 (m, 2H), 1.20-1.37 (m, 3H), 1.45-1.48 (m, 1H), 1.64-1.69 (m, 2H), 1.80-1.85 (m, 1H), 1.96-2.01 (m, 1H), 2.53-2.61 (m, 1H), 7.49-7.54 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.82 (dt, *J* = 1.6, 8.4 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 8.39 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.79 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.2, 156.1, 155.9, 146.9 (2), 141.0, 140.9, 135.0, 129.9, 129.8, 128.7, 127.2, 126.9, 126.7, 126.5, 125.5 (2), 122.2, 120.7, 98.6, 96.7, 45.8, 45.6, 26.2, 26.1, 26.0, 25.9 (2), 25.8, 25.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –153.2 (d, *J*= 7.1 Hz, 1F). HRMS (ESI) calcd for $C_{21}H_{19}N_2OFBr$ *m/z* $[M+H]^+$: 413.0659, found: 413.0662.




**10-chloro-6-fluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3w)**

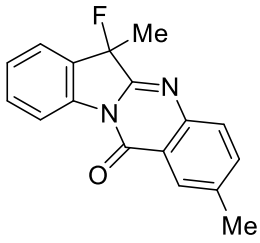
White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.04 (d, *J* = 20.4 Hz, 3H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.54-7.60 (m, 3H), 7.77-7.83 (m, 2H), 8.36 (dd, *J* = 1.6, 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 158.0, 156.2, 156.0, 146.5 (2), 137.1, 137.0, 135.0 (2), 134.7, 133.3, 133.1, 128.4, 128.3, 128.2, 127.9, 127.6, 123.3, 122.9, 122.8, 94.0, 92.2, 23.3. 23.0. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –134.5 (q, *J*= 20.4 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{11}N_2OFCl$ *m/z* $[M+H]^+$: 301.0538, found: 301.0539.




**6-fluoro-2,6-dimethylindolo[2,1-b]quinazolin-12(6H)-one (3x)**

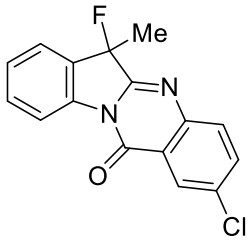
Yellow solid. $R_f$ = 0.30 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.4 Hz, 3H), 3.96 (s, 3H), 7.37-7.41 (m, 2H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 6.8 Hz, 1H), 7.78-7.80 (m, 2H), 8.56 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.7, 159.3, 154.1, 153.9, 141.6, 141.5, 139.6, 139.5, 132.0, 131.9, 130.0, 129.8, 129.6, 127.1 (2), 124.4, 124.3, 123.7, 117.5, 107.3, 94.4, 92.6, 56.1, 23.0, 22.7. $^{19}$F

NMR (376 MHz, $CDCl_3$) δ –137.0 (q, *J*= 20.4 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{14}N_2O_2F$ *m/z* $[M+H]^+$: 297.1034, found: 297.1038.



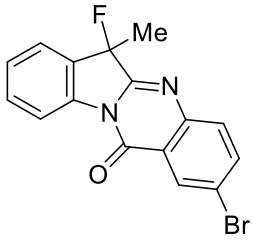

**6-fluoro-2,6-dimethylindolo[2,1-b]quinazolin-12(6H)-one (3y)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.8 Hz, 3H), 2.52 (s, 3H), 7.35-7.39 (m, 1H), 7.52-7.57 (m, 1H), 7.59-7.65 (m, 2H), 7.75 (d, *J* = 8.0 Hz, 1H), 8.18 (s, 1H), 8.53 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.4, 155.5, 155.3, 145.1, 145.0, 139.5 (2), 138.7, 136.1, 131.9 (2), 129.5, 129.3, 128.3, 127.0 (2), 126.7, 124.2, 122.3, 117.5, 94.4, 92.6, 23.0, 22.7, 21.5. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –137.5 (q, *J*= 20.5 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{14}N_2OF$ *m/z* $[M+H]^+$: 281.1085, found: 281.1089.




**2-chloro-6-fluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3z)**

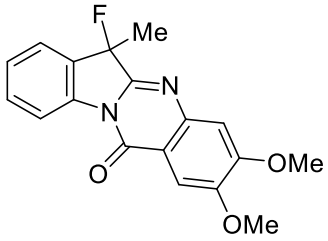
White solid. $R_f$ = 0.40 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.8 Hz, 3H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 2.4, 8.8 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 8.36 (d, *J* = 2.4 Hz, 1H), 8.52 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 158.2, 156.6, 156.4, 145.6 (2), 139.2, 139.1, 135.1, 134.3, 132.1 (2), 130.0, 129.4, 129.2, 127.4 (2), 126.6, 124.3, 123.7, 117.5, 94.5, 92.6, 23.0, 22.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.3 (q, *J*= 20.7 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{10}N_2OClFNa$ *m/z* $[M+Na]^+$: 323.0358, found: 323.0359.




**2-bromo-6-fluoro-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3aa)**

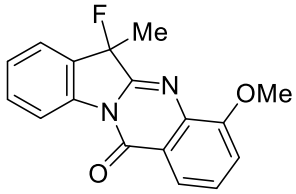
Brown solid. $R_f$ = 0.30 (PE:DCM = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.8 Hz, 3H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 8.52 (d, *J* = 8.0 Hz, 1H), 8.53

(s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 158.1, 156.7, 156.5, 146.0, 145.9, 139.2, 139.1, 137.9, 132.1 (2), 130.2, 129.8, 129.4, 129.2, 127.4 (2), 124.4, 124.0, 122.2, 117.5, 94.5, 92.7, 23.0, 22.7. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.4 (q, *J*= 20.7 Hz, 1F). HRMS (ESI) calcd for $C_{16}H_{11}N_2ONBrF$ *m/z* $[M+H]^+$: 345.0033, found: 345.0038.



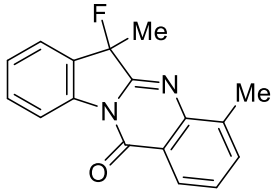

**6-fluoro-2,3-dimethoxy-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3ab)**

Yellow solid. $R_f$ = 0.20 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (d, *J* = 20.8 Hz, 3H), 4.03 (s, 3H), 4.04 (s, 3H), 7.29 (s, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.53-7.59 (m, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.74 (s, 1H), 8.55 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.4, 155.5, 155.3, 145.1, 145.0, 139.5 (2), 138.7, 136.1, 131.9 (2), 129.5, 129.3, 128.3, 127.0 (2), 126.7, 124.2, 122.3, 117.5, 94.4, 92.6, 23.0, 22.7, 21.5. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –137.5 (q, *J*= 20.5 Hz, 1F). HRMS (ESI) calcd for $C_{18}H_{16}N_2O_3F$ *m/z* $[M+H]^+$: 327.1139, found: 327.1139.




**6-fluoro-4-methoxy-6-methylindolo[2,1-b]quinazolin-12(6H)-one (3ac)**

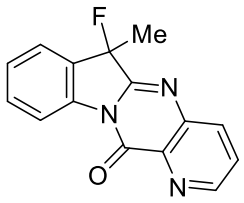
Yellow solid. $R_f$ = 0.20 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.10 (d, *J* = 20.4 Hz, 3H), 4.06 (s, 3H), 7.27 (d, *J* = 9.2 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.50-7.58 (m, 2H), 7.65 (d, *J* = 7.6 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 8.55 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.3, 155.4, 155.3, 155.1, 139.4, 139.3, 137.5, 137.4, 131.9 (2), 129.8, 129.6, 128.7, 127.2 (2), 124.3, 123.9, 118.5, 117.6, 115.4, 94.5, 92.7, 56.7, 23.1, 22.8. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –137.2 (q, *J*= 20.5 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{14}N_2O_2F$ *m/z* $[M+H]^+$: 297.1034, found: 297.1036.




**6-fluoro-4,6-dimethylindolo[2,1-b]quinazolin-12(6H)-one (3ad)**

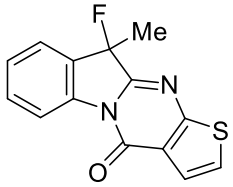
Brown solid. $R_f$ = 0.30 (PE:EtOAc = 20:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.07 (d, *J* = 20.8 Hz, 3H), 2.72 (s, 3H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J*

= 7.6 Hz, 1H), 8.25 (d, *J* = 8.0 Hz, 1H), 8.55 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.8, 154.7, 154.5, 145.6 (2), 139.6, 139.5, 137.3, 135.6, 132.0, 131.9, 129.6, 129.4, 127.8, 127.0 (2), 124.8, 124.3, 122.6, 117.5, 94.5, 92.7, 23.0, 22.7, 17.6. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –136.7 (q, *J*= 20.7 Hz, 1F). HRMS (ESI) calcd for $C_{17}H_{14}N_2OF$ *m/z* $[M+H]^+$: 281.1085, found: 281.1088.



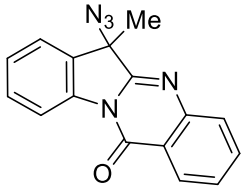

**6-fluoro-6-methylpyrido[3',2':4,5]pyrimido[1,2-a]indol-12(6H)-one (3ae)**

White solid. $R_f$ = 0.20 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.10 (d, *J* = 20.8 Hz, 3H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.51-7.59 (m, 2H), 7.66 (dd, *J* = 2.0, 7.2 Hz, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 8.73 (dd, *J* = 2.0, 8.0 Hz, 1H), 9.03 (dd, *J* = 2.0, 4.8 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.9, 159.7, 159.3, 157.6 (2), 156.1, 139.0 (2), 136.7, 132.1 (2), 129.6, 129.4, 127.7, 127.6, 124.5, 123.5, 118.1, 117.3, 94.5, 92.7, 22.7, 22.4. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –138.4 (q, *J*= 20.7 Hz, 1F). HRMS (ESI) calcd for $C_{15}H_{11}N_3OF$ *m/z* $[M+H]^+$: 268.0881, found: 268.0884.




**10-fluoro-10-methylthieno[2',3':4,5]pyrimido[1,2-a]indol-4(10H)-one (3af)**

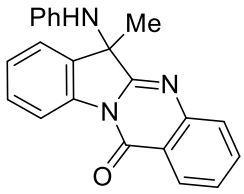
White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.04 (d, *J* = 20.8 Hz, 3H), 7.36 (d, *J* = 6.0 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.60-7.64 (m, 2H), 8.57 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.5, 157.0, 156.8, 156.1, 139.4, 132.1 (2), 129.8, 129.7, 127.4 (2), 125.6, 125.2, 124.3, 122.8, 117.9, 94.3, 92.5, 22.8, 22.5. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –140.0 (q, *J*= 20.4 Hz, 1F). HRMS (ESI) calcd for $C_{14}H_{10}N_2OFS$ *m/z* $[M+H]^+$: 273.0492, found: 273.0496.




**6-azido-6-methylindolo[2,1-b]quinazolin-12(6H)-one (5)**

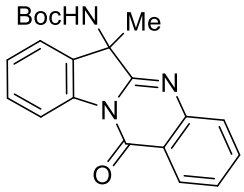
White solid. $R_f$ = 0.40 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.95 (s, 3H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.51-7.59 (m, 3H),7.81 (dt, *J* = 1.6, 8.0 Hz, 1H), 7.86 (t, *J* = 8.4 Hz, 1H), 8.41 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.57 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.6, 158.3, 147.1, 138.8, 134.8, 131.0, 130.9, 128.3, 127.9, 127.2,

127.1, 123.6, 122.1, 117.5, 65.5, 23.8. HRMS (ESI) calcd for $C_{16}H_{11}N_5ONa$ *m/z* $[M+Na]^+$: 312.0856, found: 312.0857.



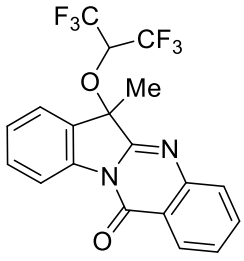

**6-methyl-6-(phenylamino)indolo[2,1-b]quinazolin-12(6H)-one (6)**

White solid. $R_f$ = 0.20 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.87 (s, 3H), 6.15 (d, *J* = 8.0 Hz, 2H), 6.59 (t, *J* = 7.2 Hz, 1H), 6.88 (t, *J* = 8.4 Hz, 2H), 7.35 (dt, *J* = 1.2, 7.6 Hz, 1H),7.49-7.54 (m, 3H), 7.73-7.75 (m, 2H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.68 (d, *J* = 8.4 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 161.4, 160.2, 147.4, 144.8, 138.3, 134.6, 134.0, 129.9, 129.2, 127.8, 127.3 (2), 127.1, 123.3, 121.8, 119.3, 117.7, 115.0, 62.6, 30.2. HRMS (ESI) calcd for $C_{22}H_{18}N_3O$ *m/z* $[M+H]^+$: 340.1444, found: 340.1448.




**tert-butyl (6-methyl-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl)carbamate (7)**

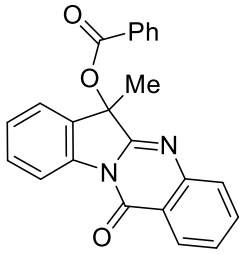
White solid. $R_f$ = 0.30 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.07 (s, 9H), 1.73 (s, 3H), 5.47 (s, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.45-7.50 (m, 2H), 7.52-7.56 (m, 1H), 7.77-7.80 (m, 2H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.59 (d, *J* = 7.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 161.4, 160.0, 153.7, 147.5, 138.8, 134.6, 129.6, 127.6, 127.2, 127.1, 126.8, 122.1, 121.9, 117.3, 80.9, 60.1, 27.9, 26.9. HRMS (ESI) calcd for $C_{21}H_{22}N_3O_3$ *m/z* $[M+H]^+$: 364.1656, found: 364.1659.



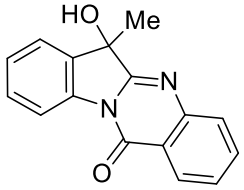

**6-((1,1,1,3,3,3-hexafluoropropan-2-yl)oxy)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (8)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 3H), 5.13-5.19 (m, 1H), 7.43 (dt, *J* = 7.2 Hz, 1H), 7.57-7.62 (m, 3H), 7.80-7.86 (m, 2H), 8.40 (d, *J* = 7.2 Hz, 1H), 8.59 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.4, 156.7, 146.7, 139.3, 134.9, 131.8, 129.4, 128.3 (2), 127.3, 127.2, 124.7, 122.3,

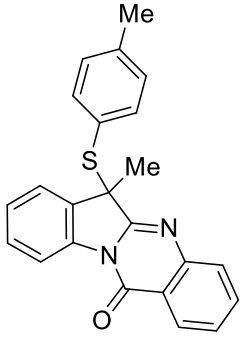
117.6, 81.7, 70.9, 70.5, 70.2, 69.9, 69.6, 23.5. $^{19}$F NMR (376 MHz, $CDCl_3$) δ –72.8 - –72.9 (m, 3F), –73.3 - –73.4 (m, 3F). HRMS (ESI) calcd for $C_{19}H_{13}F_6N_2O_2$ *m/z* $[M+H]^+$: 415.0876, found: 415.0884.




**6-methyl-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl benzoate (9)**
White solid. $R_f$ = 0.30 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.05 (s, 3H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.49-7.58 (m, 4H), 7.73-7.77 (m, 2H), 8.01 (d, *J* = 3.2 Hz, 2H), 8.45 (d, *J* = 8.0 Hz, 1H), 8.65 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.7, 159.9, 158.7, 147.3, 139.5, 134.5, 133.7, 131.4, 130.7, 130.1, 129.2, 128.5, 128.0, 127.5, 127.2, 126.8, 122.4, 122.3, 117.4, 25.4. HRMS (ESI) calcd for $C_{23}H_{16}N_2O_3Na$ *m/z* $[M+Na]^+$: 391.1053, found: 391.1057.

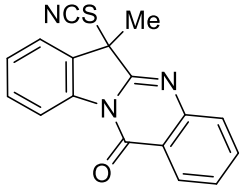



**6-hydroxy-6-methylindolo[2,1-b]quinazolin-12(6H)-one (10)**[1]
White solid. $R_f$ = 0.30 (PE:EtOAc = 3:1); $^1$H NMR (400 MHz, $CD_3OD$) δ 1.82 (s, 3H), 7.42 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.50 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.58-7.62 (m, 1H), 7.66-7.68 (m, 1H), 7.81-7.89 (m, 2H), 8.33-8.36 (m, 1H), 8.49 (d, *J* = 7.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CD_3OD$) δ 163.6, 161.2, 148.7, 139.6, 136.6, 135.9, 131.0, 128.6, 128.5, 128.2, 127.7, 124.7, 123.0, 118.0, 76.3, 26.1. HRMS (ESI) calcd for $C_{16}H_{13}N_2O_2$ *m/z* $[M+H]^+$: 265.0972, found: 265.0976.



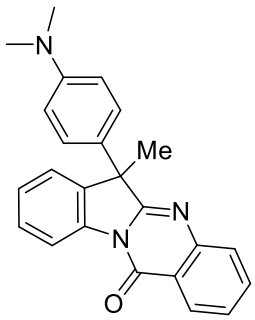

**6-methyl-6-(p-tolylthio)indolo[2,1-b]quinazolin-12(6H)-one (11)**
White solid. $R_f$ = 0.50 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.02 (s, 3H), 2.17 (s, 3H), 6.75 (d, *J* = 7.6 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 7.34-7.39 (m, 1H),

7.51-7.57 (m, 2H), 7.81 (dt, *J* = 1.6, 6.8 Hz, 1H), 7.90 (dd, *J* = 1.2, 8.0 Hz, 1H), 8.28-8.30 (m, 1H), 8.34 (dd, *J* = 1.6, 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 161.6, 159.7, 147.5, 140.3, 138.5, 136.4, 134.5, 134.0, 129.4, 129.3, 127.8, 127.1, 126.9, 126.6, 126.0, 124.0, 121.4, 116.9, 56.6, 23.4, 21.3. HRMS (ESI) calcd for $C_{23}H_{19}N_2OS$ *m/z* $[M+H]^+$: 371.1213, found: 371.1216.



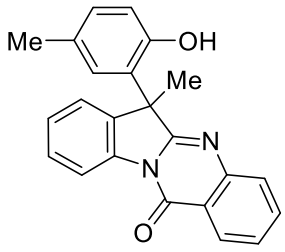

**6-methyl-6-thiocyanatoindolo[2,1-b]quinazolin-12(6H)-one (12)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.24 (s, 3H), 7.45 (dt, *J* = 0.6, 7.6 Hz, 1H), 7.57-7.62 (m, 2H), 7.70 (dd, *J* = 1.2, 7.6 Hz, 1H), 7.82-7.89 (m, 2H), 8.43 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.62 (dd, *J* = 1.2, 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.5, 157.7, 147.0, 138.8, 135.0, 131.7, 129.9, 128.3 (2), 127.4, 127.2, 123.9, 121.9, 117.7, 109.3, 56.5, 24.9. HRMS (ESI) calcd for $C_{17}H_{11}N_3OSNa$ *m/z* $[M+Na]^+$: 328.0515, found: 328.0518.




**6-(4-(dimethylamino)phenyl)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (13)**

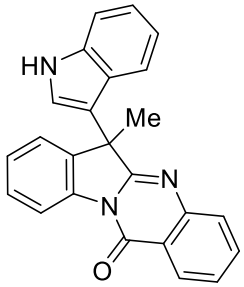
White solid. $R_f$ = 0.20 (PE:EtOAc = 8:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.03 (s, 3H), 2.90 (s, 3H), 6.63-6.67 (m, 2H), 7.18-7.21 (m, 2H), 7.33-7.35 (m, 2H), 7.45-7.50 (m, 2H), 7.72-7.75 (m, 2H), 8.41 (d, *J* = 8.0 Hz, 1H), 8.69 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.3, 160.4, 149.8, 148.0, 139.0, 137.9, 134.2, 129.5, 128.6, 127.8, 127.5, 126.8 (2), 126.7, 124.3, 121.4, 117.4, 112.5, 52.2, 40.6, 25.6. HRMS (ESI) calcd for $C_{24}H_{22}N_3O$ *m/z* $[M+H]^+$: 368.1757, found: 368.1758.




**6-(2-hydroxy-5-methylphenyl)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (14)**

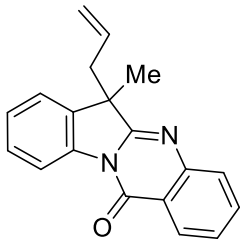
White solid. $R_f$ = 0.40 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.15 (s, 3H), 6.77 (d, *J* = 2.0 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.01 (dd, *J* = 2.0, 8.0 Hz, 1H),

7.48-7.59 (m, 4H), 7.73-7.80 (m, 2H), 8.38 (d, $J$ = 7.2 Hz, 1H), 8.69 (d, $J$ = 7.6 Hz, 1H), 11.07 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.4, 159.6, 154.4, 145.6, 139.0, 134.8, 134.6, 130.3, 129.5, 129.3, 128.4, 127.5, 127.1, 126.8, 126.6, 126.4, 126.0, 121.4, 120.6, 117.7, 53.5, 24.4, 20.8. HRMS (ESI) calcd for $C_{23}H_{19}N_2O_2$ *m/z* $[M+H]^+$: 355.1441, found: 355.1445.



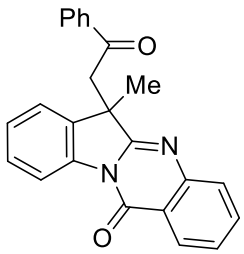

**6-(3a,7a-dihydro-1H-indol-3-yl)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (15)**

White solid. $R_f$ = 0.20 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.06 (s, 3H), 6.55 (d, $J$ = 7.6 Hz, 1H), 6.78 (t, $J$ = 7.6 Hz, 1H), 6.98 (s, 1H), 7.06 (t, $J$ = 7.6 Hz, 1H), 7.26-7.31 (m, 2H), 7.38 (d, $J$ = 8.0 Hz, 1H), 7.50 (t, $J$ = 8.0 Hz, 2H), 7.69-7.75 (m, 2H), 8.49 (d, $J$ = 8.0 Hz, 1H), 8.80 (d, $J$ = 8.0 Hz, 1H), 9.65 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.8, 160.5, 147.7, 138.8, 137.3, 137.0, 134.6, 128.9, 127.2, 127.1 (2), 125.4, 124.0, 123.7, 122.2, 121.5, 119.8, 119.2, 117.5, 116.1, 111.6, 49.0, 26.1. HRMS (ESI) calcd for $C_{24}H_{19}N_3ONa$ *m/z* $[M+Na]^+$: 388.1420, found: 388.1421.



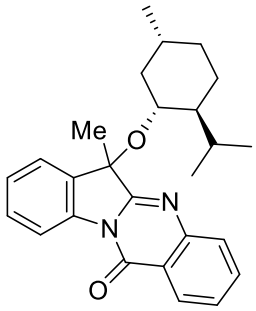

**6-allyl-6-methylindolo[2,1-b]quinazolin-12(6H)-one (16)**

White solid. $R_f$ = 0.40 (PE:EtOAc = 10:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.66 (s, 3H), 2.73-2.79 (m, 1H), 2.82-2.88 (m, 1H), 4.83 (dd, $J$ = 1.6, 10.0 Hz, 1H), 4.91 (dd, $J$ = 1.6, 16.8 Hz, 1H), 5.31-5.41 (m, 1H), 7.35 (dt, $J$ = 1.2, 7.2 Hz, 1H), 7.41-7.46 (m, 2H), 7.50-7.54 (m, 1H), 7.76-7.81 (m, 2H), 8.42 (d, $J$ = 8.0 Hz, 1H), 8.61 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 163.5, 160.3, 147.7, 139.2, 135.8, 134.4, 132.1, 128.6, 127.5, 127.0, 126.8, 126.6, 123.0, 121.5, 119.5, 117.3, 49.3, 44.8, 25.2. HRMS (ESI) calcd for $C_{19}H_{17}N_2O$ *m/z* $[M+H]^+$: 289.1335, found: 289.1336.



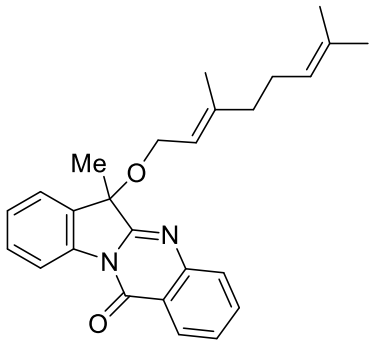
**6-methyl-6-(2-oxo-2-phenylethyl)indolo[2,1-b]quinazolin-12(6H)-one (17)**

White solid. $R_f$ = 0.20 (PE:EtOAc = 4:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.68 (s, 3H), 3.96-4.12 (m, 2H), 7.26 (dd, *J* = 1.2, 7.2 Hz, 1H), 7.32 (dd, *J* = 1.6, 7.6 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.44 (dt, *J* = 1.6, 7.6 Hz, 1H), 7.47-7.53 (m, 2H), 7.67 (dd, *J* = 1.6, 8.0 Hz, 1H), 7.73 (dt, *J* = 1.6, 6.8 Hz, 1H), 7.81 (dd, *J* = 1.2, 8.0 Hz, 2H), 8.46 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.69 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.7, 164.2, 160.4, 147.7, 139.9, 136.2, 136.0, 134.2, 133.5, 128.7 (2), 128.1, 127.2, 127.1, 126.6, 126.4, 121.8, 121.6, 117.5, 48.1, 46.3, 27.5. HRMS (ESI) calcd for $C_{24}H_{19}N_2O_2$ *m/z* $[M+H]^+$: 367.1441, found: 367.1443.




**6-((2-isopropyl-5-methylcyclohexyl)oxy)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (18)**

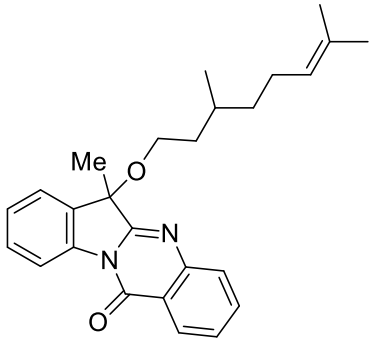
White solid. $R_f$ = 0.30 (PE:EtOAc = 20:1);$^1$H NMR (400 MHz, $CDCl_3$) δ 0.50 (d, *J* = 6.4 Hz, 3H), 0.61 (d, *J* = 6.8 Hz, 3H), 0.64-0.88 (m, 4H), 0.91 (d, *J* = 7.2 Hz, 3H), 1.07-1.12 (m, 1H), 1.28-1.35 (m, 1H), 1.41-1.45 (m, 1H), 1.50-1.54 (m, 1H), 1.82 (s, 3H), 2.36-2.45 (m, 1H), 3.06-3.12 (m, 1H), 7.39 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.48-7.57 (m, 3H), 7.80 (dt, *J* = 1.6, 7.6 Hz, 1H), 7.89 (dd, *J* = 1.6, 8.4 Hz, 1H), 8.43 (dd, *J* = 1.2, 8.0 Hz, 1H), 8.63 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 161.3, 160.0, 147.4, 139.1, 134.7, 131.1, 130.5, 128.1, 127.5, 127.0, 126.8, 124.7, 121.9, 117.6, 79.2, 75.8, 48.3, 42.6, 34.0, 31.3, 27.4, 25.1, 22.9, 22.3, 21.5, 16.3. HRMS (ESI) calcd for $C_{26}H_{31}N_2O_2$ *m/z* $[M+H]^+$: 403.2380, found: 403.2386.




**(E)-6-((3,7-dimethylocta-2,6-dien-1-yl)oxy)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (19)**

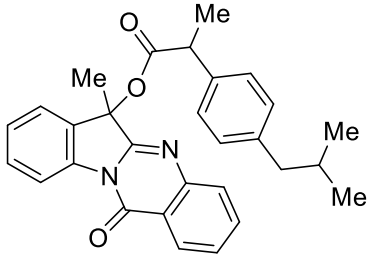
White solid. $R_f$ = 0.30 (PE:EtOAc = 15:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.30 (s, 3H), 1.50 (s, 3H), 1.62 (s, 3H), 1.77-1.91 (m, 7H), 3.60-3.70 (m, 2H), 4.92-4.95 (m, 1H), 5.22 (dt, *J* = 1.2, 7.2 Hz, 1H), 7.41 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.51 (dt, *J* = 1.2, 7.6 Hz,

1H), 7.56-7.59 (m, 2H), 7.81 (dt, $J$ = 1.6, 7.2 Hz, 1H), 7.90 (dd, $J$ = 1.2, 8.0 Hz, 1H), 8.42 (dd, $J$ = 1.6, 8.0 Hz, 1H), 8.60 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.9, 159.8, 147.4, 141.2, 139.3, 134.7, 131.7 (2), 130.6, 128.2, 127.6, 127.1, 127.0, 124.1, 124.0, 122.1, 120.1, 117.5, 80.6, 62.5, 39.5, 26.6, 26.2, 25.8, 17.8, 16.4. HRMS (ESI) calcd for $C_{26}H_{29}N_2O_2$ *m/z* $[M+H]^+$: 401.2224, found: 401.2225.




**6-((3,7-dimethyloct-6-en-1-yl)oxy)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (20)**

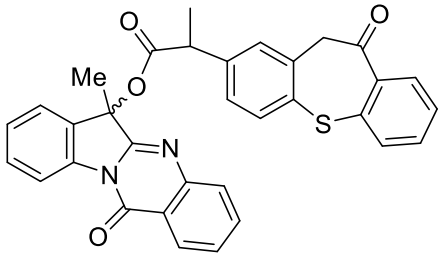
White solid. $R_f$ = 0.50 (PE:EtOAc = 5:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.73 (d, $J$ = 6.4 Hz, 3H), 0.95-1.07 (m, 1H), 1.12-1.37 (m, 2H), 1.45-1.62 (m, 5H), 1.63 (s, 3H), 1.82 (s, 3H), 1.84-1.94 (m, 2H), 2.92-3.13 (m, 2H), 4.97-5.03 (m, 1H), 7.39 (t, $J$ = 7.6 Hz, 1H), 7.50-7.58 (m, 3H), 7.81 (dt, $J$ = 1.6, 8.0 Hz, 1H), 7.89 (d, $J$ = 8.0 Hz, 1H), 8.43 (dd, $J$ = 1.6, 8.0 Hz, 1H), 8.59 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 159.9, 159.5 (2), 147.4, 139.2 (2), 134.7, 131.9, 131.2, 130.5, 128.2 (2), 127.6, 127.1, 127.0, 124.9 (2), 123.9, 122.1, 117.4, 80.9 (2), 63.6, 63.5, 37.2, 37.0 (2), 36.9, 29.3 (2), 26.4, 25.8, 25.5, 19.6, 19.4, 17.7. HRMS (ESI) calcd for $C_{26}H_{31}N_2O_2$ *m/z* $[M+H]^+$: 403.2380, found: 403.2386.




**6-methyl-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl 2-(4-isobutylphenyl)propanoate (21)**

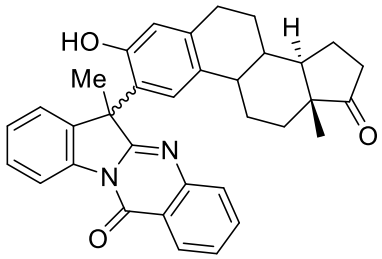
White solid. $R_f$ = 0.30 (PE:DCM = 1:2); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.89 (s, 3H), 0.91 (s, 3H), 1.43 (d, $J$ = 7.2 Hz, 3H), 1.80-1.90 (m, 4H), 2.45 (d, $J$ = 7.2 Hz, 2H), 3.73 (q, $J$ = 7.2 Hz, 1H), 7.06-7.12 (m, 4H), 7.30 (dd, $J$ = 1.2, 7.2 Hz, 1H), 7.33 (dd, $J$ = 1.6, 7.2 Hz, 1H), 7.46-7.54 (m, 2H), 7.67 (dd, $J$ = 1.2, 8.0 Hz, 1H), 7.75 (dt, $J$ = 1.6, 6.8 Hz, 1H), 8.40 (dd, $J$ = 1.2, 8.0 Hz, 1H), 8.57 (d, $J$ = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 172.9, 159.8, 158.5, 147.3, 140.7, 139.4, 136.9, 134.4, 131.4, 130.6, 129.4, 127.8, 127.4 (2), 127.2, 126.7, 122.3, 122.1, 117.4, 79.5, 45.2, 44.9, 30.3, 25.2,

22.5, 18.6. HRMS (ESI) calcd for $C_{29}H_{29}N_2O_3$ *m/z* $[M+H]^+$: 453.2173, found: 453.2177.



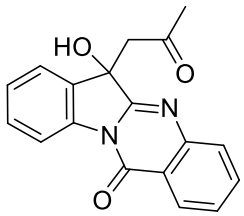

**6-methyl-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl 2-(10-oxo-10,11-dihydrodibenzo[b,f]thiepin-2-yl)propanoate (22)**

White solid. $R_f$ = 0.20 (PE:DCM = 1:3); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.29 (d, *J* = 6.8 Hz, 3H), 1.78 (s, 3H), 3.80-3.86 (m, 1H), 4.32-4.38 (m, 2H), 6.88 (dd, *J* = 1.6, 7.6 Hz, 1H), 6.96 (dd, *J* = 2.0, 8.0 Hz, 1H), 7.15-7.19 (m, 2H), 7.35 (dt, *J* = 1.2, 8.0 Hz, 1H), 7.44-7.49 (m, 2H), 7.52-7.56 (m, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.63 (dd, *J* = 1.2, 8.0 Hz, 1H), 7.77-7.79 (m, 2H), 8.25 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.56 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 191.3, 171.9, 159.7, 158.7, 147.2, 142.4, 140.3, 139.3, 138.2, 136.3, 134.5, 133.6, 132.8, 131.7 (2), 131.0, 130.7, 128.5, 127.8, 127.5, 127.3, 127.1, 126.8, 126.5, 122.3, 122.1, 117.3, 79.8, 51.1, 44.8, 25.2, 18.2. HRMS (ESI) calcd for $C_{33}H_{25}N_2O_4S$ *m/z* $[M+H]^+$: 545.1530, found: 545.1533.



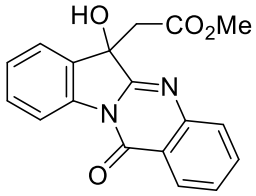

**6-((13R,14R)-3-hydroxy-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-2-yl)-6-methylindolo[2,1-b]quinazolin-12(6H)-one (23)**

White solid. $R_f$ = 0.30 (PE:EtOAc = 3:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 0.93 (s, 3H), 1.27-1.63 (m, 6H), 1.86-2.13 (m, 6H), 2.16 (s, 3H), 2.45-2.52 (m, 1H), 2.83-2.87 (m, 2H), 6.84 (s, 1H), 6.89 (s, 1H), 7.52-7.61 (m, 4H), 7.74-7.81 (m, 2H), 8.40 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.70 (d, *J* = 7.6 Hz, 1H), 11.37 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.5, 159.6, 154.6, 145.6, 139.0, 138.6, 134.9, 134.5, 131.5, 129.5, 127.5, 127.2, 126.8, 126.6, 126.0, 125.3, 124.0, 121.4, 120.9, 117.9, 53.8, 50.4, 48.1, 44.3, 38.6, 36.0, 31.7, 29.3, 26.6, 25.9, 24.6, 21.7, 14.0. HRMS (ESI) calcd for $C_{34}H_{33}N_2O_3$ *m/z* $[M+H]^+$: 517.2486, found: 517.2488.



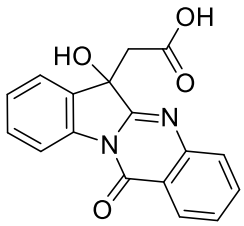
**methyl 2-(6-hydroxy-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl)acetate (24)**[2]

White solid. $R_f$ = 0.20 (PE:EtOAc = 1:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.14 (s, 3H), 3.41 (d, *J* = 17.6 Hz, 1H), 3.55 (d, *J* = 17.6 Hz, 1H), 4.92 (s, 1H), 7.16 (dd, *J* = 1.2, 7.6 Hz, 1H), 7.23-7.28 (m, 1H), 7.47-7.51 (m, 2H), 7.71-7.76 (m, 2H), 8.24 (d, *J* = 7.6 Hz, 1H), 8.35 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 206.9, 159.8, 159.7, 147.3, 139.2, 134.6, 132.2, 130.6, 127.9, 127.6, 127.2, 127.1, 123.6, 122.0, 117.1, 75.9, 50.9, 31.2.



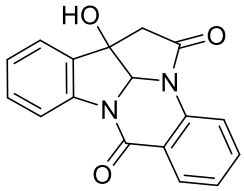
**methyl 2-(6-hydroxy-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl)acetate (25)**[3]

Pale yellow solid. $R_f$ = 0.20 (PE:EtOAc = 2:1); $^1$H NMR (400 MHz, DMSO-d6) δ 3.32 (m, 3H), 3.44-3.54 (m, 2H), 6.67 (s, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.53 (dt, *J* = 1.2, 8.0 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.90 (dt, *J* = 1.6, 8.4 Hz, 1H), 8.33 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, DMSO-d6) δ 169.9, 161.3, 159.3, 147.5, 139.7, 135.3, 133.7, 130.5, 128.0 (2), 127.1, 126.9, 124.5, 121.8, 116.4, 75.1, 51.8, 43.1. HRMS (ESI) calcd for $C_{18}H_{15}N_2O_4$ *m/z* $[M+H]^+$: 323.1026, found: 323.1027.



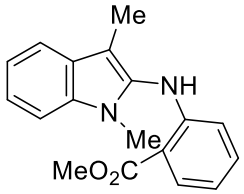
**2-(6-hydroxy-12-oxo-6,12-dihydroindolo[2,1-b]quinazolin-6-yl)acetic acid (26)**[4]

White solid. $R_f$ = 0.20 (DCM:MeOH = 10:1); $^1$H NMR (400 MHz, $CD_3OD$) δ 3.35-3.49 (m, 2H), 7.40 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.50 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.60 (dt, *J* = 1.6, 8.0 Hz, 1H), 7.67 (dd, *J* = 1.6, 7.6 Hz, 1H), 7.81-7.88 (m, 2H), 8.36 (dd, *J* = 1.6, 8.0 Hz, 1H), 8.50 (d, *J* = 8.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CD_3OD$) δ 163.1, 161.3, 148.7, 141.0, 135.9, 135.0, 131.1, 128.5, 128.4, 128.0, 127.7, 124.8, 123.1, 117.9, 76.6, 44.9.



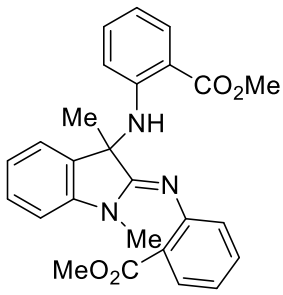
**11b-hydroxy-2a1,11b-dihydro-7H-2a,7a-diazabenzo[b]cyclopenta[lm]fluorene-2, 7(1H)-dione (27)**[3]

White solid. $R_f$ = 0.40 (PE:EtOAc = 1:1); $^1$H NMR (400 MHz, DMSO-d6) δ 3.05 (d, *J* = 18.4 Hz, 1H), 3.15 (d, *J* = 18.4 Hz, 1H), 5.80 (s, 1H), 6.72 (s, 1H), 7.23 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.41 (dt, *J* = 1.2, 7.6 Hz, 1H), 7.46 (dt, *J* = 2.0, 7.6 Hz, 1H), 7.54 (dd, *J* = 1.2, 7.6 Hz, 1H), 7.70-7.76 (m, 2H), 7.93 (d, *J* = 8.0 Hz, 1H), 8.04 (dd, *J* = 1.6, 7.6 Hz, 1H); $^{13}$C NMR (100 MHz, DMSO-d6) δ 175.8, 164.0, 145.7, 141.8, 140.7, 138.9, 135.2, 133.8, 131.4, 130.3, 130.0, 128.8, 127.4, 120.2, 87.9, 82.9, 51.2.



**methyl 2-((1,3-dimethyl-1H-indol-2-yl)amino)benzoate (29)**

White solid. $R_f$ = 0.60 (PE:EtOAc = 7:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 2.17 (s, 3H), 3.56 (s, 3H), 3.96 (s, 3H), 6.42 (dd, *J* = 1.2, 8.8 Hz, 1H), 6.73 (dt, *J* = 1.2, 8.0 Hz, 1H), 7.15 (dt, *J* = 1.2, 8.0 Hz, 1H), 7.22-7.31 (m, 3H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.99 (dd, *J* = 1.6, 8.0 Hz, 1H), 9.18 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 169.3, 150.2, 134.9, 134.8, 132.1, 131.4, 127.5, 121.7, 119.1, 118.9, 117.2, 114.1, 111.0, 109.3, 105.1, 52.0, 28.7, 8.5. HRMS (ESI) calcd for $C_{18}H_{19}N_2O_2$ *m/z* $[M+H]^+$: 295.1441, found: 295.1441.



**methyl(Z)-2-((3-((2-(methoxycarbonyl)phenyl)amino)-1,3-dimethylindolin-2-ylid ene)amino)benzoate (30)**

Brown oil. $R_f$ = 0.20 (PE:EtOAc = 7:1); $^1$H NMR (400 MHz, $CDCl_3$) δ 1.63 (s, 3H), 3.40 (s, 3H), 3.69 (s, 3H), 3.77 (s, 3H), 5.83 (d, *J* = 8.0 Hz, 1H), 6.20 (d, *J* = 8.0 Hz, 1H), 6.58 (dt, *J* = 1.2, 7.2 Hz, 1H), 6.84-6.93 (m, 3H), 7.02 (dd, *J* = 1.6, 7.6 Hz, 1H), 7.05-7.10 (m, 2H), 7.25-7.29 (m, 1H), 7.84 (dd, *J* = 1.6, 8.0 Hz, 1H), 7.88 (dd, *J* = 1.6, 8.0 Hz, 1H), 7.96 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 168.7, 166.9, 157.9, 149.2, 148.6, 143.9, 134.2, 132.1, 131.6, 130.8, 129.1, 122.7, 122.0, 121.7, 121.4, 120.5,

115.8, 113.1, 111.6, 107.4, 62.0, 51.7, 51.5, 29.2, 28.3. HRMS (ESI) calcd for $C_{26}H_{26}N_3O_4$ *m/z* $[M+H]^+$: 444.1918, found: 444.1918.

**(I) References**

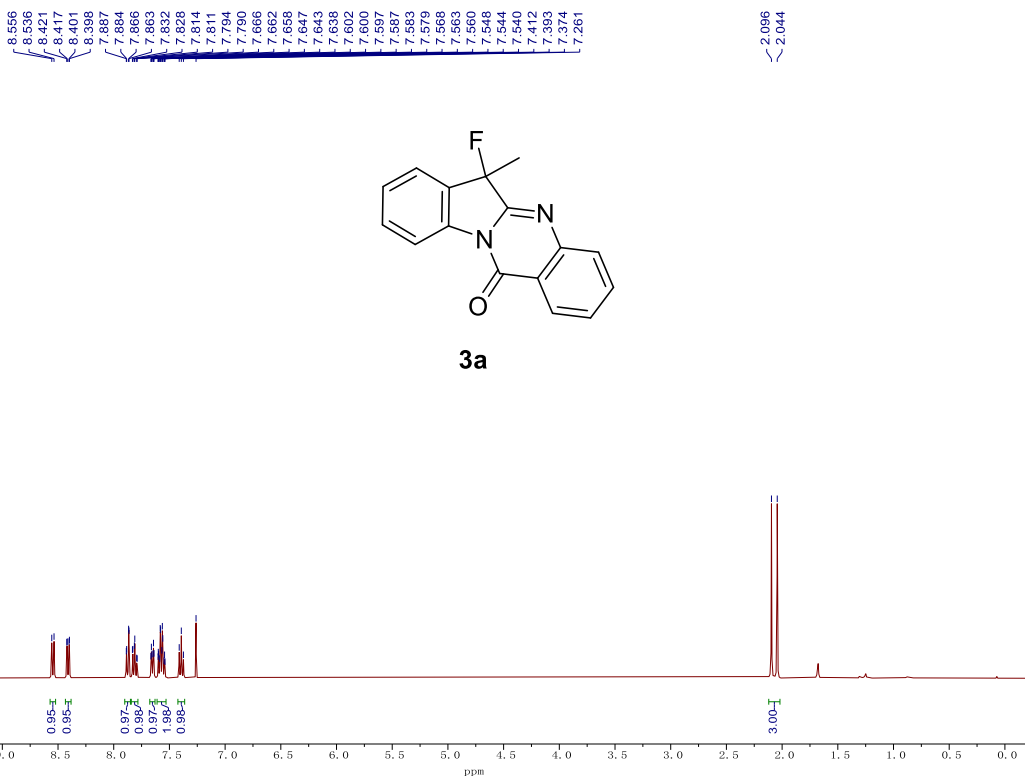

1**.** Vaidya. S.; Argade, N. *Org. Lett.* **2013**, *15*, 4006−4009.

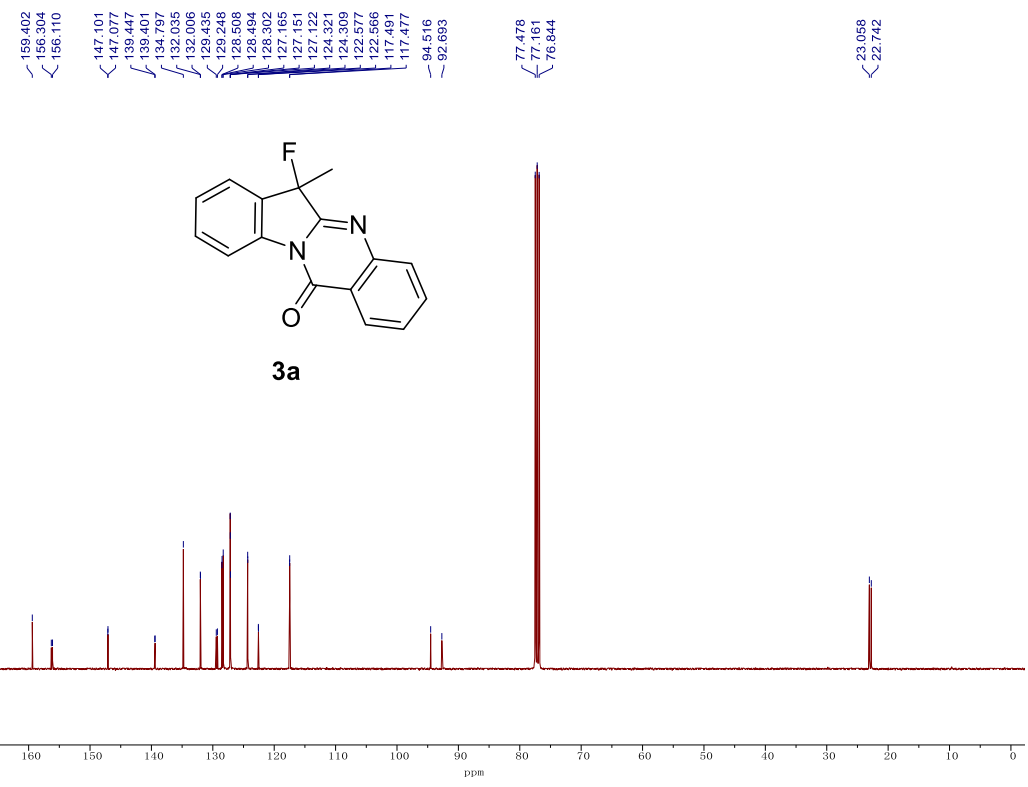
2. Jiao, C-W.; Lin, W.-C.; Wu, Y.-T.; Wu, P.-L. *J. Nat*. *Prod*. **2008**, *71*, 1275−1279.

3. Vaidya, S. D.; Argade, N. P. *Org. Lett*. **2013**, *15*, 4006–4009.

4. Reddy, U. V. S.; Chennapuram, M.; Seki, K.; Seki, C.; Anusha, B.; Kwon, E.; Okuyama, Y.; Uwai, K.; Tokiwa, M.; Takeshita, M.; Nakano, H. *Eur. J. Org. Chem.* **2017**. 3874–3885.

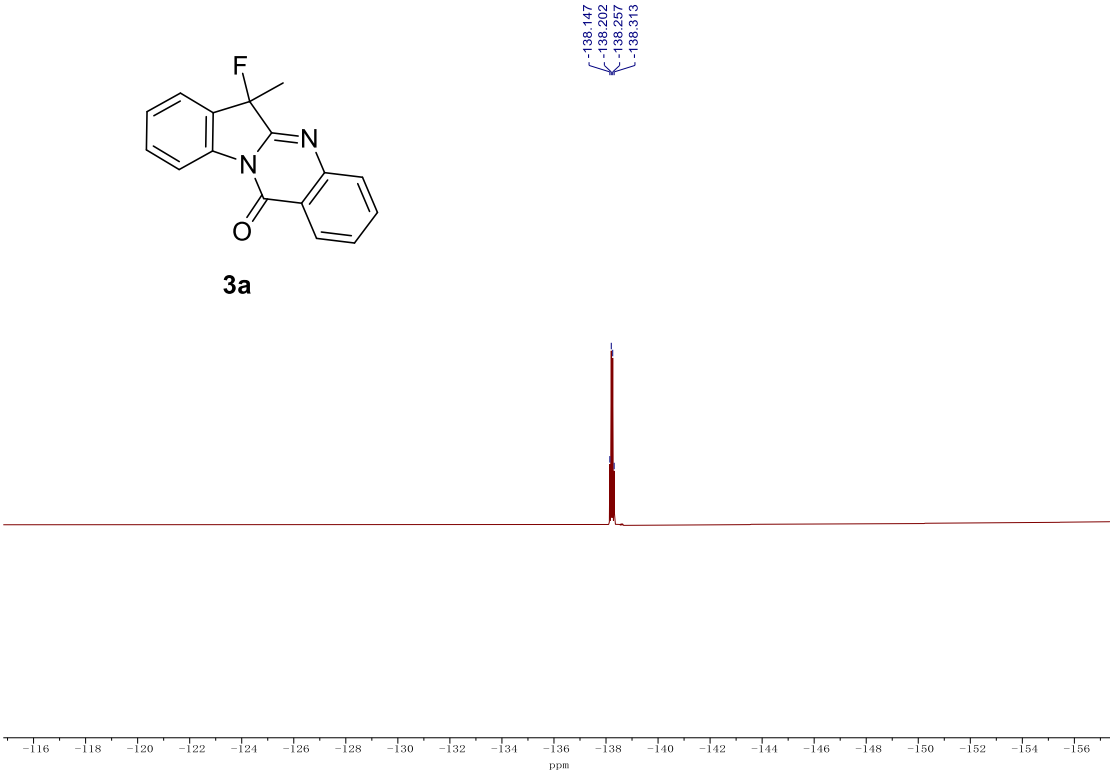
## (J) NMR Spectra



F
N
N
O

**3a**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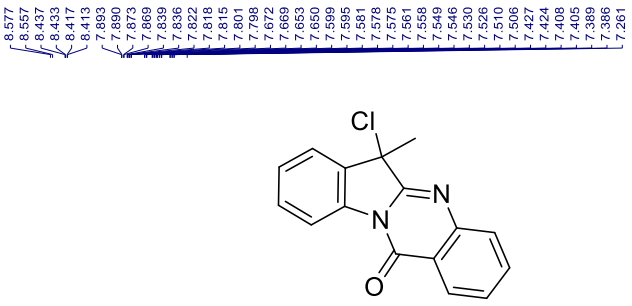
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7.798
7.672
7.669
7.653
7.650
7.599
7.595
7.581
7.578
7.575
7.561
7.558
7.549
7.546
7.530
7.526
7.510
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Cl
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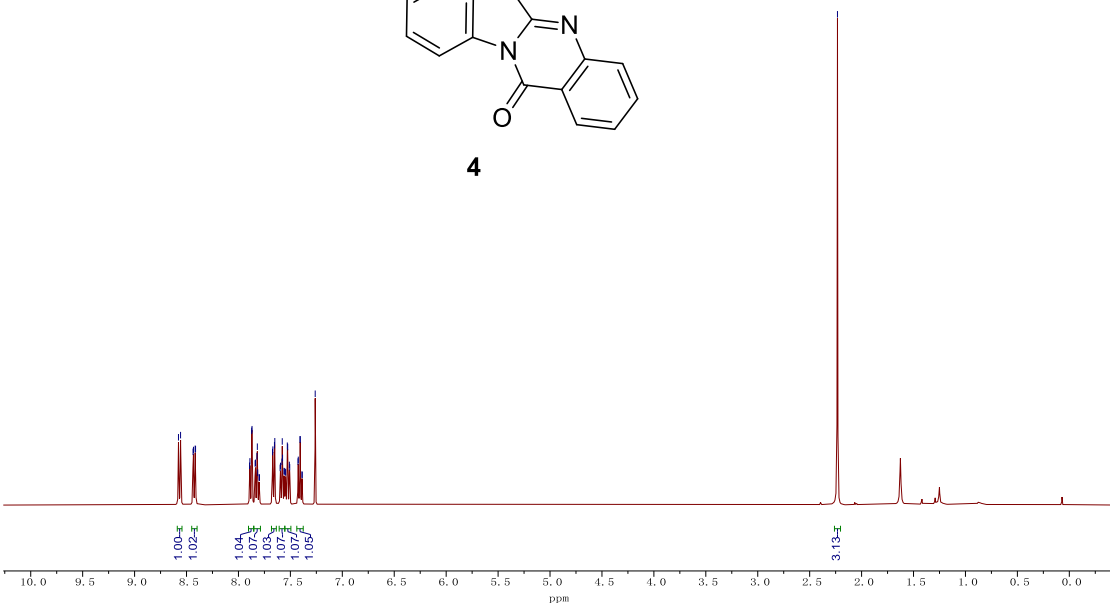
N
O

**4**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1.05
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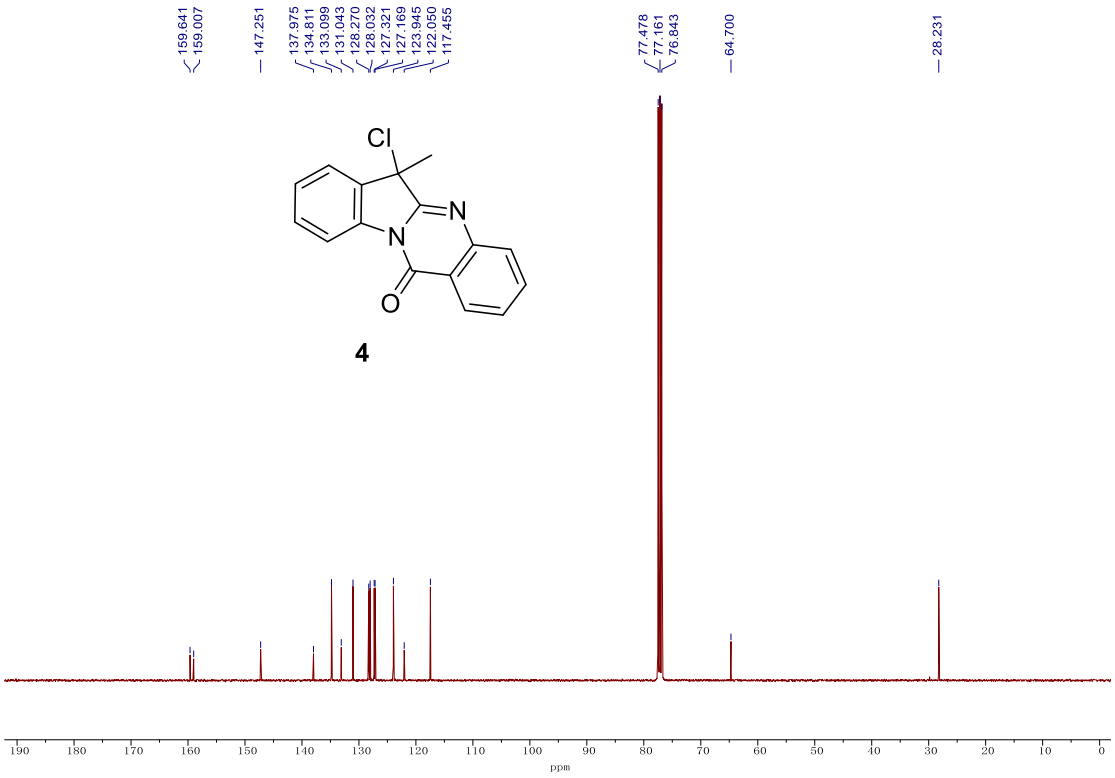
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Cl
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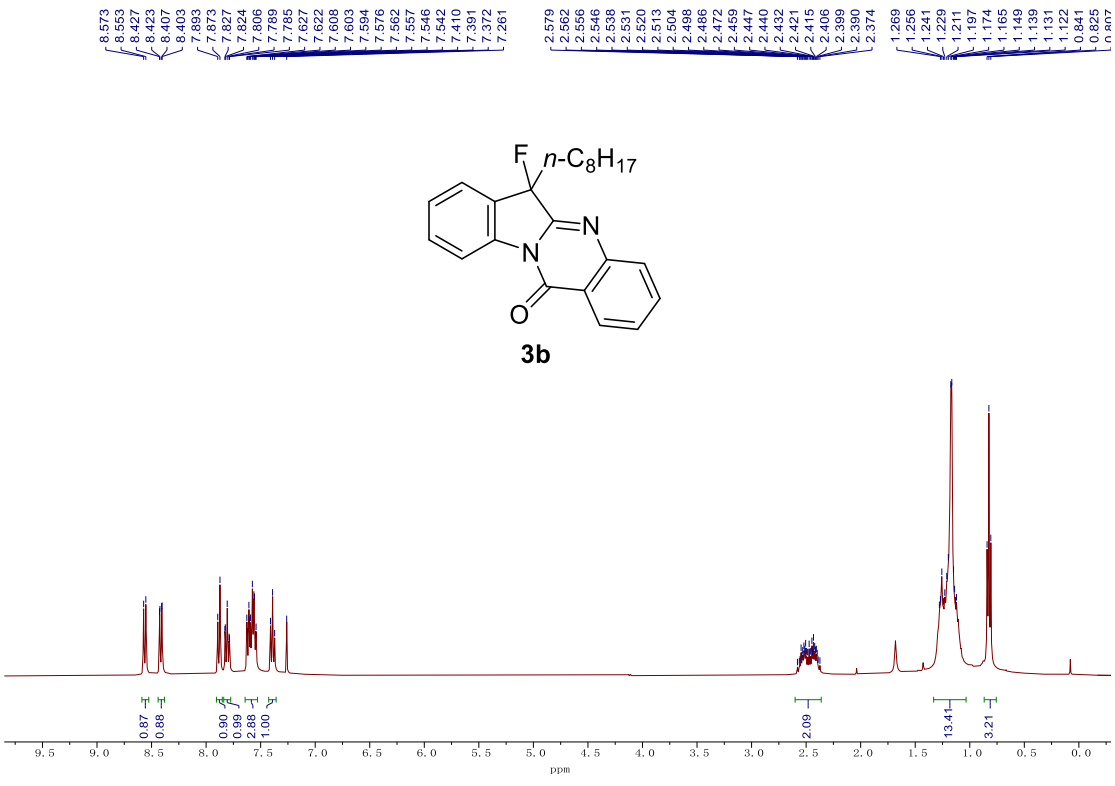
N
O
ppm

**4**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7.391
7.372
7.261
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2.415
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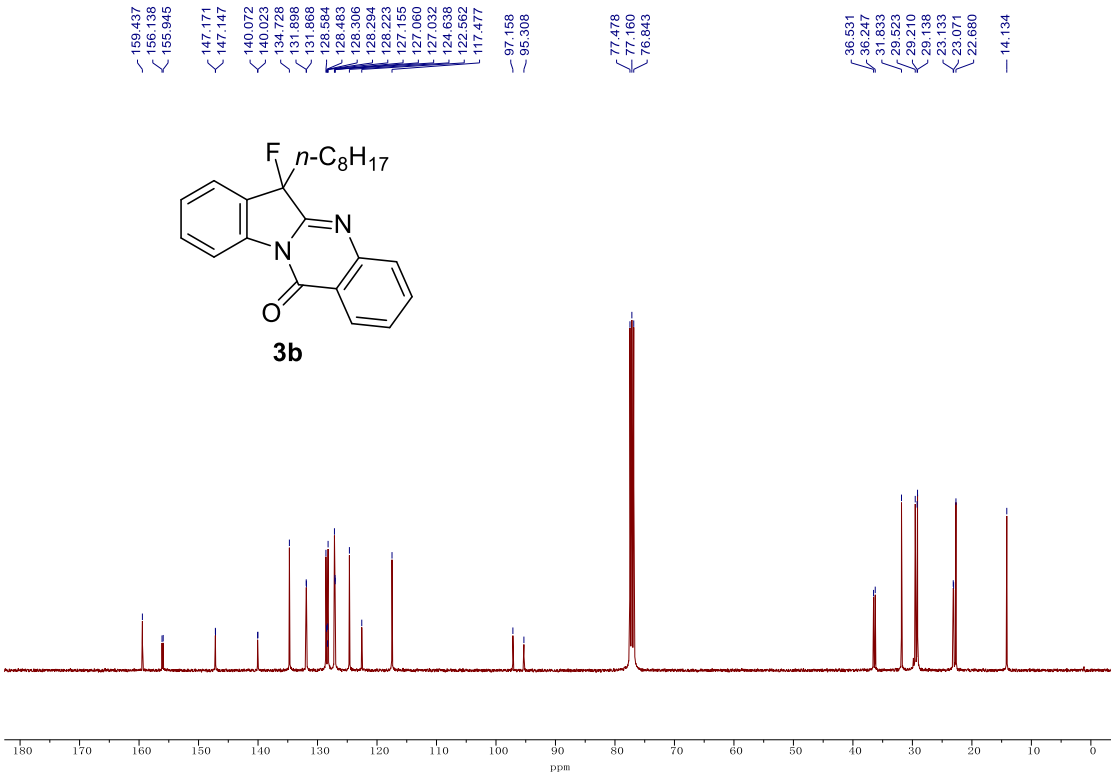
**3b**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N
N
O
3b
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50
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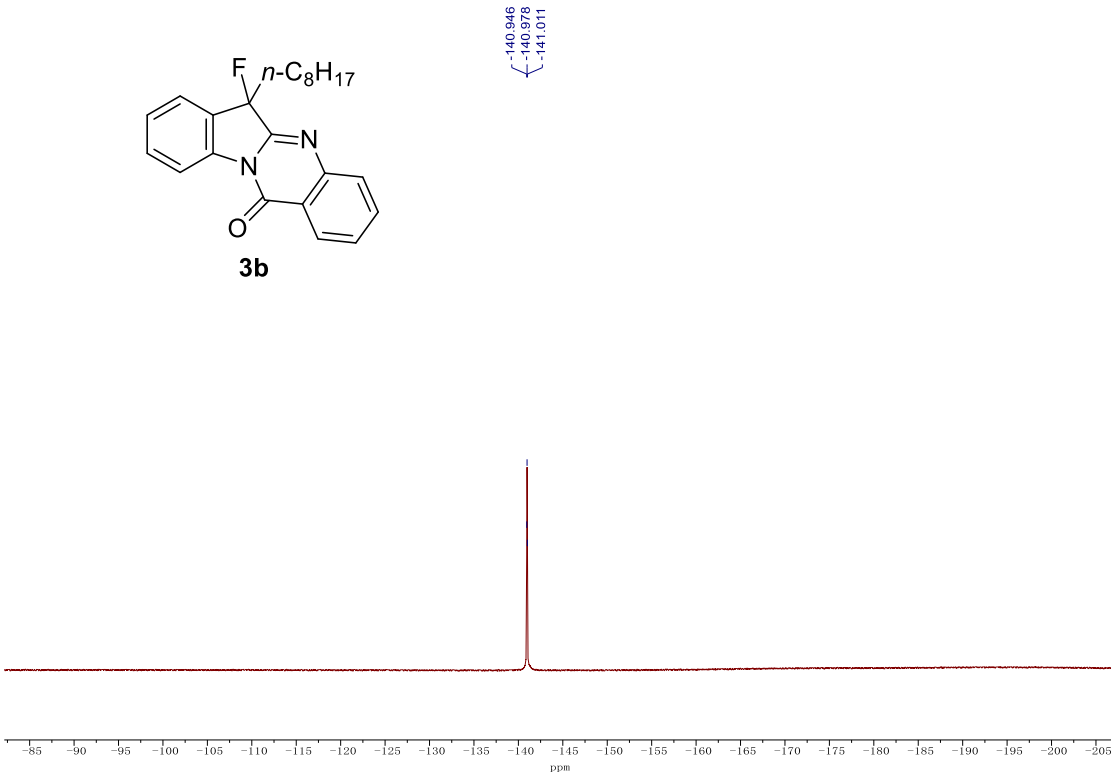
0
ppm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−110
−115
−120
−125
−130
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−155
−160
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−205
ppm


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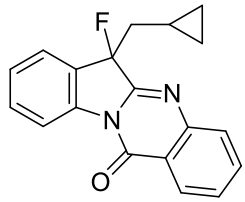
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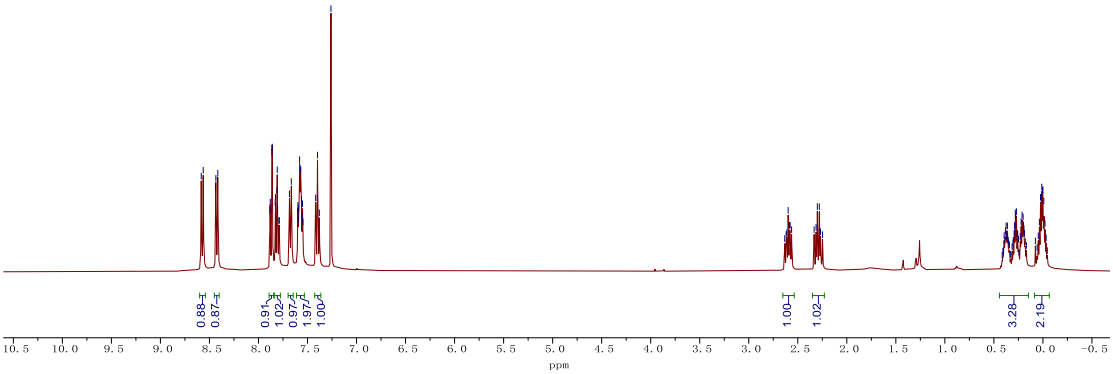
N
O

**3c**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6.0
5.5
5.0
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4.0
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ppm


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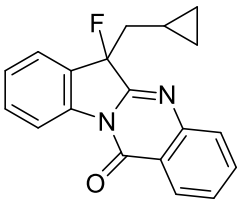
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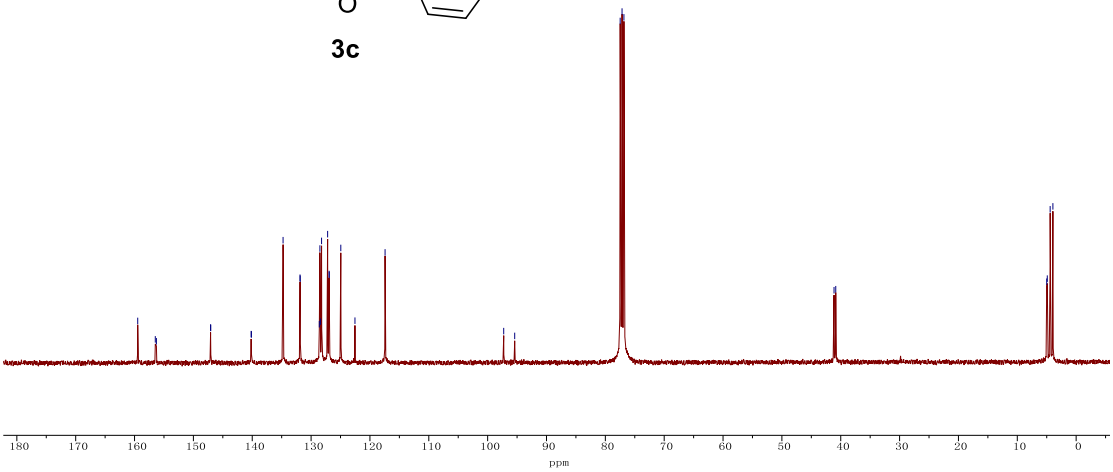
N
N
O

**3c**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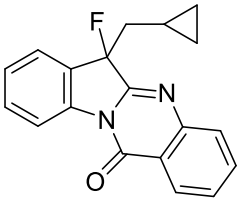
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**3c**


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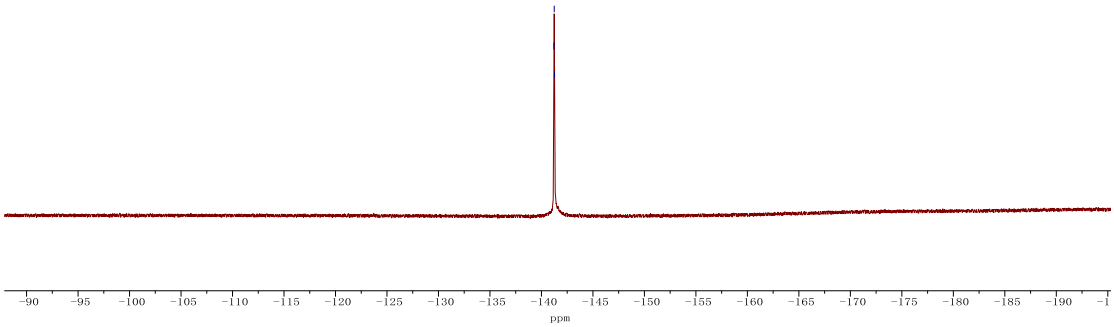
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7.236
7.232
7.228
7.217
7.213
7.209
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7.152
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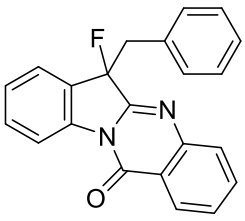
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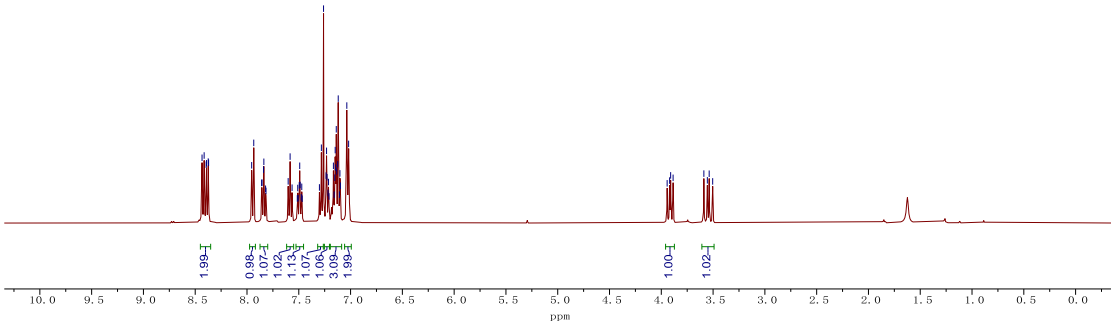
N
O

**3d**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1.13
1.07
1.06
3.09
1.99
1.00
1.02
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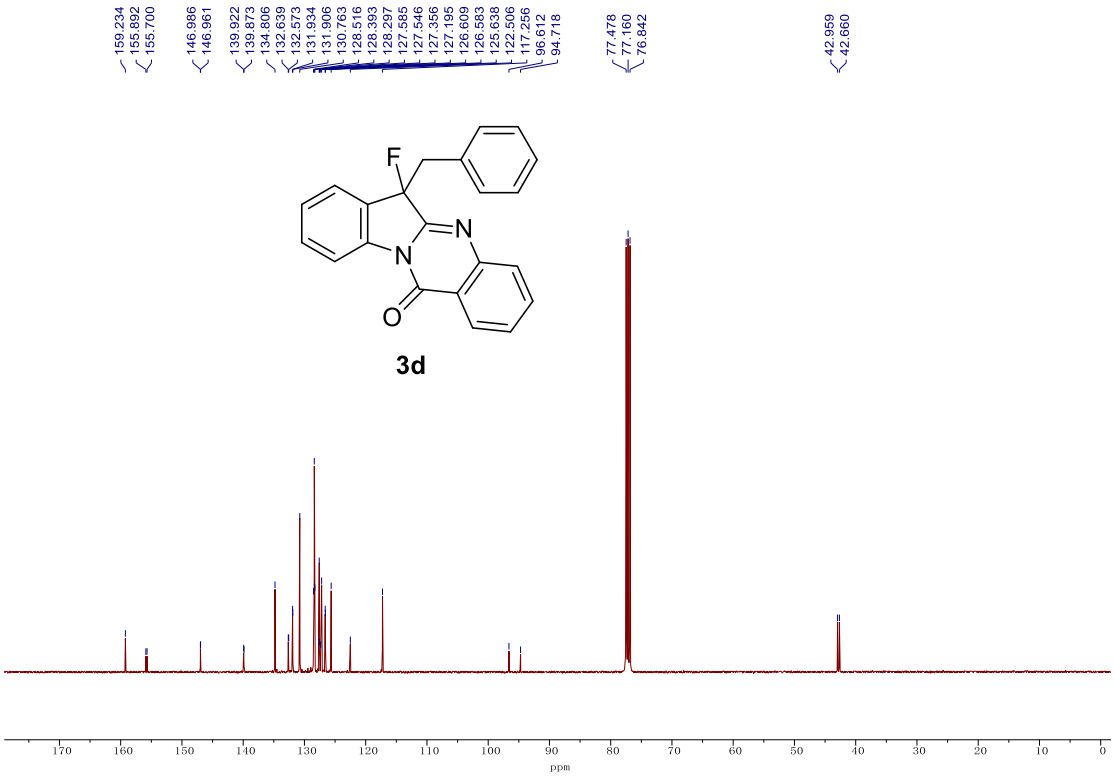
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42.660
F
N
N
O
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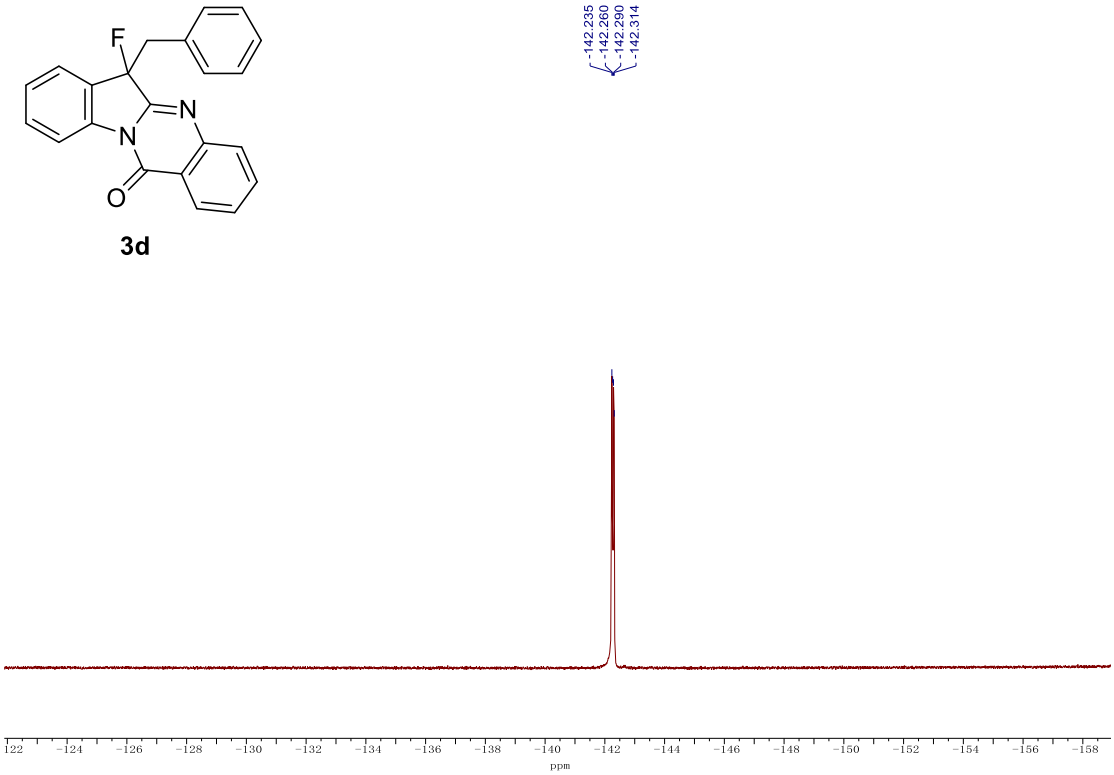
ppm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-144
-146
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-152
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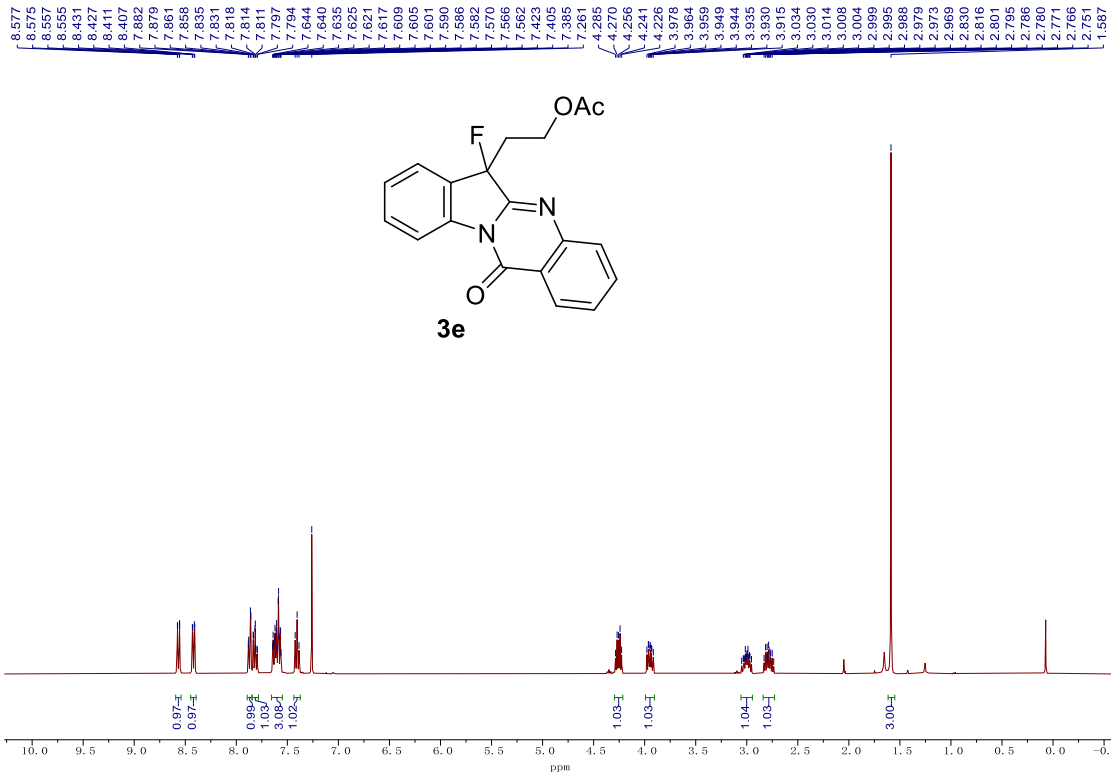
-158
ppm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7.858
7.835
7.831
7.818
7.814
7.811
7.797
7.794
7.644
7.640
7.635
7.625
7.621
7.617
7.609
7.605
7.601
7.590
7.586
7.582
7.570
7.566
7.562
7.423
7.405
7.385
7.261
4.285
4.270
4.256
4.241
4.226
3.978
3.964
3.959
3.949
3.944
3.935
3.930
3.915
3.034
3.030
3.014
3.008
3.004
2.999
2.995
2.988
2.979
2.973
2.969
2.830
2.816
2.801
2.795
2.786
2.780
2.771
2.766
2.751
1.587
OAc
F
N
N
O
3e
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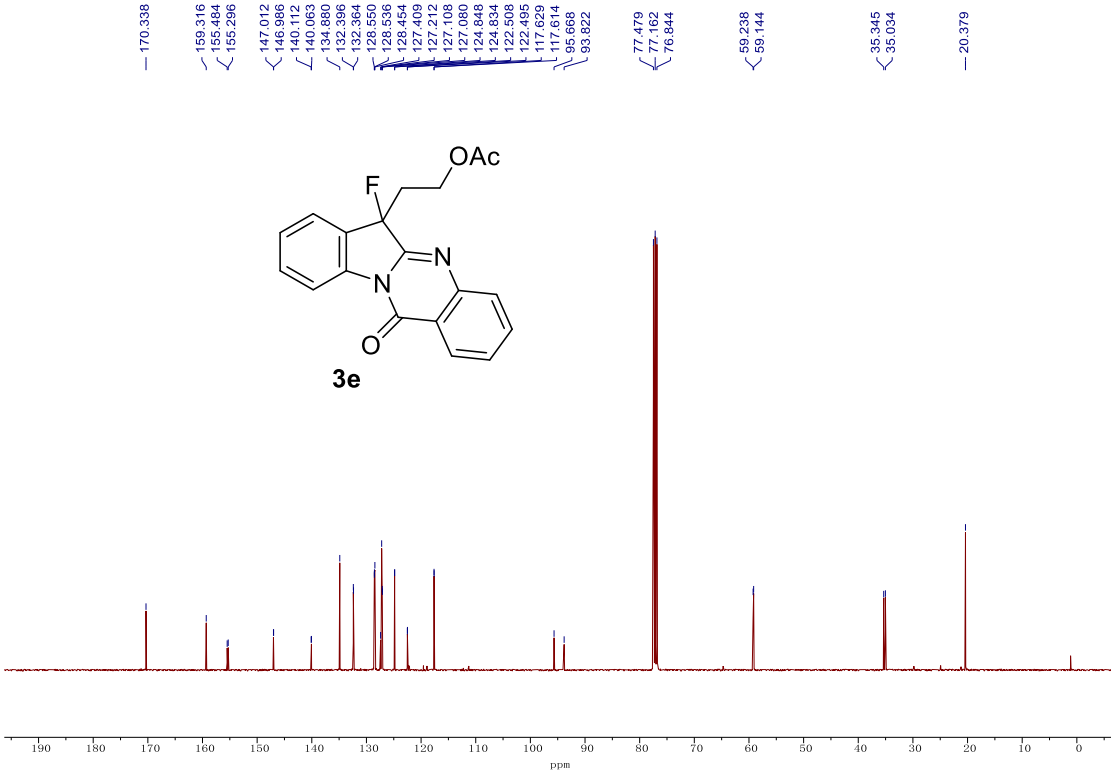
0.97
0.99
1.03
3.08
1.02
1.03
1.03
1.04
1.03
3.00
ppm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128.536
128.454
127.409
127.212
127.108
127.080
124.848
124.834
122.508
122.495
117.629
117.614
95.668
93.822
77.479
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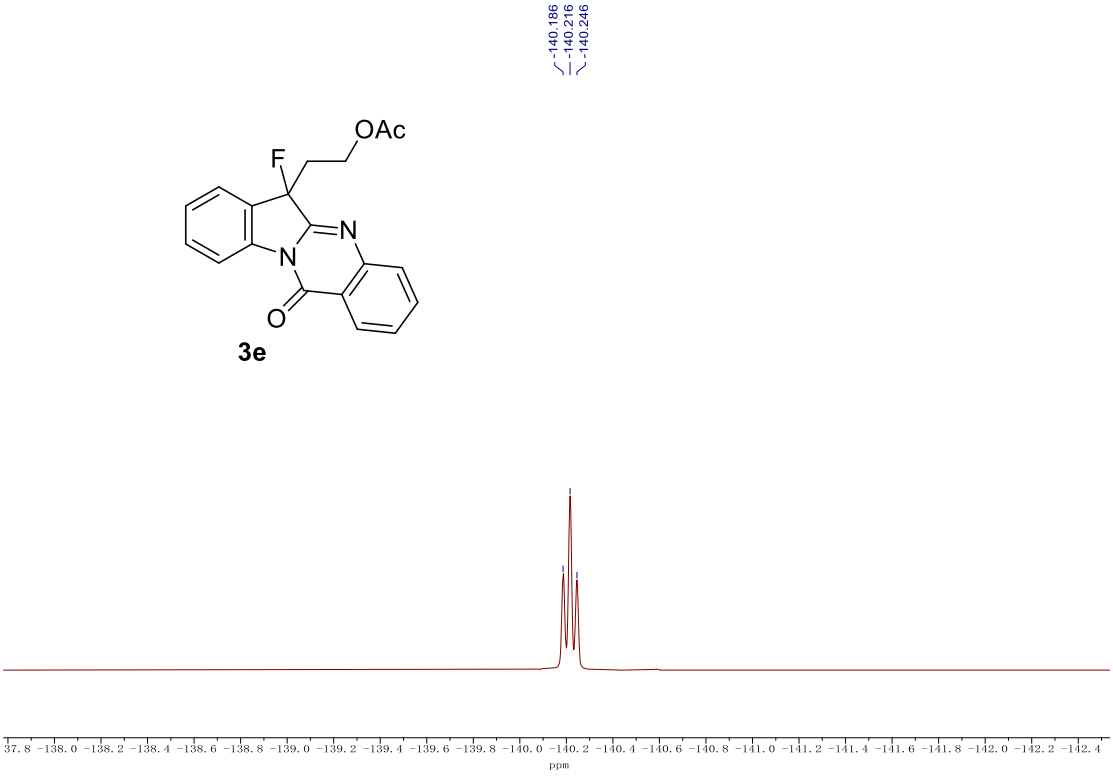
59.144
35.345
35.034
20.379
OAc
F
N
N
O
3e
ppm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-140.216
-140.246
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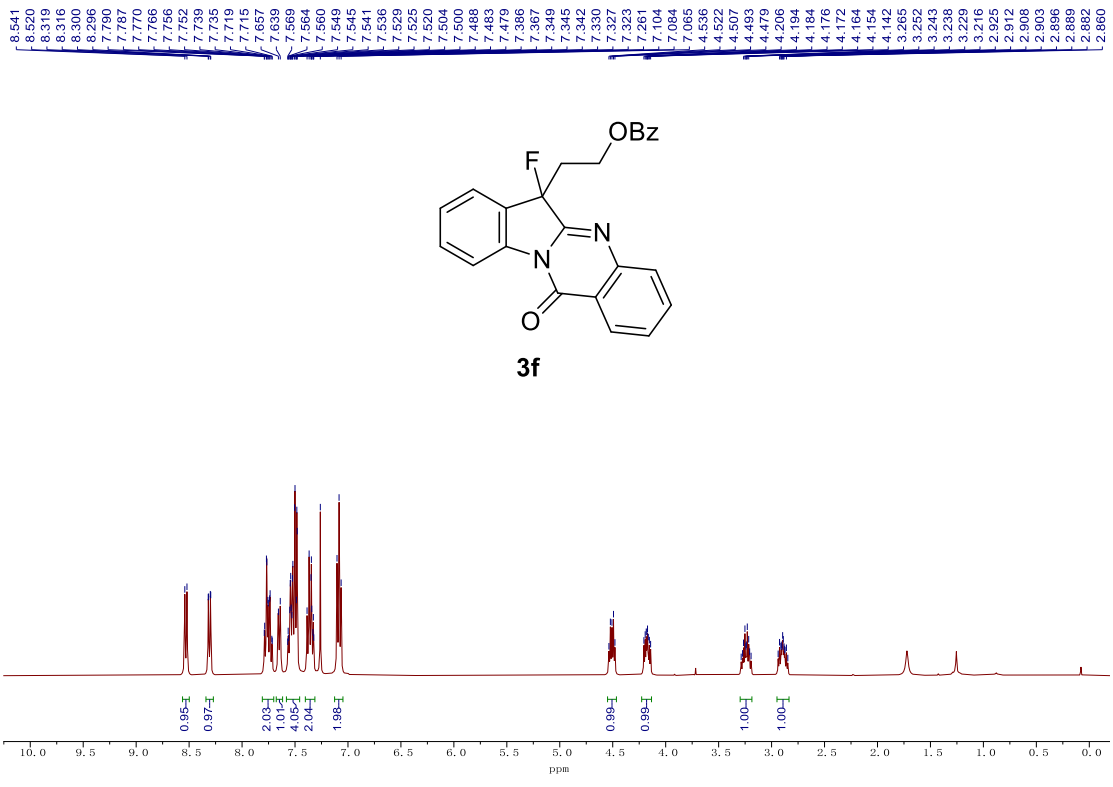
F
N
N
O
3e
37.8 -138.0 -138.2 -138.4 -138.6 -138.8 -139.0 -139.2 -139.4 -139.6 -139.8 -140.0 -140.2 -140.4 -140.6 -140.8 -141.0 -141.2 -141.4 -141.6 -141.8 -142.0 -142.2 -142.4
ppm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7.766
7.756
7.752
7.739
7.735
7.719
7.715
7.657
7.639
7.569
7.564
7.560
7.549
7.545
7.541
7.536
7.529
7.525
7.520
7.504
7.500
7.488
7.483
7.479
7.386
7.367
7.349
7.345
7.342
7.330
7.327
7.323
7.261
7.104
7.084
7.065
4.536
4.522
4.507
4.493
4.479
4.206
4.194
4.184
4.176
4.172
4.164
4.154
4.142
3.265
3.252
3.243
3.238
3.229
3.216
2.925
2.912
2.908
2.903
2.896
2.889
2.882
2.860
OBz
F
N
N
O
3f
0.95
0.97
2.03
1.01
4.05
2.04
1.98
0.99
0.99
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


165.881
159.217
155.549
155.361
146.992
146.966
140.222
140.174
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133.031
132.396
132.364
129.270
129.122
128.472
128.458
128.230
128.145
127.187
127.151
127.123
127.105
127.003
124.823
124.608
122.541
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77.478
77.160
76.843
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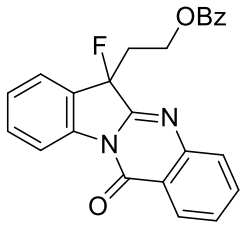
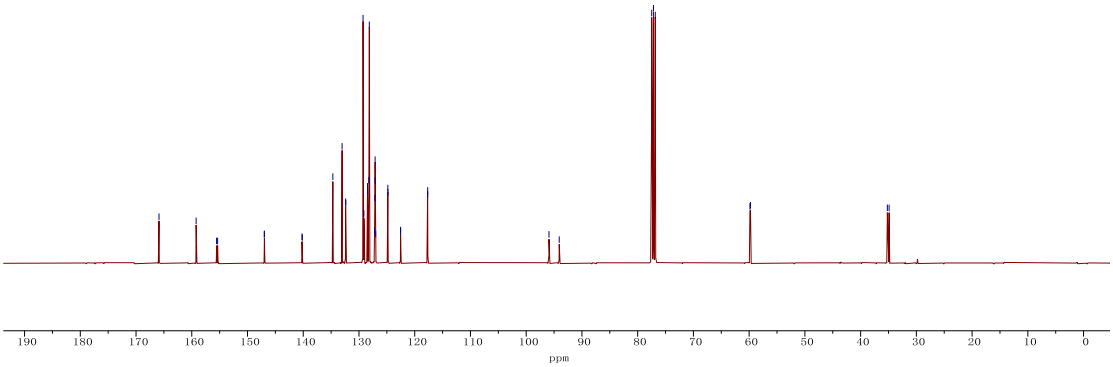
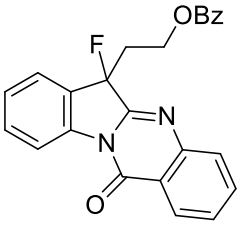
59.758
35.204
34.890


OBz
F
N
N
O

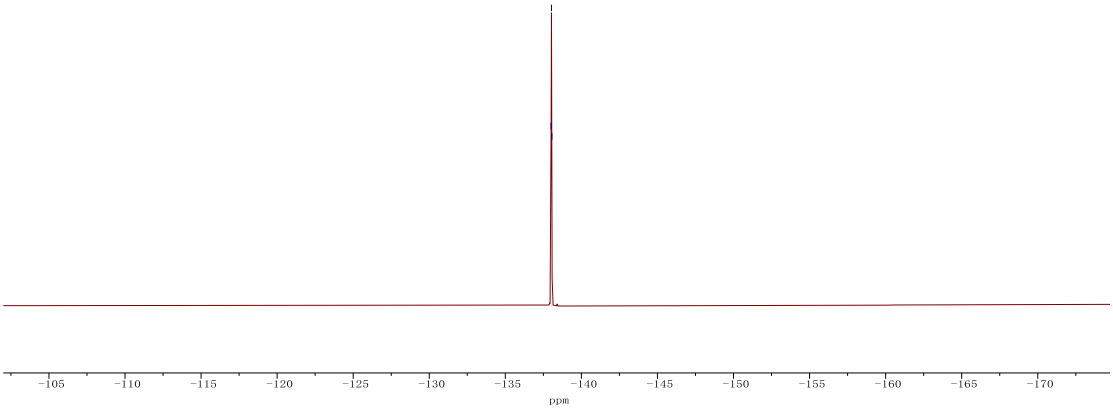
**3f**

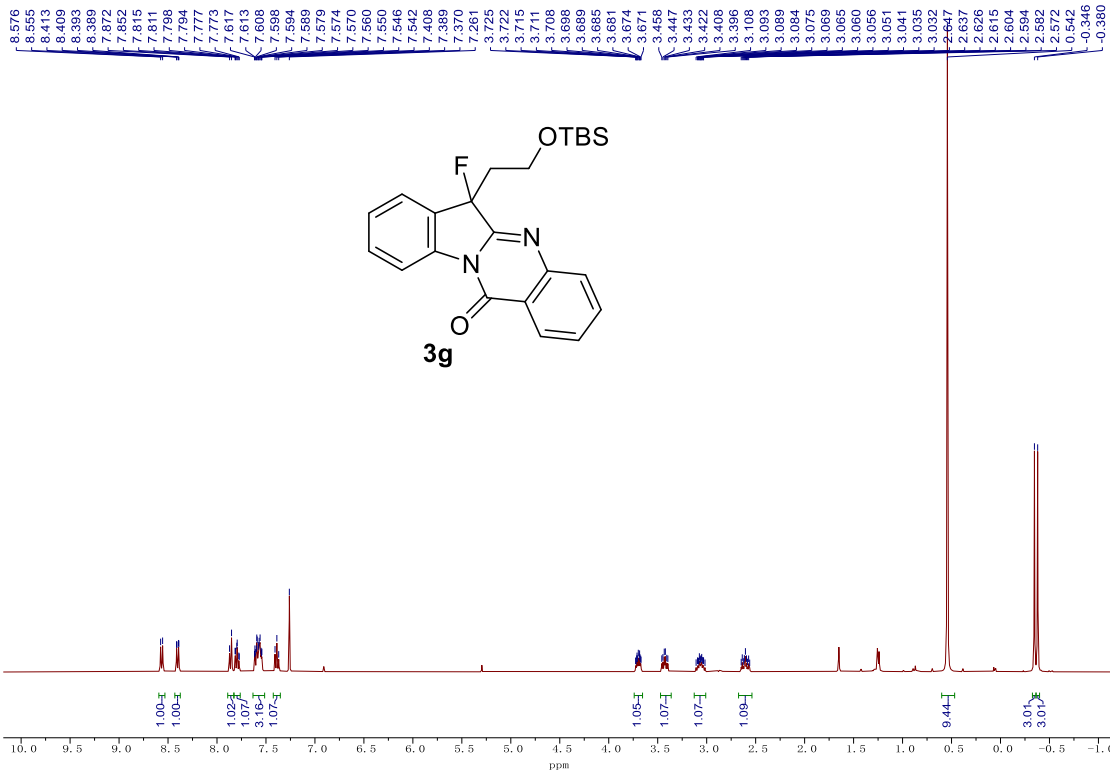

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-138.007
-138.035
-138.063

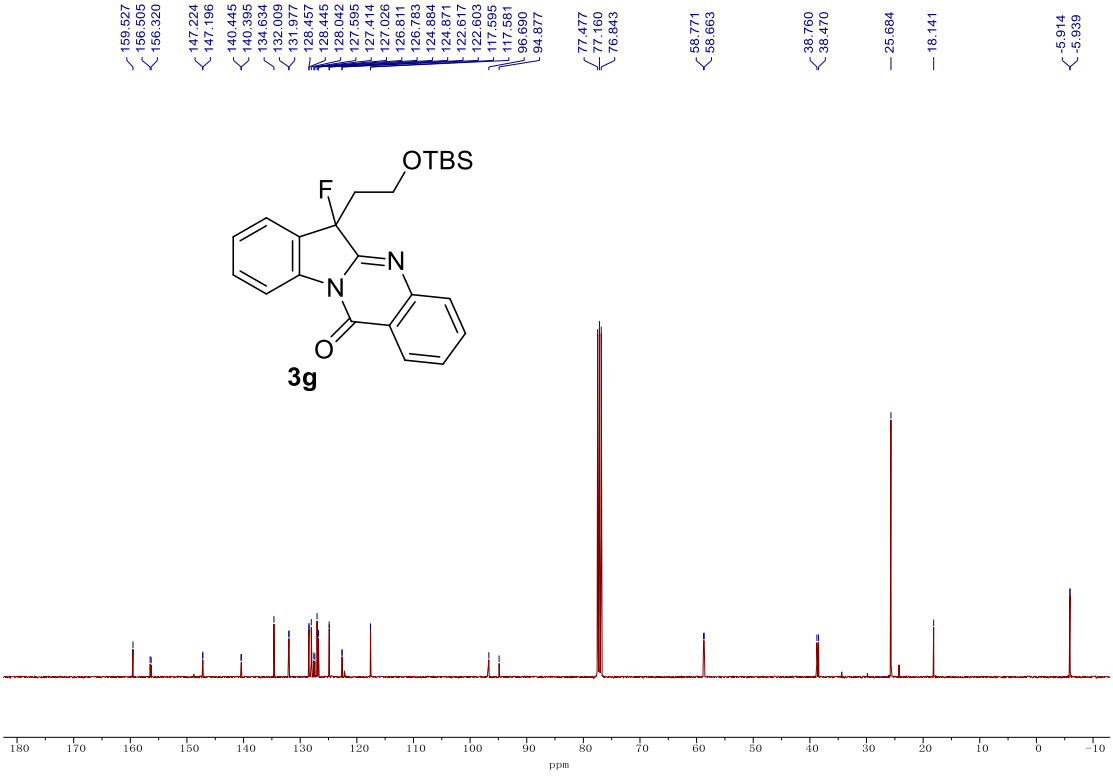

OBz
F
N
N
O

**3f**

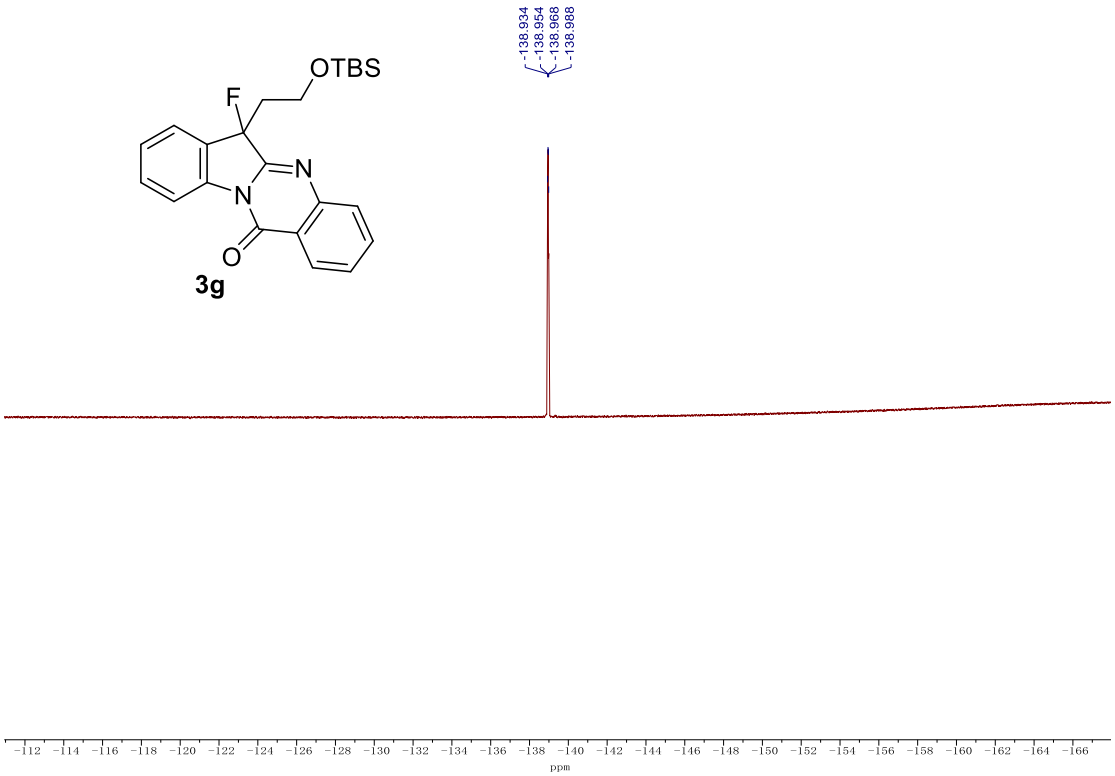

−105
−110
−115
−120
−125
−130
−135
−140
−145
−150
−155
−160
−165
−170
ppm




**3g**




**3g**


OTBS
F
N
N
O
3g
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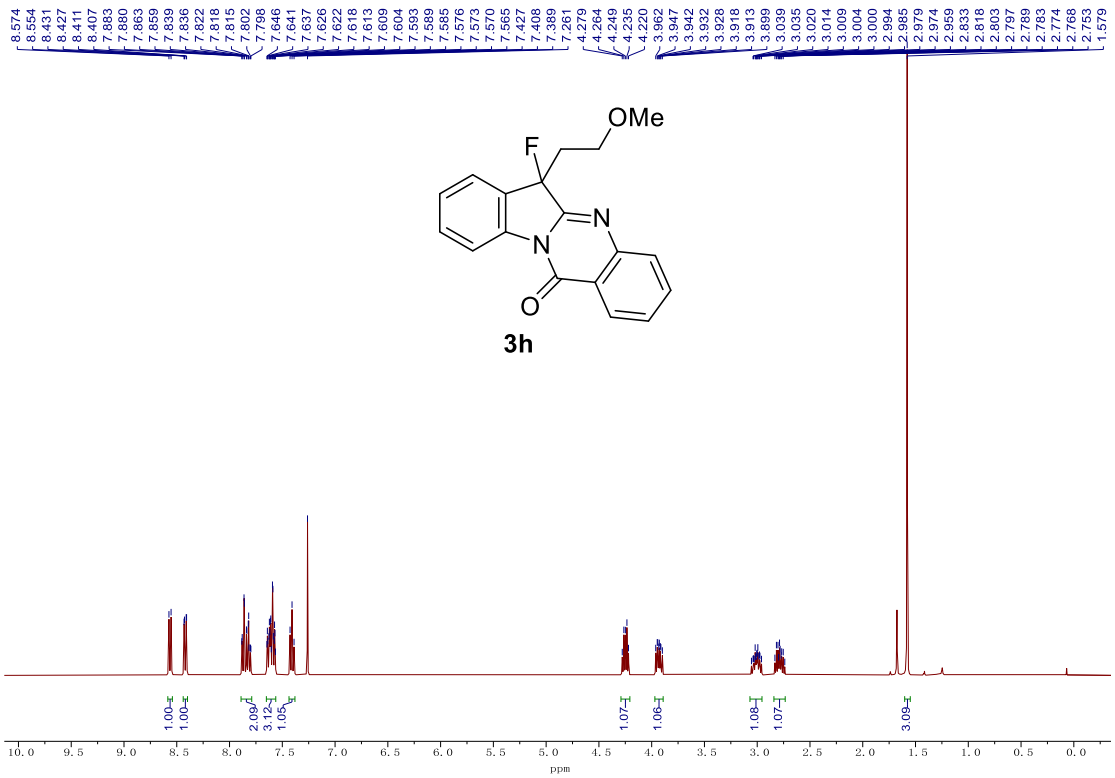
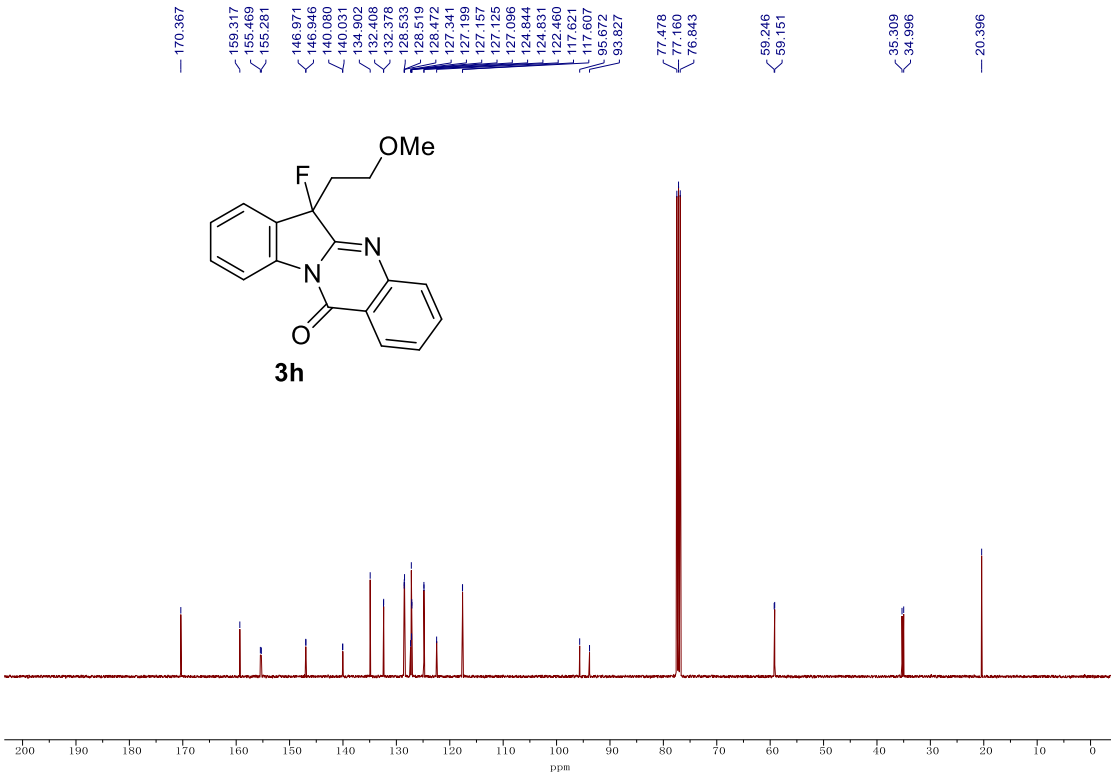
-138.988
ppm


OMe
F
N
N
O
3h
ppm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140.031
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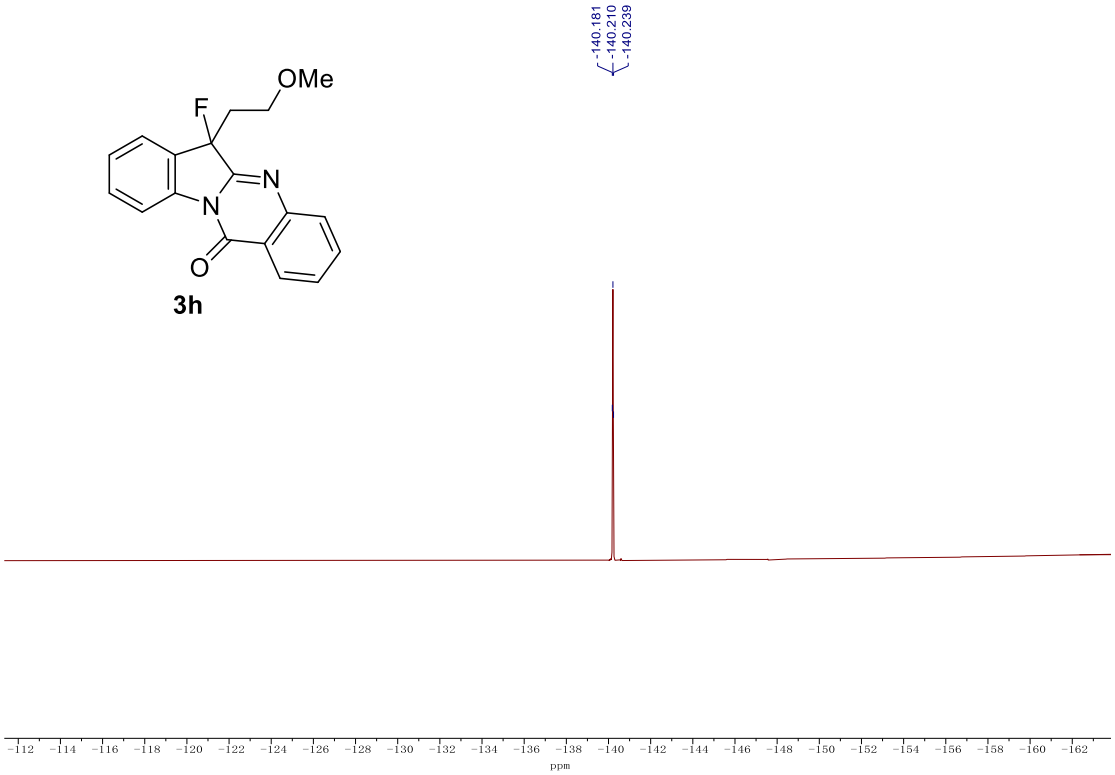
132.408
132.378
128.533
128.519
128.472
127.341
127.199
127.157
127.125
127.096
124.844
124.831
122.460
117.621
117.607
95.672
93.827
77.478
77.160
76.843
59.246
59.151
35.309
34.996
20.396
OMe
F
N
N
O
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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-140.210
-140.239
OMe
F
N
N
O
3h
-112
-114
-116
-118
-120
-122
-124
-126
-128
-130
-132
-134
-136
-138
-140
-142
-144
-146
-148
-150
-152
-154
-156
-158
-160
-162
ppm


8.580
8.560
8.429
8.409
7.883
7.863
7.846
7.842
7.829
7.825
7.808
7.805
7.638
7.621
7.603
7.584
7.435
7.416
7.397
7.261
3.690
3.677
3.664
3.651
3.638
3.626
3.480
3.465
3.454
3.439
3.429
3.414
3.188
3.173
3.161
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3.136
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3.111
3.100
3.084
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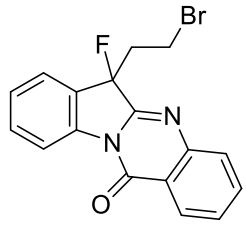
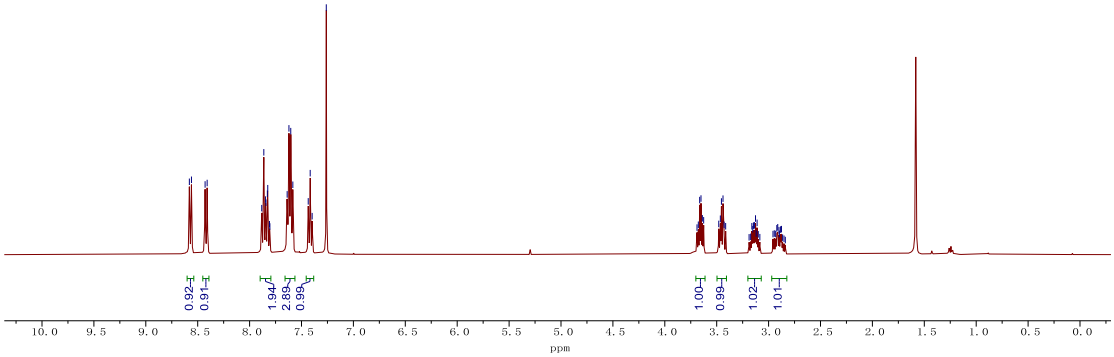
2.852
2.839


Br
F
N
N
O

**3i**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0.99
1.00
0.99
1.02
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


159.299
154.845
154.650
146.874
146.849
140.044
139.995
134.919
132.602
132.572
128.696
128.596
127.237
127.205
127.016
124.712
122.592
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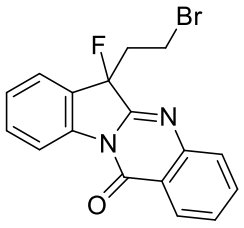
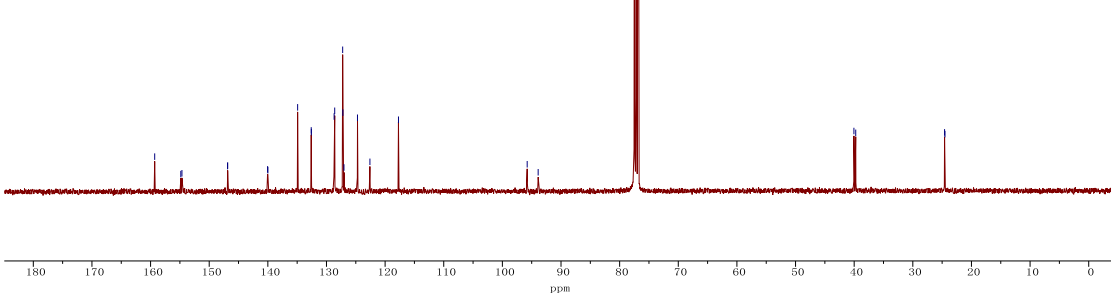
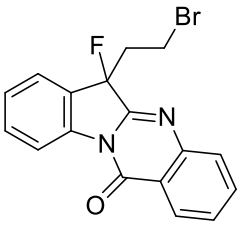
95.768
93.898
77.478
77.160
76.843
40.045
39.736
24.584
24.517


Br
F
N
N
O

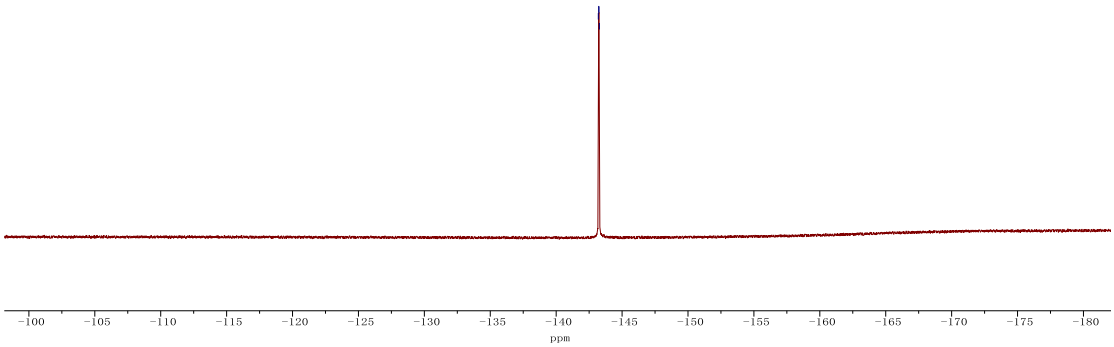
**3i**


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


Br
F
N
N
O

**3i**


-143.198
-143.226
-143.246
-143.274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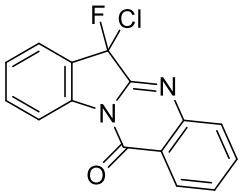
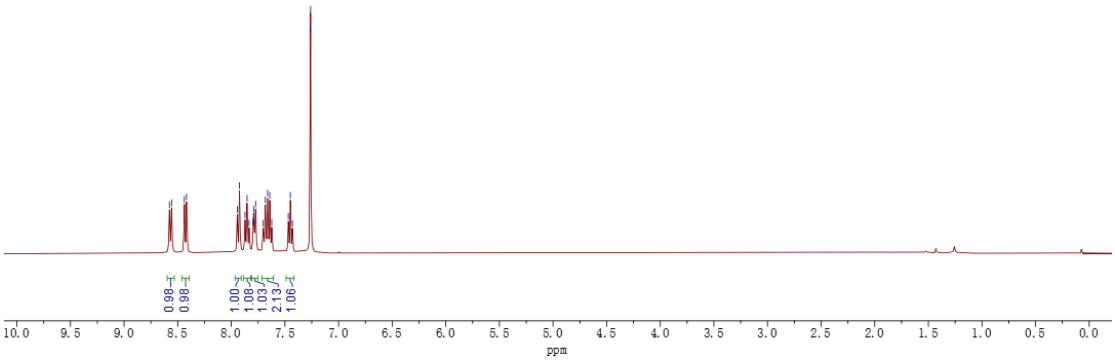
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175
-180
ppm


8.577
8.557
8.438
8.418
7.944
7.923
7.872
7.853
7.834
7.798
7.792
7.774
7.702
7.683
7.662
7.642
7.623
7.469
7.450
7.431
7.264
7.260


F
Cl
N
N
O

**3j**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2.13
1.06
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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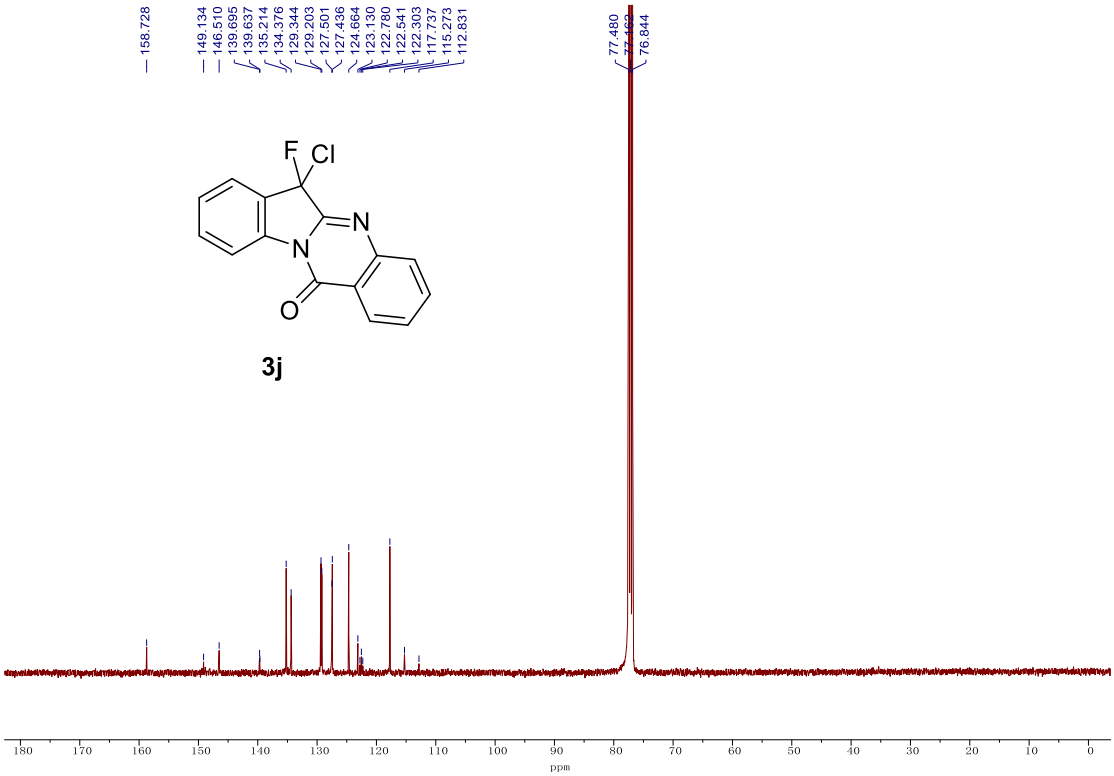
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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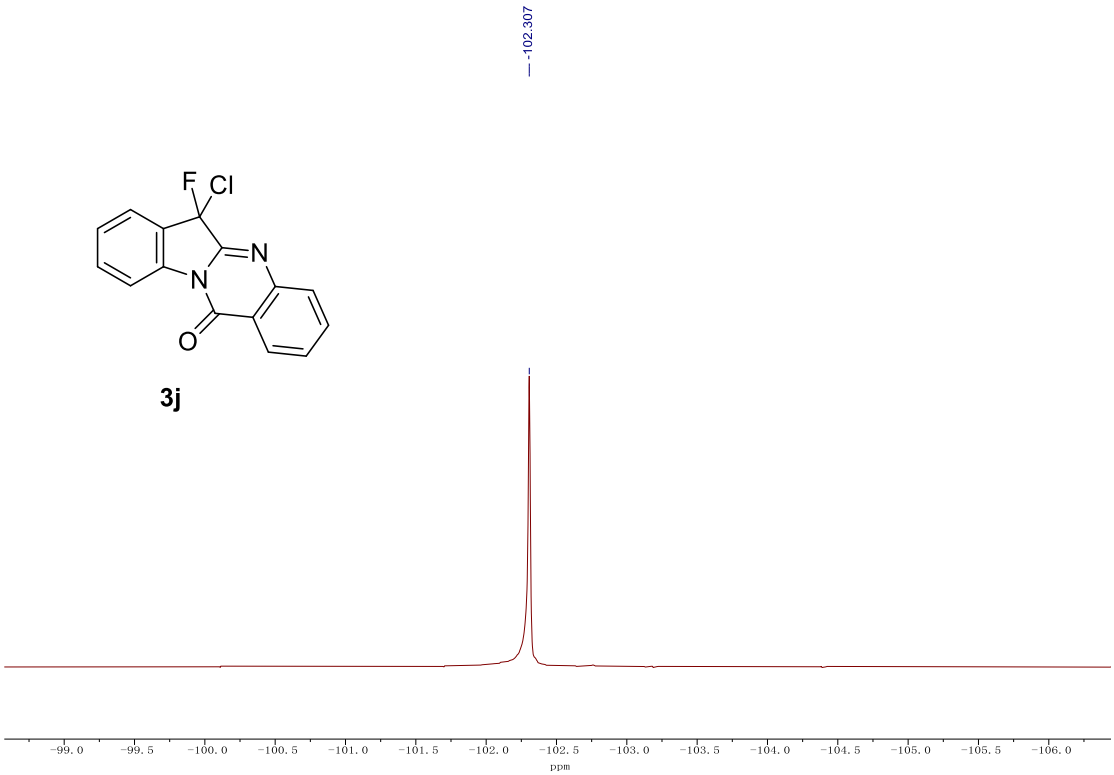
139.637
135.214
134.376
129.344
129.203
127.501
127.436
124.664
123.130
122.780
122.541
122.303
117.737
115.273
112.831
77.480
77.160
76.844
F
Cl
N
N
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

**3j**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Cl
N
N
O
-99.0
-99.5
-100.0
-100.5
-101.0
-101.5
-102.0
-102.5
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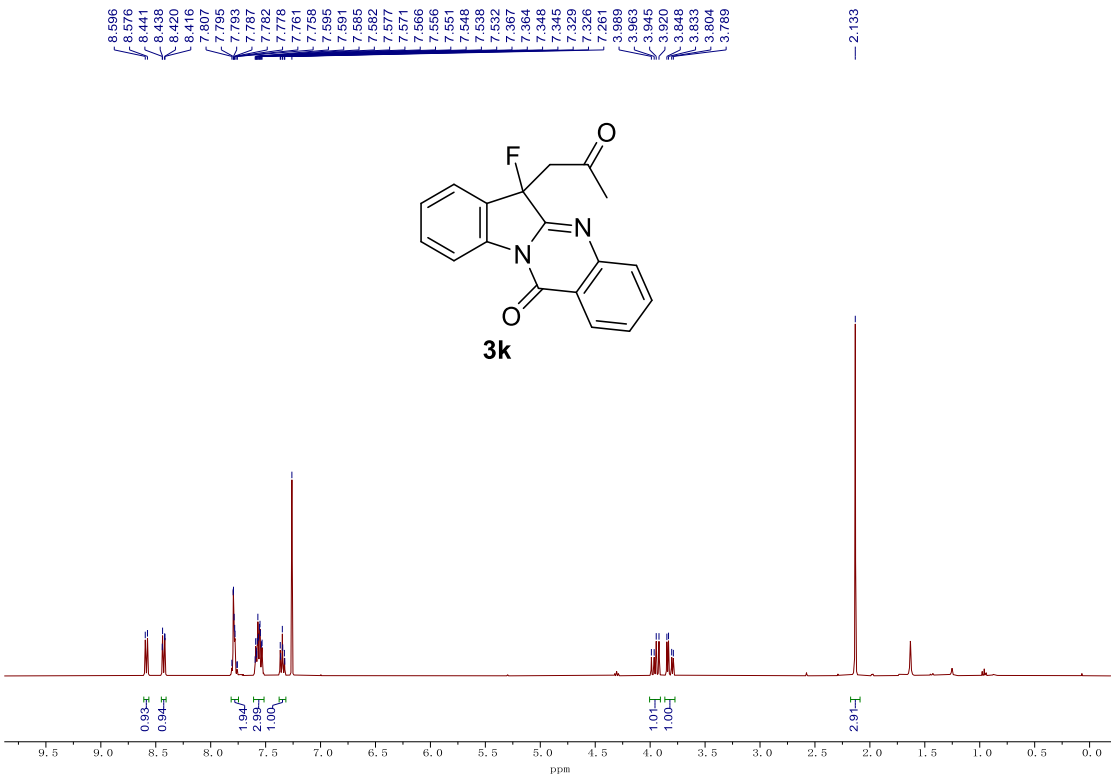
-103.5
-104.0
-104.5
-105.0
-105.5
-106.0
ppm

**3j**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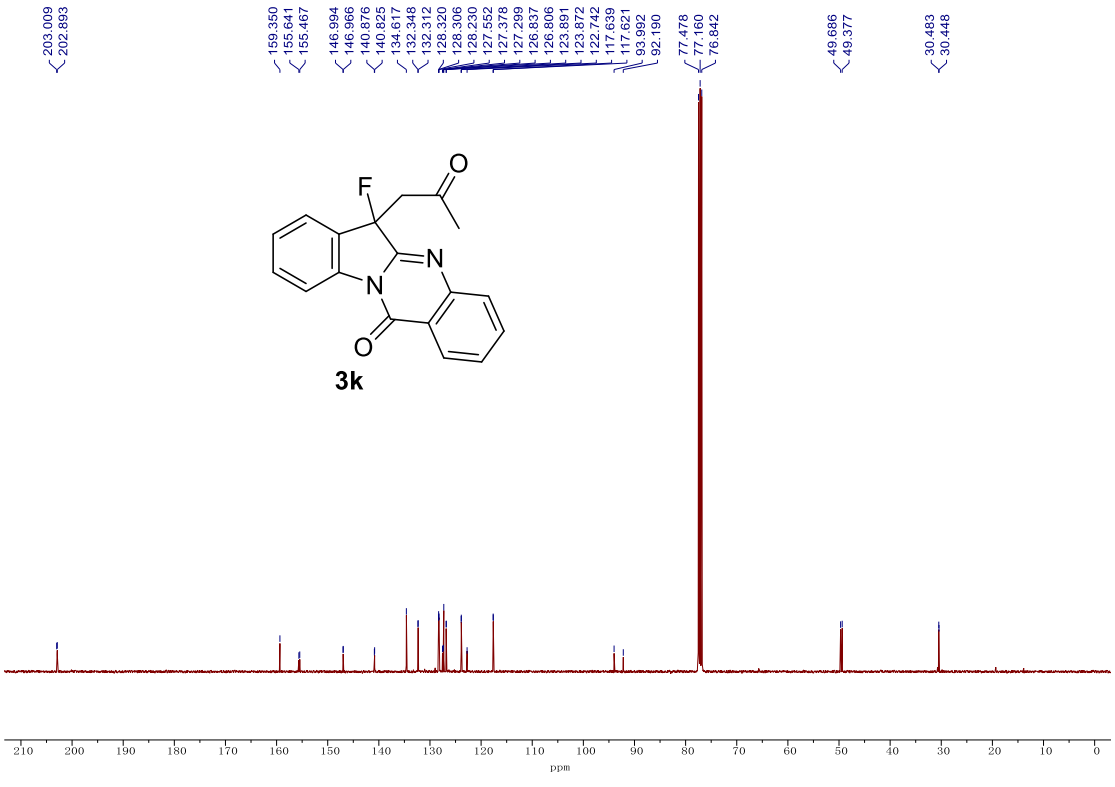
7.582
7.577
7.571
7.566
7.556
7.551
7.548
7.538
7.532
7.367
7.364
7.348
7.345
7.329
7.326
7.261
3.989
3.963
3.945
3.920
3.848
3.833
3.804
3.789
2.133
F
O
N
N
O
3k
0.93
0.94
1.94
2.99
1.00
1.01
1.00
2.91
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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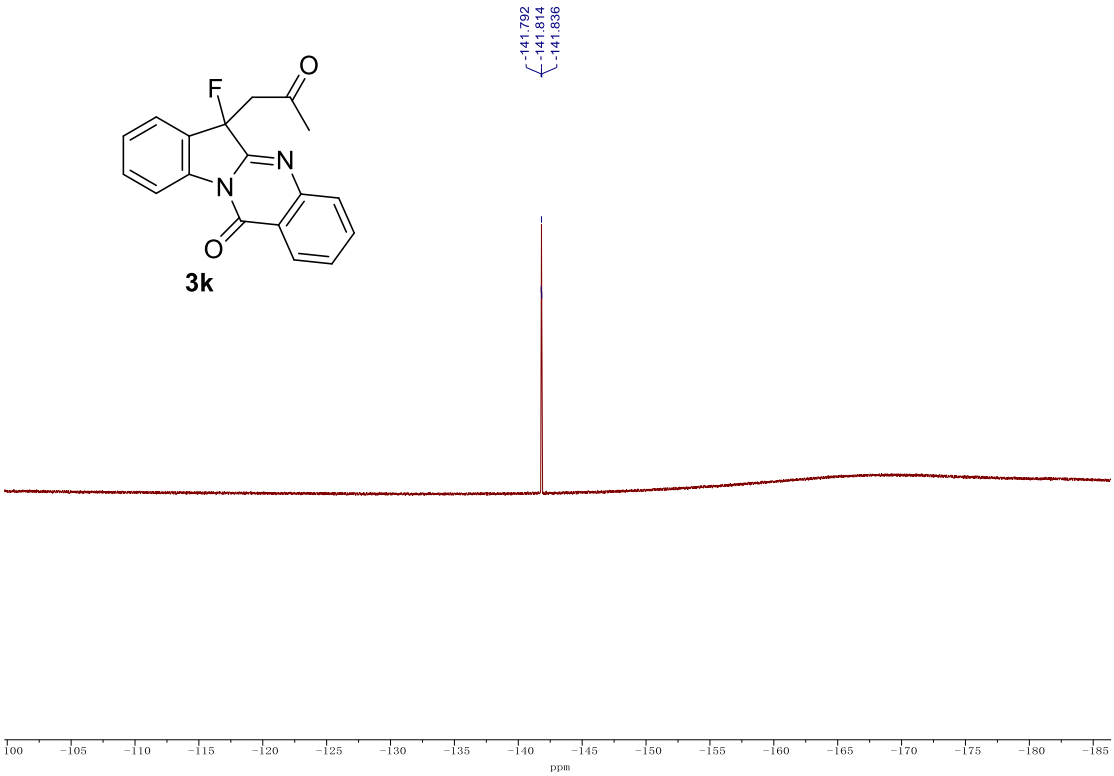
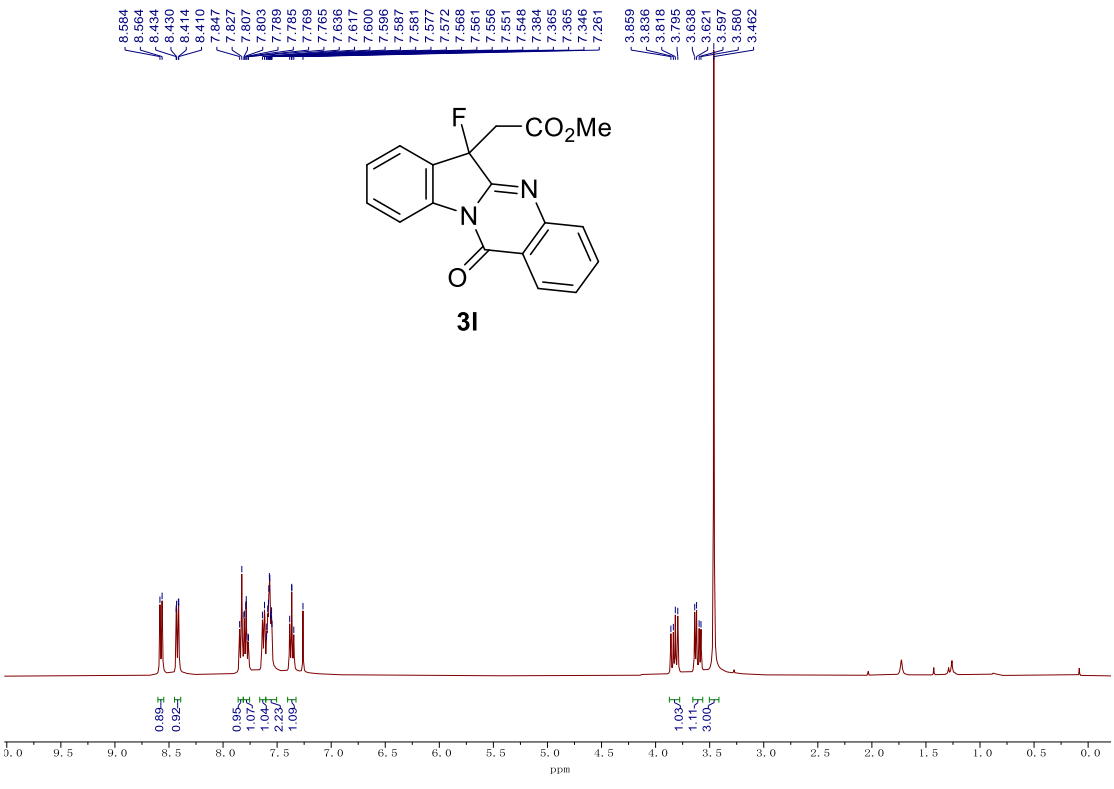
155.641
155.467
146.994
146.966
140.876
140.825
134.617
132.348
132.312
128.320
128.306
128.230
127.552
127.378
127.299
126.837
126.806
123.891
123.872
122.742
117.639
117.621
93.992
92.190
77.478
77.160
76.842
49.686
49.377
30.483
30.448
F
O
N
N
O
3k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-141.792
-141.814
-141.836
F
O
N
N
O
3k
100 −105 −110 −115 −120 −125 −130 −135 −140 −145 −150 −155 −160 −165 −170 −175 −180 −185
ppm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8.414
8.410
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7.827
7.807
7.803
7.789
7.785
7.769
7.765
7.636
7.617
7.600
7.596
7.587
7.581
7.577
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7.561
7.556
7.551
7.548
7.384
7.365
7.346
7.261
3.859
3.836
3.818
3.795
3.638
3.621
3.597
3.580
3.462
F
CO2Me
N
N
O
3l
0.89
0.92
0.95
1.07
1.04
2.23
1.09
1.03
1.11
3.00
5.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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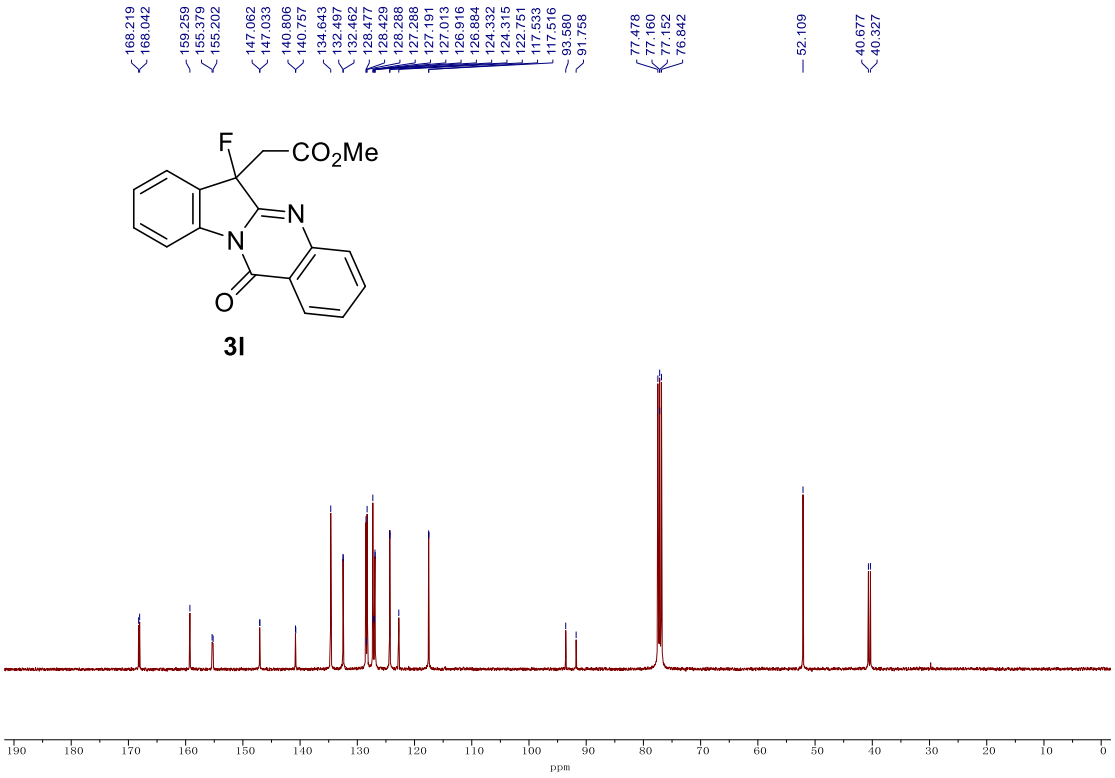
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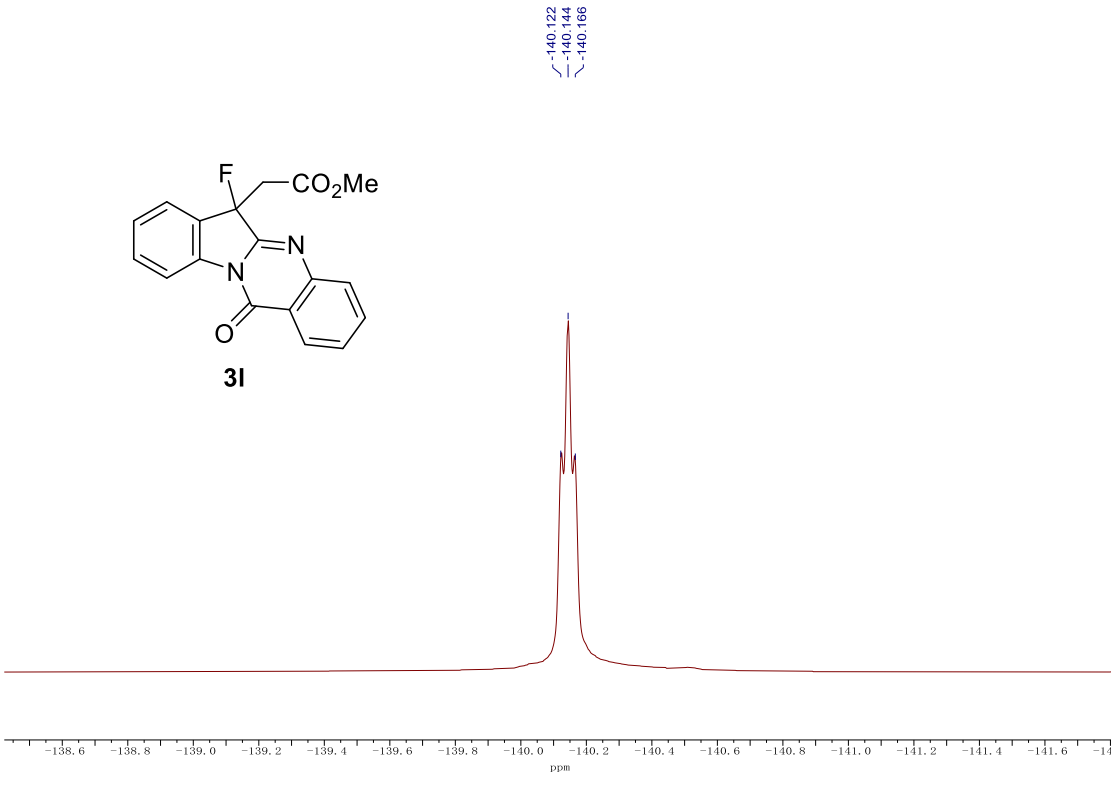
168.042
159.259
155.379
155.202
147.062
147.033
140.806
140.757
134.643
132.497
132.462
128.477
128.429
128.288
127.288
127.191
127.013
126.916
126.884
124.332
124.315
122.751
117.533
117.516
93.580
91.758
77.478
77.160
77.152
76.842
52.109
40.677
40.327
F
CO2Me
N
N
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

**3l**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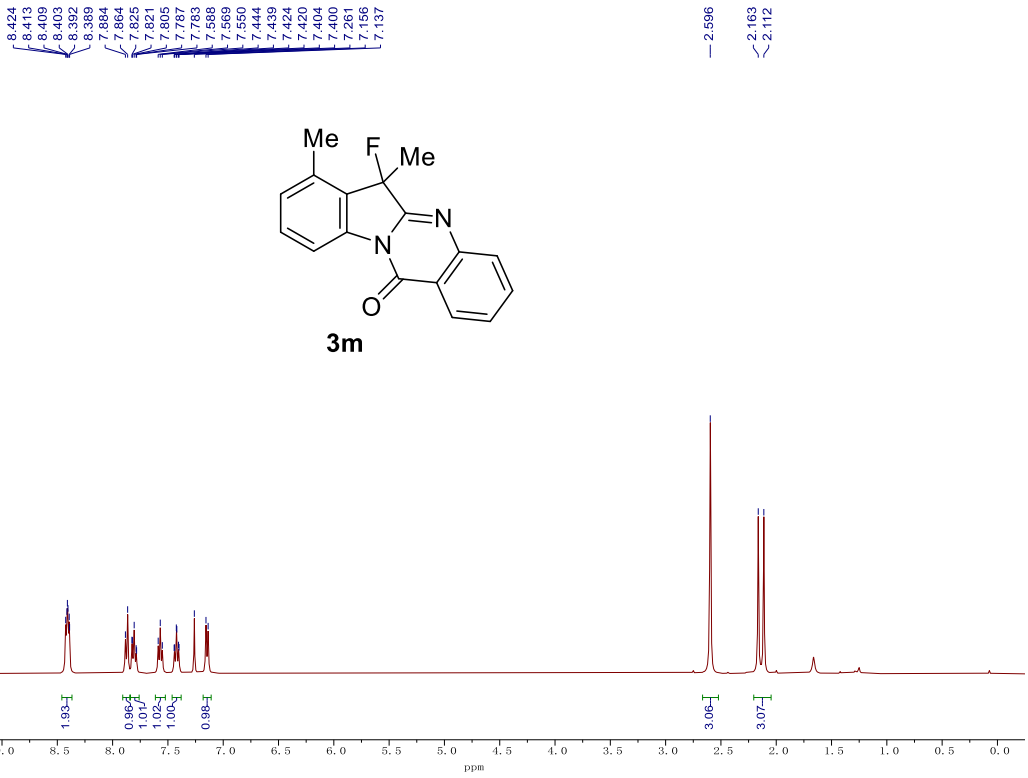
-140.144
-140.166
F
CO2Me
N
N
O
-138.6
-138.8
-139.0
-139.2
-139.4
-139.6
-139.8
-140.0
-140.2
-140.4
-140.6
-140.8
-141.0
-141.2
-141.4
-141.6
ppm

**3l**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8.409
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8.389
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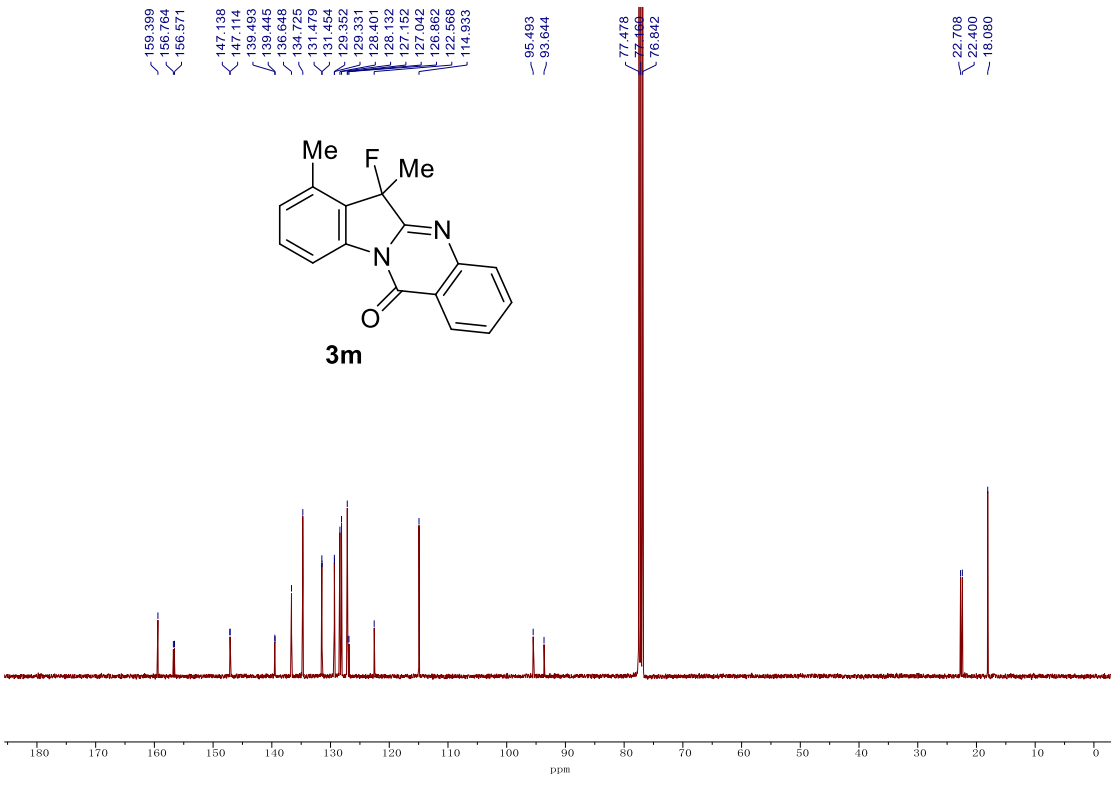
7.864
7.825
7.821
7.805
7.787
7.783
7.588
7.569
7.550
7.444
7.439
7.424
7.420
7.404
7.400
7.261
7.156
7.137
2.596
2.163
2.112
Me
F
Me
N
N
O
3m
1.93
0.96
1.01
1.02
1.00
0.98
3.06
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm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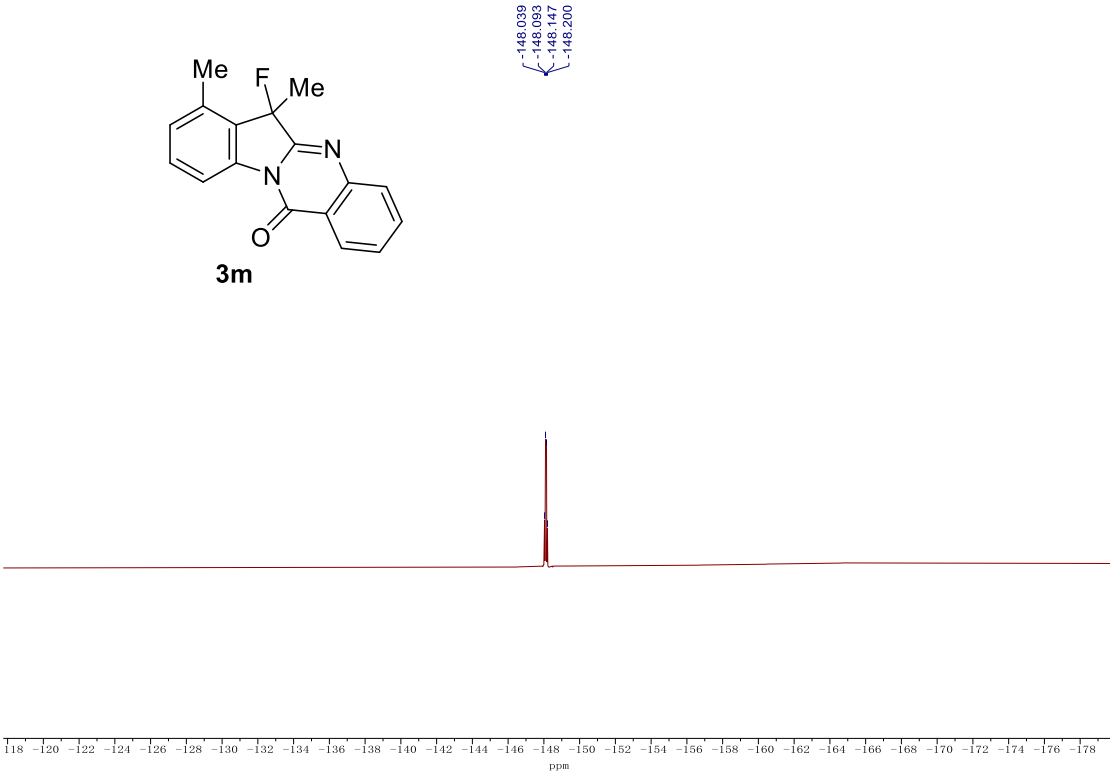
156.764
156.571
147.138
147.114
139.493
139.445
136.648
134.725
131.479
131.454
129.352
129.331
128.401
128.132
127.152
127.042
126.862
122.568
114.933
95.493
93.644
77.478
77.160
76.842
22.708
22.400
18.080
Me
F
Me
N
N
O
3m
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

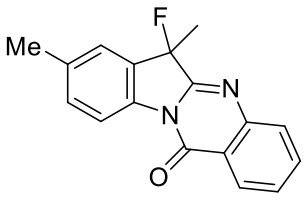
Me
F
Me
N
N
O

**3m**

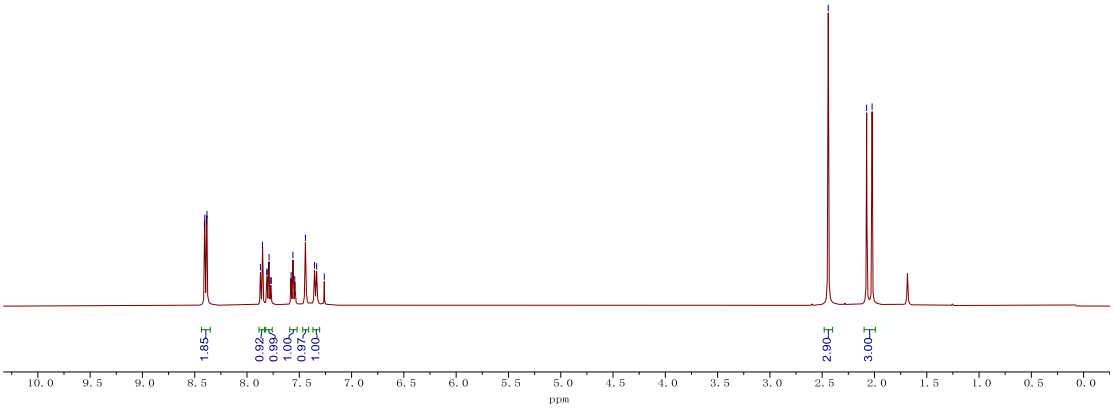

-148.039
-148.093
-148.147
-148.200
118 -120 -122 -124 -126 -128 -130 -132 -134 -136 -138 -140 -142 -144 -146 -148 -150 -152 -154 -156 -158 -160 -162 -164 -166 -168 -170 -172 -174 -176 -178
ppm

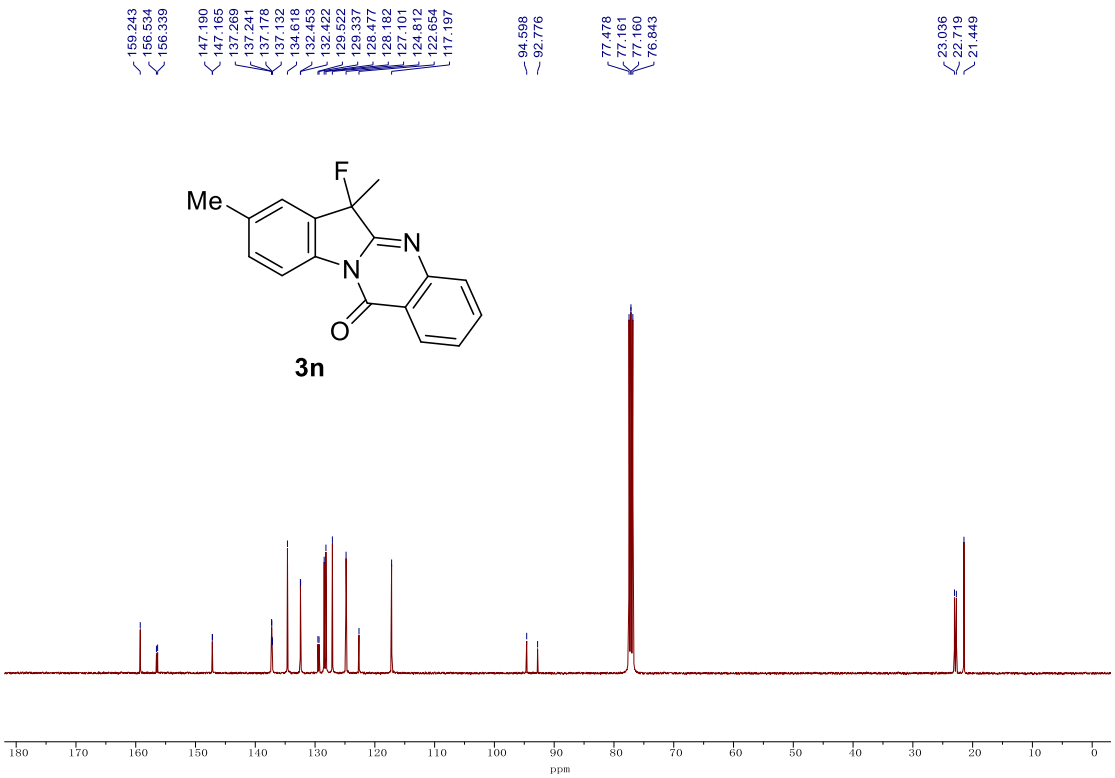

8.407
8.403
8.386
8.383
7.872
7.853
7.811
7.807
7.793
7.789
7.773
7.769
7.578
7.561
7.544
7.442
7.354
7.334
7.261

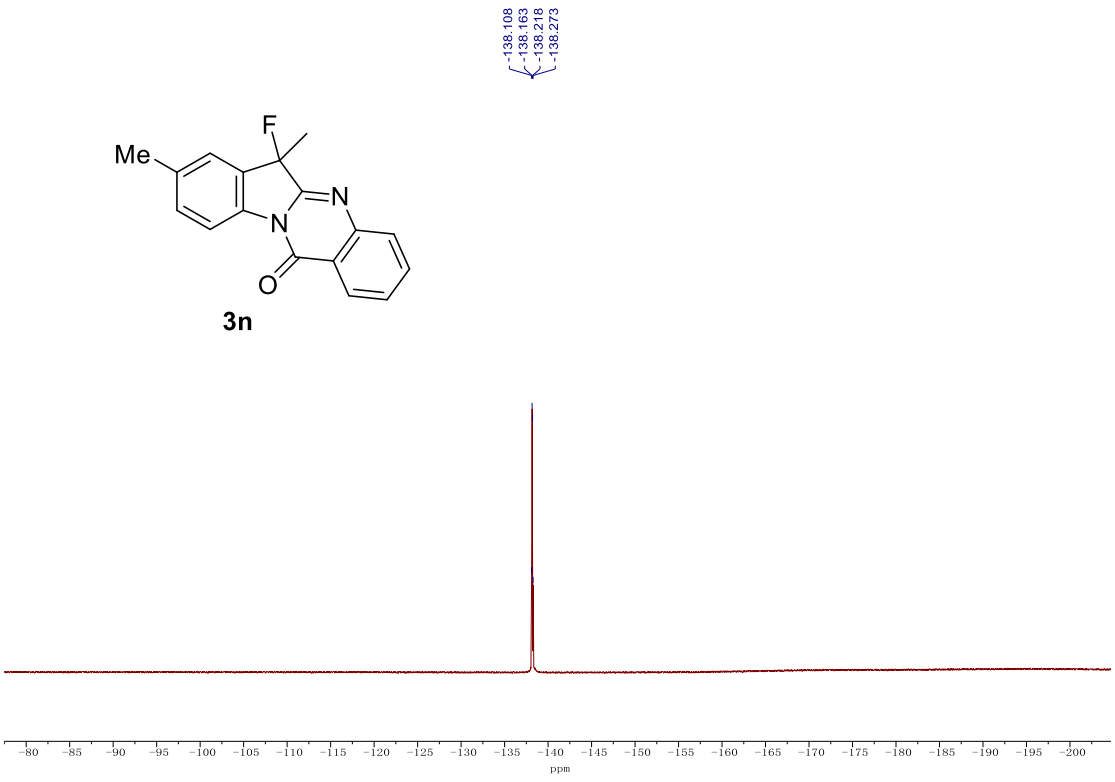

2.442
2.075
2.023

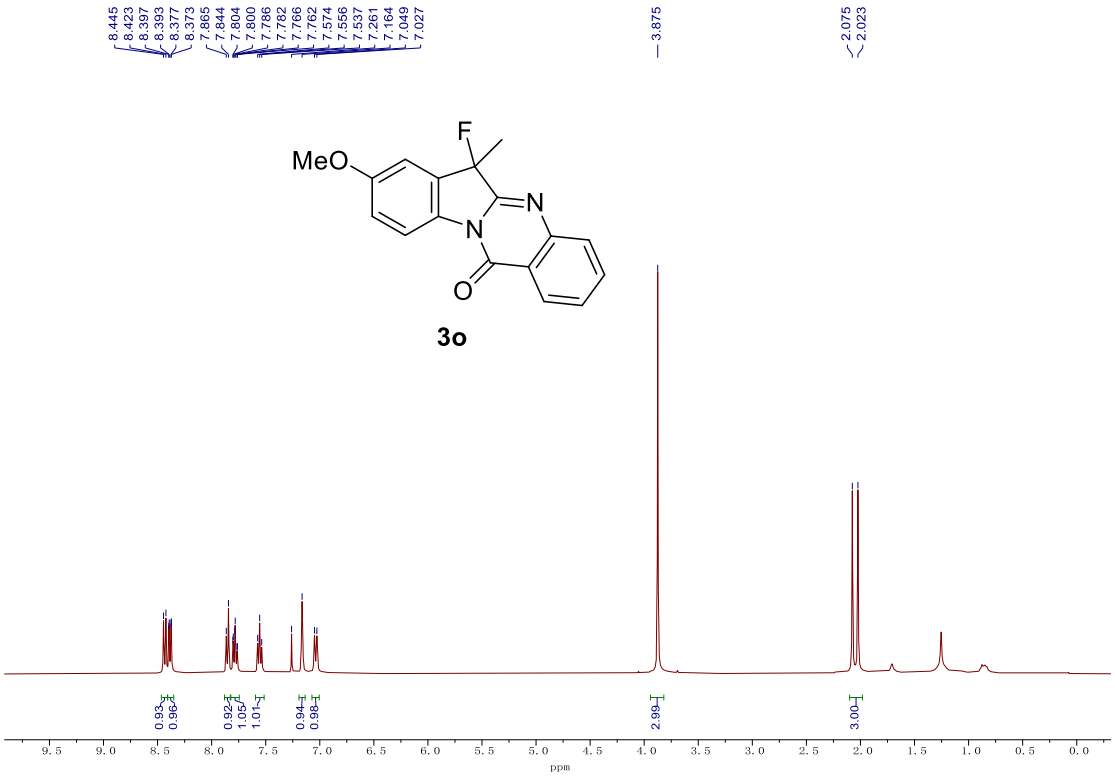

F
Me
N
N
O

**3n**

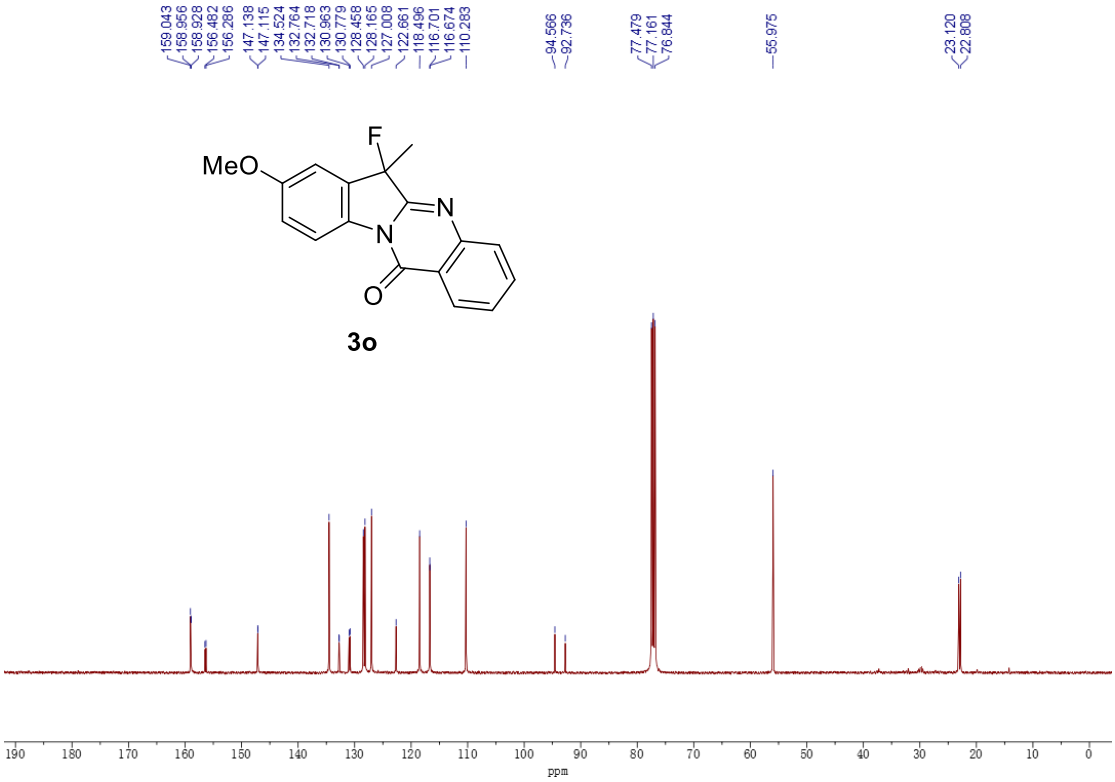

1.85
0.92
0.99
1.00
0.97
1.00
2.90
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


159.243
156.534
156.339
147.190
147.165
137.269
137.241
137.178
137.132
134.618
132.453
132.422
129.522
129.337
128.477
128.182
127.101
124.812
122.654
117.197
94.598
92.776
77.478
77.161
77.160
76.843
23.036
22.719
21.449
F
Me
N
N
O
3n
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-138.108
-138.163
-138.218
-138.273
F
Me
N
N
O
3n
−80
−85
−90
−95
−100
−105
−110
−115
−120
−125
−130
−135
−140
−145
−150
−155
−160
−165
−170
−175
−180
−185
−190
−195
−200
ppm


8.445
8.423
8.397
8.393
8.377
8.373
7.865
7.844
7.804
7.800
7.786
7.782
7.766
7.762
7.574
7.556
7.537
7.261
7.164
7.049
7.027
3.875
2.075
2.023
F
MeO
N
N
O
0.93
0.96
0.92
1.05
1.01
0.94
0.98
2.99
3.00
ppm

**3o**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158.956
158.928
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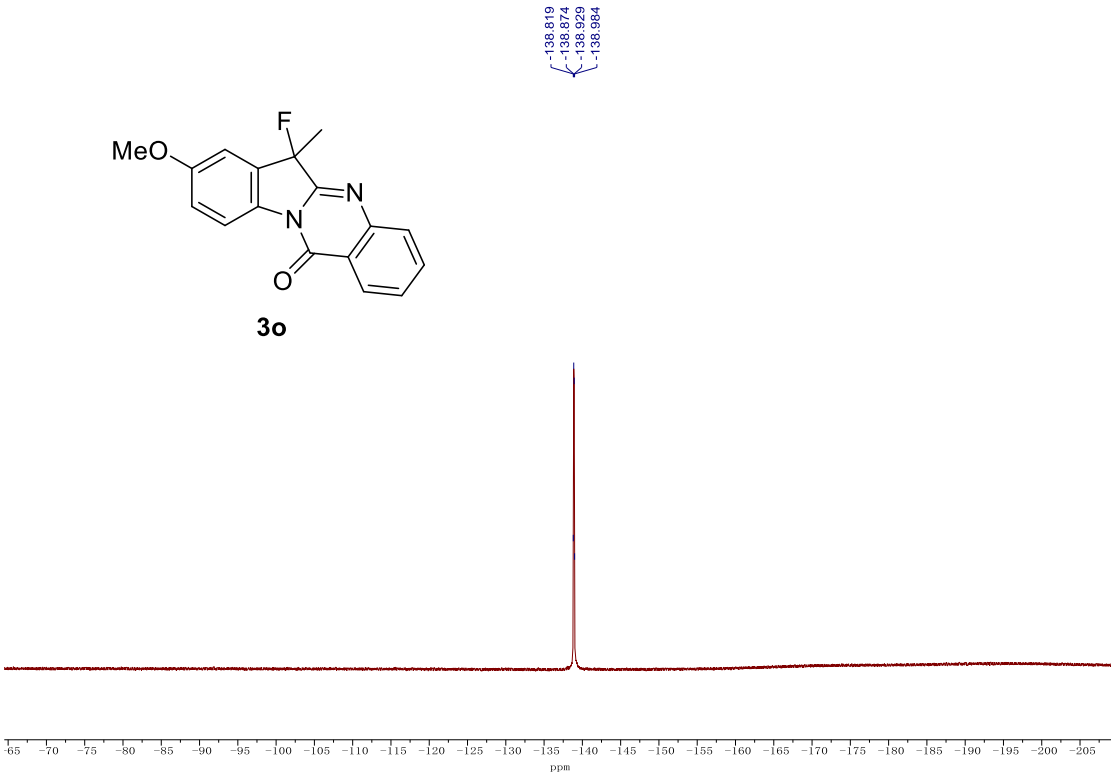
156.286
147.138
147.115
134.524
132.764
132.718
130.963
130.779
128.458
128.165
127.008
122.661
118.496
116.701
116.674
110.283
94.566
92.736
77.479
77.161
76.844
55.975
23.120
22.808
F
MeO
N
N
O
ppm

**3o**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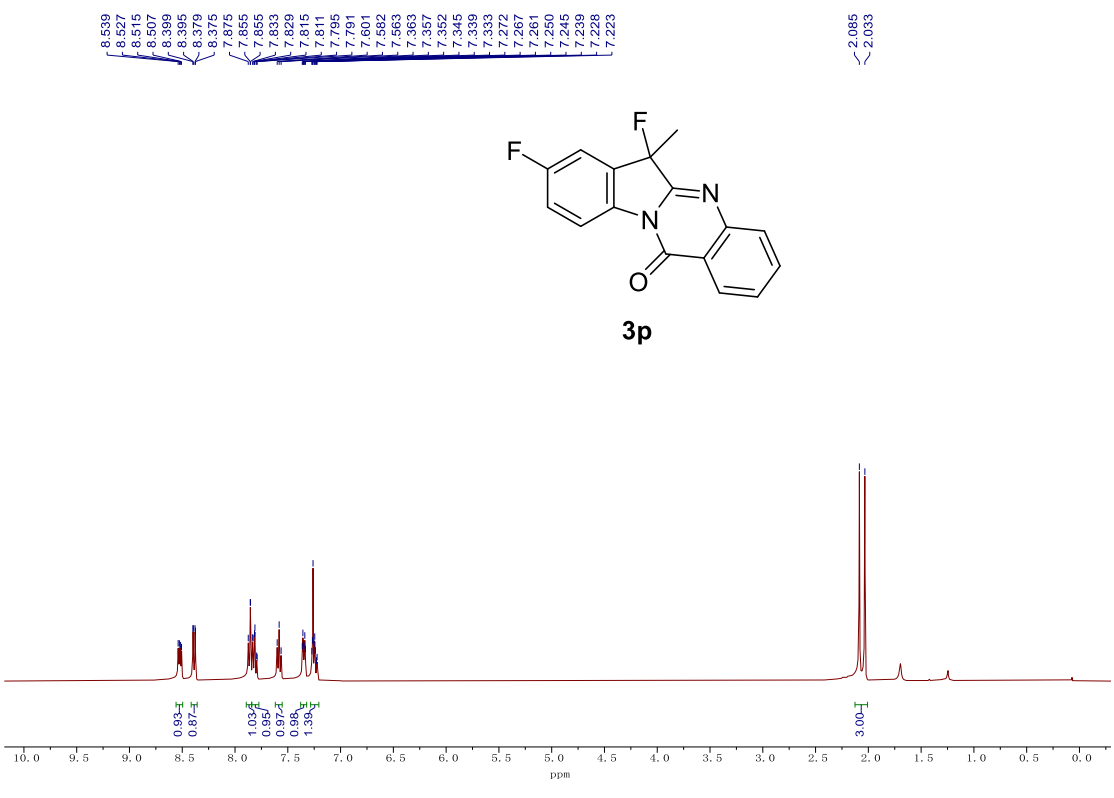
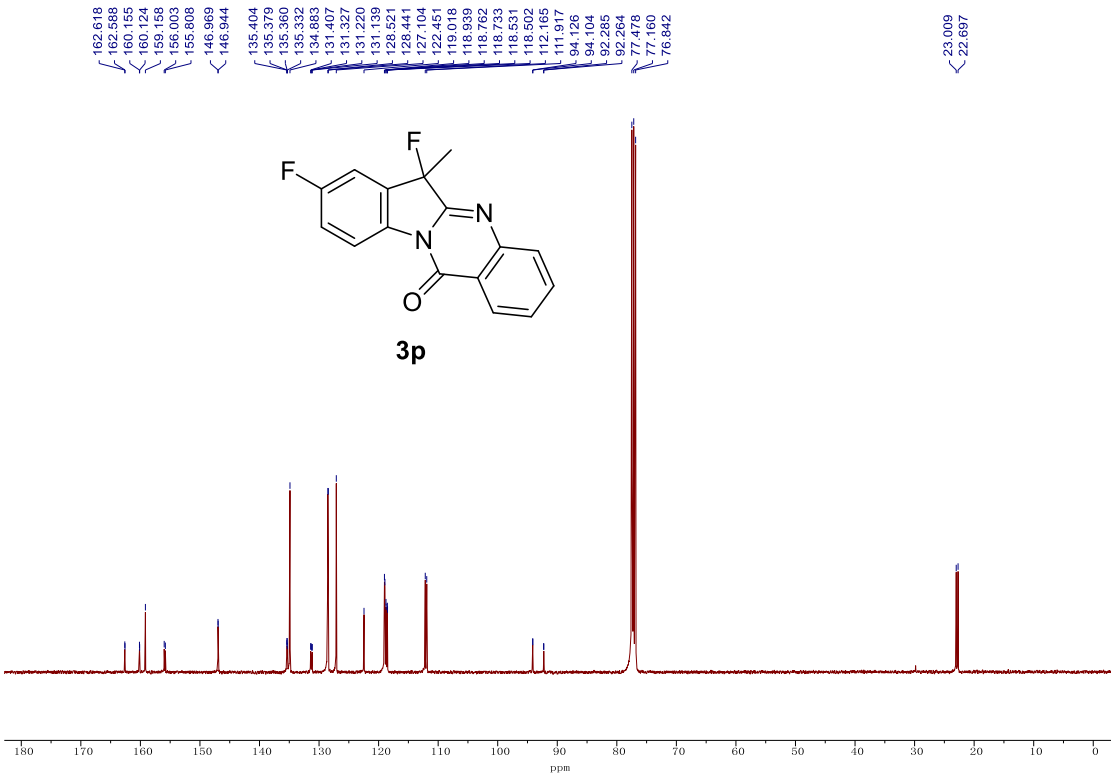
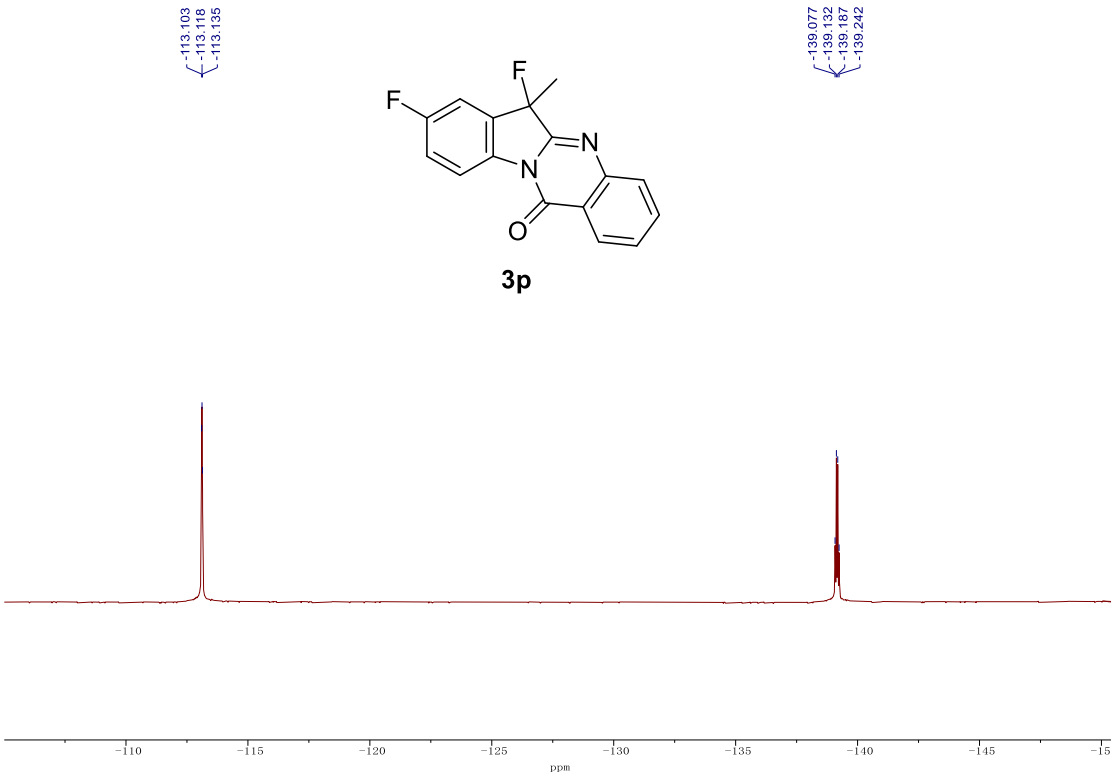
-138.874
-138.929
-138.984
F
MeO
N
N
O
ppm

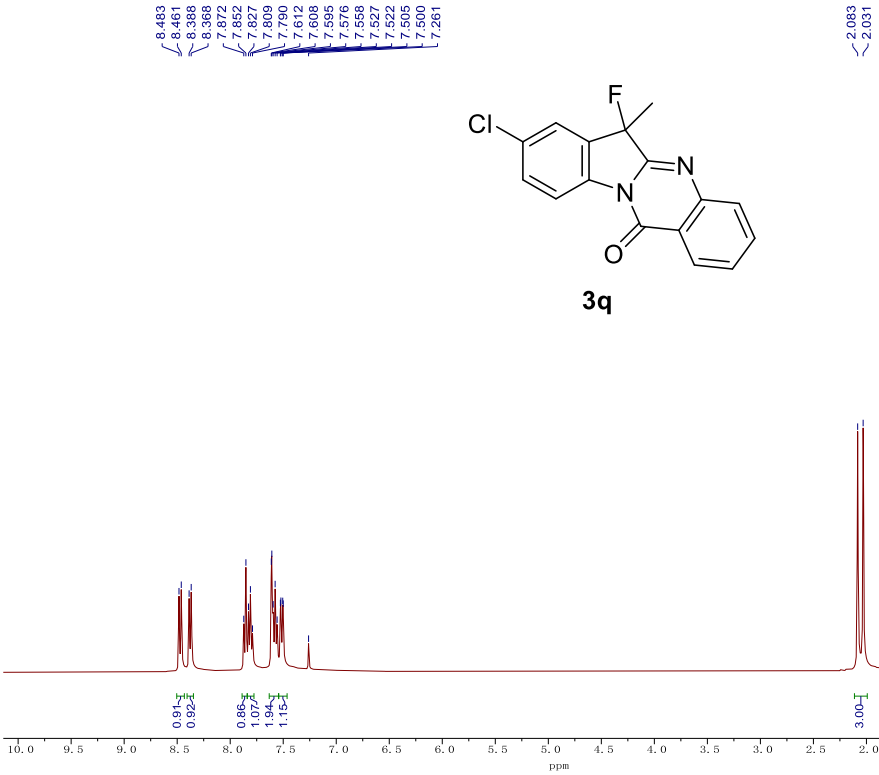
**3o**


8.539
8.527
8.515
8.507
8.399
8.395
8.379
8.375
7.875
7.855
7.855
7.833
7.829
7.815
7.811
7.795
7.791
7.601
7.582
7.563
7.363
7.357
7.352
7.345
7.339
7.333
7.272
7.267
7.261
7.250
7.245
7.239
7.228
7.223
2.085
2.033
F
F
N
N
O
0.93
0.87
1.03
0.95
0.97
0.98
1.39
3.00
ppm

**3p**


162.618
162.588
160.155
160.124
159.158
156.003
155.808
146.969
146.944
135.404
135.379
135.360
135.332
134.883
131.407
131.327
131.220
131.139
128.521
128.441
127.104
122.451
119.018
118.939
118.762
118.733
118.531
118.502
112.165
111.917
94.126
94.104
92.285
92.264
77.478
77.160
76.842
23.009
22.697
F
F
N
N
O
3p
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-113.103
-113.118
-113.135
-139.077
-139.132
-139.187
-139.242
F
F
N
N
O
3p
−110
−115
−120
−125
−130
−135
−140
−145
−15
ppm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8.388
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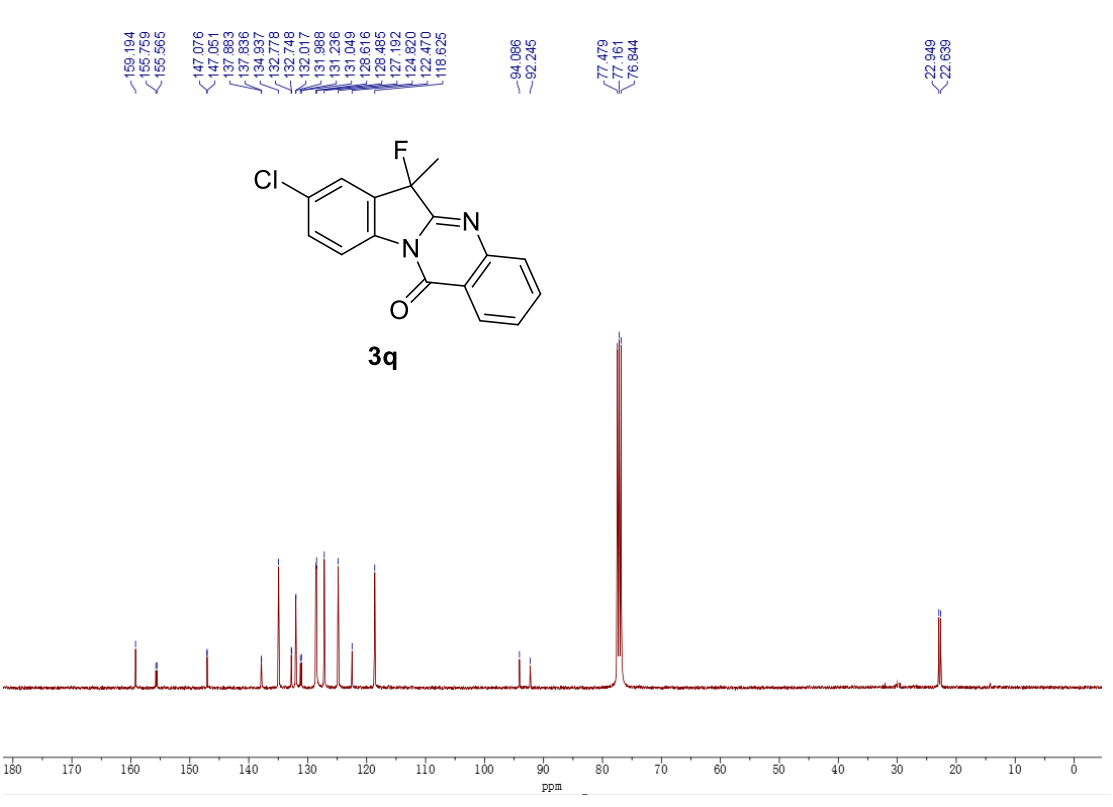
7.852
7.827
7.809
7.790
7.612
7.608
7.595
7.576
7.558
7.527
7.522
7.505
7.500
7.261
2.083
2.031
F
Cl
N
N
O
0.91
0.92
0.86
1.07
1.94
1.15
3.00
ppm

**3q**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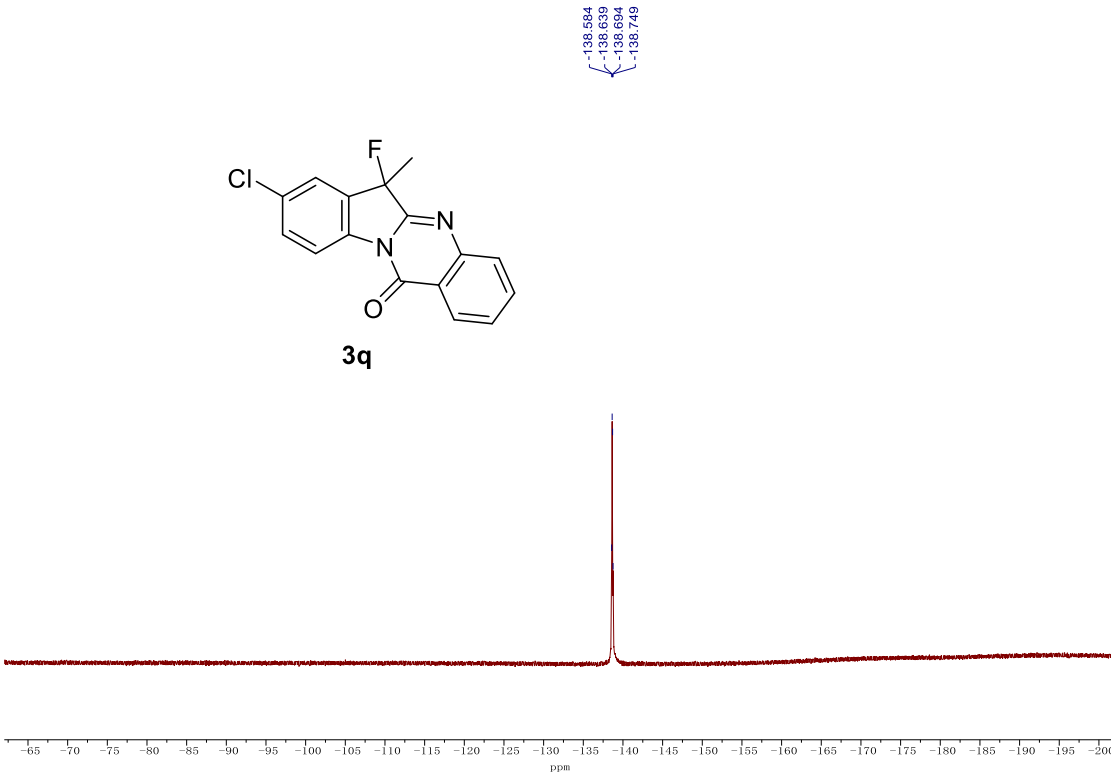
155.759
155.565
147.076
147.051
137.883
137.836
134.937
132.778
132.748
132.017
131.988
131.236
131.049
128.616
128.485
127.192
124.820
122.470
118.625
94.086
92.245
77.479
77.161
76.844
22.949
22.639
F
Cl
N
N
O
ppm

**3q**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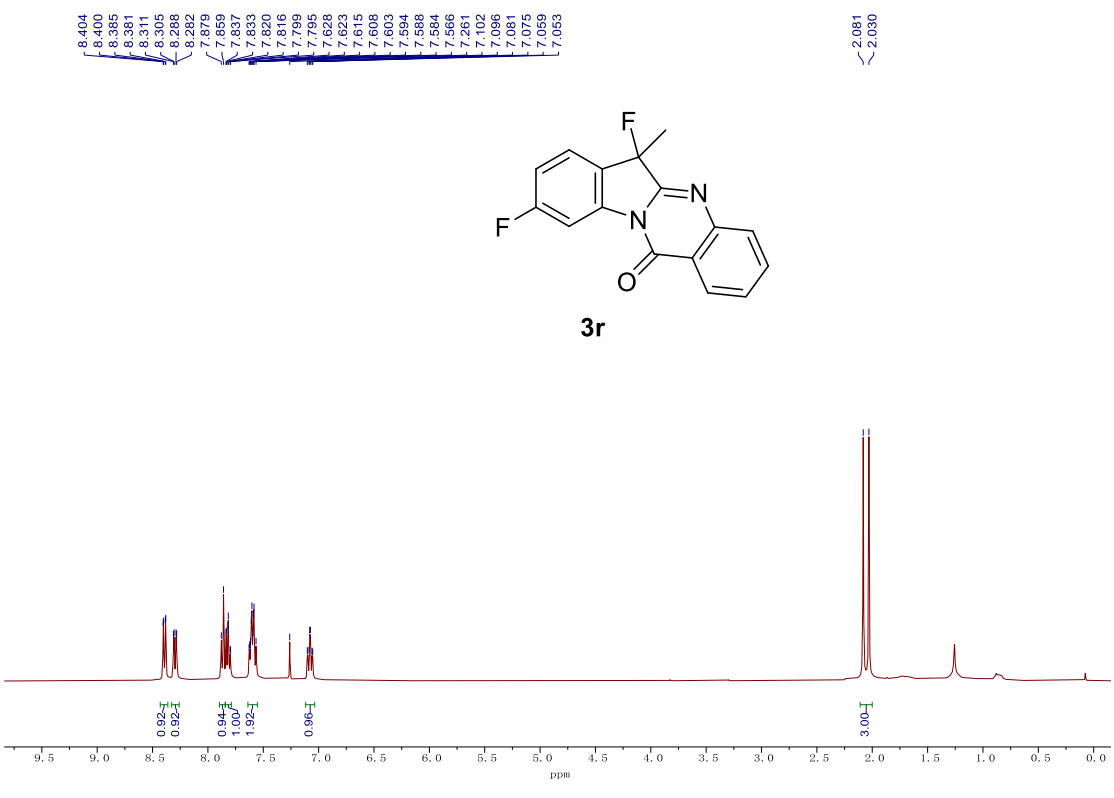
-138.639
-138.694
-138.749
F
Cl
N
N
O
ppm

**3q**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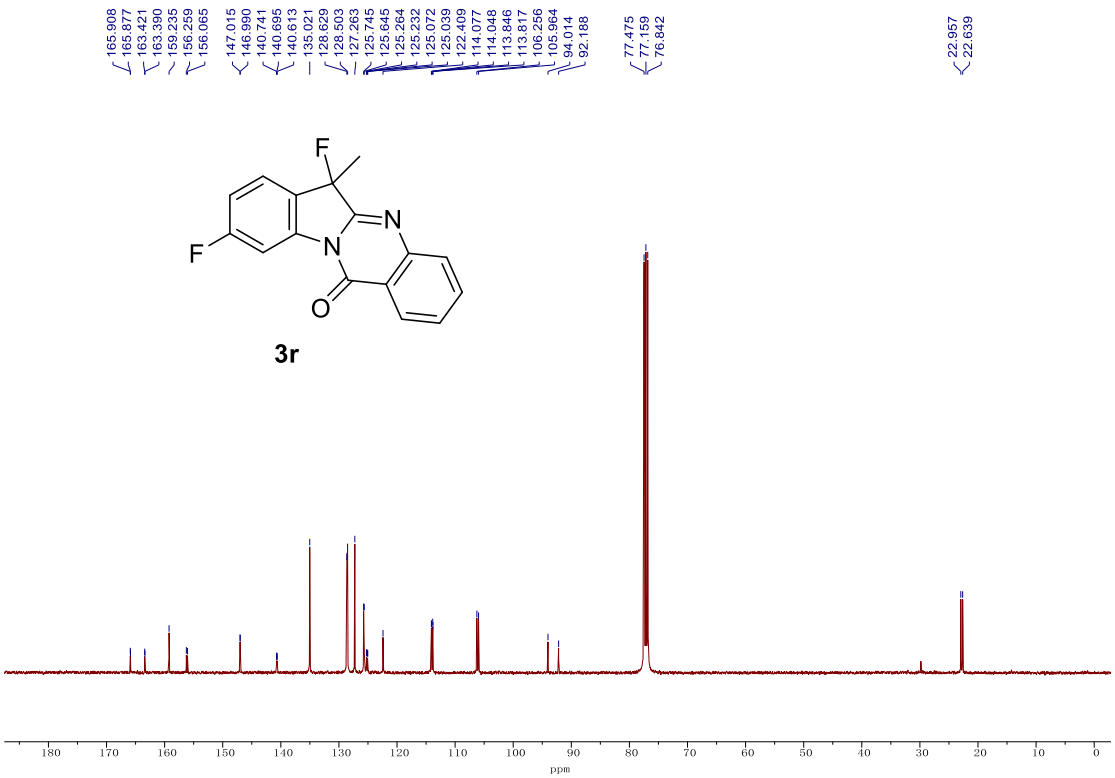
8.385
8.381
8.311
8.305
8.288
8.282
7.879
7.859
7.837
7.833
7.820
7.816
7.799
7.795
7.628
7.623
7.615
7.608
7.603
7.594
7.588
7.584
7.566
7.261
7.102
7.096
7.081
7.075
7.059
7.053
2.081
2.030
F
F
N
N
O
0.92
0.92
0.94
1.00
1.92
0.96
3.00
ppm

**3r**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165.877
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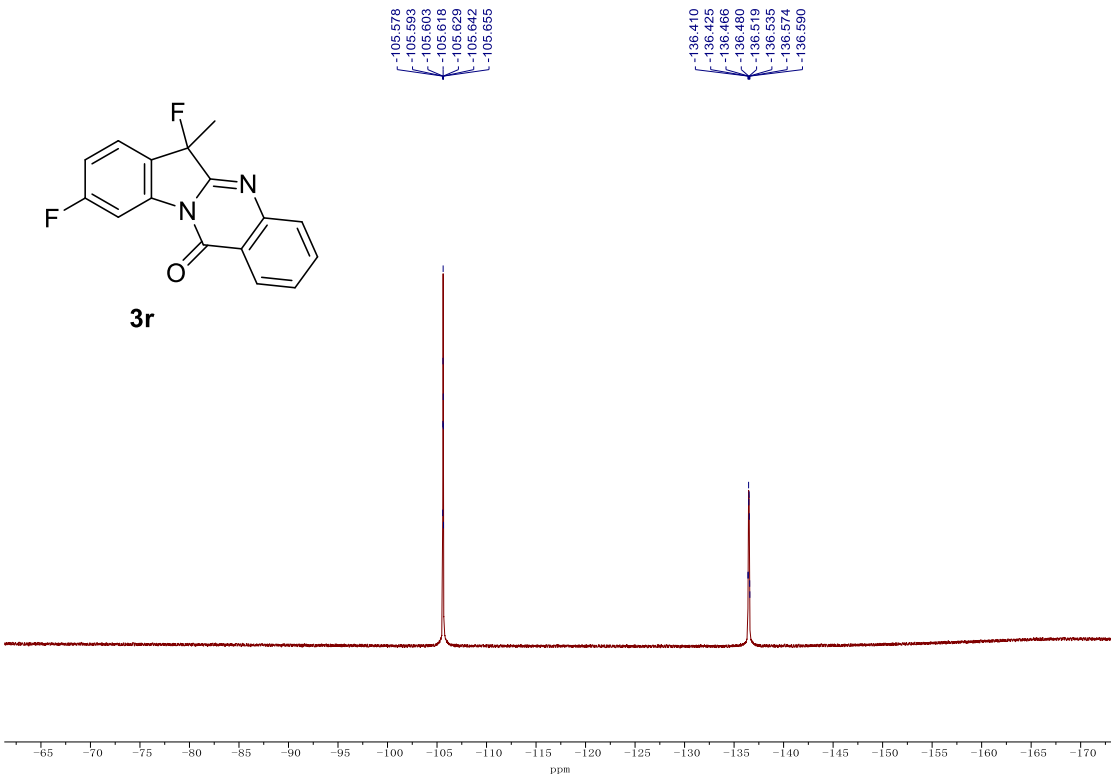
163.390
159.235
156.259
156.065
147.015
146.990
140.741
140.695
140.613
135.021
128.629
128.503
127.263
125.745
125.645
125.264
125.232
125.072
125.039
122.409
114.077
114.048
113.846
113.817
106.256
105.964
94.014
92.188
77.475
77.159
76.842
22.957
22.639
F
F
N
N
O
3r
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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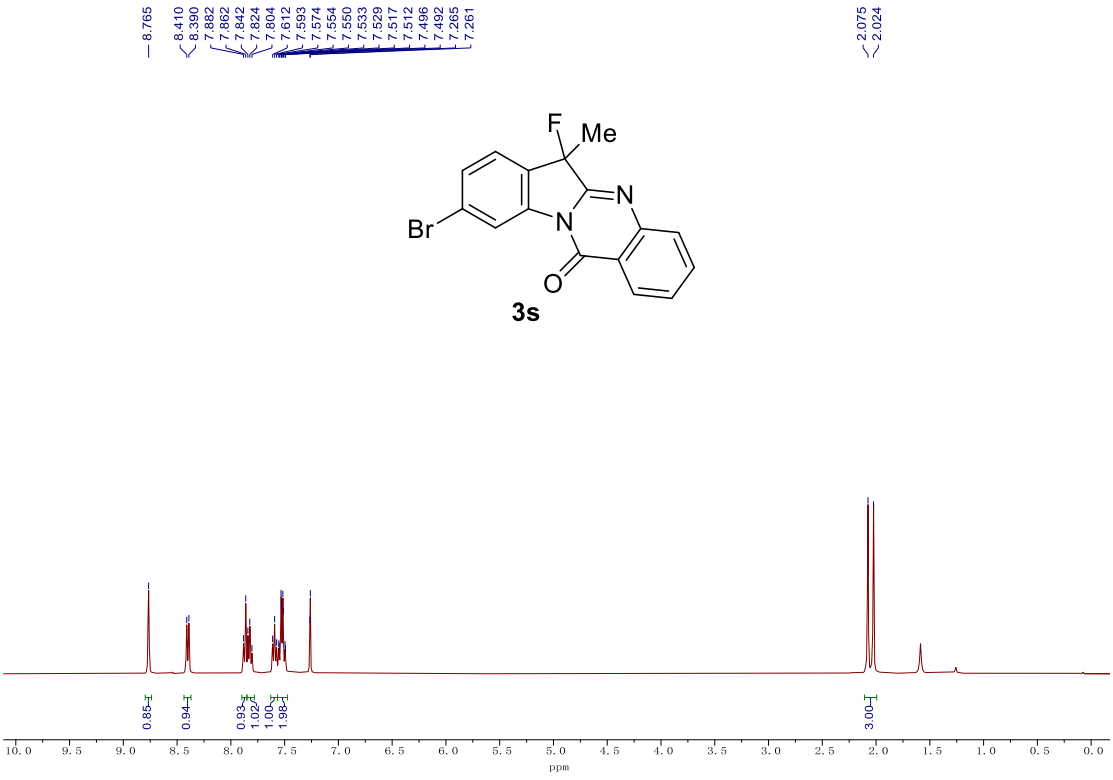
-105.593
-105.603
-105.618
-105.629
-105.642
-105.655
-136.410
-136.425
-136.466
-136.480
-136.519
-136.535
-136.574
-136.590
F
F
N
N
O
3r
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
ppm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8.410
8.390
7.882
7.862
7.842
7.824
7.804
7.612
7.593
7.574
7.554
7.550
7.533
7.529
7.517
7.512
7.496
7.492
7.265
7.261
2.075
2.024
F
Me
N
N
Br
O
3s
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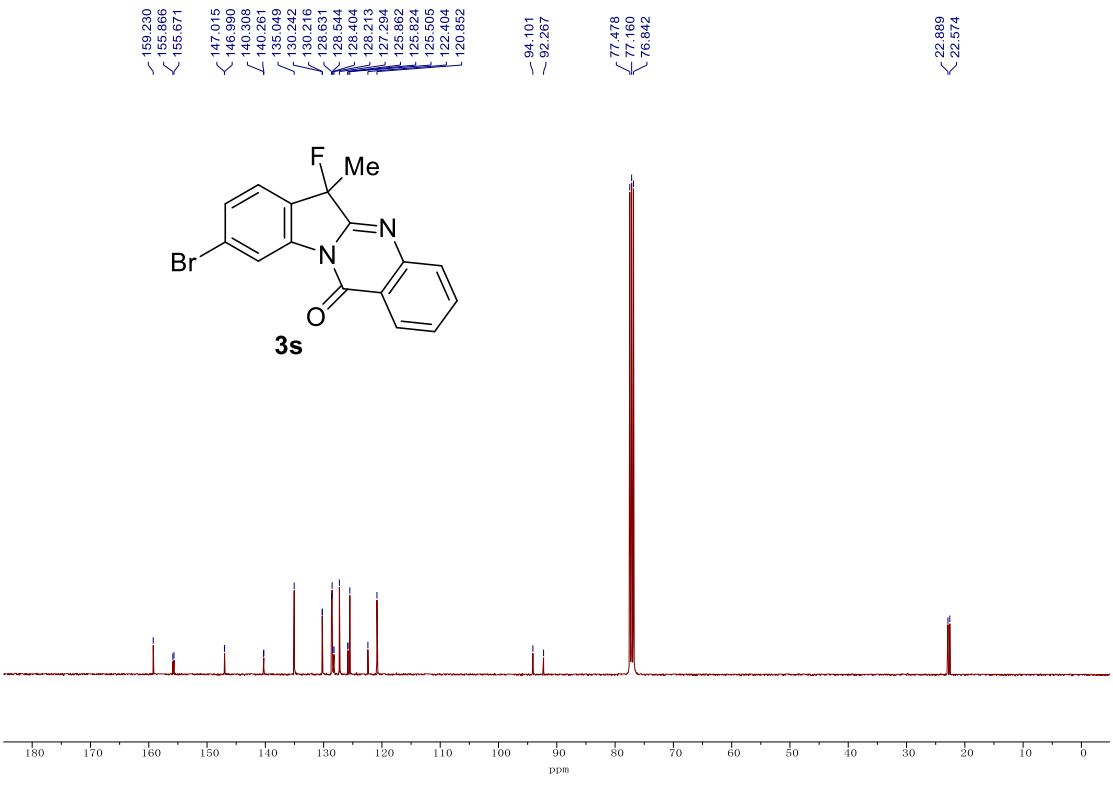
0.94
0.93
1.02
1.00
1.98
3.00
ppm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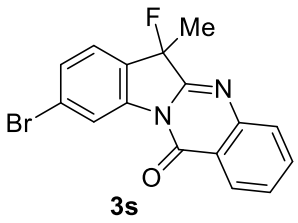
140.261
135.049
130.242
130.216
128.631
128.544
128.404
128.213
127.294
125.862
125.824
125.505
122.404
120.852
94.101
92.267
77.478
77.160
76.842
22.889
22.574
F
Me
N
N
Br
O
3s
ppm


F
Me
N
Br
N
O

**3s**


-137.947
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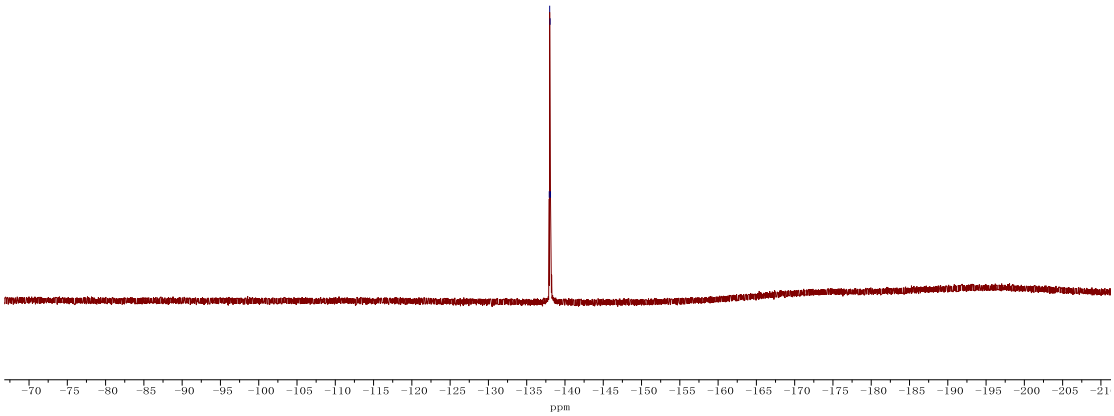
-138.056
-138.111


-70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180 -185 -190 -195 -200 -205 -21
ppm


8.801
8.414
8.410
8.394
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7.804
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7.612
7.595
7.578
7.574
7.541
7.537
7.521
7.517
7.510
7.506
7.490
7.486
7.261
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2.914
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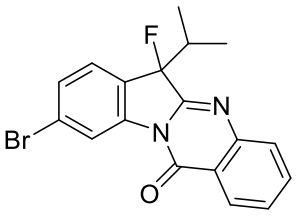
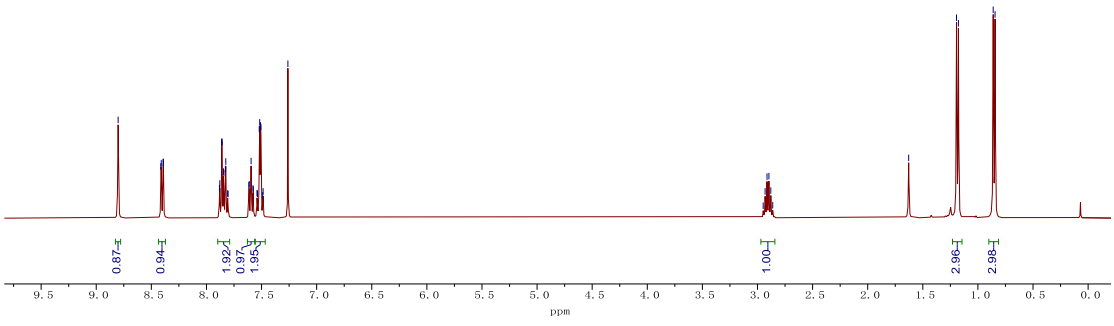
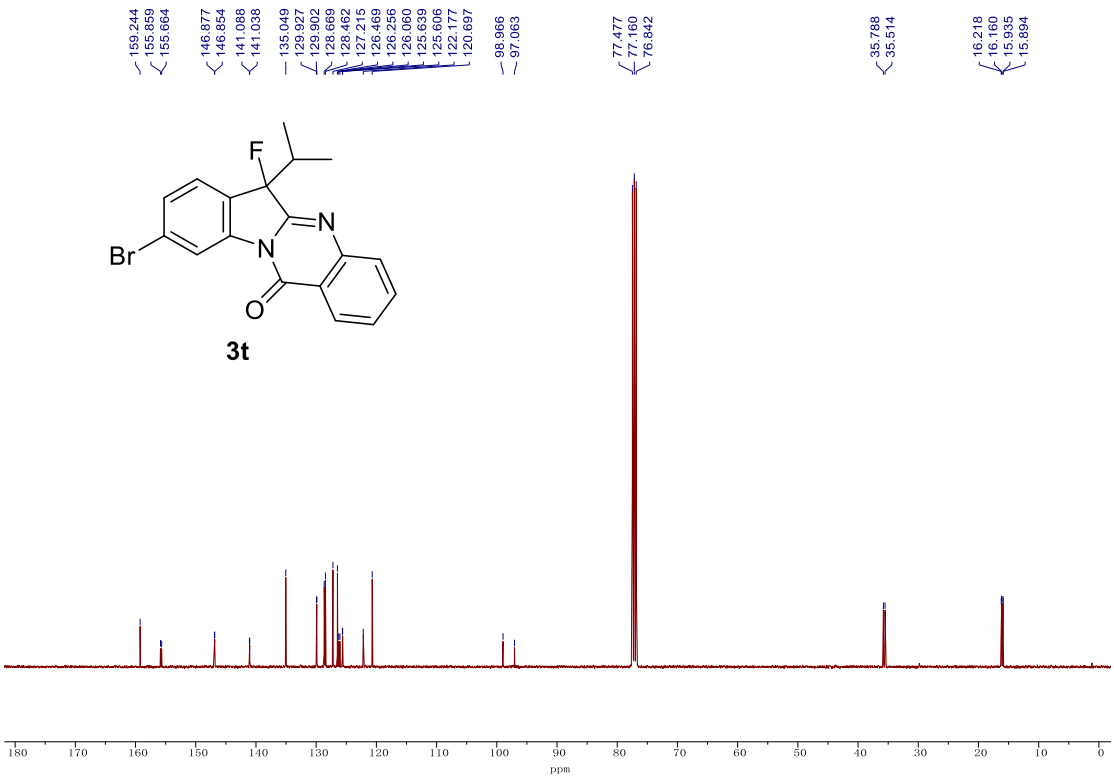
0.861
0.844


F
N
Br
N
O

**3t**


0.87
0.94
1.92
0.97
1.95
1.00
2.96
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm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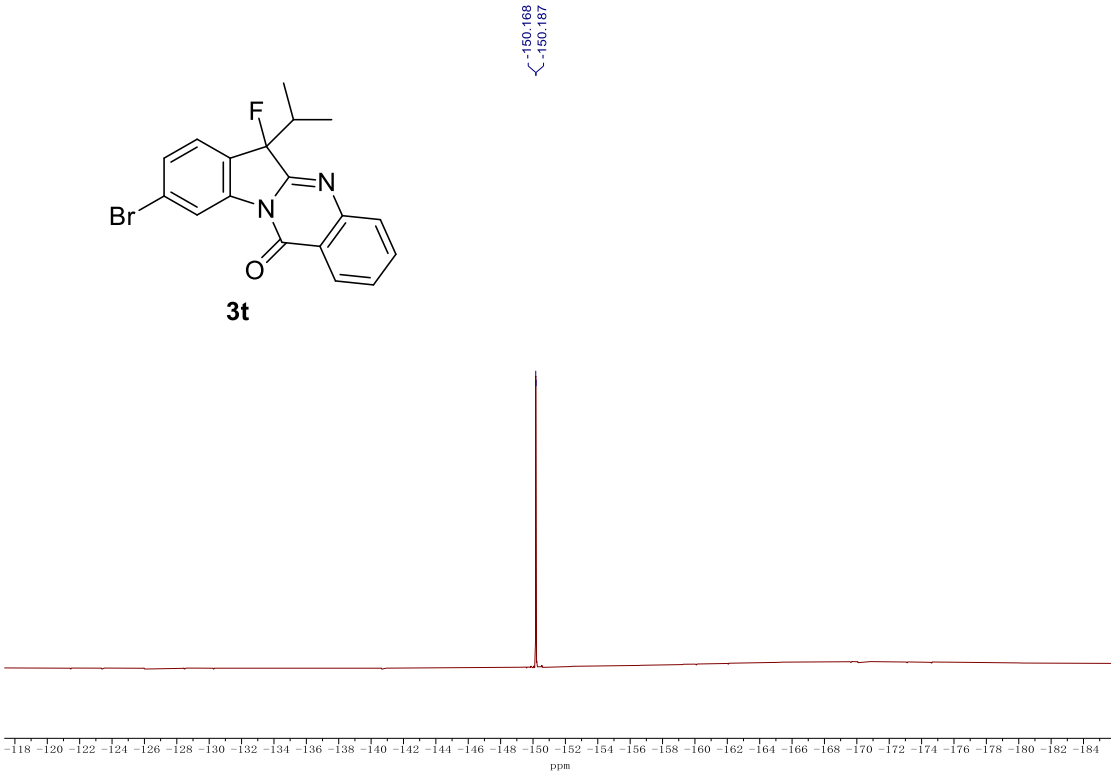
155.859
155.664
146.877
146.854
141.088
141.038
135.049
129.927
129.902
128.669
128.462
127.215
126.469
126.256
126.060
125.639
125.606
122.177
120.697
98.966
97.063
77.477
77.160
76.842
35.788
35.514
16.218
16.160
15.935
15.894
F
N
N
Br
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

**3t**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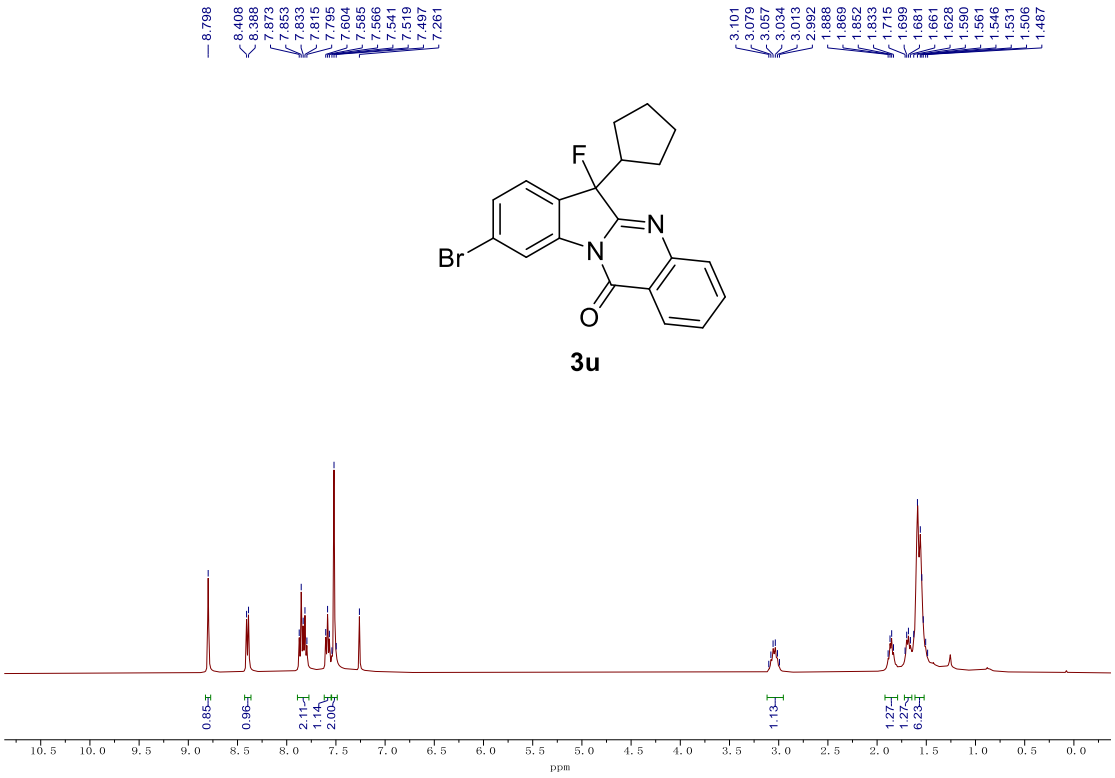
F
N
N
Br
O
−118 −120 −122 −124 −126 −128 −130 −132 −134 −136 −138 −140 −142 −144 −146 −148 −150 −152 −154 −156 −158 −160 −162 −164 −166 −168 −170 −172 −174 −176 −178 −180 −182 −184
ppm

**3t**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8.408
8.388
7.873
7.853
7.833
7.815
7.795
7.604
7.585
7.566
7.541
7.519
7.497
7.261
3.101
3.079
3.057
3.034
3.013
2.992
1.888
1.869
1.852
1.833
1.715
1.699
1.681
1.661
1.628
1.590
1.561
1.546
1.531
1.506
1.487
F
Br
N
N
O
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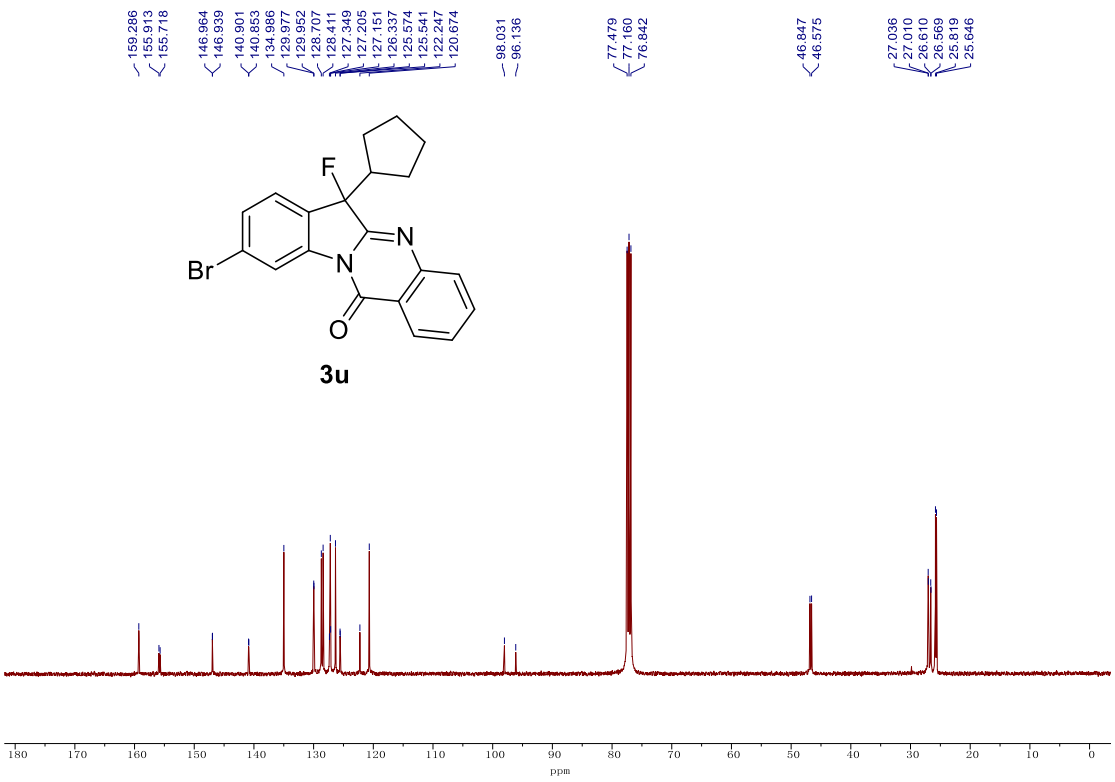
0.96
2.11
1.14
2.00
1.13
1.27
1.27
6.23
ppm

**3u**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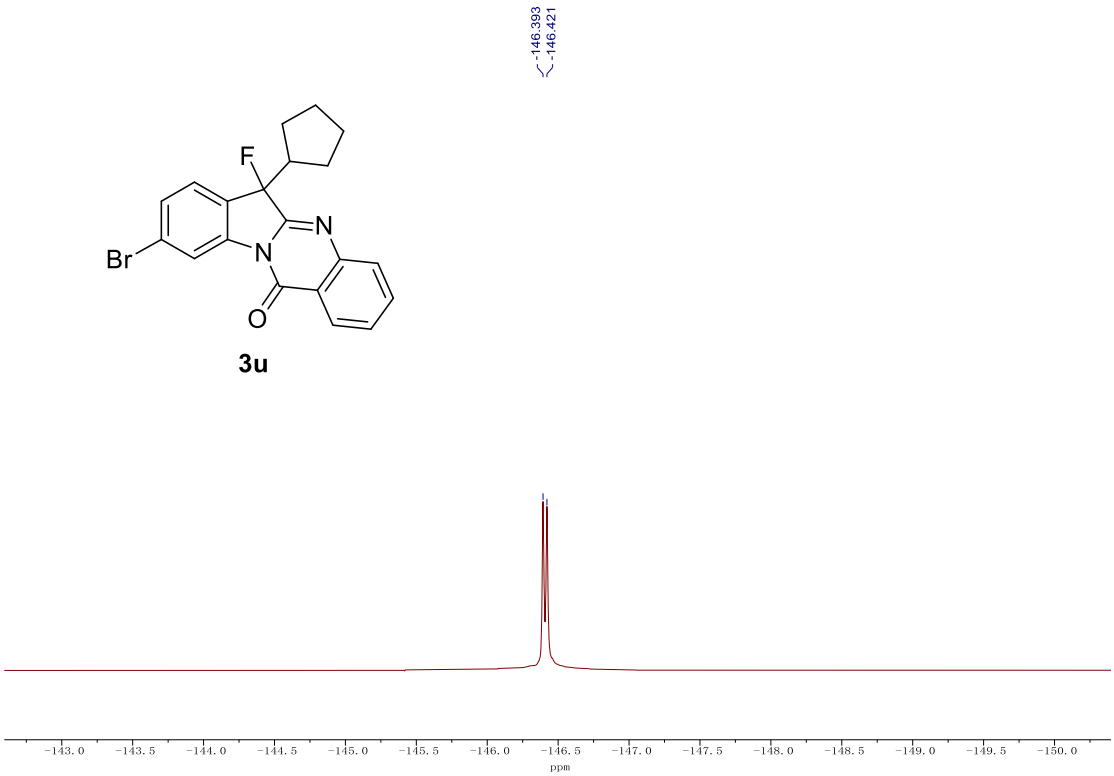
155.913
155.718
146.964
146.939
140.901
140.853
134.986
129.977
129.952
128.707
128.411
127.349
127.205
127.151
126.337
125.574
125.541
122.247
120.674
98.031
96.136
77.479
77.160
76.842
46.847
46.575
27.036
27.010
26.610
26.569
25.819
25.646
F
Br
N
N
O
ppm

**3u**

F
Br
N
N
O

**3u**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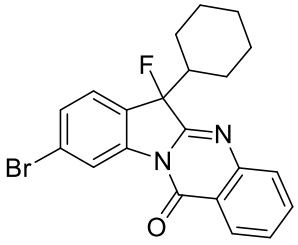
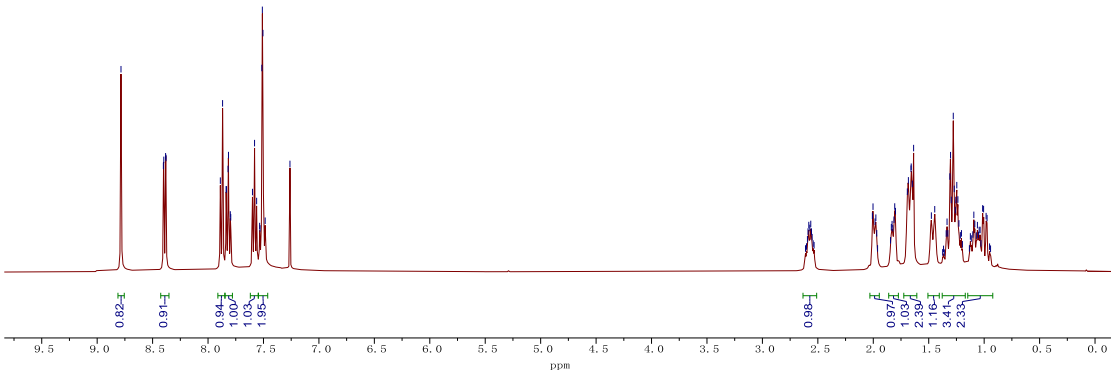
-146.421
-143.0
-143.5
-144.0
-144.5
-145.0
-145.5
-146.0
-146.5
-147.0
-147.5
-148.0
-148.5
-149.0
-149.5
-150.0
ppm


8.785
8.403
8.399
8.383
8.379
7.889
7.869
7.837
7.833
7.819
7.816
7.799
7.795
7.599
7.580
7.562
7.535
7.531
7.515
7.510
7.505
7.485
7.261
2.589
2.582
2.572
2.564
2.557
2.008
2.002
1.984
1.977
1.969
1.837
1.831
1.824
1.813
1.807
1.800
1.693
1.683
1.660
1.658
1.648
1.636
1.476
1.446
1.342
1.335
1.328
1.309
1.303
1.297
1.279
1.270
1.261
1.255
1.247
1.237
1.228
1.205
1.102
1.093
1.084
1.061
1.052
1.045
1.036
1.014
1.005
0.983
0.974


F
Br
N
N
O

**3v**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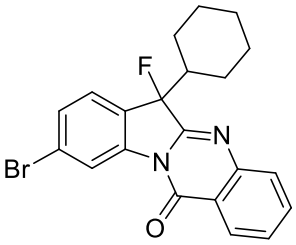
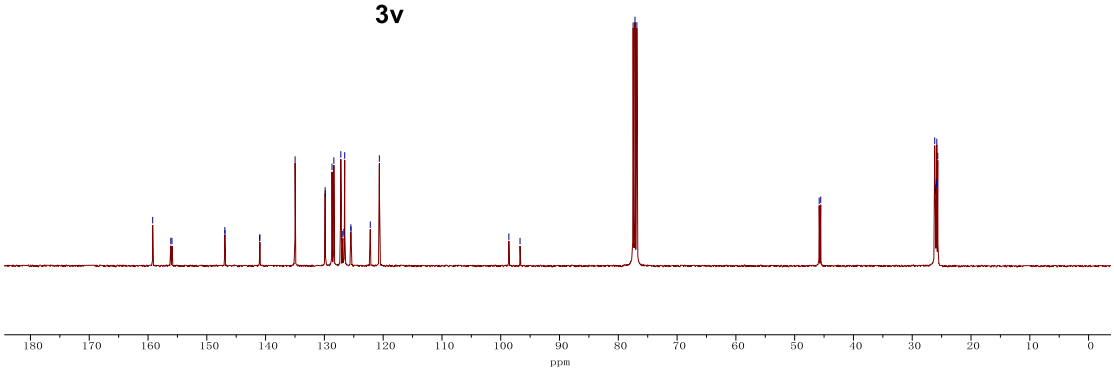
0.91
0.94
1.00
1.03
1.95
0.98
0.97
1.03
2.39
1.16
3.41
2.33
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

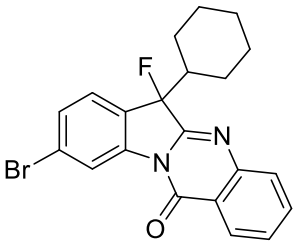

159.205
156.122
155.928
146.932
146.908
141.023
140.970
134.982
129.874
129.848
128.699
128.384
127.204
126.874
126.678
126.543
125.501
125.468
122.196
120.650
98.622
96.717
77.479
77.161
76.844
45.829
45.564
26.176
26.090
26.037
25.910
25.874
25.817
25.656


F
N
N
Br
O

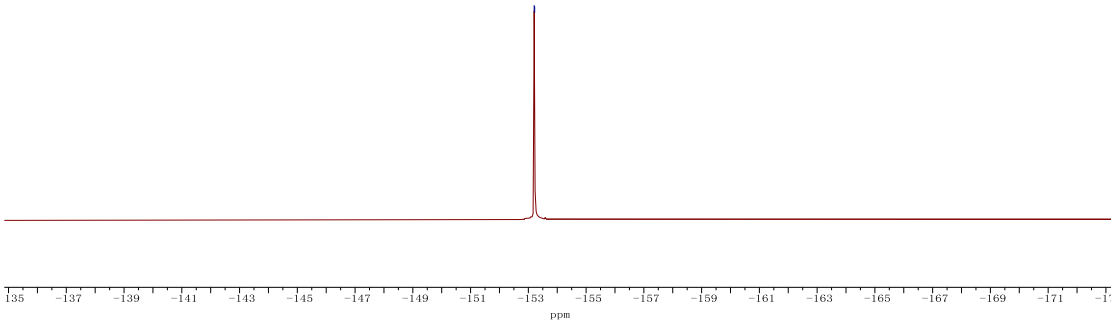
**3v**


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

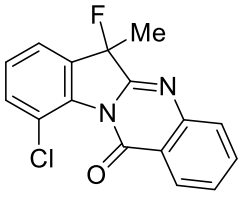

-153.201
-153.220


F
N
N
Br
O

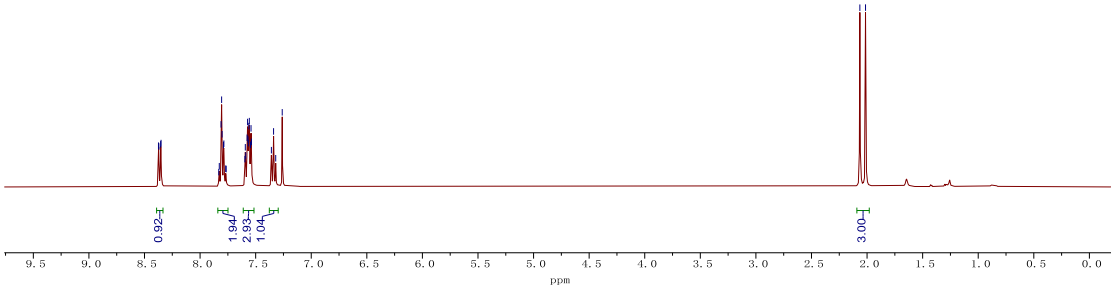
**3v**


135
137
139
141
143
145
147
149
151
153
155
157
159
161
163
165
167
169
171
ppm


8.374
8.371
8.355
8.351
7.832
7.827
7.811
7.806
7.802
7.790
7.786
7.769
7.766
7.597
7.593
7.589
7.577
7.573
7.569
7.565
7.562
7.557
7.547
7.542
7.538
7.358
7.339
7.320
7.261
2.065
2.014


F
Me
N
N
Cl
O

**3w**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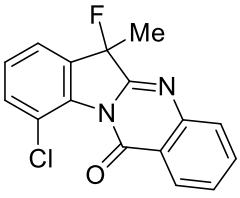
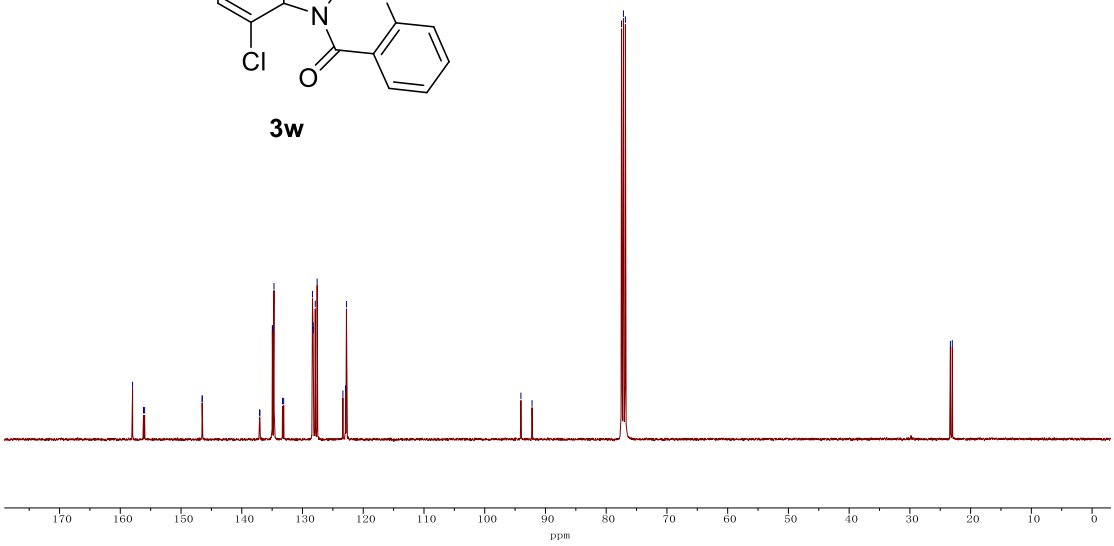
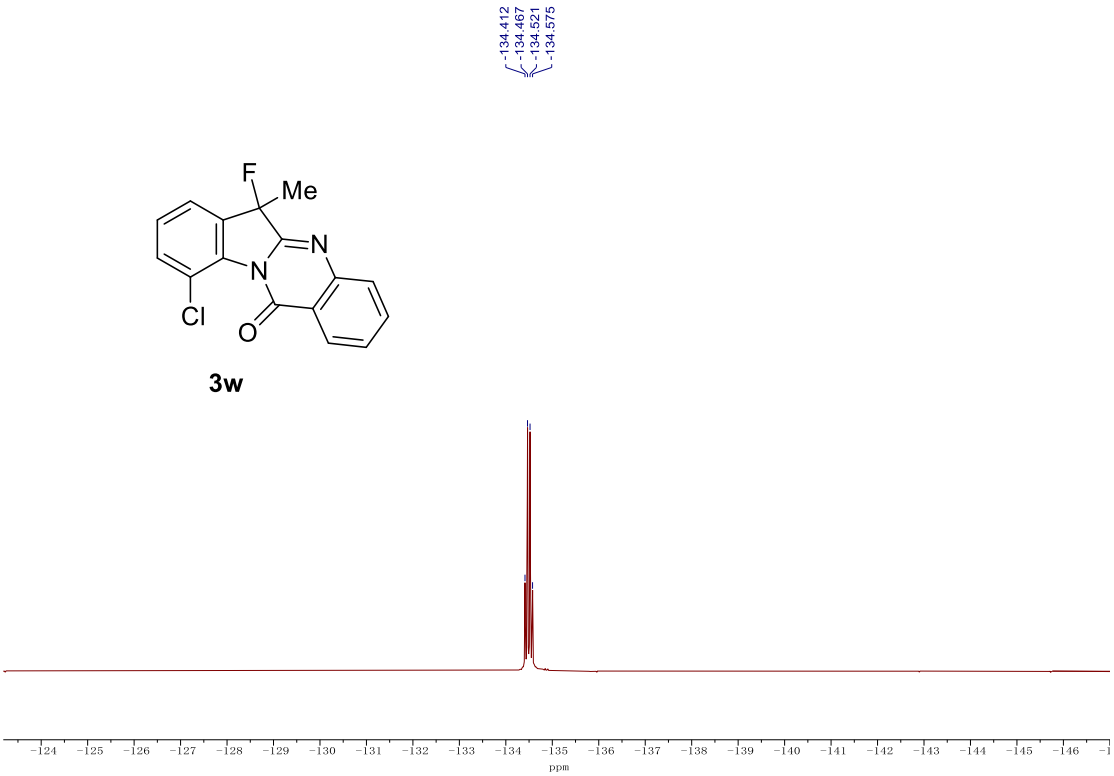
1.94
2.93
1.04
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


157.979
156.184
155.996
146.525
146.499
137.063
137.017
134.967
134.937
134.694
133.291
133.101
128.361
128.256
128.228
127.902
127.592
123.348
122.918
122.766
94.043
92.210
77.478
77.160
76.842
23.329
23.012


F
Me
N
N
Cl
O

**3w**


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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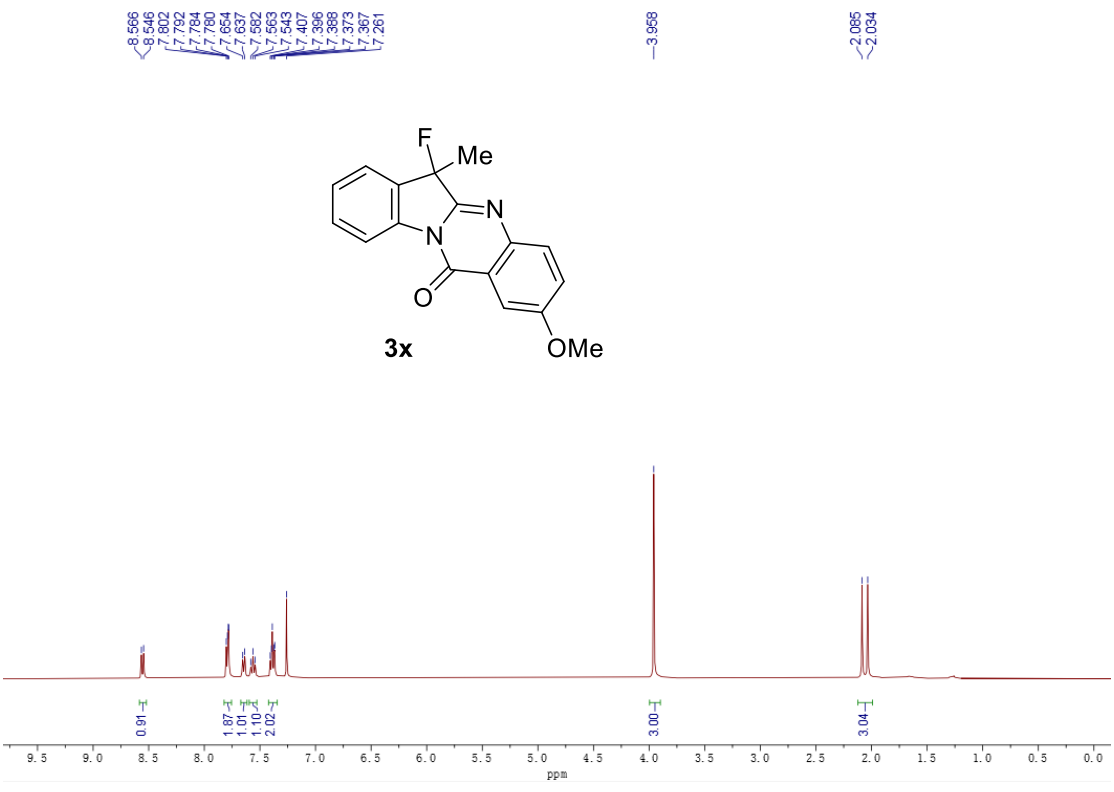
-134.467
-134.521
-134.575
F
Me
N
N
Cl
O
3w
ppm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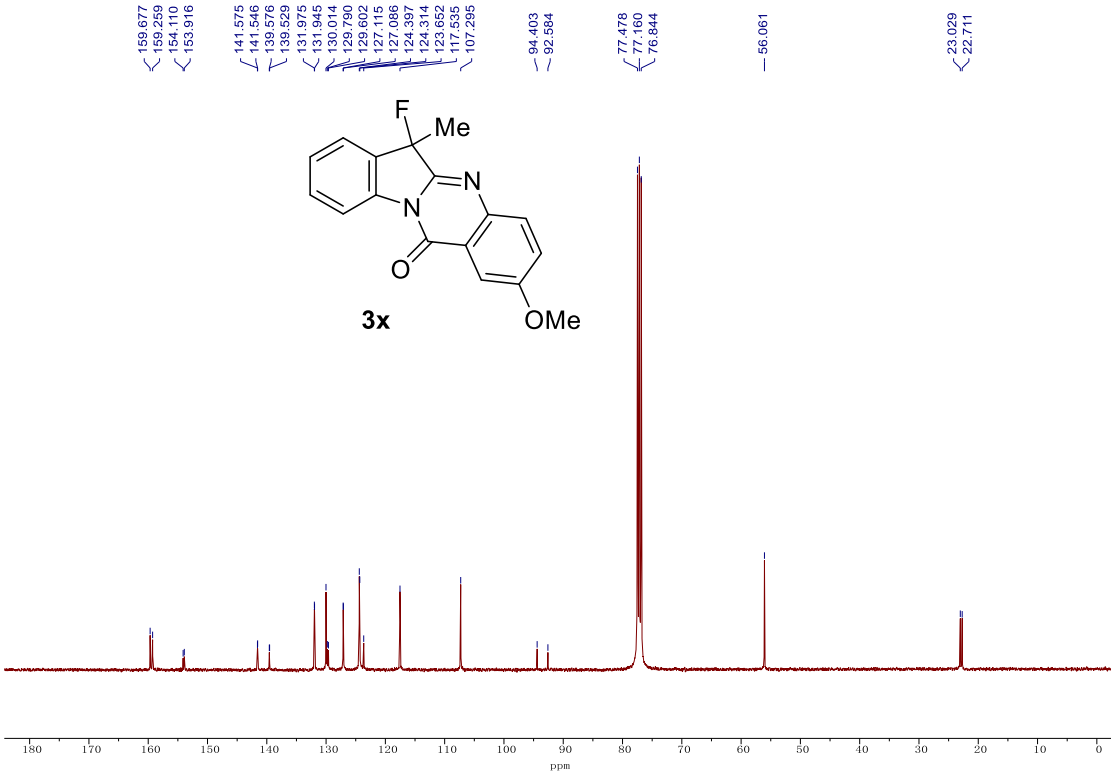
8.546
7.802
7.792
7.784
7.780
7.654
7.637
7.582
7.563
7.543
7.407
7.396
7.388
7.373
7.367
7.261
3.958
2.085
2.034
F
Me
N
N
O
3x
OMe
0.91
1.87
1.01
1.10
2.02
3.00
3.04
ppm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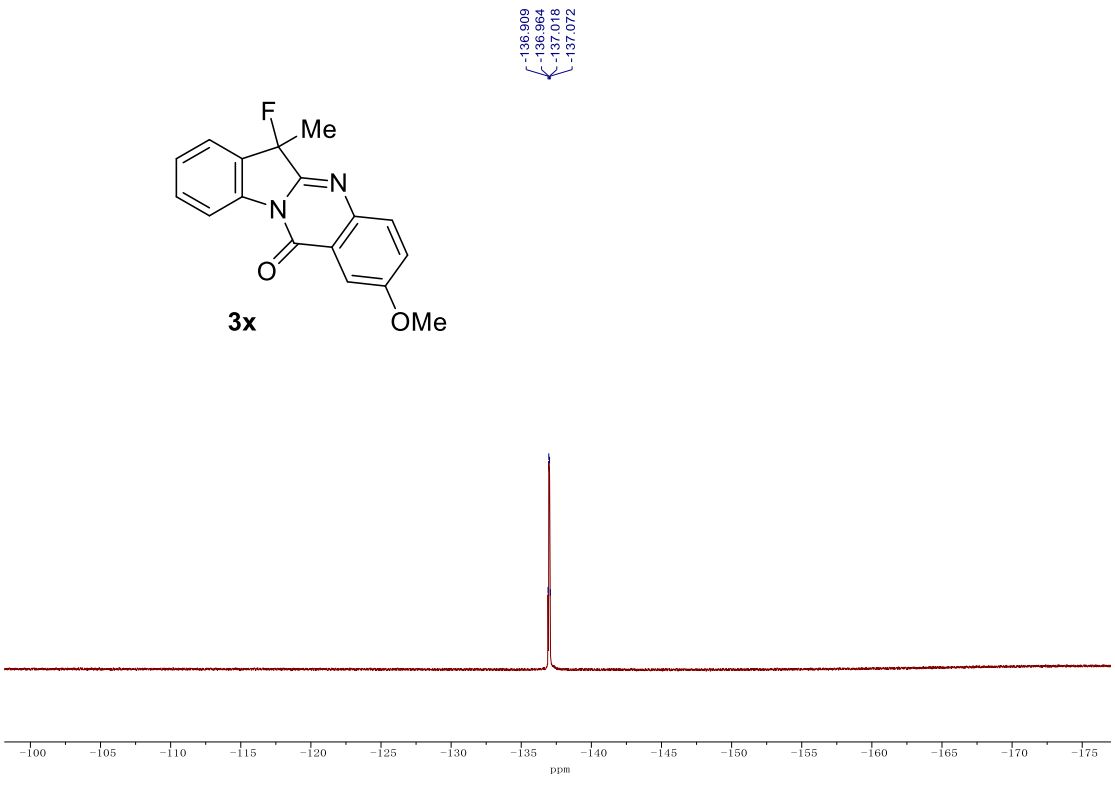
154.110
153.916
141.575
141.546
139.576
139.529
131.975
131.945
130.014
129.790
129.602
127.115
127.086
124.397
124.314
123.652
117.535
107.295
94.403
92.584
77.478
77.160
76.844
56.061
23.029
22.711
F
Me
N
N
O
OMe
3x
ppm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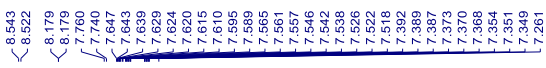
-136.964
-137.018
-137.072
F
Me
N
N
O
OMe
3x
ppm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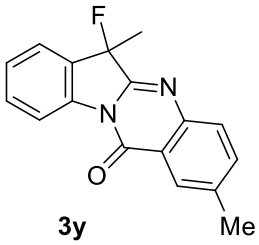
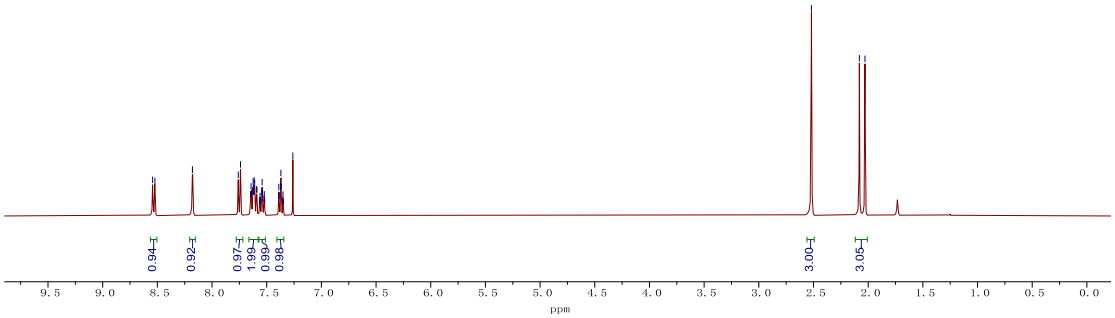
8.179
8.179
7.760
7.740
7.647
7.643
7.639
7.629
7.624
7.620
7.615
7.610
7.595
7.589
7.565
7.561
7.557
7.546
7.542
7.538
7.526
7.522
7.518
7.392
7.389
7.387
7.373
7.370
7.368
7.354
7.351
7.349
7.261
2.519
2.081
2.029


F
N
N
O
3y
Me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0.92
0.97
1.99
0.99
0.98
3.00
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


159.404
155.460
155.267
145.067
145.042
139.526
139.481
138.681
136.081
131.944
131.914
129.519
129.332
128.259
127.010
126.982
126.733
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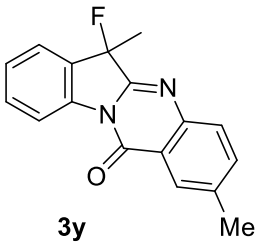
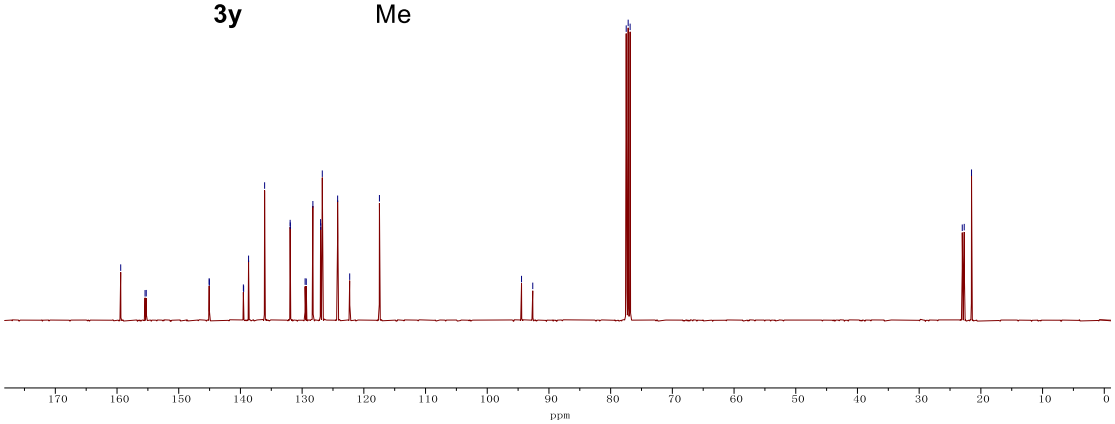
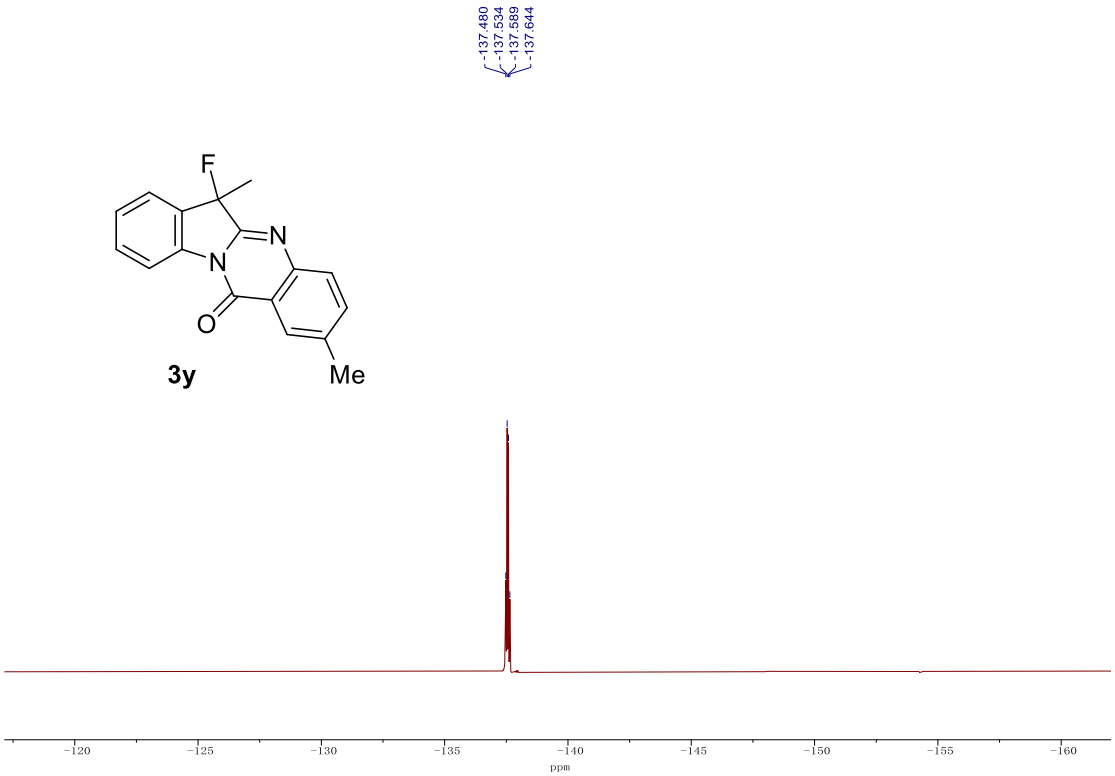
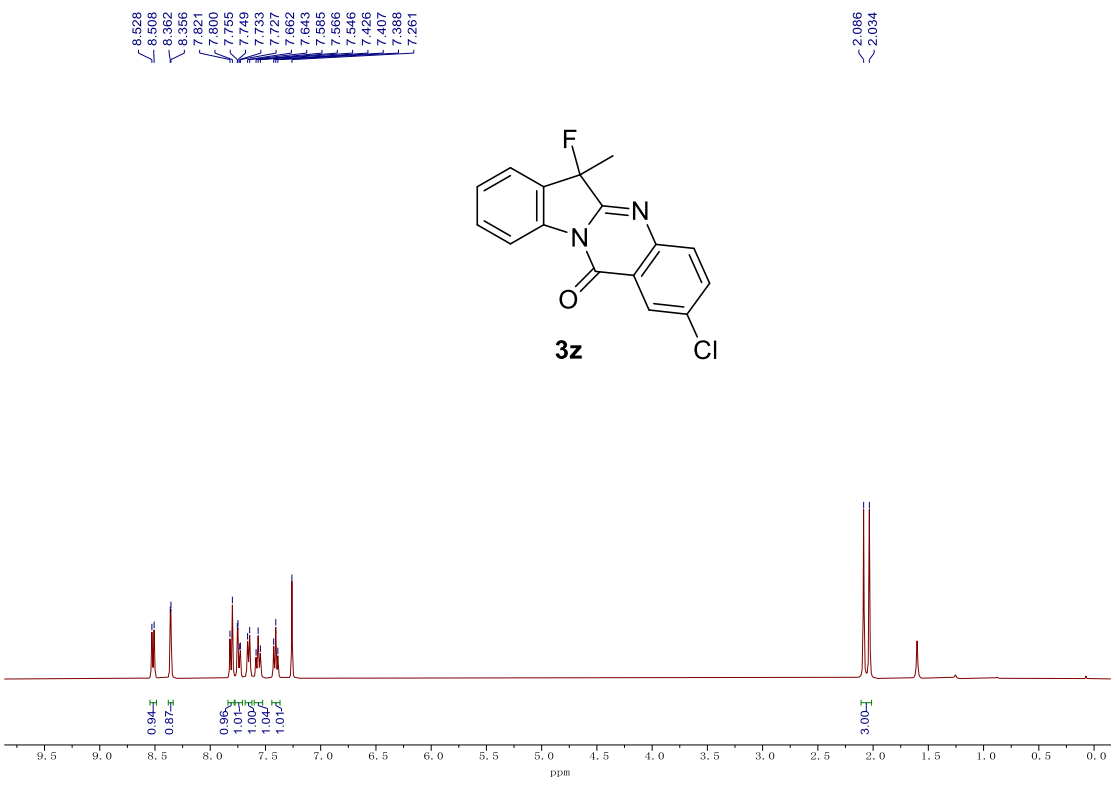
122.291
117.473
94.444
92.624
77.478
77.160
76.842
23.014
22.697
21.513


F
N
N
O
3y
Me


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-137.480
-137.534
-137.589
-137.644
F
N
N
O
3y
Me
−120
−125
−130
−135
−140
−145
−150
−155
−160
ppm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8.362
8.356
7.821
7.800
7.755
7.749
7.733
7.727
7.662
7.643
7.585
7.566
7.546
7.426
7.407
7.388
7.261
2.086
2.034
F
N
N
O
3z
Cl
0.94
0.87
0.96
1.01
1.00
1.04
1.01
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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4.0
3.5
3.0
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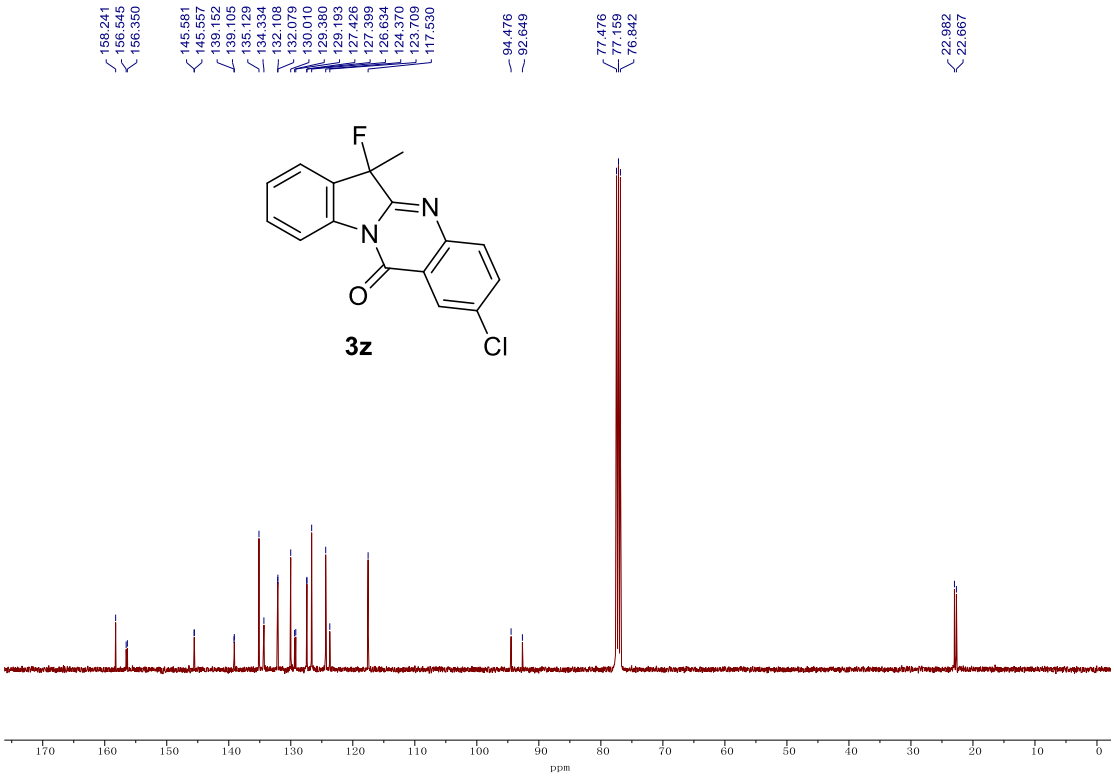
2.0
1.5
1.0
0.5
0.0
ppm


158.241
156.545
156.350
145.581
145.557
139.152
139.105
135.129
134.334
132.108
132.079
130.010
129.380
129.193
127.426
127.399
126.634
124.370
123.709
117.530
94.476
92.649
77.476
77.159
76.842
22.982
22.667
F
N
N
O
Cl
3z
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160
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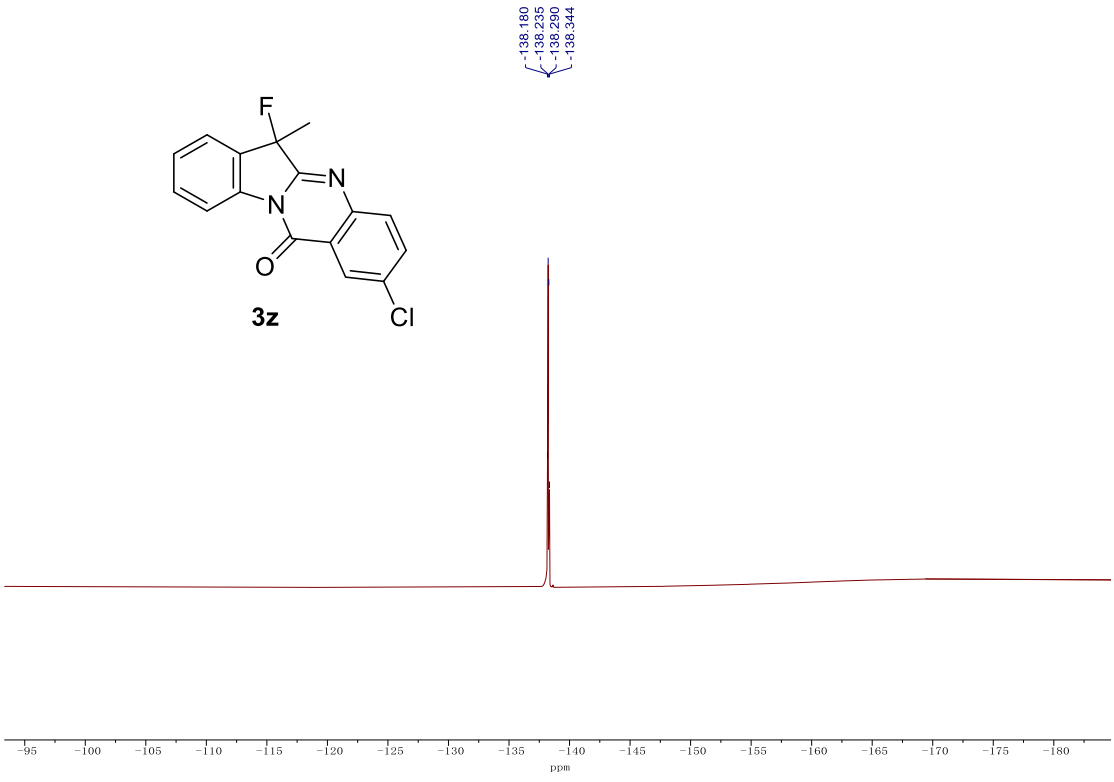
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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-138.235
-138.290
-138.344
F
N
N
O
Cl
3z
−95
−100
−105
−110
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−120
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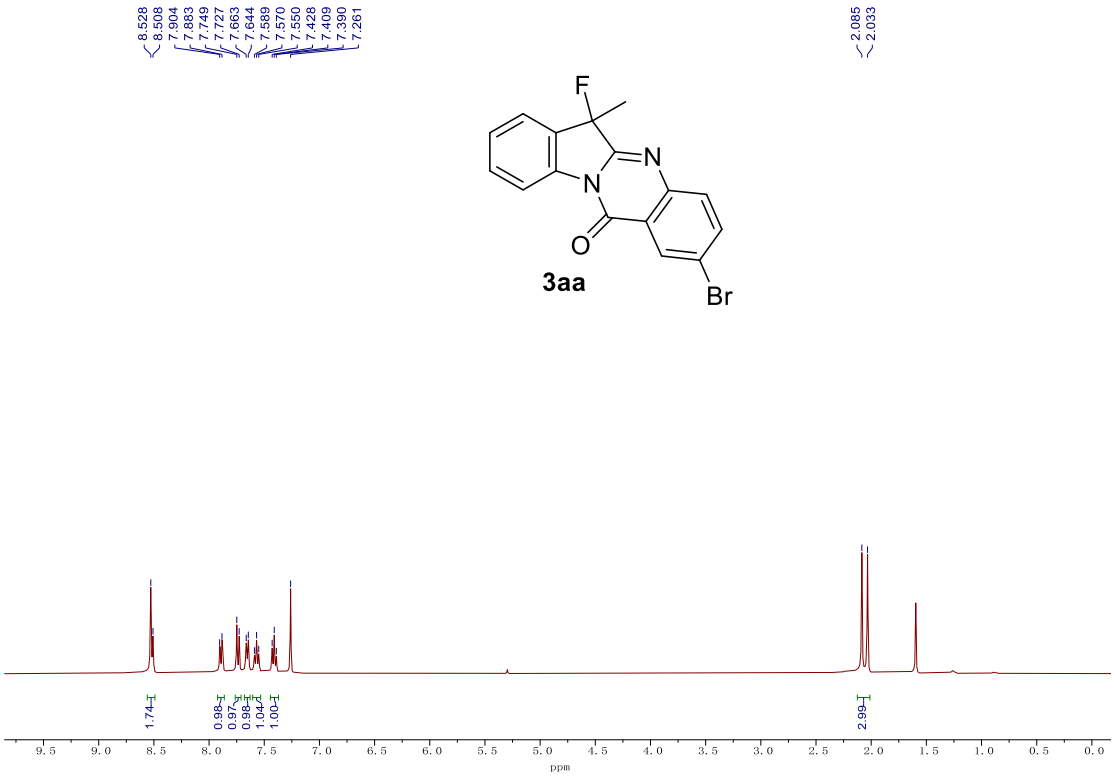
−130
−135
−140
−145
−150
−155
−160
−165
−170
−175
−180
ppm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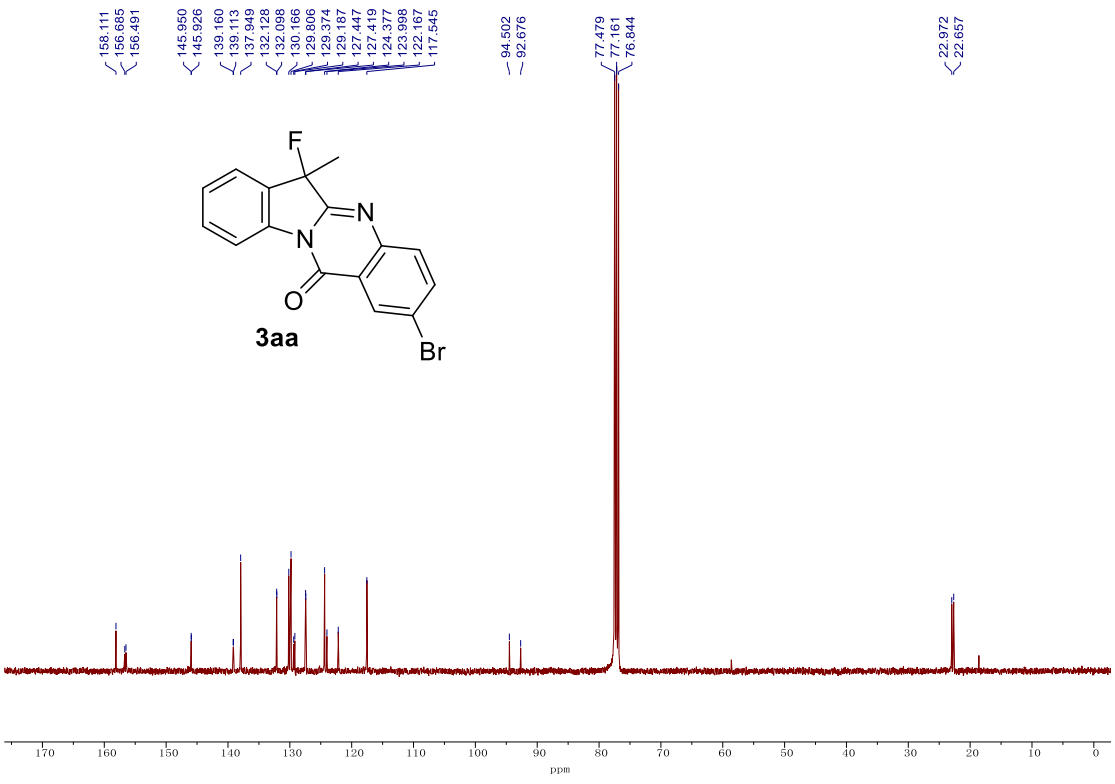
8.508
7.904
7.883
7.749
7.727
7.663
7.644
7.589
7.570
7.550
7.428
7.409
7.390
7.261
2.085
2.033
F
N
N
O
Br
3aa
1.74
0.98
0.97
0.98
1.04
1.00
2.99
ppm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156.491
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145.926
139.160
139.113
137.949
132.128
132.098
130.166
129.806
129.374
129.187
127.447
127.419
124.377
123.998
122.167
117.545
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77.479
77.161
76.644
22.972
22.657
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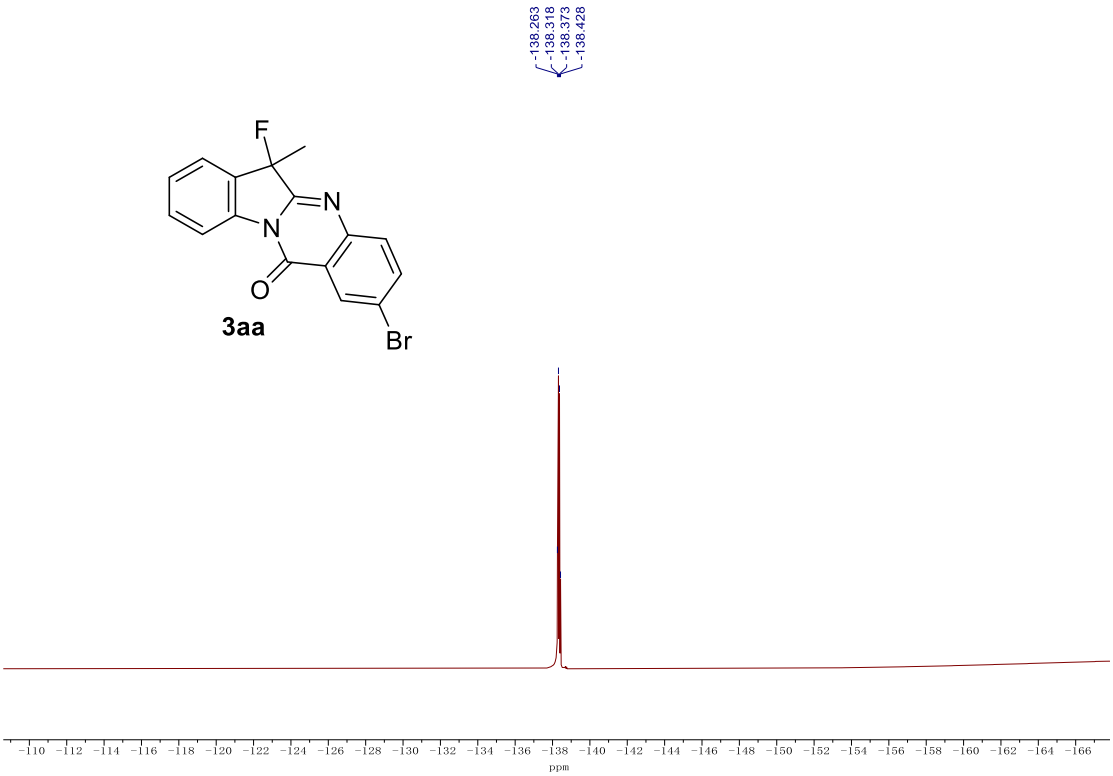
N
O
Br
3aa
ppm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N
O
Br
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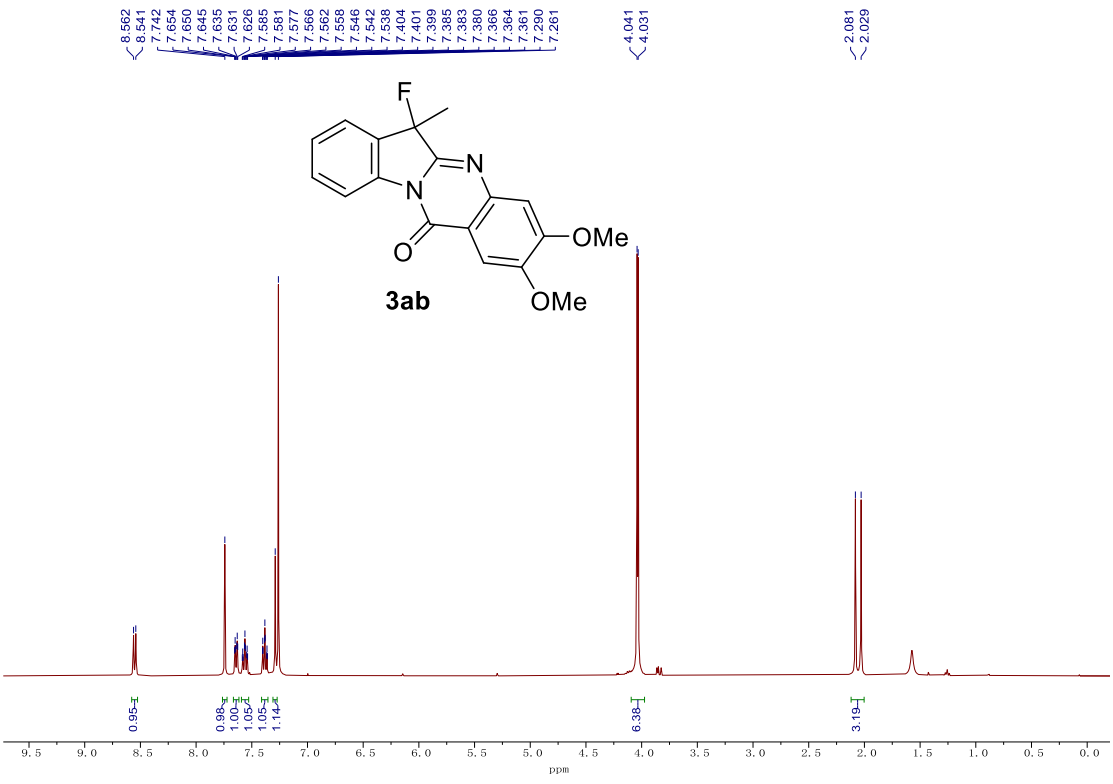
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8.541
7.742
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7.645
7.635
7.631
7.626
7.585
7.581
7.577
7.566
7.562
7.558
7.546
7.542
7.538
7.404
7.401
7.399
7.385
7.383
7.380
7.366
7.364
7.361
7.290
7.261
4.041
4.031
2.081
2.029
F
N
N
O
OMe
OMe
3ab
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1.05
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3.19
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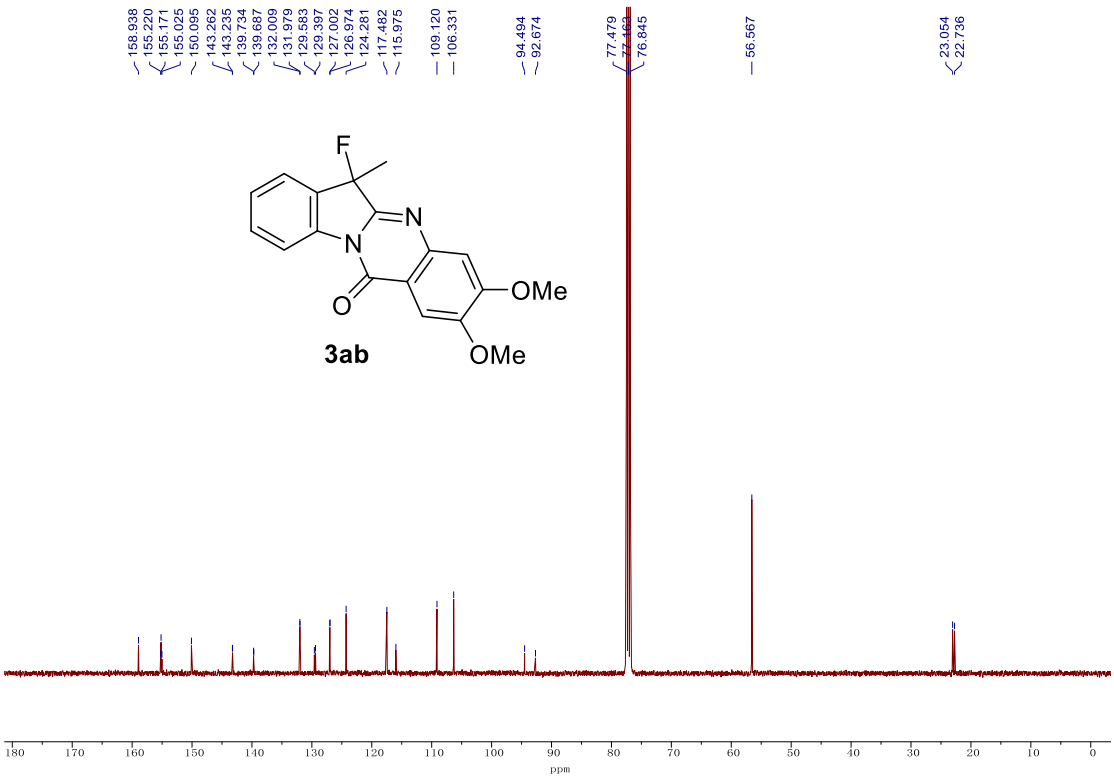
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129.397
127.002
126.974
124.281
117.482
115.975
109.120
106.331
94.494
92.674
77.479
77.163
76.845
56.567
23.054
22.736
F
N
N
O
OMe
OMe
3ab
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140
130
120
110
100
90
80
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60
50
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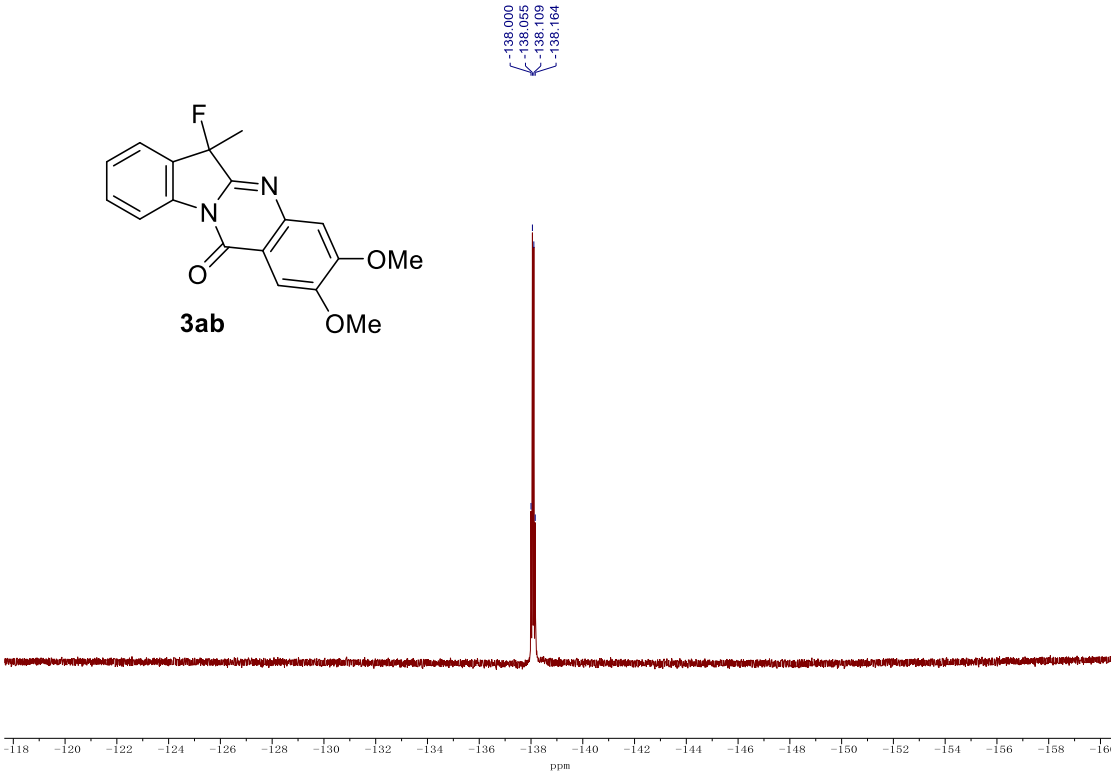
20
10
0
ppm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N
O
OMe
OMe
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-118
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-124
-126
-128
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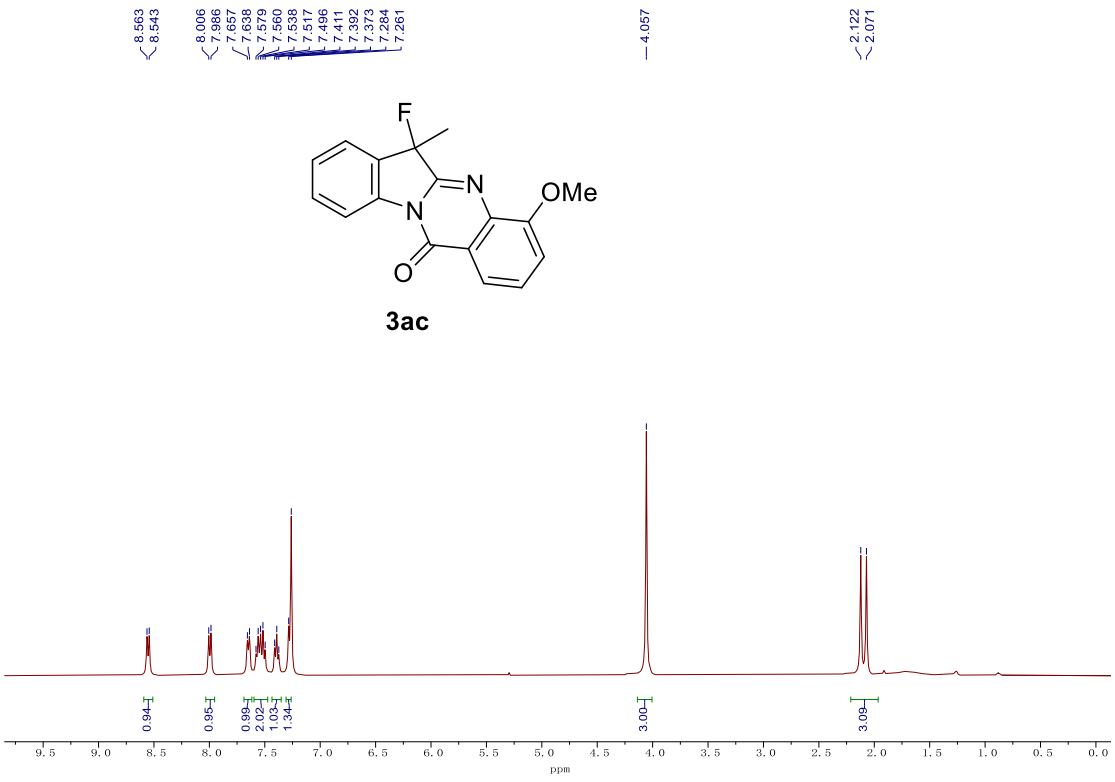
-138
-140
-142
-144
-146
-148
-150
-152
-154
-156
-158
ppm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8.543
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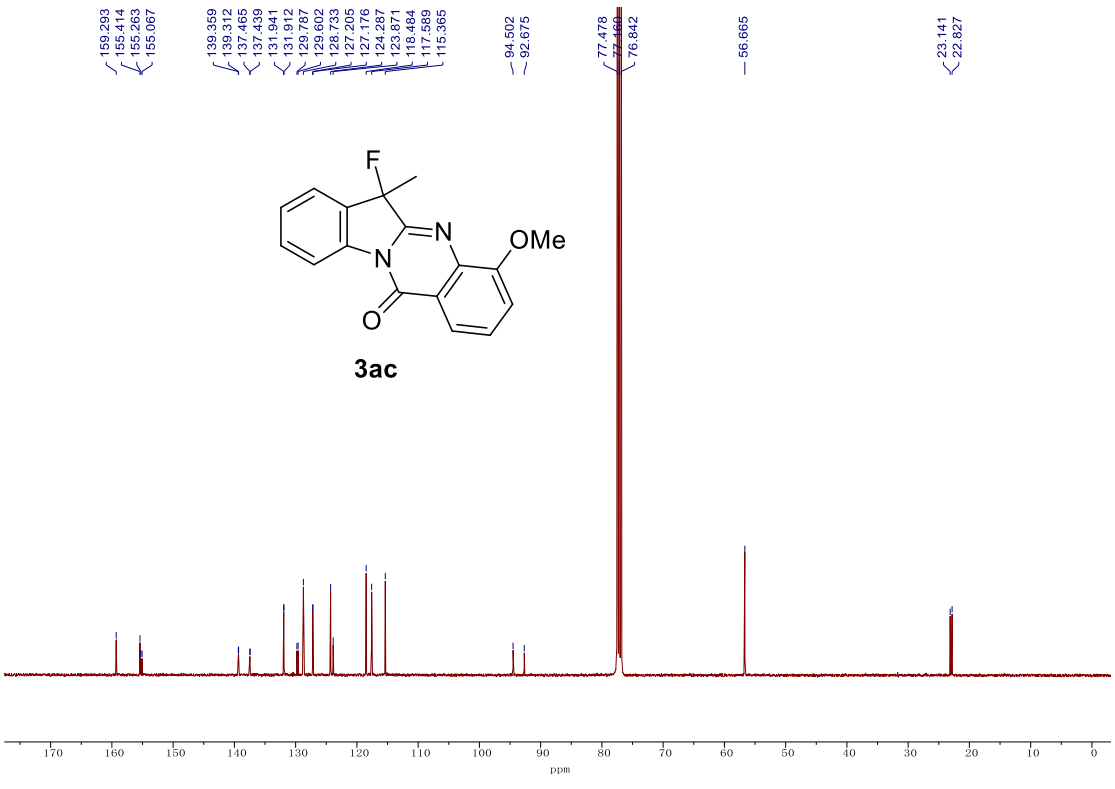
7.579
7.560
7.538
7.517
7.496
7.411
7.392
7.373
7.284
7.261
4.057
2.122
2.071
F
N
N
O
OMe
0.94
0.95
0.99
2.02
1.03
1.34
3.00
3.09
ppm

**3ac**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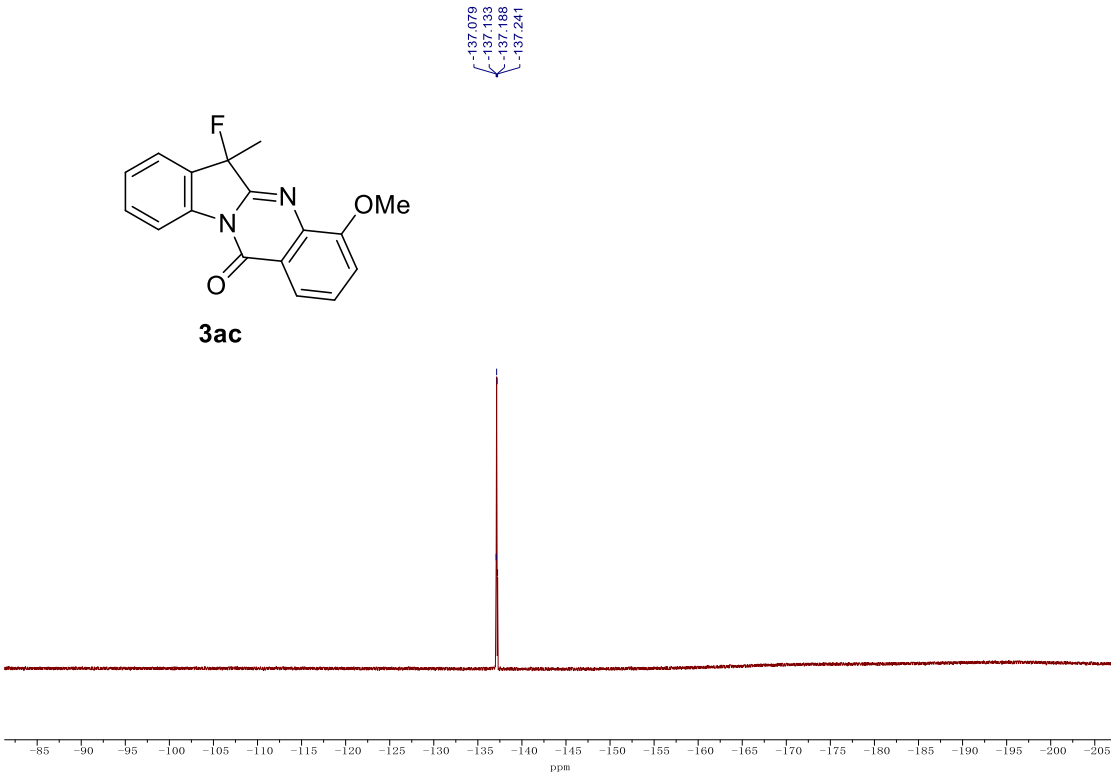
155.414
155.263
155.067
139.359
139.312
137.465
137.439
131.941
131.912
129.787
129.602
128.733
127.205
127.176
124.287
123.871
118.484
117.589
115.365
94.502
92.675
77.478
77.469
76.842
56.665
23.141
22.827
F
N
N
O
OMe
ppm

**3ac**

F
N
N
OMe
O

**3ac**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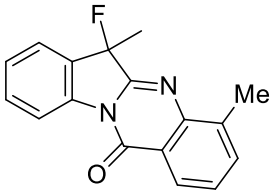
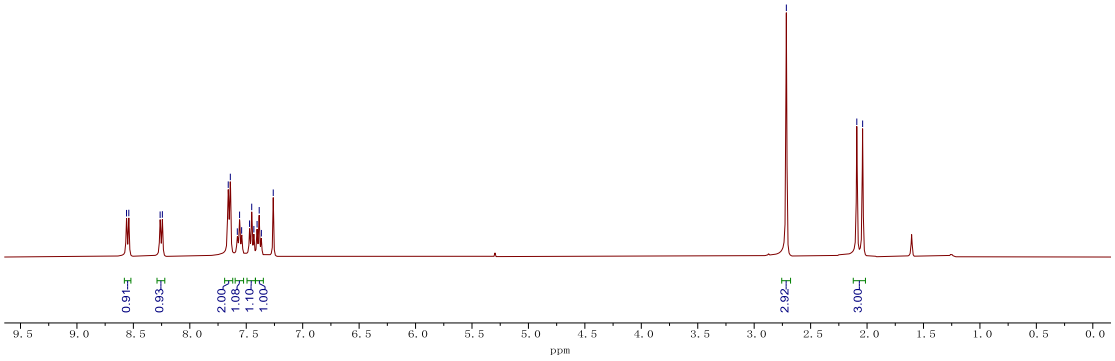
-137.133
-137.188
-137.241
-85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180 -185 -190 -195 -200 -205
ppm


8.561
8.540
8.263
8.243
7.660
7.641
7.579
7.559
7.541
7.471
7.452
7.432
7.404
7.385
7.366
7.261
2.715
2.091
2.039


F
N
N
Me
O

**3ad**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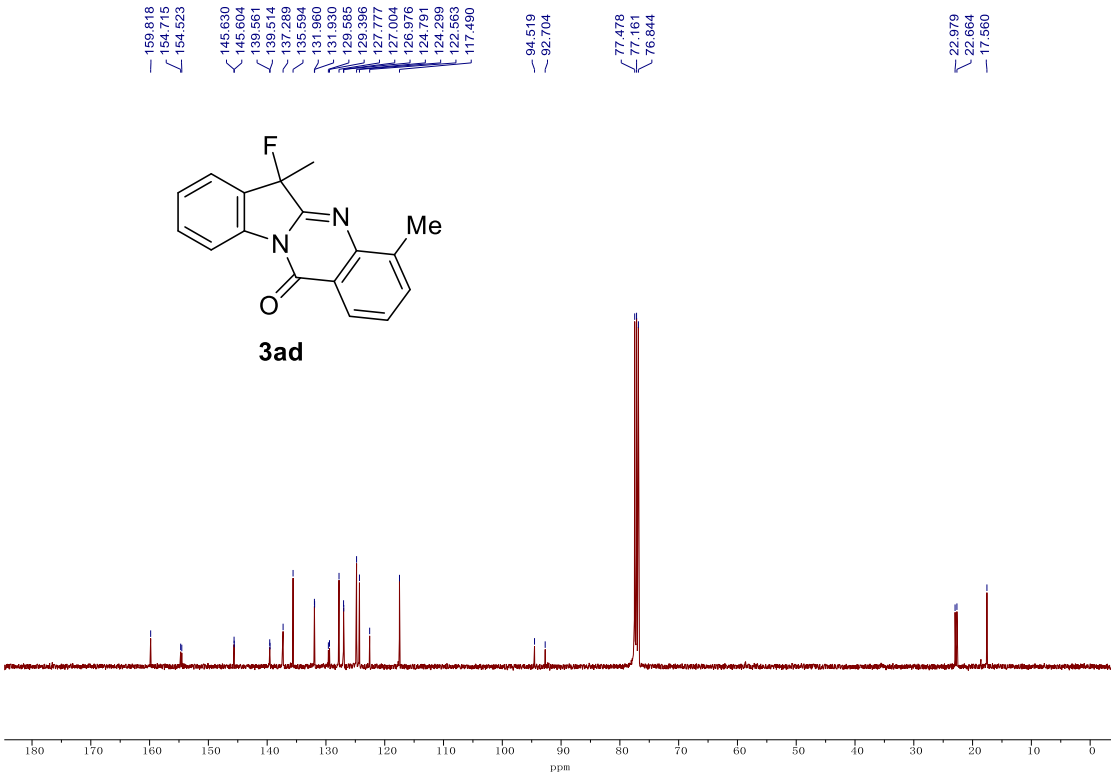
0.93
2.00
1.08
1.10
1.00
2.92
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm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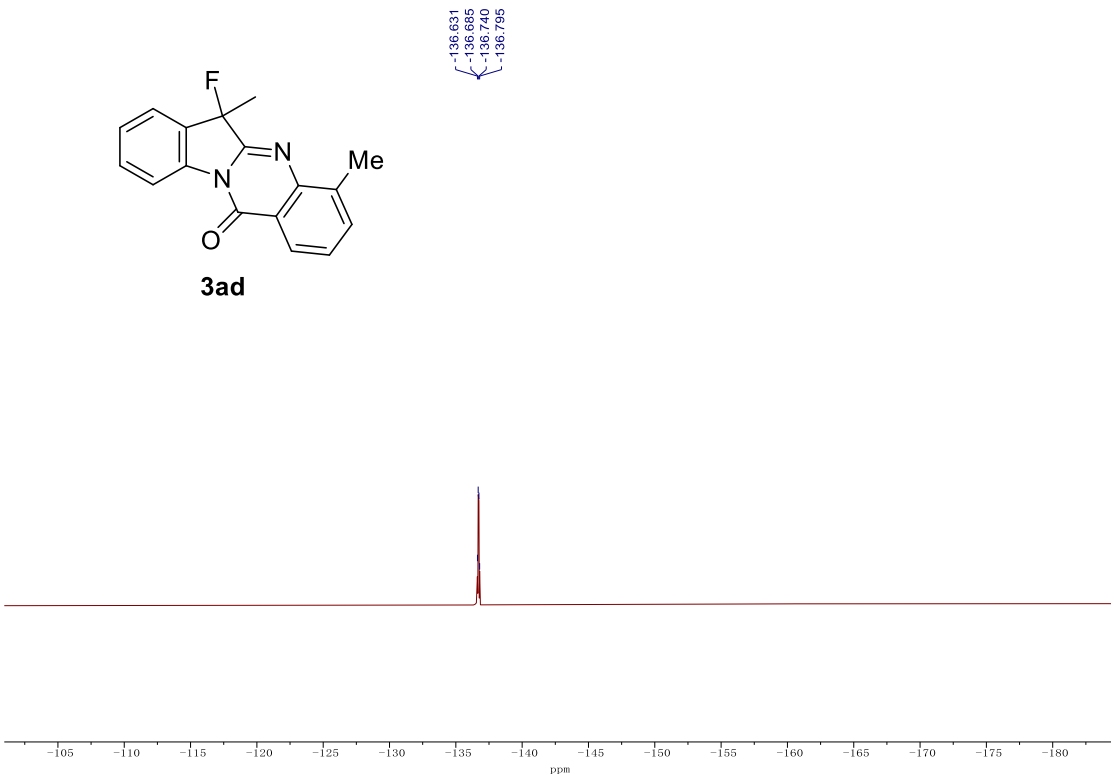
154.715
154.523
145.630
145.604
139.561
139.514
137.289
135.594
131.960
131.930
129.585
129.396
127.777
127.004
126.976
124.791
124.299
122.563
117.490
94.519
92.704
77.478
77.161
76.844
22.979
22.664
17.560
F
N
N
Me
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

**3ad**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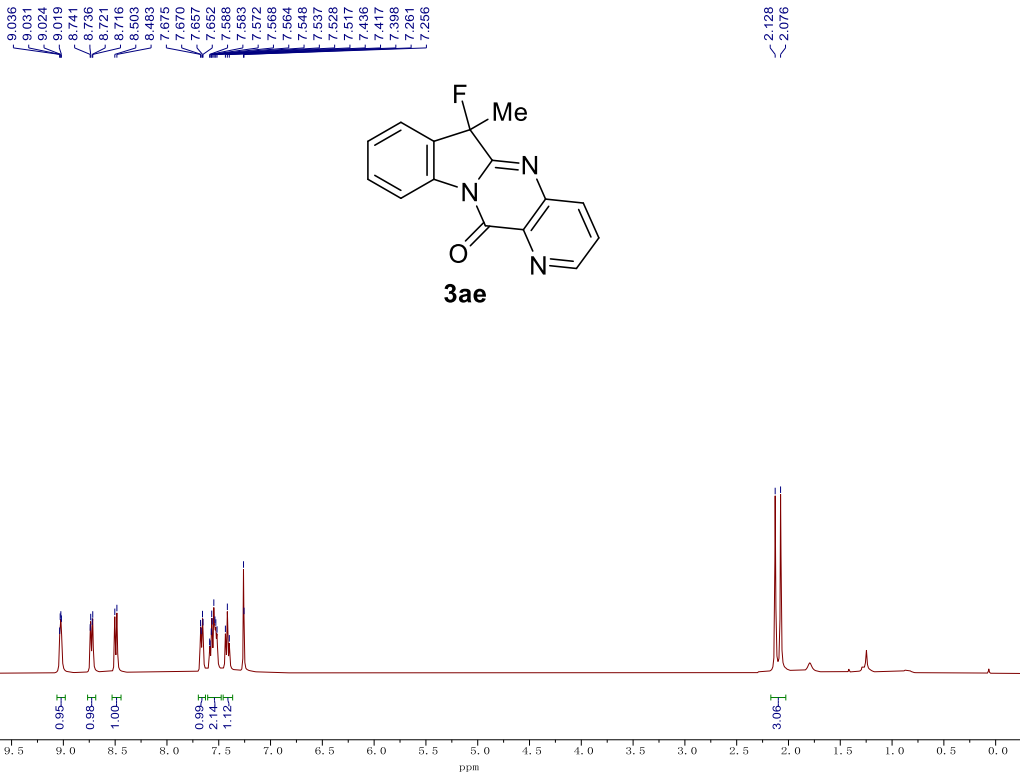
-136.685
-136.740
-136.795
F
N
N
Me
O
−105
−110
−115
−120
−125
−130
−135
−140
−145
−150
−155
−160
−165
−170
−175
−180
ppm

**3ad**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9.031
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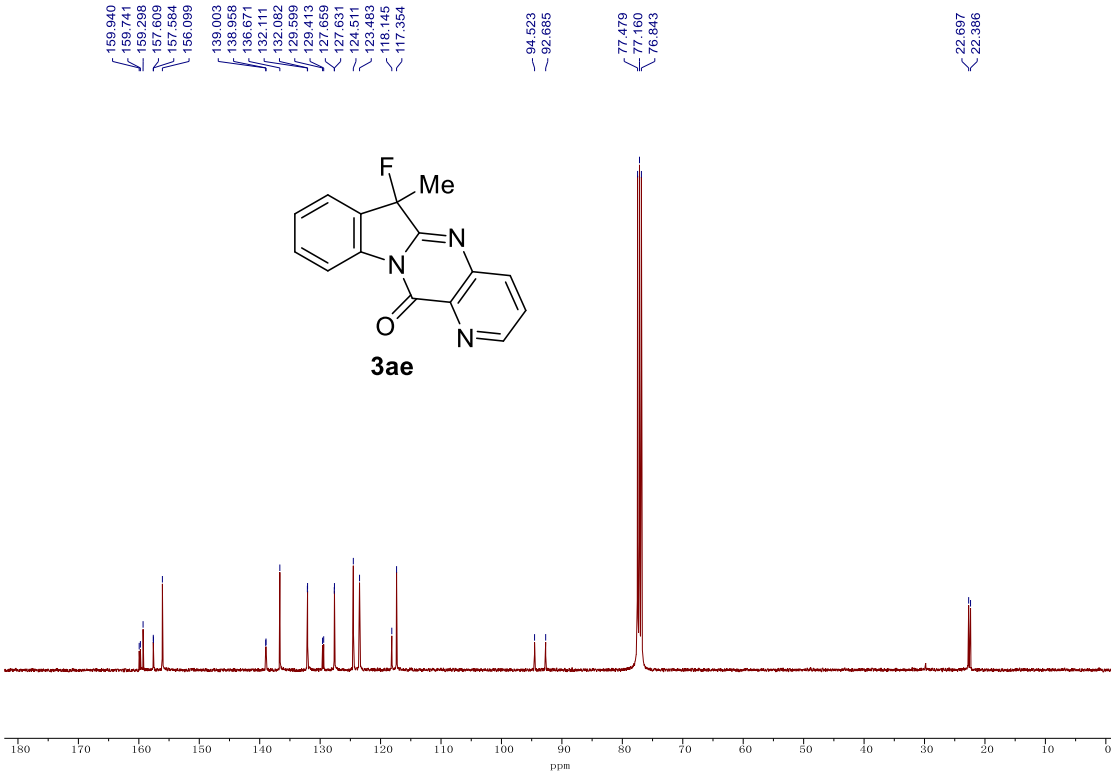
8.736
8.721
8.716
8.503
8.483
7.675
7.670
7.657
7.652
7.588
7.583
7.572
7.568
7.564
7.548
7.537
7.528
7.517
7.436
7.417
7.398
7.261
7.256
2.128
2.076
F
Me
N
N
O
N
0.95
0.98
1.00
0.99
2.14
1.12
3.06
ppm

**3ae**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132.111
132.082
129.599
129.413
127.659
127.631
124.511
123.483
118.145
117.354
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77.479
77.160
76.843
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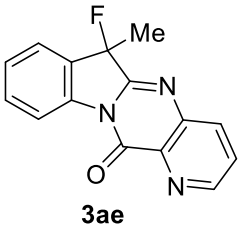
22.386
F
Me
N
N
O
N
ppm

**3ae**


F
Me
N
N
O
N

**3ae**


-138.750
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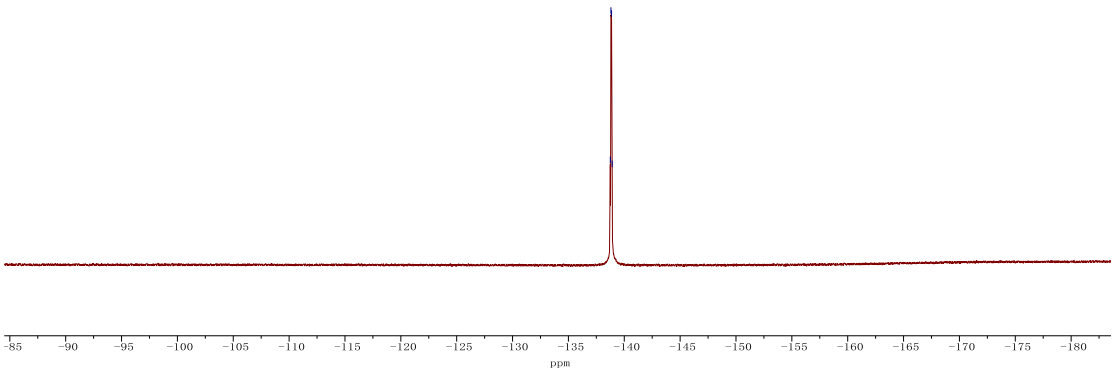
-138.860
-138.915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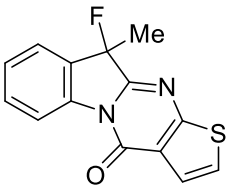
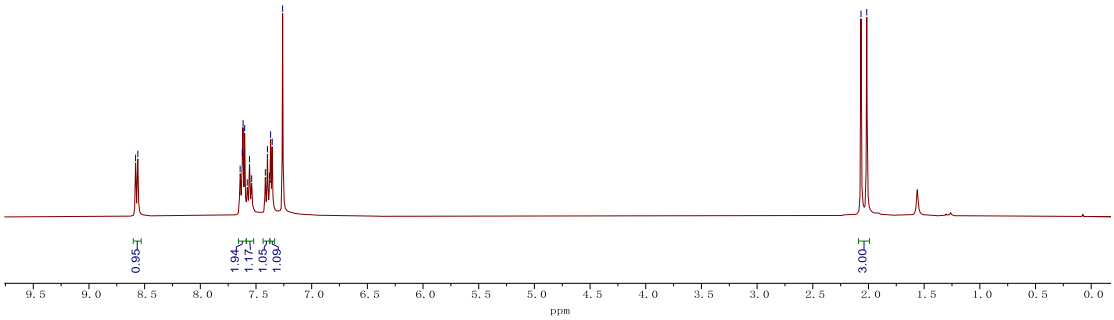
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175
-180
ppm


8.582
8.561
7.642
7.624
7.616
7.602
7.578
7.558
7.539
7.416
7.397
7.379
7.369
7.354
7.261


F
Me
N
N
S
O

**3af**


2.067
2.015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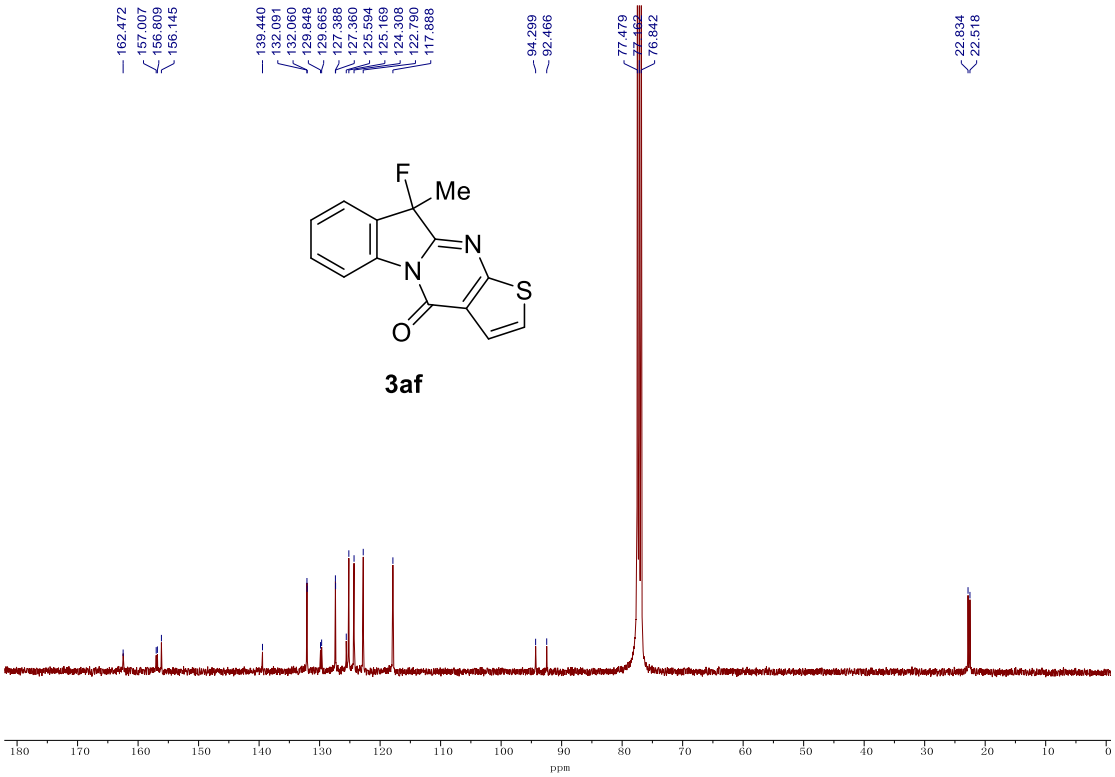
1.94
1.17
1.05
1.09
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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129.848
129.665
127.388
127.360
125.594
125.169
124.308
122.790
117.888
94.299
92.466
77.479
77.162
76.842
22.834
22.518
F
Me
N
N
S
O
3af
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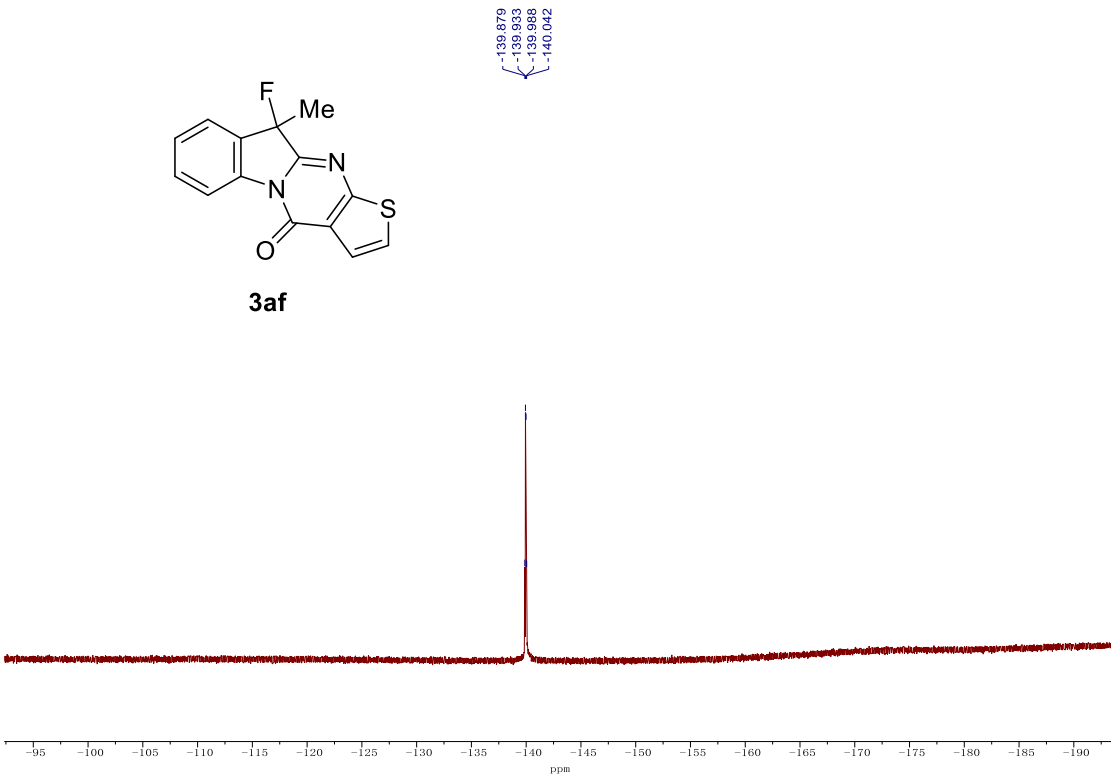
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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F
Me
N
N
S
O
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−110
−115
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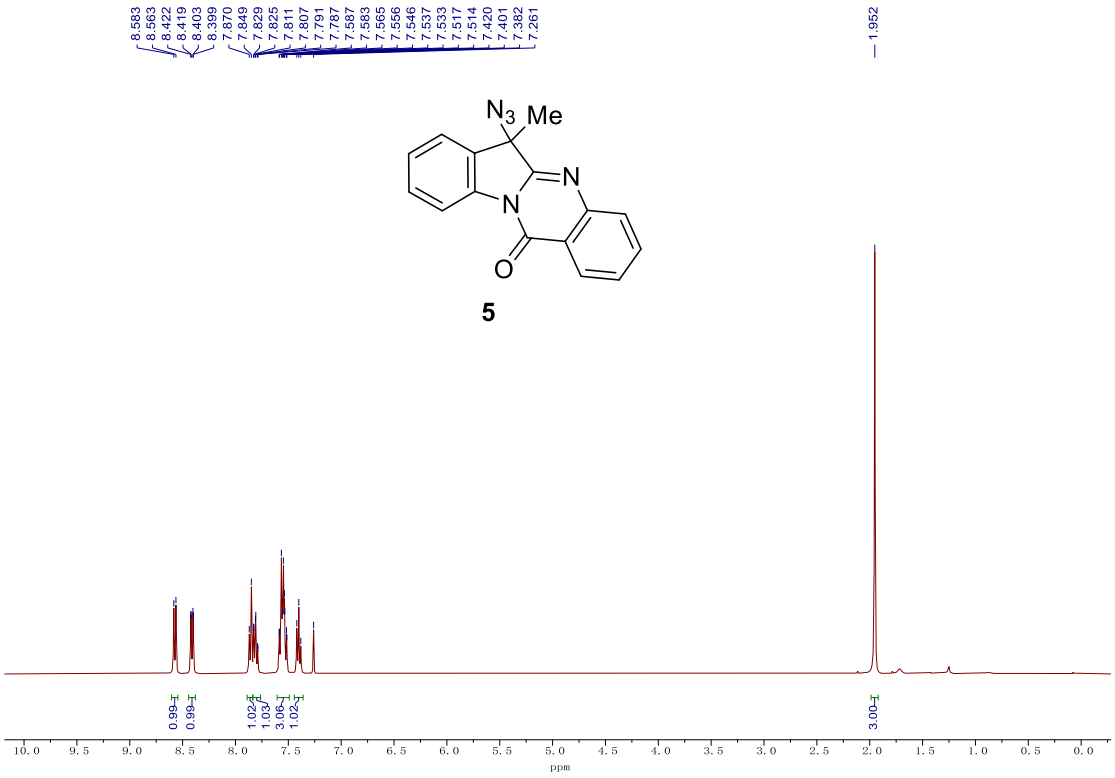
−130
−135
−140
−145
−150
−155
−160
−165
−170
−175
−180
−185
−190
ppm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8.419
8.403
8.399
7.870
7.849
7.829
7.825
7.811
7.807
7.791
7.787
7.587
7.583
7.565
7.556
7.546
7.537
7.533
7.517
7.514
7.420
7.401
7.382
7.261
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N3 Me
N
N
O
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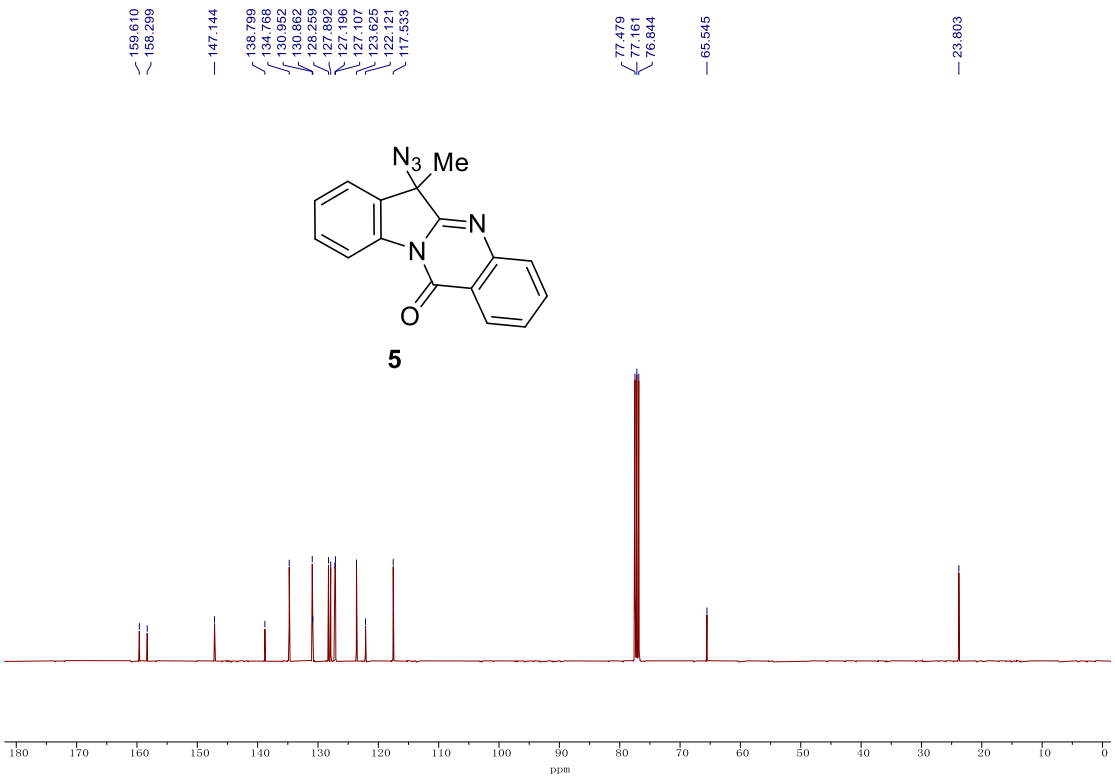
0.99
1.02
1.03
3.06
1.02
3.00
ppm

**5**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130.952
130.862
128.259
127.892
127.196
127.107
123.625
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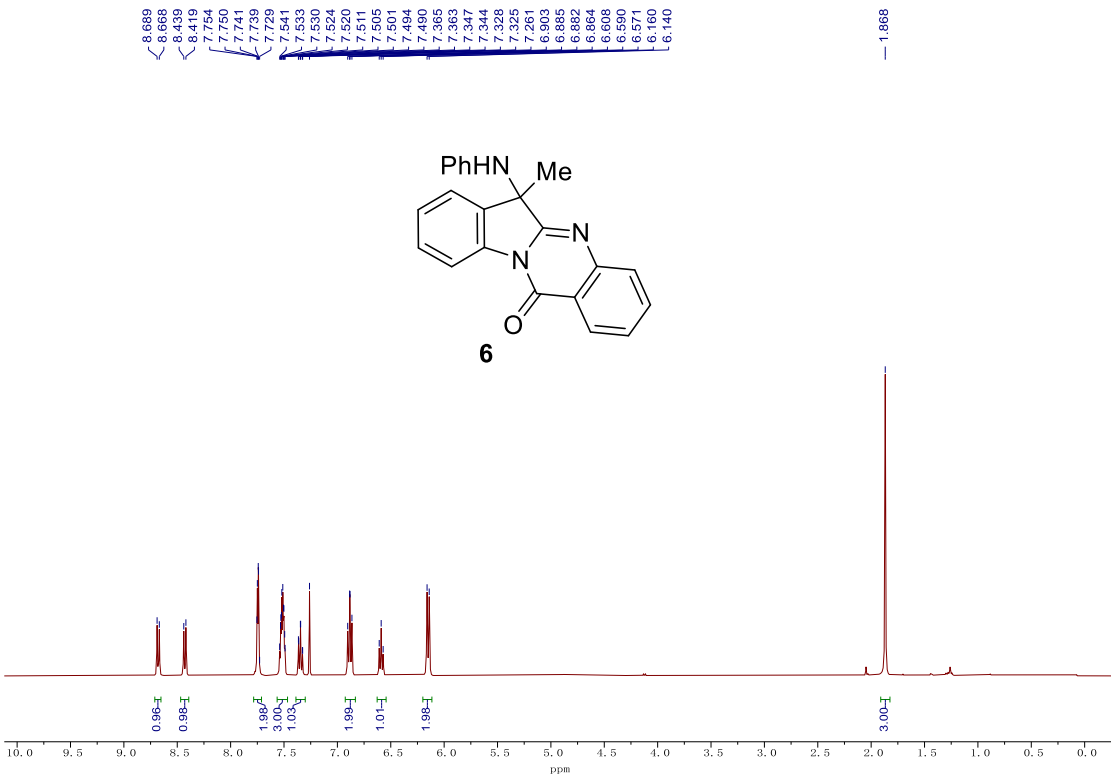
77.479
77.161
76.844
65.545
23.803
N3 Me
N
N
O
ppm

**5**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7.739
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7.533
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7.524
7.520
7.511
7.505
7.501
7.494
7.490
7.365
7.363
7.347
7.344
7.328
7.325
7.261
6.903
6.885
6.882
6.864
6.608
6.590
6.571
6.160
6.140
1.868
PhHN
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1.99
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3.00
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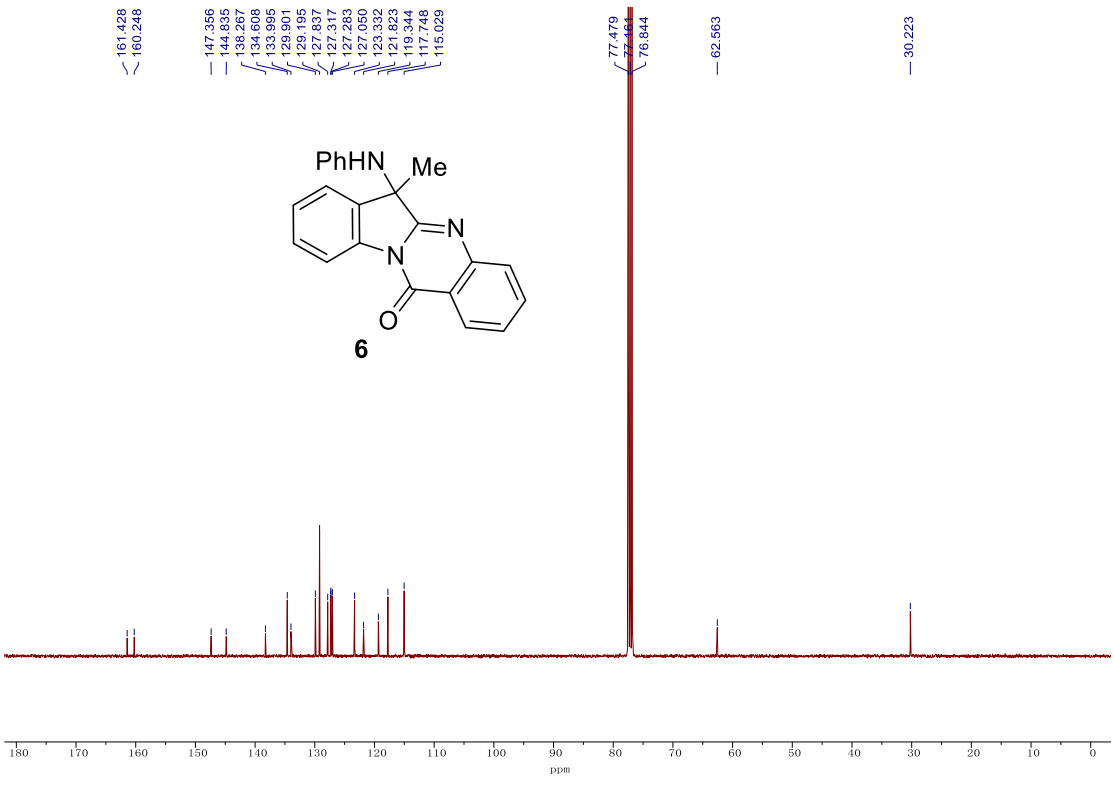
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127.837
127.317
127.283
127.050
123.332
121.823
119.344
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77.479
77.161
76.844
62.563
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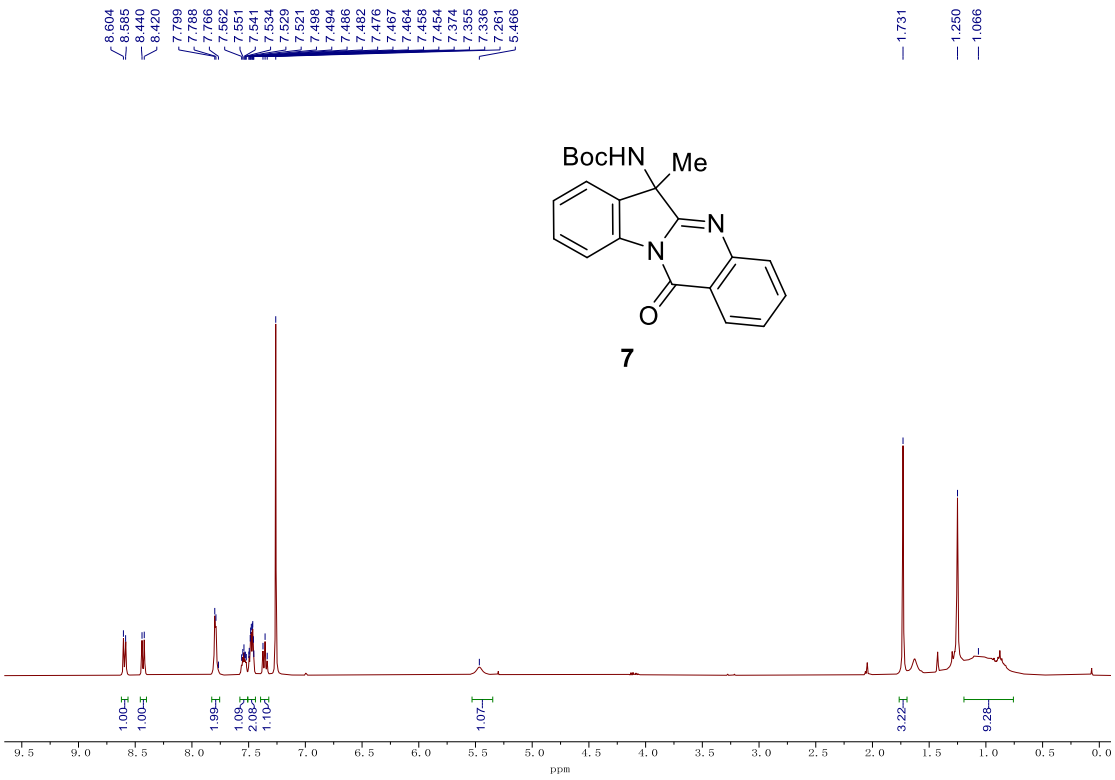
PhHN
Me
N
N
O
6
ppm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7.551
7.541
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7.529
7.521
7.498
7.494
7.486
7.482
7.476
7.467
7.464
7.458
7.454
7.374
7.355
7.336
7.261
5.466
1.731
1.250
1.066
BocHN
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N
O
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1.00
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1.10
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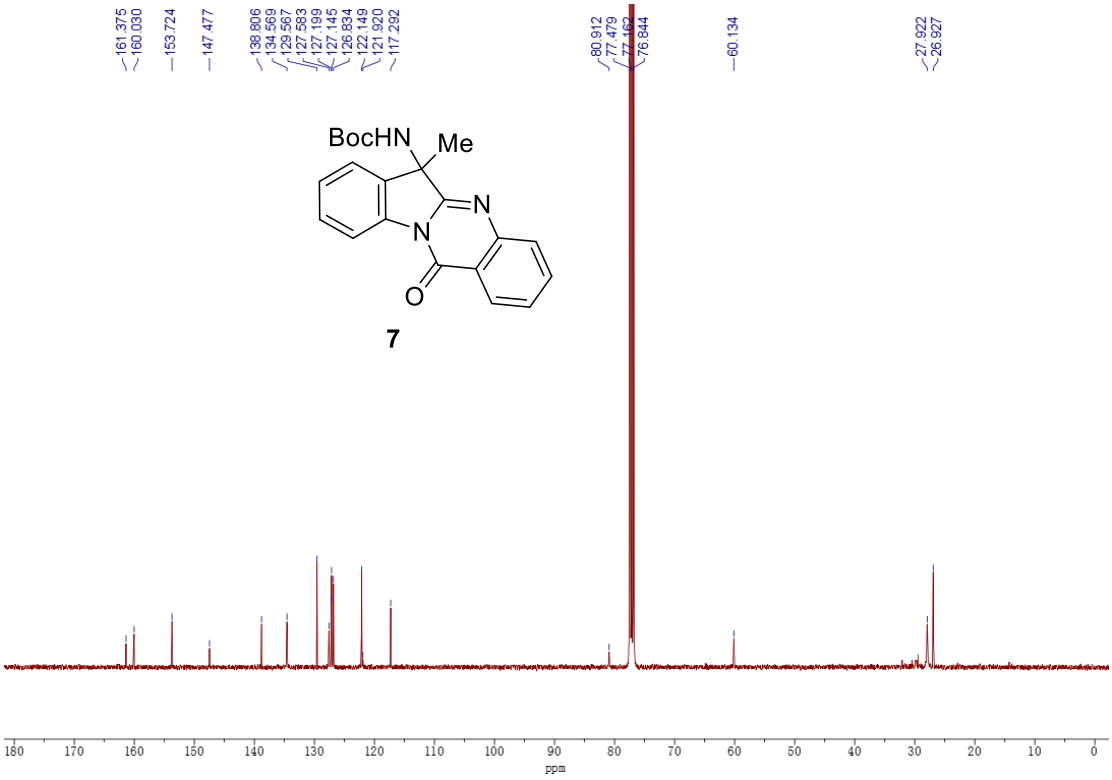
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122.149
121.920
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76.844
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BocHN
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O
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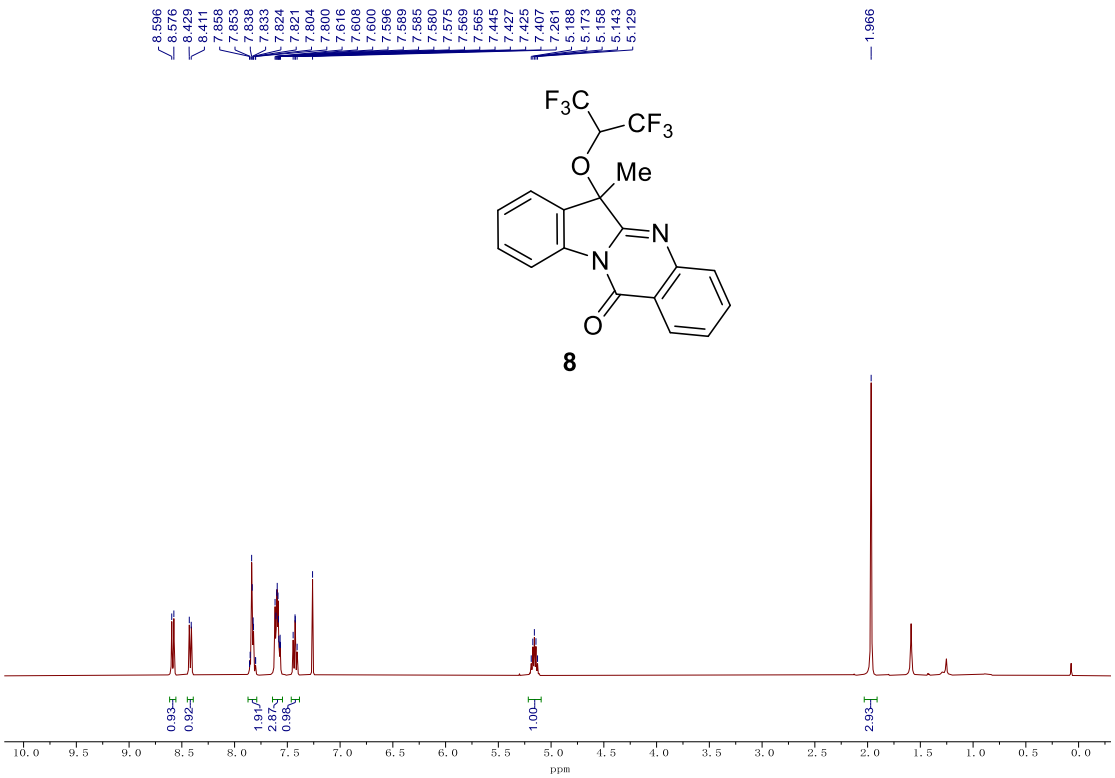
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7.800
7.616
7.608
7.600
7.596
7.589
7.585
7.580
7.575
7.569
7.565
7.445
7.427
7.425
7.407
7.261
5.188
5.173
5.158
5.143
5.129
1.966
F3C
CF3
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Me
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O
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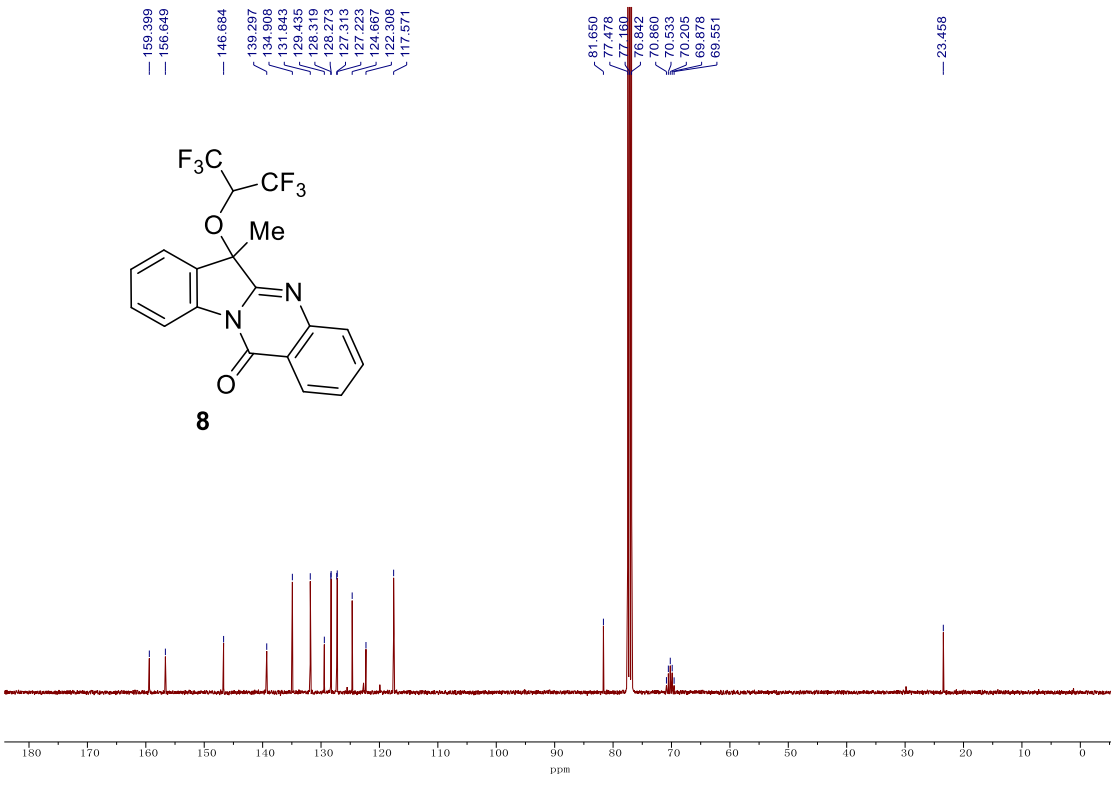
**8**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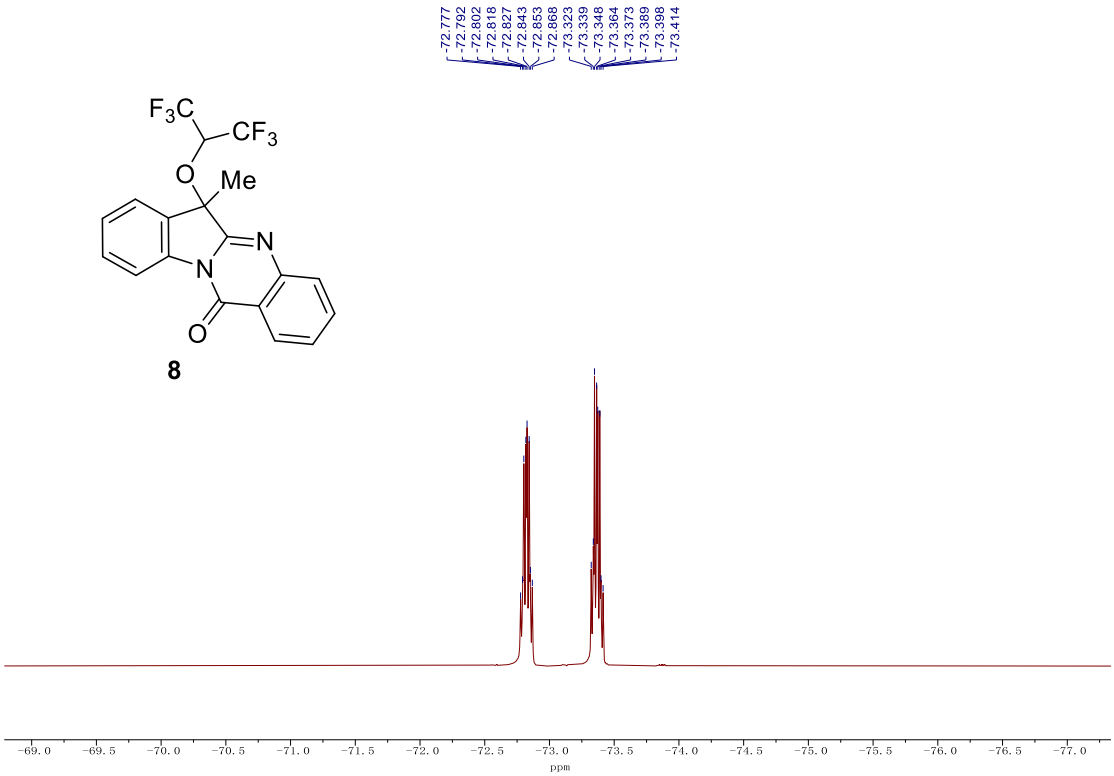
127.223
124.667
122.308
117.571
81.650
77.478
77.160
76.842
70.860
70.533
70.205
69.878
69.551
23.458
F3C
CF3
O
Me
N
N
O
ppm

**8**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CF3
O
Me
N
N
O
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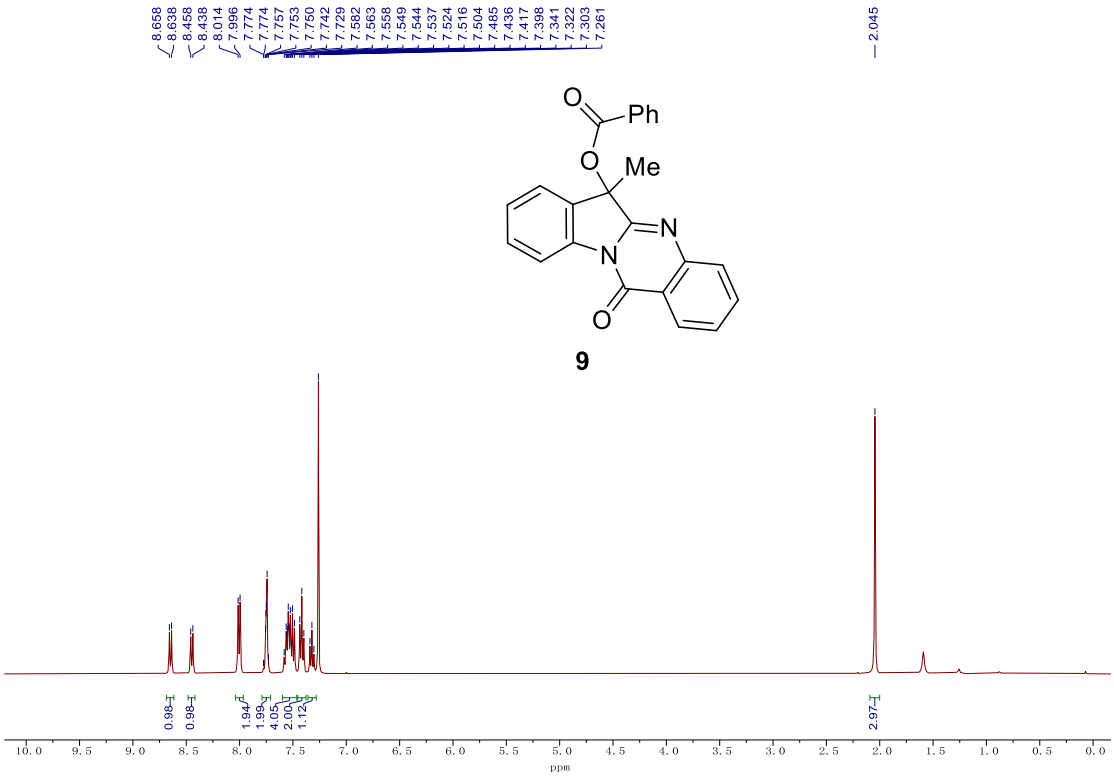
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7.485
7.436
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7.398
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7.322
7.303
7.261
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O
Ph
O
Me
N
N
O
9
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0.98
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1.99
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2.00
1.12
2.97
10.0
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9.0
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8.0
7.5
7.0
6.5
6.0
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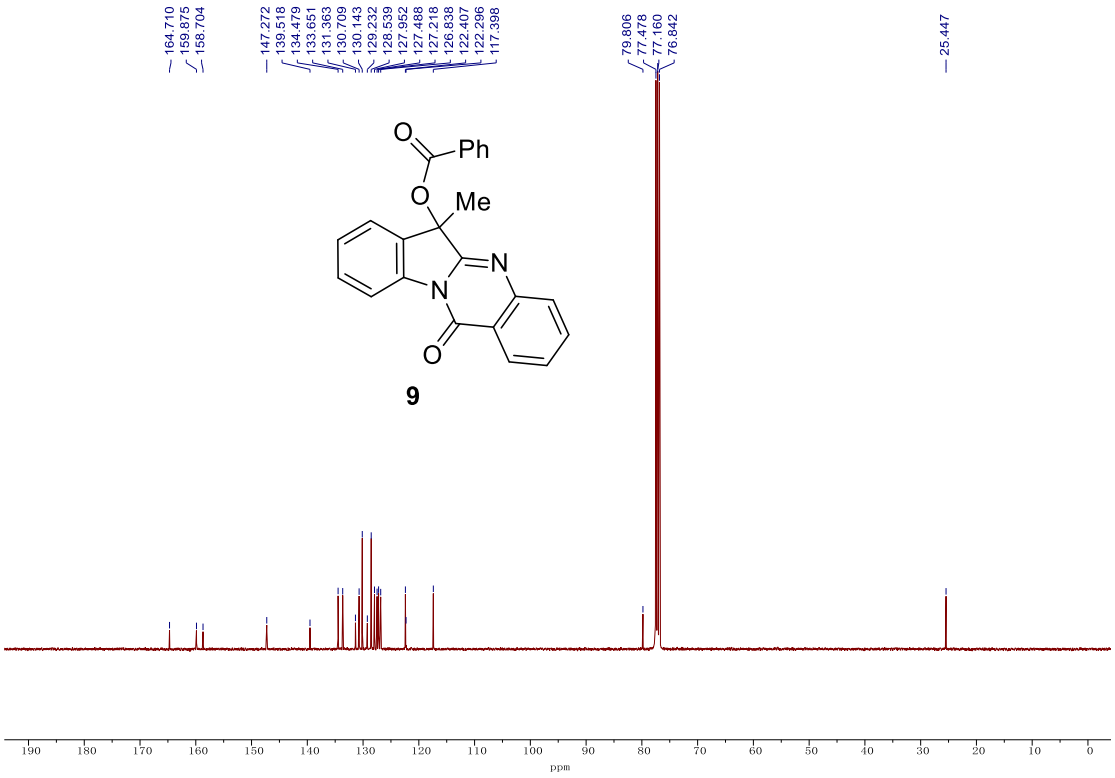
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126.838
122.407
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Me
N
N
O
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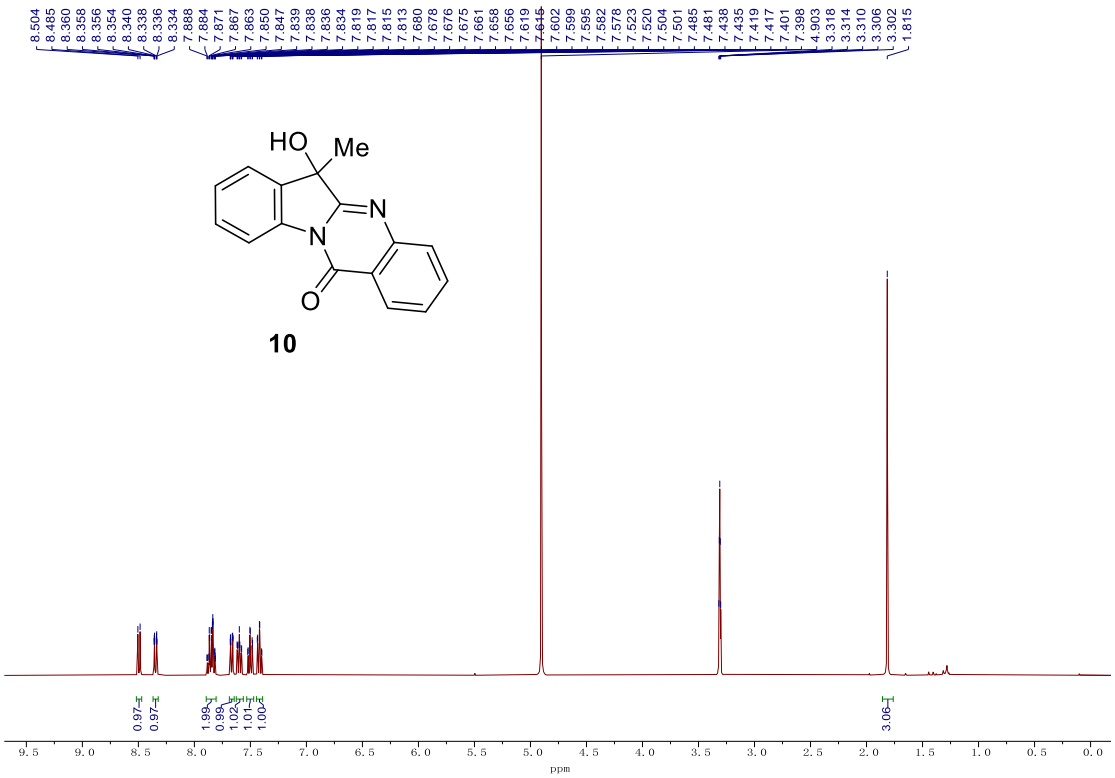
ppm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7.847
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7.619
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7.582
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7.520
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7.501
7.485
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7.419
7.417
7.401
7.398
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3.314
3.310
3.306
3.302
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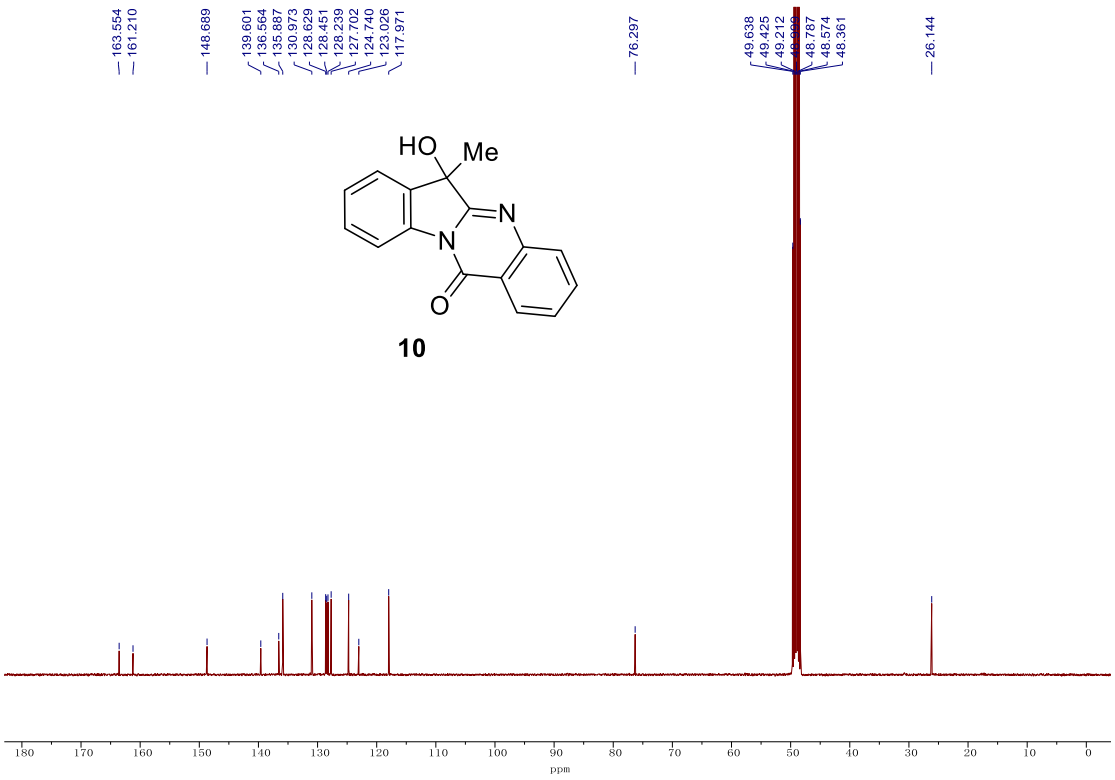
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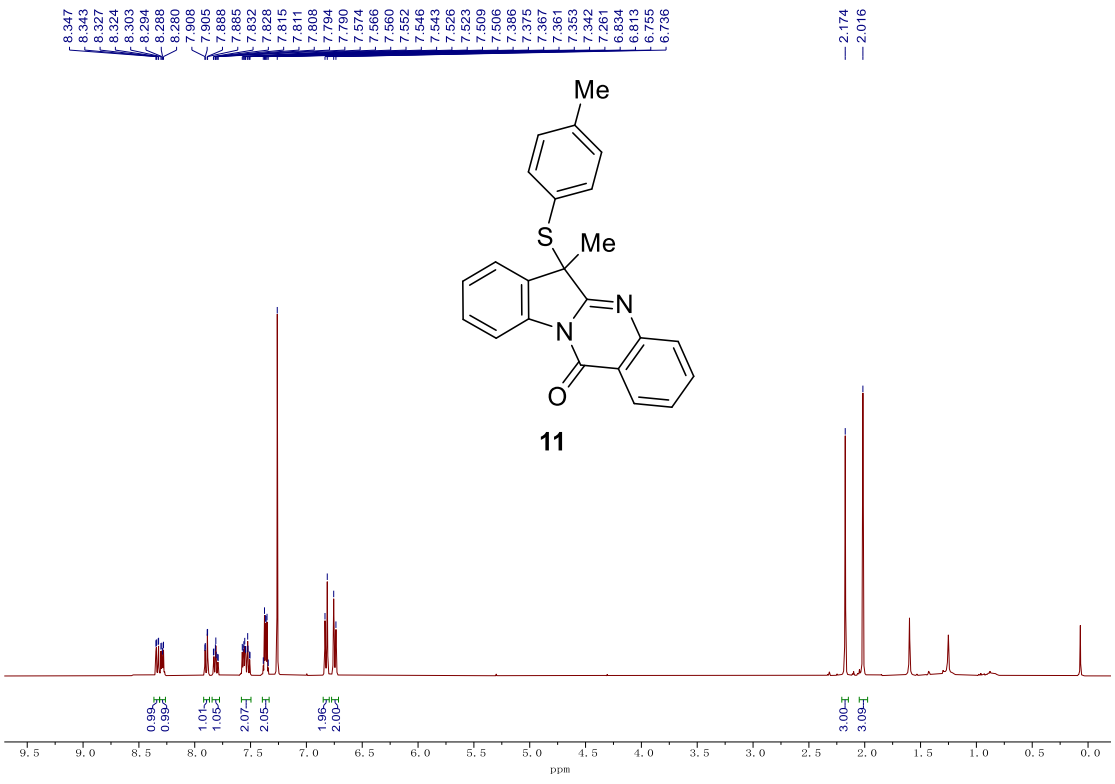
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7.828
7.815
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7.794
7.790
7.574
7.566
7.560
7.552
7.546
7.543
7.526
7.523
7.509
7.506
7.386
7.375
7.367
7.361
7.353
7.342
7.261
6.834
6.813
6.755
6.736
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Me
S
Me
N
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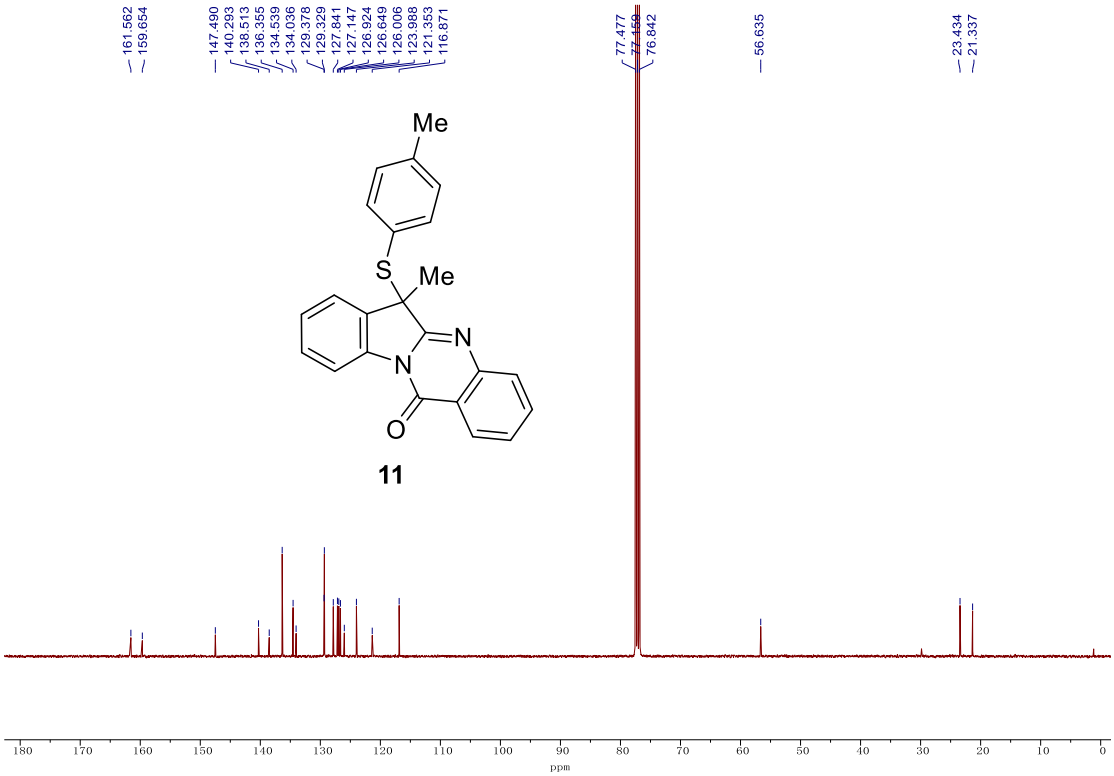
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77.159
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56.635
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Me
S
Me
N
N
O
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130
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60
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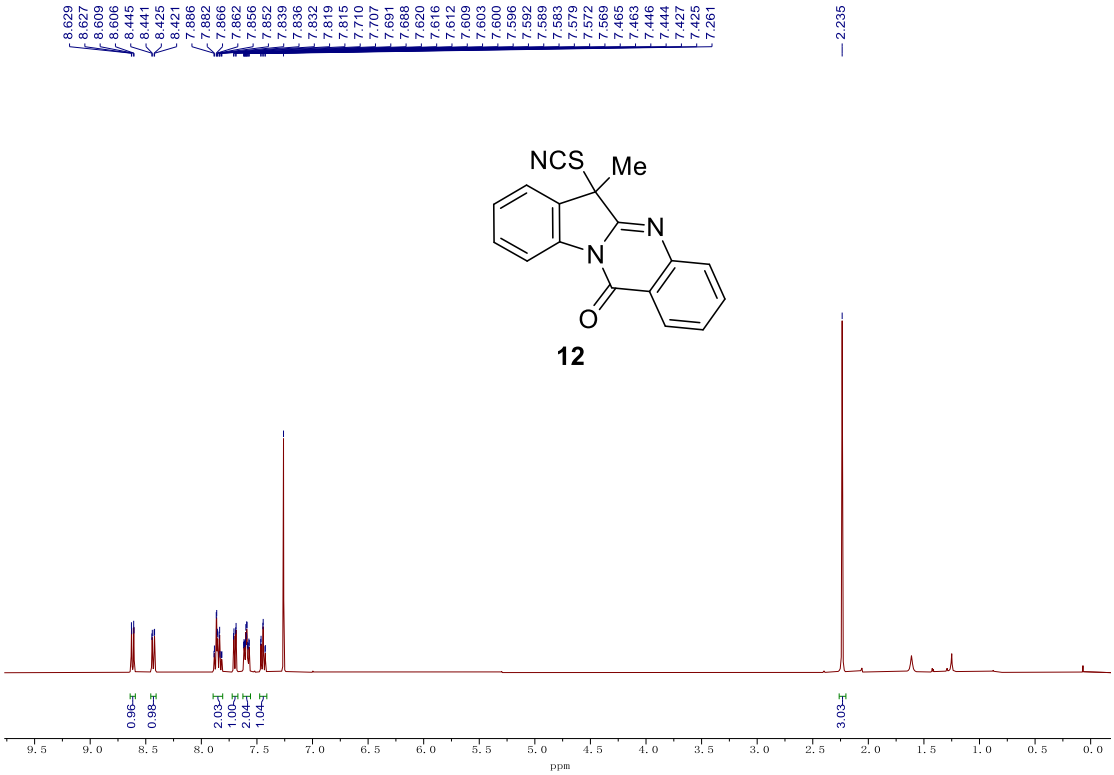
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7.616
7.612
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2.04
1.04
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7.0
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6.0
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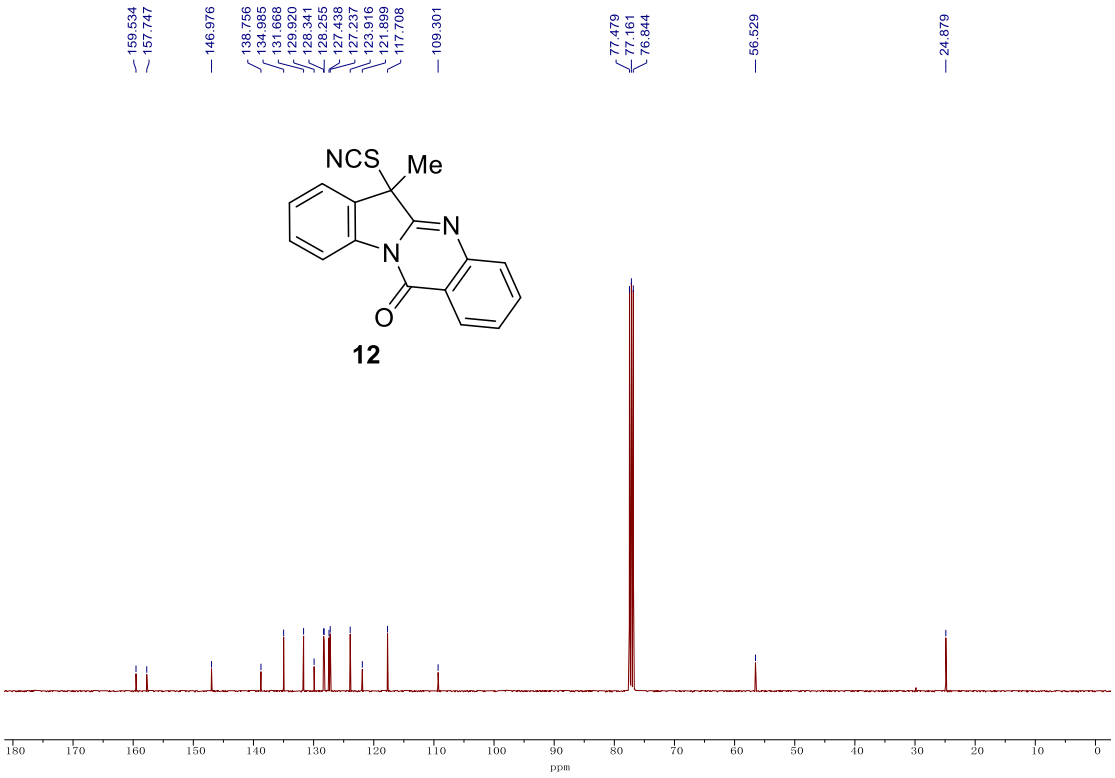
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Me
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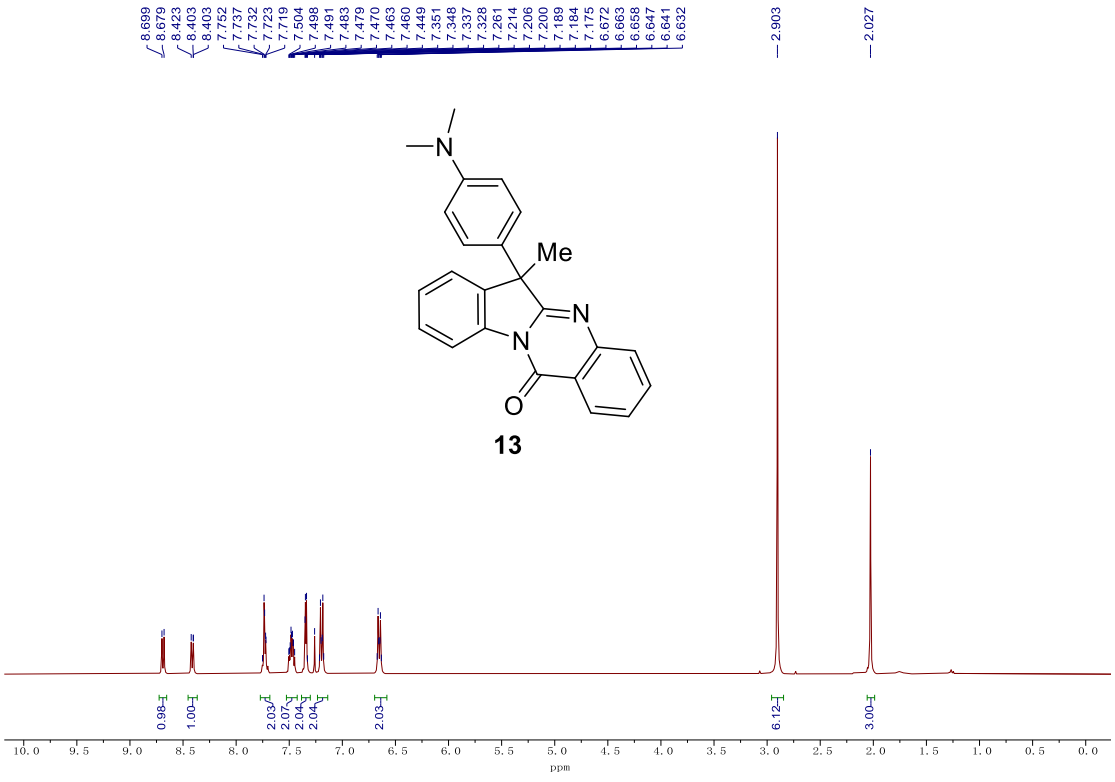
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6.0
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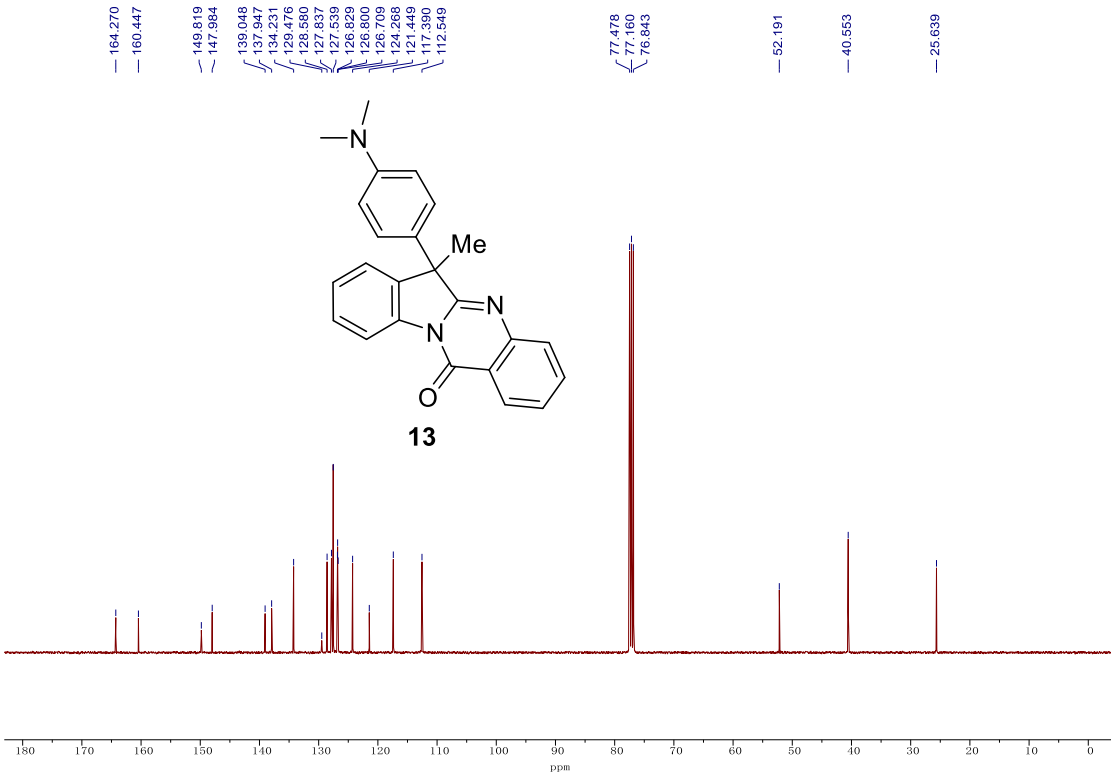
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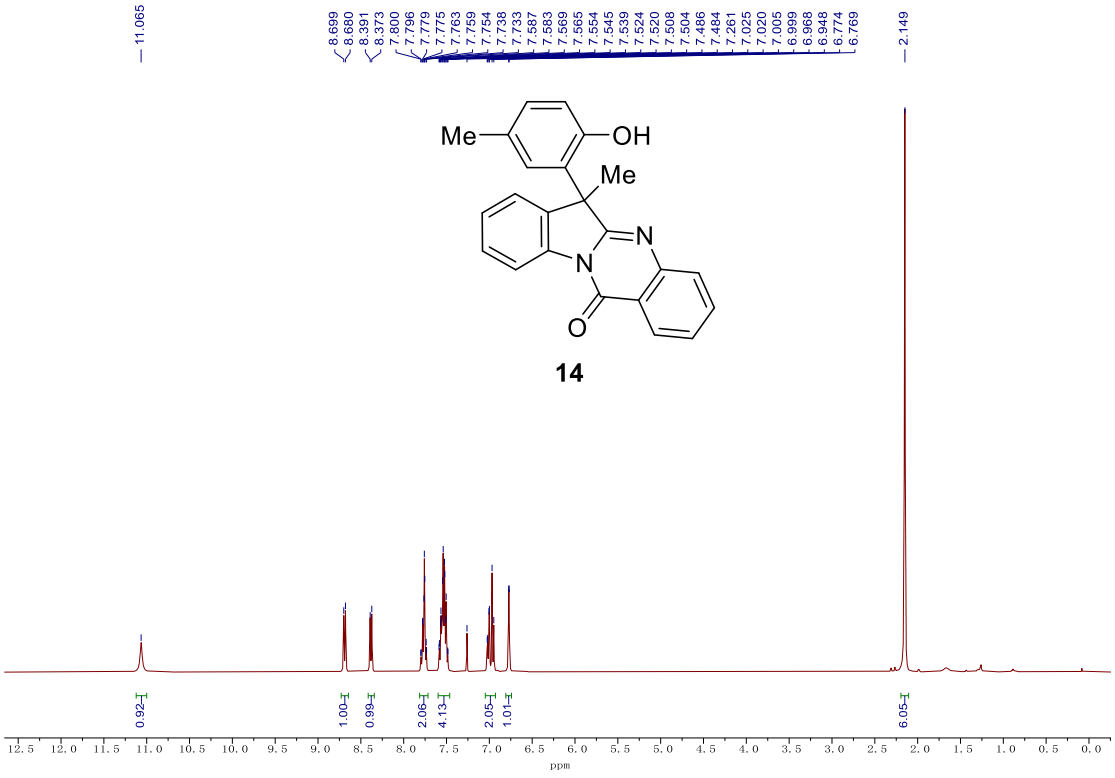
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7.520
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7.504
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7.484
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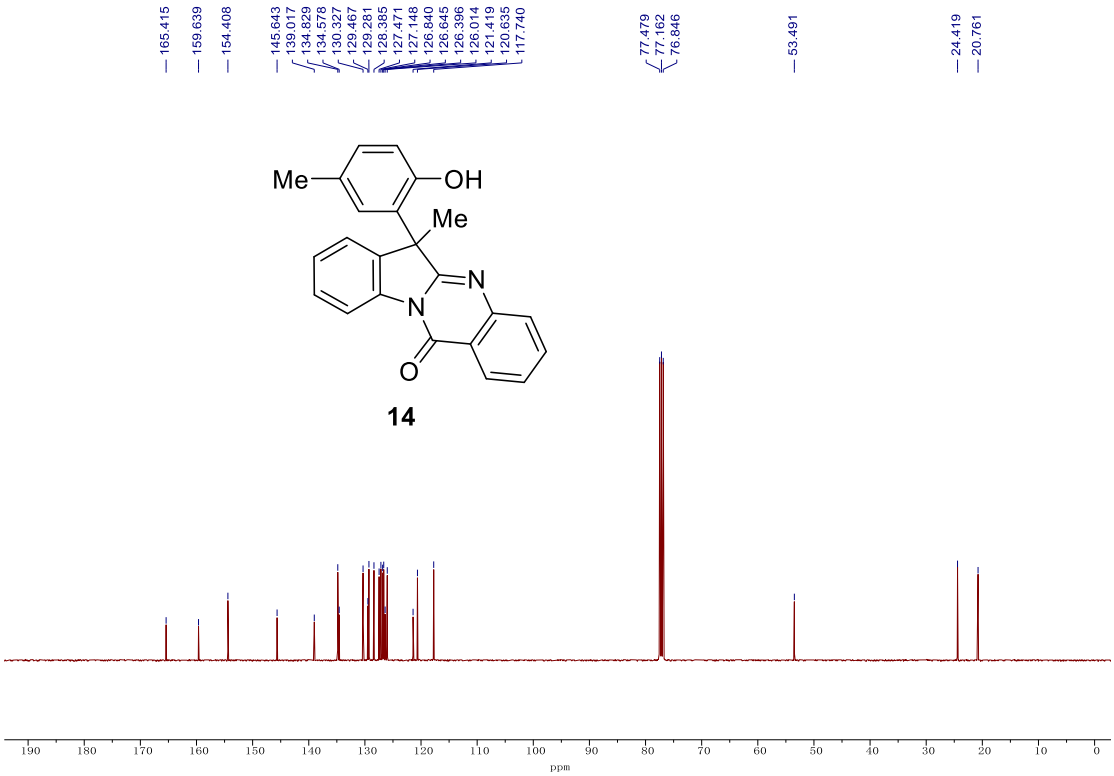
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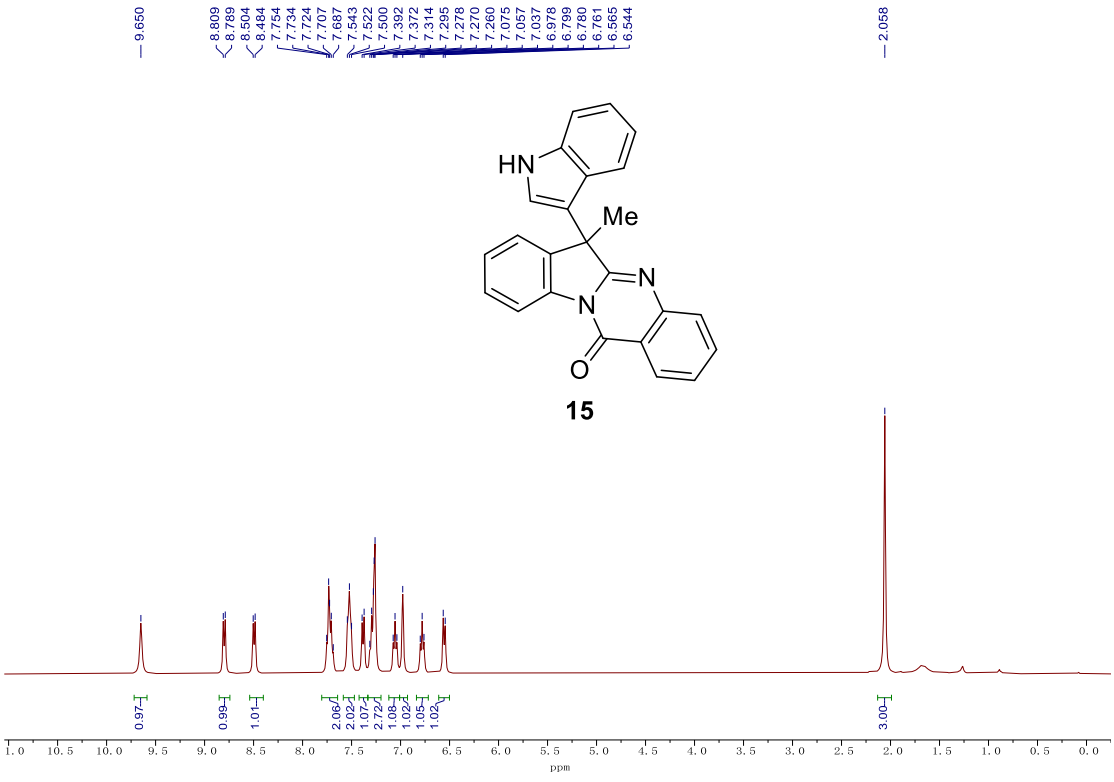
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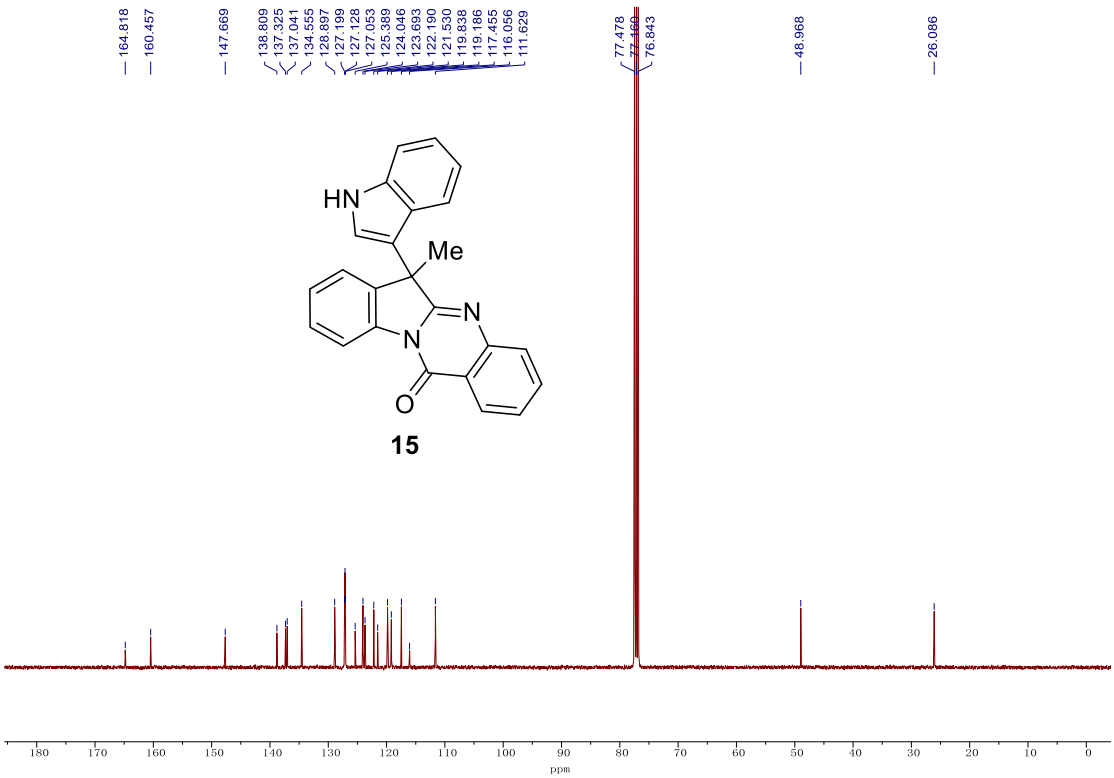
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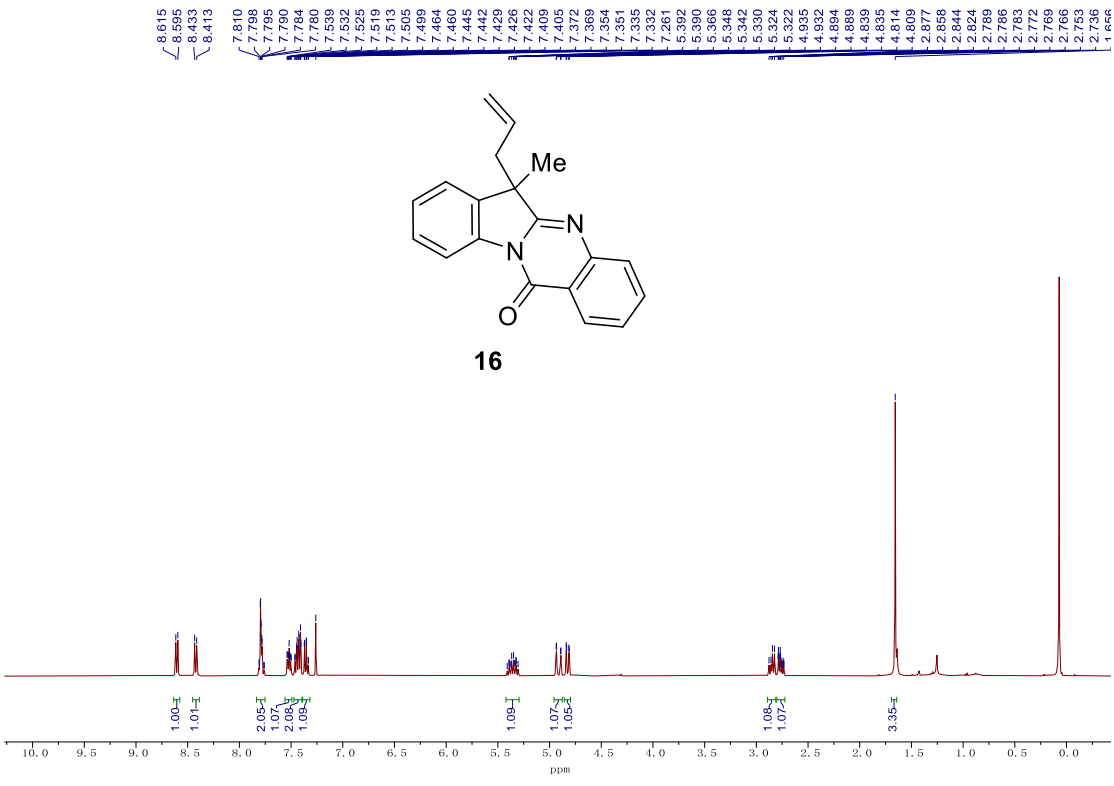
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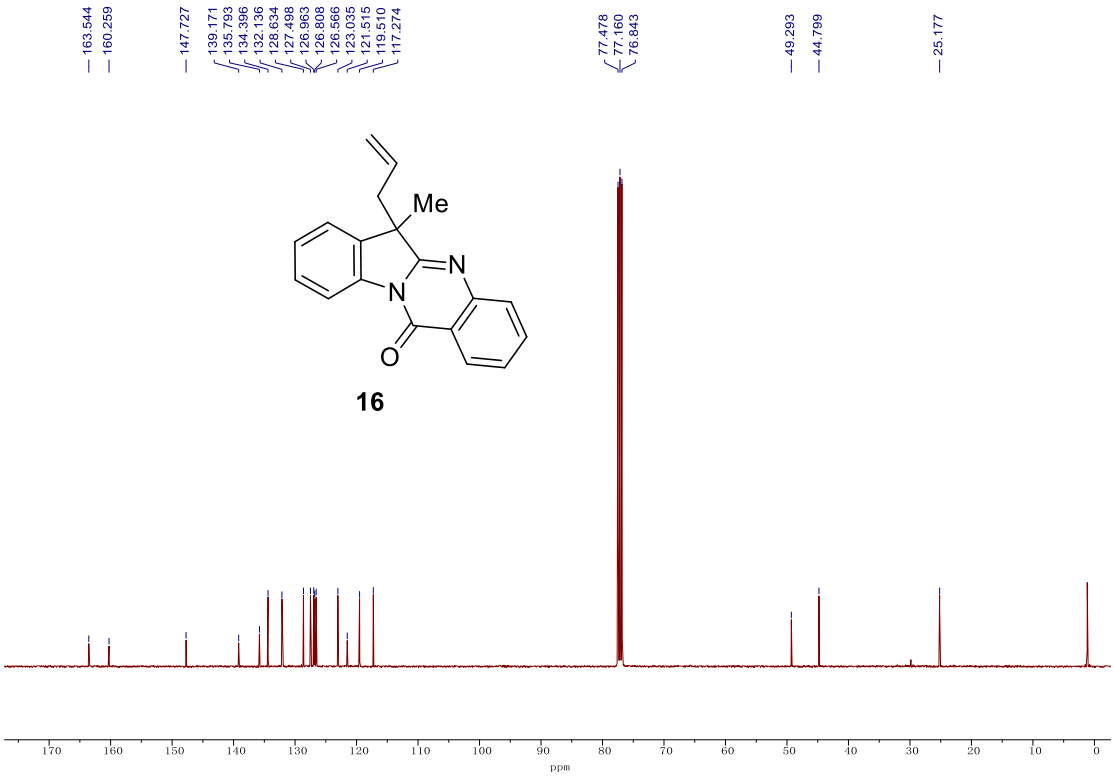
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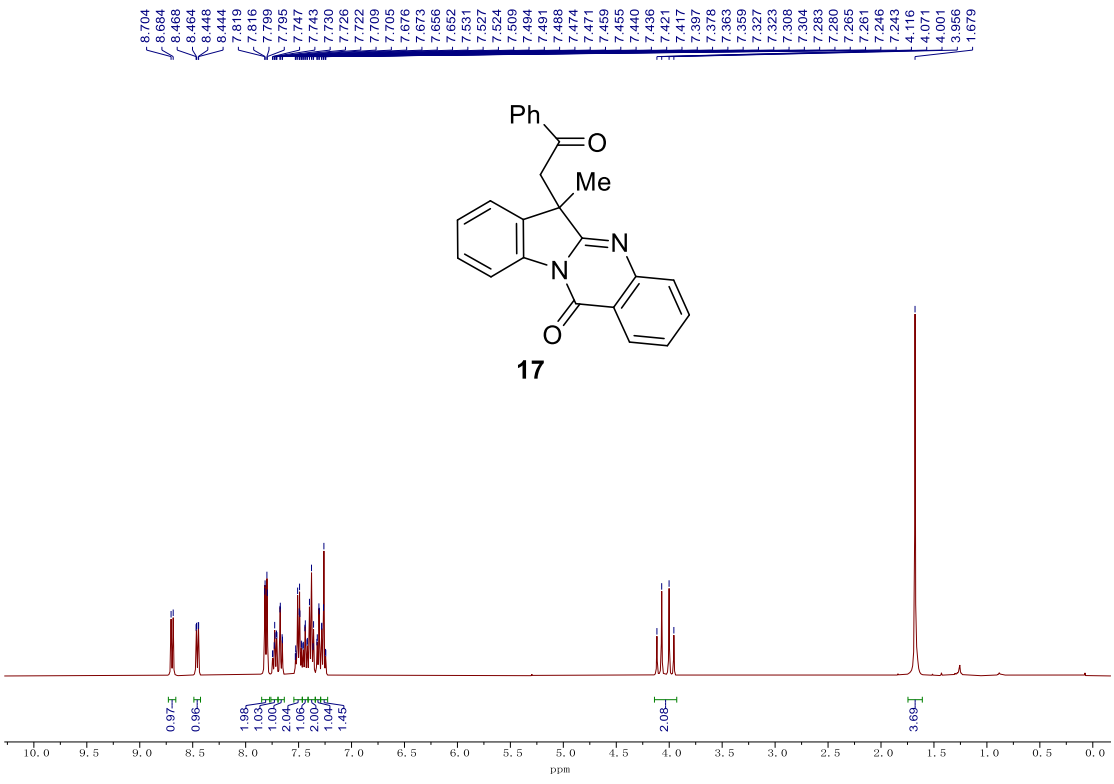
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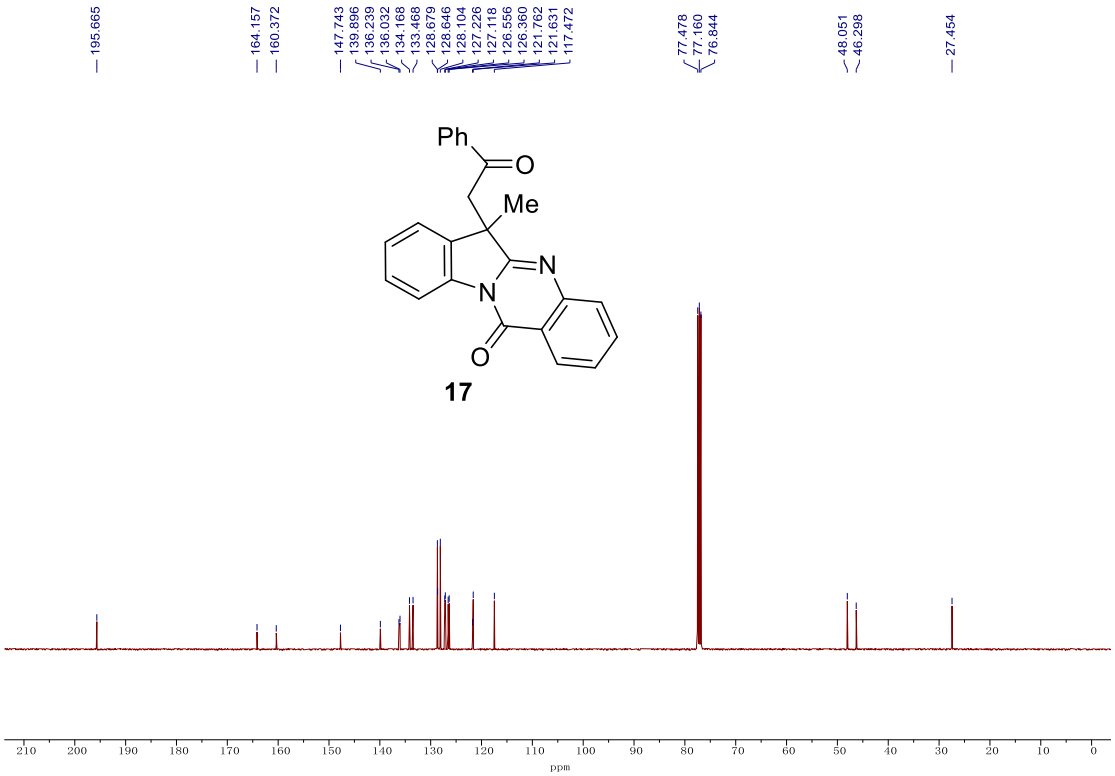
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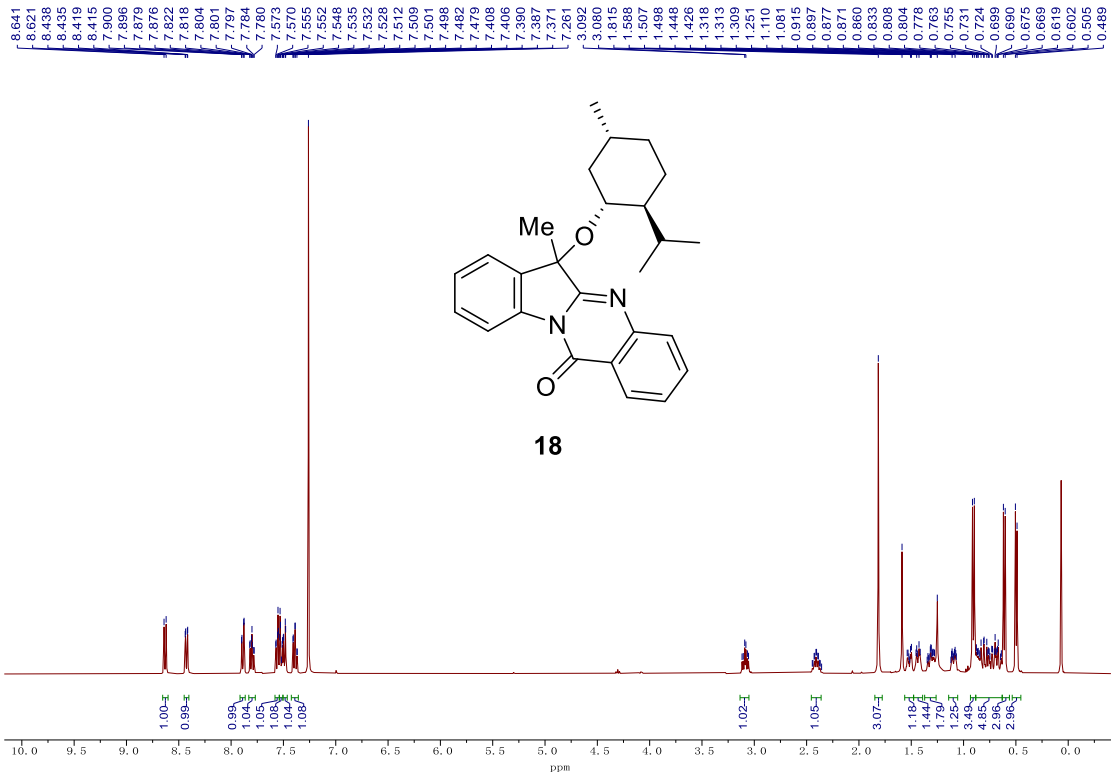
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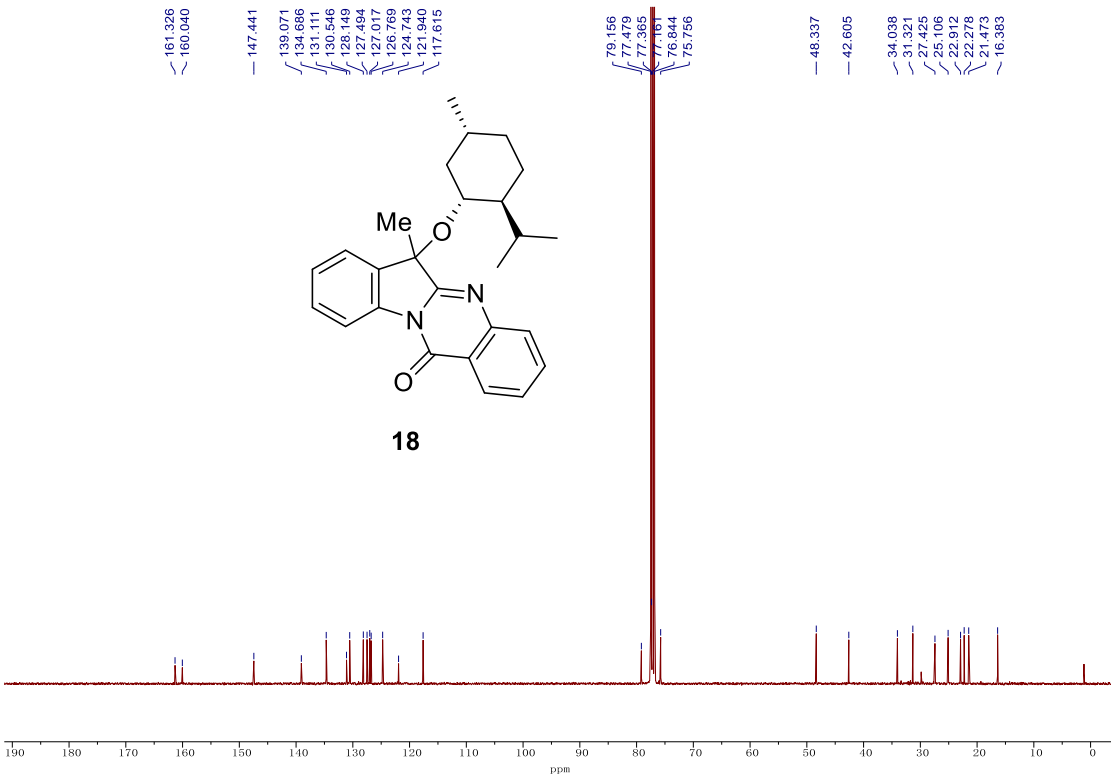
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128.149
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127.017
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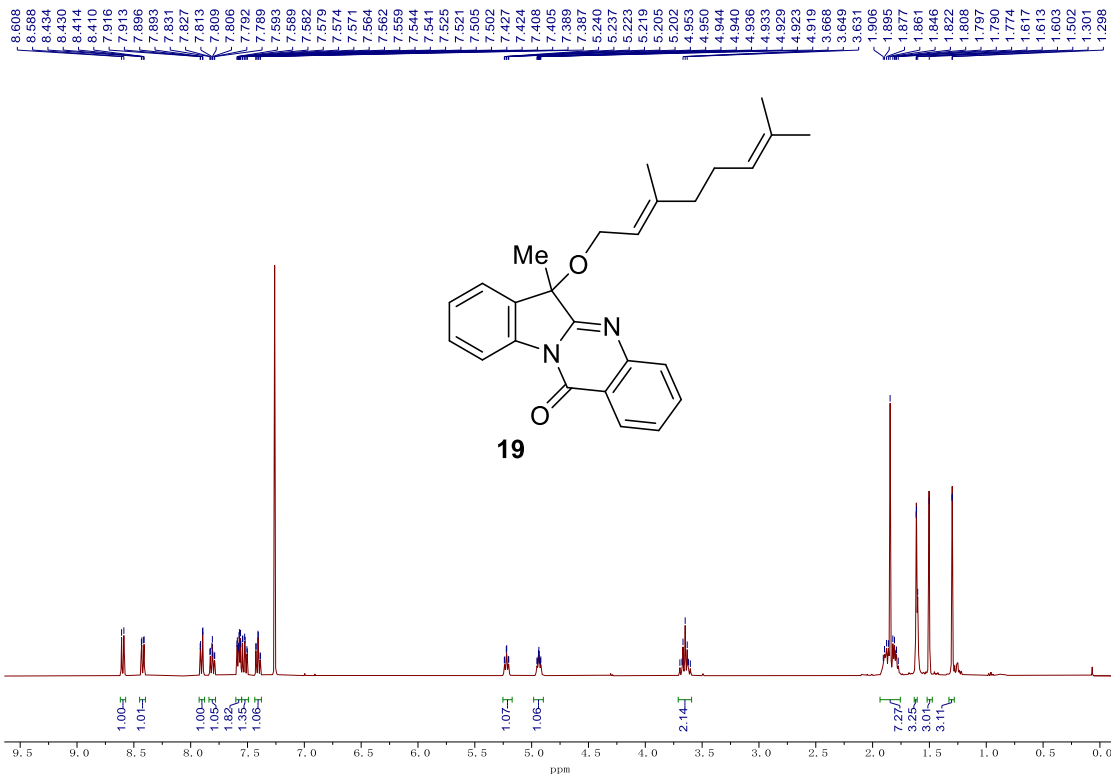
124.743
121.940
117.615
79.156
77.479
77.365
77.161
76.844
75.756
48.337
42.605
34.038
31.321
27.425
25.106
22.912
22.278
21.473
16.383
Me
O
N
N
O
18
ppm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8.414
8.410
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7.913
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7.893
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7.827
7.813
7.809
7.806
7.792
7.789
7.593
7.589
7.582
7.579
7.574
7.571
7.564
7.562
7.559
7.544
7.541
7.525
7.521
7.505
7.502
7.427
7.424
7.408
7.405
7.389
7.387
5.240
5.237
5.223
5.219
5.205
5.202
4.953
4.950
4.944
4.940
4.936
4.933
4.929
4.923
4.919
3.668
3.649
3.631
1.906
1.895
1.877
1.861
1.846
1.822
1.808
1.797
1.790
1.774
1.617
1.613
1.603
1.502
1.301
1.298
Me
O
N
N
O
19
1.00
1.01
1.00
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1.35
1.06
1.07
1.06
2.14
7.27
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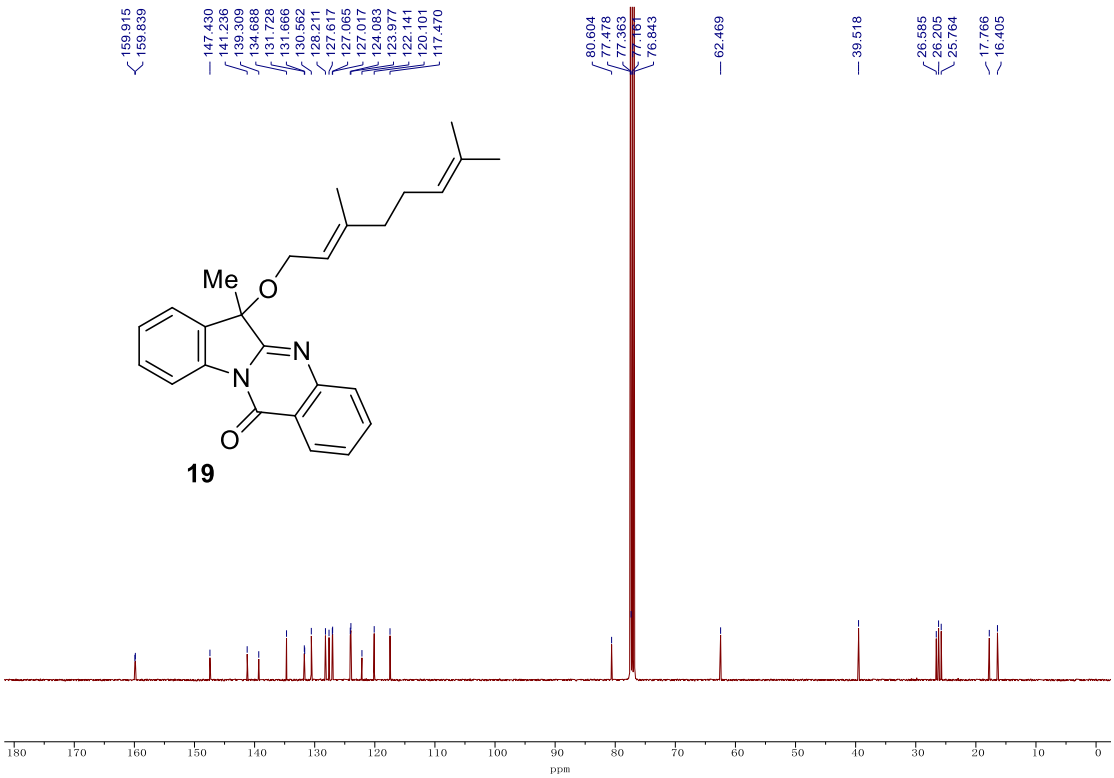
3.11
ppm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130.562
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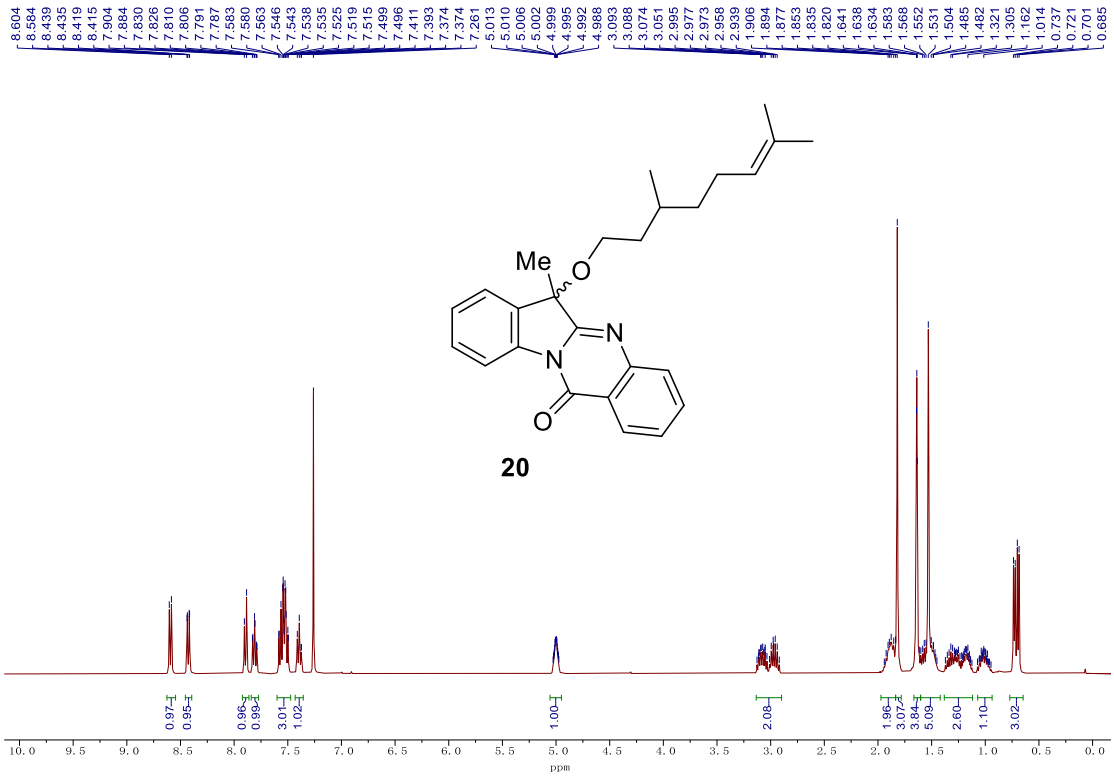
127.617
127.065
127.017
124.083
123.977
122.141
120.101
117.470
80.604
77.478
77.363
77.161
76.843
62.469
39.518
26.585
26.205
25.764
17.766
16.405
Me
O
N
N
O
19
ppm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7.884
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7.806
7.791
7.787
7.583
7.580
7.563
7.546
7.543
7.538
7.535
7.525
7.519
7.515
7.499
7.496
7.411
7.393
7.374
7.374
7.261
5.013
5.010
5.006
5.002
4.999
4.995
4.992
4.988
3.093
3.088
3.074
3.051
2.995
2.977
2.973
2.958
2.939
1.906
1.894
1.877
1.853
1.835
1.820
1.641
1.638
1.634
1.583
1.568
1.552
1.531
1.504
1.485
1.482
1.321
1.305
1.162
1.014
0.737
0.721
0.701
0.685
Me
O
N
N
O
20
0.97
0.95
0.96
0.99
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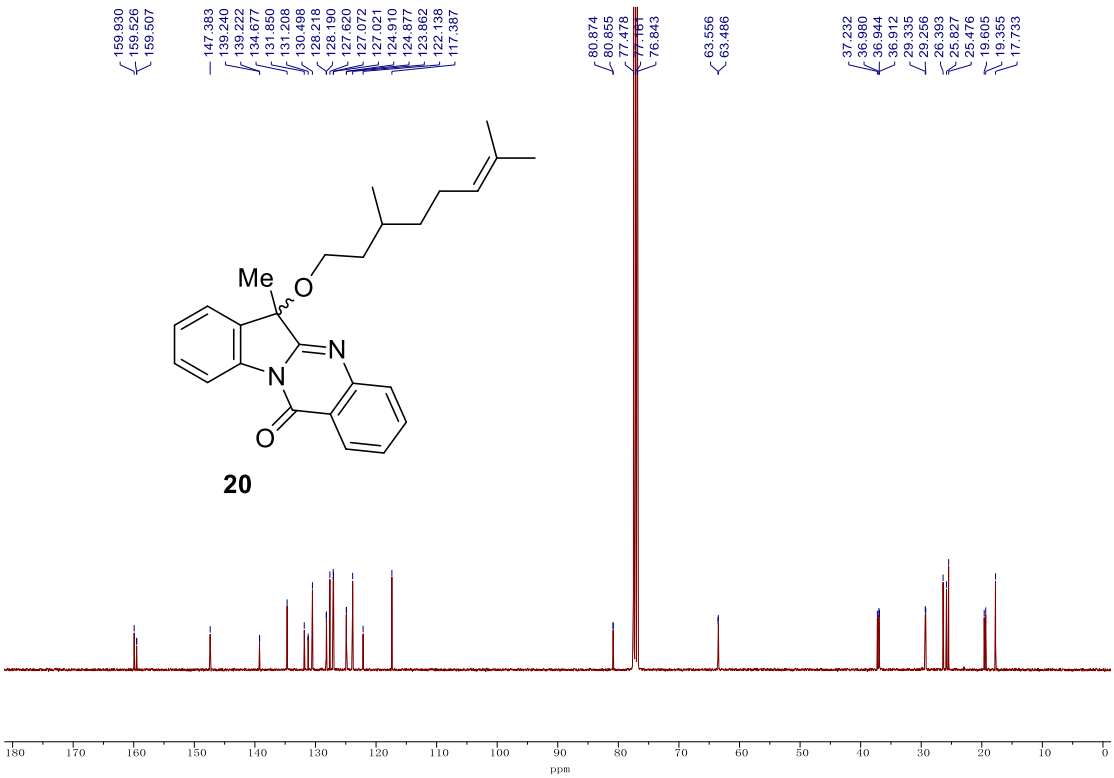
1.02
1.00
2.08
1.96
3.07
3.84
5.09
2.60
1.10
3.02
ppm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139.240
139.222
134.677
131.850
131.208
130.498
128.218
128.190
127.620
127.072
127.021
124.910
124.877
123.862
122.138
117.387
80.874
80.855
77.478
77.161
76.843
63.556
63.486
37.232
36.980
36.944
36.912
29.335
29.256
26.393
25.827
25.476
19.605
19.355
17.733
Me
O
N
N
O
20
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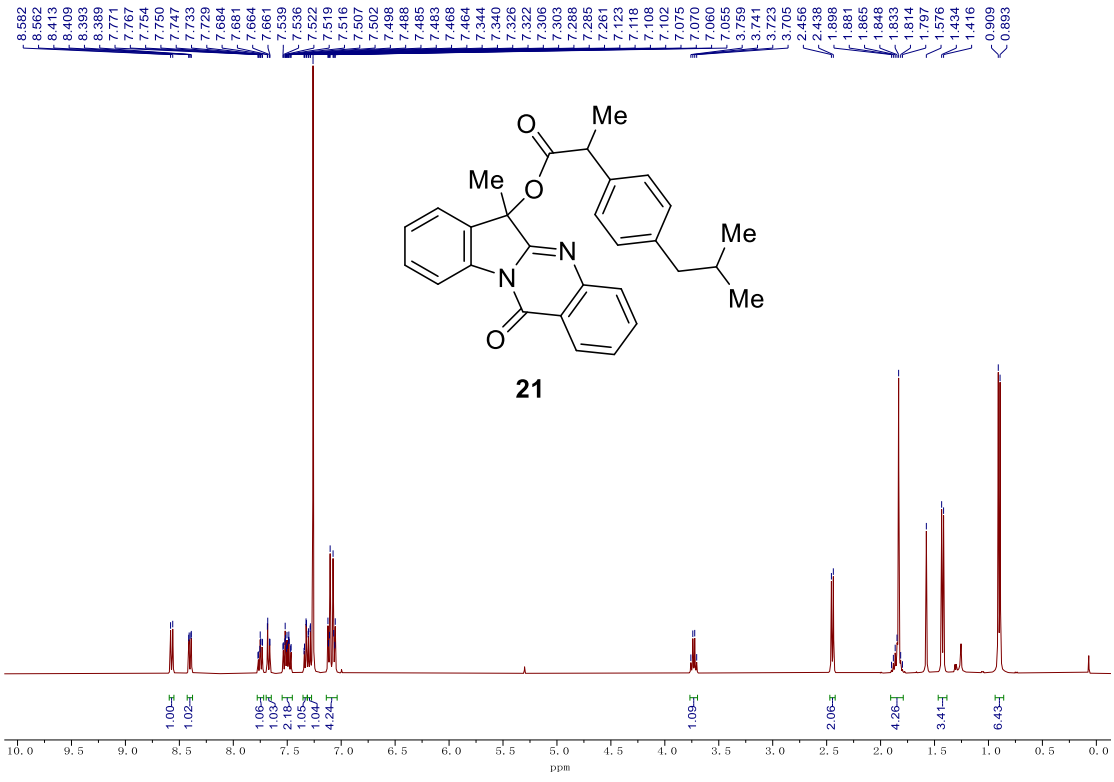
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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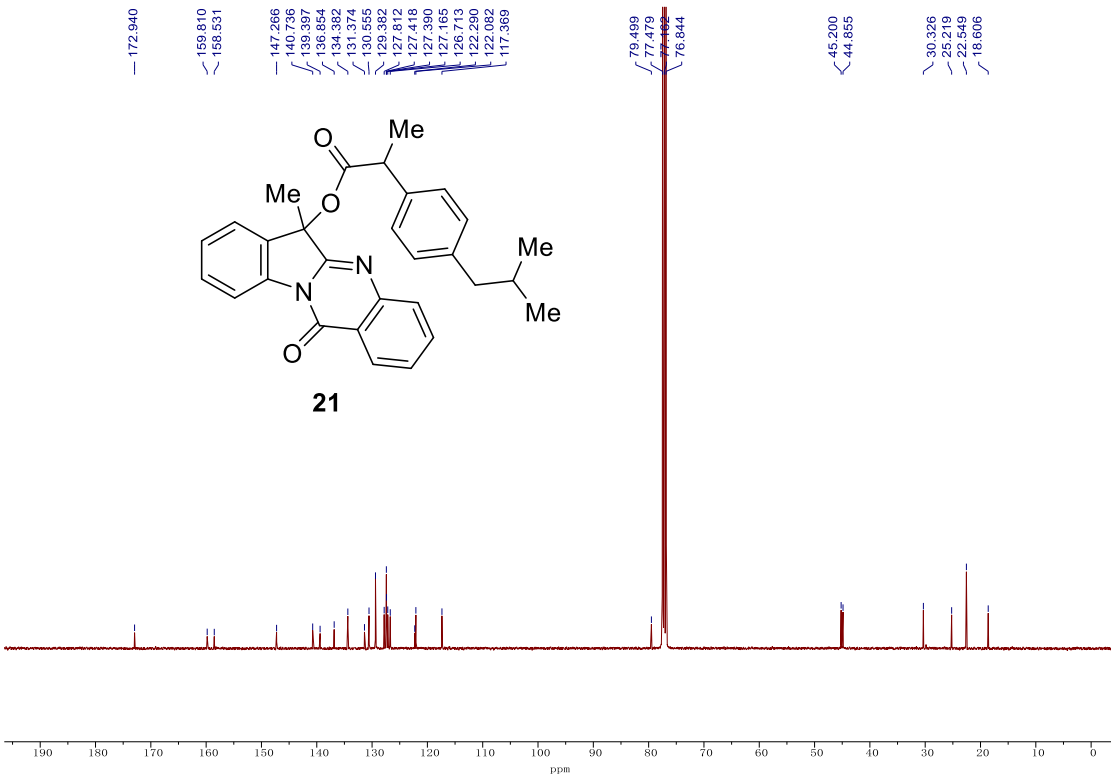
8.393
8.389
7.771
7.767
7.754
7.750
7.747
7.733
7.729
7.684
7.681
7.664
7.661
7.539
7.536
7.522
7.519
7.516
7.507
7.502
7.498
7.488
7.485
7.483
7.468
7.464
7.344
7.340
7.326
7.322
7.306
7.303
7.288
7.285
7.261
7.123
7.118
7.108
7.102
7.075
7.070
7.060
7.055
3.759
3.741
3.723
3.705
2.456
2.438
1.898
1.881
1.865
1.848
1.833
1.814
1.797
1.576
1.434
1.416
0.909
0.893
O
Me
Me
O
Me
N
N
O
21
1.00
1.02
1.06
1.03
2.18
1.05
1.04
4.24
1.09
2.06
4.26
3.41
6.43
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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158.531
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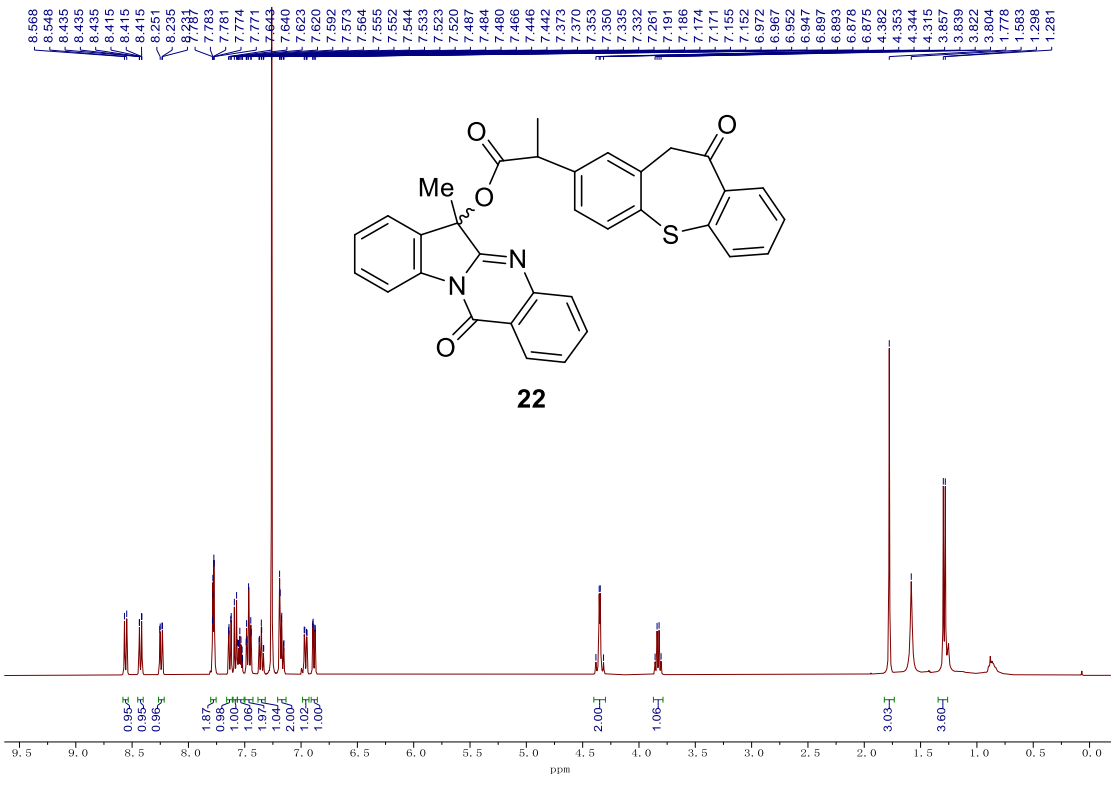
139.397
136.854
134.382
131.374
130.555
129.382
127.812
127.418
127.390
127.165
126.713
122.290
122.082
117.369
79.499
77.479
76.844
45.200
44.855
30.326
25.219
22.549
18.606
O
Me
Me
O
N
N
O
Me
Me
ppm

**21**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8.435
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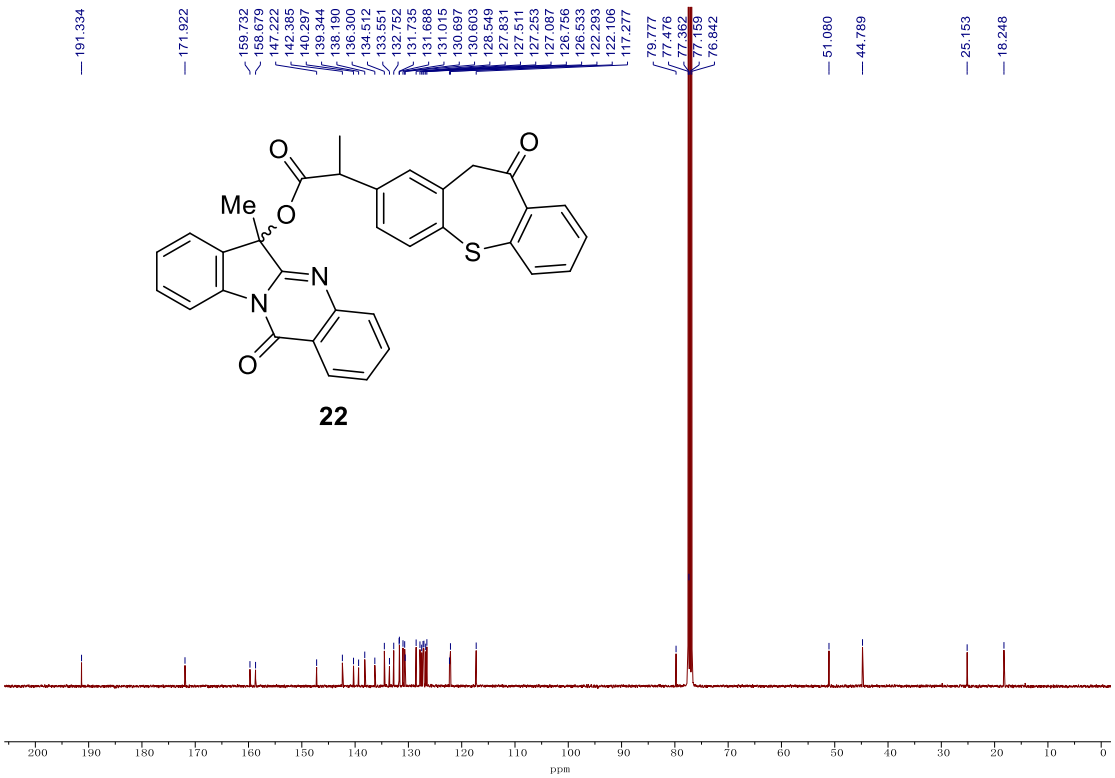
8.415
8.415
8.251
8.235
7.783
7.781
7.774
7.771
7.643
7.640
7.623
7.620
7.592
7.573
7.564
7.555
7.552
7.544
7.533
7.523
7.520
7.487
7.484
7.480
7.466
7.446
7.442
7.373
7.370
7.353
7.350
7.335
7.332
7.261
7.191
7.186
7.174
7.171
7.155
7.152
6.972
6.967
6.952
6.947
6.897
6.893
6.878
6.875
4.382
4.353
4.344
4.315
3.857
3.839
3.822
3.804
1.778
1.583
1.298
1.281
O
O
Me
O
S
N
N
O
0.95
0.95
0.96
1.87
0.98
1.00
1.06
1.97
1.04
2.00
1.02
1.00
2.00
1.06
3.03
3.60
ppm

**22**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140.297
139.344
138.190
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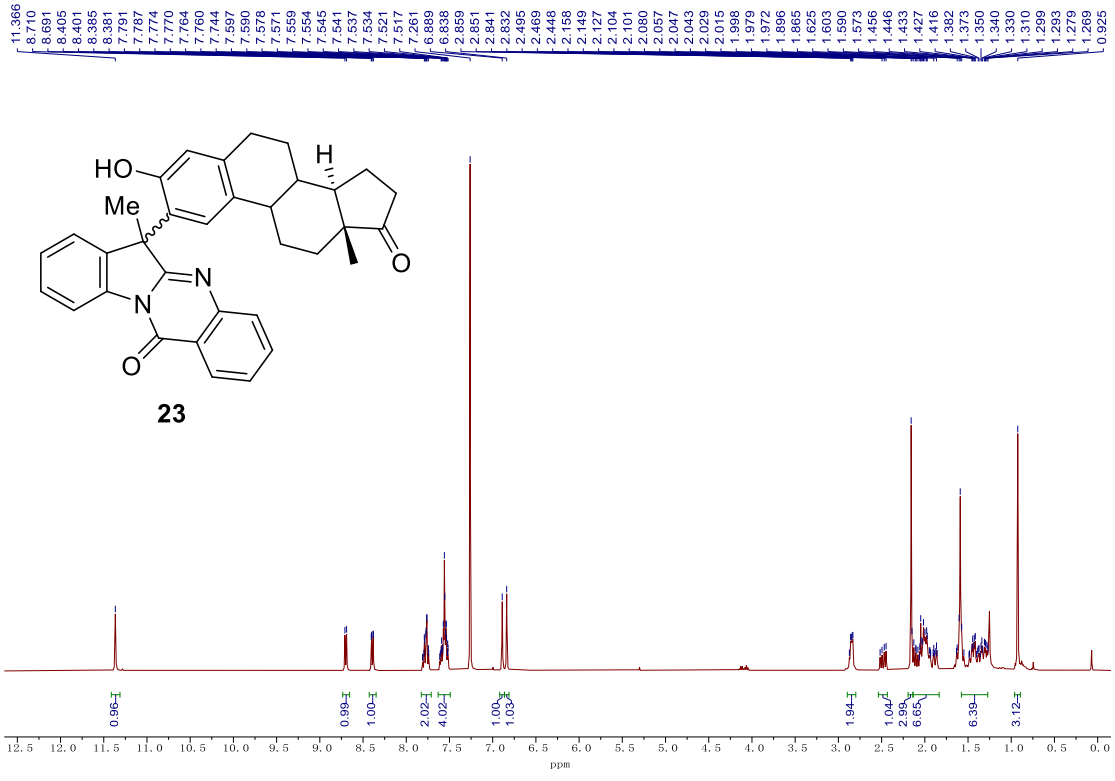
133.551
132.752
131.735
131.688
131.015
130.697
130.603
128.549
127.831
127.511
127.253
127.087
126.756
126.533
122.293
122.106
117.277
79.777
77.476
77.362
77.159
76.842
51.080
44.789
25.153
18.248
O
O
Me
O
S
N
N
O
ppm

**22**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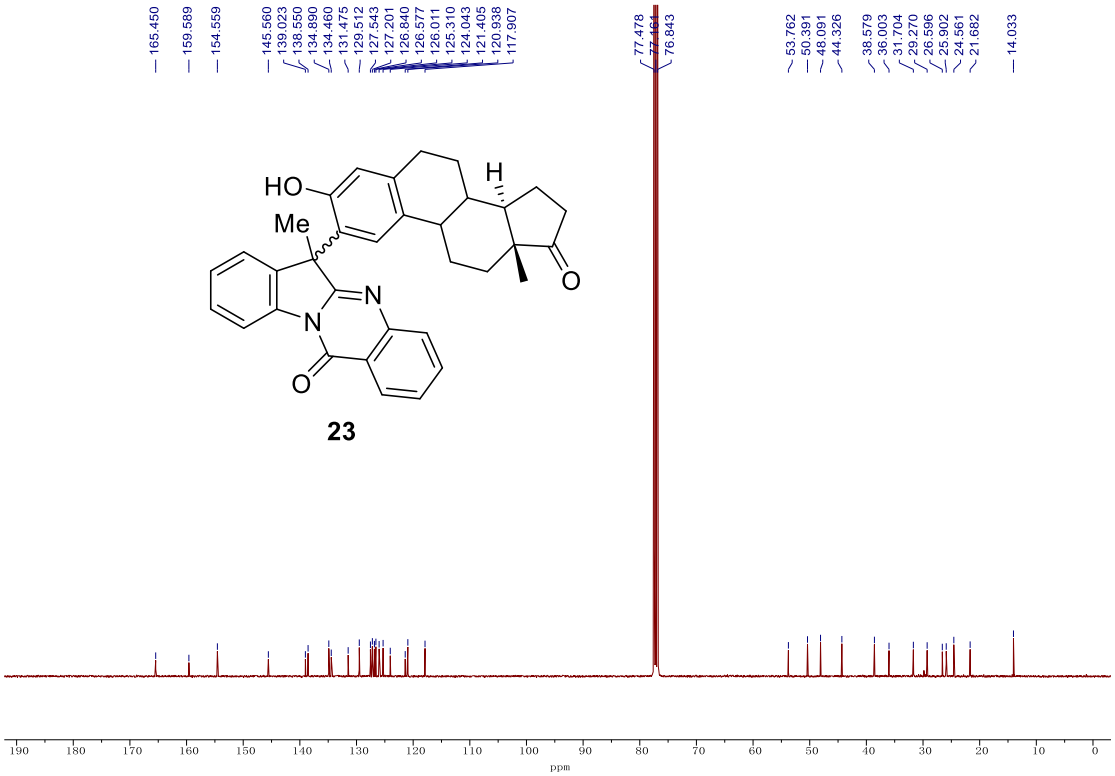
8.691
8.405
8.401
8.385
8.381
7.791
7.787
7.774
7.770
7.764
7.760
7.744
7.597
7.590
7.578
7.571
7.559
7.554
7.545
7.541
7.537
7.534
7.521
7.517
7.261
6.889
6.838
2.859
2.851
2.841
2.832
2.495
2.469
2.448
2.158
2.149
2.127
2.104
2.101
2.080
2.057
2.047
2.043
2.029
2.015
1.998
1.979
1.972
1.896
1.865
1.625
1.603
1.590
1.573
1.456
1.446
1.433
1.427
1.416
1.382
1.373
1.350
1.340
1.330
1.310
1.299
1.293
1.279
1.269
0.925
HO
Me
H
O
N
N
O
0.96
0.99
1.00
2.02
4.02
1.00
1.03
1.94
1.04
2.99
6.65
6.39
3.12
ppm

**23**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145.560
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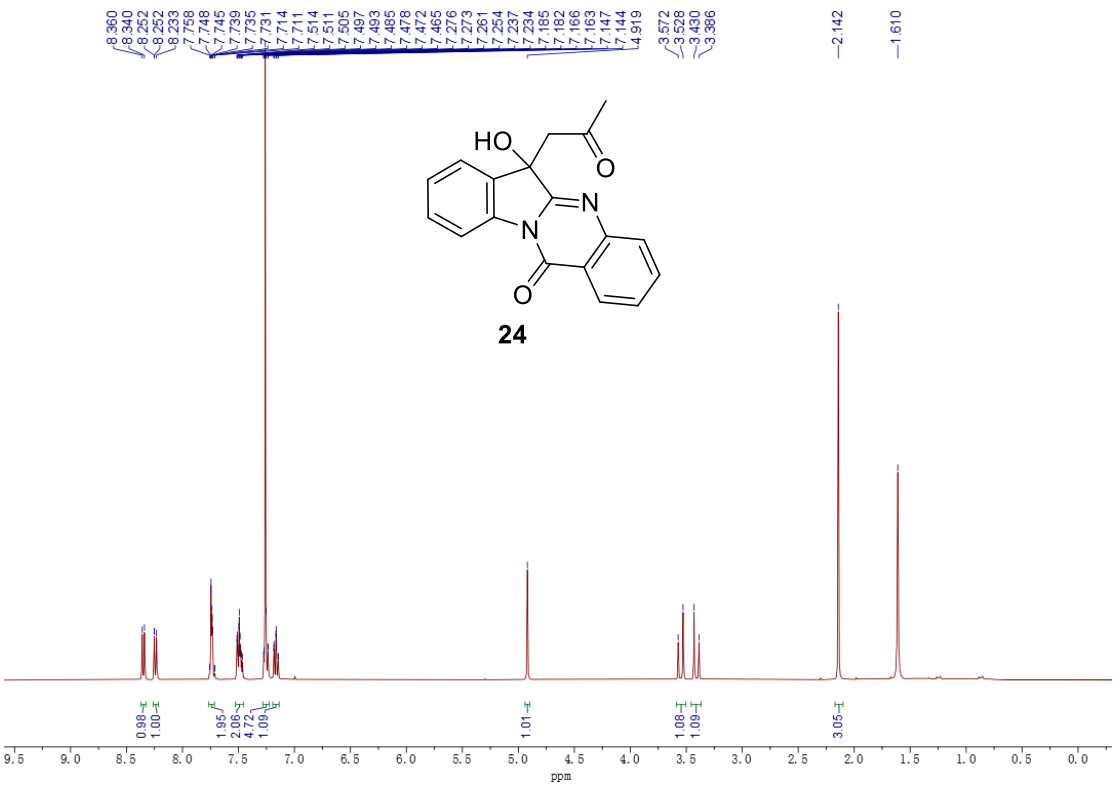
138.550
134.890
134.460
131.475
129.512
127.543
127.201
126.840
126.577
126.011
125.310
124.043
121.405
120.938
117.907
77.478
77.161
76.843
53.762
50.391
48.091
44.326
38.579
36.003
31.704
29.270
26.596
25.902
24.561
21.682
14.033
HO
Me
H
O
N
N
O
ppm

**23**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8.252
8.252
8.233
7.758
7.748
7.745
7.739
7.735
7.731
7.714
7.711
7.514
7.511
7.505
7.497
7.493
7.485
7.478
7.472
7.465
7.276
7.273
7.261
7.254
7.237
7.234
7.185
7.182
7.166
7.163
7.147
7.144
4.919
3.572
3.528
3.430
3.386
2.142
1.610
HO
O
N
N
O
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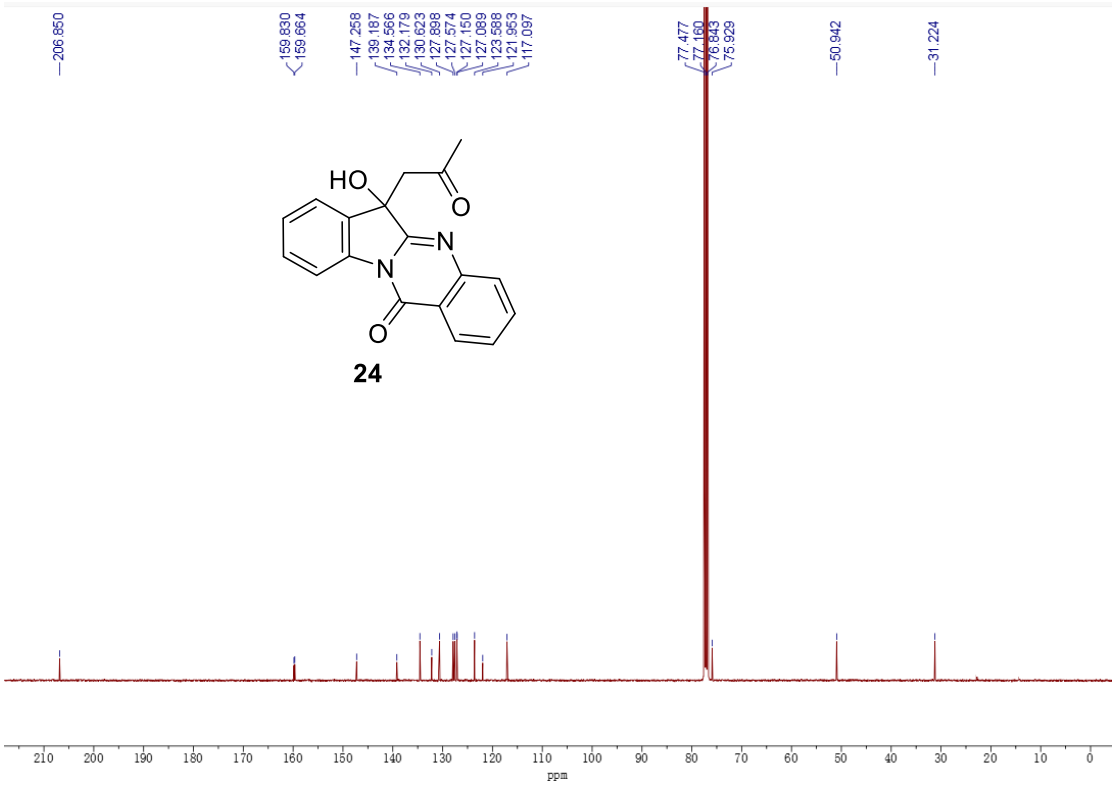
1.95
2.06
4.72
1.09
1.01
1.08
1.09
3.05
ppm

**24**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147.258
139.187
134.566
132.179
130.623
127.898
127.574
127.150
127.089
123.588
121.953
117.097
77.477
77.160
76.843
75.929
50.942
31.224
HO
O
N
N
O
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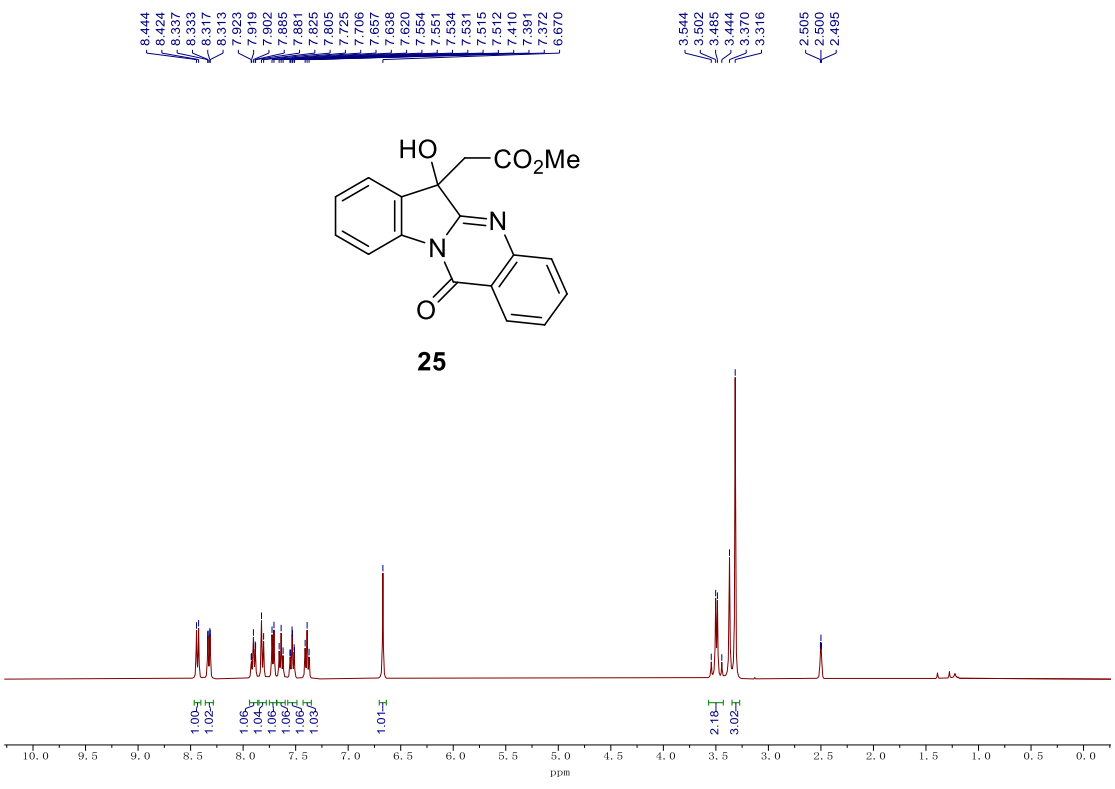
ppm

**24**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8.337
8.333
8.317
8.313
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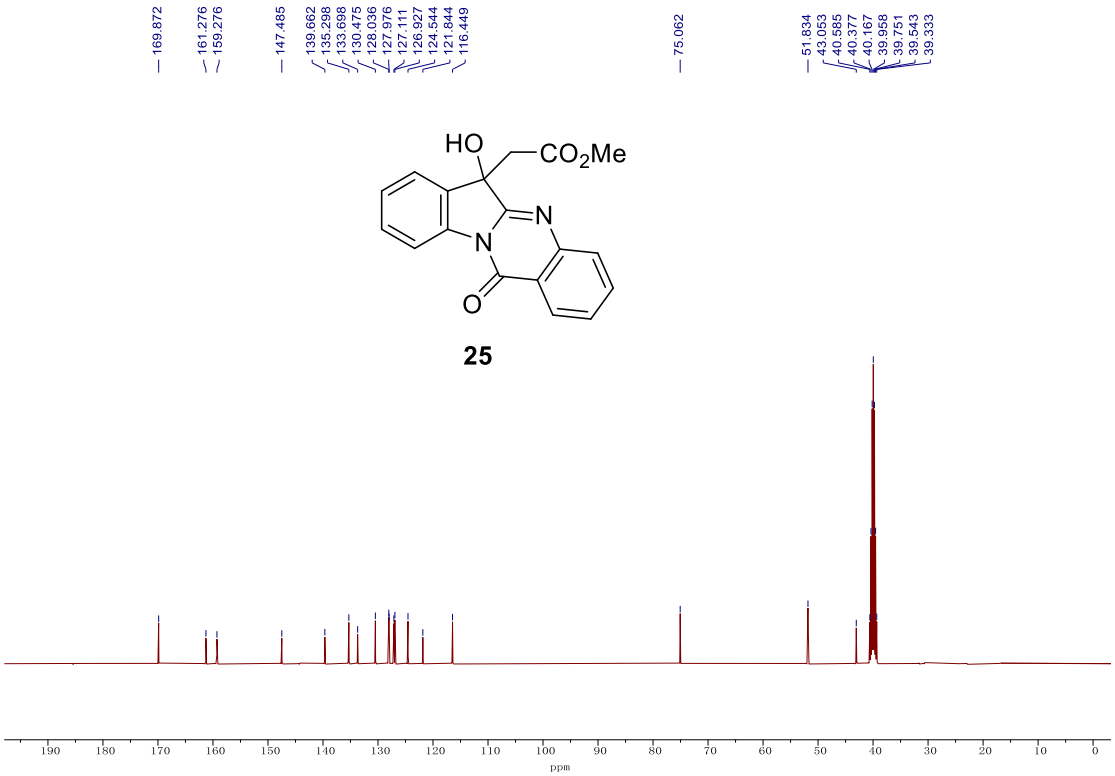
7.919
7.902
7.885
7.881
7.825
7.805
7.725
7.706
7.657
7.638
7.620
7.554
7.551
7.534
7.531
7.515
7.512
7.410
7.391
7.372
6.670
3.544
3.502
3.485
3.444
3.370
3.316
2.505
2.500
2.495
HO
CO2Me
N
N
O
1.00
1.02
1.06
1.04
1.06
1.06
1.06
1.03
1.01
2.18
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

**25**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159.276
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135.298
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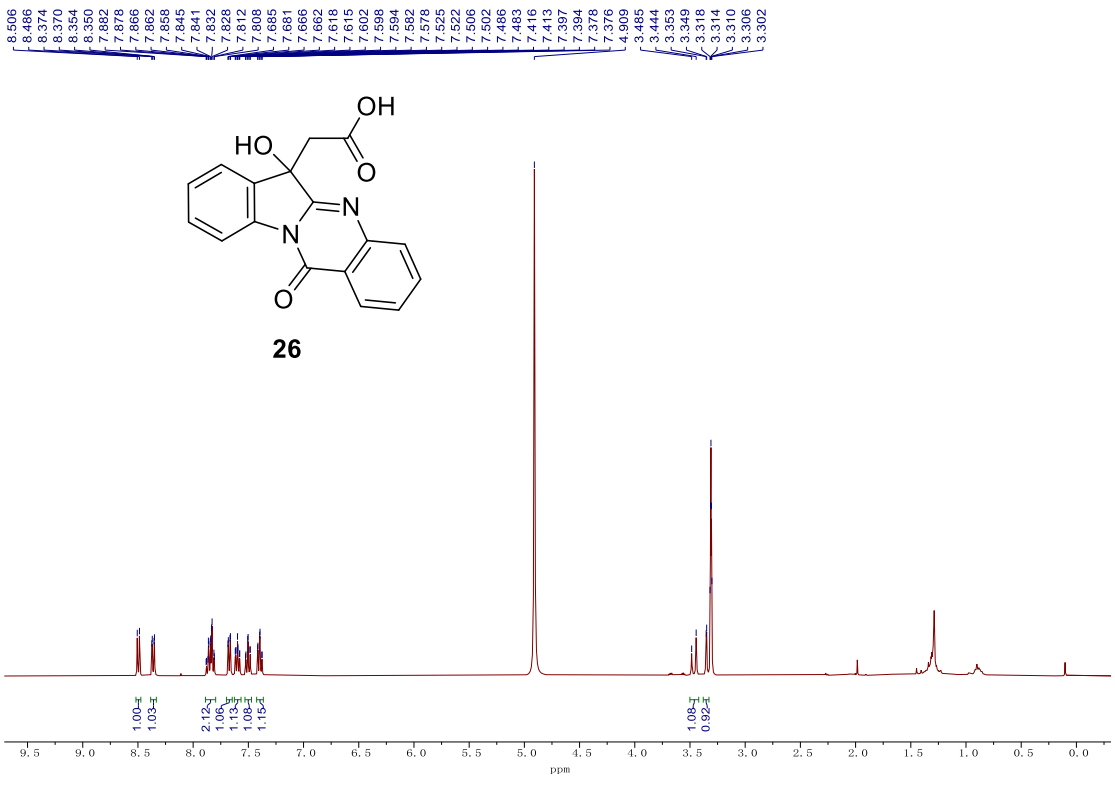
130.475
128.036
127.976
127.111
126.927
124.544
121.844
116.449
75.062
51.834
43.053
40.585
40.377
40.167
39.958
39.751
39.543
39.333
HO
CO2Me
N
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

**25**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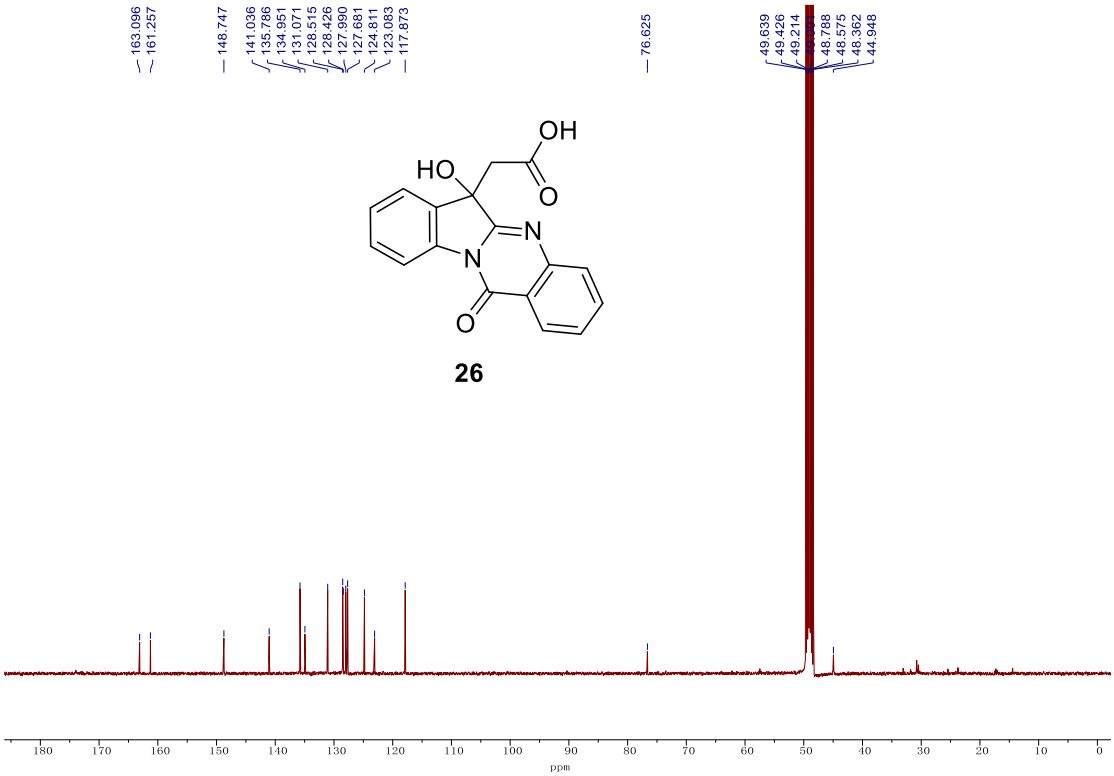
8.370
8.354
8.350
7.882
7.878
7.866
7.862
7.858
7.845
7.841
7.832
7.828
7.812
7.808
7.685
7.681
7.666
7.662
7.618
7.615
7.602
7.598
7.594
7.582
7.578
7.525
7.522
7.506
7.502
7.486
7.483
7.416
7.413
7.397
7.394
7.378
7.376
4.909
3.485
3.444
3.353
3.349
3.318
3.314
3.310
3.306
3.302
OH
HO
O
N
N
O
1.00
1.03
2.12
1.06
1.13
1.08
1.15
1.08
0.92
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

**26**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148.747
141.036
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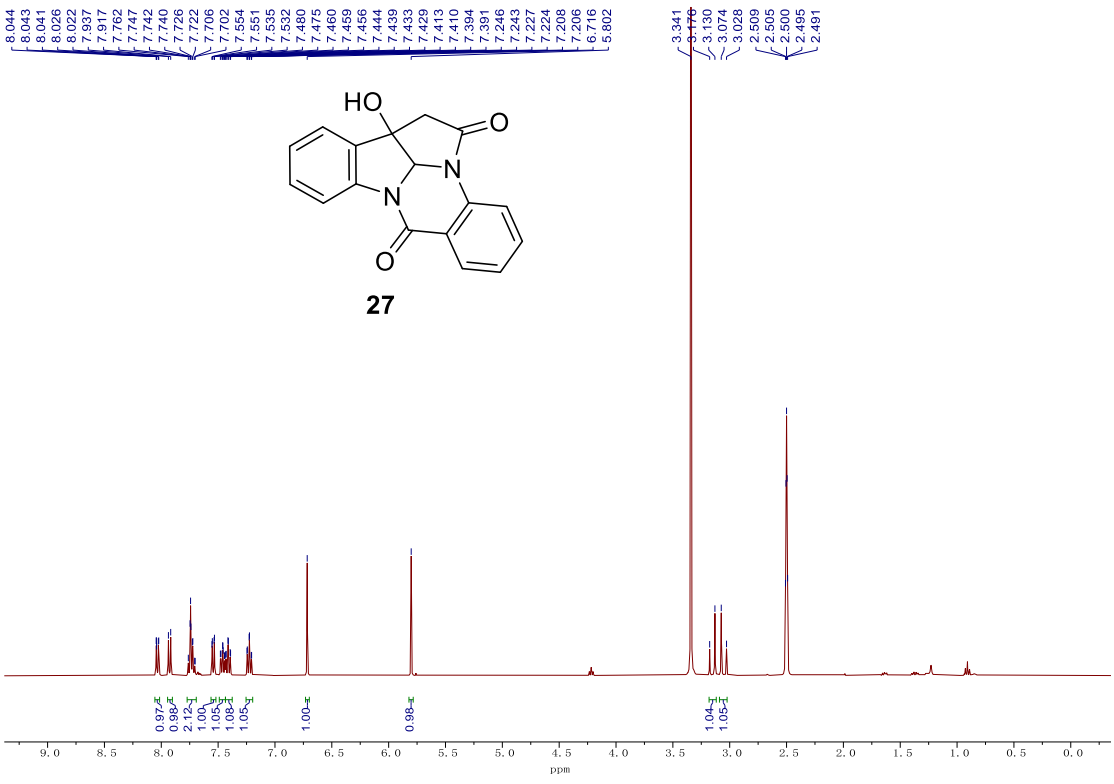
134.951
131.071
128.515
128.426
127.990
127.681
124.811
123.083
117.873
76.625
49.639
49.426
49.214
48.788
48.575
48.362
44.948
OH
HO
O
N
N
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

**26**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8.041
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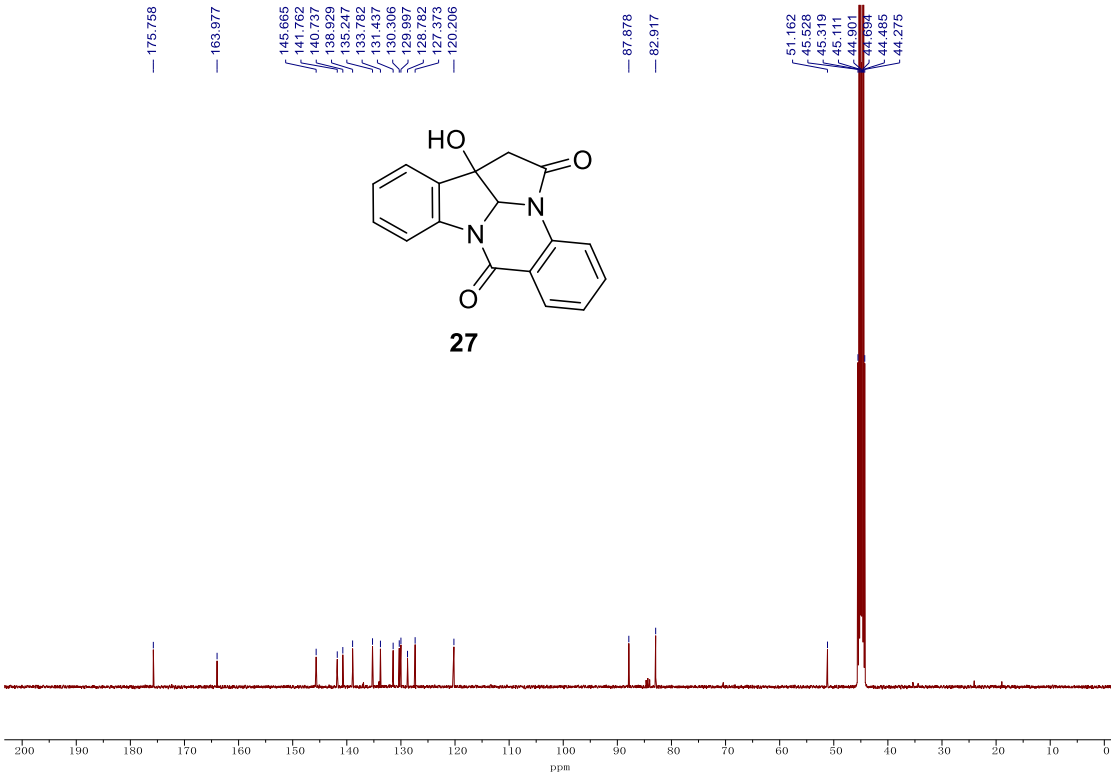
8.022
7.937
7.917
7.762
7.747
7.742
7.740
7.726
7.722
7.706
7.702
7.564
7.551
7.535
7.532
7.480
7.475
7.460
7.459
7.456
7.444
7.439
7.433
7.429
7.413
7.410
7.394
7.391
7.246
7.243
7.227
7.224
7.208
7.206
6.716
5.802
3.341
3.176
3.130
3.074
3.028
2.509
2.505
2.500
2.495
2.491
HO
O
N
N
O
0.97
0.98
2.12
1.00
1.05
1.08
1.05
1.00
0.96
1.04
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

**27**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141.762
140.737
138.929
135.247
133.782
131.437
130.306
129.997
128.782
127.373
120.206
87.878
82.917
51.162
45.528
45.319
45.111
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N
O
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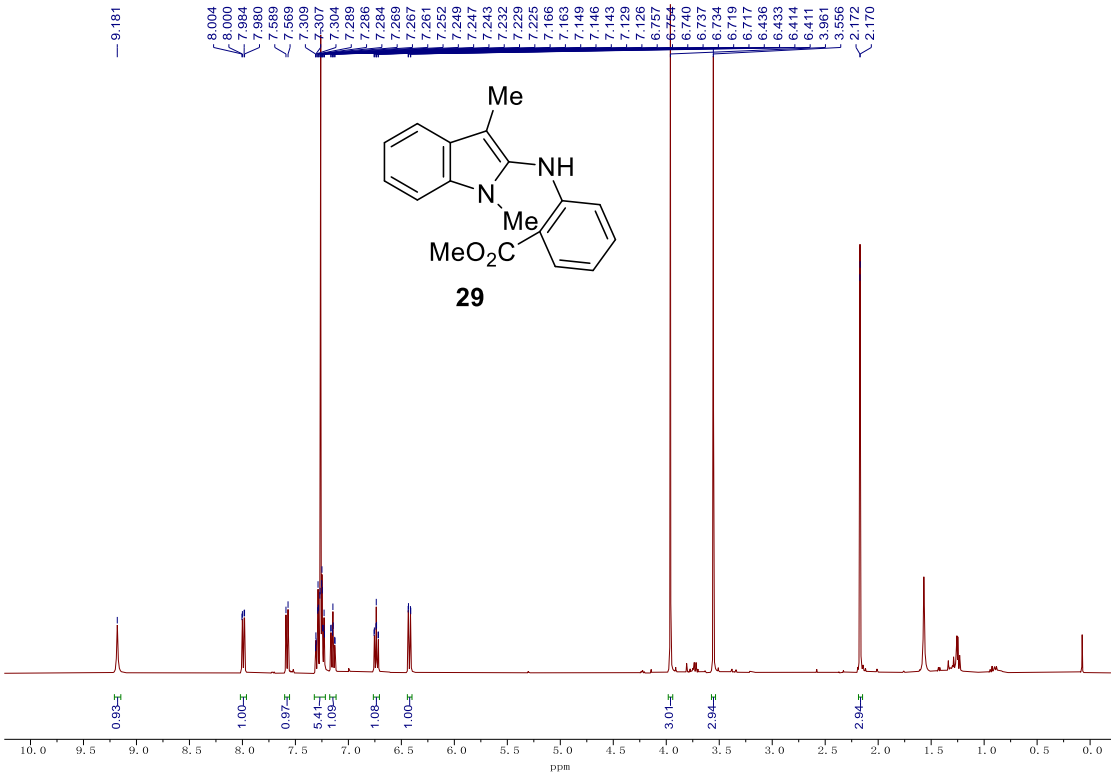
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7.267
7.261
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7.247
7.243
7.232
7.229
7.225
7.166
7.163
7.149
7.146
7.143
7.129
7.126
6.757
6.754
6.740
6.737
6.734
6.719
6.717
6.436
6.433
6.414
6.411
3.961
3.556
2.172
2.170
Me
NH
N
Me
MeO2C
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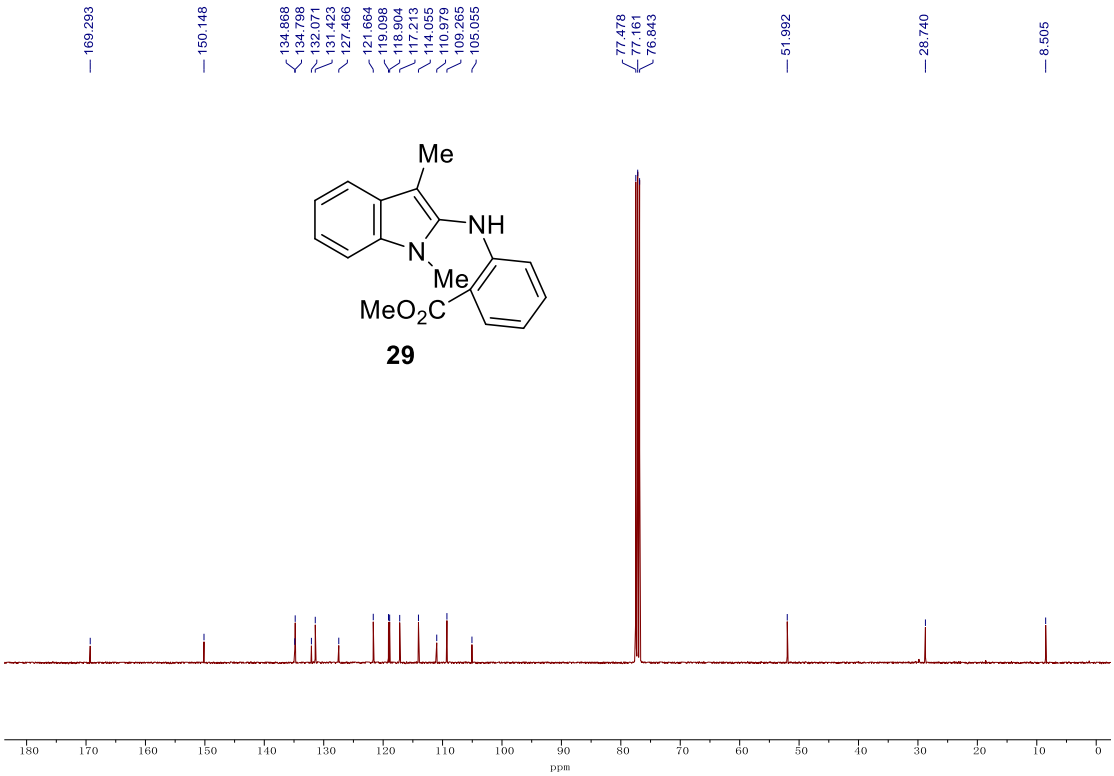
1.08
1.00
3.01
2.94
2.94
ppm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Me
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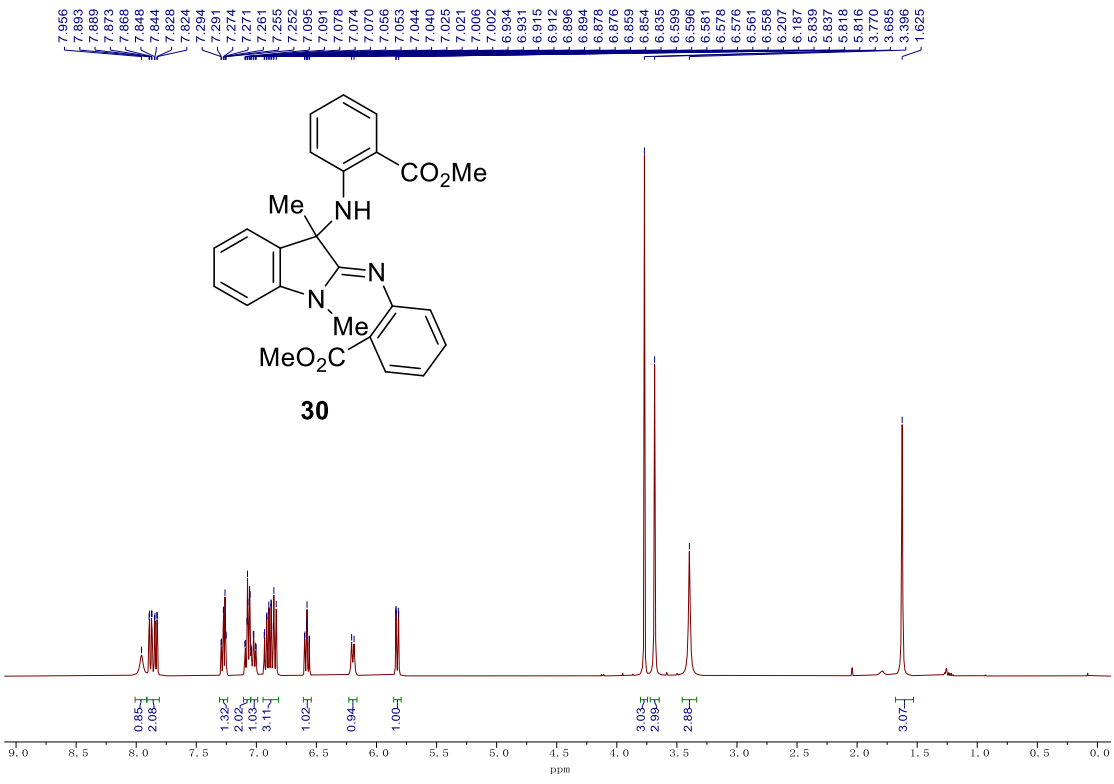
Me
MeO2C
29
ppm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7.271
7.261
7.255
7.252
7.095
7.091
7.078
7.074
7.070
7.056
7.053
7.044
7.040
7.025
7.021
7.006
7.002
6.934
6.931
6.915
6.912
6.896
6.894
6.878
6.876
6.859
6.854
6.835
6.599
6.596
6.581
6.578
6.576
6.561
6.558
6.207
6.187
5.839
5.837
5.818
5.816
3.770
3.685
3.396
1.625
CO2Me
Me
NH
N
N
Me
MeO2C
30
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3.11
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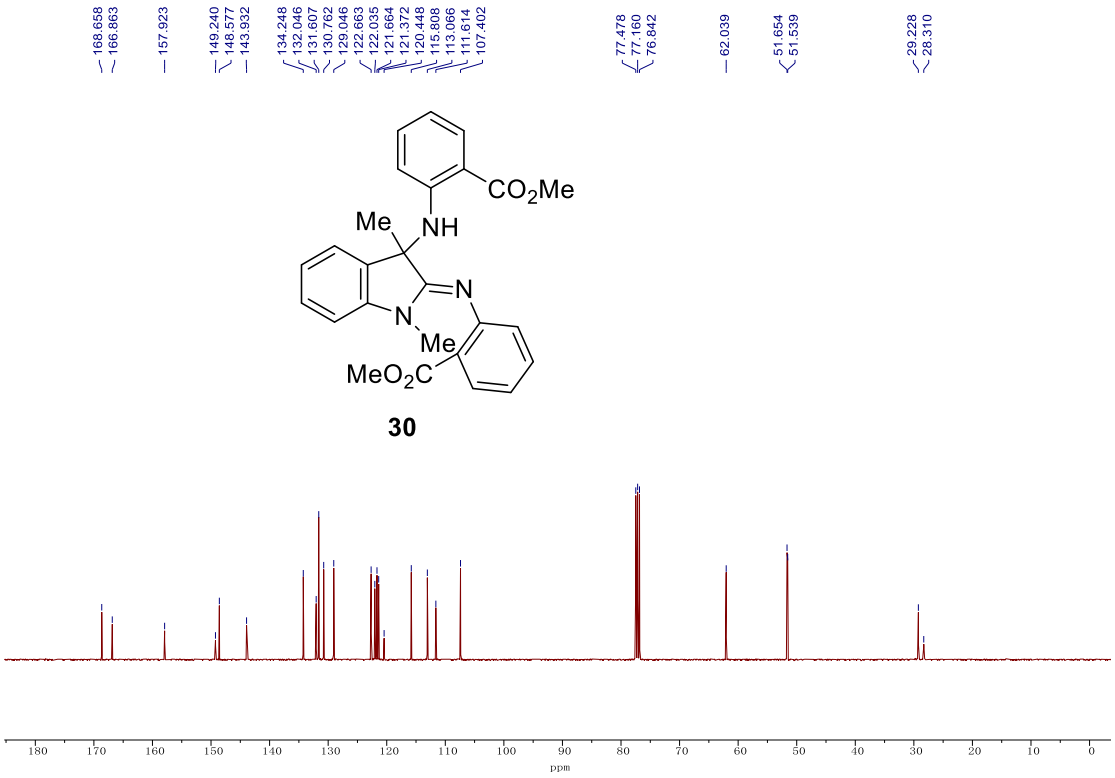
ppm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121.372
120.448
115.808
113.066
111.614
107.402
77.478
77.160
76.842
62.039
51.654
51.539
29.228
28.310
CO2Me
Me
NH
N
N
Me
MeO2C
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

**30**