

Supporting information for

Construction of heterocyclo-fused tetrahydrocarbazoles through a formal [3+3]- annulation of 2-indolylmethanols with *para*-quinone methides

Gurdeep Singh,[#] Sonam Sharma,[#] Rajat Pandey, Rekha and Ramasamy Vijaya Anand*

*Department of Chemical Sciences, Indian Institute of Science Education and Research
(IISER) Mohali, Sector 81, Knowledge City, S. A. S. Nagar, Manauli (PO), Punjab –
140306. India.*

E-mail: rvijayan@iisermohali.ac.in

[#] These authors contributed equally

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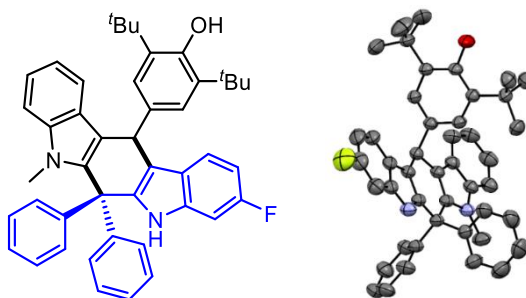
Experimental Section

1. General Information: All reactions were carried out under an argon atmosphere in an oven-dried round bottom flask. All the solvents were distilled before use and stored under an argon atmosphere. Most of the reagents and starting materials were purchased from commercial sources and used as such. 2-indolylmethanols were prepared according to the literature procedure.¹ *p*-quinone methides were prepared by following a literature procedure.² Melting points were recorded on the SMP20 melting point apparatus and are uncorrected. ¹H, ¹³C, and ¹⁹F spectra were recorded in CDCl₃ and DMSO (400, 100, and 376 MHz, respectively) on Bruker FT-NMR spectrometer. Chemical shift (δ) values are reported in parts per million relatives to TMS, and the coupling constants (*J*) are reported in Hz. High-resolution mass spectra were recorded on Waters Q-TOF Premier-HAB213 spectrometer. FT-IR spectra were recorded on a Perkin-Elmer FTIR spectrometer. Thin-layer chromatography was performed on Merck silica gel 60 F₂₅₄ TLC pellets and visualized by UV irradiation and KMnO₄ stain. Column chromatography was carried out through silica gel (100–200 mesh) using EtOAc/hexane as eluent.

2. X-ray crystallographic analysis for compound **3u**:

Table S1: Crystal data and structure refinement for compound **3u** (CCDC 2194163)

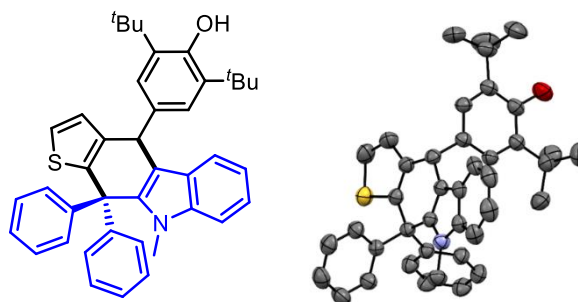
Identification code	XX-GS-40-RT
Empirical formula	C ₄₅ H ₄₃ FN ₂ O
Formula weight	646.81
Temperature/K	298.01(1)
Crystal system	triclinic
Space group	P-1
a/Å	10.7970(5)
b/Å	11.7144(5)
c/Å	17.2757(7)
α/°	109.155(4)
β/°	106.362(4)
γ/°	90.359(4)
Volume/Å ³	1968.69(16)
Z	2
ρ _{calc} /cm ³	1.091
μ/mm ⁻¹	0.068
F(000)	688.0
Crystal size/mm ³	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	5.116 to 65.482
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 16, -25 ≤ l ≤ 26
Reflections collected	29730
Independent reflections	13262 [R _{int} = 0.0326, R _{sigma} = 0.0555]
Data/restraints/parameters	13262/0/449
Goodness-of-fit on F ²	1.042
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0804, wR ₂ = 0.2270
Final R indexes [all data]	R ₁ = 0.1393, wR ₂ = 0.2817
Largest diff. peak/hole / e Å ⁻³	0.65/-0.24



3. X-ray crystallographic analysis for compound **5i**:

Table S2: Crystal data and structure refinement for compound **5i** (CCDC2194168)

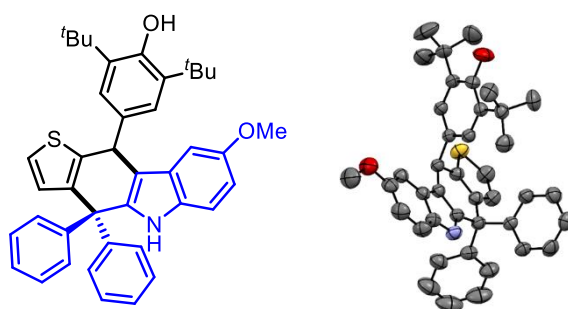
Identification code	XX GS-78_RT
Empirical formula	C ₄₂ H ₄₃ Cl ₂ NOS
Formula weight	680.73
Temperature/K	298.0(1)
Crystal system	triclinic
Space group	P-1
a/Å	9.2987(4)
b/Å	12.1896(5)
c/Å	17.6436(8)
α/°	109.223(4)
β/°	90.262(4)
γ/°	104.830(4)
Volume/Å ³	1816.78(15)
Z	2
ρ _{calc} /cm ³	1.244
μ/mm ⁻¹	0.270
F(000)	720.0
Crystal size/mm ³	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.914 to 50.108
Index ranges	-11 ≤ h ≤ 11, -14 ≤ k ≤ 14, -21 ≤ l ≤ 21
Reflections collected	25964
Independent reflections	6428 [R _{int} = 0.0417, R _{sigma} = 0.0327]
Data/restraints/parameters	6428/0/404
Goodness-of-fit on F ²	1.064
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0575, wR ₂ = 0.1586
Final R indexes [all data]	R ₁ = 0.0754, wR ₂ = 0.1808
Largest diff. peak/hole / e Å ⁻³	0.45/-0.22



4. X-ray crystallographic analysis for compound 7h:

Table S3: Crystal data and structure refinement for compound **7h** (CCDC 2194169)

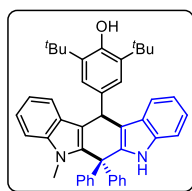
Identification code	XX-GS-61
Empirical formula	C ₄₁ H ₄₀ NO ₂ S
Formula weight	610.80
Temperature/K	298.01(1)
Crystal system	monoclinic
Space group	P21/c
a/Å	10.9175(3)
b/Å	10.7799(3)
c/Å	29.2158(10)
α/°	90
β/°	91.629(3)
γ/°	90
Volume/Å ³	3437.00(18)
Z	4
ρ _{calc} /cm ³	1.180
μ/mm ⁻¹	0.130
F(000)	1300.0
Crystal size/mm ³	0.1 × 0.1 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	5.312 to 65.554
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -44 ≤ l ≤ 43
Reflections collected	50310
Independent reflections	12028 [R _{int} = 0.0444, R _{sigma} = 0.0366]
Data/restraints/parameters	12028/0/413
Goodness-of-fit on F ²	1.026
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0656, wR ₂ = 0.1800
Final R indexes [all data]	R ₁ = 0.1093, wR ₂ = 0.2239
Largest diff. peak/hole / e Å ⁻³	0.61/-0.22



5. General procedure for the synthesis of tetrahydroindolo[2,3-*b*]carbazole derivatives (3a-x): TsOH (1.0 equiv.) was added to a solution of *p*-QM [**1a-j**] (30 mg, 1.0 equiv.) and 2-indolylmethanol [**2a-1**, **2n** & **2o**] (1.0 equiv.) in acetone (1.5 mL), and the resulting suspension was stirred at room temperature for 1 hour. After the reaction was complete (based on TLC analysis), the residue was then concentrated under reduced pressure, and the residue was then purified through a silica gel column using EtOAc/Hexane mixture as an eluent to get the pure products [**3a-x**].

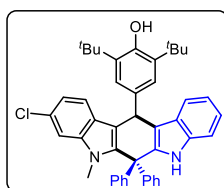
6. Characterization of products 3a to 3y

2,6-di-*tert*-butyl-4-(5-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)phenol (3a): The reaction was performed at 0.086 mmol scale of **1a**; white solid (48.9 mg,



90% yield); m. p. = 269–271 °C; R_f = 0.3 (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.68 – 7.64 (m, 3H), 7.60 (d, J = 7.9 Hz, 1H), 7.51 (d, J = 7.8 Hz, 1H), 7.44 – 7.37 (m, 5H), 7.35 – 7.32 (m, 2H), 7.30 – 7.29 (m, 1H), 7.28 – 7.23 (m, 3H), 7.21 (s, 2H), 7.14 – 7.08 (m, 2H), 7.05 – 7.01 (m, 1H), 5.75 (s, 1H), 4.97 (s, 1H), 3.30 (s, 3H), 1.35 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 152.0, 143.1, 142.4, 138.7, 138.4, 137.3, 137.1, 135.4, 135.3, 129.8, 129.3 (2C), 128.8, 128.5, 127.2, 126.6, 126.1, 125.3, 121.8, 121.5, 120.3, 120.1, 119.4, 119.0, 115.5, 114.7, 110.9, 108.8, 52.6, 39.62, 39.6, 34.3, 32.2, 30.5; FT-IR (thin film, neat): 3635, 3434, 2957, 1598, 737 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{45}\text{H}_{45}\text{N}_2\text{O}$ [$\text{M}+\text{H}$] $^+$: 629.3532; found : 629.3540.

2,6-di-*tert*-butyl-4-(3-chloro-5-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)phenol (3b): The reaction was performed at 0.079 mmol scale of **1b**; white

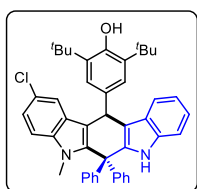


solid (50.0 mg, 96% yield); m. p. = 276–278 °C; R_f = 0.3 (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.65 (s, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 7.8 Hz, 1H), 7.41 – 7.36 (m, 5H), 7.34 – 7.24 (m, 4H), 7.22

– 7.20 (m, 2H), 7.15 (s, 2H), 7.11 – 7.07 (m, 1H), 7.01 – 6.97 (m, 2H), 5.66 (s, 1H), 4.96 (s, 1H), 3.24 (s, 3H), 1.32 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 152.1, 142.8, 142.1, 138.9, 138.4, 137.8, 137.3, 135.6, 135.0, 129.7, 129.2 (2C), 128.9, 128.6, 127.7, 127.3, 126.5, 125.3, 124.6, 121.9, 121.0, 120.1, 119.7, 119.4, 115.7, 114.3, 110.9, 109.0, 52.6, 39.52, 39.5, 34.4, 32.4, 30.5; FT-IR (thin film, neat): 3633, 3458, 2957, 1603, 733 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{45}\text{H}_{44}\text{ClN}_2\text{O}$ $[\text{M}+\text{H}]^+$: 663.3142; found : 663.3146.

2,6-di-tert-butyl-4-(2-chloro-5-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-

b]carbazol-12-yl)phenol (3c): The reaction was performed at 0.079 mmol scale of **1c**; white

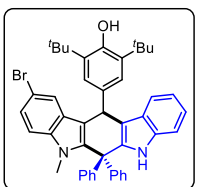


solid (49.0 mg, 94% yield); m. p. = 265–267 °C; R_f = 0.3 (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.67 (s, 1H), 7.60 – 7.58 (m, 2H), 7.55 – 7.54 (m, 1H), 7.46 – 7.39 (m, 4H), 7.37 – 7.26 (m, 5H), 7.23 (d, J =

8.0 Hz, 1H), 7.17 – 7.16 (m, 2H), 7.13 – 7.09 (m, 3H), 7.03 – 6.99 (m, 1H), 5.67 (s, 1H), 5.00 (s, 1H), 3.26 (s, 3H), 1.34 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 152.2, 142.8, 142.1, 138.5, 138.3, 137.3, 136.8, 135.6, 134.8, 129.8, 129.2 (2C), 128.9, 128.6, 127.3, 127.0, 126.5, 125.3, 124.7, 121.9, 121.7, 120.1, 119.8, 119.5, 115.3, 114.3, 110.9, 109.9, 52.6, 39.5, 39.4, 34.4, 32.4, 30.5; FT-IR (thin film, neat): 3636, 3457, 2957, 1468, 732 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{45}\text{H}_{44}\text{ClN}_2\text{O}$ $[\text{M}+\text{H}]^+$: 663.3142; found : 663.3166.

4-(2-bromo-5-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-b]carbazol-12-yl)-2,6-

di-tert-butylphenol (3d): The reaction was performed at 0.070 mmol scale of **1d**; white solid



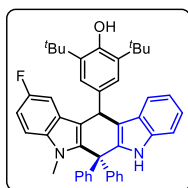
(44.8 mg, 90% yield); m. p. = 267–269 °C; R_f = 0.3 (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.74 (s, 1H), 7.67 (s, 1H), 7.60 – 7.58 (m, 2H), 7.43 – 7.32 (m, 11H), 7.17 – 7.16 (m, 2H), 7.13 – 7.08 (m, 2H), 7.03 – 7.00

(m, 1H), 5.67 (s, 1H), 5.00 (s, 1H), 3.25 (s, 3H), 1.35 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 152.2, 142.7, 142.0, 138.6, 138.1, 137.3, 137.1, 135.6, 134.8, 129.8, 129.2 (2C), 128.9, 128.6, 127.7, 127.3, 126.5, 125.3, 124.2, 122.9, 121.9, 120.1, 119.5, 115.3, 114.2, 112.3,

110.9, 110.4, 52.6, 39.45, 39.4, 34.4, 32.3, 30.5; FT-IR (thin film, neat): 3634, 3432, 2957, 1466, 1229, 737 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{45}\text{H}_{44}\text{BrN}_2\text{O}$ $[\text{M}+\text{H}]^+$: 707.2637; found : 707.2658.

2,6-di-tert-butyl-4-(2-fluoro-5-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-

b]carbazol-12-yl)phenol (3e): The reaction was performed at 0.082 mmol scale of **1e**; white



solid (44.1 mg, 83% yield); m. p. = 277–279 °C; R_f = 0.3 (15% EtOAc in

hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.63 (s, 1H), 7.60 – 7.57 (m, 2H), 7.45

(d, J = 7.8 Hz, 1H), 7.41 – 7.35 (m, 4H), 7.34 – 7.26 (m, 4H), 7.20 (d, J = 8.0

Hz, 1H), 7.15 (s, 2H), 7.14 – 7.12 (m, 1H), 7.11 – 7.07 (m, 2H), 7.01 – 6.97 (m, 1H), 6.94 –

6.89 (m, 1H), 5.63 (s, 1H), 4.96 (s, 1H), 3.26 (s, 3H), 1.32 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz,

CDCl_3) δ 157.5 (d, $J_{\text{C-F}}$ = 232.4 Hz), 152.2, 142.9, 142.2, 138.7, 138.4, 137.3, 135.6, 135.0,

134.9, 129.7, 129.2 (2C), 128.9, 128.6, 127.3, 126.5, 126.3 (d, $J_{\text{C-F}}$ = 9.9 Hz), 125.3, 121.9,

120.1, 119.4, 115.4 (d, $J_{\text{C-F}}$ = 4.7 Hz), 114.4, 110.9, 109.6 (d, $J_{\text{C-F}}$ = 26.2 Hz), 109.4 (d, $J_{\text{C-F}}$ =

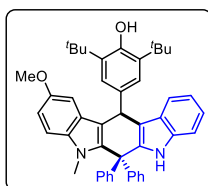
9.8 Hz), 105.1 (d, $J_{\text{C-F}}$ = 23.5 Hz), 52.7, 39.6, 39.5, 34.4, 32.5, 30.5; ^{19}F $\{^1\text{H}\}$ NMR (376 MHz,

CDCl_3) δ -125.1; FT-IR (thin film, neat): 3636, 2956, 1484, 1149, 737 cm^{-1} ; HRMS (ESI): m/z

calcd for $\text{C}_{45}\text{H}_{44}\text{FN}_2\text{O}$ $[\text{M}+\text{H}]^+$: 647.3438; found : 647.3463.

2,6-di-tert-butyl-4-(2-methoxy-5-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-

b]carbazol-12-yl)phenol (3f): The reaction was performed at 0.079 mmol scale of **1f**; white



solid (39.3 mg, 75% yield); m. p. = 159–161 °C; R_f = 0.2 (15% EtOAc in

hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.67 (s, 1H), 7.60 (d, J = 7.5 Hz,

2H), 7.40 – 7.37 (m, 5H), 7.33 – 7.25 (m, 4H), 7.22 – 7.20 (m, 1H), 7.19 (s,

2H), 7.12 – 7.07 (m, 2H), 7.00 – 6.95 (m, 2H), 6.83 (dd, J = 8.8, 2.4 Hz, 1H), 5.64 (s, 1H), 4.95

(s, 1H), 3.77 (s, 3H), 3.24 (s, 3H), 1.32 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 153.5,

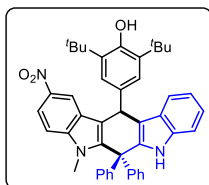
152.0, 143.0, 142.5, 138.7, 137.5, 137.3, 135.5, 135.4, 133.6, 129.8, 129.3, 128.8, 128.5, 127.2,

127.1, 126.6, 126.3, 125.4, 121.8, 120.1, 119.3, 115.1, 114.5, 111.8, 110.9, 109.6, 101.7, 55.8,

55.7, 52.7, 39.7, 34.3, 32.3, 30.5; FT-IR (thin film, neat): 3634, 2956, 1486, 1228, 736 cm^{-1} ;
HRMS (ESI): m/z calcd for $\text{C}_{46}\text{H}_{47}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 659.3638; found : 659.3655.

2,6-di-tert-butyl-4-(5-methyl-2-nitro-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-

b]carbazol-12-yl)phenol (3g): The reaction was performed at 0.076 mmol scale of **1g**; white

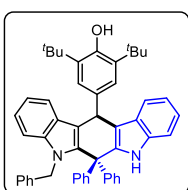


solid (37.0 mg, 72% yield); m. p. = 278–280 °C; R_f = 0.2 (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 8.53 (d, J = 2.2 Hz, 1H), 8.05 (dd, J = 9.0, 2.2 Hz, 1H), 7.70 (s, 1H), 7.59 – 7.57 (m, 2H), 7.43 – 7.25 (m, 9H),

7.22 (d, J = 8.0 Hz, 1H), 7.20 – 7.18 (m, 3H), 7.12 – 7.08 (m, 1H), 7.01 – 6.97 (m, 1H), 5.72 (s, 1H), 5.01 (s, 1H), 3.31 (s, 3H), 1.32 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 152.5, 142.1, 141.6, 141.3, 141.2, 140.1, 138.2, 137.4, 136.0, 134.4, 129.7, 129.12 (2C), 129.1, 128.8, 127.6, 126.3, 125.3, 125.2, 122.2, 120.1, 119.6, 118.2, 117.6, 117.3, 113.7, 111.0, 108.8, 52.7, 39.4, 34.4, 32.8, 30.5; FT-IR (thin film, neat): 3631, 3428, 2957, 1483, 735 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{45}\text{H}_{44}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 674.3383; found : 674.3416.

4-(5-benzyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-b]carbazol-12-yl)-2,6-di-tert-

butylphenol (3h): The reaction was performed at 0.071 mmol scale of **1h**; white solid (31.9

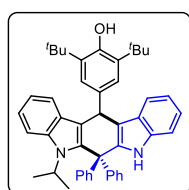


mg, 64% yield); gummy solid; R_f = 0.3 (15% EtOAc in hexane); ^1H NMR (400 MHz, DMSO-d_6) δ 10.56 (s, 1H), 7.61 (d, J = 7.6 Hz, 2H), 7.42 (d, J = 8.1 Hz, 1H), 7.29 – 7.15 (m, 9H), 7.10 (t, J = 7.5 Hz, 2H), 7.04 – 6.98 (m,

1H), 6.95 – 6.91 (m, 2H), 6.88 – 6.81 (m, 5H), 6.78 – 6.76 (m, 1H), 6.64 (s, 1H), 6.19 (d, J = 7.6 Hz, 2H), 5.72 (s, 1H), 5.14 – 5.03 (m, 2H), 1.24 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 151.7, 142.5, 141.7, 138.9, 138.7, 137.5, 137.4, 137.1, 136.4, 129.4, 128.3, 128.2, 127.5, 126.7, 126.5, 126.48, 126.13, 126.1, 125.7, 125.3, 125.1, 124.7, 121.5, 121.1, 119.7, 119.2, 119.0, 118.3, 114.3, 112.0, 111.2, 110.4, 52.2, 48.4, 48.36, 38.5, 34.6, 30.6; FT-IR (thin film, neat): 3634, 3295, 2953, 1459, 735 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{51}\text{H}_{49}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 705.3845; found : 705.3869.

2,6-di-tert-butyl-4-(5-isopropyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-

12-yl)phenol (3i): The reaction was performed at 0.080 mmol scale of **1i**; white solid (27.8



mg, 53% yield); gummy solid; $R_f = 0.3$ (15% EtOAc in hexane); ^1H NMR

(400 MHz, DMSO- d_6) δ 10.56 (s, 1H), 7.73 (d, $J = 7.8$ Hz, 2H), 7.44 – 7.33

(m, 5H), 7.30 – 7.24 (m, 5H), 7.18 – 7.12 (m, 2H), 7.08 (s, 2H), 6.99 – 6.94

(m, 1H), 6.90 – 6.84 (m, 2H), 6.78 – 6.74 (m, 1H), 6.57 (s, 1H), 5.61 – 5.60 (m, 1H), 4.20 (sept,

$J = 6.2$ Hz, 1H), 1.21 – 1.17 (m, 24H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 151.7, 143.2,

141.4, 139.5, 138.9, 137.5, 137.0, 136.5, 135.0, 129.6, 129.4, 128.3, 128.2, 127.0, 126.7, 126.5,

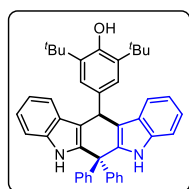
125.2, 124.6, 121.04, 121.0, 119.8, 119.1, 118.3, 118.2, 113.6, 112.4, 111.6, 111.2, 52.4, 47.8,

38.4, 34.5, 30.6; 19.9, 19.3; FT-IR (thin film, neat): 3647, 3465, 2922, 1460, 740 cm^{-1} ; HRMS

(ESI): m/z calcd for $\text{C}_{47}\text{H}_{49}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 657.3845; found : 657.3859.

2,6-di-tert-butyl-4-(6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)phenol

(3j): The reaction was performed at 0.09 mmol scale of **1a**; pale yellow solid (34.9 mg, 63%



yield); m. p. = 236–238°C; $R_f = 0.3$ (15% EtOAc in hexane); ^1H NMR (400

MHz, CDCl_3) δ 7.71 (s, 2H), 7.47 – 7.42 (m, 4H), 7.37 – 7.26 (m, 6H), 7.25 –

7.23 (m, 4H), 7.18 (s, 2H), 7.12 – 7.08 (m, 2H), 7.01 – 6.97 (m, 2H), 5.62 (s,

1H), 4.95 (s, 1H), 1.32 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 152.1, 144.8, 144.7,

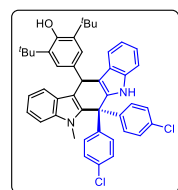
137.3, 135.8, 135.5, 135.0, 129.0 (2C), 128.8 (2C), 127.4, 127.2, 126.7, 125.3, 121.9, 120.3,

119.4, 115.7, 110.9, 52.6, 39.6, 34.4, 30.6; FT-IR (thin film, neat): 3637, 2954, 1470, 738 cm^{-1} ;

HRMS (ESI): m/z calcd for $\text{C}_{44}\text{H}_{43}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 615.3375; found : 615.336.

4-(6,6-bis(4-chlorophenyl)-5-methyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)-2,6-

di-tert-butylphenol (3k): The reaction was performed at 0.086 mmol scale of **1a**; white solid



(56.0 mg, 93% yield); m. p. = 195–197 °C; $R_f = 0.3$ (15% EtOAc in hexane); ^1H

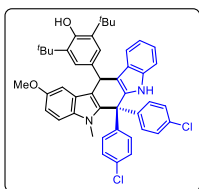
NMR (400 MHz, CDCl_3) δ 7.61 – 7.57 (m, 2H), 7.53 – 7.51 (m, 2H), 7.47 (d,

$J = 7.8$ Hz, 1H), 7.38 – 7.36 (m, 2H), 7.31 – 7.21 (m, 7H), 7.15 – 7.08 (m, 4H),

7.05 – 7.01 (m, 1H), 5.69 (s, 1H), 4.96 (s, 1H), 3.27 (s, 3H), 1.31 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 152.1, 141.5, 140.8, 138.4, 137.7, 137.4, 136.0, 135.5, 134.8, 133.4, 131.0, 130.5 (2C), 129.1, 128.8, 126.5, 126.0, 125.2, 122.2, 121.9, 120.4, 120.2, 119.7, 119.3, 116.1, 115.2, 111.0, 109.0, 51.8, 39.5, 34.3, 32.3, 30.4; FT-IR (thin film, neat): 3636, 3456, 2956, 1488, 735 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{45}\text{H}_{43}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 697.2752; found : 697.2740.

4-(6,6-bis(4-chlorophenyl)-2-methoxy-5-methyl-5,6,7,12-tetrahydroindolo[2,3-

b]carbazol-12-yl)-2,6-di-*tert*-butylphenol (3l): The reaction was performed at 0.079 mmol



scale of **1f**; white solid (42.8 mg, 74% yield); gummy solid; R_f = 0.3 (15%

EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.56 (s, 1H), 7.50 – 7.47

(m, 2H), 7.37 (d, J = 8.1 Hz, 1H), 7.35 – 7.32 (m, 2H), 7.26 – 7.21 (m, 5H),

7.13 – 7.08 (m, 4H), 7.00 – 6.96 (m, 1H), 6.95 (d, J = 2.4 Hz, 1H), 6.84 (dd, J = 8.8, 2.4 Hz,

1H), 5.59 (s, 1H), 4.95 (s, 1H), 3.76 (s, 3H), 3.22 (s, 3H), 1.29 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100

MHz, CDCl_3) δ 153.7, 152.1, 141.4, 140.9, 137.7, 137.4, 136.4, 135.6, 134.9, 133.6, 133.43,

133.4, 131.0, 130.5, 129.1, 128.8, 126.5, 126.2, 125.2, 122.2, 120.2, 119.7, 115.6, 115.1, 112.2,

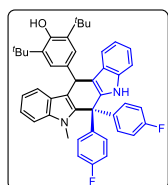
111.0, 109.8, 101.7, 55.8, 51.9, 39.64, 39.6, 34.3, 32.4, 30.5; FT-IR (thin film, neat): 3636,

2953, 1486, 1229, 739 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{46}\text{H}_{43}\text{Cl}_2\text{N}_2\text{O}_2$ $[\text{M}-\text{H}]^-$: 725.2702;

found : 725.2720.

4-(6,6-bis(4-fluorophenyl)-5-methyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)-2,6-

di-*tert*-butylphenol (3m): The reaction was performed at 0.086 mmol scale of **1a**; white solid



(48.2 mg, 84% yield); m. p. = 172–174 $^\circ\text{C}$; R_f = 0.3 (15% EtOAc in hexane);

^1H NMR (400 MHz, CDCl_3) δ 7.58 – 7.55 (m, 4H), 7.46 (d, J = 7.8 Hz, 1H),

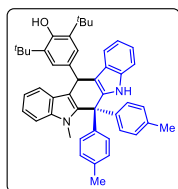
7.32 – 7.28 (m, 2H), 7.27 – 7.20 (m, 3H), 7.14 – 7.10 (m, 4H), 7.08 – 7.06 (m,

2H), 7.04 – 6.98 (m, 3H), 5.68 (s, 1H), 4.95 (s, 1H), 3.26 (s, 3H), 1.30 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR

(100 MHz, CDCl_3) δ 161.82 (d, $J_{\text{C-F}}$ = 246.2 Hz), 161.8 (d, $J_{\text{C-F}}$ = 246.4 Hz), 152.1, 138.9 (d,

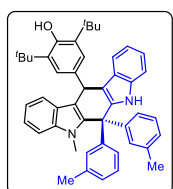
$J_{C-F} = 3.3$ Hz), 138.4, 138.3, 138.2 (d, $J_{C-F} = 3.0$ Hz), 137.4, 136.6, 135.5, 135.0, 131.4 (d, $J_{C-F} = 7.9$ Hz), 130.8 (d, $J_{C-F} = 7.8$ Hz), 126.6, 126.0, 125.2, 122.1, 121.8, 120.3, 120.2, 119.6, 119.3, 115.8 (d, $J_{C-F} = 21.2$ Hz), 115.7 (d, $J_{C-F} = 19.3$ Hz), 115.4, 114.9, 110.9, 108.9, 51.6, 39.5, 34.3, 32.2, 30.5; ^{19}F { 1H } NMR (376 MHz, $CDCl_3$) δ -114.8, -115.2; FT-IR (thin film, neat): 3636, 3457, 2958, 1504, 735 cm^{-1} ; HRMS (APCI): m/z calcd for $C_{45}H_{43}F_2N_2O$ [M+H] $^+$: 665.3343; found : 665.3365.

2,6-di-*tert*-butyl-4-(5-methyl-6,6-di-*p*-tolyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)phenol (3n): The reaction was performed at 0.086 mmol scale of **1a**; white solid (52.2 mg,



92% yield); m. p. = 267–269 °C; $R_f = 0.3$ (15% EtOAc in hexane); 1H NMR (400 MHz, DMSO- d_6) δ 10.51 (s, 1H), 7.42 (d, $J = 8.2$ Hz, 2H), 7.32 (d, $J = 7.8$ Hz, 1H), 7.24 (d, $J = 7.8$ Hz, 1H), 7.20 (d, $J = 8.2$ Hz, 1H), 7.14 – 7.10 (m, 3H), 7.09 – 7.03 (m, 6H), 7.00 – 6.96 (m, 1H), 6.89 – 6.84 (m, 2H), 6.74 (t, $J = 7.4$ Hz, 1H), 6.53 (s, 1H), 5.59 (s, 1H), 3.04 (s, 3H), 2.21 (s, 3H), 2.17 (s, 3H), 1.14 (s, 18H); ^{13}C { 1H } NMR (100 MHz, DMSO- d_6) δ 151.7, 140.4, 139.4, 139.1, 138.8, 137.9, 137.5, 137.3, 136.5, 136.0, 135.9, 129.4, 129.1, 128.8, 125.3, 124.6, 121.24, 121.2, 120.9, 119.3, 119.0, 118.99, 118.7, 118.3, 114.3, 112.0, 111.2, 109.3, 51.5, 38.6, 34.5, 31.8, 30.6, 20.6; FT-IR (thin film, neat): 3635, 3459, 2957, 1509, 734 cm^{-1} ; HRMS (APCI): m/z calcd for $C_{47}H_{49}N_2O$ [M+H] $^+$: 657.3845; found : 657.3873.

2,6-di-*tert*-butyl-4-(5-methyl-6,6-di-*m*-tolyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)phenol (3o): The reaction was performed at 0.086mmol scale of **1a**; white solid (48.2 mg,

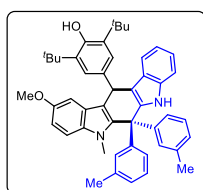


85% yield); m. p. = 247–249 °C; $R_f = 0.3$ (15% EtOAc in hexane); 1H NMR (400 MHz, DMSO- d_6) δ 10.60 (s, 1H), 7.45 (s, 1H), 7.33 (d, $J = 7.8$ Hz, 2H), 7.28 – 7.21 (m, 3H), 7.19 – 7.13 (m, 2H), 7.11 – 7.09 (m, 3H), 7.04 – 6.99 (m, 4H), 6.93 – 6.87 (m, 2H), 6.80 – 6.76 (m, 1H), 6.58 (s, 1H), 5.61 (s, 1H), 3.08 (s, 3H), 2.25 (s, 3H), 2.14 (s, 3H), 1.18 (s, 18H); ^{13}C { 1H } NMR (100 MHz, DMSO- d_6) δ 151.7, 143.4, 141.9,

139.0, 138.9, 137.9, 137.4, 137.36, 137.3, 137.1, 136.4, 129.9, 129.7, 128.3, 128.1, 127.6, 127.4, 126.8, 126.4, 125.3, 125.2, 124.6, 121.2, 120.9, 119.4, 119.0, 118.7, 118.2, 114.2, 112.1, 111.3, 109.4, 52.0, 38.6, 34.5, 31.8, 30.6, 21.52, 21.5, 21.35, 21.3; FT-IR (thin film, neat): 3643, 3432, 2953, 1460, 738 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{47}\text{H}_{49}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 657.3845; found : 657.3862.

2,6-di-*tert*-butyl-4-(2-methoxy-5-methyl-6,6-di-*m*-tolyl-5,6,7,12-tetrahydroindolo[2,3-

***b*]carbazol-12-yl)phenol (3p):** The reaction was performed at 0.079 mmol scale of **1f**; white



solid (39.8 mg, 73% yield); gummy solid; $R_f = 0.3$ (15% EtOAc in hexane);

^1H NMR (400 MHz, CDCl_3) δ 7.67 (s, 1H), 7.38 – 7.34 (m, 3H), 7.27 – 7.25

(m, 1H), 7.23 – 7.21 (m, 1H), 7.18 – 7.15 (m, 4H), 7.13 (s, 1H), 7.11 – 7.04

(m, 4H), 6.99 – 6.95 (m, 2H), 6.83 (dd, $J = 8.8, 2.5$ Hz, 1H), 5.62 (s, 1H), 4.94 (s, 1H), 3.77 (s,

3H), 3.23 (s, 3H), 2.34 (s, 3H), 2.24 (s, 3H), 1.30 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3)

δ 153.5, 152.0, 143.2, 142.6, 138.9, 138.21, 138.2, 137.8, 137.3, 135.5, 135.4, 133.6, 130.5,

129.8, 128.7, 128.2, 128.0, 127.9, 126.8, 126.7, 126.5, 126.4, 125.4, 121.6, 120.0, 119.2, 115.1,

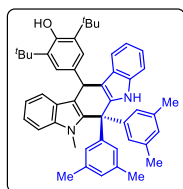
114.5, 111.6, 110.9, 109.6, 101.6, 55.8, 55.76, 52.6, 39.81, 39.8, 34.3, 32.4, 30.5, 22.0, 21.8;

FT-IR (thin film, neat): 3633, 3452, 2922, 1485, 1229, 738 cm^{-1} ; HRMS (APCI): m/z calcd for

$\text{C}_{48}\text{H}_{51}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 687.3951; found : 687.3978.

4-(6,6-bis(3,5-dimethylphenyl)-5-methyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-

***yl*)-2,6-di-*tert*-butylphenol (3q):** The reaction was performed at 0.086 mmol scale of **1a**; white



solid (53.2 mg, 90% yield); m. p. = 276–278 $^{\circ}\text{C}$; $R_f = 0.3$ (15% EtOAc in

hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.75 (s, 1H), 7.58 (d, $J = 7.8$ Hz, 1H),

7.43 (d, $J = 7.8$ Hz, 1H), 7.27 – 7.24 (m, 2H), 7.22 – 7.18 (m, 3H), 7.14 (s, 2H),

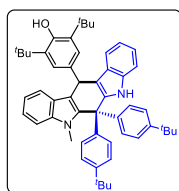
7.11 – 7.05 (m, 2H), 6.99 (t, $J = 7.4$ Hz, 1H), 6.96 (s, 1H), 6.90 – 6.87 (m, 3H), 5.68 (s, 1H),

4.93 (s, 1H), 3.28 (s, 3H), 2.30 (s, 6H), 2.22 (s, 6H), 1.29 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz,

CDCl_3) δ 151.9, 143.6, 142.6, 139.2, 138.3, 138.0, 137.8, 137.7, 137.2, 135.4, 135.3, 128.9,

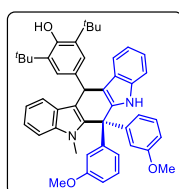
128.8, 127.6, 127.0, 126.8, 126.3, 125.3, 121.4, 121.1, 120.1, 120.0, 119.1, 118.8, 115.4, 114.4, 110.9, 108.9, 52.4, 39.7, 39.67, 34.2, 32.4, 30.5, 21.9, 21.89, 21.67, 21.66; FT-IR (thin film, neat): 3643, 3461, 2956, 1467, 738 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{49}\text{H}_{51}\text{N}_2\text{O}$ $[\text{M}-\text{H}]^-$: 683.4001; found : 683.4017.

4-(6,6-bis(4-(tert-butyl)phenyl)-5-methyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)-2,6-di-*tert*-butylphenol (3r): The reaction was performed at 0.086 mmol scale of **1a**; white



solid (39.0 mg, 61% yield); m. p. = 227–229 °C; R_f = 0.4 (15% EtOAc in hexane); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 10.66 (s, 1H), 7.56 – 7.54 (m, 2H), 7.42 – 7.37 (m, 3H), 7.34 – 7.30 (m, 3H), 7.26 (d, J = 8.3 Hz, 1H), 7.21 – 7.19 (m, 3H), 7.09 – 7.03 (m, 3H), 6.94 – 6.90 (m, 2H), 6.82 – 6.79 (m, 1H), 6.59 (s, 1H), 5.64 (s, 1H), 3.07 (s, 3H), 1.26 (s, 9H), 1.22 (s, 9H), 1.20 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, $\text{DMSO}-d_6$) δ 151.6, 148.9, 148.86, 140.3, 139.3, 138.9, 138.86, 138.8, 137.8, 137.4, 137.2, 136.5, 129.2, 128.8, 125.2, 124.9, 124.5, 121.2, 120.9, 119.3, 119.0, 118.7, 118.2, 114.2, 111.8, 111.2, 111.18, 109.2, 51.4, 38.5, 34.5, 34.2, 34.1, 31.7, 31.12, 31.1, 30.6; FT-IR (thin film, neat): 3644, 3409, 2958, 1462, 734 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{53}\text{H}_{59}\text{N}_2\text{O}$ $[\text{M}-\text{H}]^-$: 739.4627; found : 739.4635.

4-(6,6-bis(3-methoxyphenyl)-5-methyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)-2,6-di-*tert*-butylphenol (3s): The reaction was performed at 0.086 mmol scale of **1a**; white

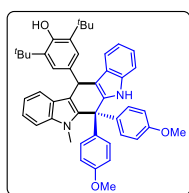


solid (45.8 mg, 77% yield); m. p. = 253–255 °C; R_f = 0.2 (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.66 (s, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.45 (d, J = 7.8 Hz, 1H), 7.29 – 7.19 (m, 5H), 7.16 – 7.14 (m, 2H), 7.12 (s, 2H), 7.10 – 7.03 (m, 2H), 6.98 (t, J = 7.4 Hz, 1H), 6.93 – 6.92 (m, 1H), 6.89 (d, J = 7.8 Hz, 1H), 6.83 – 6.80 (m, 1H), 6.77 (dd, J = 8.1, 2.2 Hz, 1H), 5.66 (s, 1H), 4.91 (s, 1H), 3.74 (s, 3H), 3.69 (s, 3H), 3.30 (s, 3H), 1.28 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 159.8, 159.7, 152.2, 145.0, 144.1, 138.45, 138.4, 137.2, 137.1, 135.4, 135.3, 129.7, 129.5, 126.7, 126.2,

125.3, 122.4, 121.8, 121.7, 121.5, 120.2, 120.1 119.3, 119.0, 116.6, 116.5, 115.7, 114.8, 111.5, 111.0, 110.9, 108.9, 55.4, 55.3, 52.5, 39.6, 34.3, 32.3, 30.5; FT-IR (thin film, neat): 3624, 3434, 2955, 1483, 736 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{47}\text{H}_{49}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$: 689.3743; found : 689.3773.

4-(6,6-bis(4-methoxyphenyl)-5-methyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)-

2,6-di-*tert*-butylphenol (3t): The reaction was performed at 0.086 mmol scale of **1a**; white

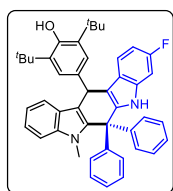


solid (48.2 mg, 81% yield); m. p. = 263–265 °C; R_f = 0.2 (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.68 (s, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.50 (d, J = 8.9 Hz, 2H), 7.46 (d, J = 7.8 Hz, 1H), 7.28 – 7.18 (m, 5H), 7.15

(s, 2H), 7.11 – 7.05 (m, 2H), 7.01 – 6.98 (m, 1H), 6.90 (d, J = 8.9 Hz, 2H), 6.82 (d, J = 8.9 Hz, 2H), 5.68 (s, 1H), 4.93 (s, 1H), 3.82 (s, 3H), 3.78 (s, 3H), 3.29 (s, 3H), 1.31 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 158.5, 158.46, 152.0, 139.4 138.3, 137.6, 137.3, 135.44, 135.4, 135.36, 134.8, 131.0, 130.3, 126.7, 126.2, 125.3, 121.6, 121.4, 120.2, 120.0, 119.3, 119.0, 115.4, 114.3, 114.1, 113.7, 110.8, 108.8, 55.44, 55.4, 51.2, 39.6, 34.3, 32.1, 30.5; FT-IR (thin film, neat): 3624, 3391, 2956, 1507, 735 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{47}\text{H}_{49}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$: 689.3743; found : 689.3766.

2,6-di-*tert*-butyl-4-(3-fluoro-7-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-

***b*]carbazol-12-yl)phenol (3u):** The reaction was performed at 0.086 mmol scale of **1a**; white

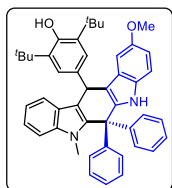


solid (36.3 mg, 65% yield); m. p. = 175–177 °C; R_f = 0.3 (15% EtOAc in hexane); ^1H NMR (400 MHz, DMSO-d_6) δ 10.76 (s, 1H), 7.59 (d, J = 7.7 Hz, 2H), 7.40 – 7.36 (m, 3H), 7.32 – 7.30 (m, 2H), 7.28 – 7.20 (m, 6H), 7.09 (s,

2H), 7.06 – 7.02 (m, 1H), 6.94 – 6.90 (m, 2H), 6.71 – 6.66 (m, 1H), 6.61 (s, 1H), 5.64 (s, 1H), 3.07 (s, 3H), 1.19 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO-d_6) δ 158.7 (d, $J_{\text{C-F}}$ = 232.2 Hz), 151.8, 142.9, 141.7, 139.5 (d, $J_{\text{C-F}}$ = 3.4 Hz), 138.9, 137.9, 137.3, 137.2, 137.0, 136.1, 129.4, 129.1, 128.5, 128.2, 127.0, 126.8, 125.2, 124.5, 119.9 (d, $J_{\text{C-F}}$ = 10.3 Hz), 119.4, 118.8, 114.2,

112.3, 109.3, 106.7 (d, $J_{C-F} = 25.4$ Hz), 97.4, 97.2, 52.1, 38.41, 38.4, 34.5, 31.7, 30.6; ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -121.6; FT-IR (thin film, neat): 3541, 3241, 2922, 1459, 738 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{45}\text{H}_{44}\text{FN}_2\text{O}$ [$\text{M}+\text{H}$] $^+$: 647.3438; found : 647.3453.

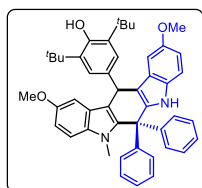
2,6-di-*tert*-butyl-4-(2-methoxy-7-methyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-12-yl)phenol (3v): The reaction was performed at 0.086 mmol scale of **1a**; white



solid (31.9 mg, 56% yield); m. p. = 248–250 °C; $R_f = 0.3$ (15% EtOAc in hexane); ^1H NMR (400 MHz, DMSO-d_6) δ 10.46 (s, 1H), 7.63 (d, $J = 7.6$ Hz, 2H), 7.40 – 7.36 (m, 2H), 7.32 – 7.30 (m, 2H), 7.28 – 7.20 (m, 6H), 7.15 (s, 2H), 7.08 – 7.02 (m, 2H), 6.92 – 6.88 (m, 1H), 6.81 (d, $J = 2.3$ Hz, 1H), 6.62 (s, 1H), 6.58 (dd, $J = 8.7, 2.4$ Hz, 1H), 5.59 (s, 1H), 3.62 (s, 3H), 3.10 (s, 3H), 1.22 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO-d_6) δ 152.7, 151.7, 143.2, 142.0, 139.4, 139.0, 137.9, 137.3, 136.4, 132.4, 129.4, 129.1, 128.4, 128.2, 126.9, 126.7, 125.5, 125.3, 124.6, 121.3, 119.3, 118.8, 114.2, 112.1, 111.9, 110.9, 109.3, 101.0, 55.1, 55.07, 52.2, 38.7, 34.5, 31.7, 30.6; FT-IR (thin film, neat): 3642, 3433, 2954, 1482, 736 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{46}\text{H}_{47}\text{N}_2\text{O}_2$ [$\text{M}+\text{H}$] $^+$: 659.3638; found : 659.3659.

2,6-di-*tert*-butyl-4-(2,10-dimethoxy-5-methyl-6,6-diphenyl-5,6,7,12-

tetrahydroindolo[2,3-*b*]carbazol-12-yl)phenol (3w): The reaction was performed at 0.086

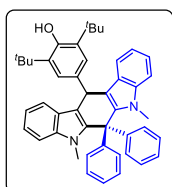


mmol scale of **1a**; white solid (45.9 mg, 84% yield); m. p. = 271–273 °C; $R_f = 0.2$ (15% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.59 – 7.56 (m, 2H), 7.51 (s, 1H), 7.38 – 7.35 (m, 4H), 7.31 – 7.23 (m, 4H), 7.20 (s, 2H), 7.11 – 7.06 (m, 2H), 6.86 (d, $J = 2.4$ Hz, 1H), 6.82 – 6.79 (m, 2H), 6.71 (dd, $J = 8.7, 2.5$ Hz, 1H), 5.57 (s, 1H), 4.96 (s, 1H), 3.72 (s, 3H), 3.70 (s, 3H), 3.23 (s, 3H), 1.31 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 153.6, 153.5, 152.0, 142.9, 142.6, 139.3, 137.5, 135.7, 135.4, 133.6, 132.3, 129.7, 129.3 (2C), 128.8, 128.5, 127.2, 127.1, 127.0, 126.3, 125.5, 114.9, 114.4, 111.8, 111.6, 109.6, 101.7, 101.6, 55.7, 55.6, 52.7, 39.9, 39.8, 34.3, 32.3, 30.6; FT-IR (thin film, neat):

3632, 3367, 2924, 1485, 737 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{47}\text{H}_{49}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$: 689.3743; found : 689.3766.

2,6-di-*tert*-butyl-4-(5,7-dimethyl-6,6-diphenyl-5,6,7,12-tetrahydroindolo[2,3-*b*]carbazol-

12-yl)phenol (3x): The reaction was performed at 0.086 mmol scale of **1a**; white solid (47.2

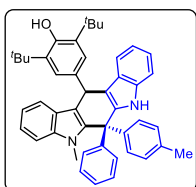


mg, 85% yield); m. p. = 195–197 °C; R_f = 0.3 (15% EtOAc in hexane); ^1H NMR (400 MHz, DMSO-d_6) δ 7.55 – 7.53 (m, 2H), 7.44 – 7.39 (m, 4H), 7.36 – 7.23 (m, 8H), 7.07 – 7.03 (m, 4H), 6.94 – 6.90 (m, 2H), 6.60 (s, 1H), 5.68 (s, 1H),

3.14 (s, 6H), 1.16 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 151.7, 142.9, 141.9, 138.92, 138.9, 138.3, 136.0, 129.2, 129.0, 128.8, 128.7, 127.2, 127.17, 125.0, 124.7, 121.4, 119.2, 118.9, 113.9, 109.5, 52.9, 38.8, 34.4, 32.4, 30.5; FT-IR (thin film, neat): 3635, 2956, 1469, 735 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{46}\text{H}_{47}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 643.3688; found : 643.3699.

2,6-di-*tert*-butyl-4-(5-methyl-6-phenyl-6-(*p*-tolyl)-5,6,7,12-tetrahydroindolo[2,3-

***b*]carbazol-12-yl)phenol (3y):** The reaction was performed at 0.086 mmol scale of **1a** and the



product was obtained as an inseparable mixture of diastereomers in the ratio of 1:1; pale yellow gummy liquid (35.5 mg, 64% yield); R_f = 0.2 (10% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.65 – 7.54 (m, 3H), 7.49 – 7.44

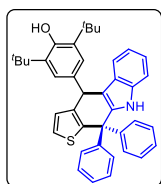
(m, 2H), 7.40 – 7.29 (m, 3H), 7.27 – 7.15 (m, 8H), 7.11 – 7.07 (m, 2H), 7.07 – 6.97 (m, 2H), 5.69 (s, 1H), 4.93 (s, 1H), 3.28 – 3.26 (m, 3H), 2.38 – 2.34 (m, 3H), 1.31 – 1.30 (m, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 152.0, 143.3, 142.6, 140.1, 139.4, 139.0, 138.8, 138.4, 138.3, 137.32, 137.31, 137.3, 137.2, 136.9, 136.85, 135.4, 135.3, 129.8, 129.7, 129.5, 129.3, 129.2, 129.17, 128.8, 128.5, 127.13, 127.12, 126.65, 126.63, 126.2, 125.3, 121.7, 121.4, 120.2, 120.1, 120.0, 119.3, 119.0, 115.5, 115.4, 114.53, 114.51, 114.4, 110.8, 108.8, 52.29, 52.27, 39.6, 34.34, 34.32, 32.22, 32.2, 30.54, 30.5, 21.1, 21.07; FT-IR (thin film, neat): 3634, 3432, 2954, 1594, 735 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{46}\text{H}_{47}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 643.3688; found : 643.3716.

7. General procedure for the synthesis of tetrahydrothieno[2,3-*b*]carbazole derivatives (5a-k): To a solution of *para*-quinone methide [**4a**] (30 mg, 1.0 equiv.) and 2-indolylmethanols [**2a-f** & **2j-n**] (1.0 equiv.) in toluene (1.5 mL), TsOH (1.0 equiv.) was added. The resulting reaction mixture was stirred at room temperature for 7 hours. After the reaction was complete (based on TLC analysis), the reaction mixture was concentrated under reduced pressure, and then the residue was purified through a silica gel column using EtOAc/Hexane mixture as an eluent to get the pure product [**5a-k**].

8. Characterization of products 5a to 5k

2,6-di-*tert*-butyl-4-(10,10-diphenyl-9,10-dihydro-4H-thieno[2,3-*b*]carbazol-4-yl)phenol

(5a): The reaction was performed at 0.10 mmol scale of **4a**; white solid (53.0 mg, 91% yield);

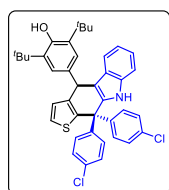


m. p. = 178–180 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.66 (s, 1H), 7.35 – 7.33 (m, 2H), 7.30 (d, J = 5.2 Hz, 1H), 7.27 – 7.21 (m, 5H), 7.19 – 7.15 (m, 2H), 7.11 – 7.09 (m, 3H), 6.96 (s, 2H), 6.94 – 6.90

(m, 1H), 6.78 – 6.75 (m, 1H), 6.70 (d, J = 5.2 Hz, 1H), 6.67 (s, 1H), 5.37 (s, 1H), 1.21 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) δ 152.1, 147.2, 146.7, 142.0, 139.8, 139.0, 137.4, 136.6, 135.7, 128.8, 128.7, 128.1, 128.0, 126.8, 126.7, 126.6, 126.1, 125.3, 124.5, 121.2, 119.1, 118.3, 112.0, 111.4, 53.6, 41.32, 41.31, 34.5, 30.5; FT-IR (thin film, neat): 3631, 3226, 2940, 1490, 735 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{40}\text{H}_{40}\text{NOS}$ [$\text{M}+\text{H}$] $^+$: 582.2831; found : 582.2828.

4-(10,10-bis(4-chlorophenyl)-9,10-dihydro-4H-thieno[2,3-*b*]carbazol-4-yl)-2,6-di-*tert*-

butylphenol (5b): The reaction was performed at 0.10 mmol scale of **4a**; white solid (55.3 mg,



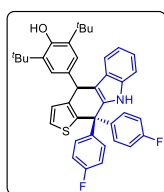
85% yield); m. p. = 246–248 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.76 (s, 1H), 7.38 – 7.35 (m, 5H), 7.32 – 7.29 (m, 2H), 7.23 – 7.21 (m, 1H), 7.14 – 7.06 (m, 3H), 6.98 – 6.94 (m, 1H), 6.89 – 6.88 (m,

2H), 6.82 – 6.79 (m, 1H), 6.76 (d, J = 5.2 Hz, 1H), 6.684 – 6.68 (m, 1H), 5.40 – 5.39 (m, 1H), 1.19 – 1.18 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) δ 152.1, 145.6, 145.0, 141.0, 140.4,

139.0, 137.4, 135.9, 135.3, 131.73, 131.7, 130.44, 130.42, 128.2, 128.1, 127.1, 126.5, 125.2, 124.3, 121.5, 119.2, 118.5, 112.5, 111.4, 52.7, 41.2, 34.5, 30.4; FT-IR (thin film, neat): 3633, 3443, 2923, 1487, 742 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{40}\text{H}_{38}\text{Cl}_2\text{NOS}$ $[\text{M}+\text{H}]^+$: 650.2051; found : 650.2074.

4-(10,10-bis(4-fluorophenyl)-9,10-dihydro-4H-thieno[2,3-b]carbazol-4-yl)-2,6-di-tert-

butylphenol (5c): The reaction was performed at 0.10 mmol scale of **4a**; white solid (53.1 mg,

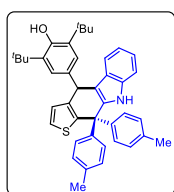


86% yield); gummy solid; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO-d_6) δ 10.74 (s, 1H), 7.38 – 7.31 (m, 3H), 7.21 (d, J = 8.0 Hz, 1H), 7.15 – 7.08 (m, 7H), 6.95 (t, J = 7.4 Hz, 1H), 6.90 – 6.87 (m, 2H), 6.81 – 6.78

(m, 1H), 6.76 – 6.72 (m, 1H), 6.68 – 6.65 (m, 1H), 5.38 (s, 1H), 1.19 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 161.0 (d, $J_{\text{C-F}}$ = 242.8 Hz), 160.9 (d, $J_{\text{C-F}}$ = 242.4 Hz), 152.1, 143.2 (d, $J_{\text{C-F}}$ = 3.2 Hz), 142.6 (d, $J_{\text{C-F}}$ = 2.9 Hz), 141.8, 140.1, 139.0, 137.4, 136.5, 135.4, 130.6, 130.5, 127.0, 126.4, 125.2, 124.3, 121.4, 119.2, 118.5, 114.92 (d, $J_{\text{C-F}}$ = 21.2 Hz), 114.87 (d, $J_{\text{C-F}}$ = 21.1 Hz), 112.2, 111.4, 52.5, 41.2, 34.5, 30.4; $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ – 116.03, –116.16; FT-IR (thin film, neat): 3643, 3463, 2922, 1504, 740 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{40}\text{H}_{36}\text{F}_2\text{NOS}$ $[\text{M}-\text{H}]^-$: 616.2486; found : 616.2504.

2,6-di-tert-butyl-4-(10,10-di-*p*-tolyl-9,10-dihydro-4H-thieno[2,3-*b*]carbazol-4-yl)phenol

(5d): The reaction was performed at 0.10 mmol scale of **4a**; white solid (48.8 mg, 80% yield);



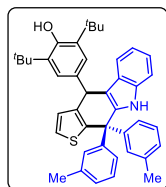
m. p. = 195–197 $^\circ\text{C}$; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO-d_6) δ 10.58 (s, 1H), 7.29 (d, J = 5.2 Hz, 1H), 7.22 – 7.18 (m, 3H), 7.10 – 7.05 (m, 5H), 6.99 – 6.97 (m, 2H), 6.95 – 6.90 (m, 3H), 6.78 – 6.75 (m, 1H),

6.69 (d, J = 5.2 Hz, 1H), 6.66 (s, 1H), 5.35 (s, 1H), 2.22 (s, 3H), 2.21 (s, 3H), 1.21 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 152.0, 144.4, 143.9, 142.5, 139.6, 138.9, 137.3, 137.1, 135.73, 135.7, 135.66, 128.7, 128.6, 128.56, 128.5, 126.8, 125.8, 125.3, 124.4, 121.1, 119.0, 118.2, 111.7, 111.3, 52.9, 41.31, 41.3, 34.5, 30.5, 20.6, 20.5; FT-IR (thin film, neat): 3644,

3462, 2923, 1457, 738 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{42}\text{H}_{44}\text{NOS}$ $[\text{M}+\text{H}]^+$: 610.3144; found : 610.3147.

2,6-di-*tert*-butyl-4-(10,10-di-*m*-tolyl-9,10-dihydro-4H-thieno[2,3-*b*]carbazol-4-yl)phenol

(5e): The reaction was performed at 0.10 mmol scale of **4a**; white solid (47.0 mg, 77% yield);



m. p. = 205–207 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz,

DMSO-d_6) δ 10.62 (s, 1H), 7.28 (d, J = 5.2 Hz, 1H), 7.19 (d, J = 8.0 Hz, 1H),

7.15 – 7.10 (m, 4H), 7.09 – 6.98 (m, 3H), 6.96 (m, 2H), 6.93 – 6.89 (m, 3H),

6.75 (t, J = 7.3 Hz, 1H), 6.67 – 6.66 (m, 2H), 5.34 (s, 1H), 2.17 (s, 3H), 2.14 (s, 3H), 1.21 (s,

18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 152.0, 147.4, 146.8, 142.1, 139.7, 139.0 (2C),

137.4, 137.0, 136.9, 136.7, 135.8, 129.33, 129.3, 129.2, 127.9, 127.3, 126.8, 126.1, 125.9,

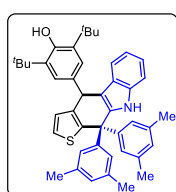
125.3, 124.5, 121.1, 119.15, 119.1, 118.3, 111.8, 111.4, 53.5, 41.34, 41.33, 34.5, 30.5, 21.45,

21.43, 21.36, 21.34; FT-IR (thin film, neat): 3643, 3459, 2923, 1484, 738 cm^{-1} ; HRMS (ESI):

m/z calcd for $\text{C}_{42}\text{H}_{44}\text{NOS}$ $[\text{M}+\text{H}]^+$: 610.3144; found : 610.3138.

4-(10,10-bis(3,5-dimethylphenyl)-9,10-dihydro-4H-thieno[2,3-*b*]carbazol-4-yl)-2,6-di-

***tert*-butylphenol (5f):** The reaction was performed at 0.10 mmol scale of **4a**; white solid (45.9



mg, 72% yield); gummy solid; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400

MHz, DMSO-d_6) δ 10.57 (s, 1H), 7.31 (d, J = 5.2 Hz, 1H), 7.20 (d, J = 8.0 Hz,

1H), 7.01 (d, J = 8.0 Hz, 1H), 6.97 (s, 2H), 6.94 – 6.91 (m, 3H), 6.86 (s, 1H),

6.80 (s, 1H), 6.77 – 6.74 (m, 1H), 6.69 – 6.68 (m, 3H), 6.66 (d, J = 5.2 Hz, 1H), 5.32 (s, 1H),

2.15 (s, 6H), 2.12 (s, 6H), 1.21 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 152.0, 147.6,

147.0, 142.1, 139.6, 139.0, 137.3, 136.8, 136.71, 136.69, 135.8, 128.1, 128.0, 126.7, 126.51,

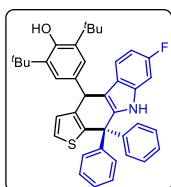
126.46, 125.8, 125.3, 124.5, 121.1, 119.1, 118.2, 111.6, 111.4, 53.3, 41.3, 34.5, 30.5, 21.34,

21.32, 21.25, 21.23; FT-IR (thin film, neat): 3646, 3433, 2922, 1458, 740 cm^{-1} ; HRMS (ESI):

m/z calcd for $\text{C}_{44}\text{H}_{48}\text{NOS}$ $[\text{M}+\text{H}]^+$: 638.3457; found : 638.3468.

2,6-di-tert-butyl-4-(7-fluoro-10,10-diphenyl-9,10-dihydro-4H-thieno[2,3-b]carbazol-4-

yl)phenol (5g): The reaction was performed at 0.10 mmol scale of **4a**; white solid (49.2 mg,

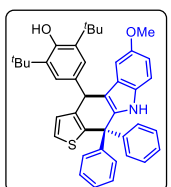


82% yield); m. p. = 115–117 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR

(400 MHz, DMSO- d_6) δ 10.81 (s, 1H), 7.37 (d, J = 5.2 Hz, 1H), 7.35 – 7.29 (m, 6H), 7.27 – 7.21 (m, 2H), 7.13 – 7.11 (m, 2H), 7.06 – 7.03 (m, 1H), 6.97 – 6.93 (m, 3H), 6.74 (d, J = 5.2 Hz, 1H), 6.72 – 6.66 (m, 2H), 5.39 (s, 1H), 1.23 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) δ 158.8 (d, $J_{\text{C-F}}$ = 233.1 Hz), 152.1, 147.0, 146.5, 141.8, 139.7, 139.1, 137.4, 137.3 (d, $J_{\text{C-F}}$ = 3.7 Hz), 135.4, 128.7, 128.6, 128.13, 128.1, 126.8, 126.7, 126.2, 124.4, 122.1, 120.0 (d, $J_{\text{C-F}}$ = 10.1 Hz), 112.1, 106.7 (d, $J_{\text{C-F}}$ = 24.3 Hz), 97.5, 97.3, 53.5, 41.1, 41.0, 34.5, 30.5; ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ –121.4; FT-IR (thin film, neat): 3643, 3463, 2922, 1460, 730 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{40}\text{H}_{37}\text{FNOS}$ [M-H] $^-$: 598.2580; found : 598.2604.

2,6-di-tert-butyl-4-(6-methoxy-10,10-diphenyl-9,10-dihydro-4H-thieno[2,3-b]carbazol-4-

yl)phenol (5h): The reaction was performed at 0.10 mmol scale of **4a**; white solid (45.2 mg,

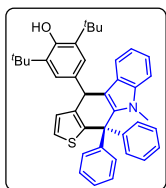


74% yield); gummy solid; R_f = 0.5 (10% EtOAc in hexane); ^1H NMR (400 MHz,

DMSO- d_6) δ 10.50 (s, 1H), 7.37 – 7.34 (m, 3H), 7.32 – 7.30 (m, 2H), 7.28 – 7.24 (m, 3H), 7.22 – 7.18 (m, 1H), 7.12 – 7.09 (m, 3H), 7.02 (s, 2H), 6.71 (s, 1H), 6.66 (d, J = 5.2 Hz, 1H), 6.62 – 6.60 (m, 2H), 5.33 (s, 1H), 3.57 (s, 3H), 1.25 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) δ 152.7, 152.0, 147.3, 146.8, 142.2, 139.9, 139.0, 136.9, 135.7, 132.4, 128.8, 128.6, 128.03, 128.0, 126.9, 126.6, 126.1, 125.6, 124.6, 112.1, 112.01, 112.0, 111.0, 101.2, 55.1, 55.0, 53.6, 41.5, 34.5, 30.5; FT-IR (thin film, neat): 3674, 3445, 2924, 1485, 737 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{41}\text{H}_{42}\text{NO}_2\text{S}$ [M+H] $^+$: 612.2936; found : 612.2931.

2,6-di-tert-butyl-4-(9-methyl-10,10-diphenyl-9,10-dihydro-4H-thieno[2,3-b]carbazol-4-

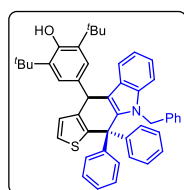
yl)phenol (5i): The reaction was performed at 0.10 mmol scale of **4a**; white solid (41.1 mg,



69% yield); m. p. = 253–255 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.59 – 7.57 (m, 2H), 7.41 – 7.38 (m, 3H), 7.36 – 7.32 (m, 2H), 7.30 – 7.26 (m, 3H), 7.24 – 7.15 (m, 3H), 7.09 (d, J = 5.2 Hz, 1H), 7.04 – 7.00 (m, 3H), 6.72 (d, J = 5.2 Hz, 1H), 5.47 (s, 1H), 4.97 (s, 1H), 3.15 (s, 3H), 1.30 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 152.2, 145.7, 145.3, 143.7, 138.8, 138.4, 137.9, 135.6, 135.2, 129.9, 129.8, 128.3, 128.1, 126.93, 126.9, 126.5, 125.8, 125.2, 125.0, 121.6, 120.2, 119.0, 113.9, 108.9, 54.2, 42.32, 42.3, 34.4, 32.1, 30.5; FT-IR (thin film, neat): 3635, 2923, 1469, 738 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{41}\text{H}_{42}\text{NOS}$ [$\text{M}+\text{H}$] $^+$: 596.2987; found : 596.2976.

4-(9-benzyl-10,10-diphenyl-9,10-dihydro-4H-thieno[2,3-*b*]carbazol-4-yl)-2,6-di-*tert*-

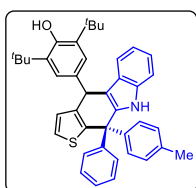
butylphenol (5j): The reaction was performed at 0.10 mmol scale of **4a**; white solid (22.2 mg,



33% yield); m. p. = 215–217 °C; R_f = 0.5 (10% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 7.54 (d, J = 7.2 Hz, 2H), 7.39 – 7.35 (m, 3H), 7.20 – 7.13 (m, 3H), 7.11 – 7.08 (m, 5H), 7.05 – 6.97 (m, 4H), 6.91 – 6.88 (m, 3H), 6.77 (d, J = 5.3 Hz, 1H), 6.25 (d, J = 7.4 Hz, 2H), 5.56 (s, 1H), 5.16 – 5.04 (m, 2H), 5.03 (s, 1H), 1.36 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 152.3, 145.8, 144.5, 143.7, 138.4, 138.2, 138.1, 137.1, 135.7, 135.3, 129.9, 129.7, 128.2, 128.1, 127.8, 126.8, 126.7, 126.3, 126.2, 126.1, 125.4, 125.3, 125.2, 122.0, 120.3, 119.4, 113.7, 110.4, 54.3, 49.1, 42.15, 42.13, 34.4, 30.5; FT-IR (thin film, neat): 3634, 2957, 1465, 732 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{47}\text{H}_{46}\text{NOS}$ [$\text{M}+\text{H}$] $^+$: 672.3300; found : 672.3315.

2,6-di-*tert*-butyl-4-(10-phenyl-10-(*p*-tolyl)-9,10-dihydro-4H-thieno[2,3-*b*]carbazol-4-

yl)phenol (5k): The reaction was performed at 0.10 mmol scale of **4a** and the product was



obtained as an inseparable mixture of diastereomers in the ratio of 1:1; pale yellow gummy liquid (50.0 mg, 84% yield); R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 10.62 (s, 1H), 7.33 – 7.31 (m, 2H), 7.27 – 7.17 (m, 5H), 7.10 – 7.05 (m, 4H), 6.98 – 6.90 (m, 4H), 6.78 – 6.75 (m, 1H), 6.70 – 6.68 (m,

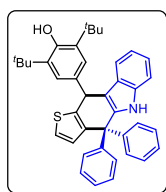
1H), 6.67 (s, 1H), 5.36 – 5.35 (m, 1H), 2.22– 2.21 (m, 3H), 1.20 (s, 18H); ¹³C {¹H} NMR (100 MHz, DMSO-d₆) δ 152.0, 147.3, 146.8, 144.4, 143.7, 142.28, 142.26, 139.77, 139.73, 139.0, 138.97, 137.4, 136.91, 136.9, 135.83, 135.8, 135.7, 128.8, 128.7, 128.63, 128.61, 128.6, 128.05, 128.0, 126.83, 126.81, 126.7, 126.6, 126.0, 125.3, 124.4, 121.1, 119.1, 118.3, 111.9, 111.3, 53.2, 41.3, 41.27, 34.5, 30.5, 20.6; FT-IR (thin film, neat): 3633, 3224, 2942, 1493, 737 cm⁻¹; HRMS (ESI): *m/z* calcd for C₄₁H₄₂NOS [M+H]⁺ : 596.2987; found : 596.2985.

9. General procedure for the synthesis of tetrahydrothieno[3,2-*b*]carbazole derivatives (7a-k): *Para*-quinone methide [6a-c] (30 mg, 1.0 equiv.) and 2-indolylmethanols [2a-e, 2i-k & 2n] (1.0 equiv.) were dissolved in acetonitrile (1.5 mL) and, then TsOH (1.0 equiv.) was added to it. The resulting reaction mixture was stirred at room temperature for an hour. The residue was then concentrated under reduced pressure, and the residue was then purified through a silica gel column using EtOAc/Hexane mixture as an eluent to get the pure products [7a-k].

10. Characterization of products 7a to 7k

2,6-di-*tert*-butyl-4-(4,4-diphenyl-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-yl)phenol

(7a): The reaction was performed at 0.10 mmol scale of 6a; white solid (51.2 mg, 88% yield);

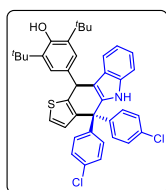


gummy solid; *R_f* = 0.6 (10% EtOAc in hexane); ¹H NMR (400 MHz, DMSO-d₆) δ 10.64 (s, 1H), 7.34 – 7.26 (m, 7H), 7.25 – 7.18 (m, 3H), 7.16 – 7.11 (m, 3H), 7.02 (s, 2H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.81 (t, *J* = 7.5 Hz, 1H), 6.75 (s, 1H),

6.68 (d, *J* = 5.3 Hz, 1H), 5.61 (s, 1H), 1.24 (s, 18H); ¹³C {¹H} NMR (100 MHz, DMSO-d₆) δ 152.3, 146.3, 146.0, 141.3, 139.3, 139.0 (2C), 137.4, 137.3, 136.4, 128.8 (2C), 128.1 (2C), 127.3, 126.4, 125.0, 124.9, 124.2, 121.1, 119.1, 118.3, 111.4, 111.3, 53.4, 40.9, 40.88, 34.5, 30.5; FT-IR (thin film, neat): 3637, 3457, 2923, 1488, 738 cm⁻¹; HRMS (ESI): *m/z* calcd for C₄₀H₄₀NOS [M+H]⁺ : 582.2831; found : 582.2820.

4-(4,4-bis(4-chlorophenyl)-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-yl)-2,6-di-*tert*-

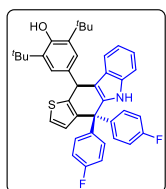
butylphenol (7b): The reaction was performed at 0.10 mmol scale of **6a**; white solid (47.5 mg,



73% yield); m. p. = 236–238 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.72 (s, 1H), 7.39 – 7.36 (m, 5H), 7.31 – 7.28 (m, 2H), 7.24 (d, J = 8.1 Hz, 1H), 7.18 (d, J = 7.9 Hz, 1H), 7.08 (d, J = 8.6 Hz, 2H), 7.01 – 6.97 (m, 1H), 6.94 (s, 2H), 6.84 (t, J = 7.4 Hz, 1H), 6.75 (s, 1H), 6.69 (d, J = 5.3 Hz, 1H), 5.62 (s, 1H), 1.22 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) δ 152.3, 144.9, 144.4, 141.9, 139.0, 138.6, 137.4, 136.6, 136.1, 131.5, 131.4, 130.6, 130.5, 128.2, 128.1, 126.9, 125.3, 125.0, 124.1, 121.4, 119.1, 118.5, 111.8, 111.4, 52.6, 40.75, 40.73, 34.5, 30.4; FT-IR (thin film, neat): 3638, 3457, 2923, 1489, 739 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{40}\text{H}_{36}\text{Cl}_2\text{NOS}$ [$\text{M}-\text{H}$] $^-$: 648.1895; found : 648.1915.

4-(4,4-bis(4-fluorophenyl)-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-yl)-2,6-di-*tert*-

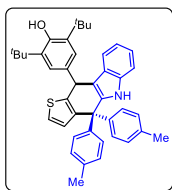
butylphenol (7c): The reaction was performed at 0.10 mmol scale of **6a**; white solid (47.0 mg,



73% yield); gummy solid; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.70 (s, 1H), 7.34 – 7.30 (m, 3H), 7.24 (d, J = 8.1 Hz, 1H), 7.17 – 7.14 (m, 2H), 7.13 – 7.07 (m, 5H), 6.98 (d, J = 7.4 Hz, 1H), 6.96 (s, 2H), 6.83 (t, J = 7.5 Hz, 1H), 6.75 (s, 1H), 6.68 (d, J = 5.3 Hz, 1H), 5.60 (s, 1H), 1.22 (s, 18H); ^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) δ 160.8 (d, $J_{\text{C-F}}$ = 242.2 Hz), 152.3, 142.4 (d, $J_{\text{C-F}}$ = 3.0 Hz), 142.0 (d, $J_{\text{C-F}}$ = 3.0 Hz), 141.6, 139.2, 139.0, 137.4, 137.2, 136.2, 130.73, 130.7, 130.6, 127.0, 125.2, 125.0, 124.1, 121.3, 119.1, 118.5, 114.9 (d, $J_{\text{C-F}}$ = 21.0 Hz), 114.8 (d, $J_{\text{C-F}}$ = 21.2 Hz), 111.5, 114.4, 52.3, 40.8, 40.78, 34.5, 30.4; ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -116.44, -116.48; FT-IR (thin film, neat): 3649, 3458, 2921, 1459, 741 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{40}\text{H}_{38}\text{F}_2\text{NOS}$ [$\text{M}+\text{H}$] $^+$: 618.2642; found : 618.2635.

2,6-di-*tert*-butyl-4-(4,4-di-*p*-tolyl-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-yl)phenol

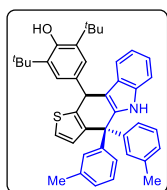
(7d): The reaction was performed at 0.10 mmol scale of **6a**; white solid (43.9 mg, 72% yield);



m. p. = 197–199 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.56 (s, 1H), 7.27 (d, J = 5.3 Hz, 1H), 7.23 – 7.20 (m, 2H), 7.18 (s, 1H), 7.13 (d, J = 7.9 Hz, 1H), 7.07 (d, J = 7.9 Hz, 4H), 7.00 – 6.93 (m, 5H), 6.80 (t, J = 7.5 Hz, 1H), 6.73 (s, 1H), 6.64 (d, J = 5.3 Hz, 1H), 5.57 (s, 1H), 2.24 (s, 3H), 2.23 (s, 3H), 1.23 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 152.2, 143.5, 143.2, 141.1, 139.8, 139.0, 137.9, 137.3, 136.4, 135.5, 135.4, 128.75, 128.7, 128.6, 127.3, 125.1, 124.6, 124.2, 121.0, 119.0, 118.2, 111.3 (2C), 111.1, 52.7, 40.9, 40.88, 34.5, 30.4, 20.52, 20.51; FT-IR (thin film, neat): 3640, 3457, 2922, 1457, 738 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{42}\text{H}_{44}\text{NOS}$ $[\text{M}+\text{H}]^+$: 610.3144; found : 610.3157.

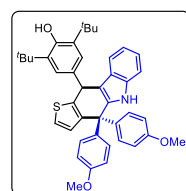
2,6-di-tert-butyl-4-(4,4-di-*m*-tolyl-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-yl)phenol

(7e): The reaction was performed at 0.10 mmol scale of **6a**; white solid (53.0 mg, 87% yield);



m. p. = 205–207 °C; R_f = 0.6 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.61 (s, 1H), 7.28 (d, J = 5.3 Hz, 1H), 7.23 (d, J = 8.1 Hz, 1H), 7.19 – 7.13 (m, 3H), 7.12 – 7.10 (m, 2H), 7.05 – 7.03 (m, 3H), 7.01 (d, J = 7.6 Hz, 1H), 6.95 (t, J = 7.4 Hz, 1H), 6.92 – 6.90 (m, 2H), 6.80 (t, J = 7.5 Hz, 1H), 6.75 (s, 1H), 6.69 (d, J = 5.3 Hz, 1H), 5.58 (s, 1H), 2.21 (s, 3H), 2.18 (s, 3H), 1.25 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 152.3, 146.5, 146.1, 141.3, 139.3, 139.0, 137.5, 137.3, 136.9 (2C), 136.4, 129.4, 129.3, 127.9, 127.4, 127.12, 127.1, 126.13, 126.1, 125.0, 124.7, 124.6, 124.2, 121.1, 119.1, 118.2, 111.4, 111.1, 53.3, 40.95, 40.93, 34.5, 30.5, 21.41, 21.4, 21.33, 21.31; FT-IR (thin film, neat): 3638, 3458, 2922, 1457, 739 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{42}\text{H}_{44}\text{NOS}$ $[\text{M}+\text{H}]^+$: 610.3144; found : 610.3148.

4-(4,4-bis(3-methoxyphenyl)-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-yl)-2,6-di-tert-

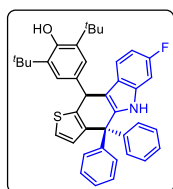


butylphenol (7f): The reaction was performed at 0.10 mmol scale of **6a**; white solid (44.3 mg, 69% yield); gummy solid; R_f = 0.4 (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.58 (s, 1H), 7.29 (d, J = 5.3 Hz, 1H), 7.23

– 7.20 (m, 3H), 7.14 (d, $J = 8.0$ Hz, 1H), 7.02 – 6.99 (m, 4H), 6.95 (t, $J = 7.7$ Hz, 1H), 6.85 – 6.82 (m, 4H), 6.80 (d, $J = 7.2$ Hz, 1H), 6.73 (s, 1H), 6.64 (d, $J = 5.3$ Hz, 1H), 5.56 (s, 1H), 3.694 (s, 3H), 3.691 (s, 3H), 1.23 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 157.7, 157.6, 152.2, 140.8, 140.2, 139.0, 138.6, 138.3, 138.2, 137.3, 136.4, 129.9, 129.8, 127.3, 125.1, 124.65, 124.6, 124.2, 121.0, 119.0, 118.2, 113.4, 111.3, 110.9, 55.1, 55.07, 52.0, 40.89, 40.87, 34.5, 30.4; FT-IR (thin film, neat): 3626, 3455, 2922, 1458, 738 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{42}\text{H}_{44}\text{NO}_3\text{S}$ $[\text{M}+\text{H}]^+$: 642.3042; found : 642.3058.

2,6-di-*tert*-butyl-4-(7-fluoro-4,4-diphenyl-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-

yl)phenol (7g): The reaction was performed at 0.10 mmol scale of **6a**; white solid (39.0 mg,

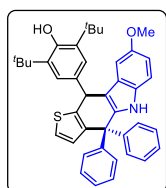


65% yield); gummy solid; $R_f = 0.6$ (10% EtOAc in hexane); ^1H NMR (400 MHz, DMSO- d_6) δ 10.76 (s, 1H), 7.30 – 7.29 (m, 6H), 7.26 (s, 1H), 7.25 – 7.19 (m, 2H), 7.11 (d, $J = 7.6$ Hz, 2H), 7.09 – 7.05 (m, 1H), 7.00 (s, 2H), 6.98 – 6.95

(m, 1H), 6.76 (s, 1H), 6.72 – 6.66 (m, 2H), 5.60 (s, 1H), 1.24 (s, 18H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) δ 158.7 (d, $J_{\text{C-F}} = 232.8$ Hz), 152.3, 146.1, 145.8, 141.2, 139.12, 139.1, 138.1 (d, $J_{\text{C-F}} = 3.4$ Hz), 137.3 (d, $J_{\text{C-F}} = 12.7$ Hz), 136.1, 128.8, 128.77, 128.1, 127.2, 126.5, 124.9, 124.2, 121.9, 119.9, 111.4, 106.7 (d, $J_{\text{C-F}} = 24.4$ Hz), 106.7 (d, $J_{\text{C-F}} = 24.5$ Hz), 97.6 (d, $J_{\text{C-F}} = 1.6$ Hz), 97.3 (d, $J_{\text{C-F}} = 1.5$ Hz), 53.4, 40.7, 40.68, 34.5, 30.5; $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ –121.47; FT-IR (thin film, neat): 3615, 3458, 2923, 1488, 736 cm^{-1} ; HRMS (APCI): m/z calcd for $\text{C}_{40}\text{H}_{39}\text{FNOS}$ $[\text{M}+\text{H}]^+$: 600.2736; found : 600.2725.

2,6-di-*tert*-butyl-4-(8-methoxy-4,4-diphenyl-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-

yl)phenol (7h): The reaction was performed at 0.10 mmol scale of **6a**; white solid (42.8 mg,



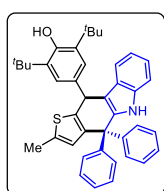
70% yield); m. p. = 246–248 $^{\circ}\text{C}$; $R_f = 0.5$ (10% EtOAc in hexane); ^1H NMR (400 MHz, CDCl_3) δ 10.46 (s, 1H), 7.35 – 7.30 (m, 5H), 7.28 – 7.24 (m, 3H), 7.23 – 7.19 (m, 1H), 7.12 – 7.10 (m, 3H), 7.05 (s, 2H), 6.76 (s, 1H), 6.69 (d, $J = 5.3$ Hz,

1H), 6.65 – 6.64 (m, 1H), 6.63 – 6.60 (m, 1H), 5.54 (s, 1H), 3.59 (s, 3H), 1.26 (s, 18H); ^{13}C

{¹H} NMR (100 MHz, CDCl₃) δ 152.7, 152.3, 146.4, 146.1, 141.3, 139.6, 139.0, 137.7, 136.4, 132.4, 128.82, 128.8, 128.06, 128.04, 127.2, 126.43, 126.4, 125.3, 124.9, 124.4, 112.0, 111.5, 110.9, 101.1, 55.12, 55.1, 53.5, 41.08, 41.04, 34.5, 30.5; FT-IR (thin film, neat): 3627, 3456, 2922, 1483, 736 cm⁻¹; HRMS (APCI): *m/z* calcd for C₄₁H₄₂NO₂S [M+H]⁺ : 612.2936; found : 612.2917.

2,6-di-*tert*-butyl-4-(2-methyl-4,4-diphenyl-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-

yl)phenol (7i): The reaction was performed at 0.095 mmol scale of **6b**; white solid (47.1 mg,



83% yield); m. p. = 273–275 °C; *R_f* = 0.6 (10% EtOAc in hexane); ¹H NMR

(400 MHz, CDCl₃) δ 7.64 (s, 1H), 7.40 – 7.38 (m, 2H), 7.34 – 7.26 (m, 8H),

7.24 – 7.21 (m, 2H), 7.10 (t, *J* = 7.2 Hz, 1H), 7.07 (s, 2H), 6.98 (t, *J* = 7.4 Hz,

1H), 6.47 (s, 1H), 5.53 (s, 1H), 5.05 (s, 1H), 2.35 (s, 3H), 1.36 (s, 18H); ¹³C {¹H} NMR (100

MHz, CDCl₃) δ 152.5, 146.2, 146.1, 140.2, 138.6, 138.4, 137.5, 137.0, 135.6, 135.5, 129.12,

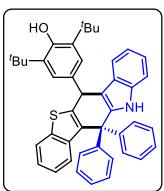
129.1, 128.43, 128.4, 126.8, 126.7, 126.3, 124.9, 124.8, 121.8, 120.1, 119.3, 113.2, 110.9, 53.8,

41.87, 41.85, 34.4, 30.5, 15.91, 15.9; FT-IR (thin film, neat): 3620, 3450, 2956, 1434, 732 cm⁻¹;

HRMS (ESI): *m/z* calcd for C₄₁H₄₂NOS [M+H]⁺ : 596.2987; found : 596.2992.

2,6-di-*tert*-butyl-4-(12,12-diphenyl-11,12-dihydro-6H-benzo[4,5]thieno[3,2-*b*]carbazol-6-

yl)phenol (7j): The reaction was performed at 0.086 mmol scale of **6c**; white solid (33.0 mg,



61% yield); gummy solid; *R_f* = 0.5 (10% EtOAc in hexane); ¹H NMR (400 MHz,

CDCl₃) δ 7.71 – 7.69 (m, 1H), 7.61 (s, 1H), 7.53 – 7.50 (m, 2H), 7.33 – 7.29 (m,

4H), 7.28 – 7.22 (m, 6H), 7.18 – 7.09 (m, 3H), 7.07 – 7.04 (m, 3H), 7.02 – 6.97

(m, 1H), 5.67 (s, 1H), 5.05 (s, 1H), 1.30 (s, 18H); ¹³C {¹H} NMR (100 MHz, CDCl₃) δ 152.8,

145.9, 143.8, 143.5, 140.3, 139.6, 138.0, 137.0, 135.9, 134.4, 132.6, 129.5, 129.4 (2C), 128.6,

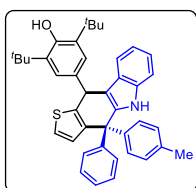
128.5, 127.1, 126.2, 125.2, 124.9, 123.4, 123.3, 122.5, 121.9, 120.0, 119.6, 112.4, 111.1, 54.1,

43.2, 43.1, 34.4, 30.4; FT-IR (thin film, neat): 3632, 3456, 2922, 1457, 739 cm⁻¹; HRMS

(APCI): *m/z* calcd for C₄₄H₄₂NOS [M+H]⁺ : 632.2987; found : 632.2999.

2,6-di-*tert*-butyl-4-(4-phenyl-4-(*p*-tolyl)-5,10-dihydro-4H-thieno[3,2-*b*]carbazol-10-

yl)phenol (**7k**): The reaction was performed at 0.10 mmol scale of **6a** and the product was



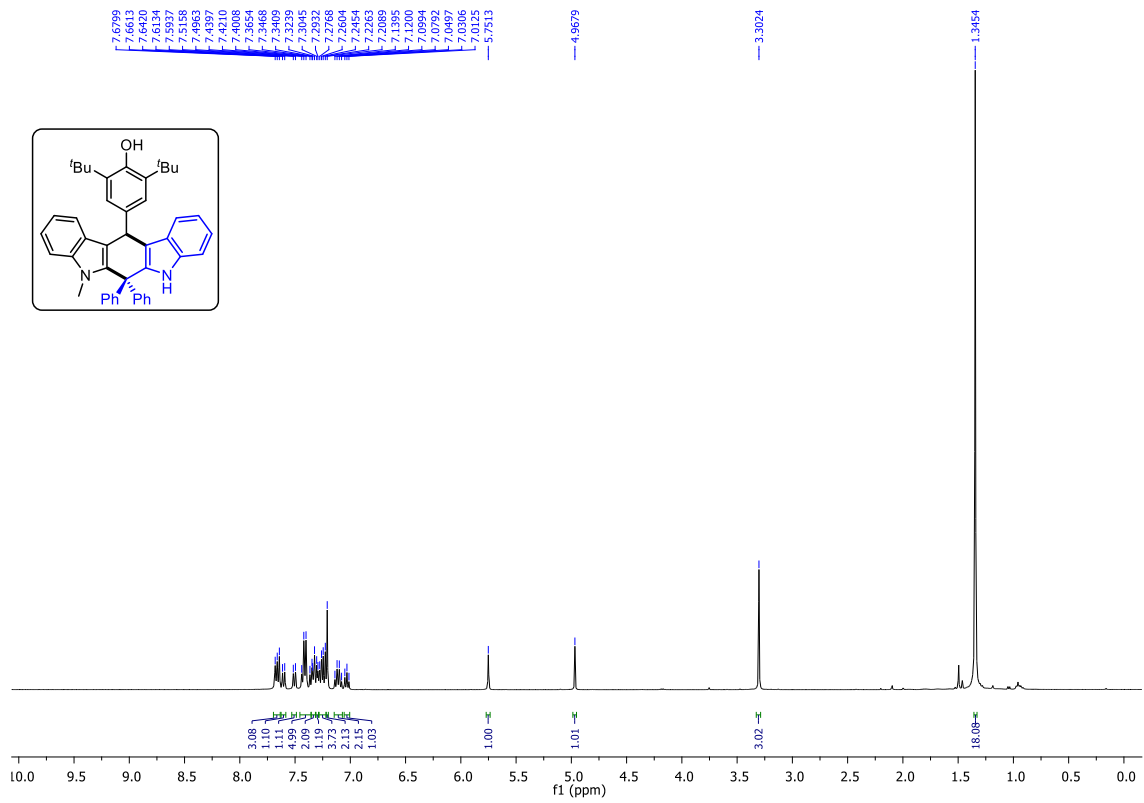
obtained as an inseparable mixture of diastereomers in the ratio of 1:1; pale yellow gummy solid (44.6 mg, 75% yield); $R_f = 0.6$ (10% EtOAc in hexane);

$^1\text{H NMR}$ (400 MHz, DMSO-d_6) δ 10.57 (s, 1H), 7.29 – 7.22 (m, 4H), 7.20 – 7.15 (m, 3H), 7.12 – 7.04 (m, 4H), 6.97 – 6.90 (m, 4H), 6.79 – 6.75 (m, 1H), 6.72 (s, 1H), 6.64 – 6.61 (m, 1H), 5.56 – 5.55 (m, 1H), 2.21 – 2.20 (m, 3H), 1.20 (s, 18H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO-d_6) δ 152.3, 146.4, 146.1, 143.4, 143.1, 141.2, 141.19, 139.6, 139.03, 139.02, 137.7, 137.6, 137.3, 136.4, 135.6, 135.5, 128.8, 128.77, 128.65, 128.1, 127.3, 126.4, 125.1, 124.8, 124.3, 121.12, 121.10, 119.1, 118.3, 111.4, 111.21, 111.2, 53.1, 40.90, 40.89, 34.5, 30.5, 20.6, 20.5; FT-IR (thin film, neat): 3635, 3454, 2920, 1484, 735 cm^{-1} ; HRMS (ESI): m/z calcd for $\text{C}_{41}\text{H}_{42}\text{NOS}$ $[\text{M}+\text{H}]^+$: 596.2987; found : 596.2994.

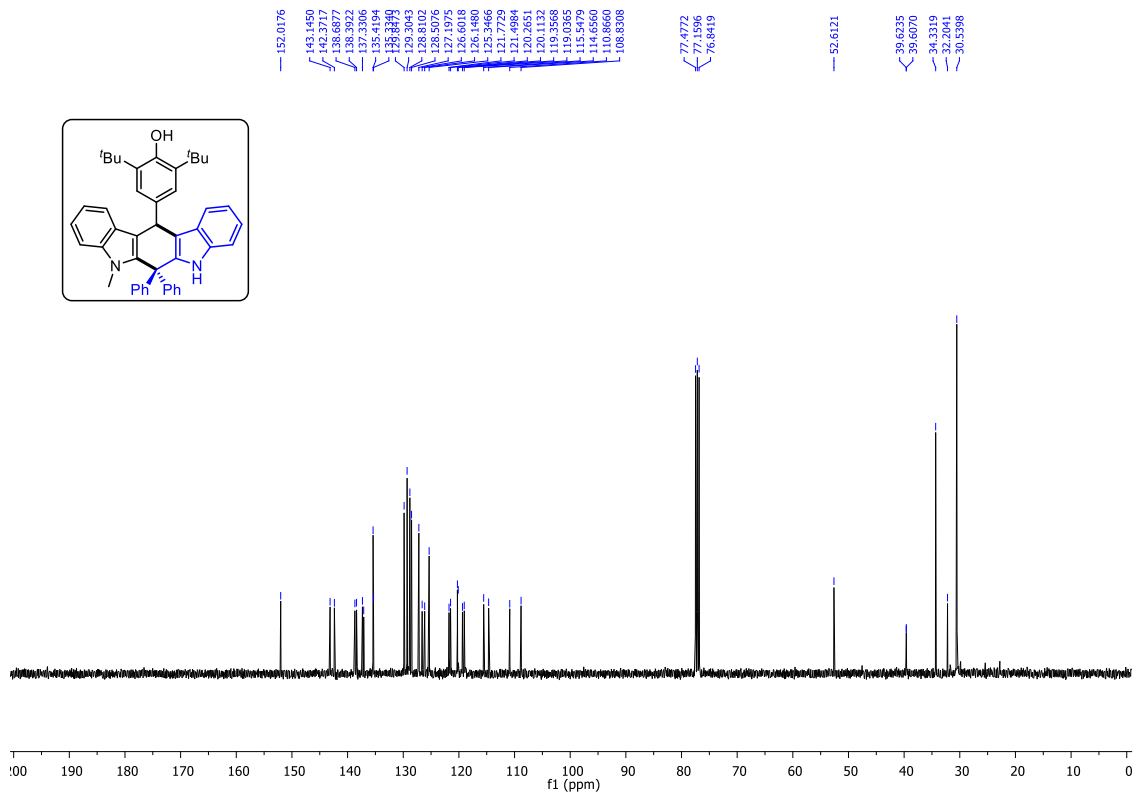
11. References:

1. T. Z. Li, S. J. Liu, Y. W. Sun, S. Deng, W. Tan, Y. Jiao, Y. C. Zhang and F. Shi, *Angew. Chemie - Int. Ed.* 2021, **60**, 2355–2363.
2. Z. Yuan, W. Wei, A. Lin and H. Yao, *Org. Lett.* 2016, **18**, 3370–3373.

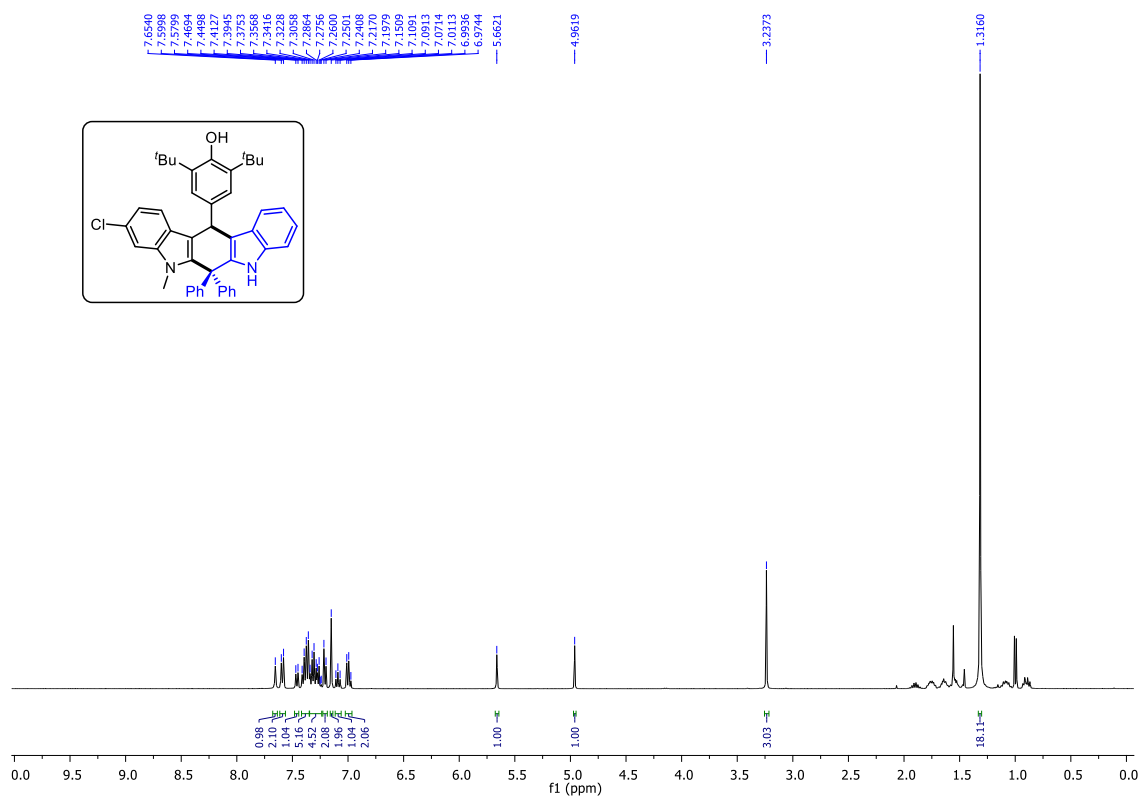
¹H NMR (400 MHz, CDCl₃) Spectrum of **3a**



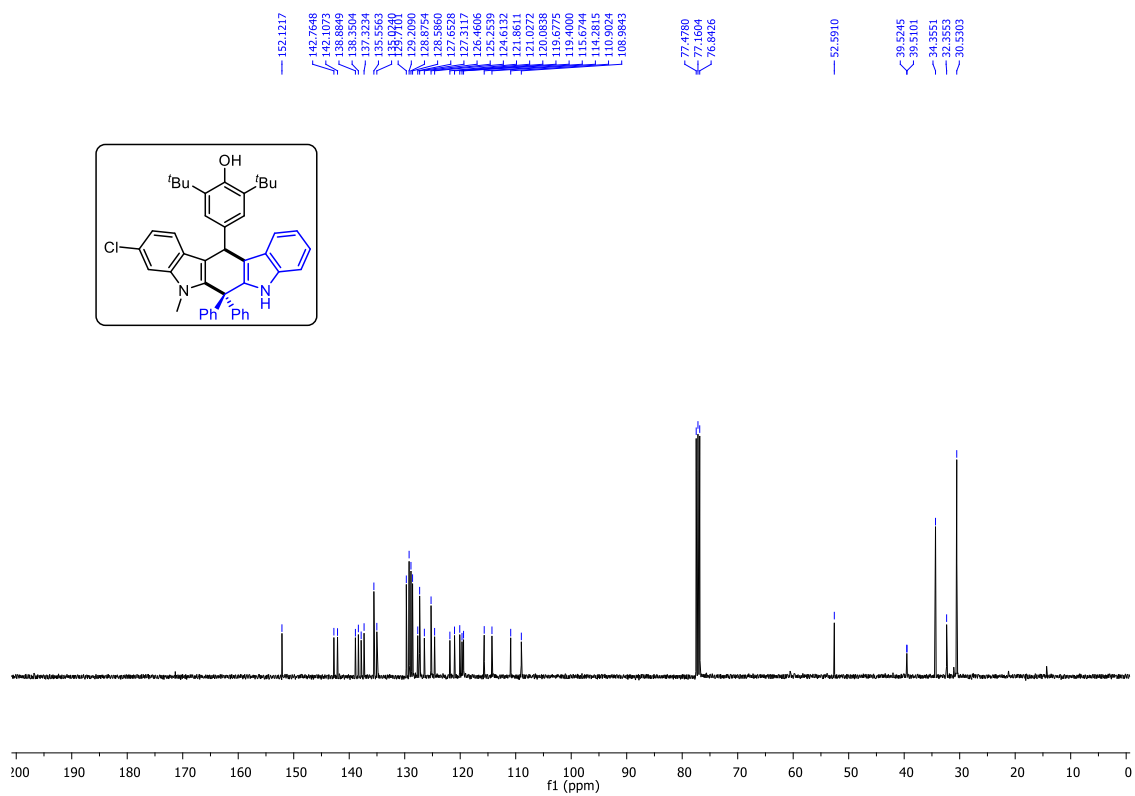
¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of **3a**



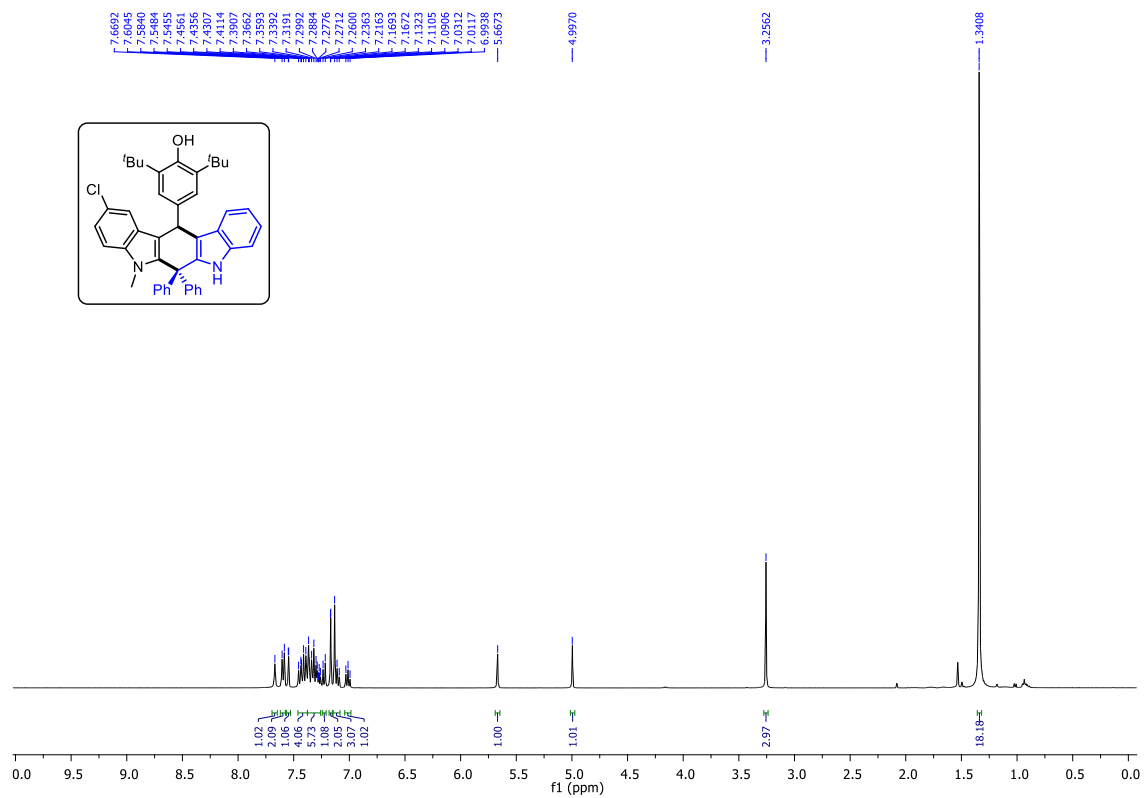
^1H NMR (400 MHz, CDCl_3) Spectrum of **3b**



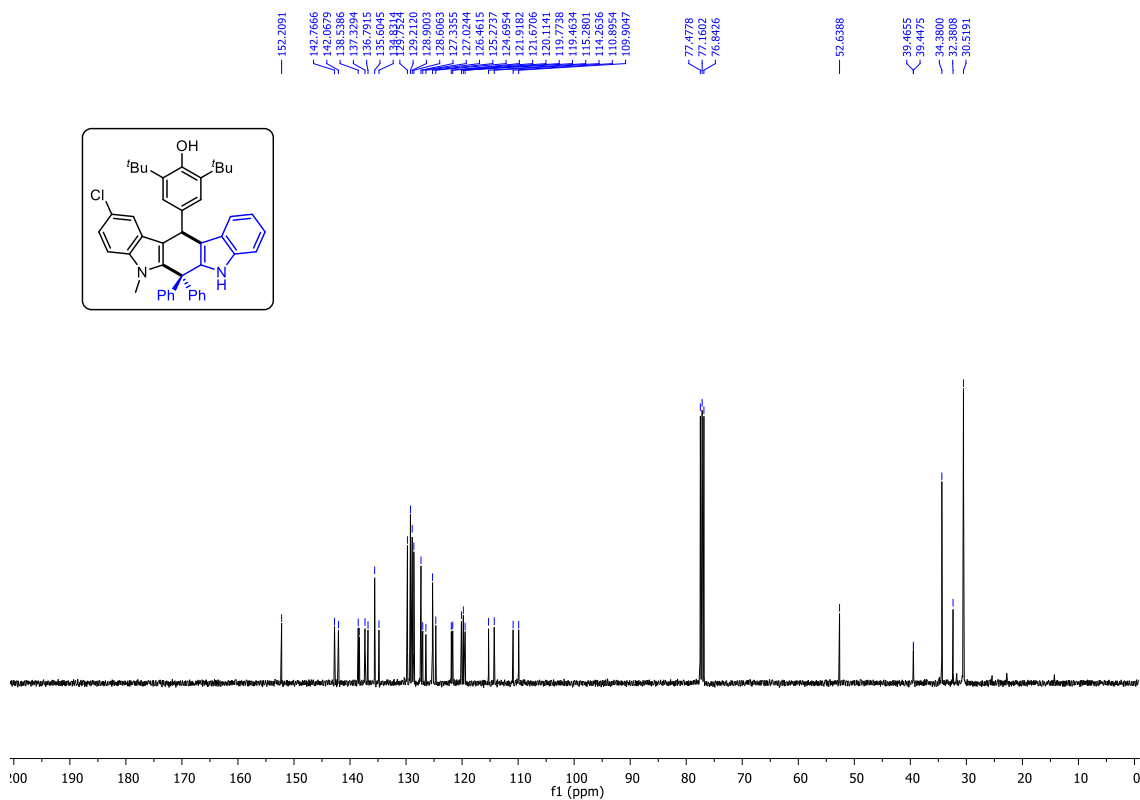
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3b**



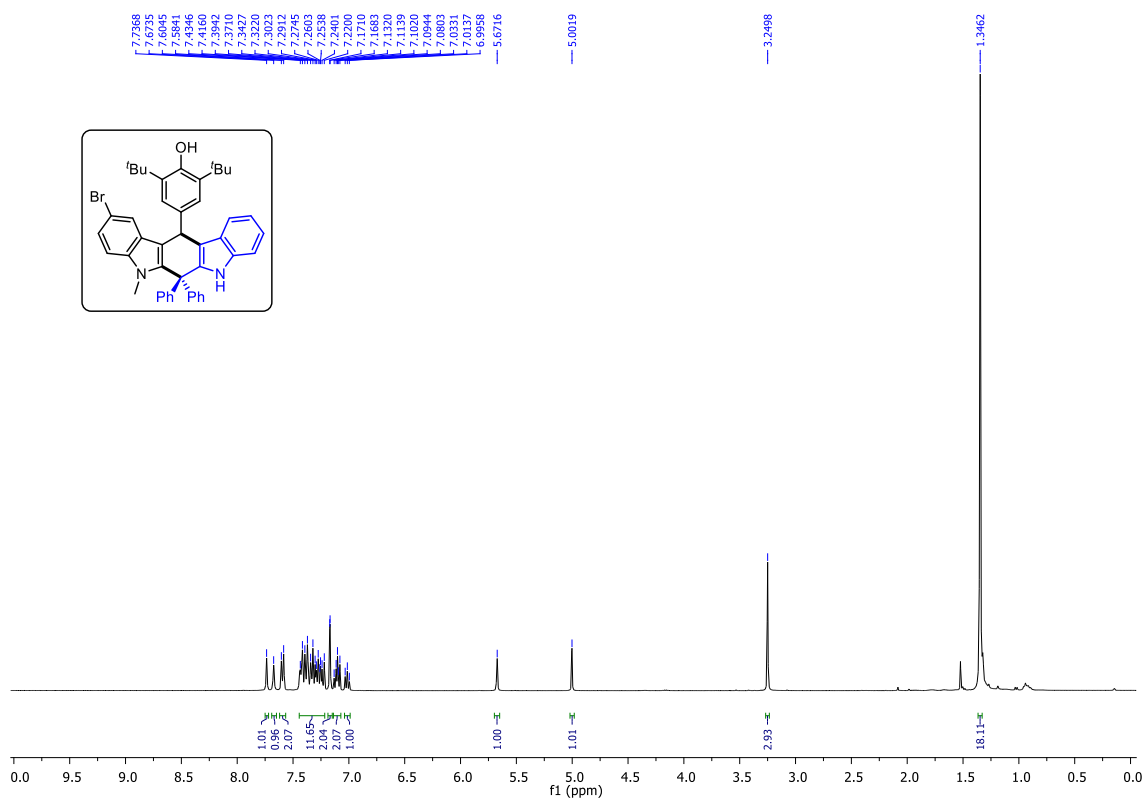
¹H NMR (400 MHz, CDCl₃) Spectrum of **3c**



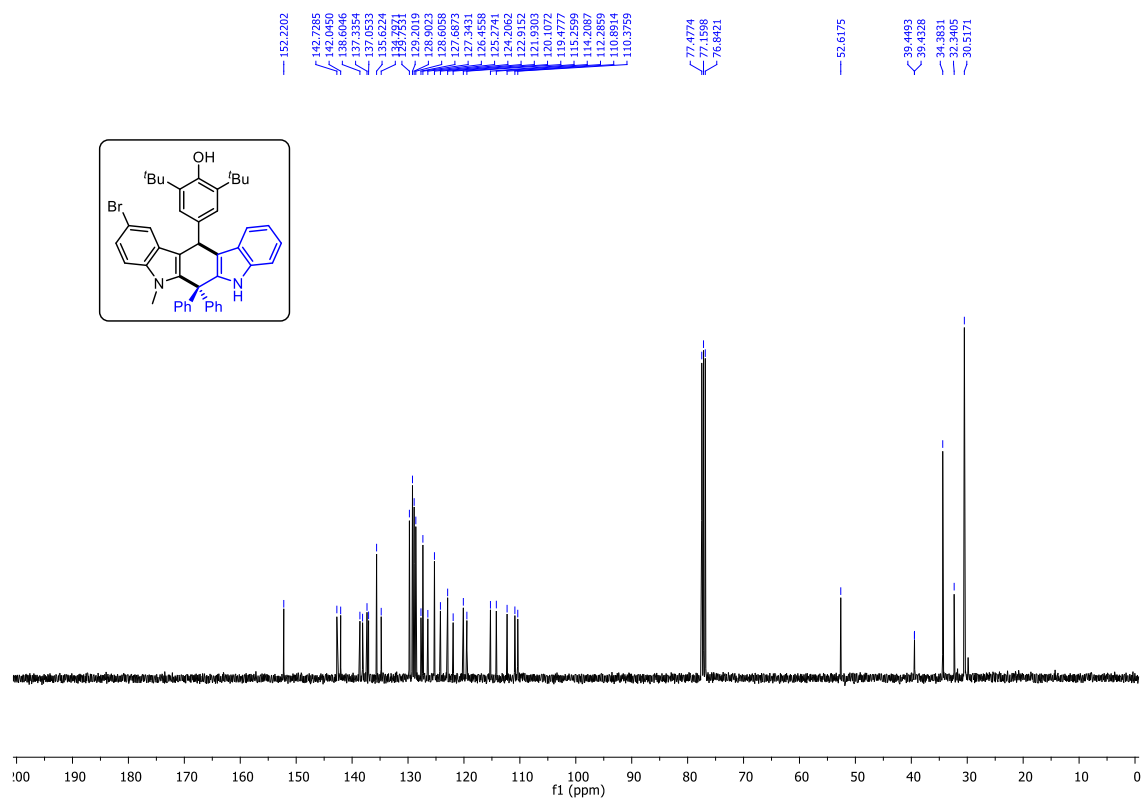
¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of **3c**



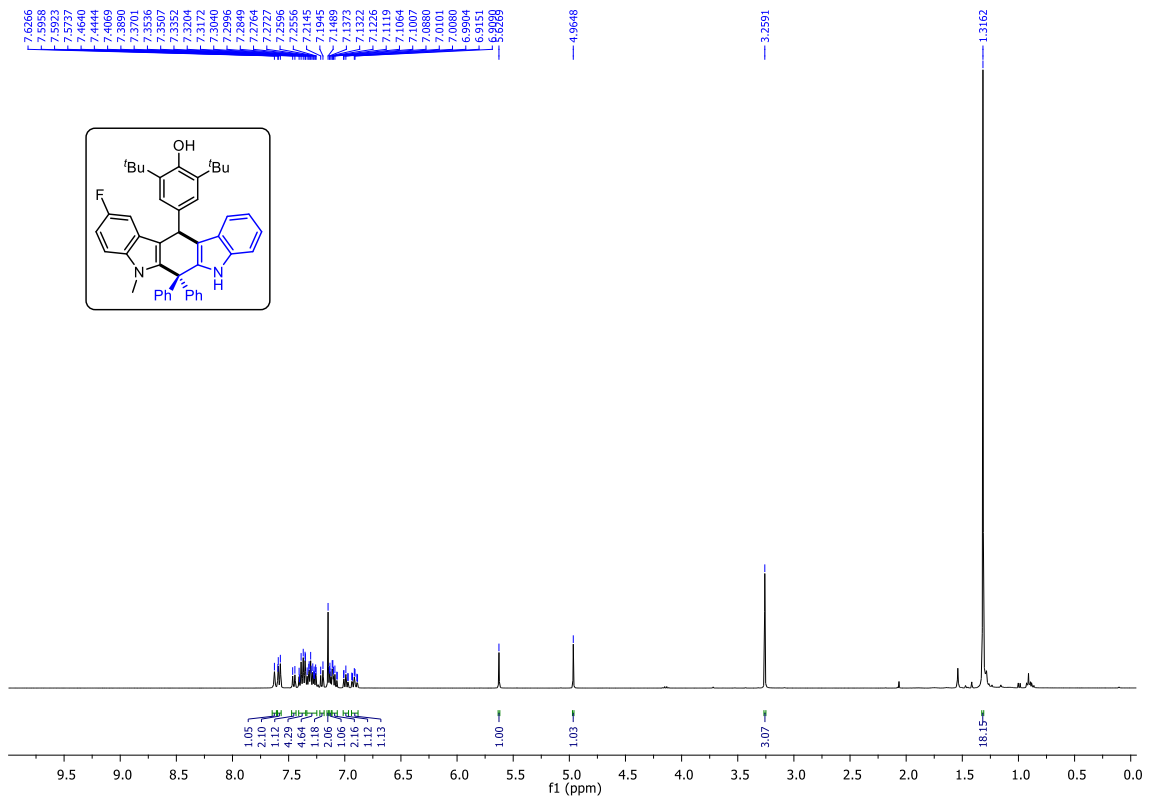
^1H NMR (400 MHz, CDCl_3) Spectrum of **3d**



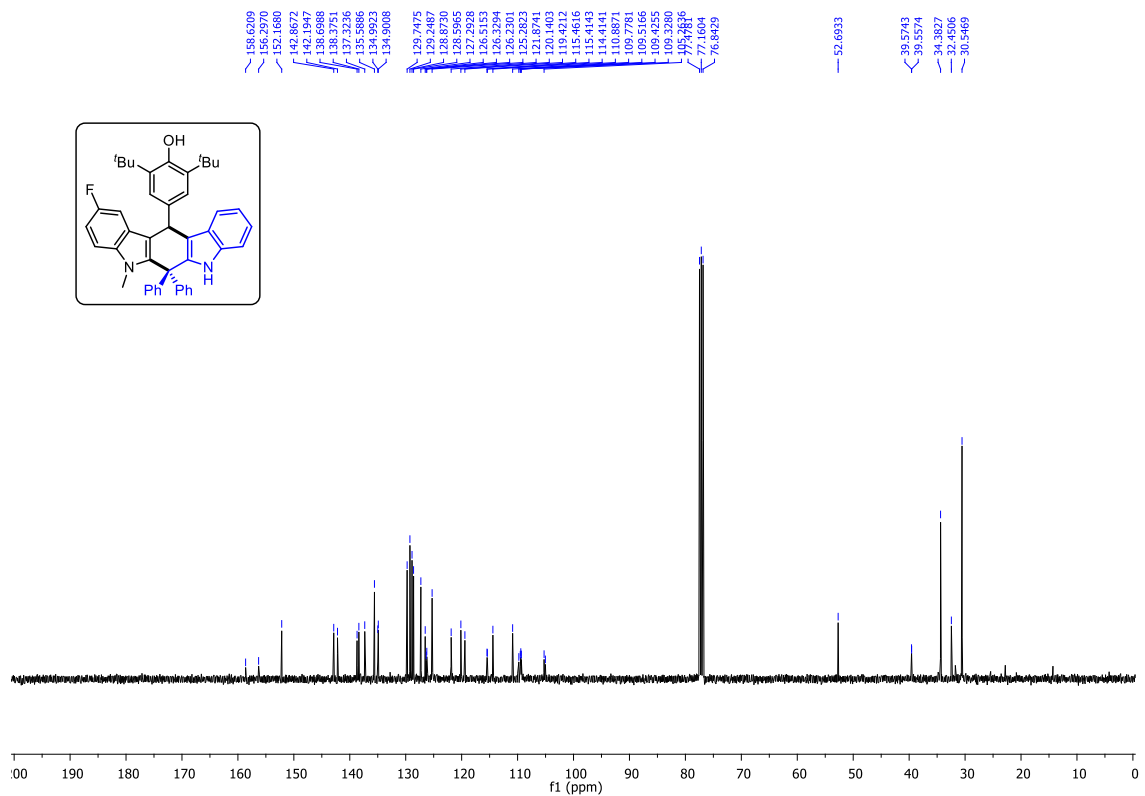
^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of **3d**



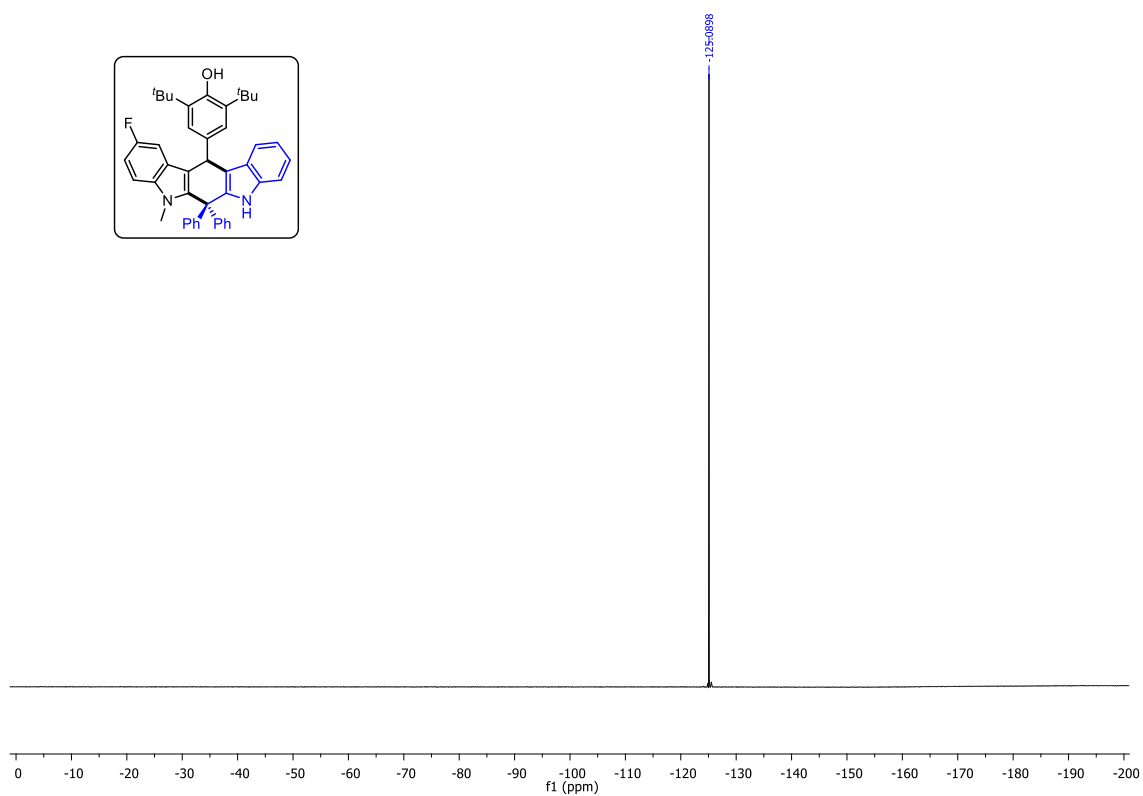
¹H NMR (400 MHz, CDCl₃) Spectrum of **3e**



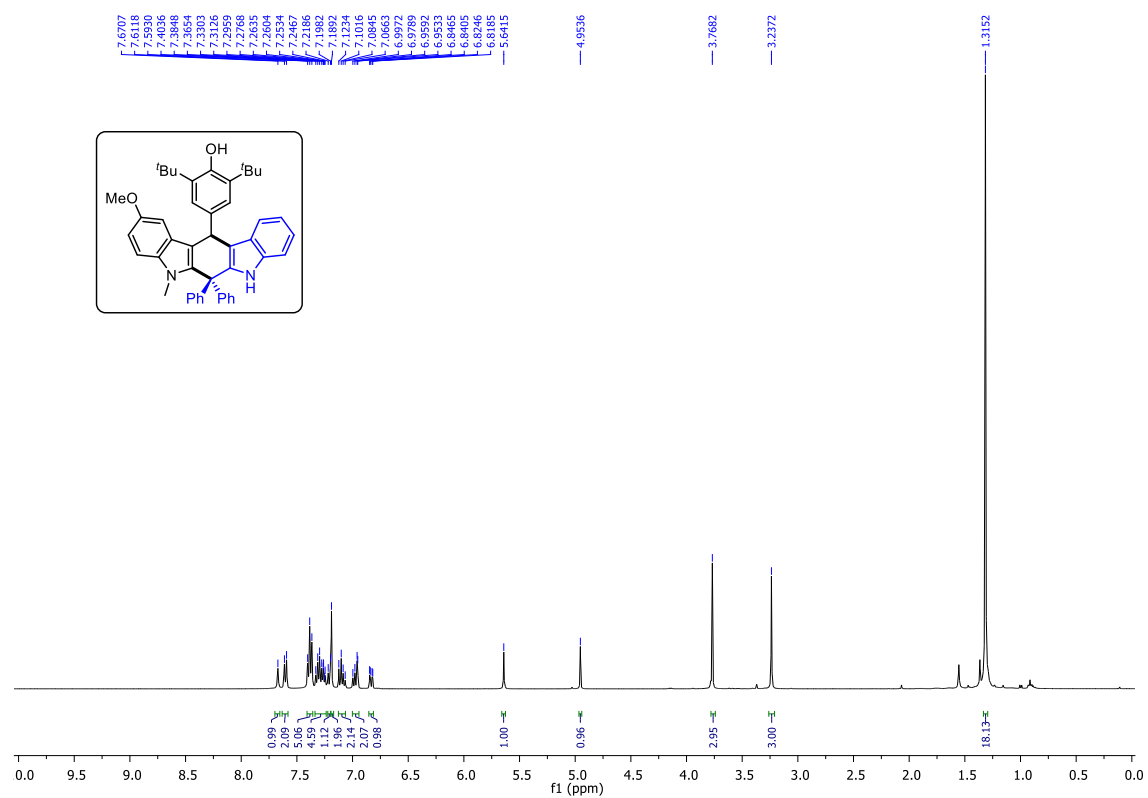
¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of **3e**



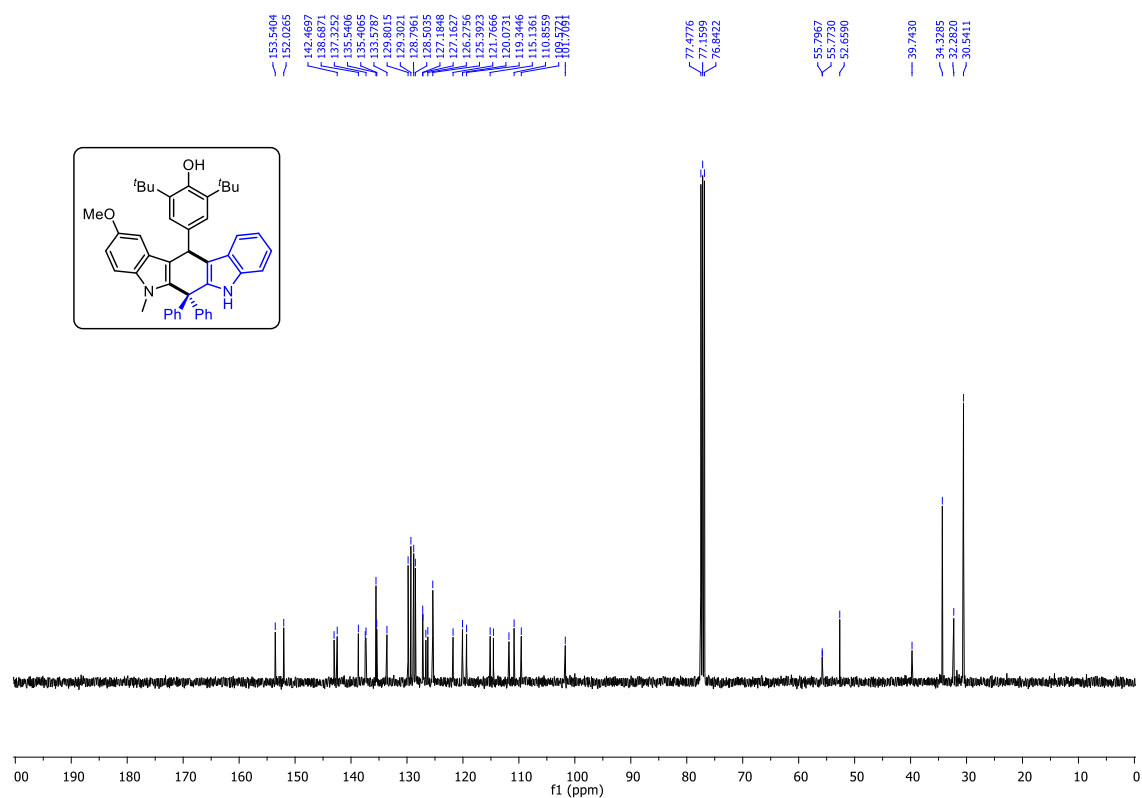
^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) Spectrum of **3e**



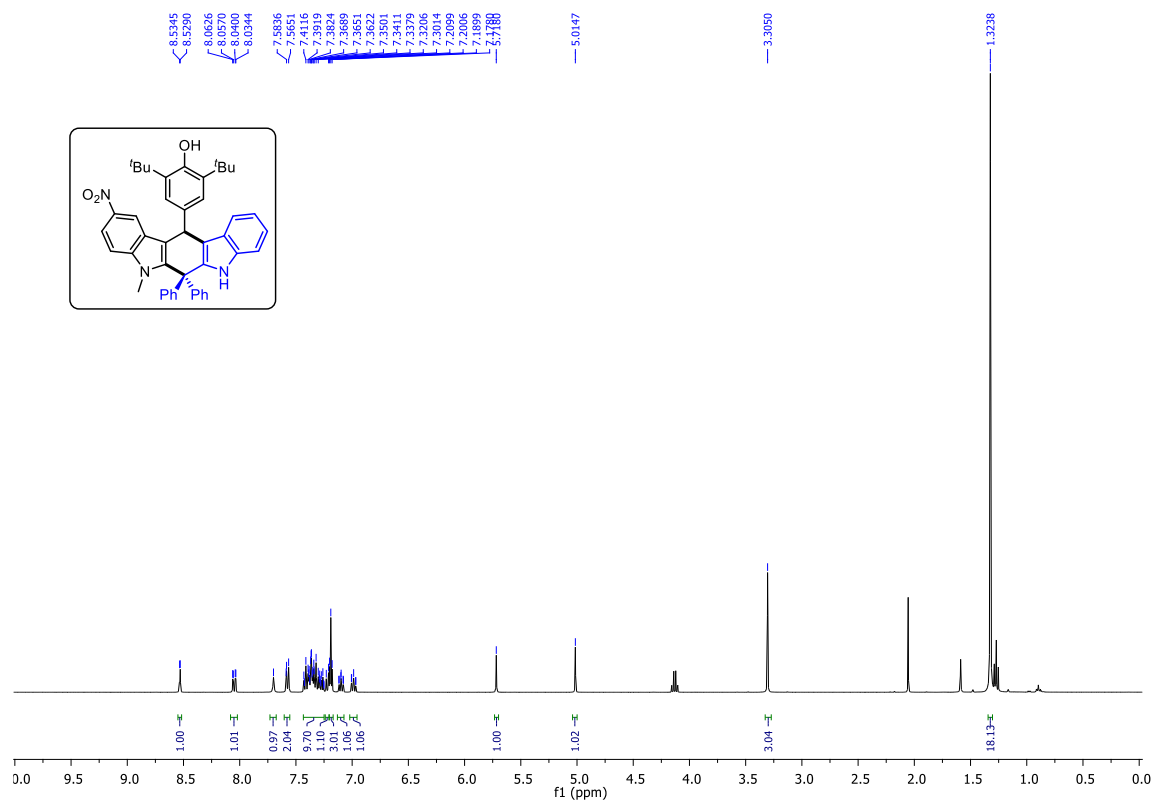
^1H NMR (400 MHz, CDCl_3) Spectrum of **3f**



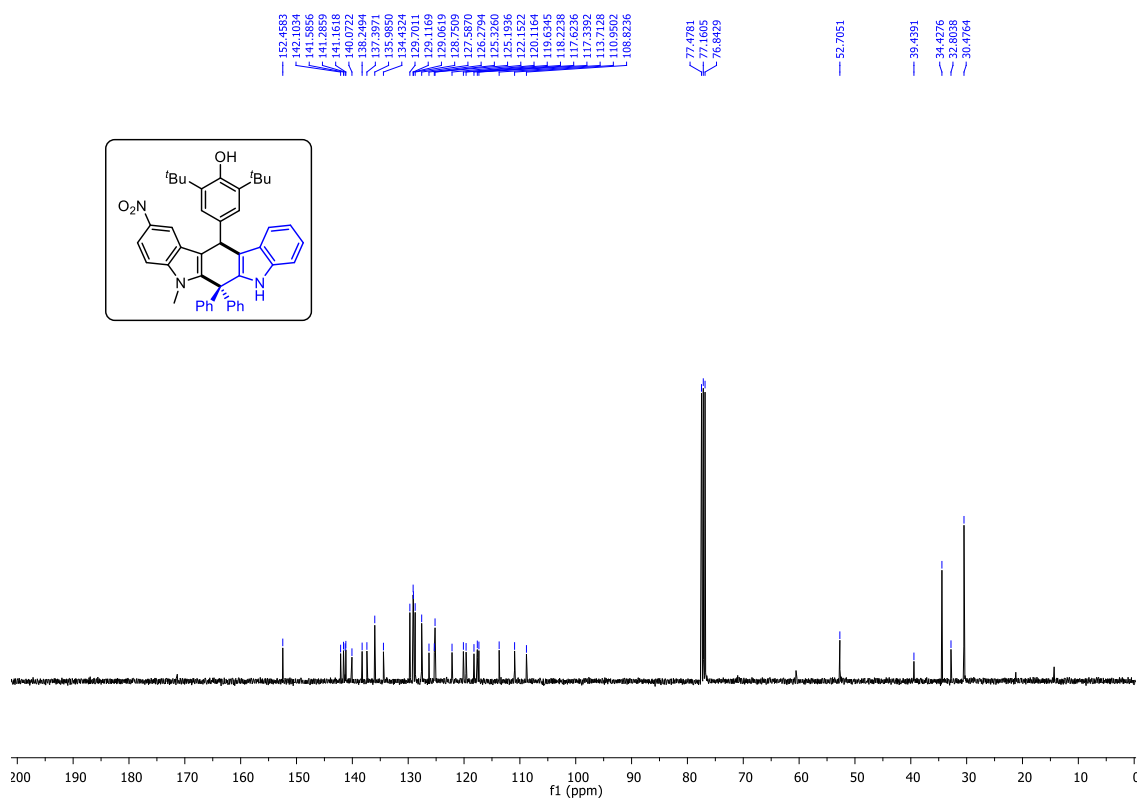
^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of **3f**



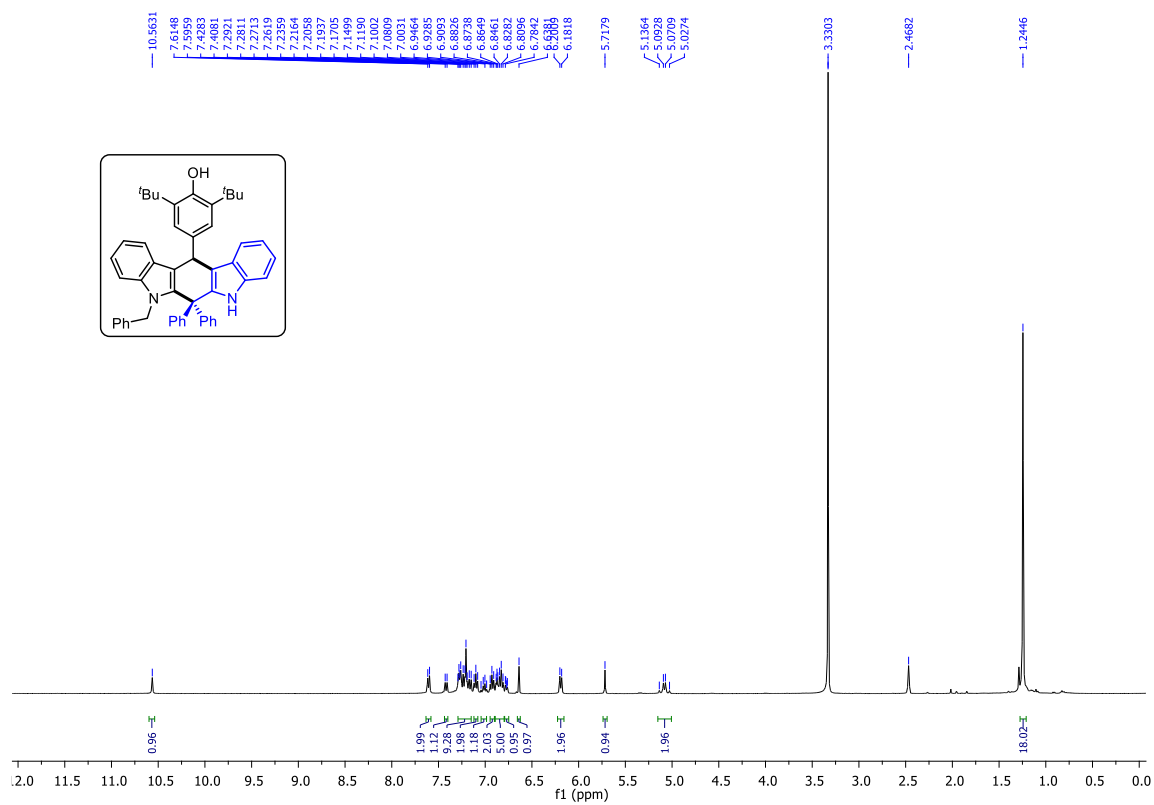
^1H NMR (400 MHz, CDCl_3) Spectrum of **3g**



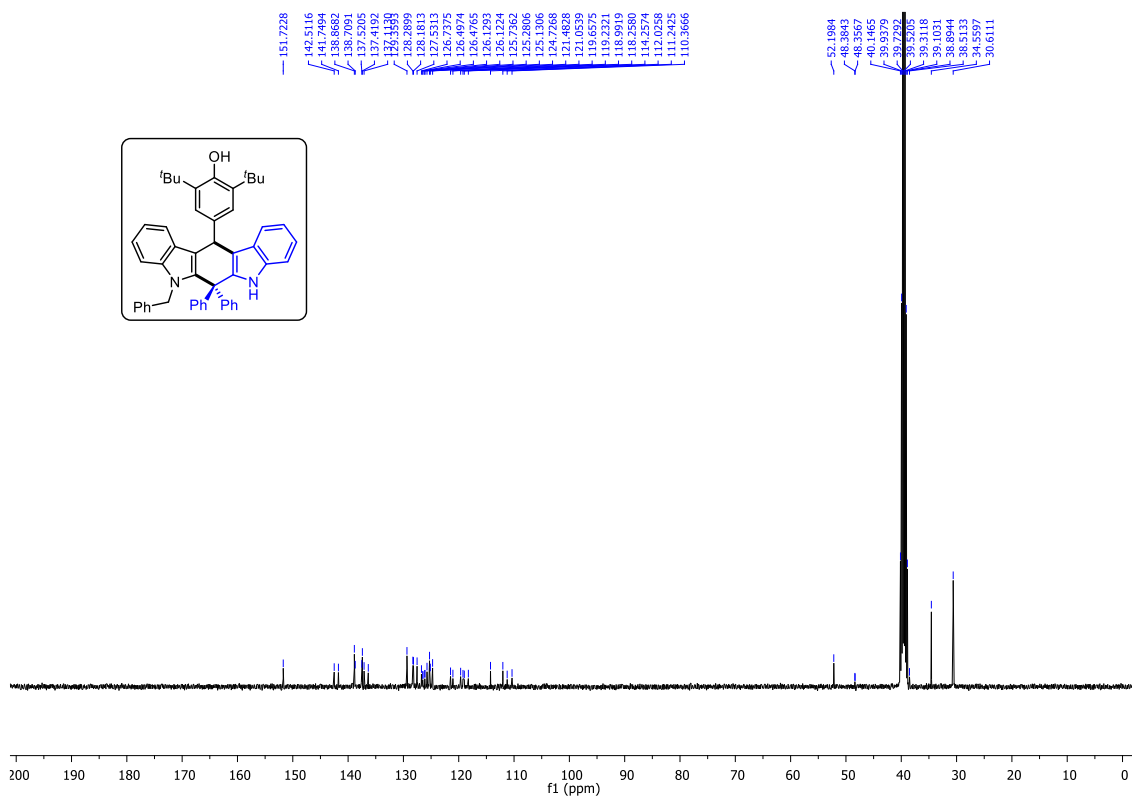
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3g**



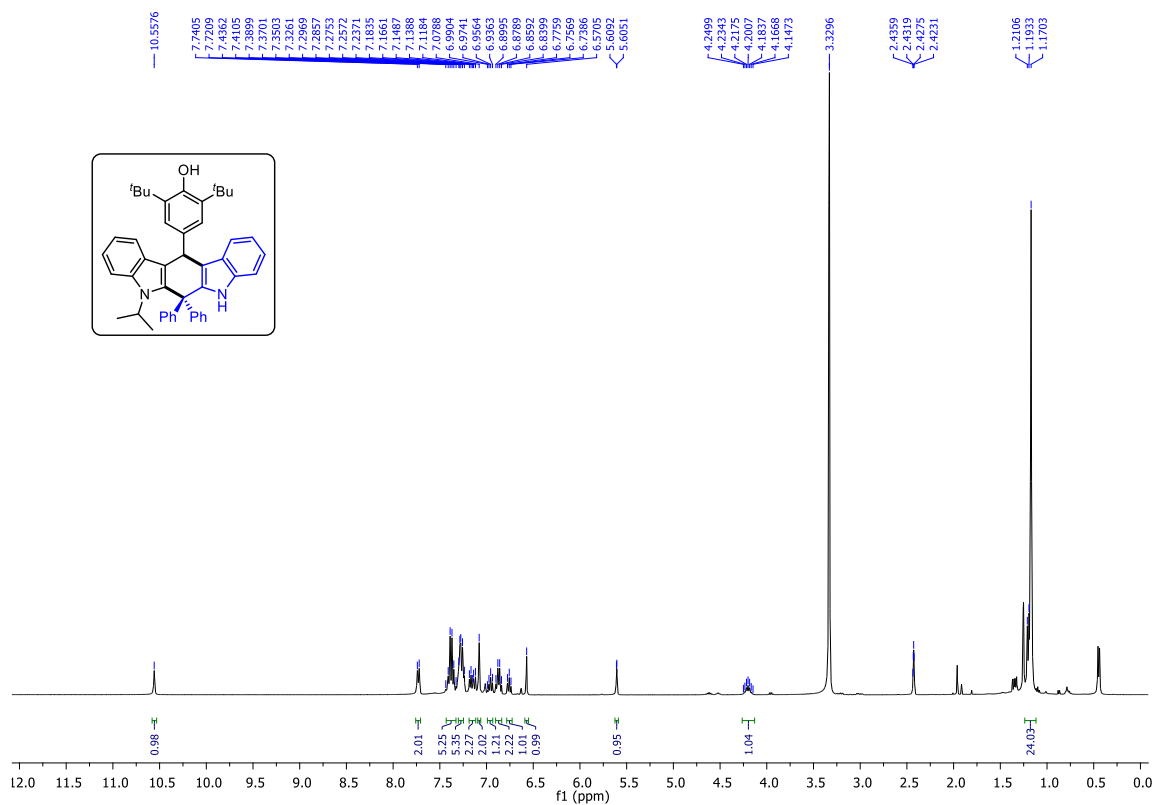
^1H NMR (400 MHz, DMSO-d_6) Spectrum of **3h**



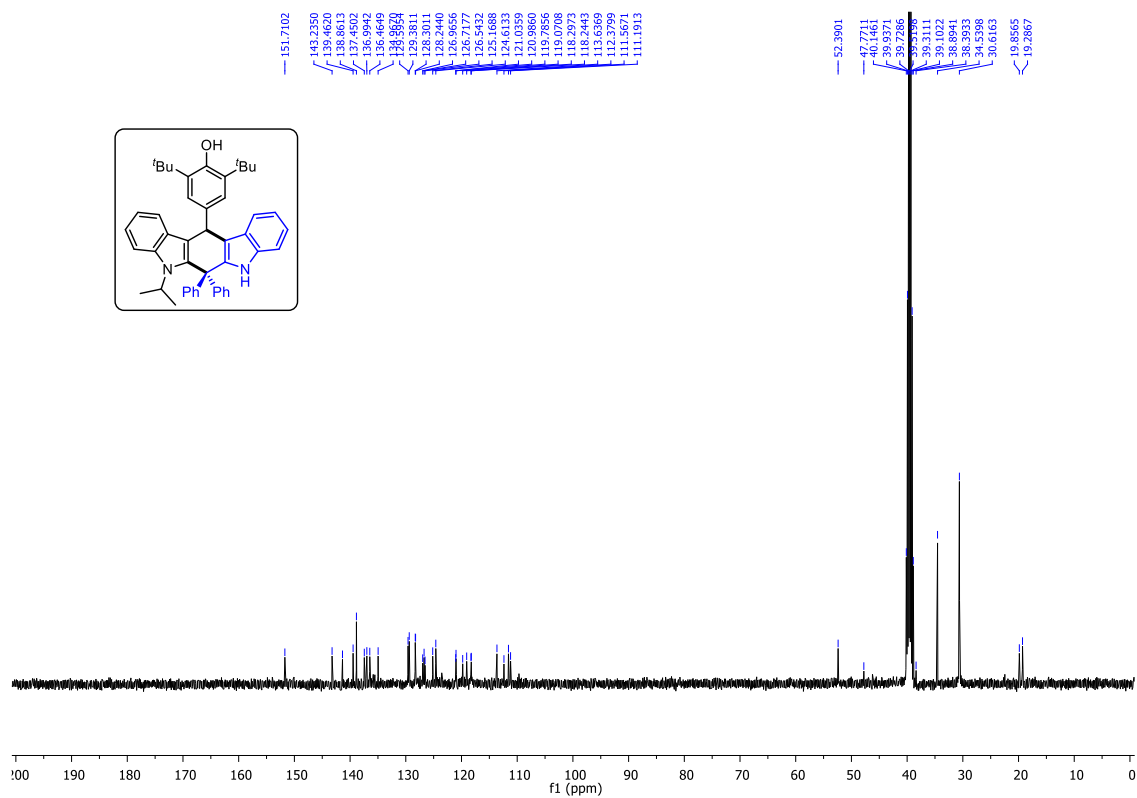
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **3h**



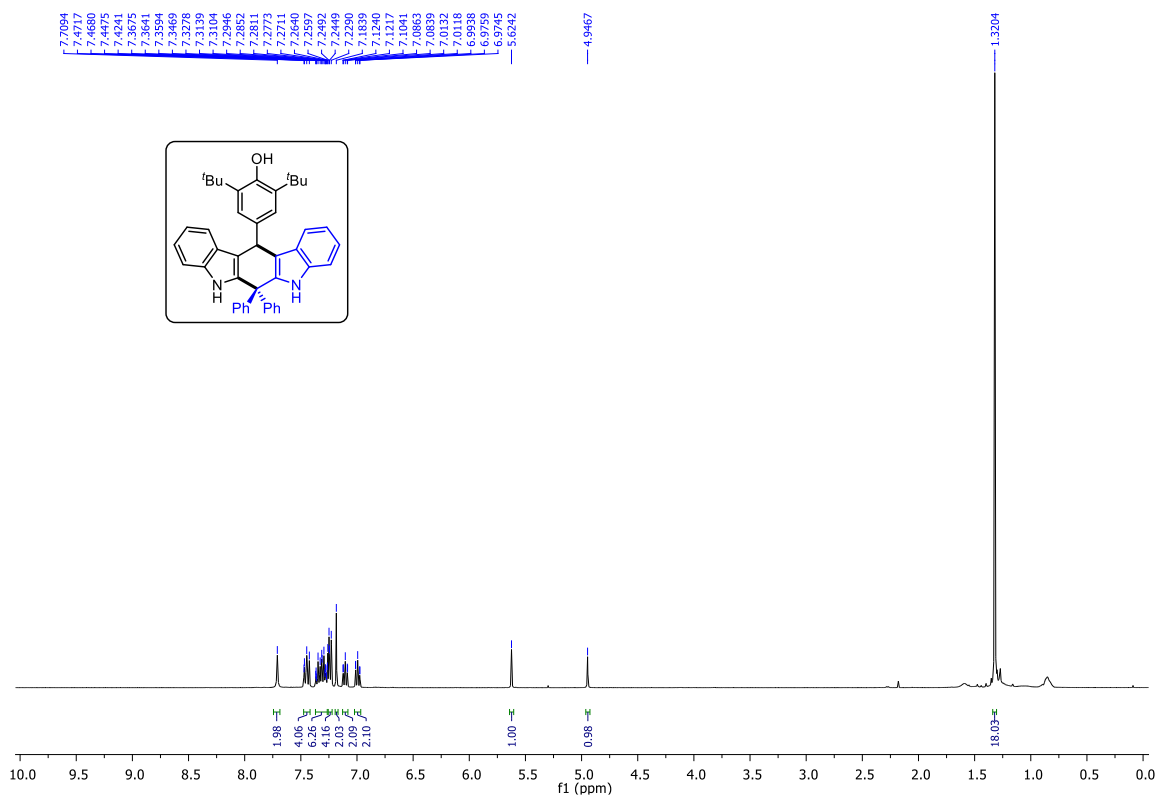
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **3i**



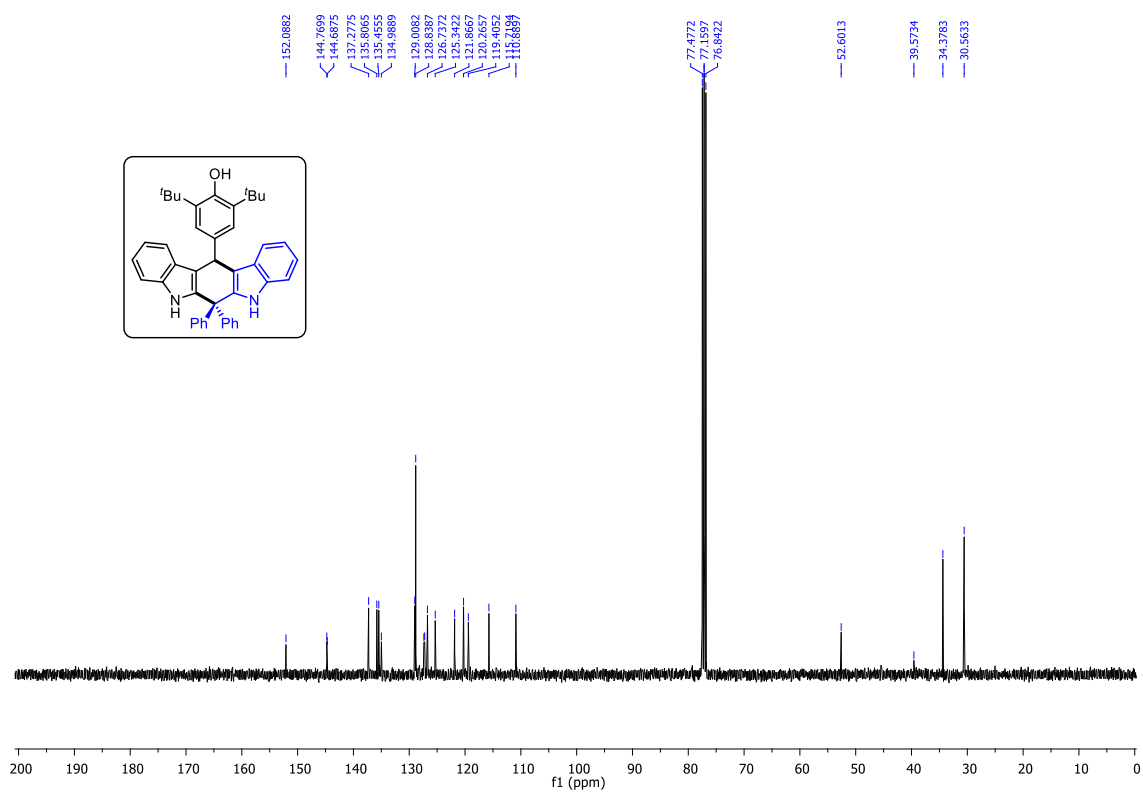
^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) Spectrum of **3i**



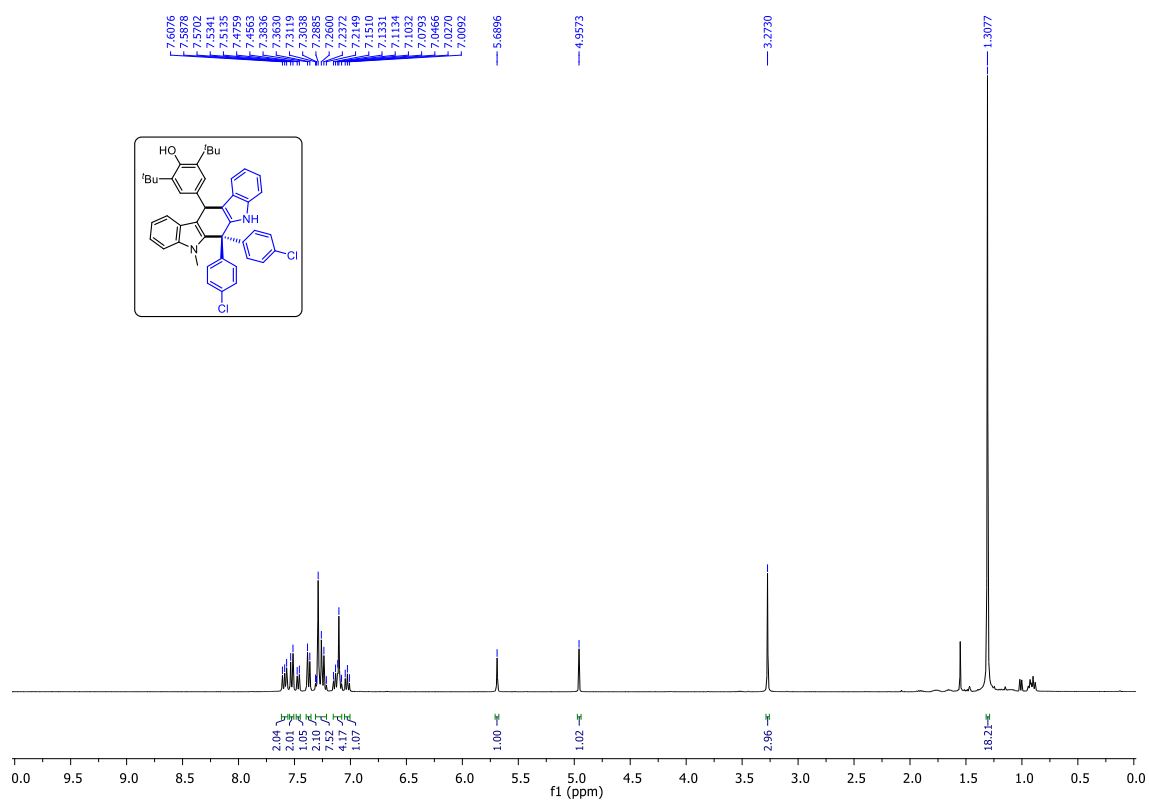
^1H NMR (400 MHz, CDCl_3) Spectrum of **3j**



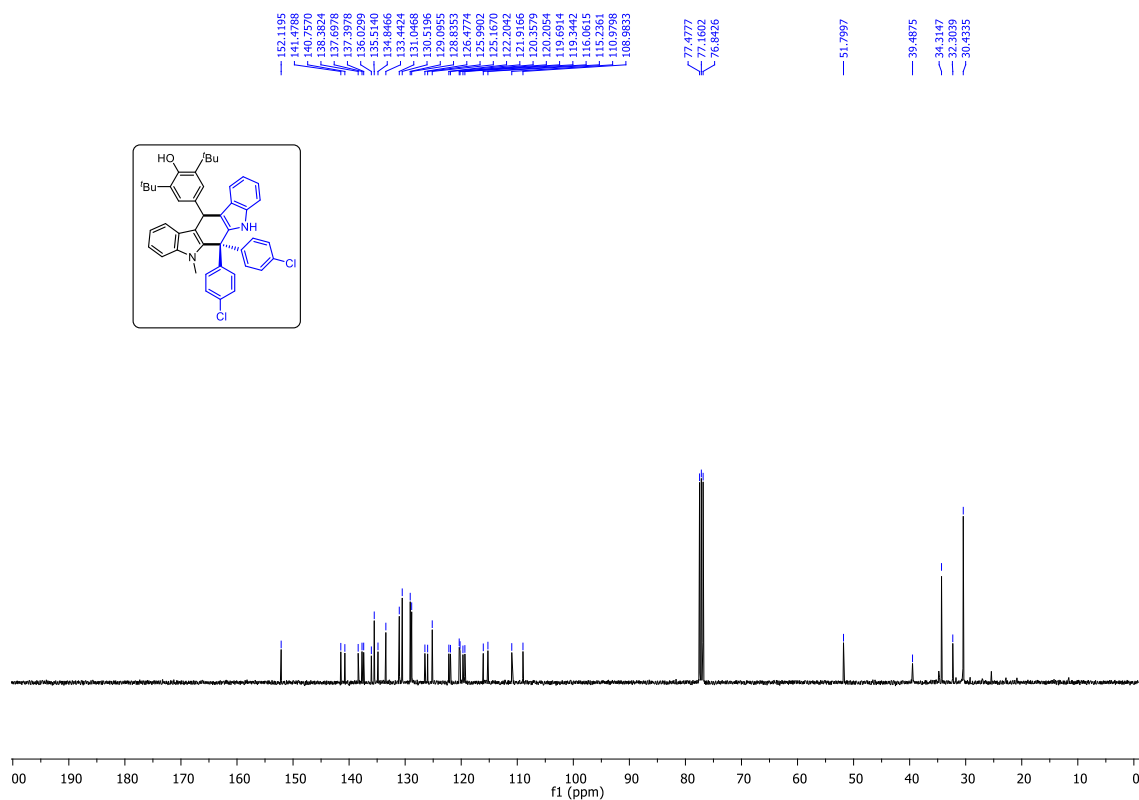
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3j**



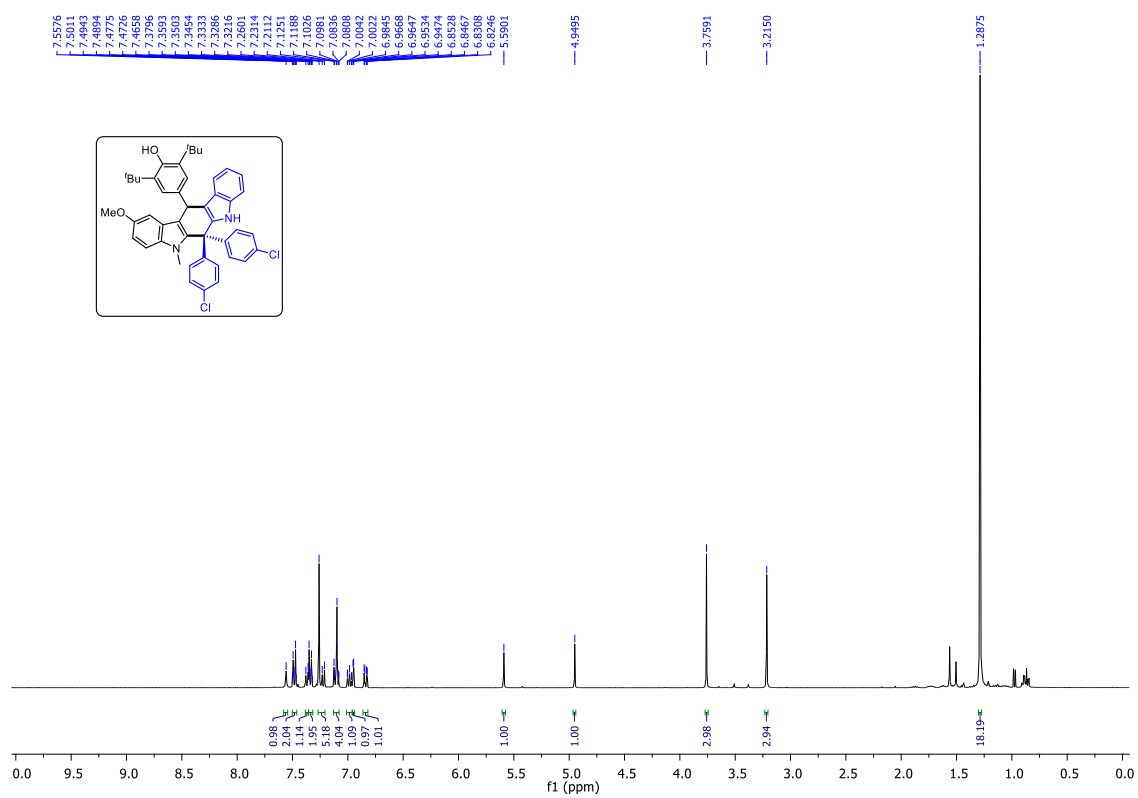
^1H NMR (400 MHz, CDCl_3) Spectrum of **3k**



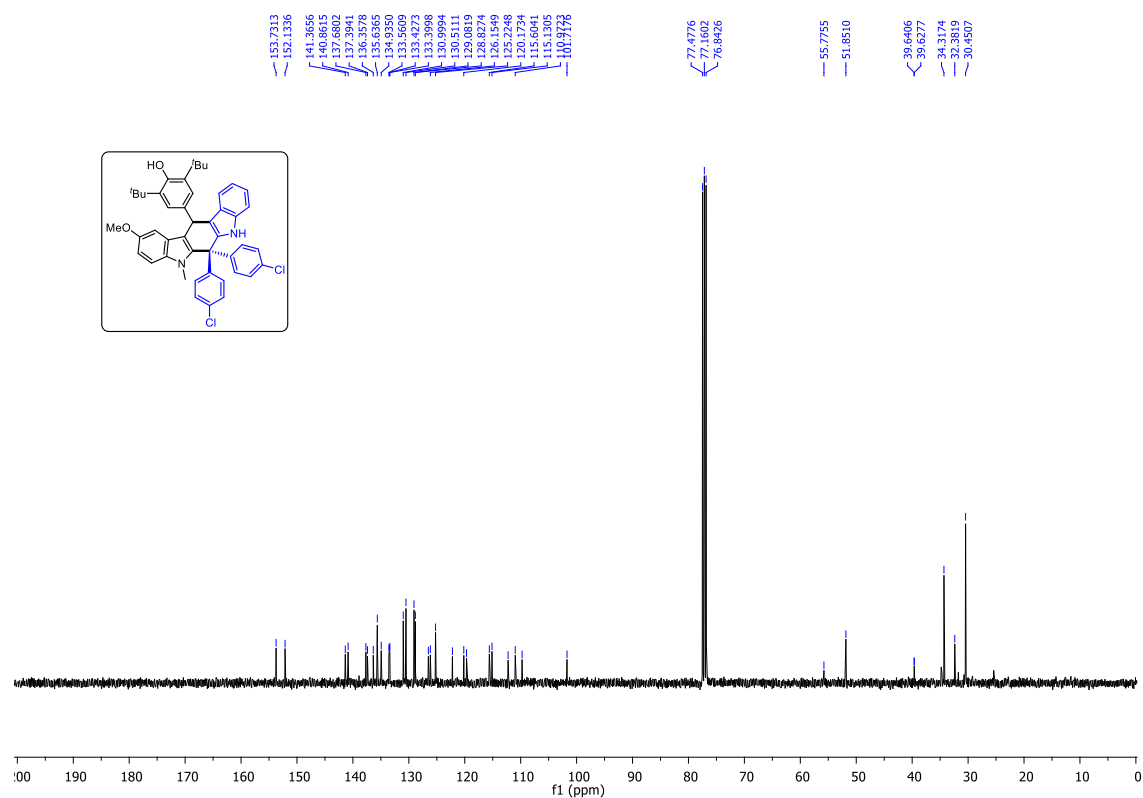
^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of **3k**



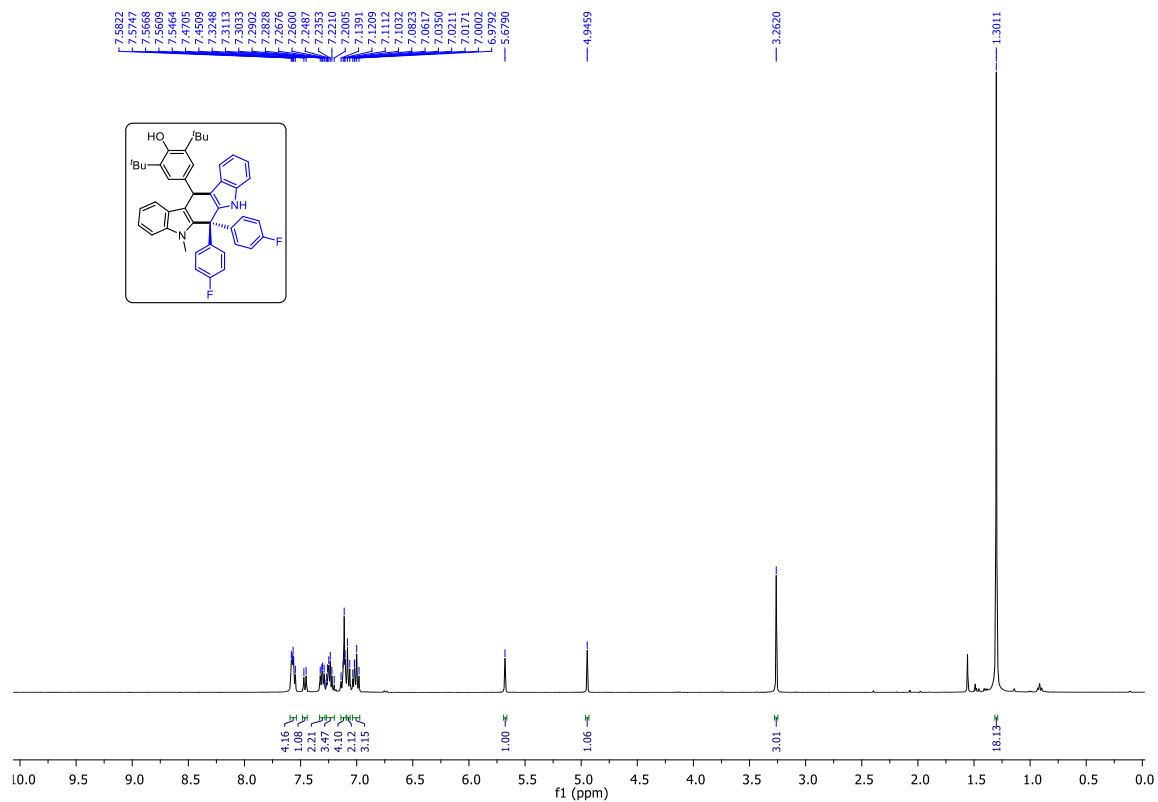
^1H NMR (400 MHz, CDCl_3) Spectrum of **3l**



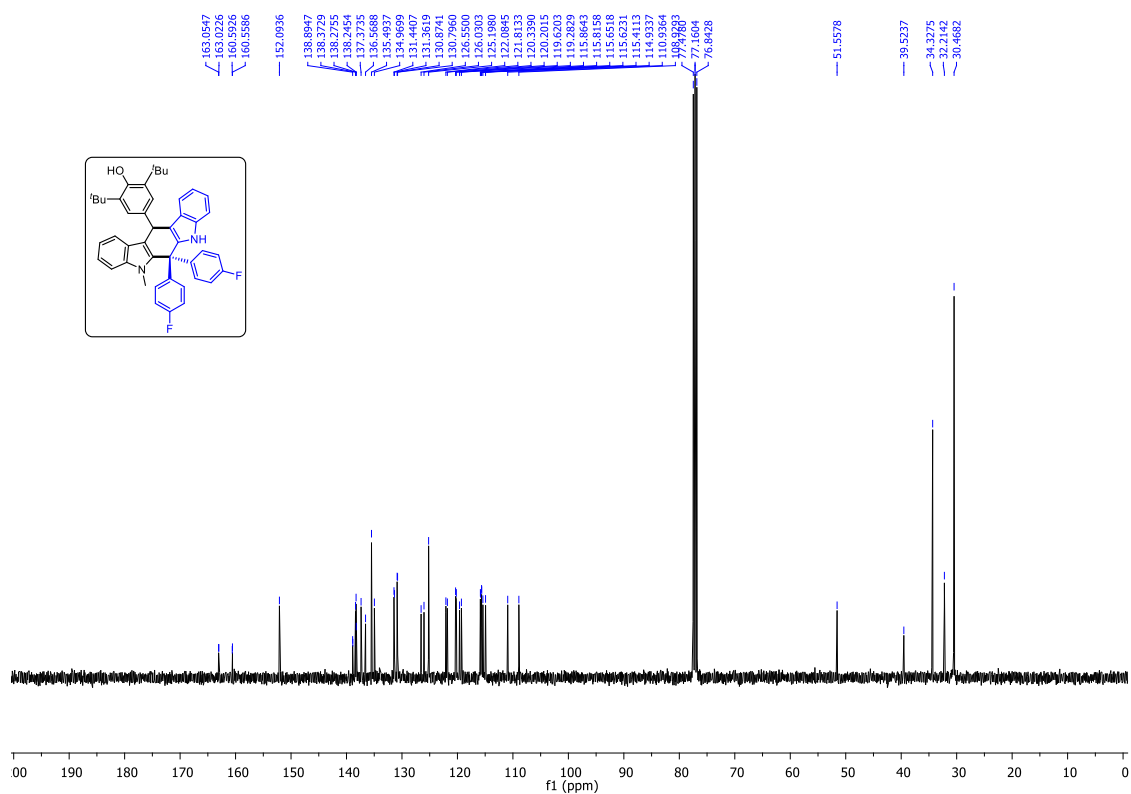
^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of **3l**



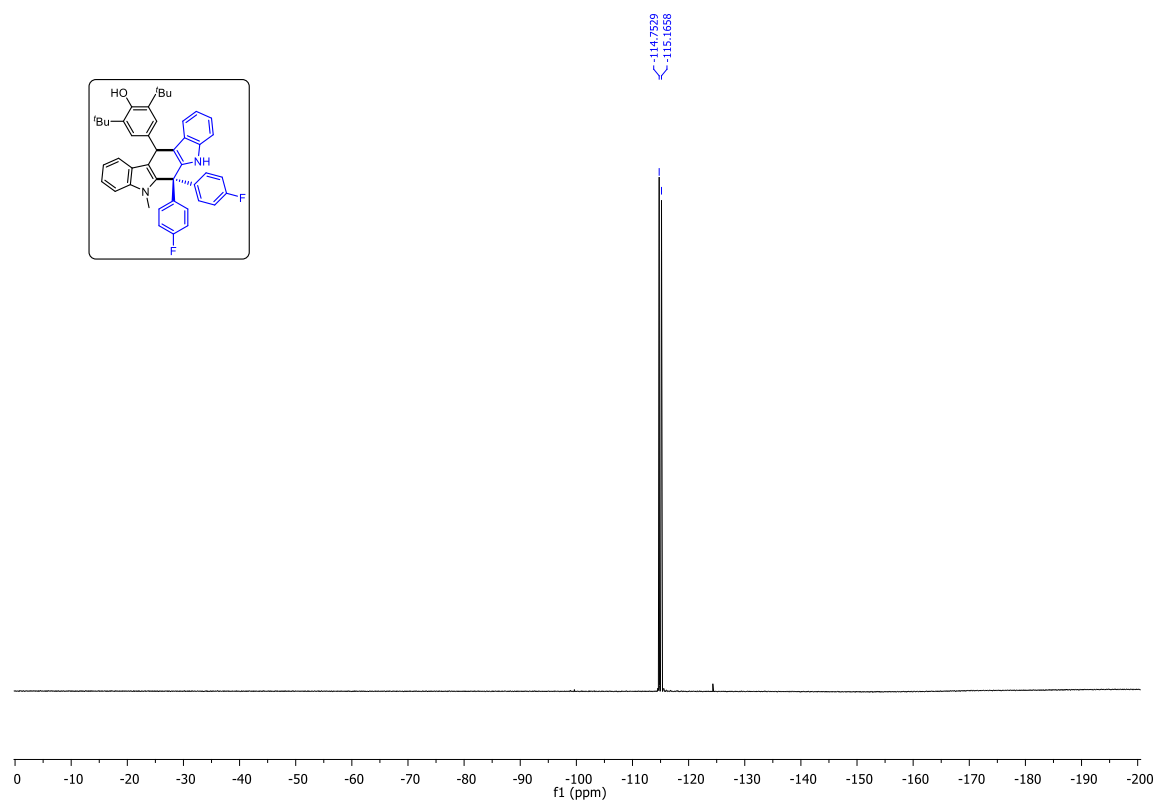
^1H NMR (400 MHz, CDCl_3) Spectrum of **3m**



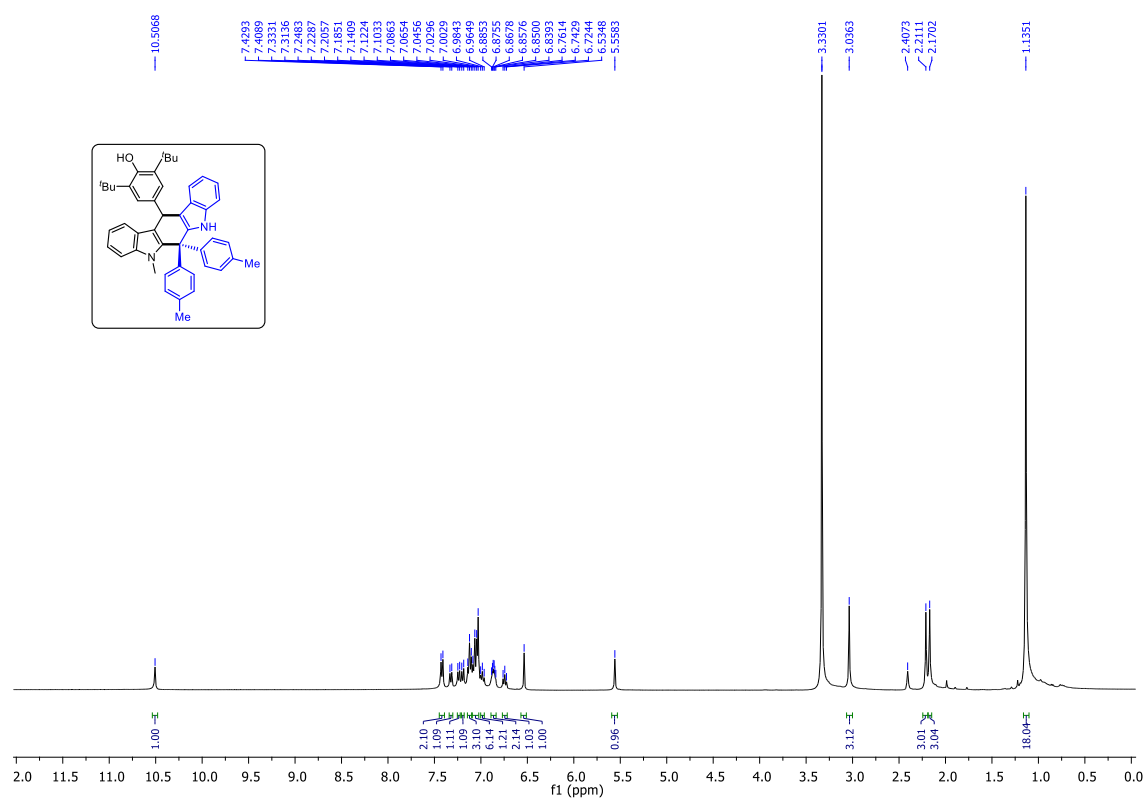
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3m**



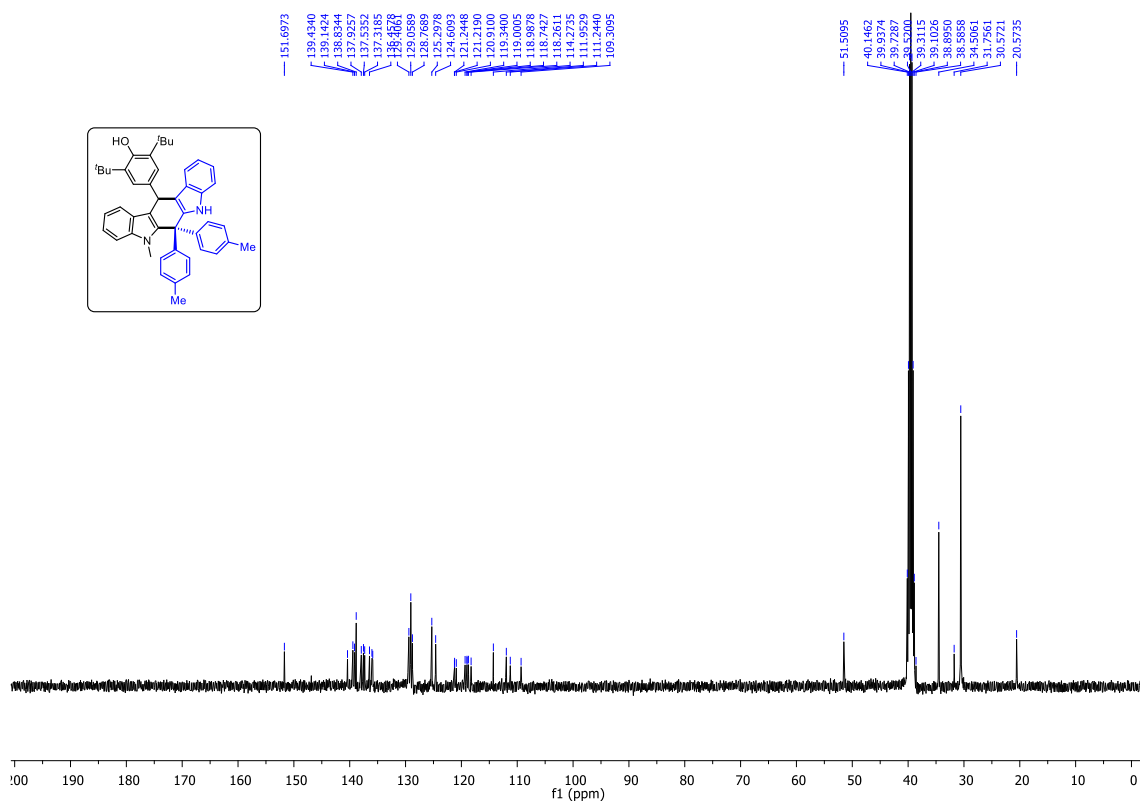
^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) Spectrum of **3m**



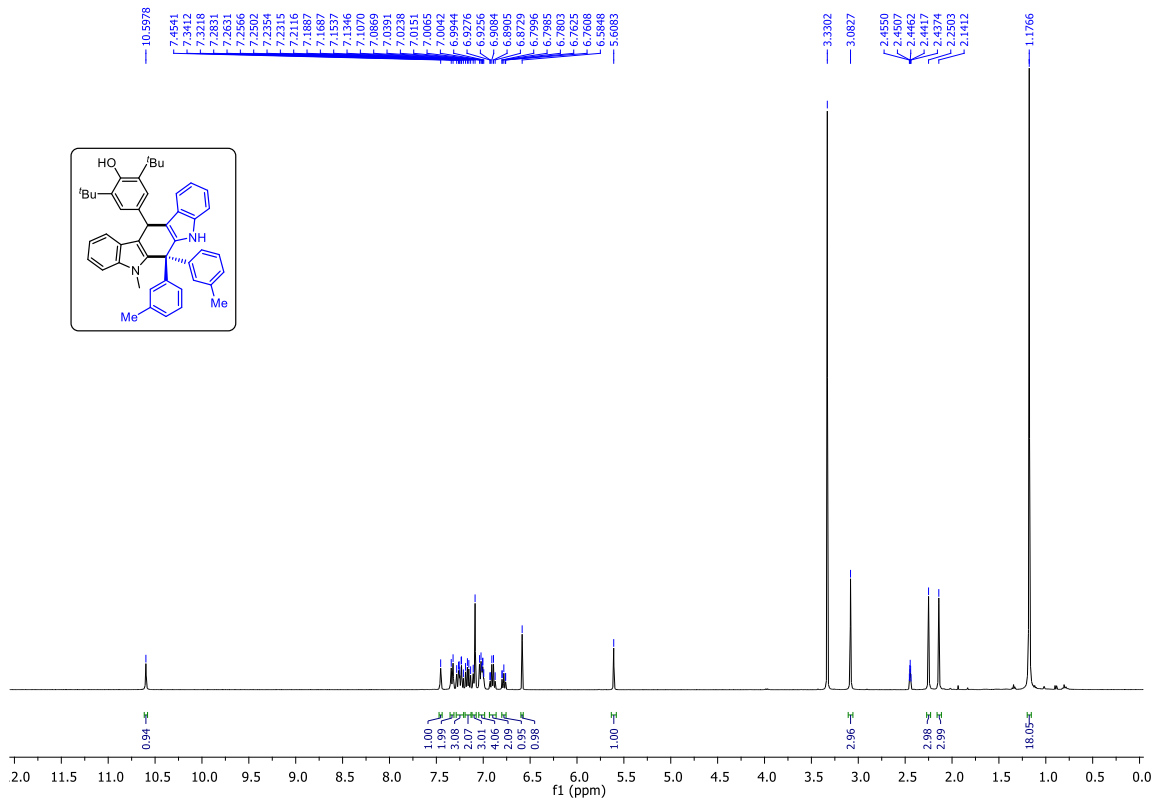
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **3n**



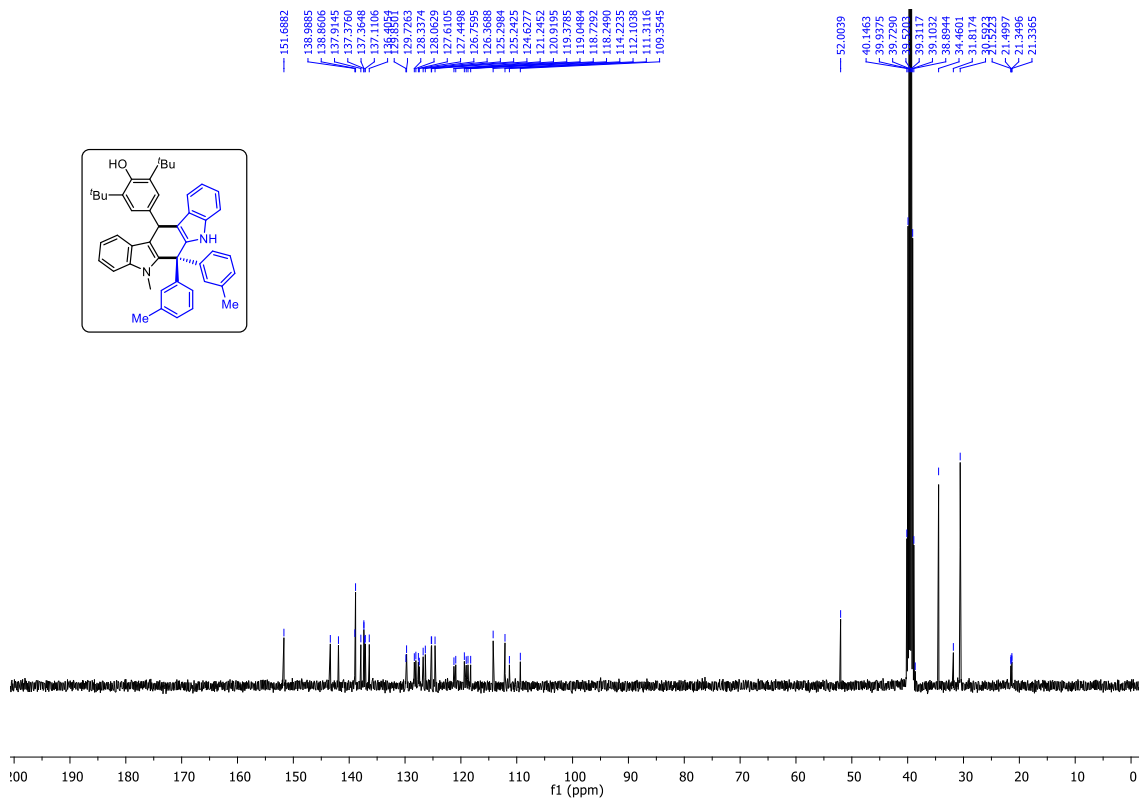
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **3n**



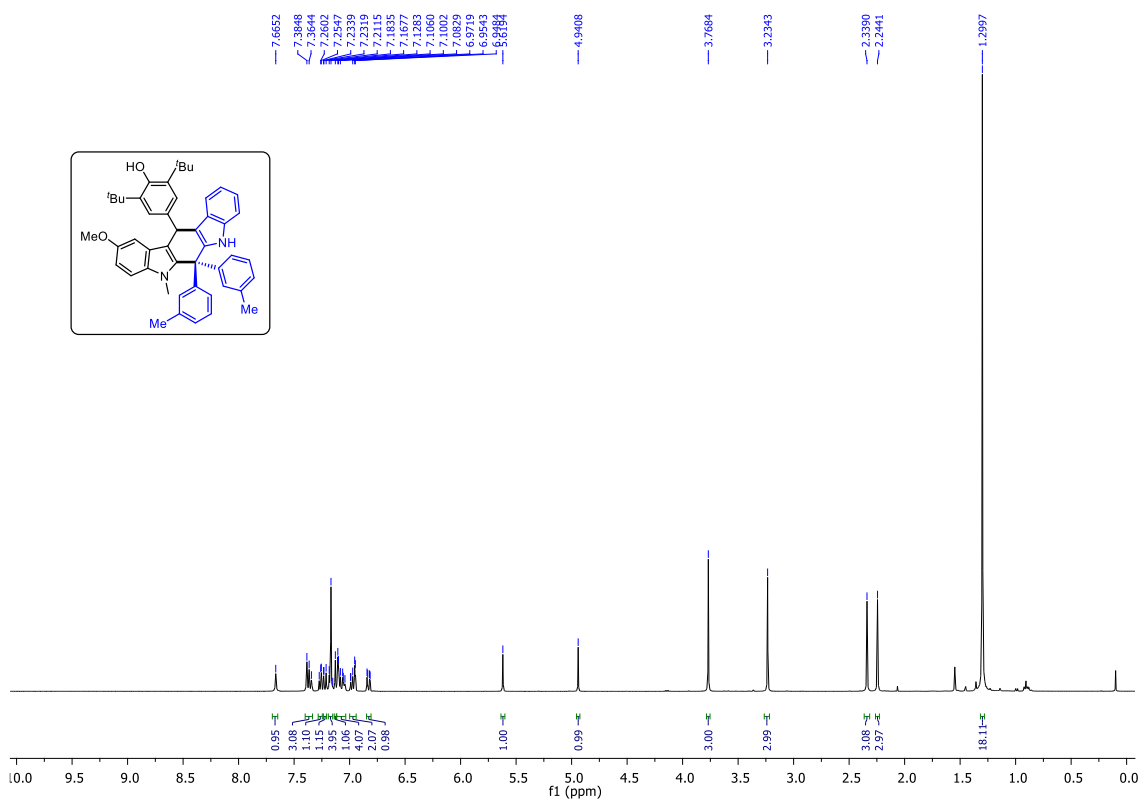
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **30**



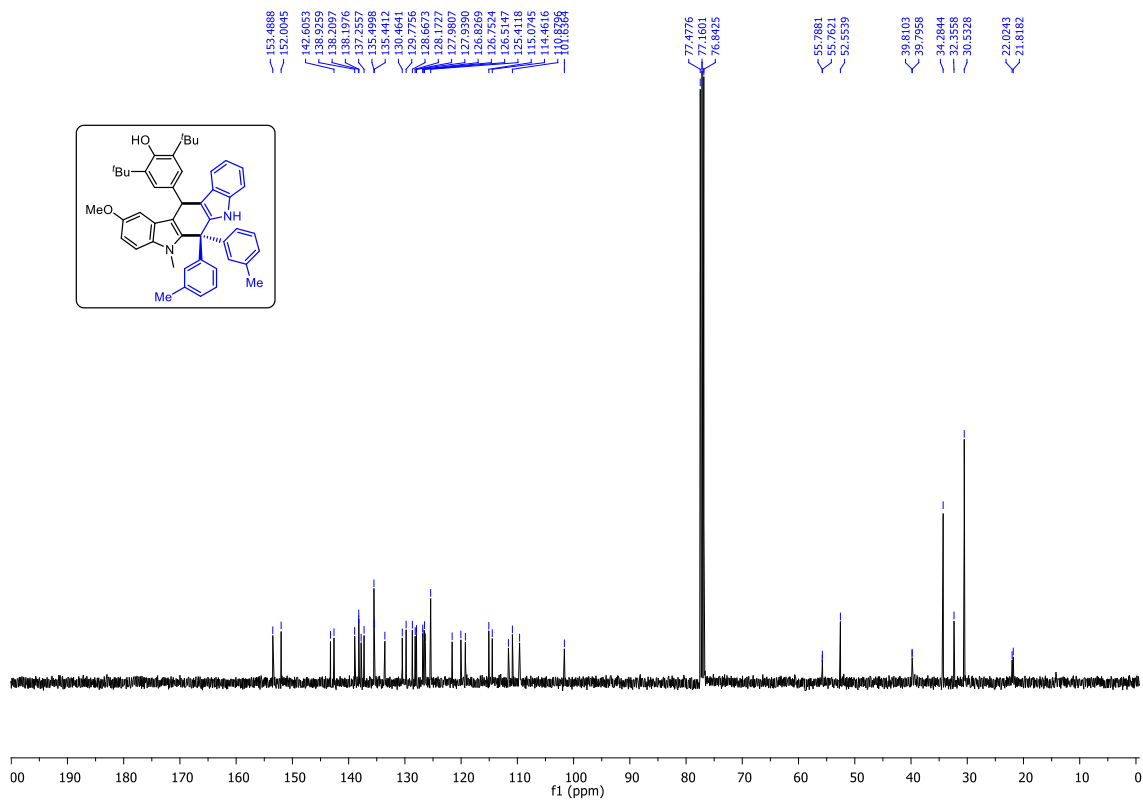
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **30**



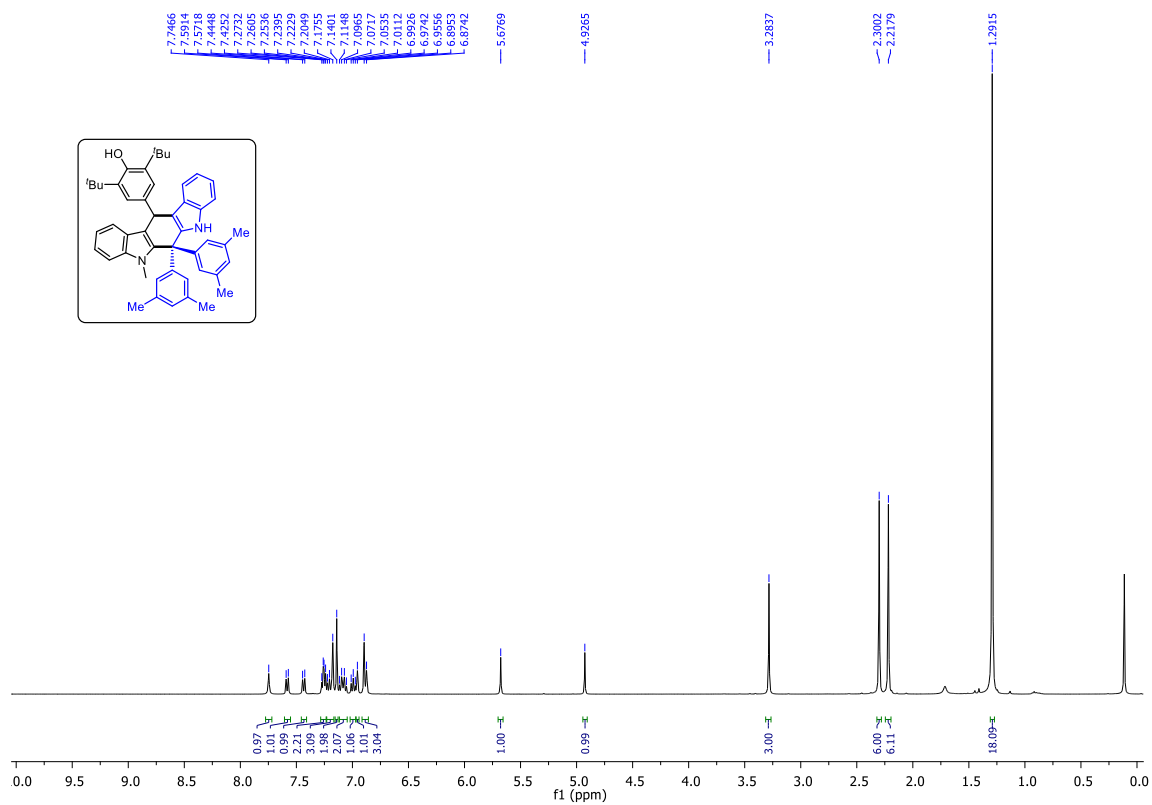
^1H NMR (400 MHz, CDCl_3) Spectrum of **3p**



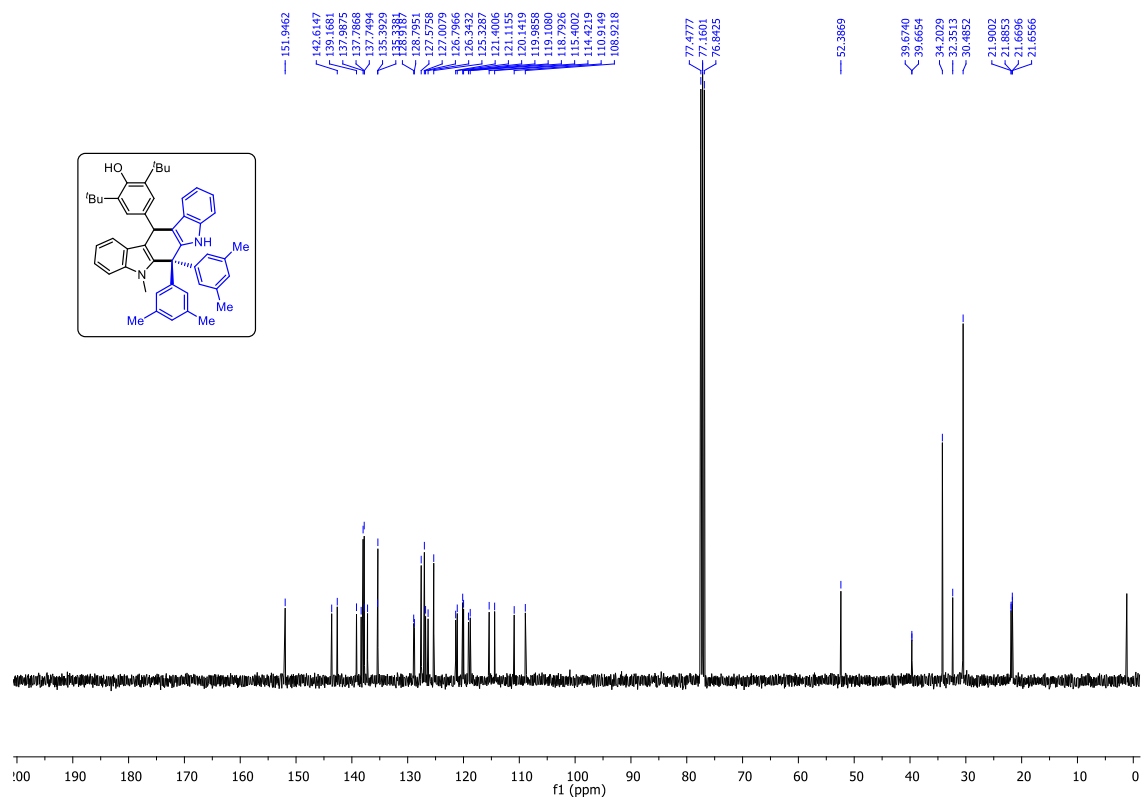
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3p**



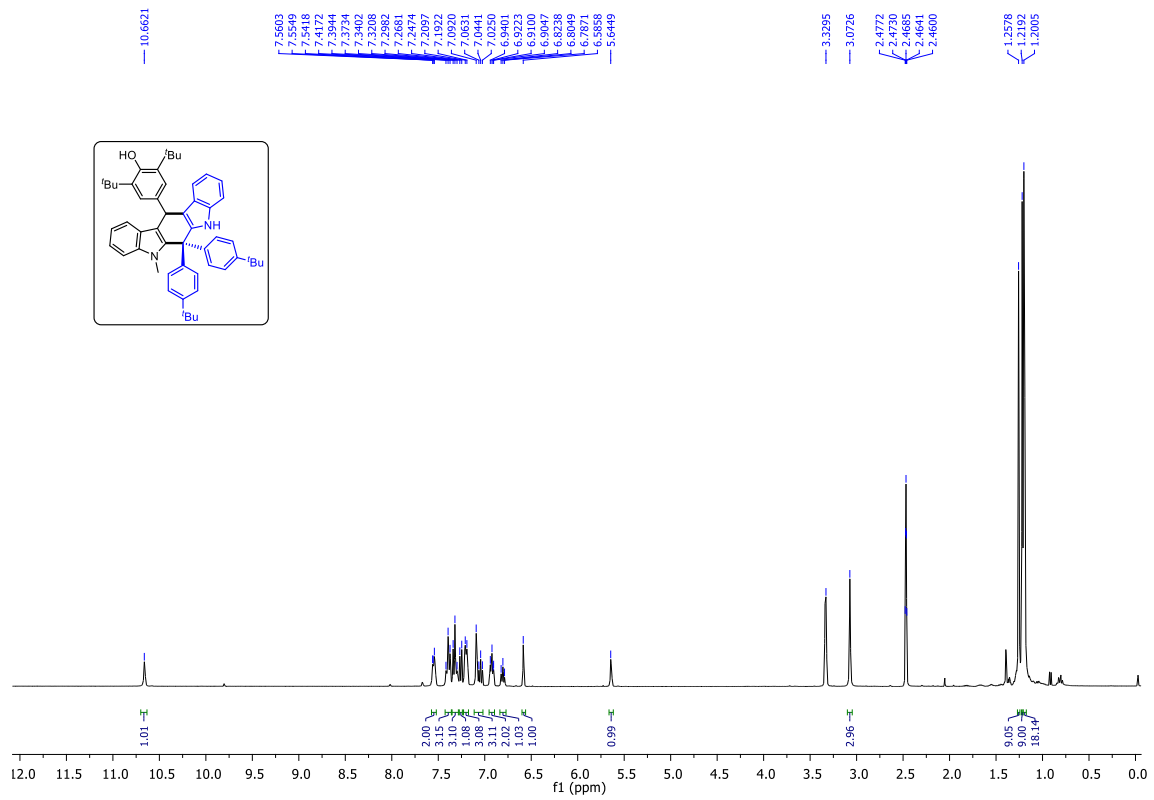
^1H NMR (400 MHz, CDCl_3) Spectrum of **3q**



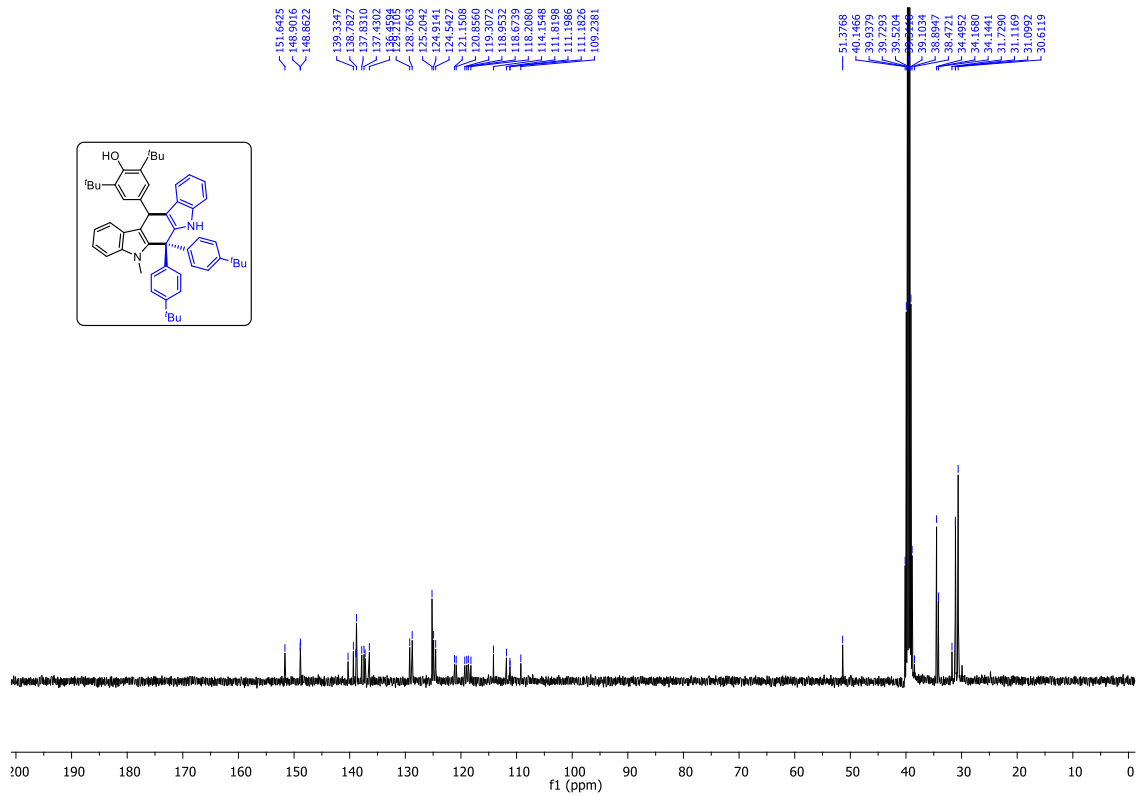
^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of **3q**



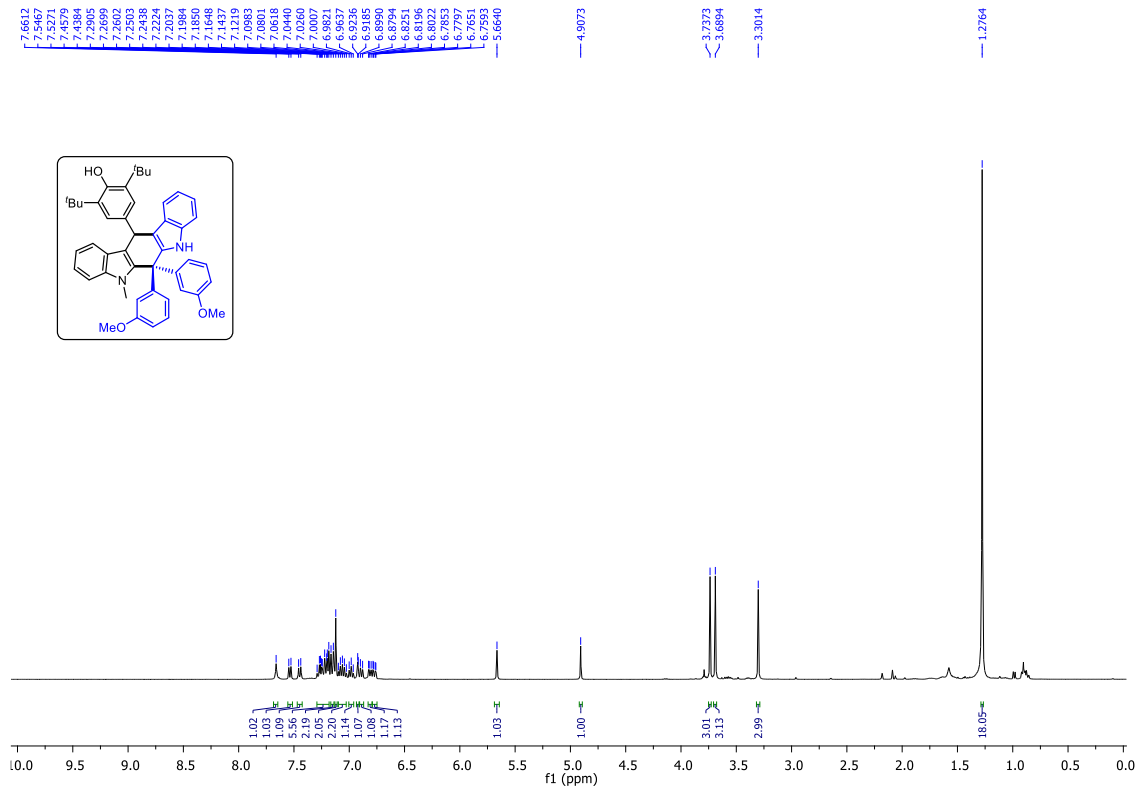
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **3r**



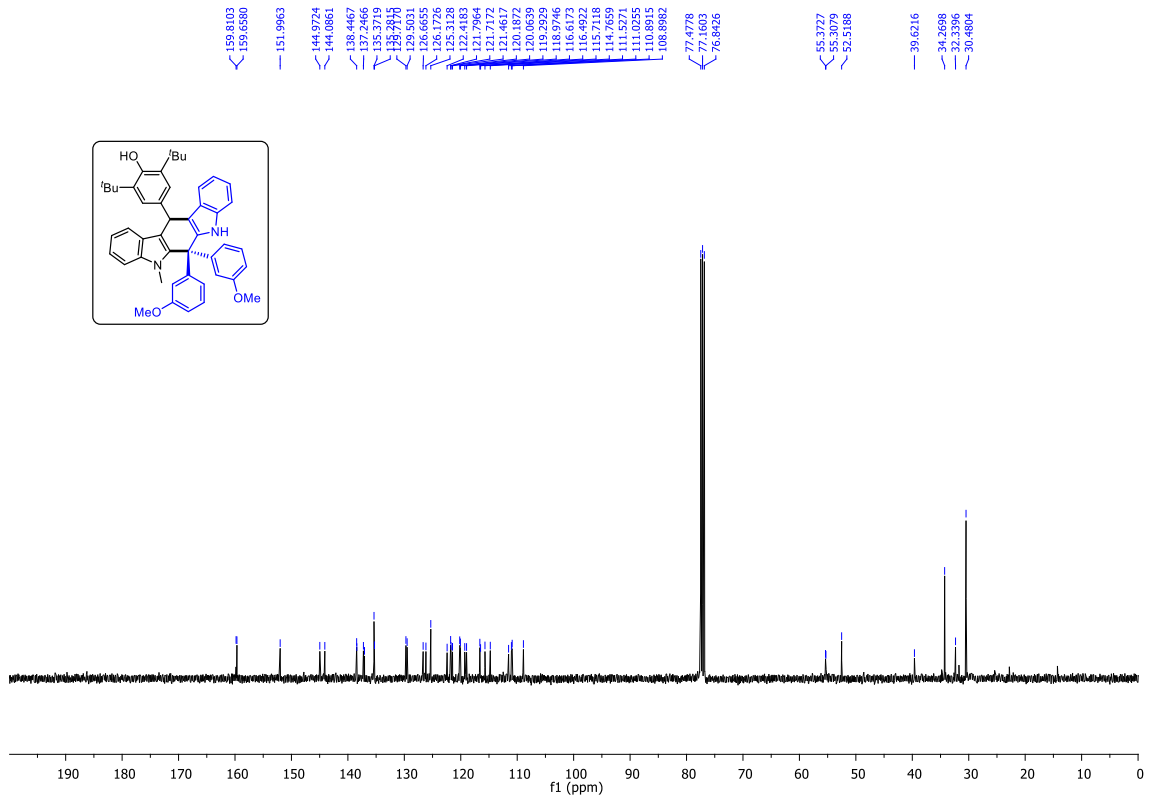
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **3r**



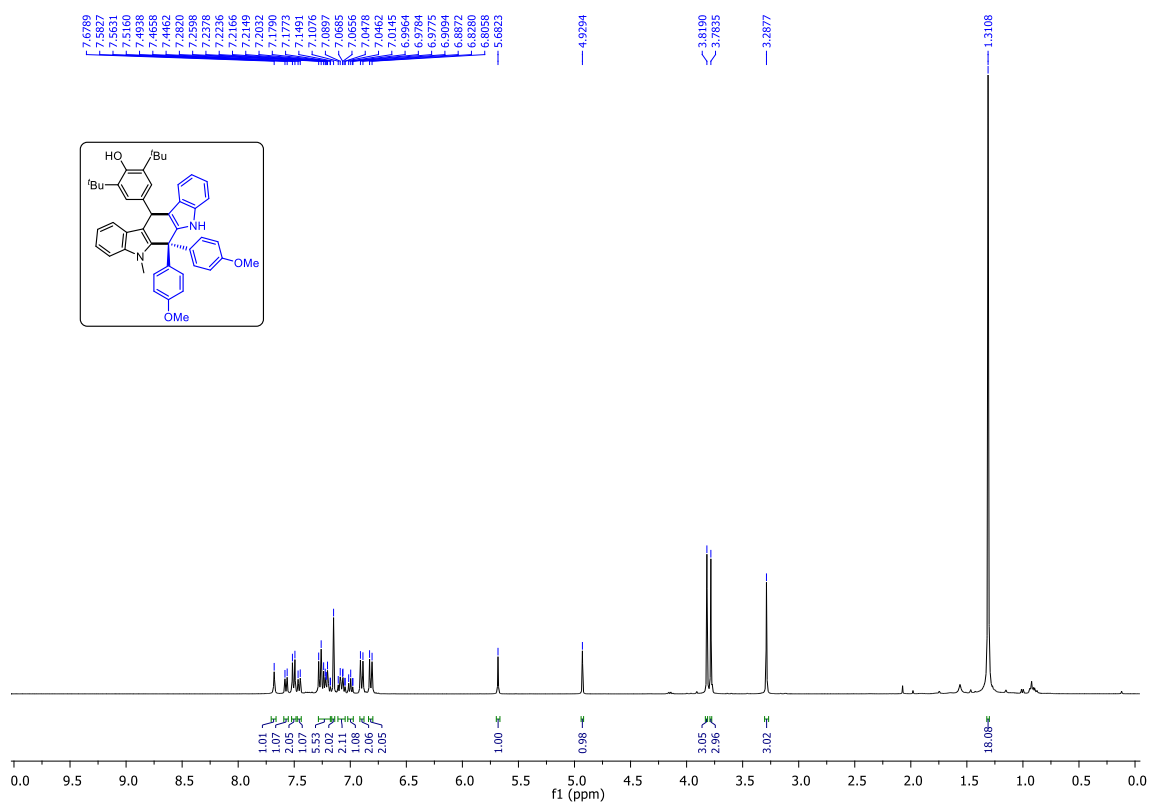
¹H NMR (400 MHz, CDCl₃) Spectrum of **3s**



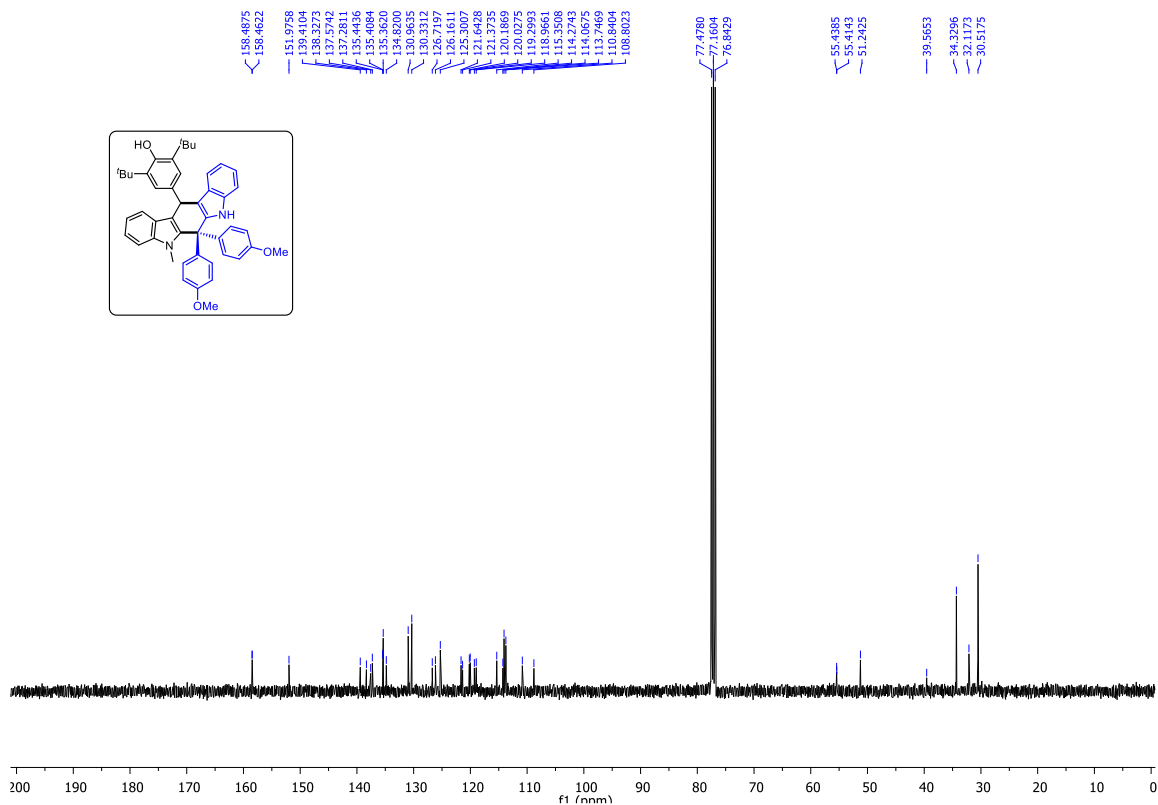
¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of **3s**



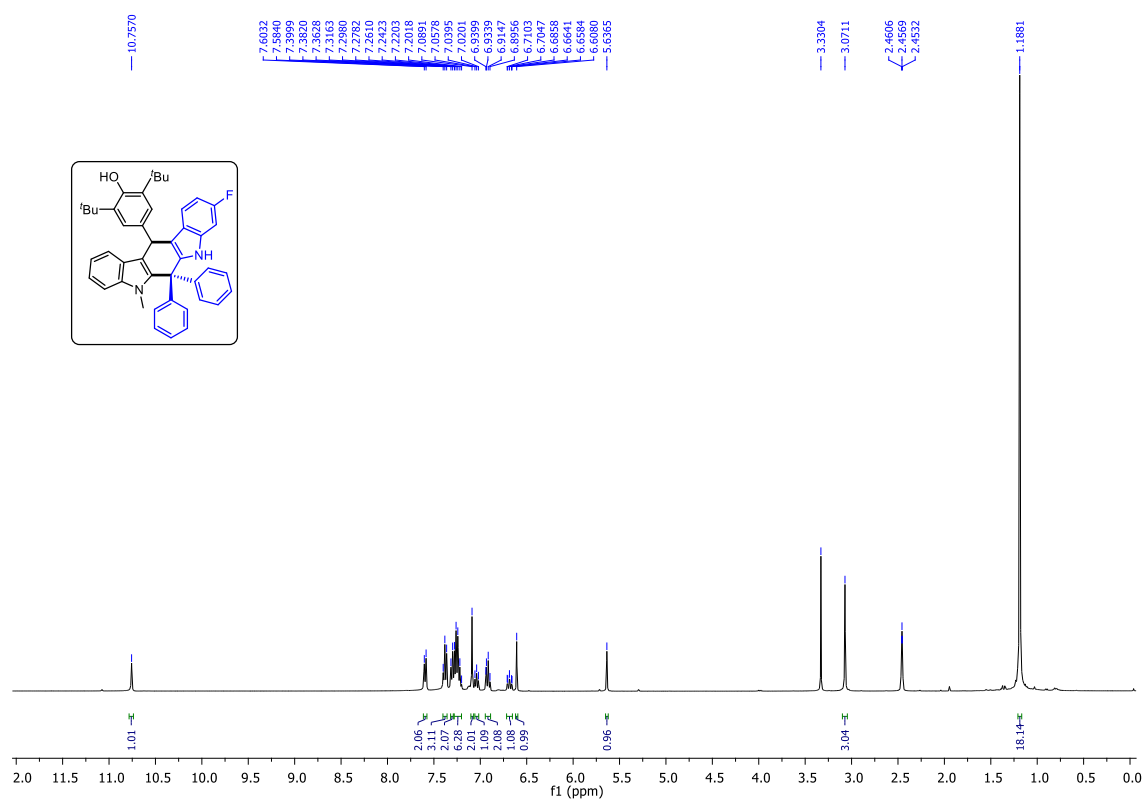
¹H NMR (400 MHz, CDCl₃) Spectrum of **3t**



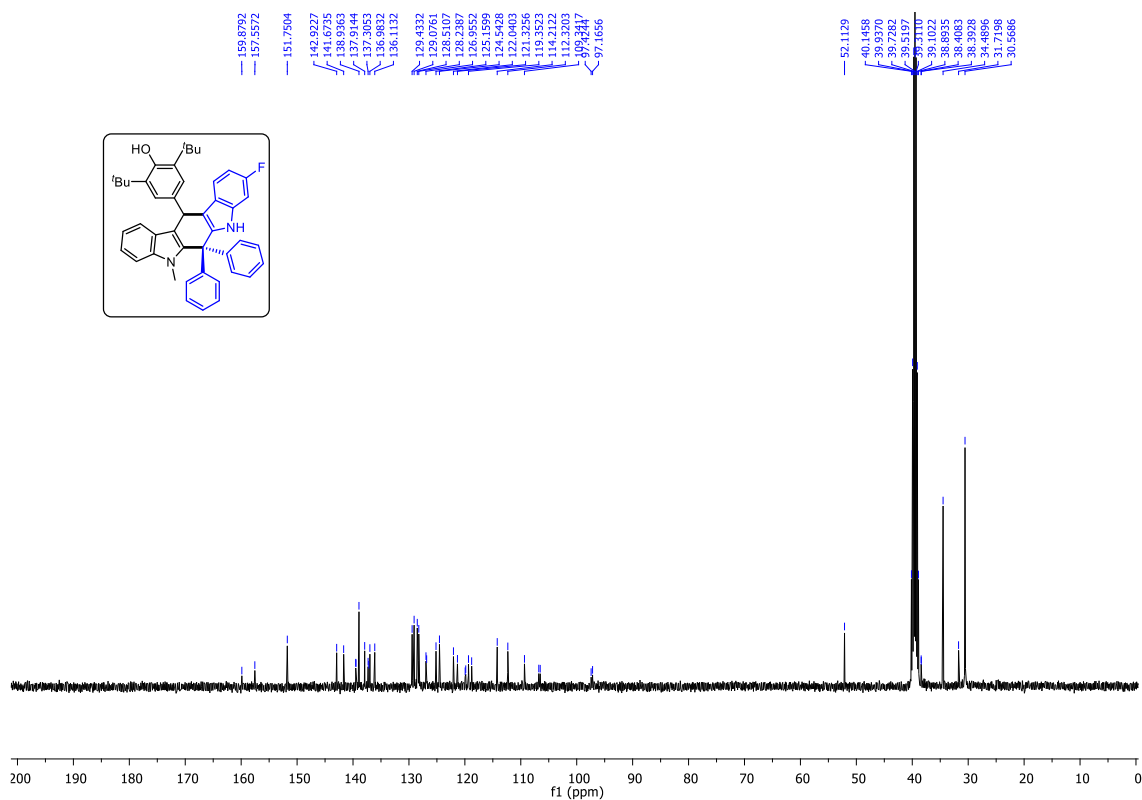
¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of **3t**



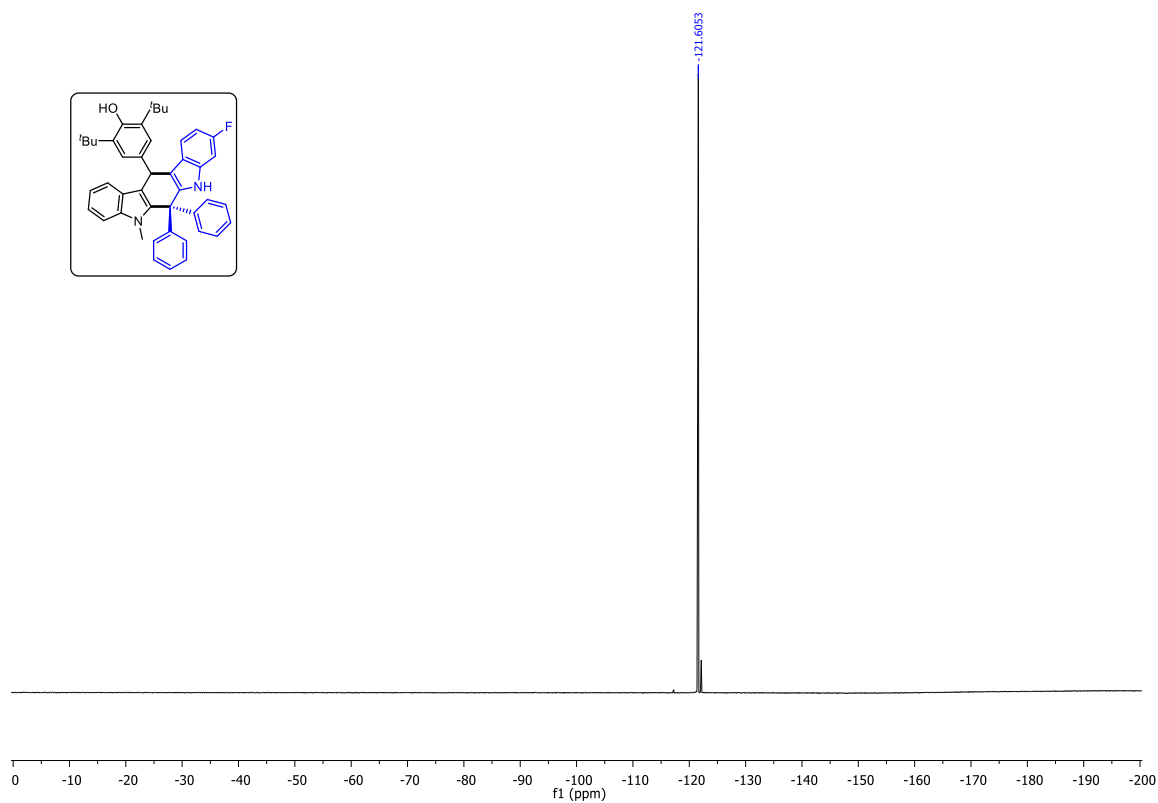
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **3u**



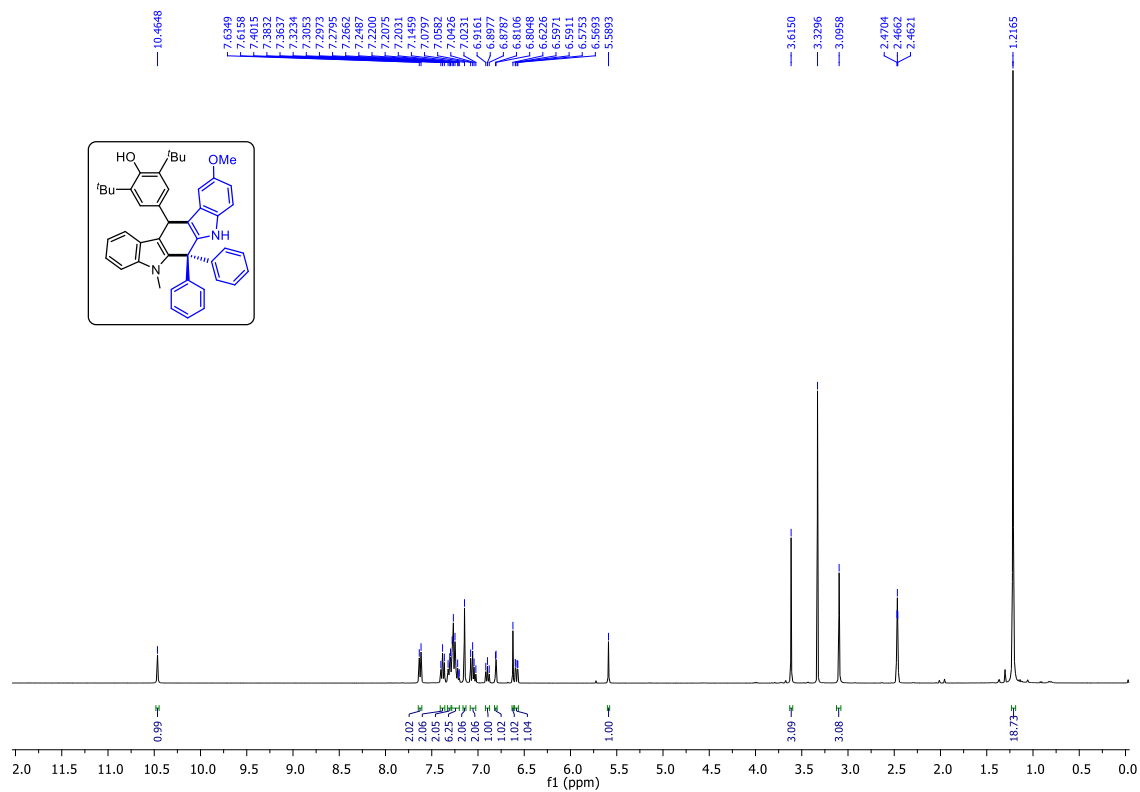
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **3u**



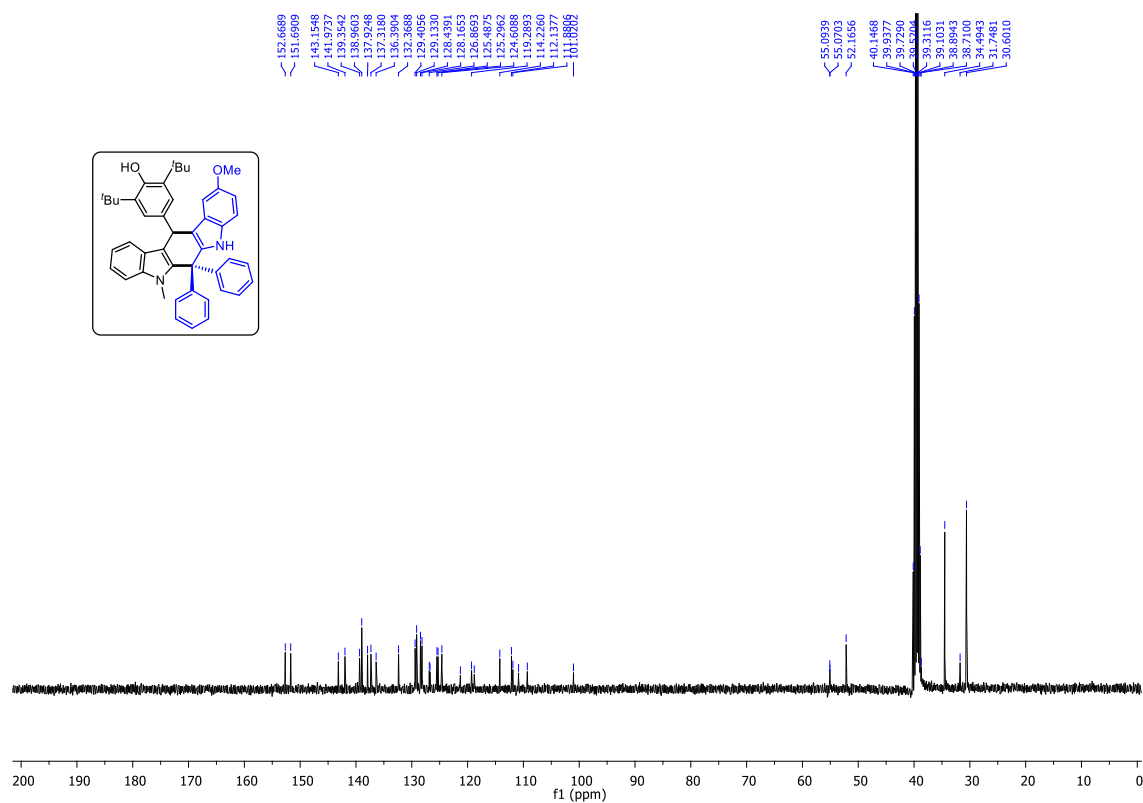
^{19}F $\{^1\text{H}\}$ NMR (376 MHz, DMSO- d_6) Spectrum of **3u**



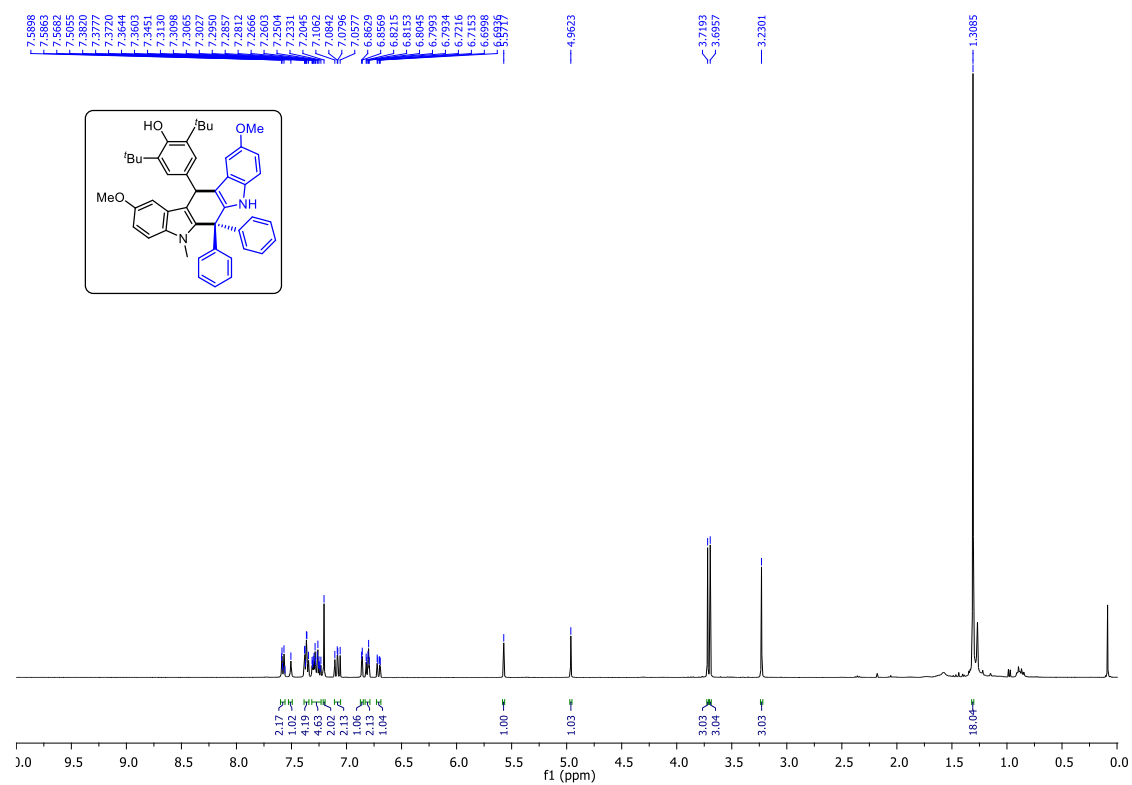
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **3v**



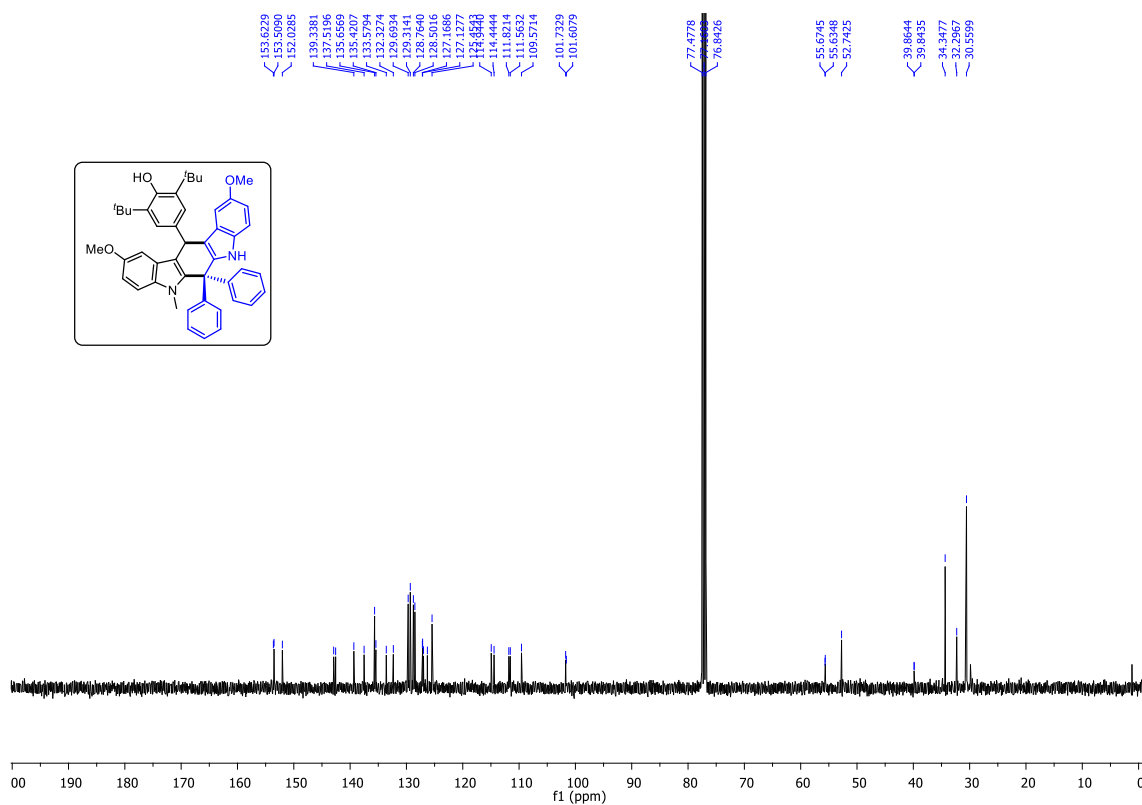
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **3v**



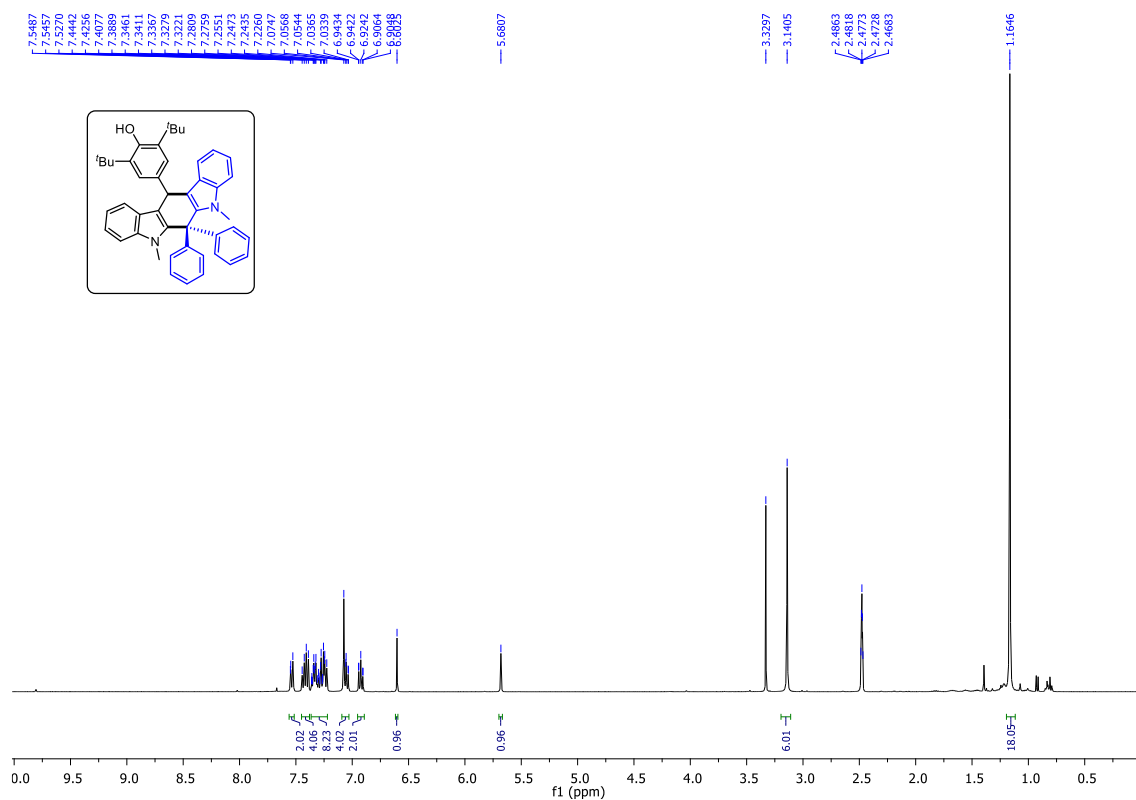
^1H NMR (400 MHz, CDCl_3) Spectrum of **3w**



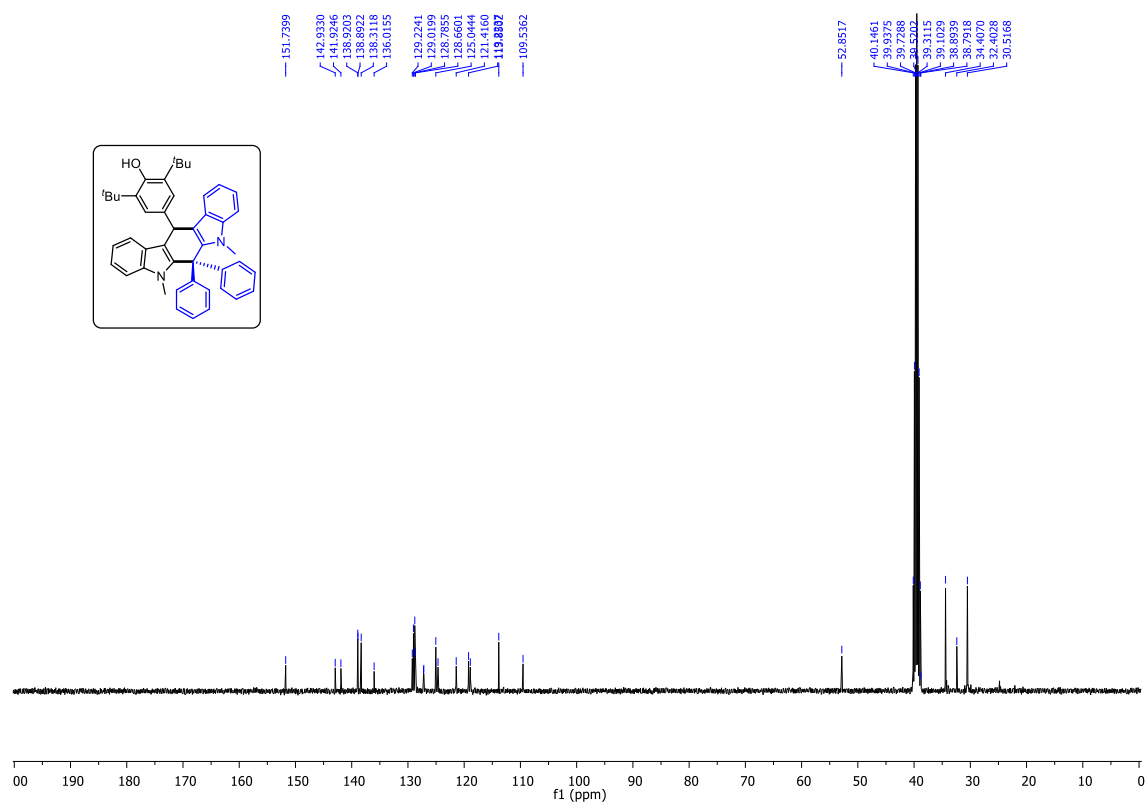
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3w**



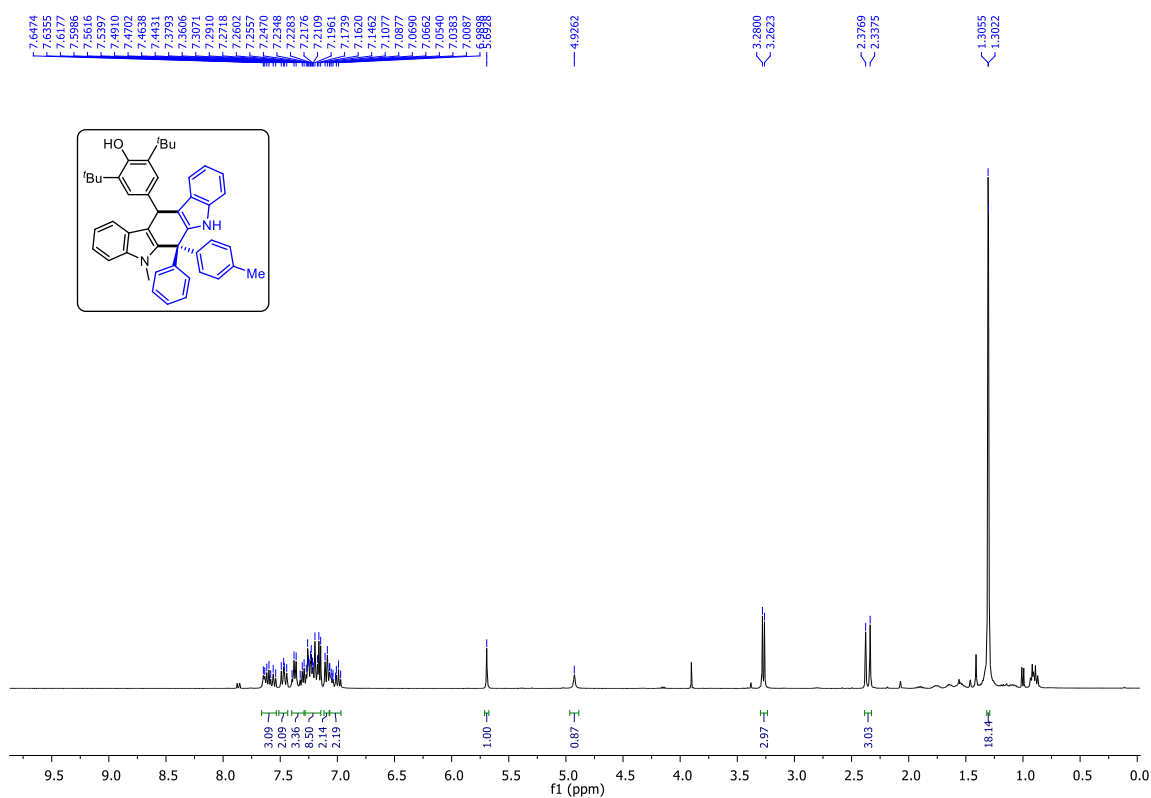
^1H NMR (400 MHz, CDCl_3) Spectrum of **3x**



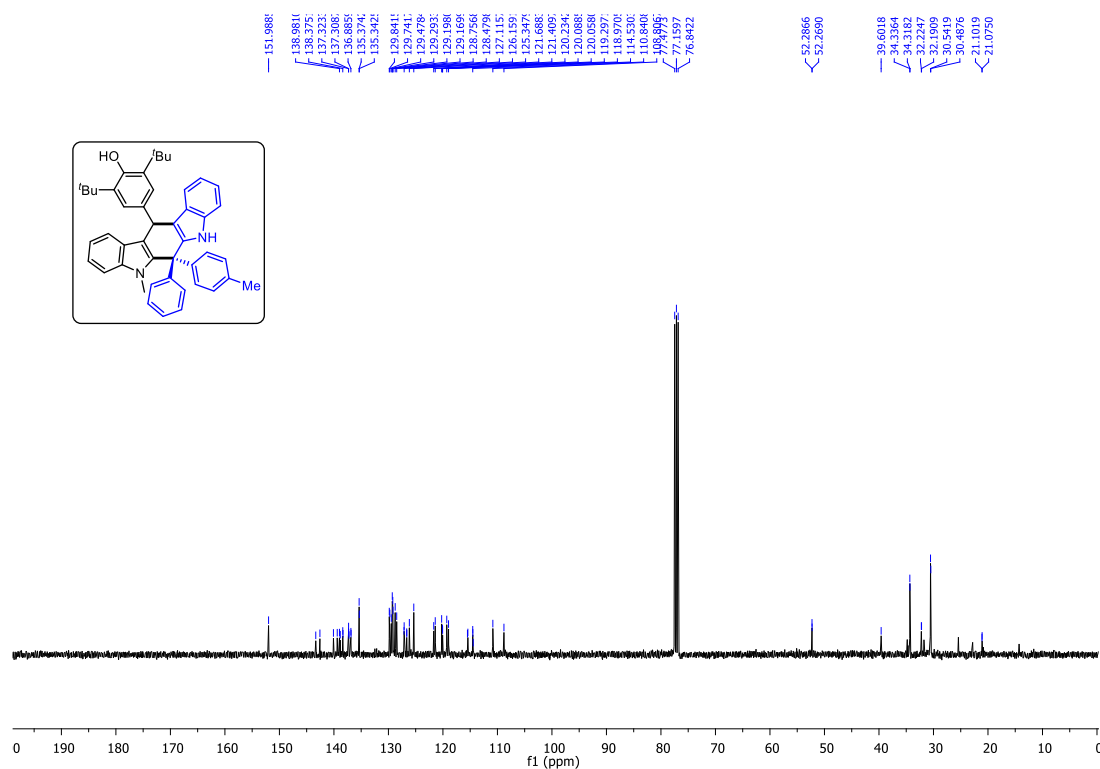
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3x**



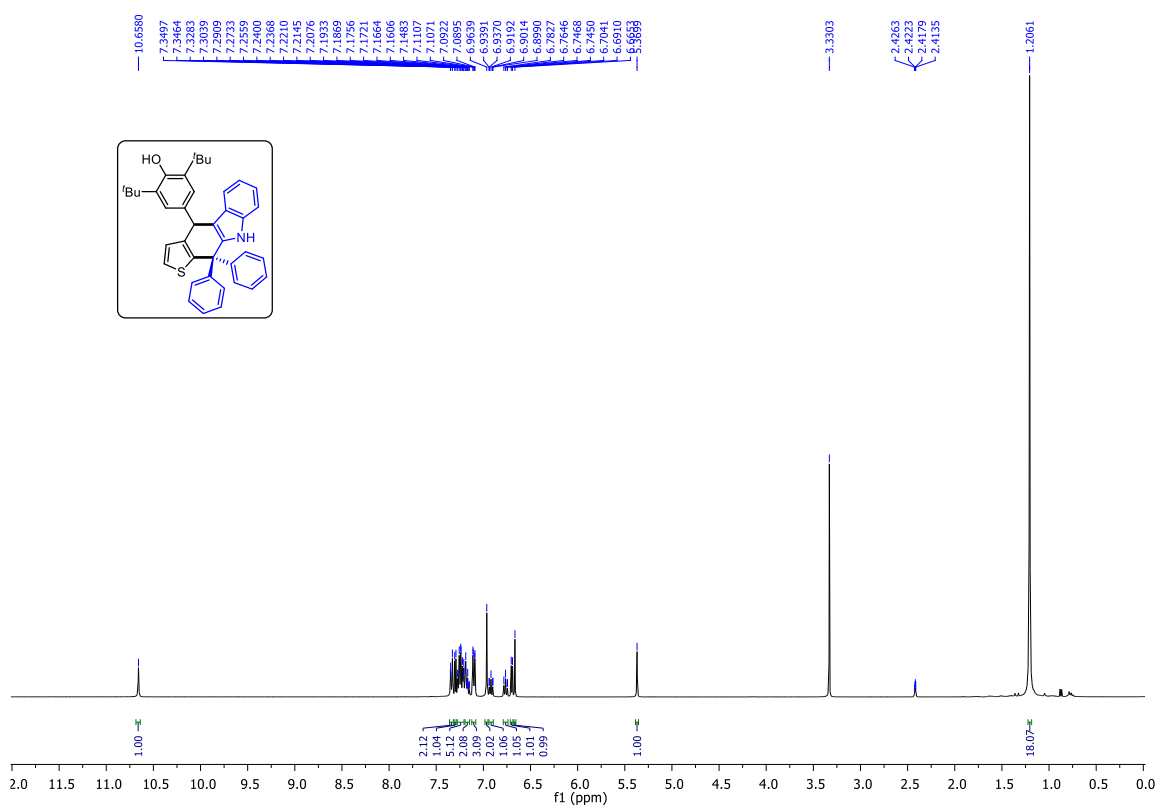
^1H NMR (400 MHz, CDCl_3) Spectrum of **3y**



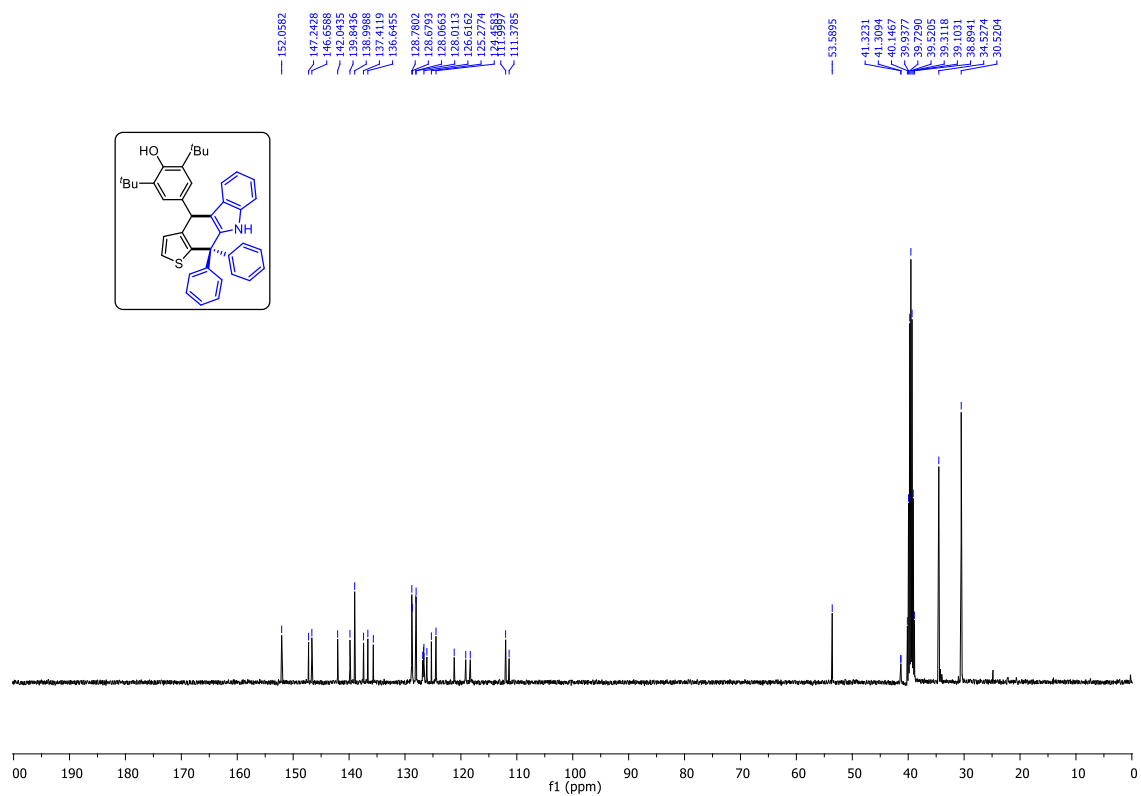
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **3y**



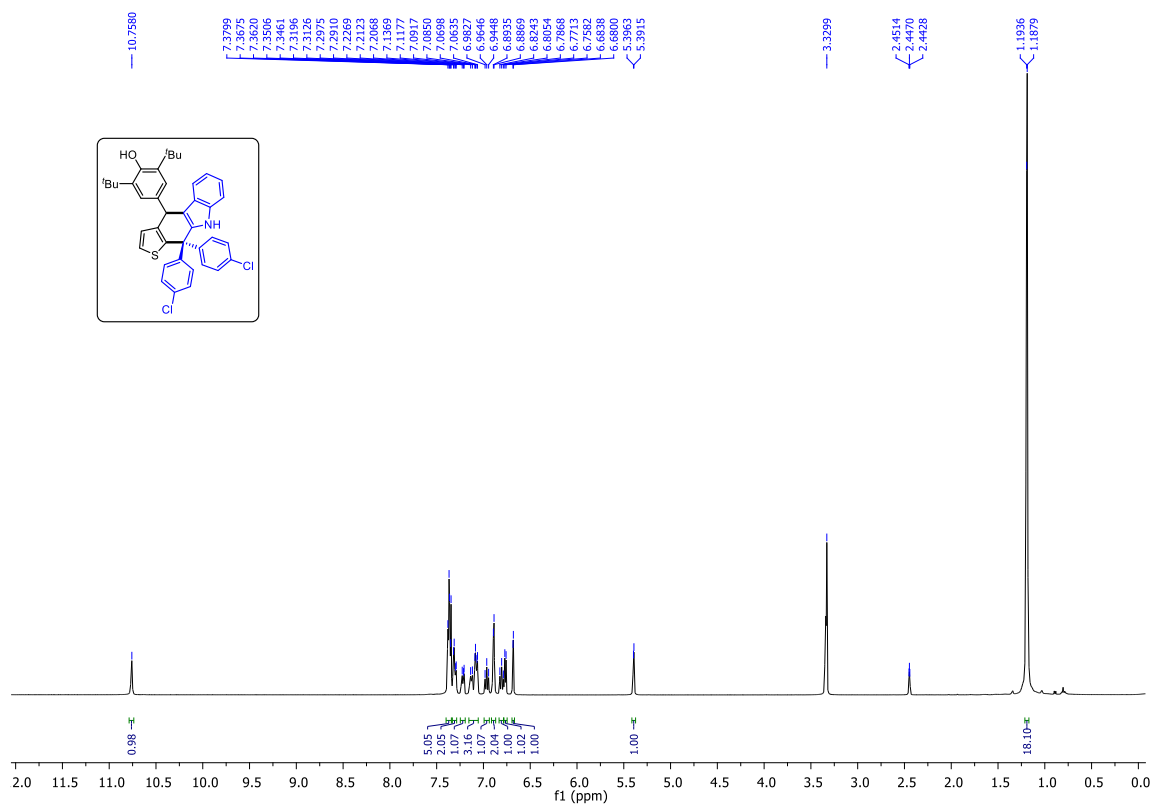
^1H NMR (400 MHz, DMSO-d_6) Spectrum of **5a**



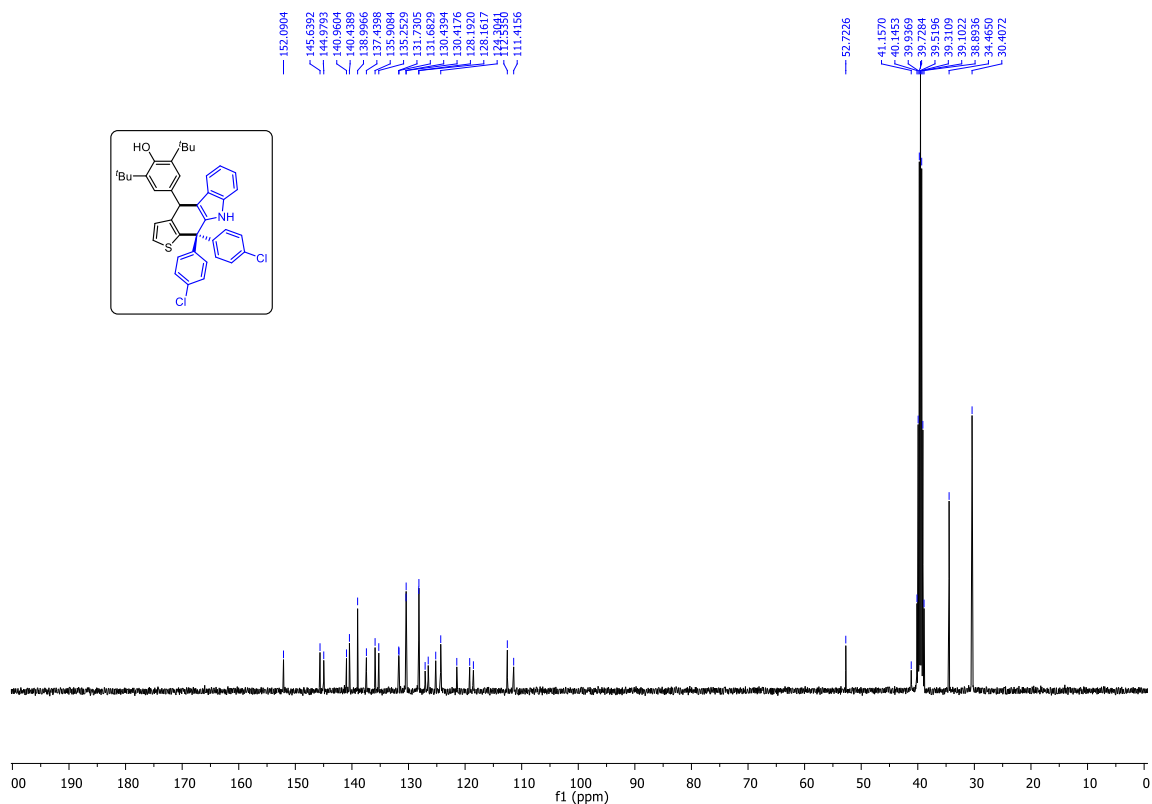
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **5a**



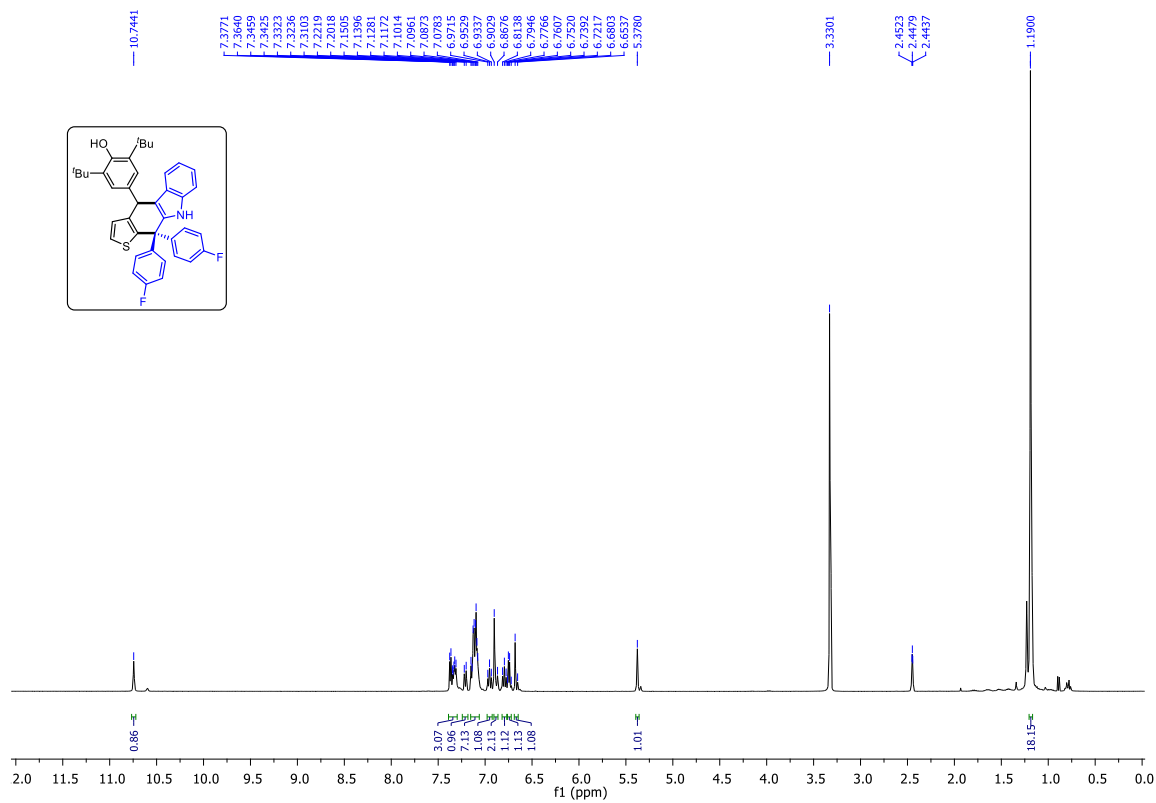
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **5b**



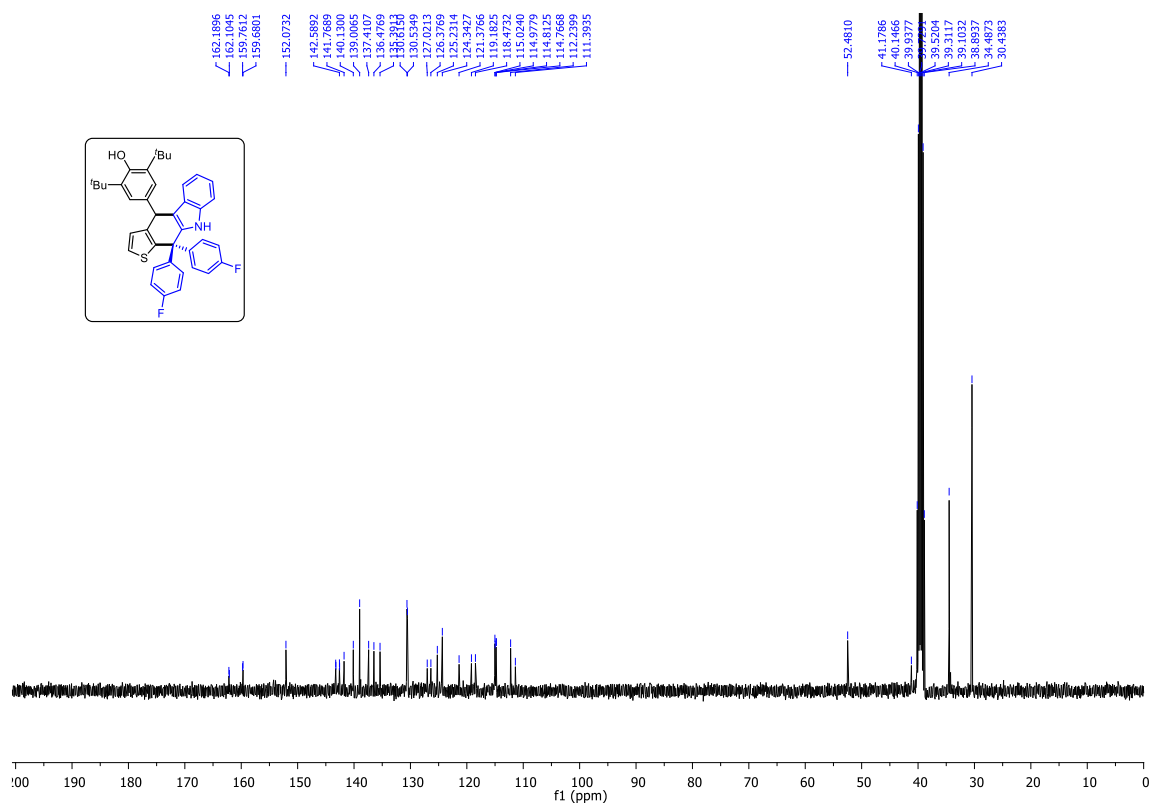
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **5b**



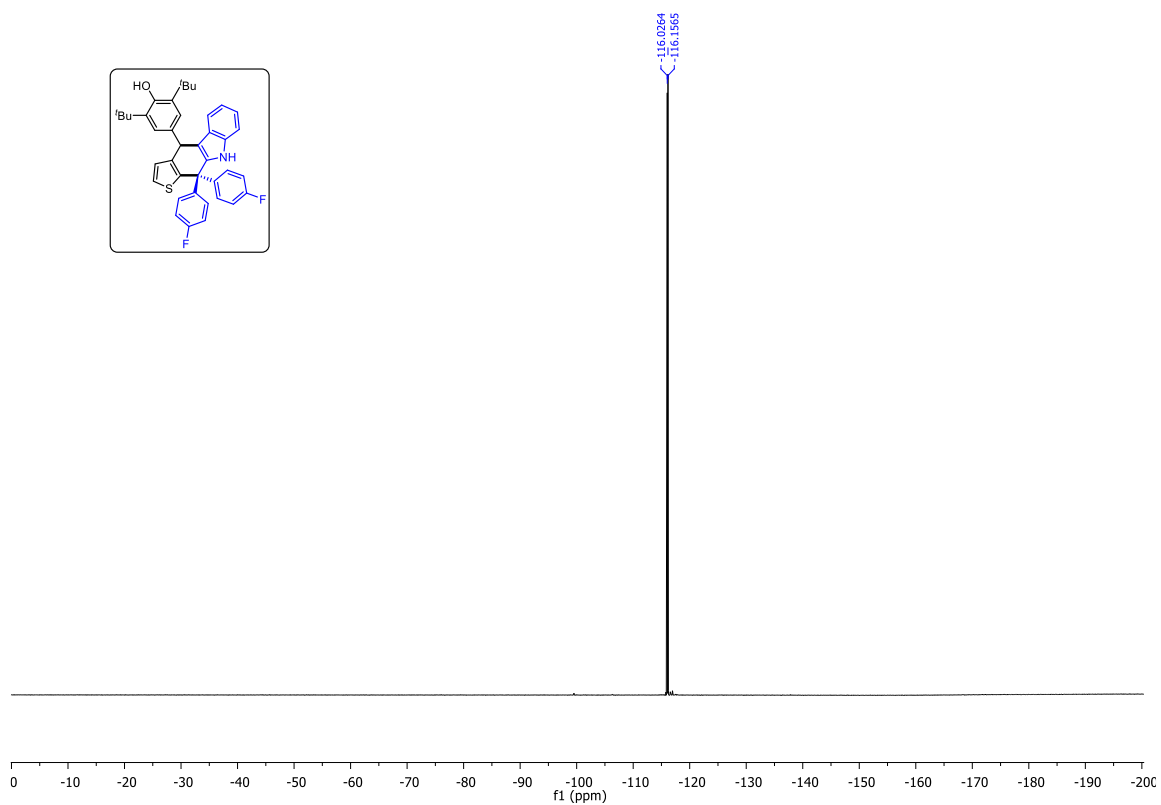
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **5c**



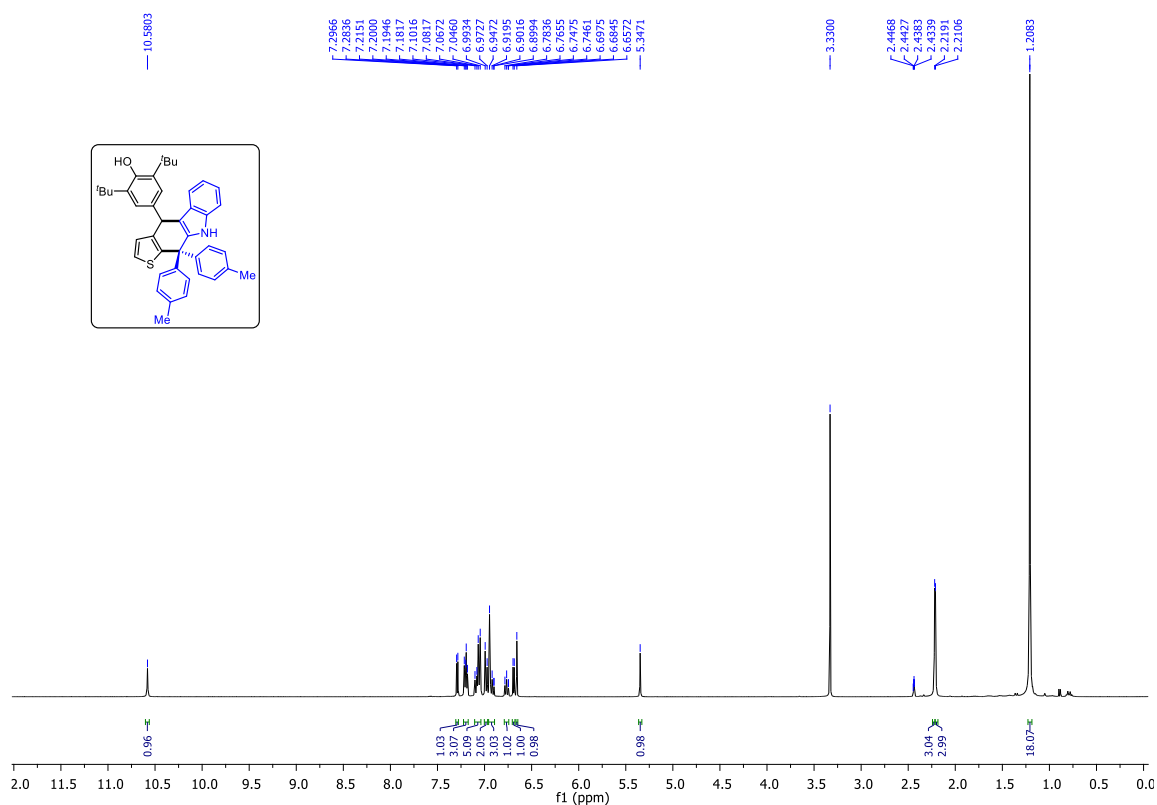
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **5c**



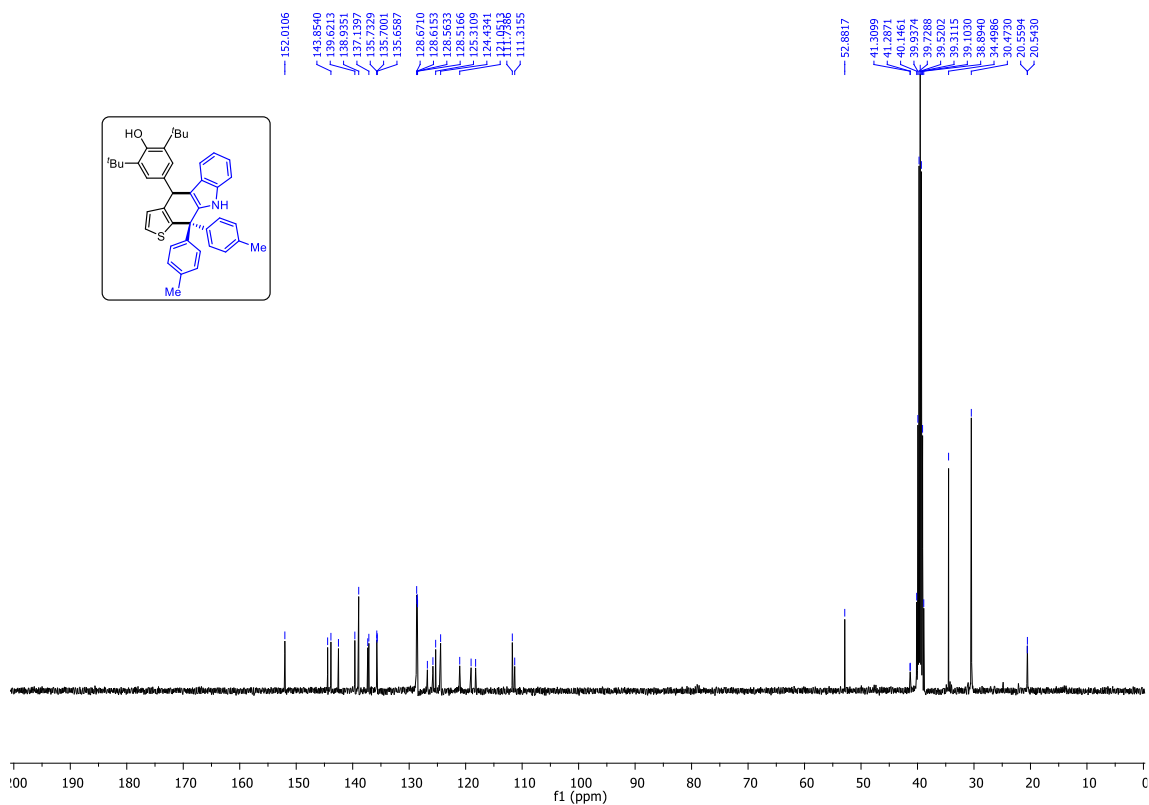
^{19}F $\{^1\text{H}\}$ NMR (376 MHz, DMSO- d_6) Spectrum of **5c**



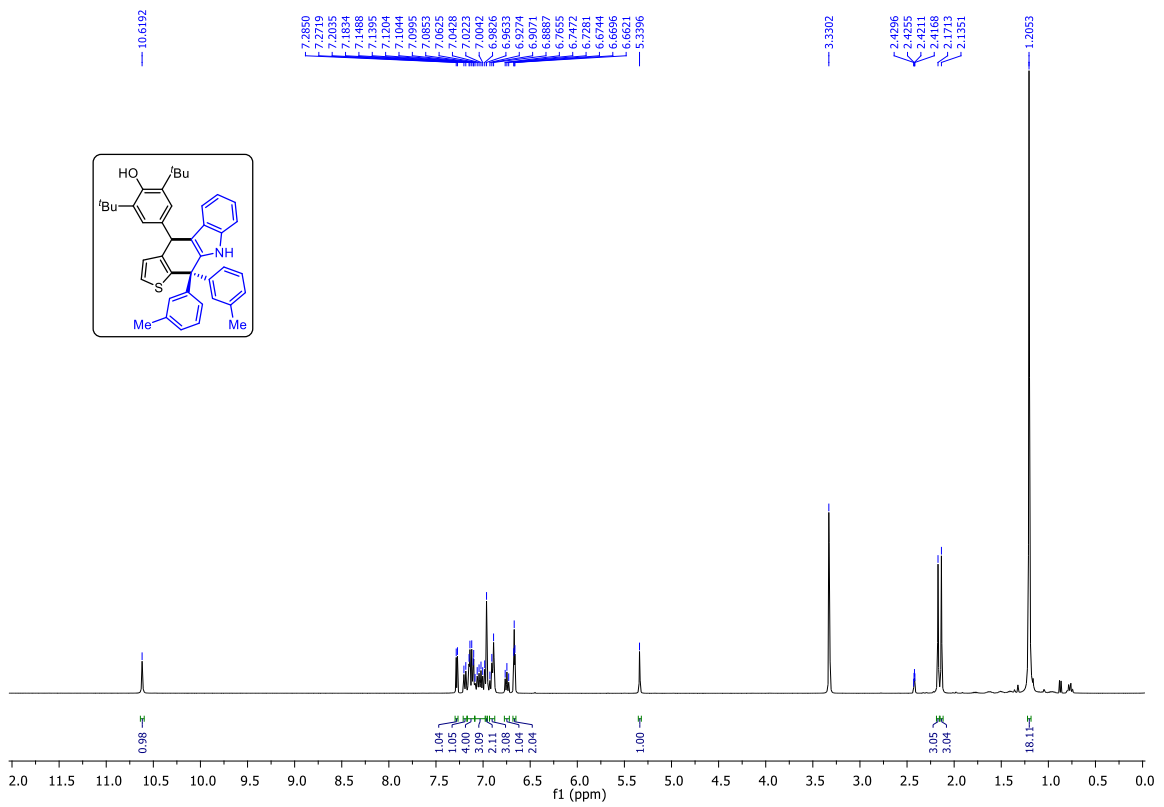
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **5d**



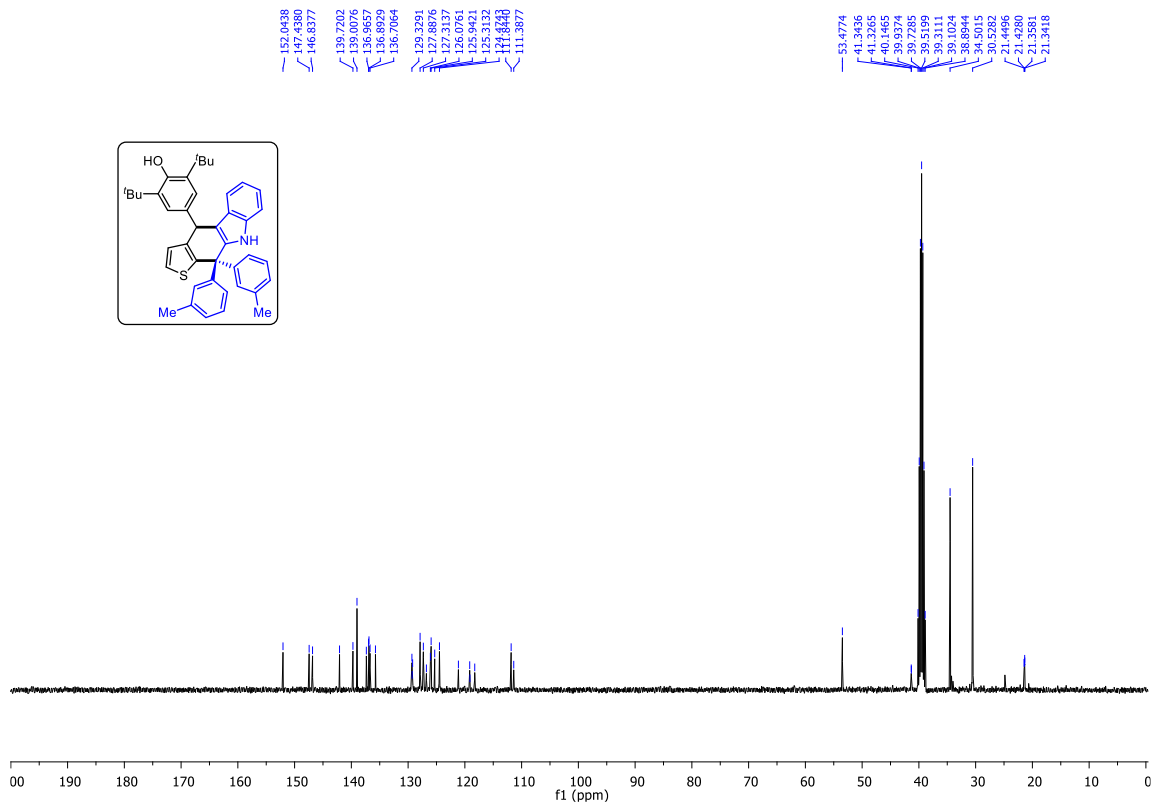
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **5d**



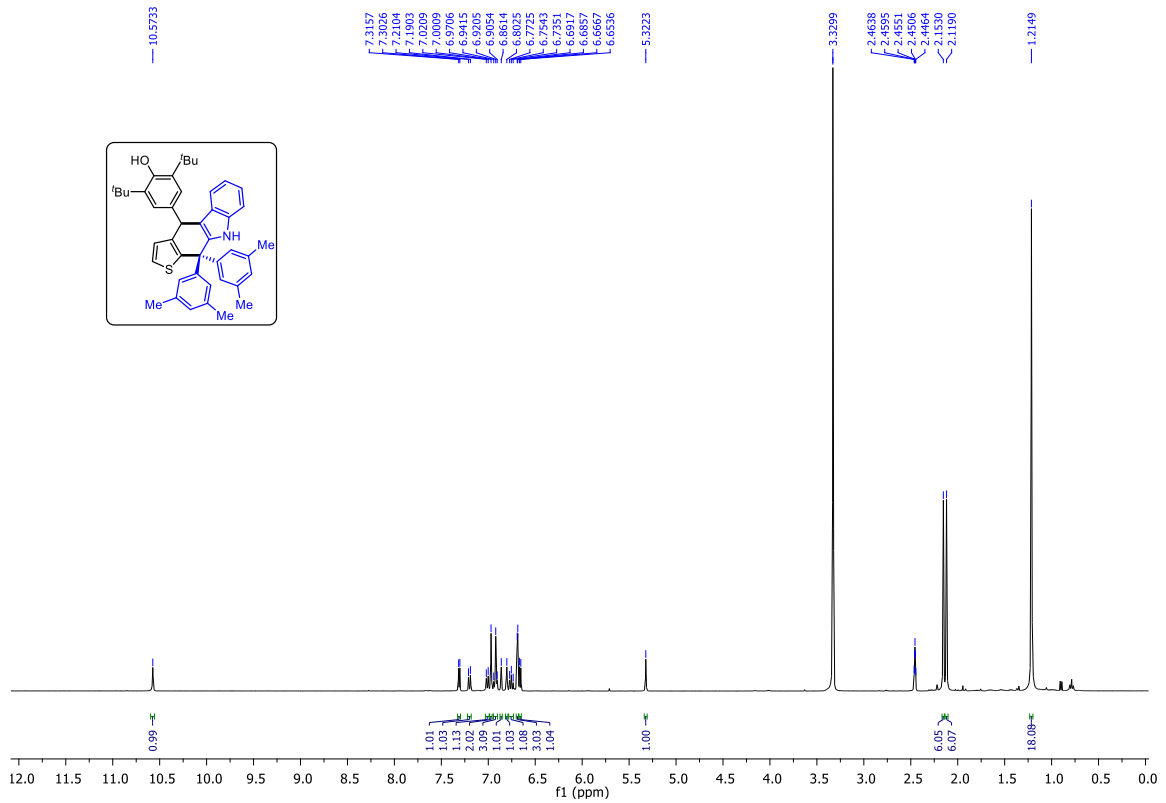
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **5e**



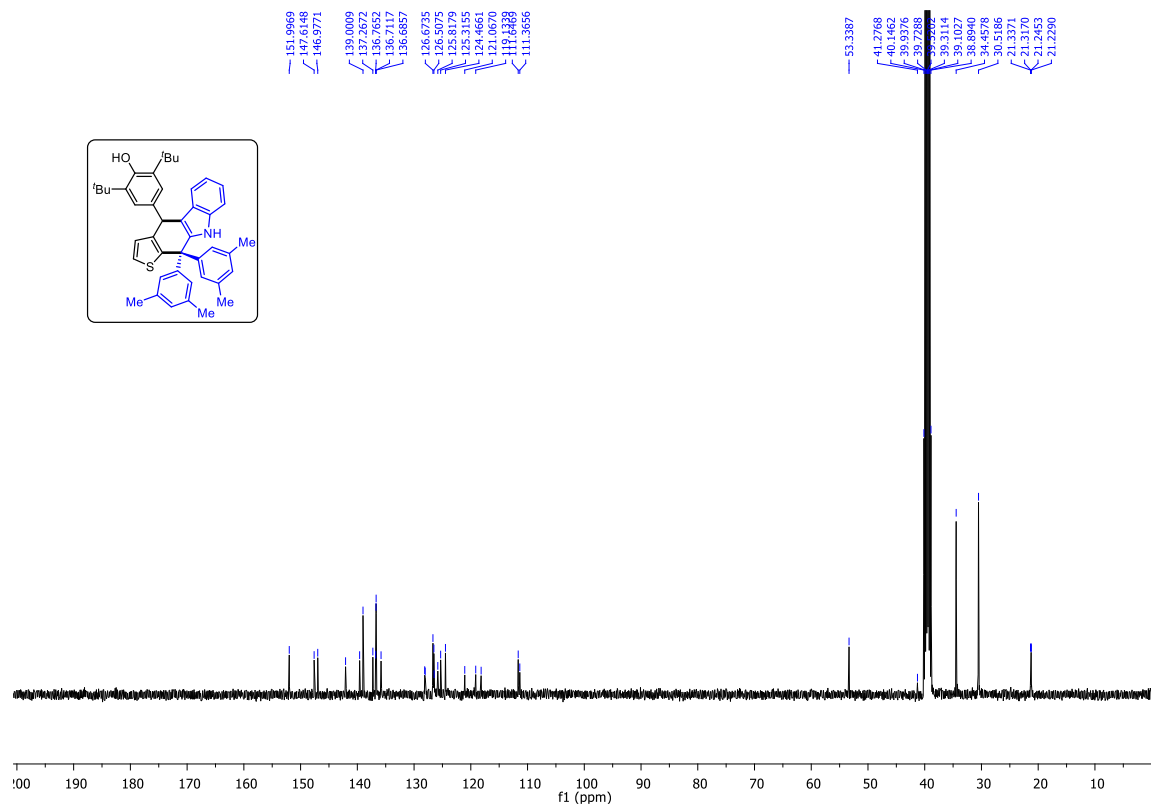
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **5e**



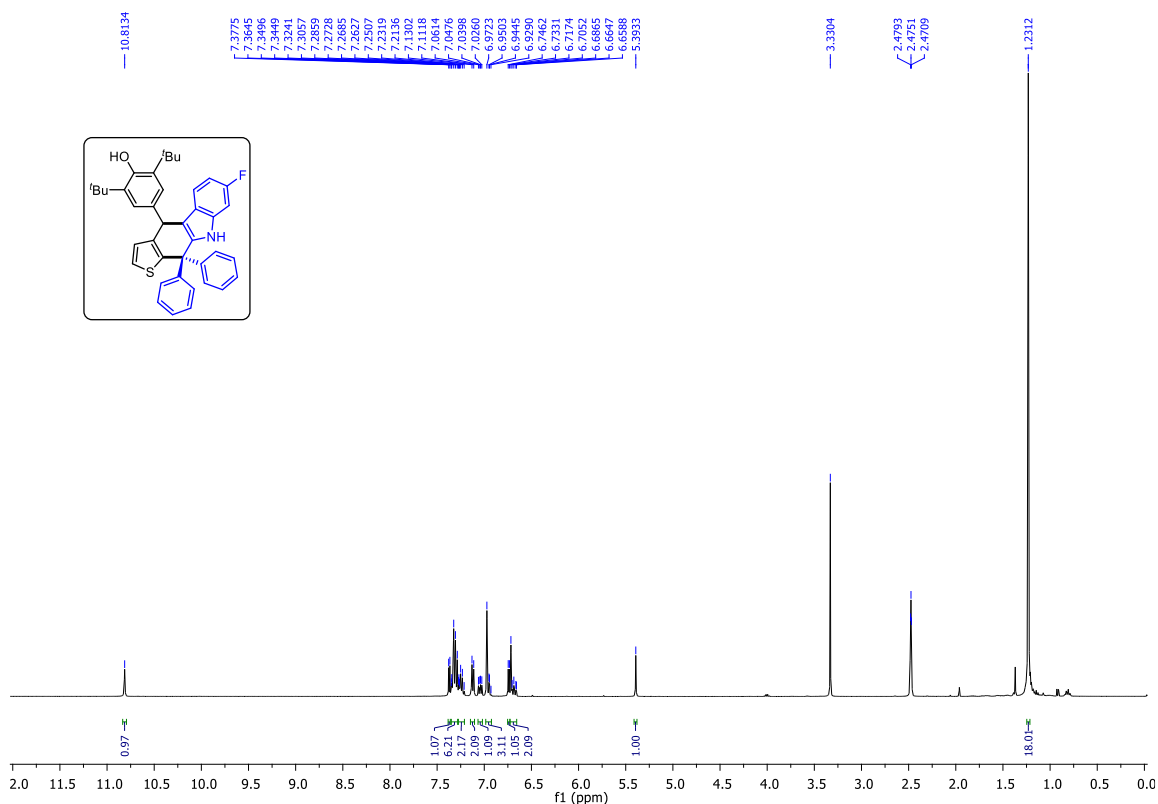
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **5f**



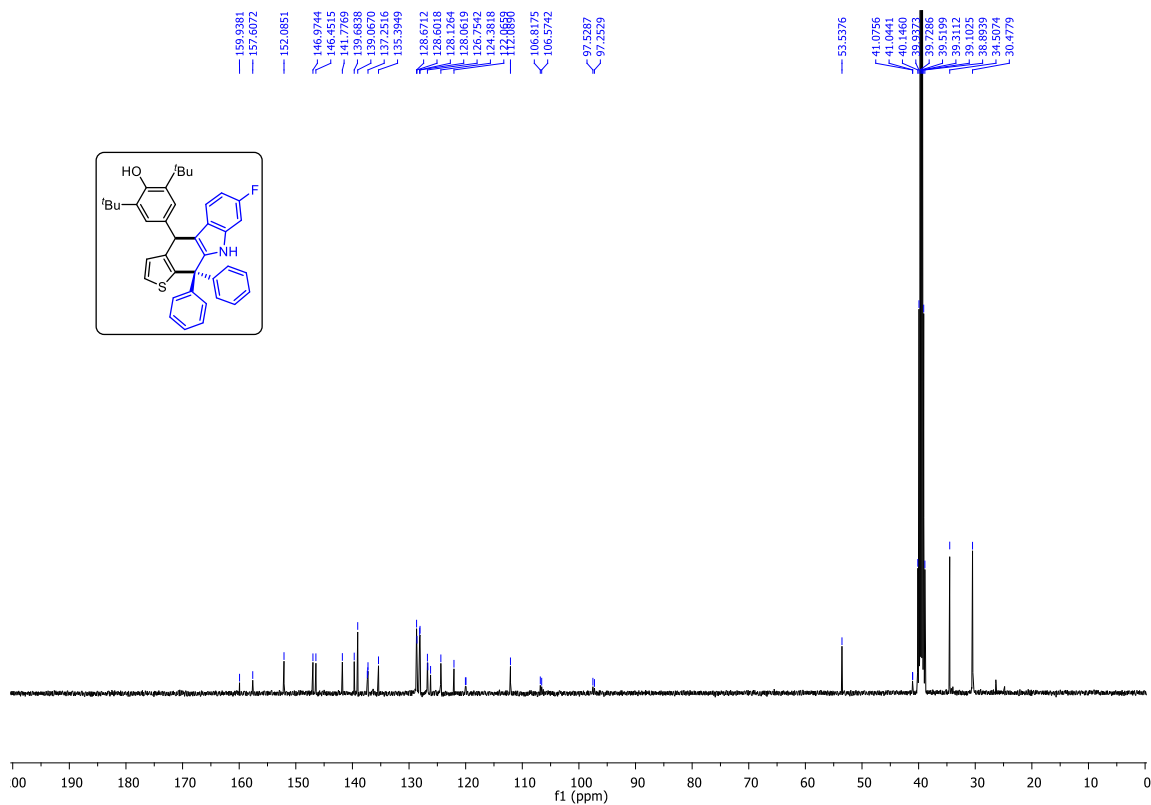
^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) Spectrum of **5f**



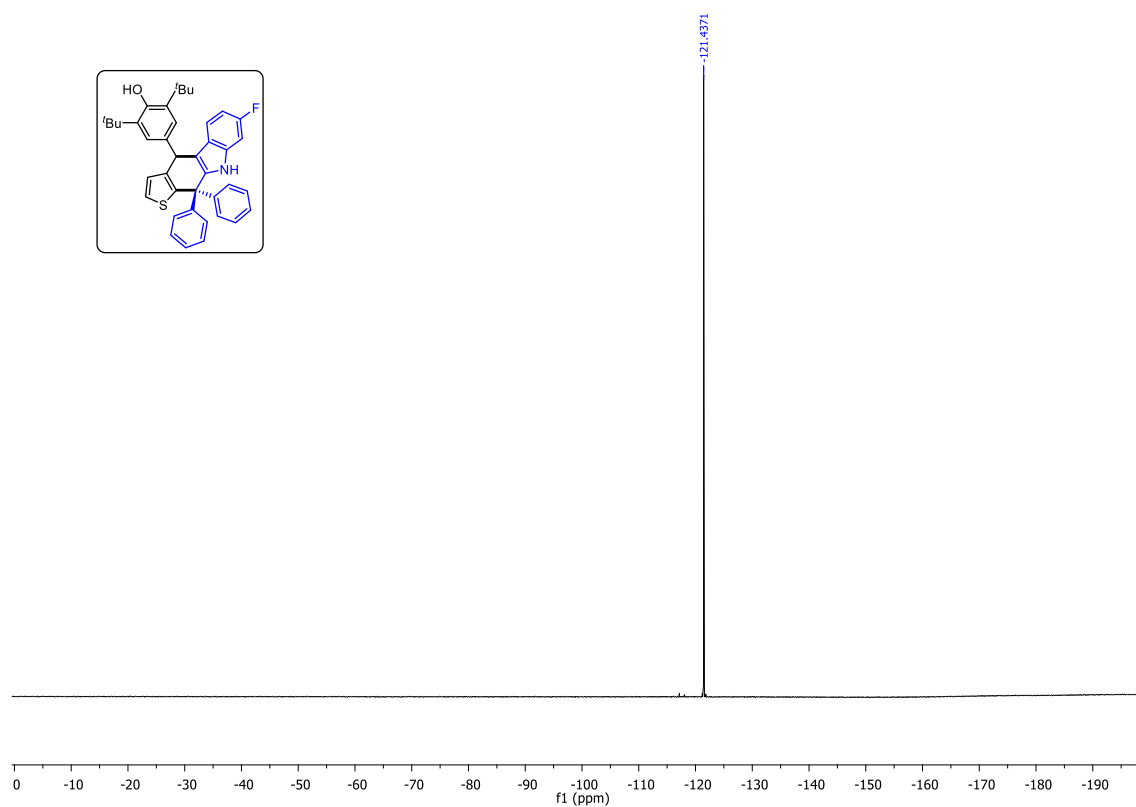
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **5g**



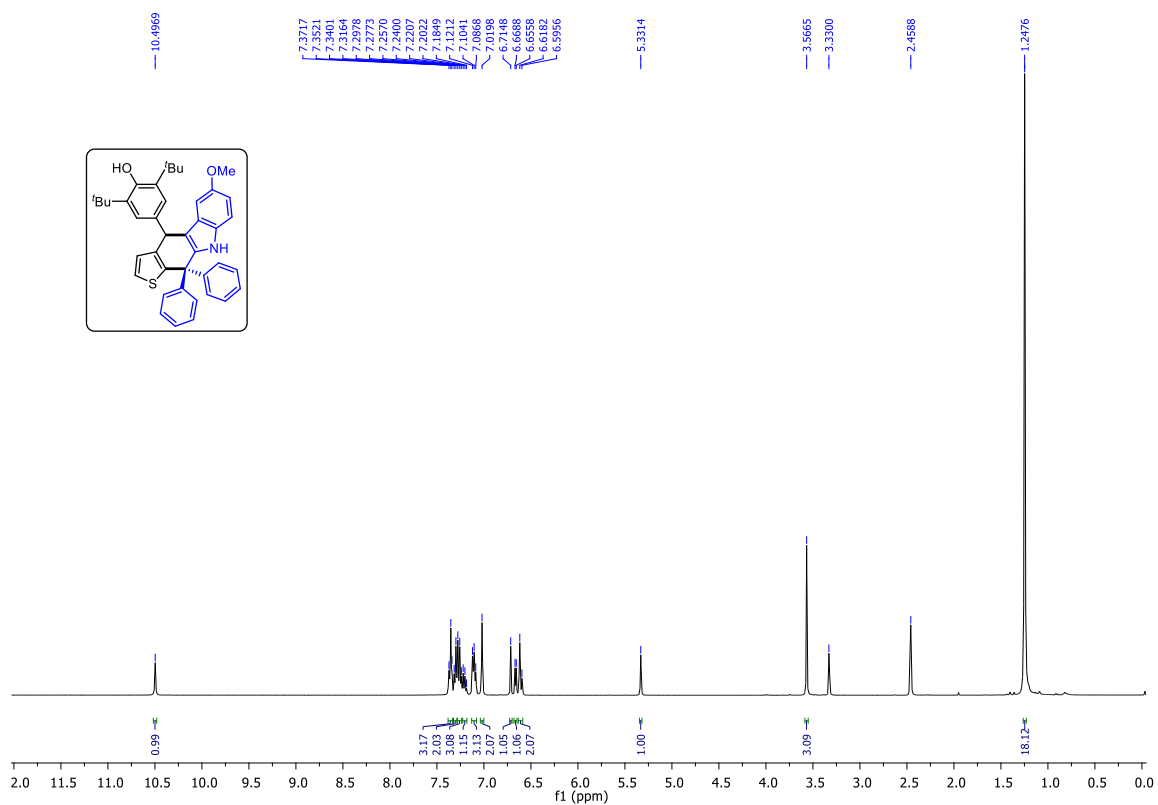
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **5g**



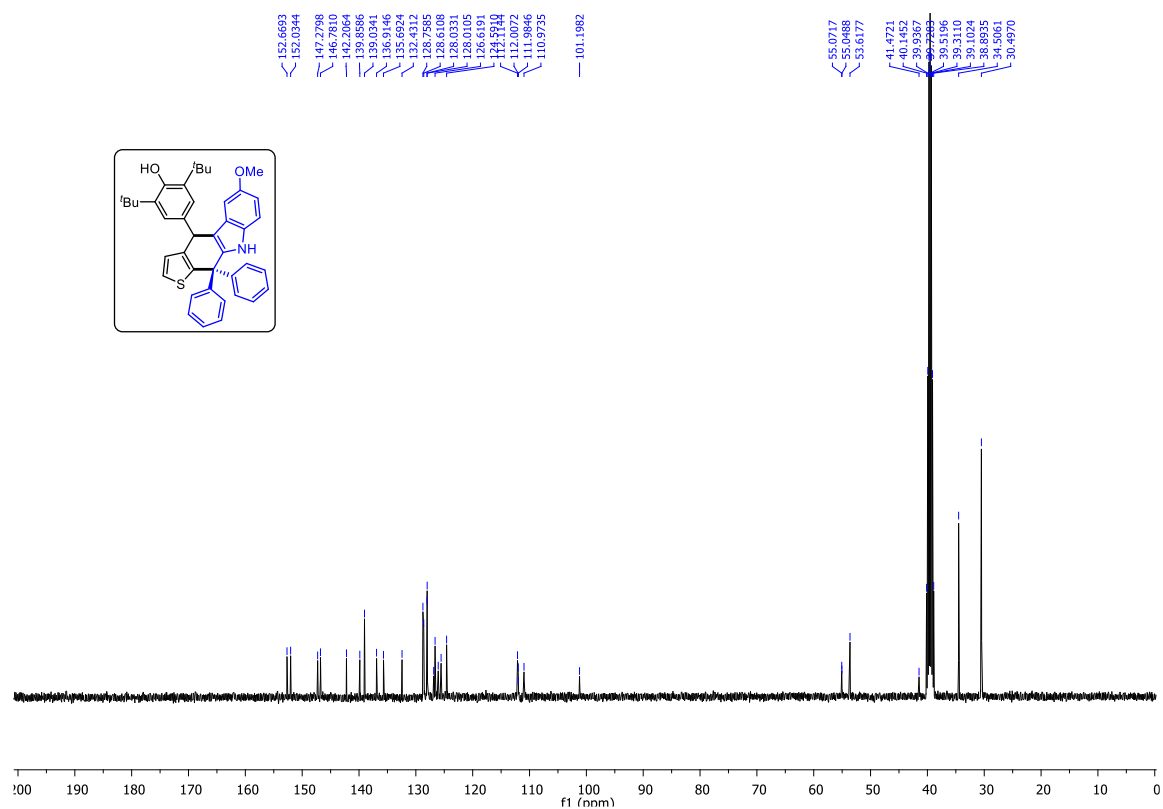
^{19}F $\{^1\text{H}\}$ NMR (376 MHz, DMSO- d_6) Spectrum of **5g**



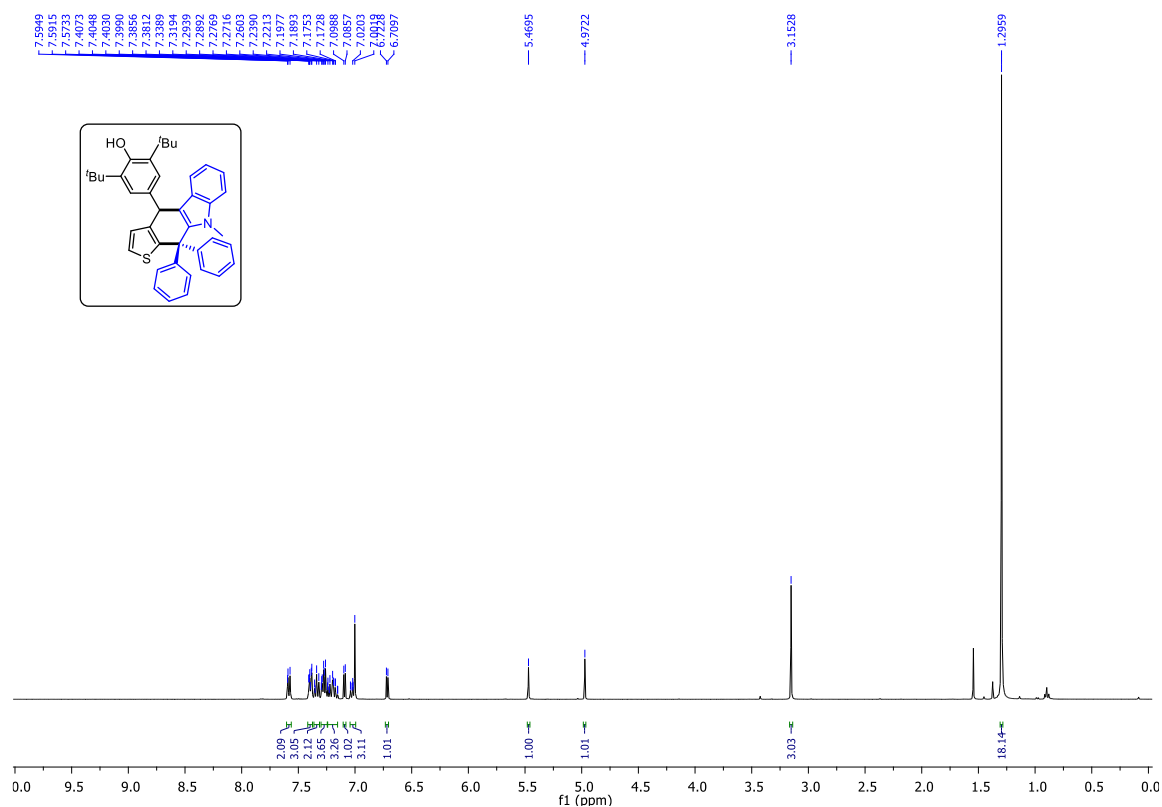
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **5h**



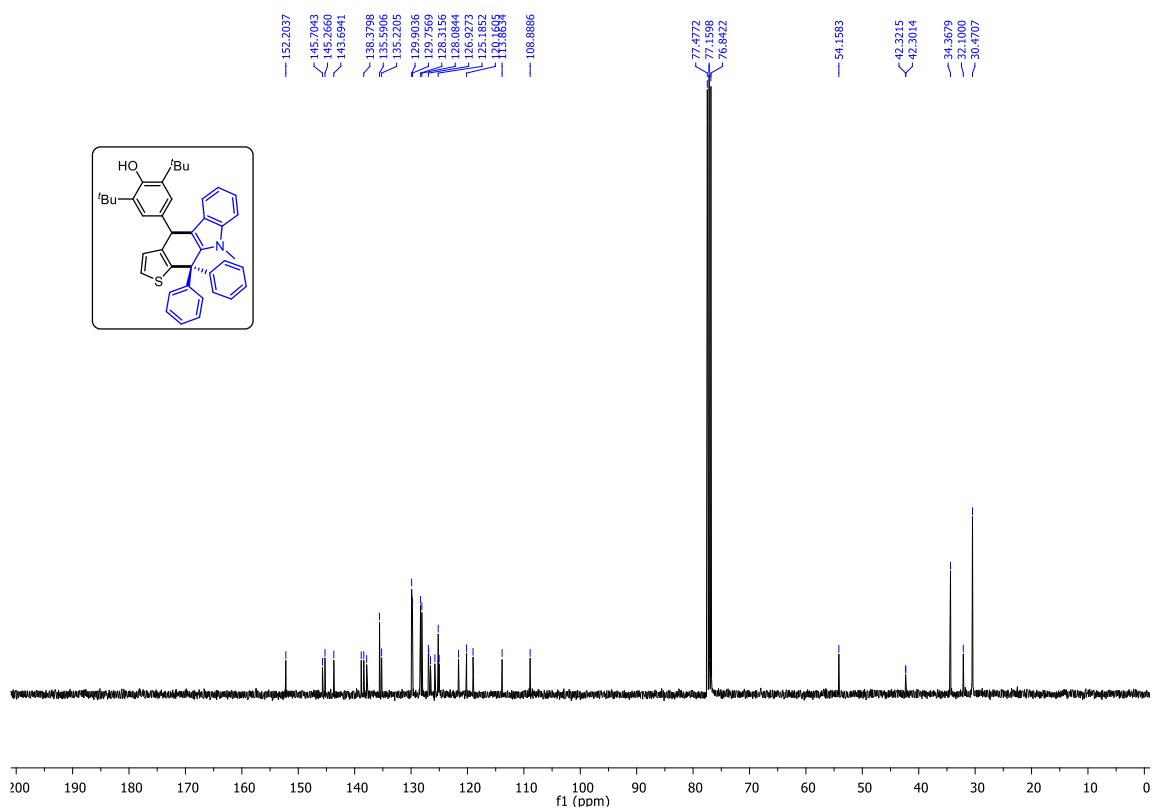
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **5h**



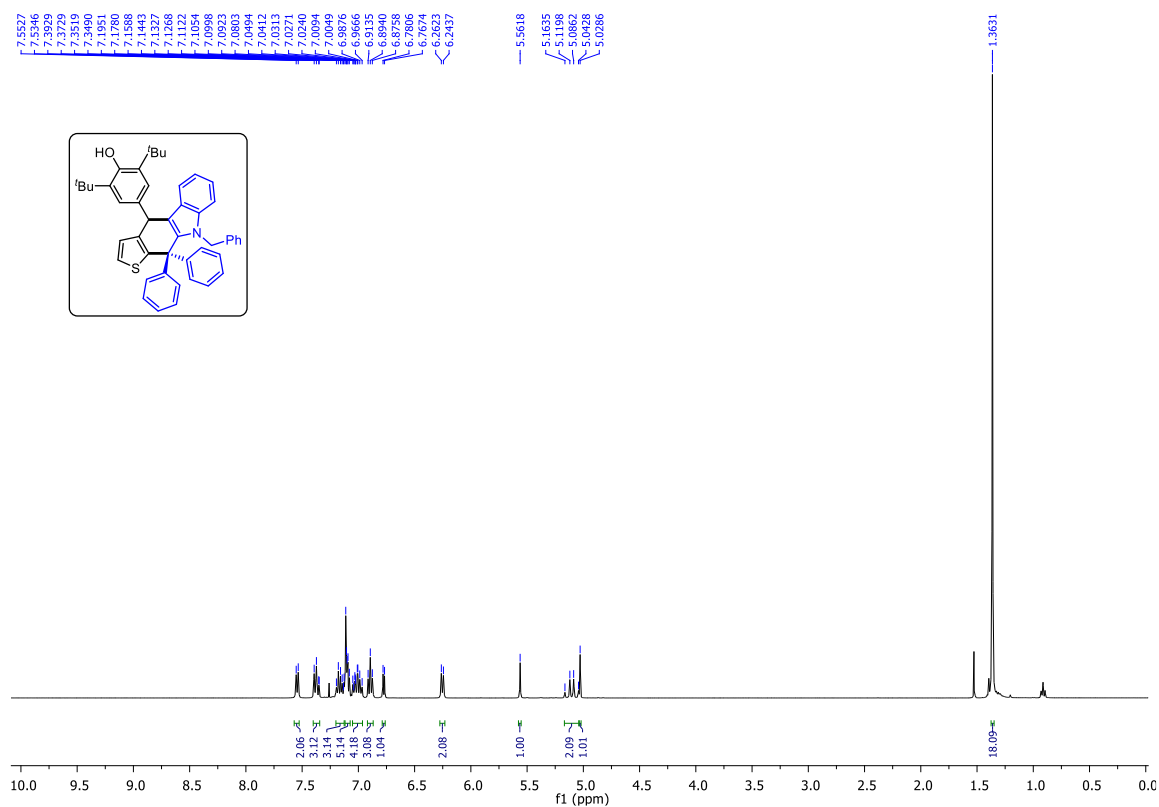
^1H NMR (400 MHz, CDCl_3) Spectrum of **5i**



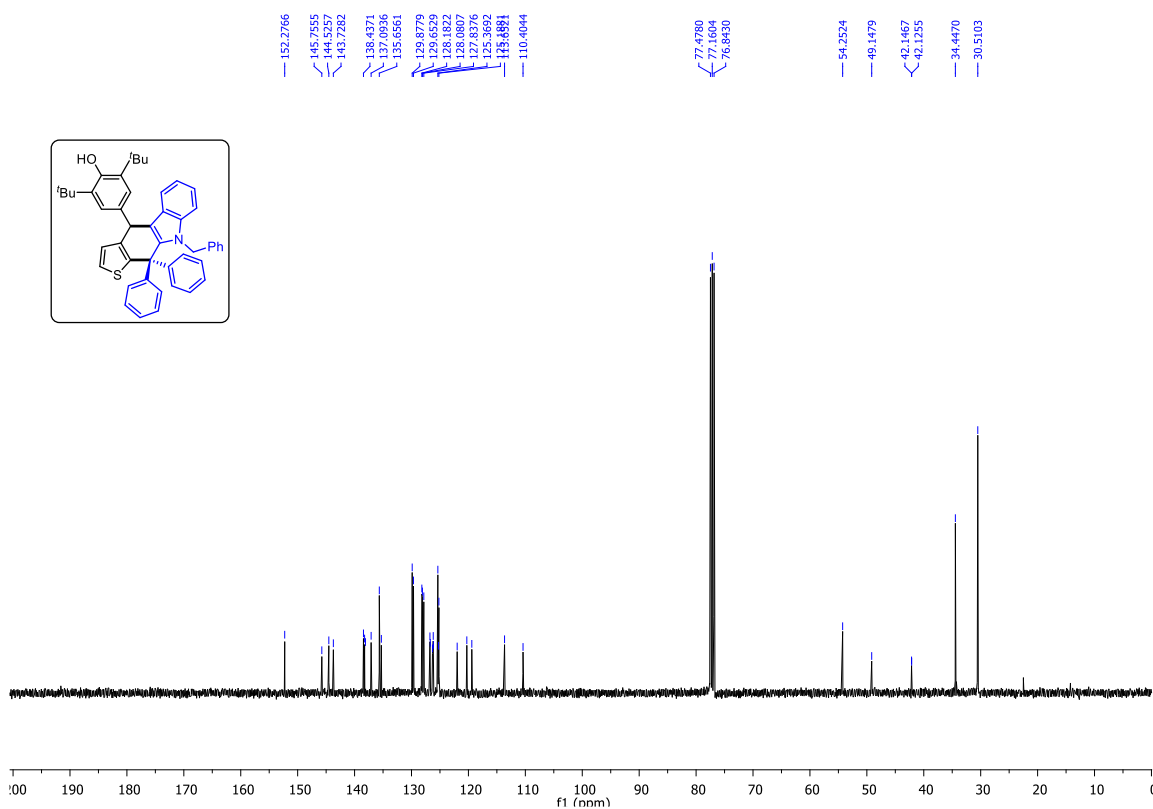
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **5i**



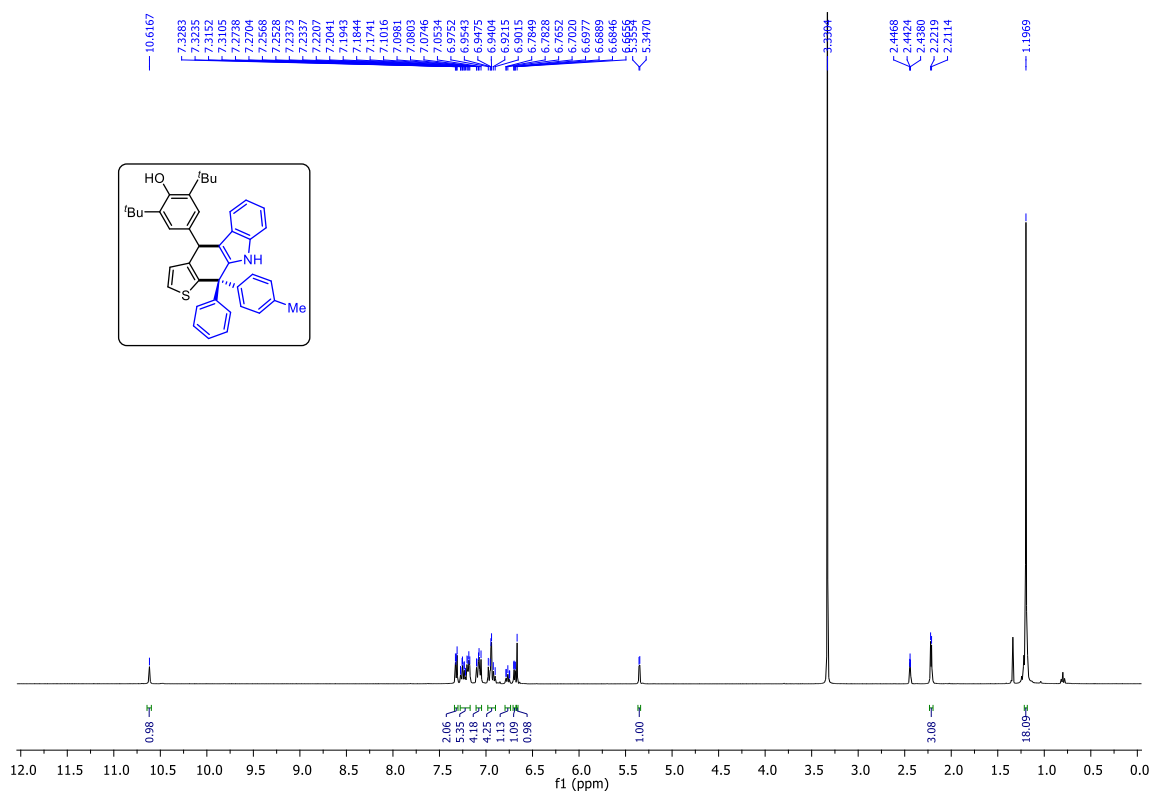
^1H NMR (400 MHz, CDCl_3) Spectrum of **5j**



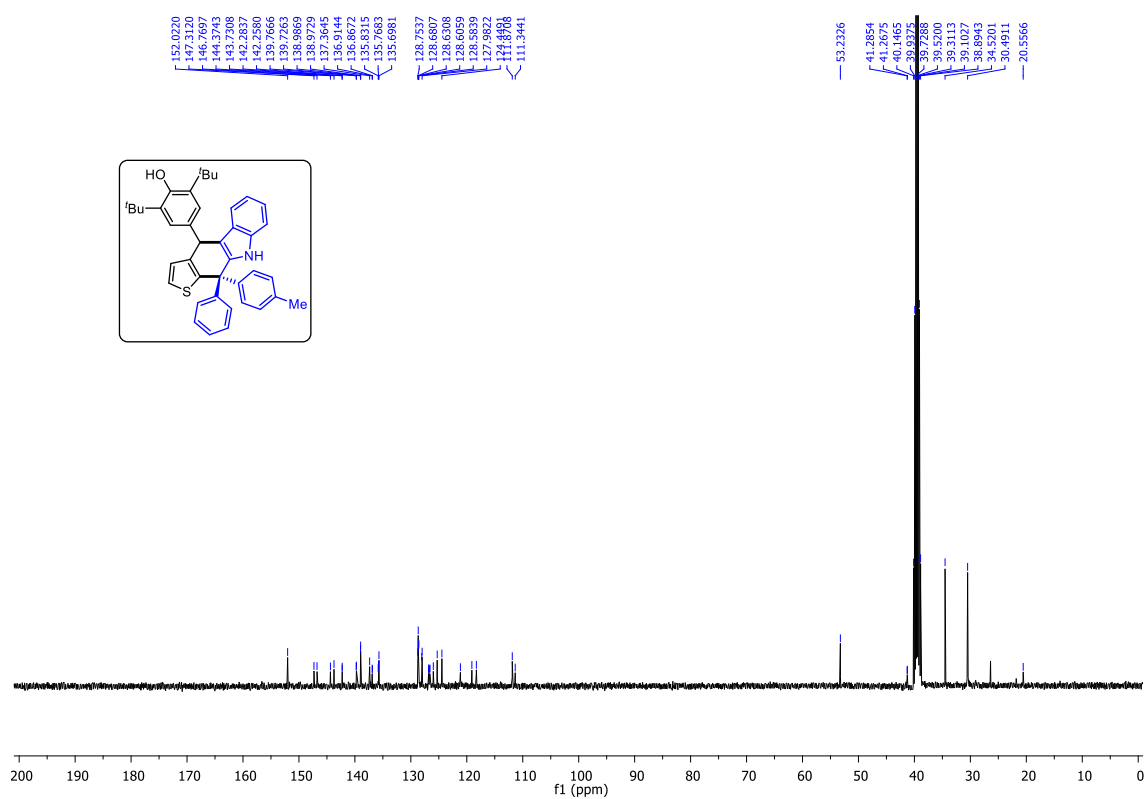
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) Spectrum of **5j**



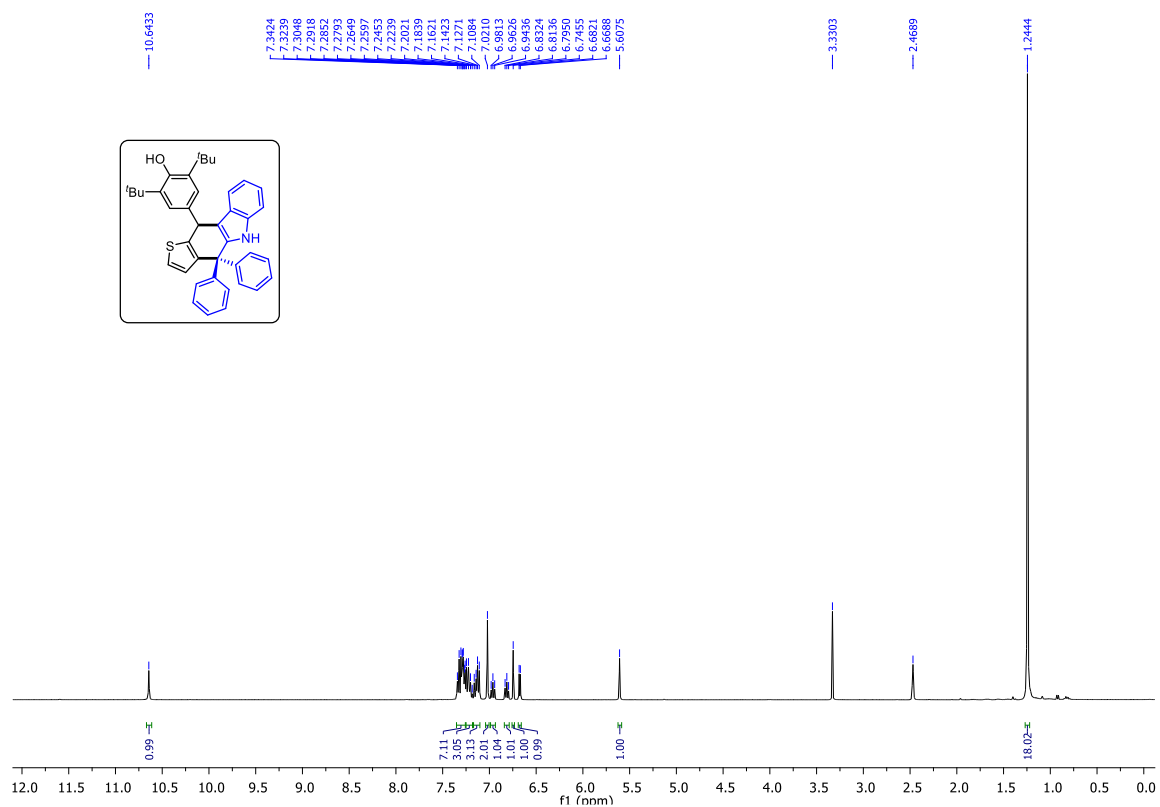
^1H NMR (400 MHz, DMSO-d_6) Spectrum of **5k**



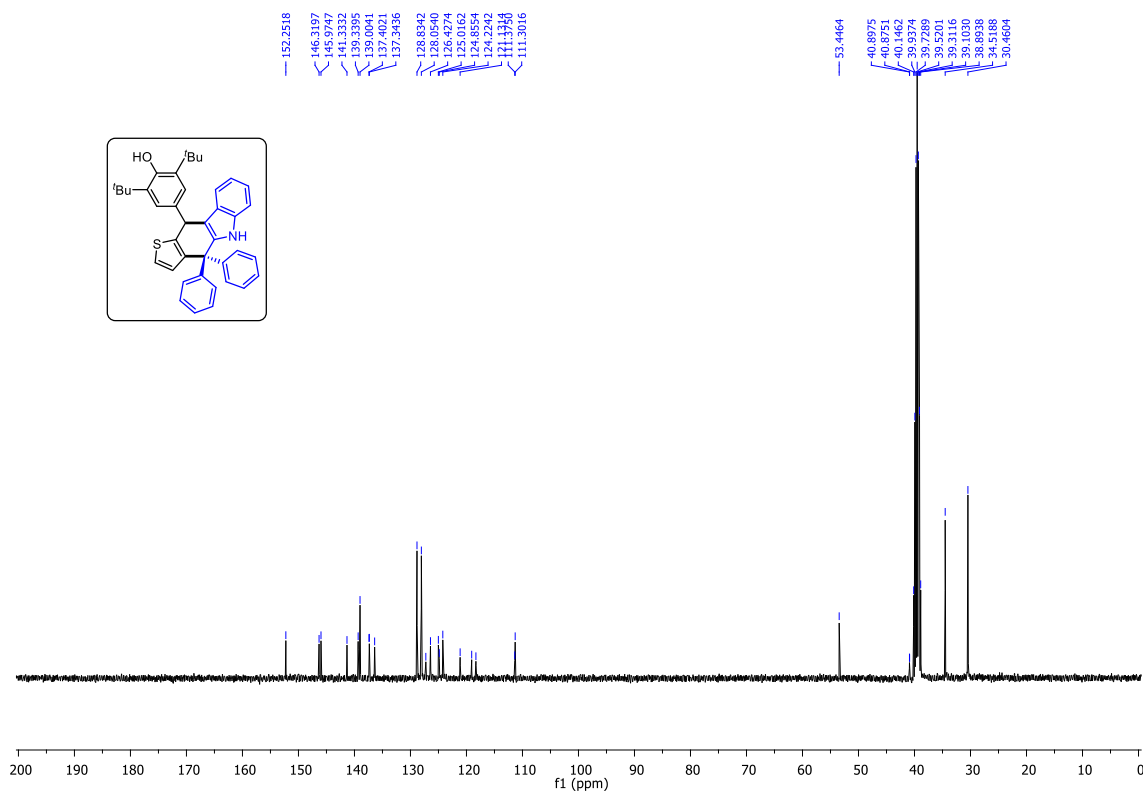
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **5k**



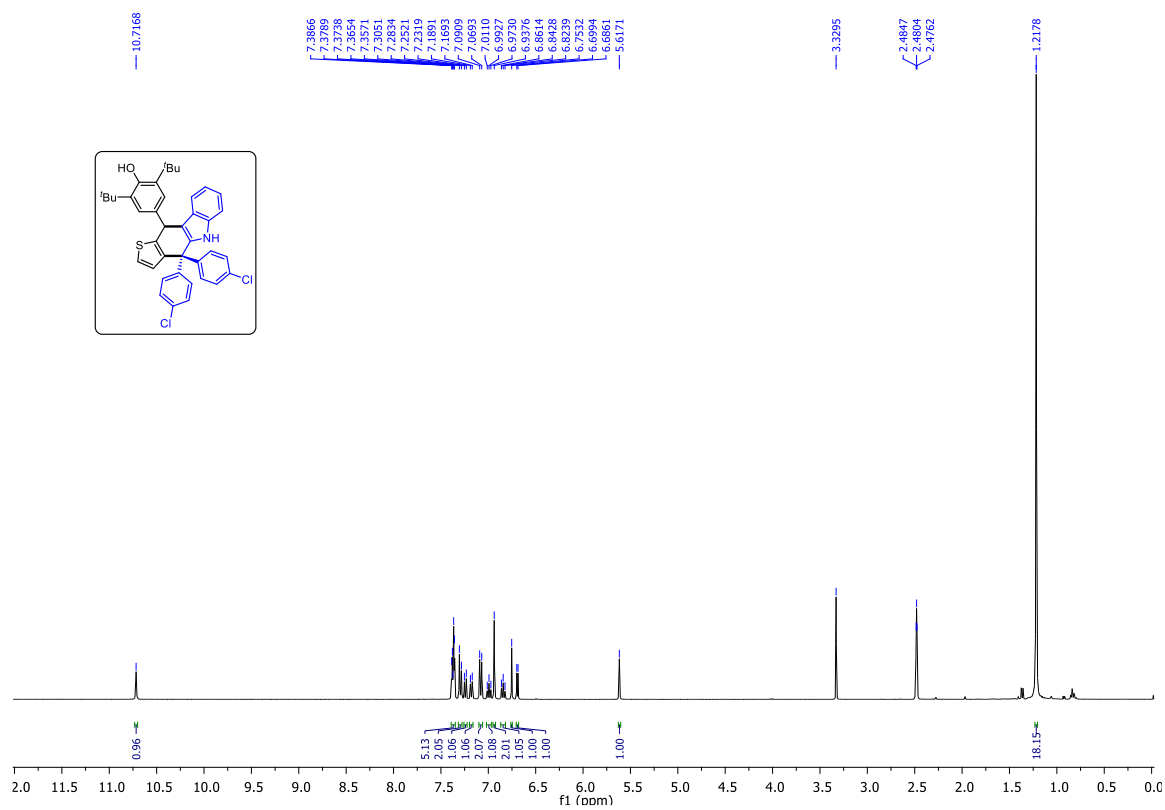
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **7a**



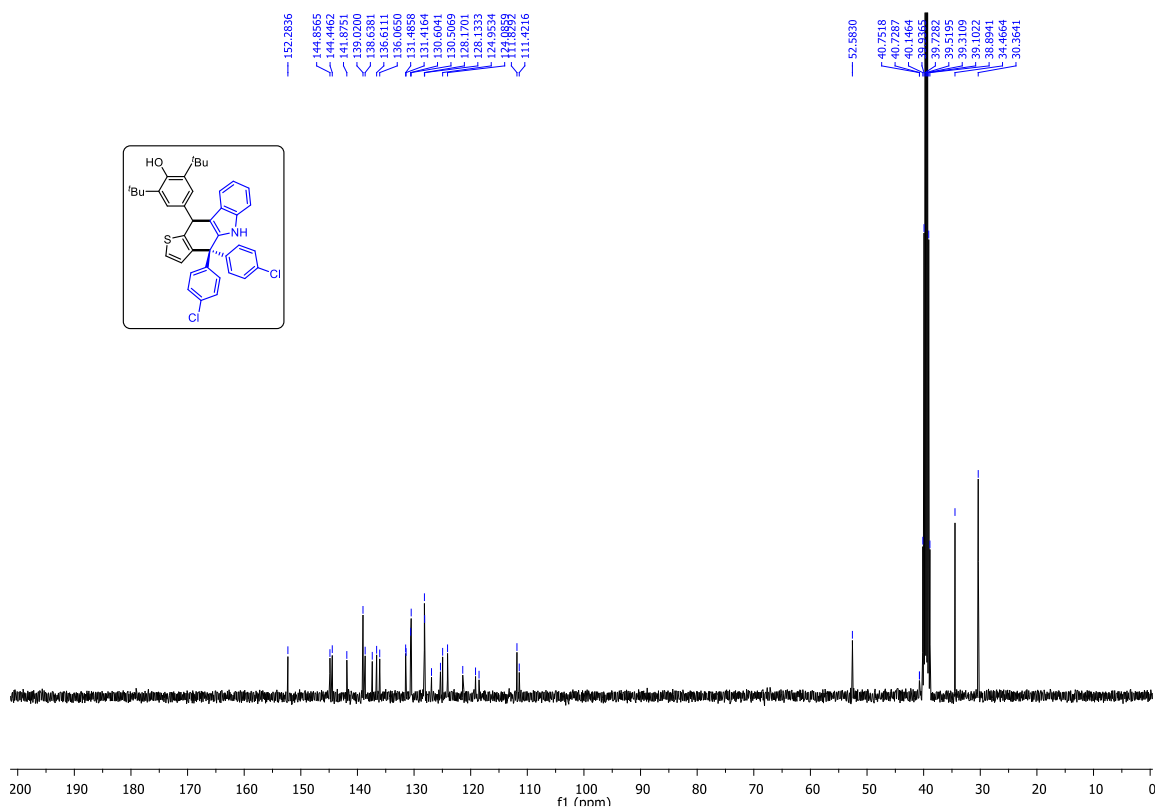
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **7a**



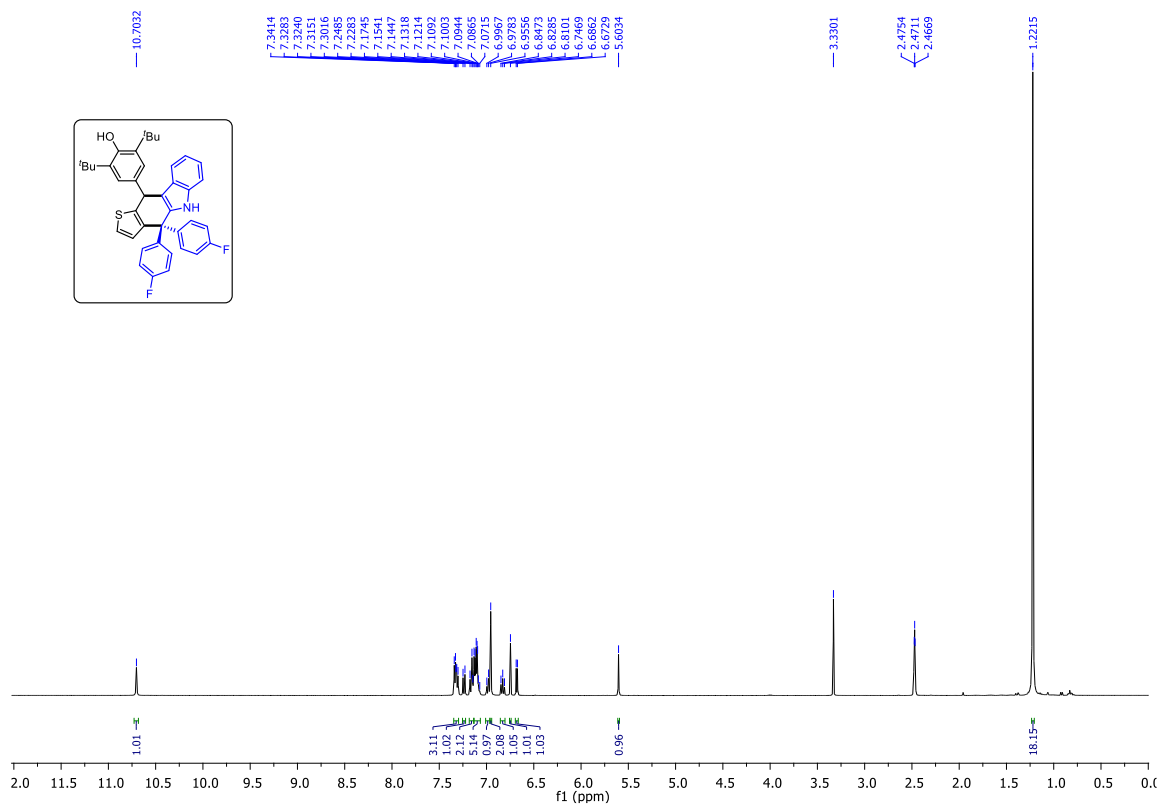
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **7b**



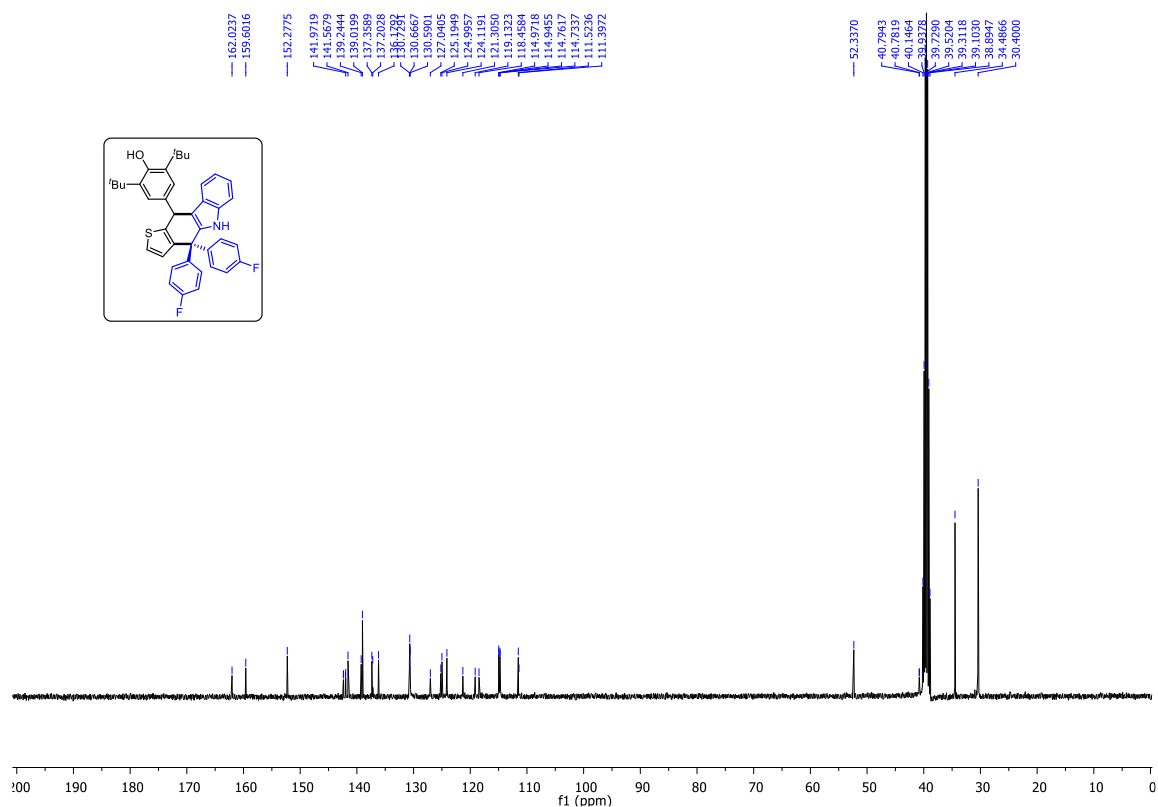
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **7b**



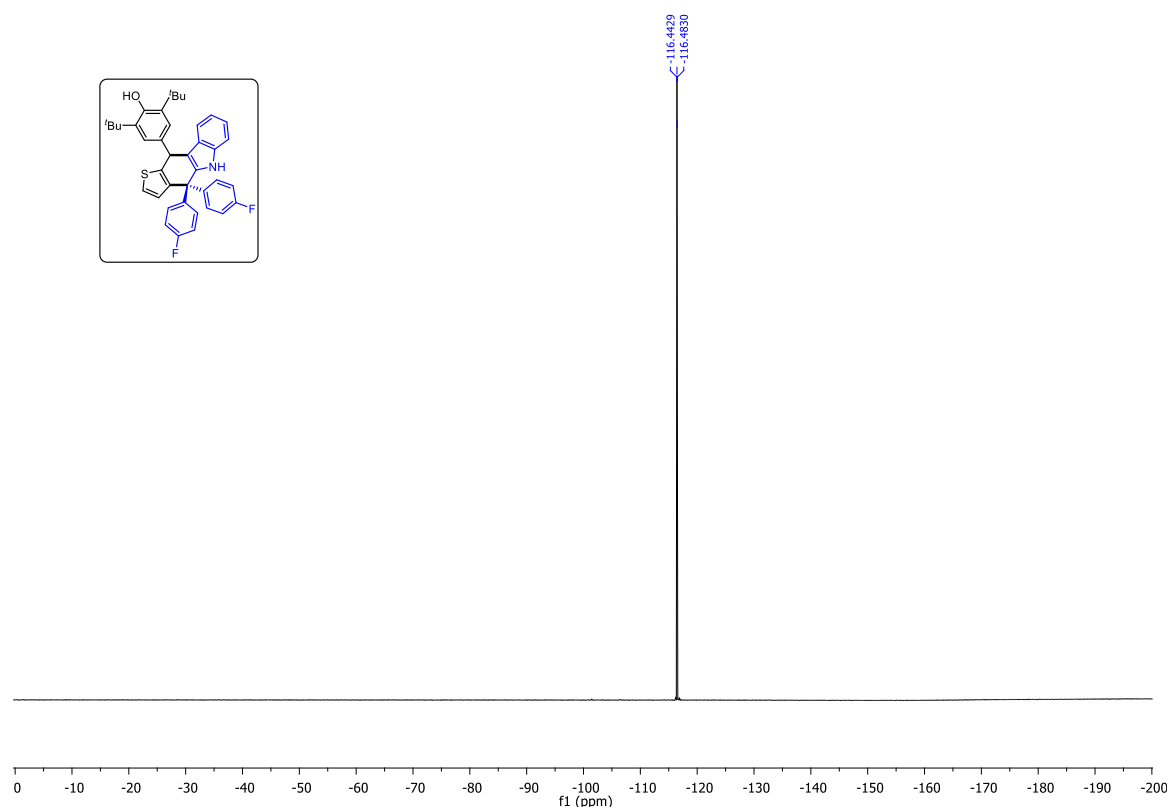
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **7c**



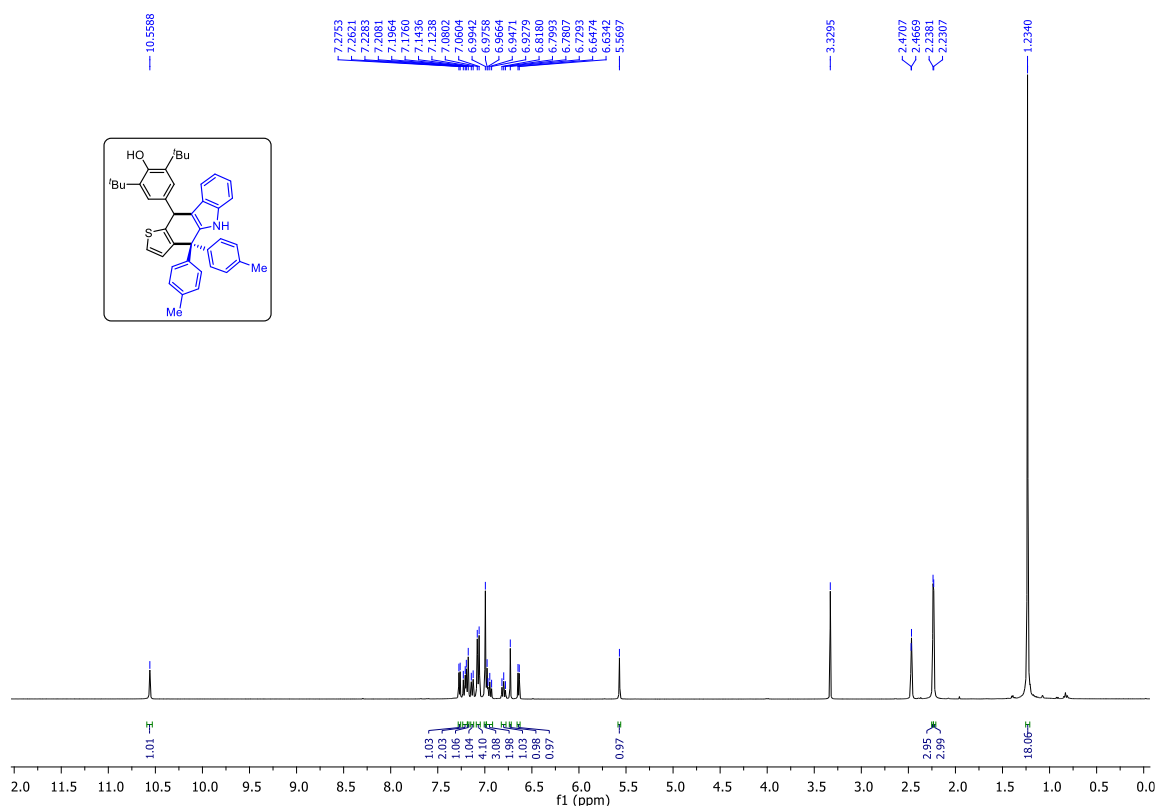
^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) Spectrum of **7c**



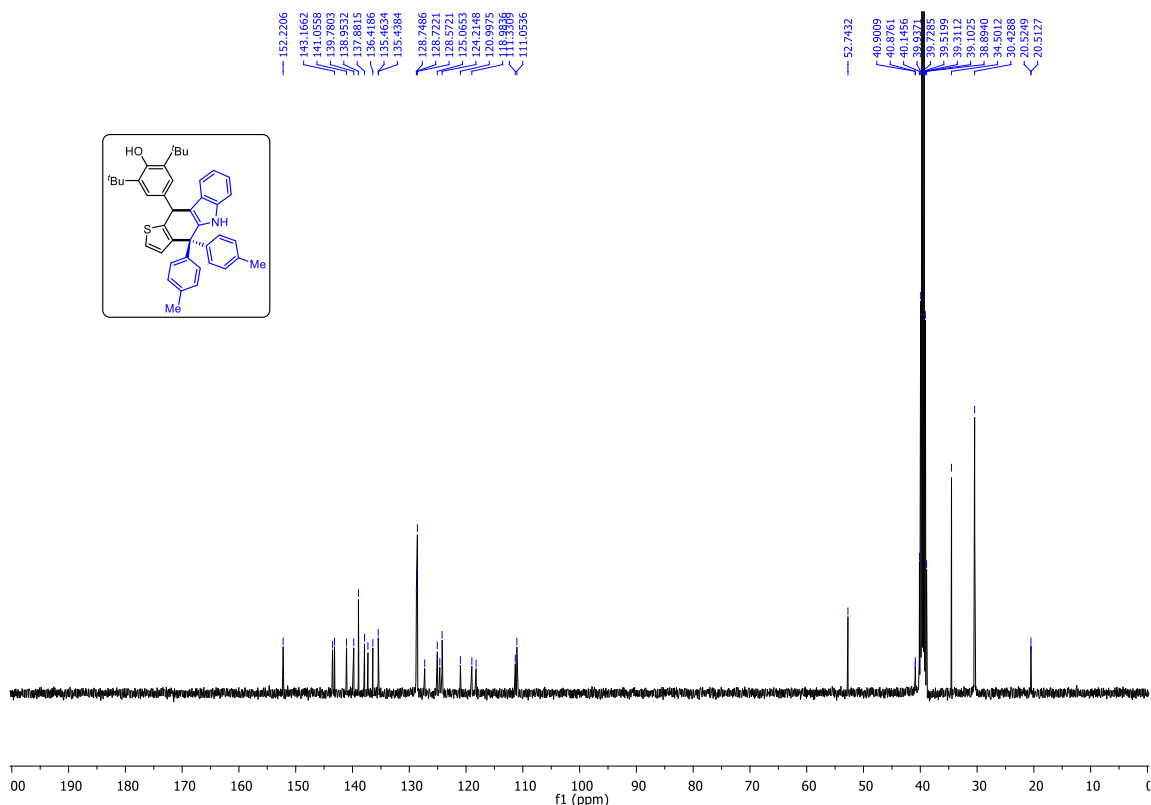
^{19}F { ^1H } NMR (376 MHz, DMSO- d_6) Spectrum of **7c**



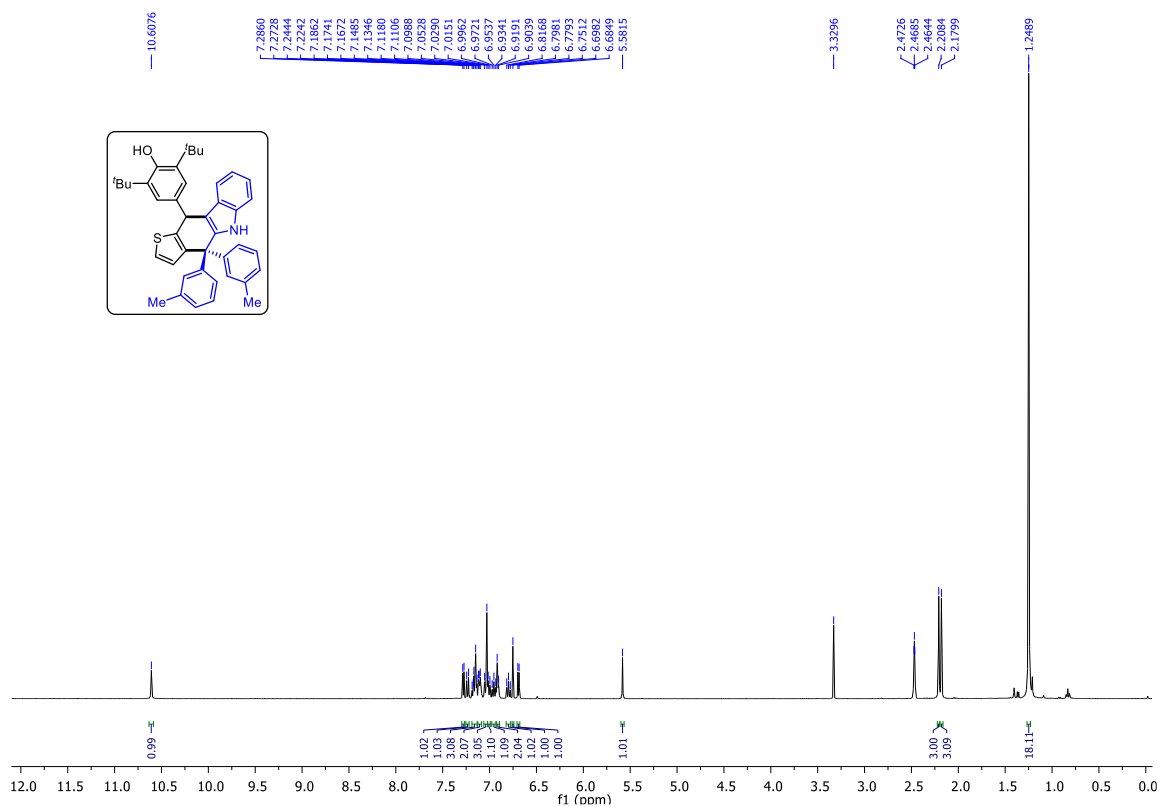
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **7d**



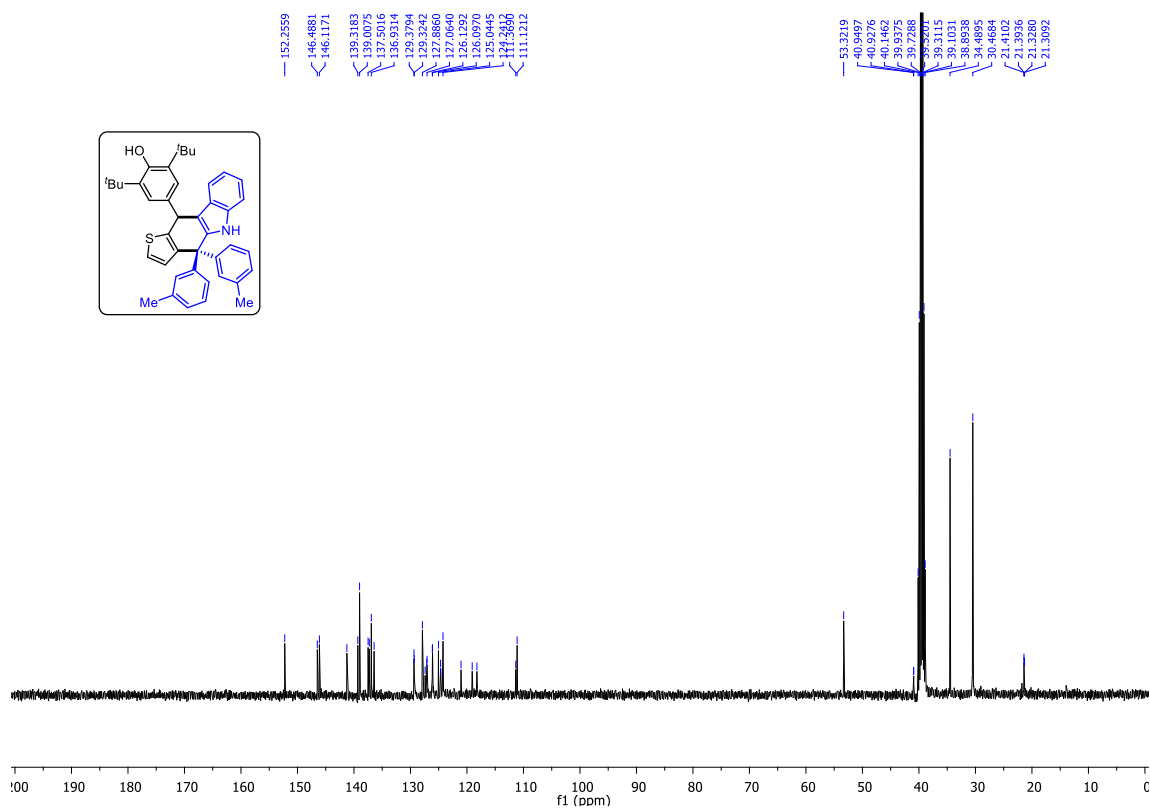
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **7d**



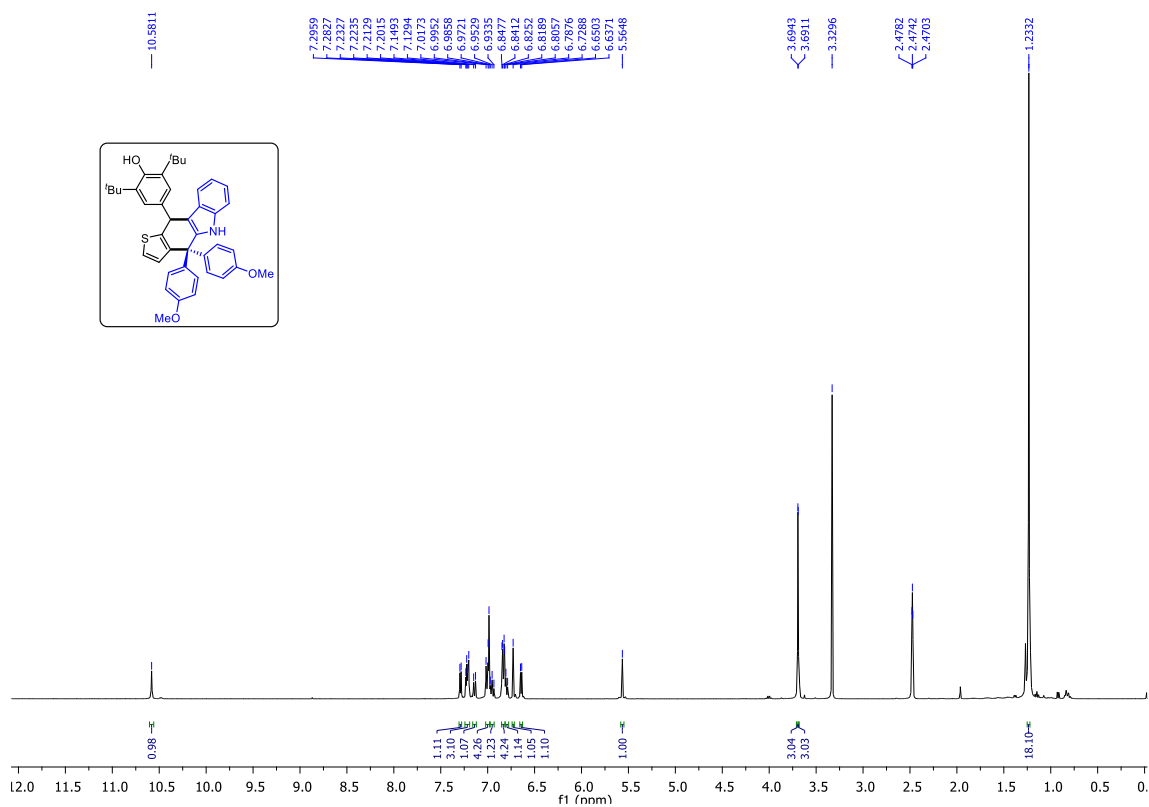
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **7e**



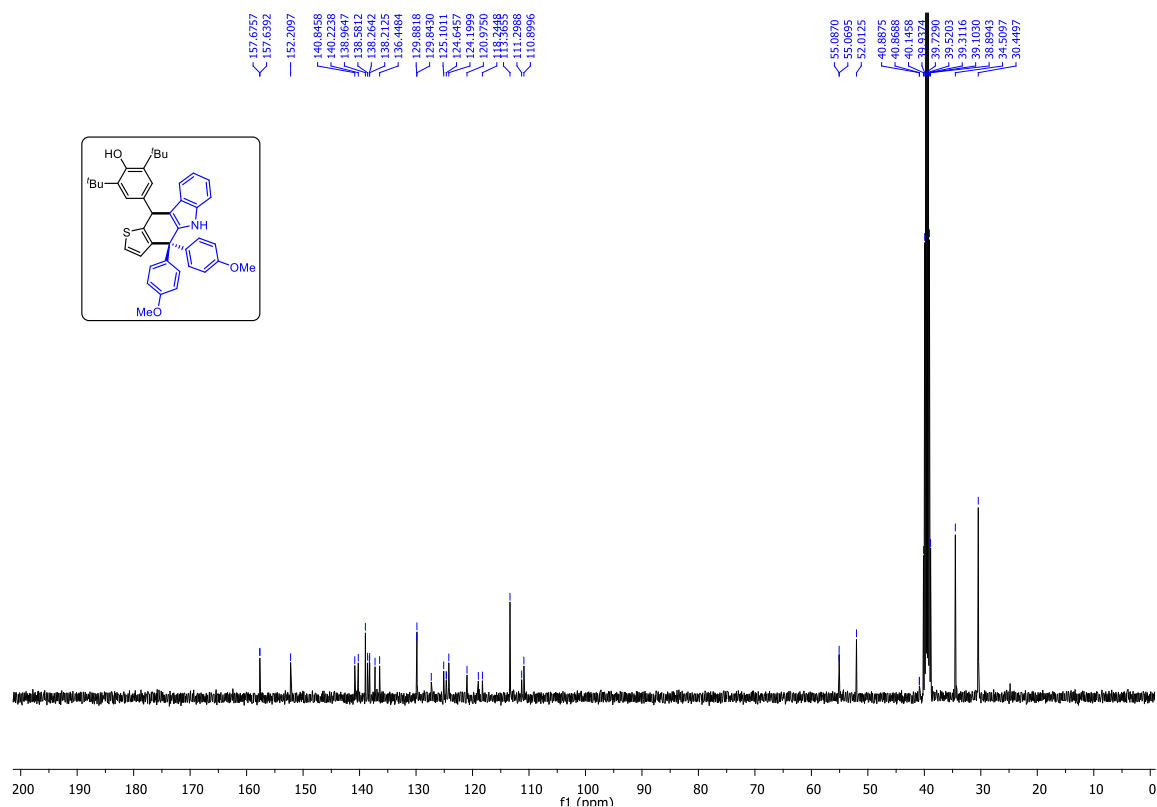
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **7e**



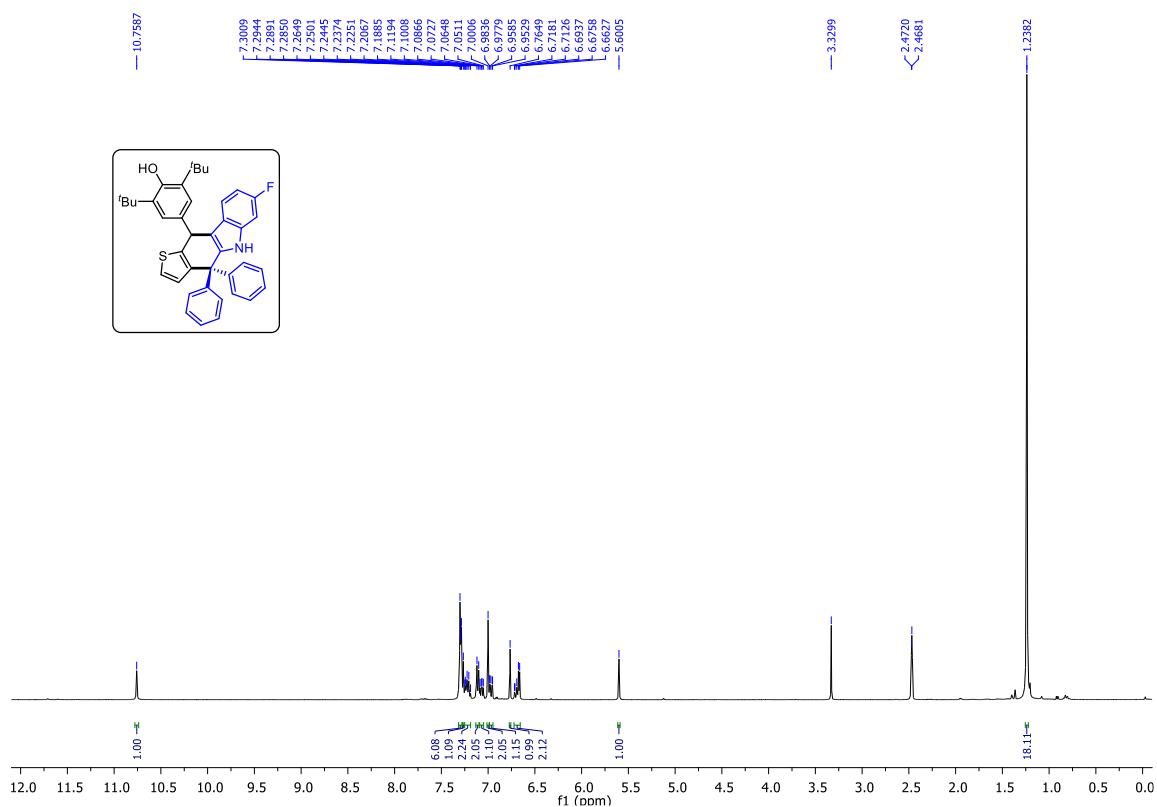
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **7f**



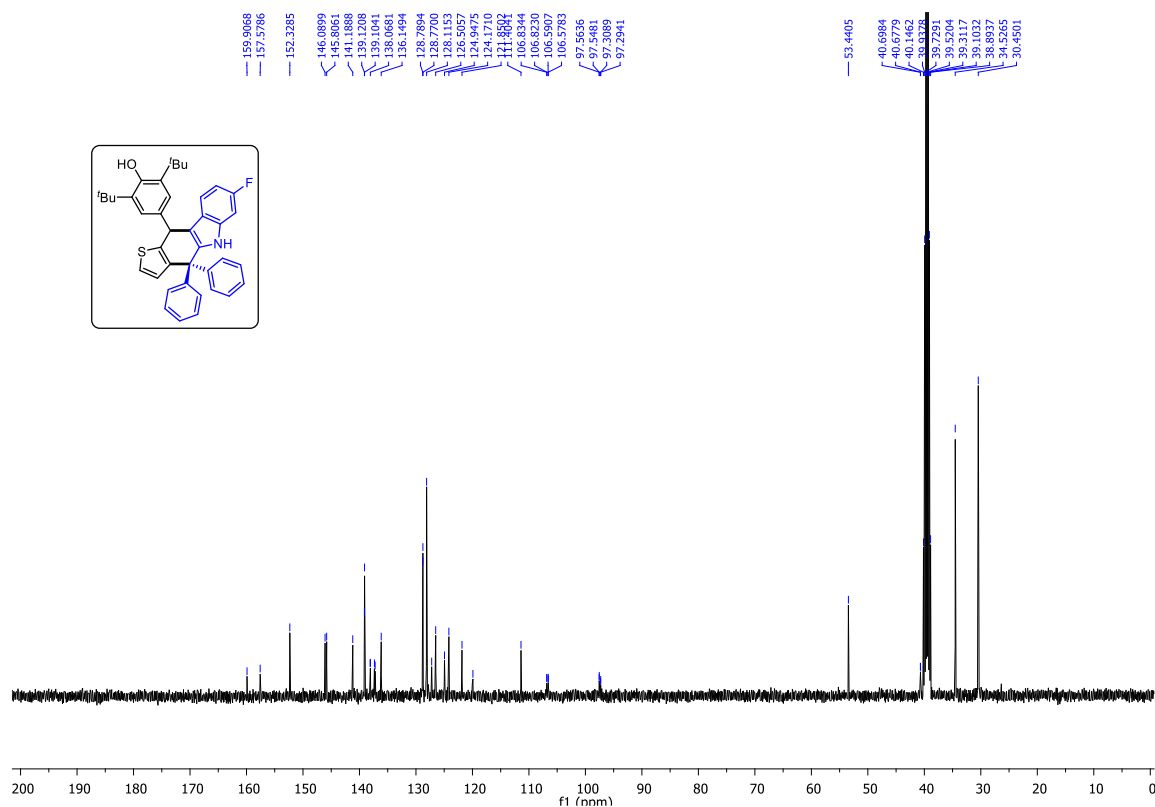
^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) Spectrum of **7f**



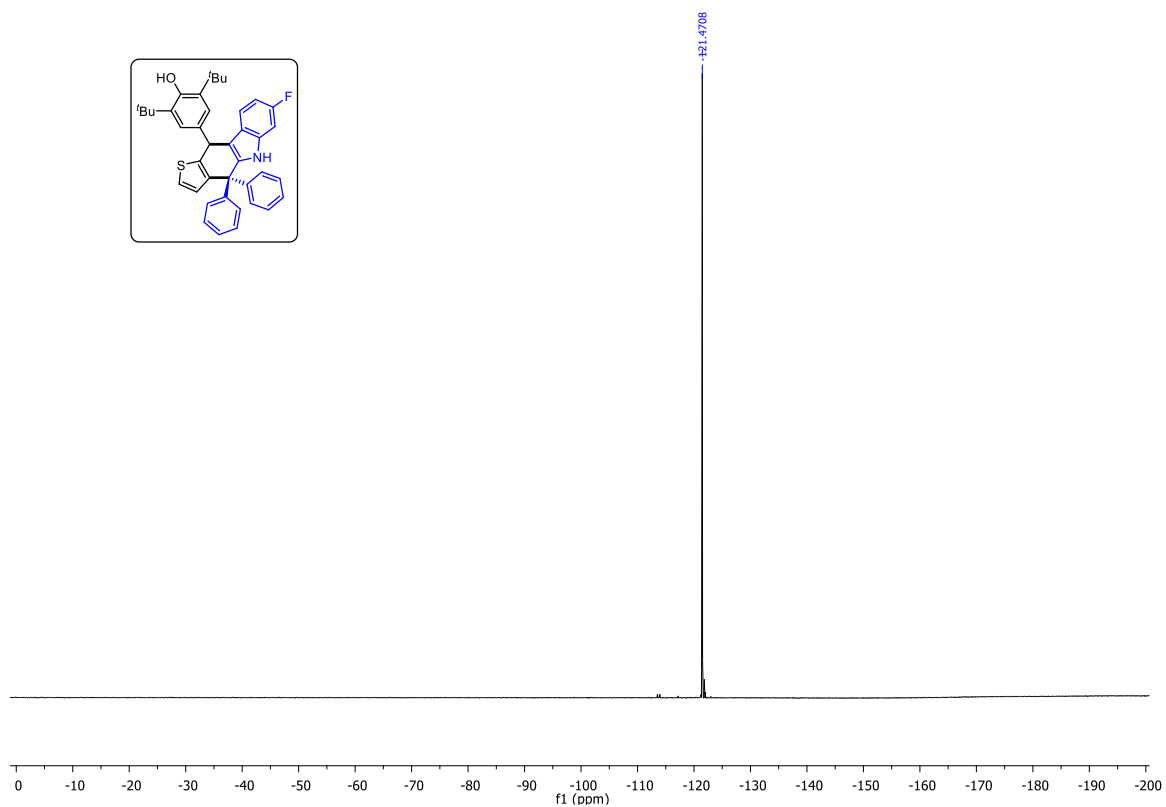
¹H NMR (400 MHz, DMSO-d₆) Spectrum of **7g**



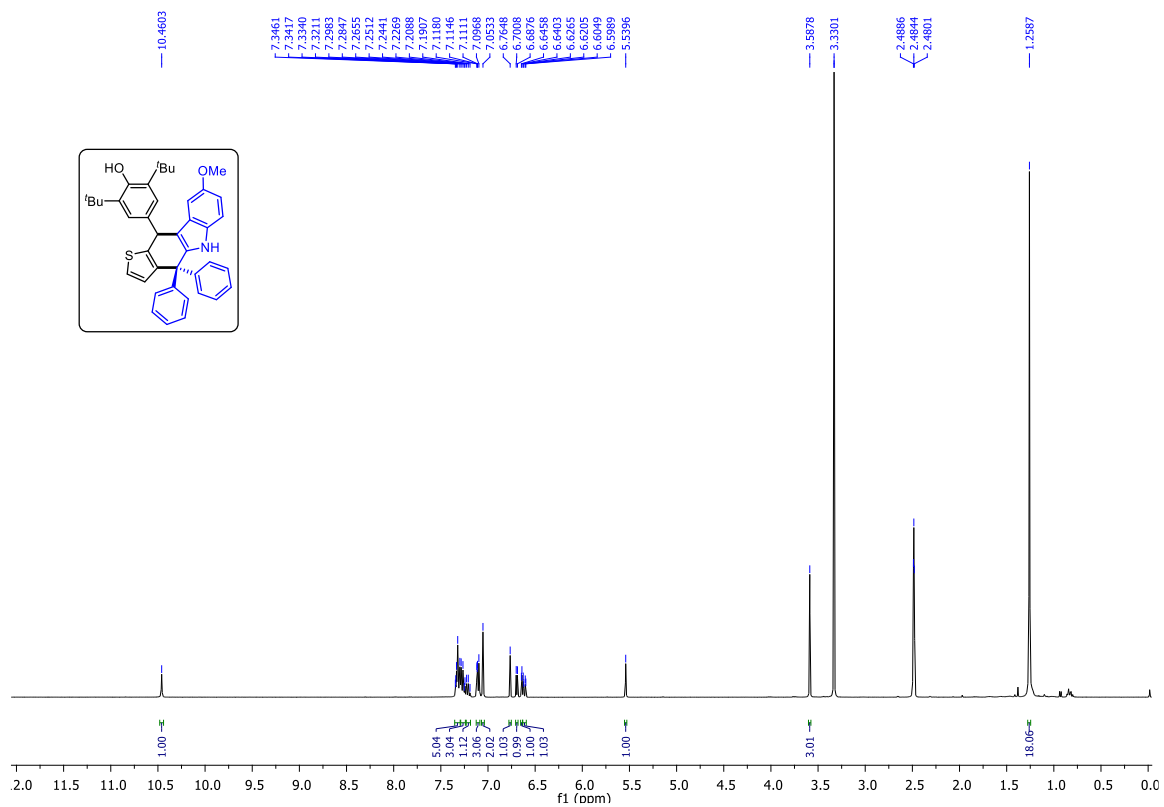
¹³C {¹H} NMR (100 MHz, DMSO-d₆) Spectrum of **7g**



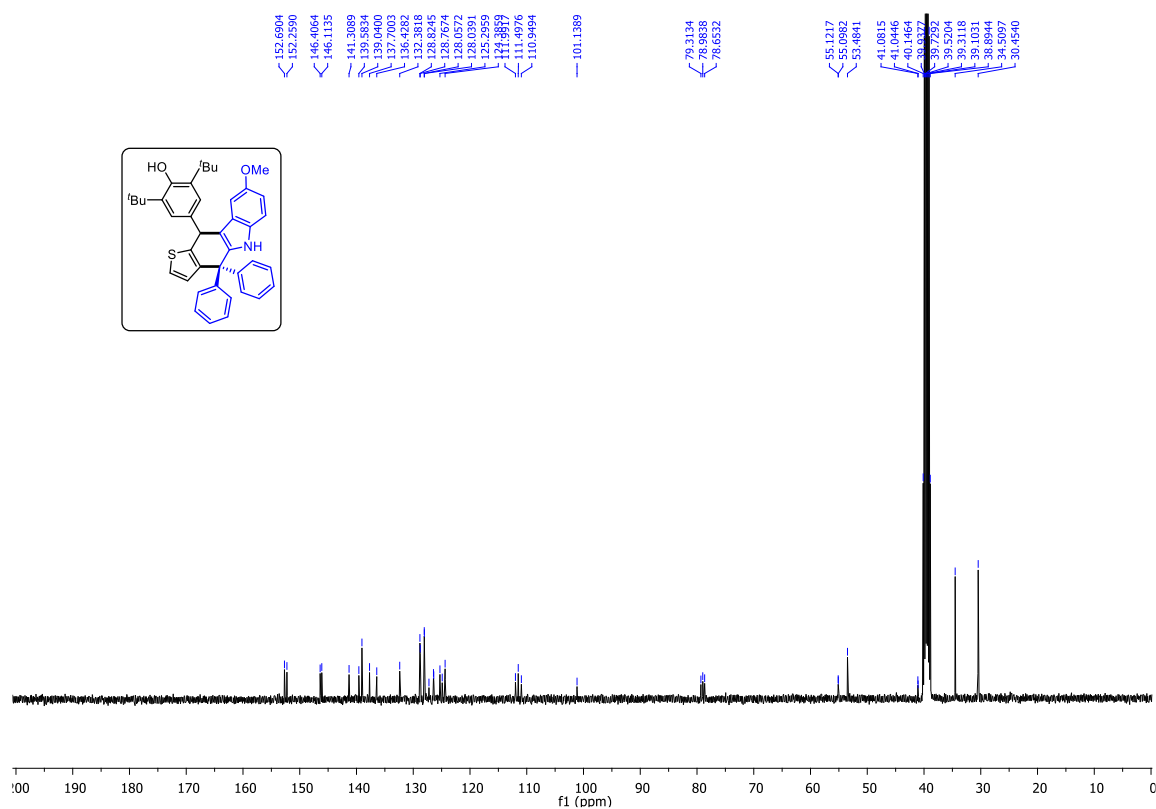
^{19}F $\{^1\text{H}\}$ NMR (376 MHz, DMSO- d_6) Spectrum of **7g**



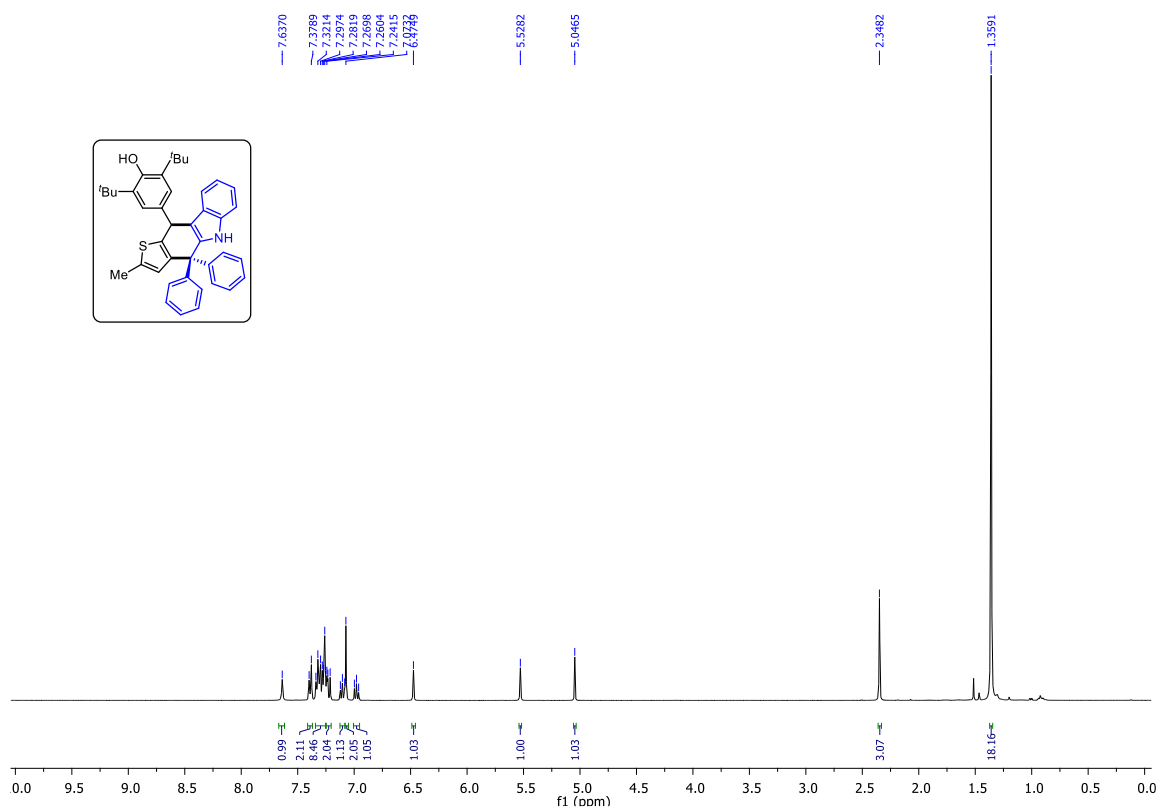
^1H NMR (400 MHz, DMSO- d_6) Spectrum of **7h**



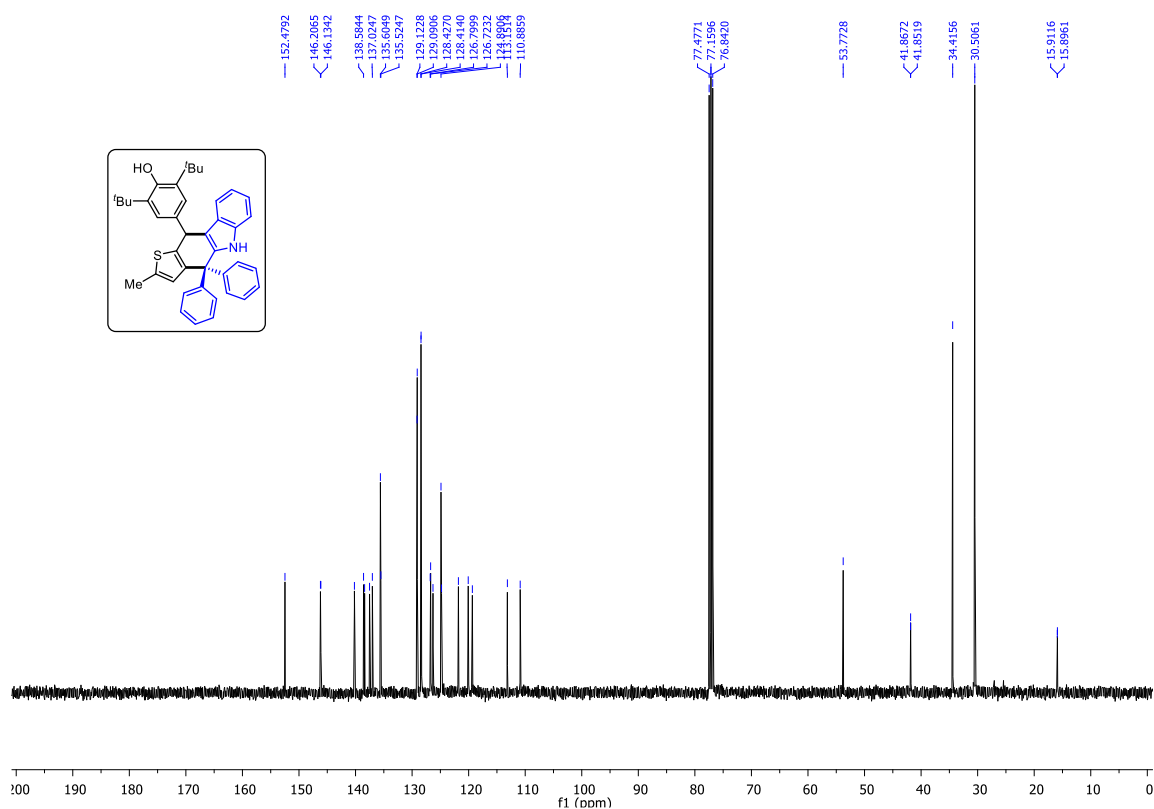
^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **7h**



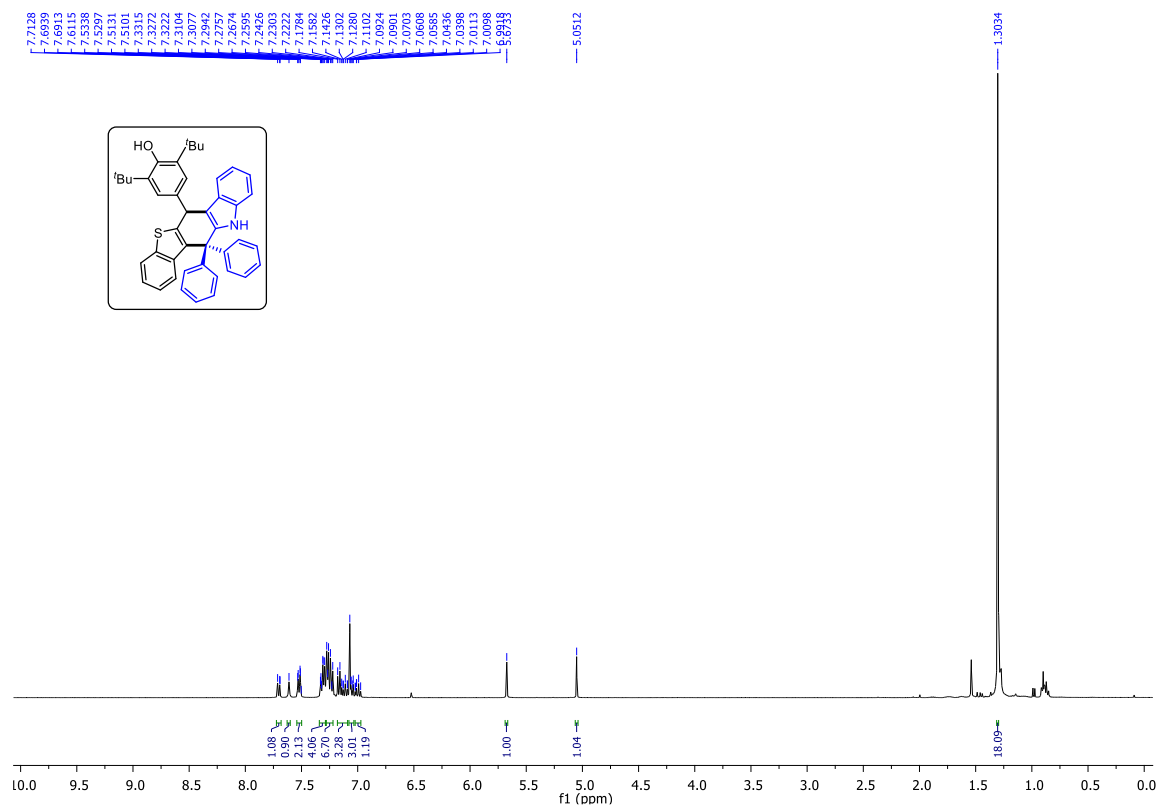
^1H NMR (400 MHz, CDCl_3) Spectrum of **7i**



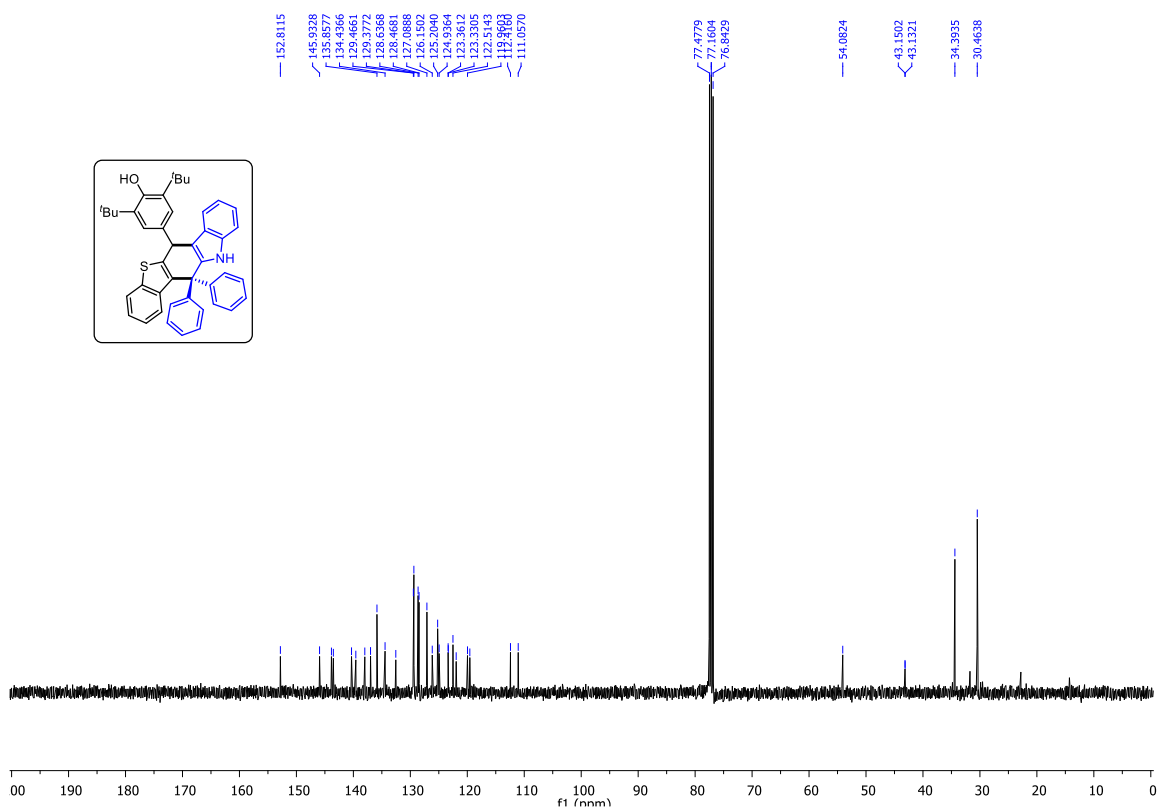
¹³C {¹H} NMR (100 MHz, CDCl₃) Spectrum of **7i**



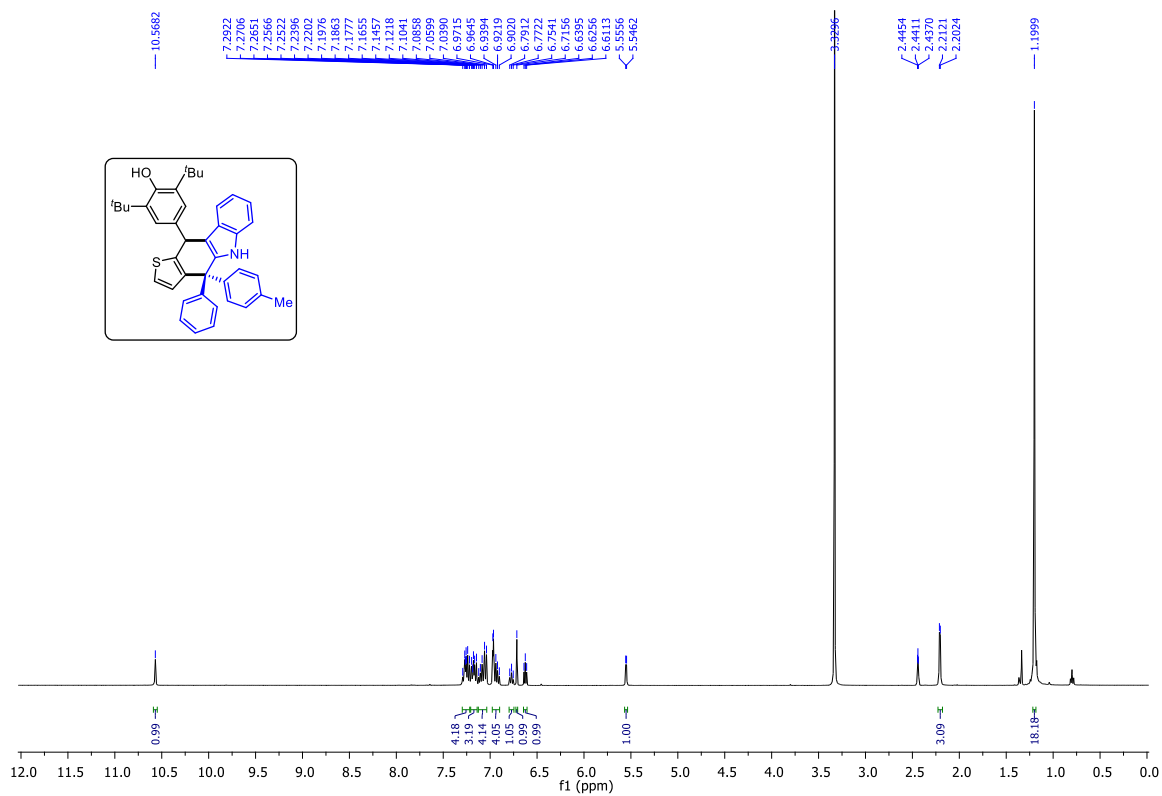
¹H NMR (400 MHz, CDCl₃) Spectrum of **7j**



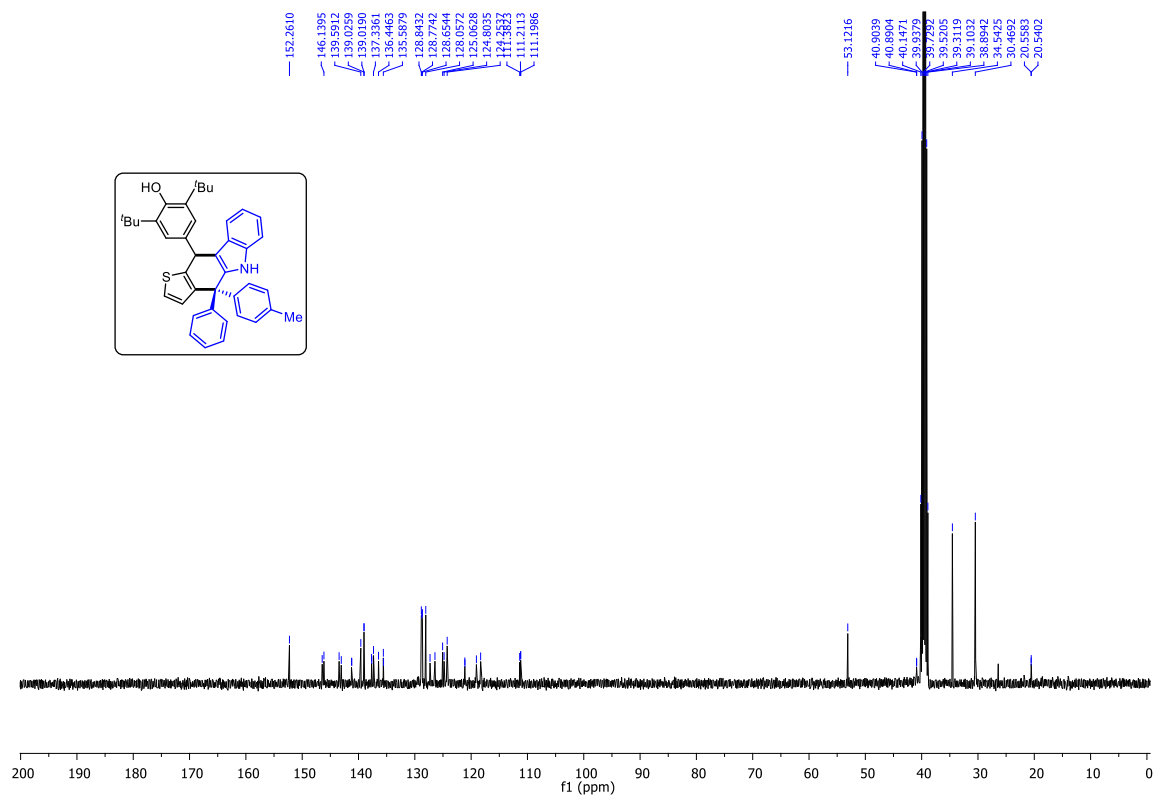
^{13}C { ^1H } NMR (100 MHz, CDCl_3) Spectrum of **7j**



^1H NMR (400 MHz, DMSO-d_6) Spectrum of **7k**



^{13}C $\{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) Spectrum of **7k**



Crude ^1H NMR (400 MHz, CDCl_3) Spectrum of **12**

