Supporting Information

Molecular Iodine-Mediated Formal [2+1+1+1] Cycloaddition Access to Pyrrolo[2,1-*a*]isoquinolins with DMSO as Methylene Source

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Supporting Information

Table of Contents

Experimental Section

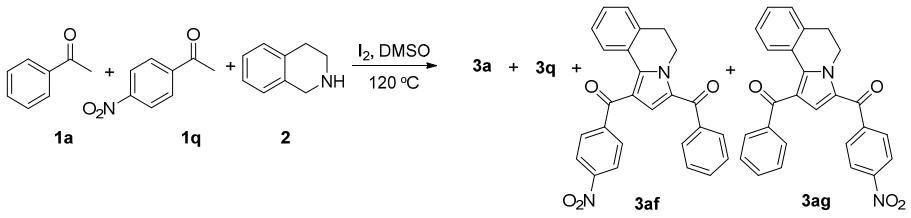
1. General methods

All of the substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Flash column chromatography was performed on silica gel (200–300 mesh). IR spectra were recorded as KBr pellets with absorption in cm^{-1}. ^{1}H NMR spectra were determined at 25 °C on a Varian Mercury 400 or 600 MHz spectrometer. Chemical shifts were provided in ppm relative to the internal standard of tetramethylsilane (TMS). ^{13}C spectra were recorded in $CDCl_3$ or DMSO-d_6 on 100/150 MHz NMR spectrometers and resonances (δ) in ppm. HRMS were obtained on an Apex-Ultra MS equipped with an atmospheric-pressure chemical ionization source. The melting points were determined using XT-4 apparatus and recorded without correction. The X-ray crystal-structures were obtained on a Bruker APEX DUO CCD system.

2. General experimental details

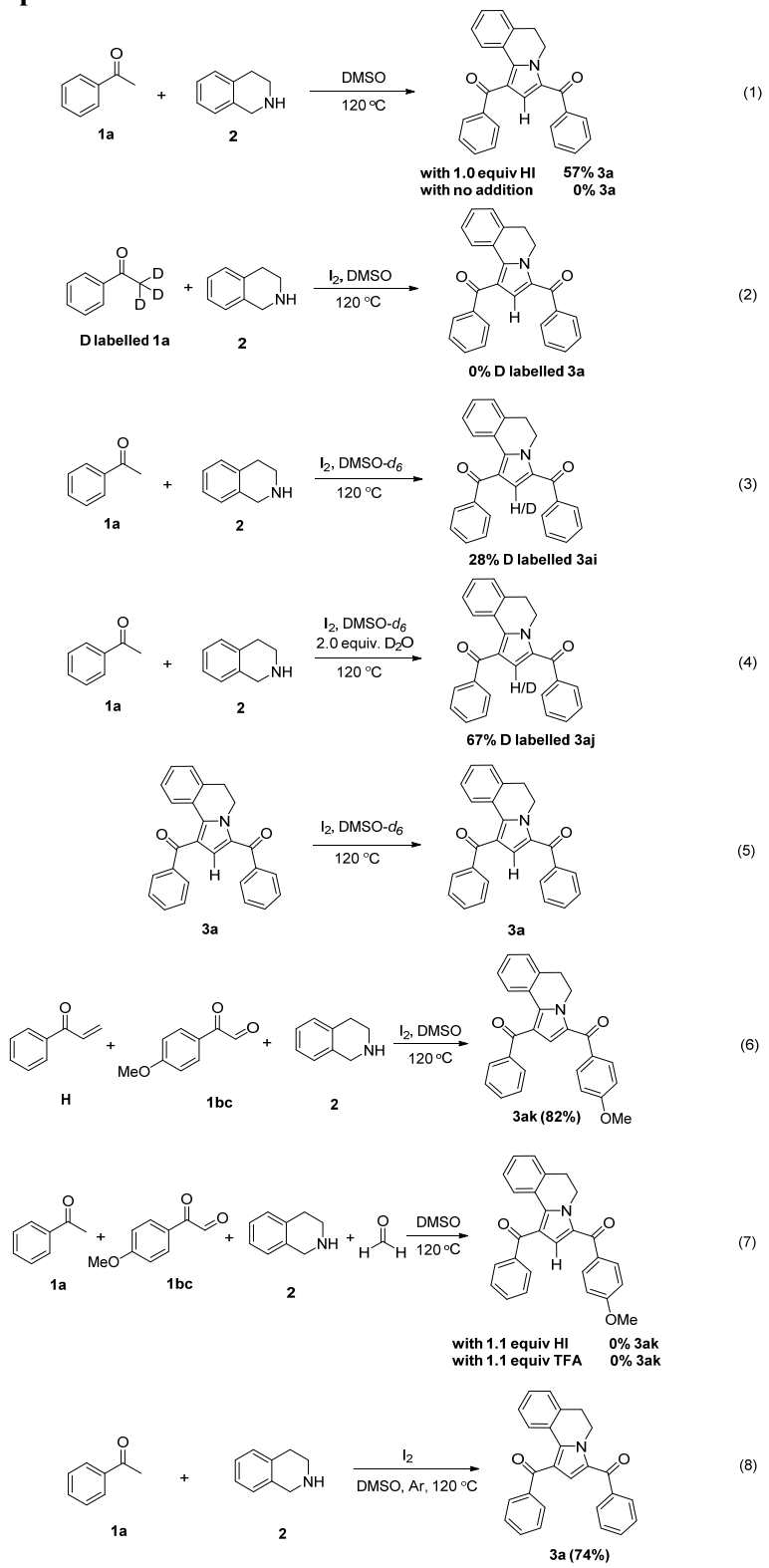
General procedure for the synthesis of desired product (**3a** as an Example). A mixture of acetophenone **1a** (120 mg, 1.0 mmol), 1,2,3,4-tetrahydroisoquinoline **2** (133 mg, 1.0 mmol), and iodine (127 mg, 0.5 mmol) was added to DMSO (5 mL) in sealed tube and stirred at 120 °C for 2.5 h. After the completion of the reaction, 30 mL of $Na_2S_2O_3$ (aq) was then added to the mixture, which was then extracted with EtOAc three times (3 × 30 mL). The product was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was then purified by column chromatography on silica gel (petroleum ether/ EtOAc = 8:1) to afford the desired product **3a**.

3. Cross-coupling experiment



We investigated the cross-coupling reaction using acetophenone **1a**, 4-NO_2-phenylmethyl ketone **1q** and **2** under the standard conditions, the reaction delivered **3a**, **3q** and another two cross-coupling products **3af** and **3ag**. The structure of **3ag** was further confirmed by single-crystal X-ray diffraction analysis (**Figure S4**).

4. Control experiments and HRMS



To gain a deeper understanding on the mechanism, several isotope labeling experiments were performed. Treating D labelled **1a**-d_3 with **2** in standard conditions, no deuterated product **3a** was

detected (eq 2). When this reaction was conducted in DMSO-d_6, we isolated 28% D labelled **3ai** (eq 3), which was confirmed by ^{1}H NMR spectra. Then we added 2.0 equiv. D_2O in DMSO-d_6 under standard conditions, 67% D labelled **3aj** was isolated (eq 4). **3a** could not transform into D labelled **3a** when heated in DMSO-d_6. These results might indicate that the C-H in the pyrrol ring of **3a** is stable, and the H-exchange might be happened during the formation of compound **E**. Furthermore, intermediate **G** was synthesized and could be converted to **3ak** in 82% yield (eq 6). It was reported that α,β-unsaturated carbonyl compound could be obtained from formaldehyde and kerones.[1] However, the reaction of formaldehyde with **1a**, **1bc** and **2** did not result in the formation of **3ak** in the presence of HI or TFA, these results confirmed that DMSO as a source of methylene. We also conducted this reaction under Ar atmosphere, and the corresponding product **3a** could be obtained in 74% yield, indicating that I_2 is the oxidant in the final oxidation process.[2]

ZKL348: HRMS (ESI) m/z calcd for $C_{24}{}^{13}C_2H_{20}NO_2^+$ $(M+H)^+$ 380.15556, found 380.15549.

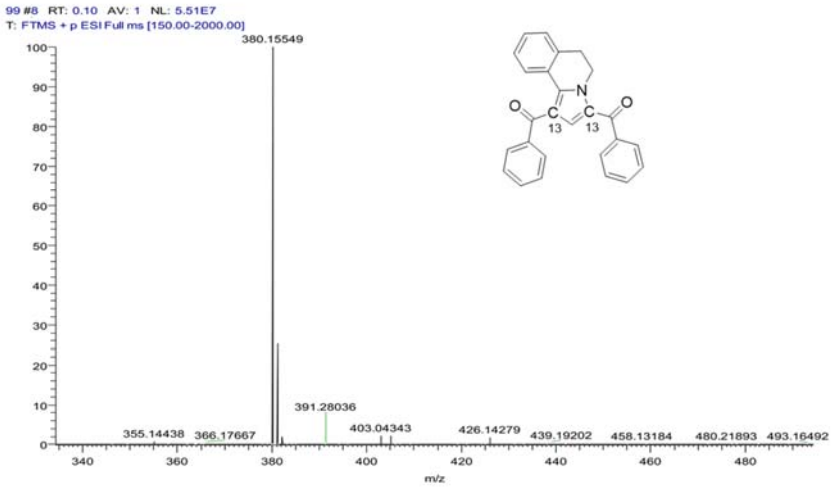


Figure S1. HRMS of **3ah**.

Reference

1. A. Bugarin, K. D. Jones and B. T. Connell, *Chem. Commun*. 2010, **46**, 1715-1717.

2. (a) Q. H. Gao, Z. Fei, Y. P. Zhu, M. Lian, F. C. Jia, M. C. Liu, N. F. She and A. X. Wu, *Tetrahedron* 2013, **69**, 22−28; (b) J. C. Xiang, M. Wang, Y. Cheng and A. X. Wu, *Org. Lett*. 2016, **18**, 24-27

5. The crystallographic data

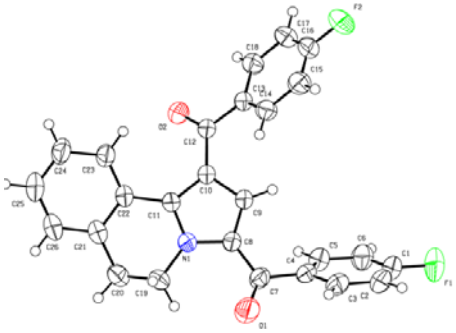


Figure S2. X-ray structural details of **3i:** (CCDC 1545082).

Empirical formula	$C_{26}H_{17}F_2NO_2$		Absorption coefficient	0.100 mm^{-1}
Formula weight	413.4		F(000)	428
Temperature	273(2) K		Crystal size	0.22 x 0.20 x 0.18 mm^3
Wavelength	0.71073 Å		Reflections collected	10962
Crystal system	Triclinic,		Independent reflections	6302 [R(int) = 0.0214]
Space group	P-1		Max. and min. transmission	0.9850 and 0.9817
Unit cell dimensions	a = 8.821(3) Å	α = 81.907(5) °	Refinement method	Full-matrix least-squares on F^2
	b = 11.239(4) Å	β = 70.268(5)°	Data / restraints / parameters	6302 / 0 / 280
	c = 11.410(4) Å	γ = 69.729(5)°	Goodness-of-fit on F^2	0.969
Volume	998.4(6) $Å^3$		Final R indices [I>2sigma(I)]	R1 = 0.0538, wR2 = 0.1776
Z	2		R indices (all data)	R1 = 0.0735, wR2 = 0.2073
Density (calculated)	1.375 Mg/m^3		Largest diff. peak and hole	0.279 and -0.314 $e.Å^{-3}$

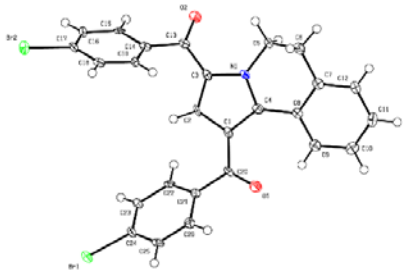


Figure S3. X-ray structural details of **3m:** (CCDC 1842947).

Empirical formula	$C_{26}H_{17}Br_2NO_2$		Absorption coefficient	3.826 mm^{-1}
Formula weight	535.2		F(000)	1064
Temperature	100(1) K		Crystal size	0.13 x 0.12 x 0.11 mm^3
Wavelength	0.71073 Å		Reflections collected	10593
Crystal system	monoclinic		Independent reflections	4967 [R(int) = 0.0555]
Space group	$P2_1/c$		Max. and min. transmission	
Unit cell dimensions	a = 8.735(8) Å	α = 90°	2Θ range for data collection	4.124 to 58.978°
	b = 22.115(14) Å	β = 107.507(9)°	Data / restraints / parameters	4967 / 0 / 280
	c = 11.575(9) Å	γ = 90°	Goodness-of-fit on F^2	1.044
Volume	2132.4(3) $Å^3$		Final R indices [I>2sigma(I)]	R1 = 0.0513, wR2 = 0.0849
Z	4		R indices (all data)	R1 = 0.0760, wR2 = 0.0961
Density (calculated)	1.667 Mg/m^3		Largest diff. peak and hole	0.82 and -0.8 $e.Å^{-3}$

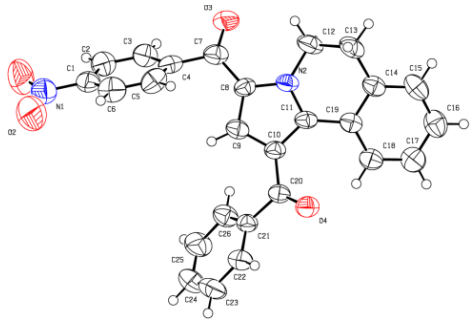
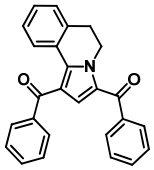


Figure S4. X-ray structural details of **3ag:** (CCDC 1555924).

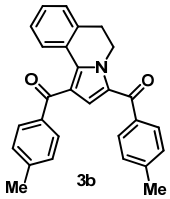
Empirical formula	$C_{26}H_{18}N_2O_4$		Absorption coefficient	0.093 mm^{-1}
Formula weight	422.42		F(000)	880
Temperature	295(2) K		Crystal size	0.130 x 0.100 x 0.030 mm^3
Wavelength	0.71073 Å		Reflections collected	10874
Crystal system	Monoclinic		Independent reflections	3543 [R(int) = 0.1139]
Space group	$P2_1/c$		Max. and min. transmission	
Unit cell dimensions	a =11.821(15) Å	α = 90 °	Refinement method	Full-matrix least-squares on F^2
	b = 9.242(11) Å	β = 92.57(2)°	Data / restraints / parameters	3543 / 0 / 290
	c = 18.97(2)Å	γ = 90°	Goodness-of-fit on F^2	1.070
Volume	2071(4) $Å^3$		Final R indices [I>2sigma(I)]	R1 = 0.0850, wR2 = 0.2373
Z	4		R indices (all data)	R1 = 0.1384, wR2 = 0.2872
Density (calculated)	1.355 Mg/m^3		Largest diff. peak and hole	0.337 and -0.353 $e.Å^{-3}$

6. Spectroscopic data



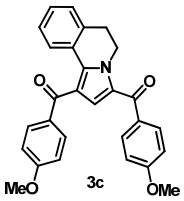
3a

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(phenylmethanone) (**3a**): light yellow solid; 150.8 mg (yield 80%); mp 127-130 °C; IR (KBr): 3717, 3042, 2933, 2847, 1629, 1473, 1426, 1320, 1288, 1271, 1137, 989, 843, 772 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.90 (d, J = 7.8 Hz, 2H), 7.82 (t, J = 7.8 Hz, 3H), 7.56-7.52 (m, 2H), 7.44 (q, J = 7.2 Hz, 4H), 7.28 (d, J = 4.8 Hz, 2H), 7.17-7.14 (m, 1H), 6.94 (s, 1H), 4.73 (t, J = 7.2 Hz, 2H), 3.15 (t, J = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.2, 186.0, 139.0, 138.6, 134.1, 132.5, 132.0, 129.8, 129.2, 129.1, 128.5, 128.2, 128.2, 127.7, 127.6, 126.9, 126.5, 126.2, 120.1, 42.8, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{20}NO_2$: 378.1489; found: 378.1490.



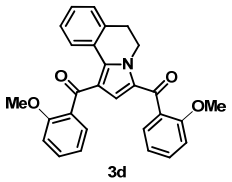
3b

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(*p*-tolylmethanone) (**3b**): Yellow solid; 151.9 mg (yield 75%); mp 138-141 °C; IR (KBr): 3453, 2922, 1627, 1605, 1529, 1478, 1419, 1385, 1266, 1218, 1174, 960, 885, 751, 617 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.81 (d, J = 7.8 Hz, 3H), 7.74 (d, J = 7.8 Hz, 2H), 7.28-7.25 (m, 3H), 7.23 (d, J = 3.6 Hz, 2H), 7.22 (s, 1H), 7.19-7.16 (m, 1H), 6.92 (s, 1H), 4.70 (t, J = 6.6 Hz, 2H), 3.14 (t, J = 6.0 Hz, 2H), 2.41 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.1, 185.9, 143.4, 142.7, 138.2, 136.5, 136.1, 134.1, 130.1, 129.5, 129.0, 129.0, 128.6, 127.6, 127.0, 126.7, 125.8, 120.3, 42.8, 29.3, 21.6, 21.6; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{28}H_{24}NO_2$: 406.1802; found: 406.1788.



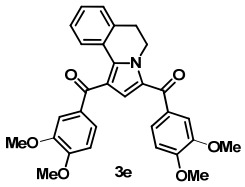
3c

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-methoxyphenyl)methanone) (**3c**): Yellow solid; 152.9 mg (yield 70%); mp 112-114 °C; IR (KBr): 3451, 2922, 1724, 1629, 1550, 1513, 1465, 1384, 1256, 1168, 1129, 762, 616, 566 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.92 (d, J = 8.4 Hz, 2H), 7.86 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 7.8 Hz, 1H), 7.28-7.24 (m, 2H), 7.17 (t, J = 7.8 Hz, 1H), 6.94 (d, J = 7.8 Hz, 2H), 6.91 (d, J = 8.4 Hz, 3H), 4.66 (t, J = 6.6 Hz, 2H), 3.86 (s, 3H), 3.85 (s, 3H), 3.13 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.3, 184.9, 163.2, 162.8, 137.6, 134.0, 132.2, 131.7, 131.6, 131.3, 128.8, 128.6, 127.6, 127.4, 126.9, 126.7, 124.9, 120.2, 113.5, 55.4, 42.8, 29.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{28}H_{24}NO_4$: 438.1700; found: 438.1698.



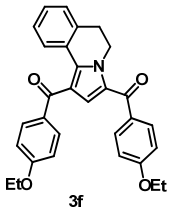
3d

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((2-methoxyphenyl)methanone) (**3d**): Yellow oil; 152.7 mg (yield 70%); IR (KBr): 3450, 2932, 1631, 1597, 1523, 1486, 1435, 1281, 1247, 1022, 960, 886, 755, 660 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.14 (d, J = 8.4 Hz, 1H), 7.43 (d, J = 7.2 Hz, 1H), 7.38-7.34 (m, 3H), 7.19 (t, J = 7.8 Hz, 2H), 6.93 (q, J = 7.8 Hz, 4H), 6.85 (d, J = 8.4 Hz, 1H), 6.91 (s, 1H), 4.79 (t, J = 6.6 Hz, 2H), 3.78 (s, 3H), 3.70 (s, 3H), 3.09 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.8, 185.7, 157.4, 156.9, 139.1, 134.4, 132.0, 131.4, 130.0, 129.9, 129.3, 129.2, 129.1, 128.3, 128.0, 127.1, 126.6, 126.6, 126.5, 122.1, 120.0, 119.7, 111.3, 55.5, 55.4, 42.5, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{28}H_{24}NO_4$: 438.1700; found: 438.1720.



3e

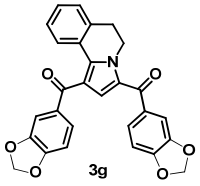
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((3,4-dimethoxyphenyl)methanone) (**3e**): Yellow solid; 186.4 mg (yield 75%); mp 145-147 °C; IR (KBr): 3447, 2957, 2924, 2852, 1628, 1595, 1511, 1450, 1266, 1169, 1137, 1023, 768 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.72 (d, J = 7.8 Hz, 1H), 7.56 (s, 1H), 7.55-7.50 (m, 2H), 7.46 (s, 1H), 7.28-7.24 (m, 2H), 7.18 (t, J = 7.2 Hz, 1H), 6.97 (s, 1H), 6.89 (d, J = 8.4 Hz, 1H), 6.84 (d, J = 8.4 Hz, 1H), 4.67 (t, J = 6.6 Hz, 2H), 3.95 (s, 6H), 3.93 (s, 3H), 3.91 (s, 3H), 3.15 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.2, 184.8, 153.0, 152.5, 148.8, 148.7, 137.7, 133.9, 131.7, 131.3, 128.8, 128.6, 127.6, 127.4, 126.9, 126.7, 125.1, 124.9, 124.0, 120.1, 111.6, 111.5, 109.7, 109.7, 56.0, 55.9, 55.9, 42.8, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{30}H_{28}NO_6$: 498.1911; found: 498.1914.



3f

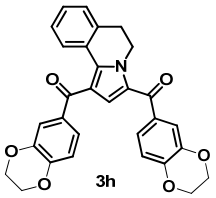
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-ethoxyphenyl)methanone) (**3f**): Light yellow solid; 174.5 mg (yield 75%); mp 135-138 °C; IR (KBr): 3443, 2926, 1624, 1600, 1508, 1445, 1394, 1306, 1253, 1168, 1114, 1042, 961, 886, 846, 764 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.90 (d, J = 8.4 Hz, 2H), 7.85 (d, J = 7.8 Hz, 2H), 7.75 (d, J = 7.8 Hz, 1H), 7.27-7.23 (m, 2H), 7.17 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 8.4 Hz, 3H), 6.89 (d, J = 8.4 Hz, 2H), 4.66 (t, J = 6.6 Hz, 2H), 4.08 (q, J = 6.0 Hz, 4H), 3.13 (t, J = 6.6 Hz, 2H), 1.43 (q, J = 6.0 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.3, 184.9, 162.6, 162.2, 137.5, 133.9, 132.2, 131.6, 131.4, 131.1, 128.7,

128.6, 127.6, 127.4, 126.9, 126.7, 124.9, 120.2, 113.9, 63.6, 63.6, 42.7, 29.3, 14.6, 14.6; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{30}H_{28}NO_4$: 466.2013; found: 466.2012.



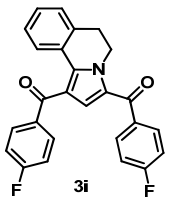
3g

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(benzo[*d*][1,3]dioxol-5-ylmethanone) (**3g**): Yellow solid; 146.5 mg (yield 63%); mp 119-121 °C; IR (KBr): 3444, 2924, 1628, 1600, 1502, 1482, 1446, 1395, 1257, 1164, 1114, 1038, 931, 765 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.71 (d, J = 7.8 Hz, 1H), 7.48 (d, J = 8.4 Hz, 1H), 7.45 (d, J = 9.6 Hz, 2H), 7.35 (s, 1H), 7.28-7.24 (m, 2H), 7.10-7.16 (m, 1H), 6.91 (s, 1H), 6.85 (d, J = 7.8 Hz, 1H), 6.80 (d, J = 8.4 Hz, 1H), 6.05 (s, 2H), 6.04 (s, 2H), 4.64 (t, J = 6.0 Hz, 2H), 3.13 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.8, 184.3, 151.5, 151.1, 147.9, 147.7, 137.8, 133.9, 133.3, 133.1, 128.9, 128.5, 127.6, 127.3, 126.9, 126.6, 126.6, 125.4, 124.9, 120.0, 109.4, 109.3, 107.6, 107.6, 42.8, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{28}H_{20}NO_6$: 466.1285; found: 466.1288.



3h

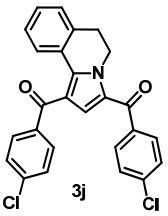
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)methanone) (**3h**): Yellow oil; 179.9 mg (yield 73%); IR (KBr): 3450, 2923, 1629, 1578, 1502, 1446, 1319, 1288, 1260, 1065, 889, 762 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.75 (d, J = 7.2 Hz, 1H), 7.49 (s, 1H), 7.45 (d, J = 8.4 Hz, 1H), 7.40 (t, J = 8.4 Hz, 2H), 7.25-7.23 (m, 2H), 7.19-7.15 (m, 1H), 6.94 (s, 1H), 6.88 (q, J = 7.8 Hz, 2H), 4.63 (t, J = 6.0 Hz, 2H), 4.28 (s, 4H), 4.76 (s, 2H), 4.25 (s, 2H), 3.11 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.0, 184.5, 147.7, 147.2, 143.1, 143.0, 137.7, 133.9, 132.4, 132.2, 128.8, 128.4, 127.6, 127.3, 126.9, 126.7, 125.0, 124.2, 123.4, 120.0, 119.3, 118.8, 116.8, 64.5, 64.5, 64.0, 64.0, 42.7, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{30}H_{24}NO_6$: 494.1598; found: 494.1625.



3i

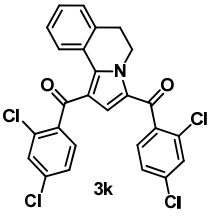
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-fluorophenyl)methanone) (**3i**): Light yellow solid; 169.4 mg (yield 82%); mp 119-121 °C; IR (KBr): 3451, 2950, 2919, 2867, 2839, 1633, 1505, 1458, 1376, 1218, 1154, 1127, 771 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.92 (t, J = 6.0 Hz, 2H), 7.86 (t, J = 6.0 Hz, 2H), 7.74 (d, J = 7.8 Hz, 1H), 7.29-7.26 (m, 2H), 7.20-7.17 (m, 1H), 7.13 (t, J = 8.4 Hz, 2H), 7.10 (t, J = 8.4 Hz, 2H), 6.91 (s, 1H), 4.69 (t, J = 6.0 Hz, 2H), 3.14 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.6, 184.4, 166.2, 165.9, 164.5,

164.2, 138.6, 135.2, 135.2, 134.8, 134.8, 134.1, 132.4, 132.3, 131.7, 131.6, 129.2, 128.4, 127.7, 127.6, 127.0, 126.3, 125.6, 119.9, 115.5, 115.3, 42.8, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{18}F_2NO_2$: 414.1300; found: 414.1308.



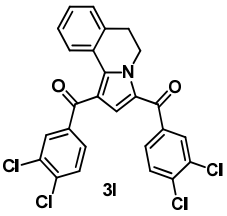
3j

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-chlorophenyl)methanone) (**3j**): Yellow solid; 183.7 mg (yield 79%); mp 147-149 °C; IR (KBr): 3440, 1629, 1587, 1480, 1445, 1398, 1263, 1215, 1193, 1089, 1013, 961, 883, 756, 565, 478 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.83 (d, J = 7.8 Hz, 2H), 7.77 (t, J = 7.8 Hz, 3H), 7.43 (d, J = 8.4 Hz, 2H), 7.39 (d, J = 7.8 Hz, 2H), 7.29 (s, 2H), 7.20-7.16 (m, 1H), 6.88 (s, 1H), 4.69 (t, J = 6.6 Hz, 2H), 3.14 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.8, 184.6, 139.0, 138.9, 138.4, 137.2, 136.9, 134.1, 131.2, 130.6, 129.4, 128.6, 128.6, 128.3, 127.7, 127.0, 126.2, 125.8, 119.8, 42.8, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{18}Cl_2NO_2$: 446.0709; found: 446.0702.



3k

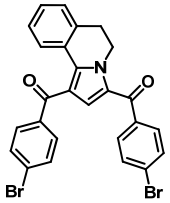
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((2,4-dichlorophenyl)methanone) (**3k**): Brown solid; 158.9 mg (yield 62%); mp 201-203 °C; IR (KBr): 3439, 1727, 1698, 1658, 1649, 1641, 1631, 1612, 1581, 1461, 1452, 1384, 1356, 670, 595 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.19 (d, J = 7.8 Hz, 1H), 7.44 (s, 1H), 7.41 (s, 1H), 7.37 (t, J = 8.4 Hz, 2H), 7.34 (d, J = 7.8 Hz, 1H), 7.31-7.28 (m, 3H), 7.27-7.25 (m, 1H), 6.53 (s, 1H), 4.78 (t, J = 6.6 Hz, 2H), 3.13 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 188.8, 183.4, 140.8, 137.8, 137.0, 136.8, 136.6, 134.6, 134.6, 132.7, 132.5, 130.6, 130.2, 130.2, 130.1, 128.5, 127.8, 127.5, 127.1, 127.0, 126.9, 126.0, 121.0, 42.9, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{16}Cl_4NO_2$: 513.9930; found: 513.9902.



3l

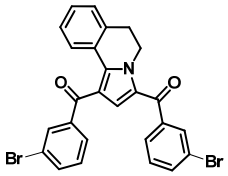
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((3,4-dichlorophenyl)methanone) (**3l**): Yellow solid; 189.8 mg (yield 74%); mp 213-215 °C; IR (KBr): 3449, 1635, 1528, 1447, 1400, 1267, 1027, 967, 910, 778, 763, 670 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.99 (s, 1H), 7.92 (s,

1H), 7.82 (d, J = 7.8 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.52 (q, J = 7.8 Hz, 2H), 7.34-7.30 (m, 2H), 7.22 (t, J = 7.2 Hz, 1H), 6.89 (s, 1H), 4.69 (t, J = 6.6 Hz, 2H), 3.15 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 189.3, 183.2, 139.5, 138.5, 138.3, 137.2, 136.6, 134.2, 133.0, 132.9, 131.6, 131.1, 130.5, 130.4, 129.7, 128.8, 128.2, 128.0, 127.8, 127.8, 127.1, 126.0, 126.0, 119.4, 42.9, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{16}Cl_4NO_2$: 513.9930; found: 513.9944.



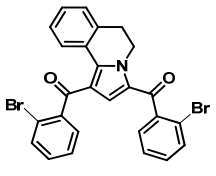
3m

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-bromophenyl)methanone) (**3m**): Yellow solid; 213.2 mg (yield 80%); mp 148-149 °C; IR (KBr): 3446, 2924, 1630, 1584, 1479, 1445, 1384, 1262, 1214, 1191, 1172, 1011, 882, 753, 563 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.78 (d, J = 7.8 Hz, 1H), 7.75 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 7.8 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.57 (d, J = 8.4 Hz, 2H), 7.30-7.27 (m, 2H), 7.22-7.19 (m, 1H), 6.87 (s, 1H), 4.69 (t, J = 6.0 Hz, 2H), 3.14 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.9, 184.8, 139.0, 137.7, 137.4, 134.2, 131.6, 131.6, 131.3, 130.7, 129.5, 128.3, 127.8, 127.7, 127.1, 127.1, 126.3, 125.9, 119.8, 42.9, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{18}Br_2NO_2$: 533.9699; found: 533.9704.



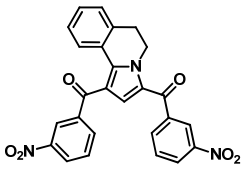
3n

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((3-bromophenyl)methanone) (**3n**): Yellow solid; 221.2 mg (yield 83%); mp 139-140 °C; IR (KBr): 3441, 1650, 1619, 1555, 1529, 1444, 1249, 1211, 1186, 1143, 967, 890, 772, 746, 710 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.05 (s, 1H), 7.96 (s, 1H), 7.86 (d, J = 7.8 Hz, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.74 (d, J = 7.2 Hz, 1H), 7.66 (d, J = 7.2 Hz, 2H), 7.36-7.28 (m, 4H), 7.21 (t, J = 7.2 Hz, 1H), 6.91 (s, 1H), 4.70 (t, J = 6.0 Hz, 2H), 3.14 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.3, 184.3, 140.8, 140.5, 139.3, 135.4, 134.9, 134.2, 132.7, 132.1, 129.9, 129.9, 129.6, 128.4, 128.1, 127.8, 127.7, 127.7, 127.1, 126.4, 126.2, 122.6, 122.5, 119.7, 42.8, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{18}Br_2NO_2$: 533.9699; found: 533.9688.



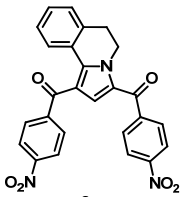
3o

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((2-bromophenyl)methanone) (**3o**): Brown solid; 186.5 mg (yield 70%); mp 136-137 °C; IR (KBr): 3450, 2926, 1642, 1586, 1429, 1384, 1221, 1027, 960, 886, 743, 638 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.27 (d, J = 7.8 Hz, 1H), 7.55 (q, J = 7.8 Hz, 2H), 7.38 (t, J = 7.8 Hz, 2H), 7.33 (t, J = 6.6 Hz, 2H), 7.31-7.27 (m, 4H), 7.23 (t, J = 7.2 Hz, 1H), 6.50 (s, 1H), 4.80 (t, J = 6.6 Hz, 2H), 3.13 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.6, 185.4, 141.4, 140.6, 140.5, 134.6, 134.5, 133.3, 133.3, 131.2, 131.1, 129.9, 129.5, 129.0, 128.6, 128.5, 128.3, 127.4, 127.0, 126.9, 126.2, 120.9, 119.9, 119.9, 42.8, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{18}Br_2NO_2$: 533.9699; found: 533.9679.



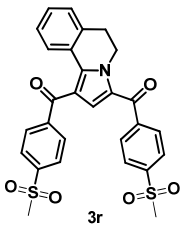
3p

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((3-nitrophenyl)methanone) (**3p**): Orange solid; 179.8 mg (yield 77%); mp 142-144 °C; IR (KBr): 3444, 1633, 1529, 1478, 1446, 1349, 1256, 1213, 1192, 762, 720 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.70 (s, 1H), 8.66 (s, 1H), 8.38 (t, J = 7.2 Hz, 2H), 8.25 (d, J = 7.2 Hz, 1H), 8.18 (d, J = 7.2 Hz, 1H), 7.86 (d, J = 7.8 Hz, 1H), 7.68 (q, J = 7.8 Hz, 2H), 7.37-7.32 (m, 2H), 7.24-7.21 (m, 1H), 6.93 (s, 1H), 4.76 (t, J = 6.6 Hz, 2H), 3.20 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 189.0, 183.1, 148.0, 147.9, 140.2, 140.0, 135.3, 134.8, 134.4, 130.0, 129.7, 128.0, 127.9, 127.1, 126.9, 126.5, 125.8, 124.6, 124.0, 119.3, 43.0, 29.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{18}N_3O_6$: 468.1190; found: 468.1182.



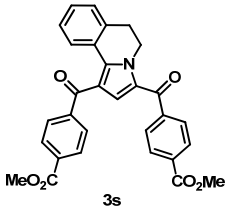
3q

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-nitrophenyl)methanone) (**3q**)**:** Orange solid; 184.5 mg (yield 79%); mp 218-221 °C; IR (KBr): 3444, 2923, 1634, 1524, 1445, 1384, 1348, 1216, 1191, 1129, 1041, 846, 771, 563 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.29 (d, J = 8.4 Hz, 2H), 8.24 (d, J = 8.4 Hz, 2H), 7.99 (d, J = 8.4 Hz, 2H), 7.95 (d, J = 9.0 Hz, 2H), 7.79 (d, J = 7.8 Hz, 1H), 7.37-7.32 (m, 2H), 7.23-7.20 (m, 1H), 6.90 (s, 1H), 4.76 (t, J = 6.6 Hz, 2H), 3.19 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 189.6, 183.7, 149.8, 149.5, 144.0, 143.6, 140.2, 134.4, 130.4, 130.0, 129.9, 128.2, 128.0, 127.8, 127.0, 126.5, 125.7, 123.5, 119.6, 43.0, 29.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{18}N_3O_6$: 468.1190; found: 468.1207.



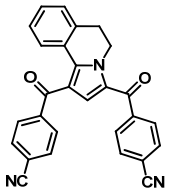
3r

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-(methylsulfonyl)phenyl)methanone) (**3r**)：Yellow solid; 183.9 mg (yield 69%); mp 160-161 °C; IR (KBr): 3440, 1636, 1523, 1445, 1397, 1301, 1153, 958, 888, 855, 779, 752, 707 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.06-7.99 (m, 6H), 7.97 (d, J = 7.8 Hz, 2H), 7.77 (d, J = 7.8 Hz, 1H), 7.35-7.30 (m, 2H), 7.21-7.17 (m, 1H), 6.87 (s, 1H), 4.74 (t, J = 6.6 Hz, 2H), 3.18 (t, J = 6.6 Hz, 2H), 3.11 (s, 3H), 3.08 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.1, 184.0, 143.5, 143.4, 143.1, 143.0, 140.0, 134.3, 130.4, 129.9, 129.8, 128.2, 127.8, 127.8, 127.4, 127.0, 126.3, 125.8, 119.6, 44.2, 42.9, 29.0; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{28}H_{23}NO_6S_2$: 534.1040; found: 534.1056.



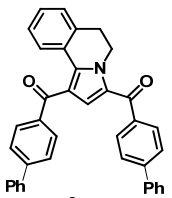
3s

dimethyl 4,4'-(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-dicarbonyl)dibenzoate (**3s**)：Yellow solid; 192.3 mg (yield 78%); mp 166-167 °C; IR (KBr): 3431, 2951, 1720, 1658, 1625, 1485, 1442, 1400, 1279, 1210, 1195, 1103, 1016, 960, 887, 778, 732 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.11 (d, J = 8.4 Hz, 2H), 8.08 (d, J = 8.4 Hz, 2H), 7.91 (d, J = 8.4 Hz, 2H), 7.86 (t, J = 8.4 Hz, 3H), 7.32-7.27 (m, 2H), 7.20 (t, J = 7.8 Hz, 1H), 6.90 (s, 1H), 4.74 (t, J = 6.6 Hz, 2H), 3.93 (s, 3H), 3.93 (s, 3H), 3.16 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.0, 185.1, 166.1, 142.6, 142.2, 139.5, 134.2, 133.3, 132.8, 129.5, 129.4, 128.9, 128.3, 127.9, 127.6, 127.0, 126.7, 126.1, 119.9, 52.3, 42.8, 29.1; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{30}H_{24}NO_6$: 494.1598; found: 494.1622.



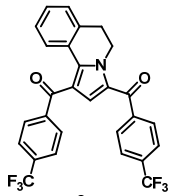
3t

4,4'-(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-dicarbonyl)dibenzonitrile (**3t**)：Yellow solid; 172.9 mg (yield 81%); mp 220-221 °C; IR (KBr): 2228, 1659, 1633, 1524, 1486, 1429, 1392, 1261, 1208, 1172, 961, 887, 859, 760 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.93 (d, J = 8.4 Hz, 2H), 7.89 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 7.8 Hz, 2H), 7.22 (d, J = 7.8 Hz, 3H), 7.34-7.30 (m, 2H), 7.21-7.17 (m, 1H), 6.87 (s, 1H), 4.73 (t, J = 6.6 Hz, 2H), 3.17 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 189.9, 183.9, 142.3, 141.9, 139.9, 134.3, 132.1, 129.9, 129.8, 129.4, 128.1, 127.9, 127.8, 127.0, 126.2, 125.7, 119.5, 117.8, 115.7, 115.3, 42.9, 29.0; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{28}H_{18}N_3O_2$: 428.1394; found: 428.1415.



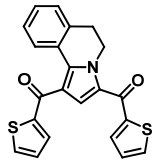
3u

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis([1,1'-biphenyl]-4-ylmethanone) (**3u**): Yellow solid; 211.7 mg (yield 80%); mp 123-124 °C; IR (KBr): 3443, 2852, 1629, 1480, 1445, 1384, 1264, 1217, 1186, 1128, 1040, 1013, 961, 886, 854, 748, 695, 563 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.00 (d, J = 7.8 Hz, 2H), 7.93 (d, J = 7.8 Hz, 2H), 7.86 (d, J = 7.8 Hz, 1H), 7.66 (t, J = 8.4 Hz, 4H), 7.61 (d, J = 7.2 Hz, 4H), 7.44 (t, J = 7.2 Hz, 4H), 7.37 (t, J = 7.2 Hz, 2H), 7.29-7.27 (m, 2H), 7.24-7.19 (m, 1H), 7.06 (s, 1H), 4.73 (t, J = 6.6 Hz, 2H), 3.16 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.8, 185.6, 145.3, 144.8, 139.8, 139.8, 138.6, 137.7, 137.3, 134.2, 130.5, 129.9, 129.1, 128.9, 128.6, 128.1, 128.0, 127.7, 127.7, 127.2, 127.2, 127.0, 127.0, 126.6, 125.9, 120.2, 42.8, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{38}H_{28}NO_2$: 530.2115; found: 530.2118.



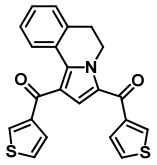
3v

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((4-(trifluoromethyl)phenyl)methanone) (**3v**)：Yellow solid; 205.2 mg (yield 80%); mp 120-121 °C; IR (KBr): 3442, 1656, 1636, 1524, 1448, 1406, 1330, 1170, 1125, 1066, 887, 852, 766 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.98 (d, J = 7.8 Hz, 2H), 7.91 (d, J = 7.8 Hz, 2H), 7.79 (d, J = 7.8 Hz, 1H), 7.72 (d, J = 7.8 Hz, 2H), 7.69 (d, J = 7.8 Hz, 2H), 7.34-7.29 (m, 2H), 7.20 (t, J = 5.4 Hz, 1H), 6.90 (s, 1H), 4.74 (t, J = 6.0 Hz, 2H), 3.17 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.7, 184.7, 142.0, 141.6, 139.7, 134.3, 134.1, 133.8, 133.6, 133.4, 130.0, 129.7, 129.4, 128.4, 127.9, 127.8, 127.1, 126.2, 126.1, 125.4, 124.5, 122.7, 119.8, 43.0, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{28}H_{18}F_6NO_2$: 514.1236; found: 514.1259.



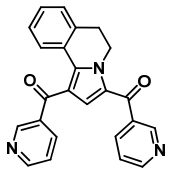
3w

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(thiophen-2-ylmethanone) (**3w**): Yellow solid; 161.4 mg (yield 83%); mp 211-212 °C; IR (KBr): 3445, 2952, 2922, 1629, 1446, 1413, 1383, 1265, 1215, 1190, 1130, 1047, 757, 562 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.90 (d, J = 7.2 Hz, 1H), 7.79 (s, 1H), 7.70 (s, 1H), 7.67-7.63 (m, 2H), 7.40 (s, 1H), 7.28-7.24 (m, 2H), 7.21 (t, J = 6.6 Hz, 1H), 7.14-7.11 (m, 2H), 4.63 (t, J = 6.0 Hz, 2H), 3.41 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 183.8, 177.0, 145.3, 144.3, 137.9, 134.1, 134.0, 133.8, 132.9, 132.7, 129.1, 128.4, 127.9, 127.8, 127.6, 127.6, 127.1, 126.7, 123.6, 120.2, 42.8, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{22}H_{16}NO_2S_2$: 390.0617; found: 390.0617.



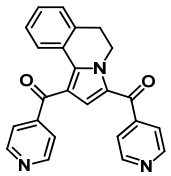
3x

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(thiophen-3-ylmethanone) (**3x**): Brown solid; 160.9 mg (yield 83%); mp 173-174 °C; IR (KBr): 3441, 3104, 1614, 1511, 1450, 1415, 1259, 1227, 1164, 975, 857, 747, 726 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.97 (d, J = 10.2 Hz, 2H), 7.82 (d, J = 7.8 Hz, 1H), 7.61 (d, J = 5.4 Hz, 1H), 7.58 (d, J = 4.8 Hz, 1H), 7.38-7.36 (m, 1H), 7.35-7.32 (m, 1H), 7.28-7.25 (m, 2H), 7.22-7.18 (m, 2H), 4.66 (t, J = 6.0 Hz, 2H), 3.12 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 185.6, 179.3, 143.0, 142.2, 137.9, 134.1, 133.7, 131.9, 129.1, 129.1, 128.2, 128.1, 127.6, 127.6, 127.0 126.6, 126.2, 124.2, 121.0, 42.8, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{22}H_{16}NO_2S_2$: 390.0617; found: 390.0626.



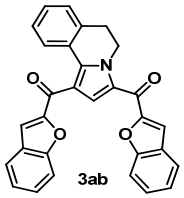
3y

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(pyridin-3-ylmethanone) (**3y**): Brown solid; 136.5 mg (yield 72%); mp 108-110 °C; IR (KBr): 3442, 1621, 1582, 1525, 1444, 1266, 1214, 1193, 959, 884, 735, 701 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 9.02 (d, J = 4.8 Hz, 2H), 8.76 (d, J = 3.6 Hz, 1H), 8.74 (d, J = 3.6 Hz, 1H), 8.19 (d, J = 7.8 Hz, 1H), 8.11 (d, J = 7.8 Hz, 1H), 7.83 (d, J = 7.8 Hz, 1H), 7.45-7.39 (m, 2H), 7.35-7.30 (m, 2H), 7.21 (t, J = 6.6 Hz, 1H), 6.97 (s, 1H), 4.74 (t, J = 6.6 Hz, 2H), 3.17 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 189.8, 183.7, 152.9, 152.5, 150.7, 150.7, 149.8, 149.7, 139.7, 136.9, 136.4, 134.6, 134.3, 134.1, 129.7, 128.3, 127.9, 127.7, 127.0, 126.5, 125.9, 123.4, 123.4, 119.7, 42.9, 29.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{24}H_{18}N_3O_2$: 380.1394; found: 380.1410.



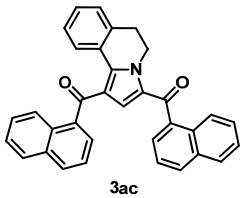
3z

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(pyridin-4-ylmethanone) (**3z**): Yellow solid; 145.9 mg (yield 77%); mp 188-189 °C; IR (KBr): 1622, 1525, 1445, 1406, 1324, 1266, 1195, 966, 889, 650 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.77 (d, J = 5.4 Hz, 2H), 8.75 (d, J = 5.4 Hz, 2H), 7.86 (d, J = 7.8 Hz, 1H), 7.63 (d, J = 5.4 Hz, 2H), 7.60 (d, J = 5.4 Hz, 2H), 7.37-7.30 (m, 2H), 7.23 (t, J = 7.2 Hz, 1H), 6.92 (s, 1H), 4.76 (t, J = 6.6 Hz, 2H), 3.17 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 190.2, 184.2, 150.5, 150.4, 145.5, 145.1, 140.4, 134.4, 130.1, 128.2, 128.0, 127.8, 127.1, 126.9, 125.8, 122.6, 122.3, 119.5, 43.0, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{24}H_{18}N_3O_2$: 380.1394; found: 380.1408.



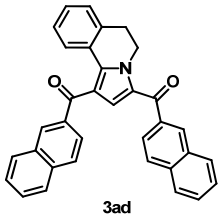
3ab

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(benzofuran-3-ylmethanone) (**3ab**): Yellow solid; 194.2 mg (yield 85%); mp 171-173 °C; IR (KBr): 3441, 1650, 1616, 1552, 1443, 1398, 1273, 1159, 1141, 853, 836, 757, 744 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.04 (s, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.72 (d, J = 7.8 Hz, 2H), 7.62 (t, J = 7.2 Hz, 2H), 7.58 (d, J = 4.8 Hz, 2H), 7.50-7.44 (m, 2H), 7.34-7.27 (m, 4H), 7.24 (t, J = 7.2 Hz, 1H), 4.74 (t, J = 6.6 Hz, 2H), 3.14 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 180.0, 173.0, 155.9, 155.6, 153.3, 153.2, 139.4, 134.3, 129.5, 128.2, 128.0, 127.9, 127.8, 127.6, 127.1, 127.1, 127.0, 126.4, 125.0, 123.9, 123.3, 123.0, 119.8, 115.7, 114.2, 112.4, 112.3, 43.0, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{30}H_{19}NO_4$: 458.1387; found: 458.1399.



3ac

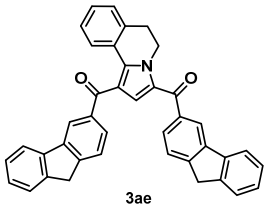
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(naphthalen-1-ylmethanone) (**3ac**): Yellow solid; 174.1 mg (yield 73%); mp 122-123 °C; IR (KBr): 3446, 2924, 2852, 1626, 1445, 1384, 1273, 1215, 1183, 1128, 1040, 760, 568, 477 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.42 (s, 1H), 8.37 (s, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.4 Hz, 2H), 7.89-8.84 (m, 4H), 7.81 (d, J = 7.8 Hz, 2H), 7.52 (q, J = 7.2 Hz, 2H), 7.48 (q, J = 7.8 Hz, 2H), 7.30-7.25 (m, 2H), 7.20-7.17 (m, 1H), 7.06 (s, 1H), 4.77 (t, J = 6.6 Hz, 2H), 3.17 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.3, 186.0, 138.6, 136.2, 135.9, 135.3, 135.0, 134.1, 132.2, 132.1, 131.8, 130.6, 129.3, 129.2, 129.1, 128.7, 128.2, 128.0, 127.7, 127.6, 127.6, 127.0, 126.6, 126.6, 126.3, 125.4, 125.3, 120.3, 42.9, 29.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{34}H_{24}NO_2$: 478.1802; found: 478.1805.



3ad

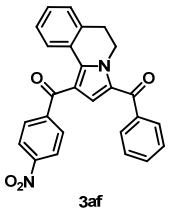
(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis(naphthalen-2-ylmethanone) (**3ad**): Yellow solid; 164.6 mg (yield 69%); mp 118-119 °C; IR (KBr): 3443, 2924, 1630, 1480, 1384, 1274, 1219, 1183, 1127, 1042, 1015, 892, 773, 693, 569 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.43 (d, J = 7.8 Hz, 1H), 8.21 (d, J = 8.4 Hz, 1H), 8.14 (d, J = 7.8 Hz, 1H), 7.88 (d, J = 8.4 Hz, 2H) 7.83 (d, J = 7.8 Hz, 2H), 7.69 (d, J = 7.2 Hz, 1H), 7.61 (d, J = 7.2 Hz, 1H), 7.54-7.50 (m, 4H), 7.36 (t, J = 7.2 Hz, 1H), 7.33 (d, J = 4.8 Hz, 2H), 7.23-7.18 (m, 1H), 6.60 (s, 1H), 4.90 (t, J = 6.6 Hz, 2H), 3.21 (t, J = 6.0 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 193.0, 187.4, 139.9, 136.8,

136.7, 134.5, 133.7, 133.6, 131.9, 131.1, 130.9, 130.7, 129.8, 129.6, 129.0, 128.3, 128.3, 128.2, 127.5, 127.4, 127.3, 127.0, 127.0, 126.5, 126.3, 126.3, 125.6, 125.6, 125.3, 124.1, 122.2, 42.9, 29.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{34}H_{24}NO_2$: 478.1802; found: 478.1800.



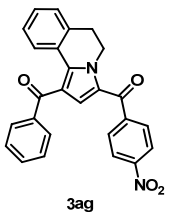
3ae

(5,6-dihydropyrrolo[2,1-*a*]isoquinoline-1,3-diyl)bis((9*H*-fluoren-3-yl)methanone) (**3ae**): Yellow solid; 143.8 mg (yield 52%); mp 253-254 °C; IR (KBr): 3441, 1637, 1623, 1605, 1446, 1433, 1423, 1387, 1264, 1150, 761, 749 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.13 (s, 1H), 8.05 (s, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 7.6 Hz, 1H), 7.83-7.76 (m, 5H), 7.56 (d, J = 6.8 Hz, 2H), 7.39 (t, J = 7.2 Hz, 2H), 7.36-7.32 (m, 2H), 7.29 (t, J = 7.2 Hz, 2H), 7.17 (t, J = 6.8 Hz, 1H), 7.03 (s, 1H), 4.74 (t, J = 6.8 Hz, 2H), 3.95 (s, 2H), 3.92 (s, 2H), 3.18 (t, J = 6.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.5, 186.1, 146.1, 145.6, 144.4, 144.2, 143.1, 143.0, 140.5, 138.2, 137.4, 137.0, 134.1, 129.5, 129.0, 128.9, 128.8, 127.9, 127.8, 127.7, 127.0, 127.0, 126.7, 126.6, 126.1, 125.8, 125.2, 125.1, 120.8, 120.7, 120.5, 119.4, 42.9, 36.9, 36.8, 29.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{40}H_{27}NO_2$: 554.2115; found: 554.2136.



3af

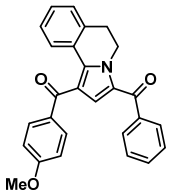
(3-benzoyl-5,6-dihydropyrrolo[2,1-*a*]isoquinolin-1-yl)(4-nitrophenyl)methanone (**3af**): 77.1 mg (yield 18%); mp 192-193 °C; IR (KBr): 1638, 1517, 1477, 1345, 1261, 1194, 1017, 959, 845, 735, 716 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.26 (d, J = 8.8 Hz, 2H), 8.00 (d, J = 8.8 Hz, 2H), 7.85 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 6.8 Hz, 2H), 7.57 (t, J = 7.6 Hz, 1H), 7.46 (t, J = 8.0 Hz, 2H), 7.33-7.31 (m, 2H), 7.23-7.19 (m, 1H), 6.89 (s, 1H), 4.72 (t, J = 6.8 Hz, 2H), 3.16 (t, J = 6.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 189.9, 186.1, 149.8, 144.1, 139.4, 138.8, 134.4, 132.3, 130.5, 129.7, 129.2, 129.0, 128.4, 127.9, 127.8, 127.0, 126.2, 126.0, 123.5, 119.2, 43.0, 29.2; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{26}H_{18}N_2O_4Na$: 445.1159; found: 445.1160.



3ag

(1-benzoyl-5,6-dihydropyrrolo[2,1-*a*]isoquinolin-3-yl)(4-nitrophenyl)methanone (**3ag**): 80 mg (yield 19%); mp 165-166 °C; IR (KBr): 1598, 1504, 1447, 1319, 1215, 1023, 948, 879, 777, 736,

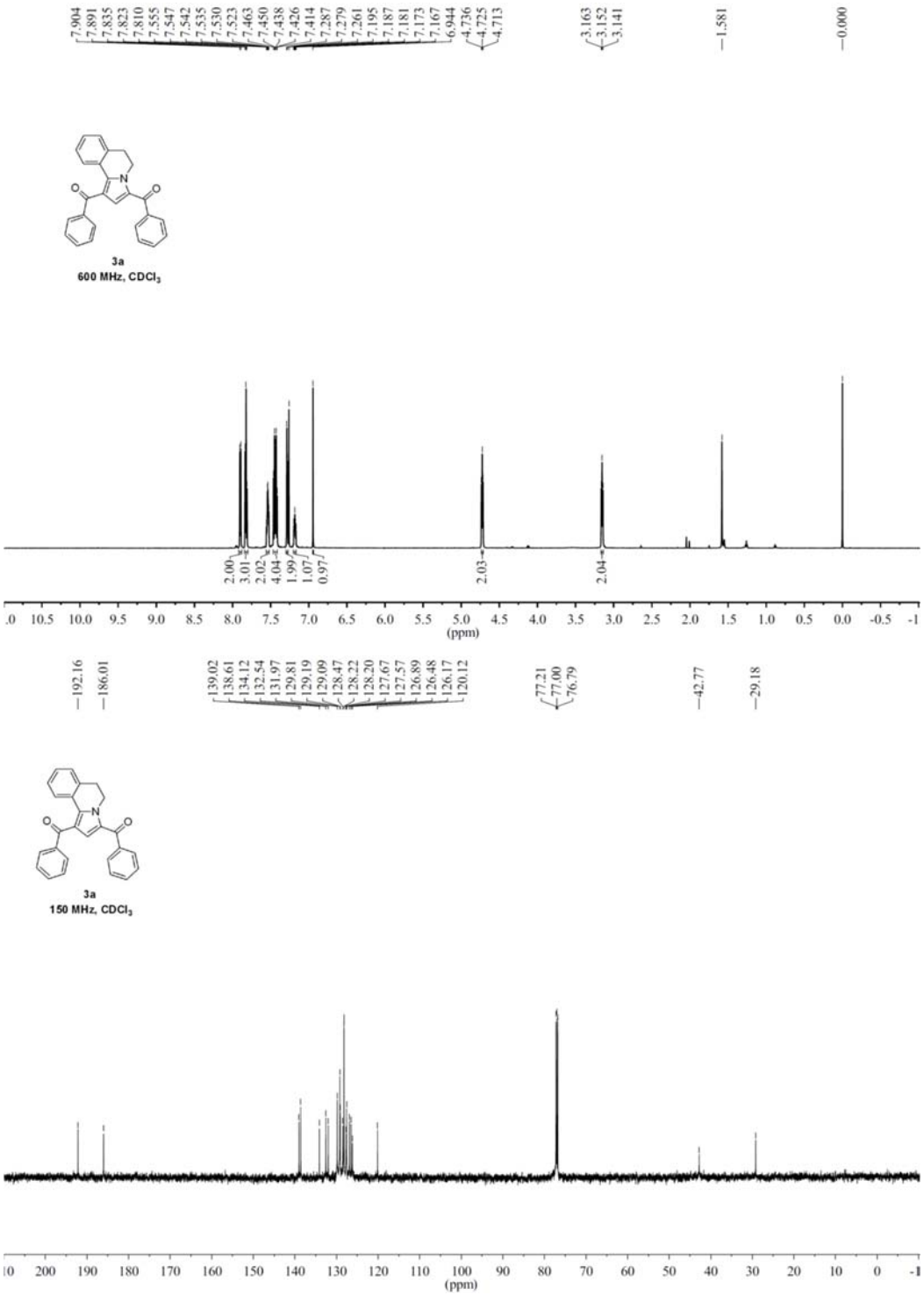
714 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 8.29 (d, J = 8.4 Hz, 2H), 7.95 (d, J = 9.0 Hz, 2H), 7.87 (d, J = 7.8 Hz, 2H), 7.78 (d, J = 7.8 Hz, 1H), 7.55 (t, J = 7.2 Hz, 1H), 7.43 (t, J = 7.8, 2H), 7.30 (d, J = 4.2, 2H), 7.20-7.17 (m, 1H), 6.90 (s, 1H), 4.76 (t, J = 6.6 Hz, 2H), 3.17 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 191.9, 183.7, 149.5, 144.5, 139.7, 138.4, 134.2, 132.9, 129.9, 129.8, 129.6, 128.4, 127.9, 127.8, 127.7, 127.1, 126.9, 126.1 123.5, 120.8, 42.9, 29.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{26}H_{19}N_2O_4$: 423.1339; found: 423.1357.

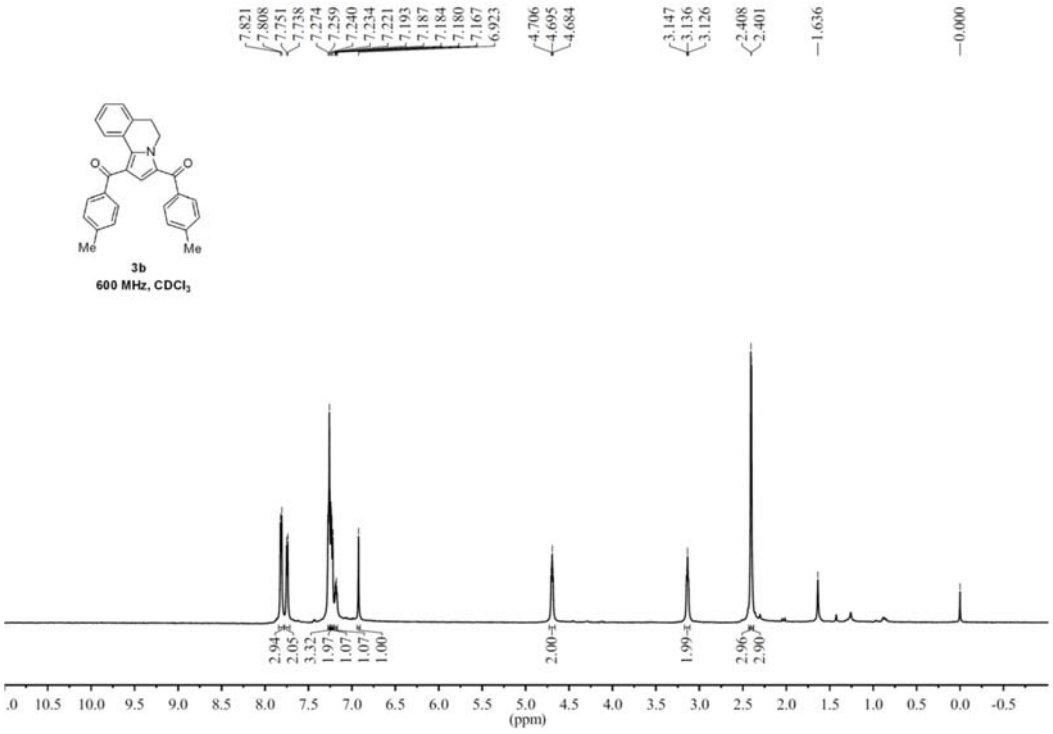


3ak

(3-benzoyl-5,6-dihydropyrrolo[2,1-*a*]isoquinolin-1-yl)(4-methoxyphenyl)methanone (**3ak**): ^1H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.91 (d, J = 7.8 Hz, 2H), 7.85 (t, J = 9.0 Hz, 3H), 7.53 (d, J = 7.2 Hz, 1H), 7.43 (t, J = 7.8 Hz, 2H), 7.28-7.24 (m, 2H), 7.19-7.16 (m, 1H), 6.94 (s, 1H), 6.93-6.91 (m, 2H), 4.66 (t, J = 7.2 Hz, 2H), 3.85 (s, 3H), 3.13 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 192.3, 184.9, 162.9, 138.8, 138.2, 134.1, 132.5, 131.6, 131.6, 129.9, 129.0, 128.8, 128.3, 127.7, 127.6, 126.9, 126.7, 125.3, 120.0, 113.5, 55.4, 42.8, 29.3; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{27}H_{21}NO_3Na$: 430.1414; found: 430.1417.

7. Appendix: spectral copies of ^{1}HNMR, and ^{13}CNMR

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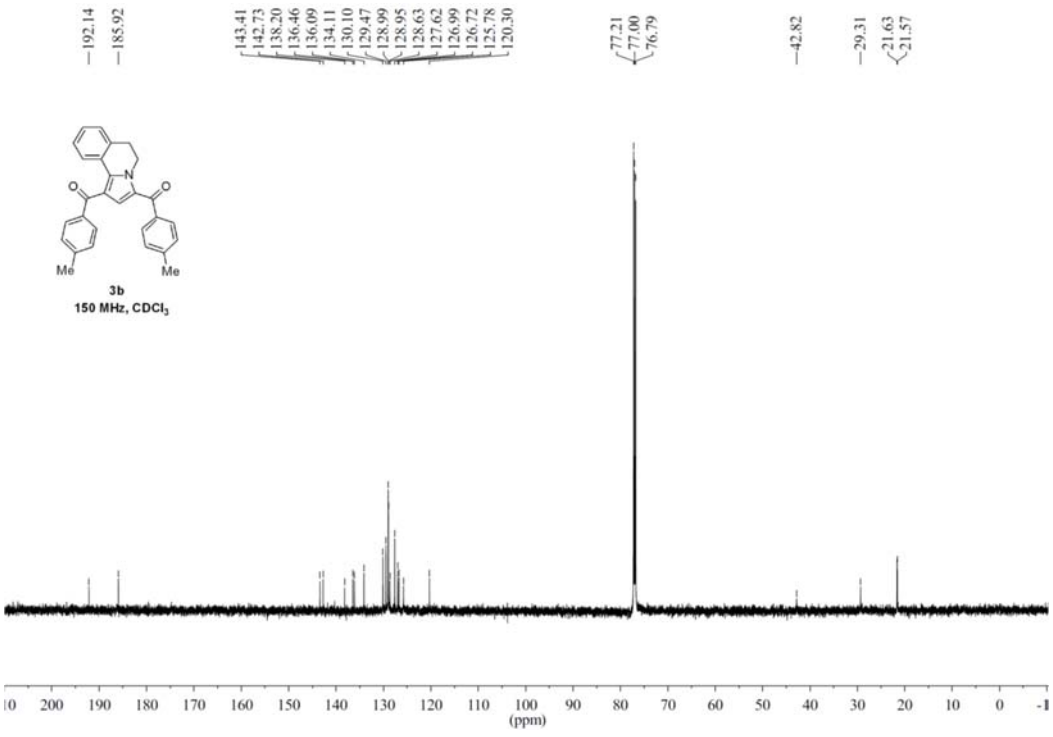
7.180
7.167
6.923
4.706
4.695
4.684
3.147
3.136
3.126
2.408
2.401
1.636
0.000
Me
Me
3b
600 MHz, CDCl3
2.94
2.05
3.32
1.97
1.07
1.07
1.00
2.00
1.99
2.96
2.90
(ppm)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136.09
134.11
130.10
129.47
128.99
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127.62
126.99
126.72
125.78
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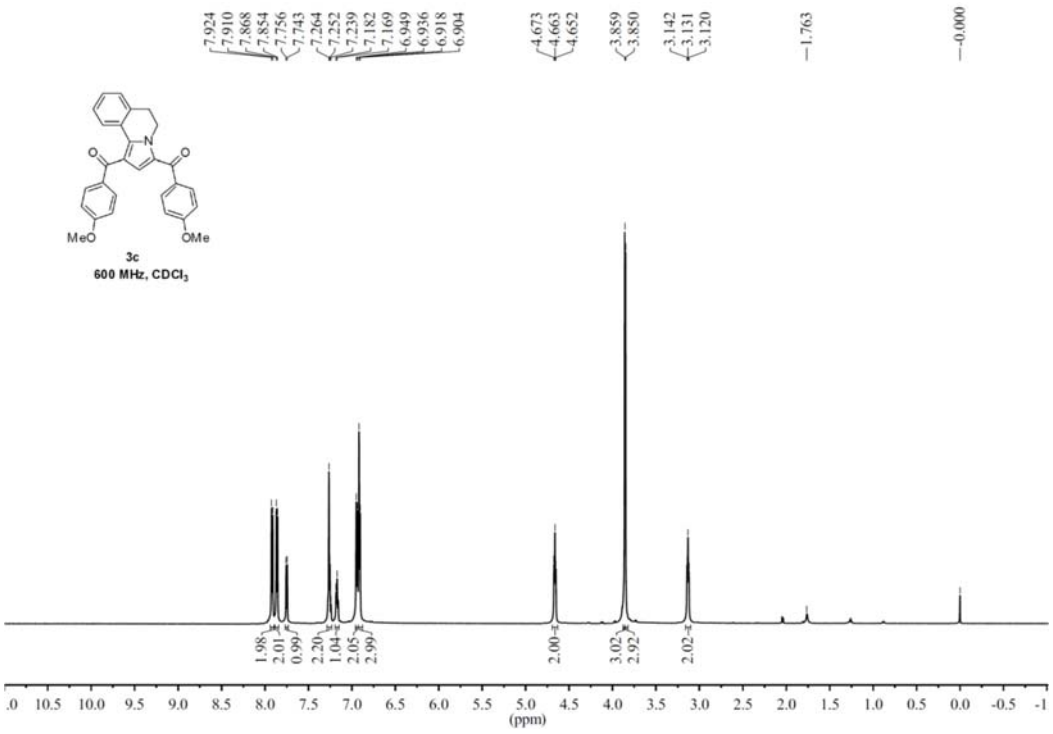
76.79
42.82
29.31
21.63
21.57
Me
Me
3b
150 MHz, CDCl3
(ppm)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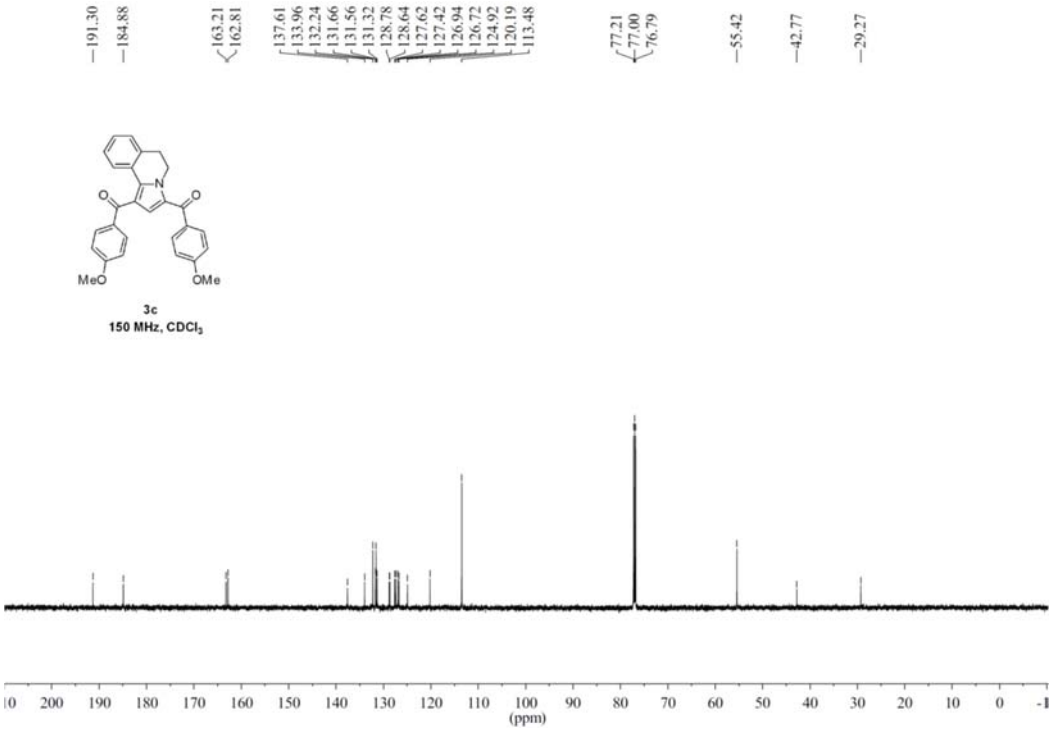
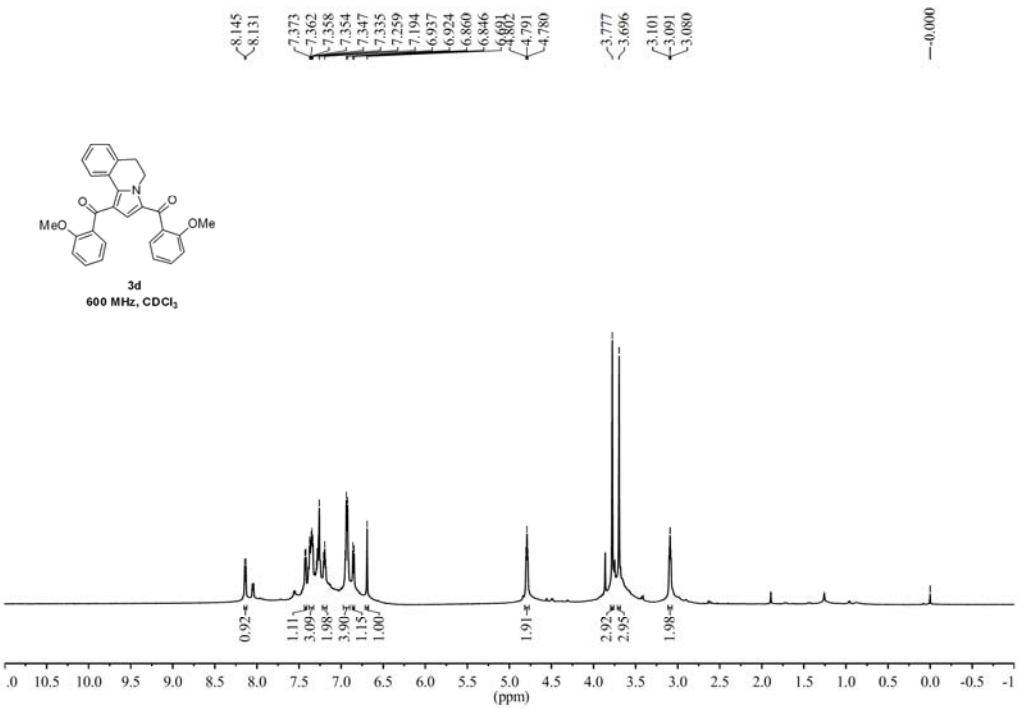
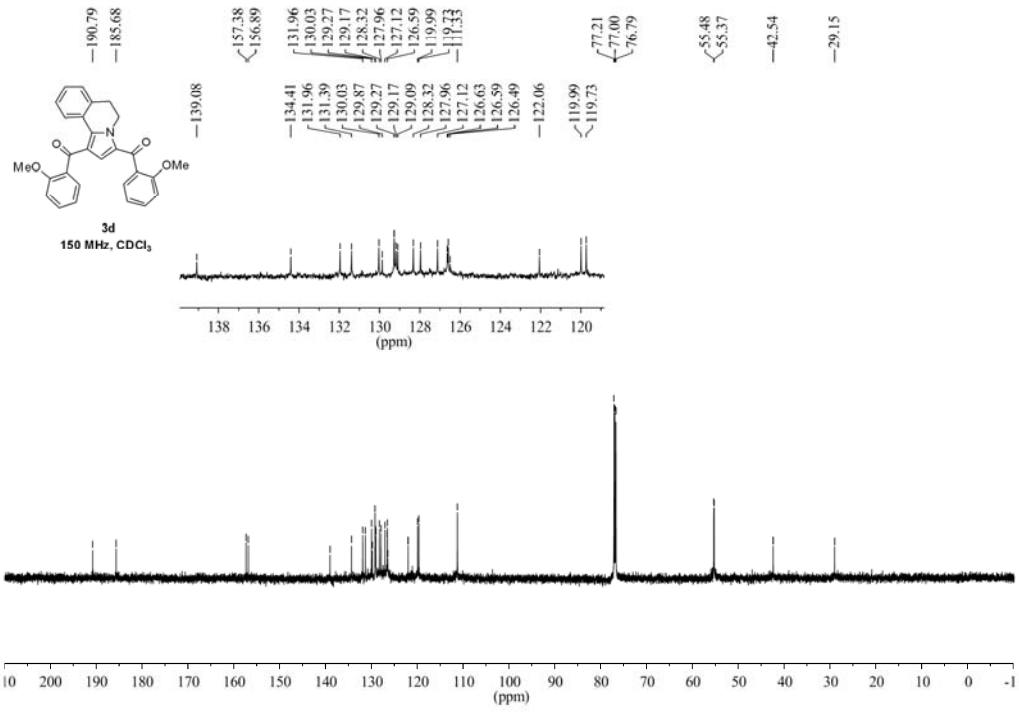
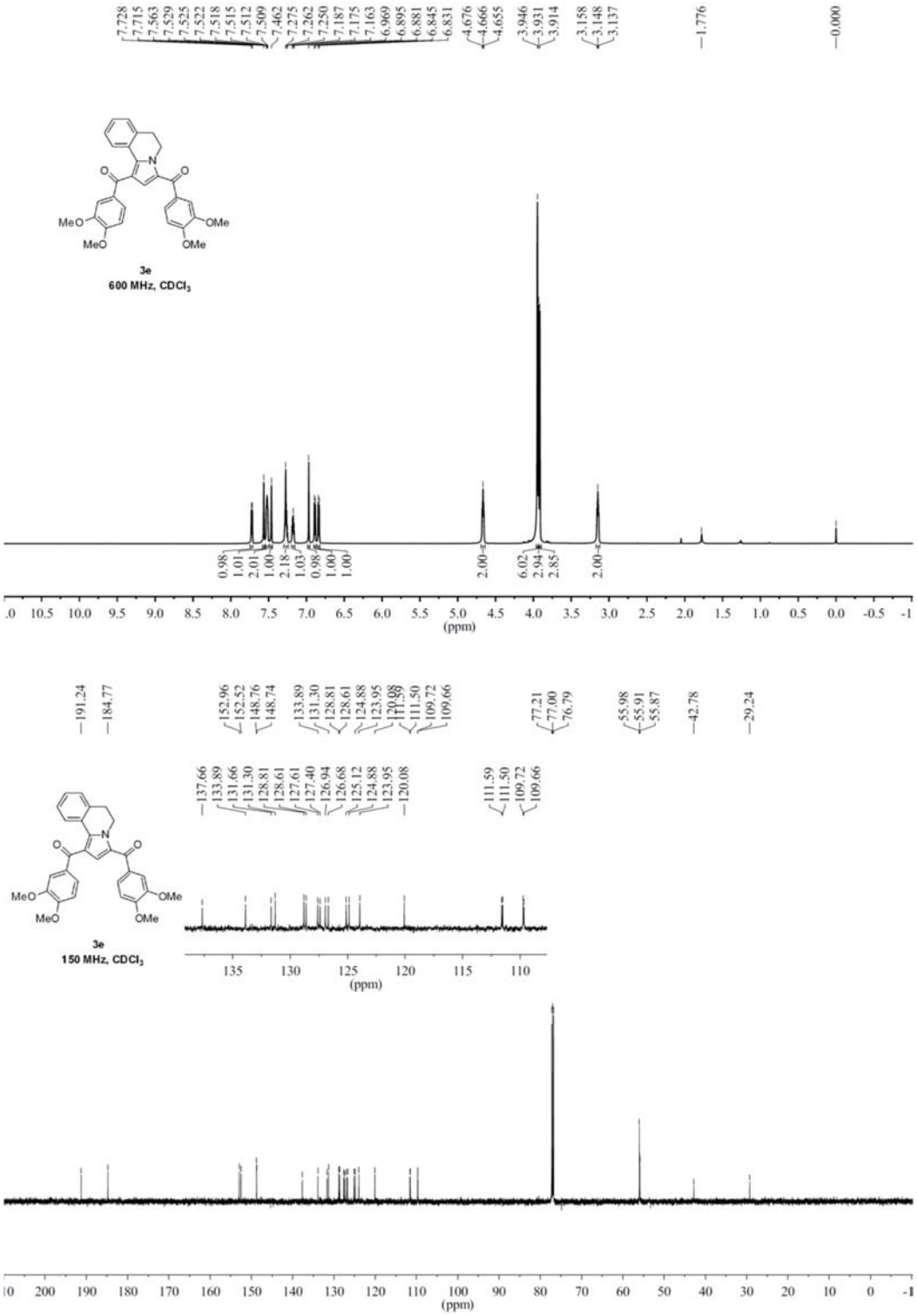
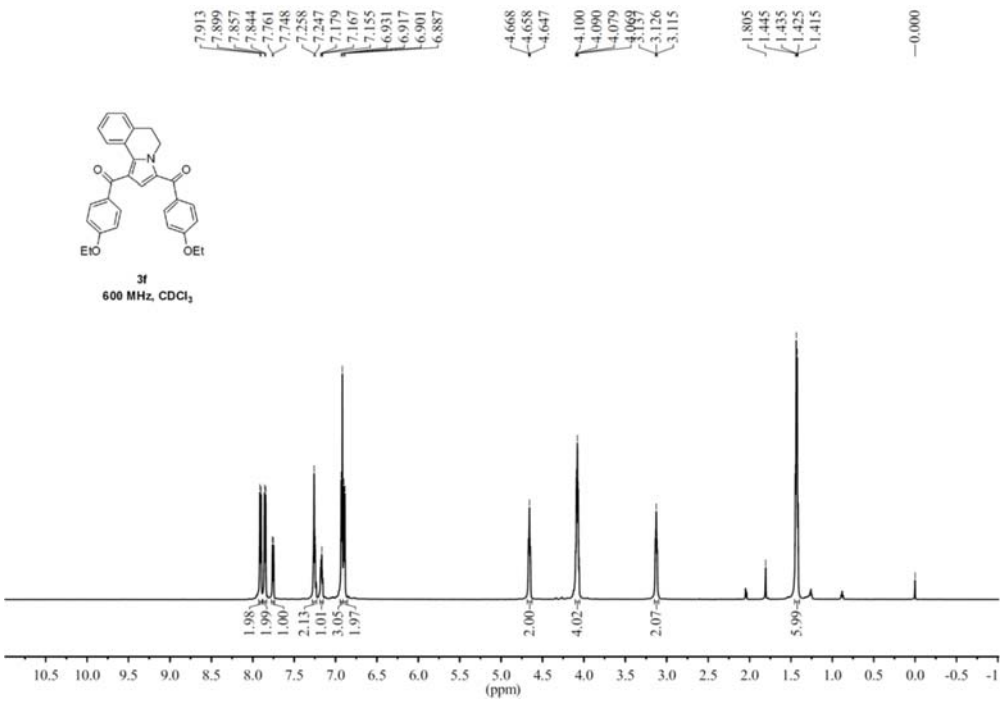
3.850
3.142
3.131
3.120
1.763
0.000
MeO
OMe
3c
600 MHz, CDCl3
1.98
2.01
0.99
2.20
1.04
2.05
2.99
2.00
3.02
2.92
2.02
(ppm)

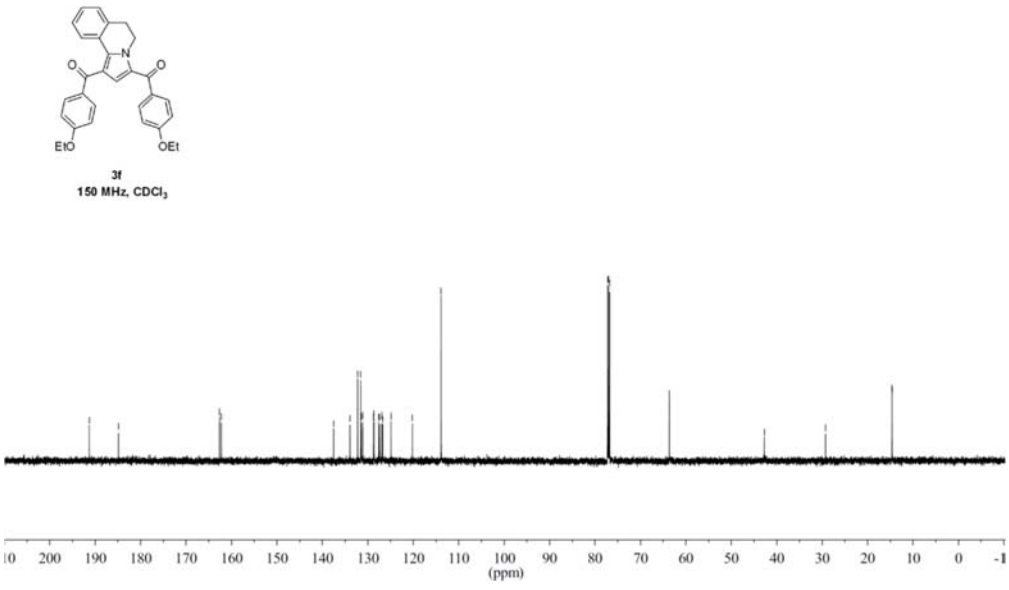

191.30
184.88
163.21
162.81
137.61
133.96
132.24
131.66
131.56
131.32
128.78
128.64
127.62
127.42
126.94
126.72
124.92
120.19
113.48
77.21
77.00
76.79
55.42
42.77
29.27
MeO
OMe
3c
150 MHz, CDCl3
(ppm)

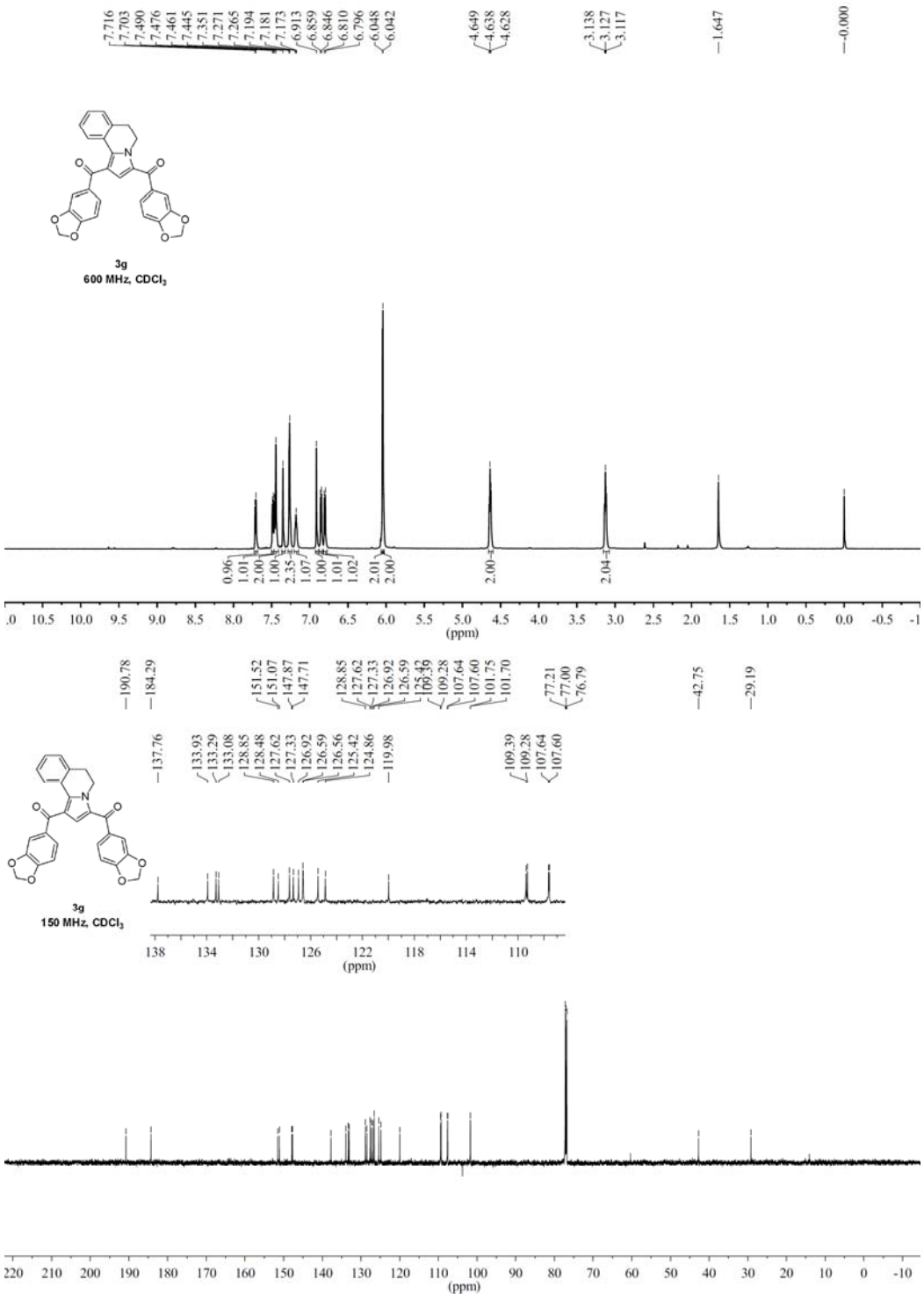

8.145
8.131
7.373
7.362
7.358
7.354
7.347
7.335
7.259
7.194
6.937
6.924
6.860
6.846
6.691
6.682
4.802
4.791
4.780
3.777
3.696
3.101
3.091
3.080
-0.000
MeO
OMe
3d
600 MHz, CDCl3
0.92
1.11
3.09
1.98
3.90
1.15
1.00
1.91
2.92
2.95
1.98
(ppm)

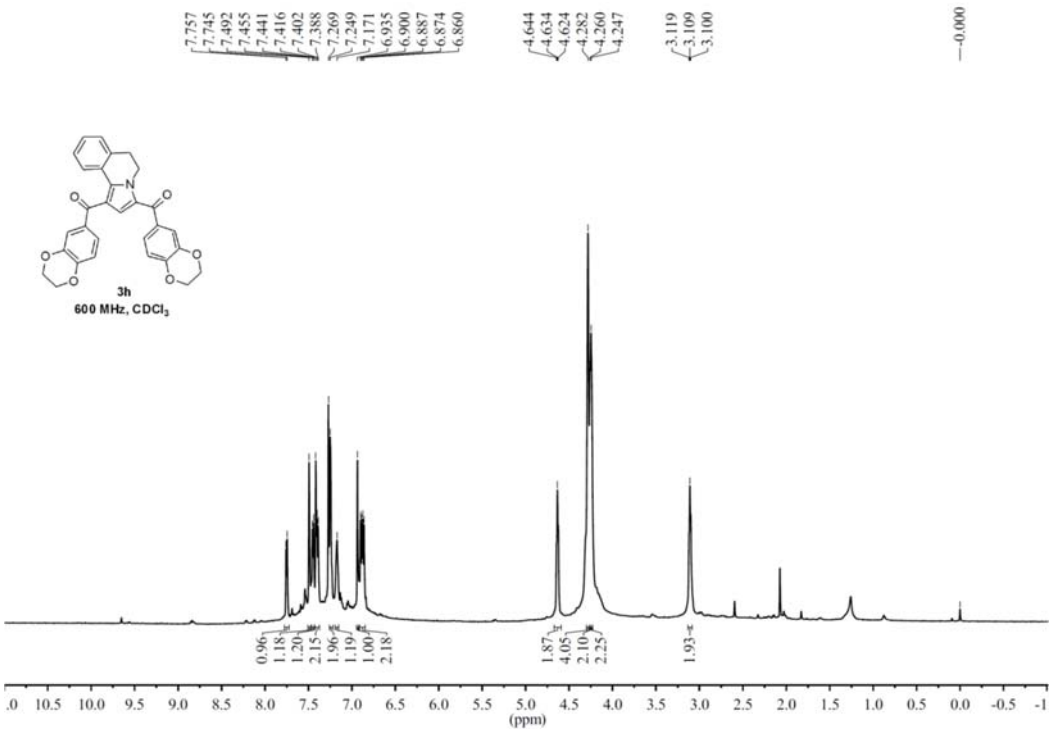

190.79
185.68
157.38
156.89
139.08
134.41
131.96
131.39
130.03
129.87
129.27
129.17
129.09
128.32
127.96
127.12
126.63
126.59
126.49
122.06
119.99
119.73
77.21
77.00
76.79
55.48
55.37
42.54
29.15
MeO
OMe
3d
150 MHz, CDCl3
(ppm)

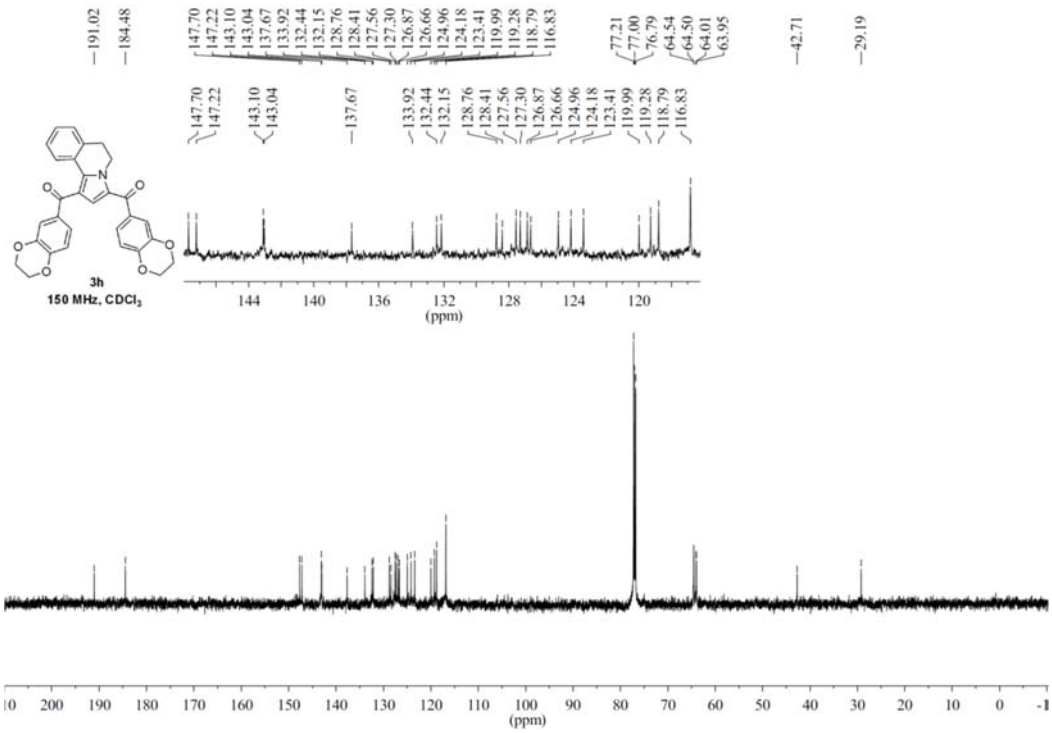

7.728
7.715
7.563
7.529
7.525
7.522
7.518
7.515
7.512
7.509
7.462
7.275
7.262
7.250
7.187
7.175
7.163
6.969
6.895
6.881
6.845
6.831
4.676
4.666
4.655
3.946
3.931
3.914
3.158
3.148
3.137
1.776
0.000
MeO
MeO
OMe
OMe
3e
600 MHz, CDCl3
0.98
1.01
2.01
1.00
2.18
1.03
0.98
1.00
1.00
2.00
6.02
2.94
2.85
2.00
(ppm)
191.24
184.77
152.96
152.52
148.76
148.74
133.89
131.30
128.81
128.61
124.88
123.95
111.50
109.72
109.66
77.21
77.00
76.79
55.98
55.91
55.87
42.78
29.24
137.66
133.89
131.66
131.30
128.81
128.61
127.61
127.40
126.94
126.68
125.12
124.88
123.95
120.08
111.59
111.50
109.72
109.66
3e
150 MHz, CDCl3
(ppm)
(ppm)

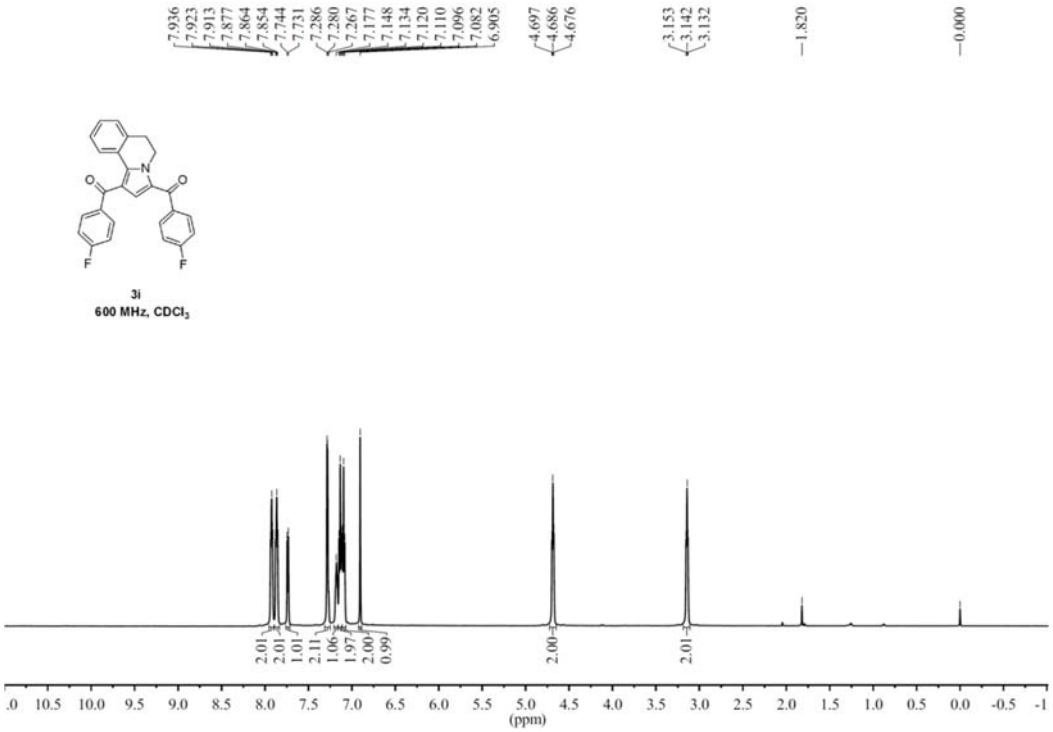

7.913
7.899
7.857
7.844
7.761
7.748
7.258
7.247
7.179
7.167
7.155
6.931
6.917
6.901
6.887
4.668
4.658
4.647
4.100
4.090
4.079
4.069
3.137
3.126
3.115
1.805
1.445
1.435
1.425
1.415
0.000
EtO
OEt
3f
600 MHz, CDCl3
1.98
1.99
1.00
2.13
1.01
3.05
1.97
2.00
4.02
2.07
5.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
(ppm)

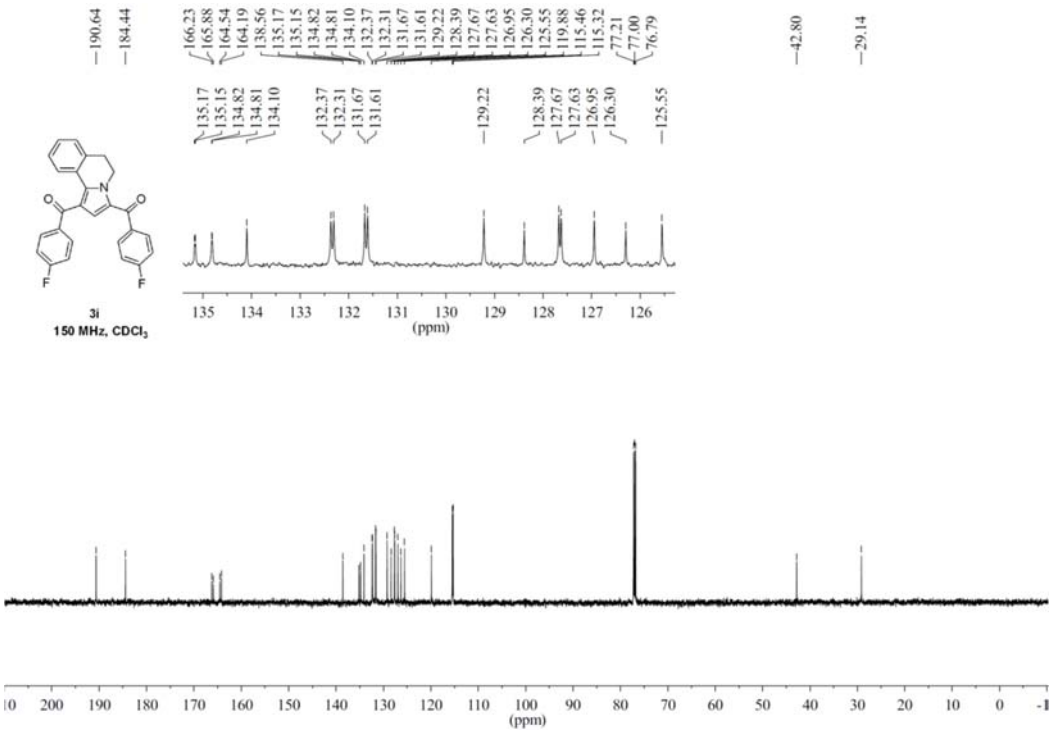

191.31
184.88
162.64
162.24
137.52
133.94
132.24
131.56
131.44
131.12
128.73
128.64
127.59
127.40
126.92
126.74
124.90
120.20
113.88
77.21
77.00
76.79
63.64
63.63
42.74
29.26
14.64
14.62
EtO
OEt
3f
150 MHz, CDCl3
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
(ppm)

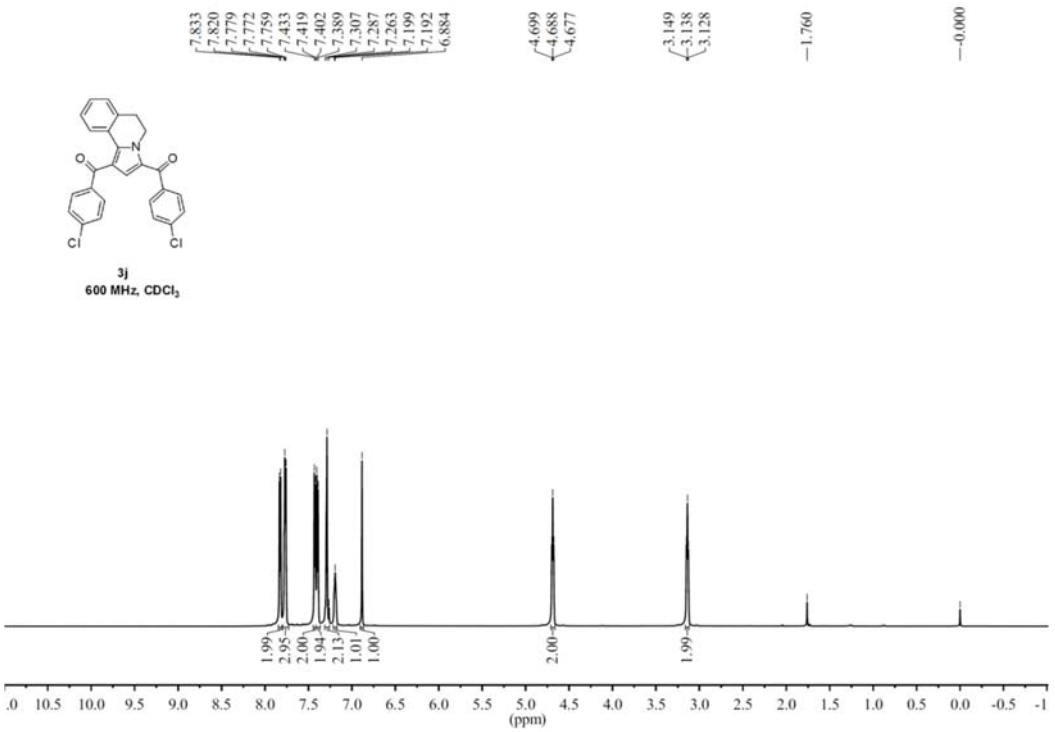

7.716
7.703
7.490
7.476
7.461
7.445
7.351
7.271
7.265
7.194
7.181
7.173
6.913
6.859
6.846
6.810
6.796
6.048
6.042
4.649
4.638
4.628
3.138
3.127
3.117
1.647
0.000
3g
600 MHz, CDCl3
0.96
1.01
2.00
1.00
2.35
1.07
1.00
1.01
1.02
2.01
2.00
2.00
2.04
(ppm)
190.78
184.29
151.52
151.07
147.87
147.71
128.85
127.62
127.33
126.92
126.59
125.42
109.28
107.64
107.60
101.75
101.70
77.21
77.00
76.79
42.75
29.19
137.76
133.93
133.29
133.08
128.85
128.48
127.62
127.33
126.92
126.59
126.56
125.42
124.86
119.98
109.39
109.28
107.64
107.60
3g
150 MHz, CDCl3
(ppm)
(ppm)

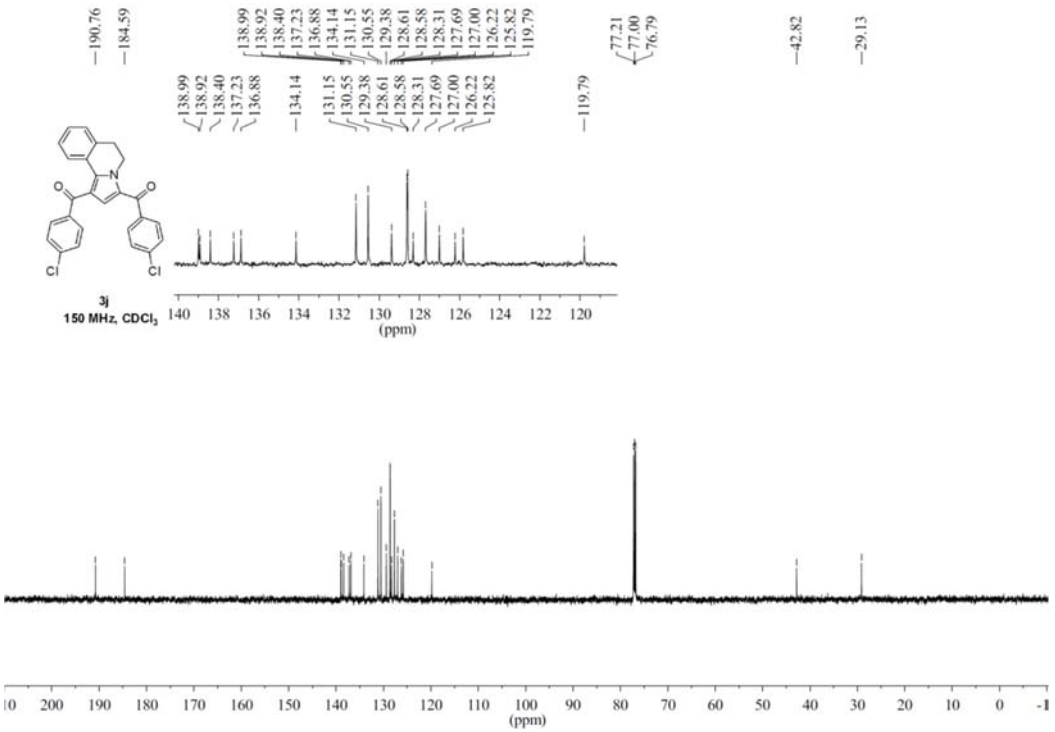

3h
600 MHz, CDCl3
(ppm)

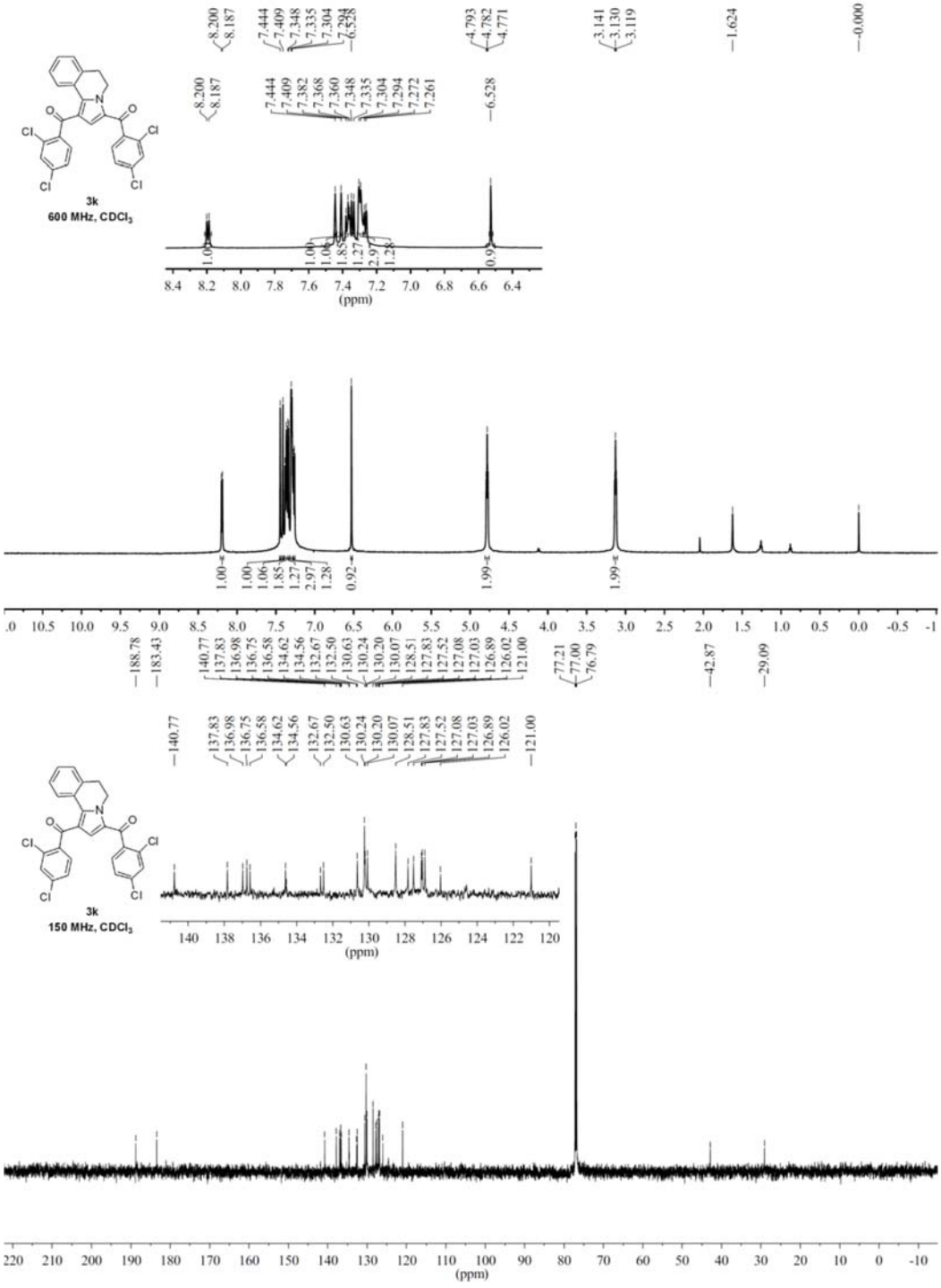

3h
150 MHz, CDCl3
(ppm)

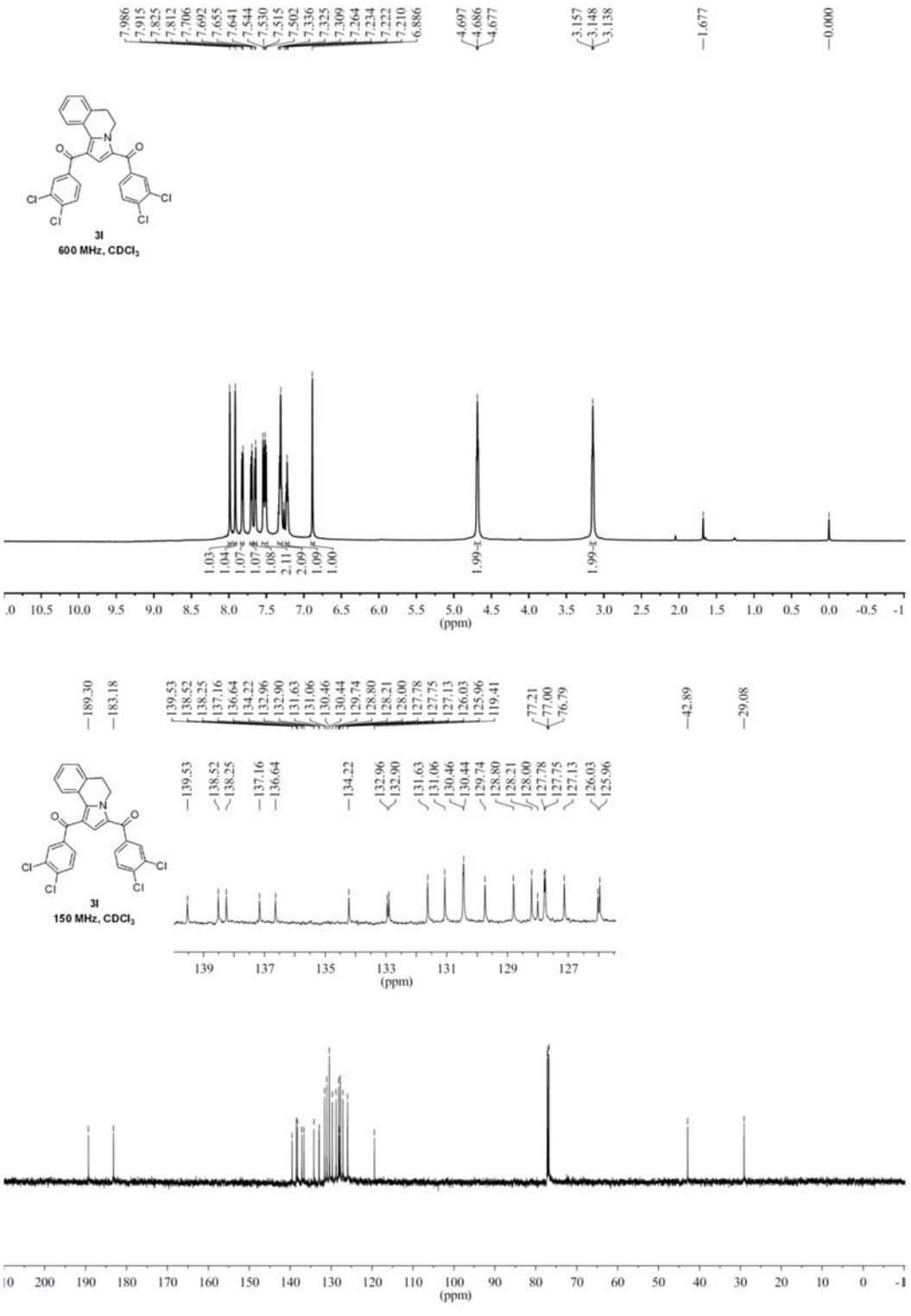

7.936
7.923
7.913
7.877
7.864
7.854
7.744
7.731
7.286
7.280
7.267
7.177
7.148
7.134
7.120
7.110
7.096
7.082
6.905
4.697
4.686
4.676
3.153
3.142
3.132
1.820
0.000
3i
600 MHz, CDCl3
2.01
2.01
1.01
2.11
1.06
1.97
2.00
0.99
2.00
2.01
(ppm)

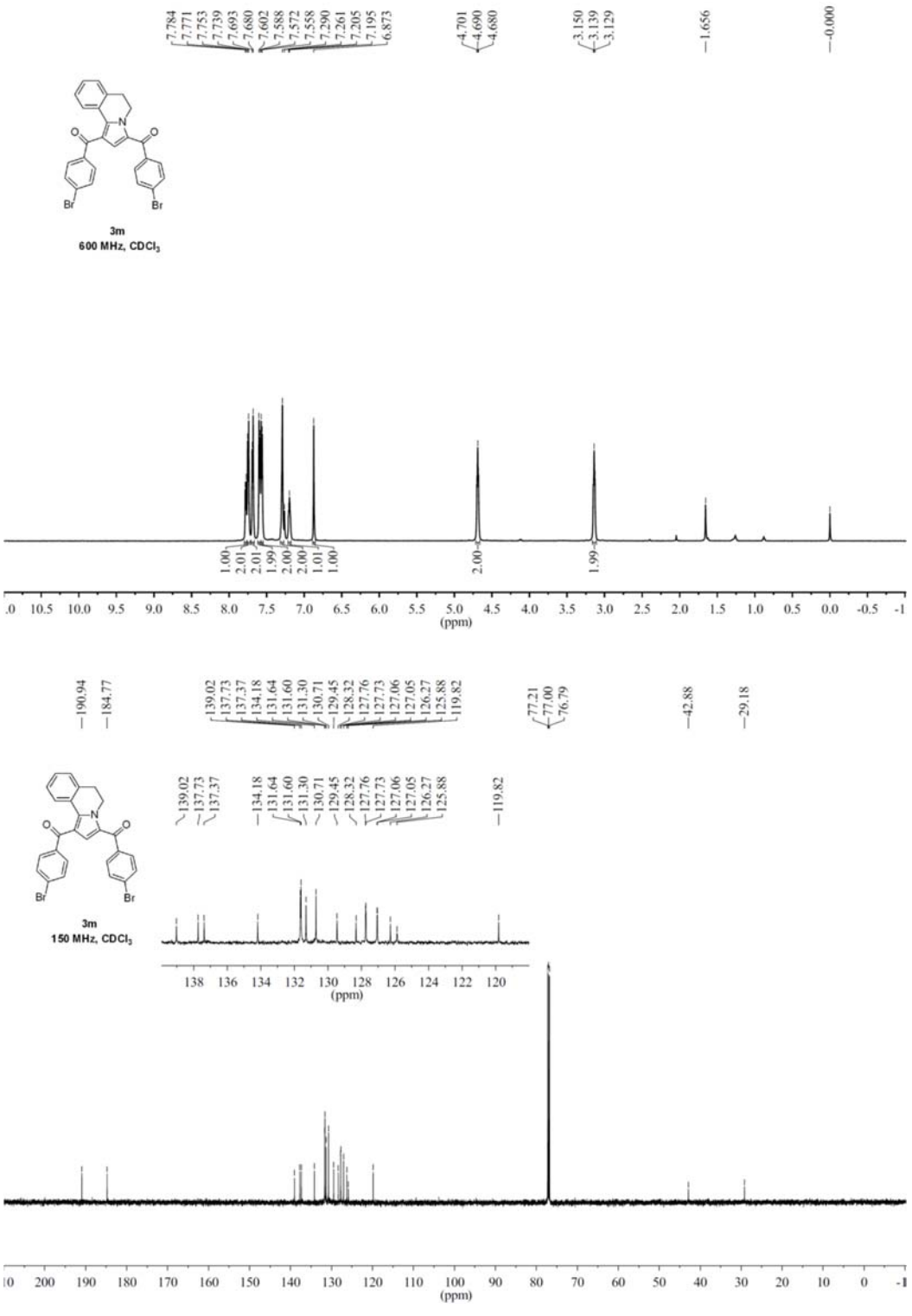

190.64
184.44
166.23
165.88
164.54
164.19
138.56
135.17
135.15
134.82
134.81
134.10
132.37
132.31
131.67
131.61
129.22
128.39
127.67
127.63
126.95
126.30
125.55
119.88
115.46
115.32
77.21
77.00
76.79
42.80
29.14
3i
150 MHz, CDCl3
(ppm)

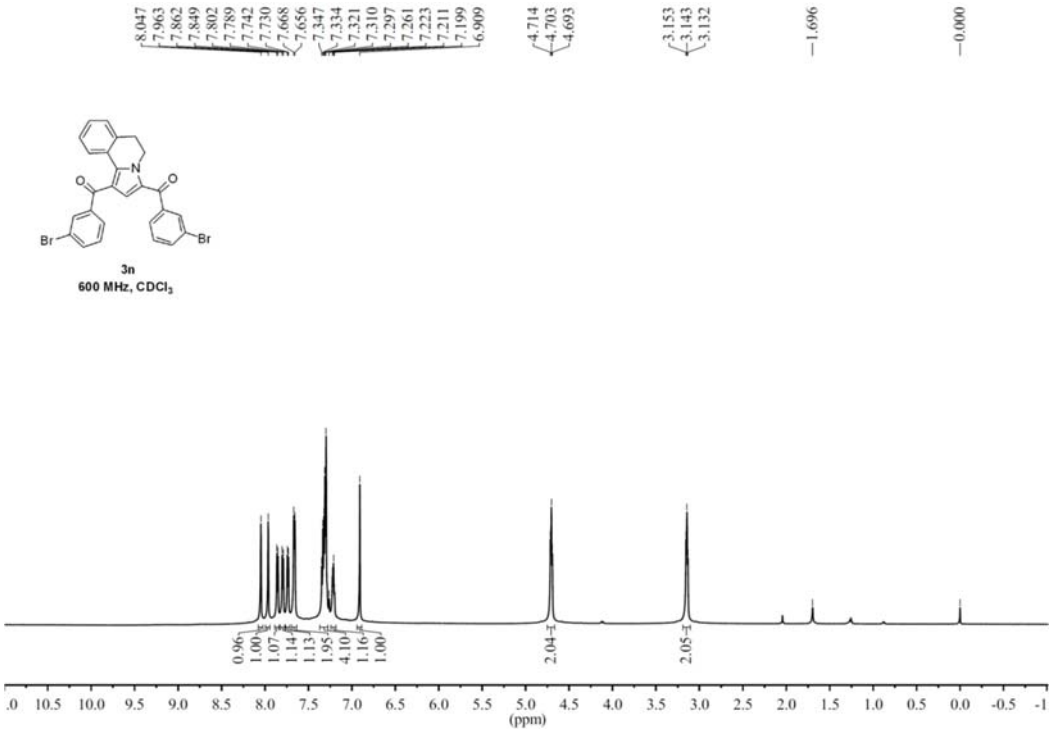

7.833
7.820
7.779
7.772
7.759
7.433
7.419
7.402
7.389
7.307
7.287
7.263
7.199
7.192
6.884
4.699
4.688
4.677
3.149
3.138
3.128
1.760
0.000
3j
600 MHz, CDCl3
1.99
2.95
2.00
1.94
2.13
1.01
1.00
2.00
1.99
(ppm)

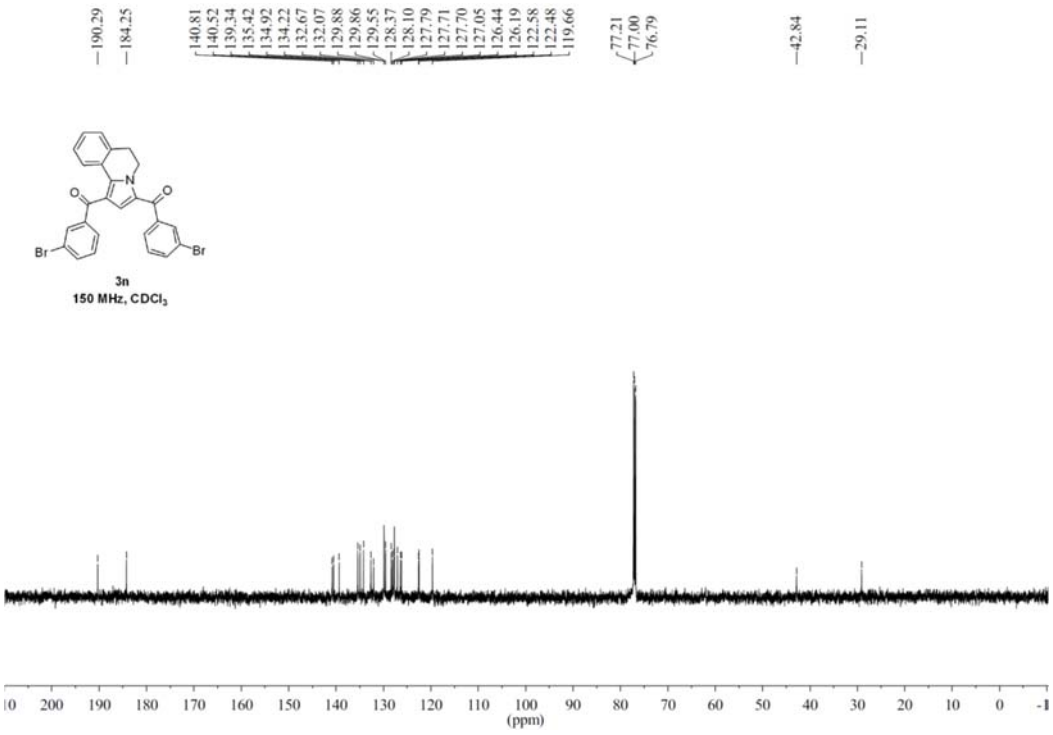

190.76
184.59
138.99
138.92
138.40
137.23
136.88
134.14
131.15
130.55
129.38
128.61
128.58
128.31
127.69
127.00
126.22
125.82
119.79
77.21
77.00
76.79
42.82
29.13
3j
150 MHz, CDCl3
(ppm)

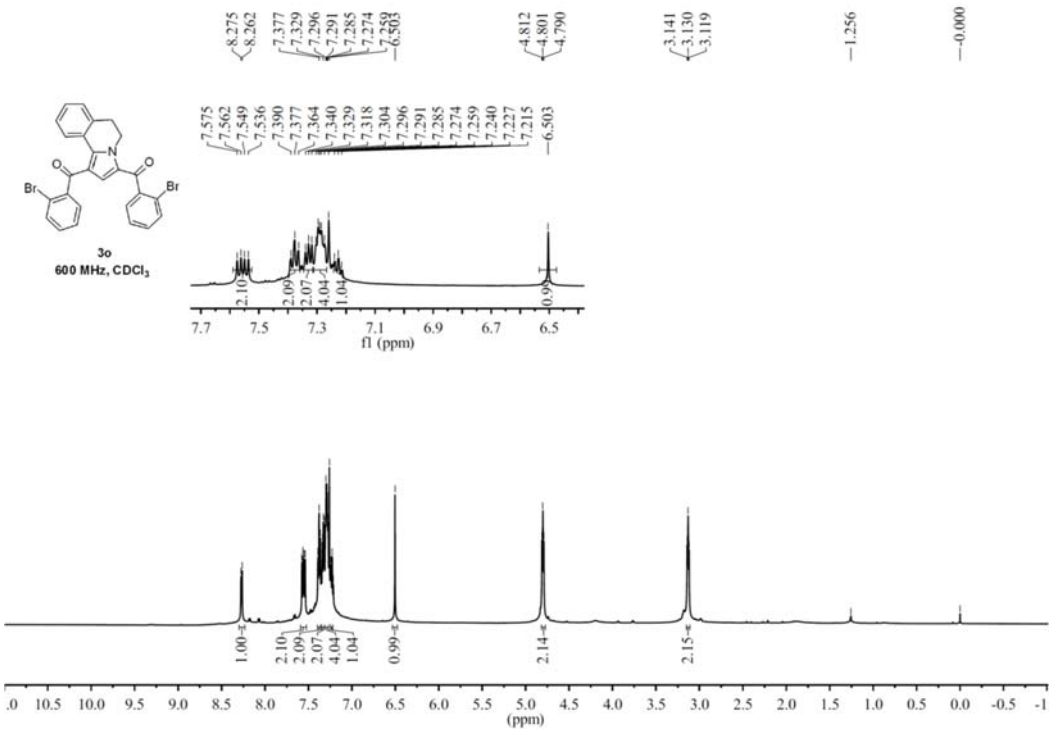

3k
600 MHz, CDCl3
3k
150 MHz, CDCl3
(ppm)

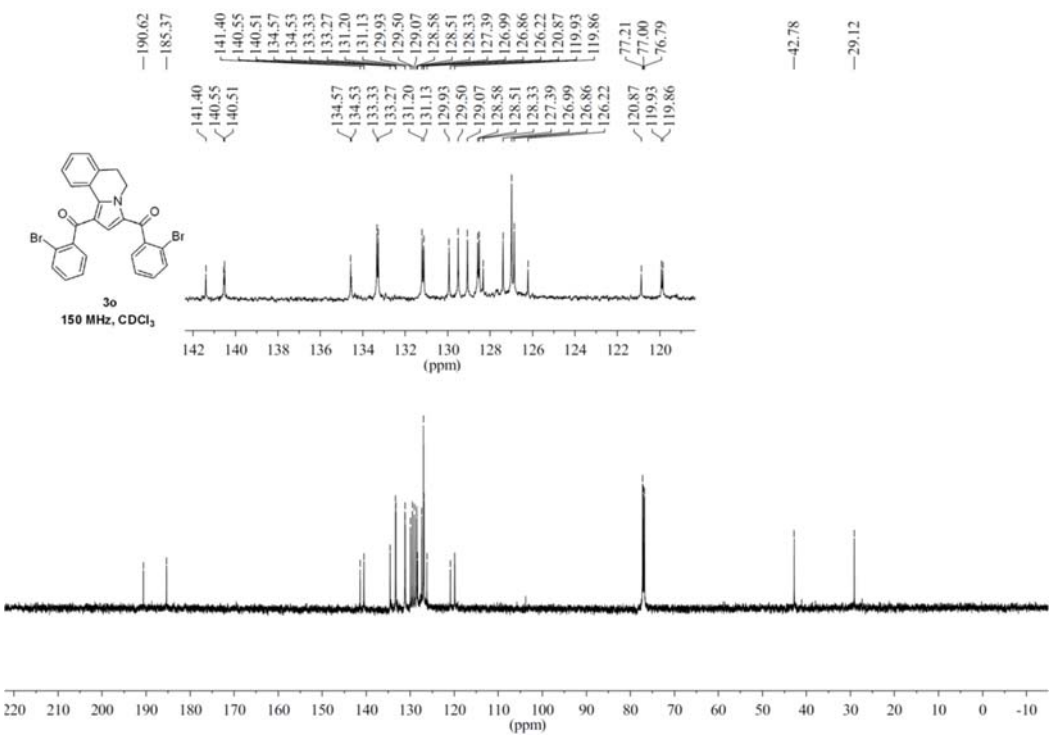

7.986
7.915
7.825
7.812
7.706
7.692
7.655
7.641
7.544
7.530
7.515
7.502
7.336
7.325
7.309
7.264
7.234
7.222
7.210
6.886
4.697
4.686
4.677
3.157
3.148
3.138
1.677
0.000
3l
600 MHz, CDCl3
1.03
1.04
1.07
1.07
1.08
2.11
2.09
1.09
1.00
1.99
1.99
(ppm)
189.30
183.18
139.53
138.52
138.25
137.16
136.64
134.22
132.96
132.90
131.63
131.06
130.46
130.44
129.74
128.80
128.21
128.00
127.78
127.75
127.13
126.03
125.96
119.41
77.21
77.00
76.79
42.89
29.08
3l
150 MHz, CDCl3
(ppm)
(ppm)

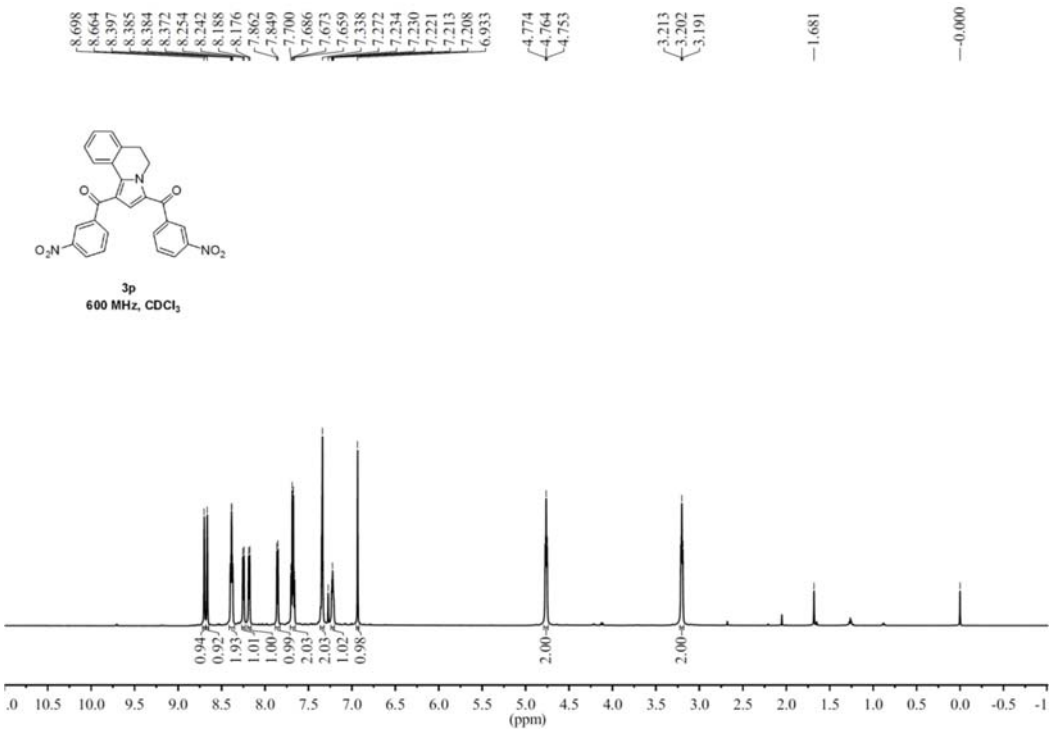

7.784
7.771
7.753
7.739
7.693
7.680
7.602
7.588
7.572
7.558
7.290
7.261
7.205
7.195
6.873
4.701
4.690
4.680
3.150
3.139
3.129
1.656
0.000
3m
600 MHz, CDCl3
1.00
2.01
2.01
1.99
2.00
2.00
1.01
1.00
2.00
1.99
(ppm)
190.94
184.77
139.02
137.73
137.37
134.18
131.64
131.60
131.30
130.71
129.45
128.32
127.76
127.73
127.06
127.05
126.27
125.88
119.82
77.21
77.00
76.79
42.88
29.18
3m
150 MHz, CDCl3
(ppm)
(ppm)

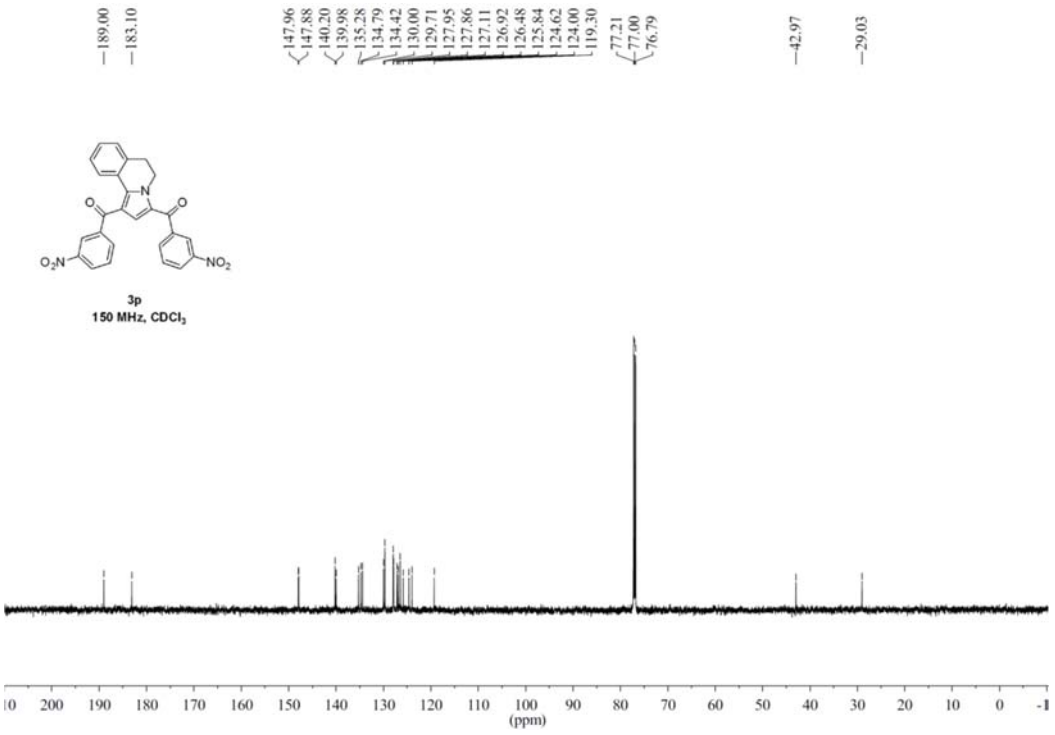

8.047
7.963
7.862
7.849
7.802
7.789
7.742
7.730
7.668
7.656
7.347
7.334
7.321
7.310
7.297
7.261
7.223
7.211
7.199
6.909
4.714
4.703
4.693
3.153
3.143
3.132
1.696
0.000
Br
Br
3n
600 MHz, CDCl3
0.96
1.00
1.07
1.14
1.13
1.95
4.10
1.16
1.00
2.04
2.05
(ppm)

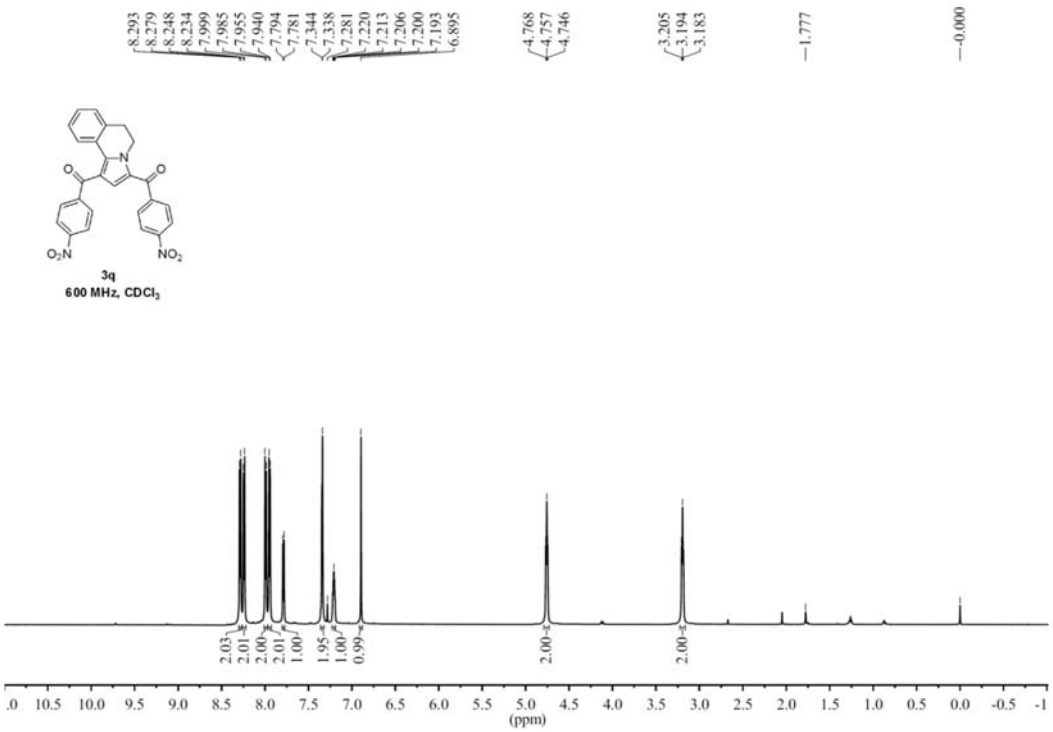

190.29
184.25
140.81
140.52
139.34
135.42
134.92
134.22
132.67
132.07
129.88
129.86
129.55
128.37
128.10
127.79
127.71
127.70
127.05
126.44
126.19
122.58
122.48
119.66
77.21
77.00
76.79
42.84
29.11
Br
Br
3n
150 MHz, CDCl3
(ppm)

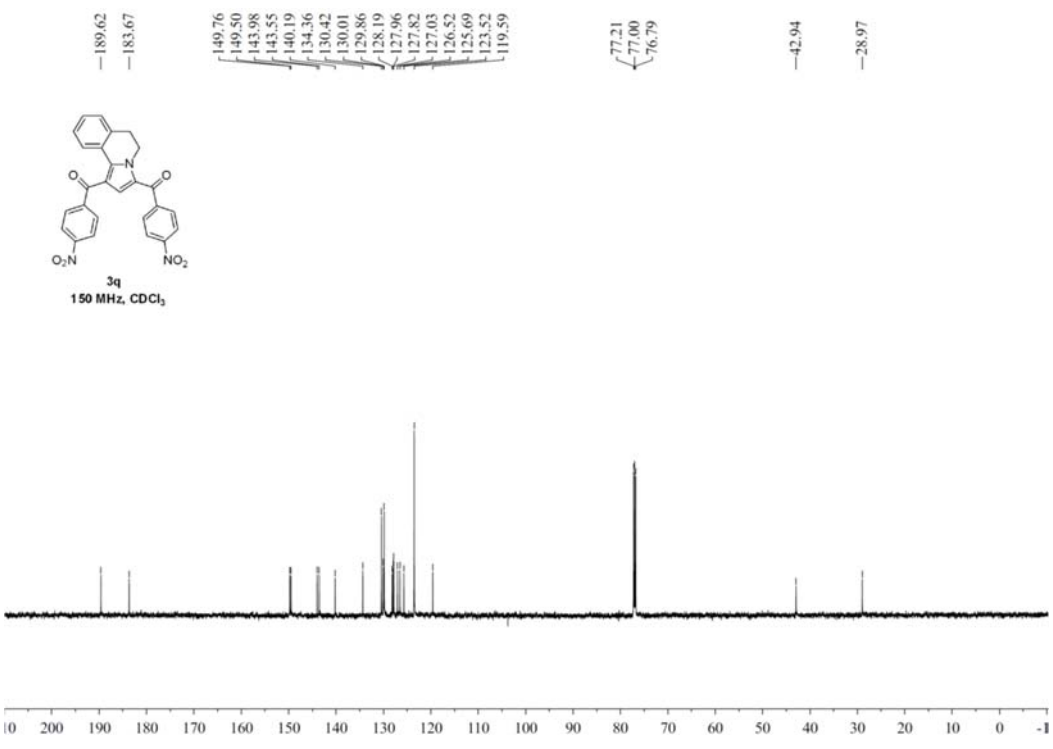

3o
600 MHz, CDCl3
f1 (ppm)
(ppm)

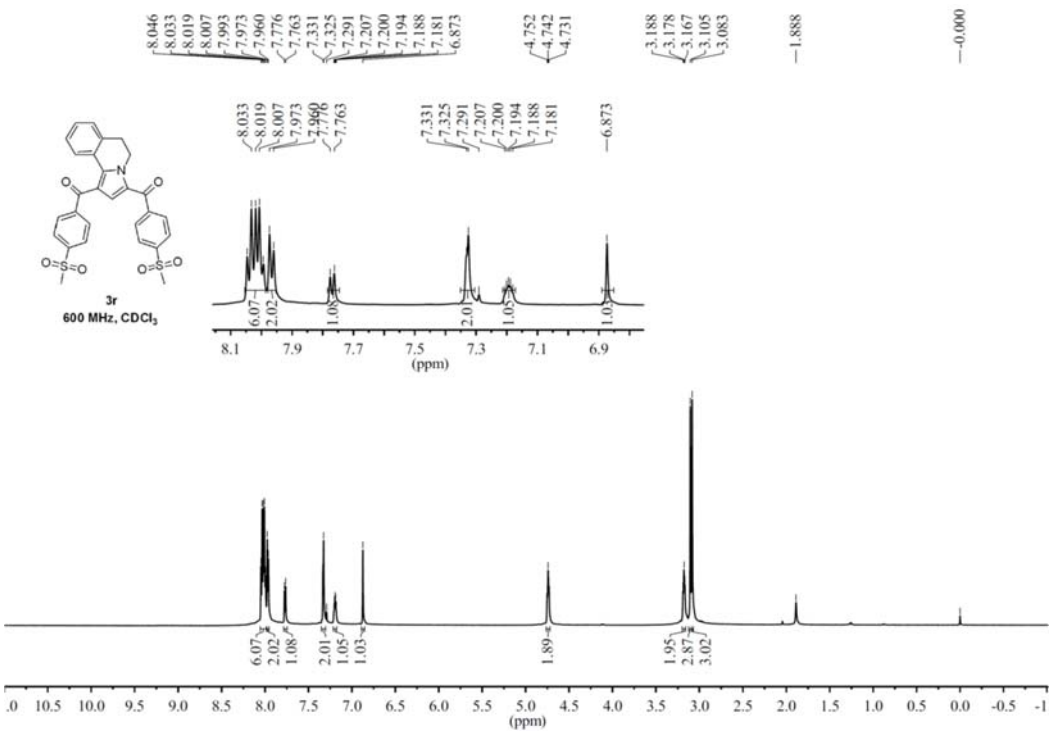

3o
150 MHz, CDCl3
(ppm)
(ppm)

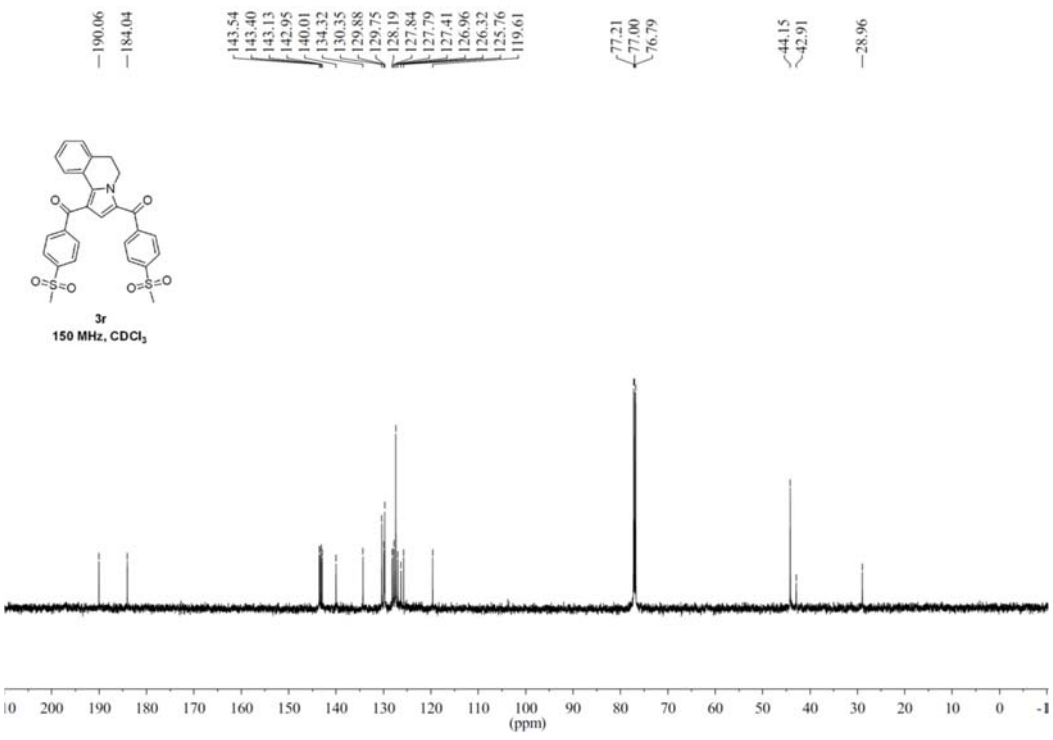

8.698
8.664
8.397
8.385
8.384
8.372
8.254
8.242
8.188
8.176
7.862
7.849
7.700
7.686
7.673
7.659
7.338
7.272
7.234
7.230
7.221
7.213
7.208
6.933
4.774
4.764
4.753
3.213
3.202
3.191
1.681
0.000
O2N
NO2
3p
600 MHz, CDCl3
0.94
0.92
1.93
1.01
1.00
0.99
2.03
2.03
1.02
0.98
2.00
2.00
(ppm)

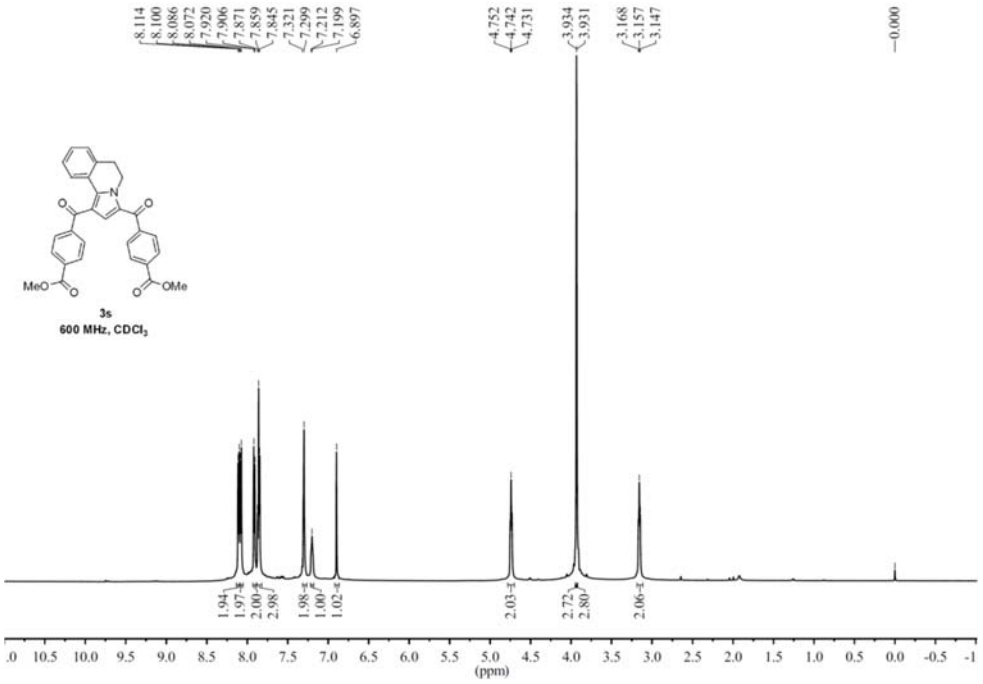

189.00
183.10
147.96
147.88
140.20
139.98
135.28
134.79
134.42
130.00
129.71
127.95
127.86
127.11
126.92
126.48
125.84
124.62
124.00
119.30
77.21
77.00
76.79
42.97
29.03
O2N
NO2
3p
150 MHz, CDCl3
(ppm)

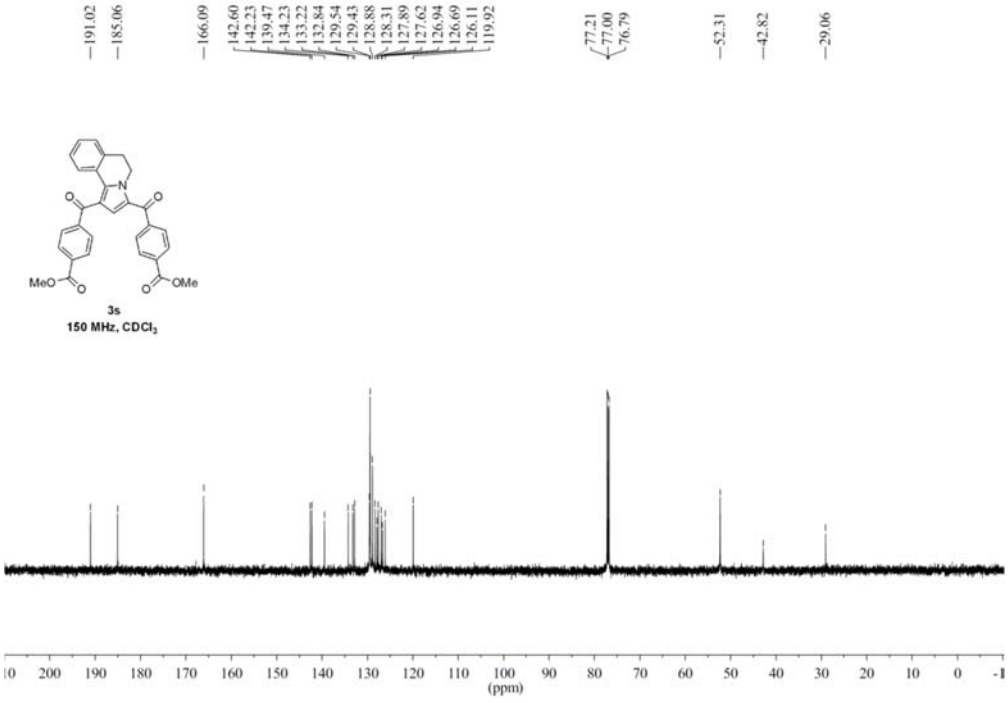

8.293
8.279
8.248
8.234
7.999
7.985
7.955
7.940
7.794
7.781
7.344
7.338
7.281
7.220
7.213
7.206
7.200
7.193
6.895
4.768
4.757
4.746
3.205
3.194
3.183
1.777
0.000
3q
600 MHz, CDCl3
2.03
2.01
2.00
2.01
1.00
1.95
1.00
0.99
2.00
2.00
(ppm)

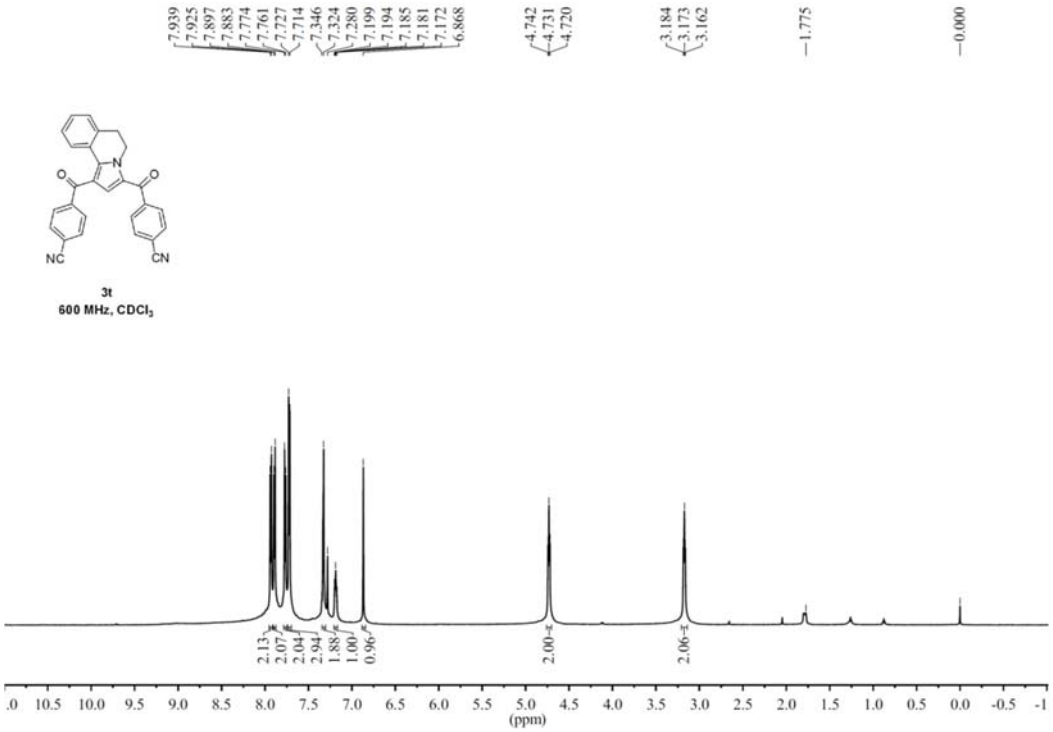

189.62
183.67
149.76
149.50
143.98
143.55
140.19
134.36
130.42
130.01
129.86
128.19
127.96
127.82
127.03
126.52
125.69
123.52
119.59
77.21
77.00
76.79
42.94
28.97
3q
150 MHz, CDCl3

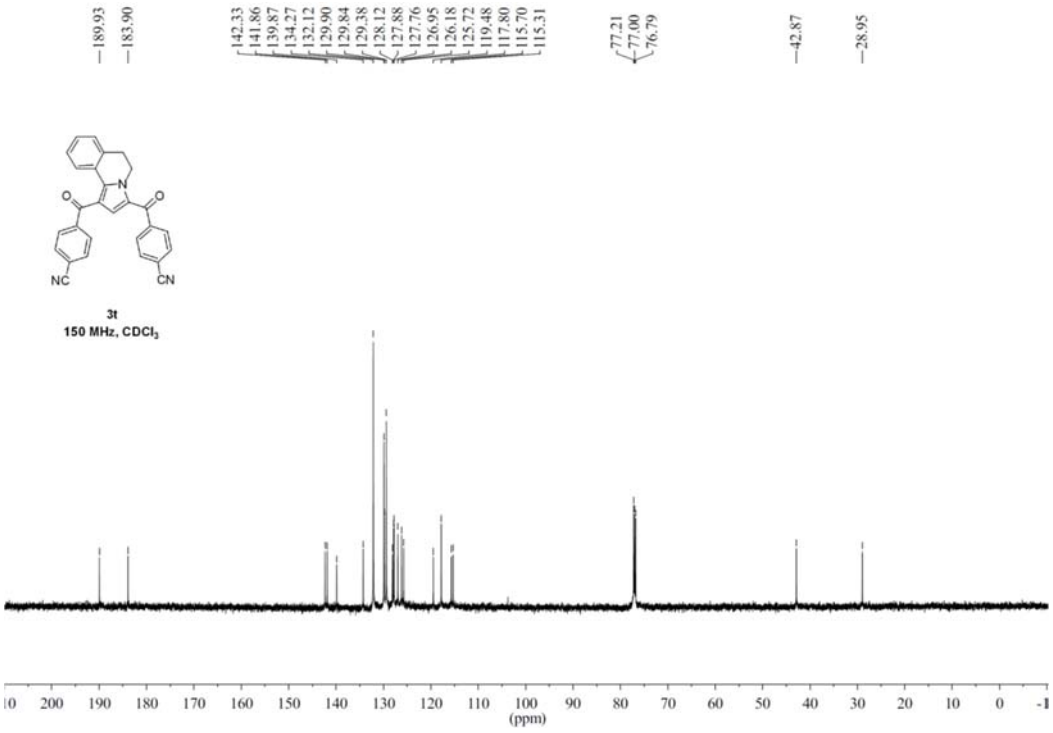

3r
600 MHz, CDCl3
(ppm)

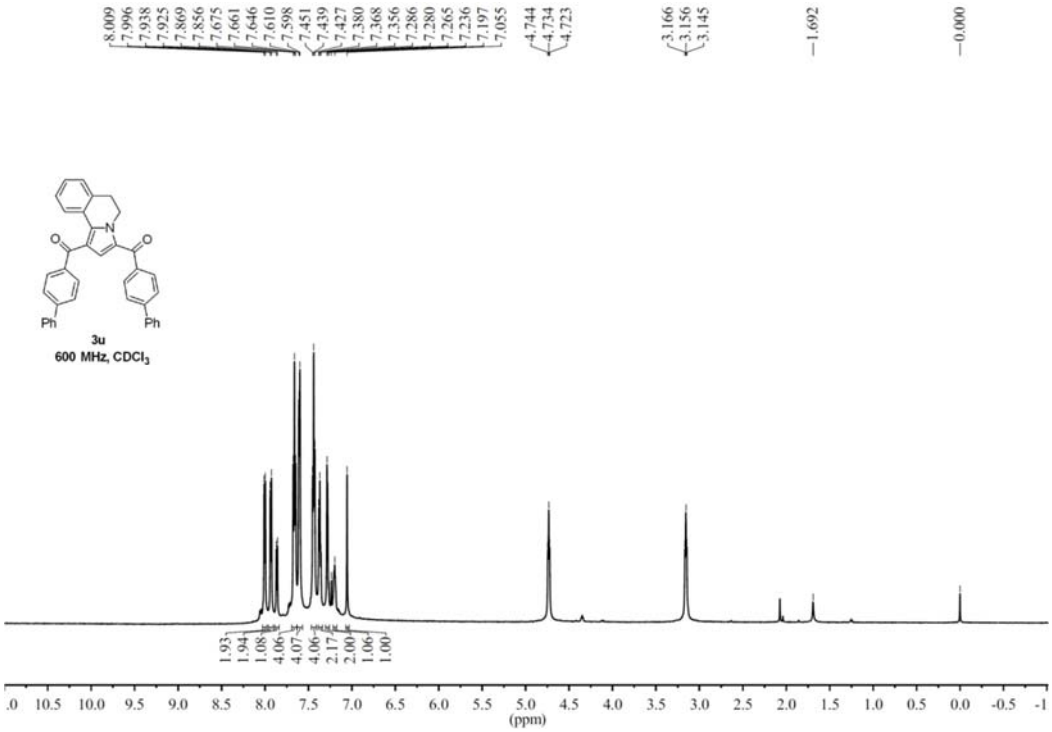

3r
150 MHz, CDCl3
(ppm)

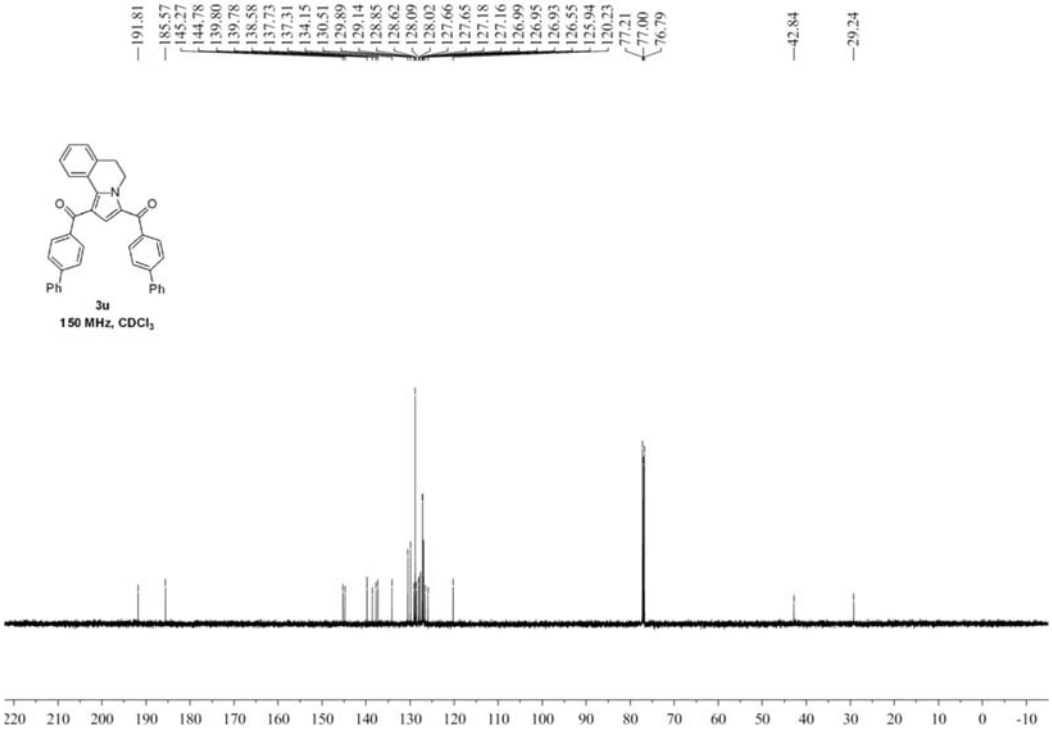

8.114
8.100
8.086
8.072
7.920
7.906
7.871
7.859
7.845
7.321
7.299
7.212
7.199
6.897
4.752
4.742
4.731
3.934
3.931
3.168
3.157
3.147
0.000
MeO
OMe
3s
600 MHz, CDCl3
1.94
1.97
2.00
2.98
1.98
1.00
1.02
2.03
2.72
2.80
2.06
(ppm)

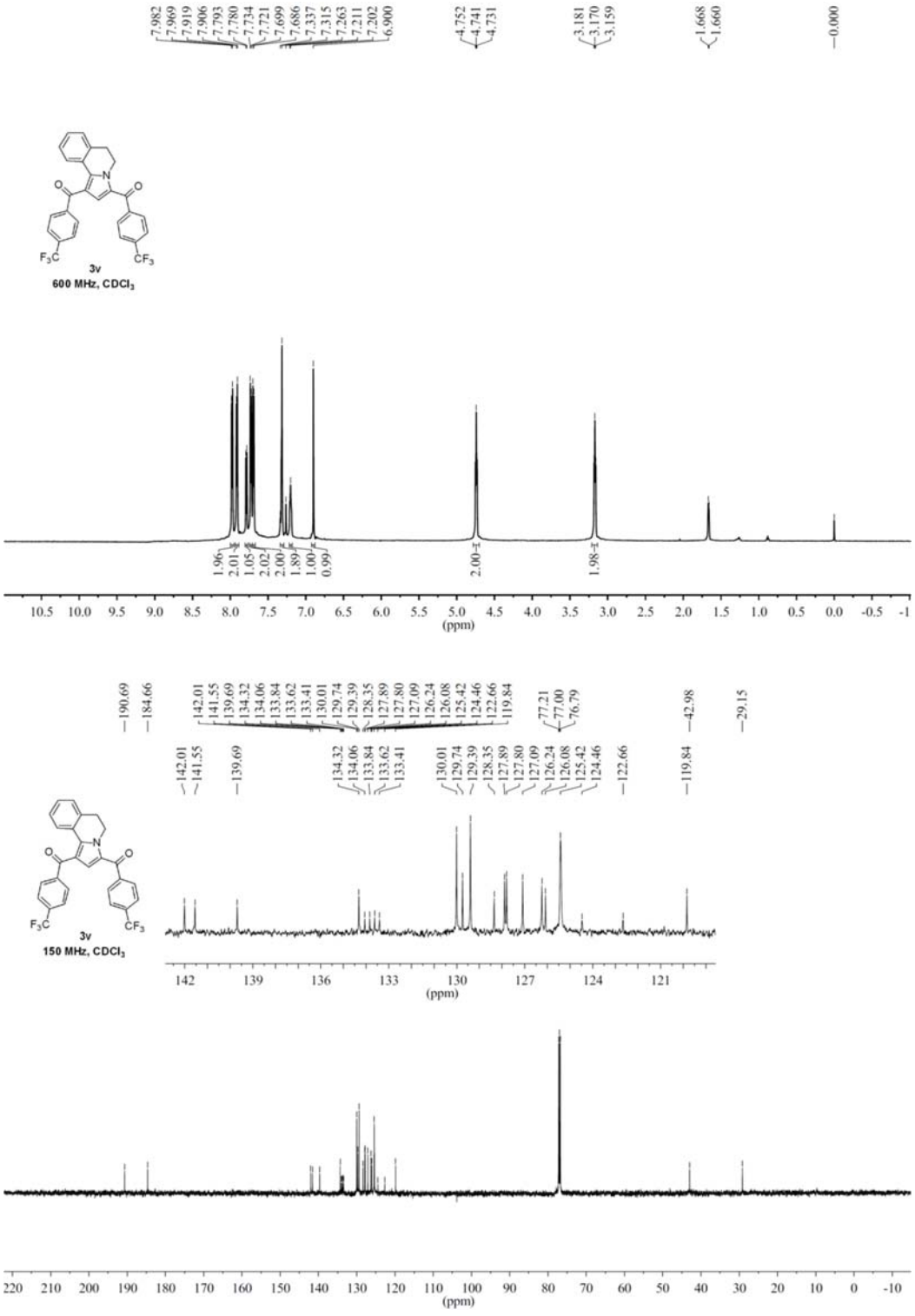

191.02
185.06
166.09
142.60
142.23
139.47
134.23
133.22
132.84
129.54
129.43
128.88
128.31
127.89
127.62
126.94
126.69
126.11
119.92
77.21
77.00
76.79
52.31
42.82
29.06
MeO
OMe
3s
150 MHz, CDCl3
(ppm)

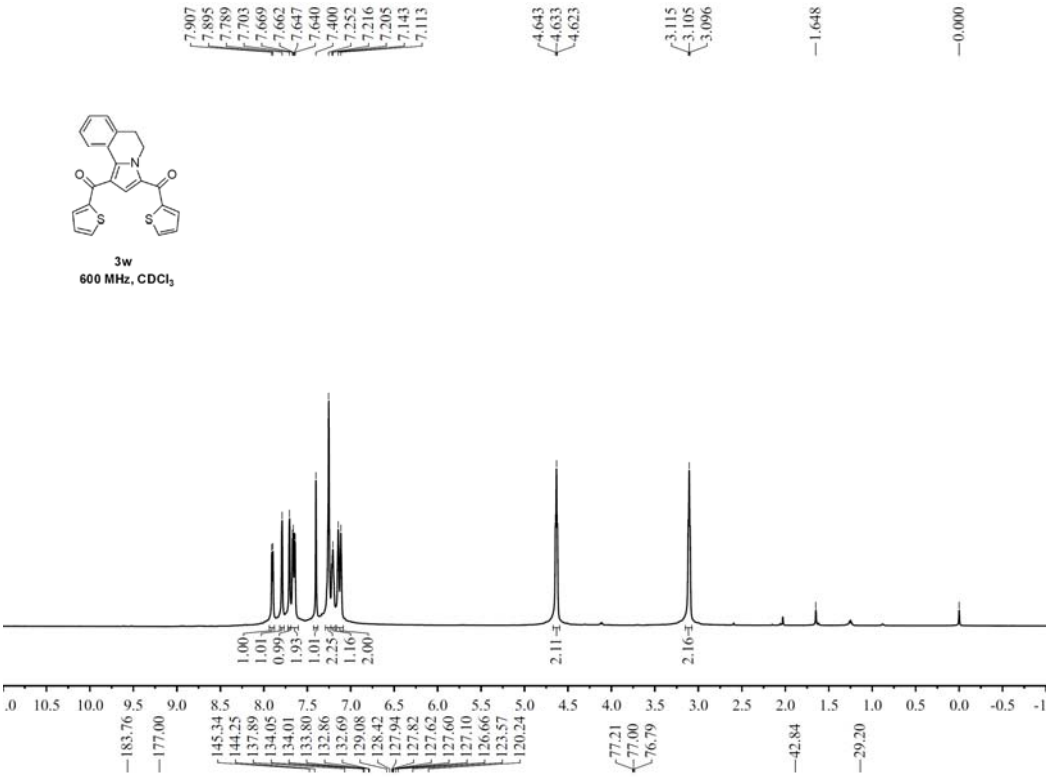

7.939
7.925
7.897
7.883
7.774
7.761
7.727
7.714
7.346
7.324
7.280
7.199
7.194
7.185
7.181
7.172
6.868
4.742
4.731
4.720
3.184
3.173
3.162
1.775
0.000
3t
600 MHz, CDCl3
2.13
2.07
2.04
2.94
1.88
1.00
0.96
2.00
2.06
(ppm)

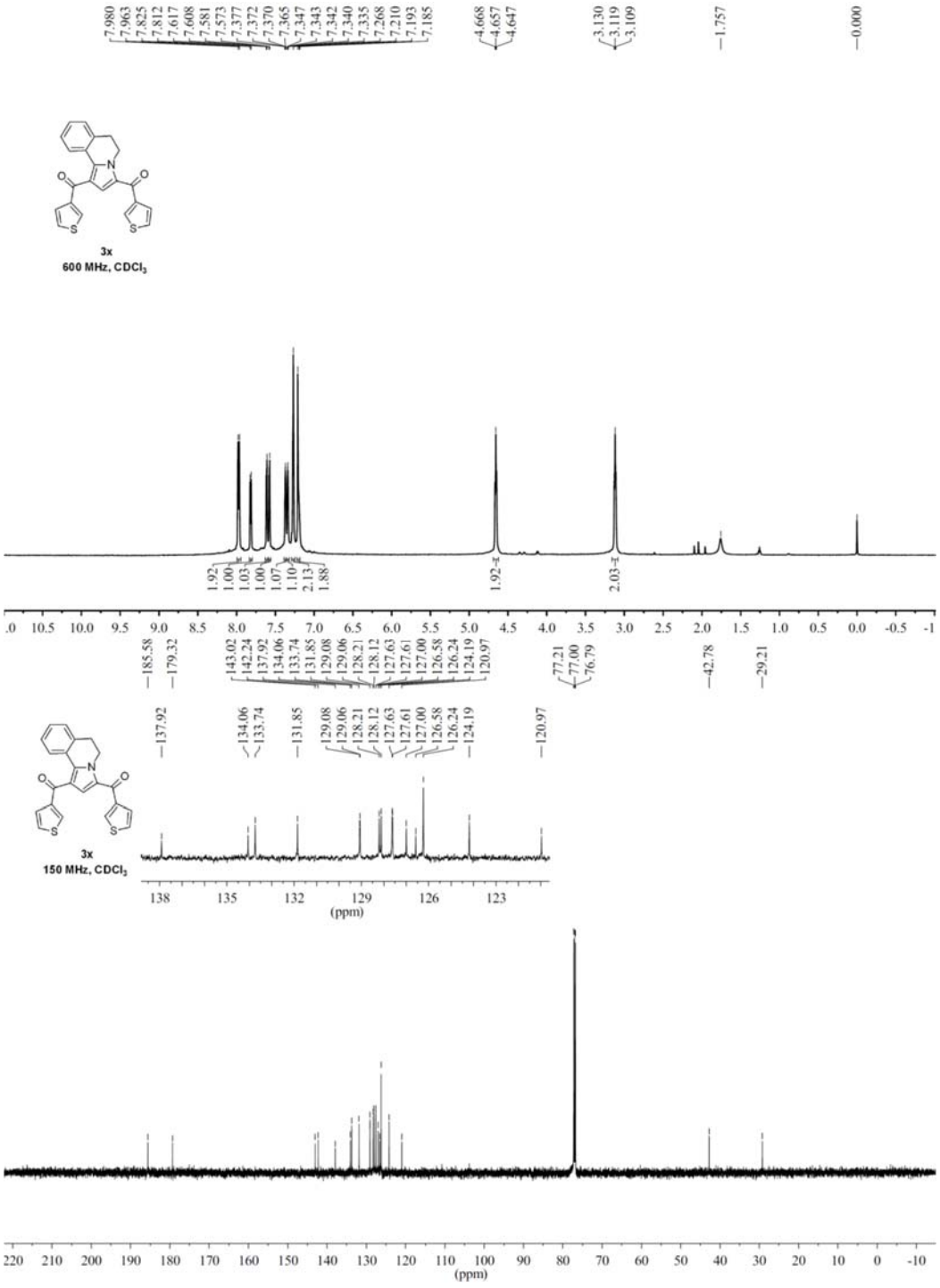

189.93
183.90
142.33
141.86
139.87
134.27
132.12
129.90
129.84
129.38
128.12
127.88
127.76
126.95
126.18
125.72
119.48
117.80
115.70
115.31
77.21
77.00
76.79
42.87
28.95
3t
150 MHz, CDCl3
(ppm)

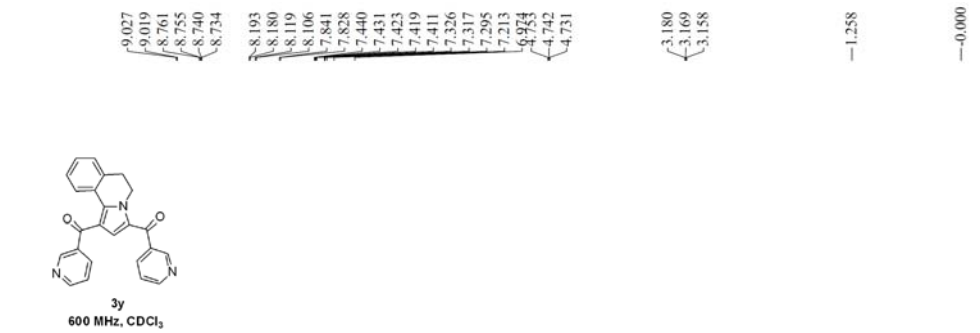

8.009
7.996
7.938
7.925
7.869
7.856
7.675
7.661
7.646
7.610
7.598
7.451
7.439
7.427
7.380
7.368
7.356
7.286
7.280
7.265
7.236
7.197
7.055
4.744
4.734
4.723
3.166
3.156
3.145
1.692
0.000
Ph
Ph
3u
600 MHz, CDCl3
1.93
1.94
1.08
4.06
4.07
4.06
2.17
2.00
1.06
1.00
(ppm)


191.81
185.57
145.27
144.78
139.80
139.78
138.58
137.73
137.31
134.15
130.51
129.89
129.14
128.85
128.62
128.09
128.02
127.66
127.65
127.18
127.16
126.99
126.95
126.93
126.55
125.94
120.23
77.21
77.00
76.79
42.84
29.24
Ph
Ph
3u
150 MHz, CDCl3

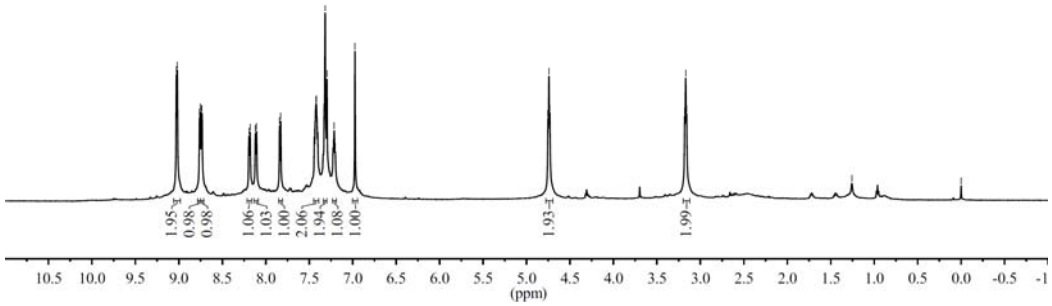

7.982
7.969
7.919
7.906
7.793
7.780
7.734
7.721
7.699
7.686
7.337
7.315
7.263
7.211
7.202
6.900
4.752
4.741
4.731
3.181
3.170
3.159
1.668
1.660
0.000
3v
600 MHz, CDCl3
1.96
2.01
1.05
2.02
2.00
1.89
1.00
0.99
2.00-I
1.98-I
(ppm)
190.69
184.66
142.01
141.55
139.69
134.32
134.06
133.84
133.62
133.41
130.01
129.74
129.39
128.35
127.89
127.80
127.09
126.24
126.08
125.42
124.46
122.66
119.84
77.21
77.00
76.79
42.98
29.15
3v
150 MHz, CDCl3
(ppm)
(ppm)

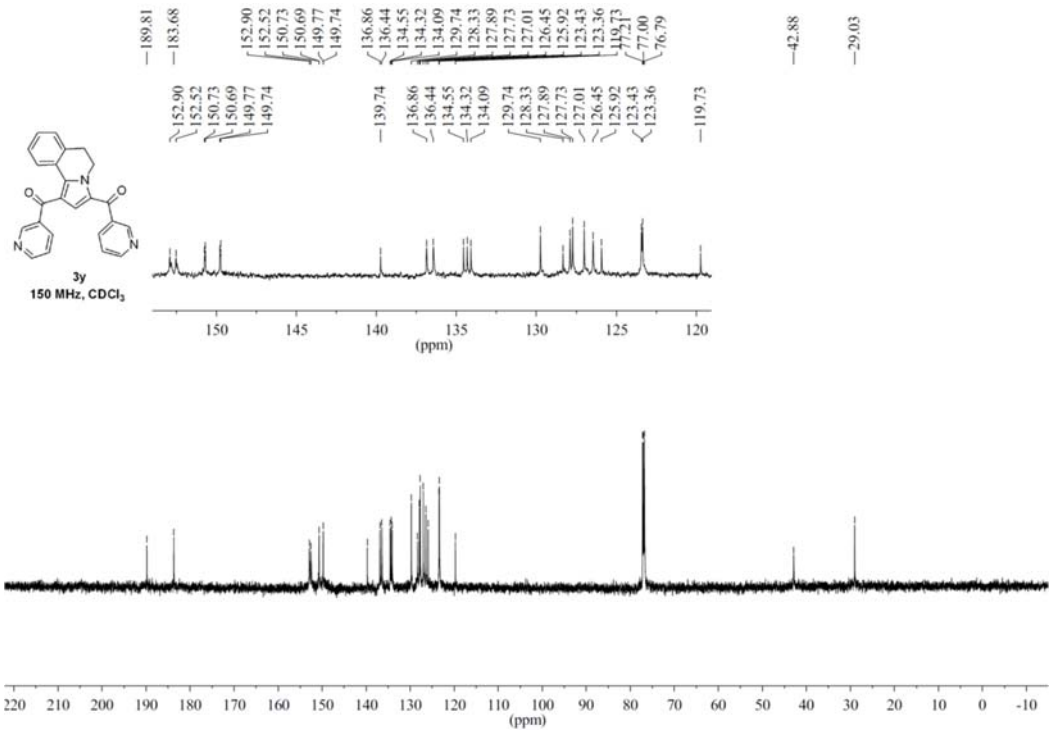

7.907
7.895
7.789
7.703
7.669
7.662
7.647
7.640
7.400
7.252
7.216
7.205
7.143
7.113
4.643
4.633
4.623
3.115
3.105
3.096
1.648
0.000
3w
600 MHz, CDCl3
1.00
1.01
0.99
1.93
1.01
2.25
1.16
2.00
2.11
2.16
183.76
177.00
145.34
144.25
137.89
134.05
134.01
133.80
132.86
132.69
129.08
128.42
127.94
127.82
127.62
127.60
127.10
126.66
123.57
120.24
77.21
77.00
76.79
42.84
29.20
3w
150 MHz, CDCl3
(ppm)


7.980
7.963
7.825
7.812
7.617
7.608
7.581
7.573
7.377
7.372
7.370
7.365
7.347
7.343
7.342
7.340
7.335
7.268
7.210
7.193
7.185
4.668
4.657
4.647
3.130
3.119
3.109
1.757
0.000
3x
600 MHz, CDCl3
1.92
1.00
1.03
1.00
1.07
1.10
2.13
1.88
1.92
2.03
185.58
179.32
143.02
142.24
137.92
134.06
133.74
131.85
129.08
129.06
128.21
128.12
127.63
127.61
127.00
126.58
126.24
124.19
120.97
77.21
77.00
76.79
42.78
29.21
3x
150 MHz, CDCl3
(ppm)
(ppm)

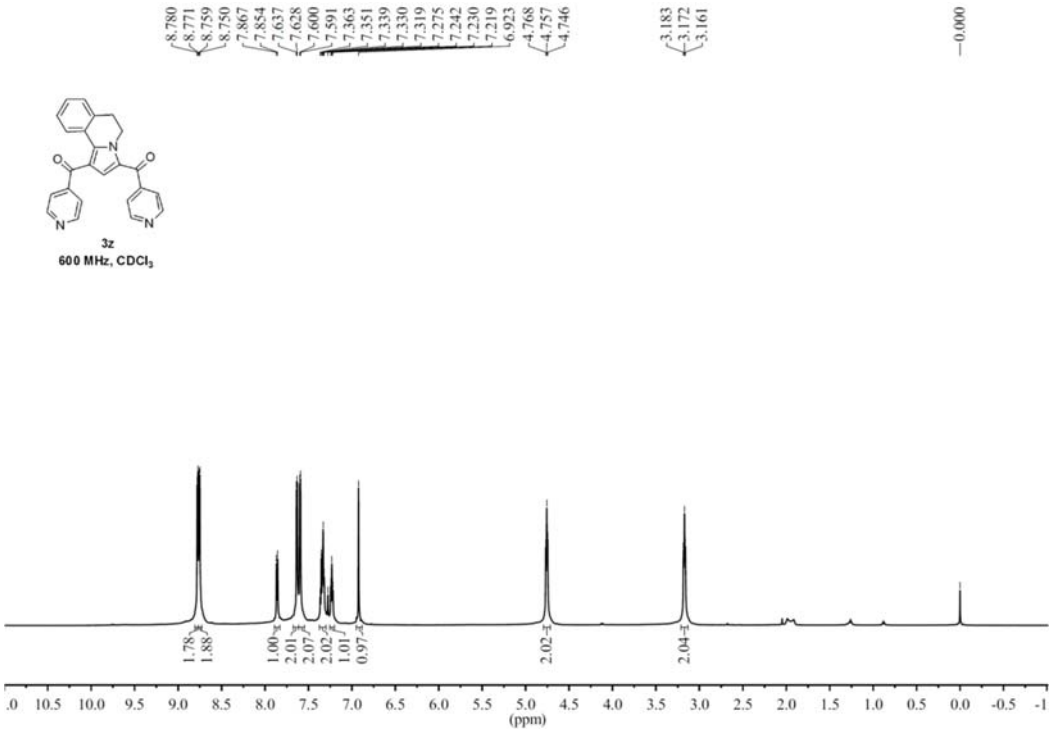


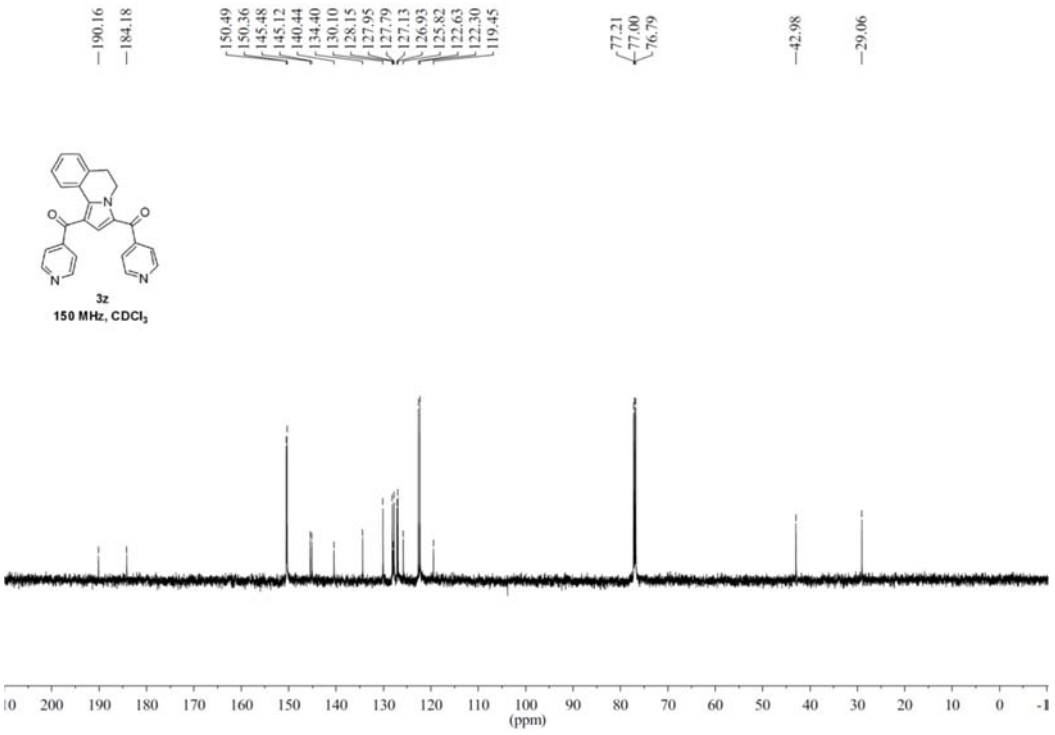
3y
600 MHz, $CDCl_3$

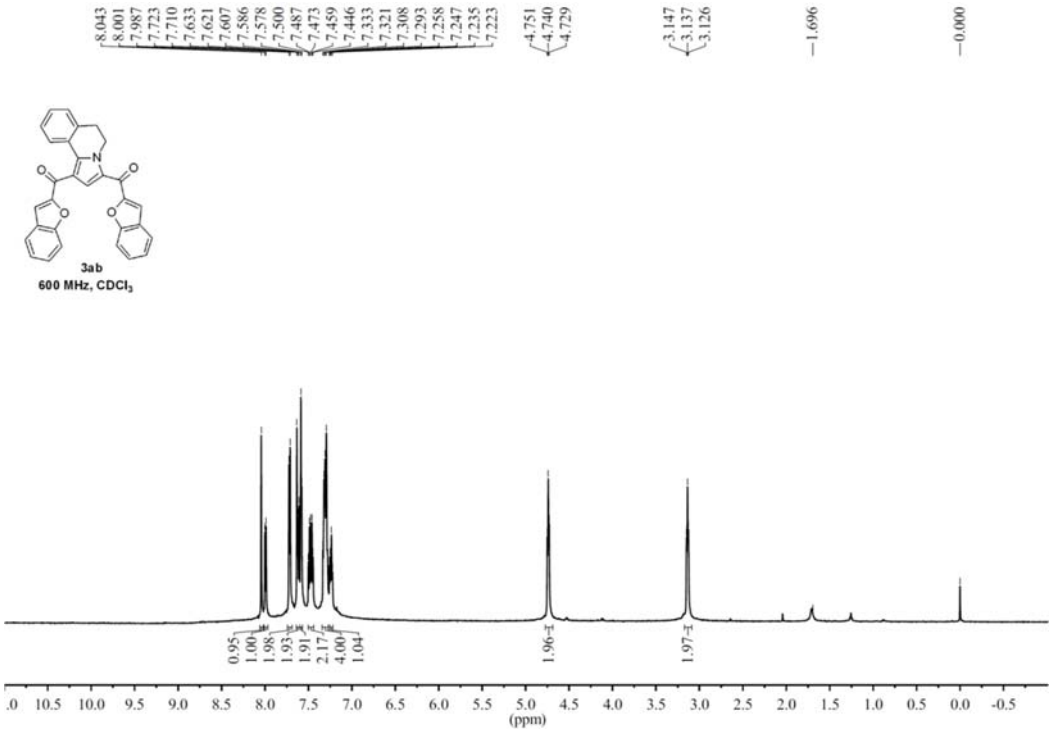


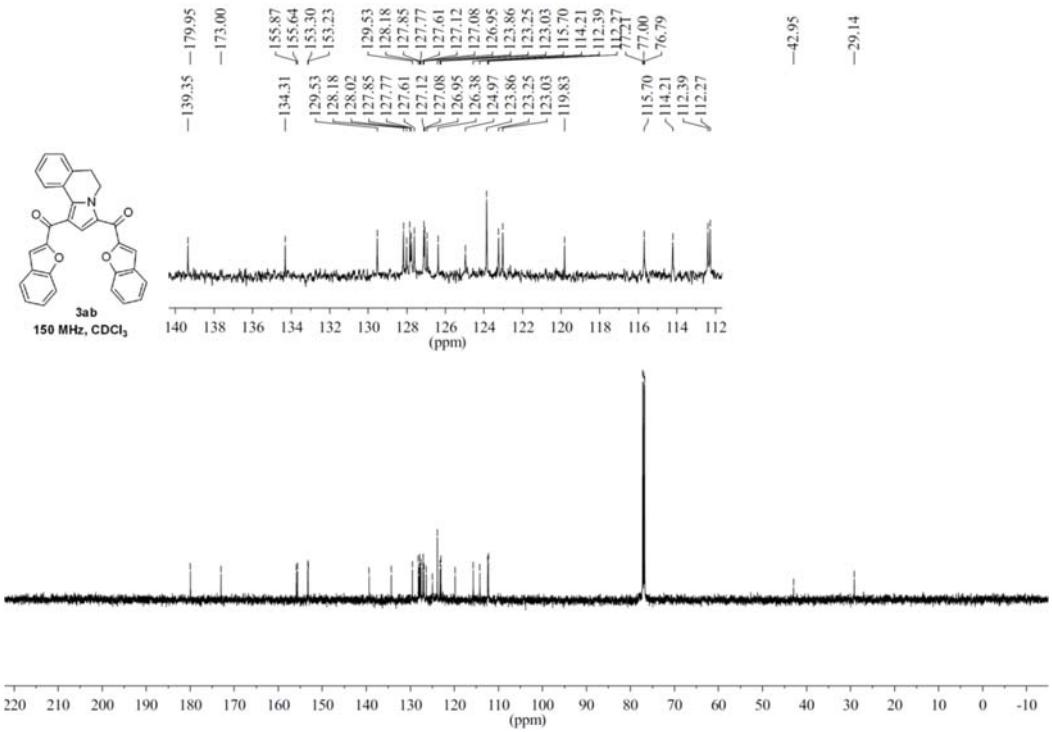


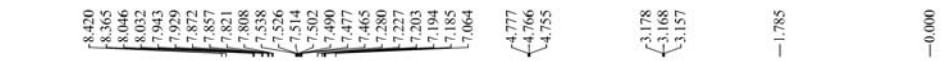
3y
150 MHz, $CDCl_3$

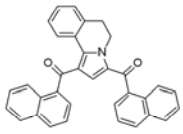

8.780
8.771
8.759
8.750
7.867
7.854
7.637
7.628
7.600
7.591
7.363
7.351
7.339
7.330
7.319
7.275
7.242
7.230
7.219
6.923
4.768
4.757
4.746
3.183
3.172
3.161
0.000
3z
600 MHz, CDCl3
1.78
1.88
1.00
2.01
2.07
2.02
1.01
0.97
2.02
2.04
(ppm)


190.16
184.18
150.49
150.36
145.48
145.12
140.44
134.40
130.10
128.15
127.95
127.79
127.13
126.93
125.82
122.63
122.30
119.45
77.21
77.00
76.79
42.98
29.06
3z
150 MHz, CDCl3
(ppm)

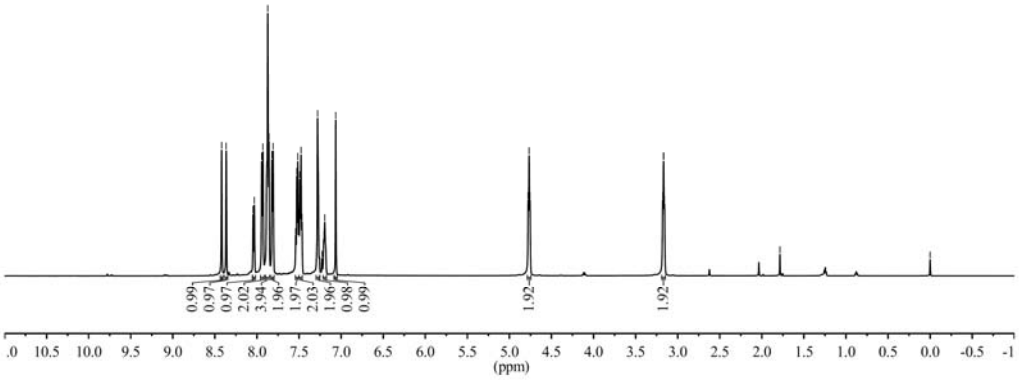

8.043
8.001
7.987
7.723
7.710
7.633
7.621
7.607
7.586
7.578
7.500
7.487
7.473
7.459
7.446
7.333
7.321
7.308
7.293
7.258
7.247
7.235
7.223
4.751
4.740
4.729
3.147
3.137
3.126
1.696
0.000
3ab
600 MHz, CDCl3
0.95
1.00
1.98
1.93
1.91
2.17
4.00
1.04
1.96
1.97
(ppm)

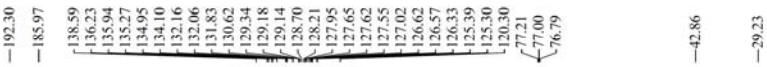

179.95
173.00
155.87
155.64
153.30
153.23
139.35
134.31
129.53
128.18
128.02
127.85
127.77
127.61
127.12
127.08
126.95
126.38
124.97
123.86
123.25
123.03
119.83
129.53
128.18
127.85
127.77
127.61
127.12
127.08
126.95
123.86
123.25
123.03
115.70
114.21
112.39
112.27
77.21
77.00
76.79
42.95
29.14
3ab
150 MHz, CDCl3
(ppm)

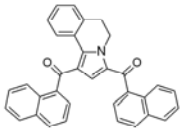




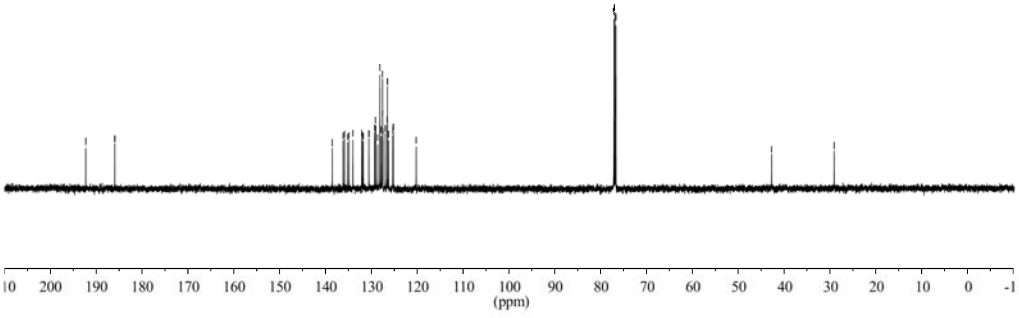
3ac
600 MHz, $CDCl_3$

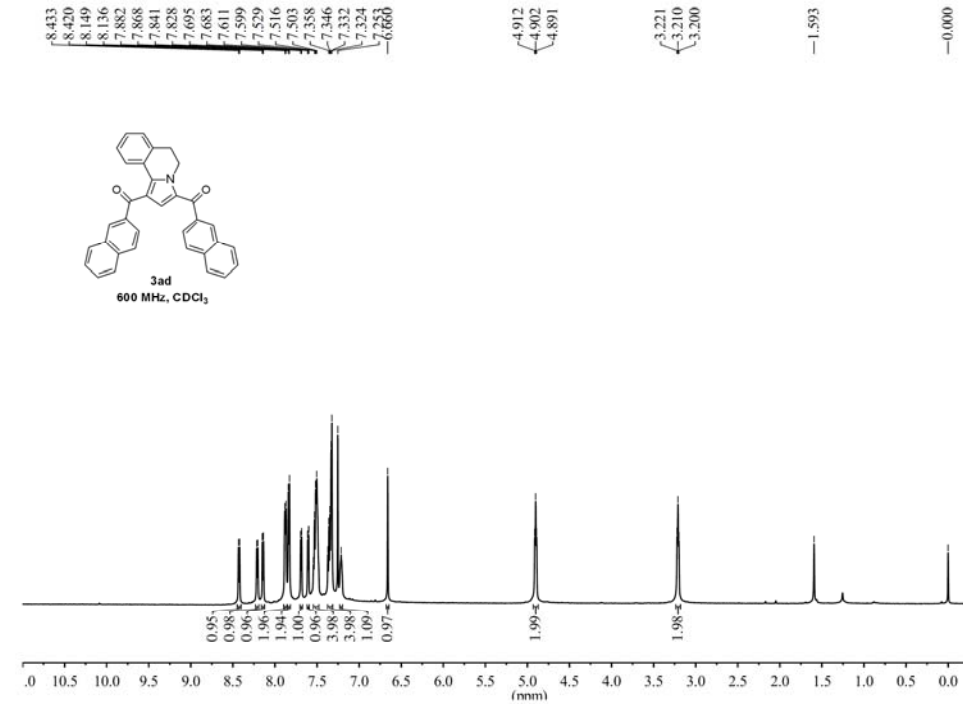


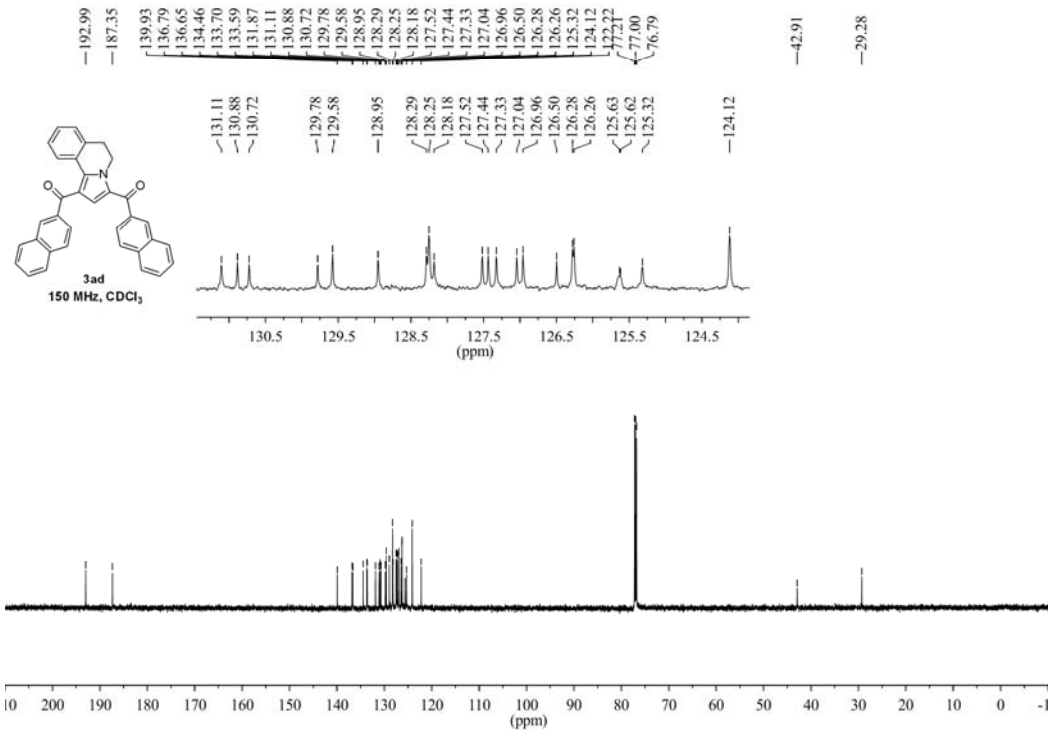


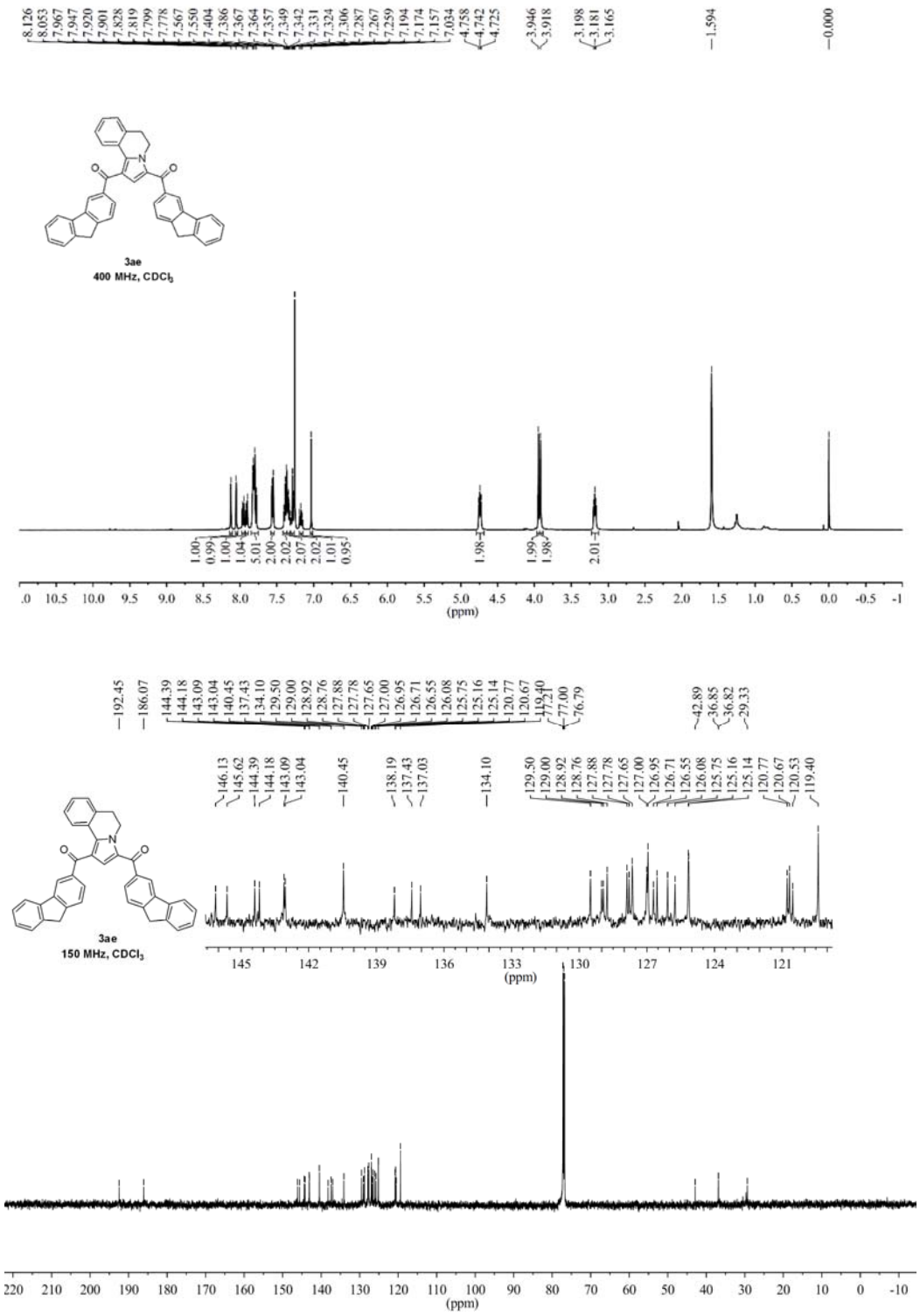


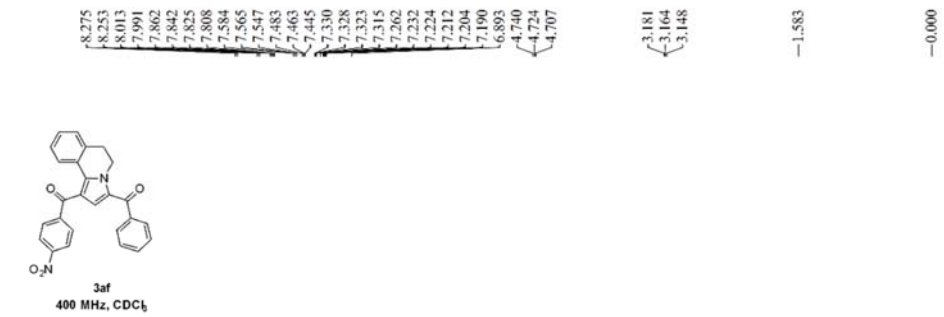
3ac
150 MHz, $CDCl_3$



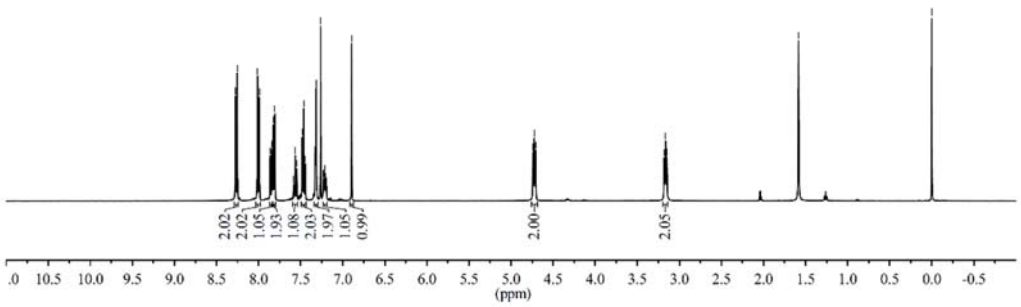

3ad
600 MHz, CDCl3
(ppm)

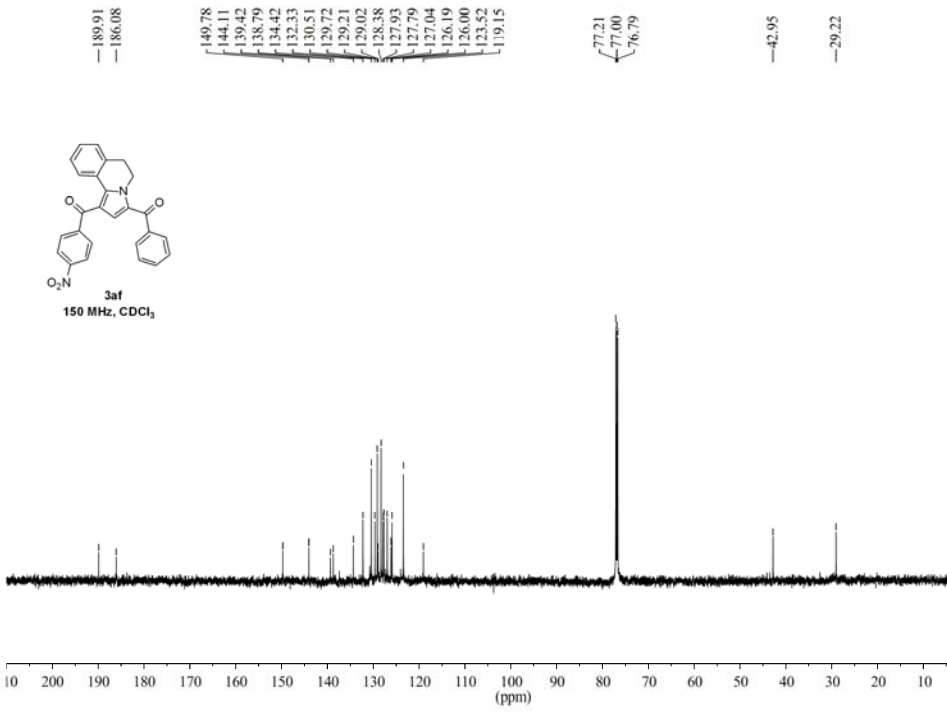

3ad
150 MHz, CDCl3
(ppm)


3ae
400 MHz, CDCl3
(ppm)
3ae
150 MHz, CDCl3
(ppm)
(ppm)

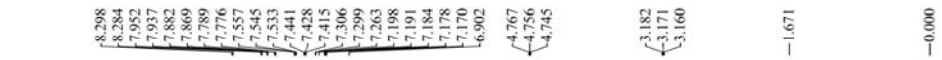


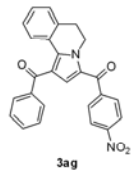
3af
400 MHz, $CDCl_3$



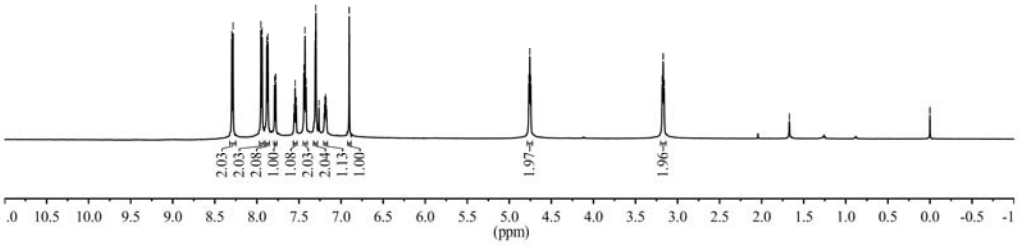


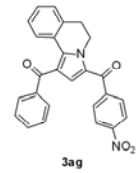
3af
150 MHz, $CDCl_3$



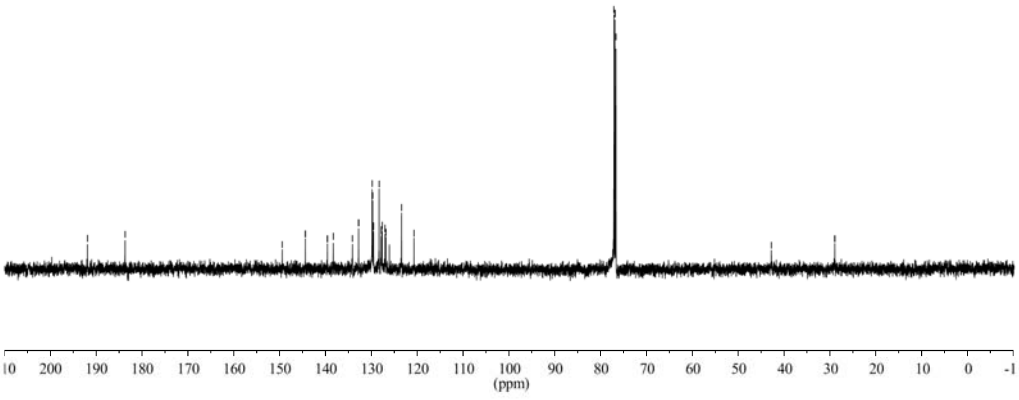


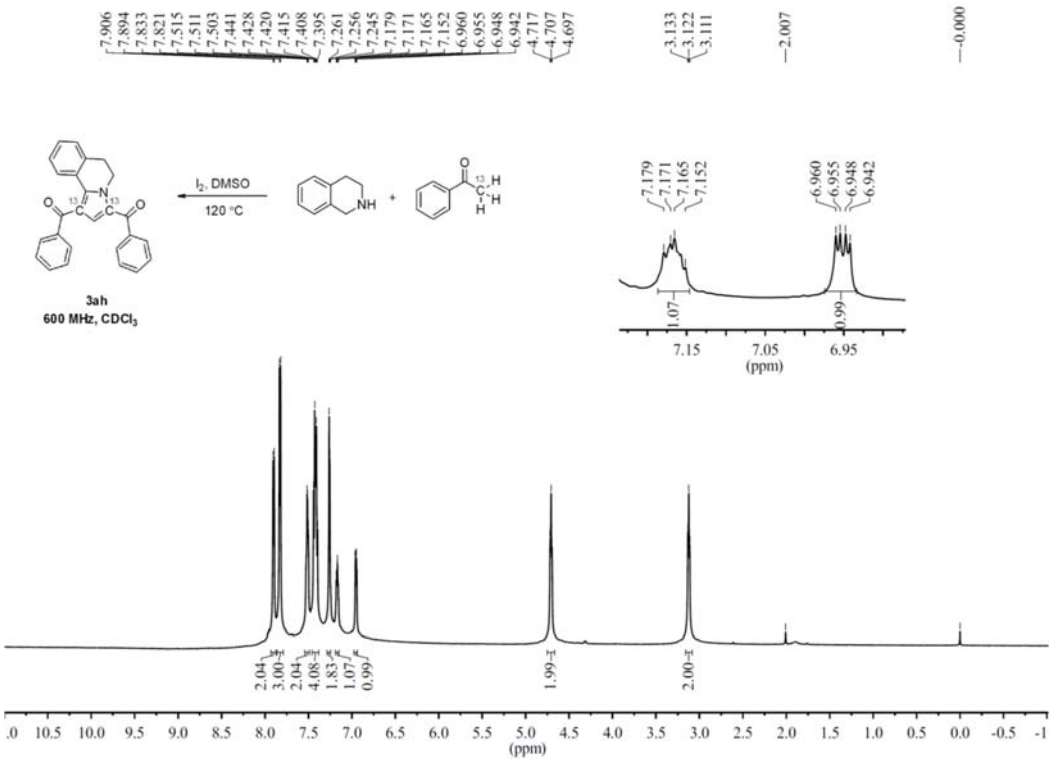
3ag
600 MHz, $CDCl_3$

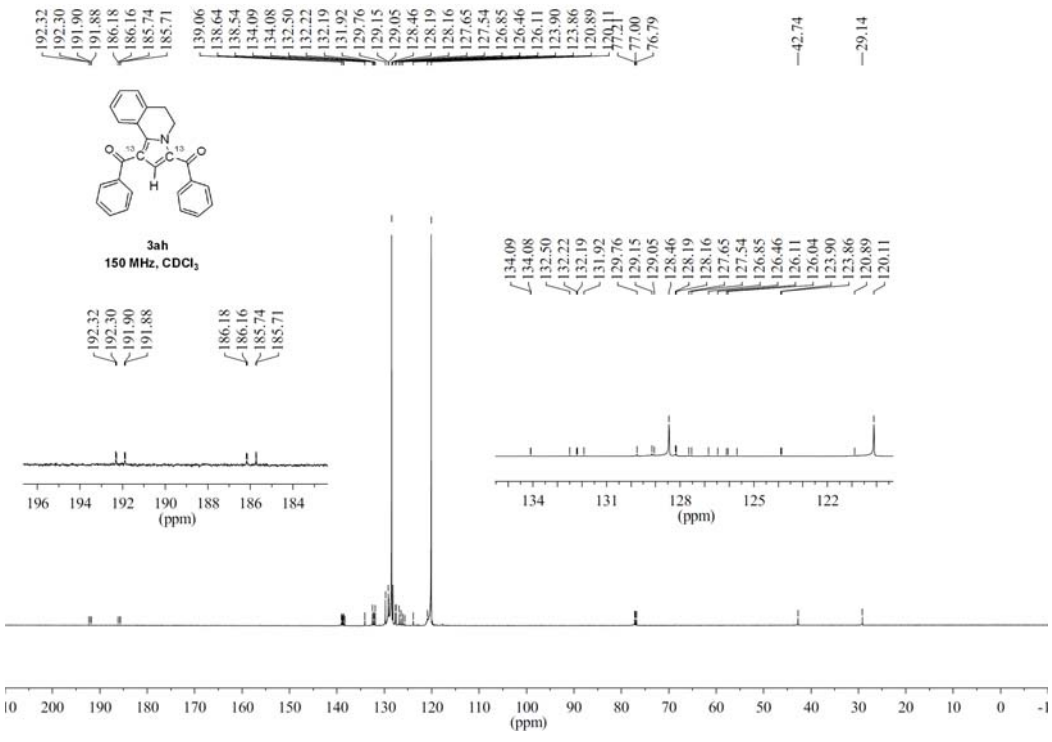


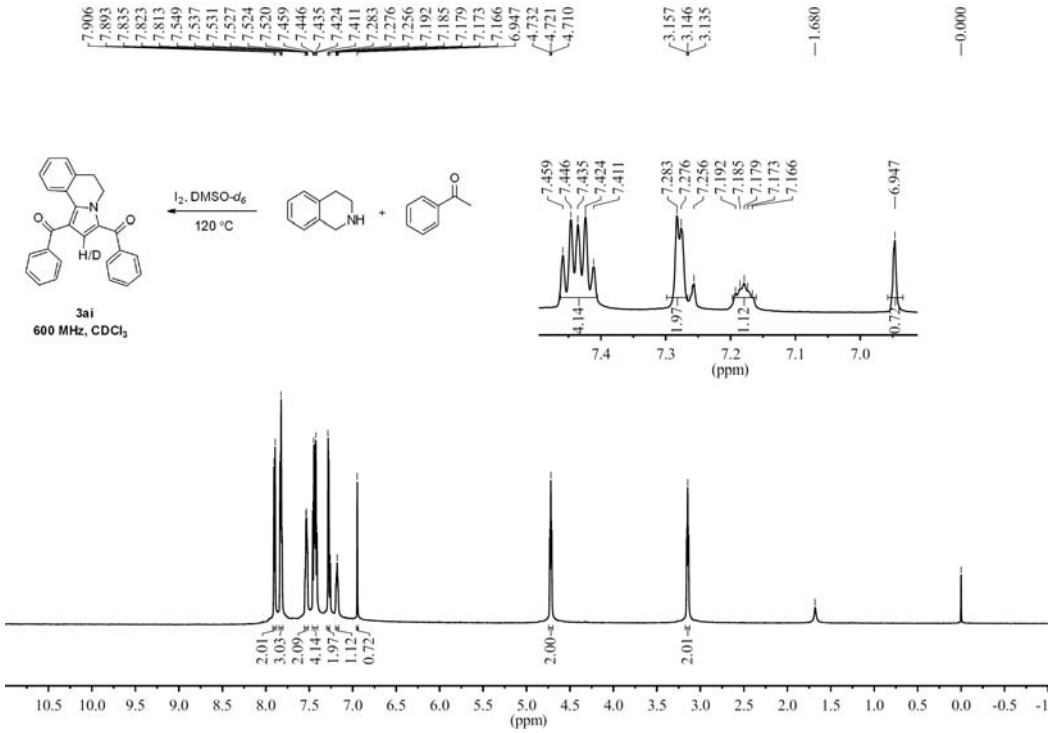


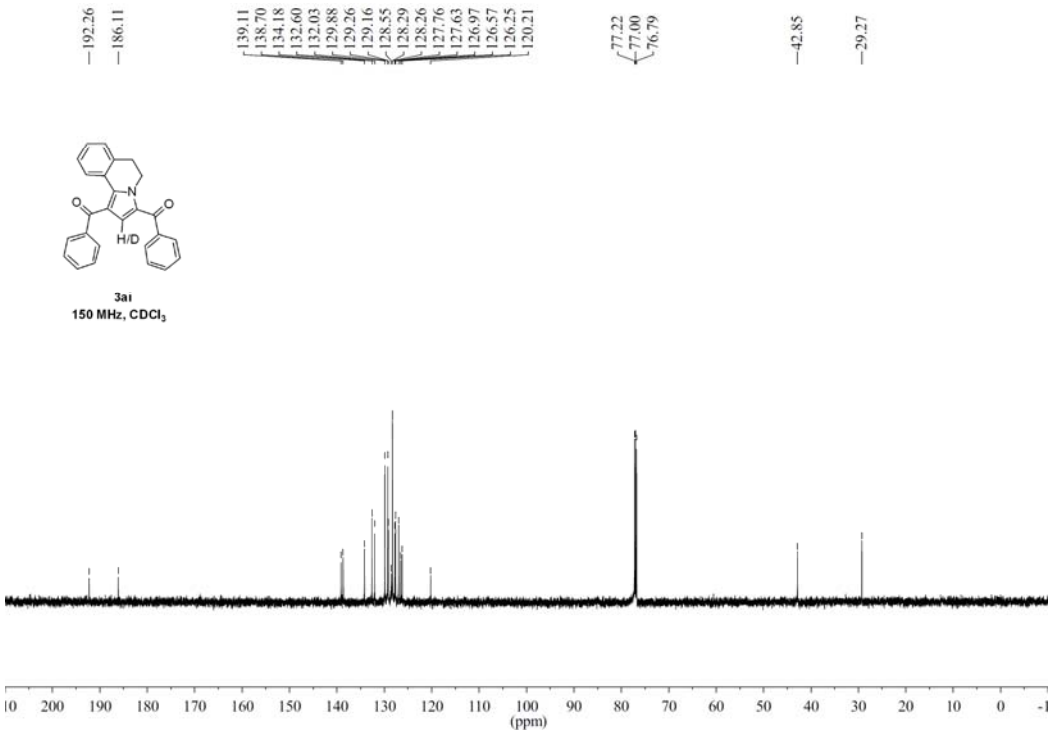
3ag
150 MHz, $CDCl_3$

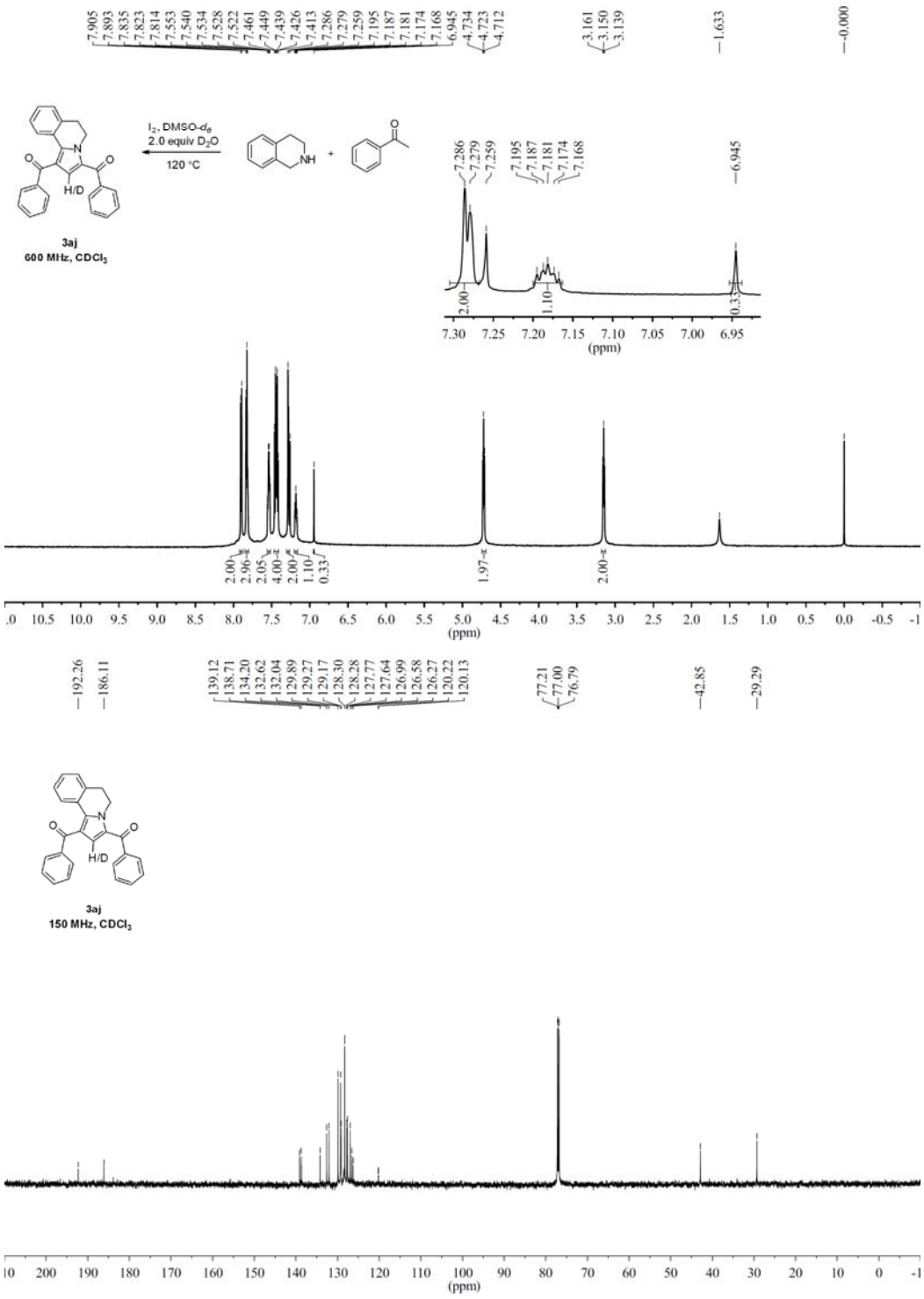


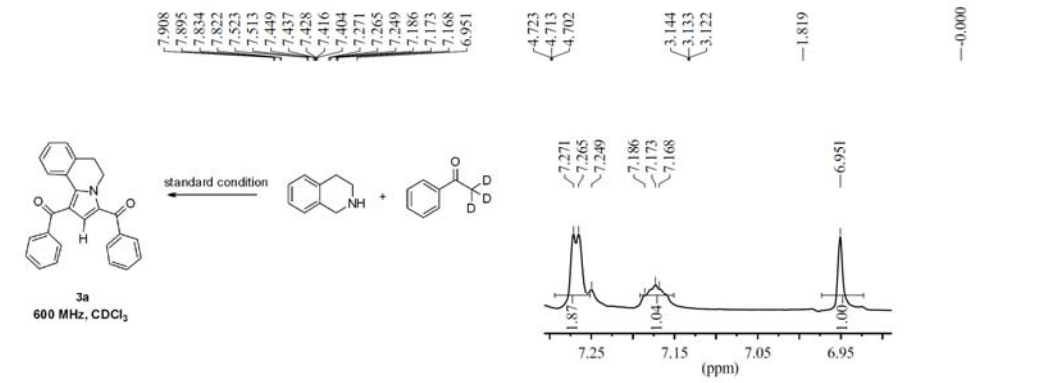

I2, DMSO
120 °C
NH
3ah
600 MHz, CDCl3
(ppm)

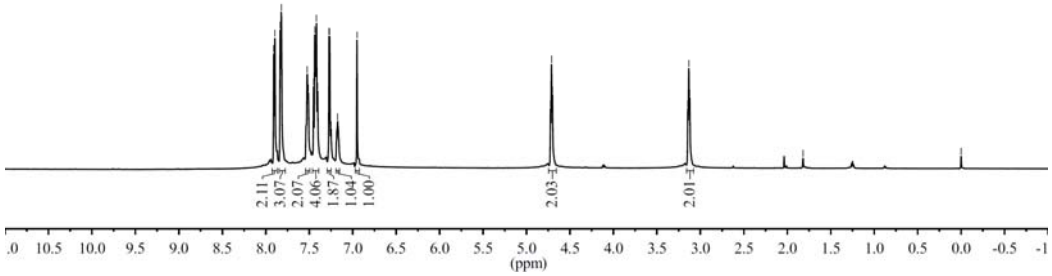

3ah
150 MHz, CDCl3
(ppm)

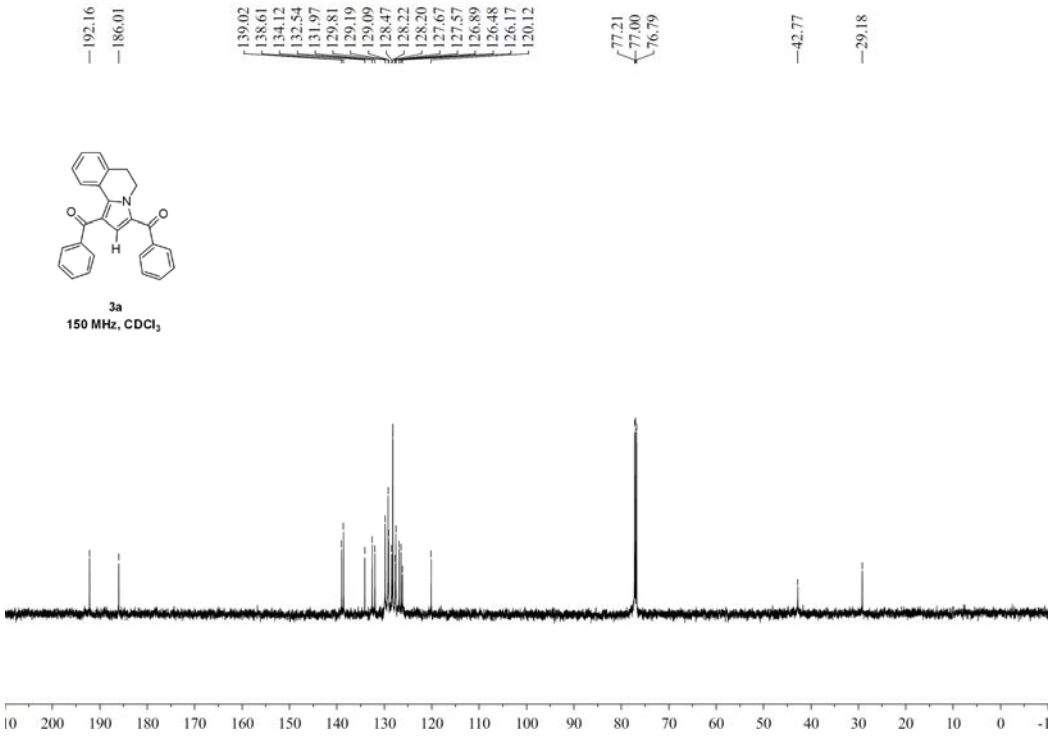

7.906
7.893
7.835
7.823
7.813
7.549
7.537
7.531
7.527
7.524
7.520
7.459
7.446
7.435
7.424
7.411
7.283
7.276
7.256
7.192
7.185
7.179
7.173
7.166
6.947
4.732
4.721
4.710
3.157
3.146
3.135
1.680
0.000
I2, DMSO-d6
120 °C
NH
H/D
3ai
600 MHz, CDCl3
2.01
3.03
2.09
4.14
1.97
1.12
0.72
2.00
2.01
(ppm)

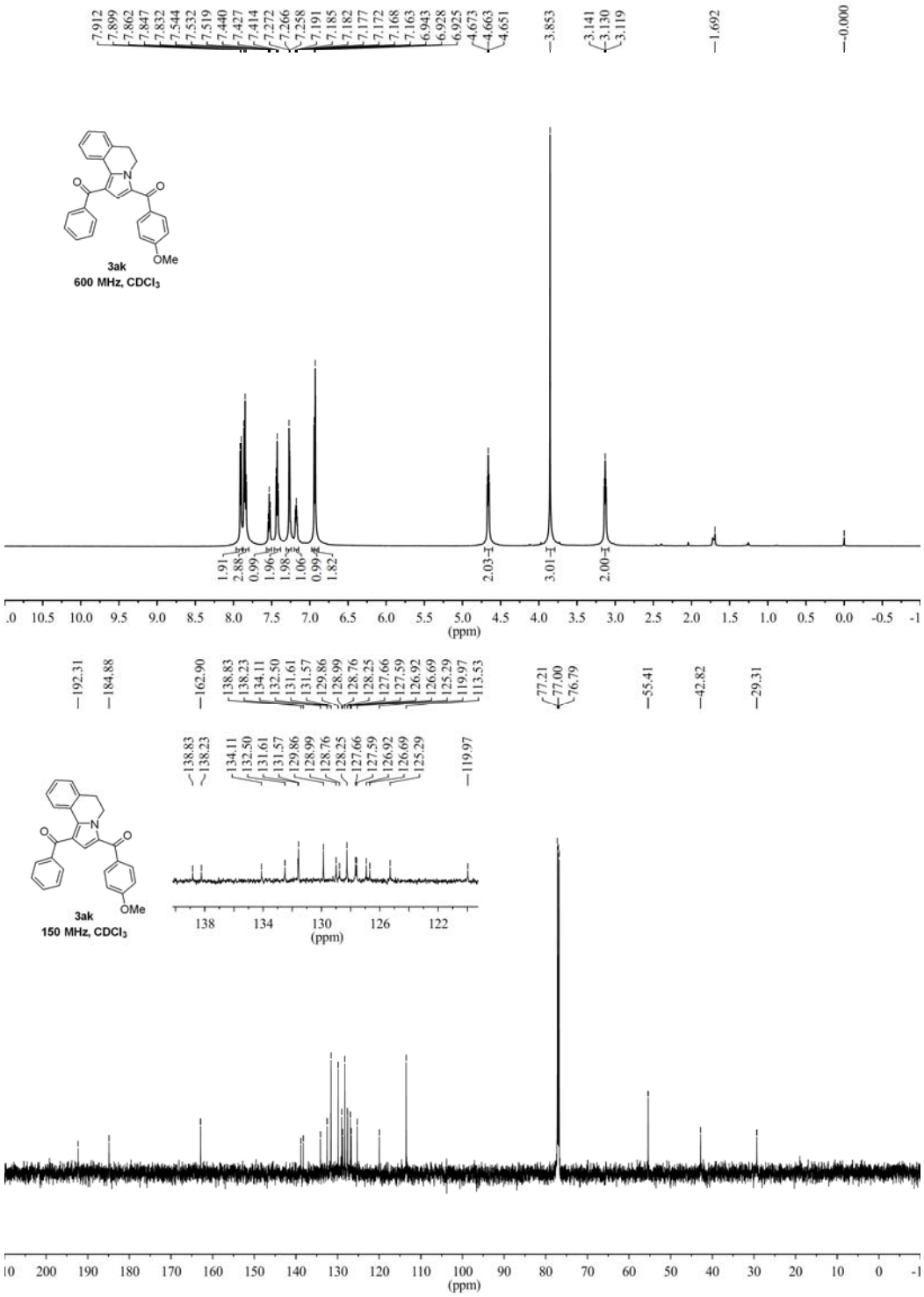

192.26
186.11
139.11
138.70
134.18
132.60
132.03
129.88
129.26
129.16
128.55
128.29
128.26
127.76
127.63
126.97
126.57
126.25
120.21
77.22
77.00
76.79
42.85
29.27
H/D
3ai
150 MHz, CDCl3
(ppm)


7.905
7.893
7.835
7.823
7.814
7.553
7.540
7.534
7.528
7.522
7.461
7.449
7.439
7.426
7.413
7.286
7.279
7.259
7.195
7.187
7.181
7.174
7.168
6.945
4.734
4.723
4.712
3.161
3.150
3.139
1.633
0.000
I2, DMSO-d6
2.0 equiv D2O
120 °C
NH
H/D
3aj
600 MHz, CDCl3
2.00
2.96
2.05
4.00
2.00
1.10
0.33
1.97
2.00
(ppm)
192.26
186.11
139.12
138.71
134.20
132.62
132.04
129.89
129.27
129.17
128.30
128.28
127.77
127.64
126.99
126.58
126.27
120.22
120.13
77.21
77.00
76.79
42.85
29.29
3aj
150 MHz, CDCl3
(ppm)


7.908
7.895
7.834
7.822
7.523
7.513
7.449
7.437
7.428
7.416
7.404
7.271
7.265
7.249
7.186
7.173
7.168
6.951
4.723
4.713
4.702
3.144
3.133
3.122
1.819
0.000
standard condition
NH
D
D
D
3a
600 MHz, CDCl3
7.271
7.265
7.249
7.186
7.173
7.168
6.951
1.87
1.04
1.00
7.25
7.15
7.05
6.95
(ppm)


2.11
3.07
2.07
4.06
1.87
1.04
1.00
2.03
2.01
(ppm)


192.16
186.01
139.02
138.61
134.12
132.54
131.97
129.81
129.19
129.09
128.47
128.22
128.20
127.67
127.57
126.89
126.48
126.17
120.12
77.21
77.00
76.79
42.77
29.18
3a
150 MHz, CDCl3


7.912
7.899
7.862
7.847
7.832
7.544
7.532
7.519
7.440
7.427
7.414
7.272
7.266
7.258
7.191
7.185
7.182
7.177
7.172
7.168
7.163
6.943
6.928
6.925
4.673
4.663
4.651
3.853
3.141
3.130
3.119
1.692
0.000
3ak
600 MHz, CDCl3
1.91
2.88
0.99
1.96
1.98
1.06
0.99
1.82
2.03
3.01
2.00
(ppm)
192.31
184.88
162.90
138.83
138.23
134.11
132.50
131.61
131.57
129.86
128.99
128.76
128.25
127.66
127.59
126.92
126.69
125.29
119.97
113.53
77.21
77.00
76.79
55.41
42.82
29.31
3ak
150 MHz, CDCl3
(ppm)