Supporting Information

Efficient approach to 2-hydroxy-2,3-dihydrofuran derivatives and its application for the synthesis of novel 4-(1*H*-pyrazol-4-yl)pyridazines

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Supporting Information

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1. General experimental: All 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}. ^1H spectra were recorded in DMSO-d_6 on 400/600 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. ^{13}C spectra were recorded in DMSO-d_6 on 100/150 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS were obtained on an apex-Ultra MS equipped with APCI. MS was recorded using ESI. Melting points were determined using an electrothermal capillary melting point apparatus and not corrected. The structures of 3aa and 4a were confirmed by X-ray diffraction.

2. General Experimental Procedure for the Synthesis of 3 (3aa as an example).

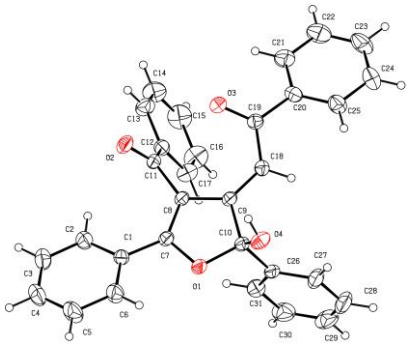
General procedure: *N*-phenacylpyridinium iodide **1a** (1.1 mmol, 1.1 equiv) with 2-benzoyl-1,4- diphenylbut-2-ene-1,4-dione **2a** (1.0 mmol, 1.0 equiv) and K_2CO_3 (1.0 mmol, 1.0 equiv) was stirred in CH_3CN (5 mL) at room temperature for 5h till almost completed conversion of the substrates by TLC analysis, then extracted with EtOAc three times (3 × 50 mL). and the combined organic extracts were then washed with brine. After drying over Na_2SO_4 and evaporation, The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 8/1) to afford the product **3aa**.

3. General Experimental Procedure for the Synthesis of 4 (4a as an example).

General procedure: (*E*)-2-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2*H*)-ylidene)-1-phenyl-ethanone **3aa** (1.0 mmol, 1.0 equiv) with 85% hydrazine hydrate (20 mmol, 20 equiv) was added and the mixture were stirred at reflux in EtOH (3 mL) for 5h till almost completed conversion of the substrates by TLC analysis, then extracted with EtOAc three times (3 × 50 mL) and the combined organic extracts were then washed with brine. After drying over Na_2SO_4 and evaporation, The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5/1) to afford the product **4a**.

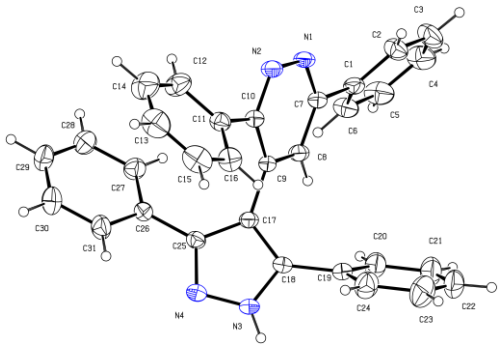
4. The crystallographic data of 3aa and 4a.

(1) Crystallographic data of **3aa** (CCDC: 1042907).



Empirical formula	$C_{31}H_{22}O_4$		Absorption coefficient	0.082 mm^{-1}
Formula weight	458.49		F(000)	480
Temperature	296(2) K		Crystal size	0.20 x 0.11 x 0.10 mm^3
Wavelength	0.71073 Å		Reflections collected	9235
Crystal system	Triclinic		Independent reflections	4703 [R(int) = 0.0305]
Space group	P-1		Max. and min. transmission	0.9918 and 0.9838
Unit cell dimensions	a = 10.992(4) Å	= 102.215(5) °	Refinement method	Full-matrix least-squares on F^2
	b = 11.214(4) Å	= 104.067(5) °	Data / restraints / parameters	4703 / 0 / 320
	c = 11.305(4) Å	= 108.292(5) °	Goodness-of-fit on F^2	1.090
Volume	1219.2(8) $Å^3$		Final R indices [I>2sigma(I)]	R1 = 0.0525, wR2 = 0.1555
Z	2		R indices (all data)	R1 = 0.0677, wR2 = 0.1652
Density (calculated)	1.249 Mg/m^3		Largest diff. peak and hole	0.390 and -0.168 $e.Å^{-3}$

(2) Crystallographic data of **4a** (CCDC: 1042908).



Empirical formula	$C_{31}H_{22}N_4$		Absorption coefficient	0.074 mm^{-1}
Formula weight	450.53		F(000)	472
Temperature	298(2) K		Crystal size	0.13 x 0.12 x 0.10 mm^3
Wavelength	0.71073 Å		Reflections collected	7751
Crystal system	Monoclinic		Independent reflections	3564 [R(int) = 0.0700]
Space group	P2(1)		Max. and min. transmission	0.9926 and 0.9904
Unit cell dimensions	a = 9.0418(19) Å	= 90°	Refinement method	Full-matrix least-squares on F^2
	b = 11.277(2) Å	= 110.94 °	Data / restraints / parameters	3564 / 1 / 320
	c = 12.649(3) Å	γ = 90 °	Goodness-of-fit on F^2	0.511
Volume	1204.5(4) $Å^3$		Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.0949
Z	2		R indices (all data)	R1 = 0.0469, wR2 = 0.1191
Density (calculated)	1.242 Mg/m^3		Largest diff. peak and hole	0.174 and -0.169 $e.Å^{-3}$

5. Spectroscopic Data:

(E)-2-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2H)-ylidene)-1-phenylethanone **(3aa)**. Yellow solid; yield 95%; mp 142-143 ^{o}C; IR (KBr): 3441, 3060, 1671, 1640, 1598, 1579, 1529, 1488, 1446, 1342, 1233, 1178, 1139, 1057, 1026, 958, 874, 768, 733, 704, 685, 651 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d$_6$): δ (ppm) 8.95 (s, 1H), 7.95 (d, *J* = 7.2 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 2H), 7.67 (d, *J* = 7.8 Hz, 2H), 7.64 (d, *J* = 7.8 Hz, 2H), 7.54-7.45 (m, 6H), 7.42-7.38 (m, 6H), 6.68 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d$_6$): δ (ppm) 190.1, 187.0, 167.7, 159.5, 140.6, 138.8, 137.7, 132.8, 132.7, 131.8, 129.1, 128.8(3), 128.8(1), 128.7, 128.6, 128.5(6), 128.5, 128.1, 127.6, 124.9, 113.7, 112.0, 110.1; HRMS (ESI): m/z [M+H]$^{+}$ calcd for $C_{31}H_{23}O_4$: 459.1591; found: 459.1591.

(E)-2-(4-benzoyl-2-hydroxy-5-phenyl-2-(p-tolyl)furan-3(2H)-ylidene)-1-phenylethanone **(3ab)**. Yellow solid; yield 91%; mp 94-95 ^{o}C; IR (KBr): 3426, 3059, 1645, 1597, 1579, 1534, 1488, 1447, 1385, 1344, 1233, 1178, 1141, 1074, 1054, 955, 878, 819, 776, 720, 689 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d$_6$): δ (ppm) 8.86 (s, 1H), 7.93 (d, *J* = 7.8 Hz, 2H), 7.66-7.63 (m, 4H), 7.58 (d, *J* = 7.8 Hz, 2H), 7.52-7.46 (m, 3H), 7.42-7.38 (m, 6H), 7.32 (d, *J* = 7.8 Hz, 2H), 6.64 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ (ppm) 190.2, 187.0, 167.8, 159.8, 138.9, 138.6, 137.9, 137.7, 132.8, 132.7, 131.9, 129.4, 128.9, 128.7, 128.6(0), 128.5(7), 128.1, 127.7, 124.9, 113.7, 111.8, 110.5, 110.4, 20.9; HRMS (ESI): m/z [M+H]$^{+}$ calcd for $C_{32}H_{25}O_4$: 473.1747; found: 473.1746.

(E)-2-(4-benzoyl-2-hydroxy-2-(4-methoxyphenyl)-5-phenylfuran-3(2H)-ylidene)-1-phenylethanone **(3ac)**. Yellow solid; yield 92%; mp 64-66 ^{o}C; IR (KBr): 3442, 3061, 1652, 1597, 1579, 1510, 1448, 1315, 1259, 1170, 1023, 739, 690 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d$_6$): δ (ppm) 8.94 (s, 1H), 8.02 (d, *J* = 6.0 Hz, 2H), 7.70-7.69 (m, 5H), 7.49-7.47 (m, 4H), 7.45-7.39 (m, 6H), 7.09 (d, *J* = 7.2 Hz, 2H), 6.71 (s, 1H), 3.78 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d$_6$) δ (ppm) 190.2, 187.1, 167.8, 159.8, 138.9, 137.8, 134.0, 132.8, 132.7, 131.8, 129.0, 128.8(3), 128.7(5), 128.7, 128.5, 128.1, 127.7, 126.5, 114.1, 113.8, 111.8, 110.6, 110.4, 55.2; HRMS (ESI): m/z [M+H]$^{+}$ calcd for $C_{32}H_{25}O_5$: 489.1697; found: 489.1695.

(E)-2-(4-benzoyl-2-(4-chlorophenyl)-2-hydroxy-5-phenylfuran-3(2H)-ylidene)-1-phenylethanone **(3ad)**. Yellow solid; yield 95%; mp 143-144 ^{o}C; IR (KBr): 3441, 3203, 1642, 1560, 1579, 1529, 1489, 1447, 1385, 1344, 1322, 1217, 1142, 1096, 1076, 1039, 1013, 896, 787, 703, 676 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d$_6$): δ (ppm) 9.03 (s, 1H), 7.95-7.92 (m, 2H), 7.73-7.71 (m, 2H),

7.66-7.64 (m, 4H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.53-7.48 (m, 3H), 7.43-7.41 (m, 6H), 6.67 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.1, 187.1(3), 187.0(7), 167.5, 159.0, 139.7, 139.6, 138.7, 137.6, 133.9, 132.9(0), 132.8(6), 132.0, 129.0, 128.9, 128.7, 128.6, 128.5, 128.1, 127.8, 127.1, 113.7, 109.6; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}ClO_4$: 493.1201; found: 493.1199.

(E)-2-(4-benzoyl-2-(4-bromophenyl)-2-hydroxy-5-phenylfuran-3(2H)-ylidene)-1-phenylethanone **(3ae)**. Yellow solid; yield 90%; mp 149-151 ^{o}C; IR (KBr): 3440, 1643, 1596, 1579, 1528, 1489, 1448, 1385, 1344, 1234, 1219, 1171, 1141, 1076, 1056, 1039, 1011, 928, 896, 740, 651 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 9.03 (s, 1H), 7.93-7.89 (m, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.66-7.65 (m, 5H), 7.53-7.48 (m, 4H), 7.43-7.41(m, 6H), 6.67 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.1, 187.1(3), 187.0(7), 167.6, 159.0, 140.0, 138.7, 137.6, 132.9, 132.8, 132.0, 131.9, 128.9, 128.7, 128.6(4), 128.6(1), 128.5, 128.2, 127.8, 127.4, 122.6, 113.8, 109.6; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}BrO_4$: 537.0696; found: 537.0698.

(E)-2-(4-benzoyl-2-(3,4-dichlorophenyl)-2-hydroxy-5-phenylfuran-3(2H)-ylidene)-1-phenylethanone **(3af)**. Yellow solid; yield 92%; mp 142-144 ^{o}C; IR (KBr): 3442, 3184, 1642, 1575, 1528, 1483, 1442, 1405, 1340, 1231, 1171, 1025, 965, 928, 875, 783, 684, 642; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 9.19 (s, 1H), 7.92 (d, *J* = 10.2 Hz, 2H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.55-7.48 (m, 4H), 7.43-7.40 (m, 6H), 6.74 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.0, 187.4, 187.3, 167.2, 158.3(1), 158.2(6), 158.2, 141.5, 138.6, 137.5, 132.9, 132.0, 131.6, 131.3, 128.9, 128.7(1), 128.6(6), 128.6, 128.3(5), 128.3(3), 128.2, 127.9, 127.2, 125.6, 113.8; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{21}Cl_2O_4$: 527.0811; found: 527.0811.

(E)-2-(4-benzoyl-2-hydroxy-2-(4-nitrophenyl)-5-phenylfuran-3(2H)-ylidene)-1-phenylethanone **(3ag)**. Yellow solid; yield 85%; mp 91-93 ^{o}C; IR (KBr): 3441, 1644, 1597, 1579, 1525, 1489, 1448, 1385, 1346, 1233, 1173, 1140, 1024, 883, 853, 651; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 9.28 (s, 1H), 8.39 (d, *J* = 9.0 Hz, 2H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.67-7.66 (m, 4H), 7.54-7.50 (m, 3H), 7.44-7.40 (m, 6H), 6.72 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.0, 187.1, 167.5, 158.3, 148.0, 147.1, 138.6, 137.5, 133.0, 132.1, 129.0, 128.7(3), 128.6(9), 128.6(5), 128.3, 128.2, 127.9, 126.7, 124.3, 123.4, 113.8, 109.2, 109.1; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}NO_6$: 504.1442; found: 504.1438.

(E)-2-(4-benzoyl-2-hydroxy-5-phenyl-2-(thiophen-3-yl)furan-3(2H)-ylidene)-1-phenylethanone **(3ah)**. Yellow solid; yield 94%; mp 148-149 ^{o}C; IR (KBr): 3423, 2978, 1687, 1664, 1638, 1596, 1579, 1533, 1488, 1449, 1419, 1385, 1264, 1246, 1232, 1195, 1182, 1169, 1076, 1054, 1024, 967, 863, 731, 688, 661; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.86 (s, 1H), 7.92 (d, J = 7.2 Hz, 2H), 7.82 (s, 1H), 7.69 (d, J = 7.8 Hz, 2H), 7.65-7.64 (m, 2H), 7.54-7.45 (m, 4H), 7.43-7.38 (m, 6H), 7.33 (d, J = 4.8 Hz, 1H), 6.78 (s, 1H).; ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.1, 187.1(2), 187.0(6), 167.3, 158.9, 158.8, 142.2, 142.1, 138.7, 137.7, 132.8, 131.8, 128.8, 128.7, 128.6, 128.1, 127.8, 125.3, 123.5, 113.5, 111.8, 109.0, 108.9; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{29}H_{21}O_4S$: 465.1155; found: 465.1155.

(E)-2-(4-benzoyl-2-hydroxy-2-(naphthalen-2-yl)-5-phenylfuran-3(2H)-ylidene)-1-phenylethanone **(3ai)**. Yellow solid; yield 94%; mp 168-169 ^{o}C; IR (KBr): 3237, 3057, 1638, 1575, 1531, 1484, 1386, 1342, 1227, 1176, 1147, 1024, 949, 877, 824, 746, 686, 640, 478; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 9.12 (s, 1H), 8.38 (s, 1H), 8.12-7.93 (m, 5H), 7.77-7.73 (m, 3H), 7.64 (t, J = 8.4 Hz, 2H), 7.59-7.54 (m, 2H), 7.51-7.47 (m, 2H), 7.46-7.43 (m, 5H), 7.39-7.31 (m, 2H), 6.75 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.2, 187.1(1), 187.0(5), 167.9, 159.6, 159.5, 138.8, 138.0, 137.9, 137.6, 133.1, 132.8, 132.7, 132.6, 131.9, 128.9, 128.7, 128.6, 128.2, 127.7, 127.6, 126.9, 126.7, 124.1, 122.9, 113.9, 112.2, 110.4, 110.3; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{35}H_{25}O_4$: 509.1747; found: 509.1743.

(E)-2-(2-(benzofuran-2-yl)-4-benzoyl-2-hydroxy-5-phenylfuran-3(2H)-ylidene)-1-phenylethanon **(3aj)**. Yellow solid; yield 93%; mp 57-59 ^{o}C; IR (KBr): 3324, 3059, 1673, 1638, 1576, 1532, 1487, 1447, 1404, 1337, 1307, 1245, 1174, 1133, 1054, 871, 828, 743, 694, ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 9.40 (s, 1H), 8.02 (d, J = 7.8 Hz, 2H), 7.78 (d, J = 7.8 Hz, 1H), 7.71-7.67 (m, 5H), 7.54-7.50 (m, 3H), 7.48-7.44 (m, 3H), 7.43-7.38 (m, 4H), 7.33-7.31 (m, 2H), 6.86 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.0, 187.2, 167.2, 156.5, 154.8, 154.3, 138.7, 137.5, 133.0, 132.9, 132.0, 128.9, 128.7(4), 128.6(7), 128.5, 128.2, 127.8, 127.2, 125.5, 123.5, 122.2, 113.8, 112.5, 111.7, 106.2, 105.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{33}H_{23}O_5$: 499.1540; found: 499.1539.

(E)-2-(2-hydroxy-4-(4-methoxybenzoyl)-5-(4-methoxyphenyl)-2-phenylfuran-3(2H)-ylidene)-1-phe nylethanon **(3ak)**. Yellow solid; yield 87%; mp 71-73 ^{o}C; IR (KBr): 3442, 2840, 1663, 1598, 1508, 1452, 1421, 1316, 1259, 1170, 1023, 842, 706; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.81 (s,

1H), 7.87 (d, *J* = 6.0 Hz, 2H), 7.65-7.62 (m, 5H), 7.52-7.49 (m, 3H), 7.45-7.39 (m, 4H), 6.99 (d, *J* = 7.2 Hz, 2H), 6.94 (d, *J* = 7.8 Hz, 2H), 6.55 (s, 1H), 3.77 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 189.3, 186.7, 167.2, 162.8, 162.0, 160.2, 141.0, 138.0, 132.5, 132.1, 130.9, 130.1, 129.0, 128.8, 128.6, 127.6, 124.9, 120.8, 114.4, 113.8, 112.6, 110.6, 109.9, 55.5, 55.4; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{33}H_{27}O_6$: 519.1802; found: 519.1810.

(E)-2-(4-acetyl-2-(4-bromophenyl)-2-hydroxy-5-phenylfuran-3(2H)-ylidene)-1-phenylethanone **(3al)**. Yellow solid; yield 93%; mp 116-118 ^{o}C; IR (KBr): 3248, 3064, 1658, 1635, 1577, 1487, 1448, 1400, 1236, 1204, 1174, 1104, 1072, 1049, 1011, 897, 825, 780, 763, 690, 640; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.93 (s, 1H), 7.80 (d, *J* = 7.8 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.40-7.36 (m, 4H), 6.51 (s, 1H), 2.21 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 189.2, 187.5, 187.4, 174.8, 158.7, 158.6, 139.7, 139.0, 137.7, 132.6, 131.6, 128.5, 128.3, 128.1, 127.4, 122.5, 114.2, 110.7, 110.6, 14.8; HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{26}H_{19}BrNaO_4$: 497.0359; found: 497.0360.

(E)-2-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2H)-ylidene)-1-(4-methoxyphenyl)ethanone **(3ba)**. Yellow solid; yield 89%; mp 63-64 ^{o}C; IR (KBr): 3425, 3061, 1658, 1597, 1448, 1419, 1389, 1315, 1257, 1169, 1021, 835, 690; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.88 (s, 1H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.72 (d, *J* = 7.2 Hz, 2H), 7.67-7.65 (m, 4H), 7.53-7.51 (m, 2H), 7.46-7.39 (m, 7H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.67 (s, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.1, 185.6, 167.0, 162.8, 158.7, 140.9(4), 140.8(8), 138.8, 132.7, 131.8, 130.5, 130.1, 129.1, 128.8, 128.7, 128.6, 128.5, 128.1, 125.0, 113.9, 113.7, 112.2, 110.2, 55.5; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{32}H_{25}O_5$: 489.1697; found: 489.1694.

(E)-2-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2H)-ylidene)-1-(4-chlorophenyl)ethanone **(3ca)**. Yellow solid; yield 91%; mp 130-131 ^{o}C; IR (KBr): 3323, 3063, 2804, 2589, 1667, 1633, 1587, 1525, 1486, 1445, 1410, 1341, 1236, 1171, 1091, 1061, 950, 874, 812, 784, 734, 684, 527, 474; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.95 (s, 1H), 7.90 (d, *J* = 7.8 Hz, 2H), 7.69-7.63 (m, 6H), 7.53-7.45 (m, 7H), 7.44-7.39 (m, 4H), 6.63 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.1, 186.0, 185.9, 168.0, 160.1, 140.6, 138.7, 137.6, 136.2, 132.8, 131.9, 129.6, 129.1, 128.9, 128.8(2), 128.7(7), 128.5, 128.1, 125.0, 113.7, 111.6, 110.3, 110.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}ClO_4$: 493.1201; found: 493.1200.

(E)-2-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2H)-ylidene)-1-(4-bromophenyl)ethanone **(3da)**. Yellow solid; yield 90%; mp 79-80 ^{o}C; IR (KBr): 3381, 3060, 1655, 1581, 1527, 1486, 1446, 1397, 1340, 1315, 1237, 1175, 1050, 1026, 1005, 948, 873, 818, 778, 736, 690; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.93 (s, 1H), 7.89 (d, *J* = 7.8 Hz, 2H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.64-7.60 (m, 4H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.52-7.45 (m, 5H), 7.44-7.39 (m, 4H), 6.61 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 190.0, 186.1, 168.0, 160.1, 140.5, 138.6, 136.6, 132.8(2), 132.8(1), 131.9, 131.7, 129.7, 129.1, 128.9, 128.8, 128.5(2), 128.4(9), 128.1, 126.8, 124.9, 113.7, 111.5, 110.3; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}BrO_4$: 537.0696; found: 537.0704.

(E)-2-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2H)-ylidene)-1-(4-nitrophenyl)ethanone **(3ea)**. Yellow solid; yield 88%; mp 80-82 ^{o}C; IR (KBr): 3414, 3062, 1658, 1597, 1525, 1488, 1447, 1392, 1343, 1228, 1053, 1020, 947, 849, 692; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 9.03 (s, 1H), 8.22 (d, *J* = 9.0 Hz, 2H), 7.93 (d, *J* = 5.4 Hz, 2H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 6.6 Hz, 2H), 7.66 (d, *J* = 6.6 Hz, 2H), 7.53-7.46 (m, 5H), 7.43-7.41 (m, 4H), 6.67 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 190.1, 185.7, 168.9, 161.2, 149.5, 142.4, 140.3, 138.5, 132.9, 132.1, 129.2, 129.1, 128.9, 128.8, 128.6, 128.4, 128.2, 124.9, 123.9, 123.8, 113.8, 111.2, 110.6; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}NO_6$: 504.1442; found: 504.1439.

(E)-2-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2H)-ylidene)-1-(thiophen-2-yl)ethanone **(3fa)**: Yellow solid; yield 93%; mp 155-156 ^{o}C; IR (KBr): 3519, 3062, 1659, 1598, 1528, 1447, 1410, 1355, 1236, 1144, 1062, 1015, 965, 941, 878, 845, 774, 689; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.91 (s, 1H), 7.89 (d, *J* = 7.8 Hz, 2H), 7.86 (d, *J* = 4.8 Hz, 1H), 7.78 (s, 1H), 7.68 (d, *J* = 7.8 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.52-7.47 (m, 4H), 7.46-7.40 (m, 5H), 7.13 (t, *J* = 4.2 Hz, 1H), 6.58 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 190.0, 179.4, 167.5, 159.3, 145.2, 140.6, 138.8, 134.7, 132.8, 132.1, 131.9, 129.1, 128.9, 128.8, 128.7, 128.6, 128.5, 128.0, 124.9, 113.8, 111.5, 110.3, 110.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{29}H_{21}O_4S$: 465.1155; found: 465.1154.

(E)-1-(4-benzoyl-2-hydroxy-2,5-diphenylfuran-3(2H)-ylidene)propan-2-one **(3ga)**: Yellow solid; yield 90%; mp 114-115 ^{o}C; IR (KBr): 3180, 1675, 1638, 1578, 1542, 1489, 1448, 1402, 1354, 1323, 1261, 1209, 1074, 1044, 956, 879, 776, 693; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 8.78 (s, 1H), 7.88 (t, *J* =7.2 Hz, 2H), 7.62-7.59 (m, 3H), 7.52-7.48 (m, 3H), 7.46-7.42 (m, 3H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.21-7.19 (m, 1H), 5.95 (s, 1H), 1.88 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 194.6, 190.0, 166.7, 156.8, 140.7, 138.9, 136.1, 132.7, 131.7,

129.0, 128.8, 128.7, 128.6, 128.5, 127.9, 124.9, 113.6, 109.8, 109.7, 30.3; HRMS (ESI): m/z $[M+Na]^+$ calcd for $C_{26}H_{20}NaO_4$: 419.1259; found: 419.1259.

4-(3,5-diphenyl-1H-pyrazol-4-yl)-3,6-diphenylpyridazine **(4a)**. Yellow solid; yield 76%; mp 271-272 ^oC; IR (KBr): 3447, 3064, 3023, 1575, 1482, 1445, 1395, 1149, 1070, 1025, 986, 959, 915, 837, 767, 693; ^1H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.65 (s, 1H), 8.16 (s, 1H), 8.13 (d, J = 7.8 Hz, 2H), 7.56-7.53 (m, 3H), 7.33 (m, 3H), 7.27-7.25 (m, 5H), 7.23 (d, J = 7.8 Hz, 1H), 7.18 (d, J = 4.2 Hz, 2H), 7.13 (t, J = 7.8 Hz, 2H), 7.07 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 159.5, 156.9, 149.8, 141.7, 136.7, 135.6, 133.0, 132.9, 130.3, 129.2, 128.9, 128.7, 128.6(1), 128.5(9), 128.5, 128.3, 127.7, 127.4, 127.3, 127.1(8), 127.1(7), 126.9, 111.9; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4$: 451.1917; found: 451.1916.

4-(3,5-diphenyl-1H-pyrazol-4-yl)-6-phenyl-3-(p-tolyl)pyridazine **(4b)**. Yellow solid; yield 70%; mp 280-281 ^oC; IR (KBr): 3066, 3022, 2913, 2865, 1581, 1486, 1443, 1398, 1180, 1151, 1068, 1023, 986, 956, 915, 824, 766, 729, 693, 609, 562, 508; ^1H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.62 (s, 1H), 8.15-8.13 (m, 3H), 7.53-7.52 (m, 3H), 7.32 (m, 3H), 7.28-7.26 (m, 5H), 7.19 (s, 2H), 7.01 (s, 2H), 6.94 (d, J = 7.8 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 159.4, 156.6, 149.6, 141.4, 137.6, 135.6, 133.8, 133.0, 132.7, 130.1, 129.1, 128.7, 128.6, 128.4, 128.3, 128.2, 127.5, 127.2, 127.1, 127.0, 126.8, 111.9, 20.8; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{32}H_{25}N_4$: 465.2074; found: 465.2072.

3-(4-bromophenyl)-4-(3,5-diphenyl-1H-pyrazol-4-yl)-6-phenylpyridazine **(4c)**. Yellow solid; yield 60%; mp 135-136 ^oC; IR (KBr): 3421, 3029, 1657, 1586, 1484, 1443, 1394, 1178, 1148, 1070, 1005, 962, 910, 830, 764, 735, 693, 508; ^1H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.66 (s, 1H), 8.12 (s, 1H), 8.07 (d, J = 6.0 Hz, 2H), 7.55-7.51 (m, 3H), 7.30-7.29 (m, 5H), 7.26-7.17 (m, 7H), 6.94 (d, J = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 158.4, 157.0, 149.7, 135.8, 135.5, 132.6, 131.6, 131.3, 130.6, 130.4, 130.3, 129.2, 128.8, 128.6, 128.5, 128.4, 128.2, 127.4, 127.1, 126.9, 125.7, 122.0, 111.4; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}BrN_4$: 529.1022; found: 529.1027.

4-(3,5-diphenyl-1H-pyrazol-4-yl)-3-(4-nitrophenyl)-6-phenylpyridazine **(4d)**. Yellow solid; yield 55%; mp 297-298 ^oC; IR (KBr): 3441, 3105, 3031, 2953, 2879, 1680, 1599, 1577, 1513, 1444, 1401, 1343, 1177, 1138, 1104, 1069, 1006, 962, 915, 854, 766, 694, 517; ^1H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.68 (s, 1H), 8.14 (s, 1H), 8.08 (d, J = 4.8 Hz, 2H), 7.96 (d, J = 8.4 Hz, 2H),

7.55-7.54 (m, 3H), 7.37-7.32 (m, 3H), 7.28-7.24 (m, 3H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.18-7.15 (m, 4H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 157.5(4), 157.4(9), 149.9, 146.8, 143.2, 142.0, 135.4, 132.8, 132.7, 130.5, 129.7, 129.2, 128.9, 128.7, 128.5, 128.4, 127.7, 127.5, 127.1, 127.0, 122.7, 111.0; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}N_5O_2$: 496.1768; found: 496.1771.

4-(3,5-diphenyl-1H-pyrazol-4-yl)-3-(naphthalen-2-yl)-6-phenylpyridazine **(4e)**. Yellow solid; yield 65%; mp >300 ^{o}C; IR (KBr): 3448, 3140, 3057, 3020, 1568, 1475, 1444, 1396, 958, 913, 862, 820, 762, 692, 617, 516, 477; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.60 (s, 1H), 8.24 (s, 1H), 8.17 (d, *J* = 6.0 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.56-7.50 (m, 5H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 6.0 Hz, 1H), 7.22-7.21 (m, 8H), 7.13 (d, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 159.4, 156.8, 149.8, 141.7, 135.6, 134.3, 133.0, 132.3(3), 132.3(1), 130.3, 129.2, 128.8, 128.6, 128.6(3), 128.5(6), 128.5, 128.4(3), 128.3(7), 128.2, 127.6, 127.4, 127.3, 127.2(0), 127.1(9), 126.9, 126.7, 126.2, 125.7, 111.8; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{35}H_{25}N_4$: 501.2074; found: 501.2076.

4-(3,5-diphenyl-1H-pyrazol-4-yl)-3-phenyl-6-(p-tolyl)pyridazine **(4f)**. Yellow solid; yield 70%; mp >300 ^{o}C; IR (KBr): 3441, 3061, 3022, 2867, 1570, 1489, 1445, 1397, 1181, 1150, 1066, 1020, 954, 914, 872, 838, 812, 781, 756, 725, 694, 664, 512; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.60 (s, 1H), 8.25 (d, *J* = 7.2 Hz, 1H), 8.12 (s, 1H), 8.03 (d, *J* = 7.8 Hz, 2H), 7.60-7.55 (m, 1H), 7.34 (d, *J* = 7.8 Hz, 2H), 7.32 (s, 2H), 7.26 (m, 4H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.17 (s, 2H), 7.12 (t, *J* = 7.8 Hz, 2H), 7.06 (d, *J* = 7.2 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ (ppm) 159.2, 156.7, 149.6, 141.5, 140.0, 136.7, 135.9, 133.0, 132.8, 132.7, 130.1, 129.8, 129.1, 128.8, 128.6, 128.5, 128.4, 128.1, 127.6, 127.2(4), 127.1(7), 126.7, 111.8, 21.0; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{32}H_{25}N_4$: 465.2074; found: 465.2079.

4-(3,5-diphenyl-1H-pyrazol-4-yl)-6-(4-methoxyphenyl)-3-phenylpyridazine **(4g)**. Yellow solid; yield 73%; mp 284-285 ^{o}C; IR (KBr): 3062, 3020, 2043, 1956, 1891, 1764, 1607, 1516, 1490, 1446, 1399, 1303, 1255, 1175, 1072, 1021, 956, 915, 833, 782, 756, 695, 663, 590, 519; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.62 (s, 1H), 8.11 (s, 1H), 8.10 (s, 2H), 7.32 (m, 3H), 7.27 (m, 4H), 7.23-7.19 (m, 3H), 7.13 (d, *J* = 7.2 Hz, 2H), 7.10 (d, *J* = 5.4 Hz, 2H), 7.09-7.06 (m, 3H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 161.0, 158.8, 156.4, 149.7, 149.6, 141.6, 141.4, 136.8, 133.0, 132.6, 128.7, 128.6, 128.4, 128.3(4), 128.2(9), 128.0, 127.9, 127.5, 127.2, 126.2, 114.5, 111.9, 55.3; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{32}H_{25}N_4O$: 481.2023; found: 481.2026.

6-(4-chlorophenyl)-4-(3,5-diphenyl-1H-pyrazol-4-yl)-3-phenylpyridazine **(4h)**. Yellow solid; yield 71%; mp 135-136 ^{o}C; IR (KBr): 3306, 3218, 3017, 2874, 1661, 1615, 1559, 1485, 1398, 1347, 1116, 1094, 988, 882, 839, 803, 729, 675, 533, 445; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.60 (s, 1H), 8.22 (s, 1H), 8.17 (d, J = 8.4 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.32 (m, 3H), 7.25-7.22 (m, 6H), 7.17 (s, 2H), 7.12 (t, J = 7.8 Hz, 2H), 7.05 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 159.5, 157.2, 155.7, 149.6, 141.5, 136.5, 135.1, 134.4, 132.9, 129.5, 129.1, 128.8, 128.6, 128.3, 128.2, 127.6, 127.2, 127.0, 111.6; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{22}ClN_4$: 485.1528; found: 485.1532.

4-(3,5-diphenyl-1H-pyrazol-4-yl)-6-(naphthalen-2-yl)-3-phenylpyridazine **(4i)**. Yellow solid; yield 58%; mp 263-264 ^{o}C; IR (KBr): 3024, 2867, 1948, 1571, 1493, 1443, 1396, 1271, 1238, 1179, 1156, 1129, 1070, 1030, 997, 955, 912, 858, 802, 754, 731, 693, 569, 516, 474; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.68 (s, 1H), 8.75 (s, 1H), 8.37 (d, J = 10.2 Hz, 2H), 8.10 (d, J = 8.4 Hz, 1H), 8.05-8.04 (m, 1H), 8.01-7.99 (m, 1H), 7.62-7.58 (m, 2H), 7.34 (m, 5H), 7.28 (m, 3H), 7.26-7.25 (m, 3H), 7.18-7.34 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 159.4, 156.8, 149.6, 141.7, 141.5, 136.7, 133.6, 133.0, 132.9, 132.8, 128.8, 128.7(2), 128.6(8), 128.6, 128.4(3), 128.4(0), 128.3(6), 128.2, 127.6(4), 127.5(8), 127.2(9), 127.2(7), 127.2(3), 127.1(5), 126.8(0), 126.7(9), 126.7, 124.0, 111.8; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{35}H_{25}N_4$: 501.2074; found: 501.2073.

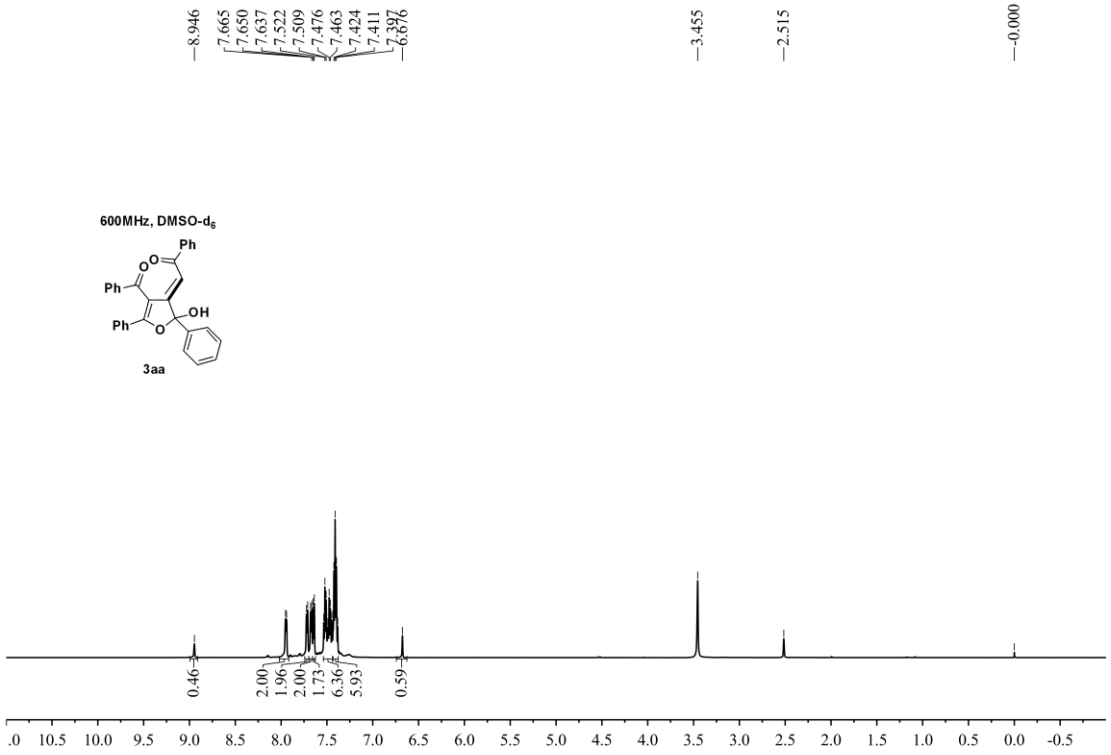
6-(3,4-dichlorophenyl)-4-(3,5-diphenyl-1H-pyrazol-4-yl)-3-phenylpyridazine **(4j)**. Yellow solid; yield 67%; mp >300 ^{o}C; IR (KBr): 3139, 3092, 3024, 2873, 1949, 1886, 1681, 1569, 1490, 1443, 1396, 1268, 1135, 1066, 1028, 994, 955, 910, 855, 813, 772, 694, 545, 513, 441; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.59 (s, 1H), 8.41 (s, 1H), 8.34 (s, 1H), 8.16 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.32 (m, 3H), 7.24-7.22 (m, 6H), 7.14-7.11 (m, 4H), 7.03 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 159.8, 154.7, 149.6, 141.6, 136.4, 136.1, 133.1, 133.0, 132.0, 131.2, 128.6, 128.5, 128.4, 128.3(4), 128.2(6), 127.6, 127.5, 127.4, 127.1, 126.9, 111.5; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{21}Cl_2N_4$: 519.1138 ; found: 519.1139.

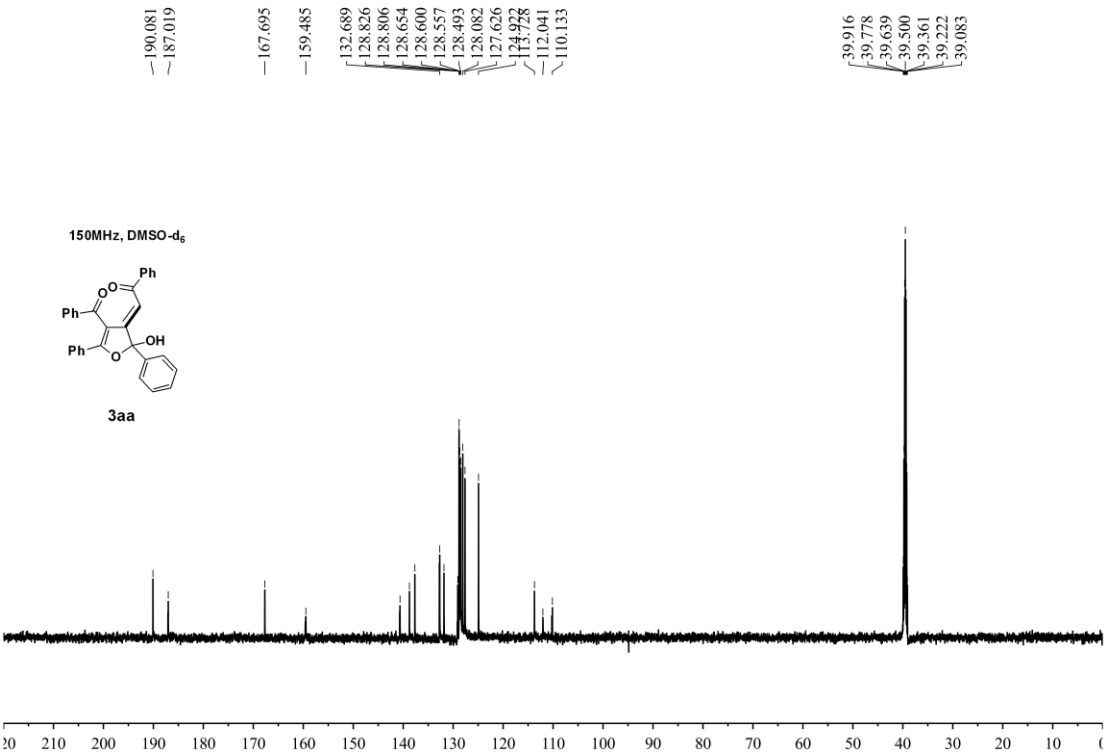
6-(benzofuran-2-yl)-4-(3,5-diphenyl-1H-pyrazol-4-yl)-3-phenylpyridazine **(4k)**. Yellow solid; yield 72%; mp 294-295 ^{o}C; IR (KBr): 3675, 3107, 3028, 2872, 1947, 1886, 1742, 1696, 1659, 1652, 1600, 1567, 1497, 1445, 1398, 1340, 1311, 1256, 1179, 1147, 1065, 1031, 999, 956, 914, 834, 734, 691, 619, 516, 417; ^{1}H NMR (600 MHz, DMSO-d_6): δ (ppm) 13.62 (s, 1H), 8.10 (s, 1H),

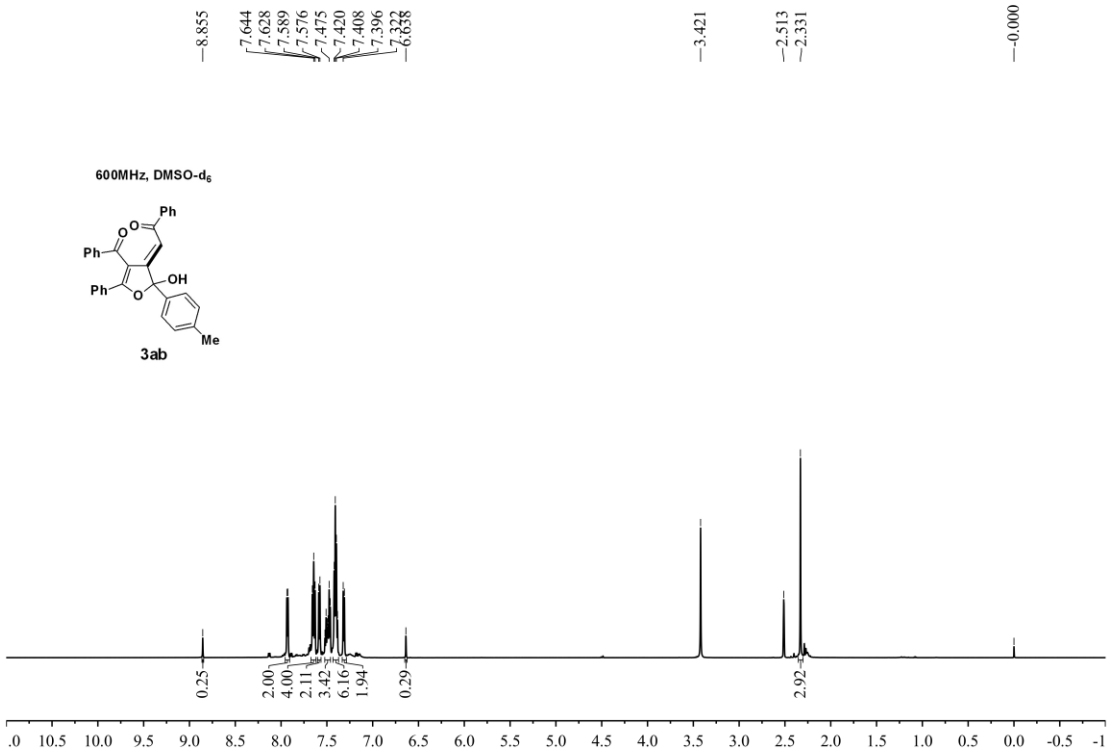
7.89 (s, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.42 (t, J = 7.8 Hz, 1H), 7.36-7.32 (m, 4H), 7.25 (m, 6H), 7.16-7.12 (m, 4H), 7.05 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 159.7, 155.0, 151.8, 150.1, 149.7, 141.8, 136.5, 132.9, 128.8(3), 128.7(7), 128.7, 128.5(3), 128.4(6), 128.4(2), 128.3(6), 128.1, 127.6, 127.2, 126.2, 125.9, 123.8(1), 123.7(7), 122.3(1), 122.2(7), 111.7, 111.2, 107.0; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{33}H_{23}N_4O$: 491.1866; found: 491.1866.

6. Spectral copies of ^{1}H NMR, and ^{13}C NMR.

(1) Spectral copies of 1,4-Enediones



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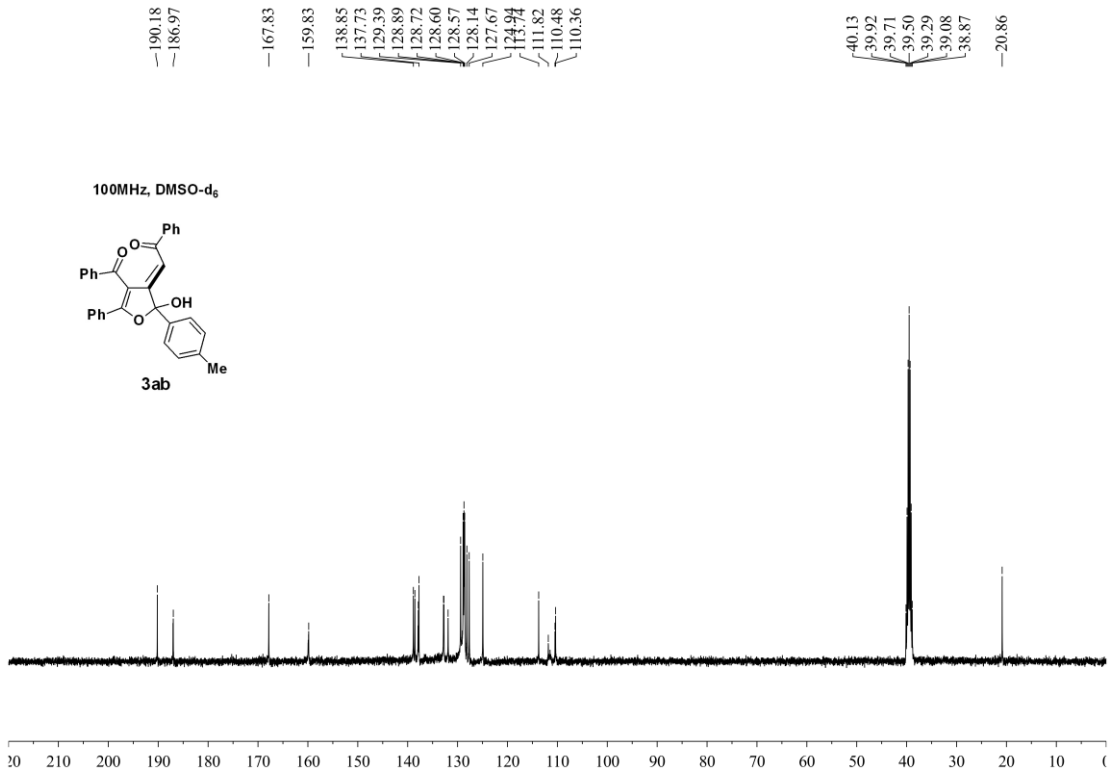
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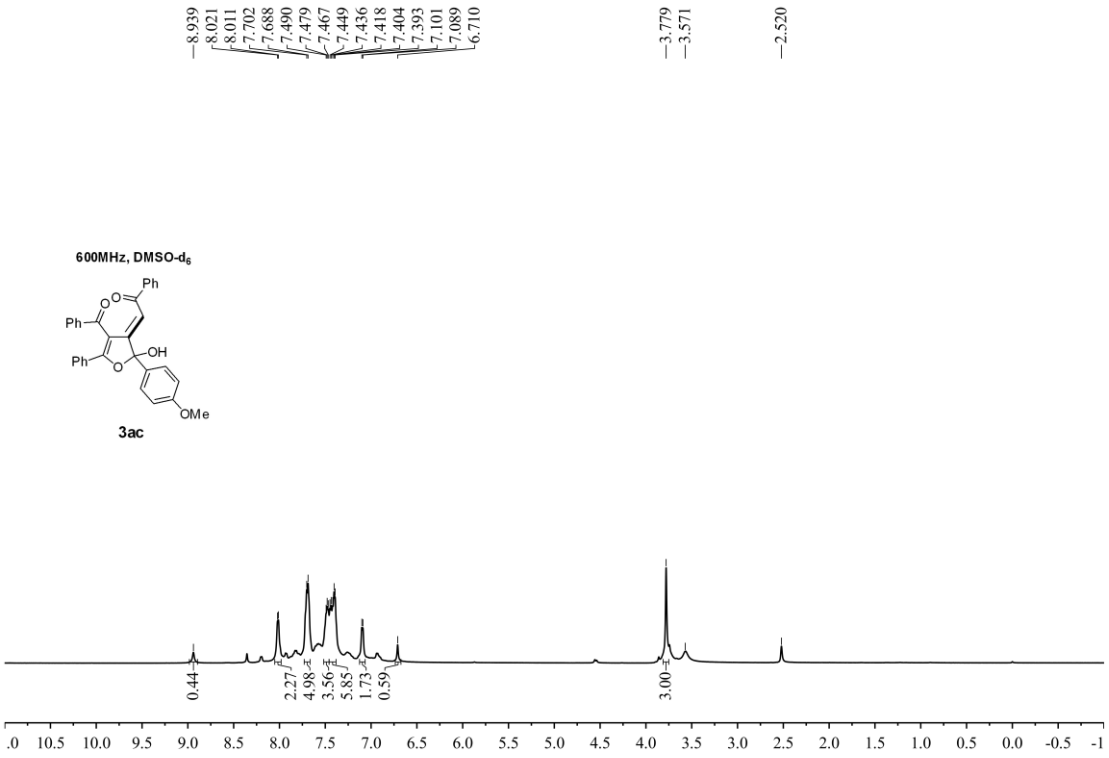
100MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
Me
3ab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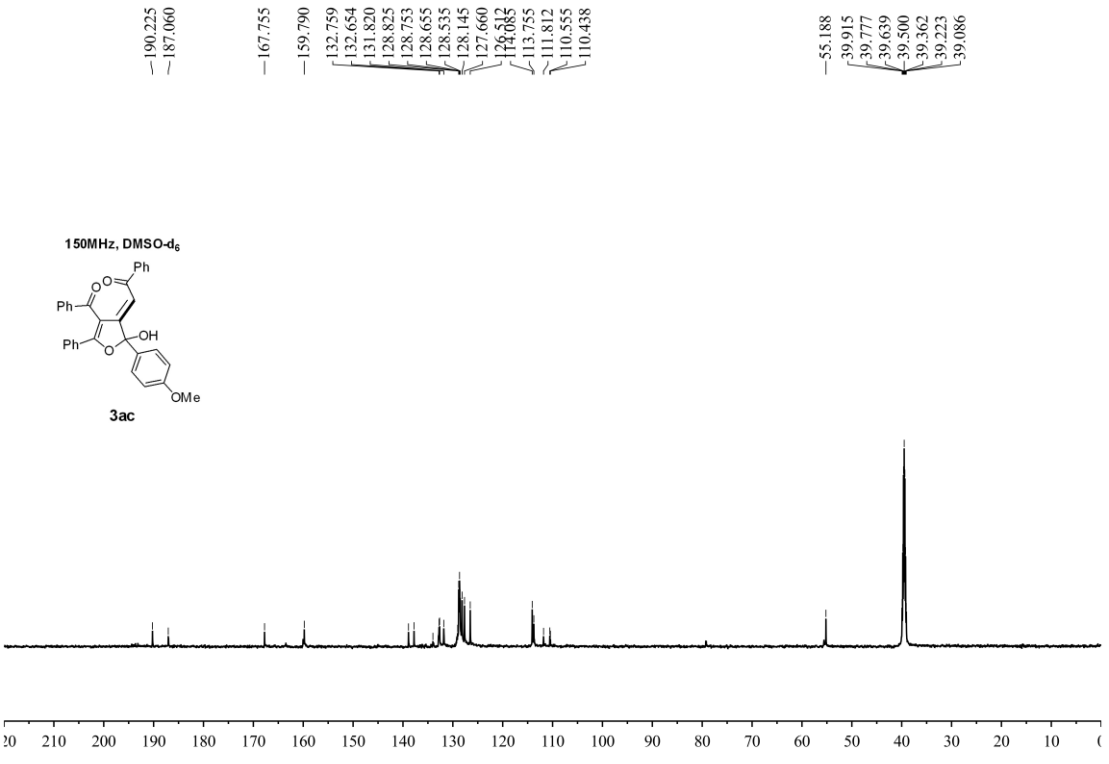
8.021
8.011
7.702
7.688
7.490
7.479
7.467
7.449
7.436
7.418
7.404
7.393
7.101
7.089
6.710
3.779
3.571
2.520
600MHz, DMSO-d6
Ph
O
Ph
O
Ph
OH
O
OMe
3ac
0.44
2.27
4.98
3.56
5.85
1.73
0.59
3.00
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1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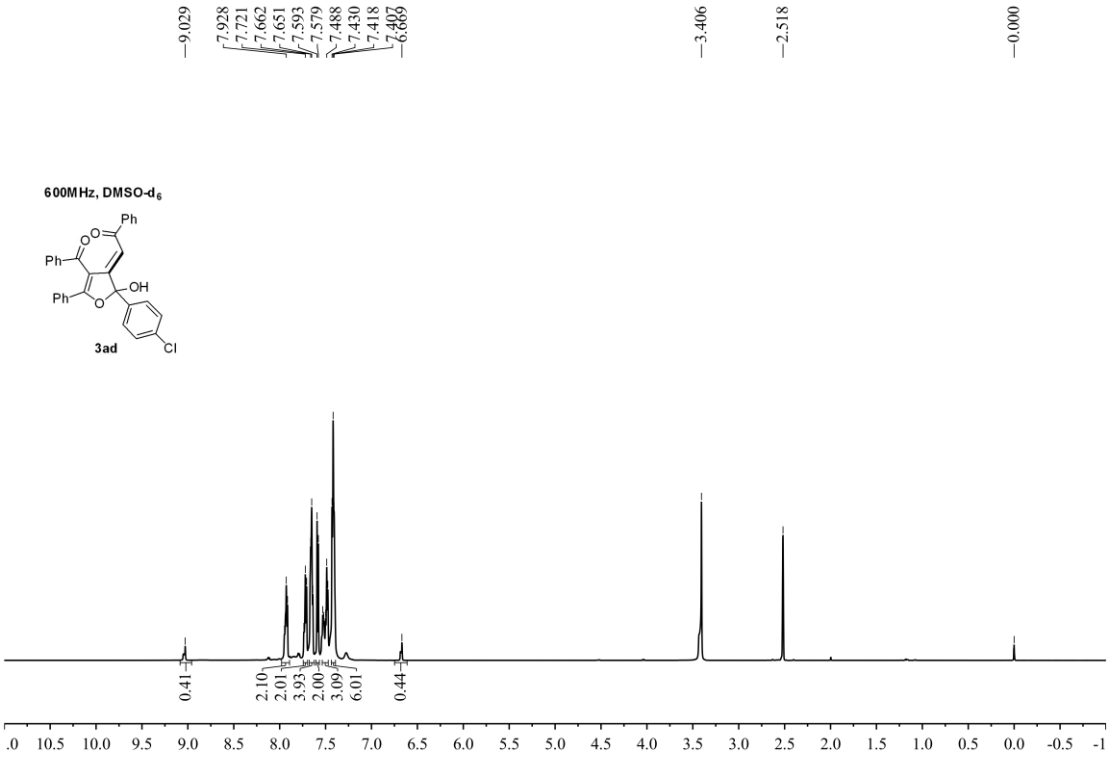
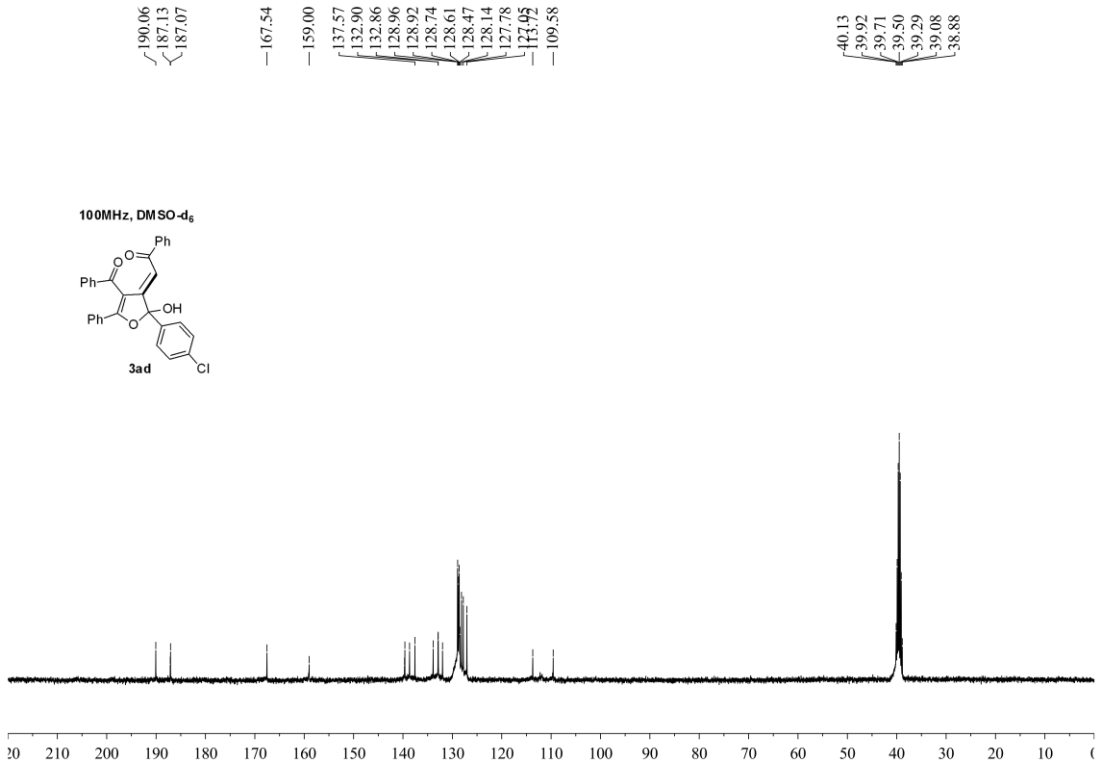
187.060
167.755
159.790
132.759
132.654
131.820
128.825
128.753
128.655
128.535
128.145
127.660
126.612
114.085
113.755
111.812
110.555
110.438
55.188
39.915
39.777
39.639
39.500
39.362
39.223
39.086
150MHz, DMSO-d6
Ph
O
Ph
O
Ph
OH
O
OMe
3ac
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


9.029
7.928
7.721
7.662
7.651
7.593
7.579
7.488
7.430
7.418
7.407
6.669
3.406
2.518
0.000
600MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
Cl
3ad
0.41
2.10
2.01
3.93
2.00
3.09
6.01
0.44
.0 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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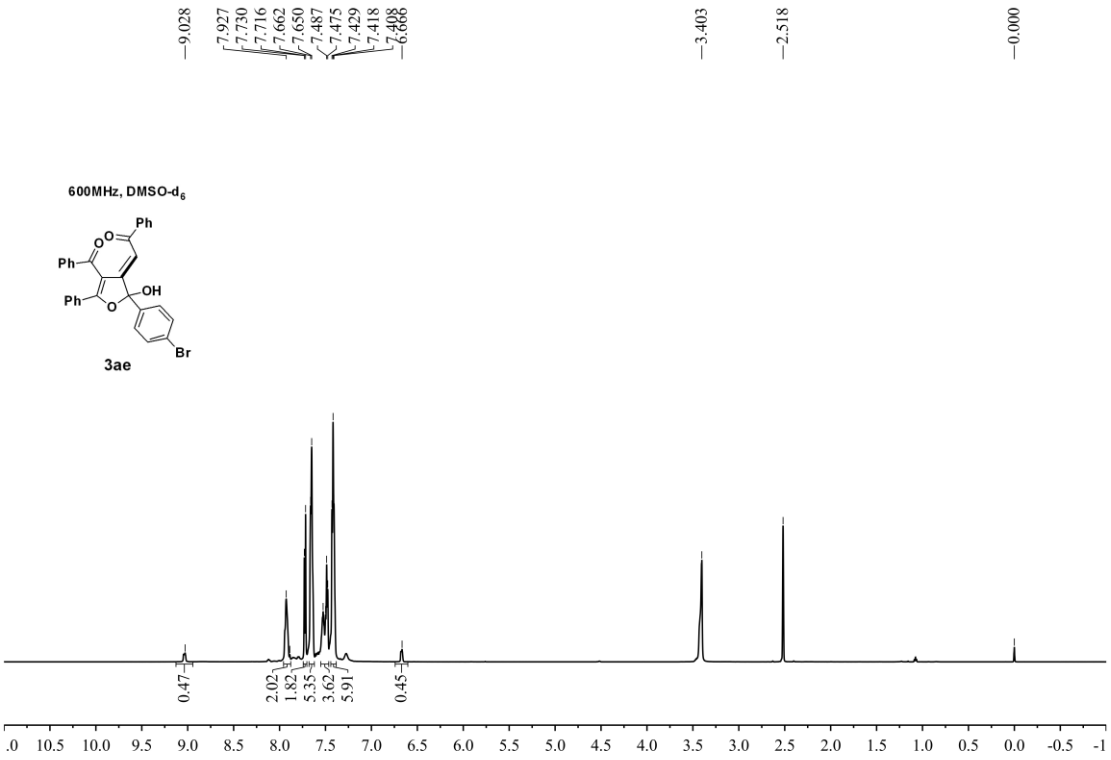
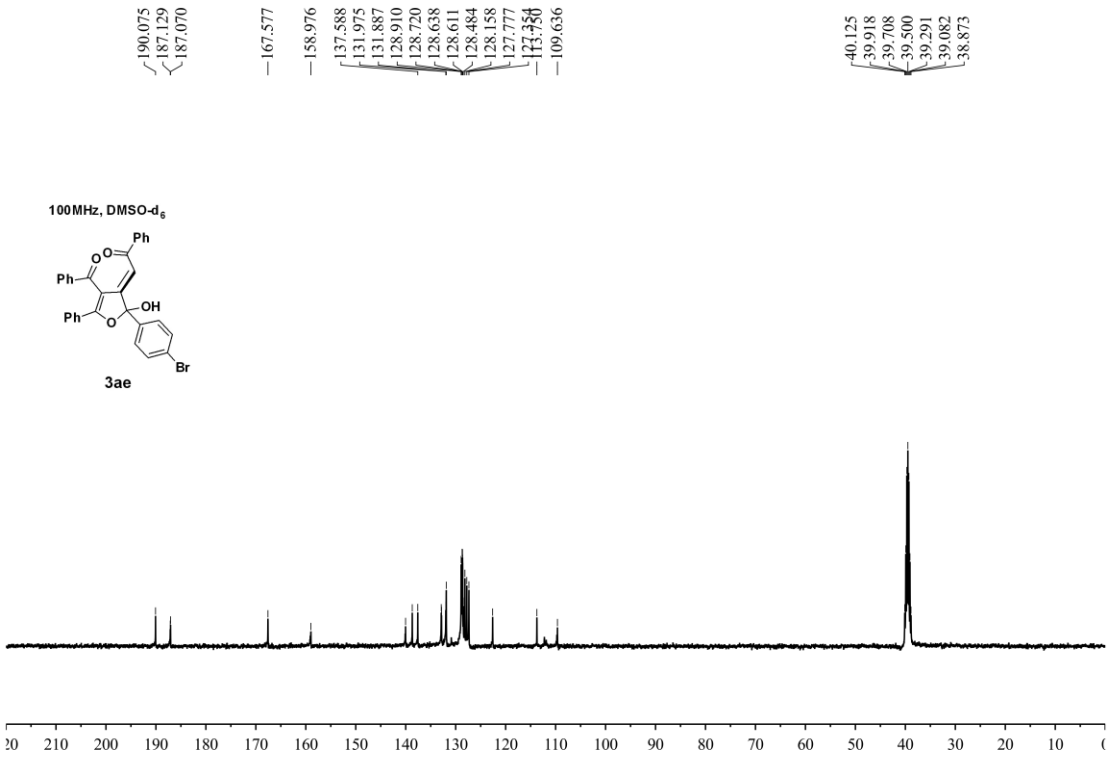
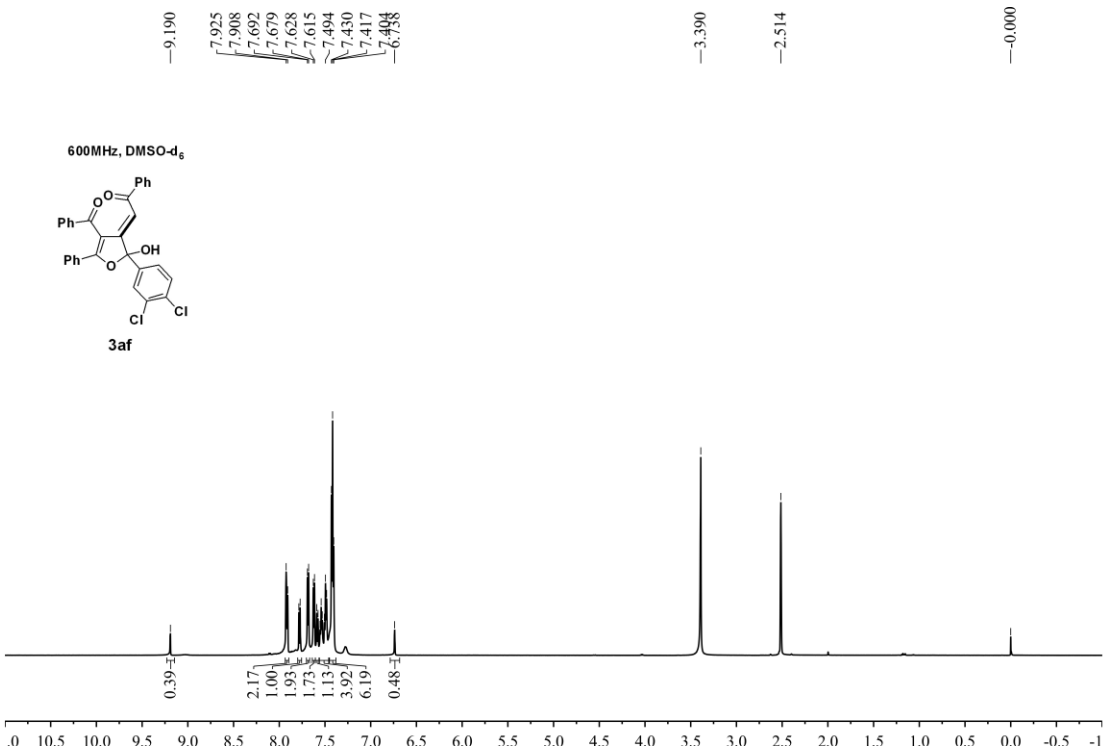
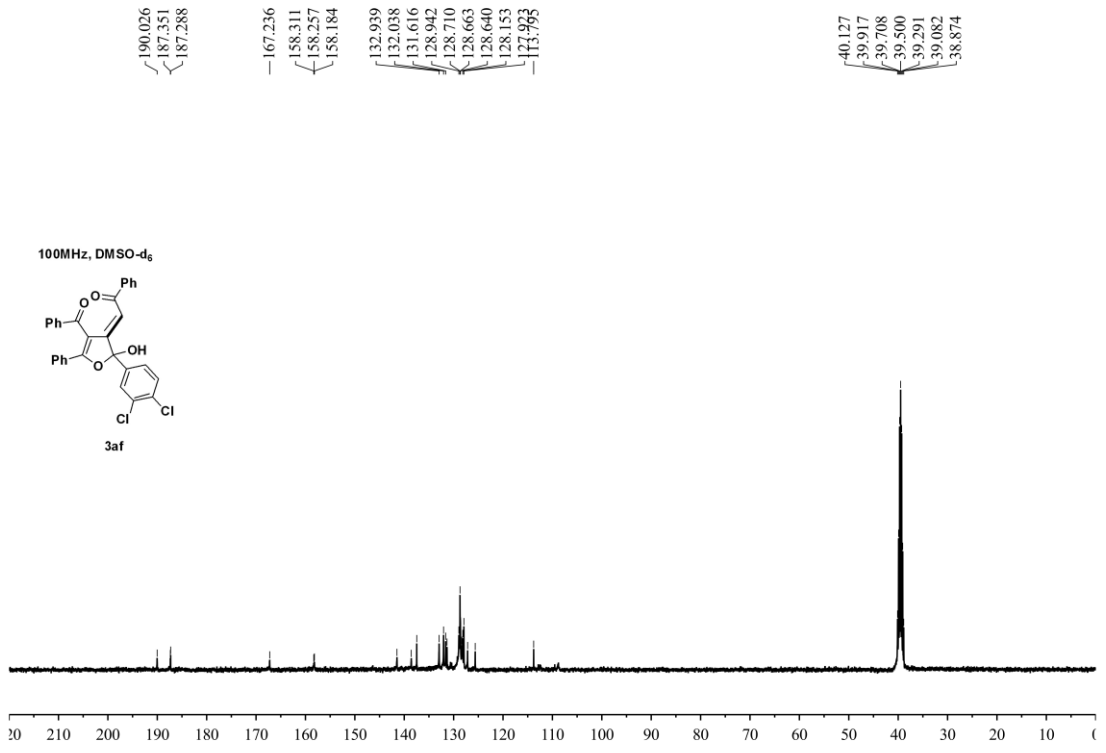
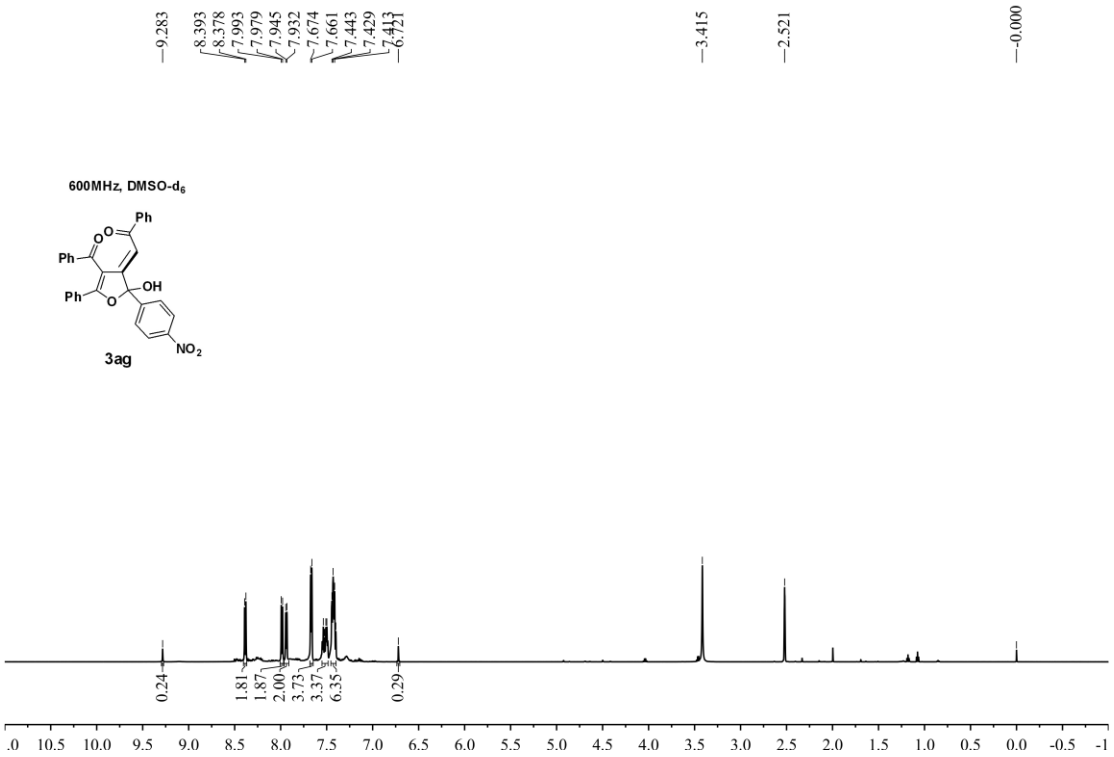
187.13
187.07
167.54
159.00
137.57
132.90
132.86
128.96
128.92
128.74
128.61
128.47
128.14
127.78
109.58
40.13
39.92
39.71
39.50
39.29
39.08
38.88
100MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
Cl
3ad
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

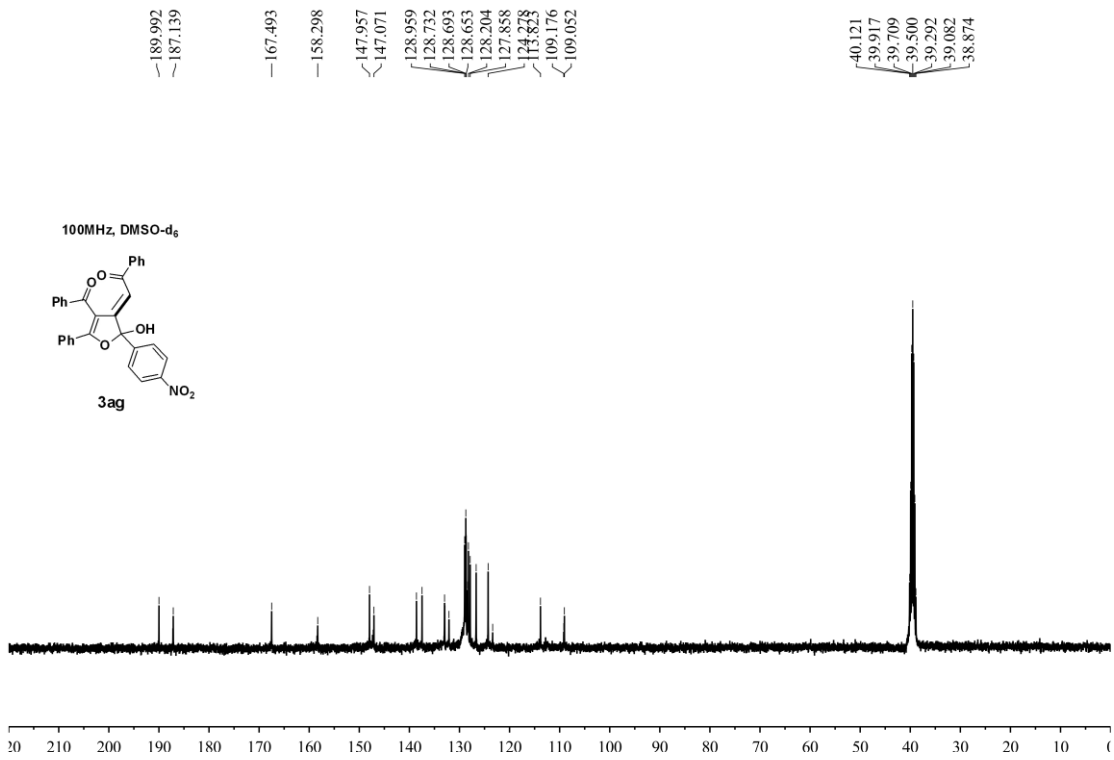

9.028
7.927
7.730
7.716
7.662
7.650
7.487
7.475
7.429
7.418
7.408
6.666
3.403
2.518
0.000
600MHz, DMSO-d6
Ph
O
Ph
Ph
O
OH
Br
3ae
0.47
2.02
1.82
5.35
3.62
5.91
0.45
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


190.075
187.129
187.070
167.577
158.976
137.588
131.975
131.887
128.910
128.720
128.638
128.611
128.484
128.158
127.777
115.750
109.636
40.125
39.918
39.708
39.500
39.291
39.082
38.873
100MHz, DMSO-d6
Ph
O
Ph
Ph
O
OH
Br
3ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

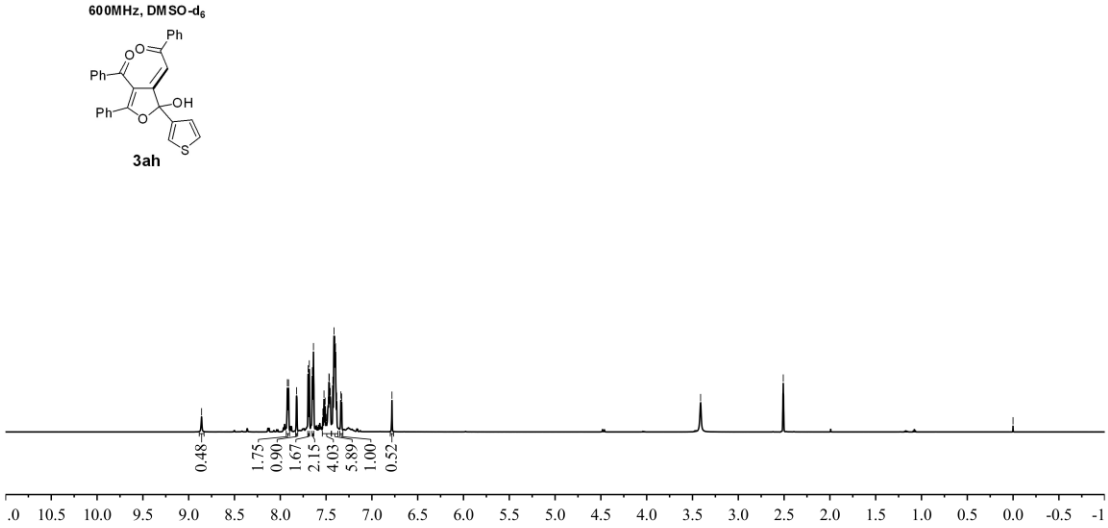

9.190
7.925
7.908
7.692
7.679
7.628
7.615
7.494
7.430
7.417
7.404
6.938
3.390
2.514
0.000
600MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
Cl
Cl
3af
0.39
2.17
1.00
1.93
1.73
1.13
3.92
6.19
0.48

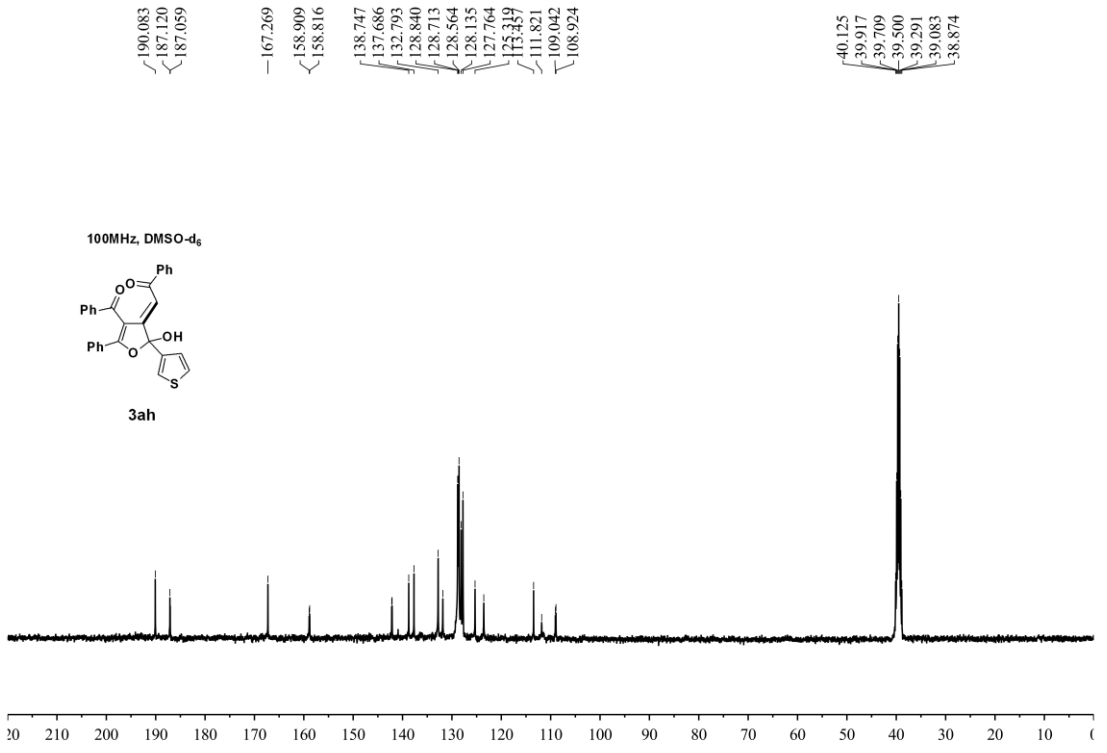

190.026
187.351
187.288
167.236
158.311
158.257
158.184
132.939
132.038
131.616
128.942
128.710
128.663
128.640
128.153
127.923
113.795
40.127
39.917
39.708
39.500
39.291
39.082
38.874
100MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
Cl
Cl
3af

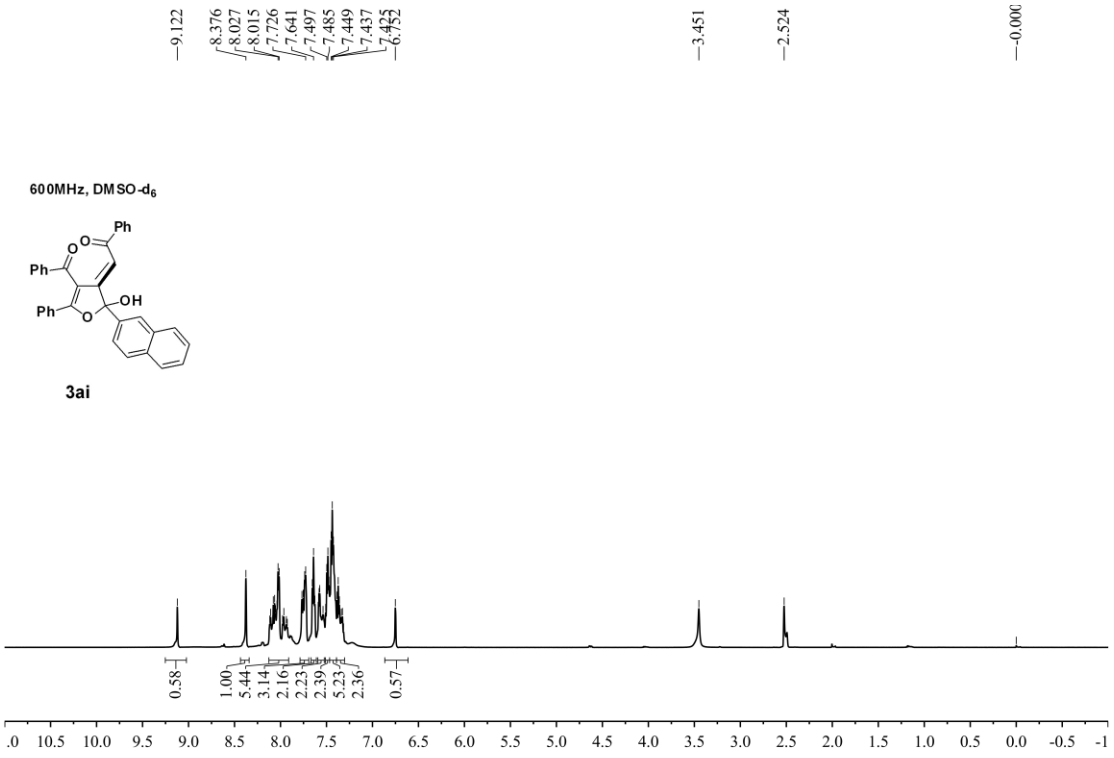

9.283
8.393
8.378
7.993
7.979
7.945
7.932
7.674
7.661
7.443
7.429
6.721
3.415
2.521
0.000
600MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
NO2
3ag
0.24
1.81
1.87
2.00
3.73
3.37
6.35
0.29
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

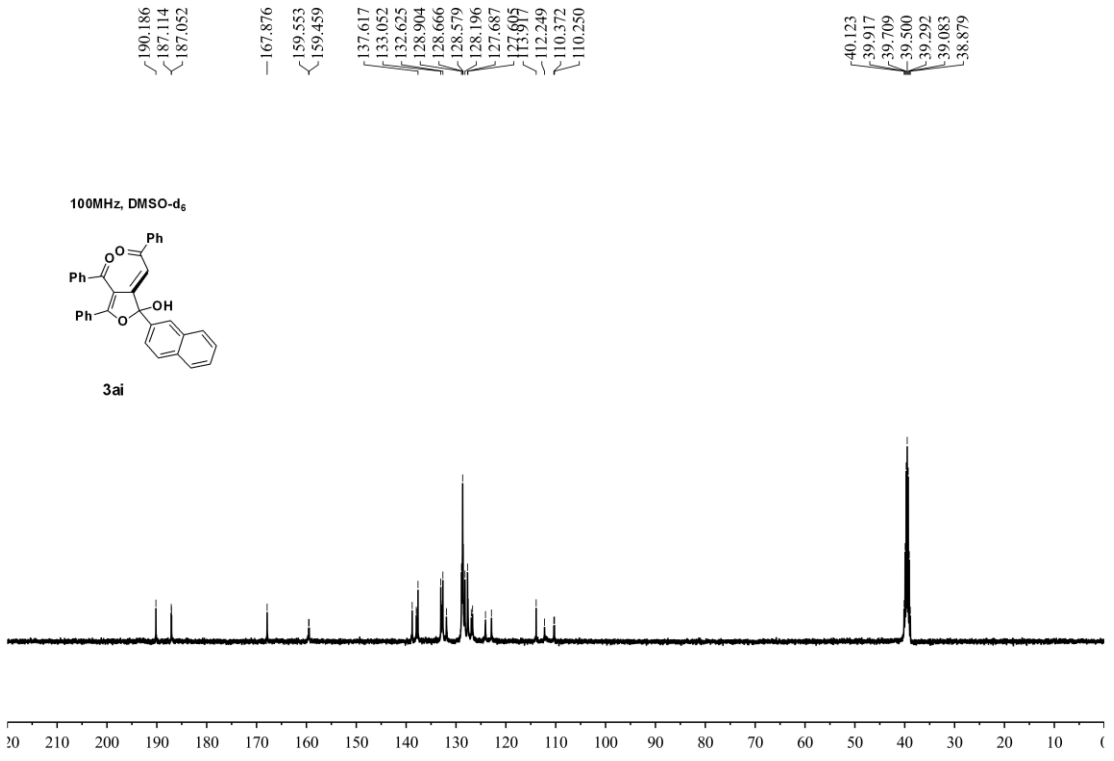

189.992
187.139
167.493
158.298
147.957
147.071
128.959
128.732
128.693
128.653
128.204
127.858
124.278
113.823
109.176
109.052
40.121
39.917
39.709
39.500
39.292
39.082
38.874
100MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
NO2
3ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

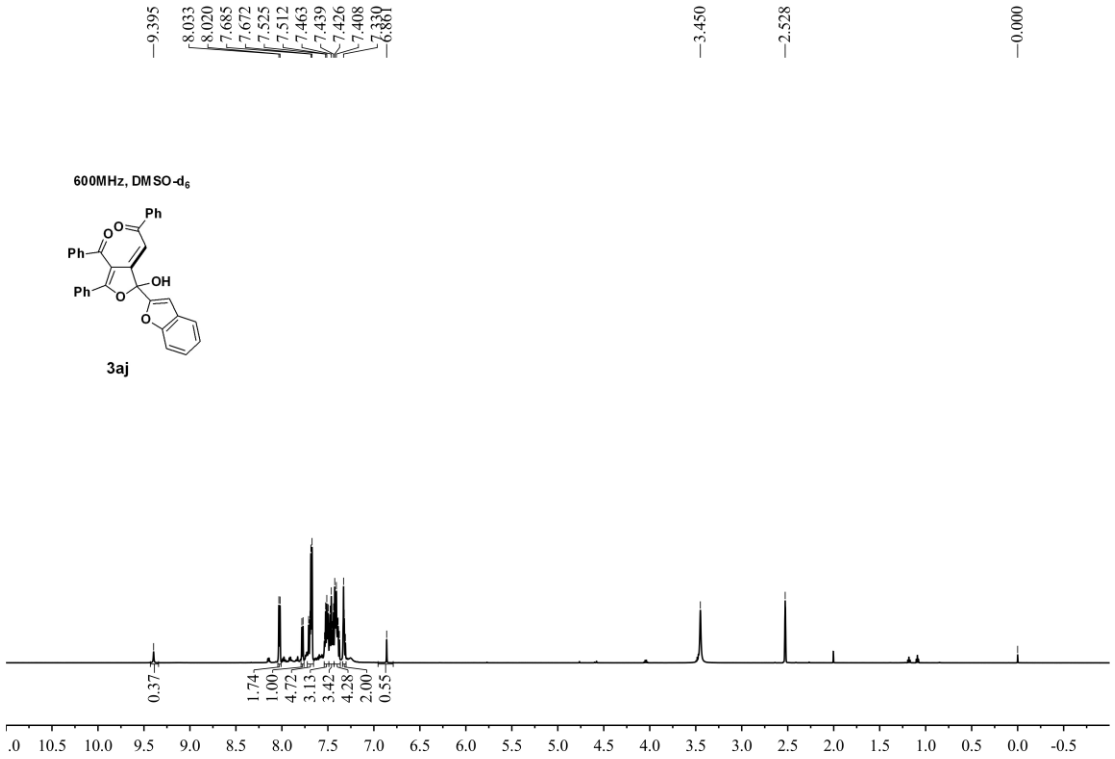

8.859
7.696
7.683
7.650
7.647
7.638
7.469
7.413
7.404
7.397
6.781
3.411
2.509
0.001

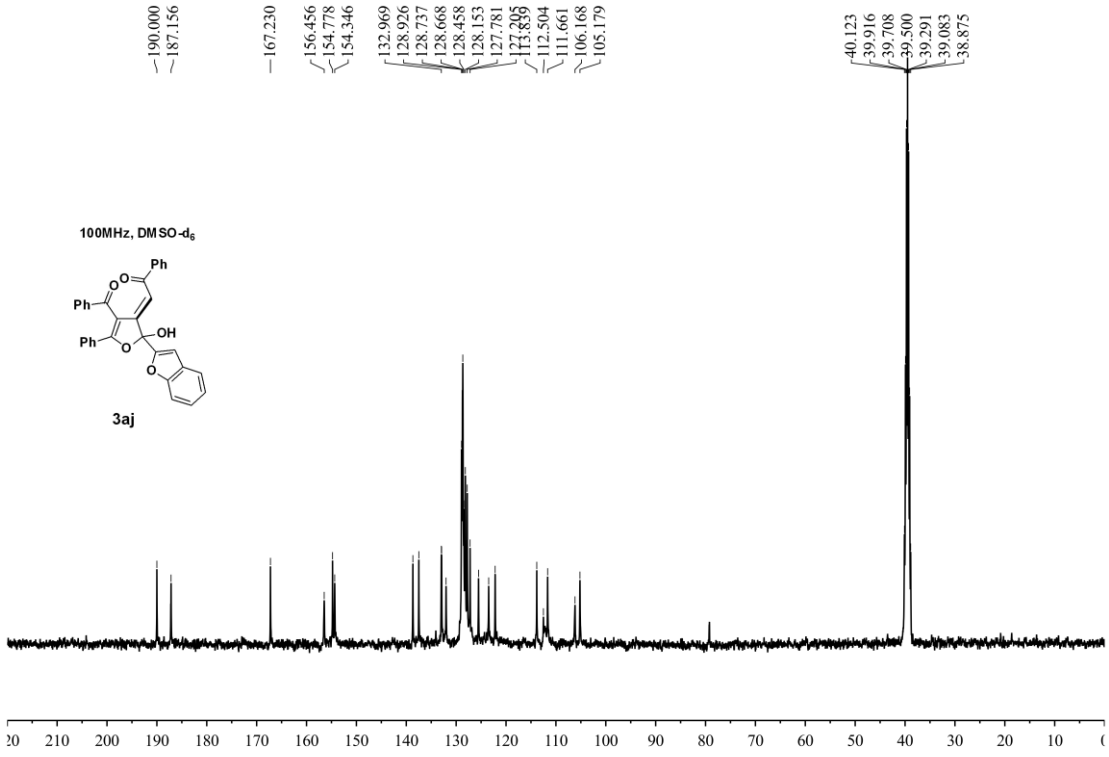

600MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
S
3ah
0.48
1.75
0.90
1.67
2.15
4.03
5.89
1.00
0.52
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1

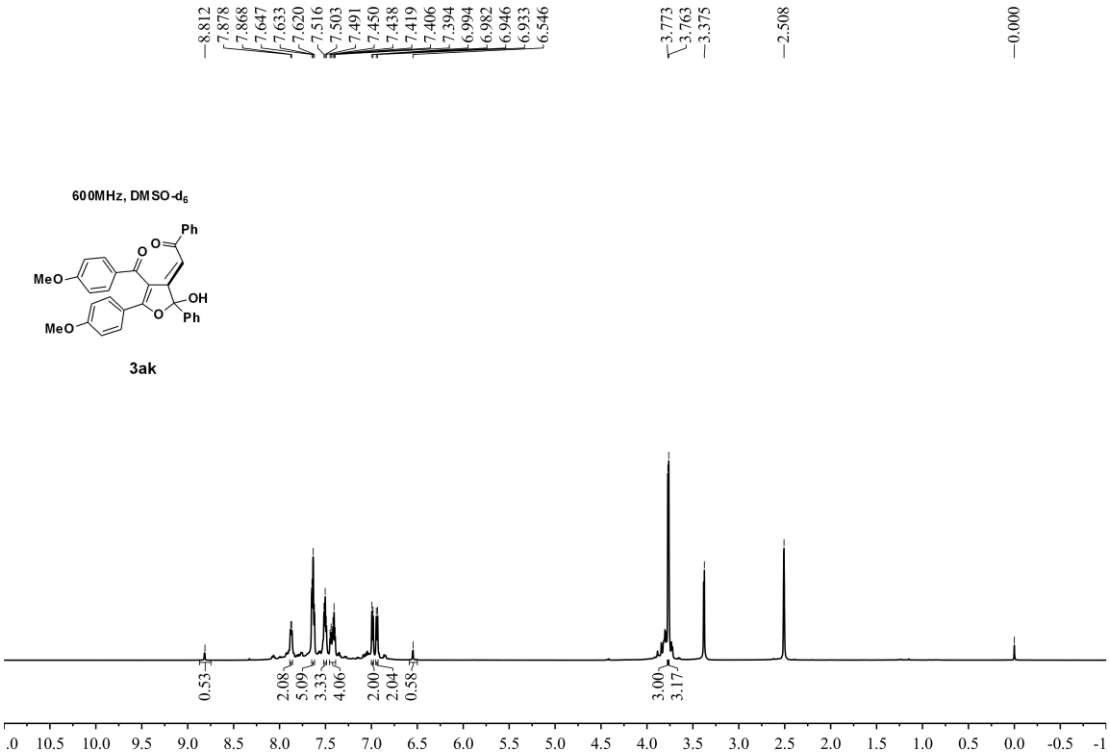

190.083
187.120
187.059
167.269
158.909
158.816
138.747
137.686
132.793
128.840
128.713
128.564
128.135
127.764
125.319
113.457
111.821
109.042
108.924
40.125
39.917
39.709
39.500
39.291
39.083
38.874
100MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
S
3ah
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

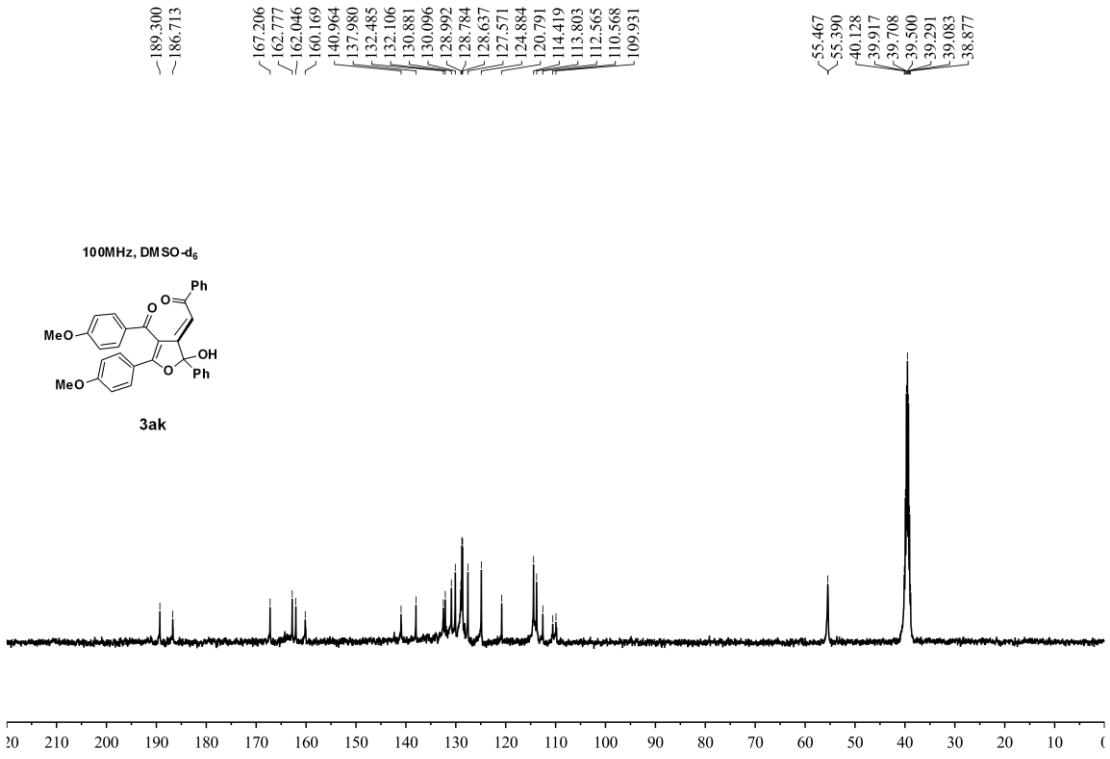

9.122
8.376
8.027
8.015
7.726
7.641
7.497
7.485
7.449
7.437
7.425
6.752
3.451
2.524
0.000
600MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
3ai
0.58
1.00
5.44
3.14
2.16
2.23
2.39
5.23
2.36
0.57
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

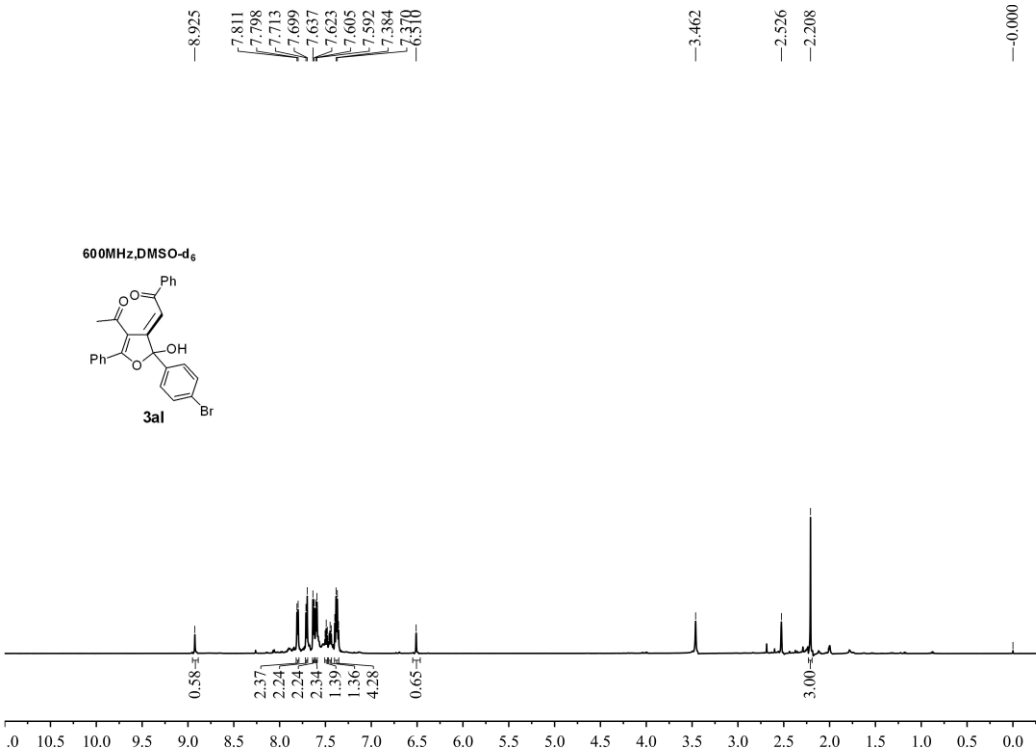

190.186
187.114
187.052
167.876
159.553
159.459
137.617
133.052
132.625
128.904
128.666
128.579
128.196
127.687
112.249
110.372
110.250
40.123
39.917
39.709
39.500
39.292
39.083
38.879
100MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
3ai
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

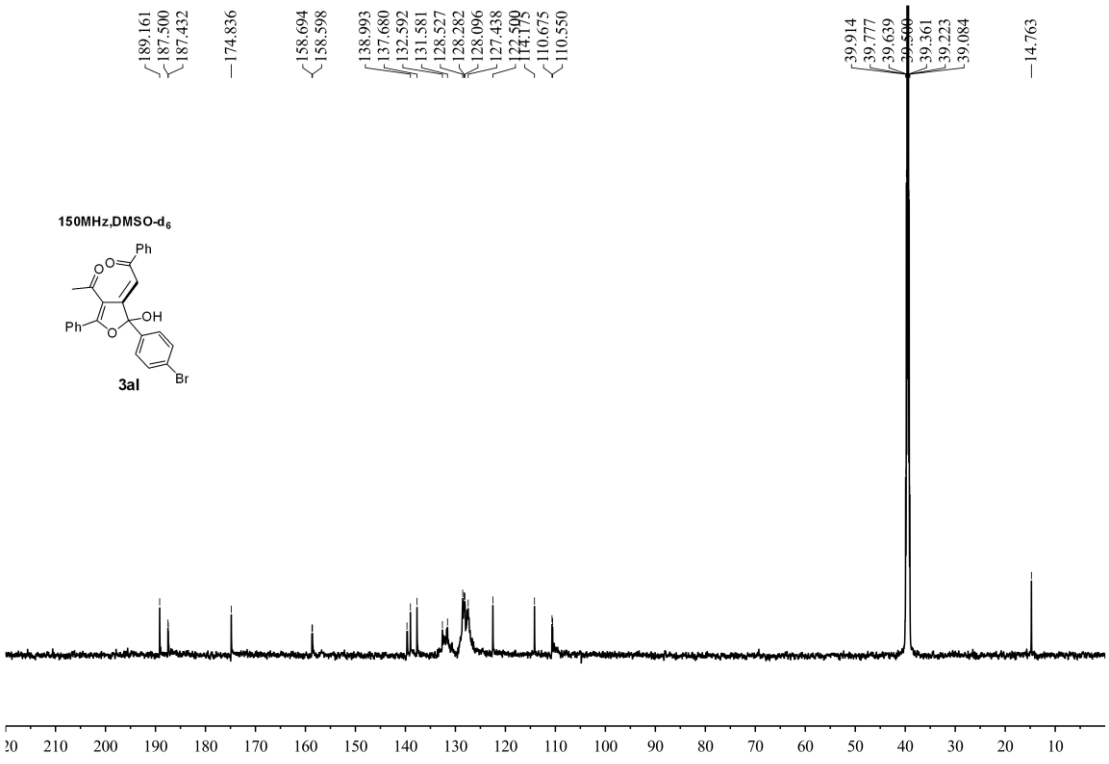

9.395
8.033
8.020
7.685
7.672
7.525
7.512
7.463
7.439
7.426
7.408
7.330
6.861
3.450
2.528
0.000
600MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
O
3aj
0.37
1.74
1.00
4.72
3.13
3.42
4.28
2.00
0.55
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


190.000
187.156
167.230
156.456
154.778
154.346
132.969
128.926
128.737
128.668
128.458
128.153
127.781
112.504
111.661
106.168
105.179
40.123
39.916
39.708
39.500
39.291
39.083
38.875
100MHz, DMSO-d6
Ph
O
Ph
OH
Ph
O
O
3aj
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

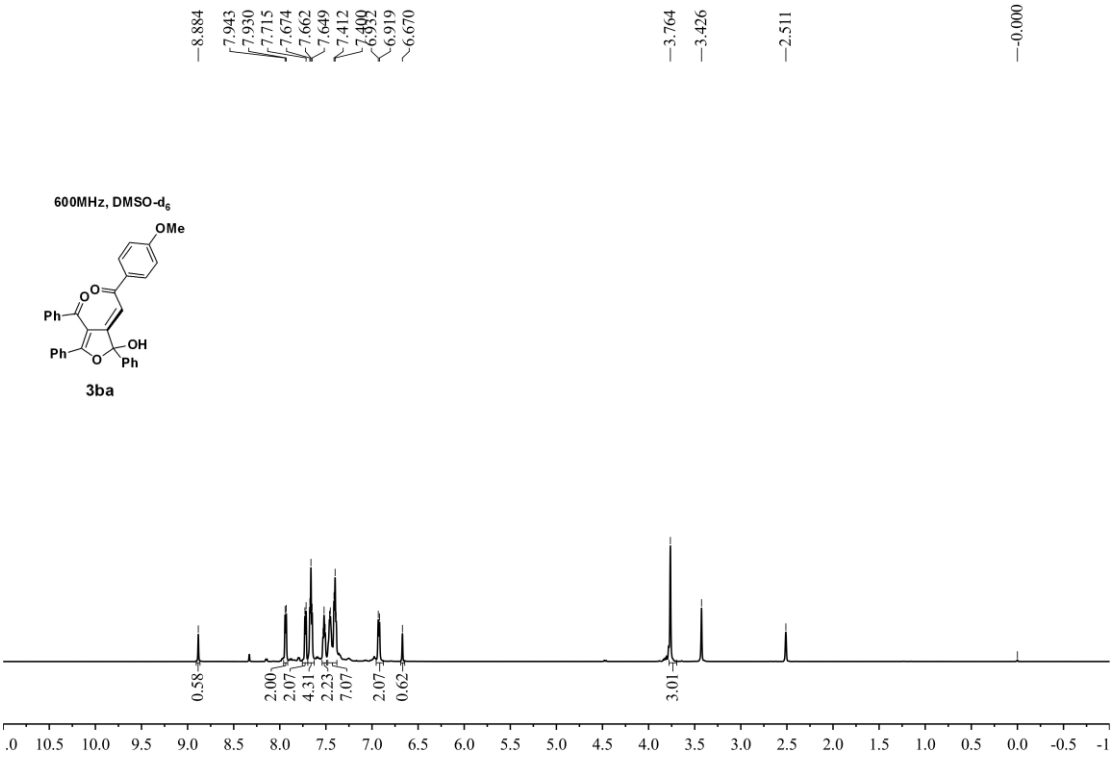

8.812
7.878
7.868
7.647
7.633
7.620
7.516
7.503
7.491
7.450
7.438
7.419
7.406
7.394
6.994
6.982
6.946
6.933
6.546
3.773
3.763
3.375
2.508
0.000
600MHz, DMSO-d6
Ph
O
MeO
OH
Ph
O
MeO
3ak
0.53
2.08
5.09
3.33
4.06
2.00
2.04
0.58
3.00
3.17
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1

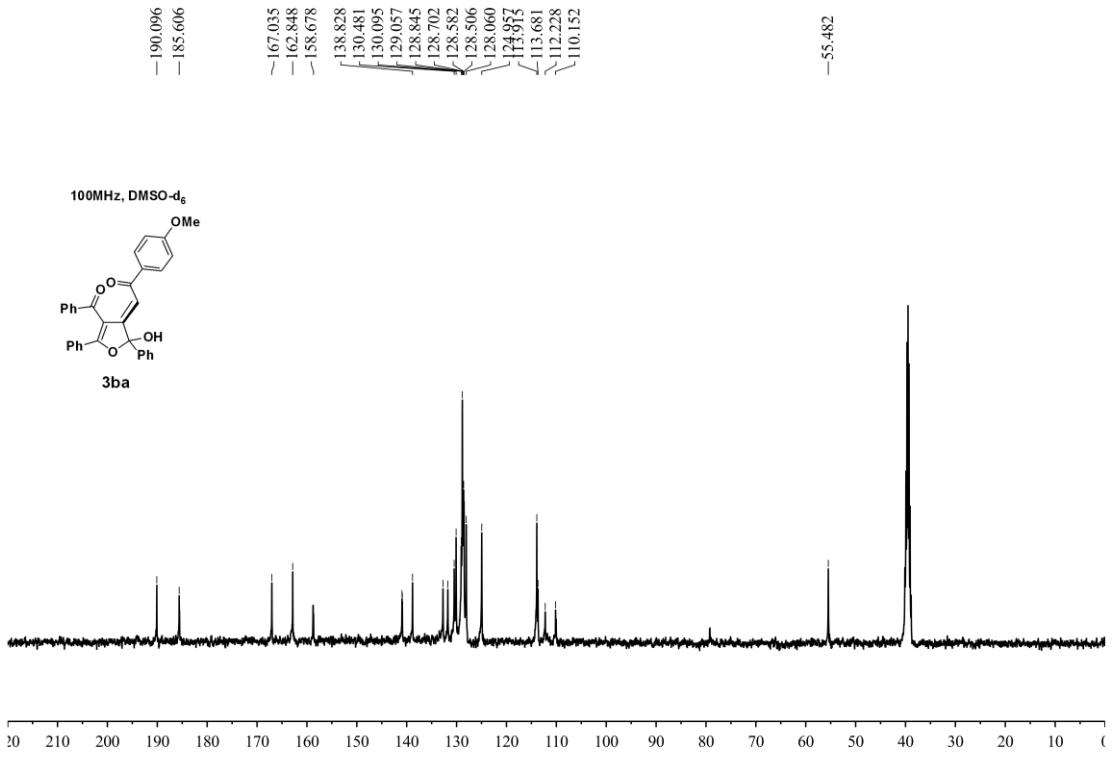

189.300
186.713
167.206
162.777
162.046
160.169
140.964
137.980
132.485
132.106
130.881
130.096
128.992
128.784
128.637
127.571
124.884
120.791
114.419
113.803
112.565
110.568
109.931
55.467
55.390
40.128
39.917
39.708
39.500
39.291
39.083
38.877
100MHz, DMSO-d6
Ph
O
MeO
OH
Ph
O
MeO
3ak
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

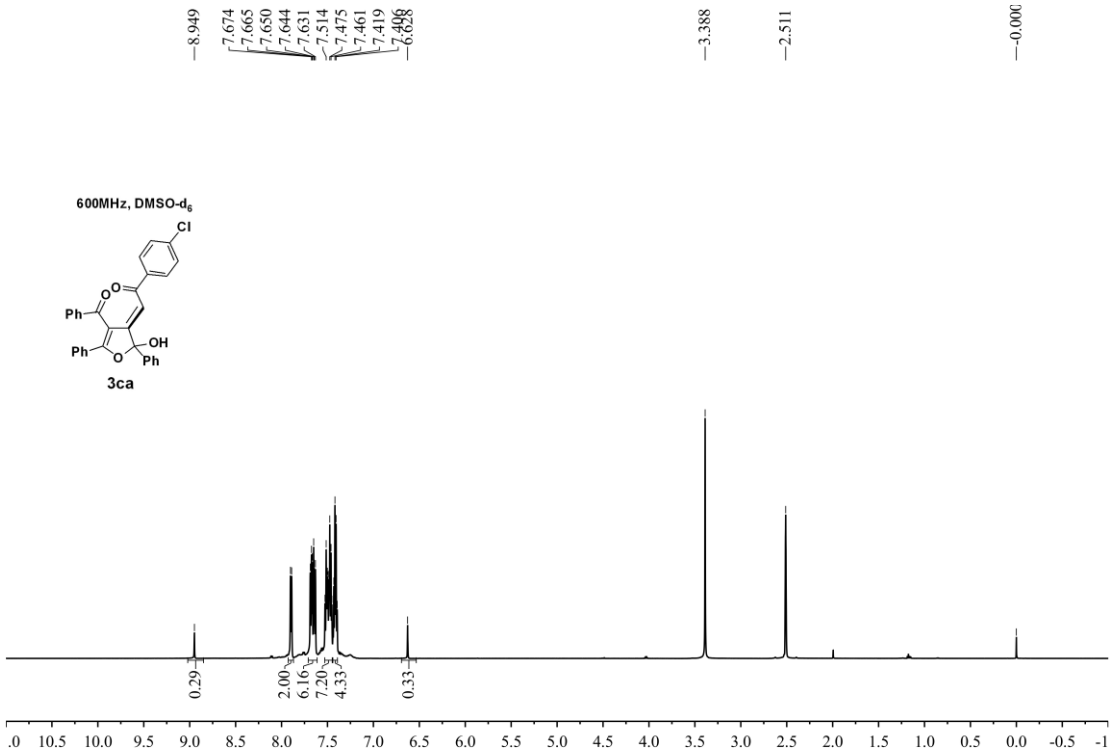

8.925
7.811
7.798
7.713
7.699
7.637
7.623
7.605
7.592
7.384
7.370
6.510
3.462
2.526
2.208
0.000
600MHz,DMSO-d6
Ph
O
O
Ph
OH
O
Br
3al
0.58
2.37
2.24
2.24
2.34
1.39
1.36
4.28
0.65
3.00

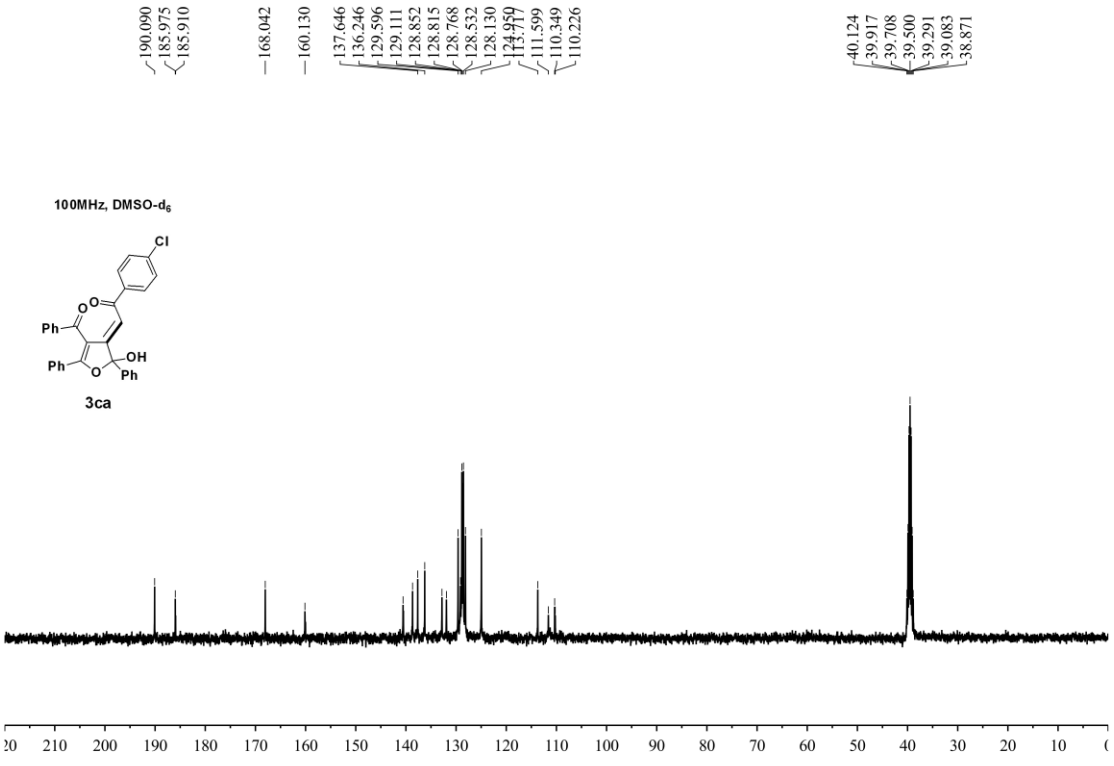

189.161
187.500
187.432
174.836
158.694
158.598
138.993
137.680
132.592
131.581
128.527
128.282
128.096
127.438
122.500
114.175
110.675
110.550
39.914
39.777
39.639
39.500
39.361
39.223
39.084
14.763
150MHz,DMSO-d6
Ph
O
O
Ph
OH
O
Br
3al

(2) Spectral copies of phenacyl pyridinium halides.

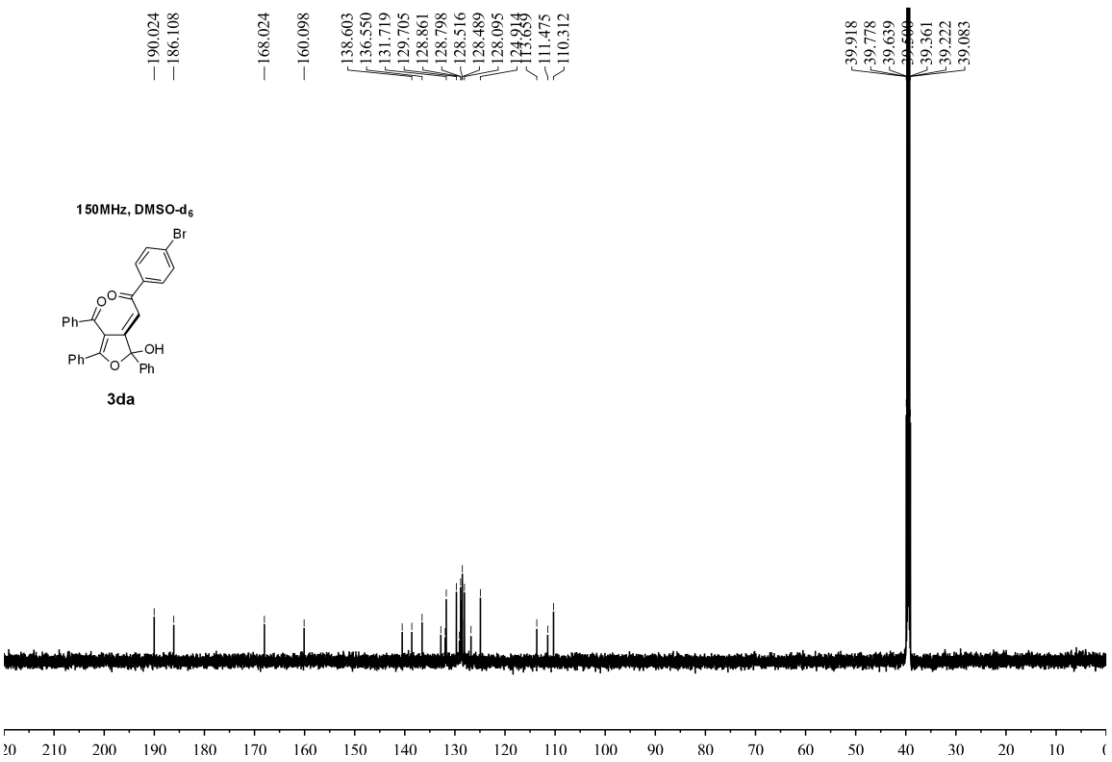


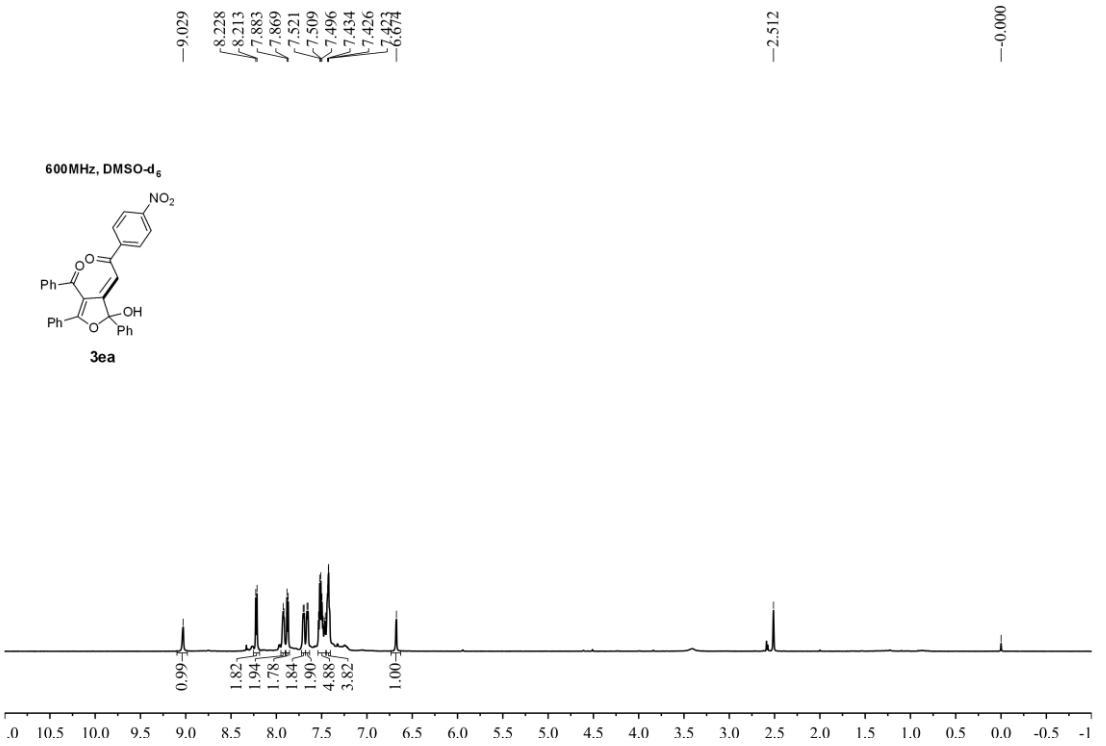


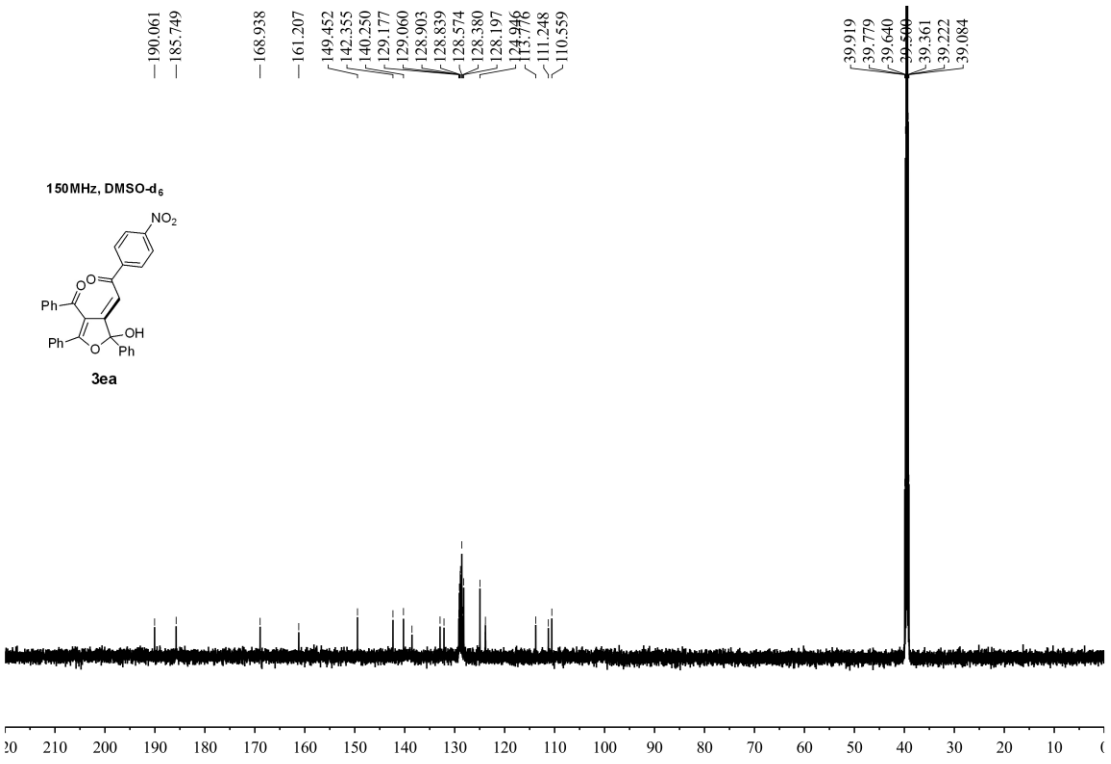

600MHz, DMSO-d6
3ca
8.949
7.674
7.665
7.650
7.644
7.631
7.514
7.475
7.461
7.419
7.406
6.628
3.388
2.511
0.000
0.29
2.00
6.16
7.20
4.33
0.33


100MHz, DMSO-d6
3ca
190.090
185.975
185.910
168.042
160.130
137.646
136.246
129.596
129.111
128.852
128.815
128.768
128.532
128.130
124.950
113.717
111.599
110.349
110.226
40.124
39.917
39.708
39.500
39.291
39.083
38.871

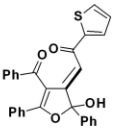

8.930
7.895
7.882
7.667
7.639
7.626
7.603
7.578
7.510
7.415
7.403
6.608
3.368
2.508
0.000
600MHz, DMSO-d6
Br
O
O
Ph
Ph
O
OH
Ph
3da
1.00
2.13
2.14
4.37
2.05
5.12
4.17
1.00


190.024
186.108
168.024
160.098
138.603
136.550
131.719
129.705
128.861
128.798
128.516
128.489
128.095
124.914
113.659
111.475
110.312
39.918
39.778
39.639
39.500
39.361
39.222
39.083
150MHz, DMSO-d6
Br
O
O
Ph
Ph
O
OH
Ph
3da

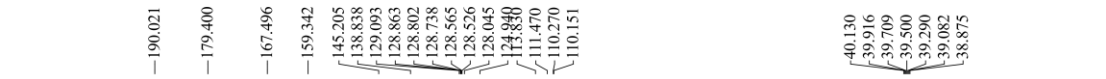

9.029
8.228
8.213
7.883
7.869
7.521
7.509
7.496
7.434
7.426
7.423
6.674
2.512
0.000
600MHz, DMSO-d6
NO2
Ph
O
OH
Ph
O
Ph
3ea
0.99
1.82
1.94
1.78
1.84
1.90
4.88
3.82
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


190.061
185.749
168.938
161.207
149.452
142.355
140.250
129.177
129.060
128.903
128.839
128.574
128.380
128.197
124.946
113.778
111.248
110.559
39.919
39.779
39.640
39.500
39.361
39.222
39.084
150MHz, DMSO-d6
NO2
Ph
O
OH
Ph
O
Ph
3ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

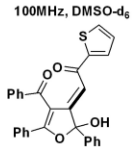
600MHz, DMSO-d_6



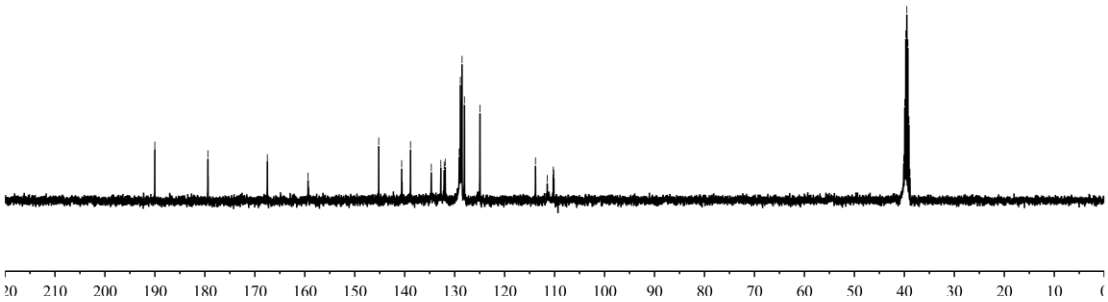
3fa

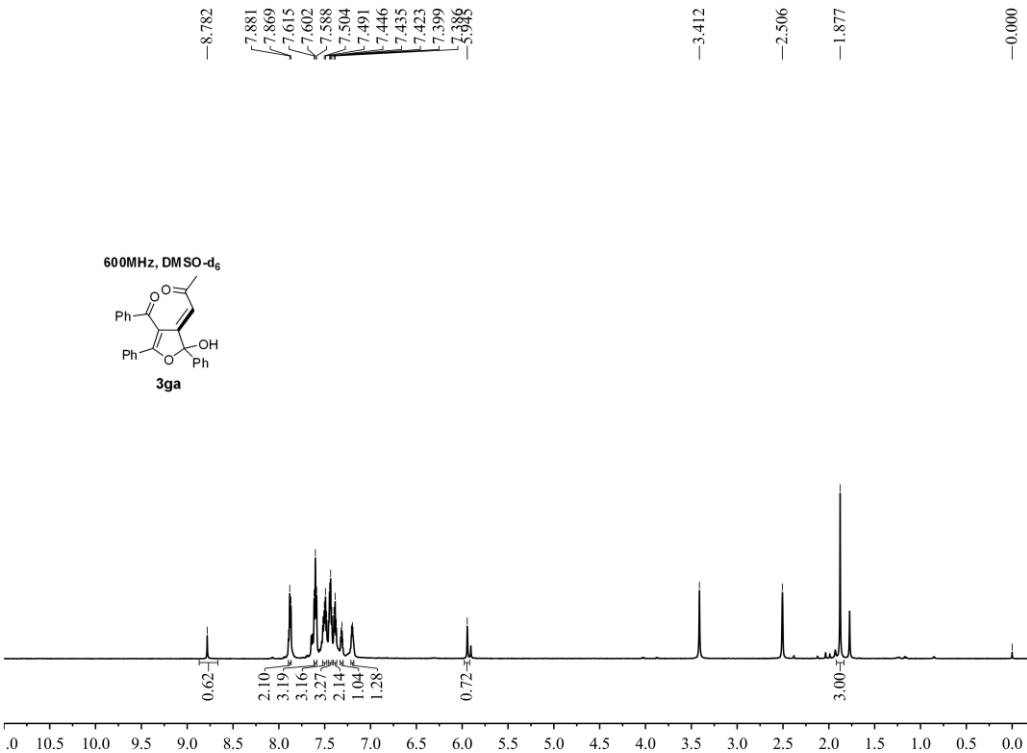


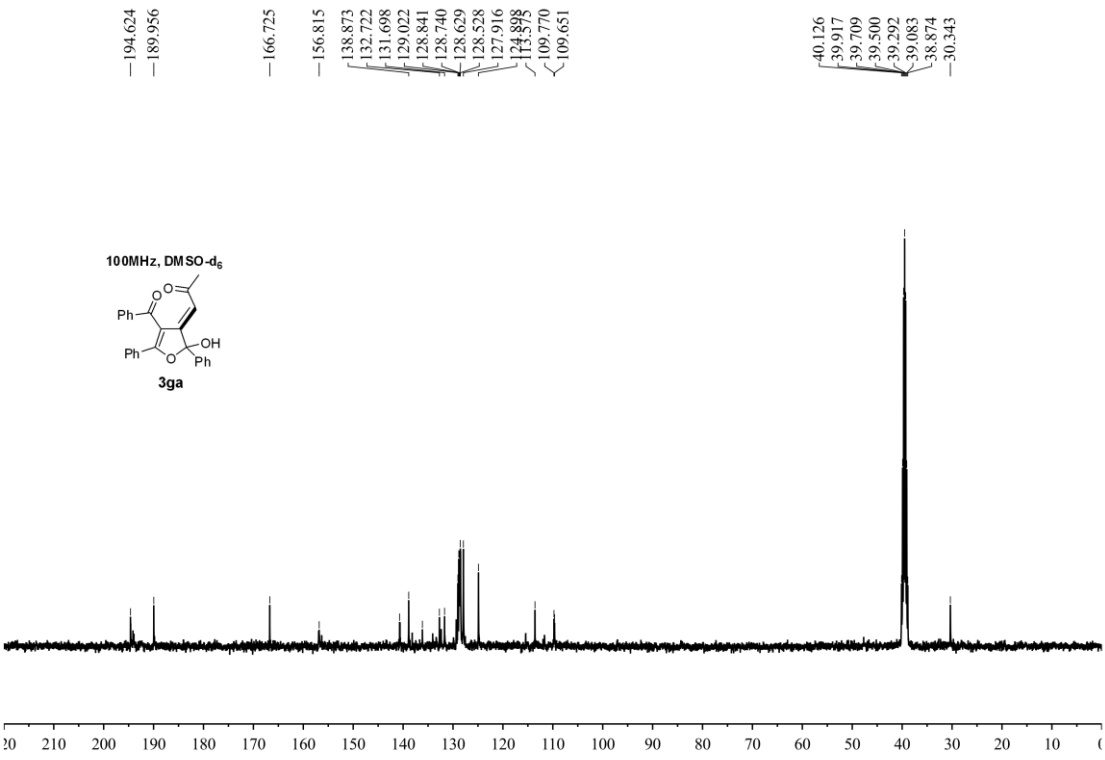
100MHz, DMSO-d_6



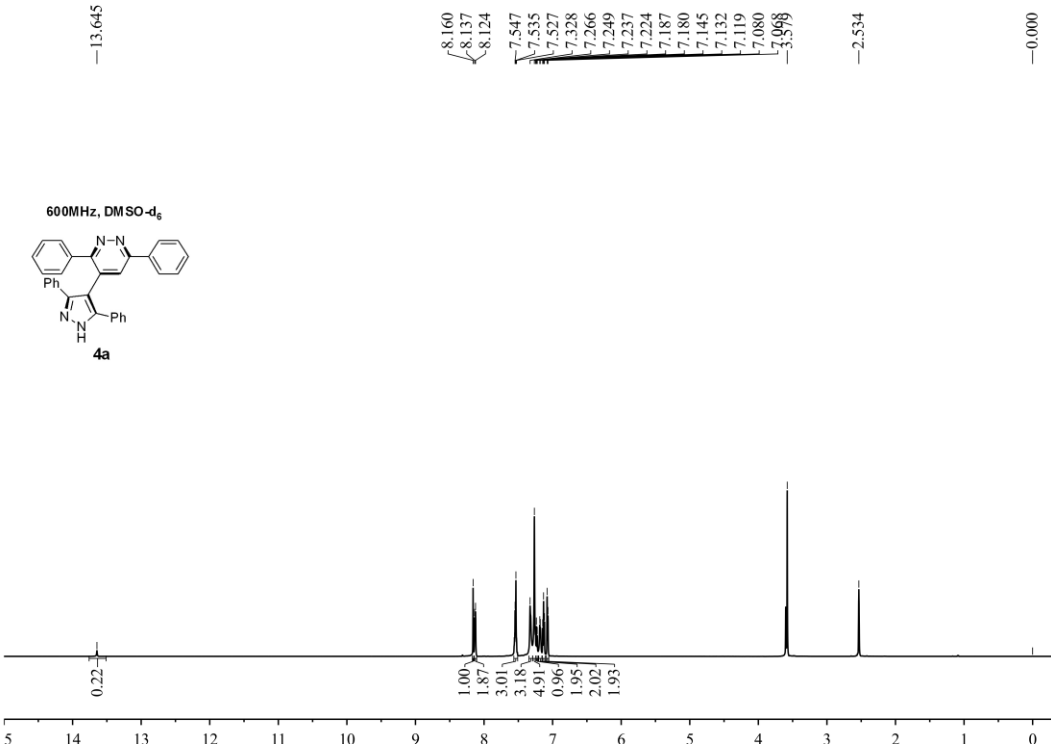
3fa

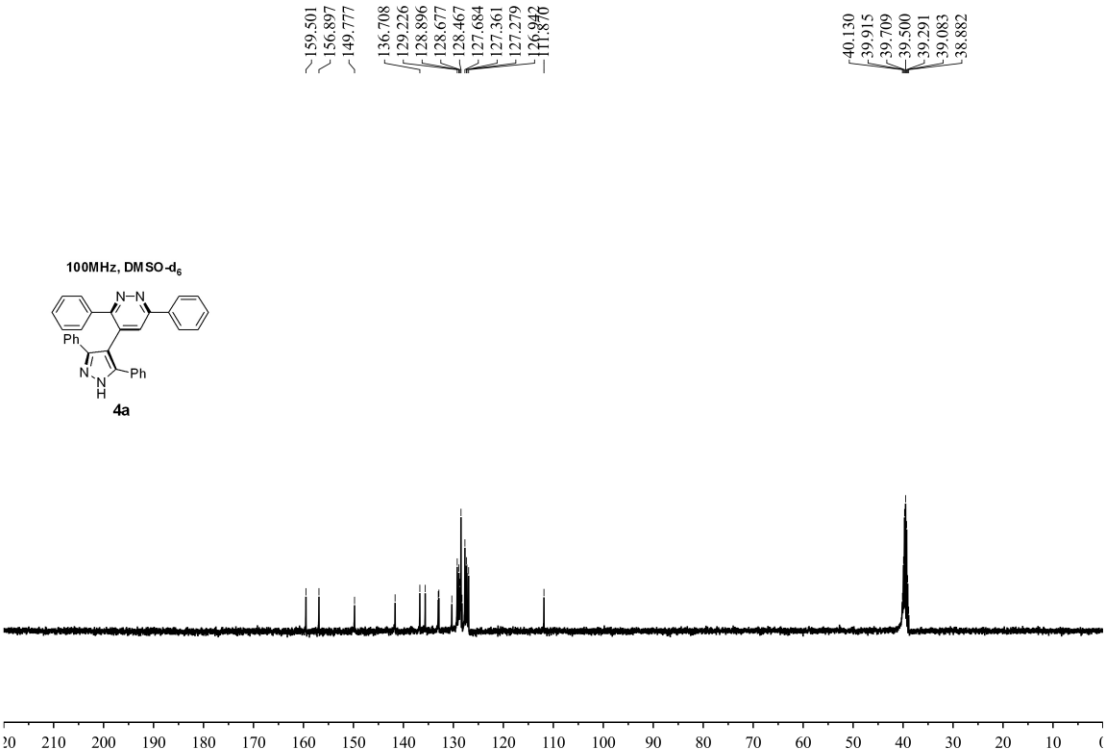


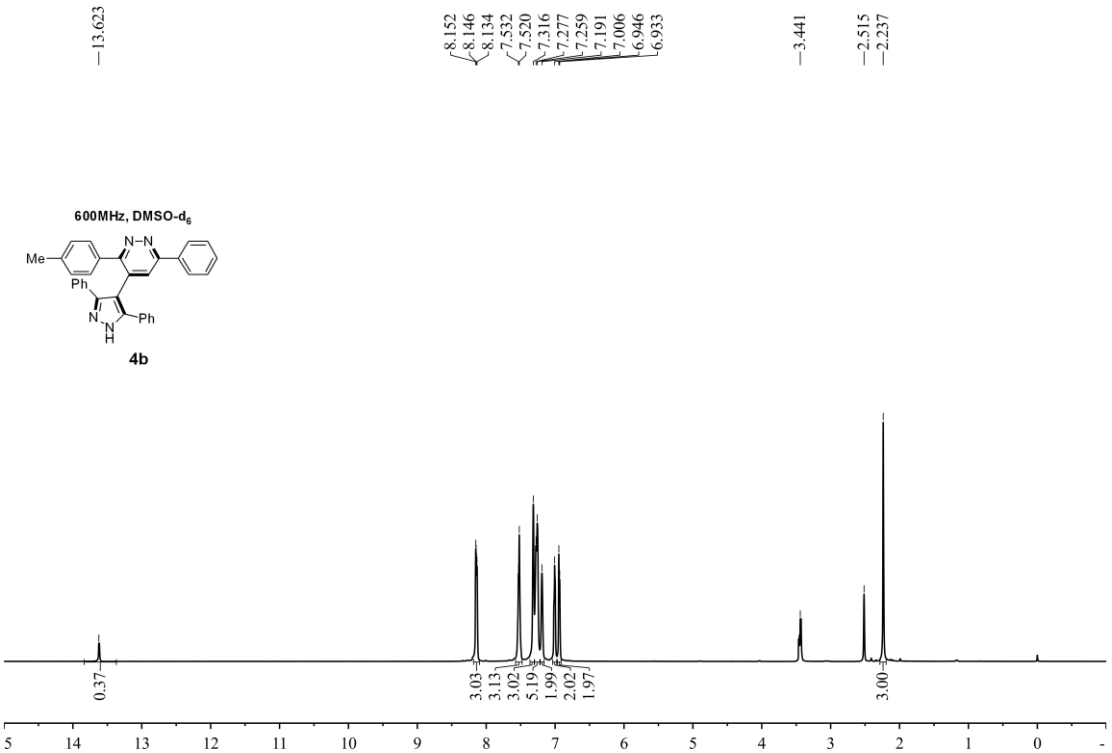

8.782
7.881
7.869
7.615
7.602
7.588
7.504
7.491
7.446
7.435
7.423
7.399
5.943
3.412
2.506
1.877
0.000
600MHz, DMSO-d6
Ph
O
OH
Ph
O
Ph
3ga
0.62
2.10
3.19
3.16
3.27
2.14
1.04
1.28
0.72
3.00

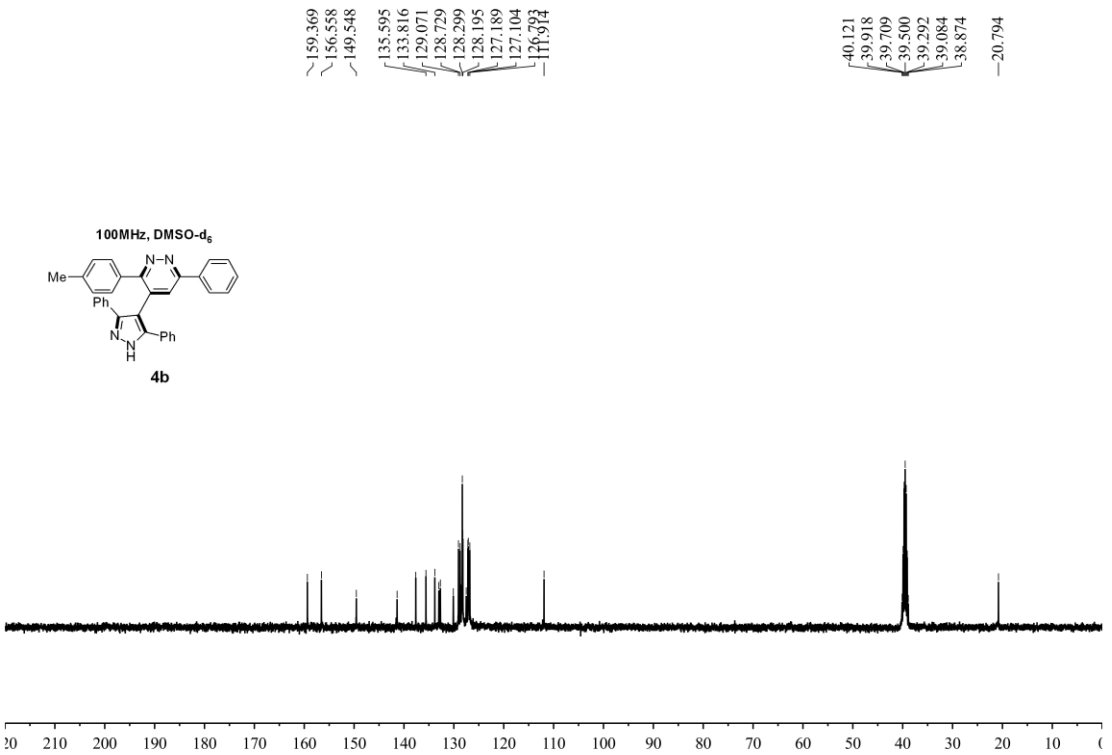

194.624
189.956
166.725
156.815
138.873
132.722
131.698
129.022
128.841
128.740
128.629
128.528
127.916
109.770
109.651
40.126
39.917
39.709
39.500
39.292
39.083
38.874
30.343
100MHz, DMSO-d6
Ph
O
OH
Ph
O
Ph
3ga

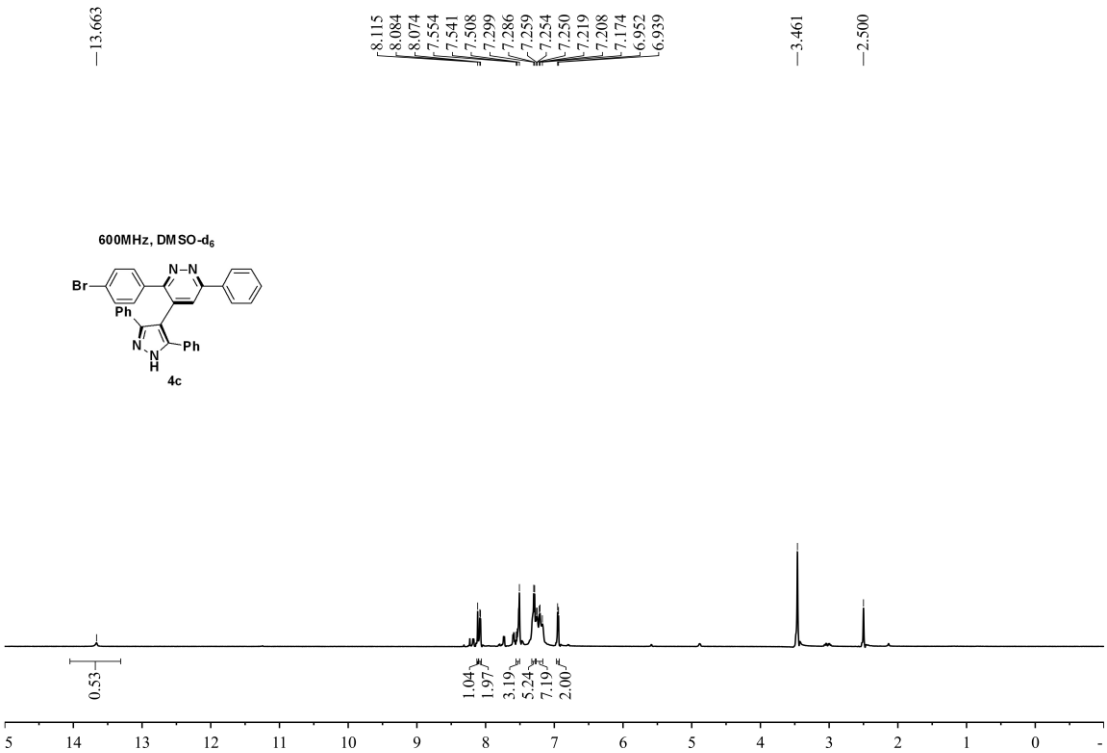
(3) Spectral copies of 4-(1H-pyrazol-4-yl)pyridazine derivatives.

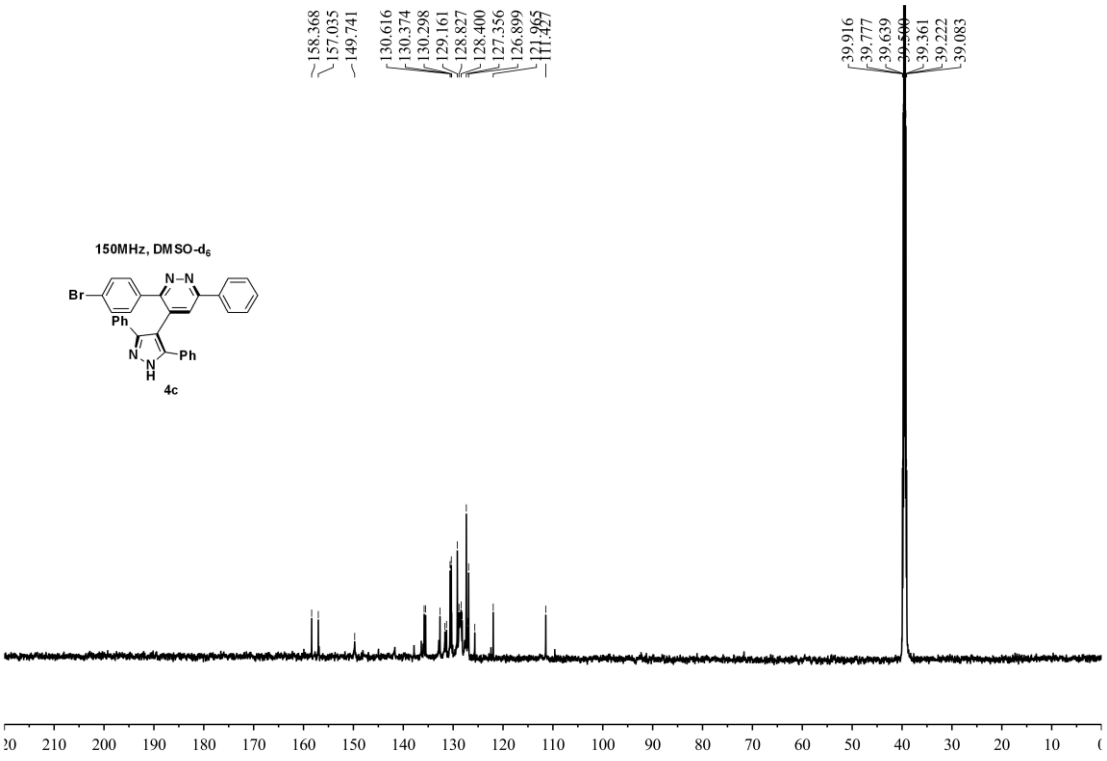




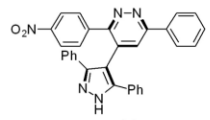

13.623
8.152
8.146
8.134
7.532
7.520
7.316
7.277
7.259
7.191
7.006
6.946
6.933
3.441
2.515
2.237
600MHz, DMSO-d6
Me
Ph
Ph
4b
0.37
3.03
3.13
3.02
5.19
1.99
2.02
1.97
3.00


159.369
156.558
149.548
135.595
133.816
129.071
128.729
128.299
128.195
127.189
127.104
126.793
111.914
40.121
39.918
39.709
39.500
39.292
39.084
38.874
20.794
100MHz, DMSO-d6
Me
Ph
Ph
4b

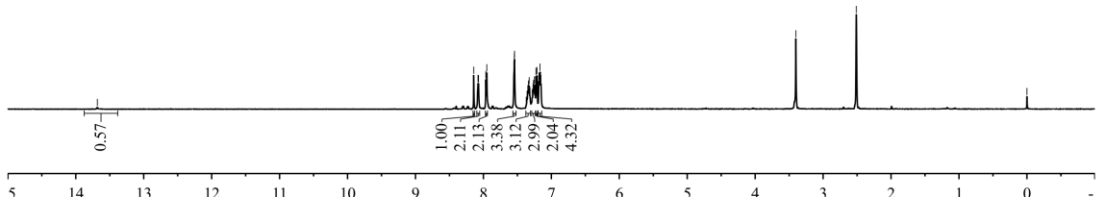

13.663
8.115
8.084
8.074
7.554
7.541
7.508
7.299
7.286
7.259
7.254
7.250
7.219
7.208
7.174
6.952
6.939
3.461
2.500
600MHz, DMSO-d6
Br
Ph
N–N
N
N
H
Ph
4c
0.53
1.04
1.97
3.19
5.24
7.19
2.00

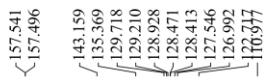

158.368
157.035
149.741
130.616
130.374
130.298
129.161
128.827
128.400
127.356
126.899
121.965
111.427
39.916
39.777
39.639
39.361
39.222
39.083
150MHz, DMSO-d6
Br
Ph
N–N
N
N
H
Ph
4c

600MHz, DMSO-d_6

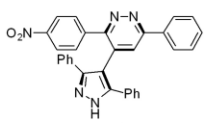


4d

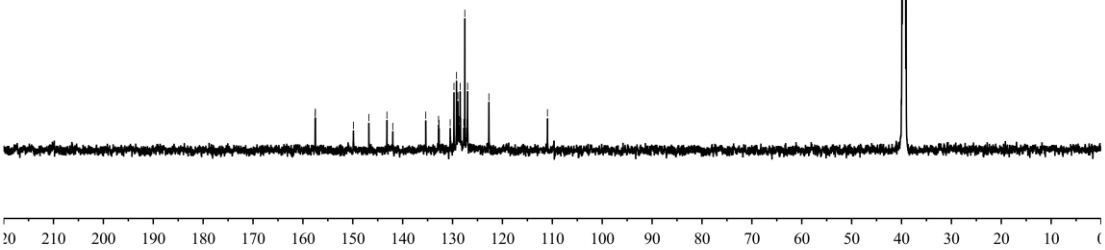


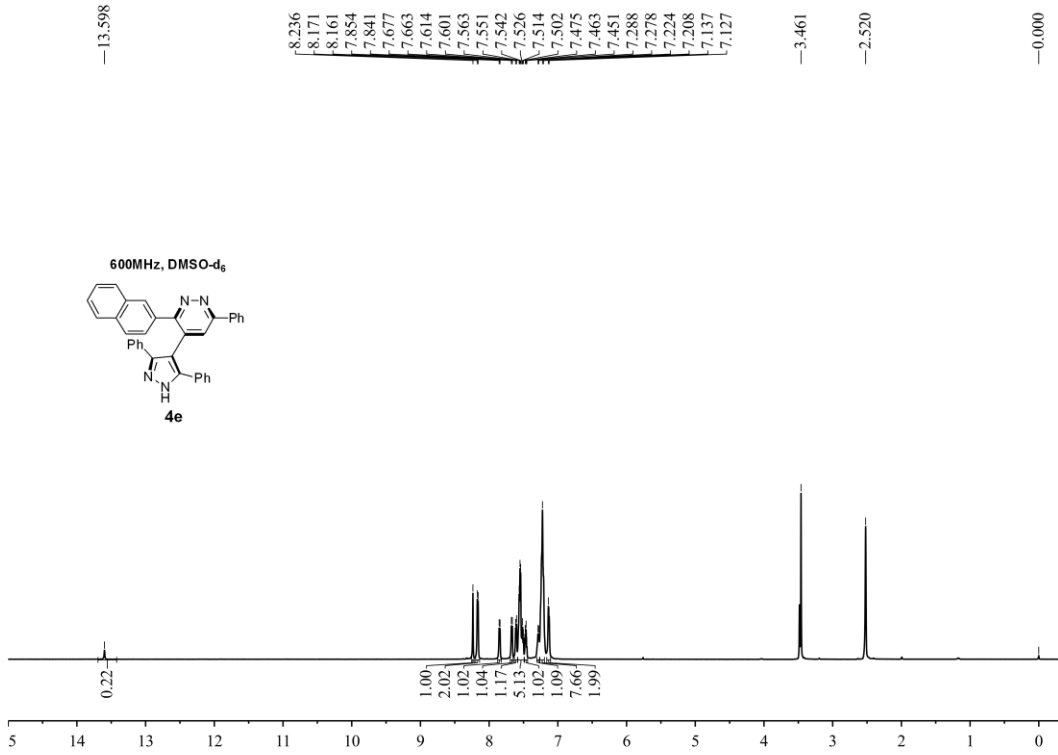


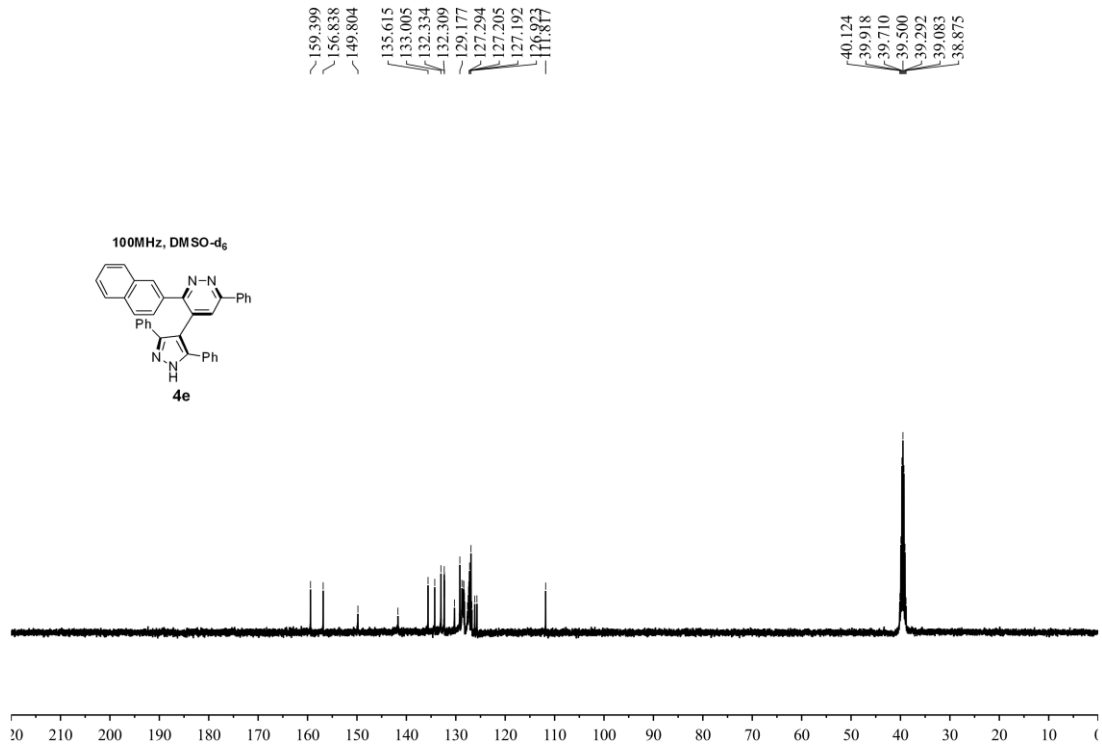
150MHz, DMSO-d_6



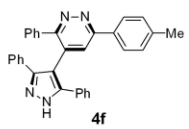
4d



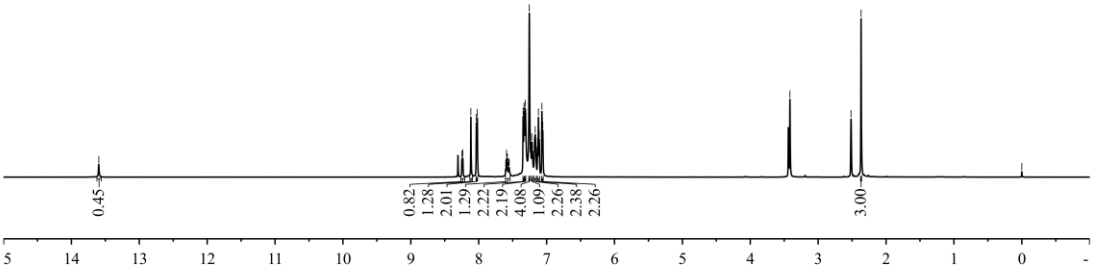

13.598
8.236
8.171
8.161
7.854
7.841
7.677
7.663
7.614
7.601
7.563
7.551
7.542
7.526
7.514
7.502
7.475
7.463
7.451
7.288
7.278
7.224
7.208
7.137
7.127
3.461
2.520
0.000
600MHz, DMSO-d6
4e
0.22
1.00
2.02
1.02
1.04
1.17
5.13
1.02
1.09
7.66
1.99

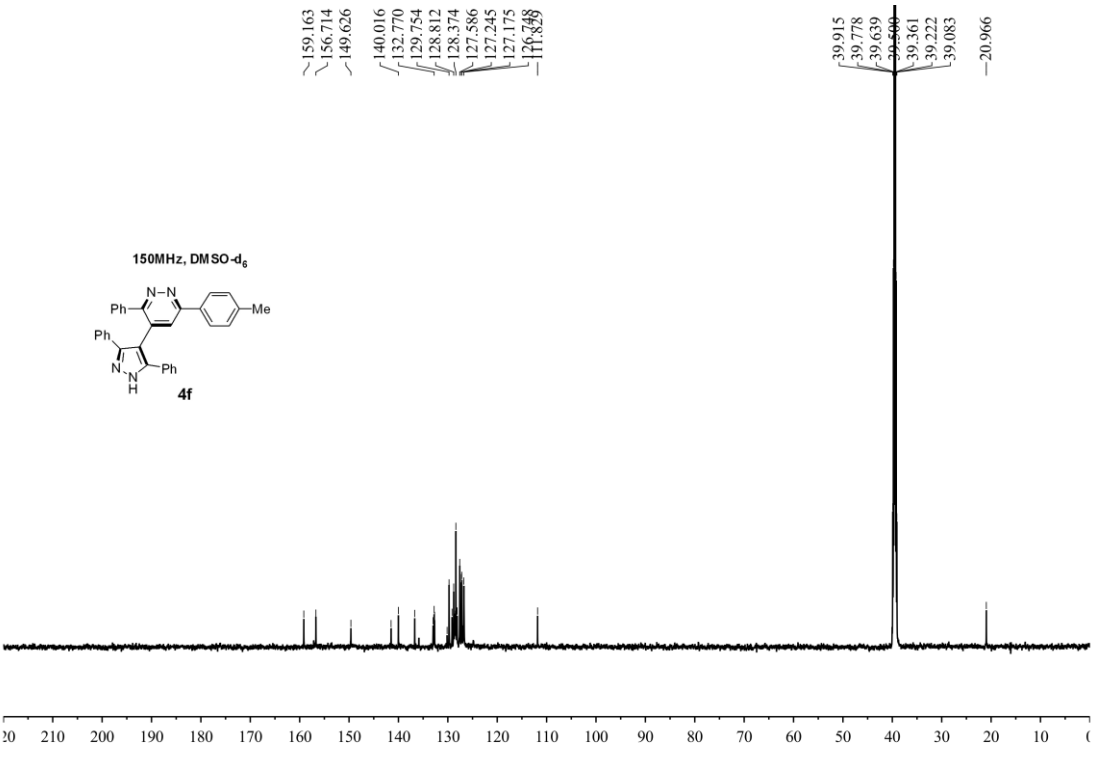

159.399
156.838
149.804
135.615
133.005
132.334
132.309
129.177
127.294
127.205
127.192
126.923
111.817
40.124
39.918
39.710
39.500
39.292
39.083
38.875
100MHz, DMSO-d6
4e

600MHz, DMSO-d_6



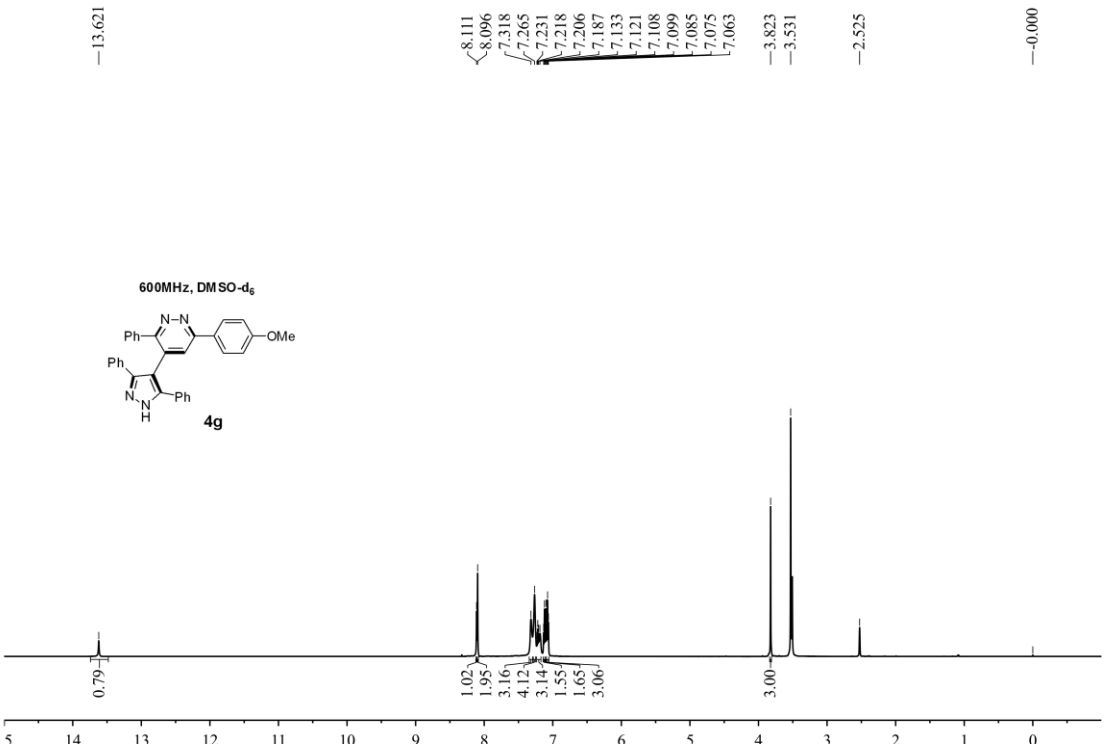
4f

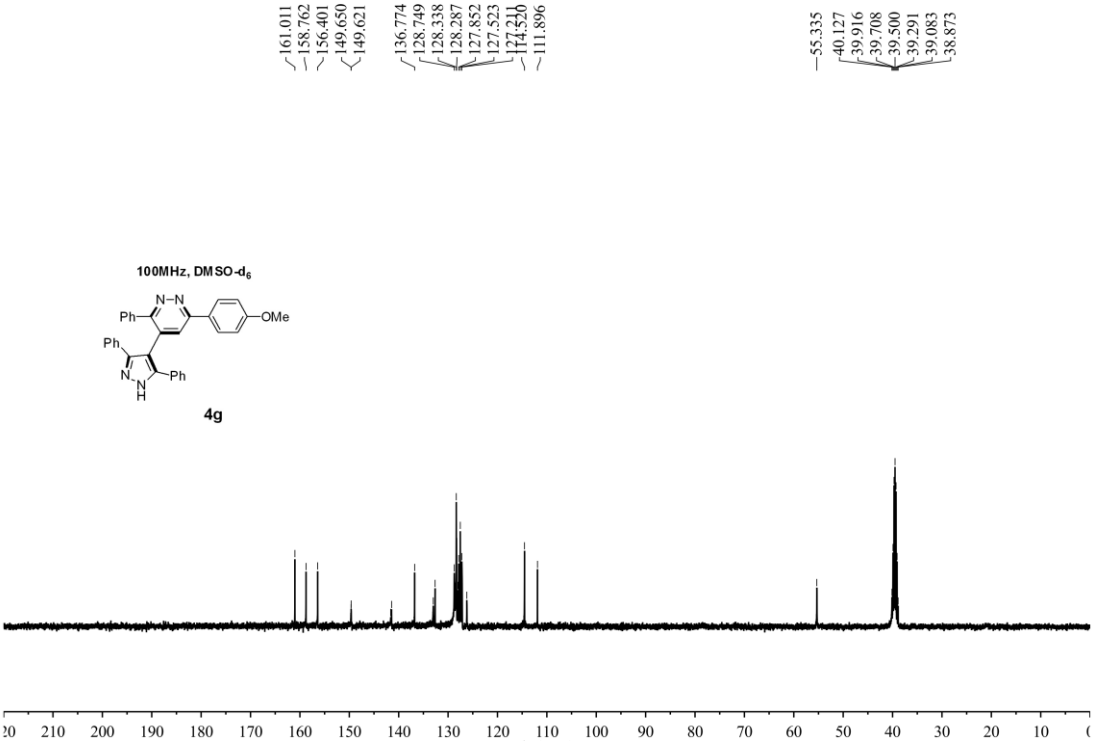


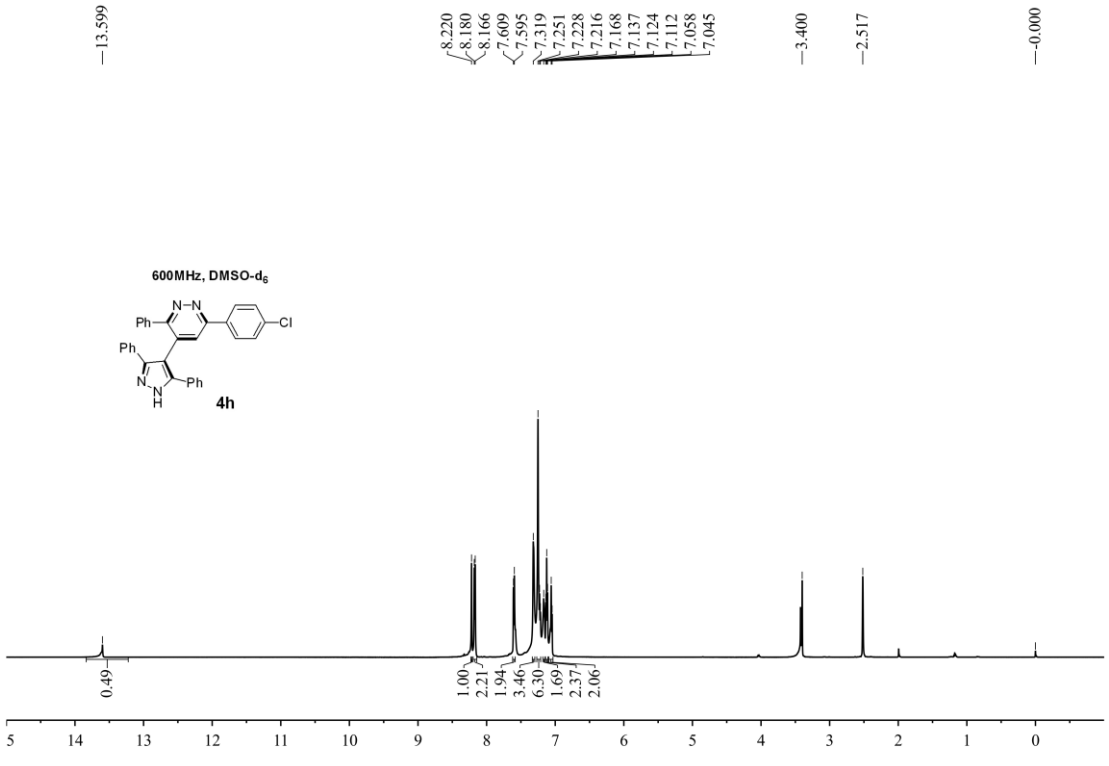


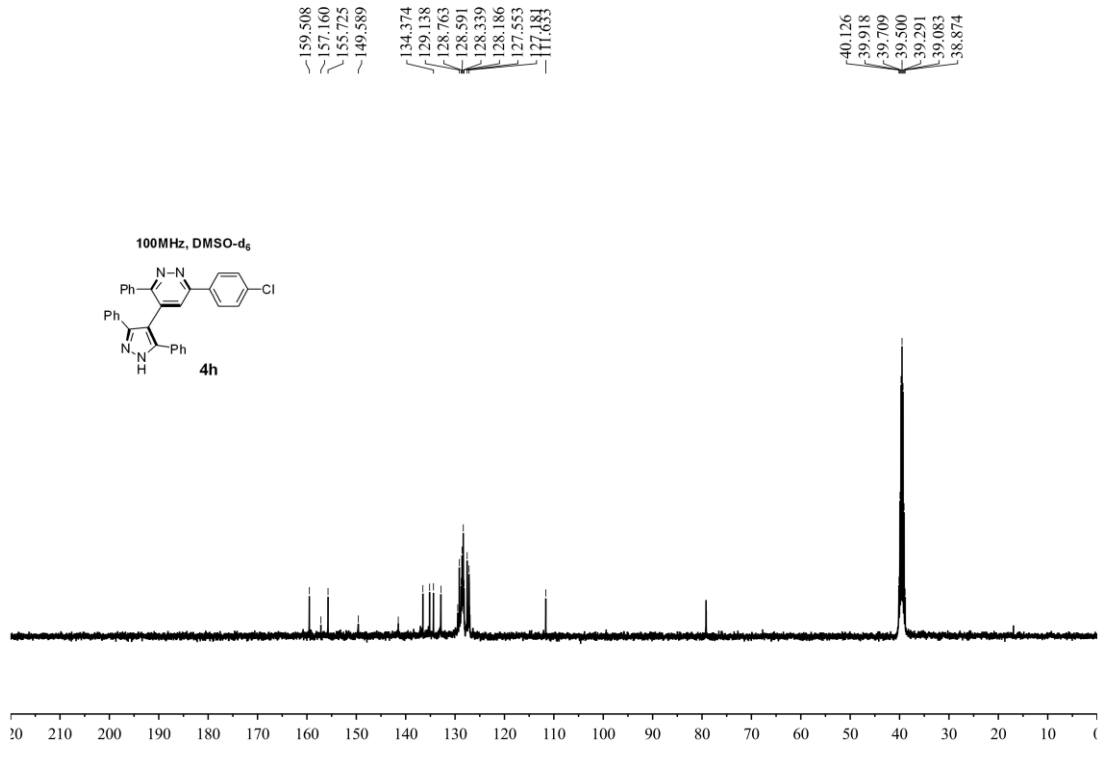
150MHz, DMSO-d_6

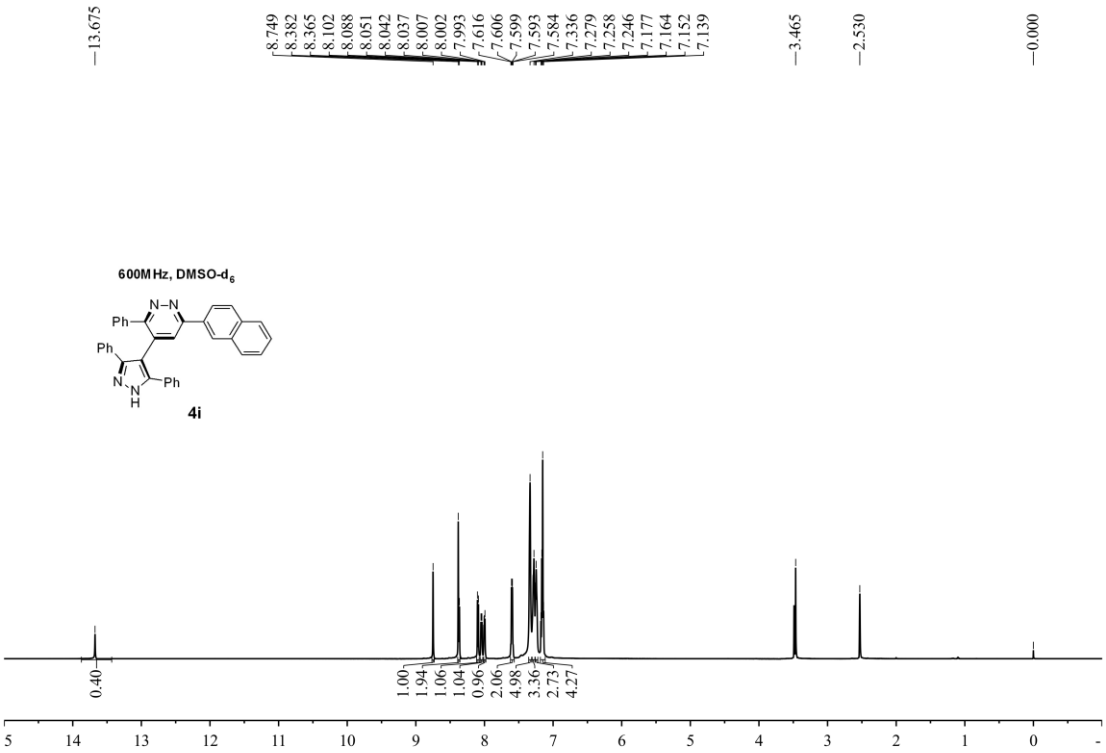
4f

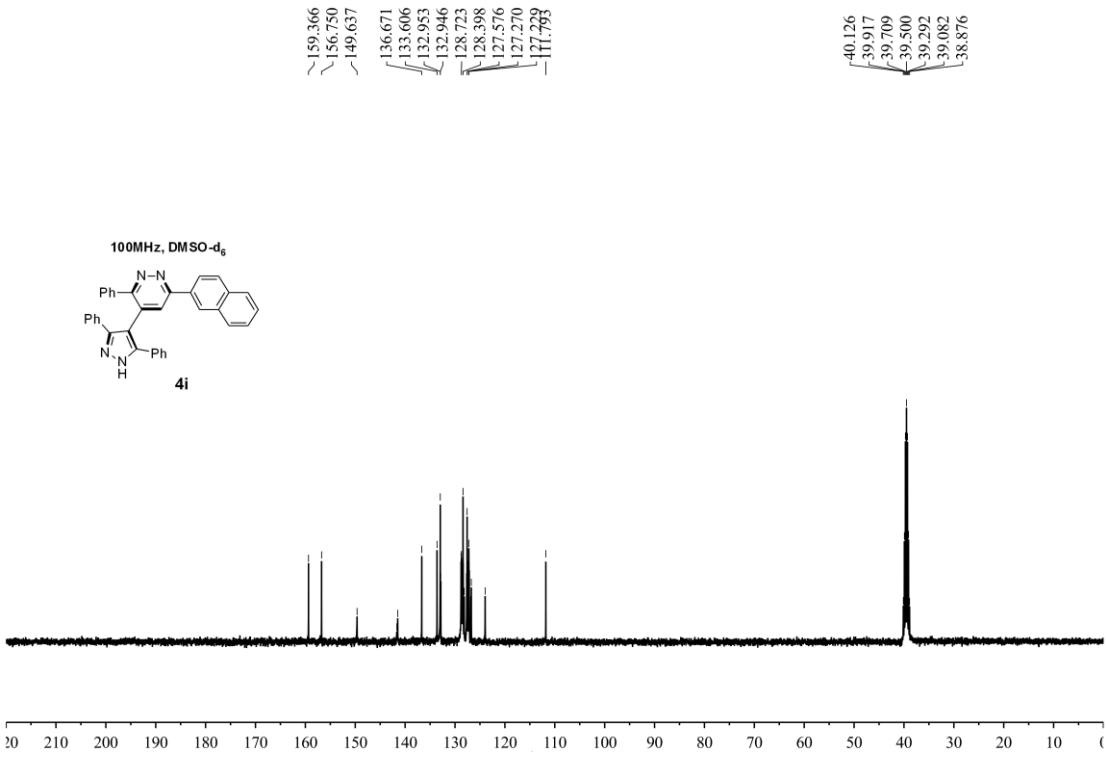

13.621
8.111
8.096
7.318
7.265
7.231
7.218
7.206
7.187
7.133
7.121
7.108
7.099
7.085
7.075
7.063
3.823
3.531
2.525
0.000
600MHz, DMSO-d6
Ph
N–N
OMe
Ph
N
N
H
Ph
4g
0.79
1.02
1.95
3.16
4.12
3.14
1.55
1.65
3.06
3.00

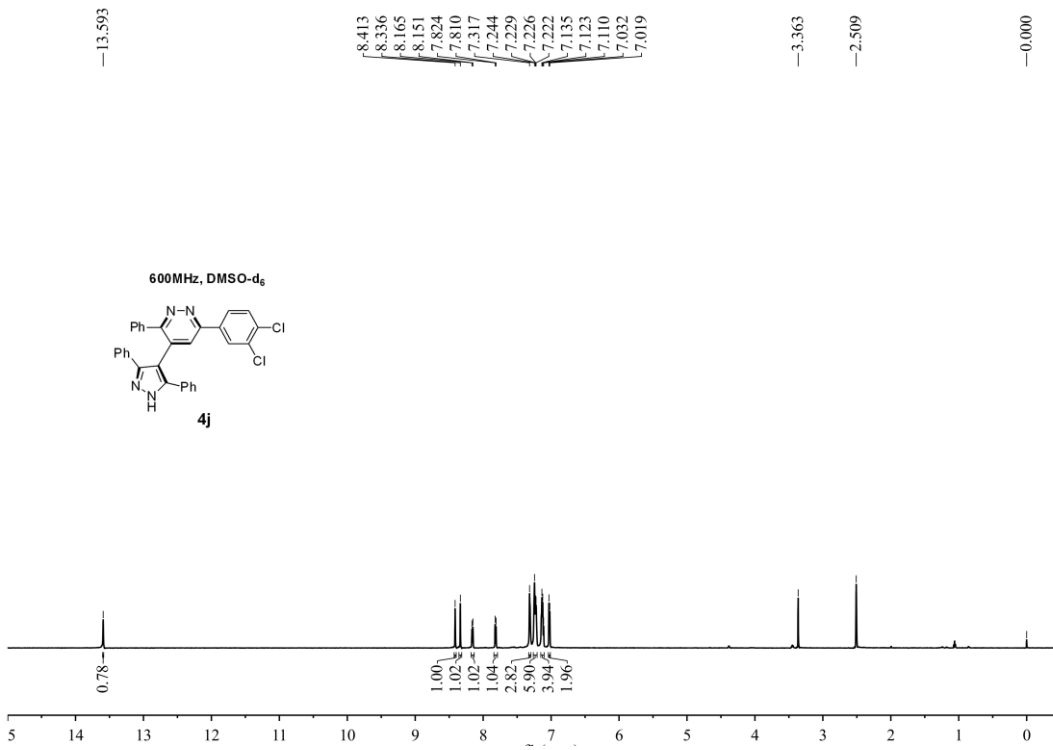

161.011
158.762
156.401
149.650
149.621
136.774
128.749
128.338
128.287
127.852
127.523
127.211
114.520
111.896
55.335
40.127
39.916
39.708
39.500
39.291
39.083
38.873
100MHz, DMSO-d6
Ph
N–N
OMe
Ph
N
N
H
Ph
4g

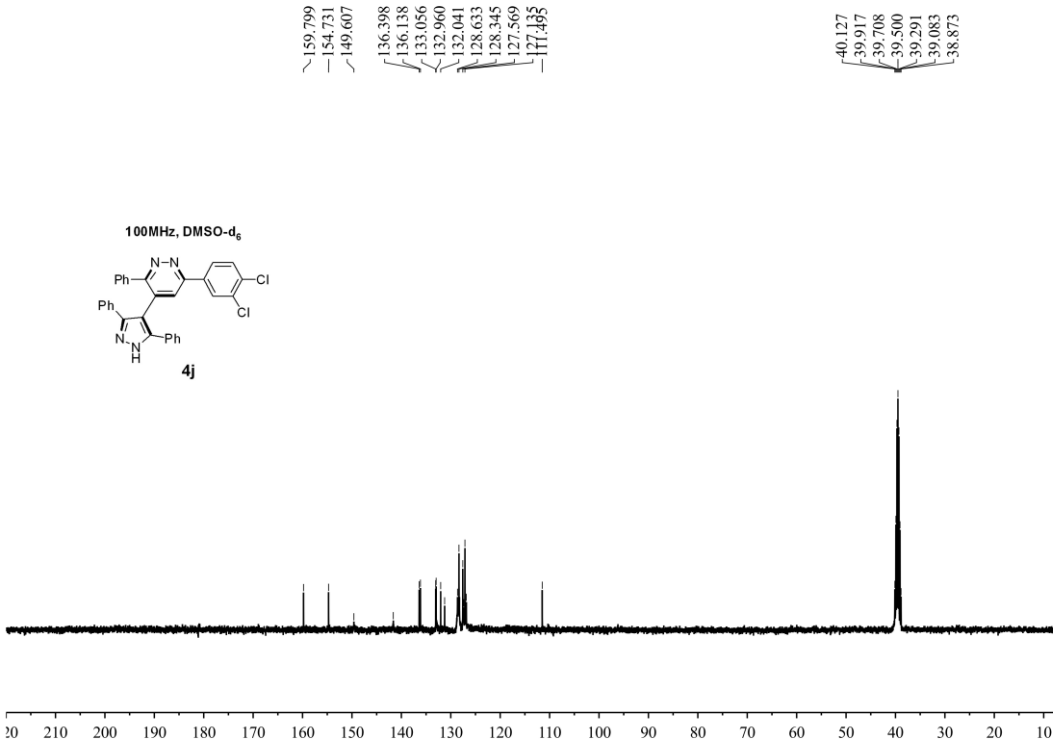

13.599
8.220
8.180
8.166
7.609
7.595
7.319
7.251
7.228
7.216
7.168
7.137
7.124
7.112
7.058
7.045
3.400
2.517
0.000
600MHz, DMSO-d6
4h
0.49
1.00
2.21
1.94
3.46
6.30
1.69
2.37
2.06

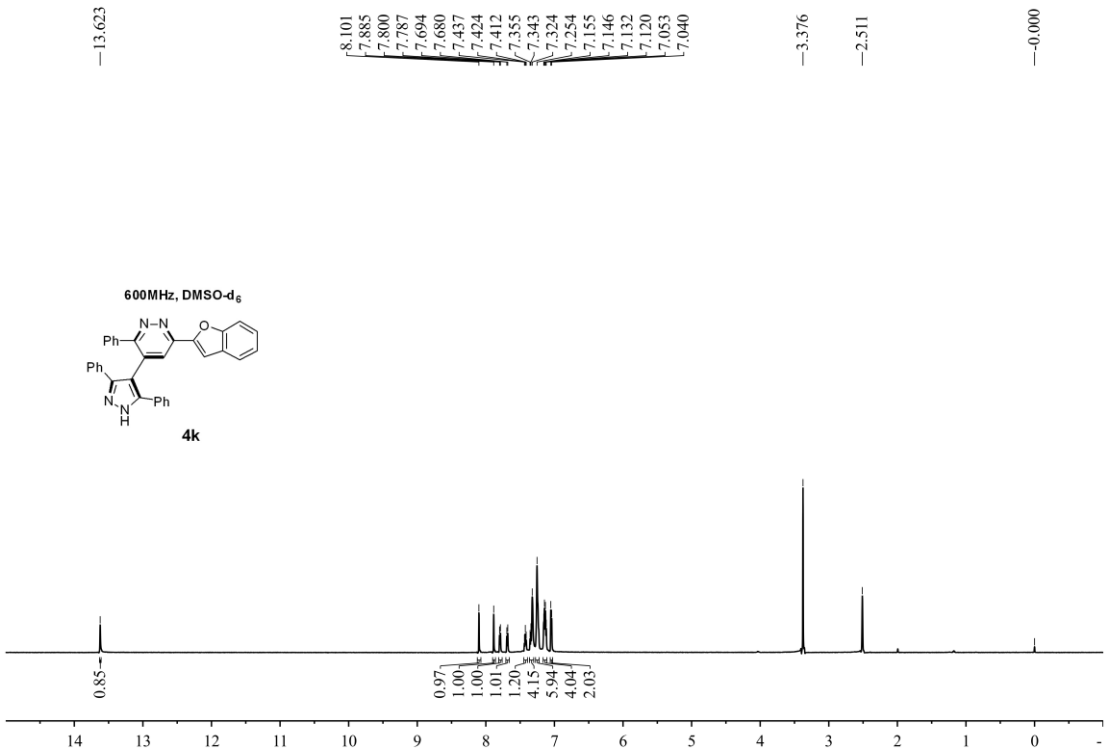

159.508
157.160
155.725
149.589
134.374
129.138
128.763
128.591
128.339
128.186
127.553
127.181
117.633
40.126
39.918
39.709
39.500
39.291
39.083
38.874
100MHz, DMSO-d6
4h

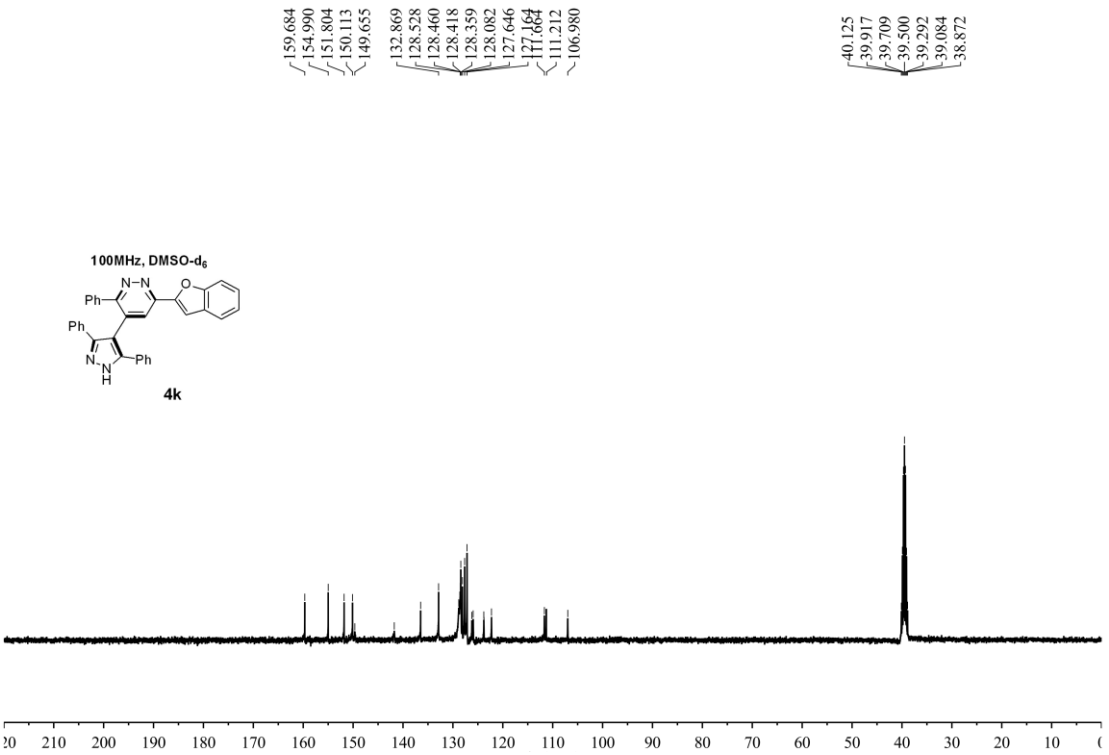

13.675
8.749
8.382
8.365
8.102
8.088
8.051
8.042
8.037
8.007
8.002
7.993
7.616
7.606
7.599
7.593
7.584
7.336
7.279
7.258
7.246
7.177
7.164
7.152
7.139
3.465
2.530
0.000
600MHz, DMSO-d6
4i
0.40
1.00
1.94
1.06
1.04
0.96
2.06
4.98
3.36
2.73
4.27


159.366
156.750
149.637
136.671
133.606
132.953
132.946
128.723
128.398
127.576
127.270
127.229
111.793
40.126
39.917
39.709
39.500
39.292
39.082
38.876
100MHz, DMSO-d6
4i


13.593
8.413
8.336
8.165
8.151
7.824
7.810
7.317
7.244
7.229
7.226
7.222
7.135
7.123
7.110
7.032
7.019
3.363
2.509
0.000
600MHz, DMSO-d6
4j
0.78
1.00
1.02
1.02
1.04
2.82
5.90
3.94
1.96


159.799
154.731
149.607
136.398
136.138
133.056
132.960
132.041
128.633
128.345
127.569
127.135
111.495
40.127
39.917
39.708
39.500
39.291
39.083
38.873
100MHz, DMSO-d6
4j


13.623
8.101
7.885
7.800
7.787
7.694
7.680
7.437
7.424
7.412
7.355
7.343
7.324
7.254
7.155
7.146
7.132
7.120
7.053
7.040
3.376
2.511
0.000
600MHz, DMSO-d6
4k
0.85
0.97
1.00
1.00
1.01
1.20
4.15
5.94
4.04
2.03


159.684
154.990
151.804
150.113
149.655
132.869
128.528
128.460
128.418
128.359
128.082
127.646
111.604
111.212
106.980
40.125
39.917
39.709
39.500
39.292
39.084
38.872
100MHz, DMSO-d6
4k