

Supporting Information

Acid/base-controlled chemodivergent synthesis of two differently functionalized tetrahydroimidazo[1,2-*a*]pyridines

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General methods

All reagents and solvents were obtained from commercial suppliers and used without further purification. All reagents were weighed and handled in air at room temperature. Chromatography refers to open column chromatography on silica gel (100-200 mesh). Melting points were recorded on a RY-1 microscopic melting apparatus and uncorrected. ^1H NMR spectra were recorded on 500 MHz and ^{13}C NMR spectra were recorded on 125 MHz by using a Bruker Avance 500 spectrometer. Chemical shifts are reported in δ (ppm) relative to tetramethylsilane (TMS). IR spectra were recorded on a Nicolet iS10 FT-IR spectrometer and only major peaks are reported in cm^{-1} . Mass spectra were performed on an Ultima Global spectrometer with an ESI source. The X-ray single-crystal diffraction was performed on Saturn 724+ instrument. The starting materials KTAs **1**¹ and HKAs **3**² were synthesized according to the literatures.

General experimental procedures of compounds 5 (5a for example)

A solution of **1a** (0.5 mmol), **2a** (0.5 mmol) and **3a** (0.5 mmol) in CH_3OH (2 mL) was heated to refluxing for 8 h. After completion of the reaction as indicated by TLC, the precipitate was filtered and washed with CH_3OH to give the intermediate **4a**. Then **4a** was dissolved in DMF (2 mL), and Na_2CO_3 (1.0 mmol) was added. The mixture was stirred at 100 °C for 2 h, quenched with saturated NH_4Cl and extracted with EtOAc (3 \times 10 mL). The combined organic phase was concentrated under vacuum, and the residue was purified by flash column chromatography (petroleum ether/EtOAc, 2: 1, v/v) to afford the products **5a**.

General experimental procedures of compounds 6 (6a for example)

A solution of **1a** (0.5 mmol), **2a** (0.5 mmol) and **3a** (0.5 mmol) in CH_3OH (2 mL) was heated to refluxing for 8 h. Then 20% H_2SO_4 (0.2 eq) was added and the mixture was heated to refluxing for additional 2 h. Water was added to the mixture and the precipitate was filtered, washed with petroleum ether/EtOAc (5: 1) and dried to afford the products **6a**.

Reference:

1. (a) X. Feng, J. J. Wang, Z. Xun, Z. B. Huang and D. Q. Shi, *J. Org. Chem.*, **2015**, *80*, 1025; (b) R. Gomper and H. Schaefer, *Chem. Ber.*, **1967**, *100*, 591.
2. (a) X. Chen, L. Zhu, L. Fang, S. Yan and J. Lin, *RSC Adv.*, **2014**, *4*, 9926; (b) Z. J. Li and D. Charles, *Synth. Commun.*, **2001**, *31*, 527; (c) Z. T. Huang and M. X. Wang, *Synthesis*, **1992**, *12*, 1273.

7-(4-Chlorophenyl)-8-(2,5-dichlorobenzoyl)-5-hydroxy-*N*,5-diphenyl-1,2,3,5,6,7-hexahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (4a)
(CCDC 858868)

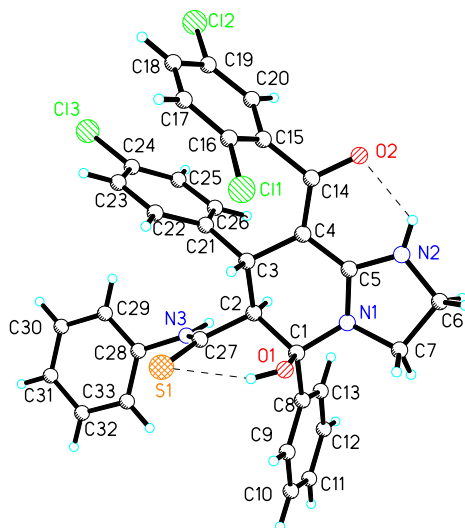


Figure S1. X-Ray Structure of **4a**

(6-Benzoyl-7-(4-methoxyphenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5c)
(CCDC 878006)

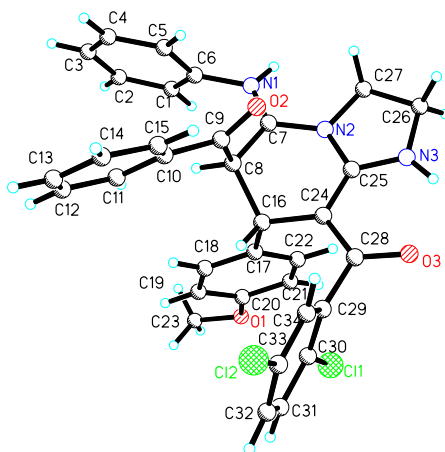


Figure S2. X-Ray Structure of **5c**

7-(3-Chlorophenyl)-8-(2,5-dichlorobenzoyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6h)

(CCDC 1003512)

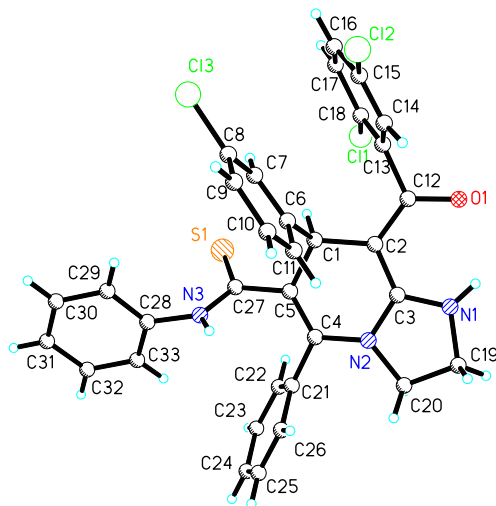
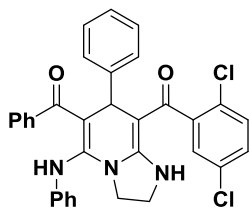


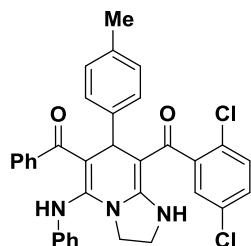
Figure S3. X-Ray Structure of **6h**

(6-Benzoyl-7-phenyl-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5a)



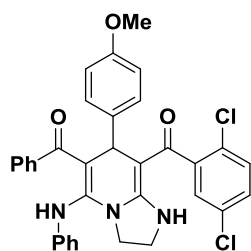
Light yellow powder; mp 235–237 °C; IR (KBr) ν 3442, 1683, 1629, 1595, 1534, 1498, 1486, 1458, 760, 699 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.58–3.85 (m, 1H, NH), 3.94–3.95 (m, 2H, CH₂), 4.13–4.14 (m, 2H, CH₂), 4.49 (s, 1H, CH), 6.05–6.25 (m, 3H, ArH), 6.89–7.64 (m, 15H, ArH), 9.49 (s, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 42.7, 43.4, 44.4, 60.2 (2C), 120.3 (4C), 123.7 (2C), 126.7 (2C), 127.5 (2C), 128.2 (2C), 129.2 (2C), 129.5 (4C), 131.4 (2C), 134.3 (2C), 148.5 (2C), 149.9, 157.2, 184.4 (2C); HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₃H₂₆N₃O₂Cl₂, 566.1402; found 566.1415.

(6-Benzoyl-5-(phenylamino)-7-(*p*-tolyl)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5b)



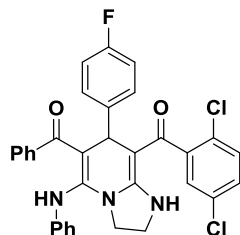
Light yellow powder; mp 219–220 °C; IR (KBr) ν 3441, 1678, 1629, 1595, 1527, 1496, 1486, 1456, 817, 755, 700 cm^{-1} ; ^1H NMR (CDCl₃, 500 MHz) δ 2.32 (s, 3H, CH₃), 3.57–3.90 (m, 1H, NH), 4.00–4.12 (m, 2H, CH₂), 4.27–4.40 (m, 2H, CH₂), 4.58 (s, 1H, CH), 6.32–7.04 (m, 12H, ArH), 7.35–7.53 (m, 5H, ArH), 9.53 (s, 1H, NH); ^{13}C NMR (CDCl₃, 125 MHz) δ 21.0, 42.0, 42.9, 44.4, 51.8 (2C), 120.4 (4C), 123.4 (2C), 126.2 (2C), 128.1 (2C), 128.9 (2C), 129.0 (4C), 129.4 (2C), 131.8 (2C), 134.4 (2C), 136.8 (2C), 148.1, 150.0, 186.4 (2C); HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₄H₂₈N₃O₂Cl₂, 580.1559; found 580.1562.

(6-Benzoyl-7-(4-methoxyphenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5c)



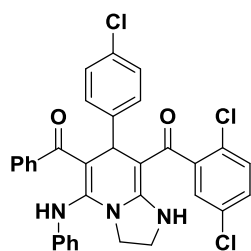
Light yellow powder; mp 203–205 °C; IR (KBr) ν 3439, 1685, 1628, 1595, 1530, 1500, 1485, 1457, 826, 754, 691 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.55–3.88 (m, 4H, $\text{OCH}_3 + \text{NH}$), 4.02–4.11 (m, 2H, CH_2), 4.27–4.40 (m, 2H, CH_2), 4.56 (s, 1H, CH), 6.32–6.35 (m, 3H, ArH), 6.71–7.06 (m, 9H, ArH), 7.34–7.55 (m, 5H, ArH), 9.52 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 41.8, 43.0, 44.5, 55.4, 114.2 (2C), 120.5 (4C), 123.5 (2C), 127.5 (4C), 128.2 (2C), 128.9 (2C), 129.1 (4C), 131.9 (2C), 134.6 (2C), 148.2 (2C), 150.1, 158.7, 186.6 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{34}\text{H}_{28}\text{N}_3\text{O}_3\text{Cl}_2$, 596.3033; found 596.3040.

(6-Benzoyl-7-(4-fluorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5d)



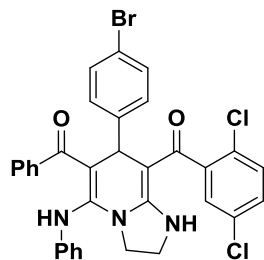
Light yellow powder; mp 206–208 °C; IR (KBr) ν 3445, 1683, 1630, 1596, 1526, 1505, 1487, 1457, 760, 696 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.59–3.89 (m, 1H, NH), 4.00–4.12 (m, 2H, CH_2), 4.29–4.40 (m, 2H, CH_2), 4.52 (s, 1H, CH), 6.15–6.48 (m, 3H, ArH), 6.78–7.07 (m, 9H, ArH), 7.36–7.54 (m, 5H, ArH), 9.52 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 41.9, 43.0, 44.5, 115.7 ($^2J_{\text{C-F}} = 241.9$ Hz) (2C), 120.3 (4C), 123.6 (2C), 128.0 (3C), 129.1 (4C), 129.2 (4C), 132.0 (2C), 134.5 (2C), 141.1 (2C), 148.1, 149.8, 161.9 ($^1J_{\text{C-F}} = 246.2$ Hz), 186.5 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{25}\text{N}_3\text{O}_2\text{Cl}_2\text{F}$, 584.1308, found 584.1315.

(6-Benzoyl-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5e)



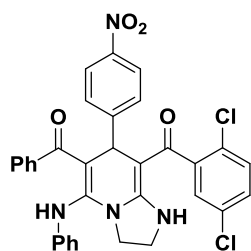
Light yellow powder; mp 216–218 °C; IR (KBr) ν 3442, 1681, 1630, 1595, 1532, 1498, 1488, 1457, 841, 764, 701 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.57–3.88 (m, 1H, NH), 4.01–4.13 (m, 2H, CH_2), 4.28–4.40 (m, 2H, CH_2), 4.52 (s, 1H, CH), 6.32–6.35 (m, 3H, ArH), 6.72–7.22 (m, 9H, ArH), 7.35–7.54 (m, 5H, ArH), 9.53 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 41.8, 43.0, 44.4, 120.2 (4C), 123.6 (2C), 127.8 (4C), 129.1 (4C), 129.1 (4C), 131.0 (2C), 132.0 (2C), 133.0 (2C), 134.3 (2C), 147.9, 149.6, 186.4 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{25}\text{N}_3\text{O}_2\text{Cl}_3$, 600.1012, found 600.1025.

(6-Benzoyl-7-(4-bromophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5f)



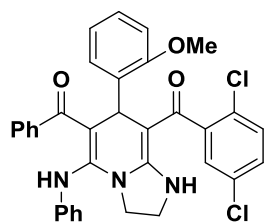
Light yellow powder; mp 222–224 °C; IR (KBr) ν 3445, 1683, 1633, 1595, 1525, 1497, 1486, 1457, 764, 700 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.56–3.86 (m, 1H, NH), 4.01–4.11 (m, 2H, CH_2), 4.28–4.40 (m, 2H, CH_2), 4.52 (s, 1H, CH), 6.32–6.35 (m, 3H, ArH), 6.66–6.73 (m, 2H, ArH), 6.98–7.13 (m, 5H, ArH), 7.37–7.54 (m, 7H, ArH), 9.52 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 42.0, 43.0, 44.5, 120.3 (4C), 121.1 (2C), 123.7 (2C), 128.2 (4C), 129.1 (4C), 129.2 (4C), 131.9 (4C), 134.4 (2C), 148.0, 149.7, 186.5 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{25}\text{N}_3\text{O}_2\text{Cl}_2\text{Br}$, 644.0507, found 644.0518.

(6-Benzoyl-7-(4-nitrophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5g)



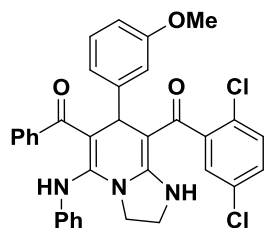
Light yellow powder; mp 243–245 °C; IR (KBr) ν 3443, 1684, 1633, 1596, 1522, 1497, 1488, 1457, 837, 767, 697 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.72–3.98 (m, 1H, NH), 4.04–4.14 (m, 2H, CH_2), 4.32–4.42 (m, 2H, CH_2), 4.52 (s, 1H, CH), 6.33 (s, 3H, ArH), 6.95–7.08 (m, 7H, ArH), 7.47–7.62 (m, 5H, ArH), 8.12 (s, 2H, ArH), 9.55 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 42.3, 43.0, 44.5, 120.1 (3C), 123.8 (2C), 124.1 (2C), 127.6 (4C), 129.2 (4C), 132.2 (2C), 134.1 (2C), 147.0 (2C), 147.7 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{25}\text{N}_4\text{O}_4\text{Cl}_2$, 611.1253; found 611.1269.

(6-Benzoyl-7-(2-methoxyphenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5h)



Light yellow powder; mp 264–266 °C; IR (KBr) ν 3282, 1681, 1629, 1596, 1545, 1494, 1485, 1458, 764, 695 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.53 (s, 3H, OCH_3), 4.00–4.37 (m, 5H, $\text{CH}_2 + \text{NH}$), 4.70 (s, 1H, CH), 6.22 (d, $J = 7.60$ Hz, 3H, ArH), 6.79–7.25 (m, 9H, ArH), 7.37–7.73 (m, 5H, ArH), 9.48 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 43.1, 44.2, 50.1, 54.8, 110.3 (2C), 120.3 (3C), 120.9 (2C), 123.3 (2C), 126.9 (2C), 128.4 (2C), 128.6 (2C), 128.8 (3C), 131.6 (2C), 134.6 (2C), 141.0 (2C), 148.2 (2C), 150.8, 155.9, 186.2 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{34}\text{H}_{28}\text{N}_3\text{O}_3\text{Cl}_2$, 596.1508; found 596.1515.

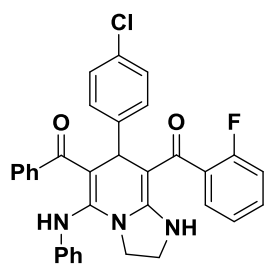
(6-Benzoyl-7-(3-methoxyphenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5i)



Light yellow powder; mp 218–220 °C; IR (KBr) ν 3327, 1683, 1624, 1597, 1529, 1495, 1486, 1456, 777, 751, 695 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.58–3.92 (m,

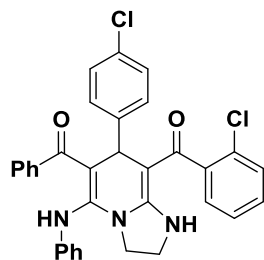
4H, OCH₃ + NH), 4.01–4.16(m, 2H, CH₂), 4.28–4.41 (m, 2H, CH₂), 4.59 (s, 1H, CH), 6.25–6.50 (m, 5H, ArH), 6.78–7.20 (m, 7H, ArH), 7.36–7.55 (m, 5H, ArH), 9.54 (s, 1H, NH); ¹³C NMR (CDCl₃, 125 MHz) δ 42.4, 42.9, 44.4, 55.2, 111.8 (2C), 113.0 (2C), 118.7 (2C), 120.4 (3C), 123.4 (2C), 128.1 (3C), 128.9 (3C), 129.0 (3C), 129.8 (2C), 131.9 (2C), 134.5 (2C), 148.1, 149.8, 186.4 (2C); HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₄H₂₈N₃O₃Cl₂, 596.1508; found 596.1519.

(6-Benzoyl-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2-fluorophenyl)methanone (5j)



Yellow powder; mp 224–225 °C; IR (KBr) ν 3296, 1681, 1637, 1621, 1594, 1511, 1493, 1457, 780, 760, cm⁻¹; ¹H NMR (CDCl₃, 500 MHz) δ 3.89 (s, 1H, NH), 3.97–4.38 (m, 4H, CH₂), 4.53–4.56 (m, 1H, CH), 6.37–6.45 (m, 3H, ArH), 6.64–6.79 (m, 4H, ArH), 6.94–7.21 (m, 6H, ArH), 7.36–7.57 (m, 5H, ArH), 9.53 (s, 1H, NH); ¹³C NMR (CDCl₃, 125 MHz) δ 41.7, 42.9, 44.4, 51.9, 85.8, 115.5 (²J_{C-F} = 21.6 Hz) (2C), 120.3 (2C), 120.7, 123.4, 123.6, 127.8 (2C), 128.1 (2C), 128.9 (3C), 129.1 (2C), 129.8 (³J_{C-F} = 7.1 Hz) (2C), 132.8, 133.4, 134.7, 138.1, 141.0, 149.9, 157.7, 158.0 (¹J_{C-F} = 241.9 Hz), 186.4, 195.4; HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₃H₂₆N₃O₂ClF, 550.1698, found 550.1685.

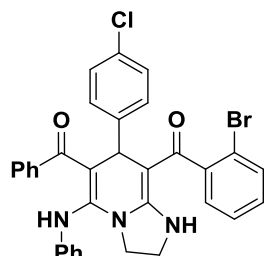
(6-Benzoyl-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2-chlorophenyl)methanone (5k)



Light yellow powder; mp 194–196 °C; IR (KBr) ν 3442, 1682, 1629, 1594, 1526, 1496, 1488, 1456, 816, 758, 738, 700 cm⁻¹; ¹H NMR (CDCl₃, 500 MHz) δ 3.67–3.90 (m, 1H, NH), 4.00–4.13 (m, 2H, CH₂), 4.25–4.39 (m, 2H, CH₂), 4.51 (s, 1H, CH), 6.20–6.50 (m, 3H, ArH), 6.59–7.20 (m, 10H, ArH), 7.43–7.55 (m, 5H, ArH), 9.56 (s, 1H, NH); ¹³C NMR (CDCl₃, 125 MHz) δ 41.9, 43.0, 44.4, 51.9, 85.5, 120.3 (3C),

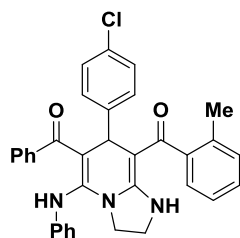
123.5 (2C), 127.9 (3C), 128.2 (3C), 128.8 (3C), 129.0 (2C), 129.1 (4C), 132.8, 133.5, 134.6, 148.1, 149.8, 157.8, 188.4 (2C); HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{33}H_{26}N_3O_2Cl_2$, 566.1402; found 566.1410.

(6-Benzoyl-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2-bromophenyl)methanone (5l)



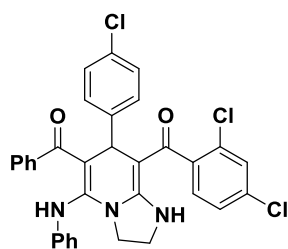
Yellow powder; mp 190–192 °C; IR (KBr) ν 3245, 1680, 1653, 1627, 1594, 1528, 1485, 1455, 816, 756, 692 cm^{-1} ; 1H NMR ($CDCl_3$, 500 MHz) δ 3.64–3.89 (m, 1H, NH), 4.00–4.50 (m, 4H, CH_2), 4.50 (s, 1H, CH), 6.23–6.37 (m, 3H, ArH), 6.63–7.25 (m, 10H, ArH), 7.34–7.56 (m, 5H, ArH), 9.57 (s, 1H, NH); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 42.0, 43.0, 44.5, 120.3 (3C), 123.6 (2C), 126.6 (2C), 127.6 (2C), 128.0 (2C), 128.4 (2C), 128.9 (2C), 129.1 (3C), 132.1 (2C), 133.6 (2C), 134.5 (2C), 148.0 (2C), 149.8, 157.9, 189.2 (2C); HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{33}H_{26}N_3O_2ClBr$, 610.0897, found 610.0885.

(6-Benzoyl-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(*o*-tolyl)methanone (5m)



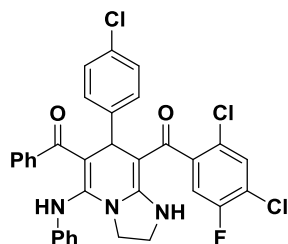
Yellow powder; mp 170–172 °C; IR (KBr) ν 3306, 1683, 1629, 1595, 1524, 1487, 1456, 779, 695, cm^{-1} ; 1H NMR ($CDCl_3$, 500 MHz) δ 1.72 (s, 3H, CH_3), 3.79 (s, 1H, NH), 3.99–4.11 (m, 2H, CH_2), 4.23–4.39 (m, 2H, CH_2), 4.46 (s, 1H, CH), 6.22–6.35 (m, 3H, ArH), 6.60–7.19 (m, 10H, ArH), 7.38–7.57 (m, 5H, ArH), 9.58 (s, 1H, NH); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 18.4, 42.2, 42.9, 44.4, 51.9, 85.7, 120.4 (2C), 123.5, 124.6, 125.1, 127.7 (2C), 127.9 (2C), 128.1 (2C), 128.8 (2C), 128.9 (2C), 129.1 (2C), 130.0, 132.7, 133.5, 134.4, 140.5, 142.0, 148.1, 149.9, 157.4, 192.6, 195.2; HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{34}H_{29}N_3O_2Cl$, 546.1948, found 546.1936.

(6-Benzoyl-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,4-dichlorophenyl)methanone (5n)



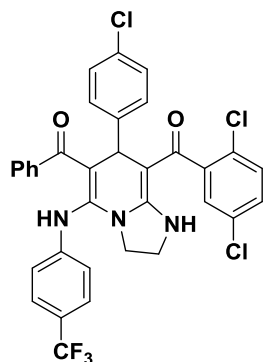
Light yellow powder; mp 218–220 °C; IR (KBr) ν 3308, 1684, 1625, 1595, 1531, 1498, 1487, 1454, 824, 776, 764, 702 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.65–3.85 (m, 1H, NH), 3.99–4.10 (m, 2H, CH_2), 4.23–4.38 (m, 2H, CH_2), 4.53 (s, 1H, CH), 6.10–6.40 (m, 3H, ArH), 6.78–7.23 (m, 9H, ArH), 7.39–7.67 (m, 5H, ArH), 9.55 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 41.8, 43.0, 44.4, 120.2 (3C), 123.6 (2C), 127.8 (3C), 128.2 (3C), 128.9 (2C), 129.1 (3C), 133.0 (2C), 133.7 (2C), 134.1 (2C), 134.4 (2C), 147.9 (2C), 149.6, 158.0, 187.0 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{25}\text{N}_3\text{O}_2\text{Cl}_3$, 600.1012; found 600.1009.

(6-Benzoyl-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,4-dichloro-5-fluorophenyl)methanone (5o)



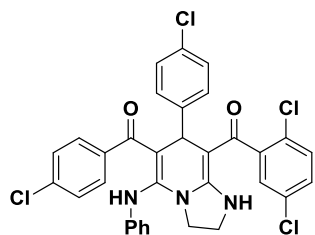
Light yellow powder; mp 250–252 °C; IR (KBr) ν 3282, 1683, 1628, 1594, 1542, 1500, 1488, 1459, 849, 781, 694 cm^{-1} ; ^1H NMR ($\text{DMSO-}d_6$, 500 MHz) δ 3.62–3.79 (m, 1H, NH), 3.91–4.12 (m, 4H, CH_2), 4.46 (s, 1H, CH), 5.92–6.30 (m, 3H, ArH), 6.91–7.08 (m, 5H, ArH), 7.32–7.66 (m, 8H, ArH), 9.48 (s, 1H, NH); ^{13}C NMR ($\text{DMSO-}d_6$, 125 MHz) δ 42.0, 43.5, 44.5, 120.0, 120.2 (4C), 123.7 (2C), 128.4 (4C), 128.8 (4C), 129.1 (2C), 129.5 (4C), 132.1, 134.1, 134.5, 148.4, 149.6, 155.7 ($^1J_{\text{C-F}} = 249.1$ Hz), 157.2, 183.3 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{24}\text{N}_3\text{O}_2\text{Cl}_3\text{F}$, 618.0918; found 618.0925.

(6-Benzoyl-7-(4-chlorophenyl)-5-((4-(trifluoromethyl)phenyl)amino)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5p)



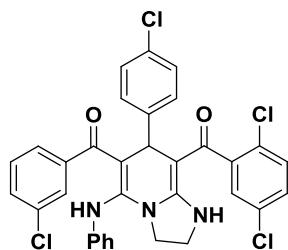
Light yellow powder; mp 204–206 °C; IR (KBr) ν 3440, 1683, 1630, 1612, 1533, 1492, 1457, 1324, 858, 778, 689 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.62–3.93 (m, 1H, NH), 4.02–4.12 (m, 2H, CH_2), 4.26–4.40 (m, 2H, CH_2), 5.20 (s, 1H, CH) 6.30–6.44 (m, 3H, ArH), 6.76–7.25 (m, 6H, ArH), 7.34–7.55 (m, 7H, ArH), 9.53 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 42.0, 43.0, 44.5, 120.6 (4C), 124.4 ($^1J_{\text{C-F}} = 326.0$ Hz), 125.6 ($^2J_{\text{C-F}} = 85.7$ Hz), 126.4 (4C), 127.8 (4C), 129.1 (3C), 129.2 (4C), 132.1 (2C), 133.2 (2C), 134.0 (2C), 149.9, 151.2, 186.7 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{34}\text{H}_{24}\text{N}_3\text{O}_2\text{Cl}_3\text{F}_3$, 668.0886; found 668.0895.

(6-(4-Chlorobenzoyl)-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5q)



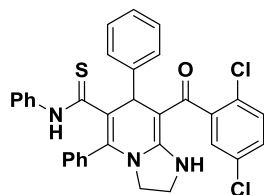
Light yellow powder; mp 224–226 °C; IR (KBr) ν 3442, 1683, 1629, 1590, 1527, 1498, 1487, 1457, 816, 781, 701 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.52–3.84 (m, 1H, NH), 4.01–4.11 (m, 2H, CH_2), 4.27–4.39 (m, 2H, CH_2), 4.46 (s, 1H, CH), 6.33 (s, 3H, ArH), 6.69–7.25 (m, 9H, ArH), 7.27–7.48 (m, 4H, ArH), 9.52 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 42.0, 43.0, 44.5, 120.2 (4C), 123.7 (3C), 127.8 (3C), 129.0 (3C), 129.2 (3C), 129.2 (4C), 129.4 (2C), 132.2 (2C), 133.2 (2C), 148.0, 149.3, 186.4 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{24}\text{N}_3\text{O}_2\text{Cl}_4$, 634.0623; found 634.0631.

(6-(3-Chlorobenzoyl)-7-(4-chlorophenyl)-5-(phenylamino)-1,2,3,7-tetrahydroimidazo[1,2-a]pyridin-8-yl)(2,5-dichlorophenyl)methanone (5r)



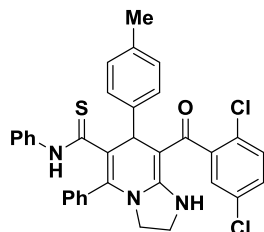
Light yellow powder; mp 215–217 °C; IR (KBr) ν 3439, 1684, 1629, 1590, 1527, 1498, 1487, 1456, 816, 781, 700 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.52–3.84 (m, 1H, NH), 4.03–4.09 (m, 2H, CH_2), 4.28–4.39 (m, 2H, CH_2), 4.46 (s, 1H, CH), 6.33 (s, 3H, ArH), 6.69–7.22 (m, 9H, ArH), 7.32–7.48 (m, 4H, ArH), 9.52 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 41.9, 42.9, 44.4, 120.2 (5C), 123.6 (4C), 127.7 (5C), 129.1 (6C), 132.1 (2C), 132.6 (2C), 133.1 (2C), 147.9, 149.3, 186.3 (2C); HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{24}\text{N}_3\text{O}_2\text{Cl}_4$, 634.0623; found 634.0630.

8-(2,5-Dichlorobenzoyl)-N,5,7-triphenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6a)



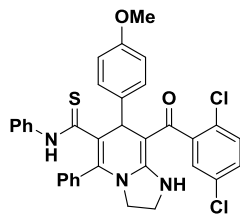
Yellow powder; mp 189–191 °C; IR (KBr) ν 3382, 1643, 1606, 1497, 1480, 1453, 1441, 1289, 765, 700 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.22–3.24 (m, 1H, CH₂), 3.78–3.79 (m, 3H, CH₂), 5.12–5.54 (m, 1H, NH), 6.05–7.68 (m, 18H, ArH), 9.38 (s, 1H, CH), 10.18–10.42 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 43.1, 45.6, 46.8, 87.8 (2C), 123.9, 124.7 (3C), 126.3, 126.6, 127.9 (4C), 128.1 (2C), 128.4 (4C), 128.6 (2C), 129.1 (2C), 130.7, 131.5, 133.4, 139.1, 143.2, 157.1, 185.7, 197.7; HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₃H₂₆N₃OSCl₂, 582.1174; found 582.1185.

8-(2,5-Dichlorobenzoyl)-N,5-diphenyl-7-(*p*-tolyl)-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6b)



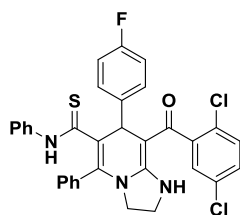
Yellow green powder; mp 227–229 °C; IR (KBr) ν 3384, 1643, 1605, 1508, 1479, 1451, 1289, 761, 700 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 2.18 (s, 3H, CH₃), 3.10–3.12 (m, 1H, CH₂), 3.66–3.68 (m, 3H, CH₂), 4.98–5.60 (m, 1H, NH), 5.93–7.56 (m, 17H, ArH), 9.26 (s, 1H, CH), 10.00–10.50 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 21.1, 43.1, 45.1, 46.8, 87.9 (2C), 124.7 (2C), 126.6 (2C), 127.8 (2C), 128.4 (3C), 128.7 (3C), 128.9 (2C), 129.1 (2C), 130.7 (2C), 131.5 (2C), 133.4 (2C), 135.1 (2C), 139.1 (2C), 185.8, 197.7; HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₄H₂₈N₃OCl₂S, 596.1330; found 596.1337.

8-(2,5-Dichlorobenzoyl)-7-(4-methoxyphenyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6c)



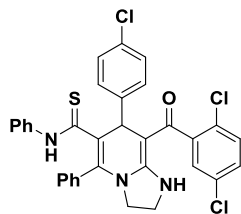
Yellow green powder; mp 212–214 °C; IR (KBr) ν 3440, 1639, 1606, 1508, 1498, 1479, 1287, 763, 700 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.11–3.13 (m, 1H, CH₂), 3.60–3.75 (m, 6H, CH₂ + CH₃), 4.96–5.60 (m, 1H, NH), 5.74–7.57 (m, 17H, ArH), 9.26 (s, 1H, CH), 10.15–10.25 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 43.1, 44.6, 46.8, 55.4, 88.0 (2C), 113.6 (2C), 124.7 (3C), 126.6 (3C), 128.4 (4C), 128.6 (2C), 128.9 (4C), 129.1 (3C), 130.7, 131.5, 133.5, 139.2, 158.0, 185.9, 197.8; HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₄H₂₈N₃O₂Cl₂S, 612.1279; found 612.1285.

8-(2,5-Dichlorobenzoyl)-7-(4-fluorophenyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6d)



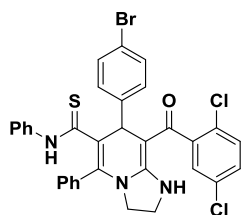
Yellow powder; mp 172–174 °C; IR (KBr) ν 3439, 1643, 1601, 1504, 1479, 1452, 1290, 763, 697 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.23–3.24 (m, 1H, CH₂), 3.78–3.83 (m, 3H, CH₂), 5.13–5.27 (m, 1H, NH), 6.11–7.66 (m, 17H, ArH), 9.40 (s, 1H, CH), 10.26–10.38 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 43.1, 44.8, 46.7, 87.6, 114.7 ($^2J_{\text{C-F}} = 20.7$ Hz) (2C), 124.7 (3C), 126.7 (2C), 127.2 (2C), 128.5 (4C), 128.6 (2C), 129.0, 129.2 (2C), 129.7 (2C), 130.6, 131.6, 133.3, 139.1, 143.3, 157.0, 161.1 ($^1J_{\text{C-F}} = 241.9$ Hz), 185.8, 197.6; HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₃H₂₅N₃OSC₂F, 600.1079; found 600.1082.

7-(4-Chlorophenyl)-8-(2,5-dichlorobenzoyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6e)



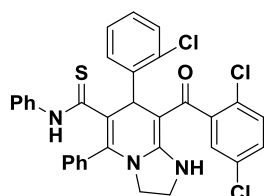
Yellow powder; mp 208–210 °C; IR (KBr) ν 3379, 1643, 1604, 1497, 1481, 1451, 1443, 1288, 765, 704 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.07–3.20 (m, 1H, CH₂), 3.63–3.75 (m, 3H, CH₂), 5.02–5.13 (m, 1H, NH), 6.02–7.55 (m, 17H, ArH), 9.30 (s, 1H, CH), 10.18–10.22 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 43.2, 44.9, 46.7, 79.6, 87.3, 124.7 (3C), 126.7, 128.1 (3C), 128.5 (3C), 128.9 (2C), 129.2 (2C), 129.7 (3C), 130.6 (2C), 131.0 (2C), 131.6 (2C), 133.3 (2C), 139.1, 185.7, 197.5; HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for C₃₃H₂₅N₃OCl₃S, 616.0784; found 616.0796.

7-(4-Bromophenyl)-8-(2,5-dichlorobenzoyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-a]pyridine-6-carbothioamide (6f)



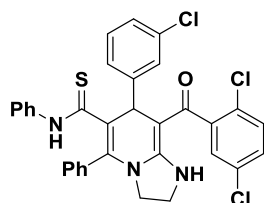
Yellow powder; mp 224–226 °C; IR (KBr) ν 3442, 1640, 1605, 1497, 1481, 1451, 1446, 1289, 816, 745, 704 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.19–3.29 (m, 1H, CH₂), 3.70–3.85 (m, 3H, CH₂), 5.11–5.25 (m, 1H, NH), 6.12–7.64 (m, 17H, ArH), 9.40 (s, 1H, CH), 10.29–10.38 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 43.2, 45.1, 46.8, 87.3 (2C), 119.6 (2C), 124.7 (3C), 126.7, 127.3, 127.5, 128.5 (3C), 128.5, 128.7, 128.9, 129.2, 130.1 (3C), 130.6, 131.0 (3C), 131.7, 133.3, 139.1, 157.0, 185.7, 197.5; HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for C₃₃H₂₅N₃OSCl₂Br, 660.0279; found 660.0285.

7-(2-Chlorophenyl)-8-(2,5-dichlorobenzoyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-a]pyridine-6-carbothioamide (6g)



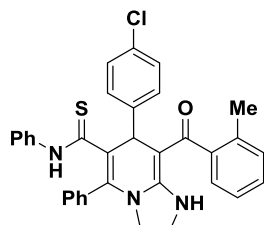
Yellow powder; mp 193–195 °C; IR (KBr) ν 3386, 1644, 1606, 1497, 1480, 1445, 1442, 1289, 761 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.27–3.30 (m, 1H, CH₂), 3.77–3.78 (m, 3H, CH₂), 5.37–5.54 (m, 1H, NH), 5.93–7.60 (m, 17H, ArH), 9.36–9.40 (m, 1H, CH), 10.47–10.78 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 42.6, 43.3, 46.7, 88.4 (2C), 124.4, 124.8, 126.5 (2C), 127.9 (3C), 128.5 (4C), 128.8, 129.1 (3C), 130.5 (3C), 131.1, 131.8 (3C), 133.2, 139.3, 143.3, 157.5, 185.6, 197.1; HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₃H₂₆N₃OSCl₃, 616.0784; found 616.0775.

7-(3-Chlorophenyl)-8-(2,5-dichlorobenzoyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-a]pyridine-6-carbothioamide (6h)



Yellow green powder; mp 164–166 °C; IR (KBr) ν 3445, 1644, 1606, 1497, 1479, 1444, 1290, 769, 703 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 3.24–3.25 (m, 1H, CH₂), 3.77–3.84 (m, 3H, CH₂), 5.10–5.35 (m, 1H, NH), 6.15–7.63 (m, 17H, ArH), 9.41 (s, 1H, CH), 10.30–10.40 (m, 1H, NH); ^{13}C NMR (DMSO- d_6 , 125 MHz) δ 43.2, 45.5, 46.7, 87.1 (2C), 122.8, 124.7 (2C), 126.3, 126.7 (3C), 127.8, 128.5 (4C), 128.9, 129.2 (3C), 129.9, 130.6, 131.1, 131.7, 132.8, 133.2, 139.0, 143.1, 149.1, 156.9, 185.7, 197.5; HRMS (ESI-TOF, [M + H]⁺) calcd for C₃₃H₂₅N₃OSCl₃, 616.0784; found 616.0796.

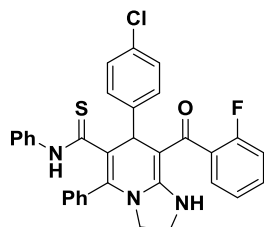
7-(4-Chlorophenyl)-8-(2-methylbenzoyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-a]pyridine-6-carbothioamide (6i)



Yellow powder; mp 235–237 °C; IR (KBr) ν 3244, 1645, 1606, 1499, 1475, 1452, 1363, 785, 699 cm^{-1} ; ^1H NMR (DMSO- d_6 , 500 MHz) δ 1.78 (s, 3H, CH₃), 3.12–3.14 (m, 1H, CH₂), 3.67–3.71 (m, 3H, CH₂), 5.14 (s, 1H, NH), 6.70–7.58 (m, 18H, ArH), 9.31 (s, 1H, CH), 10.20 (s, 1H, NH); ^{13}C NMR (CDCl₃, 125 MHz) δ 18.6, 42.7, 46.0, 46.8, 88.7 (2C), 123.8, 125.3 (2C), 125.6, 126.8, 127.9, 128.1 (2C), 128.2, 128.5 (2C),

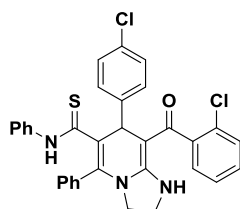
128.8, 129.0 (2C), 129.2, 129.4, 129.7, 130.1, 131.0, 131.9, 133.3, 134.3, 137.7, 141.5, 145.3, 156.8, 194.3 197.0; HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{34}H_{29}N_3OSCl$, 562.1720, found 562.1725.

7-(4-Chlorophenyl)-8-(2-fluorobenzoyl)-*N*,5-diphenyl-1,2,3,7-tetrahydroimidazo [1,2-*a*]pyridine-6-carbothioamide (6j)



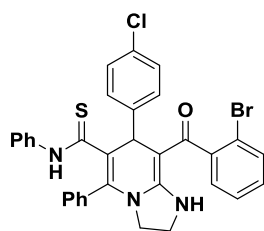
Yellow powder; mp 217–219 °C; IR (KBr) ν 3370, 1640, 1606, 1497, 1479, 1452, 782, 759, 703 cm^{-1} ; 1H NMR ($CDCl_3$, 500 MHz) δ 3.18–3.34 (m, 1H, CH_2), 3.61–3.92 (m, 3H, CH_2), 5.39 (s, 1H, NH), 6.59–7.22 (m, 13H, ArH), 7.42–7.57 (m, 6H, ArH), 9.49 (s, 1H, NH); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 42.7, 45.4, 46.8, 88.9 (2C), 115.7 ($^2J_{C-F}$ = 21.7 Hz) (2C), 123.8, 124.0, 125.3, 127.0, 128.0, 128.2 (3C), 128.6 (3C), 128.7 (2C), 128.9, 129.2, 129.5, 129.8, 130.6, 132.0, 133.1, 137.6, 145.0, 157.1, 158.4 ($^1J_{C-F}$ = 241.9 Hz), 188.1, 197.7; HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{33}H_{26}N_3OSClF$, 566.1469, found 566.1475.

8-(2-Chlorobenzoyl)-7-(4-chlorophenyl)-*N*,5-diphenyl-1,2,3,7-tetrahydroimidazo [1,2-*a*]pyridine-6-carbothioamide (6k)



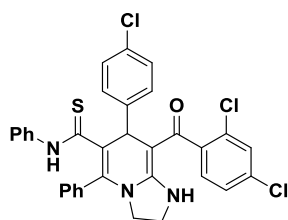
Yellow green powder; mp 241–243 °C; IR (KBr) ν 3441, 1636, 1606, 1497, 1478, 1442, 1290, 760, 703 cm^{-1} ; 1H NMR ($DMSO-d_6$, 500 MHz) δ 3.05–3.15 (m, 1H, CH_2), 3.60–3.75 (m, 3H, CH_2), 5.05–5.14 (m, 1H, NH), 6.21–7.54 (m, 18H, ArH), 9.29 (s, 1H, CH), 10.02–10.33 (m, 1H, NH); ^{13}C NMR ($DMSO-d_6$, 125 MHz) δ 43.1, 45.2, 46.8, 87.4 (2C), 123.5, 124.7 (3C), 126.7 (2C), 128.0 (3C), 128.5 (4C), 128.7, 128.9, 129.2, 129.7 (3C), 130.6, 130.7, 131.5, 133.4, 139.1, 141.5, 156.9, 187.8, 197.7; HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{33}H_{26}N_3OCl_2S$, 582.1174; found 582.1170.

8-(2-Bromobenzoyl)-7-(4-chlorophenyl)-*N*,5-diphenyl-1,2,3,7-tetrahydroimidazo [1,2-*a*]pyridine-6-carbothioamide (6l)



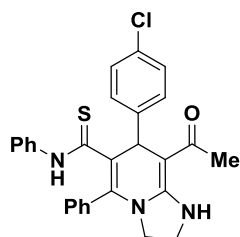
Yellow powder; mp 221–222 °C; IR (KBr) ν 3278, 1633, 1601, 1498, 1477, 1442, 780, 760 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.20–3.38 (m, 1H, CH_2), 3.70–3.88 (m, 3H, CH_2), 5.12–5.40 (m, 1H, NH), 6.33–7.11 (m, 11H, ArH), 7.41–7.58 (m, 8H, ArH), 9.45 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 42.7, 45.9, 46.9, 88.1 (2C), 119.5, 124.0 (2C), 125.5, 127.0 (3C), 128.2 (3C), 128.6 (4C), 128.9 (3C), 129.2 (2C), 129.5 (2C), 129.8, 132.0, 133.1, 137.5, 157.2, 190.9, 197.7; HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{26}\text{N}_3\text{O}\text{SClBr}$, 626.0668, found 626.0675.

7-(4-Chlorophenyl)-8-(2,4-dichlorobenzoyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-a]pyridine-6-carbothioamide (6m)



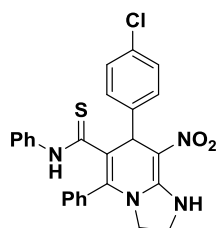
Light yellow powder; mp 183–185 °C; IR (KBr) ν 3441, 1643, 1606, 1497, 1481, 1443, 1290, 825, 749, 705 cm^{-1} ; ^1H NMR ($\text{DMSO}-d_6$, 500 MHz) δ 3.05–3.18 (m, 1H, CH_2), 3.63–3.75 (m, 3H, CH_2), 5.05–5.12 (m, 1H, NH), 6.23–7.54 (m, 17H, ArH), 9.29 (s, 1H, CH), 10.10–10.35 (m, 1H, NH); ^{13}C NMR ($\text{DMSO}-d_6$, 125 MHz) δ 43.2, 45.5, 46.8, 87.3 (2C), 123.3, 124.8 (3C), 126.7 (2C), 128.1 (3C), 128.5 (4C), 128.7 (2C), 128.9, 129.2 (2C), 129.6 (3C), 130.6, 130.9, 133.3, 139.1, 157.0, 186.4, 197.5; HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{33}\text{H}_{25}\text{N}_3\text{OCl}_3\text{S}$, 616.0784; found 616.0789.

8-Acetyl-7-(4-chlorophenyl)-N,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-a]pyridine-6-carbothioamide (6n)



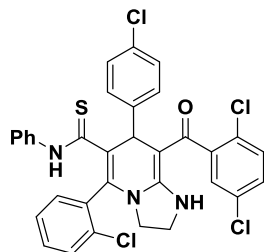
Yellow powder; mp 233–235 °C; IR (KBr) ν 3295, 3055, 2879, 1652, 1612, 1479, 1367, 837, 750 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 1.92 (s, 3H, CH_3), 3.10–3.22 (m, 1H, CH_2), 3.60–3.78 (m, 3H, CH_2), 5.66 (s, 1H, NH), 6.69–6.70 (m, 2H, ArH), 7.12–7.25 (m, 4H, ArH), 7.35–7.68 (m, 9H, ArH), 9.25 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 26.7, 42.5, 45.8, 46.8, 87.4 (2C), 124.1, 124.6, 127.1, 128.0 (2C), 128.6 (3C), 128.7 (4C), 129.4, 129.8, 131.4, 132.3, 133.4, 137.7, 144.8, 155.8, 194.4, 198.3; HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{28}\text{H}_{25}\text{N}_3\text{OSCl}$, 486.1407, found 486.1425.

7-(4-Chlorophenyl)-8-nitro-*N*,5-diphenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6o)



Light yellow powder; mp 209–211 °C; IR (KBr) ν 3421, 3351, 3250, 3061, 2884, 1637, 1602, 1488, 1456, 1377, 850, 768 cm^{-1} ; ^1H NMR ($\text{DMSO-}d_6$, 500 MHz) δ 3.26–3.33 (m, 1H, CH_2), 3.70–3.80 (m, 3H, CH_2), 5.69 (s, 1H, NH), 6.75 (d, $J = 7.70$ Hz, 2H, ArH), 7.09–7.62 (m, 12H, ArH), 9.32 (s, 1H, CH), 10.45 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 45.8, 47.6, 49.9, 108.1 (2C), 124.9, 126.9 (2C), 129.1 (2C), 129.7, 130.6 (3C), 130.8 (3C), 131.3, 131.7, 132.2 (2C), 132.8, 133.7, 135.0, 141.2, 144.2, 155.1, 198.6; HRMS (ESI-TOF, $[\text{M} + \text{H}]^+$) calcd for $\text{C}_{26}\text{H}_{22}\text{N}_4\text{O}_2\text{SCl}$, 489.1152, found 489.1165.

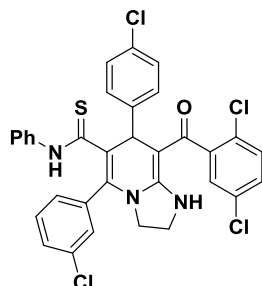
5-(2-Chlorophenyl)-7-(4-chlorophenyl)-8-(2,5-dichlorobenzoyl)-*N*-phenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6p)



Yellow powder; mp 213–215 °C; IR (KBr) ν 3440, 3360, 3046, 2898, 1653, 1609, 1510, 1488, 1363, 808, 751 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 3.30–3.36 (m, 1H, CH_2), 3.64–3.66 (m, 1H, CH_2), 3.79–3.89 (m, 2H, CH_2), 5.08 (s, 1H, NH), 6.21–7.85 (m, 17H, ArH), 9.41 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 125 MHz) δ 43.0, 44.1, 45.3,

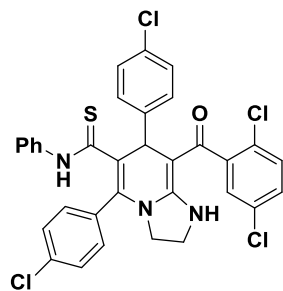
87.9 (2C), 123.7 (3C), 125.8, 127.1 (2C), 128.3 (3C), 128.6 (3C), 129.0 (3C), 130.0, 130.5, 131.3, 131.4, 132.0, 132.4, 133.4, 137.6, 141.9, 144.9, 156., 188.3, 197.0; HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{33}H_{24}N_3OSCl_4$, 650.0394, found 650.0383.

5-(3-Chlorophenyl)-7-(4-chlorophenyl)-8-(2,5-dichlorobenzoyl)-*N*-phenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6q)



Yellow powder; mp 173-175 °C; IR (KBr) ν 3440, 2919, 2847, 1644, 1608, 1494, 1452, 1361, 818, 691 cm^{-1} ; 1H NMR ($CDCl_3$, 500 MHz) δ 3.29–3.31 (m, 1H, CH_2), 3.75–3.86 (m, 3H, CH_2), 5.13 (s, 1H, NH), 6.64–7.17 (m, 11H, ArH), 7.27–7.56 (m, 6H, ArH), 9.45 (s, 1H, NH); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 42.6, 45.2, 46.7, 88.2 (2C), 123.7 (2C), 124.7, 125.6, 127.0, 127.5, 128.3 (3C), 128.6 (3C), 128.9 (3C), 129.7 (2C), 130.6 (2C), 131.1, 132.3 (2C), 135.6, 137.4, 141.7, 157.2, 187.7, 197.2; HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{33}H_{24}N_3OSCl_4$, 650.0394, found 650.0399.

5,7-Bis(4-chlorophenyl)-8-(2,5-dichlorobenzoyl)-*N*-phenyl-1,2,3,7-tetrahydroimidazo[1,2-*a*]pyridine-6-carbothioamide (6r)

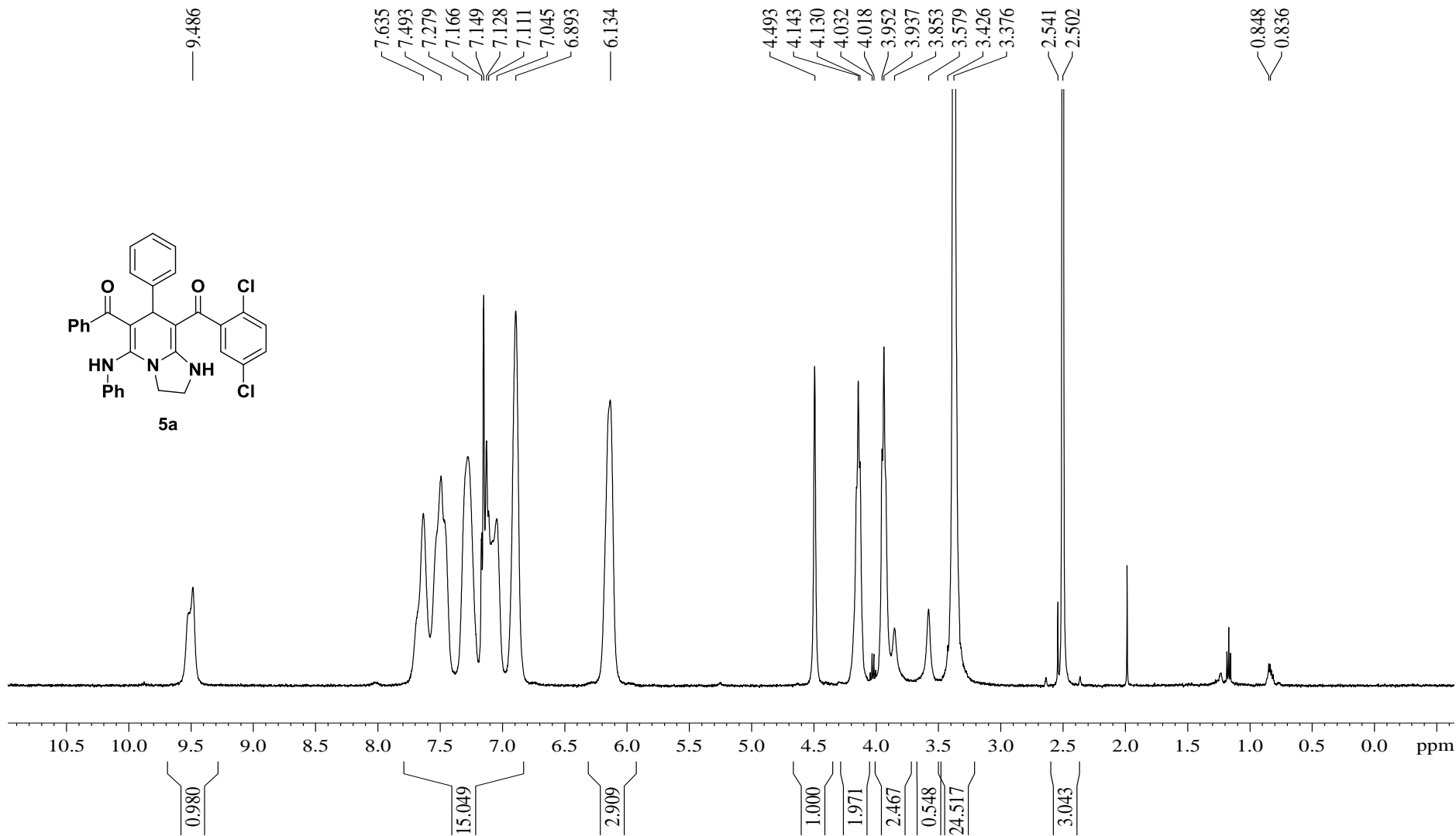
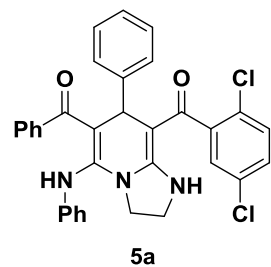


Yellow powder; mp 164–166 °C; IR (KBr) ν 3441, 2921, 2884, 1644, 1605, 1494, 1453, 1361, 816, 694 cm^{-1} ; 1H NMR ($CDCl_3$, 500 MHz) δ 3.28–3.30 (m, 1H, CH_2), 3.67–3.86 (m, 3H, CH_2), 5.00–5.40 (m, 1H, NH), 6.19–6.98 (m, 12H, ArH), 7.33–7.56 (m, 5H, ArH), 9.44 (s, 1H, NH); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 42.7, 45.4, 46.8, 88.2 (2C), 122.7, 123.8 (2C), 125.8, 127.2, 128.4 (3C), 128.7 (4C), 129.1 (3C), 129.5, 129.8, 129.9, 130.1, 130.8, 131.2, 132.4, 132.7, 135.7, 137.3, 157.2, 188.2, 197.4; HRMS (ESI-TOF, $[M + H]^+$) calcd for $C_{33}H_{24}N_3OSCl_4$, 650.0386, found 650.0399.

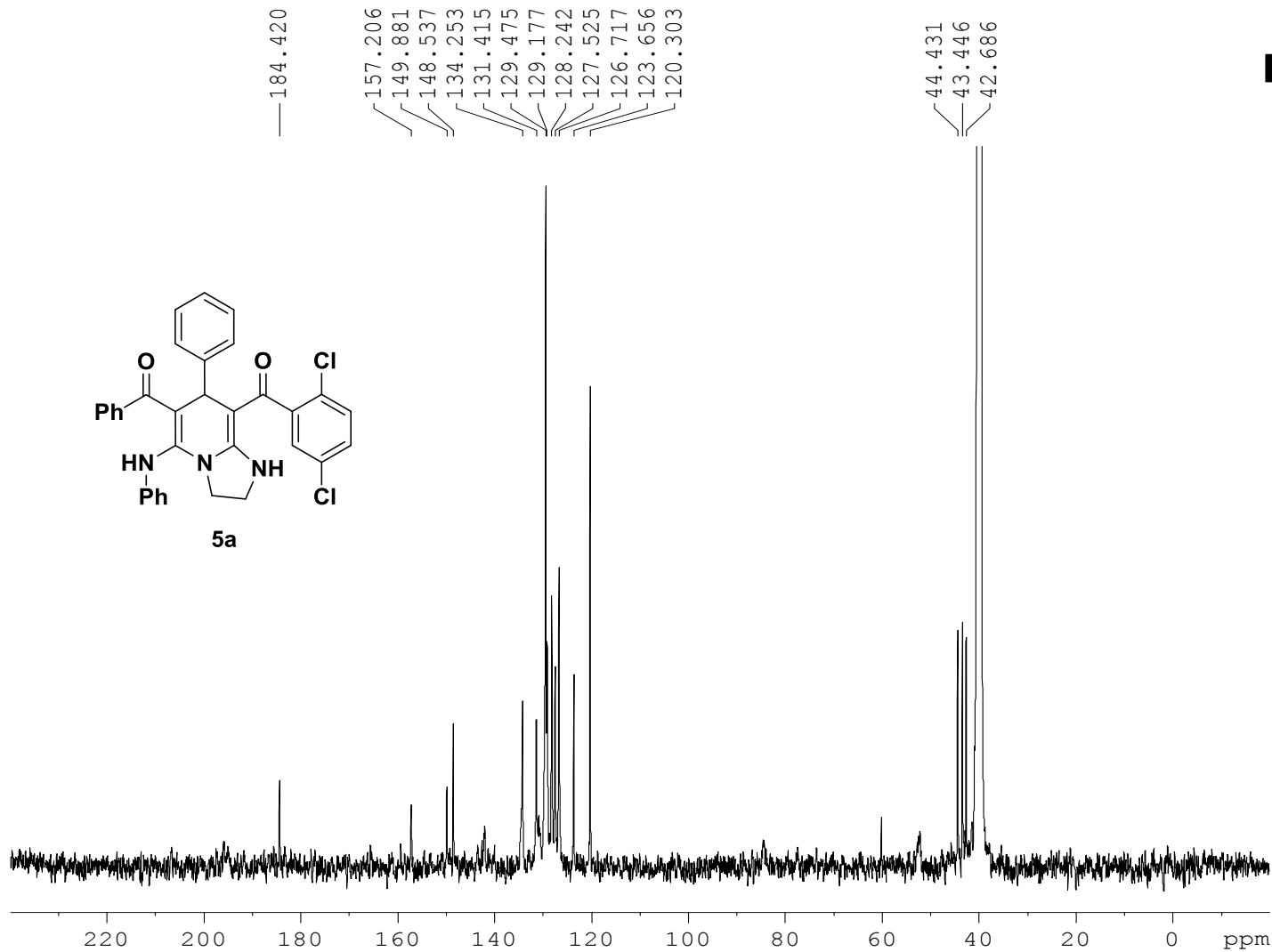
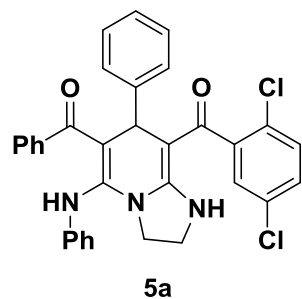
SP-E-9

1H

2012 04 24



SP-E-9 13C 1D 2012 04 29



NAM SP-E-
EXPNO 2
PROCNO 1
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Time_ 21.35
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2061
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1620
DW 15.300 usec
DE 6.00 usec
TE 299.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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SFO1 125.7464750 MHz

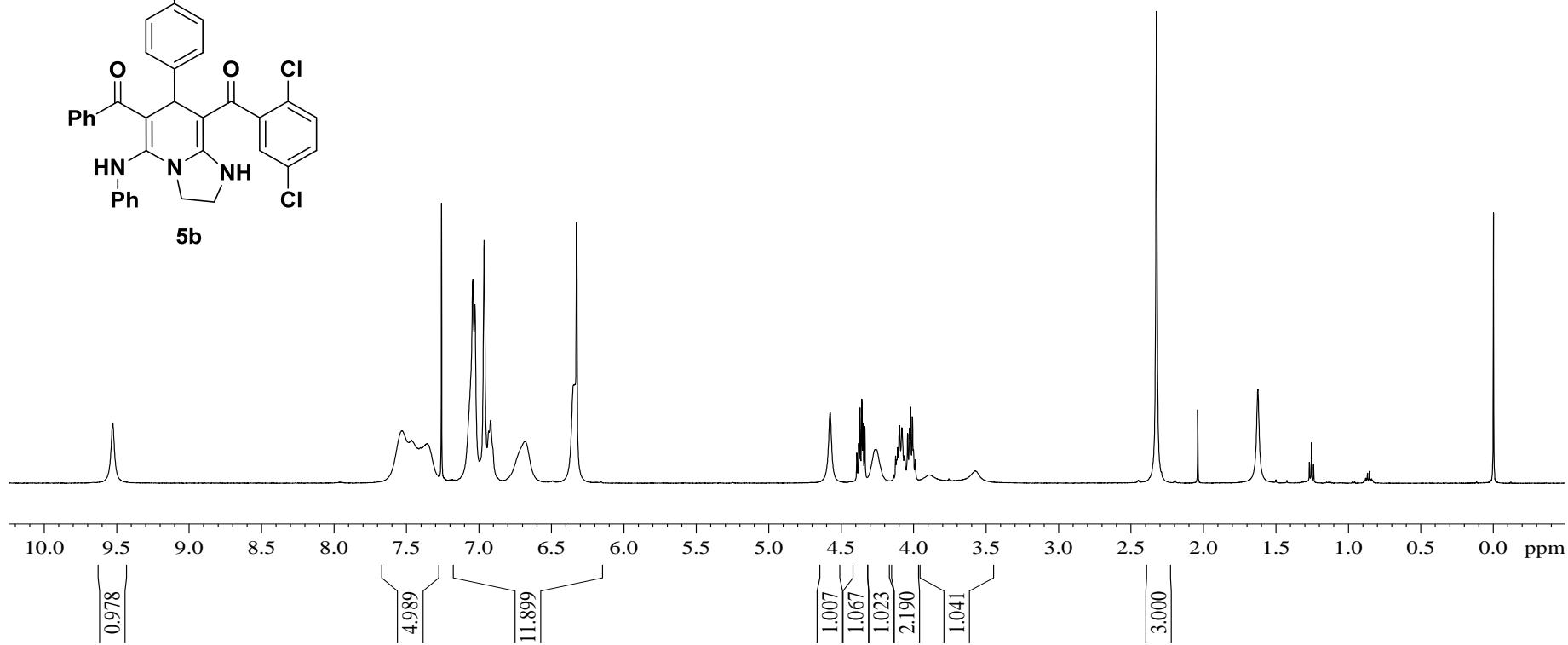
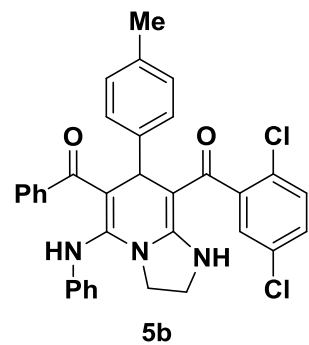
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PL12 17.66 dB
PL13 17.66 dB
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SI 32768
SF 125.7326485 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 2.00

SP-E-3

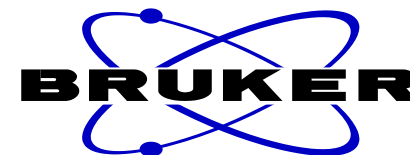
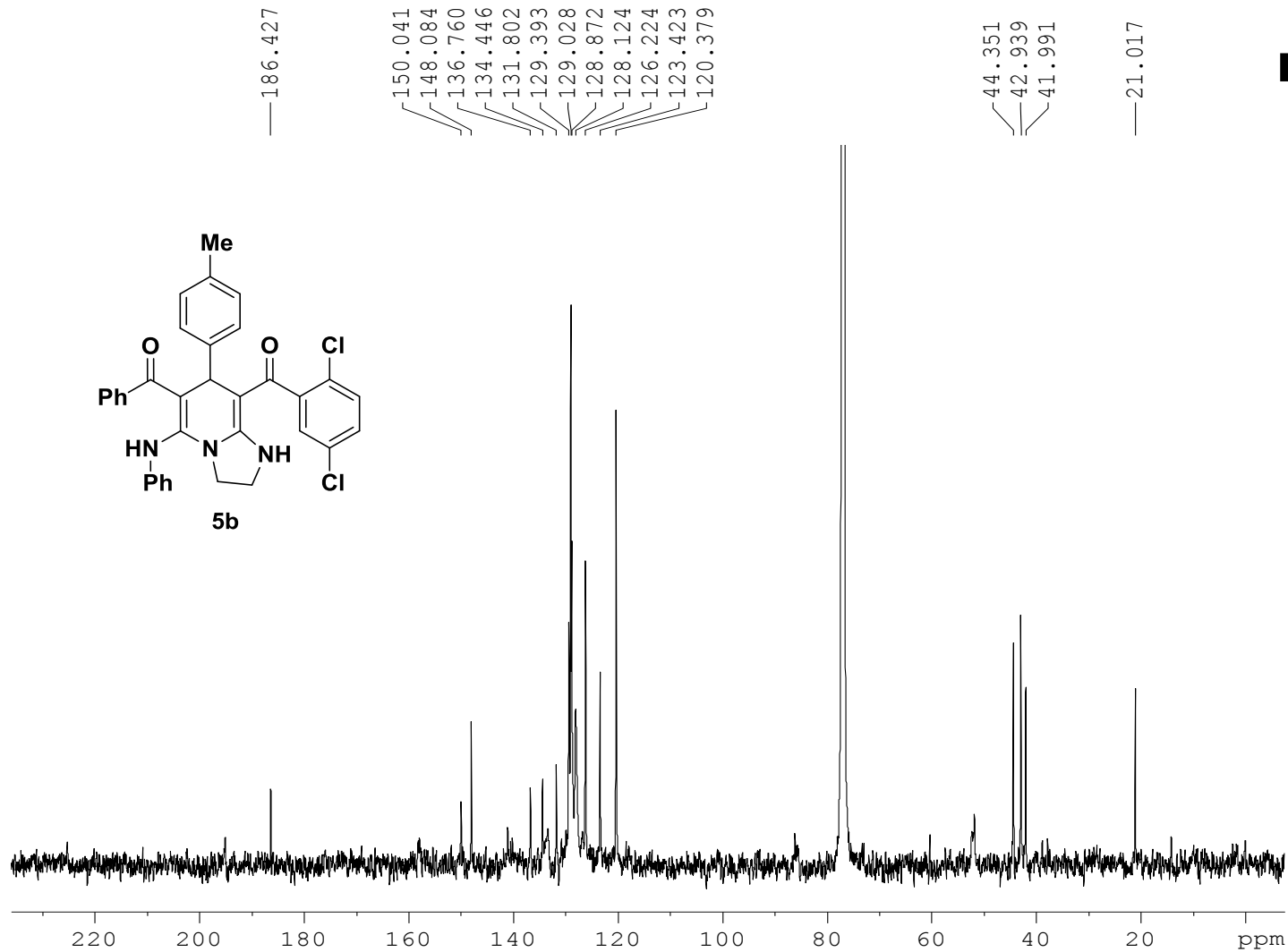
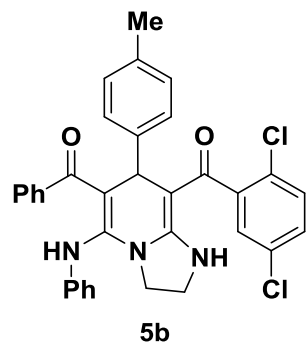
1H 1D 2014 07 03

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SP-E-3 13C 1D 2012 04 28

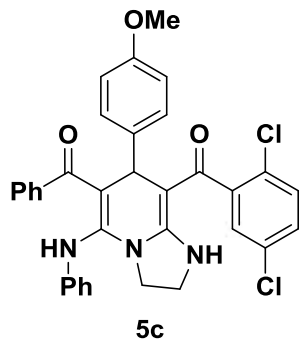
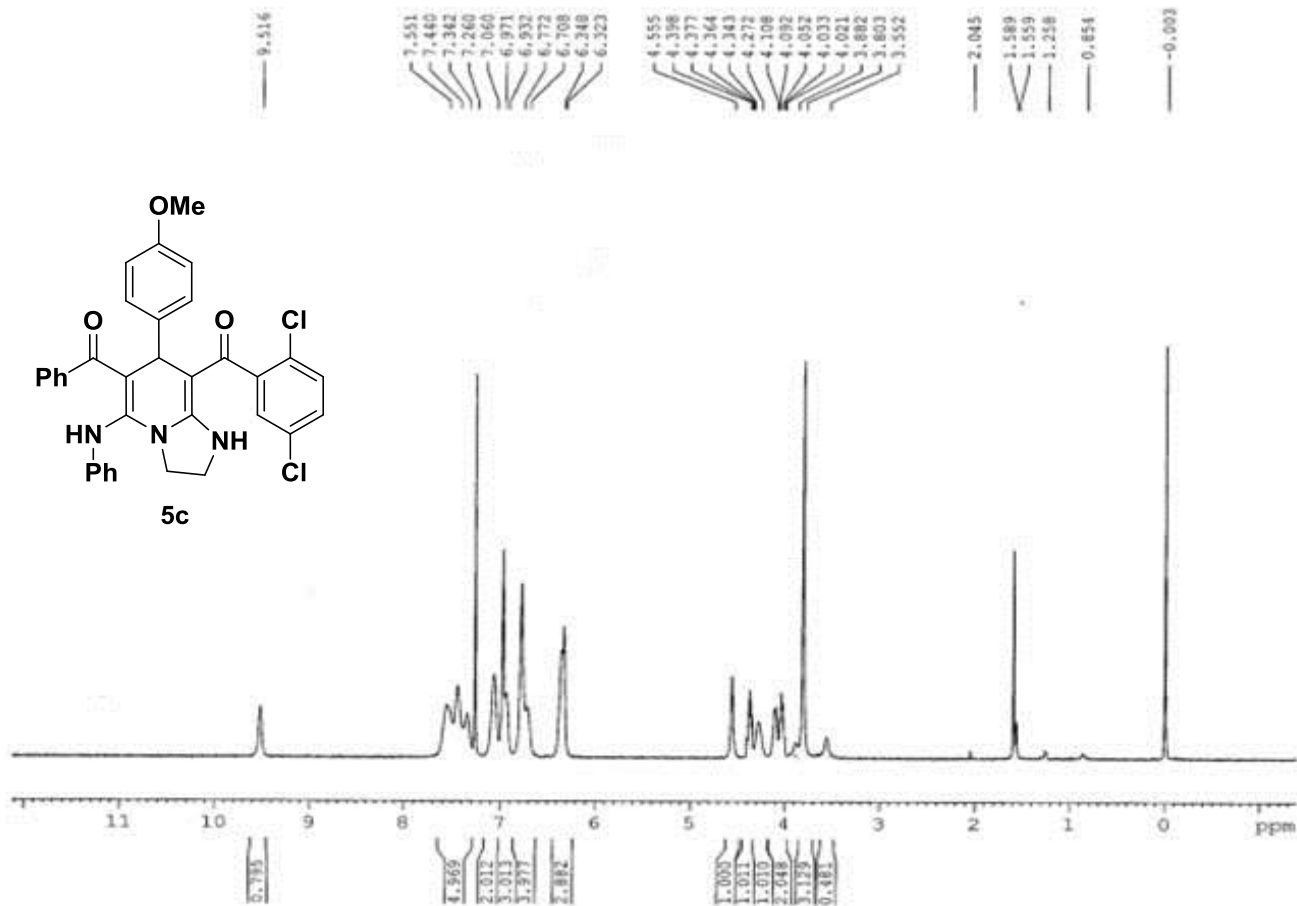


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PROCNO 1
Date_ 20120428
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PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1705
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1620
DW 15.300 usec
DE 6.00 usec
TE 297.4 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326507 MHz
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SSB 0
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GB 0
PC 2.00

SP-E-2 1H 2011 12 16



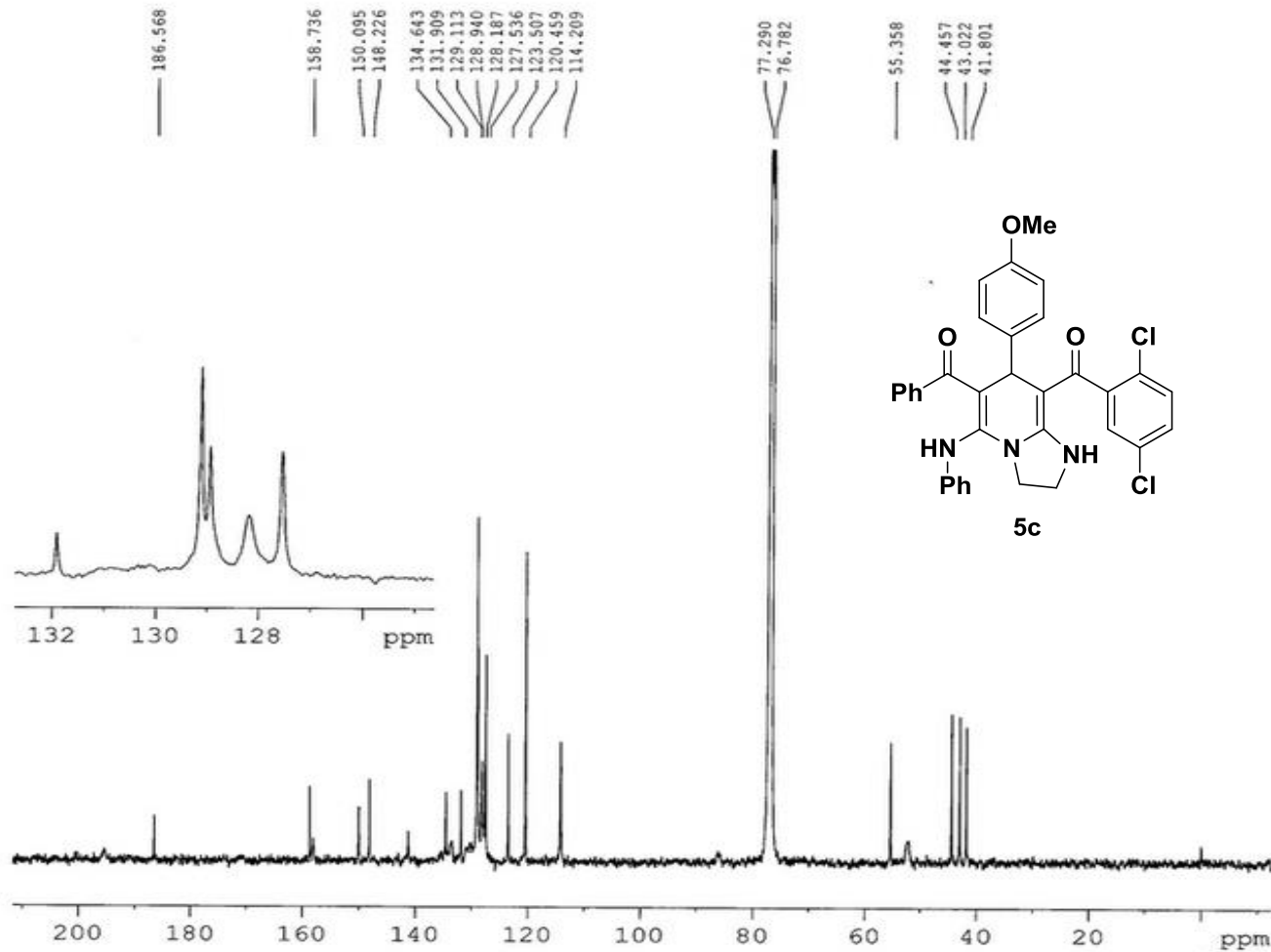
Current Data Parameters
NAME SP-E-2
EXPNO 1
PROCNO 1

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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 1
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 1.6385000 sec
RG 362
DW 50.000 usec
DE 6.00 usec
TE 293.4 K
D1 2.00000000 sec
YD0 1

----- CHANNEL f1 -----
NUC1 1H
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PL1 2.20 dB
SFO1 500.0335010 MHz

F2 - Processing parameters
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SF 500.0300103 MHz
WDW EM
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GB 0
PC 2.00

SP-E-2 13C 1D 2011 12 20



Current Data Parameters
 NAME SP-E-2
 EXPNO 2
 PROCNO 1

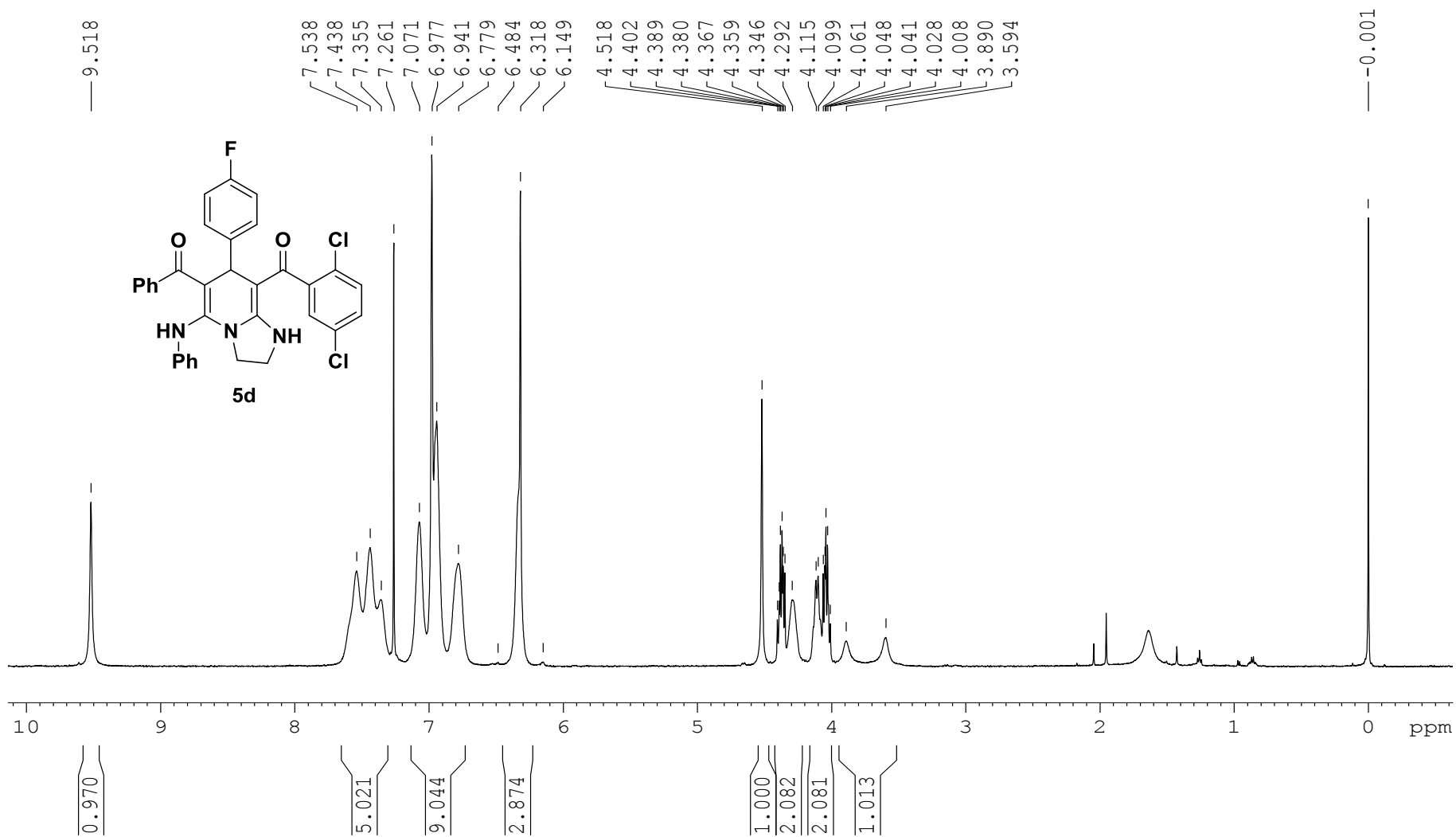
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 TD 65536
 SOLVENT CDCl3
 NS 15020
 DS 2
 SWH 32679.738 Hz
 FIDRES 0.498653 Hz
 AQ 1.0027661 sec
 RG 18400
 DW 15.300 usec
 DE 6.00 usec
 TE 294.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

----- CHANNEL f1 -----
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 PL1 2.00 dB
 SFO1 125.7464750 MHz

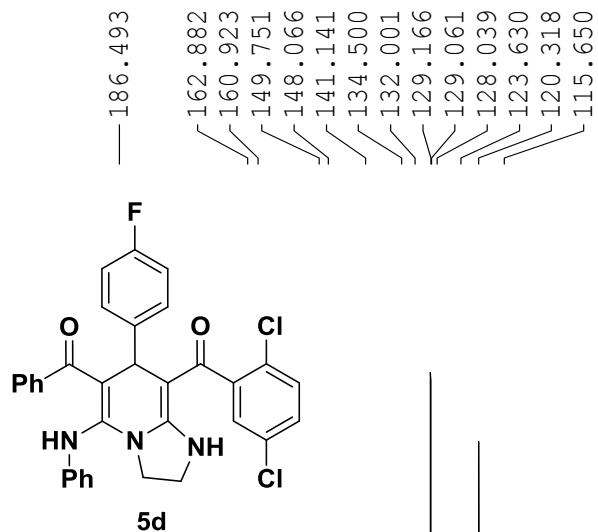
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 PL2 2.60 dB
 PL12 17.66 dB
 PL13 17.66 dB
 SFO2 500.0355000 MHz

F2 - Processing parameters
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 SF 125.7326387 MHz
 WDW EM
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 CB 0
 PC 2.00

SP-E-31 1H 1D 2013 05 08

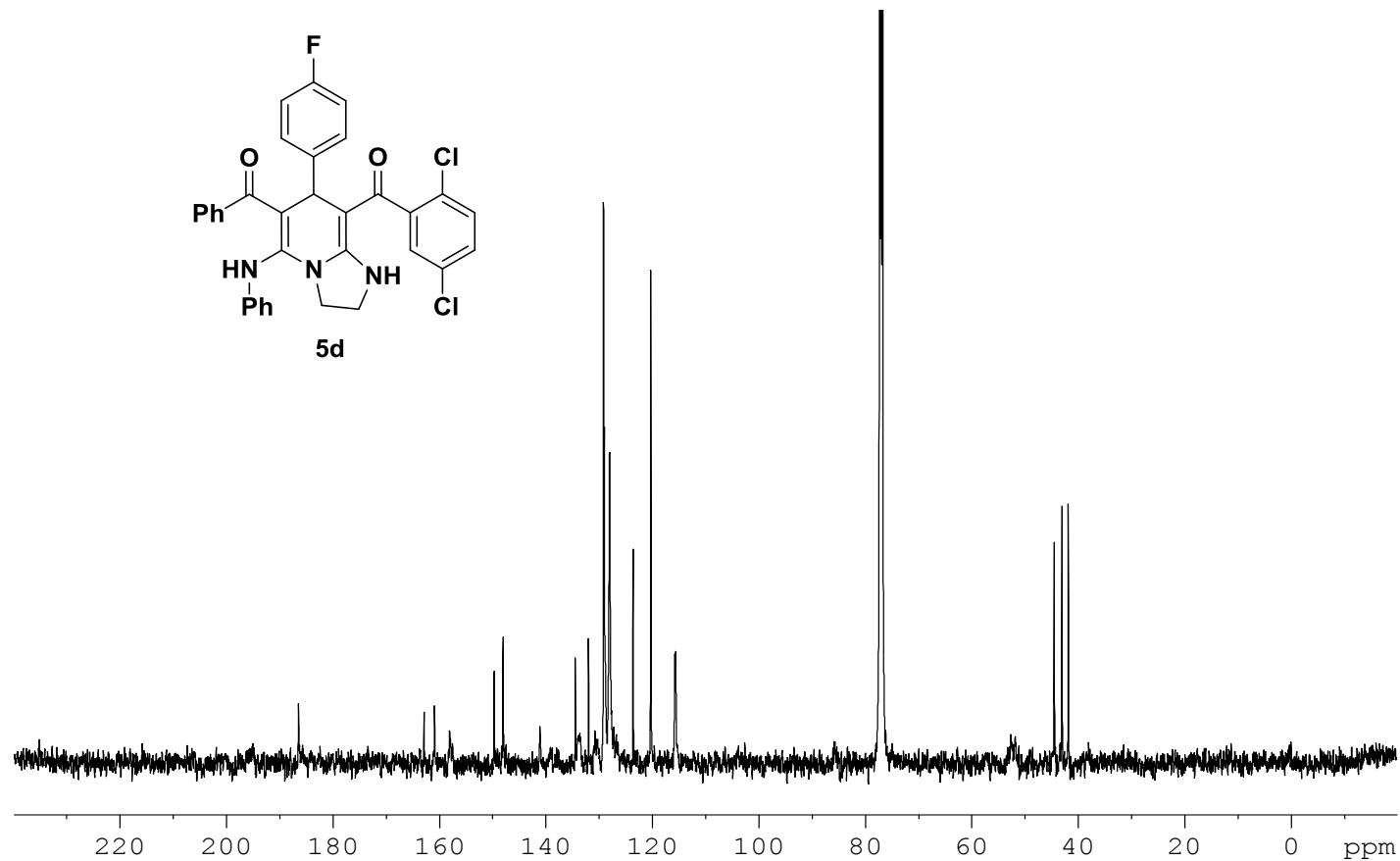


sp-e-31 13C 2013 05 07



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PROCNO         1
Date_          20130509
Time           18.28
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DS             2
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FIDRES         0.498653 Hz
AQ            1.0027661 sec
RG            1820
DW            15.300 usec
DE            6.00 usec
TE            299.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           20

===== CHANNEL f1 =====
NUC1           13C
P1            12.20 usec
PL1           3.00 dB
SFO1          125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2           1H
PCPD2          80.00 usec
PL2            2.00 dB
PL12          17.70 dB
PL13          17.70 dB
SFO2          500.0355000 MHz
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SP-E-1

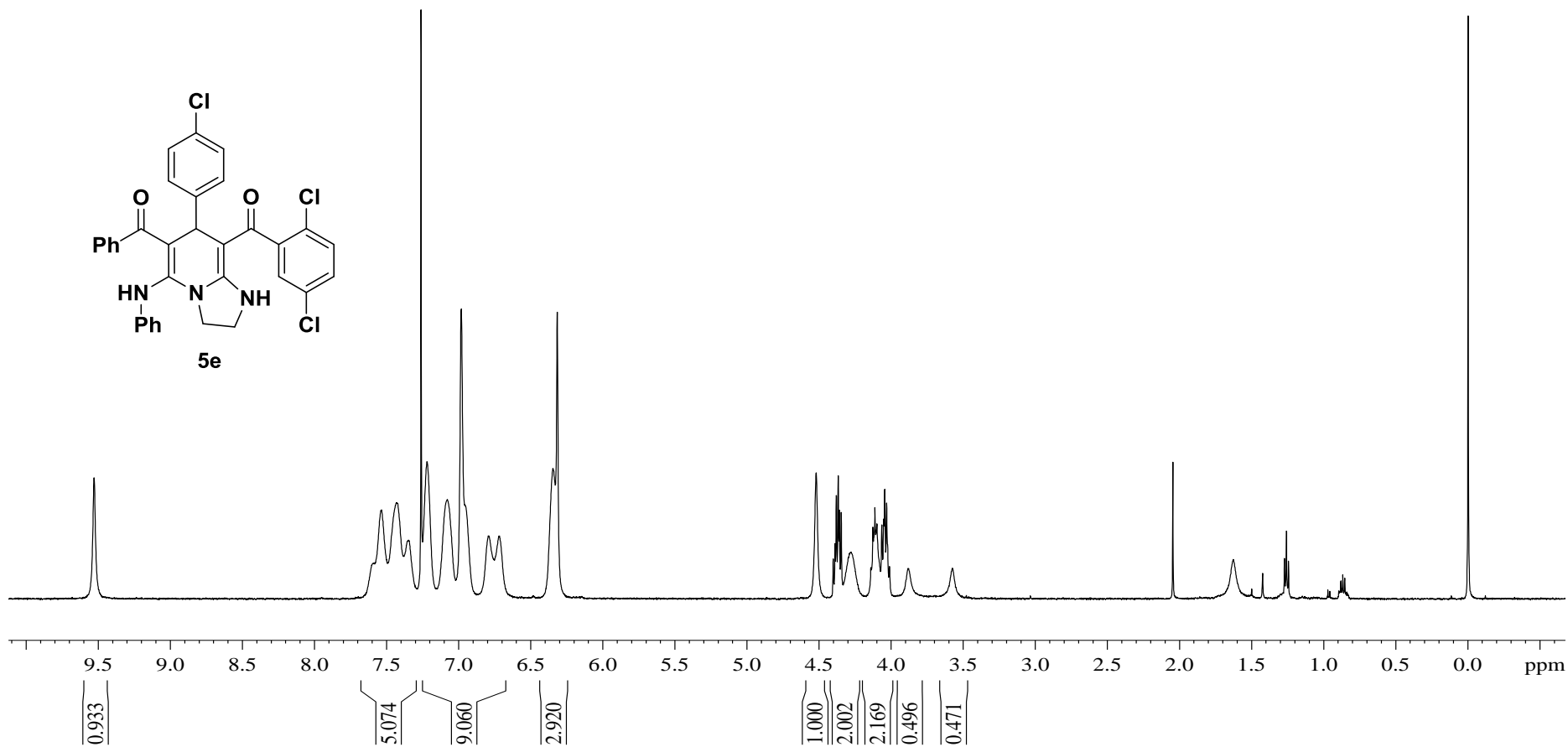
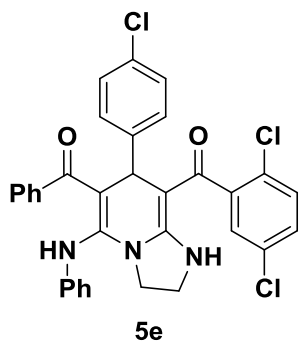
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2012 03 20

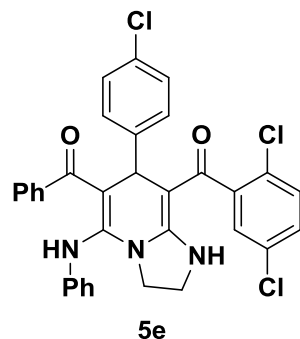
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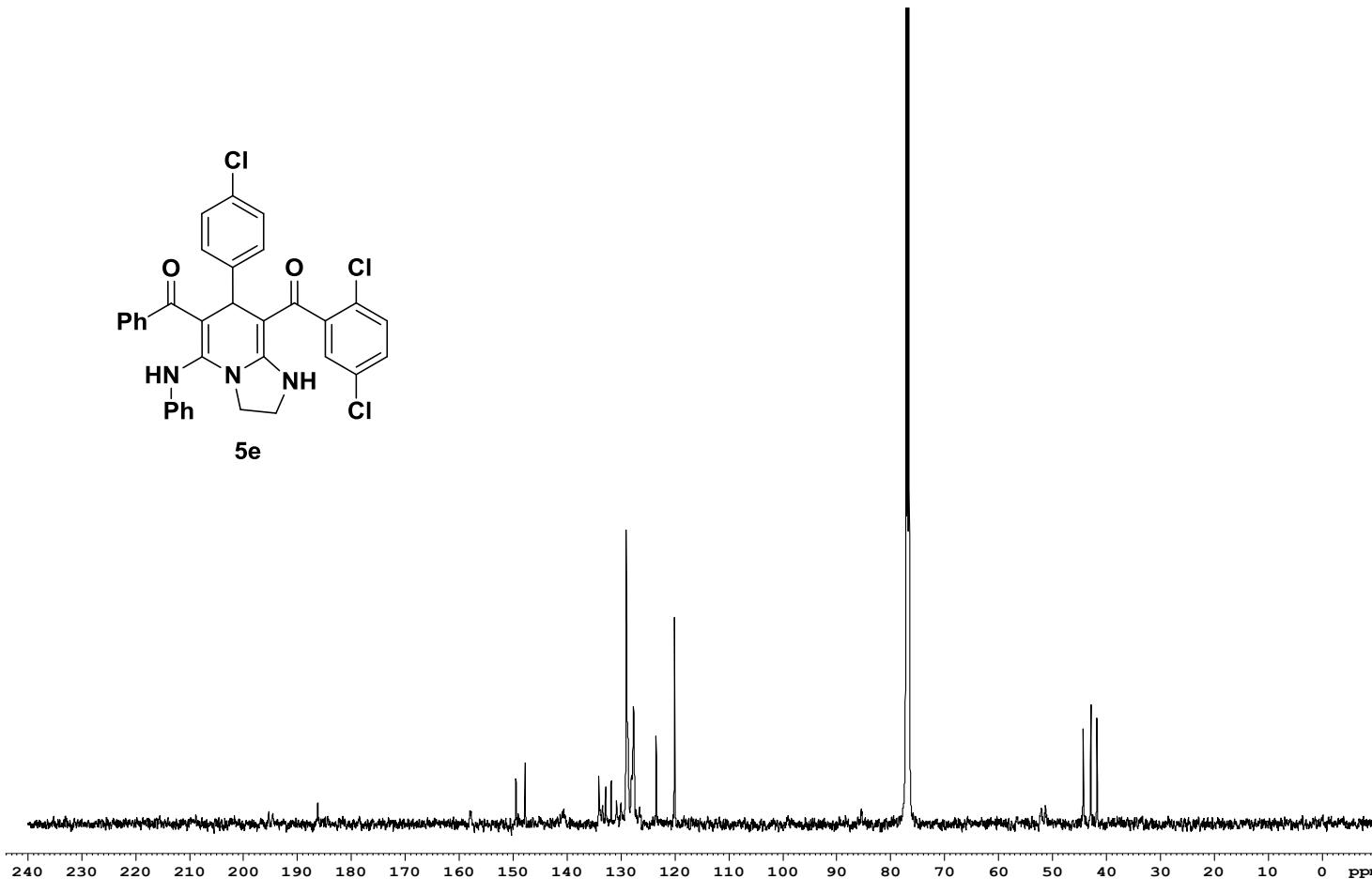


SP-E-1 13C 1D 2012 03 23



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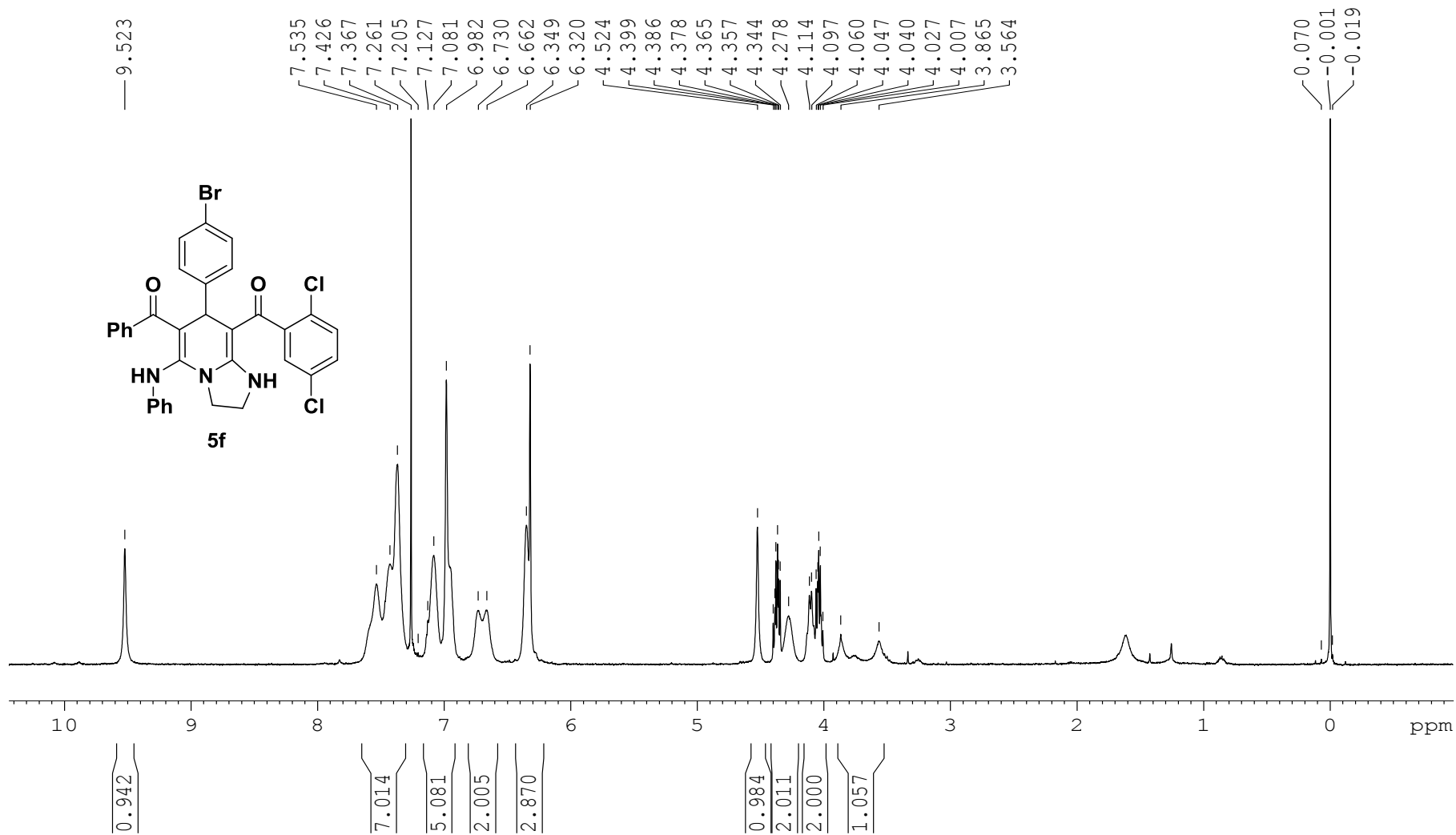


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Time 18.12
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PULPROG zgpg30
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SOLVENT CDCl3
NS 3572
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 14600
DW 15.300 usec
DE 6.00 usec
TE 293.7 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326507 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 2.00

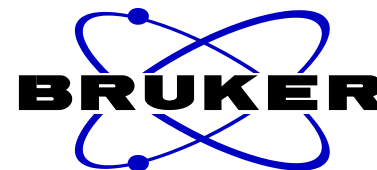
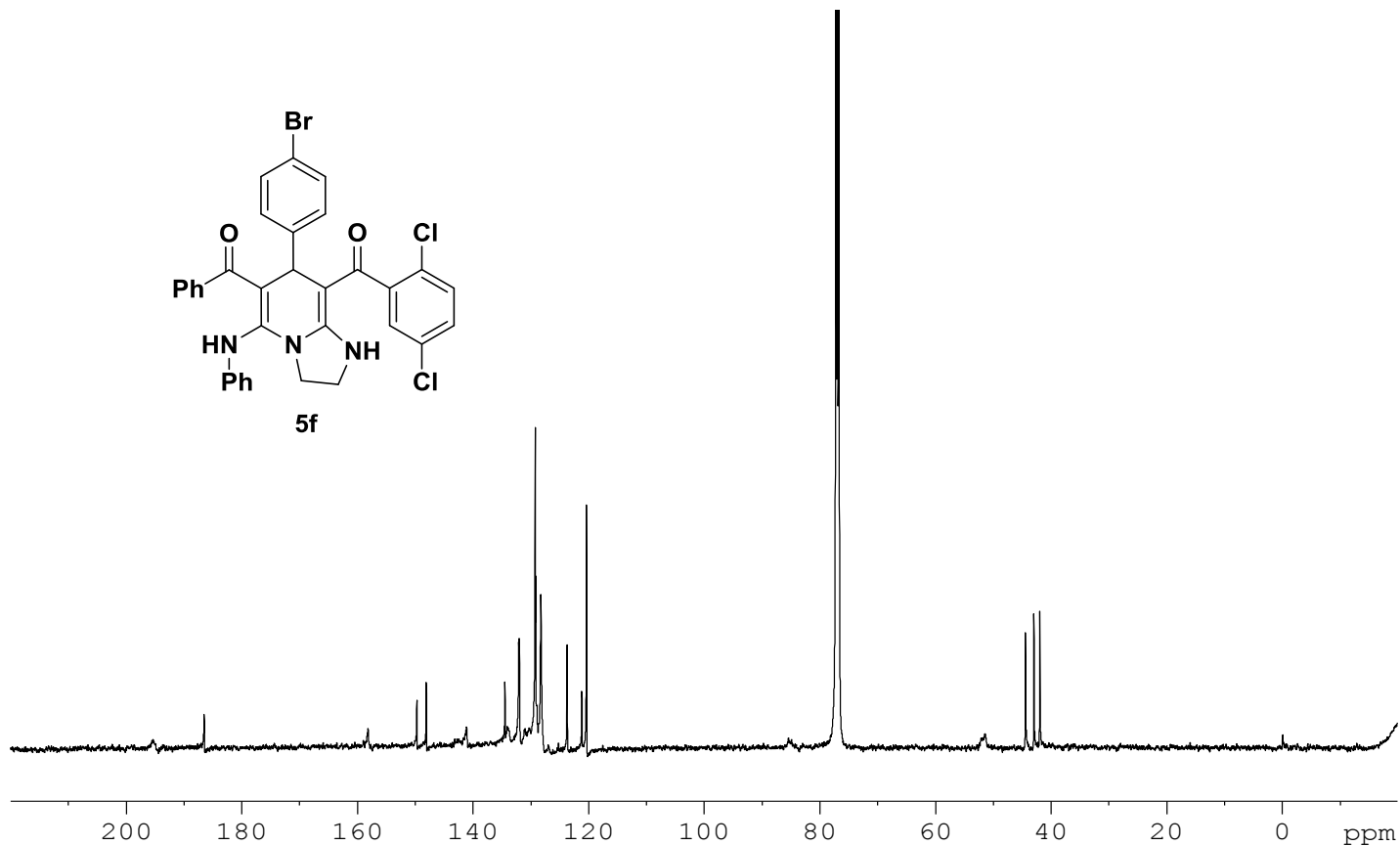
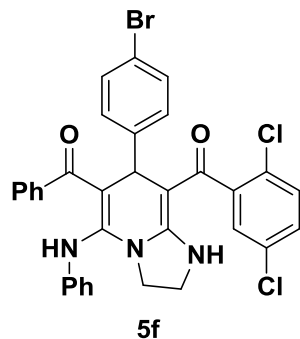
SP-E-32 1H 1D 2013 05 08



sp-e-32 13C 2013 05 09

186.451
149.655
148.025
134.432
131.942
129.193
129.100
128.211
123.659
121.131
120.317

44.509
43.039
42.031



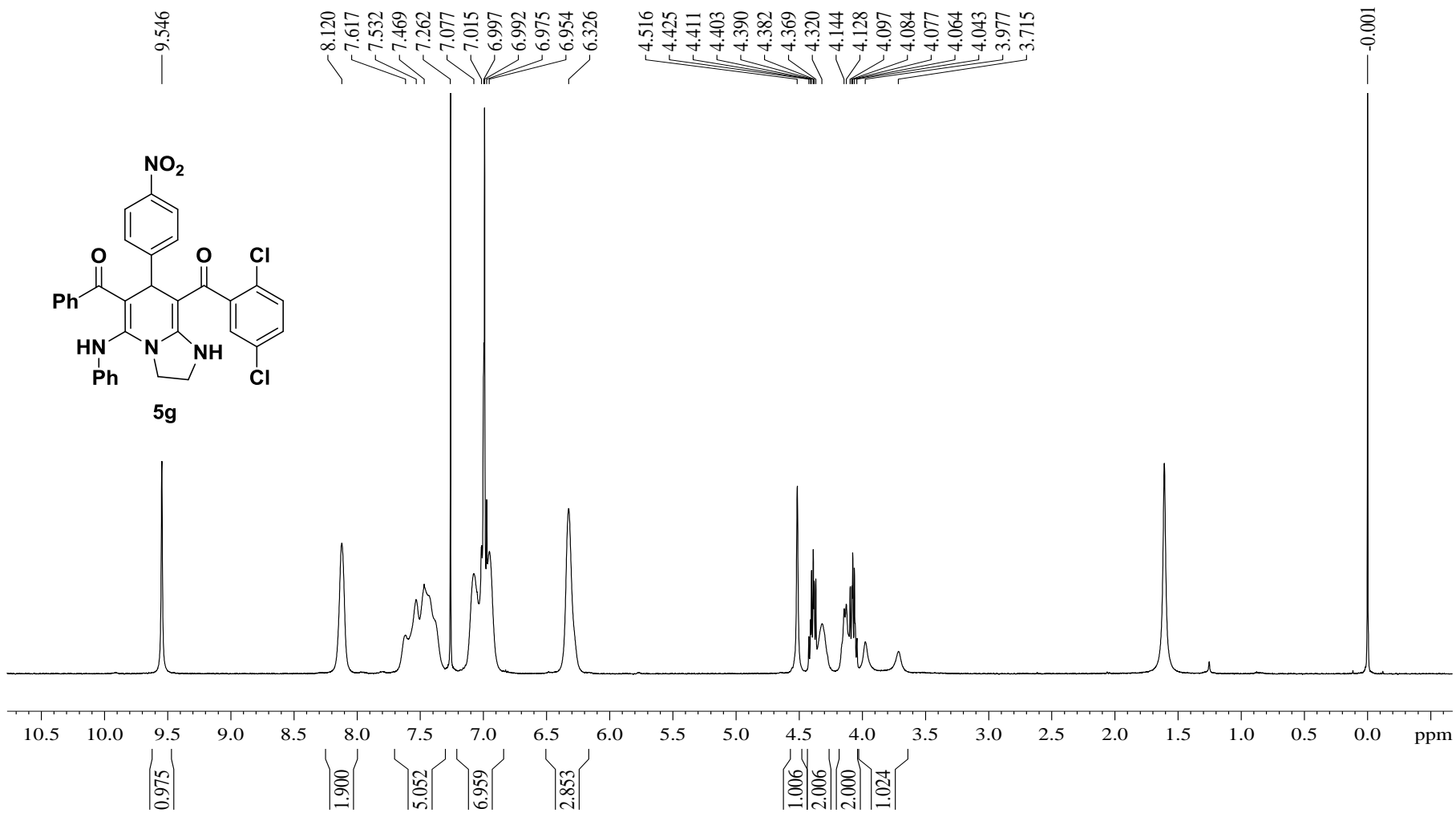
NAME SP-E-32
EXPNO 2
PROCNO 1
Date_ 20130509
Time_ 22.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 11882
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1820
DW 15.300 usec
DE 6.00 usec
TE 299.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20

=====
CHANNEL f1
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326392 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.00

SP-E-4

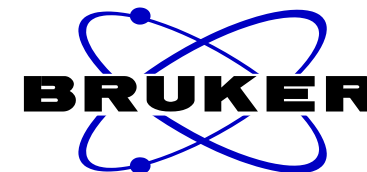
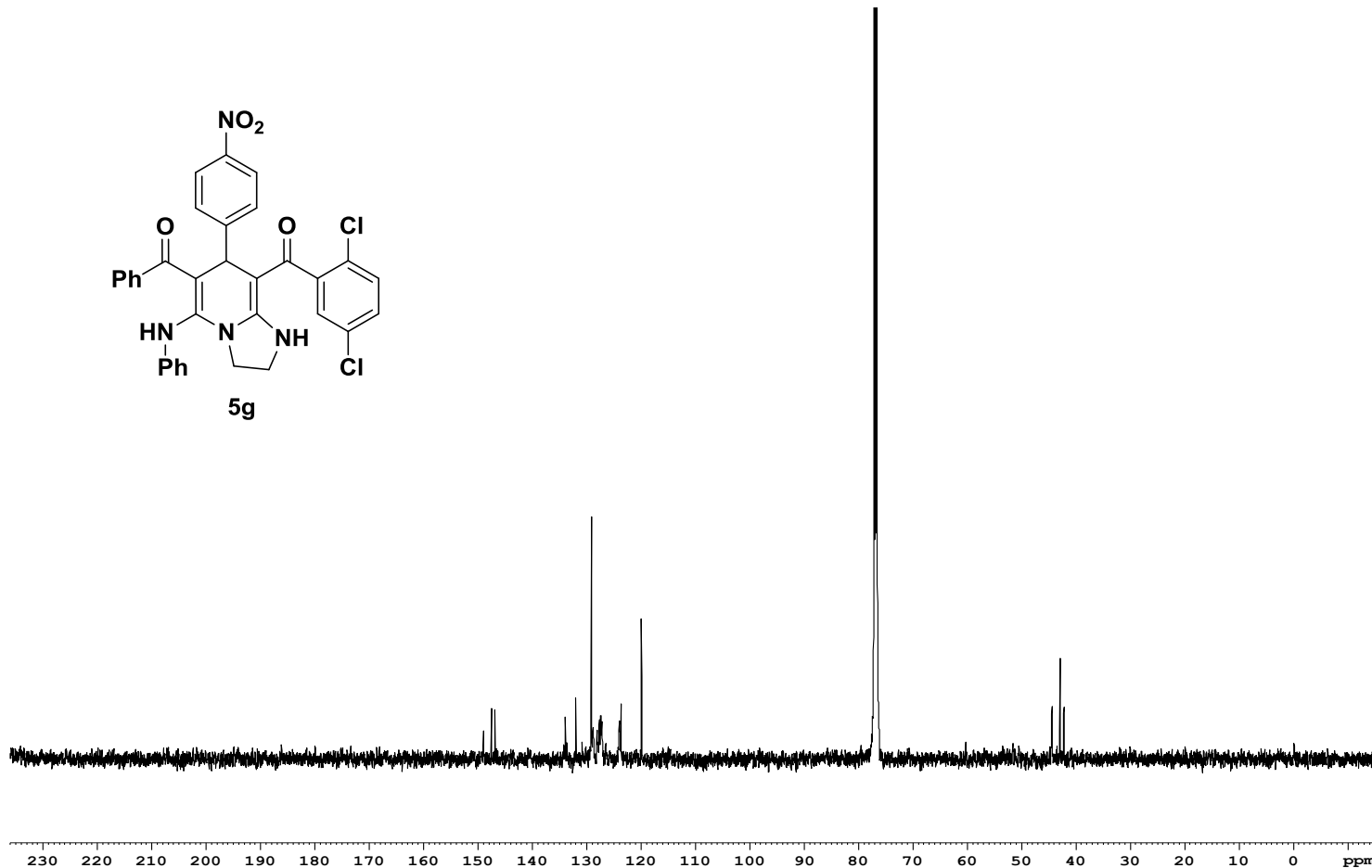
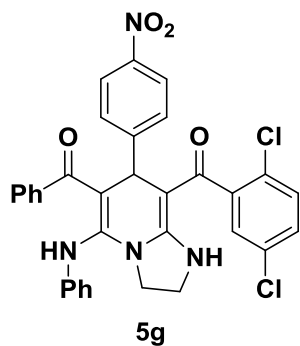
1H 1D 2014 07 07



SP-E-4 13C 1D 2012 03 26

147.655
147.009
134.050
132.156
129.246
127.551
124.055
123.814
120.050

44.528
43.036
42.321



NAME SP-E-4
EXPNO 2
PROCNO 1
Date_ 20120326
Time 16.42
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2859
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1150
DW 15.300 usec
DE 6.00 usec
TE 293.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

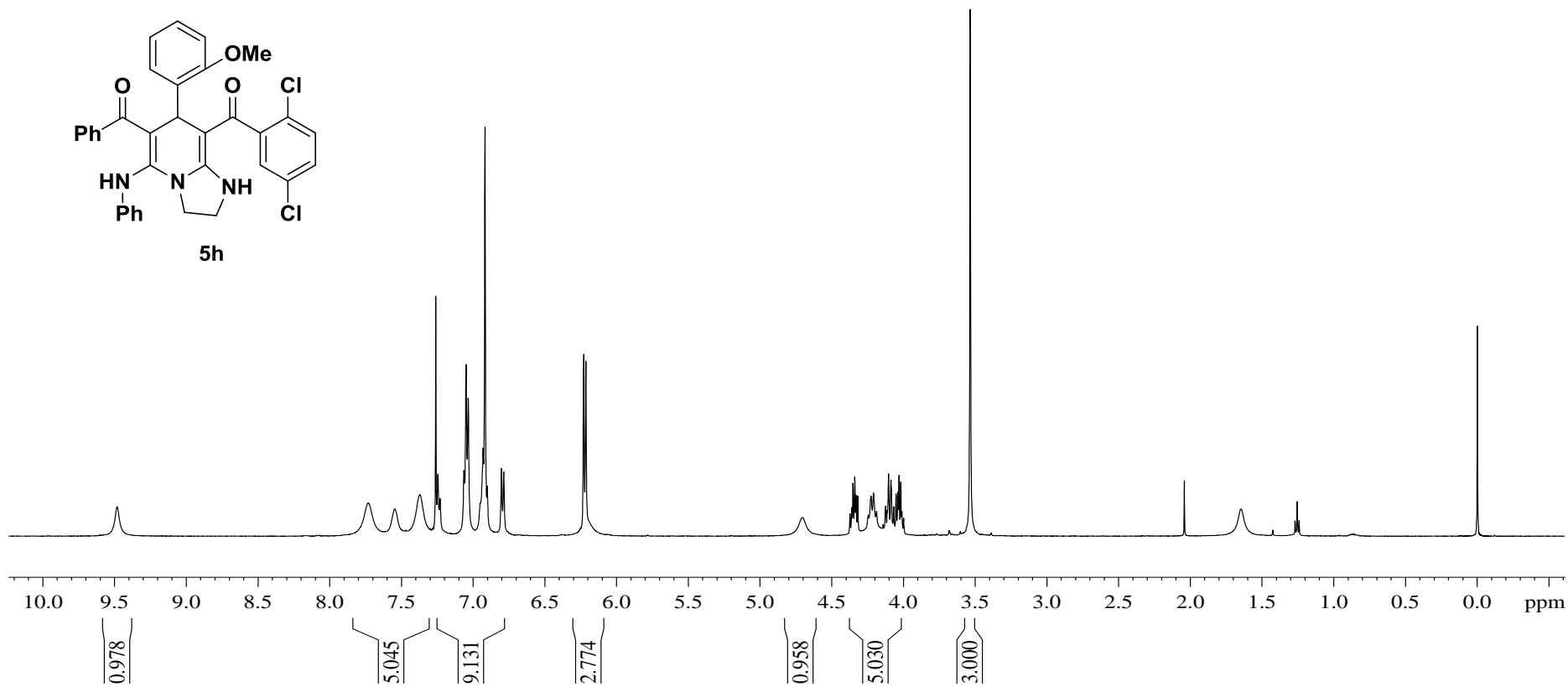
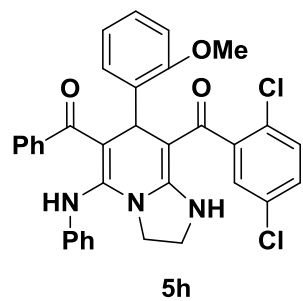
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326507 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00

SP-E-18

1H 1D 2014 07 11

9.482

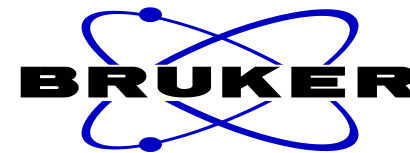
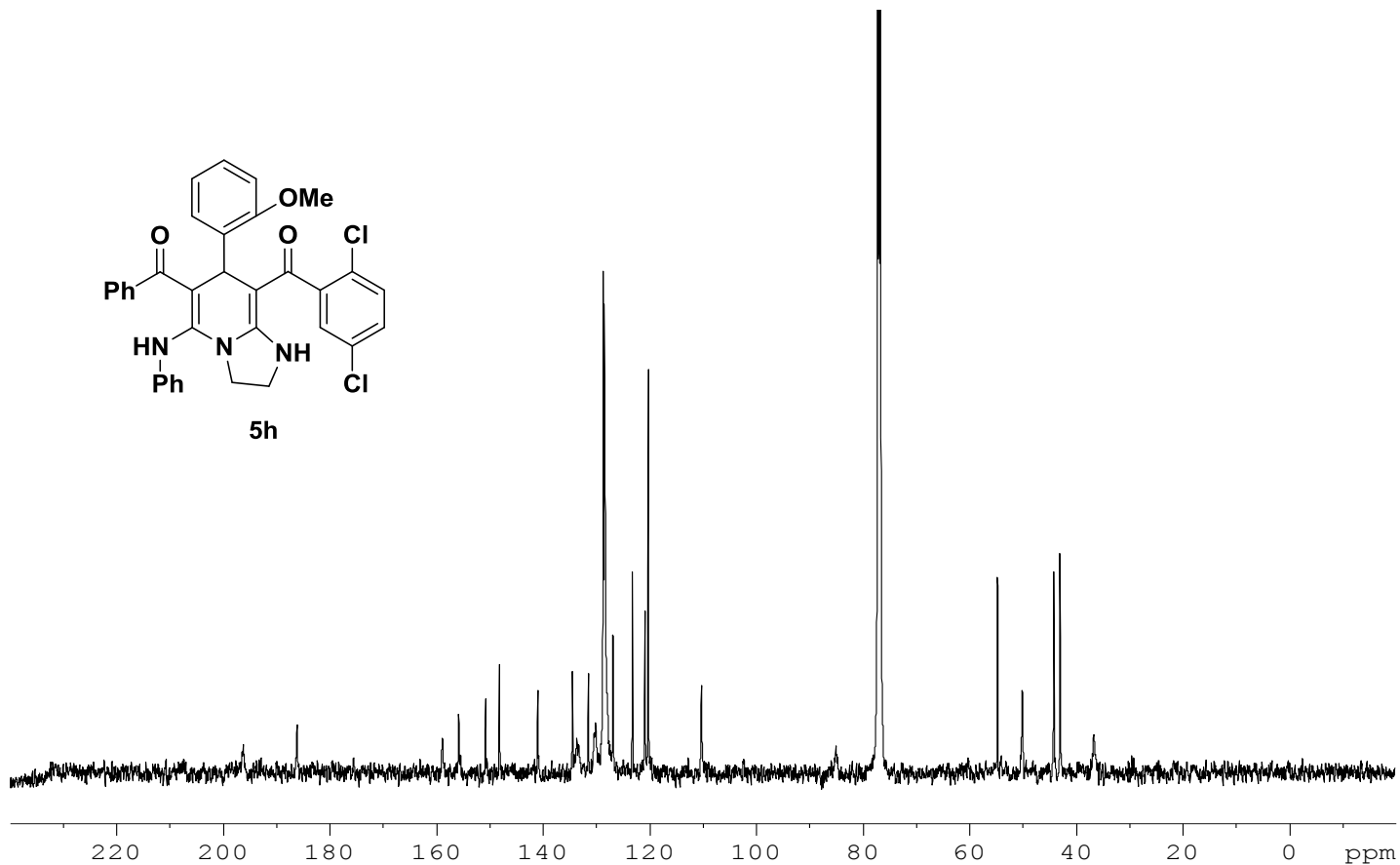
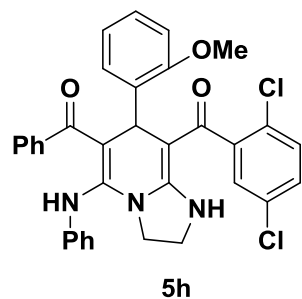
7.732 7.547 7.372 7.260 7.246 7.231 7.064 7.049 7.034 6.949 6.930 6.901 6.802 6.786 6.229 6.213 4.704 4.372 4.360 4.351 4.339 4.330 4.318 4.245 4.225 4.208 4.188 4.141 4.126 4.123 4.112 4.103 4.087 4.067 4.051 4.039 4.030 4.018 4.010 3.998 3.534



SP-E-18 13C 1D 2012 05 27

186.182
158.934
155.879
150.835
148.237
141.039
134.550
131.555
130.230
128.787
128.588
128.427
126.926
123.307
120.928
120.306
110.322

54.781
50.128
44.235
43.071



NAME SP-E-18
EXPNO 2
PROCNO 1
Date_ 20120527
Time_ 14.16
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 890
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 2050
DW 15.300 usec
DE 6.00 usec
TE 292.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

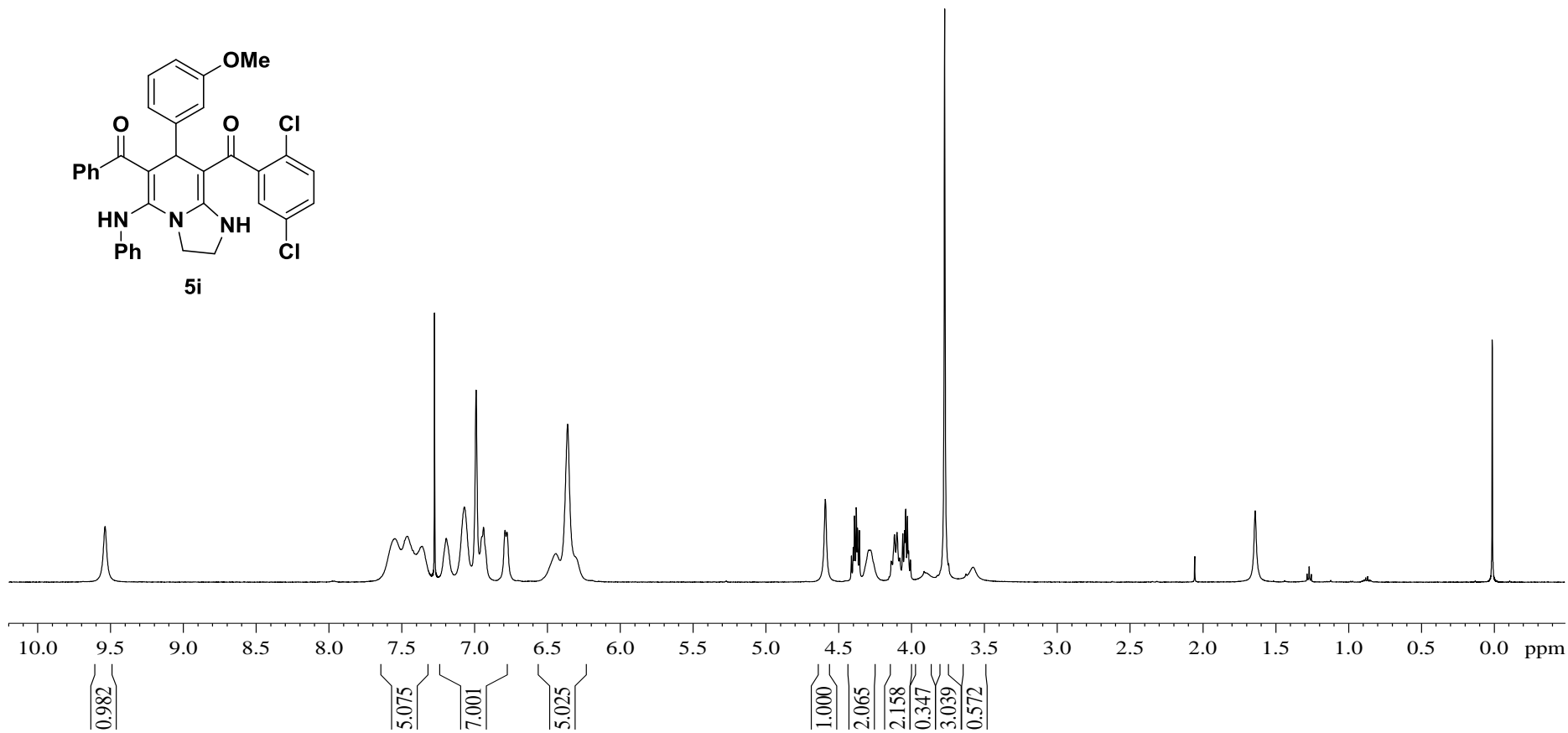
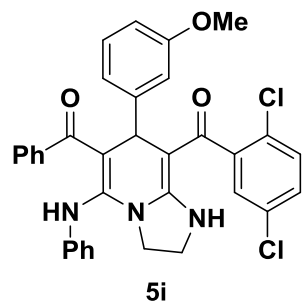
=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326518 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 2.00

SP-E-8

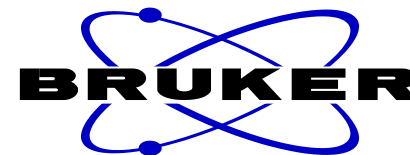
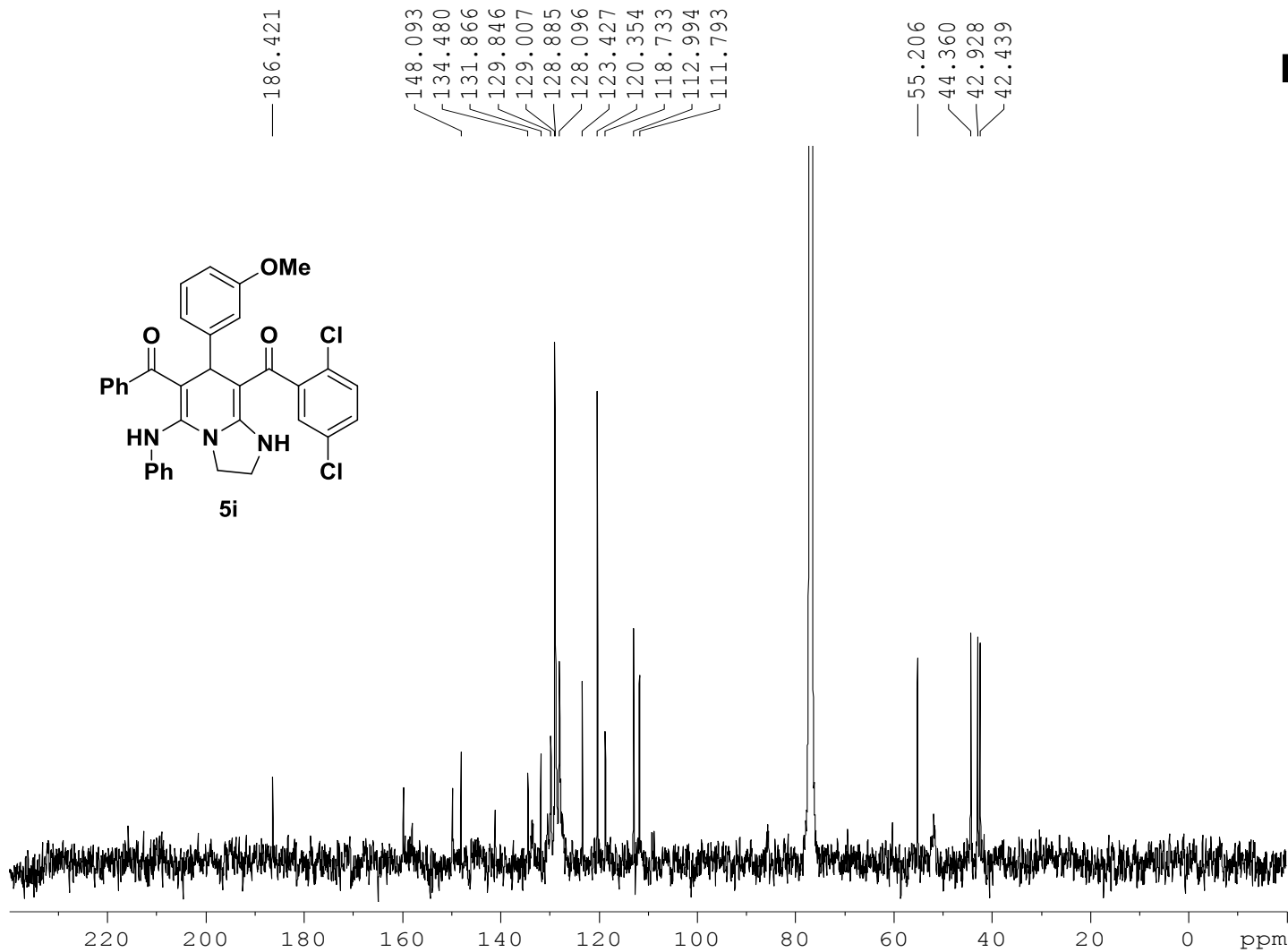
1H 1D 2014 07 08

9.538

7.548 7.462 7.360 7.275 7.195 7.070 6.990 6.938 6.791 6.777 6.442 6.361 4.593 4.414 4.402 4.393 4.380 4.372 4.360 4.295 4.285 4.156 4.141 4.119 4.101 4.083 4.062 4.050 4.042 4.029 4.022 4.009 3.915 3.747 3.628 3.579



SP-E-8 13C 1D 2012 04 28

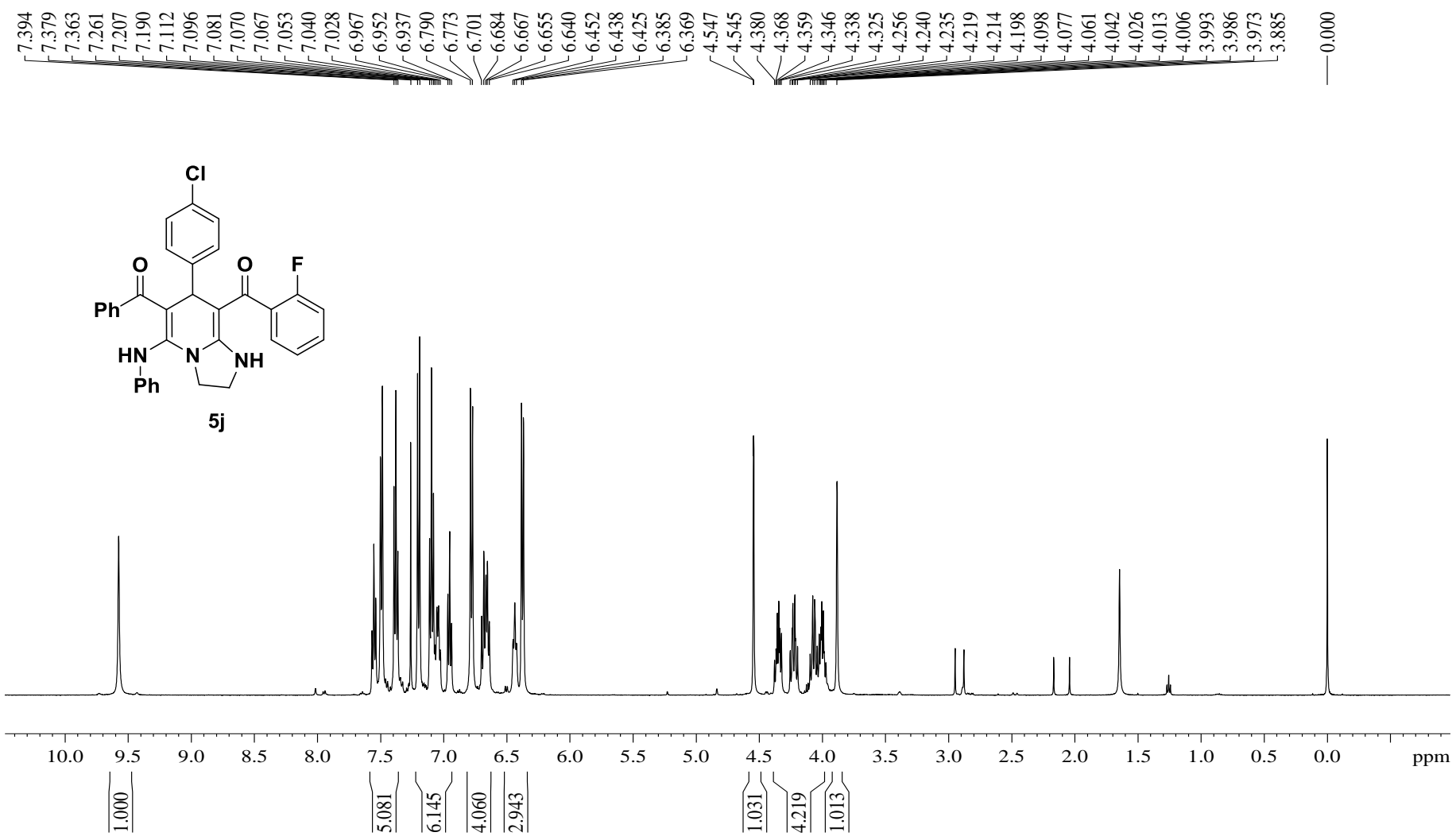


NAME SP-E-8
EXPNO 2
PROCNO 1
Date_ 20120428
Time_ 17.59
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 994
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1620
DW 15.300 usec
DE 6.00 usec
TE 299.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

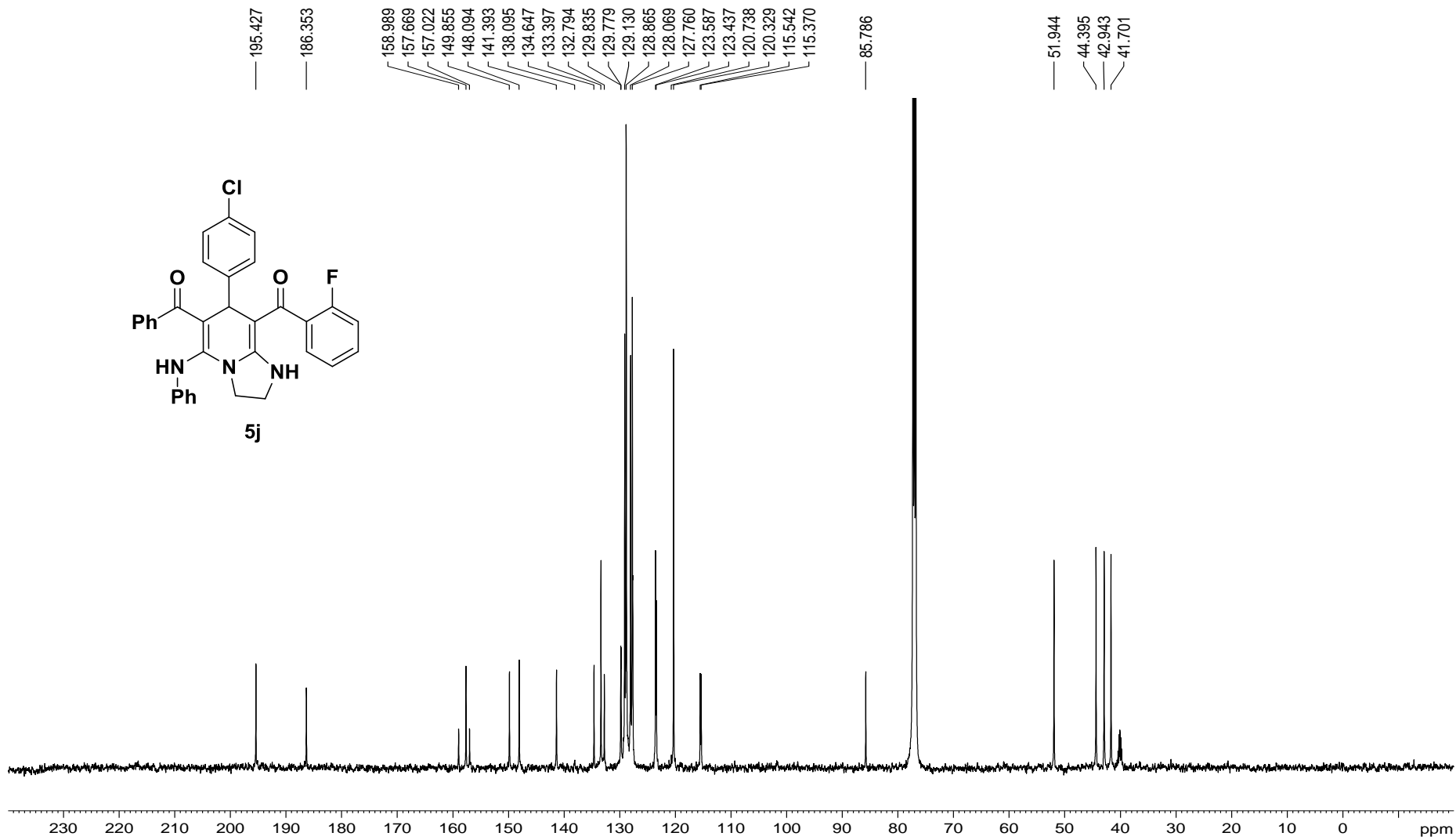
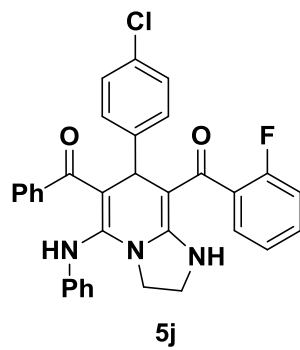
==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326507 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 2.00

ZKL-J-2 1H 1D 2014 04 15



KL-J-2 13C 1D 2014 05 1

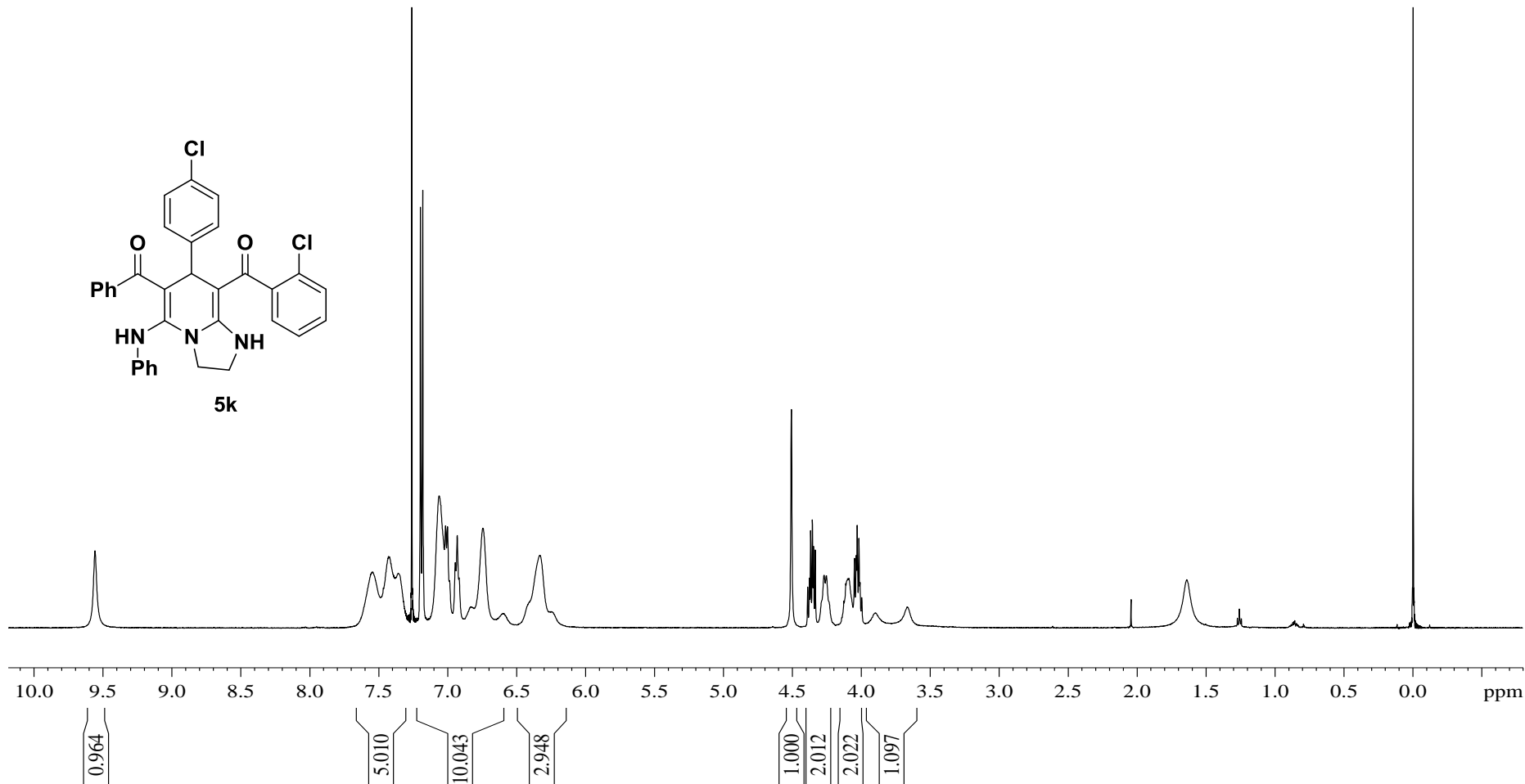
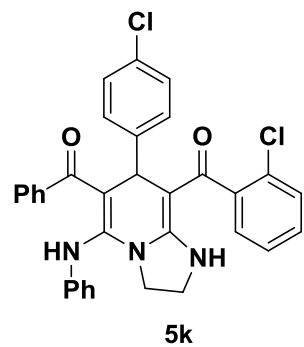


SP-E-6

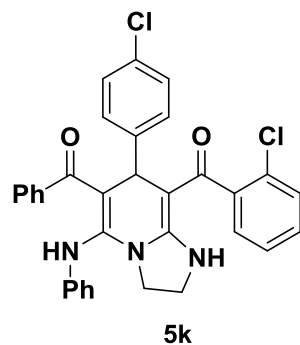
1H 1D 2014 07 11

9.558

7.547
7.428
7.360
7.308
7.198
7.181
7.062
7.016
7.001
6.945
6.931
6.917
6.834
6.745
6.590
6.331
4.507
4.389
4.376
4.367
4.355
4.346
4.334
4.270
4.253
4.127
4.113
4.090
4.050
4.037
4.029
4.017
4.010
3.997
3.896
3.667

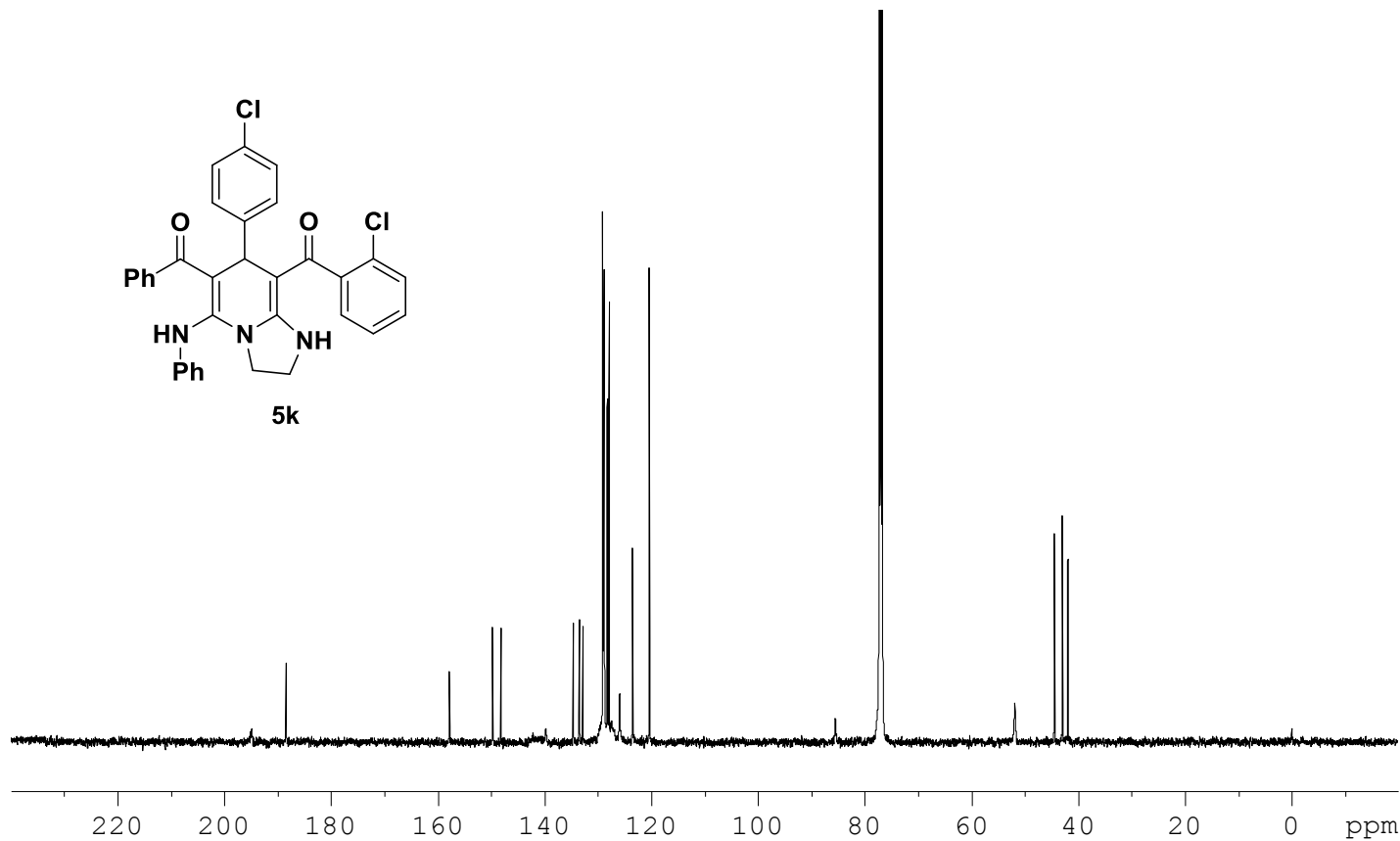


SP-E-6 13C 1D 2012 05 05



188.425
157.829
149.768
148.125
134.603
133.458
132.828
129.091
128.990
128.822
128.238
127.900
123.515
120.342

51.874
44.441
42.957
41.923



NAME SP-E-6
EXPNO 2
PROCNO 1
Date_ 20120506
Time_ 9.02
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12799
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 11500
DW 15.300 usec
DE 6.00 usec
TE 301.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

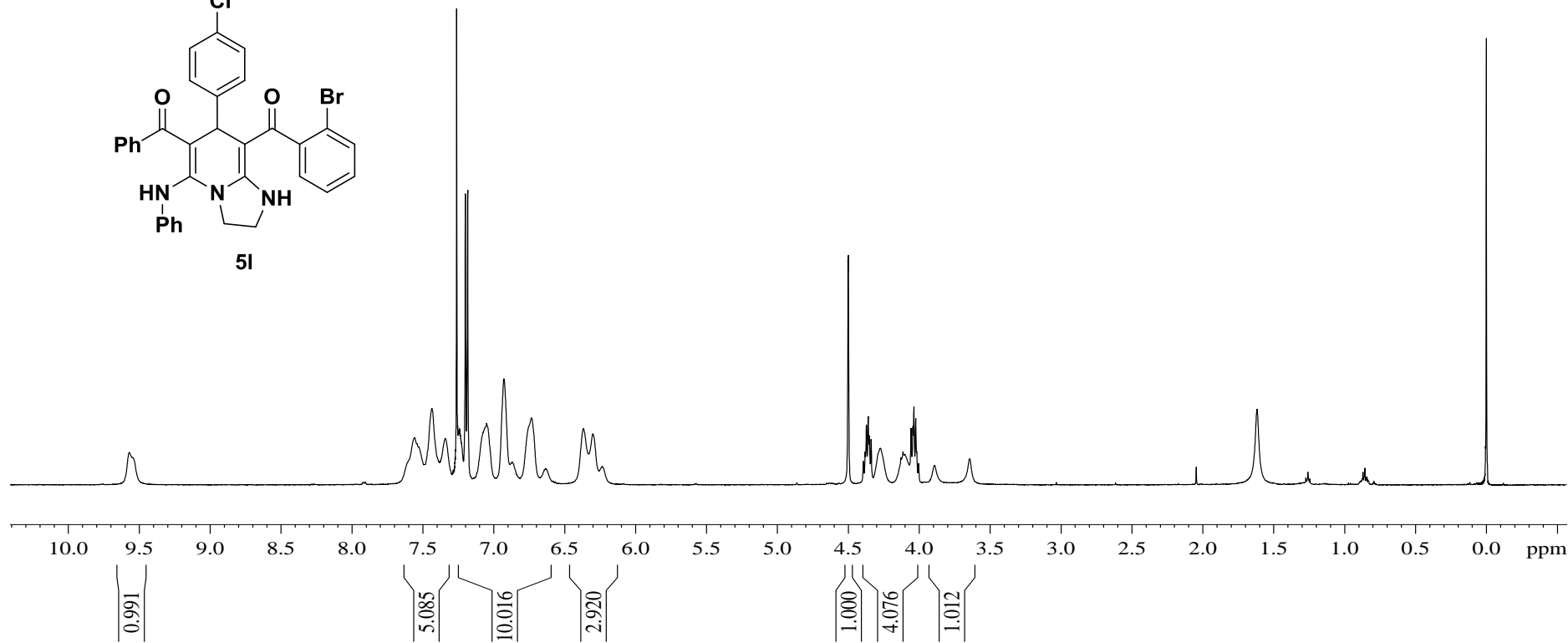
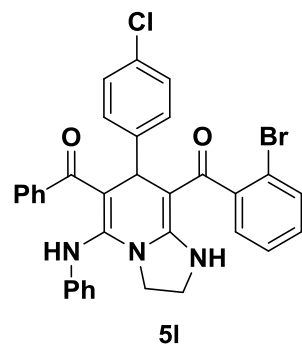
===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

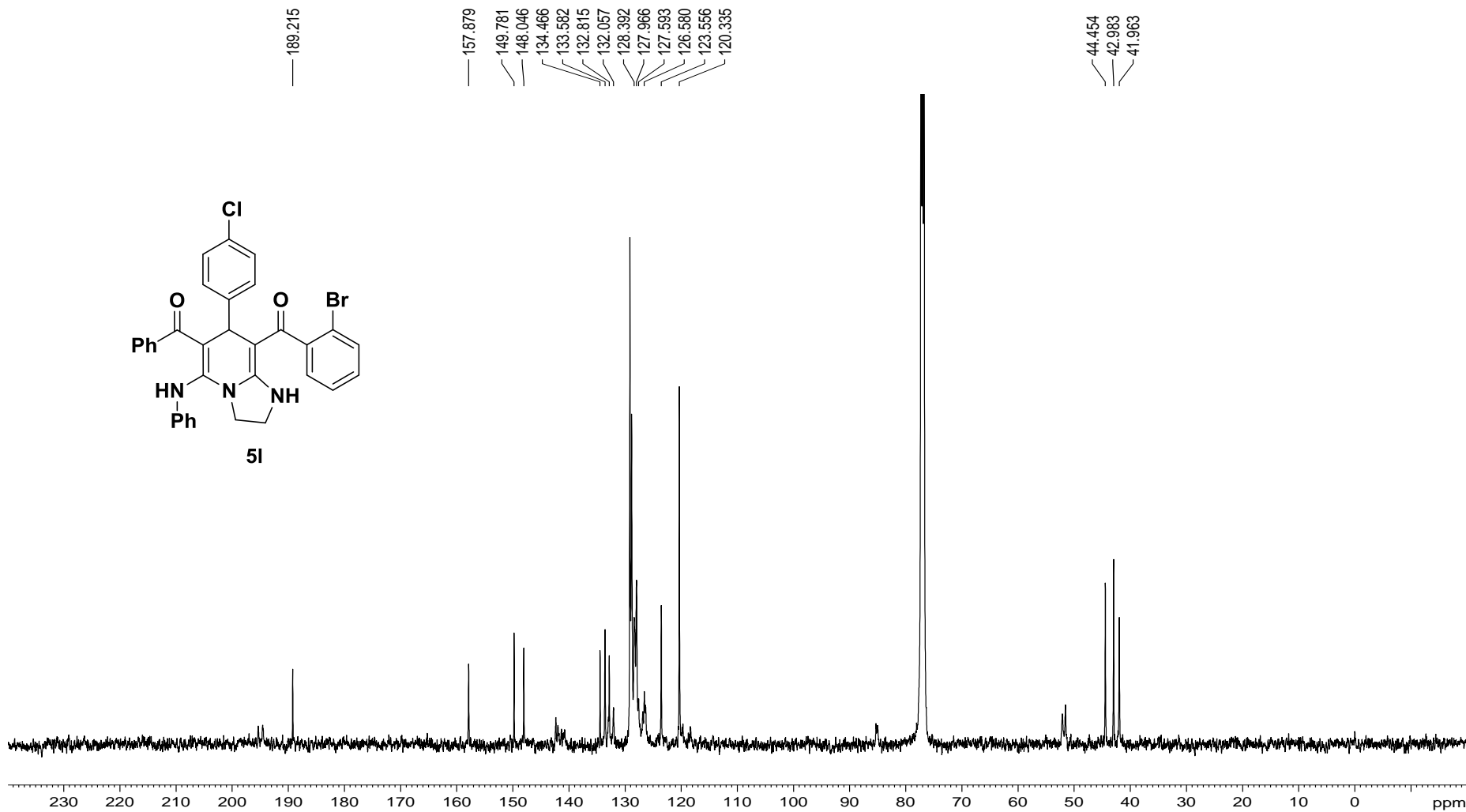
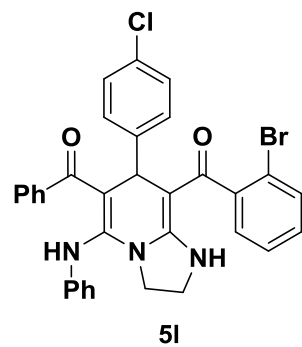
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326440 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00

ZKL-J-1 1H 1D 2014 04 15

9.569

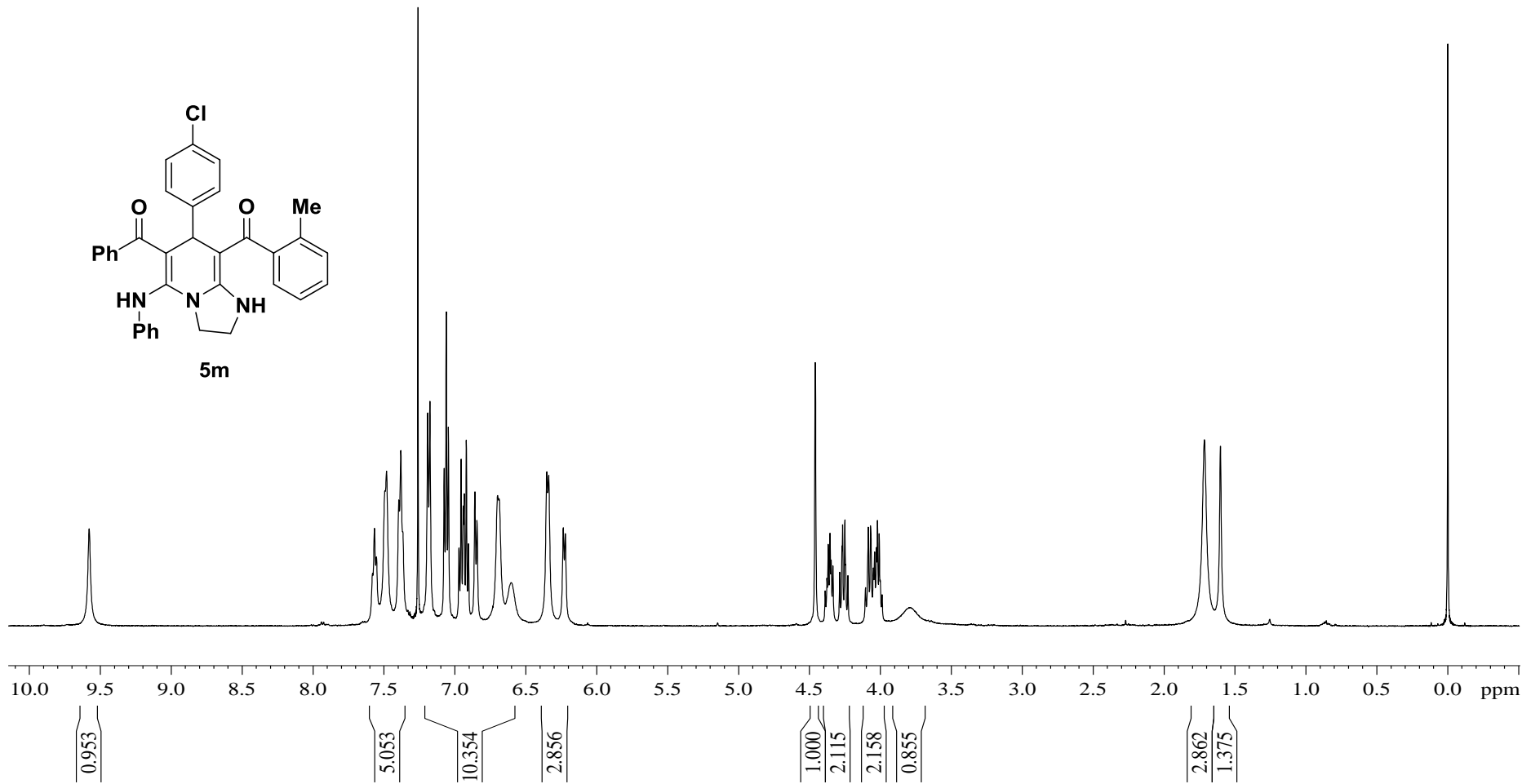
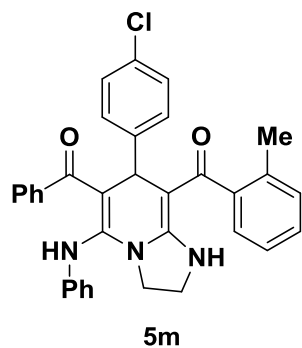
7.558 7.435 7.341 7.251 7.249 7.246 7.244 7.241 7.200 7.183 7.050 6.927 6.870 6.734 6.633 6.368 6.300 6.234 4.501 4.499 4.393 4.380 4.371 4.359 4.351 4.338 4.273 4.114 4.056 4.044 4.036 4.024 4.003 3.891 3.644





ZKL-J-3a 1H 1D 2014 06 09

9.578
7.567
7.553
7.482
7.395
7.381
7.191
7.176
7.075
7.060
7.045
6.971
6.956
6.940
6.934
6.919
6.904
6.858
6.843
6.700
6.605
6.353
6.340
6.237
6.223
4.460
4.390
4.378
4.369
4.356
4.348
4.336
4.288
4.272
4.267
4.251
4.230
4.106
4.086
4.070
4.050
4.042
4.029
4.021
4.009
3.989
3.793
1.716



195.192
192.591

157.415
149.859
148.124
142.029
140.527
134.399
133.524
132.713
129.956
129.056
128.859
128.783
128.123
127.883
127.692
125.103
124.628
123.448
120.351

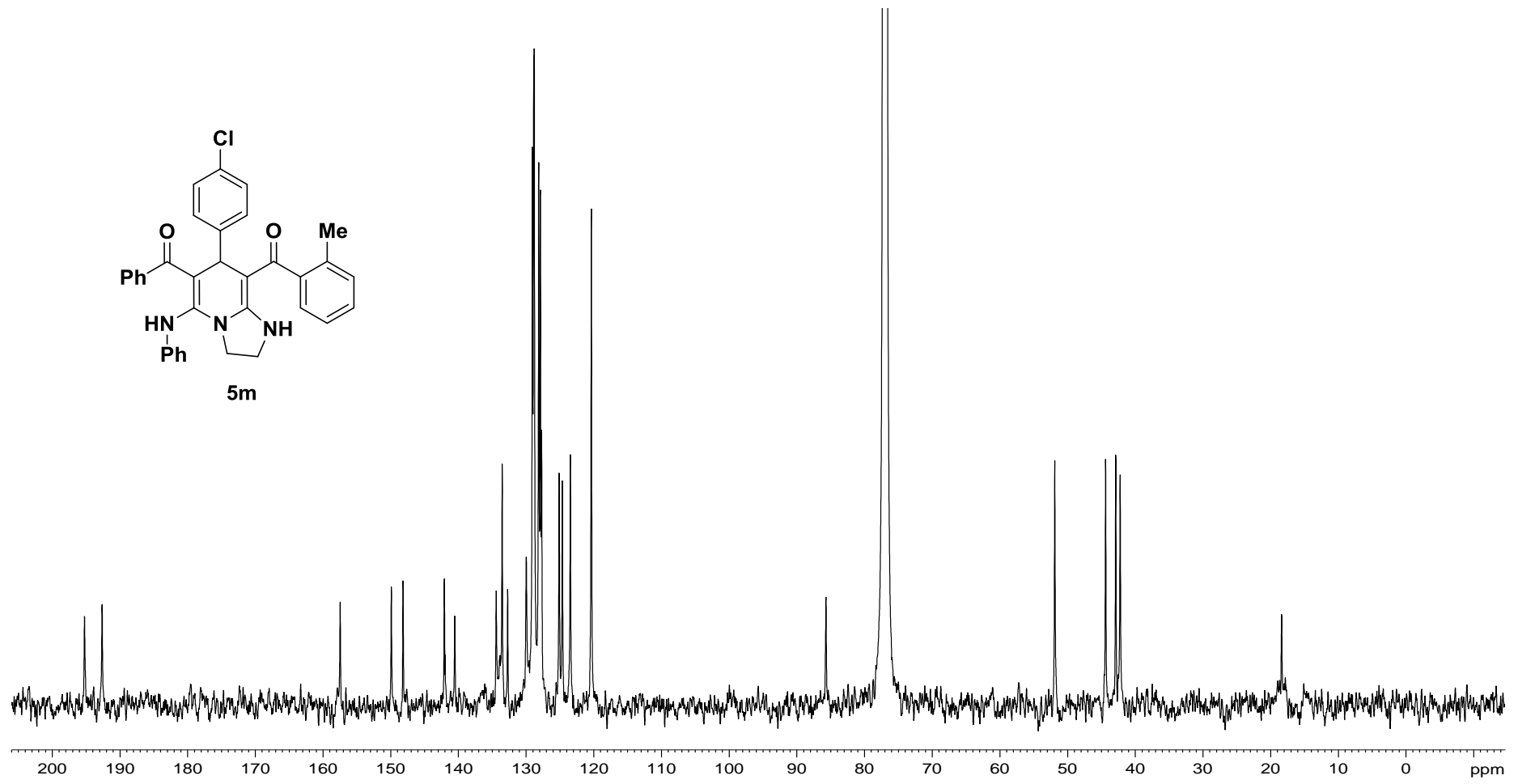
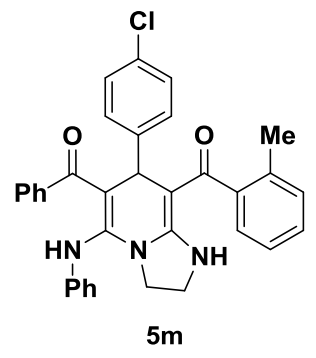
85.684

77.216
76.963
76.709

51.875

44.364
42.875
42.219

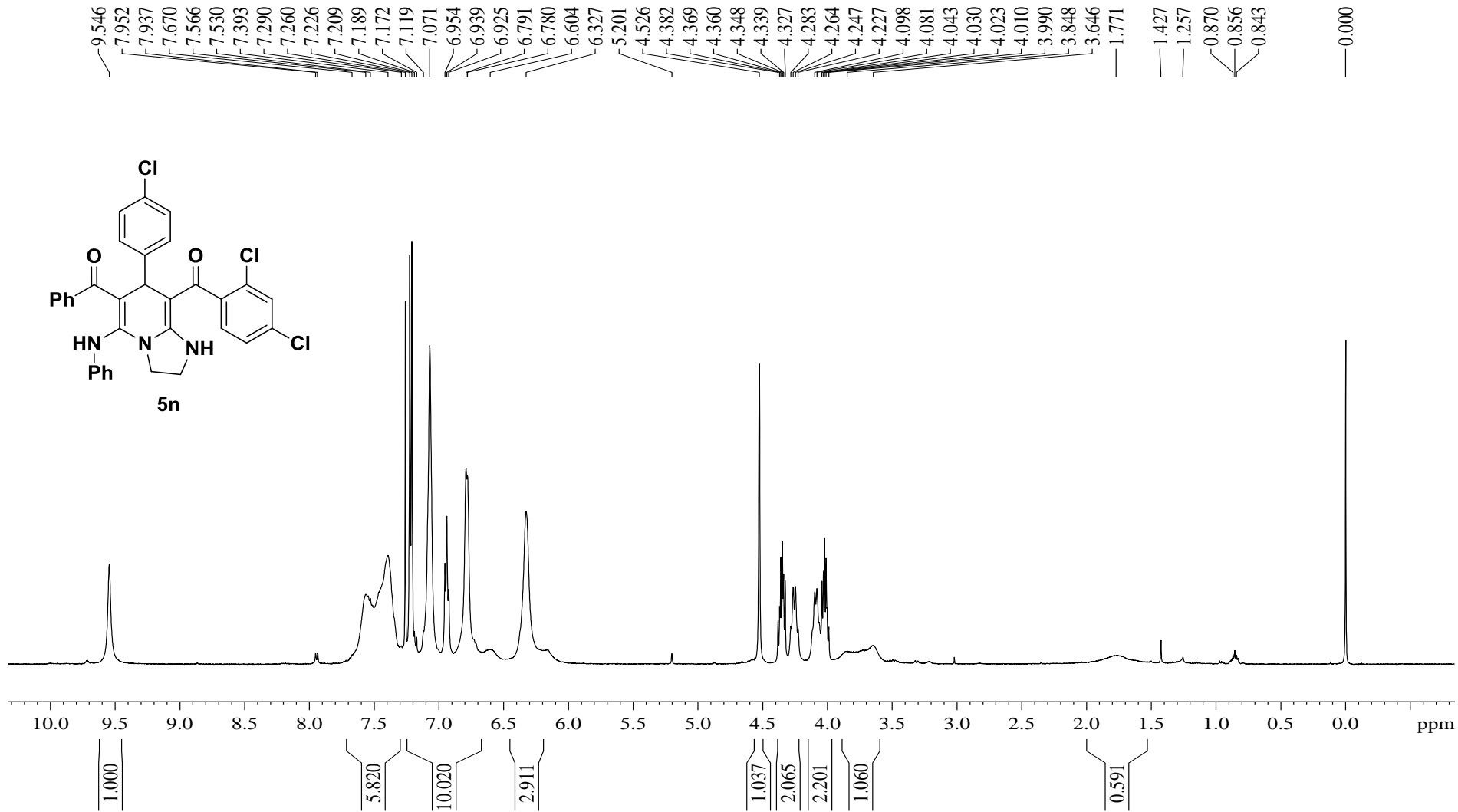
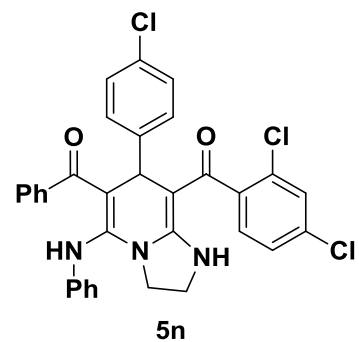
18.365

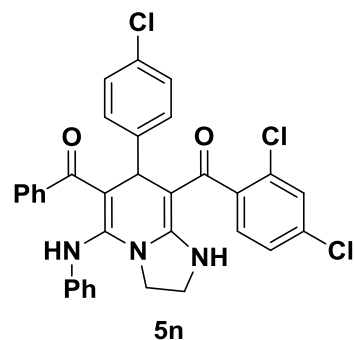
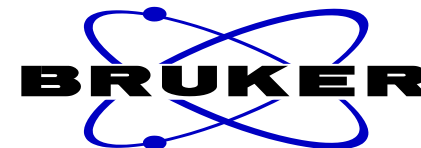


SP-E-20

1H

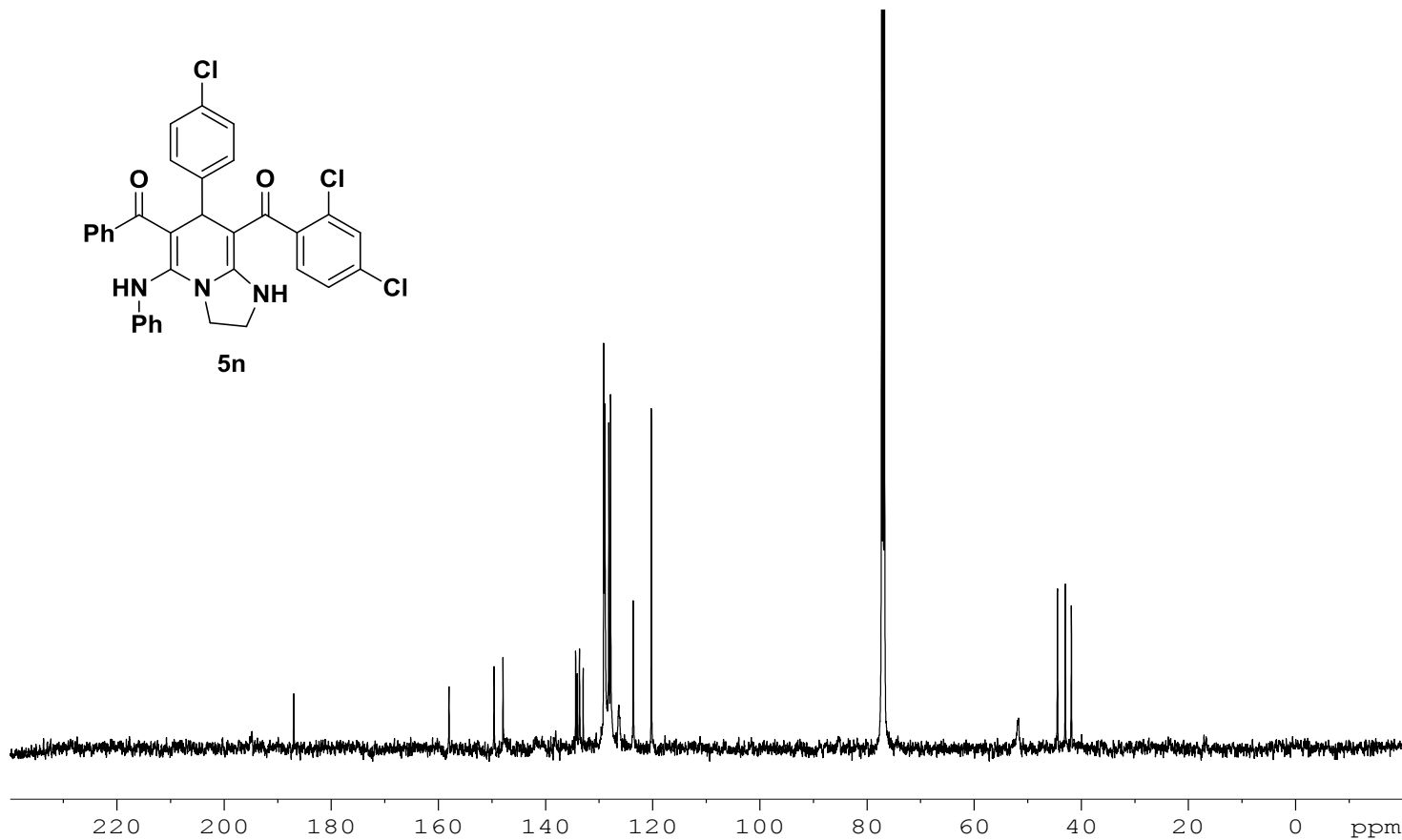
2012 06 28





186.994
 158.012
 149.595
 147.942
 134.379
 134.088
 133.658
 132.971
 129.135
 128.939
 128.188
 127.849
 126.303
 123.617
 120.245

44.440
 42.979
 41.840



```

NAME          SP-E-20
EXPNO         2
PROCNO        1
Date_         20130621
Time_         17.00
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            920
DS            2
SWH           32679.738 Hz
FIDRES        0.498653 Hz
AQ            1.0027661 sec
RG            1820
DW            15.300 usec
DE            6.00 usec
TE            299.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           20
    
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            12.20 usec
PL1           3.00 dB
SFO1          125.7464750 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           2.00 dB
PL12          17.70 dB
PL13          17.70 dB
SFO2          500.0355000 MHz
SI            32768
SF            125.7326474 MHz
WDW           EM
SSB           0
LB            6.00 Hz
GB            0
PC            1.00
    
```

SP-E-15

1H

2012 05 14

9.482

7.655

7.469

7.325

7.082

6.976

6.964

6.913

6.171

4.465

4.120

4.106

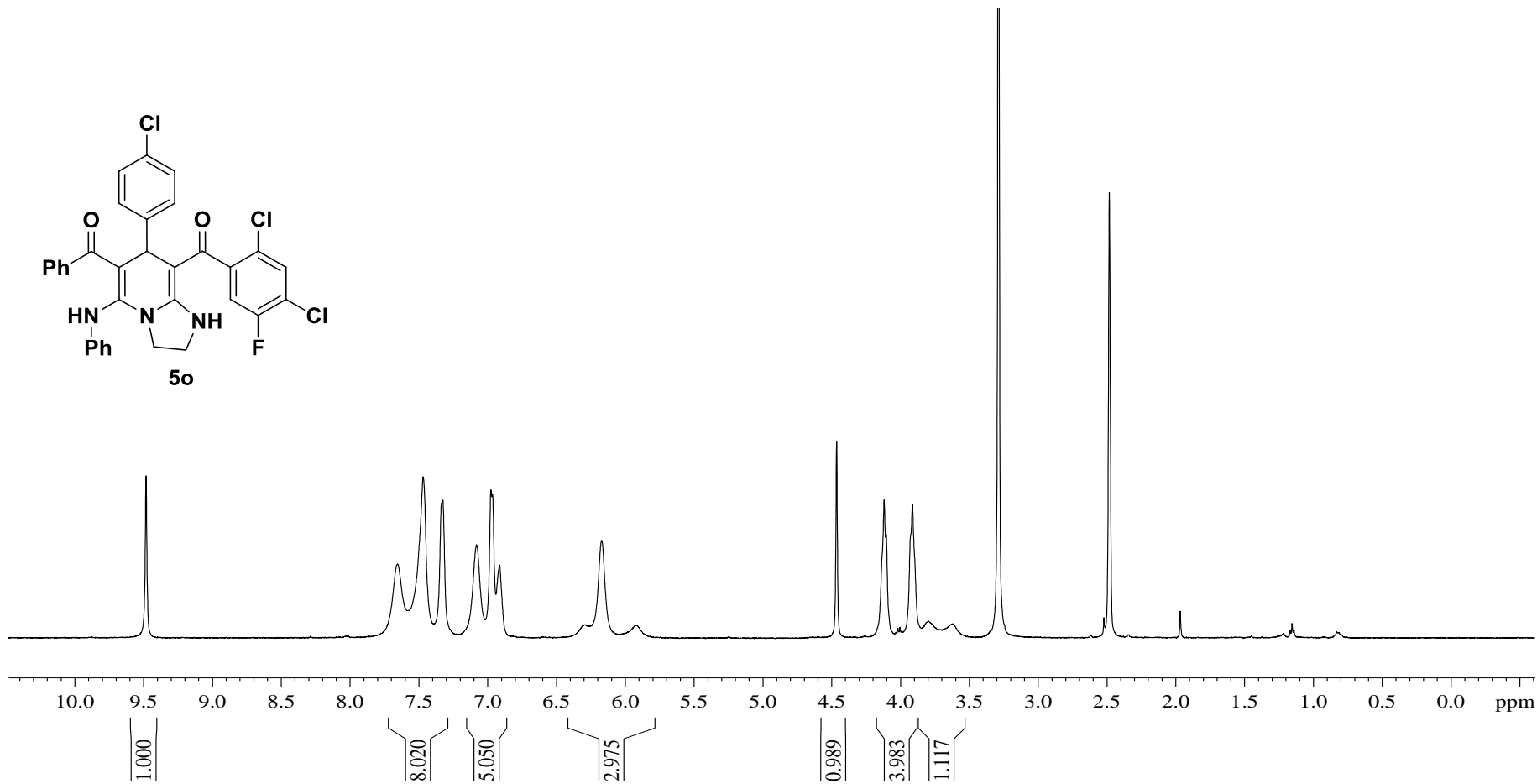
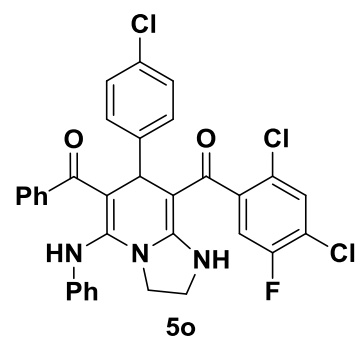
3.914

3.794

2.523

2.484

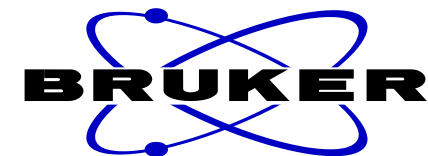
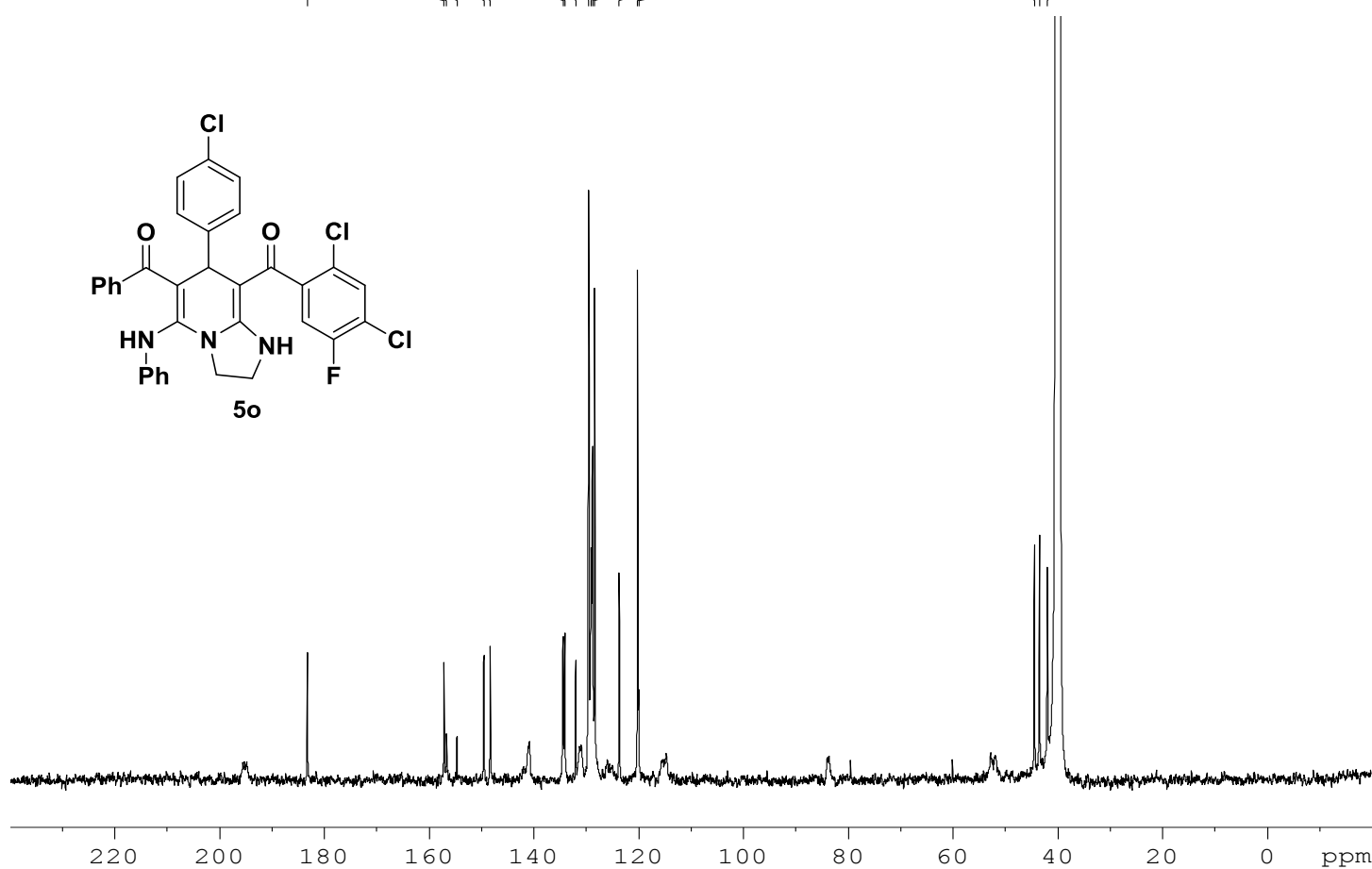
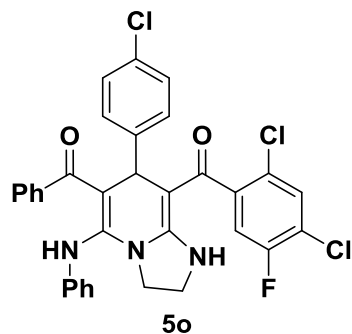
1.968



SP-E-15 13C 1D 2012 05 15

183.281
157.194
156.706
154.717
149.578
148.353
134.463
134.125
132.054
129.527
129.071
128.833
128.411
123.730
120.214
120.018

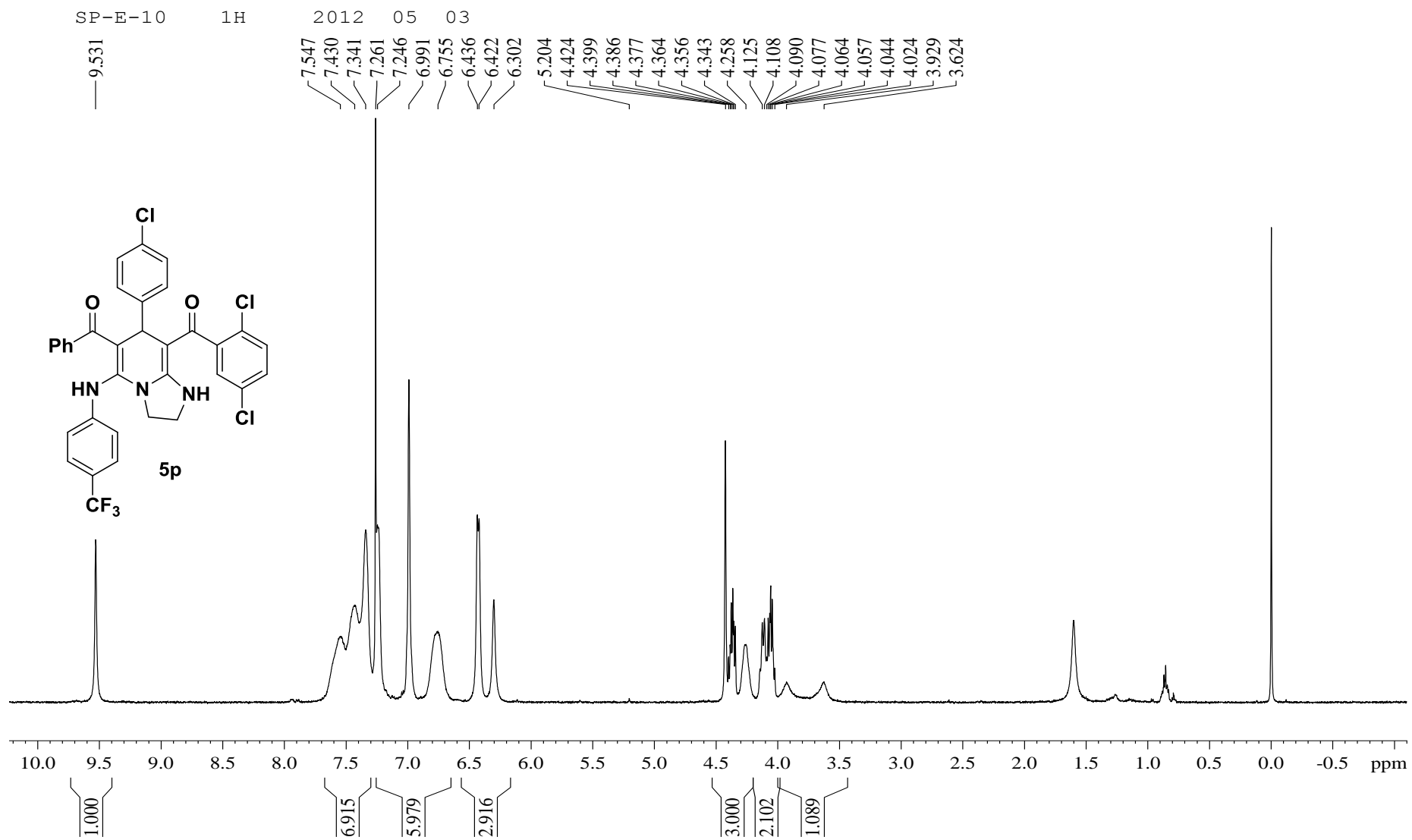
44.464
43.481
41.992



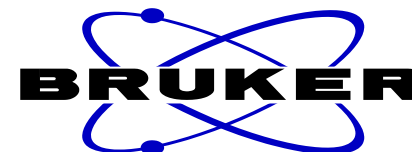
NAME SP-E-15
EXPNO 2
PROCNO 1
Date_ 20120515
Time_ 21.59
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 11304
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 2050
DW 15.300 usec
DE 6.00 usec
TE 296.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.20 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326518 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 2.00



SP-E-10 13C 1D 2012 05 05



NAME SP-E-10
EXPNO 2
PROCNO 1
Date_ 20120506
Time_ 10.15
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1271
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 11500
DW 15.300 usec
DE 6.00 usec
TE 300.3 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

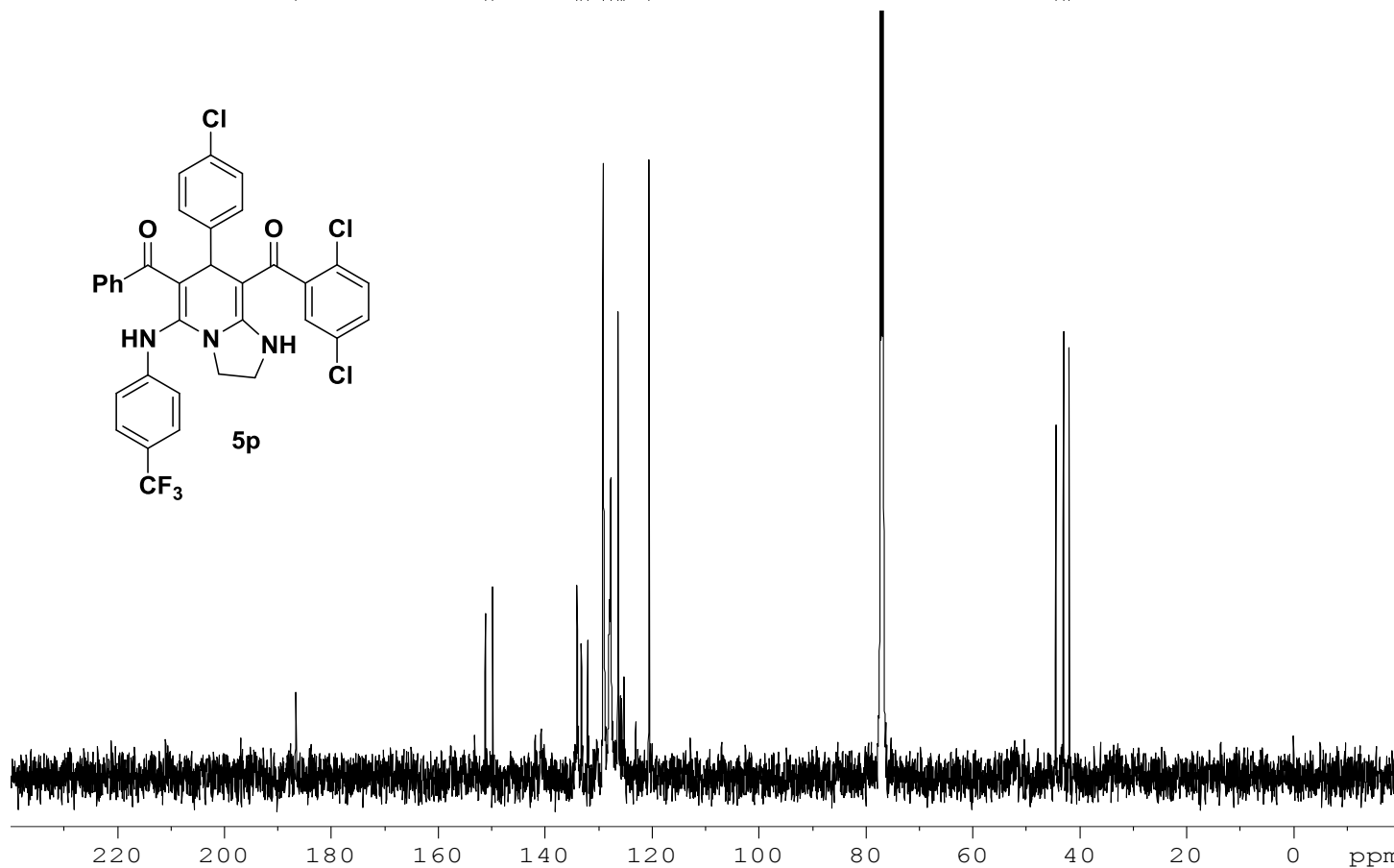
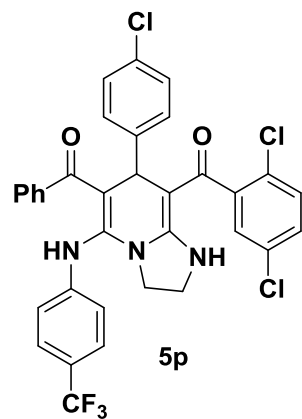
==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326440 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00

186.693

151.220
149.858
134.040
133.239
132.068
129.199
127.753
126.390
125.679
125.254
120.601

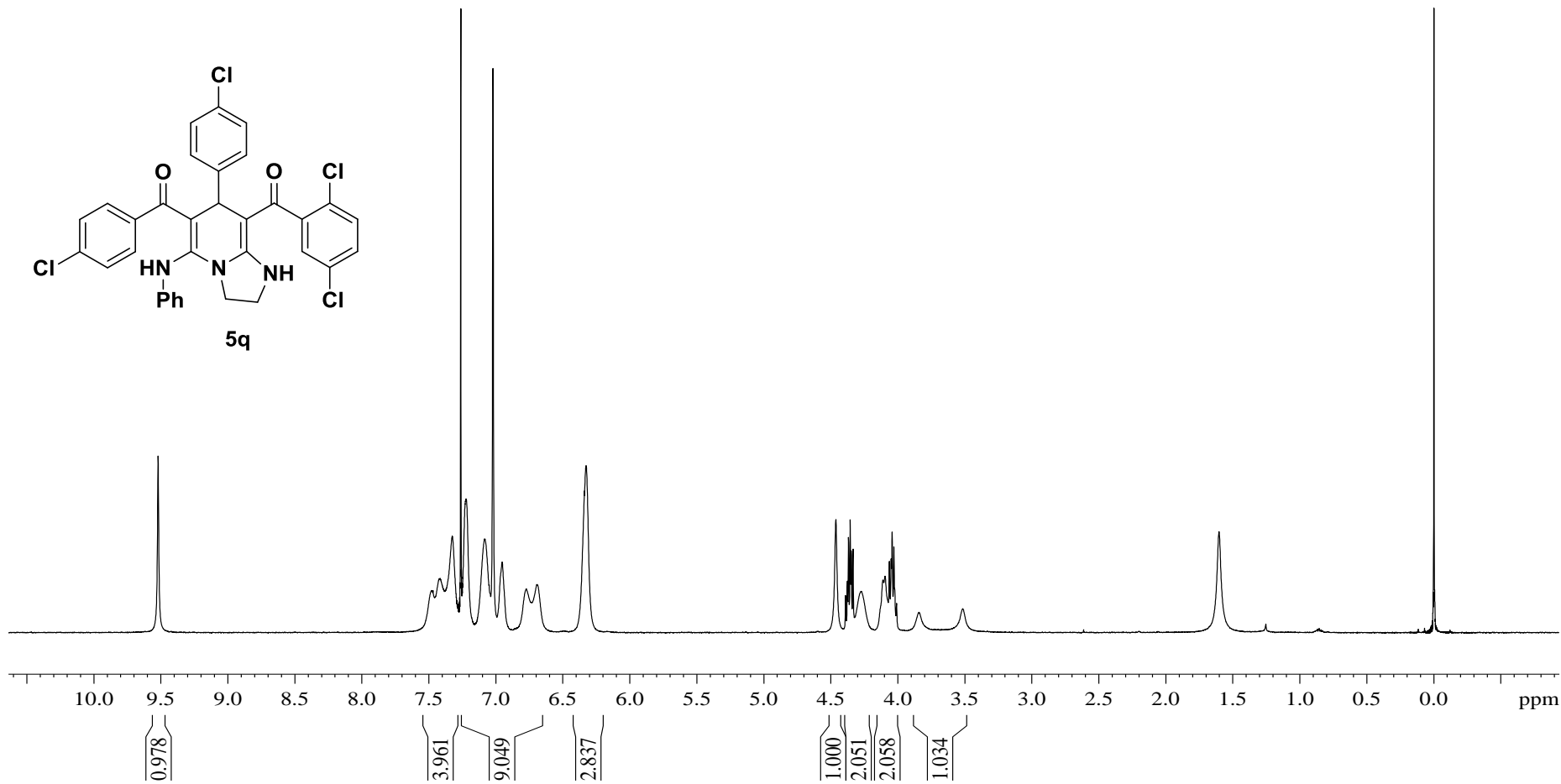
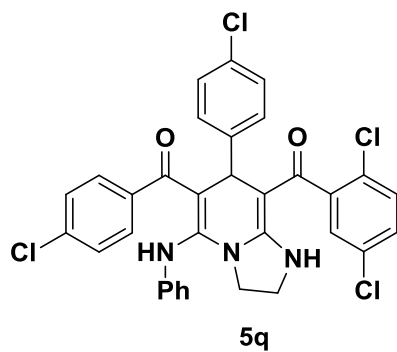
44.455
43.036
41.961



SP-E-13

1H 1D 2014 07 11

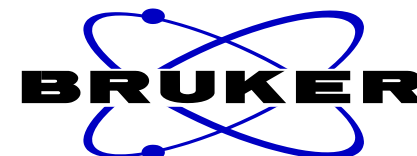
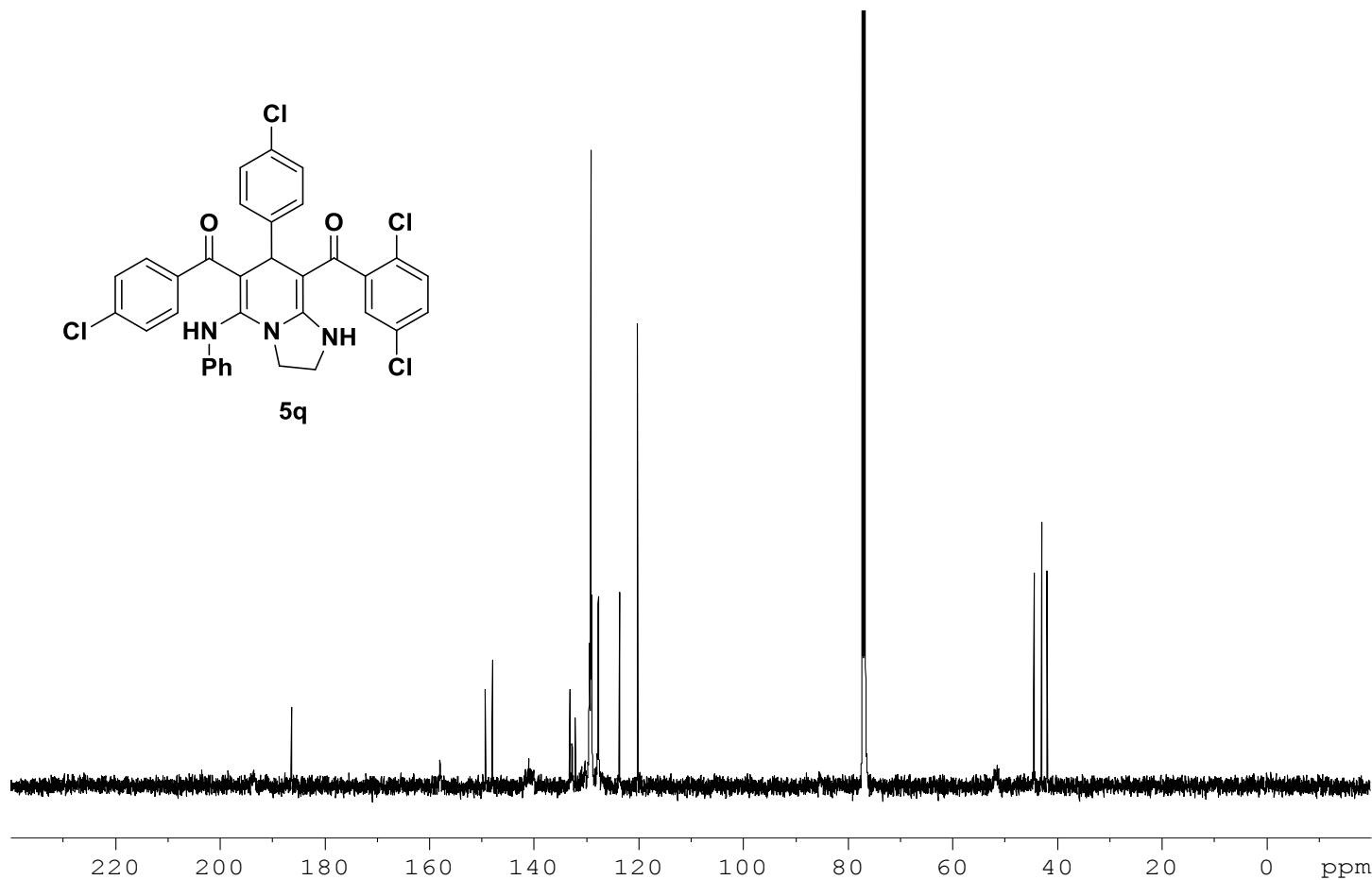
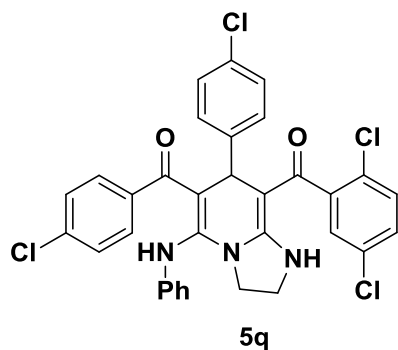
9.520
7.480
7.468
7.415
7.323
7.289
7.287
7.284
7.282
7.279
7.277
7.274
7.272
7.269
7.266
7.256
7.253
7.251
7.248
7.221
7.083
6.953
6.771
6.690
6.327
4.463
4.391
4.378
4.369
4.356
4.348
4.335
4.273
4.112
4.096
4.064
4.050
4.043
4.030
4.010
3.844
3.517



SP-E-13 13C 1D 2012 05 09

186.396
149.329
148.003
133.175
132.152
129.432
129.194
129.160
129.028
127.755
123.684
120.247

44.477
42.990
41.984



NAME SP-E-13
EXPNO 2
PROCNO 1
Date_ 20120509
Time_ 16.46
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1890
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 11500
DW 15.300 usec
DE 6.00 usec
TE 301.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.60 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326440 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 2.00

SP-E-16

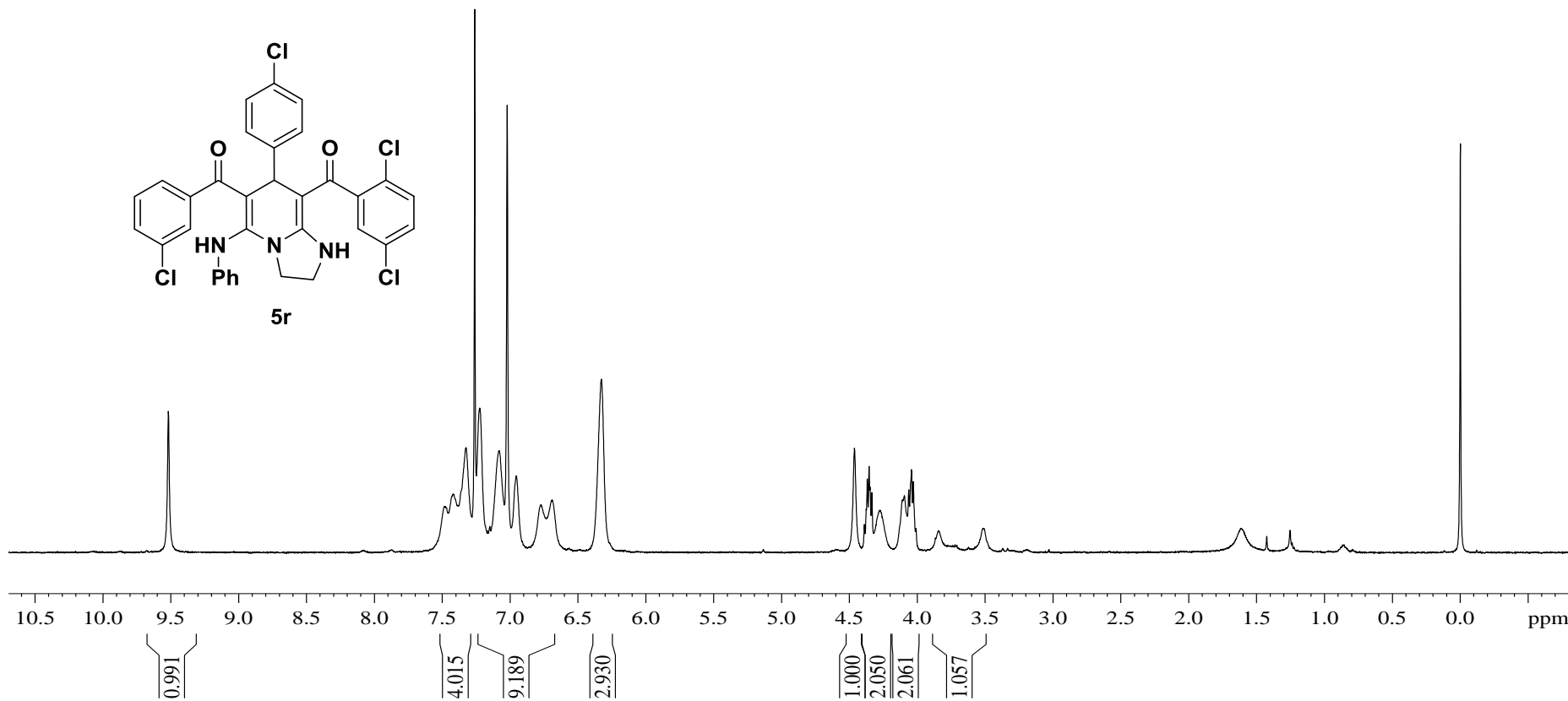
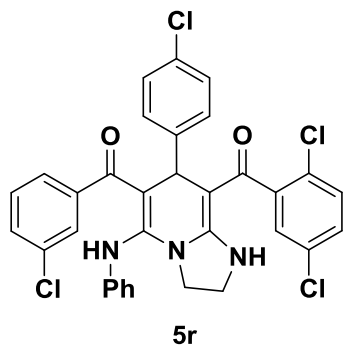
1H

2012 05 23

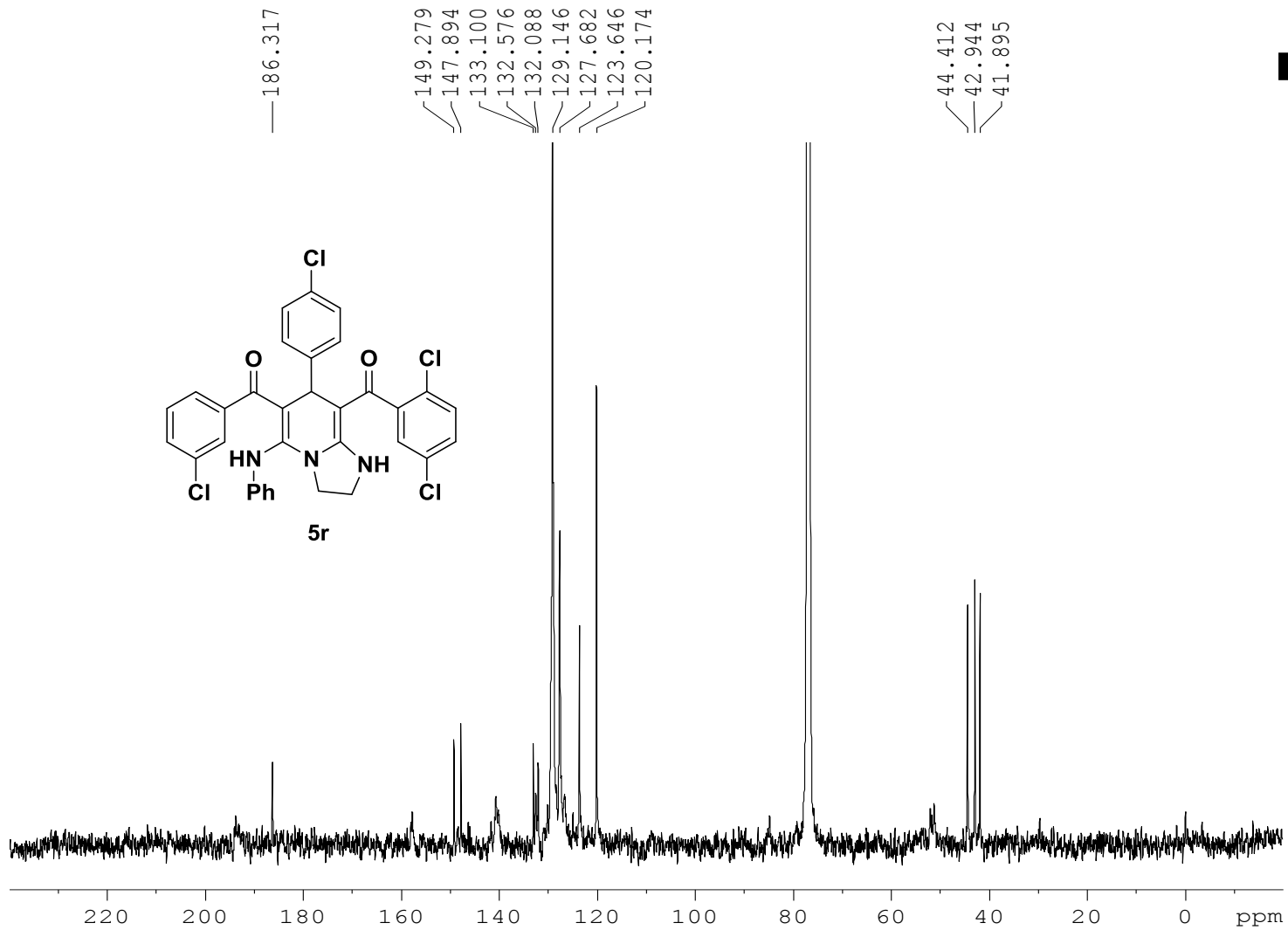
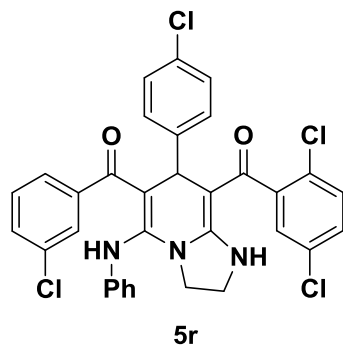
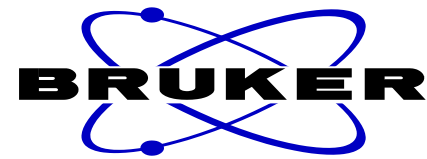
9.517

7.482
7.420
7.323
7.223
7.080
6.955
6.771
6.689
6.327

4.464
4.391
4.369
4.356
4.336
4.275
4.095
4.064
4.044
4.031
3.844
3.515



SP-E-16 13C 1D 2012 05 27

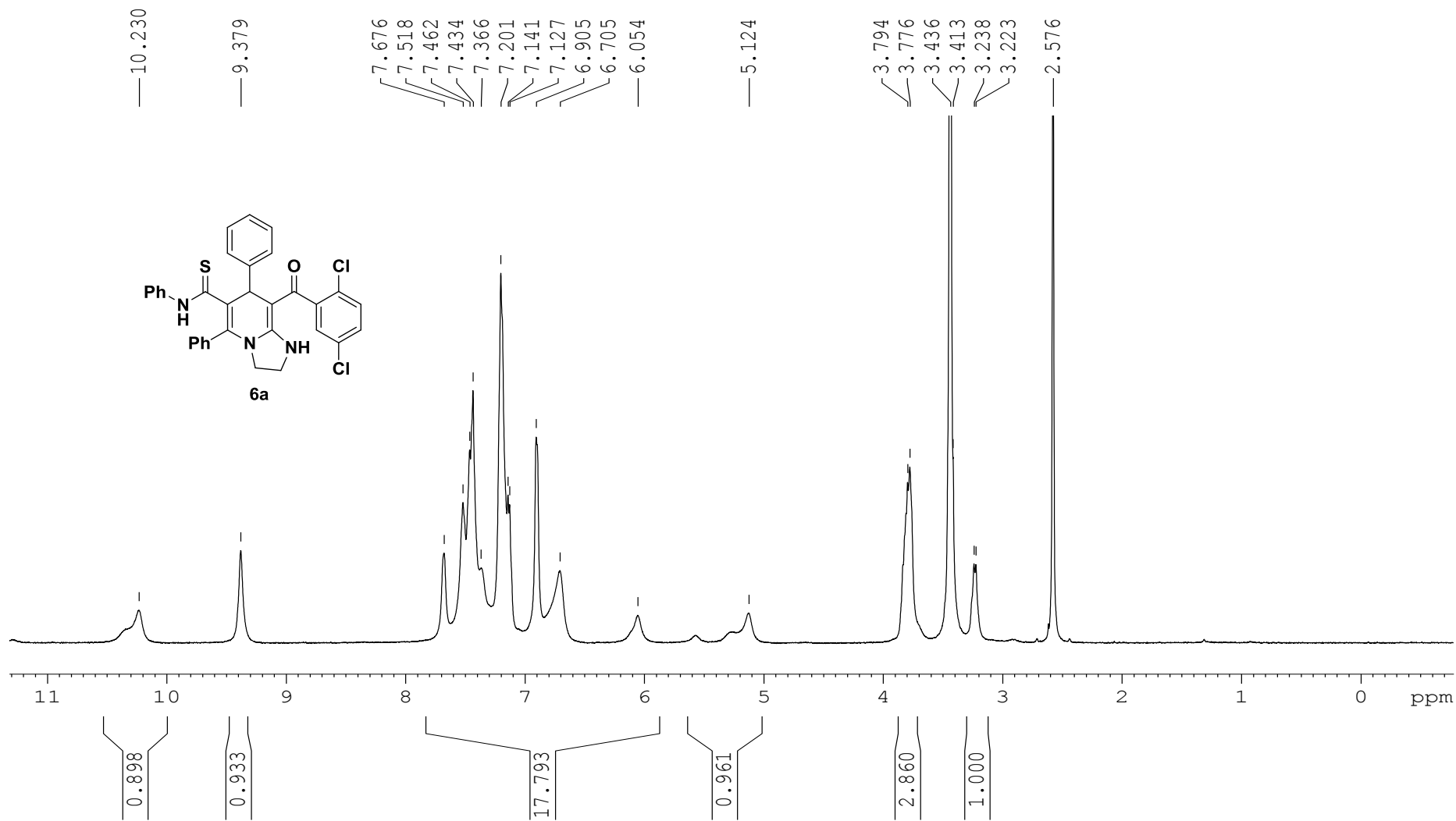


NAME SP-E-16
EXPNO 2
PROCNO 1
Date_ 20120527
Time_ 13.08
INSTRUM av500
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3752
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 2050
DW 15.300 usec
DE 6.00 usec
TE 292.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 2.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.20 dB
PL12 17.66 dB
PL13 17.66 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326518 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 2.00

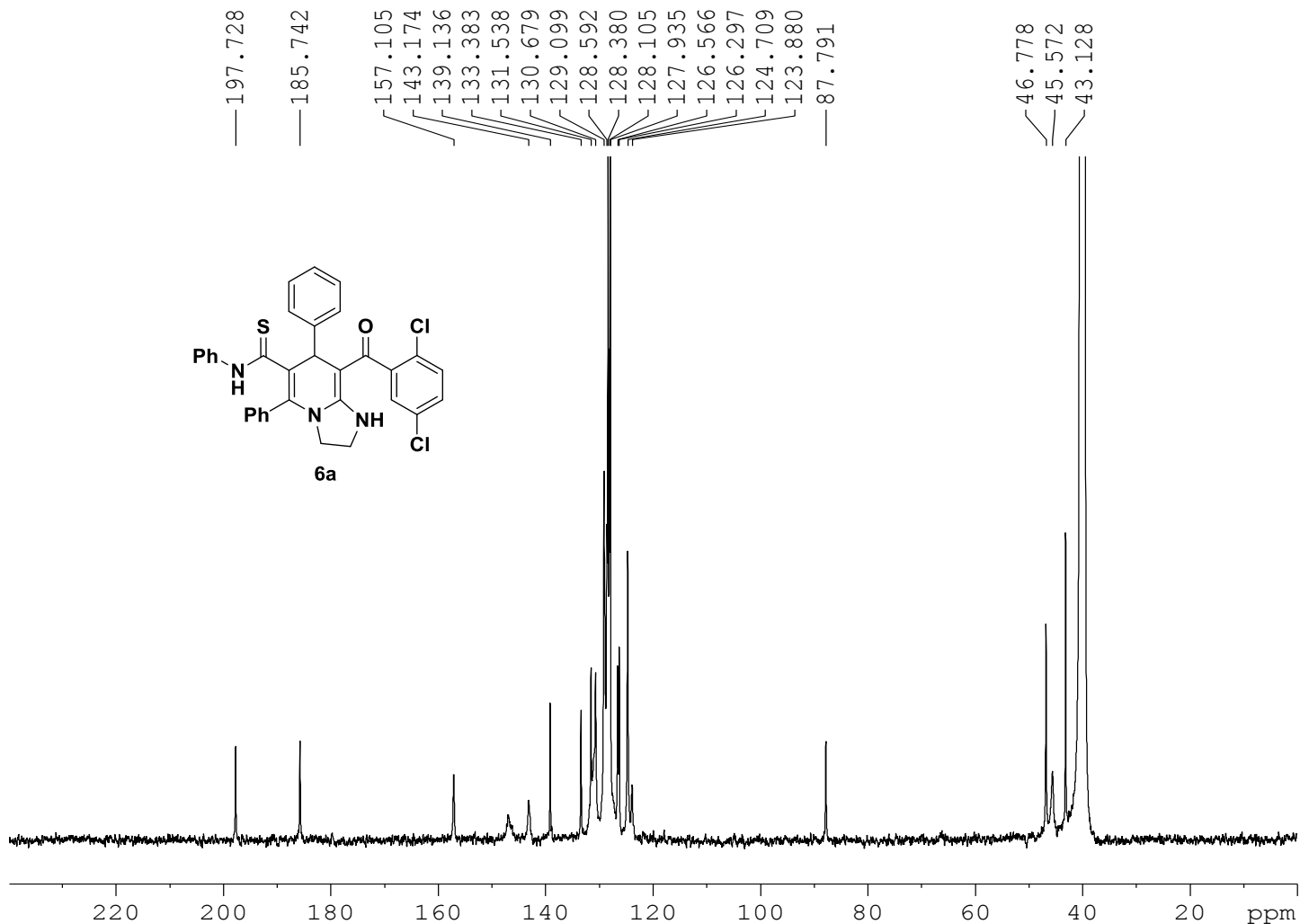
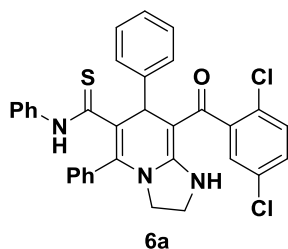
SP-P-7 1H 1D 2013 04 25



SP-P-7

13C

2013 04 29



```

NAME          SP-P-7
EXPNO         2
PROCNO        1
Date_         20130429
Time_         11.19
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            20000
DS            2
SWH           32679.738 Hz
FIDRES        0.498653 Hz
AQ            1.0027661 sec
RG            1820
DW            15.300 usec
DE            6.00 usec
TE            297.8 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.899999998 sec
TD0           20
    
```

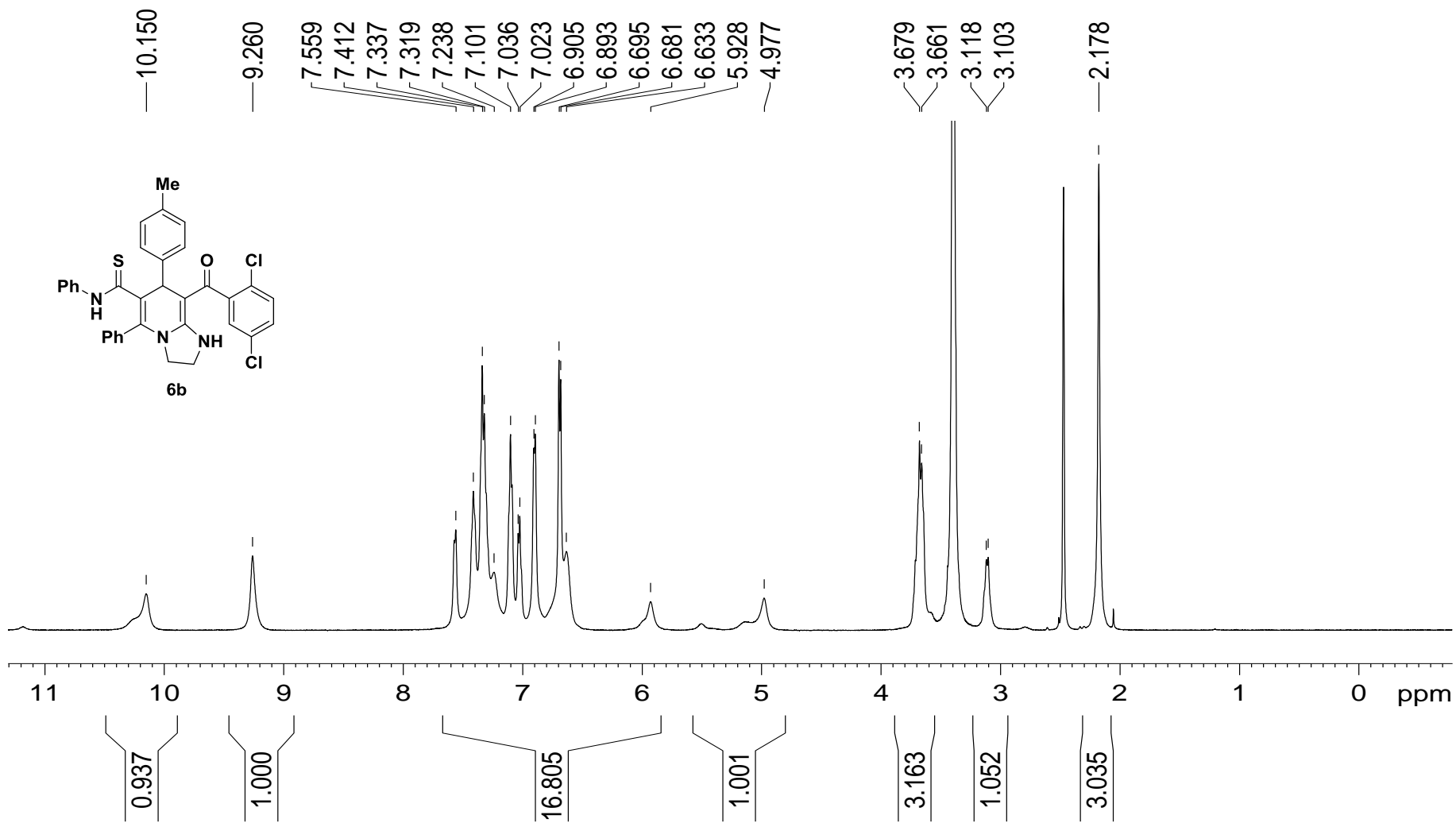
```

===== CHANNEL f1 =====
NUC1          13C
P1            12.20 usec
PL1           3.00 dB
SFO1          125.7464750 MHz
    
```

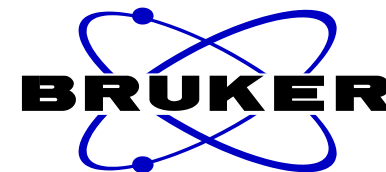
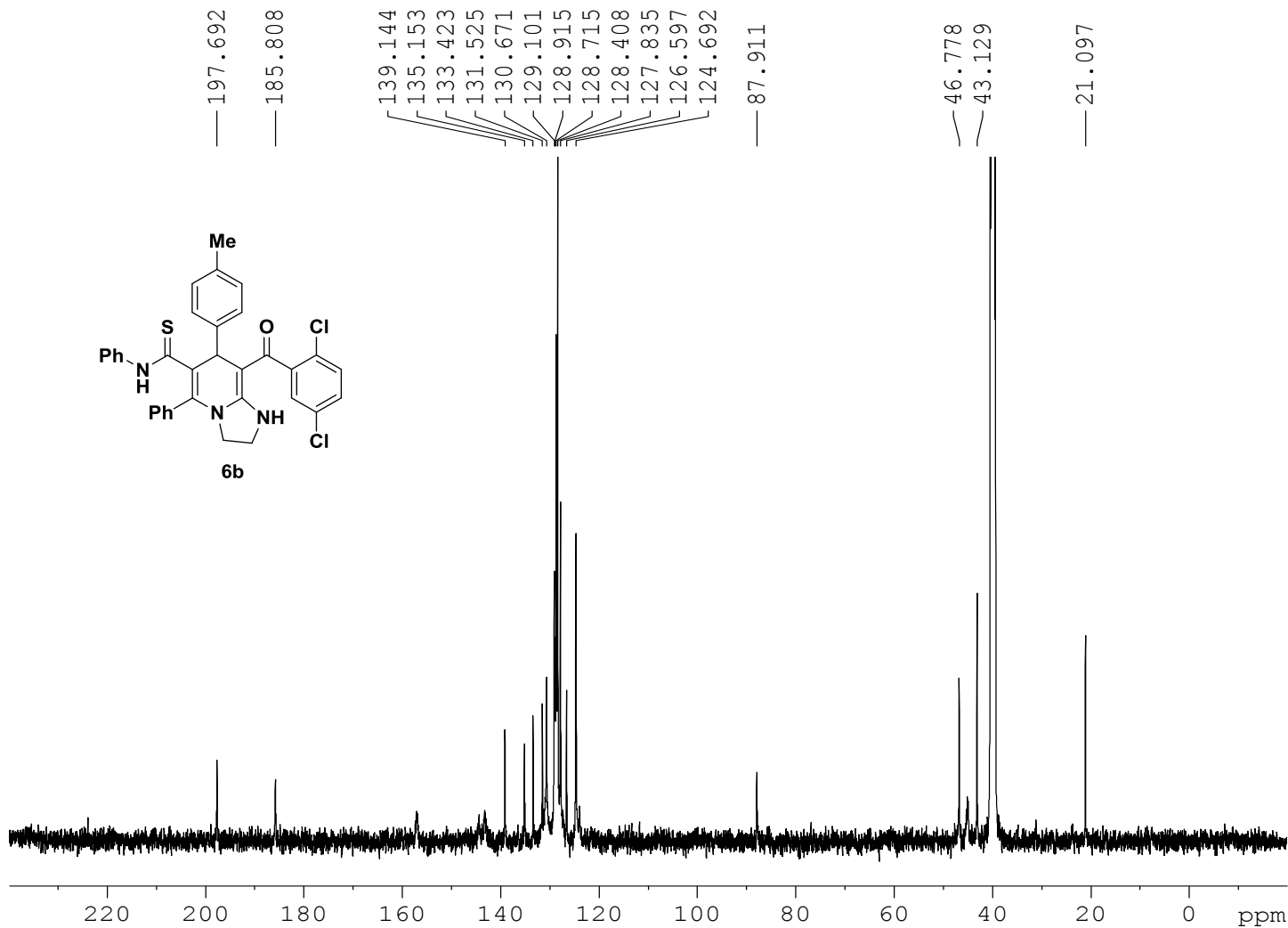
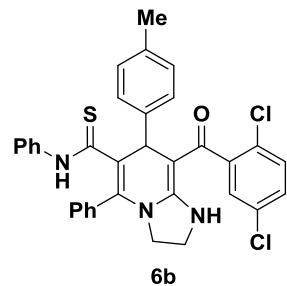
```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           2.00 dB
PL12          17.70 dB
PL13          17.70 dB
SFO2          500.0355000 MHz
SI            32768
SF            125.7326486 MHz
WDW           EM
SSB           0
LB            8.00 Hz
GB            0
PC            1.00
    
```

SP-P-3 1H 1D 2013 01 03



SP-P-3 13C 1D 2013 01 04

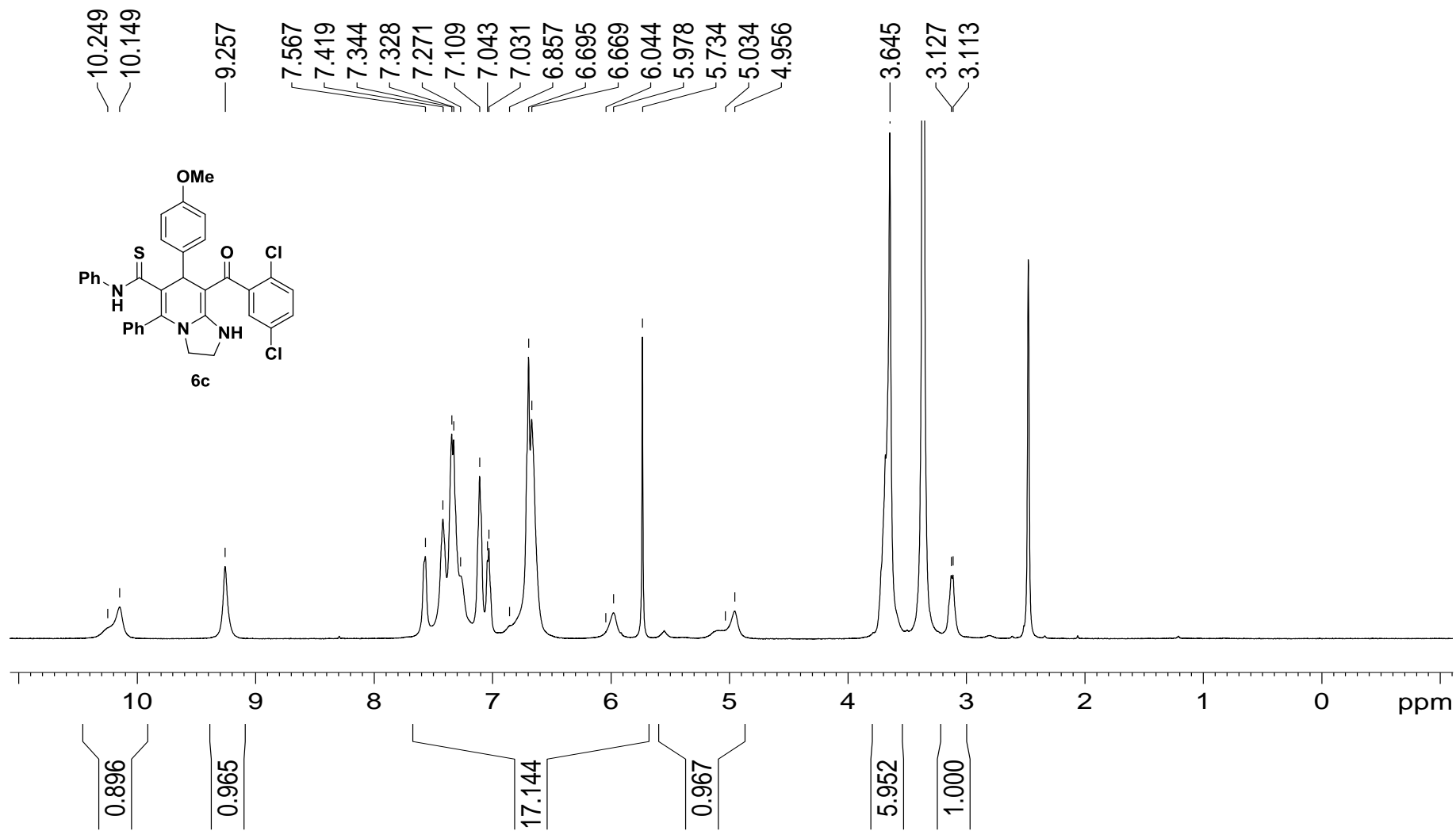


NAME SP-P-3
EXPNO 2
PROCNO 1
Date_ 20121226
Time_ 19.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2365
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 11500
DW 15.300 usec
DE 6.00 usec
TE 292.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 10

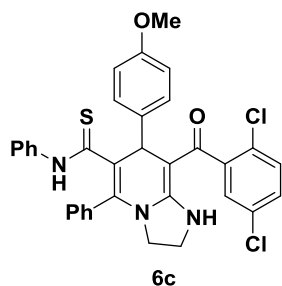
==== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326455 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00

SP-P-2a 1H 1D 2013 1 11



SP-P-2a 13C 1D 2013 01 17



197.792

185.852

157.962

139.168

133.454

131.540

130.674

129.089

128.923

128.630

128.405

126.583

124.704

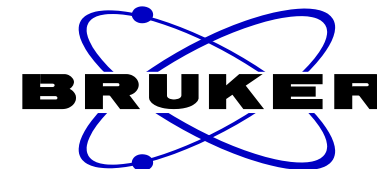
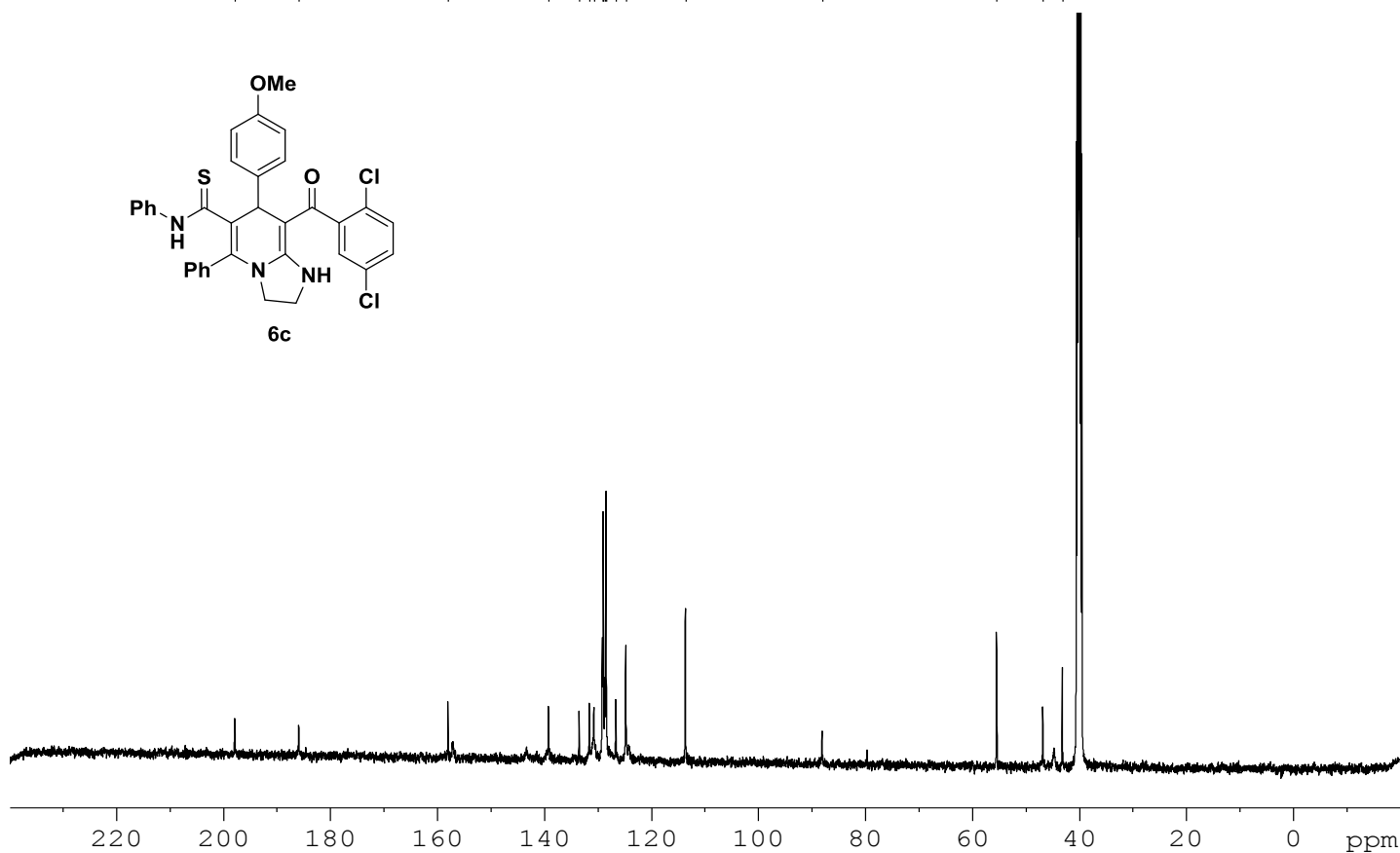
113.586

88.021

55.428

46.785

43.123

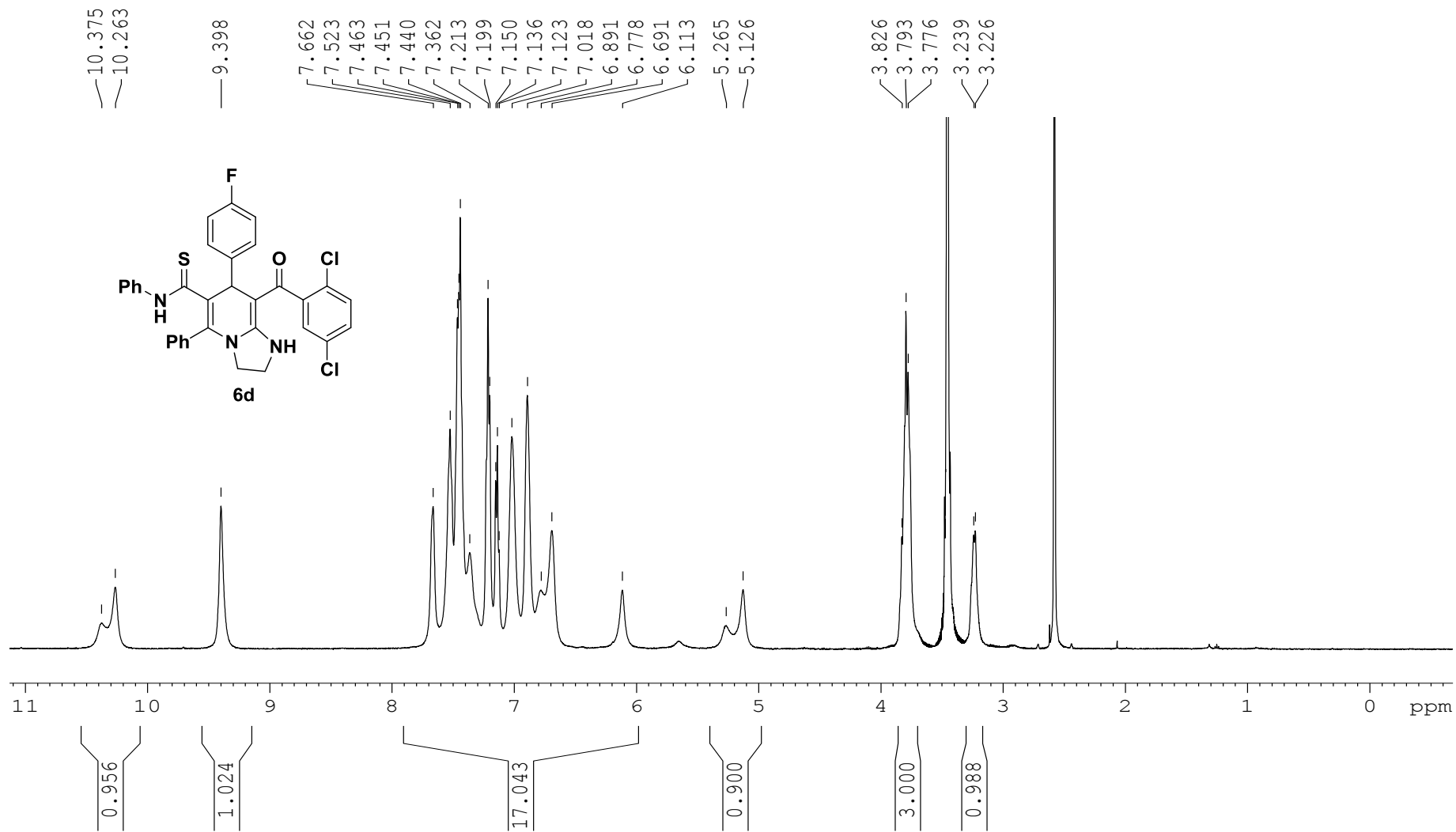


NAME SP-P-2a
EXPNO 2
PROCNO 1
Date_ 20130117
Time_ 16.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2245
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 5790
DW 15.300 usec
DE 6.00 usec
TE 294.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 8

===== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326455 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00

SP-P-9 1H 1D 2013 04 23



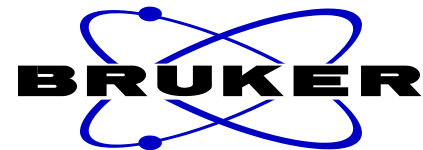
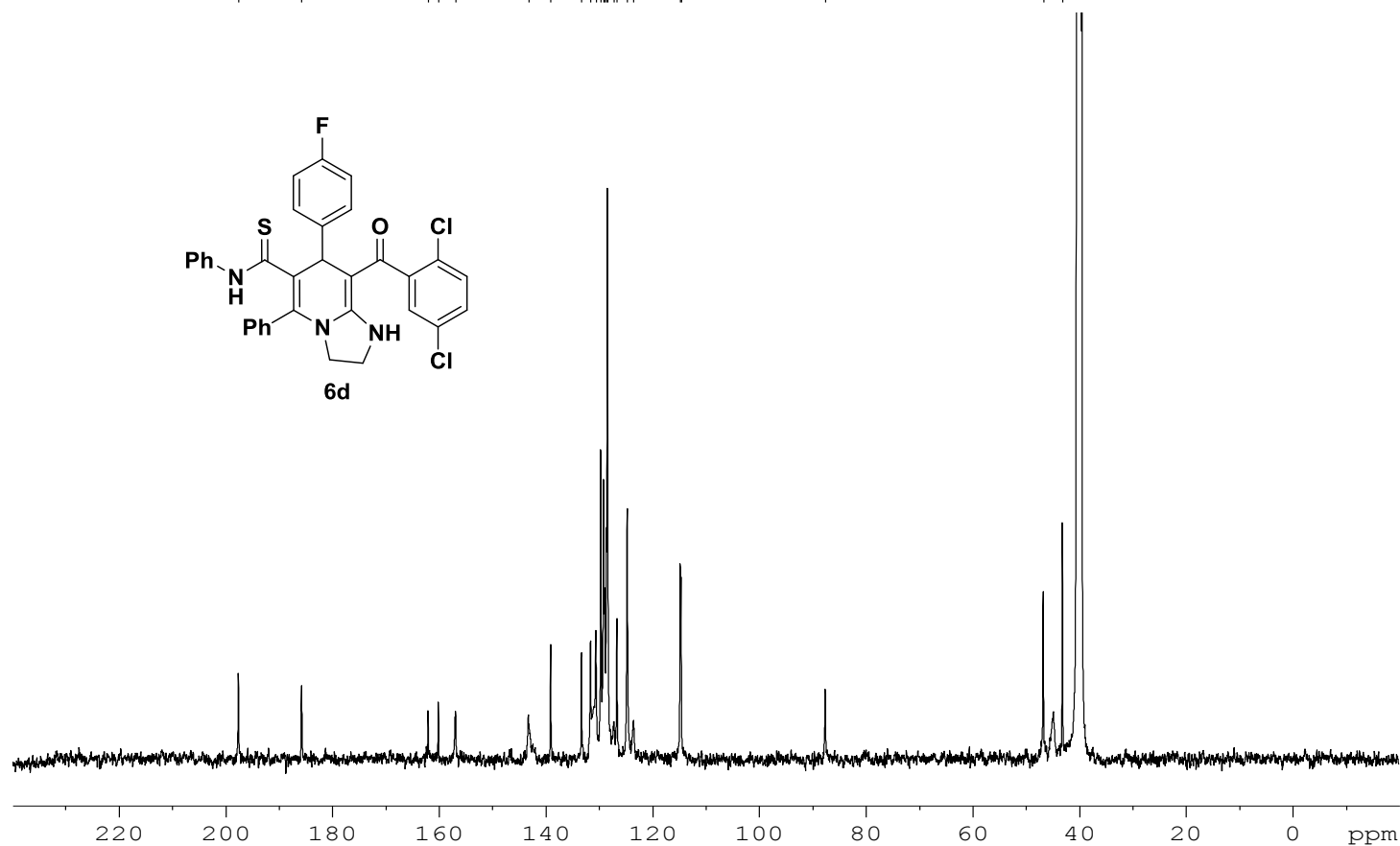
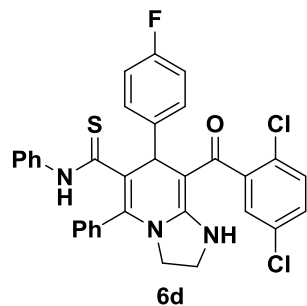
SP-P-9

13C

2013 04 28

197.634
185.780
162.075
160.151
156.947
143.248
139.085
133.320
131.608
130.604
129.695
129.156
128.974
128.633
128.457
127.225
126.658
124.737
123.548
114.803
114.638
87.604

46.748
43.149

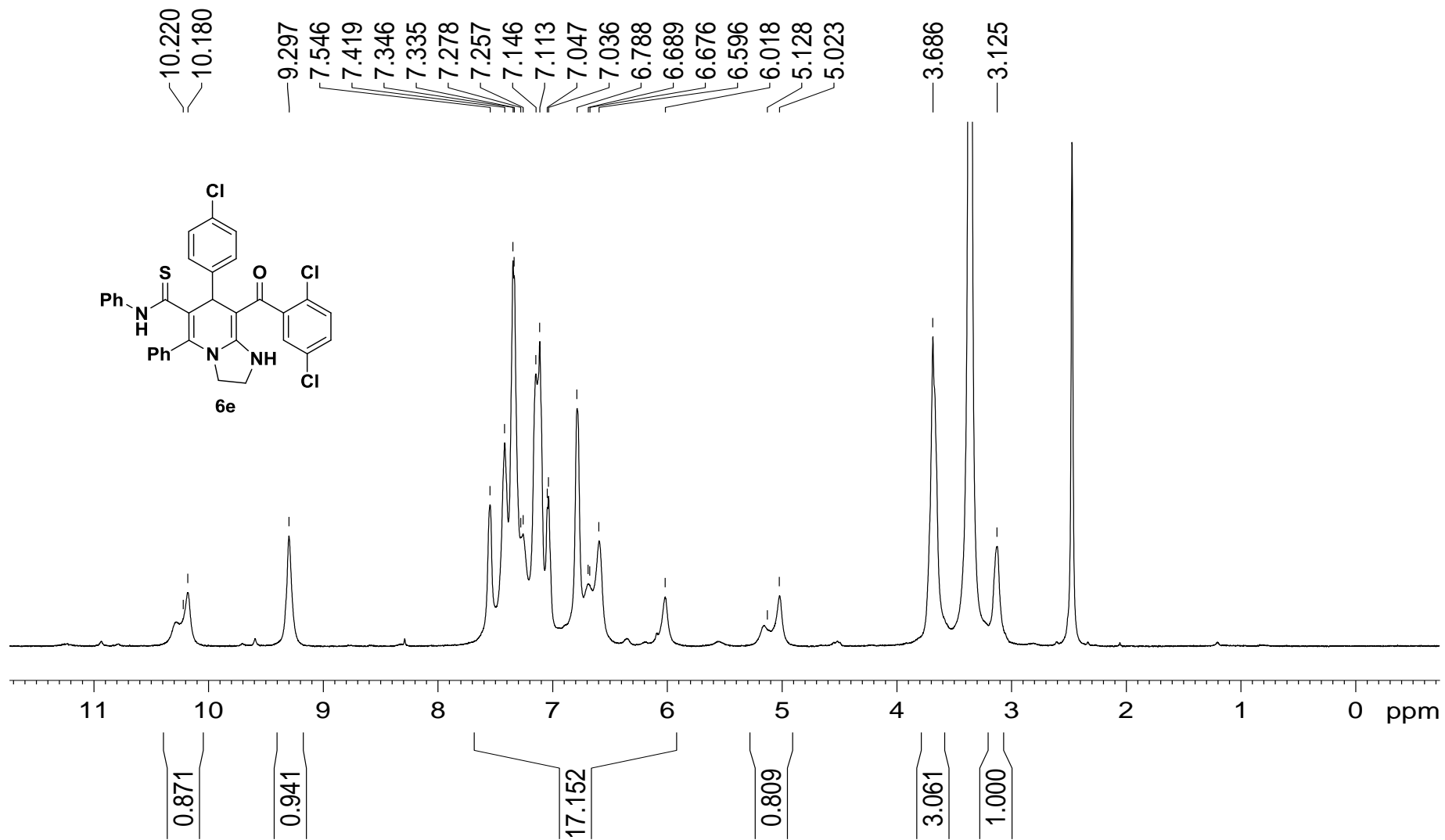


NAME SP-P-9
EXPNO 2
PROCNO 1
Date_ 20130428
Time_ 17.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2780
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1820
DW 15.300 usec
DE 6.00 usec
TE 299.1 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 20

==== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

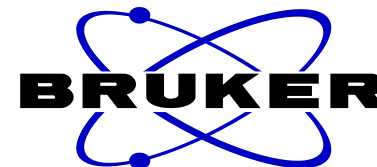
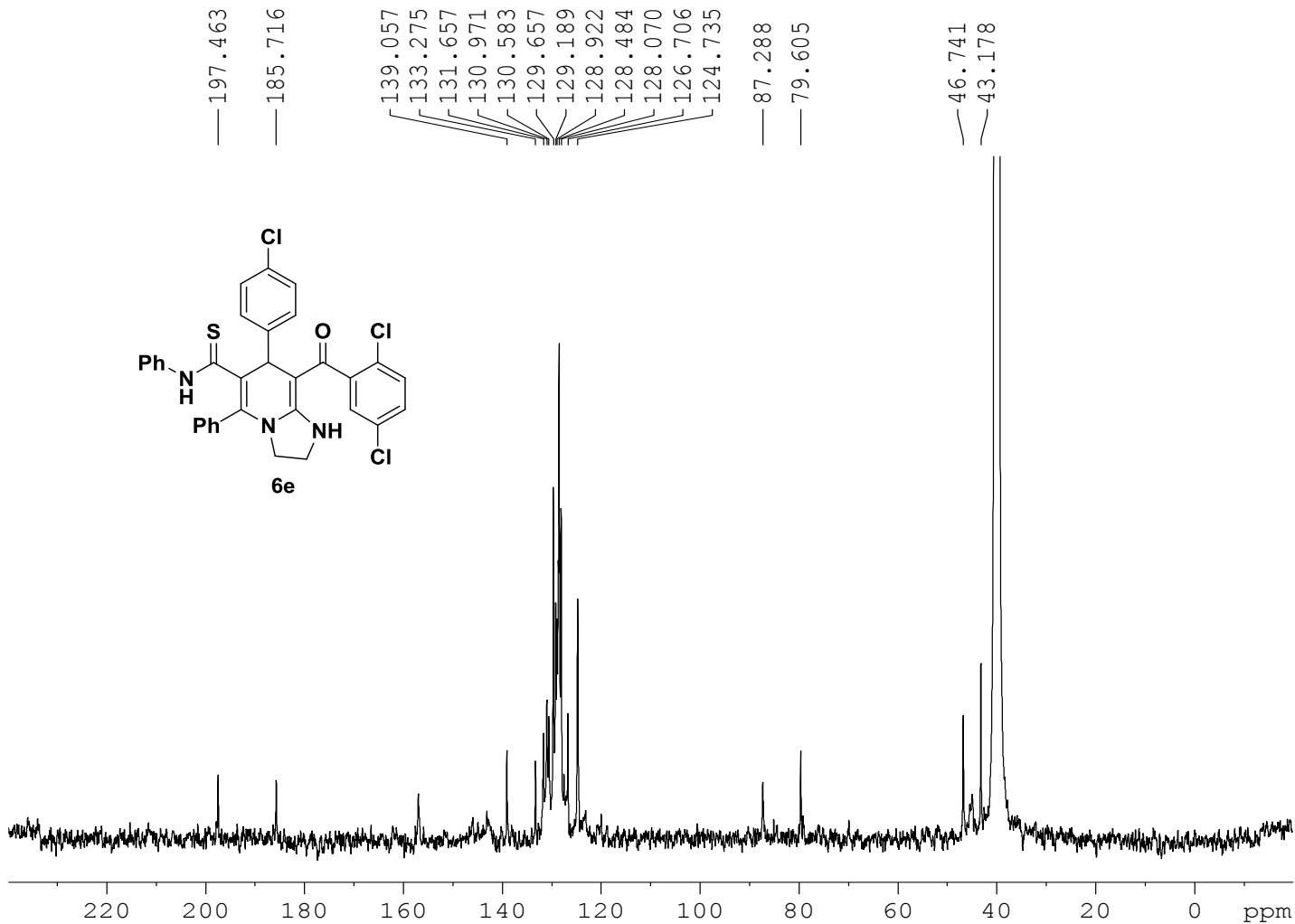
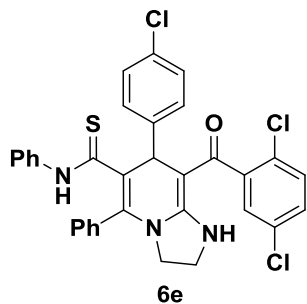
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326474 MHz
WDW EM
SSB 0
LB 8.00 Hz
GB 0
PC 1.00

SP-P-1b 1H 1D 2013 1 11



SP-P-1b

13C 1D 2013 01 18

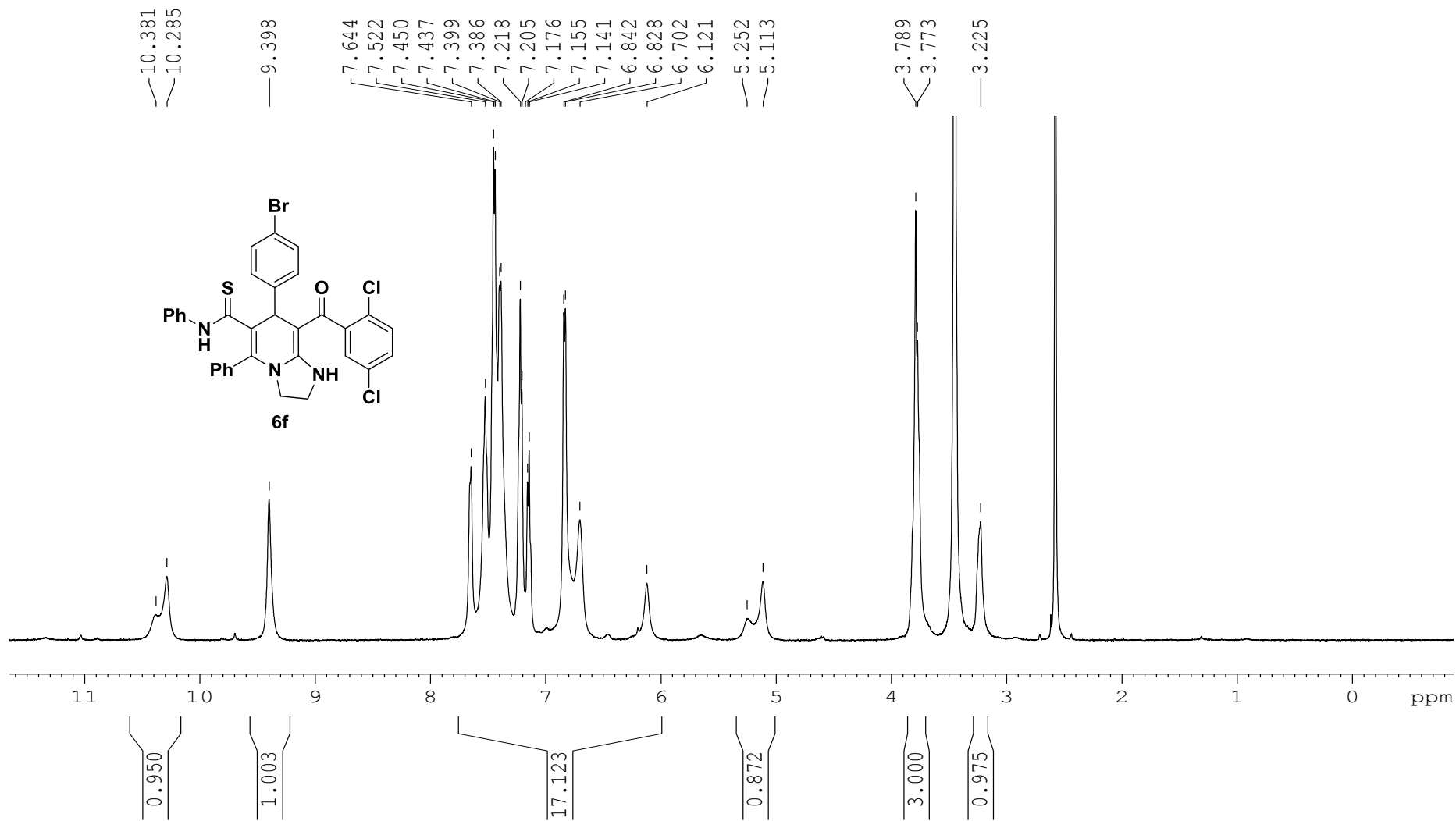


NAME SP-P-1b
EXPNO 21
PROCNO 1
Date_ 20130118
Time 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5326
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 5790
DW 15.300 usec
DE 6.00 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326455 MHz
WDW EM
SSB 0
LB 12.00 Hz
GB 0
PC 2.00

SP-P-8 1H 1D 2013 04 23



SP-P-8

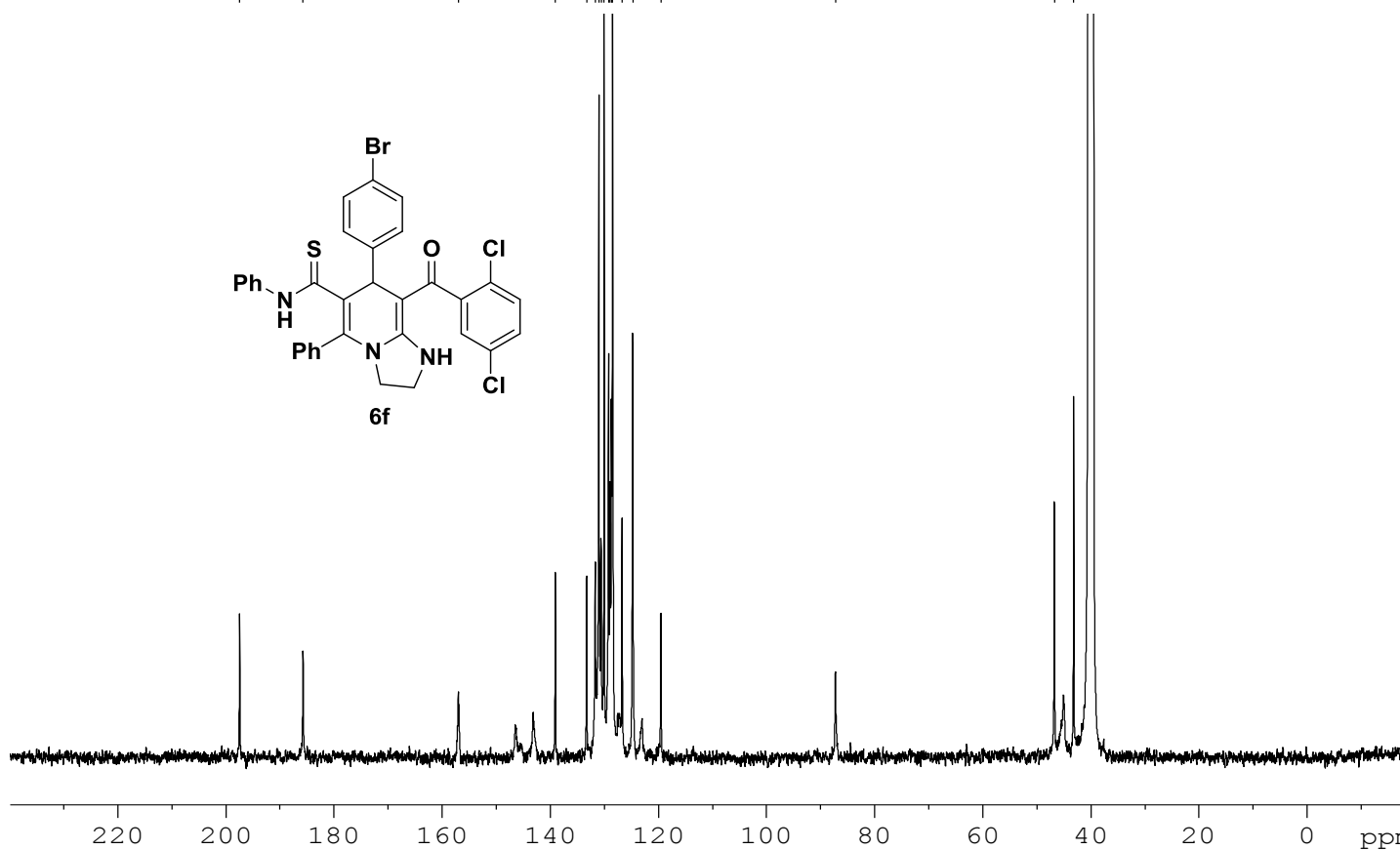
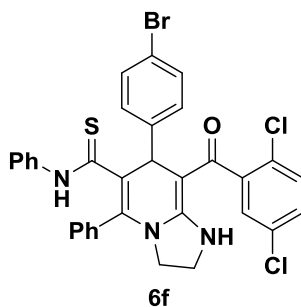
13C

2013 04 24



197.456
185.736
156.972
139.074
133.283
131.673
130.999
130.591
130.052
129.203
128.927
128.679
128.495
126.716
124.741
119.553
87.252

46.758
43.191

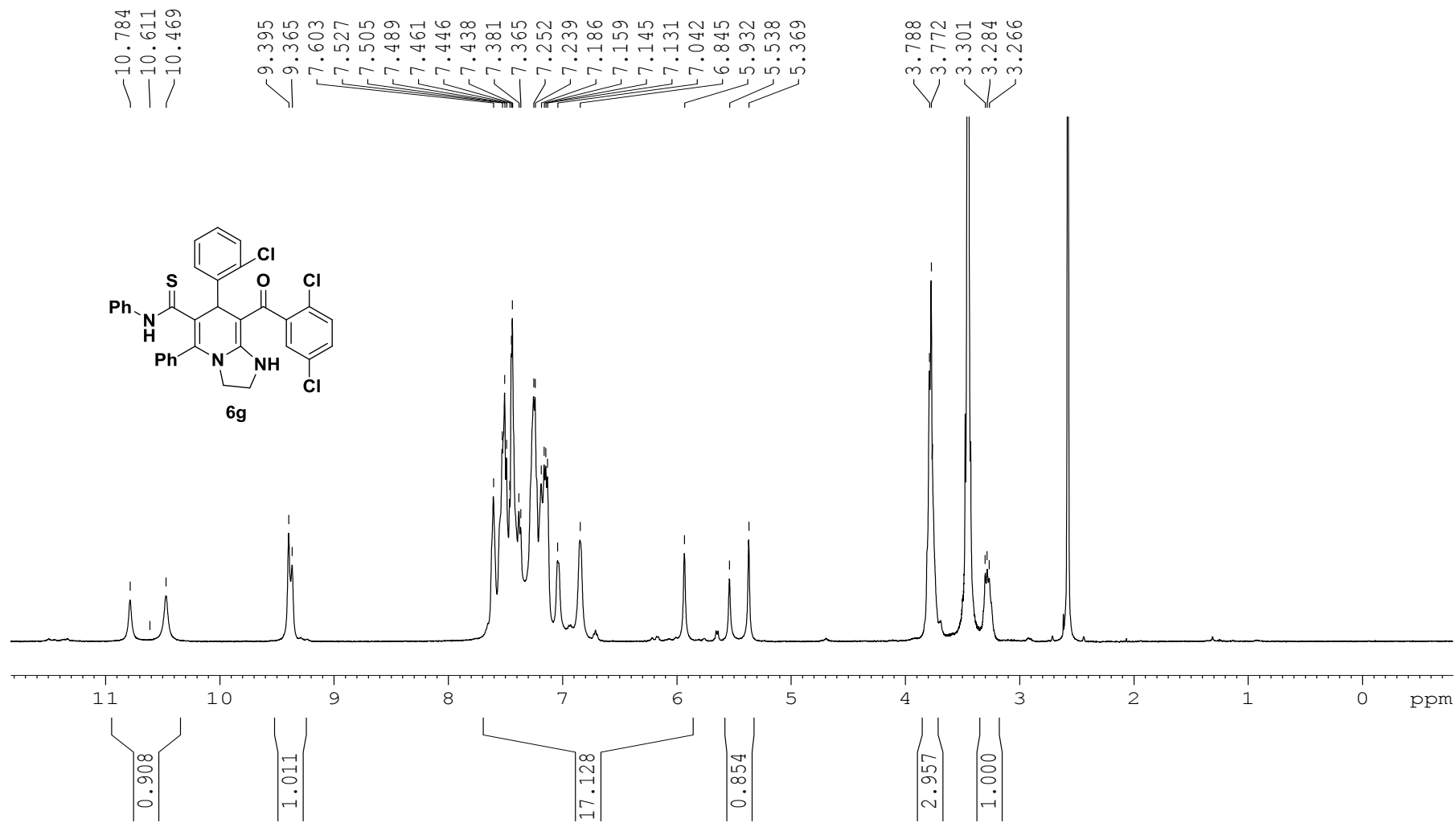


NAME SP-P-8
EXPNO 2
PROCNO 1
Date_ 20130424
Time_ 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 13565
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1820
DW 15.300 usec
DE 6.00 usec
TE 296.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20

==== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326450 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.00

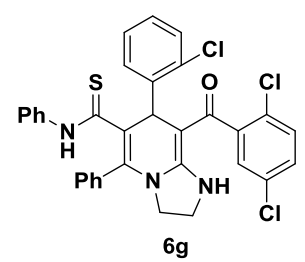
SP-P-6 1H 1D 2013 04 15



SP-P-6

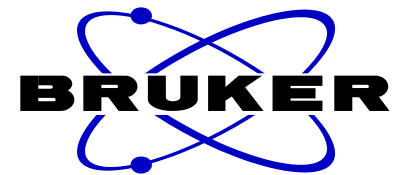
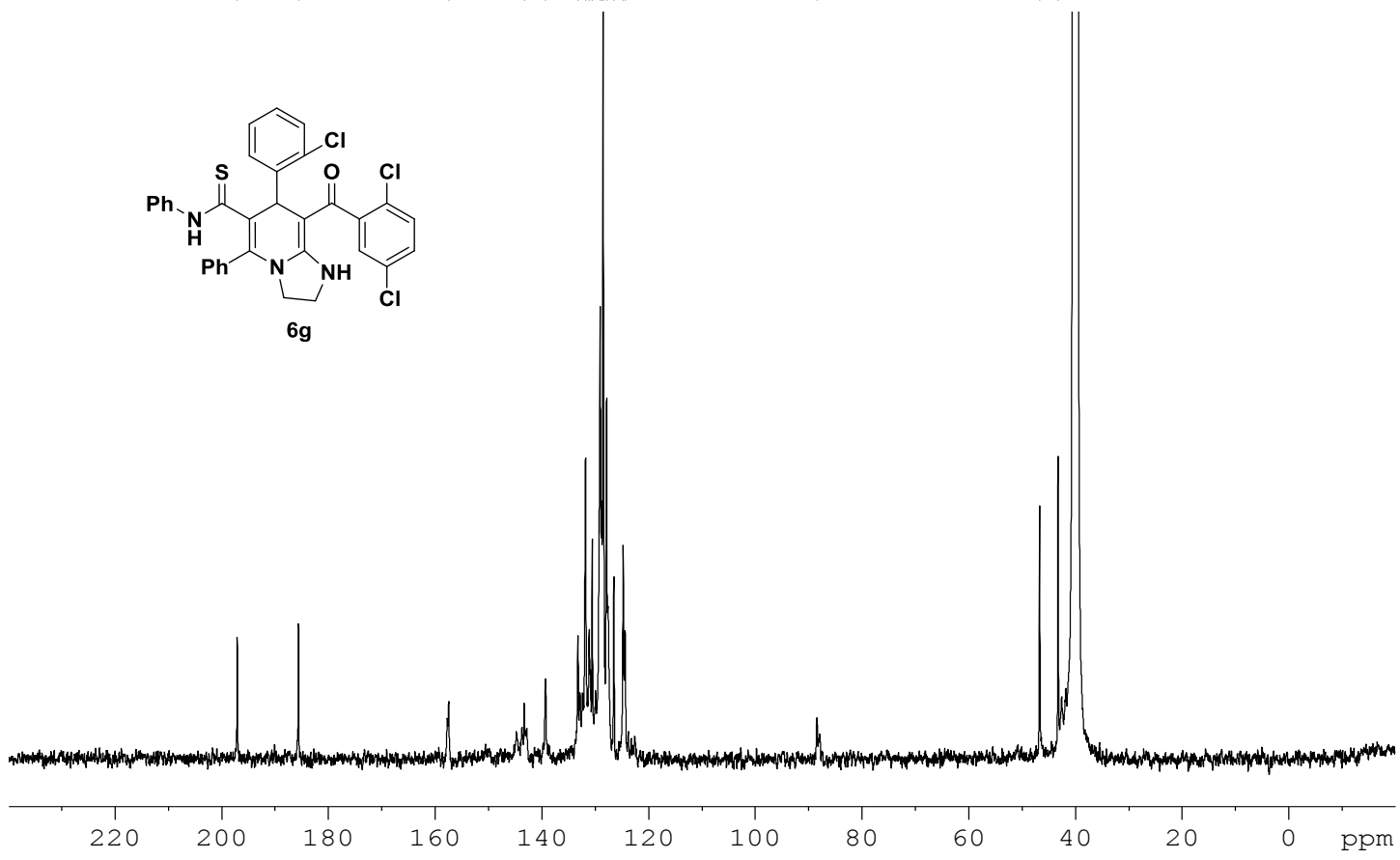
13C

2013 04 27



197.094
185.608
157.455
143.307
139.295
133.220
131.818
131.113
130.542
129.089
128.778
128.495
127.879
126.512
124.777
124.403
88.433

46.702
43.251

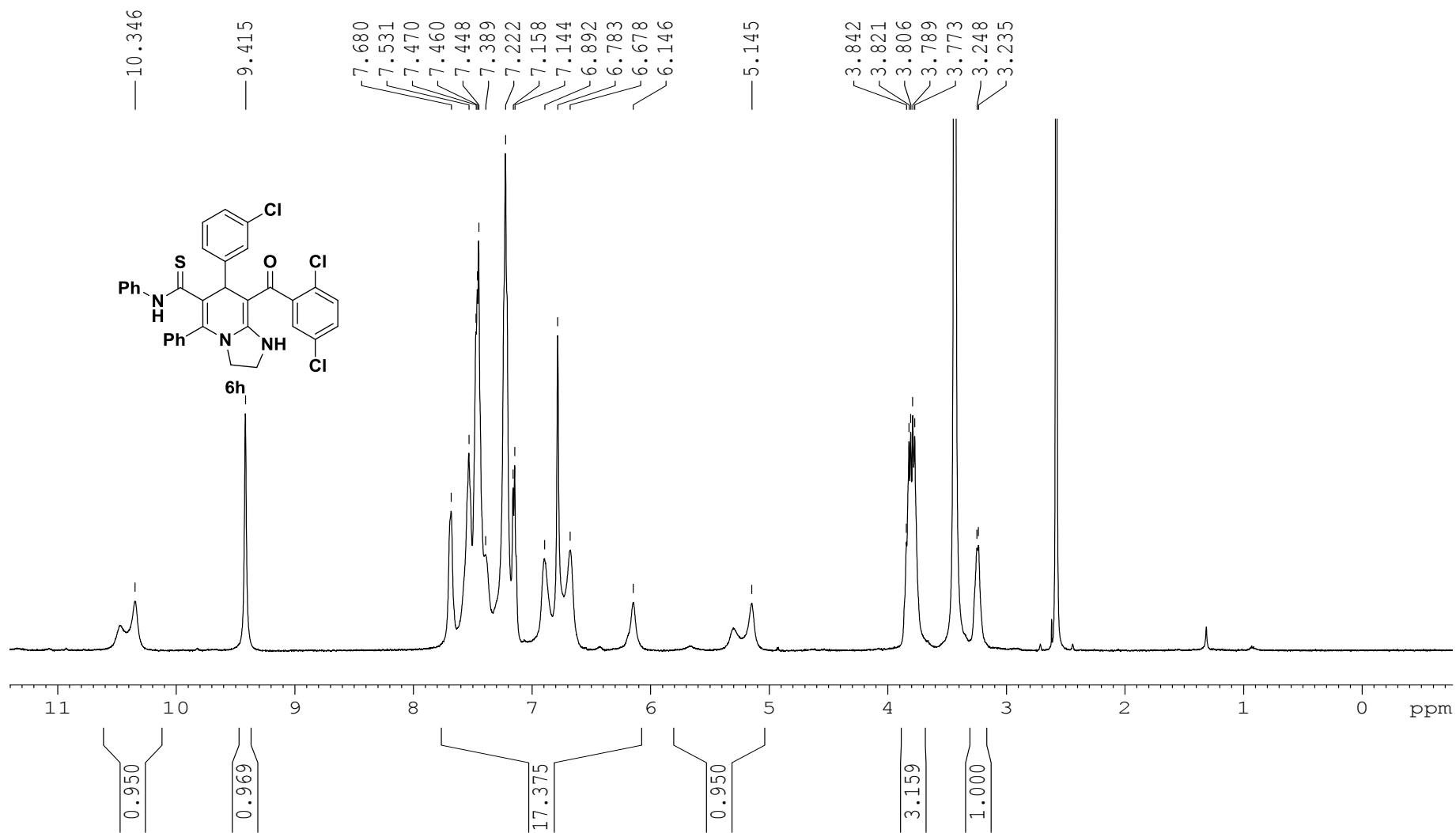


```
NAME          SP-P-6
EXPNO         2
PROCNO        1
Date_         20130427
Time_         21.27
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            11755
DS            2
SWH           32679.738 Hz
FIDRES        0.498653 Hz
AQ            1.0027661 sec
RG            1820
DW            15.300 usec
DE            6.00 usec
TE            296.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           20

===== CHANNEL f1 =====
NUC1           13C
P1             12.20 usec
PL1            3.00 dB
SFO1          125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2            2.00 dB
PL12           17.70 dB
PL13           17.70 dB
SFO2          500.0355000 MHz
SI            32768
SF            125.7326450 MHz
WDW            EM
SSB            0
LB             8.00 Hz
GB             0
PC             1.00
```

P-P-10 1H 1D 2013 04 2.

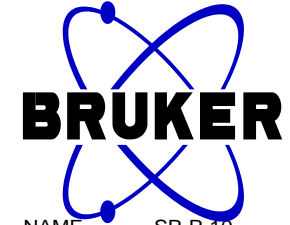
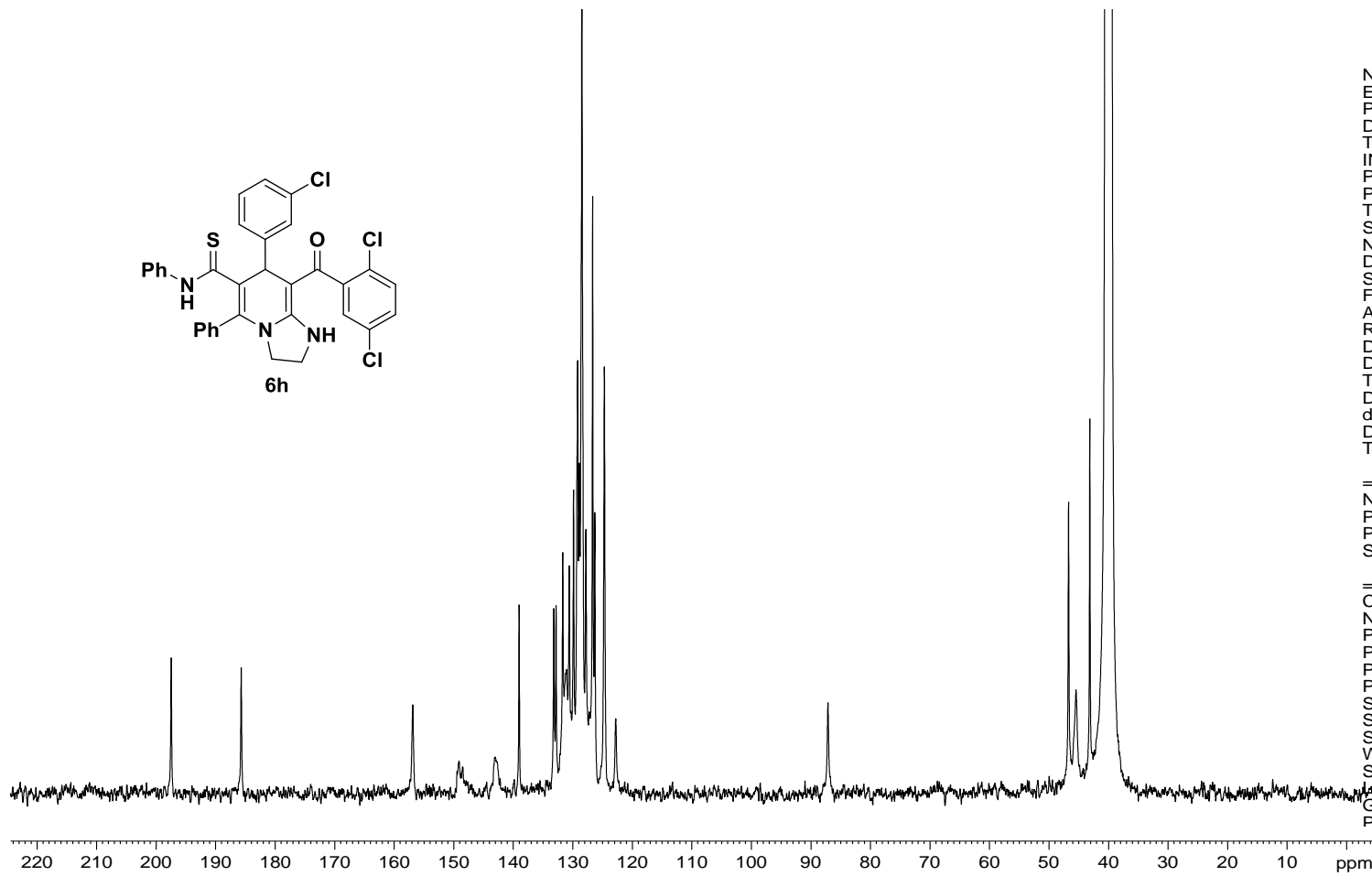
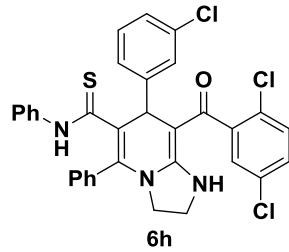


SP-P-10 13C 2013 05 01

197.446
185.687
156.903
149.139
143.071
139.035
133.223
132.837
131.710
131.069
130.621
129.893
129.200
128.933
128.483
127.819
126.687
126.321
124.720
122.810

87.149

46.715
45.462
43.152
40.489
40.328
40.164
39.999
39.833
39.669
39.506

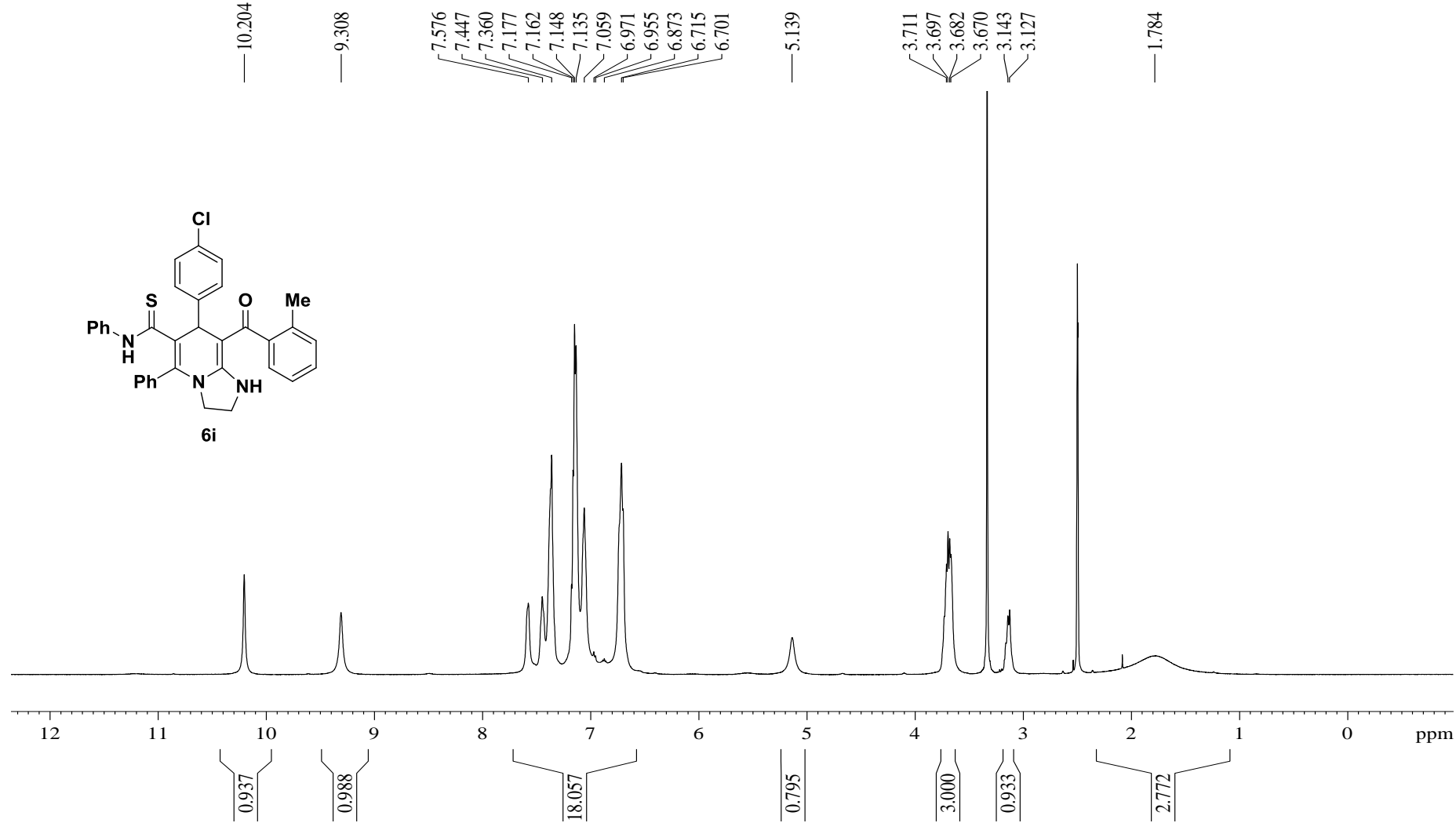


NAME SP-P-10
EXPNO 2
PROCNO 1
Date_ 20130501
Time 18.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15437
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 1820
DW 15.300 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 20

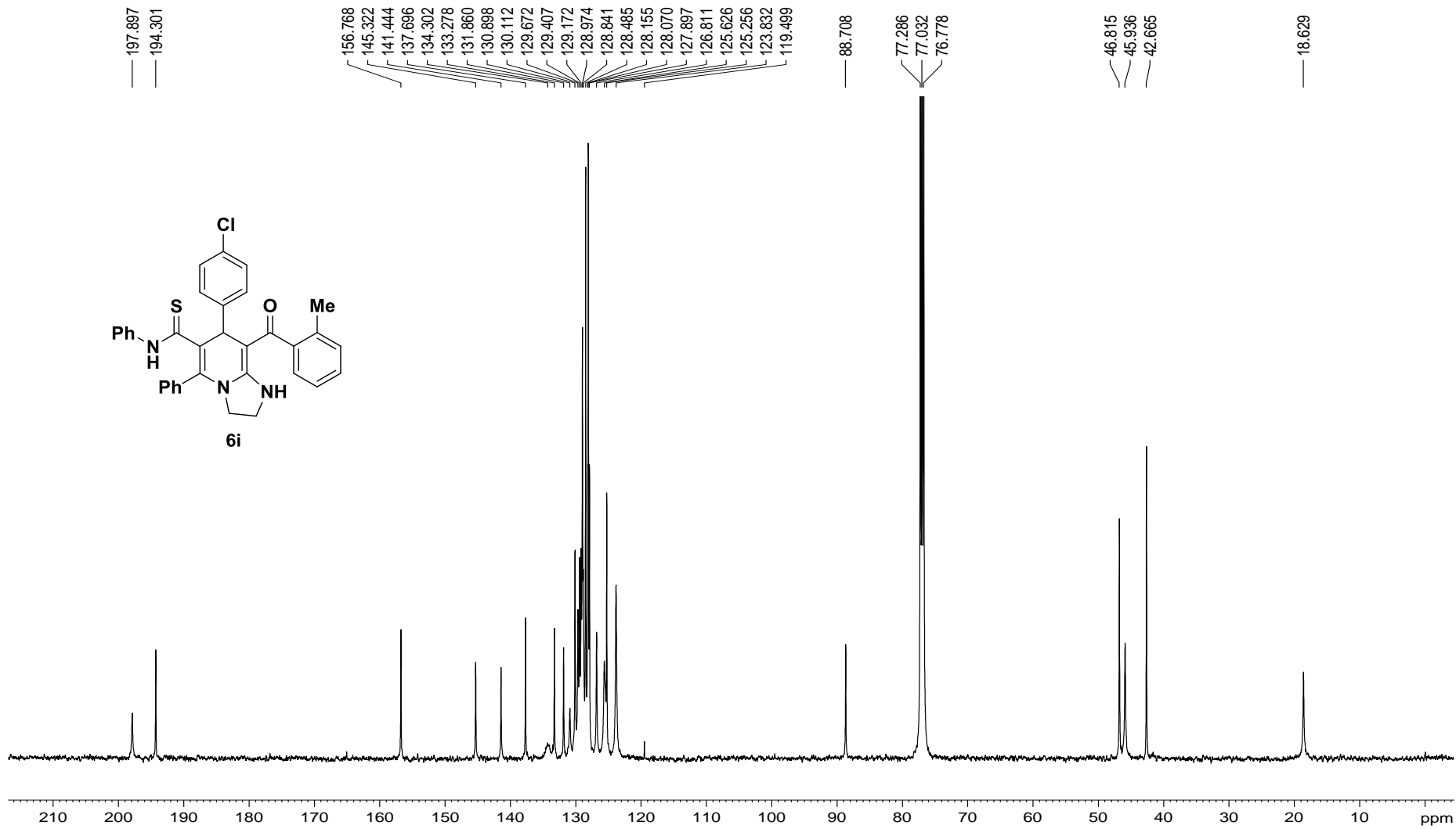
===== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326495 MHz
WDW EM
SSB 0
LB 12.00 Hz
GB 0
PC 2 00

ZKL-s-3d 1H 1D 2014 05 19



KL-S-3 13C 1D 2014 05 1



ZKL-S-2 1H 1D 2014 05 09

9.493

7.570

7.417

7.260

7.223

7.064

7.005

6.932

6.859

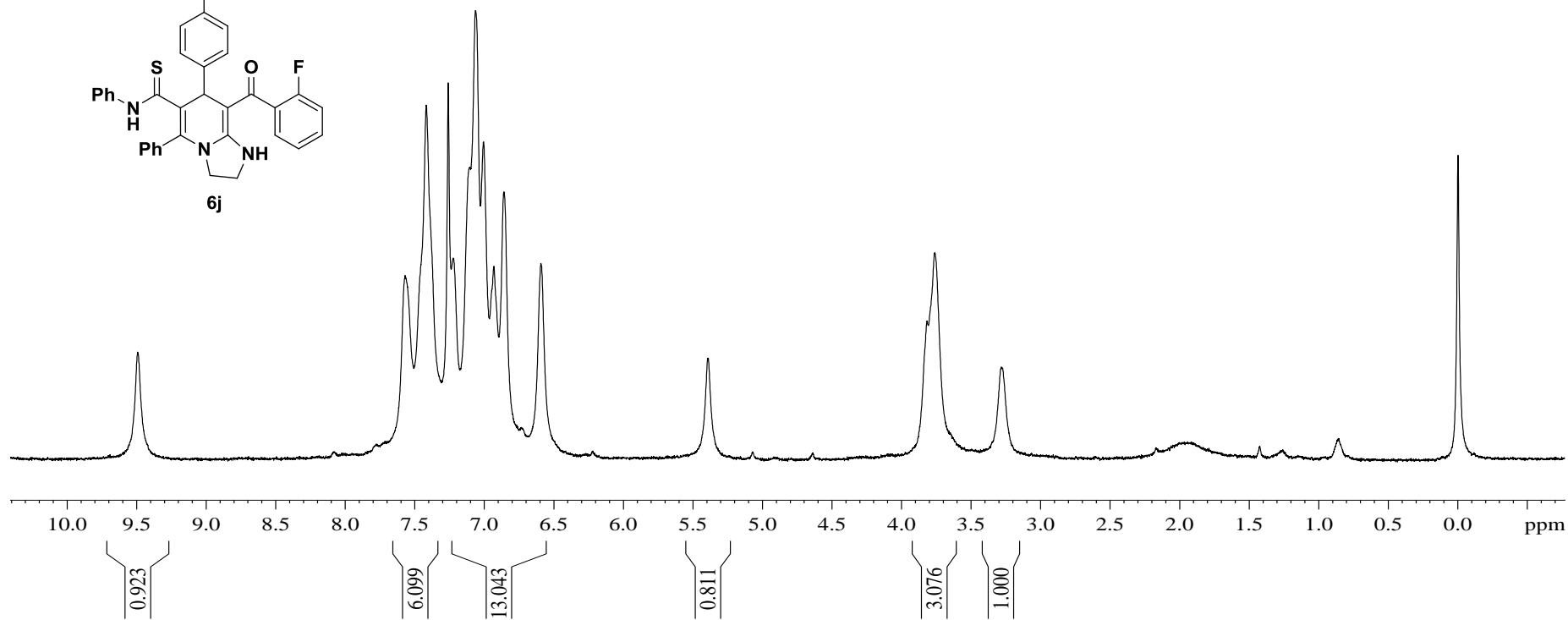
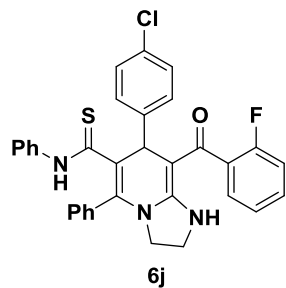
6.593

5.392

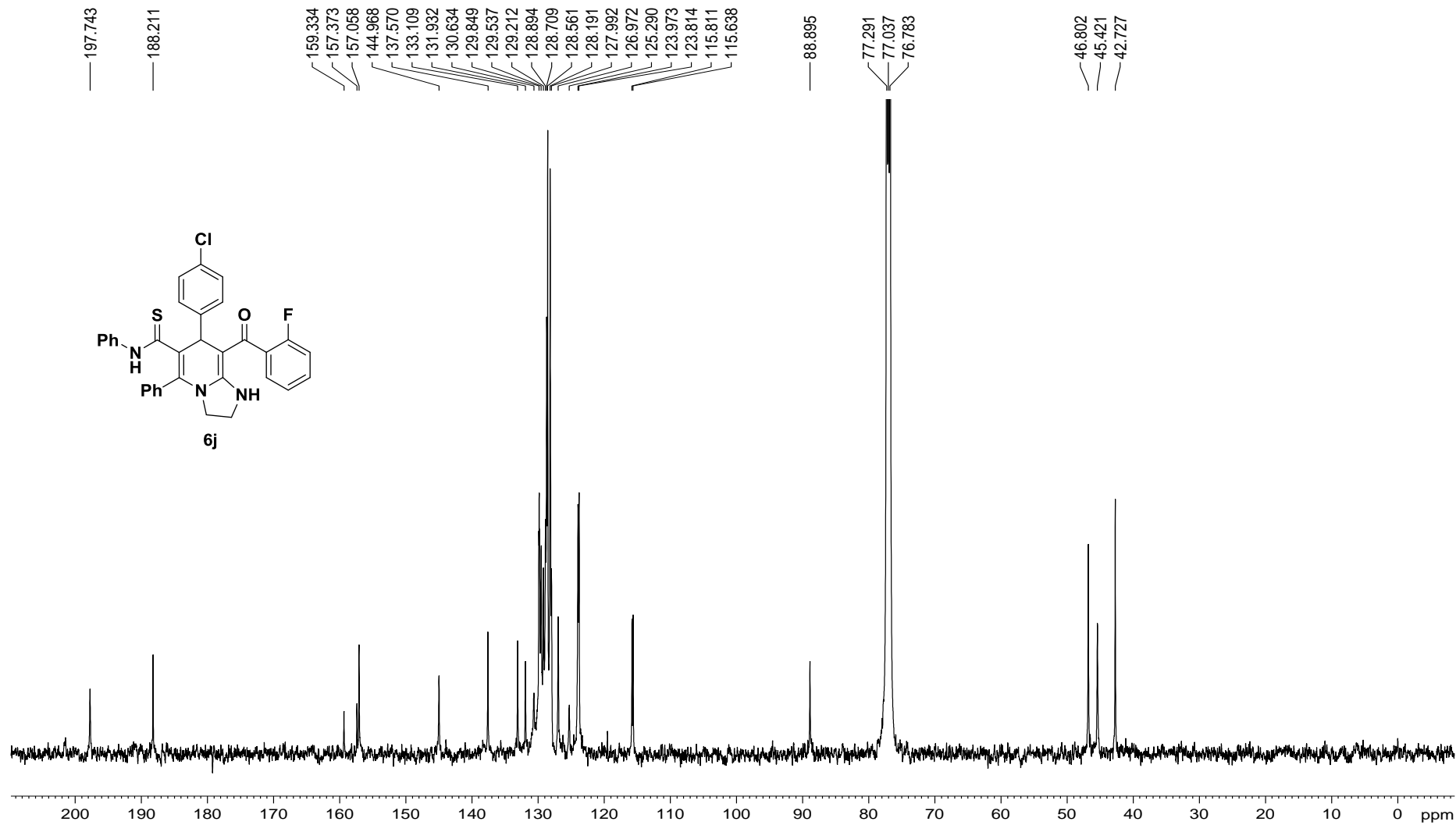
3.760

3.282

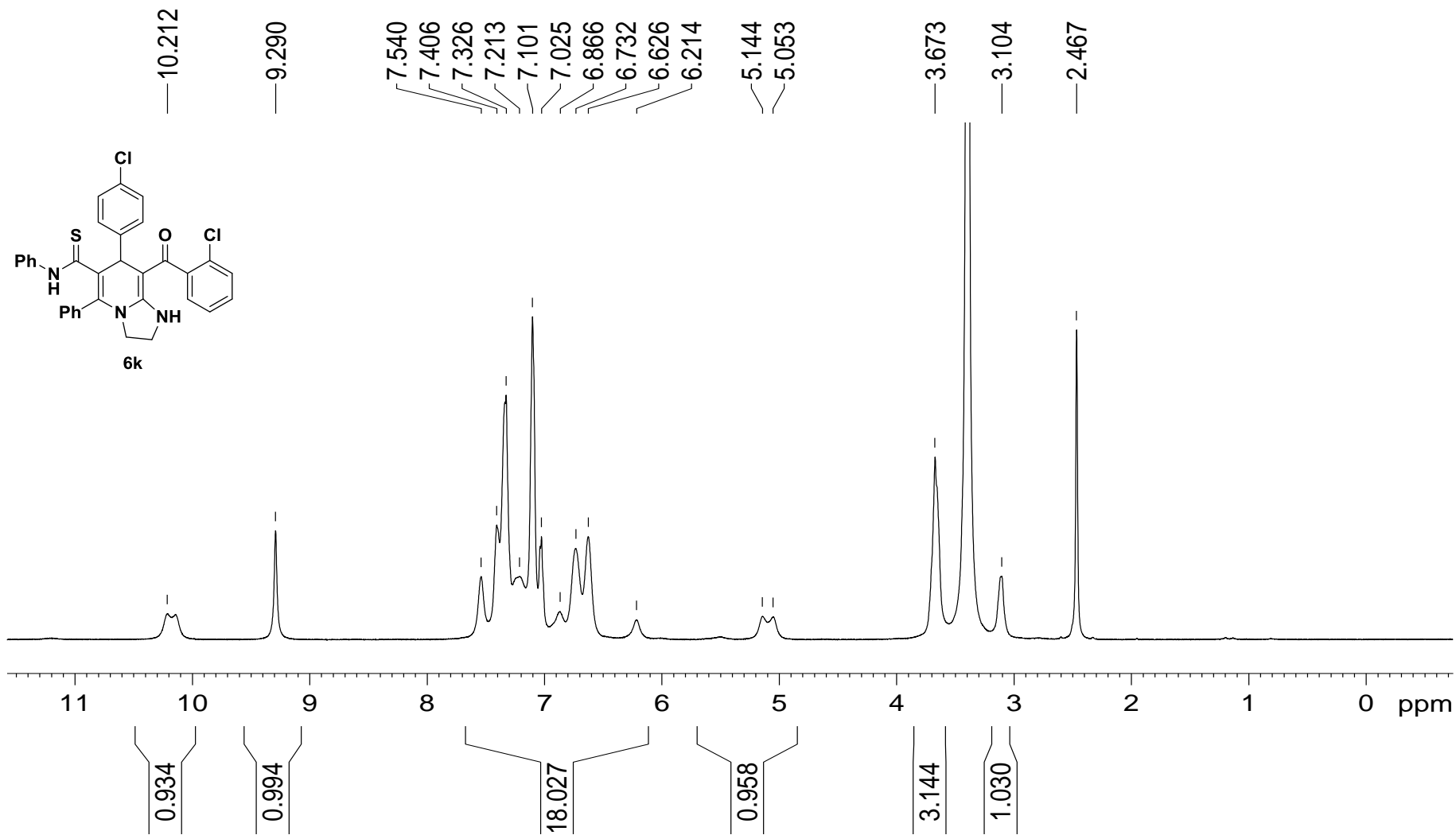
-0.001



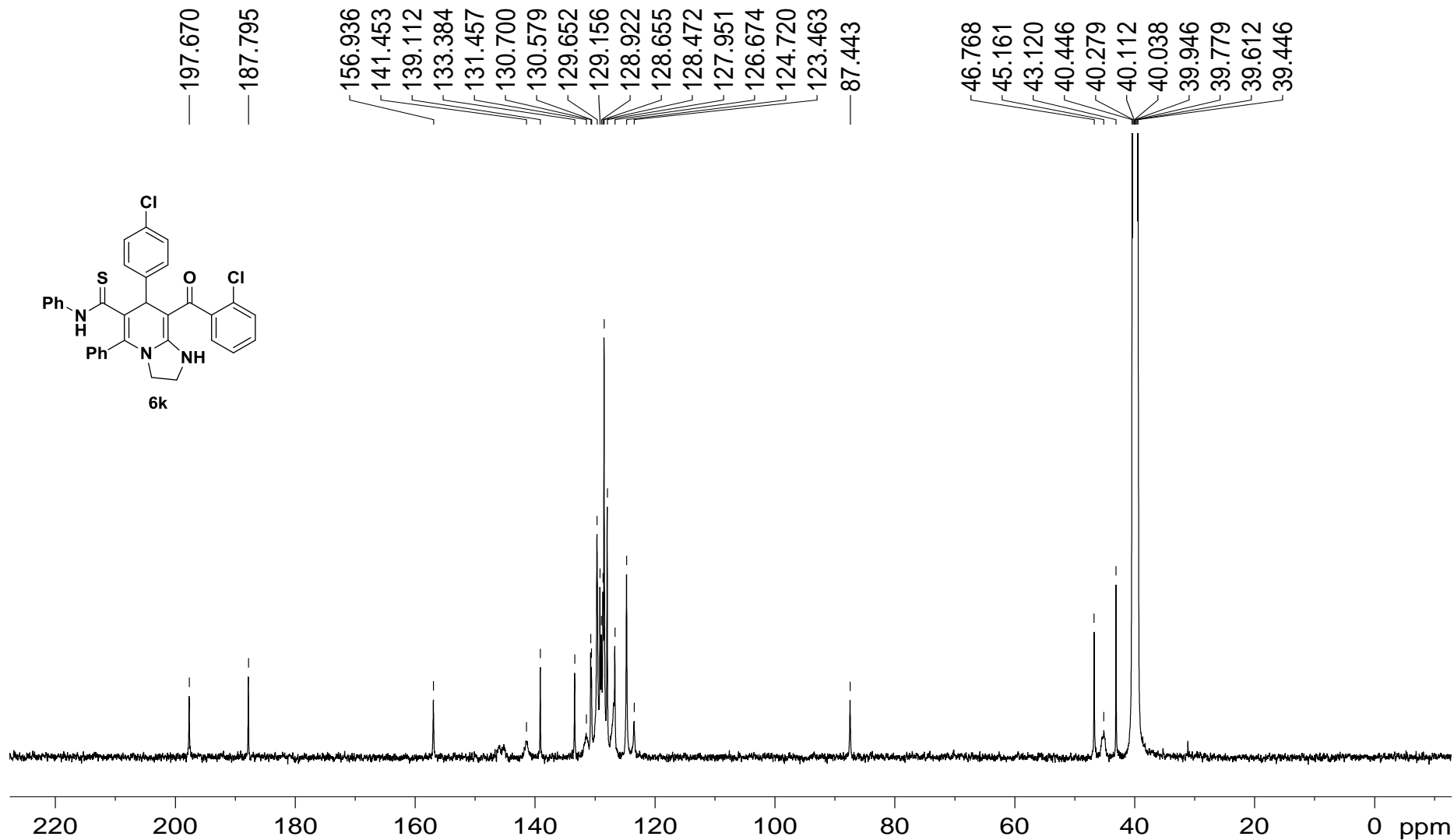
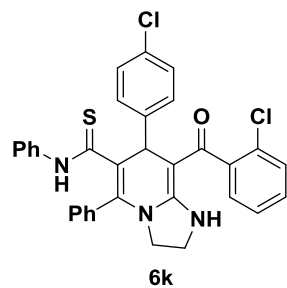
KL-s-2 13C 1D 2014 05 1



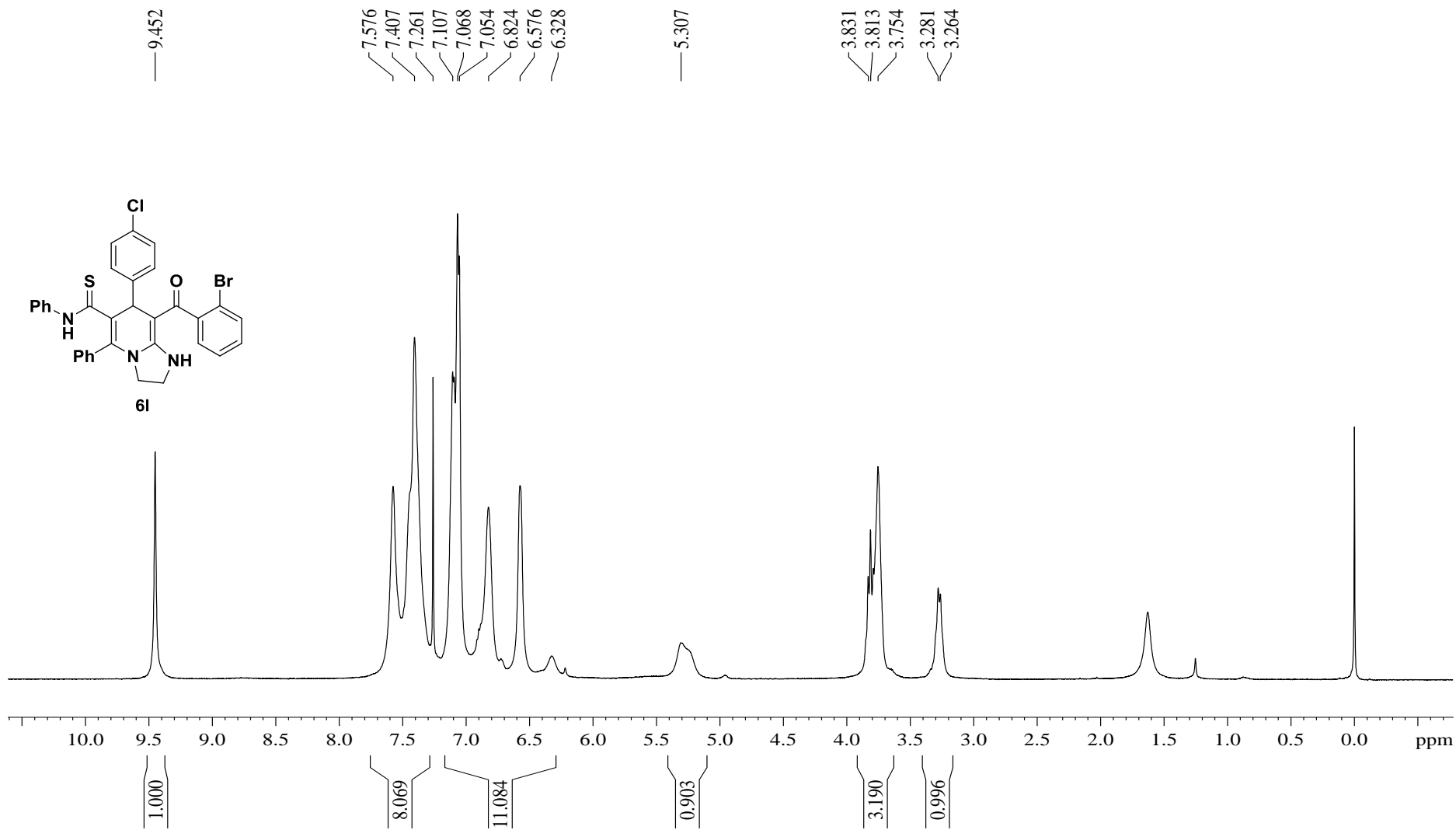
SP-P-4 1H 1D 2013 01 07



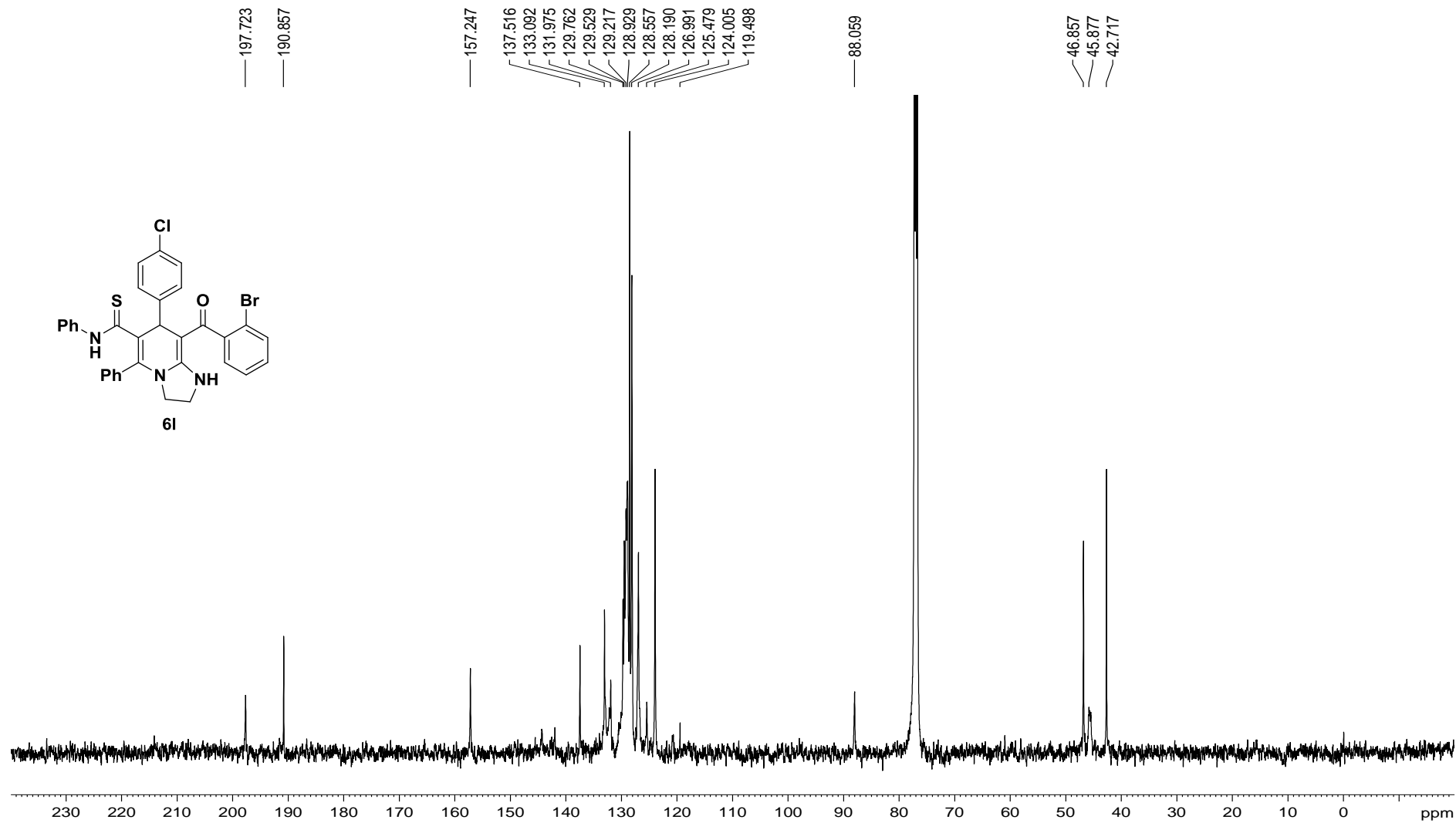
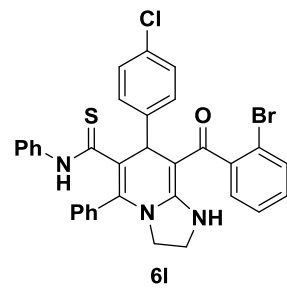
SP-P-4 13C 1D 2013 01 09



ZKL-S-1 1H 1D 2014 04 29



KL-s-1 13C 1D 2014 05 0



SP-P-5

1H 1D 2013 01 09

10.231

9.293

7.541

7.415

7.345

7.335

7.142

7.116

7.101

7.052

7.039

6.789

6.633

6.231

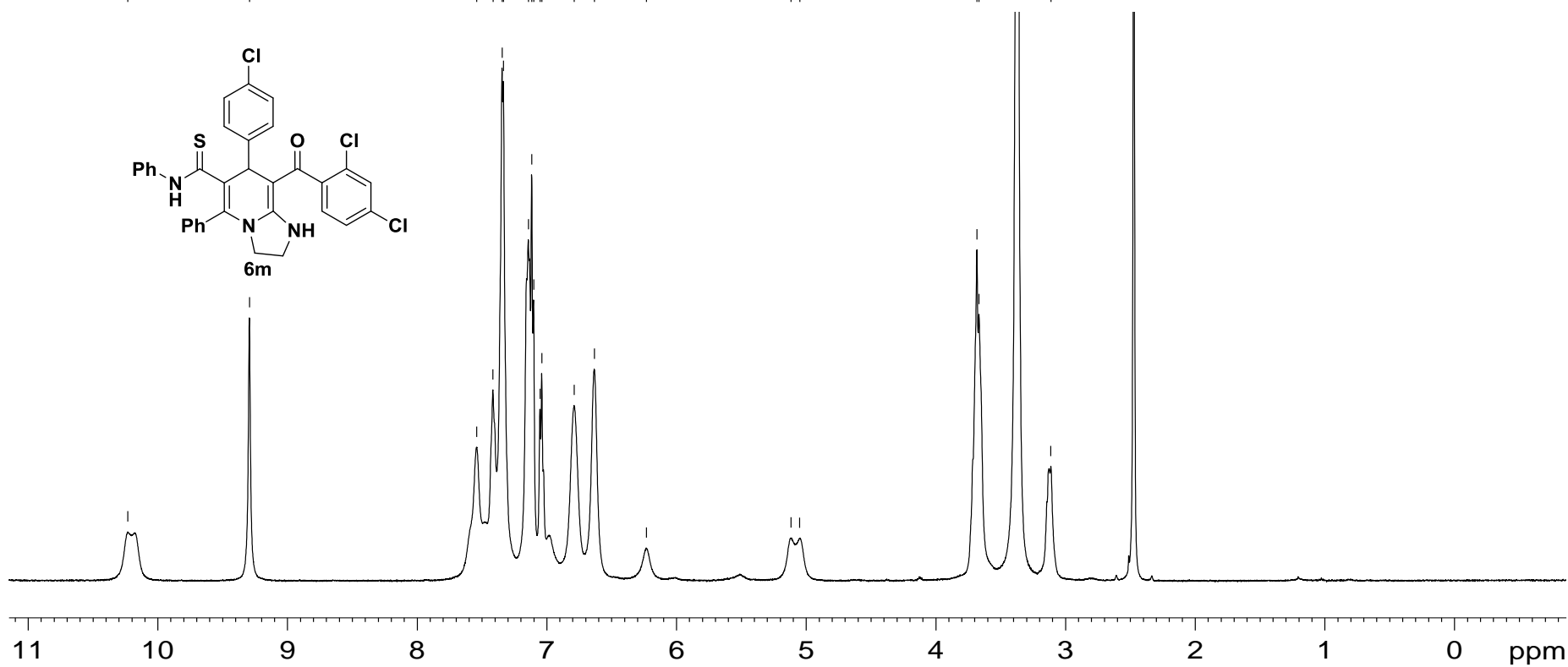
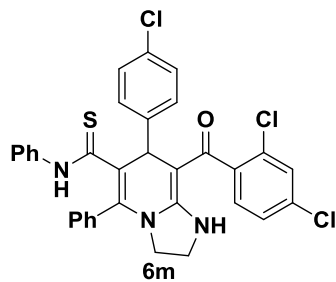
5.117

5.050

3.684

3.668

3.113



0.941

1.005

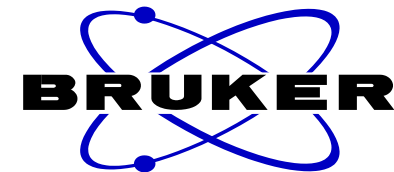
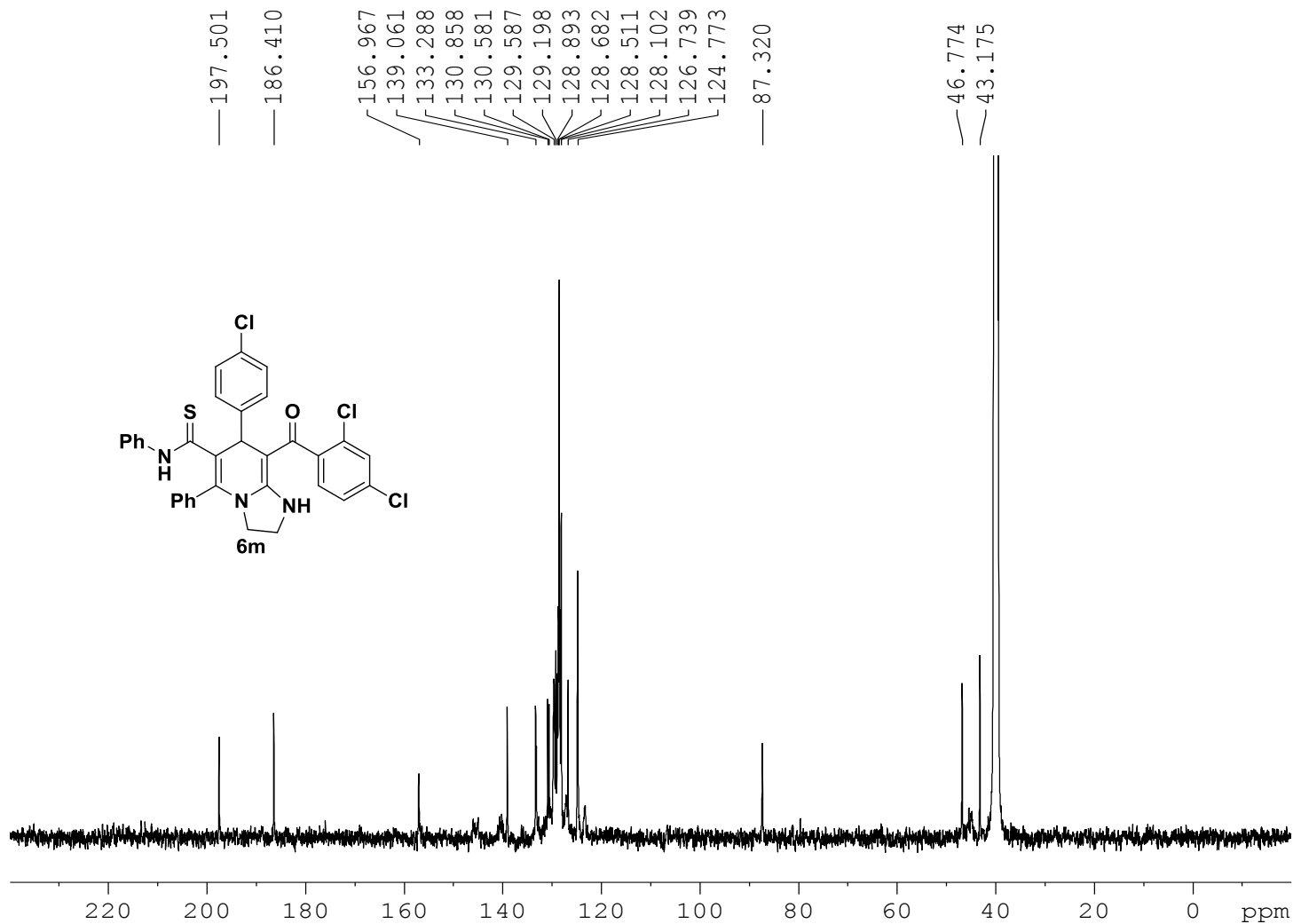
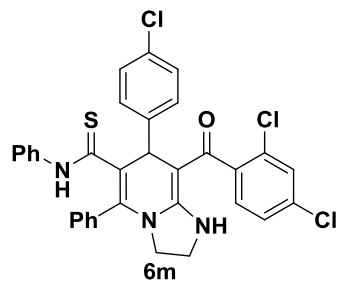
16.917

0.991

3.130

1.059

SP-P-5 13C 1D 2013 01 10

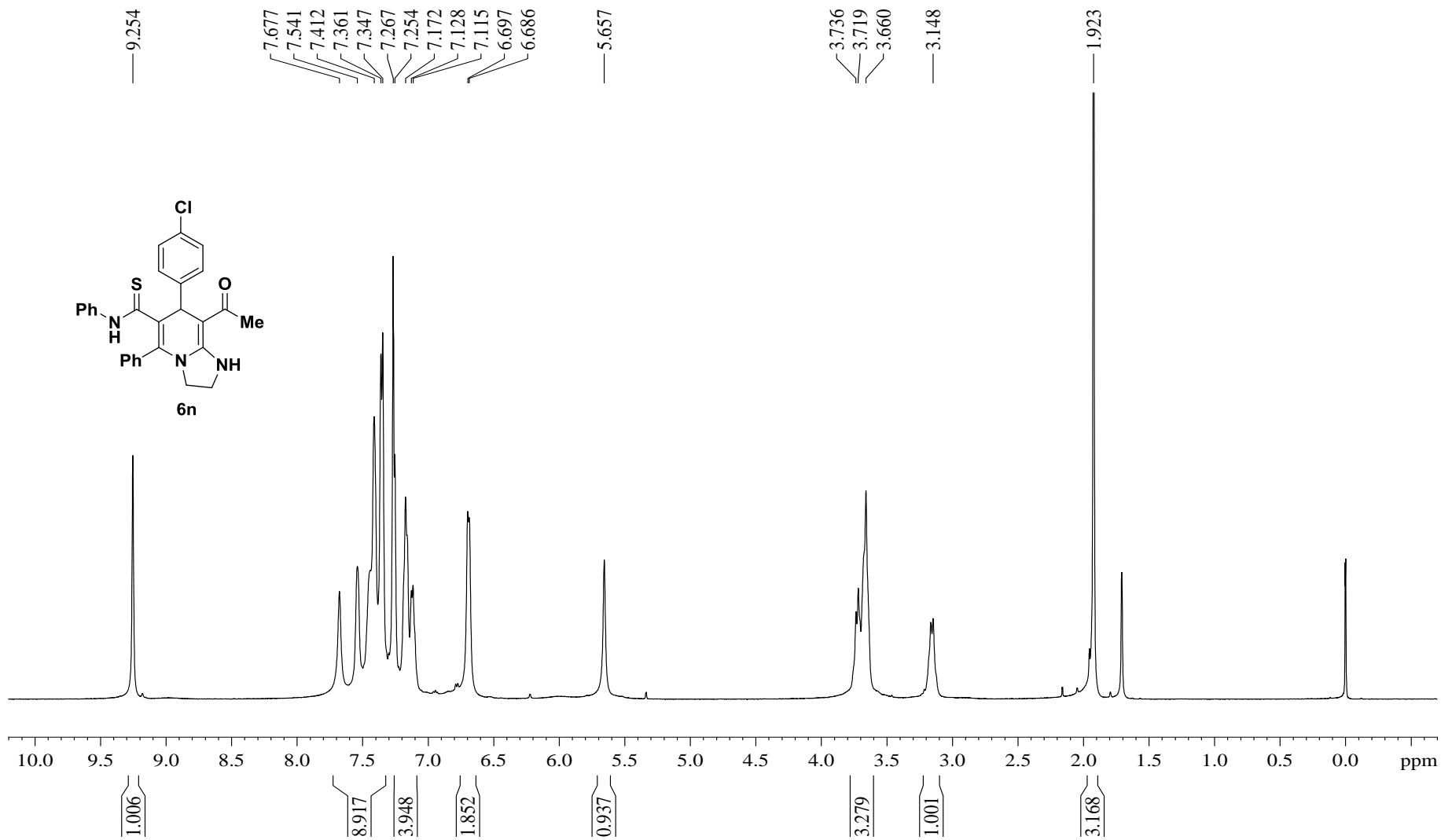
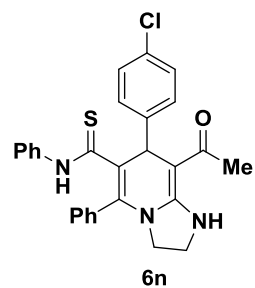


NAME SP-P-5
EXPNO 2
PROCNO 1
Date_ 20130110
Time_ 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1968
DS 2
SWH 32679.738 Hz
FIDRES 0.498653 Hz
AQ 1.0027661 sec
RG 5790
DW 15.300 usec
DE 6.00 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 3.00 dB
SFO1 125.7464750 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 500.0355000 MHz
SI 32768
SF 125.7326455 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 2.00

ZKL-S-6 1H 1D 2014 06 09



L-S-6 13C 1D 2014 06

198.299
194.354

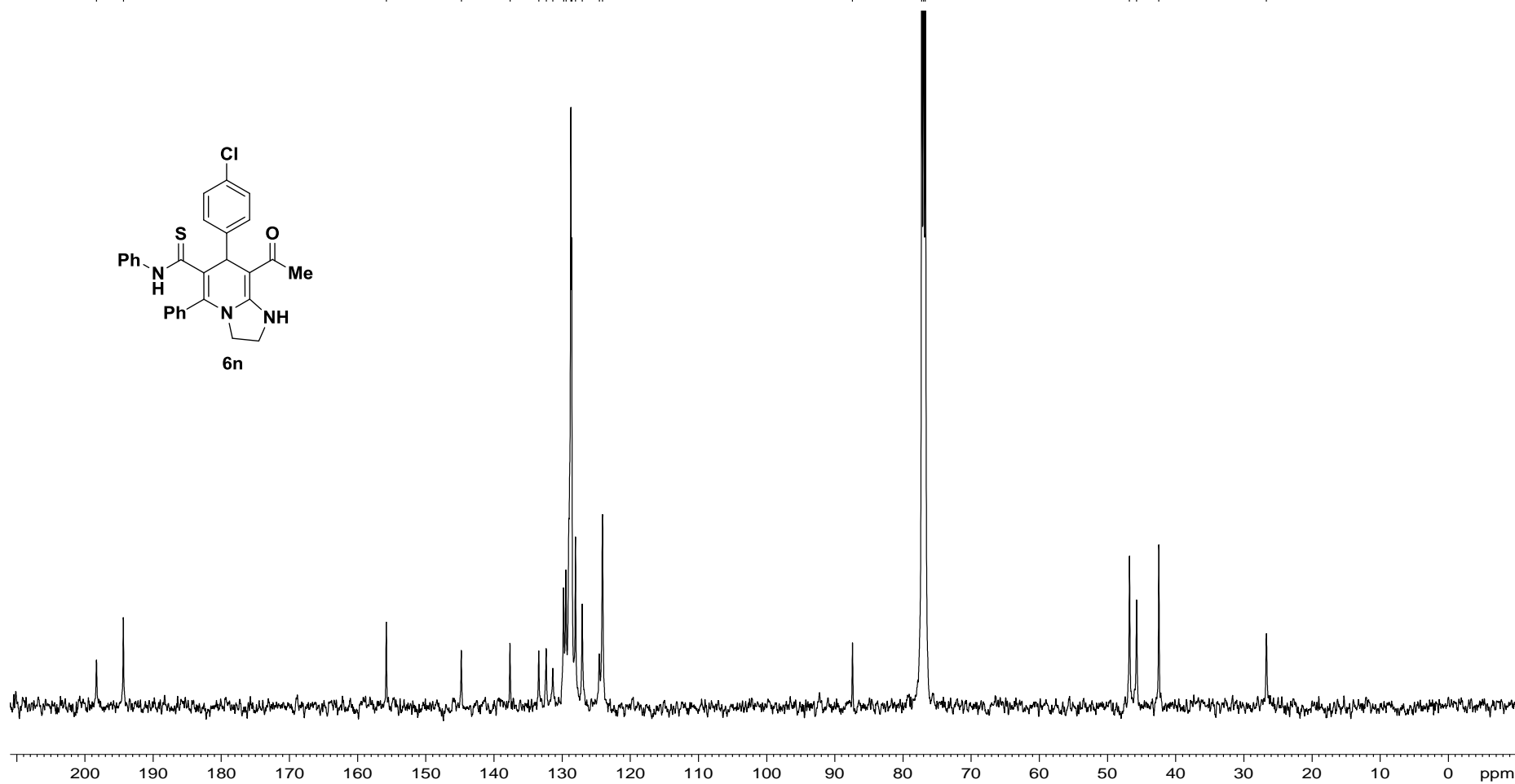
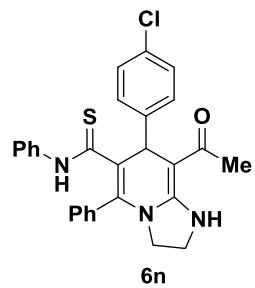
155.779
144.785
137.641
133.417
132.330
131.355
129.778
129.438
128.704
128.585
128.029
127.042
124.542
124.070

87.426

77.251
76.998
76.744

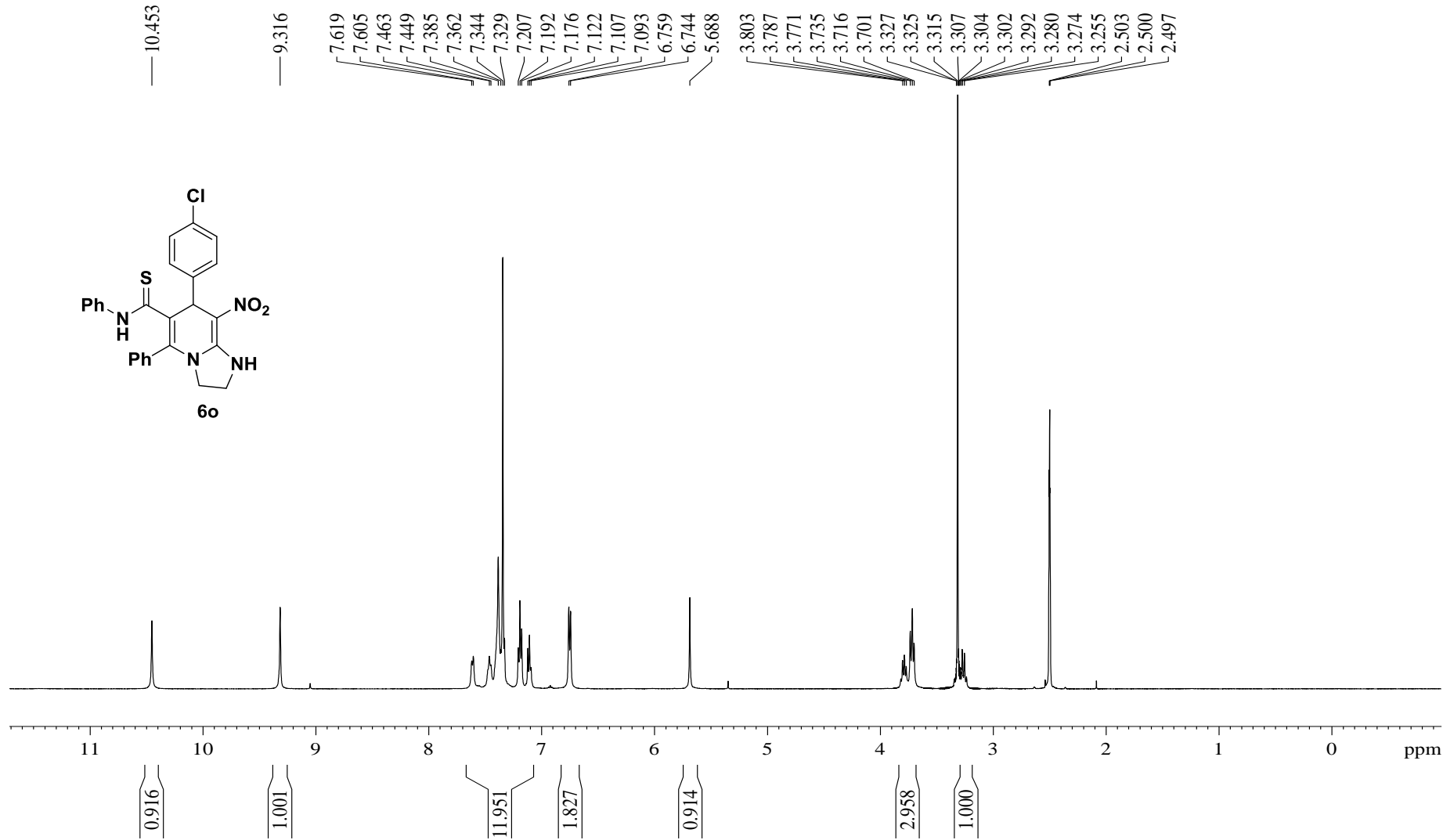
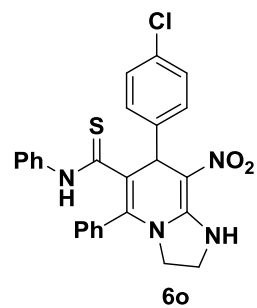
46.795
45.756
42.490

26.709



ZKL-S-7

1H 1D 2014 06 13

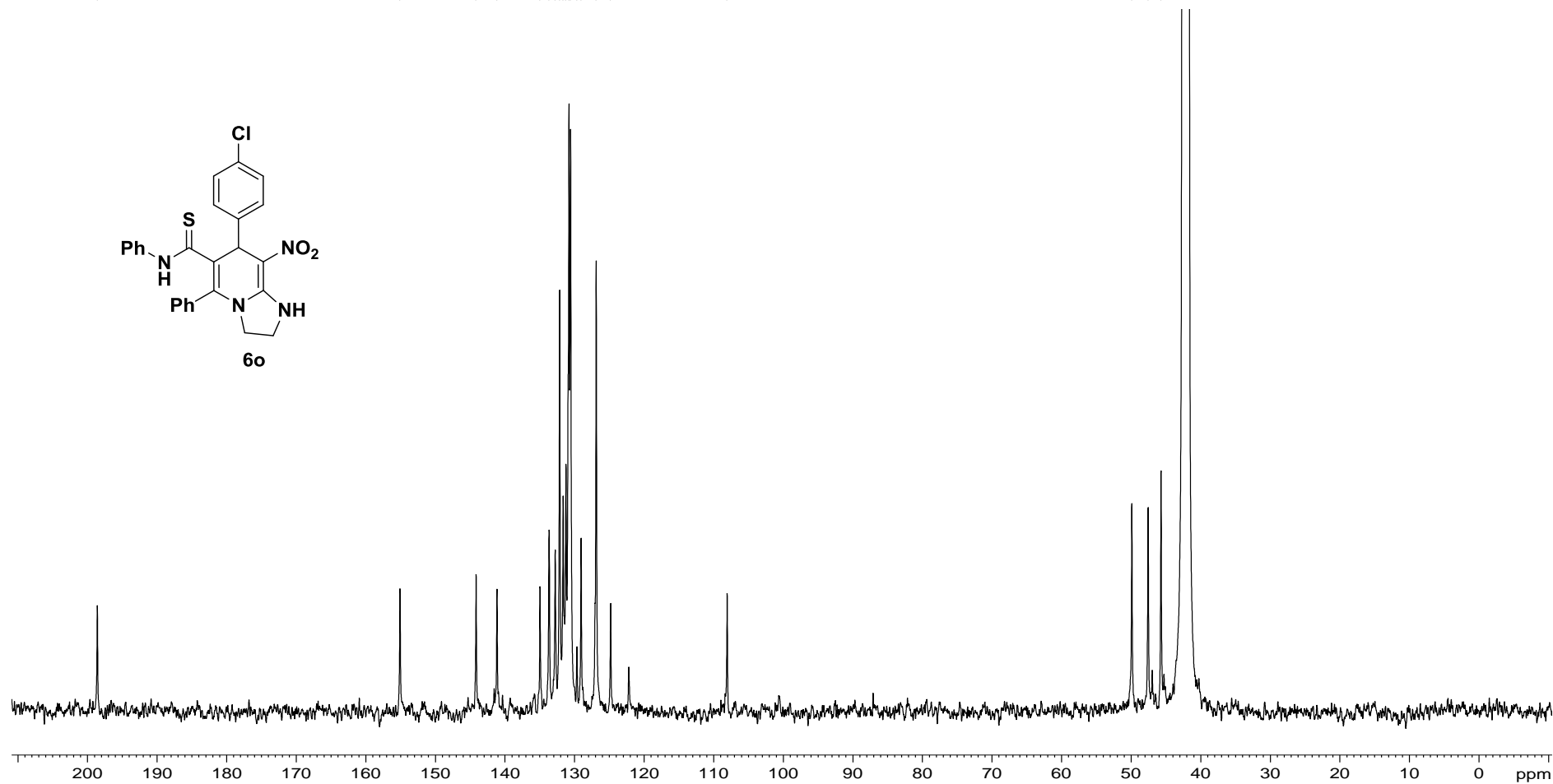
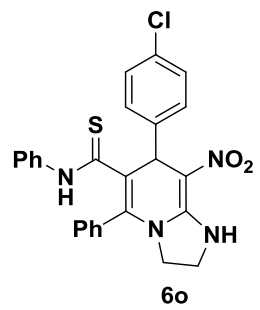


ZKL-S-7 13C 1D 2014 06 18

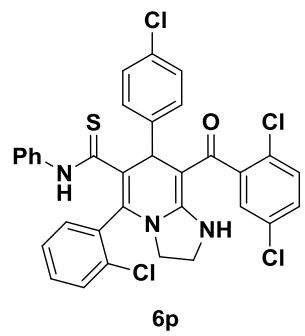
198.593

155.116
144.189
141.190
134.997
133.685
132.817
132.180
131.673
131.272
130.835
130.605
129.694
129.095
126.922
124.847
108.100

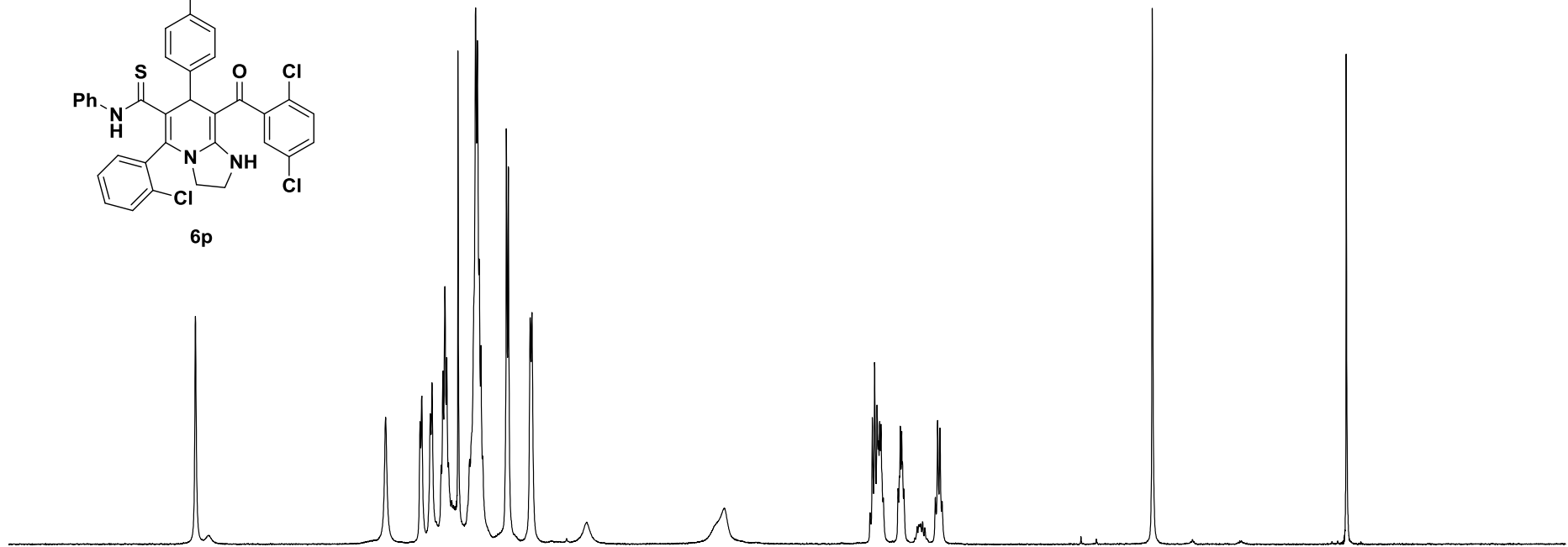
49.933
47.596
45.748



ZKL-S-8a 1H 1D 2014 06 09



9.407
7.852
7.570
7.556
7.487
7.473
7.398
7.383
7.367
7.353
7.339
7.313
7.166
7.087
7.072
6.865
6.848
6.670
6.656
6.209
5.083
3.893
3.874
3.856
3.836
3.824
3.815
3.804
3.785
3.664
3.646
3.635
3.616
3.359
3.341
3.322
3.304



10 9 8 7 6 5 4 3 2 1 0 -1 ppm

0.849
16.712
0.869
2.000
0.885
0.863

KL-S-8a 13C 1D 2014 06 1

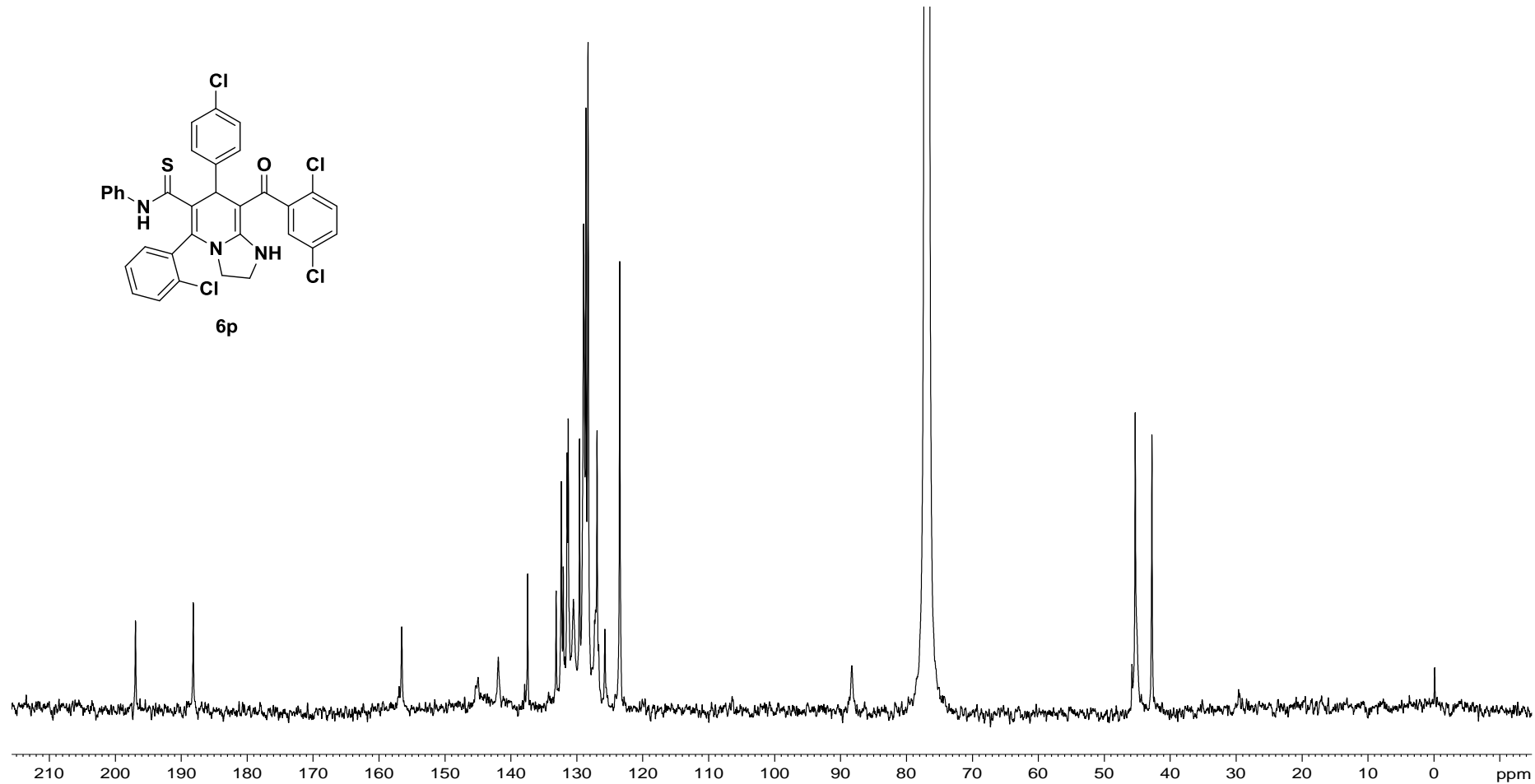
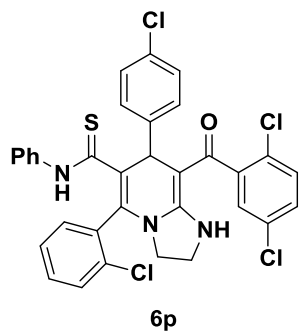
197.041

188.326

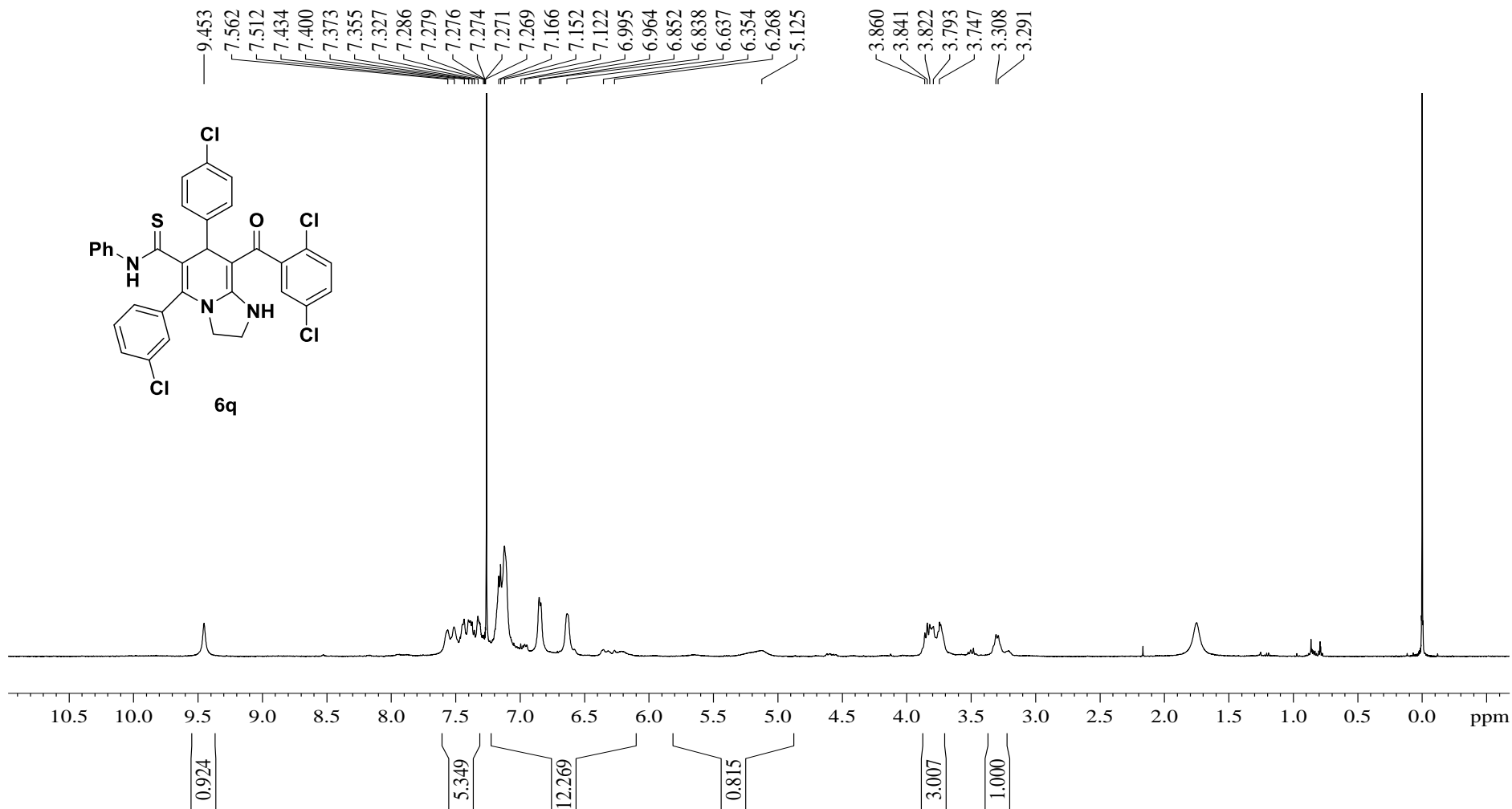
156.875
144.939
141.908
137.550
133.382
132.434
132.032
131.440
131.345
130.516
129.971
128.977
128.645
128.290
127.129
125.803
123.719

87.911

45.282
44.145
43.008



ZKL-S-5 1H 1D 2014 06 09



ZKL-S-5 13C 1D 2014 06 13

197.221

187.707

157.145

141.719

137.396

135.570

132.292

131.073

130.643

129.668

128.900

128.610

128.291

127.445

127.024

125.569

124.694

123.729

88.248

77.255

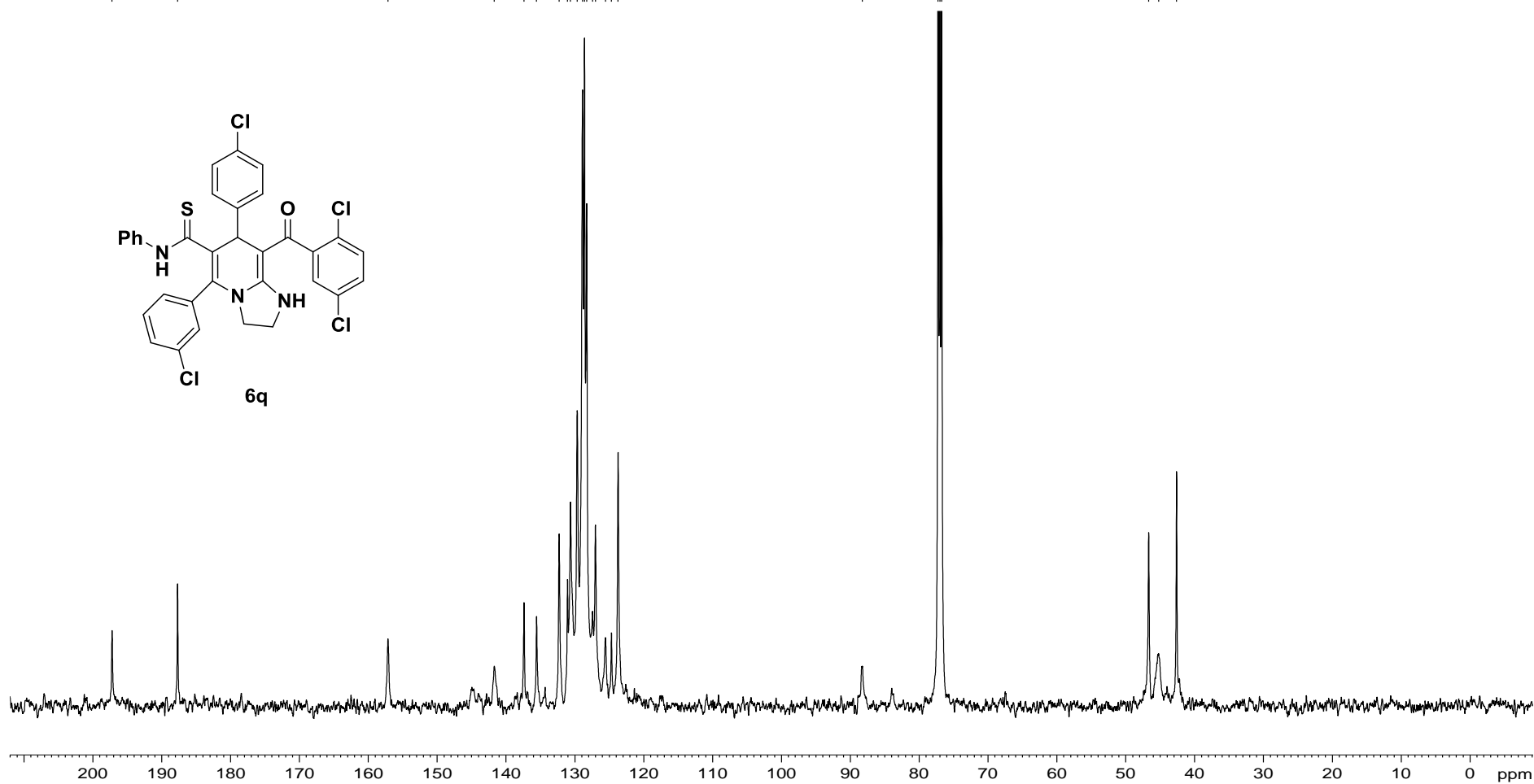
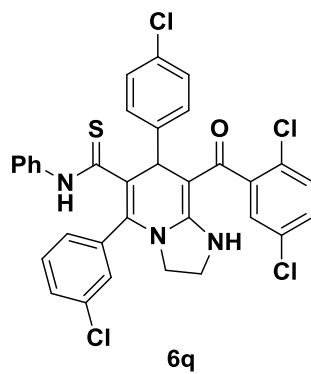
77.002

76.749

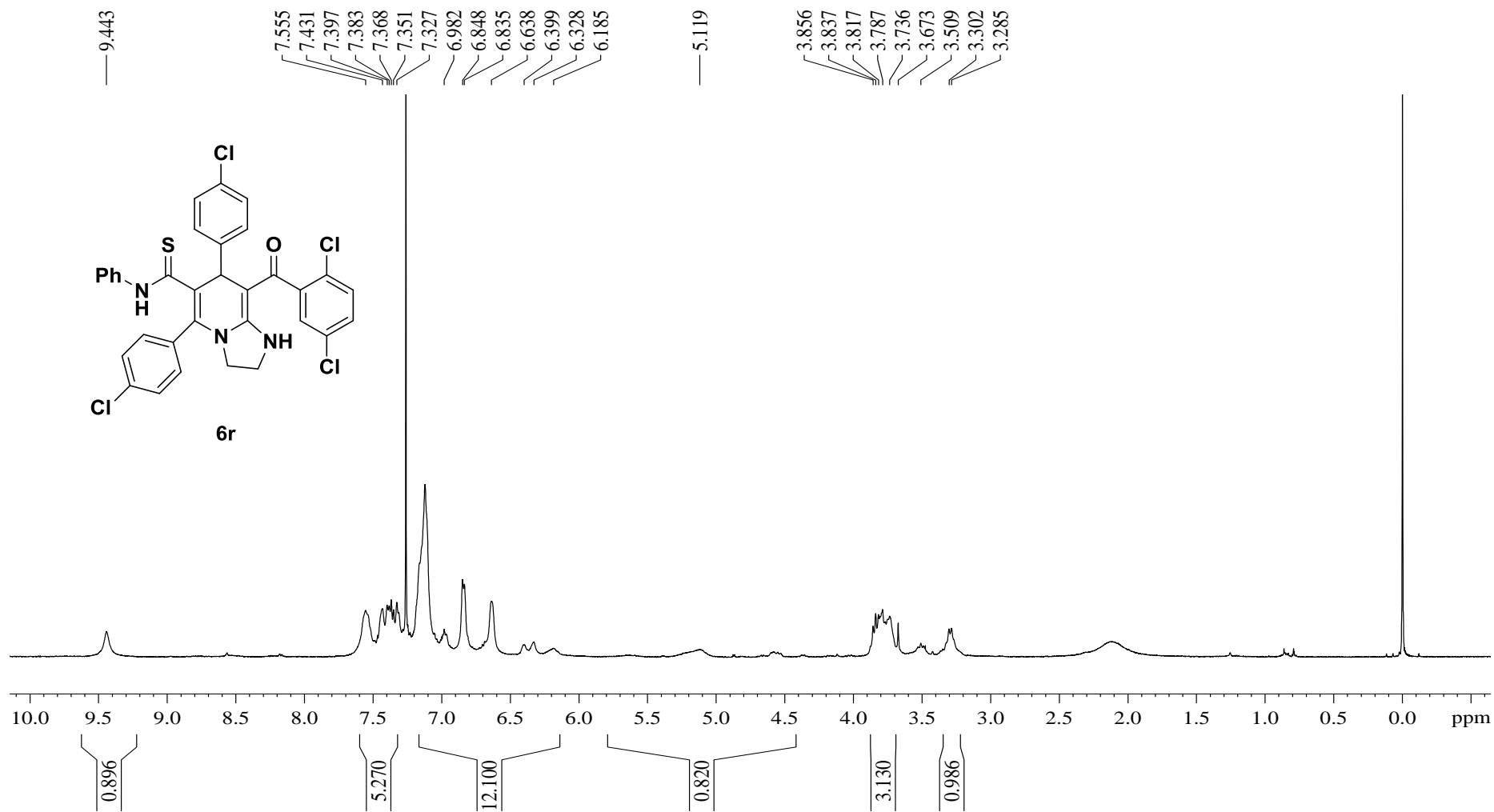
46.676

45.238

42.627



ZKL-S-4 1H 1D 2014 06 09



L-S-4 13C 1D 2014 06

197.374

188.194

157.174

137.345

135.700

132.660

132.381

131.176

130.765

130.104

129.884

129.752

129.487

129.061

128.738

128.415

127.167

125.815

123.818

122.657

88.171

46.810

42.697

45.356

