Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Acid-promoted rapid solvent-free access to substituted 1,4-dihydropyridines from β-ketothioamides

M. Li,* Ke-Na Sun and Li-Rong Wen*

State Key Laboratory Base of Eco-Chemical Engineering, College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042, China

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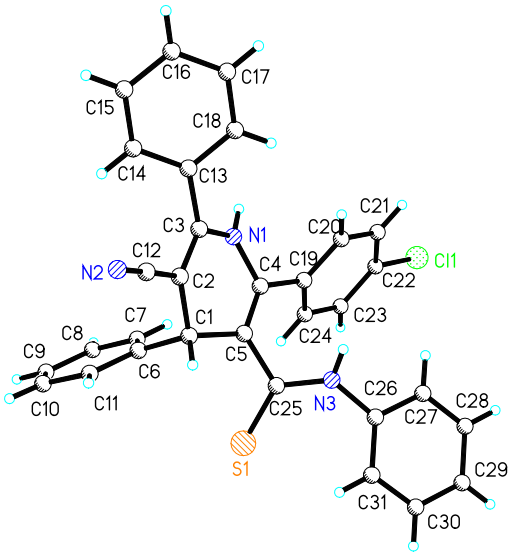
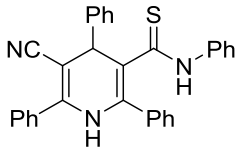
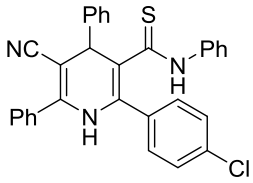


Figure S1. X-ray crystal structure of **4b**

Characterization data of compounds 4

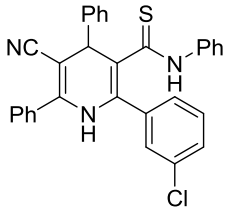


5-Cyano-*N*,2,4,6-tetraphenyl-1,4-dihydropyridine-3-carbothioamide (4a). Yellow powder (216.0 mg, 92%); mp: 206−208 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.69 (1H, s, C(=S)-NH), 9.48 (1H, s, C=C-NH), 7.66 (2H, d, J = 6.95 Hz, ArH), 7.60 (2H, d, J = 6.55 Hz, ArH), 7.51−7.47 (5H, m, ArH), 7.41−7.34 (5H, m, ArH), 7.27 (1H, t, J = 7.23 Hz, ArH), 7.20 (2H, t, J = 7.50 Hz, ArH), 7.09 (1H, t, J = 7.28 Hz, ArH), 7.03 (2H, d, J = 7.45 Hz, ArH), 5.08 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.9, 150.0, 145.1, 139.4, 135.4, 134.8, 133.4, 130.9, 129.5, 129.2, 128.9, 128.6, 128.5, 128.2, 127.3, 126.5, 124.2, 121.3, 114.5, 82.0, 46.2; HRMS (ESI-TOF): calcd for $C_{31}H_{24}N_3S$ $[M + H]^+$, 470.1691, found 470.1695.

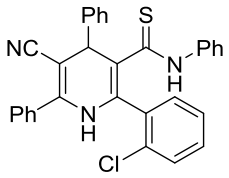


2-(4-Chlorophenyl)-5-cyano-*N*,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4b). Yellow powder (209.2 mg, 83%); mp: 207−209 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.81 (1H, s, C(=S)-NH), 9.47 (1H, s, C=C-NH), 7.63 (2H, d, J = 7.55 Hz, ArH), 7.58 (2H, d, J = 6.35 Hz, ArH), 7.50 (3H, t, J = 7.05 Hz, ArH), 7.45 (4H, t, J = 8.53 Hz, ArH), 7.37 (2H, t, J = 7.28 Hz, ArH), 7.26 (1H, d, J = 7.05 Hz, ArH), 7.22 (2H, t, J = 7.68 Hz, ArH), 7.11 (1H, d, J = 7.10 Hz, ArH),

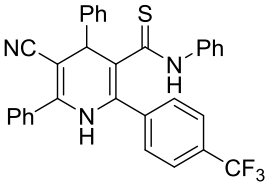
7.07 (2H, d, *J* = 7.20 Hz, ArH), 5.56 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.6, 149.9, 144.8, 139.3, 133.9, 133.5, 133.3, 131.3, 130.9, 129.1, 128.9, 128.8, 128.7, 128.4, 128.2, 127.4, 126.6, 124.0, 121.0, 115.0, 82.0, 46.2; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1325.



2-(3-Chlorophenyl)-5-cyano-*N*,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4c). Yellow powder (191.5 mg, 76%); mp: 189−191 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.79 (1H, s, C(=S)-NH), 9.43 (1H, s, C=C-NH), 7.66 (1H, s, ArH), 7.59 (3H, d, *J* = 6.85 Hz, ArH), 7.52 (3H, t, *J* = 6.60 Hz, ArH), 7.47 (2H, d, *J* = 7.50 Hz, ArH), 7.42−7.38 (4H, m, ArH), 7.28 (1H, t, *J* = 7.15 Hz, ArH), 7.23 (2H, t, *J* = 7.48 Hz, ArH), 7.12 (1H, t, *J* = 7.25 Hz, ArH), 7.01 (2H, d, *J* = 7.20 Hz, ArH), 5.14 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.8, 149.9, 144.6, 139.2, 136.5, 133.4, 132.8, 130.8, 130.1, 129.3, 129.1, 128.8, 128.7, 128.3, 127.8, 127.4, 126.6, 124.2, 121.0, 115.6, 82.1, 46.4; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1312.

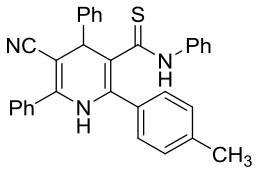


2-(2-Chlorophenyl)-5-cyano-*N*,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4d). Yellow powder (156.3 mg, 62%); mp: 128−130 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.53 (1H, broad, s, C(=S)-NH), 9.40 (1H, s, C=C-NH), 7.55 (3H, broad, s, ArH), 7.50−7.48 (6H, broad, m, ArH), 7.43 (2H, t, *J* = 7.30 Hz, ArH), 7.39−7.30 (4H, m, ArH), 7.23 (2H, t, *J* = 3.83 Hz, ArH), 7.12 (1H, t, *J* = 7.00 Hz, ArH), 7.04 (1H, broad, s, ArH), 5.27 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.8, 149.4, 144.6, 144.4, 139.2, 133.4, 132.7, 131.1, 130.8, 129.6, 129.1, 128.9, 128.7, 128.4, 128.2, 128.0, 127.5, 124.4, 123.9, 119.9, 81.2, 46.6; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1296, found 504.1289.

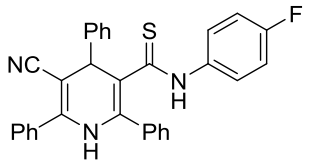


5-Cyano-*N*,4,6-triphenyl-2-(4-(trifluoromethyl)phenyl)-1,4-dihydropyridine-3-carbothioamide (4e). Yellow powder (182.8 mg, 68%); mp: 171−173 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.81 (1H, s, C(=S)-NH), 9.49 (1H, s, C=C-NH), 7.83 (2H, s, ArH), 7.79 (2H, s, ArH), 7.61 (2H, d, *J* = 6.50 Hz, ArH) 7.54−7.48 (5H, m, ArH), 7.40 (2H, t, *J* = 7.23 Hz, ArH), 7.29 (1H, t, *J* = 6.98 Hz, ArH), 7.21 (2H, t, *J* = 6.85 Hz, ArH), 7.12 (1H, t, *J* = 6.95 Hz, ArH), 7.00 (2H, s, ArH), 5.16 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.5, 149.9, 144.6, 139.0 (d, $^2J_{C\text{-}F}$ = 42.0 Hz), 133.3, 130.9, 130.3, 129.6, 129.1, 128.9, 128.6, 128.3, 127.4, 126.6, 125.2, 124.5 (d,

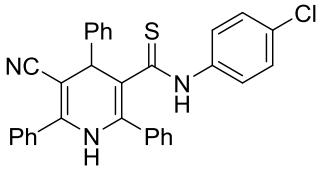
$^{1}J_{C\text{-}F}$ = 271.6 Hz), 124.0, 121.0, 115.9, 82.1, 46.3; HRMS (ESI-TOF): calcd for $C_{32}H_{23}N_3SF_3$ [M + H]$^+$, 538.1565, found 538.1562.



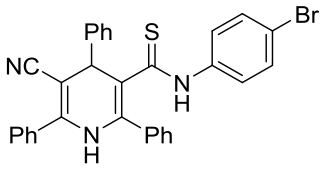
5-Cyano-*N*,4,6-triphenyl-2-(*p*-tolyl)-1,4-dihydropyridine-3-carbothioamide (4f). Yellow powder (227.3 mg, 94%); mp: 170−172 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.69 (1H, s, C(=S)-NH), 9.42 (1H, s, C=C-NH), 7.57 (2H, d, J = 5.90 Hz, ArH), 7.54 (2H, d, J = 7.45 Hz, ArH), 7.49 (3H, t, J = 6.60 Hz, ArH), 7.45 (2H, d, J = 7.60 Hz, ArH), 7.36 (2H, t, J = 7.38 Hz, ArH), 7.25 (1H, d, J = 7.30 Hz, ArH), 7.19 (4H, t, J = 7.25 Hz, ArH), 7.08 (3H, t, J = 6.85 Hz, ArH), 5.02 (1H, s, Ar-CH), 2.26 (3H, s, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.0, 149.9, 145.1, 139.5, 138.9, 135.5, 133.4, 131.9, 130.8, 129.3, 129.2, 128.8, 128.5, 128.1, 127.2, 126.4, 124.1, 121.3, 114.1, 82.0, 46.2, 21.3; HRMS (ESI-TOF): calcd for $C_{32}H_{26}N_3S$ [M + H]$^+$, 484.1847, found 484.1852.



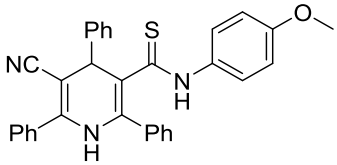
5-Cyano-*N*-(4-fluorophenyl)-2,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4g). Yellow powder (219.4 mg, 90%); mp: 187−189 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.68 (1H, s, C(=S)-NH), 9.47 (1H, s, C=C-NH), 7.64 (2H, d, J = 6.75 Hz, ArH), 7.59 (2H, d, J = 6.90 Hz, ArH), 7.51 (3H, t, J = 7.15 Hz, ArH), 7.47 (2H, d, J = 7.60 Hz, ArH), 7.42−7.37 (5H, m, ArH), 7.27 (1H, t, J = 7.15 Hz, ArH), 7.07−7.02 (4H, m, ArH), 5.07 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.2, 160.1 (d, $^{1}J_{C\text{-}F}$ = 244.3 Hz) , 150.0, 144.9, 135.7, 135.4, 134.7, 133.4, 130.8, 129.4, 129.1, 128.9, 128.4, 128.1, 127.3, 126.2, 121.2, 115.4 (d, $^{2}J_{C\text{-}F}$ = 22.3 Hz), 114.4, 82.0, 46.2; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SF$ [M + H]$^+$, 488.1597, found 488.1602.



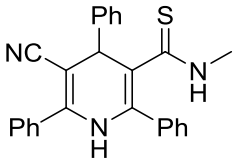
***N*-(4-Chlorophenyl)-5-cyano-2,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4h).** Yellow powder (216.7 mg, 86%); mp: 216−219 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.76 (1H, s, C(=S)-NH), 9.56 (1H, s, C=C-NH), 7.63 (2H, d, J = 5.30 Hz, ArH), 7.60 (2H, d, J = 6.40 Hz, ArH), 7.51 (3H, t, J = 6.90 Hz, ArH), 7.47 (2H, d, J = 7.60 Hz, ArH), 7.39−7.33 (5H, m, ArH), 7.27 (3H, d, J = 7.90 Hz, ArH), 7.14 (2H, d, J = 6.70 Hz, ArH), 5.05 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.2, 149.9, 145.0, 138.3, 136.0, 134.7, 133.3, 130.9, 130.1, 129.5, 129.4, 129.2, 128.9, 128.6, 128.4, 128.1, 127.3, 125.4, 121.1, 114.3, 82.2, 46.1; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1305.



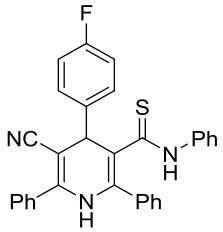
***N*-(4-Bromophenyl)-5-cyano-2,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4i).** Yellow powder (205.7 mg, 75%); mp: 223−224 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.73 (1H, s, C(=S)-NH), 9.53 (1H, s, C=C-NH), 7.62 (2H, s, ArH), 7.59 (2H, d, J = 6.40 Hz, ArH), 7.51 (3H, t, J = 6.38 Hz, ArH), 7.47 (2H, d, J = 7.55 Hz, ArH), 7.39−7.34 (7H, m, ArH), 7.26 (1H, t, J = 7.10 Hz, ArH), 7.09 (2H, s, ArH), 5.05 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.2, 149.8, 145.0, 138.7, 136.0, 134.6, 133.3, 131.4, 130.8, 129.3, 129.1, 128.8, 128.4, 128.0, 127.3, 125.7, 121.1, 118.4, 114.4, 82.2, 46.1; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SBr$ [M + H]$^+$, 548.0796, found 548.0781.



5-Cyano-*N*-(4-methoxyphenyl)-2,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4j). Yellow powder (232.3 mg, 93%); mp: 209−211 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.56 (1H, s, C(=S)-NH), 9.40 (1H, s, C=C-NH), 7.65 (2H, d, J = 7.30 Hz, ArH), 7.59 (2H, d, J = 6.80 Hz, ArH), 7.51−7.47 (5H, m, ArH), 7.41−7.36 (5H, m, ArH), 7.26 (1H, t, J = 7.20 Hz, ArH), 6.91 (2H, d, J = 8.65 Hz, ArH), 6.76 (2H, d, J = 8.70 Hz, ArH), 5.09 (1H, s, Ar-CH), 3.67 (3H, s, OCH_3); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.2, 157.6, 150.0, 144.9, 134.7, 133.4, 132.3, 130.8, 129.3, 129.1, 128.8, 128.3, 128.2, 127.2, 125.5, 121.2, 114.6, 113.7, 81.8, 55.6, 46.2; HRMS (ESI-TOF): calcd for $C_{32}H_{26}N_3OS$ [M + H]$^+$, 500.1797, found 500.1789.

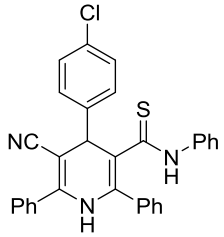


5-Cyano-*N*-methyl-2,4,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4k). Yellow powder (163.0 mg, 80%); mp: 163−165 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 9.20 (2H, s, C=C-NH and C(=S)-NH), 7.55 (2H, d, J = 7.35 Hz, ArH), 7.51−7.45 (5H, m, ArH), 7.37−7.34 (7H, m, ArH), 7.25 (1H, t, J = 6.58 Hz, ArH), 5.07 (1H, s, Ar-CH), 2.49 (3H, s, NH-CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.5, 150.0, 144.9, 134.7, 133.5, 130.6, 129.0, 128.9, 128.7, 128.2, 128.0, 127.3, 121.2, 114.7, 81.6, 46.2, 32.3; HRMS (ESI-TOF): calcd for $C_{26}H_{22}N_3S$ [M + H]$^+$, 408.1534, found 408.1542.

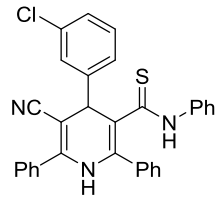


5-Cyano-4-(4-fluorophenyl)-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4l).

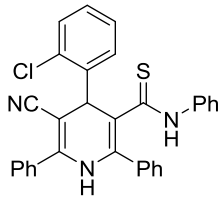
Yellow powder (207.2 mg, 85%); mp: 228−231 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.73 (1H, s, C(=S)-NH), 9.51 (1H, s, C=C-NH), 7.64 (2H, d, J = 6.95 Hz, ArH), 7.60 (2H, d, J = 6.65 Hz, ArH), 7.51−7.49 (5H, m, ArH), 7.40 (2H, t, J = 6.98 Hz, ArH), 7.36 (1H, d, J = 6.95 Hz, ArH), 7.21 (4H, t, J = 7.93 Hz, ArH), 7.11 (1H, t, J = 7.20 Hz, ArH), 7.03 (2H, d, J = 7.40 Hz, ArH), 5.09 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.4, 162.2 (d, $^1J_{C\text{-}F}$ = 242.6 Hz), 150.6, 141.8, 139.9, 135.8, 135.2, 133.9, 131.4, 130.6, 129.9, 129.7, 129.4, 129.1, 128.9, 127.0, 124.6, 121.6, 116.0 (d, $^2J_{C\text{-}F}$ = 20.7 Hz), 115.0, 82.5, 46.1; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SF$ [M + H]$^+$, 488.1597, found 488.1586.



4-(4-Chlorophenyl)-5-cyano-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4m). Yellow powder (229.3 mg, 91%); mp: 215−217 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.76 (1H, s, C(=S)-NH), 9.58 (1H, s, C=C-NH), 7.65 (2H, d, J = 6.90 Hz, ArH), 7.61 (2H, d, J = 6.50 Hz, ArH), 7.53-7.48 (5H, m, ArH), 7.45 (2H, d, J = 8.35 Hz, ArH), 7.41 (2H, t, J = 7.23 Hz, ArH), 7.37 (1H, d, J = 6.90 Hz, ArH), 7.22 (2H, t, J = 7.58 Hz, ArH), 7.11 (1H, t, J = 7.35 Hz, ArH), 7.06 (2H, d, J = 7.65 Hz, ArH), 5.07 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.6, 150.2, 144.0, 139.4, 135.8, 134.7, 133.3, 132.0, 131.0, 130.0, 129.5, 129.3, 129.0, 128.9, 128.7, 128.5, 126.6, 124.1, 121.2, 114.0, 81.6, 45.6; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1309.

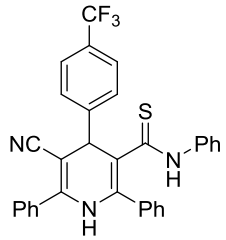


4-(3-Chlorophenyl)-5-cyano-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4n). Yellow powder (196.6 mg, 78%); mp: 204−206 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.83 (1H, s, C(=S)-NH), 9.62 (1H, s, C=C-NH), 7.66 (2H, d, J = 7.35 Hz, ArH), 7.61 (2H, d, J = 6.60 Hz, ArH), 7.52 (3H, t, J = 6.75 Hz, ArH), 7.48 (1H, s, ArH), 7.42 (4H, t, J = 7.55 Hz, ArH), 7.37 (1H, d, J = 7.05 Hz, ArH), 7.35 (1H, d, J = 3.55 Hz, ArH), 7.22 (2H, t, J = 7.58 Hz, ArH), 7.12 (1H, t, J = 7.25 Hz, ArH), 7.06 (2H, d, J = 7.65 Hz, ArH), 5.08 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.5, 150.4, 147.4, 139.4, 136.0, 134.6, 133.6, 133.2, 131.1, 130.8, 129.7, 129.5, 129.3, 129.0, 128.7, 128.5, 127.9, 127.4, 127.0, 126.6, 124.1, 121.1, 113.6, 81.4, 45.8; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1299.

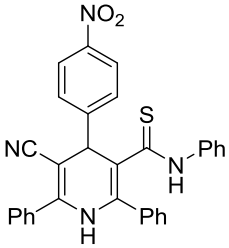


4-(2-Chlorophenyl)-5-cyano-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4o). Yellow powder (151.2 mg, 60%); mp: 203−205 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.81

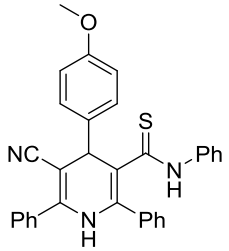
(1H, s, C(=S)-NH), 9.57 (1H, s, C=C-NH), 7.71 (1H, d, *J* = 7.50 Hz, ArH), 7.67 (2H, d, *J* = 7.15 Hz, ArH), 7.57 (2H, d, *J* = 6.85 Hz, ArH), 7.50 (3H, t, *J* = 7.65 Hz, ArH), 7.43−7.36 (5H, m, ArH), 7.27 (1H, t, *J* = 7.23 Hz, ArH), 7.20 (2H, t, *J* = 7.58 Hz, ArH), 7.09 (3H, t, *J* = 9.18 Hz, ArH), 5.60 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.2, 150.4, 142.8, 139.4, 136.4, 134.7, 133.3, 132.1, 131.3, 131.0, 129.7, 129.6, 129.5, 129.3, 129.0, 128.7, 128.5, 128.2, 126.5, 124.0, 120.8, 113.9, 81.3, 42.3; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ $[M + H]^+$, 504.1301, found 504.1322.



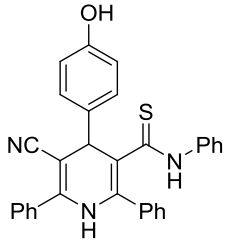
5-Cyano-*N*,2,6-triphenyl-4-(4-(trifluoromethyl)phenyl)-1,4-dihydropyridine-3-carbothioamide (4p). Yellow powder (231.2 mg, 86%); mp: 253−255 °C. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.79 (1H, s, C(=S)-NH), 9.68 (1H, s, C=C-NH), 7.77 (2H, d, *J* = 8.10 Hz, ArH), 7.70−7.66 (4H, m, ArH) 7.61 (2H, d, *J* = 6.65 Hz, ArH), 7.54−7.51 (3H, m, ArH), 7.43−7.37 (3H, m, ArH), 7.21 (2H, t, *J* = 7.55 Hz, ArH), 7.12−7.06 (3H, m, ArH), 5.13 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.4, 150.6, 149.6, 139.4, 136.5, 134.6, 133.2, 131.2, 129.7, 129.6, 129.3, 129.0, 128.9, 128.7, 128.6, 128.0 (q, $^2J_{C\text{-}F}$ = 31.7 Hz), 126.6, 125.0 (d, $^1J_{C\text{-}F}$ = 240.0 Hz), 121.1, 113.4, 81.3, 46.0; HRMS (ESI-TOF): calcd for $C_{32}H_{23}N_3SF_3$ $[M + H]^+$, 538.1565, found 538.1552.



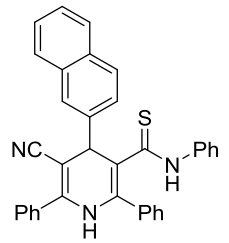
5-Cyano-4-(4-nitrophenyl)-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4q). Yellow powder (234.1 mg, 91%); mp: 258−260 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.84 (1H, s, C(=S)-NH), 9.77 (1H, s, C=C-NH), 8.28 (2H, d, *J* = 8.50 Hz, ArH), 7.75 (2H, d, *J* = 8.55 Hz, ArH), 7.68 (2H, d, *J* = 7.15 Hz, ArH), 7.61 (2H, t, *J* = 6.65 Hz, ArH), 7.54−7.50 (3H, m, ArH), 7.42 (2H, t, *J* = 7.05 Hz, ArH), 7.37 (1H, t, *J* = 7.13 Hz, ArH), 7.21 (2H, t, *J* = 7.40 Hz, ArH), 7.10 (3H, d, *J* = 6.85 Hz, ArH), 5.16 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.1, 152.5, 150.7, 147.0, 139.4, 136.9, 134.5, 133.0, 131.2, 129.8, 129.6, 129.3, 129.0, 128.7, 128.6, 126.6, 124.3, 123.9, 120.9, 112.9, 80.9, 45.9; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_4O_2S$ $[M + H]^+$, 515.1542, found 515.1550.



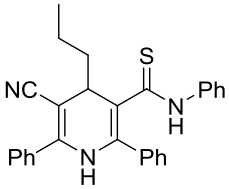
5-Cyano-4-(4-methoxyphenyl)-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4r). Yellow powder (204.8 mg, 82%); mp: 235−238 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.67 (1H, s, C(=S)-NH), 9.41 (1H, s, C=C-NH), 7.63 (2H, s, ArH), 7.58 (2H, s, ArH), 7.51 (3H, s, ArH), 7.38 (5H, d, J =7.05 Hz, ArH), 7.20 (2H, d, J = 6.35 Hz, ArH), 7.10 (1H, t, J = 6.25 Hz, ArH), 7.05 (2H, d, J = 5.45 Hz, ArH), 6.94 (2H, d, J = 7.55 Hz, ArH), 5.03 (1H, s, Ar-CH), 3.75 (1H, s, OCH_3); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.1, 158.7, 149.8, 139.5, 137.4, 135.0, 134.9, 133.5, 130.9, 129.4, 129.3, 129.2, 128.9, 128.6, 128.4, 126.5, 124.2, 121.4, 115.0, 114.2, 82.4, 55.5, 45.5; HRMS (ESI-TOF): calcd for $C_{32}H_{26}N_3OS$ $[M + H]^+$, 500.1797, found 500.1785.



5-Cyano-4-(4-hydroxyphenyl)-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4s). Yellow powder (220.9 mg, 91%); mp: 178−180 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.63 (1H, s, C(=S)-NH), 9.33 (1H, s, C=C-NH), 9.31 (1H, s, OH), 7.63 (2H, d, J = 6.55 Hz, ArH), 7.59 (2H, d, J = 6.40 Hz, ArH),7.53−7.49 (3H, m, ArH) 7.40−7.33 (3H, m, ArH), 7.26(2H, d, J = 8.15 Hz, ArH) 7.21 (2H, t, J = 7.43 Hz, ArH), 7.10 (1H, t, J = 7.13 Hz, ArH), 7.03 (2H, d, J = 7.25 Hz, ArH), 6.75 (2H, d, J = 8.15 Hz, ArH), 5.00 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.3, 156.8, 149.7, 139.4, 135.7, 135.0, 134.4, 133.6, 130.8, 129.3, 129.2, 128.9, 128.6, 128.4, 126.5, 124.3, 121.5, 115.6, 82.5, 45.6; HRMS (ESI-TOF): calcd for $C_{31}H_{24}N_3OS$ $[M + H]^+$, 486.1640, found 486.1629.

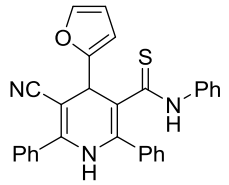


5-Cyano-4-(naphthalen-2-yl)-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4t). Yellow powder (220.9 mg, 85%); mp: 237−240 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.78 (1H, s, C(=S)-NH), 9.55 (1H, s, C=C-NH), 7.94 (2H, broad, s, ArH), 7.89 (2H, broad, s, ArH), 7.73−7.69 (3H, m, ArH),7.61 (2H, broad, s, ArH) 7.51 (5H, broad, s, ArH), 7.41 (2H, t, J = 6.20 Hz, ArH) 7.37 (1H, d, J = 6.30 Hz, ArH), 7.16 (2H, t, J = 6.95 Hz, ArH), 7.08 (1H, t, J = 6.60 Hz, ArH), 7.01 (2H, d, J = 6.60 Hz, ArH), 5.28 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.9, 150.2, 142.5, 139.4, 135.5, 134.9, 133.5, 132.8, 131.0, 129.5, 129.3, 129.0, 128.7, 128.5, 128.0, 127.0, 126.6, 126.3, 124.2, 121.4, 114.5, 82.0, 46.5; HRMS (ESI-TOF): calcd for $C_{35}H_{26}N_3S$ $[M + H]^+$, 520.1847, found 520.1839.

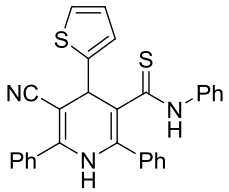


5-Cyano-*N*,2,6-triphenyl-4-propyl-1,4-dihydropyridine-3-carbothioamide (4u). Yellow

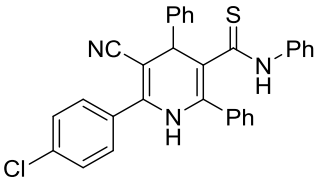
powder (189.5 mg, 87%); mp: 208−211 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.79 (1H, s, C(=S)-NH), 9.53 (1H, s, C=C-NH), 7.65 (2H, s, ArH), 7.58 (2H, d, J = 6.55 Hz, ArH), 7.54(3H, t, J = 2.48 Hz, ArH), 7.38 (2H, t, J = 6.75 Hz, ArH), 7.34 (1H, d, J = 7.30 Hz, ArH), 7.24 (4H, s, ArH), 7.13−7.12 (1H, m, ArH), 3.67 (1H, s, C_3H_7-*CH*), 1.92−1.90 (1H, m, CH_3-*CH_2*), 1.74−1.69 (2H, m, C_2H_5-*CH_2*), 1.53−1.47 (1H, m, CH_3-*CH_2*), 0.99 (3H, t, J = 7.18 Hz, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.1, 151.0, 139.8, 136.8, 135.1, 133.5, 131.1, 129.5, 129.1, 128.7, 128.6, 126.4, 124.0, 122.0, 114.8, 79.8, 18.6, 14.7; HRMS (ESI-TOF): calcd for $C_{28}H_{26}N_3S$ $[M + H]^+$, 436.1847, found 436.1859.



5-Cyano-4-(furan-2-yl)-*N*,2,6-triphenyl-1,4-dihydropyridine-3-carbothioamide (4v). Yellow powder (188.4 mg, 82%); mp: 216−218 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.80 (1H, s, C(=S)-NH), 9.65 (1H, s, C=C-NH), 7.63-7.60 (5H, m, ArH), 7.52 (3H, d, J = 6.70 Hz, ArH), 7.39 (2H, t, J = 7.10 Hz, ArH), 7.36 (1H, d, J = 7.00 Hz, ArH), 7.22 (2H, t, J = 7.25 Hz, ArH), 7.17 (2H, d, J = 6.85 Hz, ArH), 7.11 (1H, t, J = 6.98 Hz, ArH), 6.42 (1H, s, O-CH=*CH*), 6.34 (1H, s, O-C=CH), 5.17 (1H, s, C_4H_4O-*CH*); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.4, 156.8, 150.8, 142.9, 139.7, 136.4, 134.7, 133.3, 131.1, 129.6, 129.4, 129.0, 128.7, 128.6, 126.5, 124.0, 121.1, 111.9, 111.1, 107.0, 79.1; HRMS (ESI-TOF): calcd for $C_{29}H_{22}N_3SO$ $[M + H]^+$, 460.1484, found 460.1490.

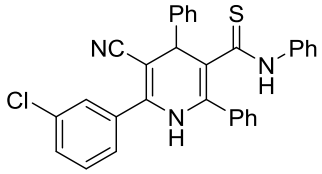


5-Cyano-*N*,2,6-triphenyl-4-(thiophen-2-yl)-1,4-dihydropyridine-3-carbothioamide (4w). Yellow powder (202.1 mg, 85%); mp: 198−200 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.71 (1H, s, C(=S)-NH), 9.85 (1H, s, C=C-NH), 7.65-7.62 (4H, m, ArH), 7.56 (3H, s, ArH), 7.43−7.35 (4H, m, ArH), 7.22 (2H, t, J = 7.00 Hz, ArH), 7.18 (2H, s, ArH), 7.11 (2H, t, J = 6.00 Hz, ArH), 7.02 (1H, t, J = 3.70 Hz, ArH), 5.26 (1H, s, C_4H_4S-*CH*); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.1, 150.3, 149.4, 139.7, 136.7, 134.5, 133.1, 131.1, 129.6, 129.3, 129.0, 128.6, 128.5, 127.2, 126.3, 125.3, 124.6, 123.9, 121.0, 114.1, 81.2; HRMS (ESI-TOF): calcd for $C_{29}H_{22}N_3S_2$ $[M + H]^+$, 476.1255, found 476.1240.

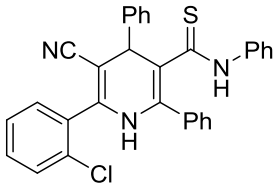


6-(4-Chlorophenyl)-5-cyano-*N*,2,4-triphenyl-1,4-dihydropyridine-3-carbothioamide (4y). Yellow powder (229.3 mg, 91%); mp: 214−217 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.70 (1H, s, C(=S)-NH), 9.50 (1H, s, C=C-NH), 7.65 (2H, d, J = 6.80 Hz, ArH), 7.62 (2H, d, J = 8.50 Hz, ArH), 7.57 (2H, d, J = 8.40 Hz, ArH), 7.47 (2H, d, J = 7.45 Hz, ArH), 7.41−7.37 (5H, m, ArH), 7.27 (1H, t, J = 7.10 Hz, ArH), 7.20 (2H, t, J = 7.53 Hz, ArH), 7.10 (1H, t, J = 7.20 Hz, ArH), 7.02

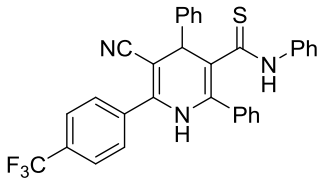
(2H, d, J = 7.40 Hz, ArH), 5.10 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.8, 148.9, 144.8, 139.3, 135.5, 135.0, 134.7, 132.2, 131.1, 129.4, 128.9, 128.8, 128.5, 128.4, 128.2, 127.3, 126.5, 124.1, 121.0, 114.7, 82.4, 46.2; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1312.



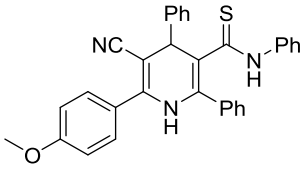
6-(3-Chlorophenyl)-5-cyano-*N*,2,4-triphenyl-1,4-dihydropyridine-3-carbothioamide (4z). Yellow powder (224.3 mg, 89%); mp: 193−195 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.66 (1H, s, C(=S)-NH), 9.46 (1H, s, C=C-NH), 7.62-7.59 (4H, m, ArH), 7.56 (2H, broad, s, ArH), 7.48 (2H, broad, s, ArH), 7.39 (5H, broad, s, ArH), 7.28 (1H, broad, s, ArH), 7.20 (2H, broad, s, ArH), 7.10 (1H, broad, s, ArH), 6.98 (2H, broad, s, ArH), 5.15 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.0, 148.7, 144.8, 139.4, 135.5, 134.8, 134.6, 133.5, 130.9, 130.8, 129.4, 129.0, 128.7, 128.5, 128.2, 127.5, 126.6, 124.3, 120.9, 115.0 82.8, 46.4; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1309.



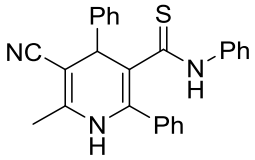
6-(2-Chlorophenyl)-5-cyano-*N*,2,4-triphenyl-1,4-dihydropyridine-3-carbothioamide (4aa). Yellow powder (211.7 mg, 84%); mp: 234−236 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.63 (1H, s, C(=S)-NH), 9.42 (1H, s, C=C-NH), 7.58 (4H, broad, s, ArH), 7.52 (3H, broad, s, ArH), 7.45−7.27 (7H, m, ArH), 7.18 (2H, broad, s, ArH), 7.09 (1H, broad, s, ArH), 6.93 (2H, broad, s, ArH), 5.30 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.2, 147.8, 144.5, 139.2, 134.7, 133.2, 132.9, 131.8, 130.0, 129.1, 128.7, 128.3, 127.8, 127.4, 126.6, 124.4, 120.1, 115.3, 84.3, 46.5; HRMS (ESI-TOF): calcd for $C_{31}H_{23}N_3SCl$ [M + H]$^+$, 504.1301, found 504.1316.



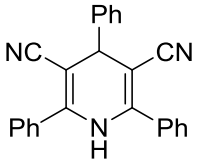
5-Cyano-*N*,2,4-triphenyl-6-(4-(trifluoromethyl)phenyl)-1,4-dihydropyridine-3-carbothioamide (4bb). Yellow powder (182.8 mg, 68%); mp: 223−226 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.73 (1H, s, C(=S)-NH), 9.55 (1H, s, C=C-NH), 7.87 (2H, broad, s, ArH), 7.82 (2H, broad, s, ArH), 7.64 (2H, broad, s, ArH), 7.48 (2H, broad, s, ArH), 7.39 (5H, broad, s, ArH), 7.28 (1H, broad, s, ArH), 7.20 (2H, broad, s, ArH), 7.10 (1H, broad, s, ArH), 7.00 (2H, broad, s, ArH), 5.16 (1H, s, Ar-CH); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.9, 148.8, 144.7, 139.3, 137.5, 134.7, 130.9 (d, $^2J_{C\text{-}F}$ = 31.7 Hz), 130.4, 129.6, 129.4, 129.0, 128.7, 128.5, 127.5, 126.6, 125.9, 124.5 (d, $^1J_{C\text{-}F}$ = 272.7 Hz), 124.3, 120.8, 114.9, 83.1, 46.3; HRMS (ESI-TOF): calcd for $C_{32}H_{23}N_3SF_3$ [M + H]$^+$, 538.1565, found 538.1572.



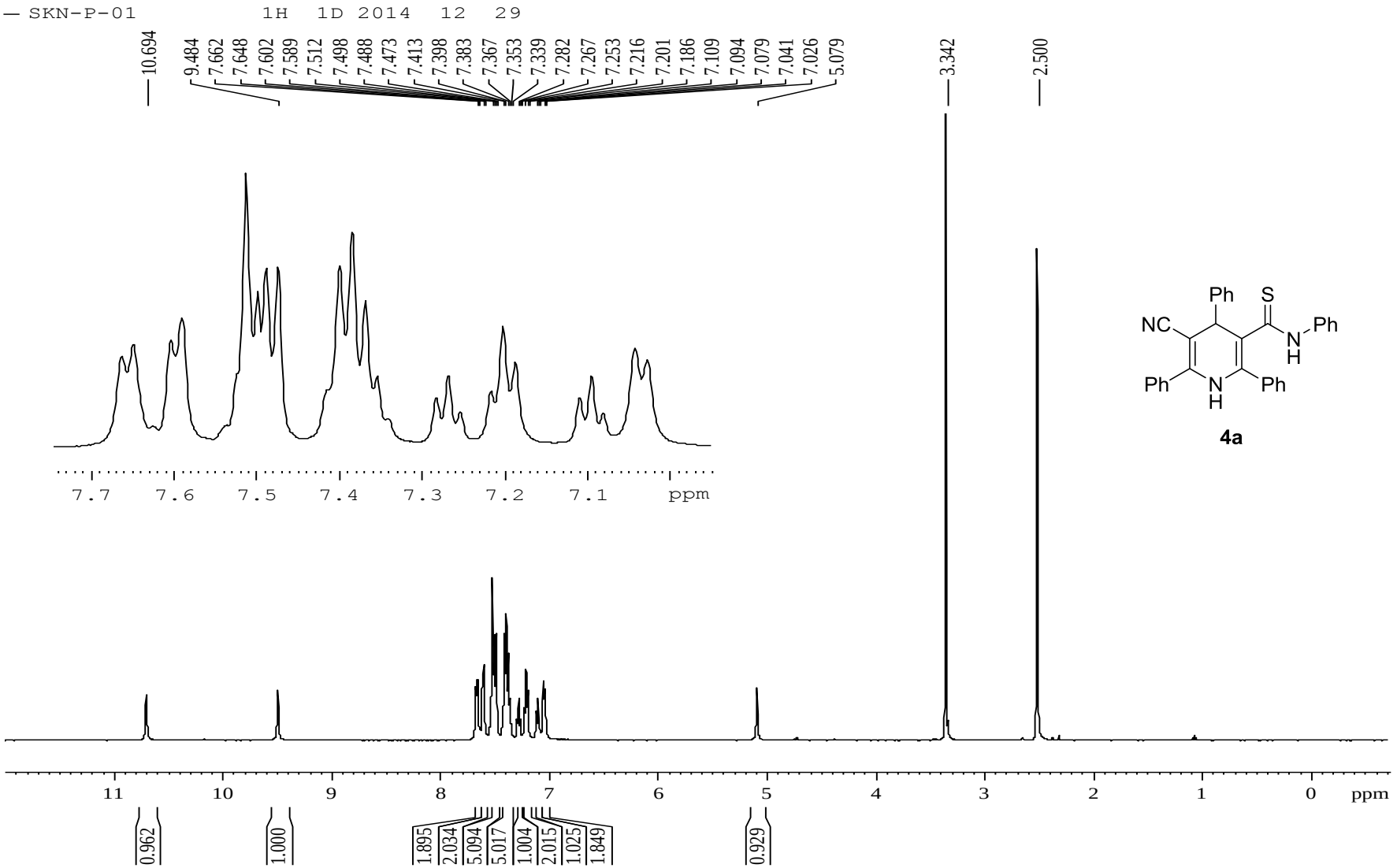
5-Cyano-6-(4-methoxyphenyl)-*N*,2,4-triphenyl-1,4-dihydropyridine-3-carbothioamide (4cc). Yellow powder (224.8 mg, 90%); mp: 232−234 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.69 (1H, s, C(=S)-NH), 9.46 (1H, s, C=C-NH), 7.66 (2H, broad, s, ArH), 7.54 (2H, d, J = 5.75 Hz, ArH), 7.46 (2H, broad, s, ArH), 7.39−7.37 (5H, m, ArH), 7.25 (1H, broad, s, ArH), 7.20 (2H, broad, s, ArH), 7.06 (5H, broad, s, ArH), 4.99 (1H, s, Ar-CH), 3.80 (3H, s, OCH_3); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 196.9, 161.5, 149.7, 145.3, 139.6, 136.1, 134.9, 130.9, 129.6, 128.9, 128.7, 128.6, 128.1, 127.3, 126.5, 125.5, 124.1, 121.8, 114.3, 81.1, 55.9, 46.1; HRMS (ESI-TOF): calcd for $C_{32}H_{26}N_3OS$ $[M + H]^+$, 500.1797, found 500.1796.



5-Cyano-6-methyl-*N*,2,4-triphenyl-1,4-dihydropyridine-3-carbothioamide (4dd). Yellow powder (173.2 mg, 85%); mp: 195−197 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm) 10.56 (1H, s, C(=S)-NH), 8.94 (1H, s, C=C-NH), 7.56 (2H, d, J = 6.70 Hz, ArH), 7.42−7.33 (7H, m, ArH), 7.24 (1H, t, J = 6.80 Hz, ArH), 7.17 (2H, t, J = 7.40 Hz, ArH), 7.08 (1H, t, J = 7.05 Hz, ArH), 6.90 (2H, d, J = 7.65 Hz, ArH), 5.13 (1H, d, J = 5.75 Hz, Ar-CH), 2.09 (3H, s, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) 197.5, 148.0, 144.7, 139.2, 135.1, 133.3, 129.2, 128.9, 128.7, 128.4, 127.2, 126.5, 124.3, 120.8, 115.4, 81.8, 46.0, 18.1; HRMS (ESI-TOF): calcd for $C_{26}H_{22}N_3S$ $[M + H]^+$, 408.1534, found 408.1542.



2,4,6-Triphenyl-1,4-dihydropyridine-3,5-dicarbonitrile (6). White powder (25.2 mg, 35%); ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.60 (4H, d, J = 6.75 Hz, ArH), 7.54−7.47 (6H, m, ArH), 7.46−7.43 (4H, m, ArH), 7.38-7.37 (1H, m, ArH), 6.38 (1H, s, C=C-NH), 4.61 (1H, s, Ar-CH).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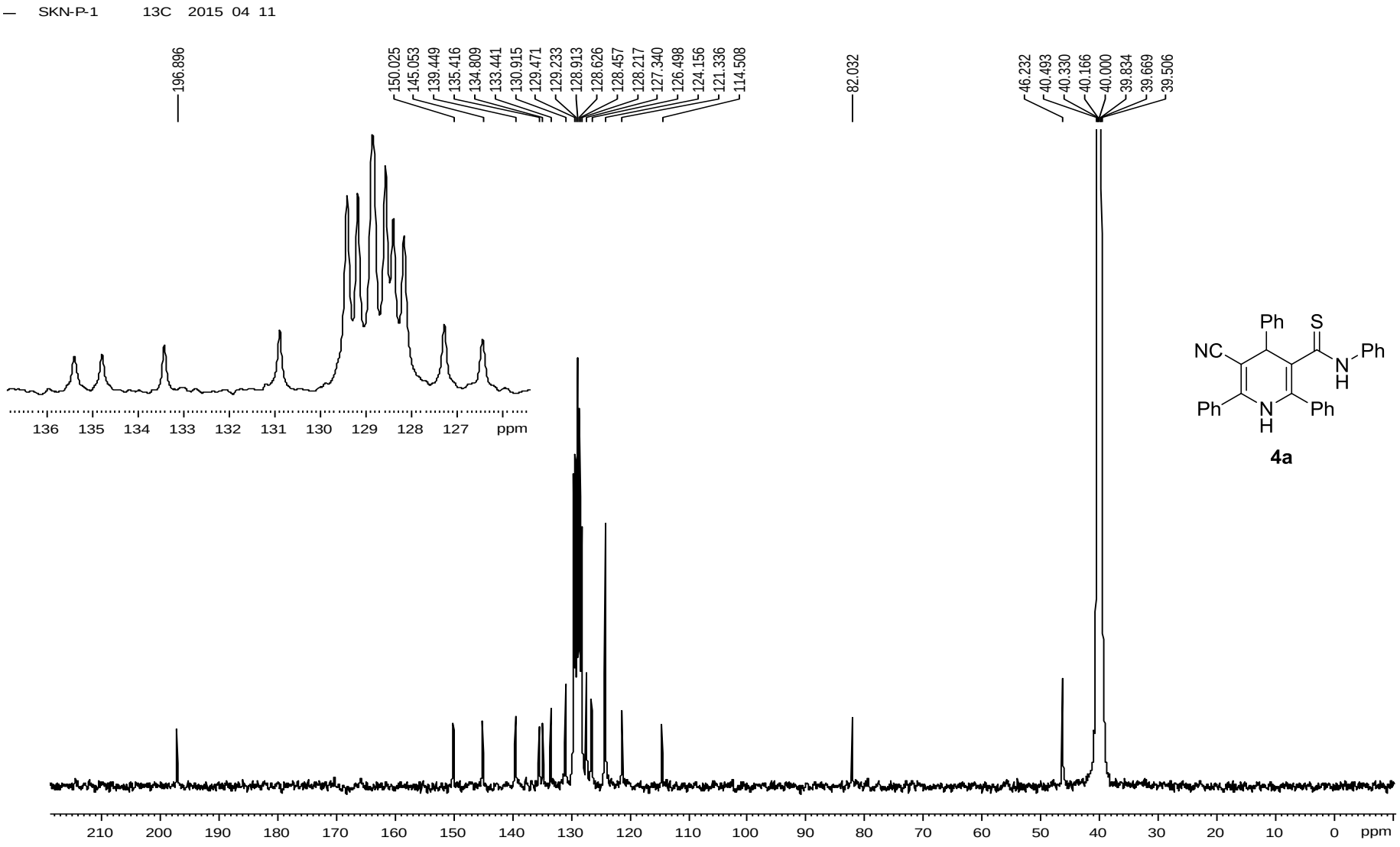
9.484
7.662
7.648
7.602
7.589
7.512
7.498
7.488
7.473
7.413
7.398
7.383
7.367
7.353
7.339
7.282
7.267
7.253
7.216
7.201
7.186
7.109
7.094
7.079
7.041
7.026
5.079
3.342
2.500
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.962
1.000
1.895
2.034
5.094
5.017
1.004
2.015
1.025
1.849
0.929

Ph
S
NC
N
H
Ph
Ph
N
H
Ph

4a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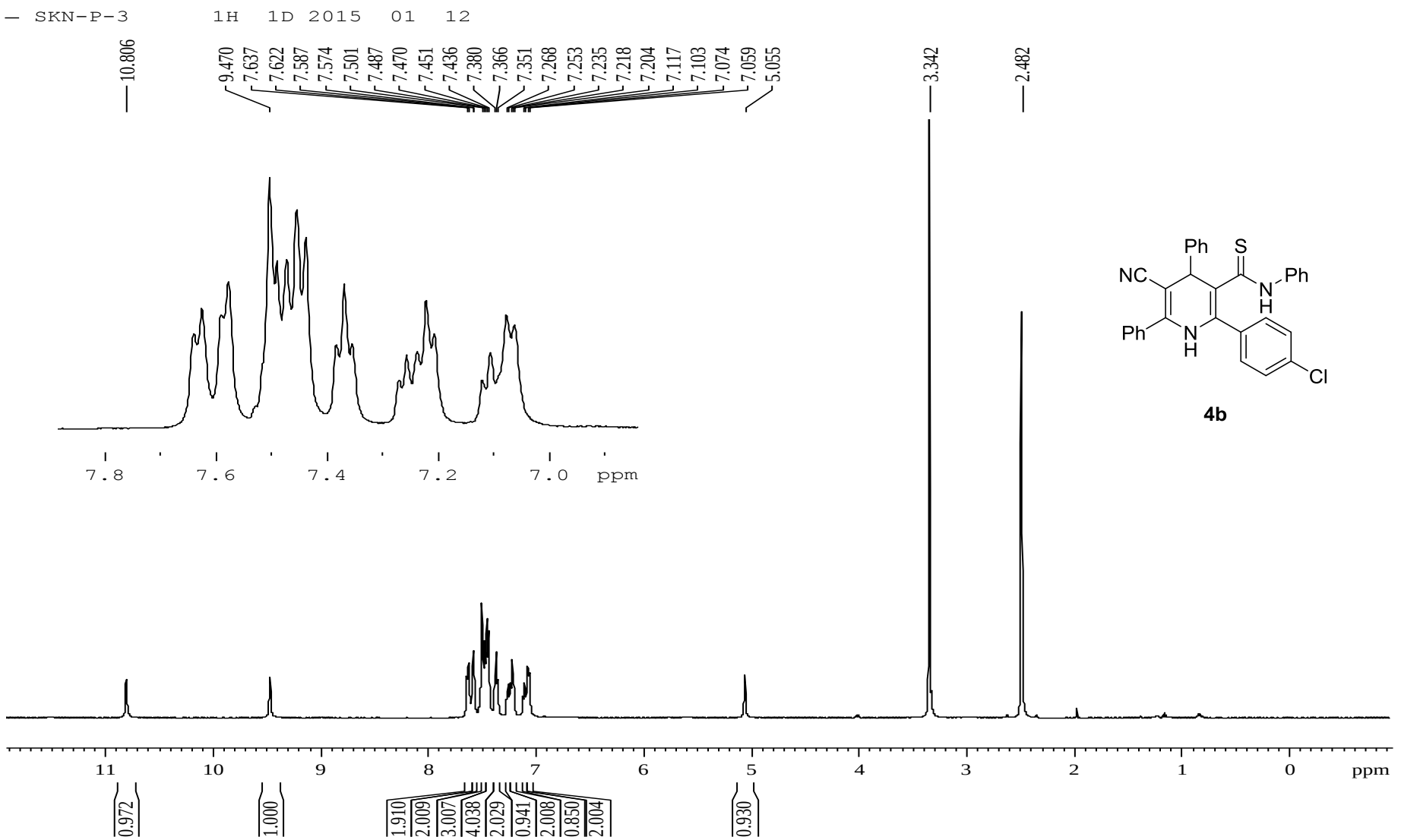
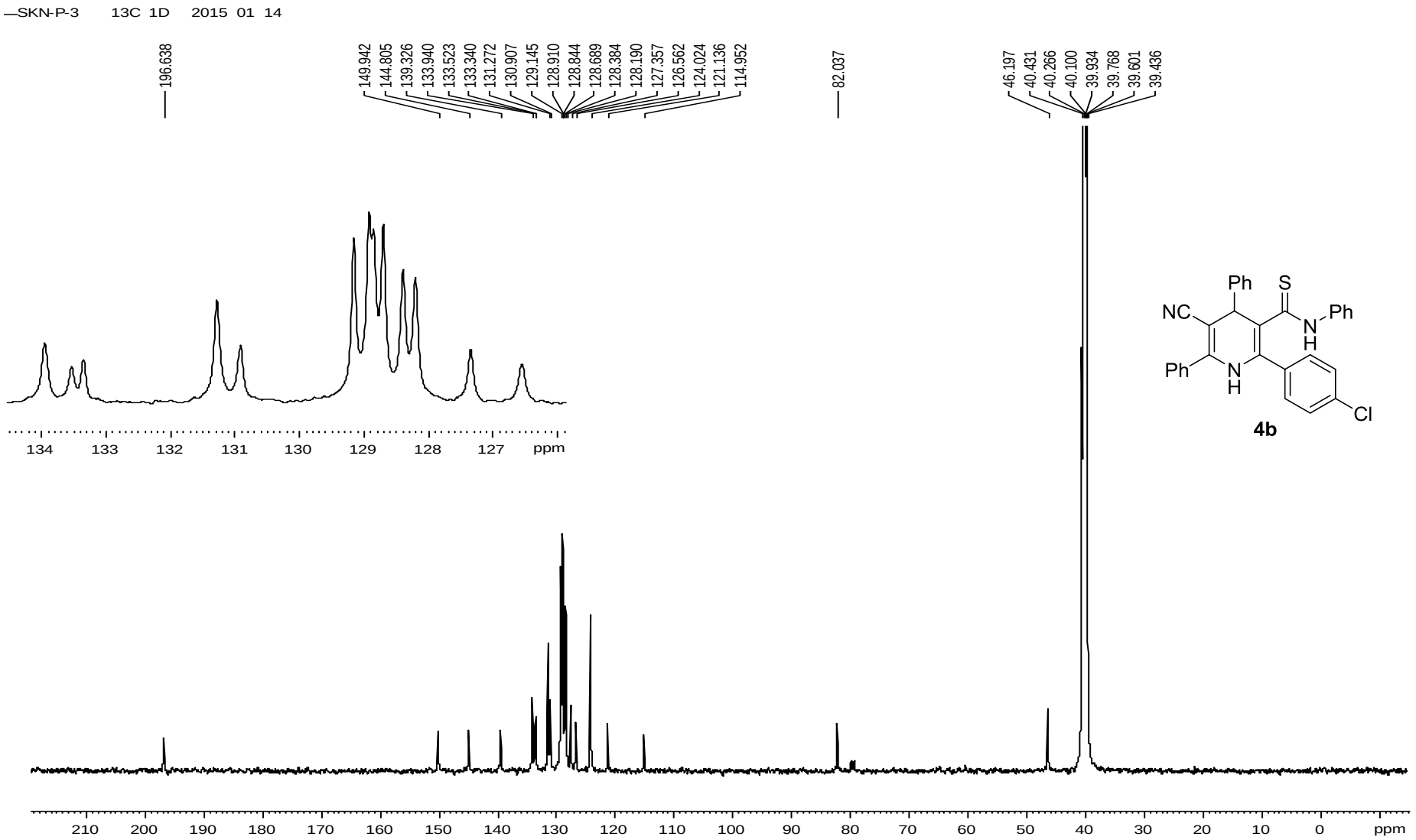
196.896
150.025
145.053
139.449
135.416
134.809
133.441
130.915
129.471
129.233
128.913
128.626
128.457
128.217
127.340
126.498
124.156
121.336
114.508
82.032
46.232
40.493
40.330
40.166
40.000
39.834
39.669
39.506
136 135 134 133 132 131 130 129 128 127 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Ph
Ph
N
H
Ph

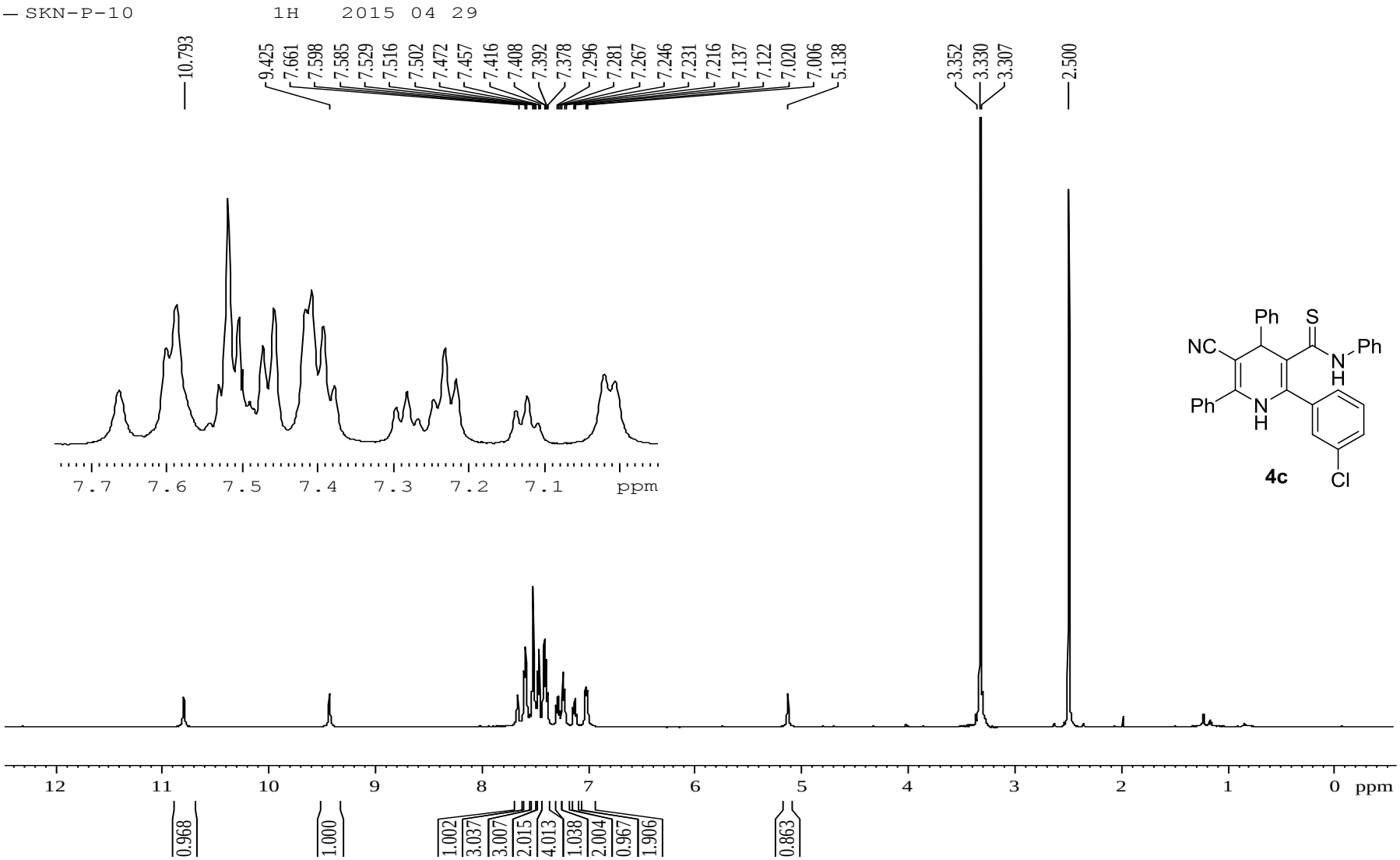
4a

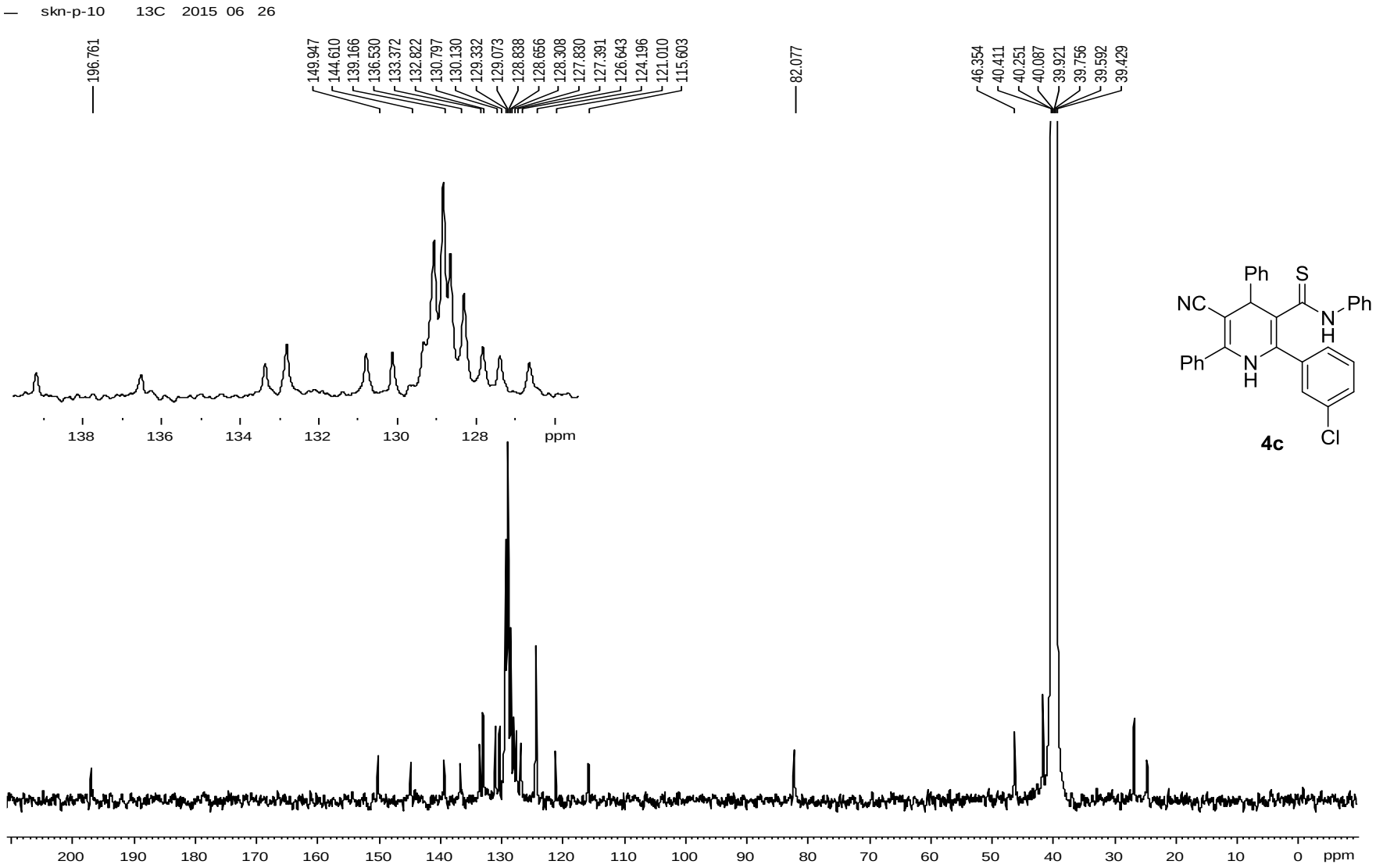

— SKN-P-3 1H 1D 2015 01 12
10.806
9.470
7.637
7.622
7.587
7.574
7.501
7.487
7.470
7.451
7.436
7.380
7.366
7.351
7.268
7.253
7.235
7.218
7.204
7.117
7.103
7.074
7.059
5.055
3.342
2.482
7.8
7.6
7.4
7.2
7.0
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.972
1.000
1.910
2.009
3.007
4.038
2.029
0.941
2.008
0.850
2.004
0.930

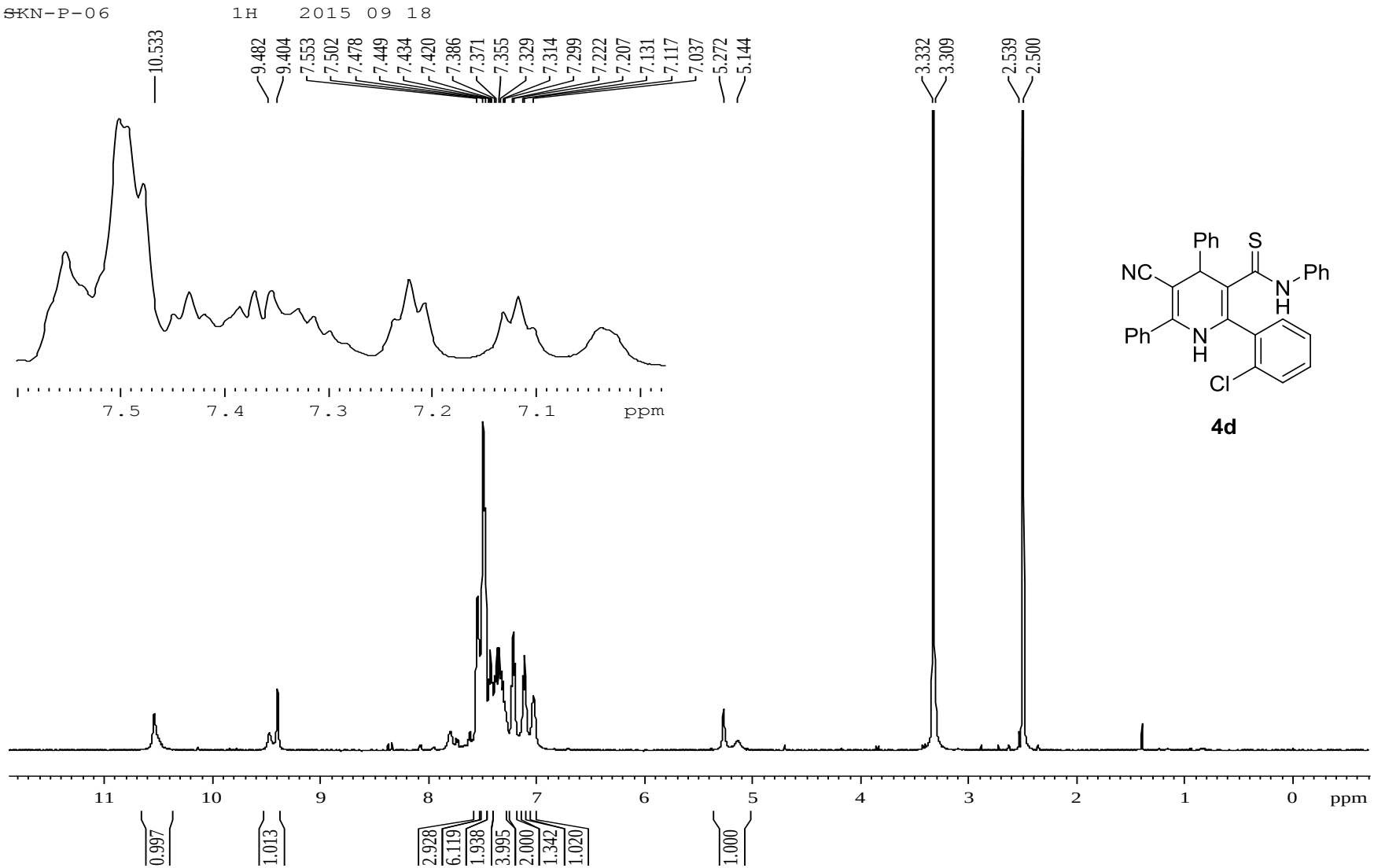
Ph
S
NC
N
H
Ph
Ph
N
H
Cl

4b

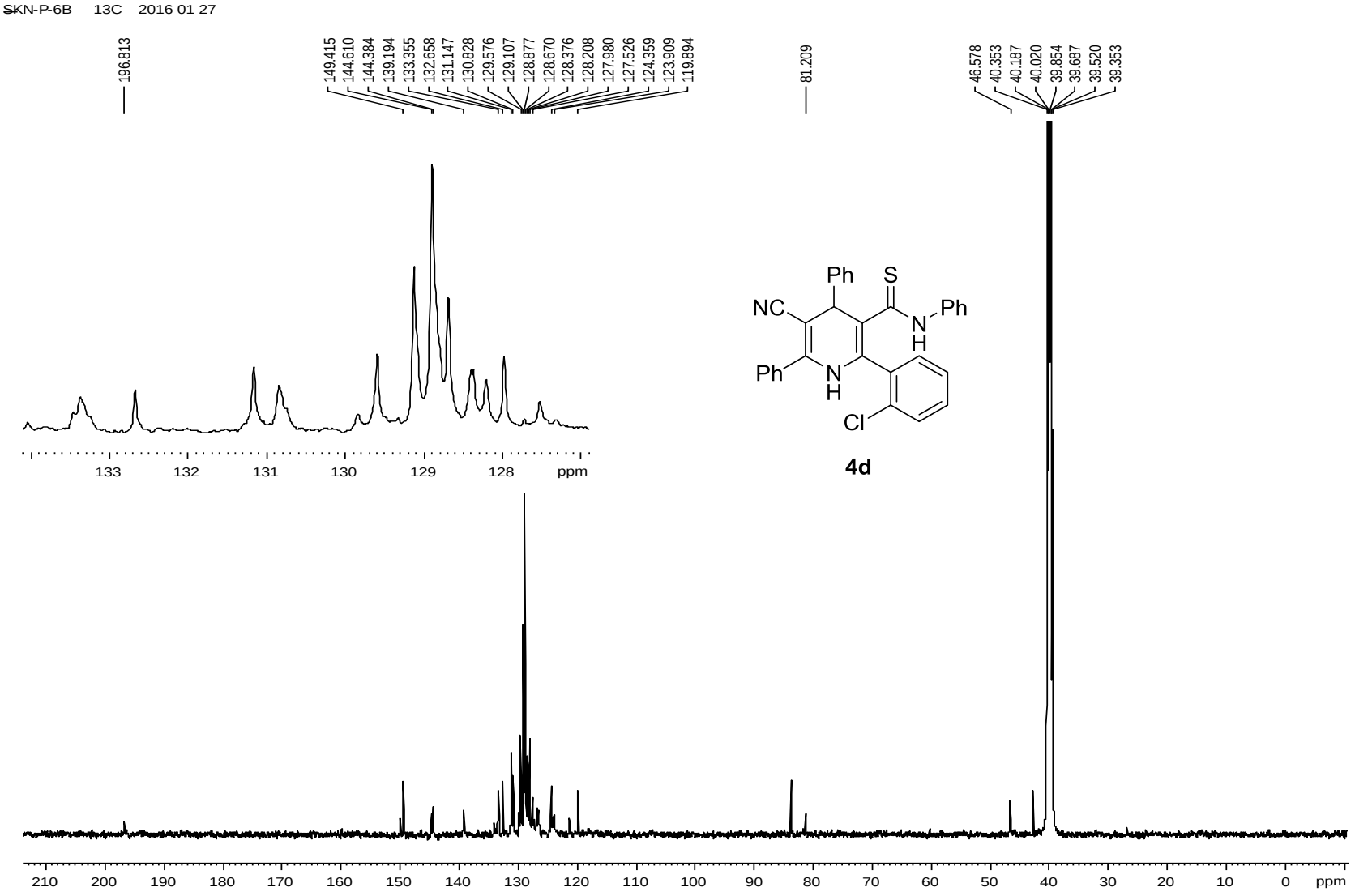

SKN-P-3 13C 1D 2015 01 14
196.638
149.942
144.805
139.326
133.940
133.523
133.340
131.272
130.907
129.145
128.910
128.844
128.689
128.384
128.190
127.357
126.562
124.024
121.136
114.952
82.037
46.197
40.431
40.266
40.100
39.934
39.768
39.601
39.436
134 133 132 131 130 129 128 127 ppm
Ph
S
NC
N
H
Ph
Ph
N
H
Cl
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

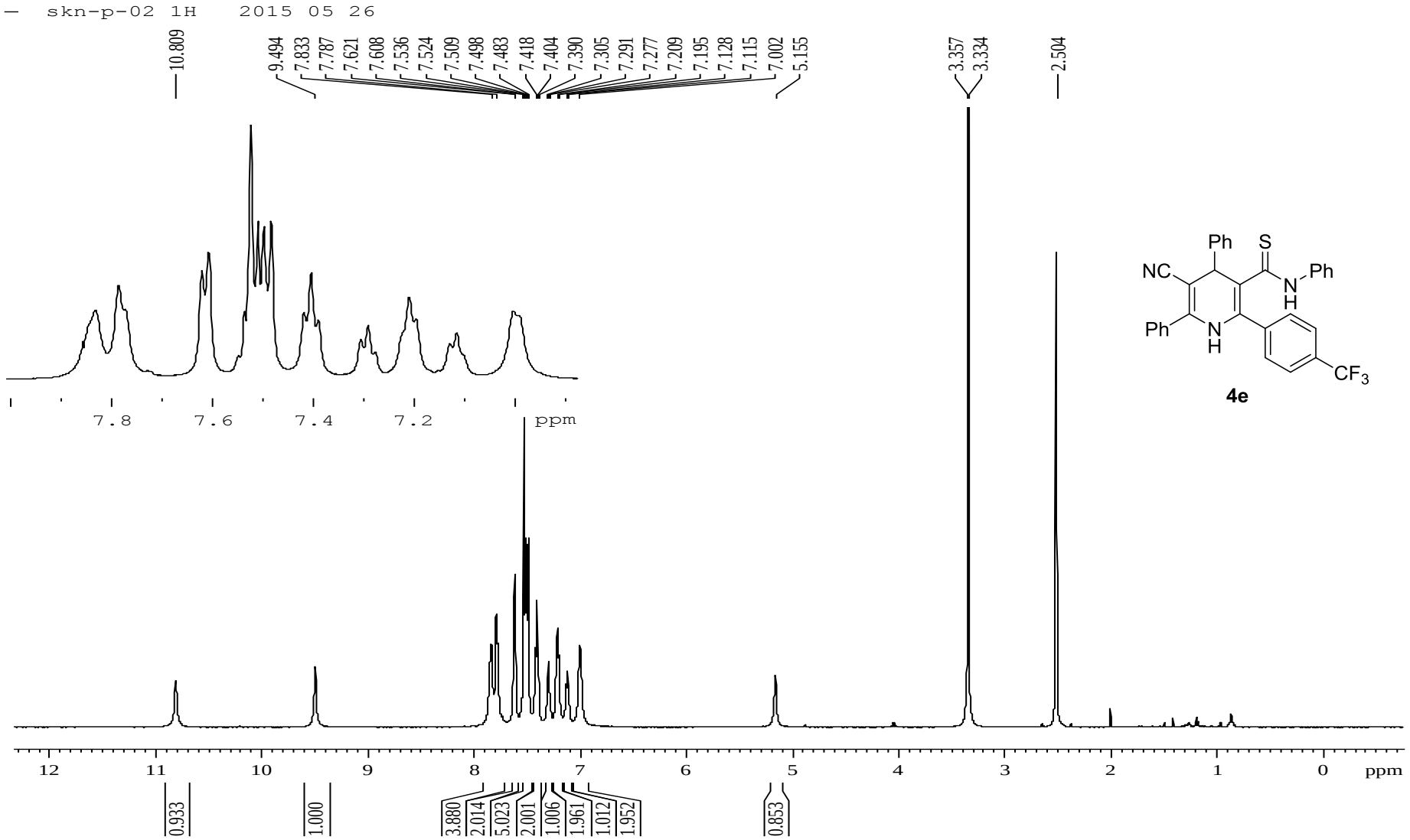

SKN-P-10 1H 2015 04 29
10.793
9.425
7.661
7.598
7.585
7.529
7.516
7.502
7.472
7.457
7.416
7.408
7.392
7.378
7.296
7.281
7.267
7.246
7.231
7.216
7.137
7.122
7.020
7.006
5.138
3.352
3.330
3.307
2.500
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.968
1.000
1.002
3.037
3.007
2.015
4.013
1.038
2.004
0.967
1.906
0.863
Ph
S
NC
N
H
Ph
Ph
N
H
Cl
4c


skn-p-10 13C 2015 06 26
196.761
149.947
144.610
139.166
136.530
133.372
132.822
130.797
130.130
129.332
129.073
128.838
128.656
128.308
127.830
127.391
126.643
124.196
121.010
115.603
82.077
46.354
40.411
40.251
40.087
39.921
39.756
39.592
39.429
138
136
134
132
130
128
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
Ph
S
NC
N
H
Ph
Ph
N
H
Cl
4c


SKN-P-06 1H 2015 09 18
10.533
9.482
9.404
7.553
7.502
7.478
7.449
7.434
7.420
7.386
7.371
7.355
7.329
7.314
7.299
7.222
7.207
7.131
7.117
7.037
5.272
5.144
3.332
3.309
2.539
2.500
7.5
7.4
7.3
7.2
7.1
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.997
1.013
2.928
6.119
1.938
3.995
2.000
1.342
1.020
1.000
Ph
S
NC
N
H
Ph
Ph
N
H
Cl

4d


SKN-P-6B 13C 2016 01 27
196.813
149.415
144.610
144.384
139.194
133.355
132.658
131.147
130.828
129.576
129.107
128.877
128.670
128.376
128.208
127.980
127.526
124.359
123.909
119.894
81.209
46.578
40.353
40.187
40.020
39.854
39.687
39.520
39.353
133
132
131
130
129
128
ppm
Ph
S
NC
N
H
Ph
Ph
N
H
Cl
4d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


skn-p-02 1H 2015 05 26
10.809
9.494
7.833
7.787
7.621
7.608
7.536
7.524
7.509
7.498
7.483
7.418
7.404
7.390
7.305
7.291
7.277
7.209
7.195
7.128
7.115
7.002
5.155
3.357
3.334
2.504
7.8
7.6
7.4
7.2
ppm
Ph
S
NC
N
H
Ph
Ph
N
H
CF3
4e
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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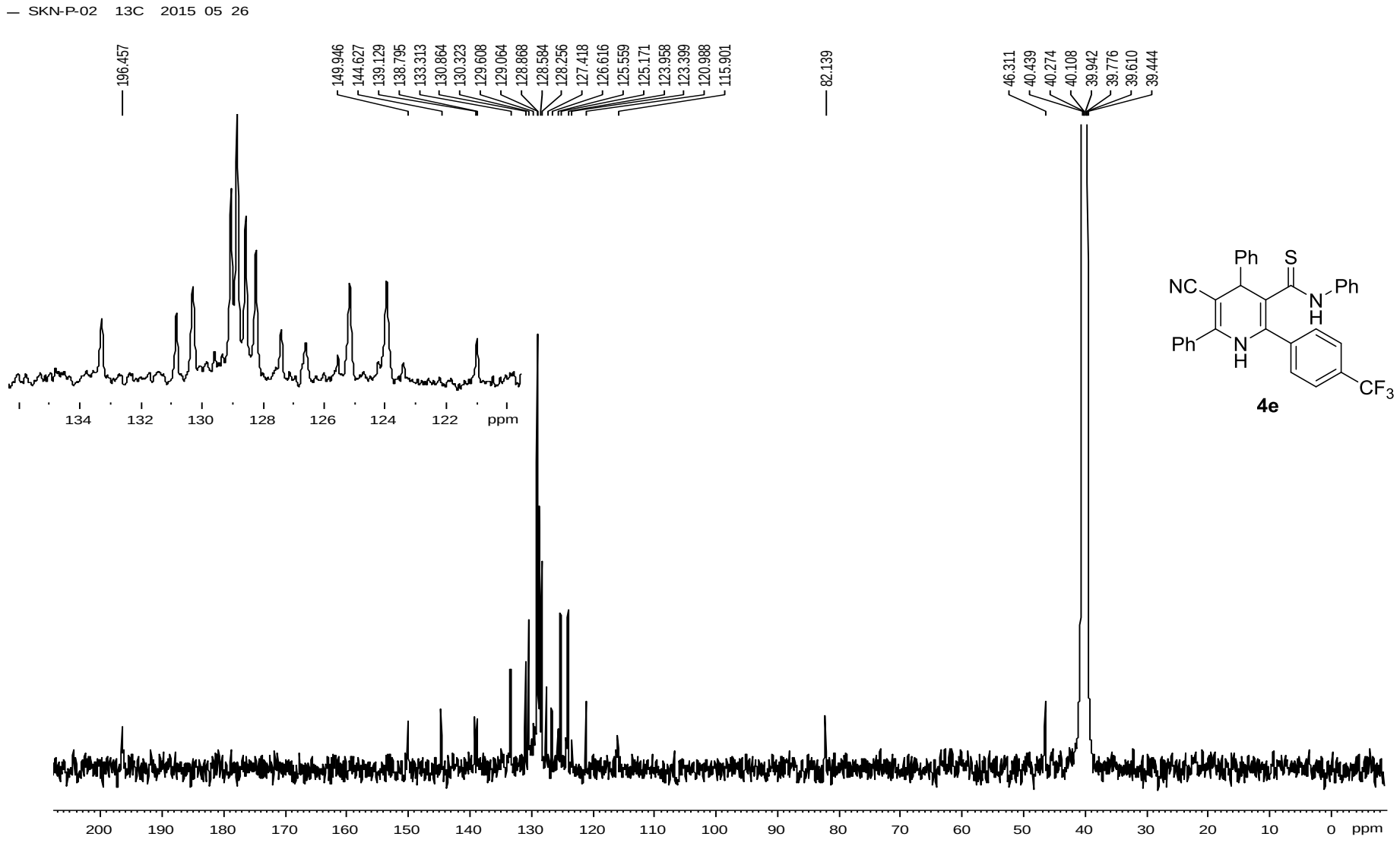
3.880
2.014
5.023
2.001
1.006
1.961
1.012
1.952
0.853


— SKN-P-02 13C 2015 05 26
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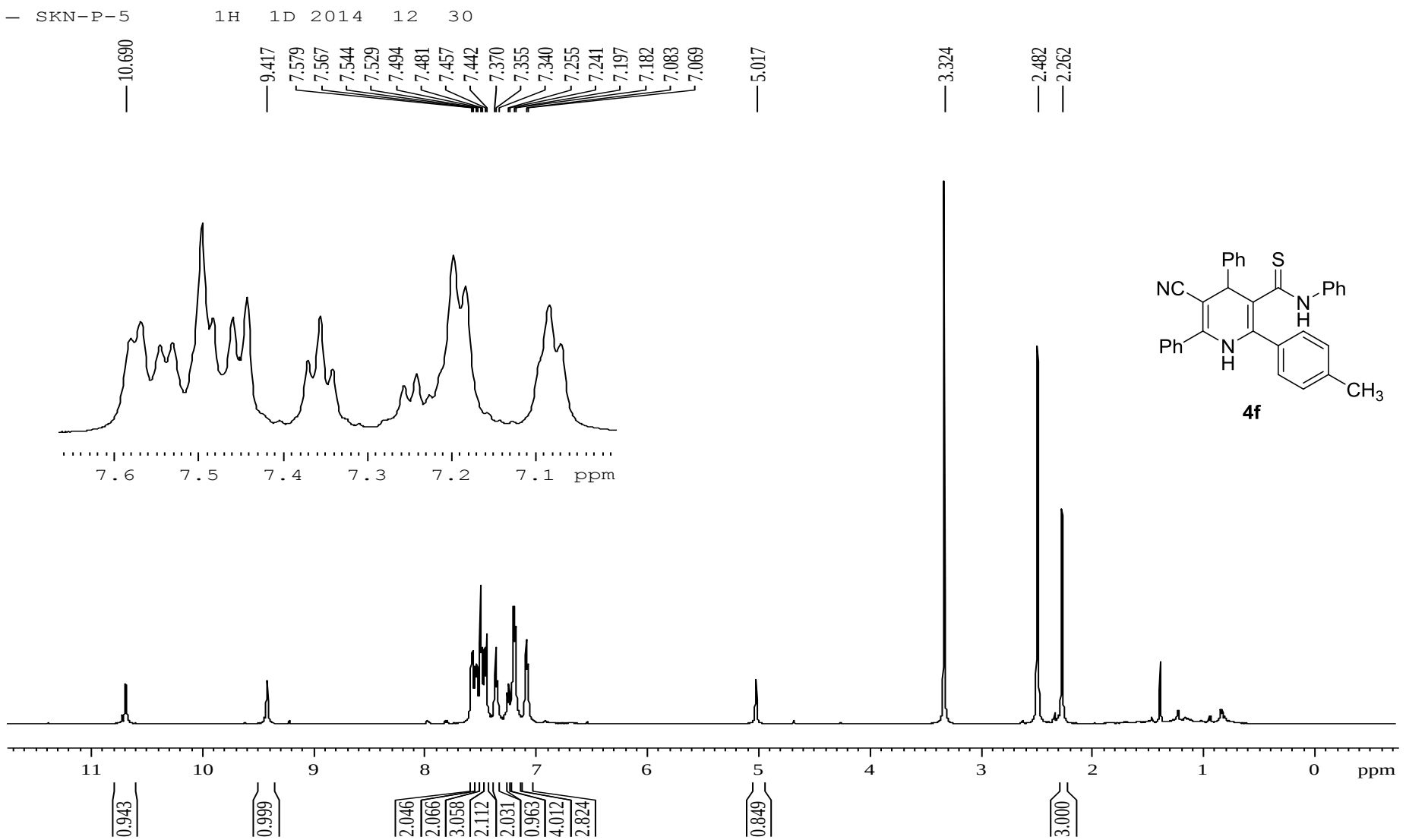
144.627
139.129
138.795
133.313
130.864
130.323
129.608
129.064
128.868
128.584
128.256
127.418
126.616
125.559
125.171
123.958
123.399
120.988
115.901
82.139
46.311
40.439
40.274
40.108
39.942
39.776
39.610
39.444
134 132 130 128 126 124 122 ppm
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Ph
Ph
N
H
CF3
4e


— SKN-P-5 1H 1D 2014 12 30
10.690
9.417
7.579
7.567
7.544
7.529
7.494
7.481
7.457
7.442
7.370
7.355
7.340
7.255
7.241
7.197
7.182
7.083
7.069
5.017
3.324
2.482
2.262
7.6 7.5 7.4 7.3 7.2 7.1 ppm
Ph
S
NC
N
H
Ph
Ph
N
H
CH3
4f
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.943
0.999
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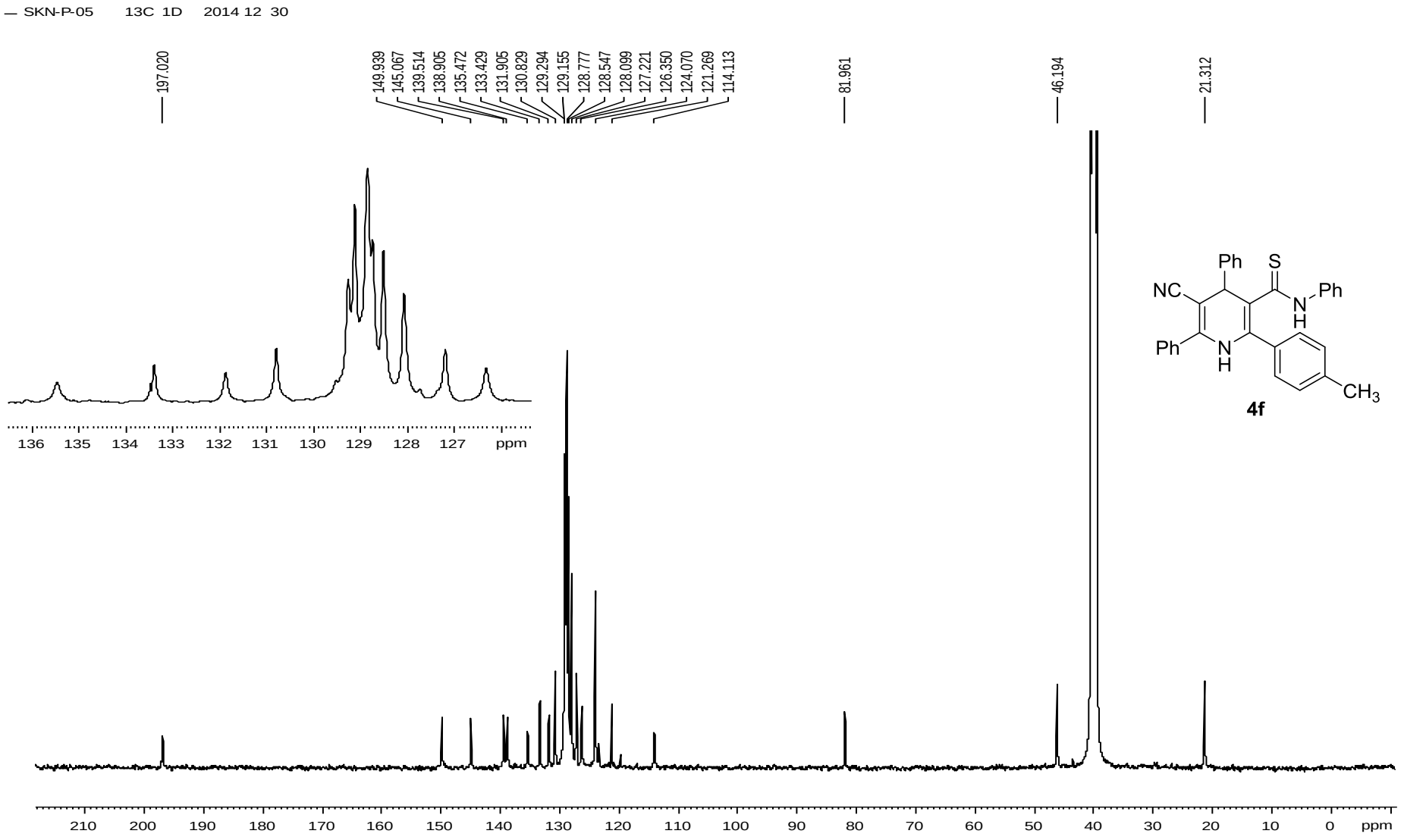
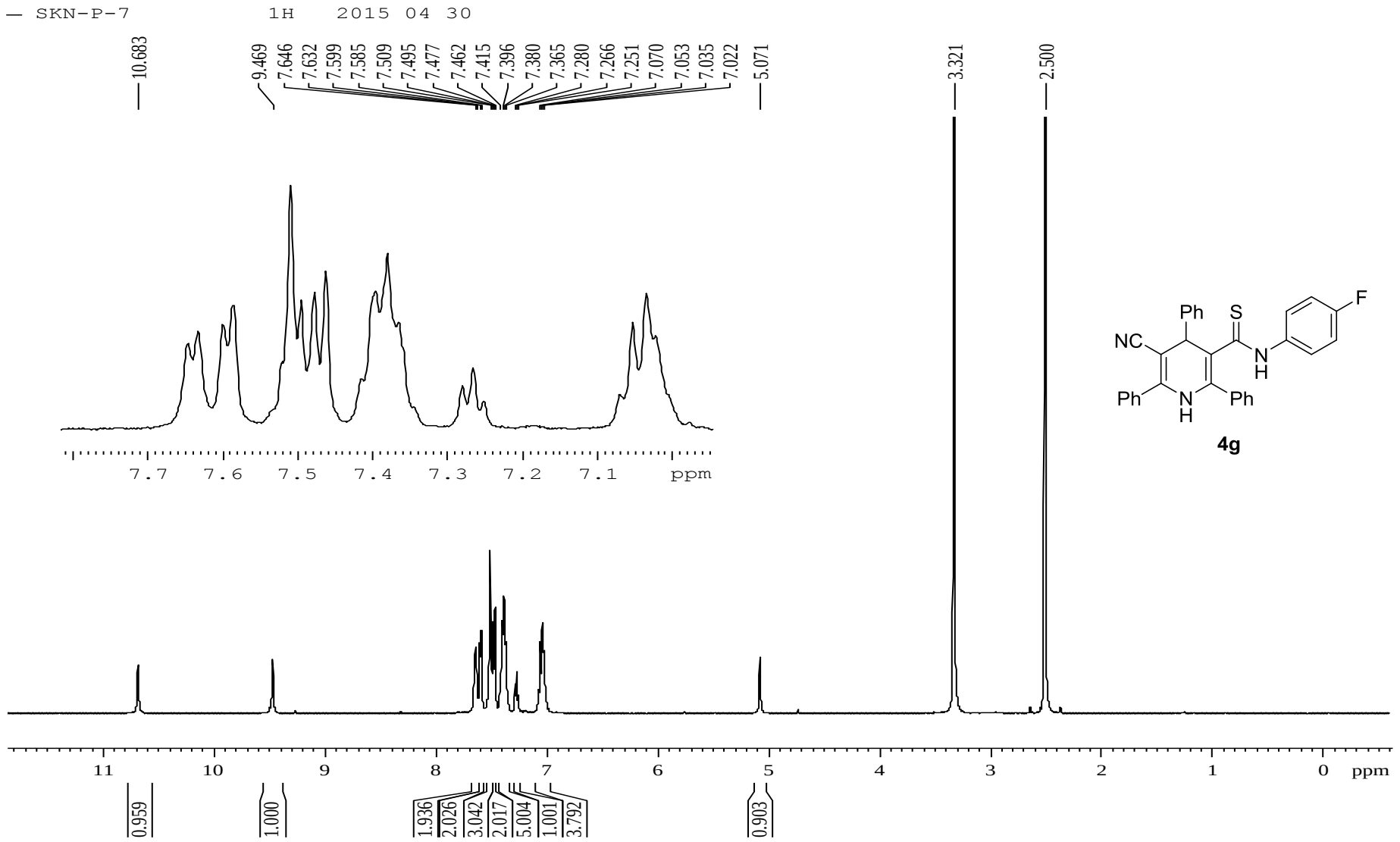
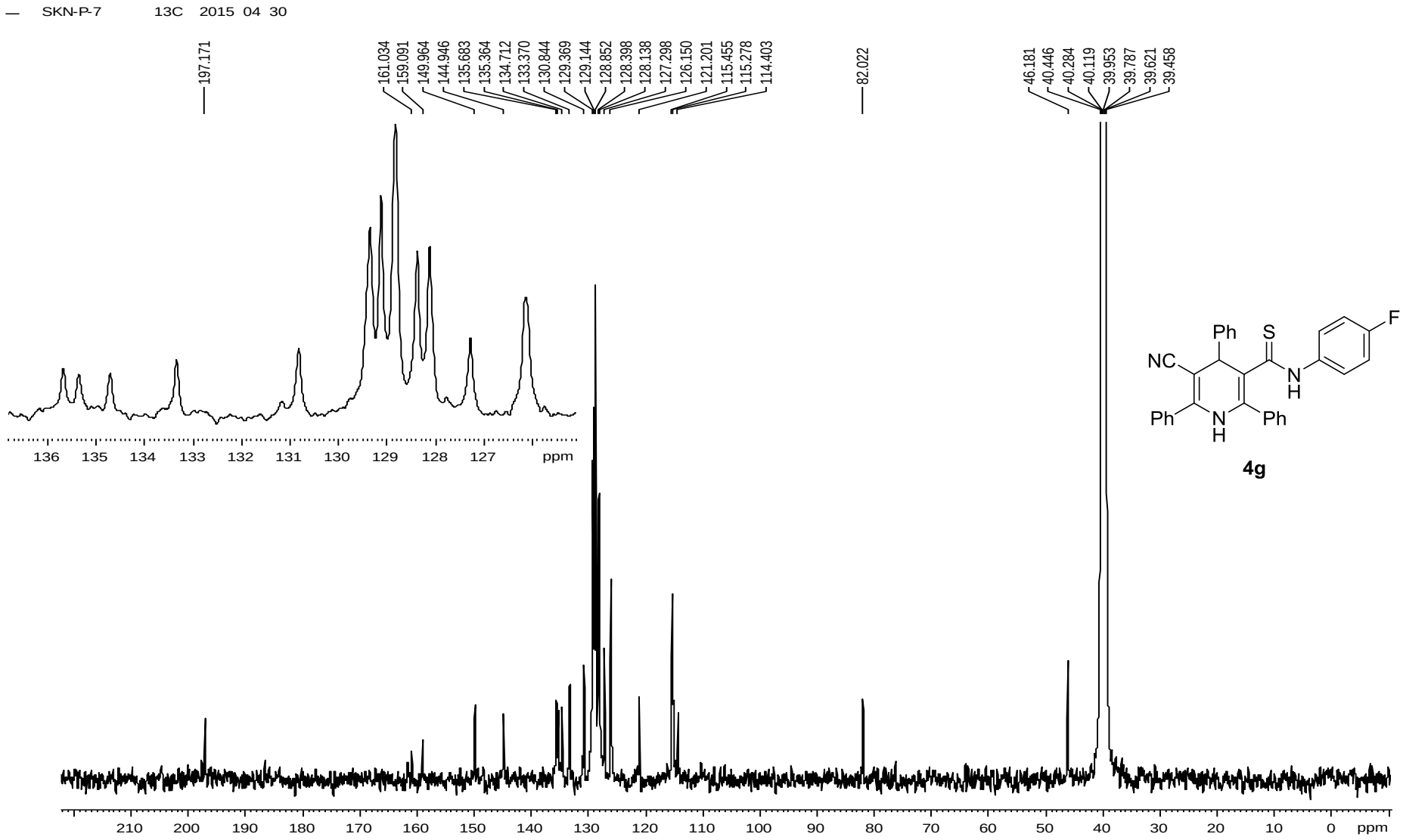
2.066
3.058
2.112
2.031
0.963
4.012
2.824
0.849
3.000


SKN-P-05 13C 1D 2014 12 30
197.020
149.939
145.067
139.514
138.905
135.472
133.429
131.905
130.829
129.294
129.155
128.777
128.547
128.099
127.221
126.350
124.070
121.269
114.113
81.961
46.194
21.312
136 135 134 133 132 131 130 129 128 127 ppm
Ph
S
NC
N
H
Ph
Ph
N
H
CH3
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


SKN-P-7 1H 2015 04 30
10.683
9.469
7.646
7.632
7.599
7.585
7.509
7.495
7.477
7.462
7.415
7.396
7.380
7.365
7.280
7.266
7.251
7.070
7.053
7.035
7.022
5.071
3.321
2.500
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.959
1.000
1.936
2.026
3.042
2.017
5.004
1.001
3.792
0.903
Ph
S
NC
N
H
F
Ph
N
H
Ph

4g


SKN-P-7 13C 2015 04 30
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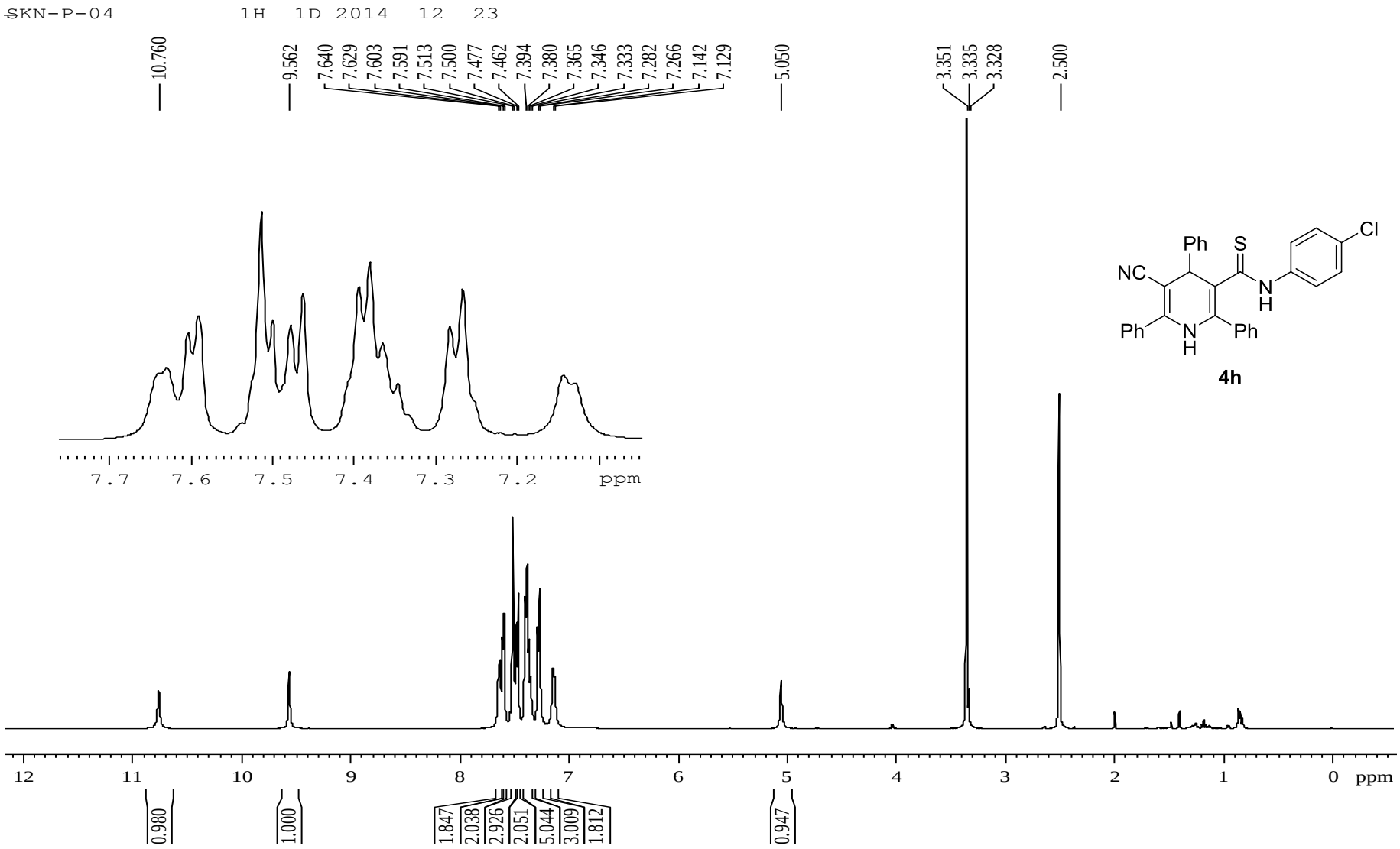
161.034
159.091
149.964
144.946
135.683
135.364
134.712
133.370
130.844
129.369
129.144
128.852
128.398
128.138
127.298
126.150
121.201
115.455
115.278
114.403
82.022
46.181
40.446
40.284
40.119
39.953
39.787
39.621
39.458
136 135 134 133 132 131 130 129 128 127 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
F
Ph
N
H
Ph
4g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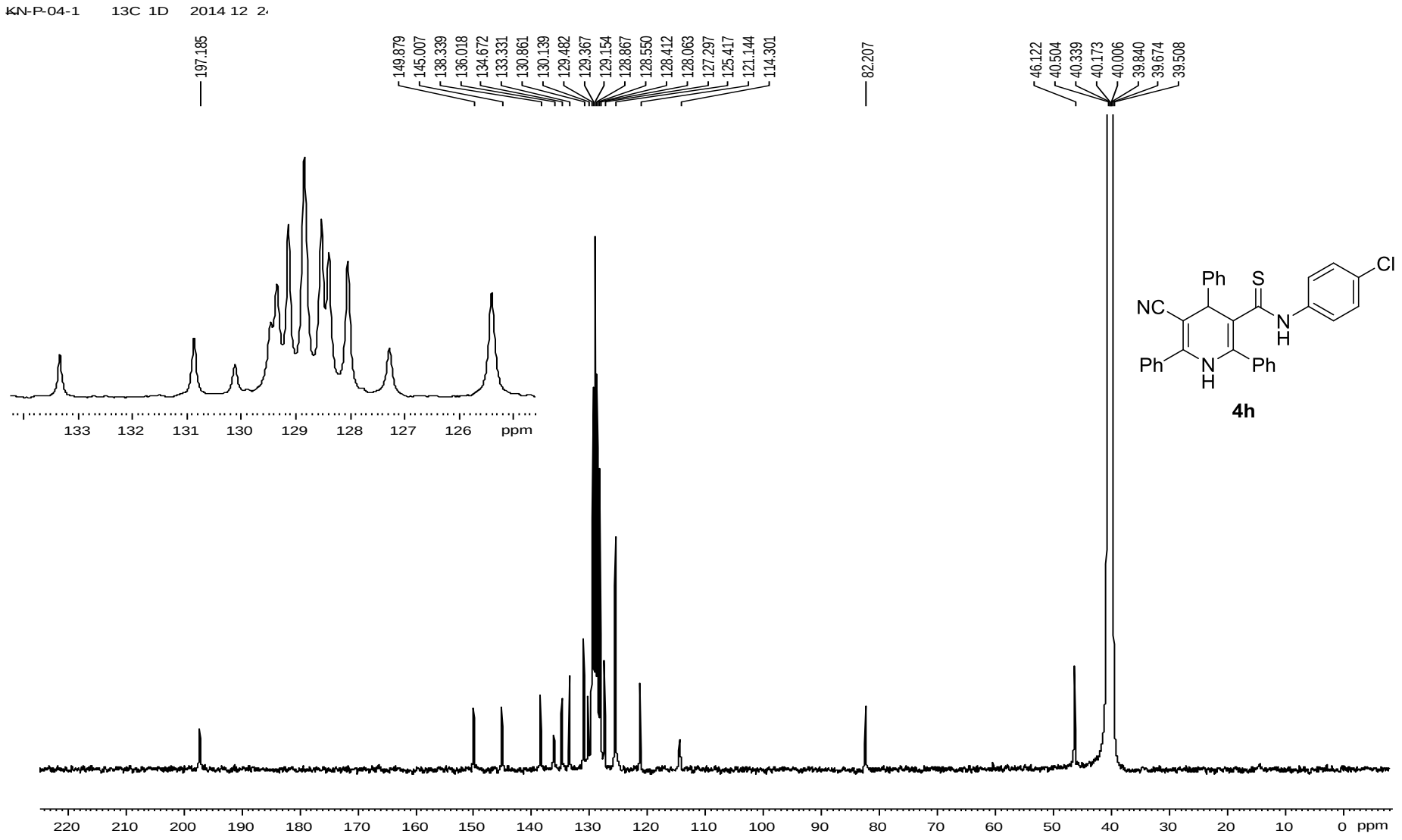
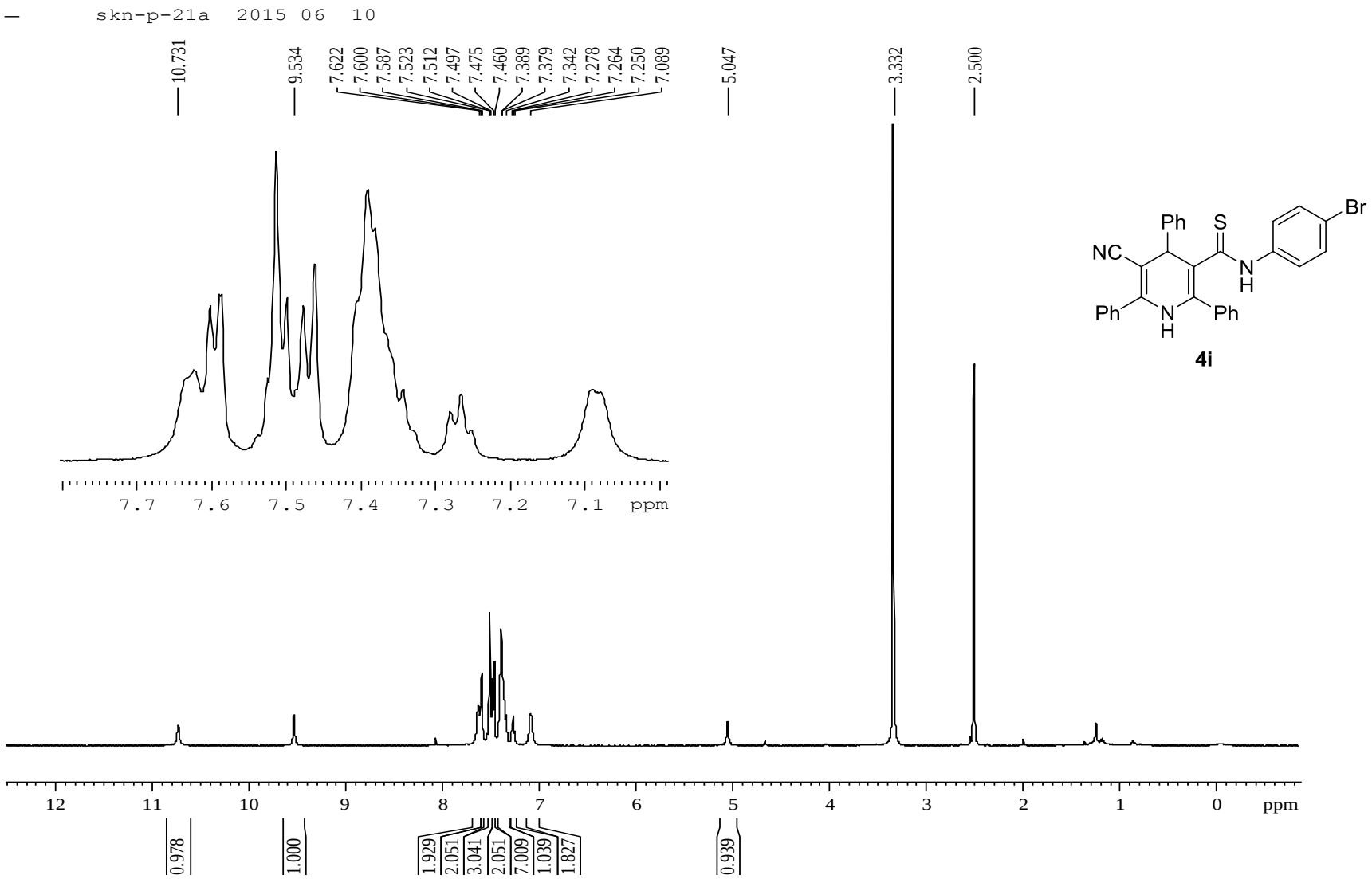
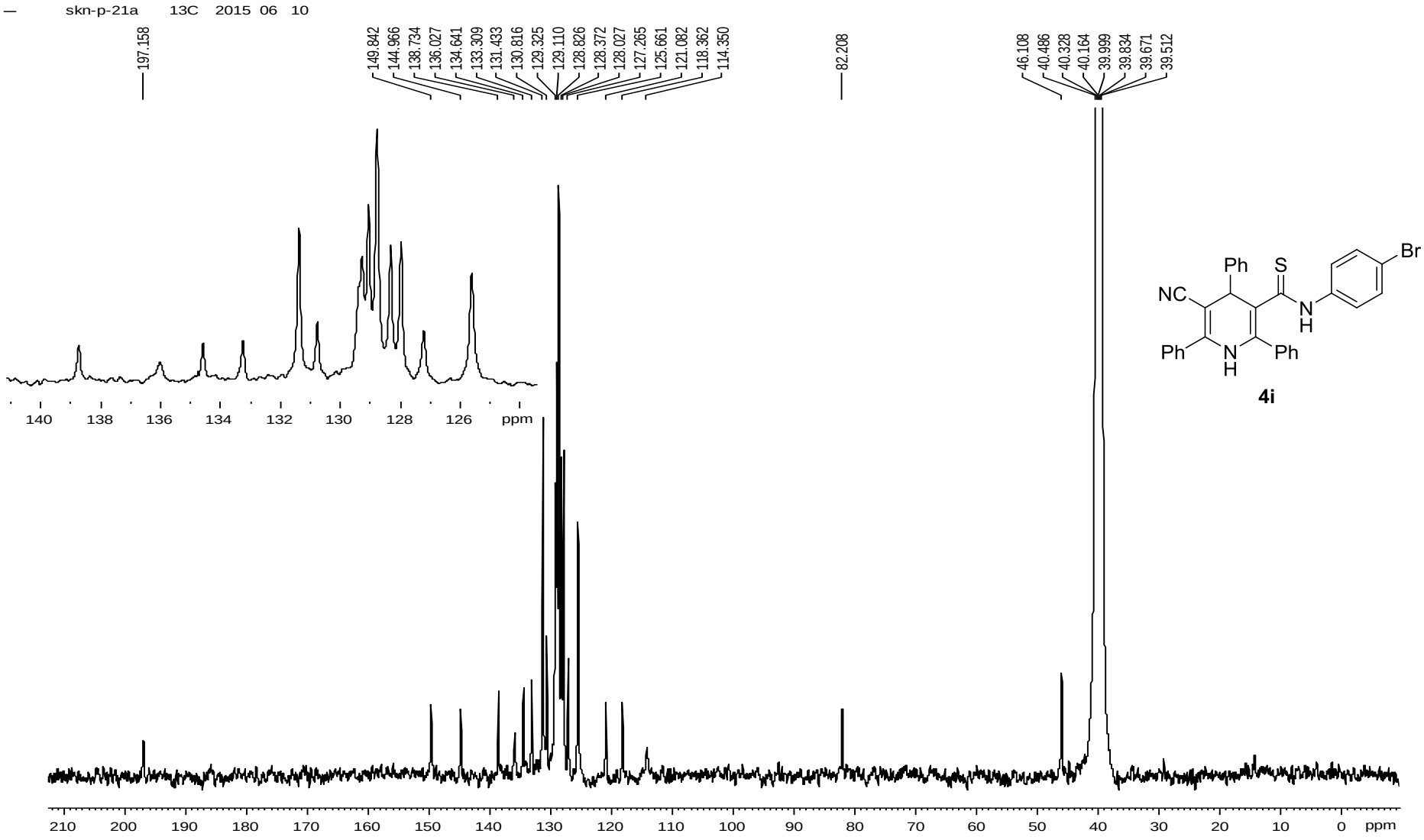
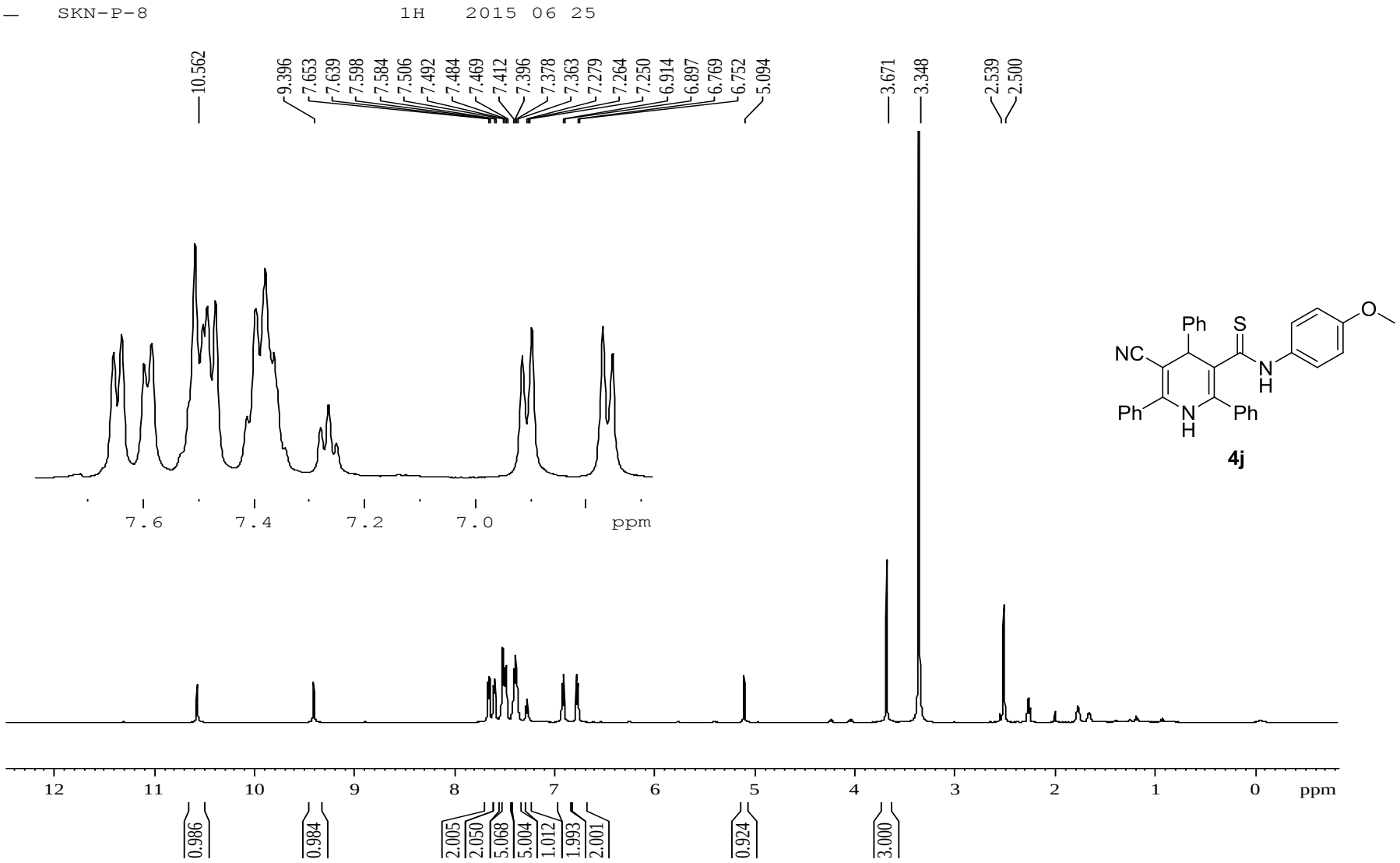
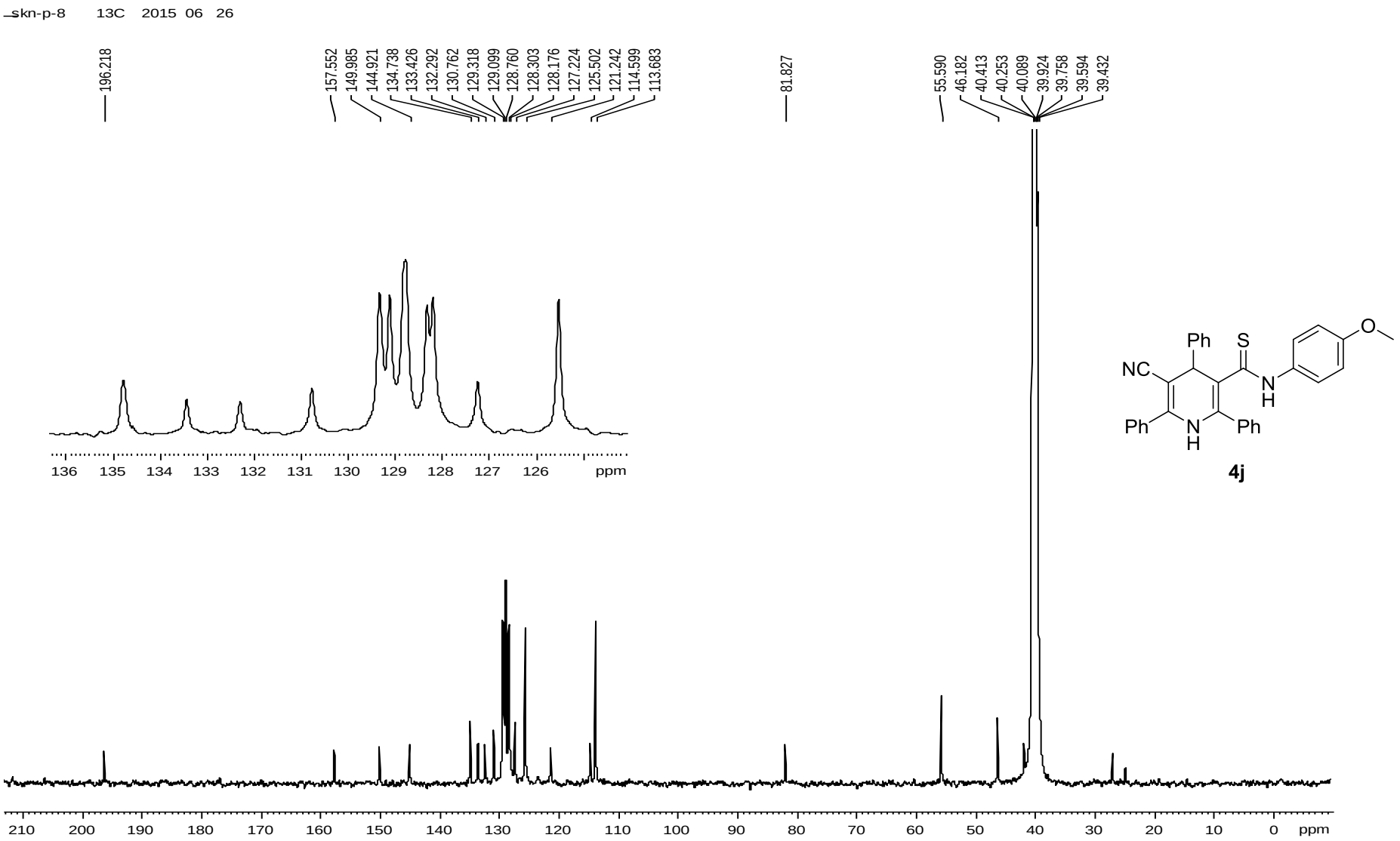
7.640
7.629
7.603
7.591
7.513
7.500
7.477
7.462
7.394
7.380
7.365
7.346
7.333
7.282
7.266
7.142
7.129
5.050
3.351
3.335
3.328
2.500
7.7 7.6 7.5 7.4 7.3 7.2 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.980
1.000
1.847
2.038
2.926
2.051
5.044
3.009
1.812
0.947
Ph
S
NC
N
H
Cl
Ph
N
H
Ph
4h

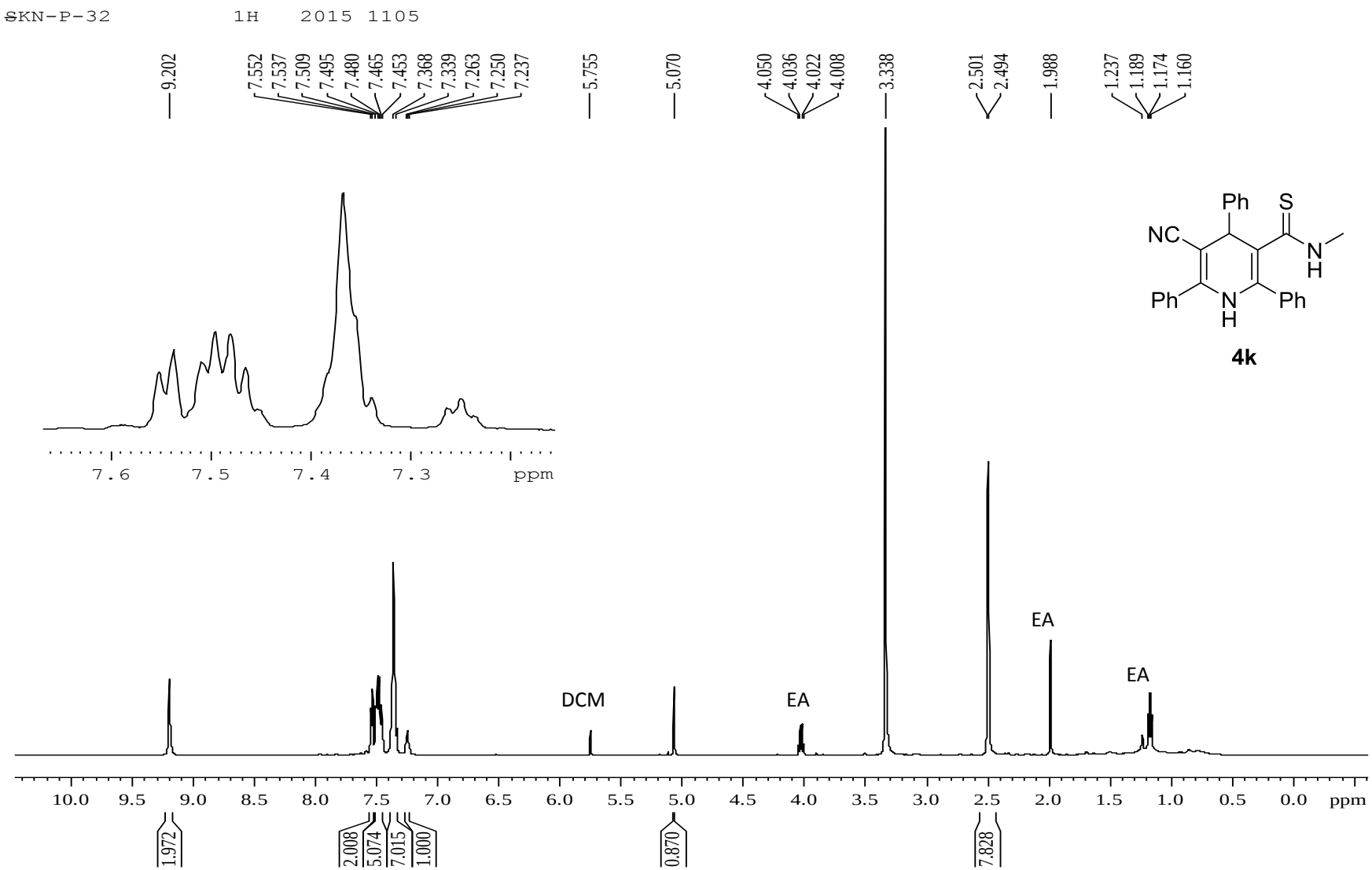

KN-P-04-1 13C 1D 2014 12 2
197.185
149.879
145.007
138.339
136.018
134.672
133.331
130.861
130.139
129.482
129.367
129.154
128.867
128.550
128.412
128.063
127.297
125.417
121.144
114.301
82.207
46.122
40.504
40.339
40.173
40.006
39.840
39.674
39.508
133 132 131 130 129 128 127 126 ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Cl
Ph
N
H
Ph
4h


skn-p-21a 2015 06 10
10.731
9.534
7.622
7.600
7.587
7.523
7.512
7.497
7.475
7.460
7.389
7.379
7.342
7.278
7.264
7.250
7.089
5.047
3.332
2.500
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.978
1.000
1.929
2.051
3.041
2.051
7.009
1.039
1.827
0.939
NC
Ph
S
N
H
Br
Ph
N
H
Ph
4i


skn-p-21a 13C 2015 06 10
197.158
149.842
144.966
138.734
136.027
134.641
133.309
131.433
130.816
129.325
129.110
128.826
128.372
128.027
127.265
125.661
121.082
118.362
114.350
82.208
46.108
40.486
40.328
40.164
39.999
39.834
39.671
39.512
140 138 136 134 132 130 128 126 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Br
Ph
N
H
Ph
4i

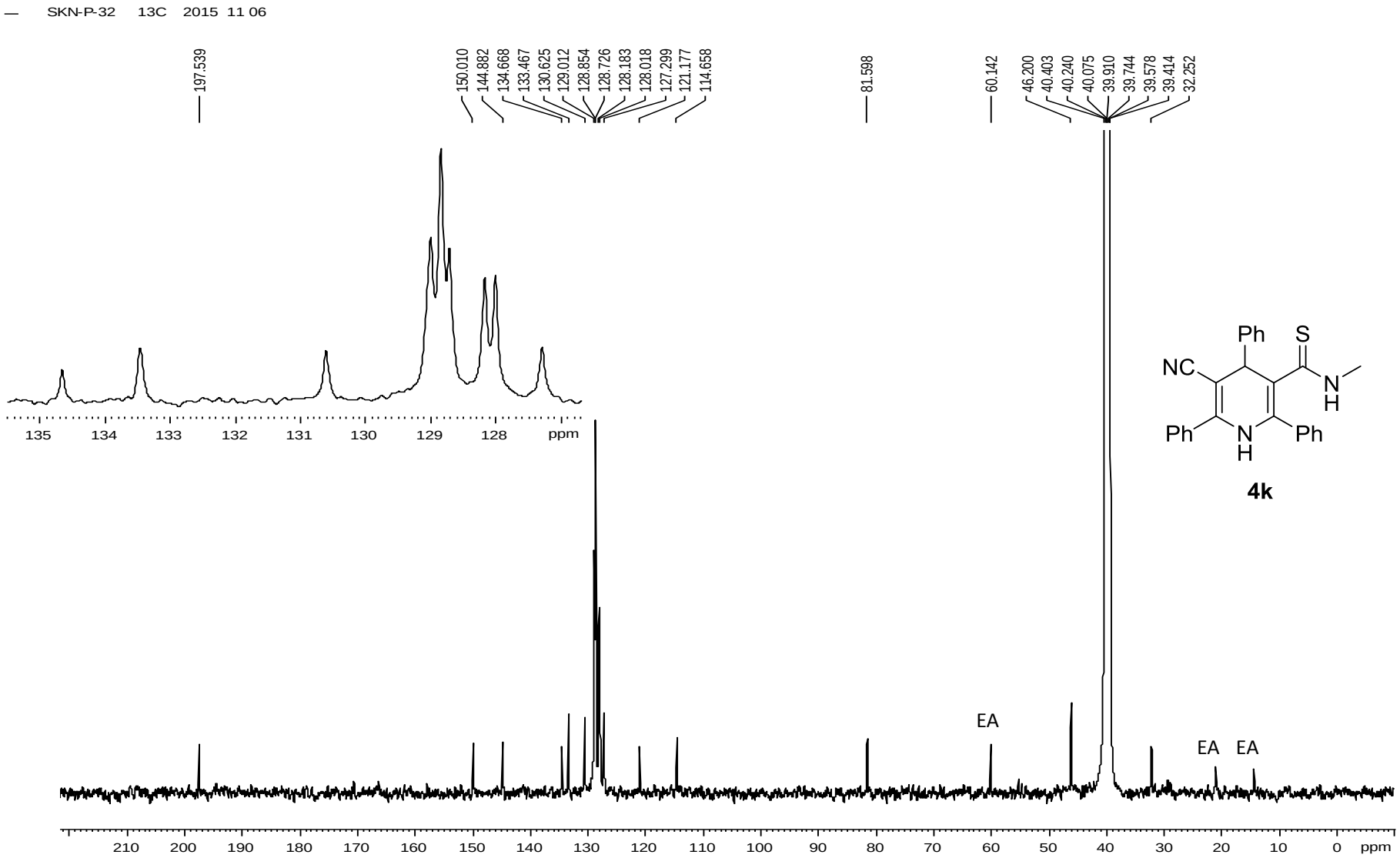

SKN-P-8 1H 2015 06 25
10.562
9.396
7.653
7.639
7.598
7.584
7.506
7.492
7.484
7.469
7.412
7.396
7.378
7.363
7.279
7.264
7.250
6.914
6.897
6.769
6.752
5.094
3.671
3.348
2.539
2.500
7.6
7.4
7.2
7.0
ppm
NC
Ph
S
N
H
O
Ph
N
H
Ph
4j
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.986
0.984
2.005
2.050
5.068
5.004
1.012
1.993
2.001
0.924
3.000

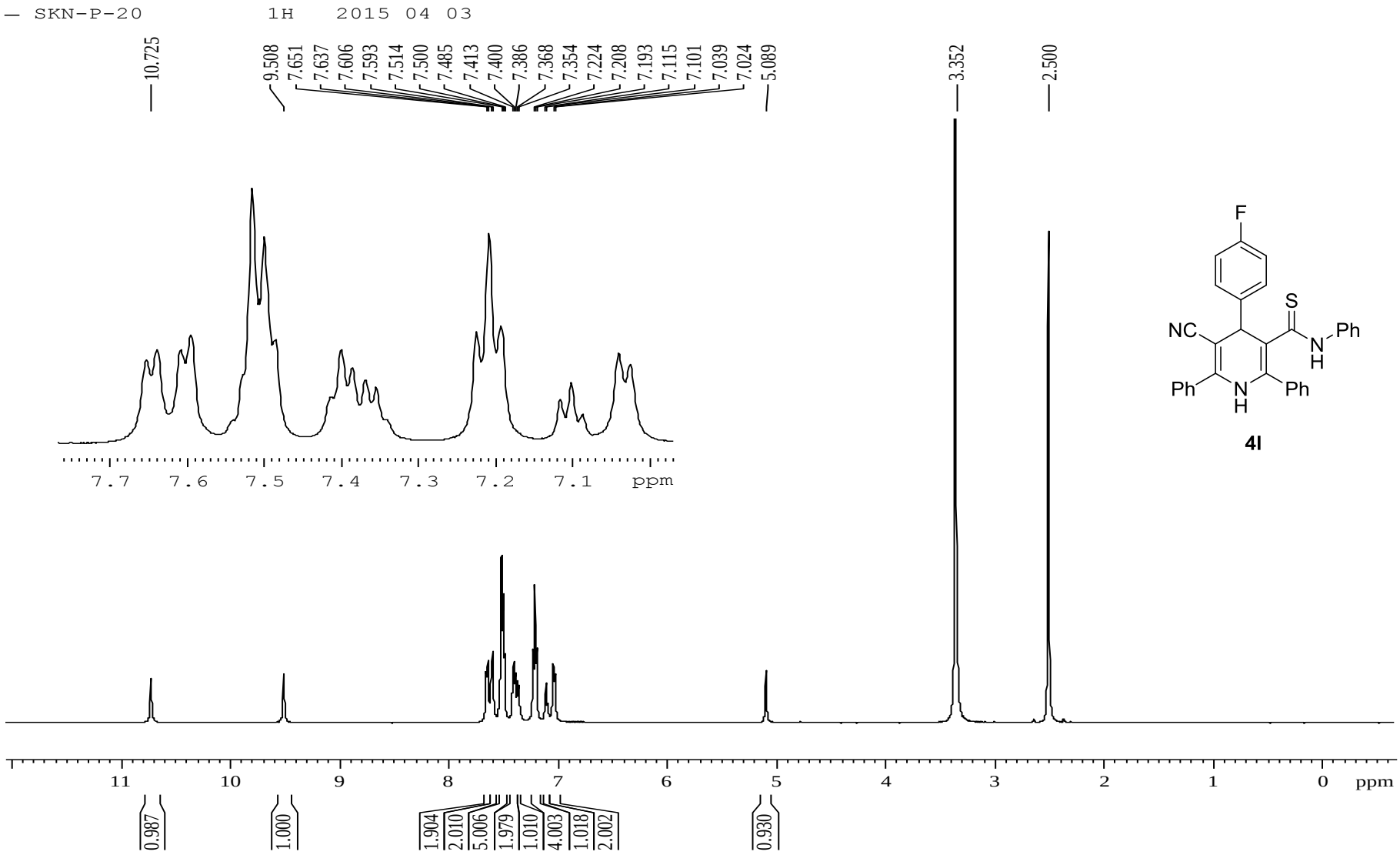

_skn-p-8 13C 2015 06 26
196.218
157.552
149.985
144.921
134.738
133.426
132.292
130.762
129.318
129.099
128.760
128.303
128.176
127.224
125.502
121.242
114.599
113.683
81.827
55.590
46.182
40.413
40.253
40.089
39.924
39.758
39.594
39.432
136 135 134 133 132 131 130 129 128 127 126 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
O
Ph
N
H
Ph
4j


SKN-P-32 1H 2015 1105
9.202
7.552
7.537
7.509
7.495
7.480
7.465
7.453
7.368
7.339
7.263
7.250
7.237
5.755
5.070
4.050
4.036
4.022
4.008
3.338
2.501
2.494
1.988
1.237
1.189
1.174
1.160
7.6
7.5
7.4
7.3
ppm
DCM
EA
EA
EA
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.972
2.008
5.074
7.015
1.000
0.870
7.828

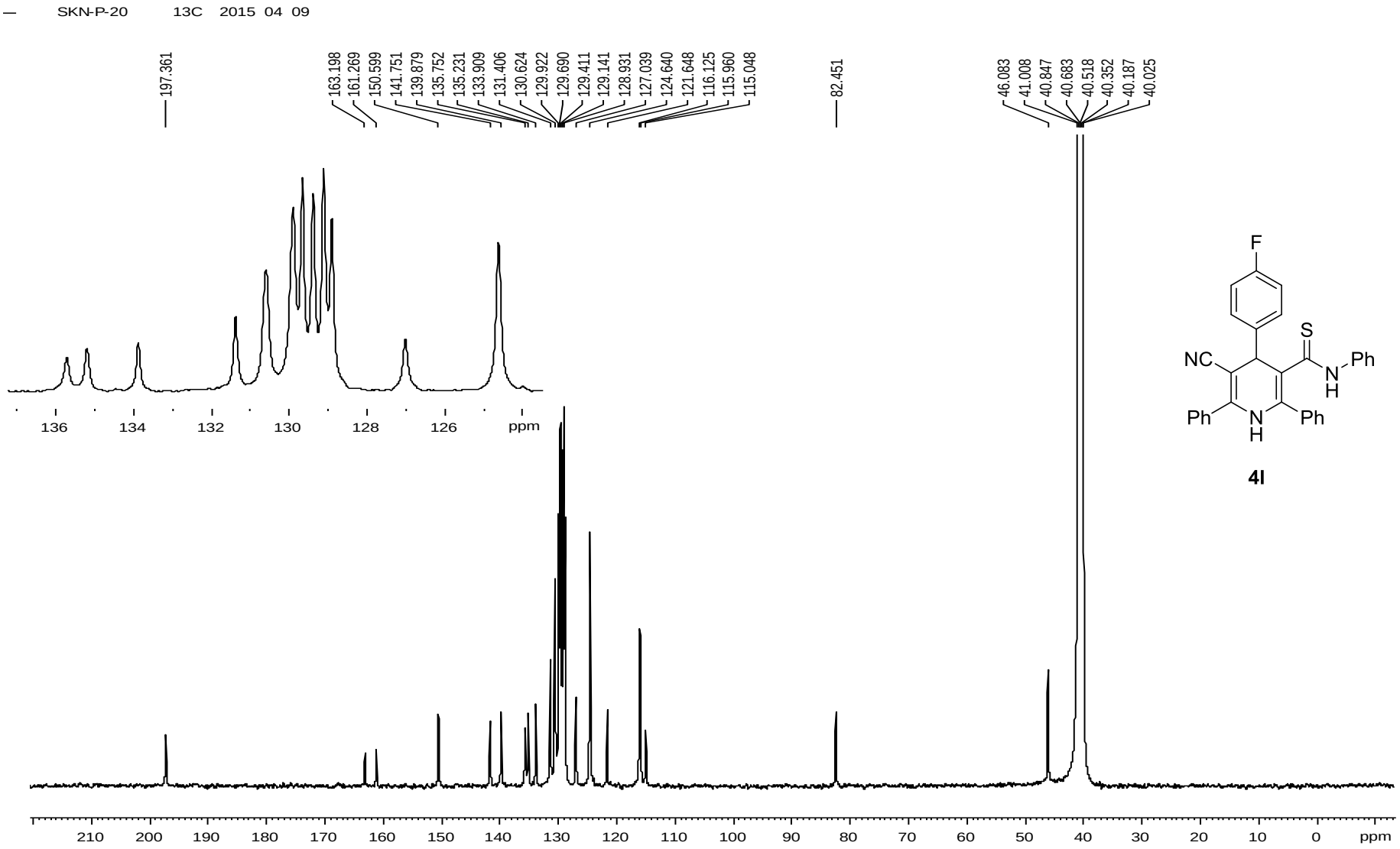
Ph
S
NC
N
H
Ph
N
H
Ph

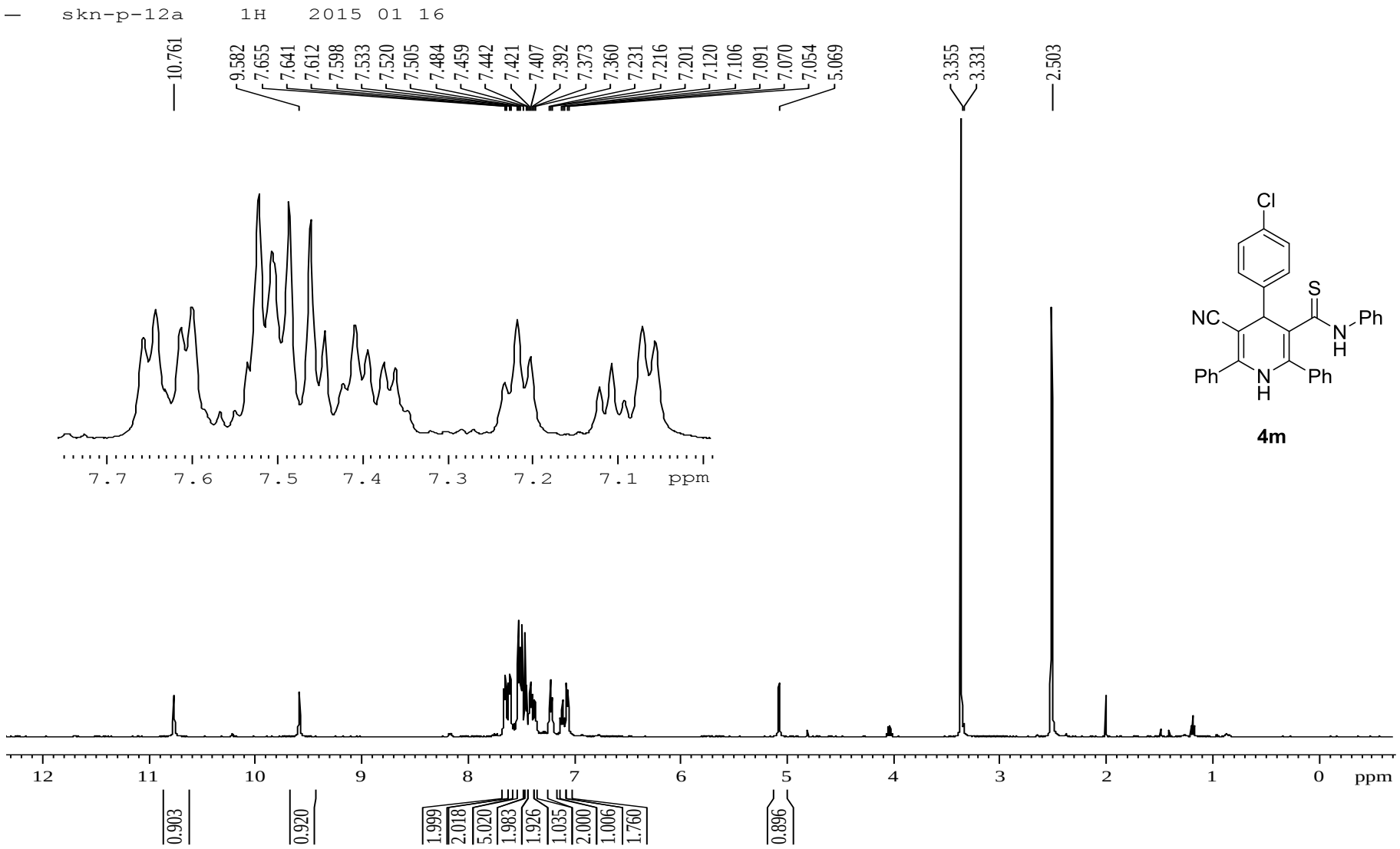
4k


SKN-P-32 13C 2015 11 06
197.539
150.010
144.882
134.668
133.467
130.625
129.012
128.854
128.726
128.183
128.018
127.299
121.177
114.658
81.598
60.142
46.200
40.403
40.240
40.075
39.910
39.744
39.578
39.414
32.252
135 134 133 132 131 130 129 128 ppm
EA
EA EA
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Ph
N
H
Ph
4k

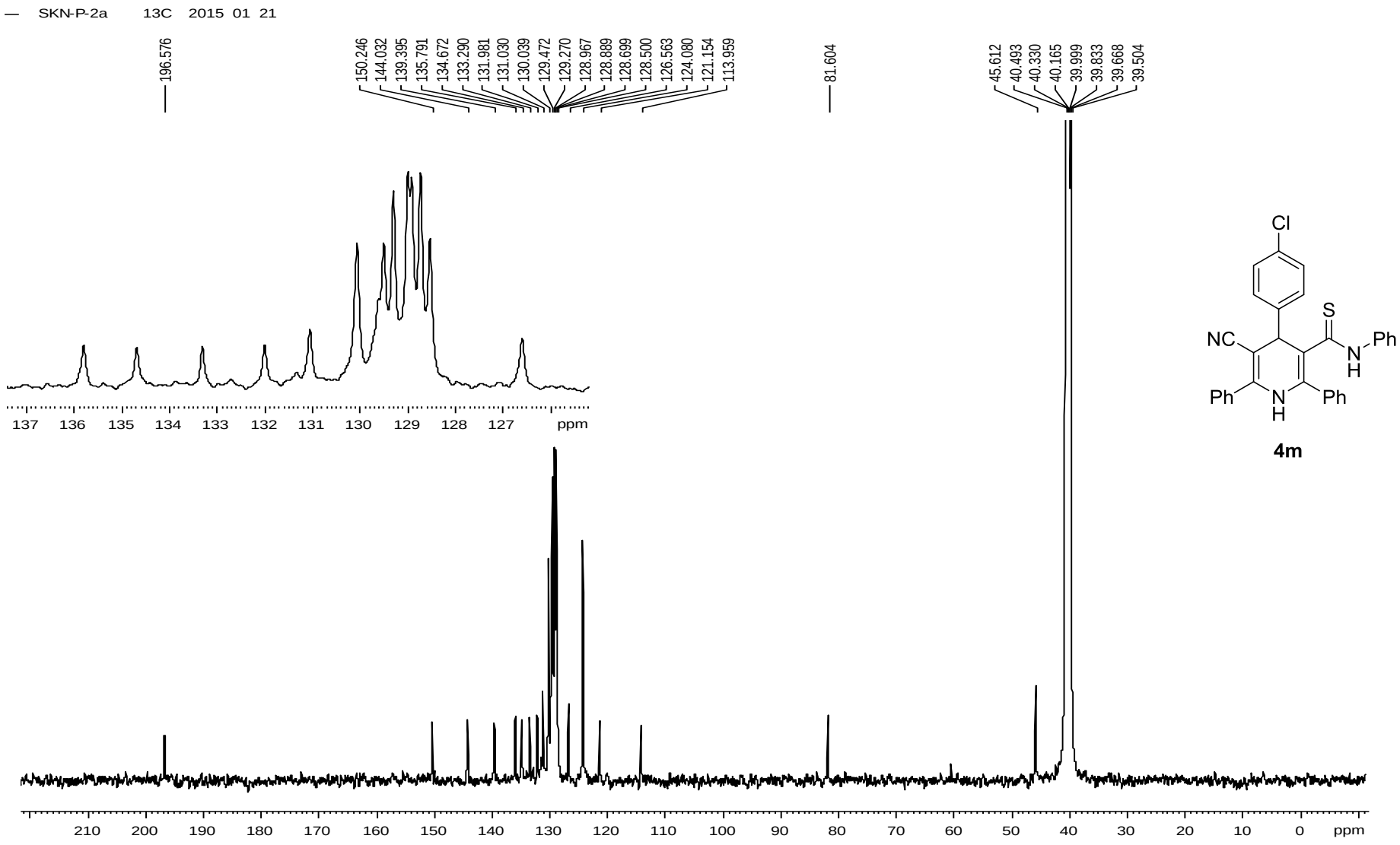

SKN-P-20 1H 2015 04 03
10.725
9.508
7.651
7.637
7.606
7.593
7.514
7.500
7.485
7.413
7.400
7.386
7.368
7.354
7.224
7.208
7.193
7.115
7.101
7.039
7.024
5.089
3.352
2.500
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.987
1.000
1.904
2.010
5.006
1.979
1.010
4.003
1.018
2.002
0.930
F
S
NC
N
H
Ph
Ph
N
H
Ph

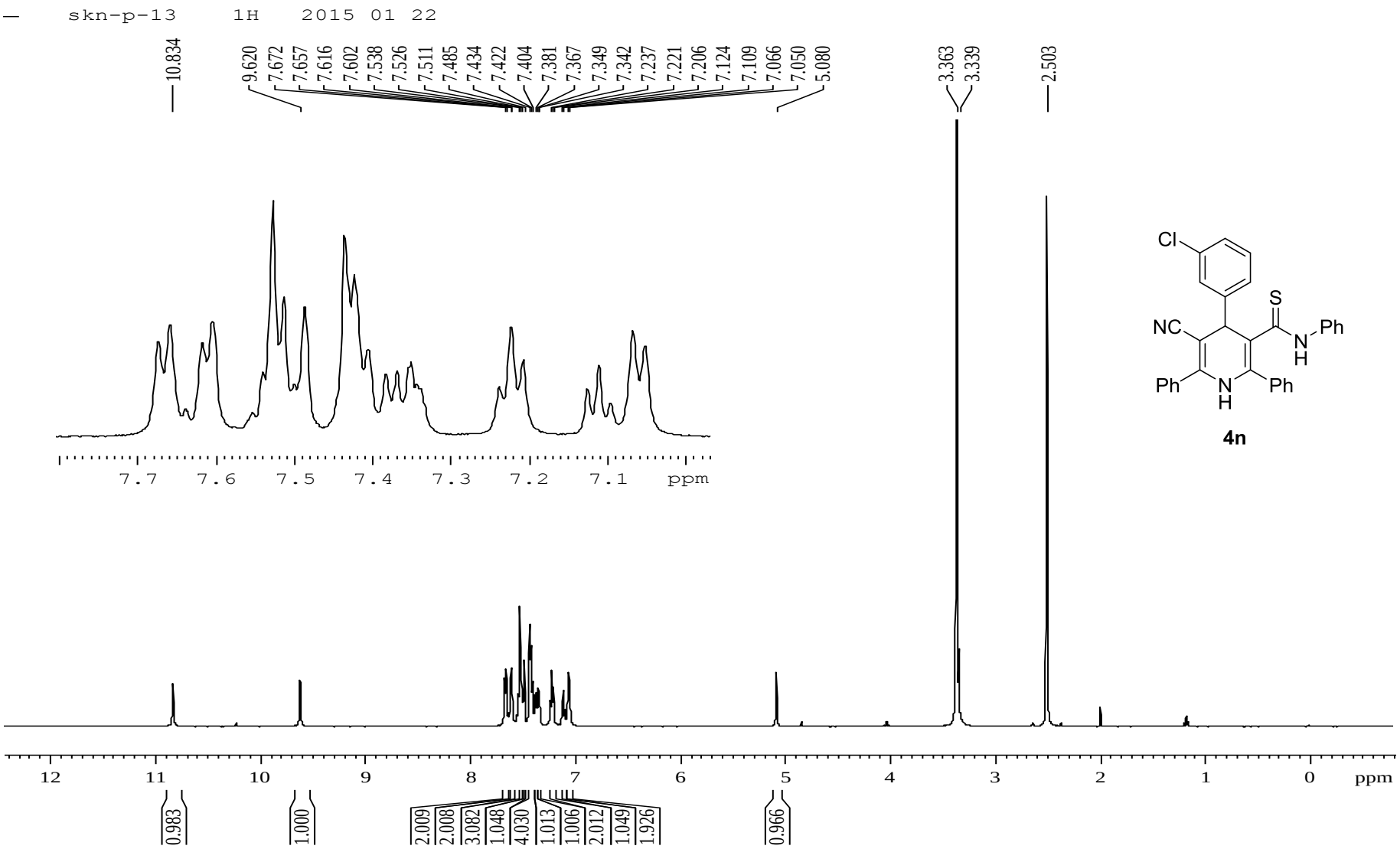
4l

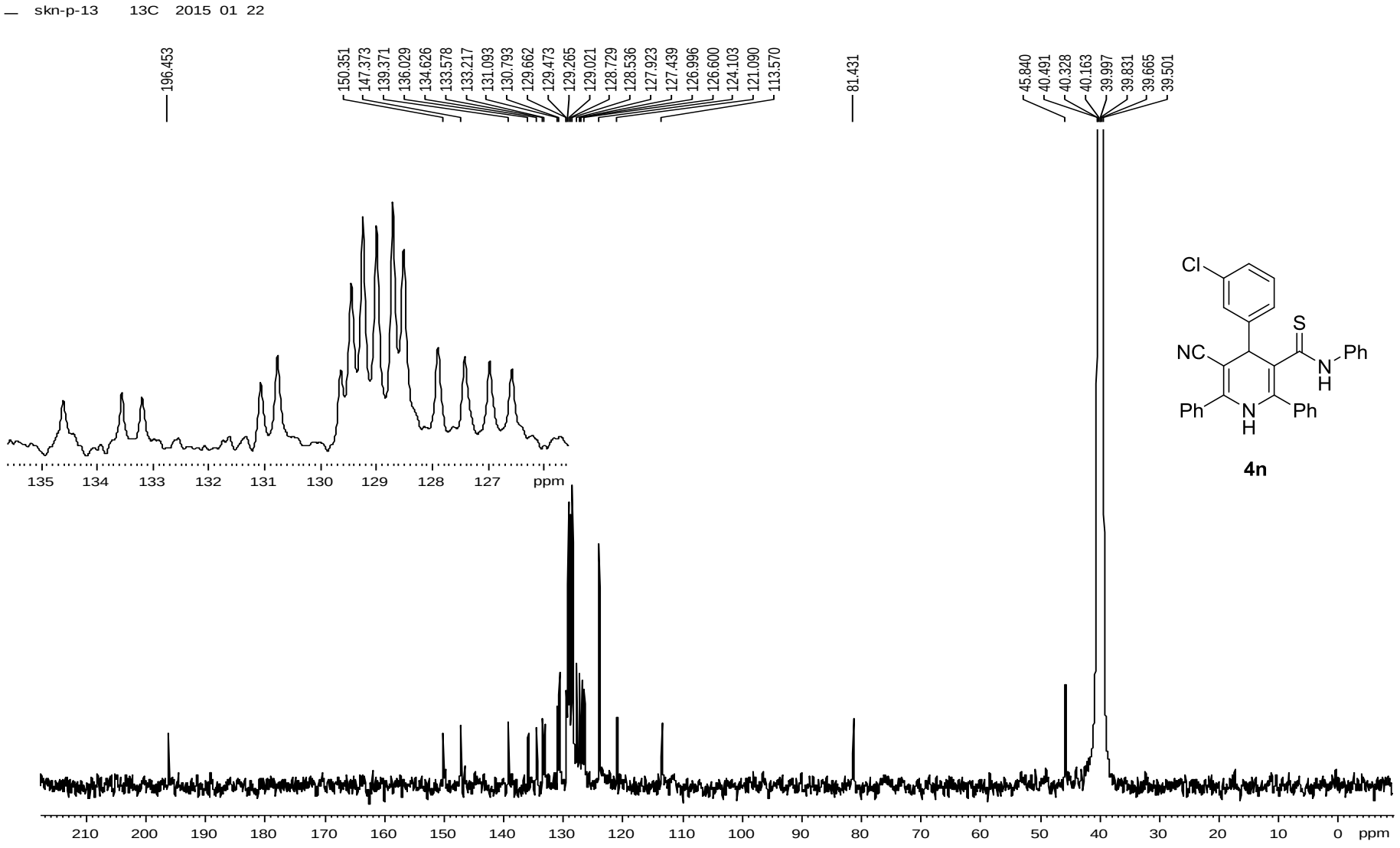

SKN-P-20 13C 2015 04 09
197.361
163.198
161.269
150.599
141.751
139.879
135.752
135.231
133.909
131.406
130.624
129.922
129.690
129.411
129.141
128.931
127.039
124.640
121.648
116.125
115.960
115.048
82.451
46.083
41.008
40.847
40.683
40.518
40.352
40.187
40.025
136
134
132
130
128
126
ppm
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
F
S
NC
N
H
Ph
Ph
N
H
Ph
4l


skn-p-12a 1H 2015 01 16
10.761
9.582
7.655
7.641
7.612
7.598
7.533
7.520
7.505
7.484
7.459
7.442
7.421
7.407
7.392
7.373
7.360
7.231
7.216
7.201
7.120
7.106
7.091
7.070
7.054
5.069
3.355
3.331
2.503
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.903
0.920
1.999
2.018
5.020
1.983
1.926
1.035
2.000
1.006
1.760
0.896
Cl
S
NC
N
H
Ph
Ph
N
H
Ph

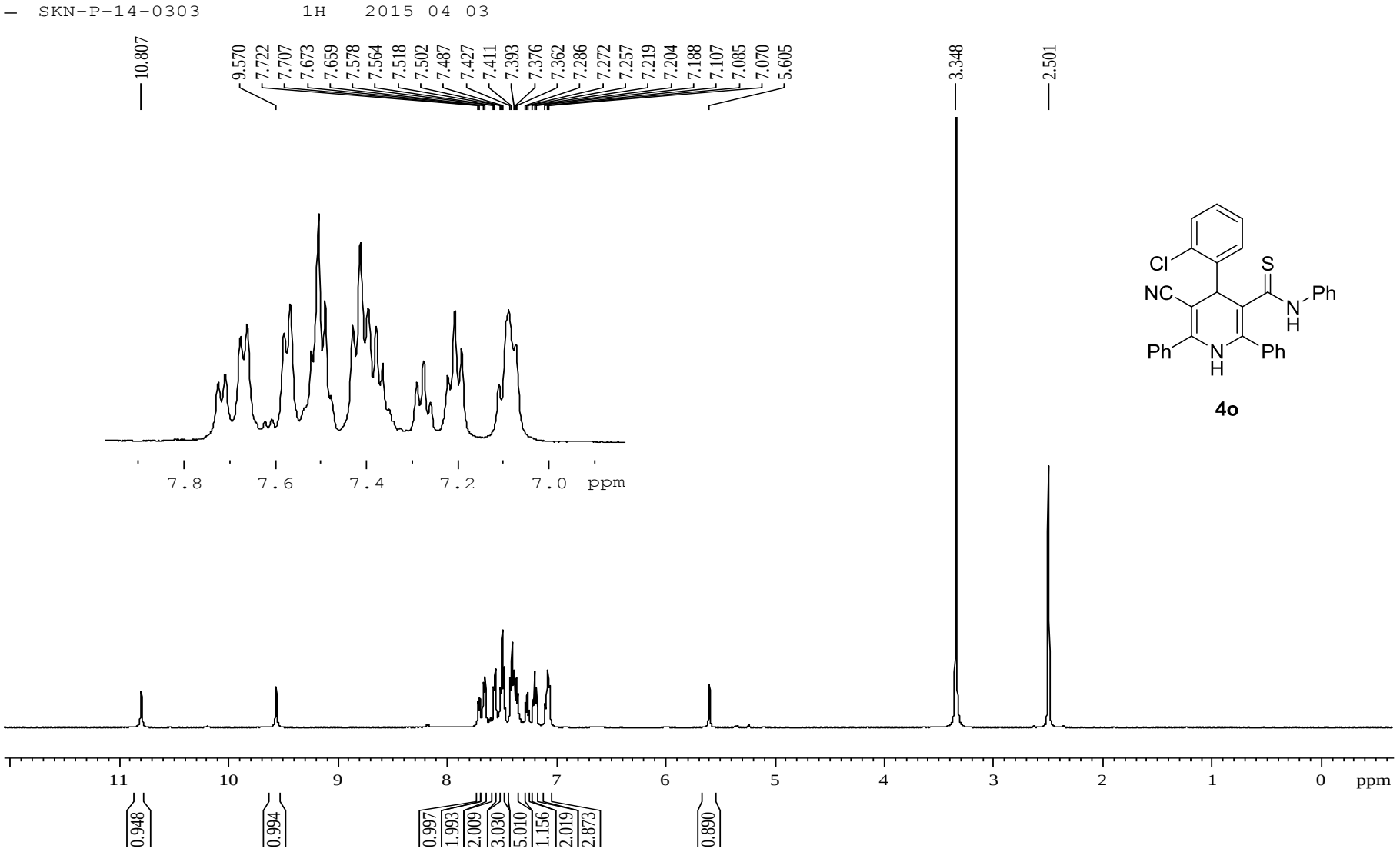
4m


SKN-P-2a 13C 2015 01 21
196.576
150.246
144.032
139.395
135.791
134.672
133.290
131.981
131.030
130.039
129.472
129.270
128.967
128.889
128.699
128.500
126.563
124.080
121.154
113.959
81.604
45.612
40.493
40.330
40.165
39.999
39.833
39.668
39.504
137 136 135 134 133 132 131 130 129 128 127 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Cl
S
NC
N
H
Ph
Ph
N
H
Ph
4m

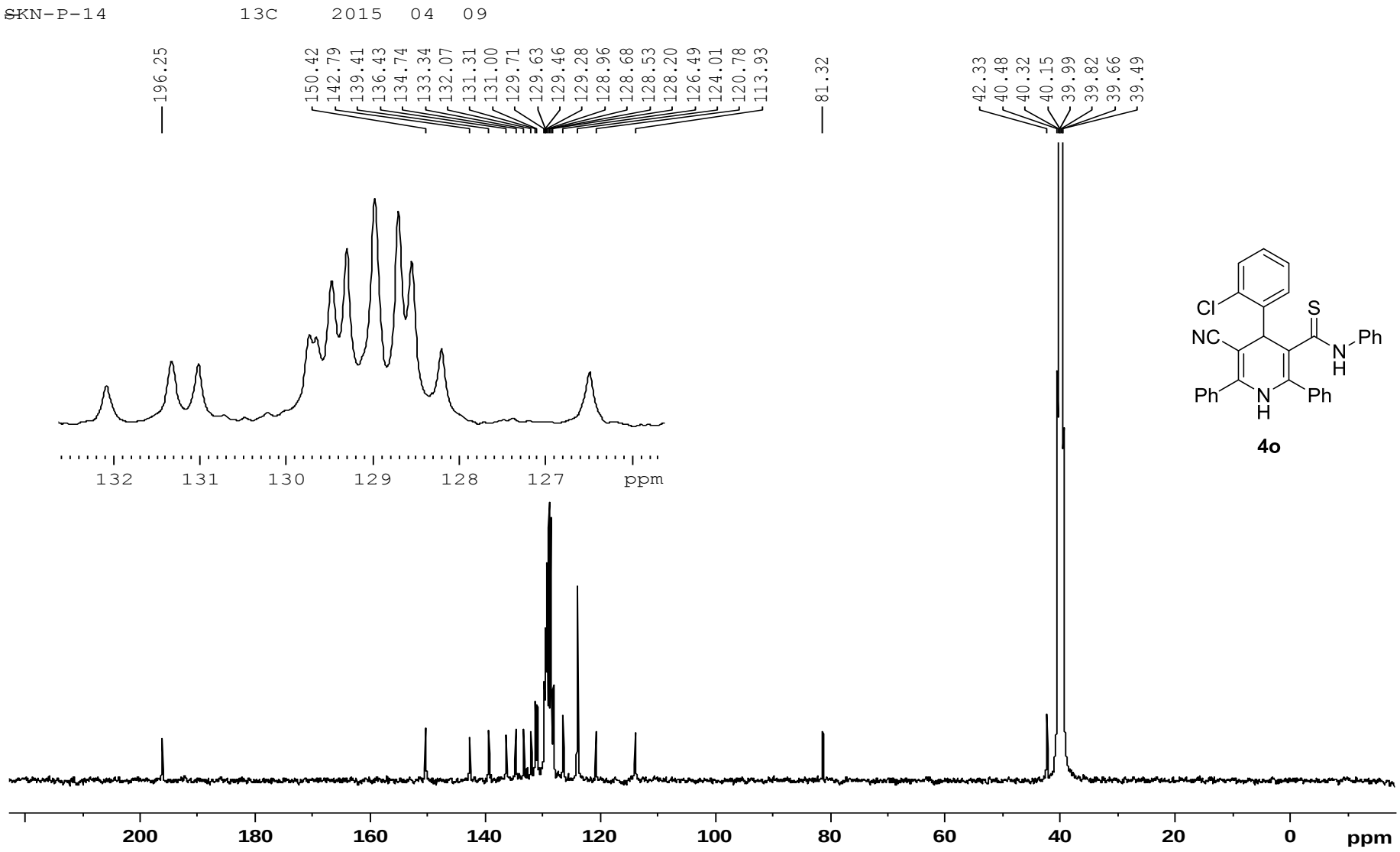

skn-p-13 1H 2015 01 22
10.834
9.620
7.672
7.657
7.616
7.602
7.538
7.526
7.511
7.485
7.434
7.422
7.404
7.381
7.367
7.349
7.342
7.237
7.221
7.206
7.124
7.109
7.066
7.050
5.080
3.363
3.339
2.503
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.983
1.000
2.009
2.008
3.082
1.048
4.030
1.013
1.006
2.012
1.049
1.926
0.966
Cl
S
NC
N
H
Ph
Ph
N
H
Ph
4n

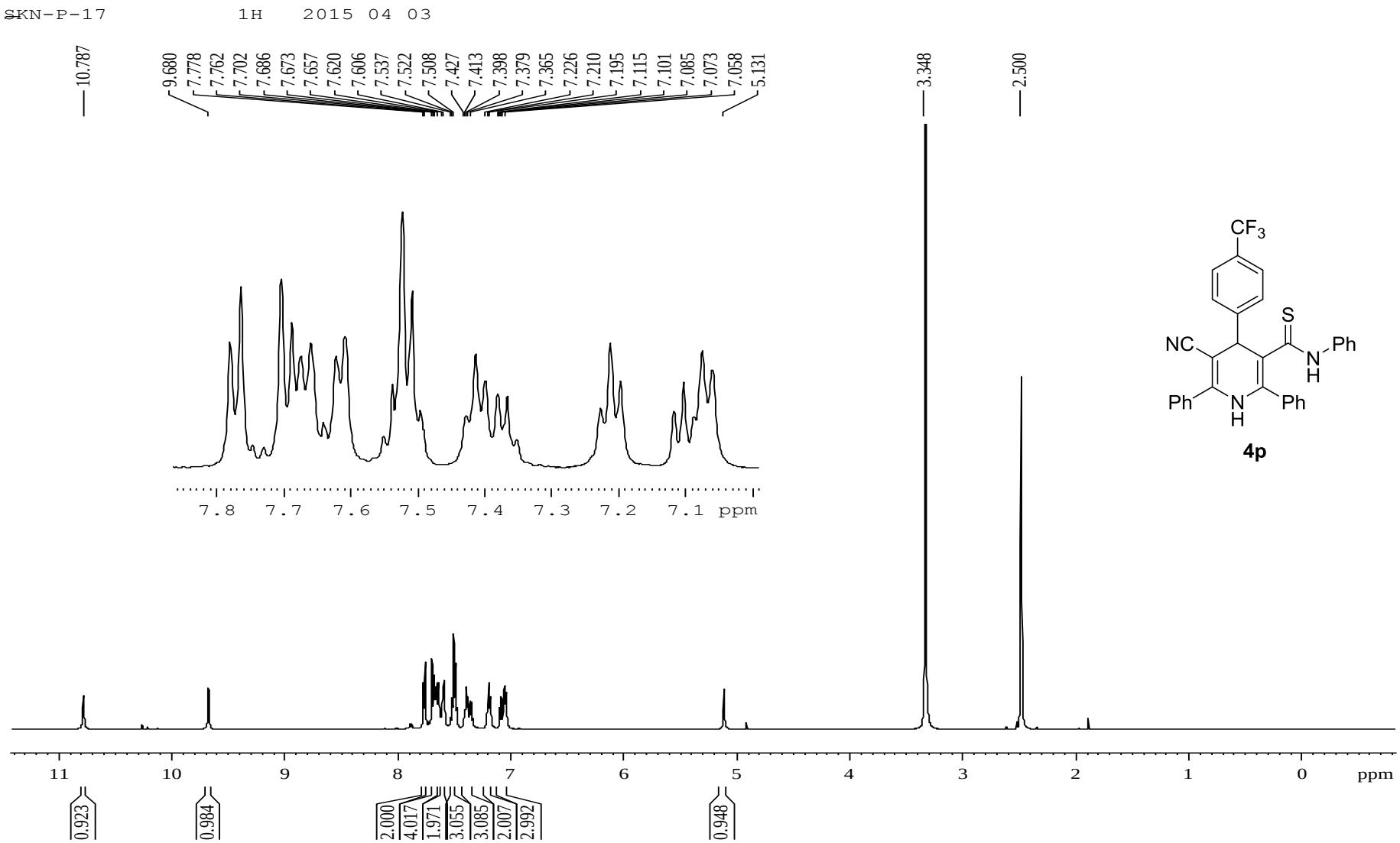

skn-p-13 13C 2015 01 22
196.453
150.351
147.373
139.371
136.029
134.626
133.578
133.217
131.093
130.793
129.662
129.473
129.265
129.021
128.729
128.536
127.923
127.439
126.996
126.600
124.103
121.090
113.570
81.431
45.840
40.491
40.328
40.163
39.997
39.831
39.665
39.501
135 134 133 132 131 130 129 128 127 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Cl
S
NC
N
H
Ph
Ph
N
H
Ph

4n


SKN-P-14-0303 1H 2015 04 03
10.807
9.570
7.722
7.707
7.673
7.659
7.578
7.564
7.518
7.502
7.487
7.427
7.411
7.393
7.376
7.362
7.286
7.272
7.257
7.219
7.204
7.188
7.107
7.085
7.070
5.605
3.348
2.501
7.8
7.6
7.4
7.2
7.0
ppm
Cl
S
NC
N
H
Ph
Ph
N
H
Ph
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.948
0.994
0.997
1.993
2.009
3.030
5.010
1.156
2.019
2.873
0.890

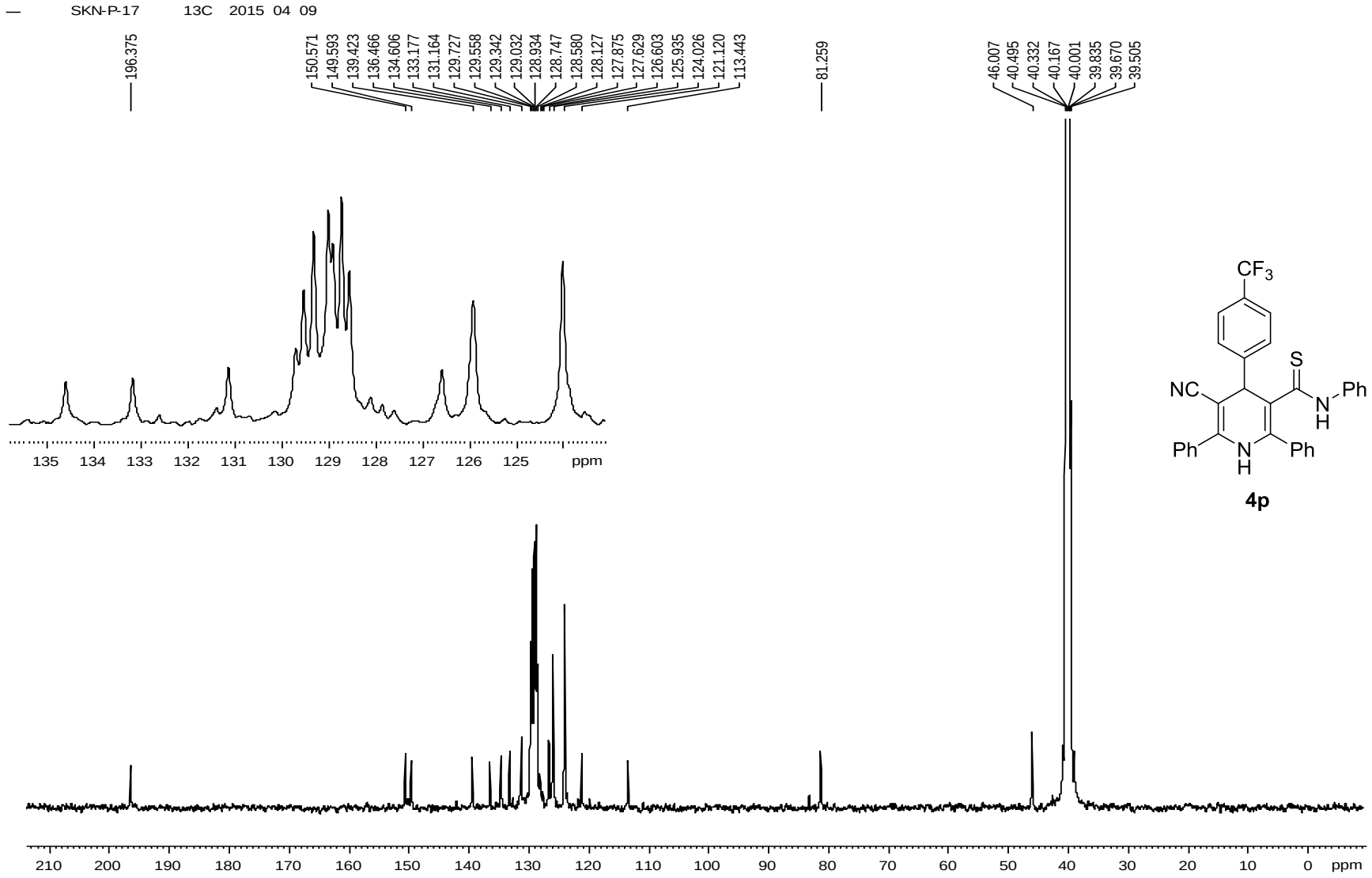
4o


SKN-P-14 13C 2015 04 09
196.25
150.42
142.79
139.41
136.43
134.74
133.34
132.07
131.31
131.00
129.71
129.63
129.46
129.28
128.96
128.68
128.53
128.20
126.49
124.01
120.78
113.93
81.32
42.33
40.48
40.32
40.15
39.99
39.82
39.66
39.49
132 131 130 129 128 127 ppm
Cl
S
NC
Ph
N
H
Ph
N
H
Ph
4o
200 180 160 140 120 100 80 60 40 20 0 ppm

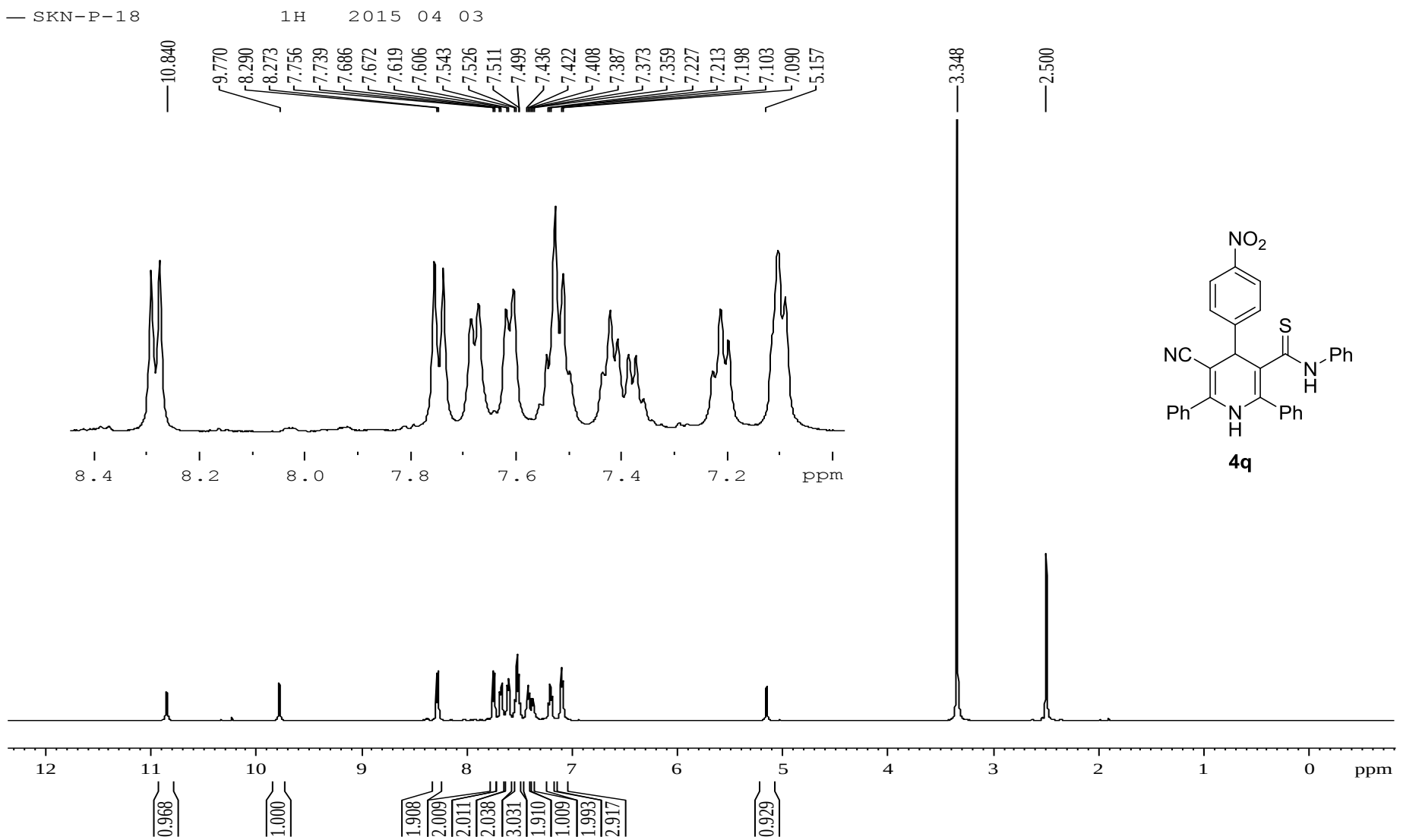

SKN-P-17 1H 2015 04 03
10.787
9.680
7.778
7.762
7.702
7.686
7.673
7.657
7.620
7.606
7.537
7.522
7.508
7.427
7.413
7.398
7.379
7.365
7.226
7.210
7.195
7.115
7.101
7.085
7.073
7.058
5.131
3.348
2.500
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.923
0.984
2.000
4.017
1.971
3.055
3.085
2.007
2.992
0.948

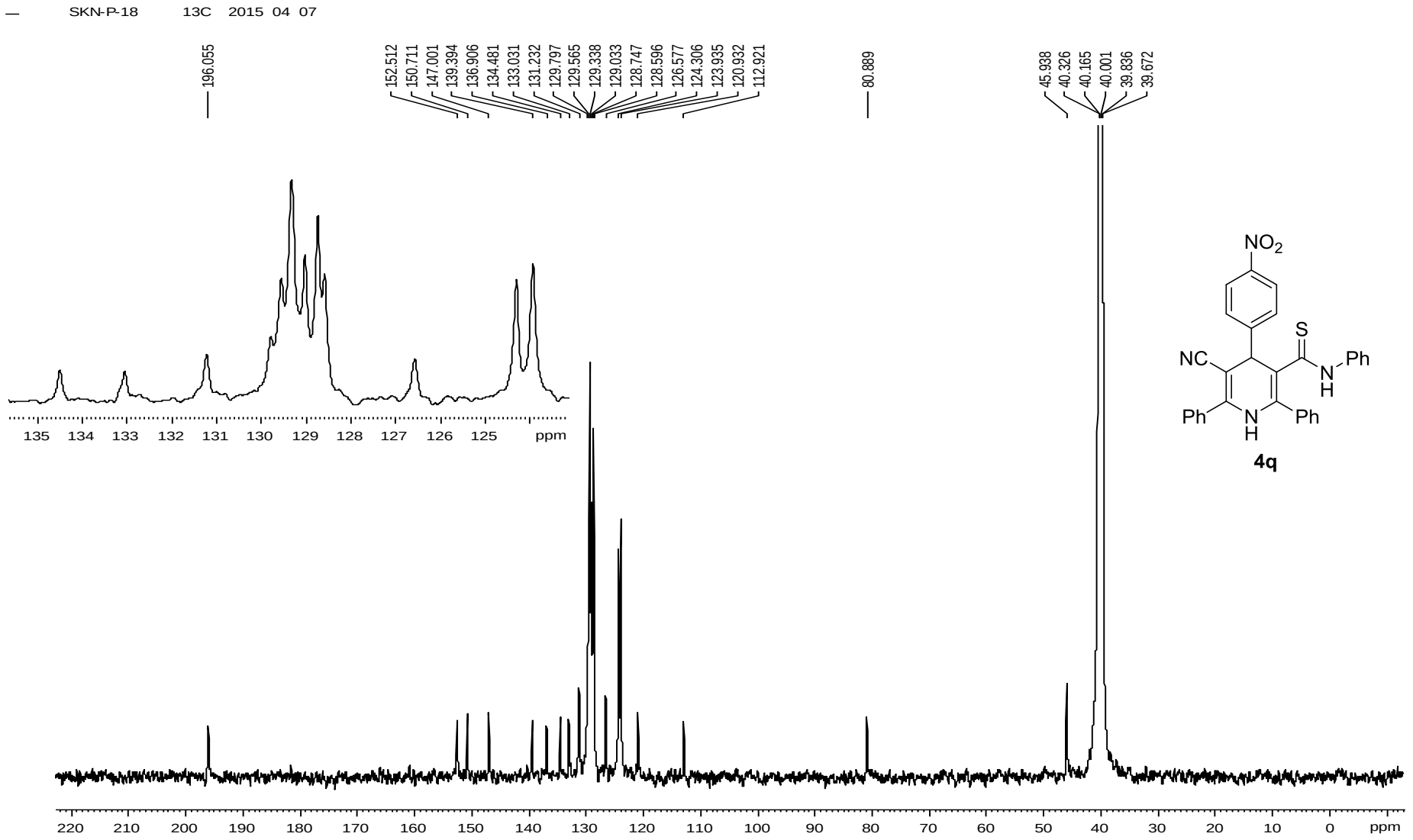
CF3
S
NC
N
H
Ph
Ph
N
H
Ph

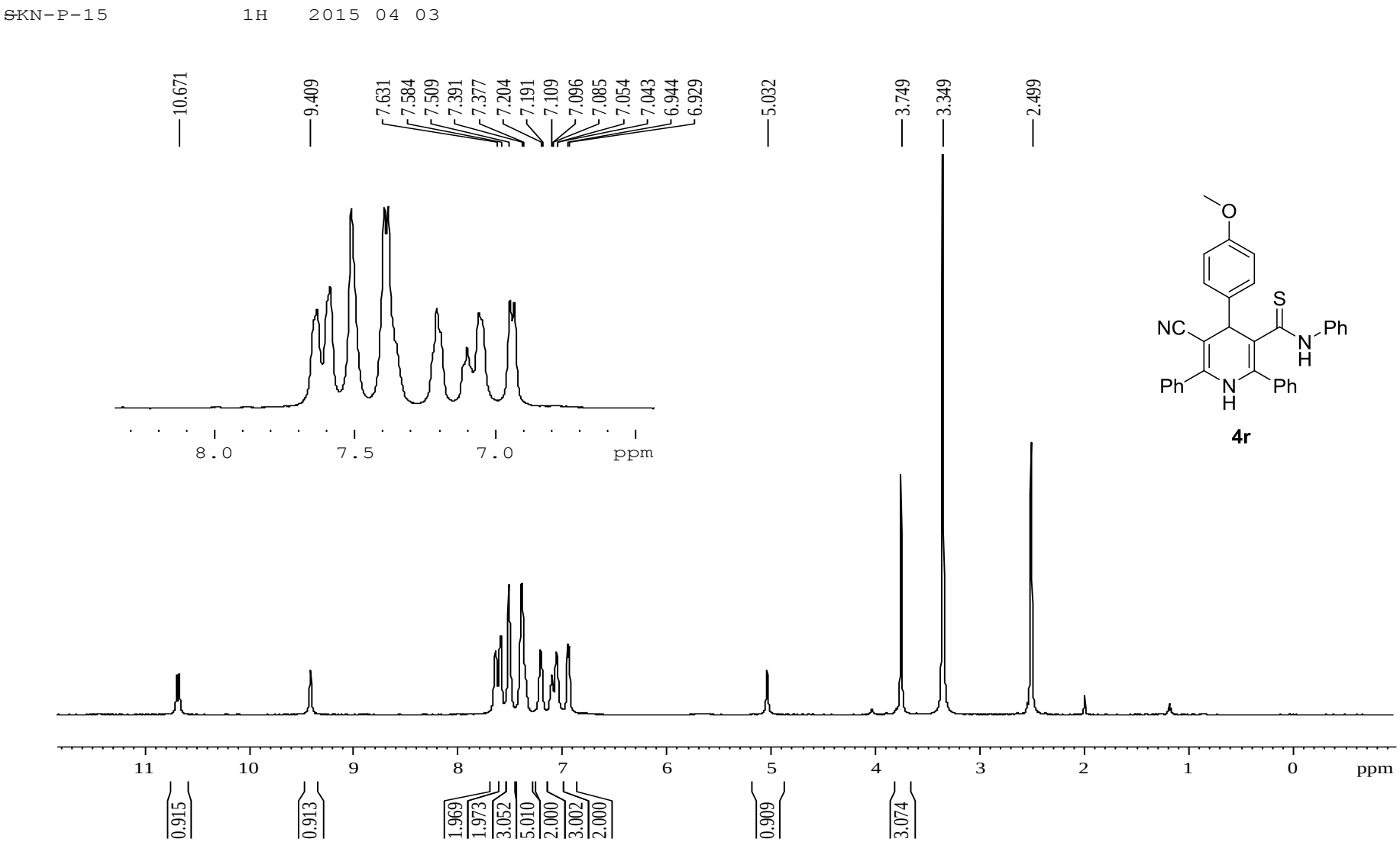
4p

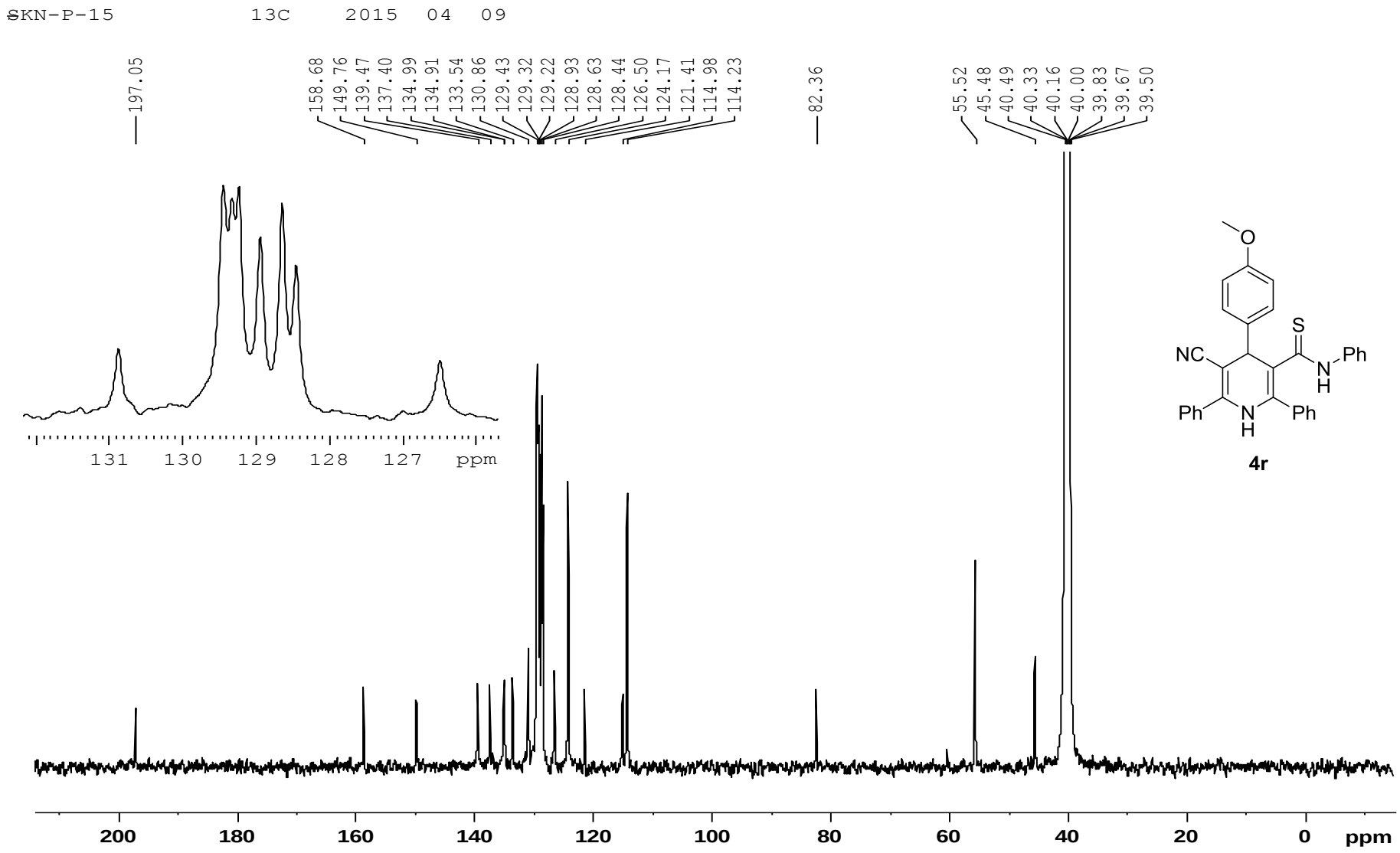

SKN-P-17 13C 2015 04 09
196.375
150.571
149.593
139.423
136.466
134.606
133.177
131.164
129.727
129.558
129.342
129.032
128.934
128.747
128.580
128.127
127.875
127.629
126.603
125.935
124.026
121.120
113.443
81.259
46.007
40.495
40.332
40.167
40.001
39.835
39.670
39.505
135 134 133 132 131 130 129 128 127 126 125 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
CF3
S
NC
N
H
Ph
Ph
N
H
Ph

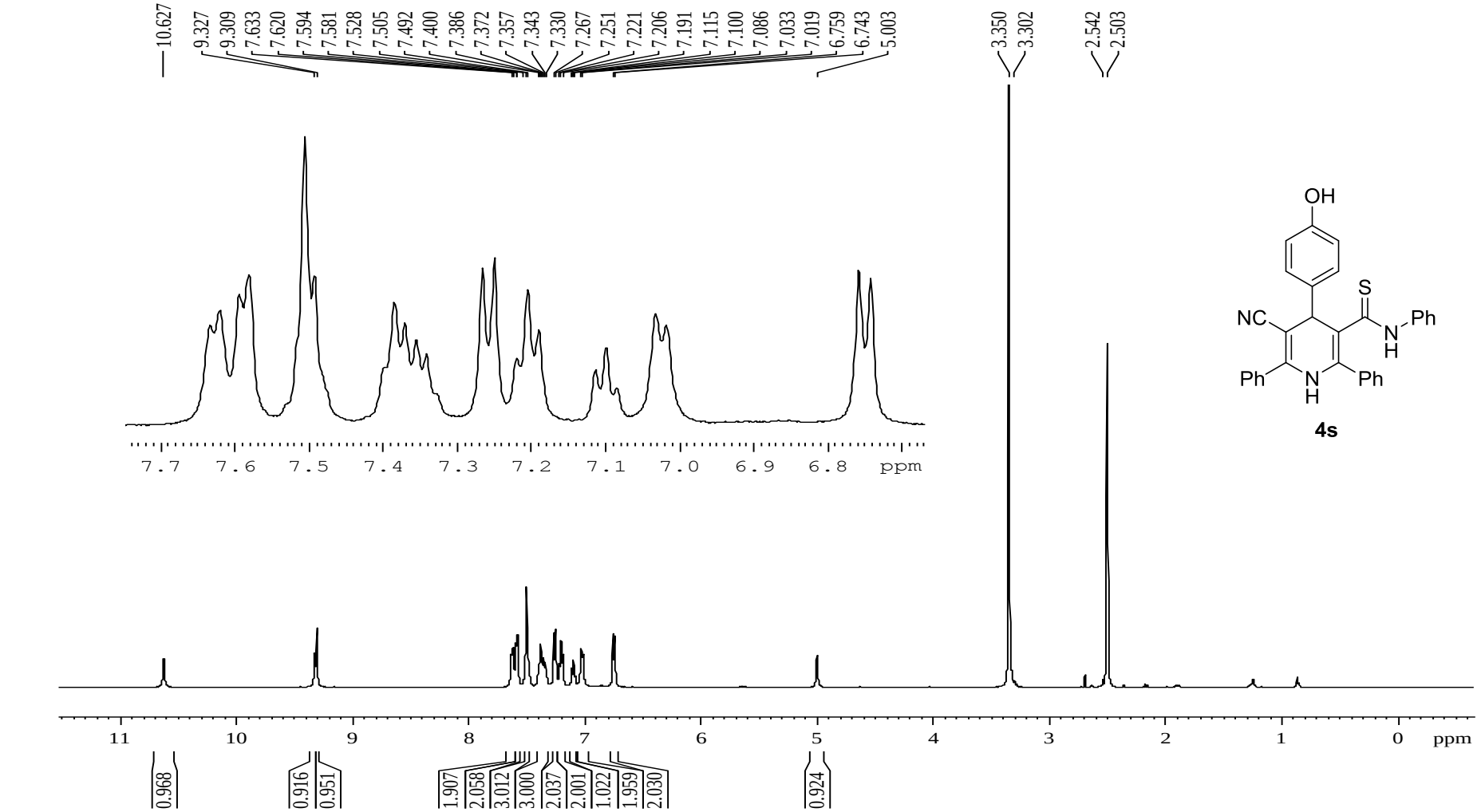
4p

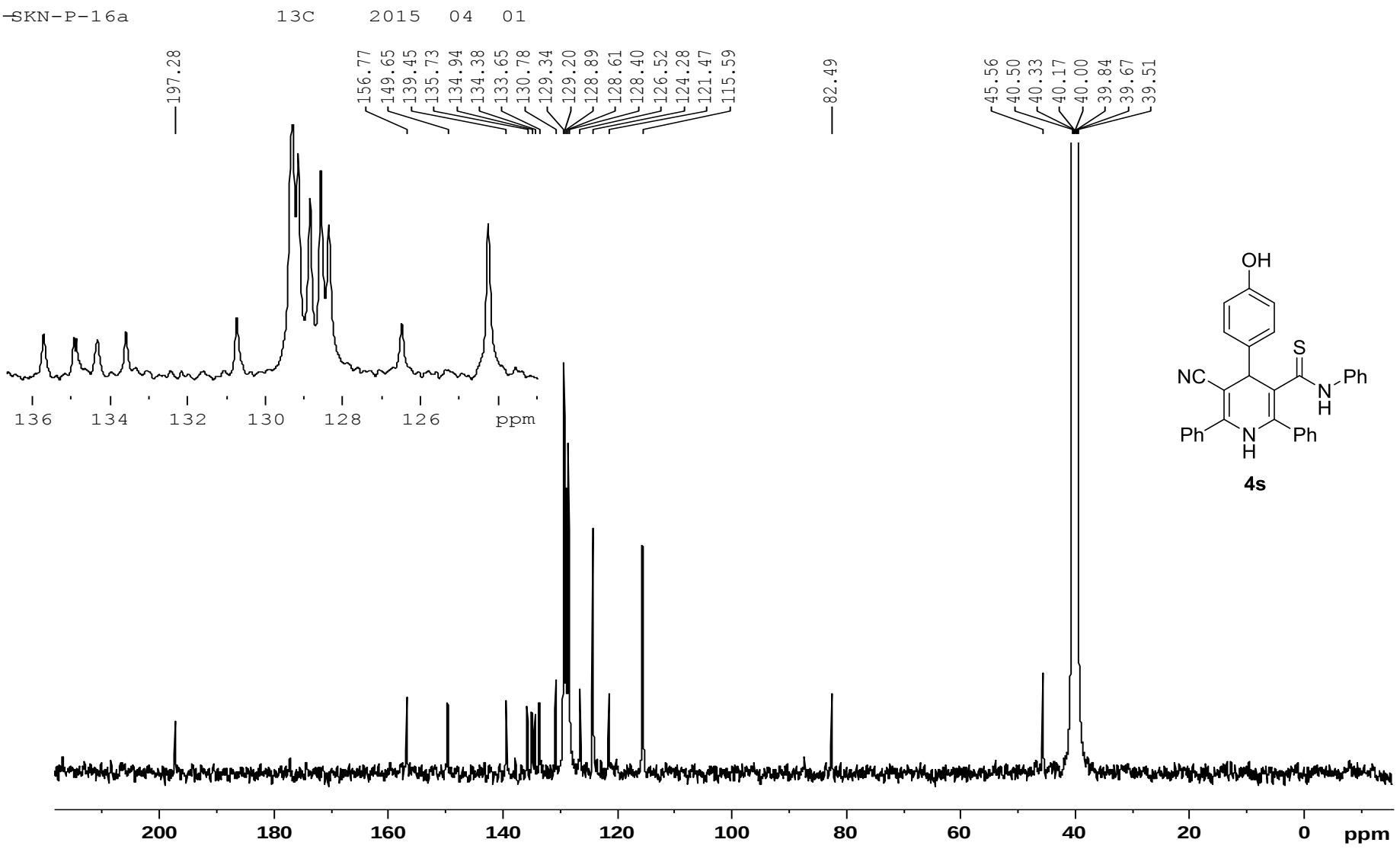

SKN-P-18 1H 2015 04 03
10.840
9.770
8.290
8.273
7.756
7.739
7.686
7.672
7.619
7.606
7.543
7.526
7.511
7.499
7.436
7.422
7.408
7.387
7.373
7.359
7.227
7.213
7.198
7.103
7.090
5.157
3.348
2.500
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.968
1.000
1.908
2.009
2.011
2.038
3.031
1.910
1.009
1.993
2.917
0.929
NO2
S
NC
Ph
N
H
Ph
N
H
Ph
4q

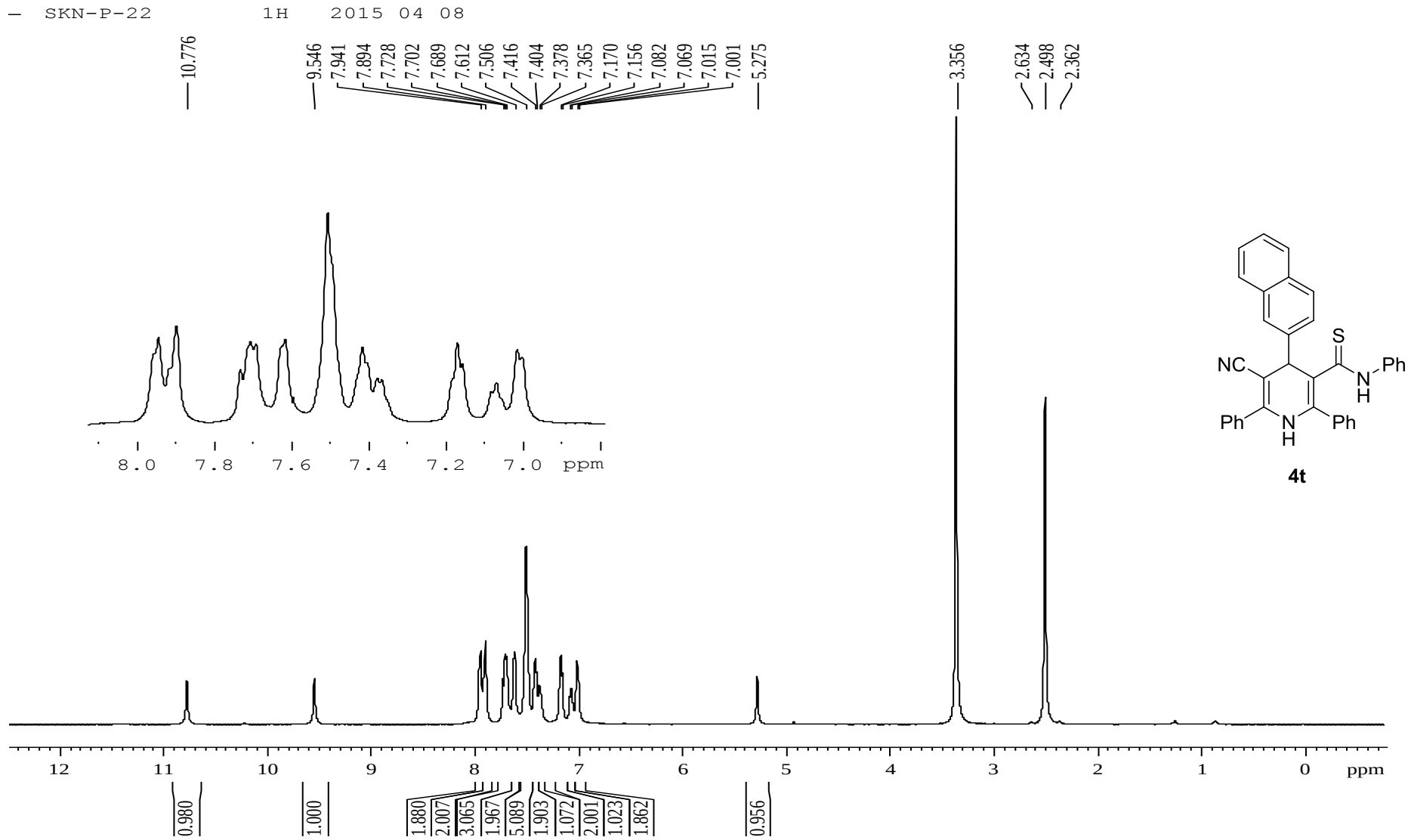

SKN-P-18 13C 2015 04 07
196.055
152.512
150.711
147.001
139.394
136.906
134.481
133.031
131.232
129.797
129.565
129.338
129.033
128.747
128.596
126.577
124.306
123.935
120.932
112.921
80.889
45.938
40.326
40.165
40.001
39.836
39.672
135 134 133 132 131 130 129 128 127 126 125 ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
NO2
S
NC
N
H
Ph
N
H
Ph
Ph
4q


SKN-P-15 1H 2015 04 03
10.671
9.409
7.631
7.584
7.509
7.391
7.377
7.204
7.191
7.109
7.096
7.085
7.054
7.043
6.944
6.929
5.032
3.749
3.349
2.499
8.0
7.5
7.0
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.915
0.913
1.969
1.973
3.052
5.010
2.000
3.002
2.000
0.909
3.074
O
S
NC
N
H
Ph
Ph
N
H
Ph
4r

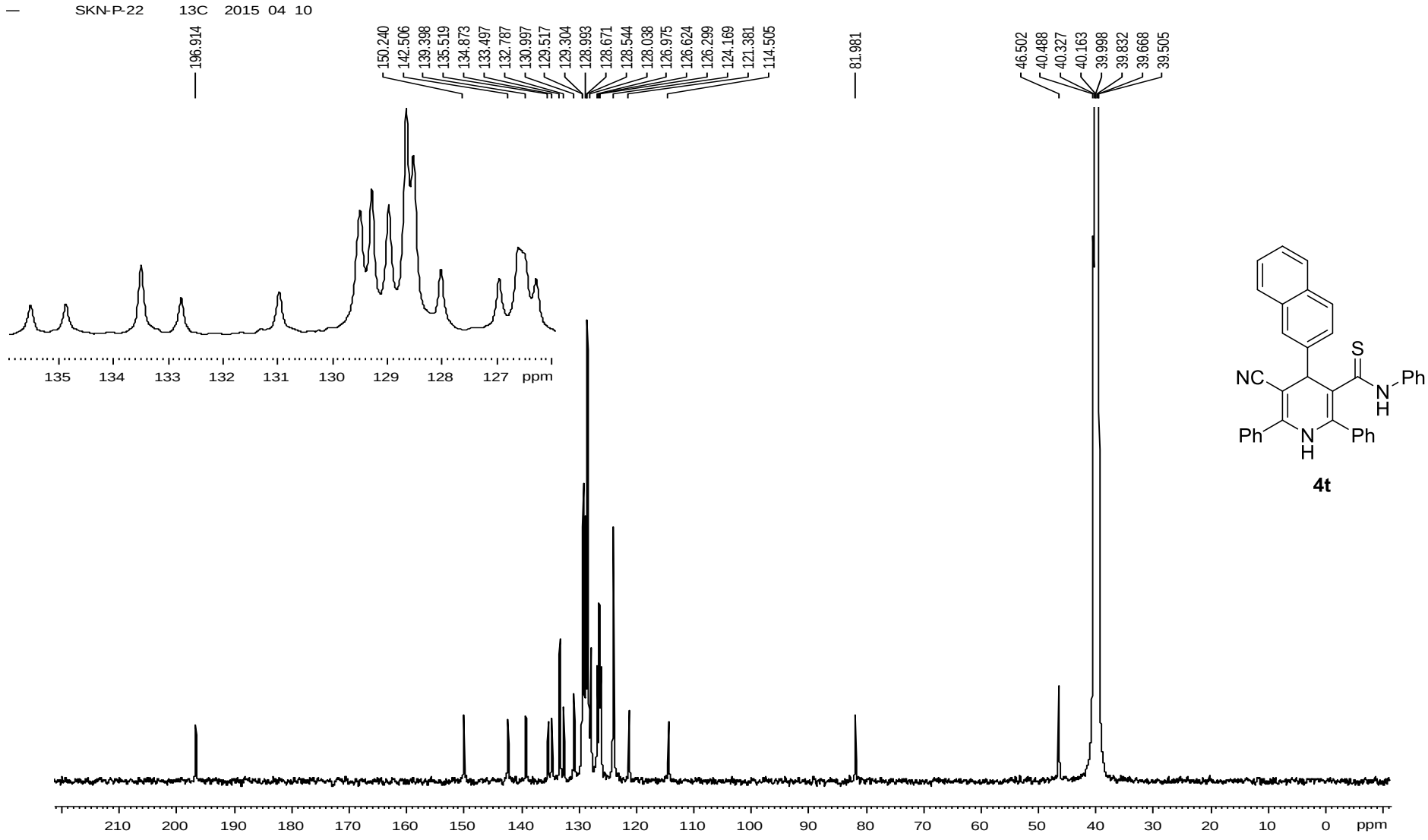

SKN-P-15 13C 2015 04 09
197.05
158.68
149.76
139.47
137.40
134.99
134.91
133.54
130.86
129.43
129.32
129.22
128.93
128.63
128.44
126.50
124.17
121.41
114.98
114.23
82.36
55.52
45.48
40.49
40.33
40.16
40.00
39.83
39.67
39.50
131 130 129 128 127 ppm
O
S
NC
Ph
N
H
Ph
N
H
Ph
4r
200 180 160 140 120 100 80 60 40 20 0 ppm


skn-p-16A 1H 2015 03 31
10.627
9.327
9.309
7.633
7.620
7.594
7.581
7.528
7.505
7.492
7.400
7.386
7.372
7.357
7.343
7.330
7.267
7.251
7.221
7.206
7.191
7.115
7.100
7.086
7.033
7.019
6.759
6.743
5.003
3.350
3.302
2.542
2.503
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.968
0.916
0.951
1.907
2.058
3.012
3.000
2.037
2.001
1.022
1.959
2.030
0.924
OH
S
NC
N
H
Ph
Ph
N
H
Ph
4s

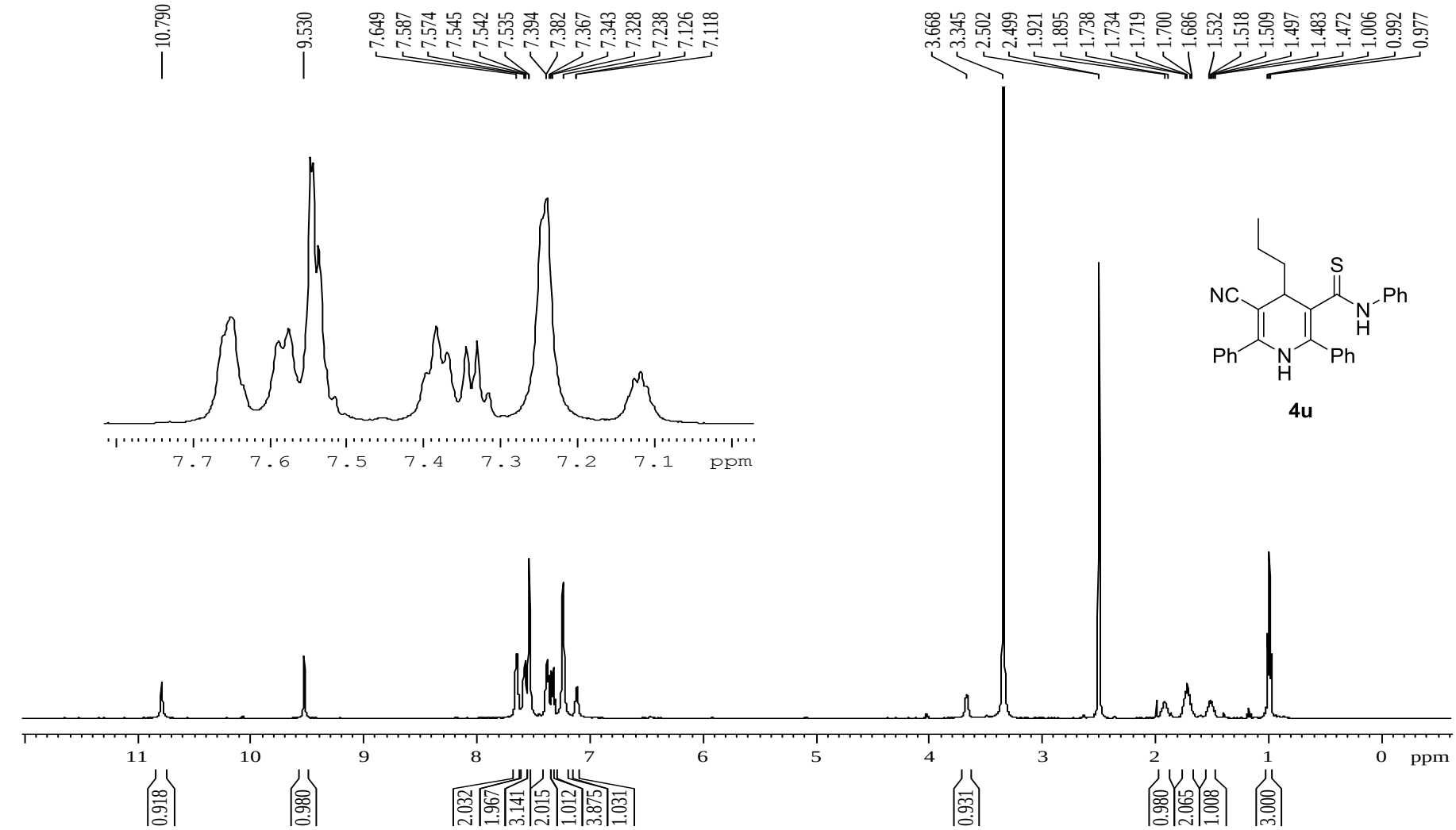

SKN-P-16a 13C 2015 04 01
197.28
156.77
149.65
139.45
135.73
134.94
134.38
133.65
130.78
129.34
129.20
128.89
128.61
128.40
126.52
124.28
121.47
115.59
82.49
45.56
40.50
40.33
40.17
40.00
39.84
39.67
39.51
136
134
132
130
128
126
ppm
OH
S
NC
Ph
N
H
Ph
N
H
Ph
4s
200
180
160
140
120
100
80
60
40
20
0
ppm

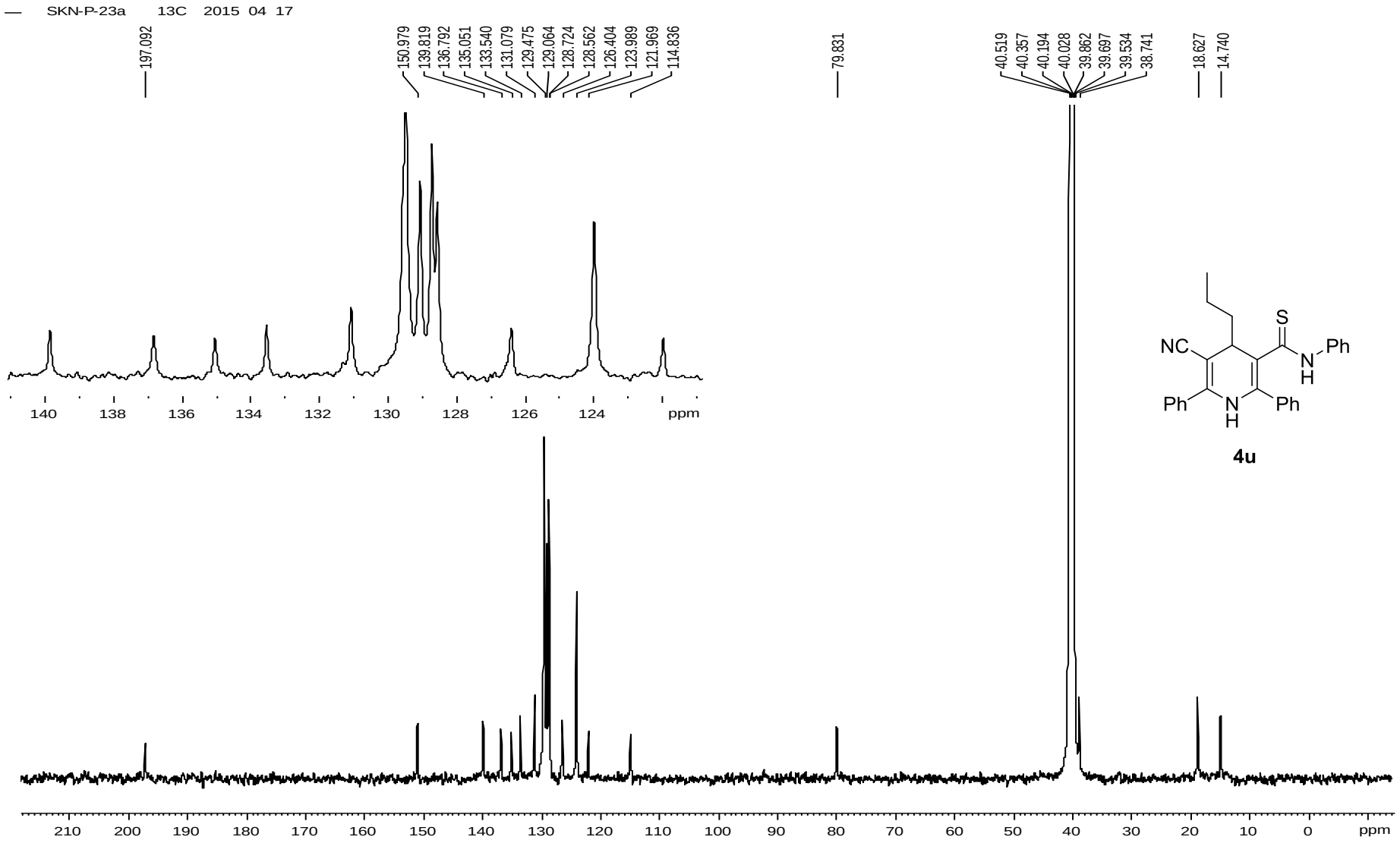

SKN-P-22 1H 2015 04 08
10.776
9.546
7.941
7.894
7.728
7.702
7.689
7.612
7.506
7.416
7.404
7.378
7.365
7.170
7.156
7.082
7.069
7.015
7.001
5.275
3.356
2.634
2.498
2.362
8.0 7.8 7.6 7.4 7.2 7.0 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.980
1.000
1.880
2.007
3.065
1.967
5.089
1.903
1.072
2.001
1.023
1.862
0.956
NC
S
N
H
Ph
Ph
N
H
Ph

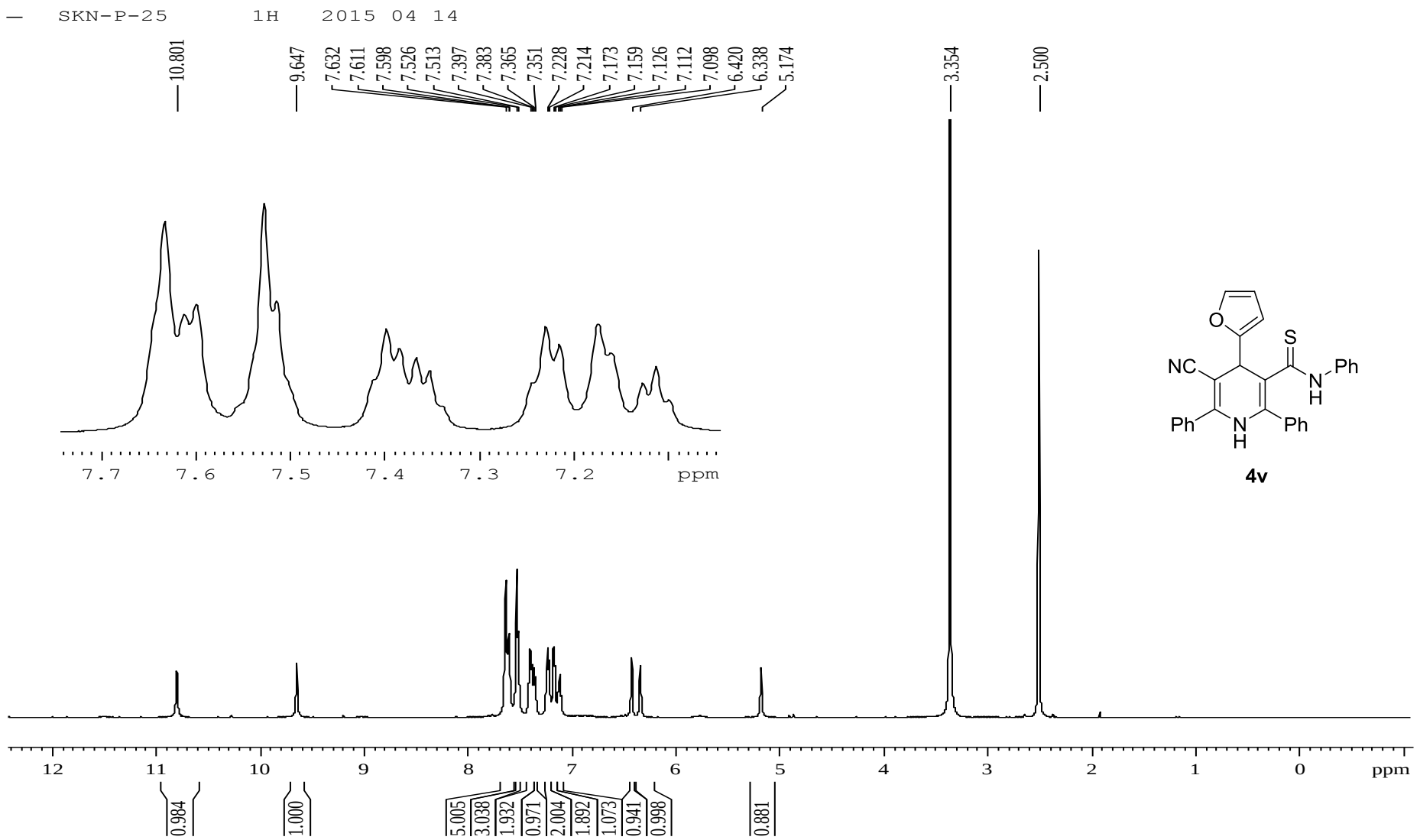
4t


SKN-P-22 13C 2015 04 10
196.914
150.240
142.506
139.398
135.519
134.873
133.497
132.787
130.997
129.517
129.304
128.993
128.671
128.544
128.038
126.975
126.624
126.299
124.169
121.381
114.505
81.981
46.502
40.488
40.327
40.163
39.998
39.832
39.668
39.505
135 134 133 132 131 130 129 128 127 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
NC
S
N
H
Ph
Ph
N
H
Ph
Ph

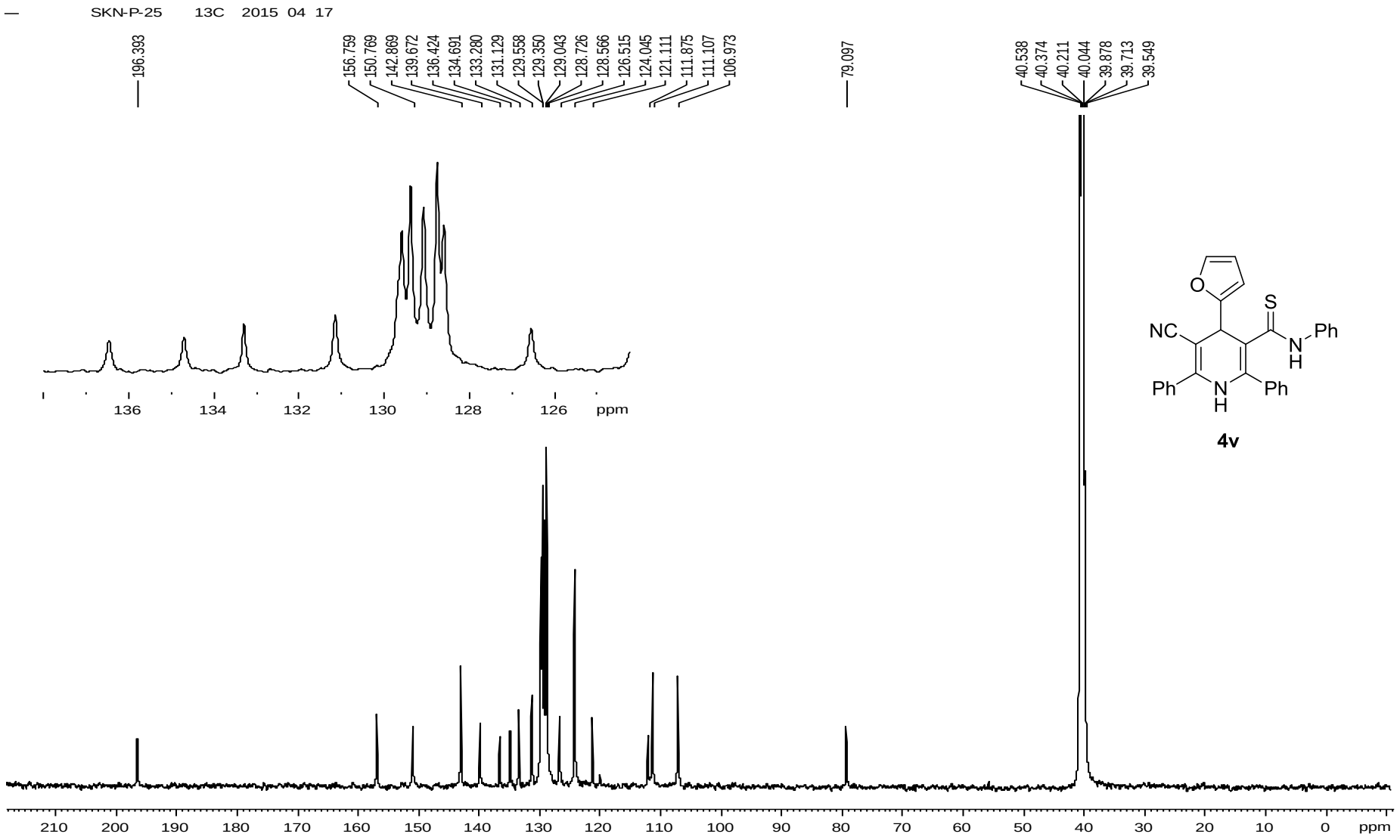
4t


SKN-P-23a 1H 2015 04 16
10.790
9.530
7.649
7.587
7.574
7.545
7.542
7.535
7.394
7.382
7.367
7.343
7.328
7.238
7.126
7.118
3.668
3.345
2.502
2.499
1.921
1.895
1.738
1.734
1.719
1.700
1.686
1.532
1.518
1.509
1.497
1.483
1.472
1.006
0.992
0.977
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.918
0.980
2.032
1.967
3.141
2.015
1.012
3.875
1.031
0.931
0.980
2.065
1.008
3.000
NC
S
N
H
Ph
Ph
N
H
Ph
4u

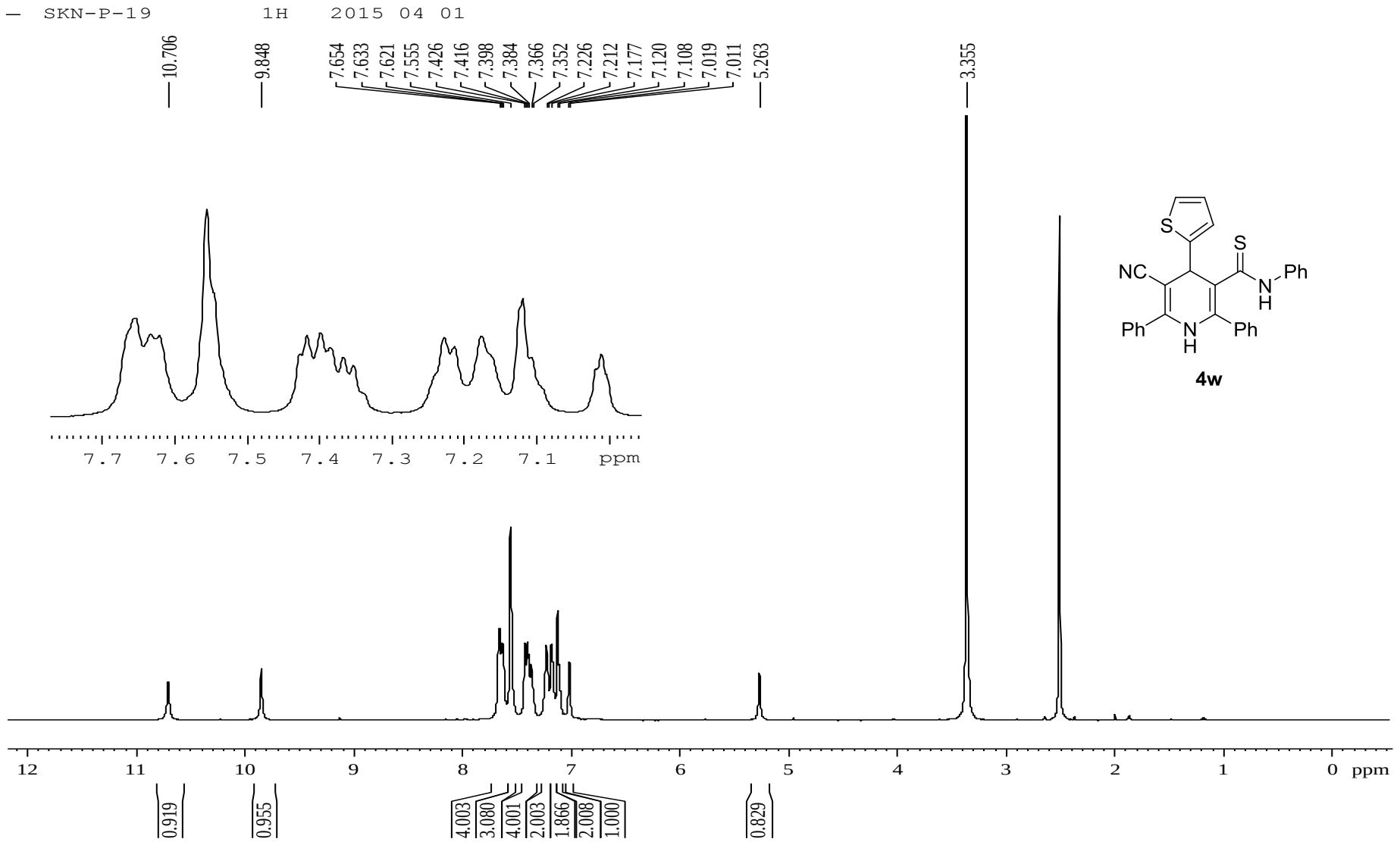

SKN-P-23a 13C 2015 04 17
197.092
150.979
139.819
136.792
135.051
133.540
131.079
129.475
129.064
128.724
128.562
126.404
123.989
121.969
114.836
79.831
40.519
40.357
40.194
40.028
39.862
39.697
39.534
38.741
18.627
14.740
140 138 136 134 132 130 128 126 124 ppm
NC
S
N
H
Ph
Ph
N
H
Ph
4u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

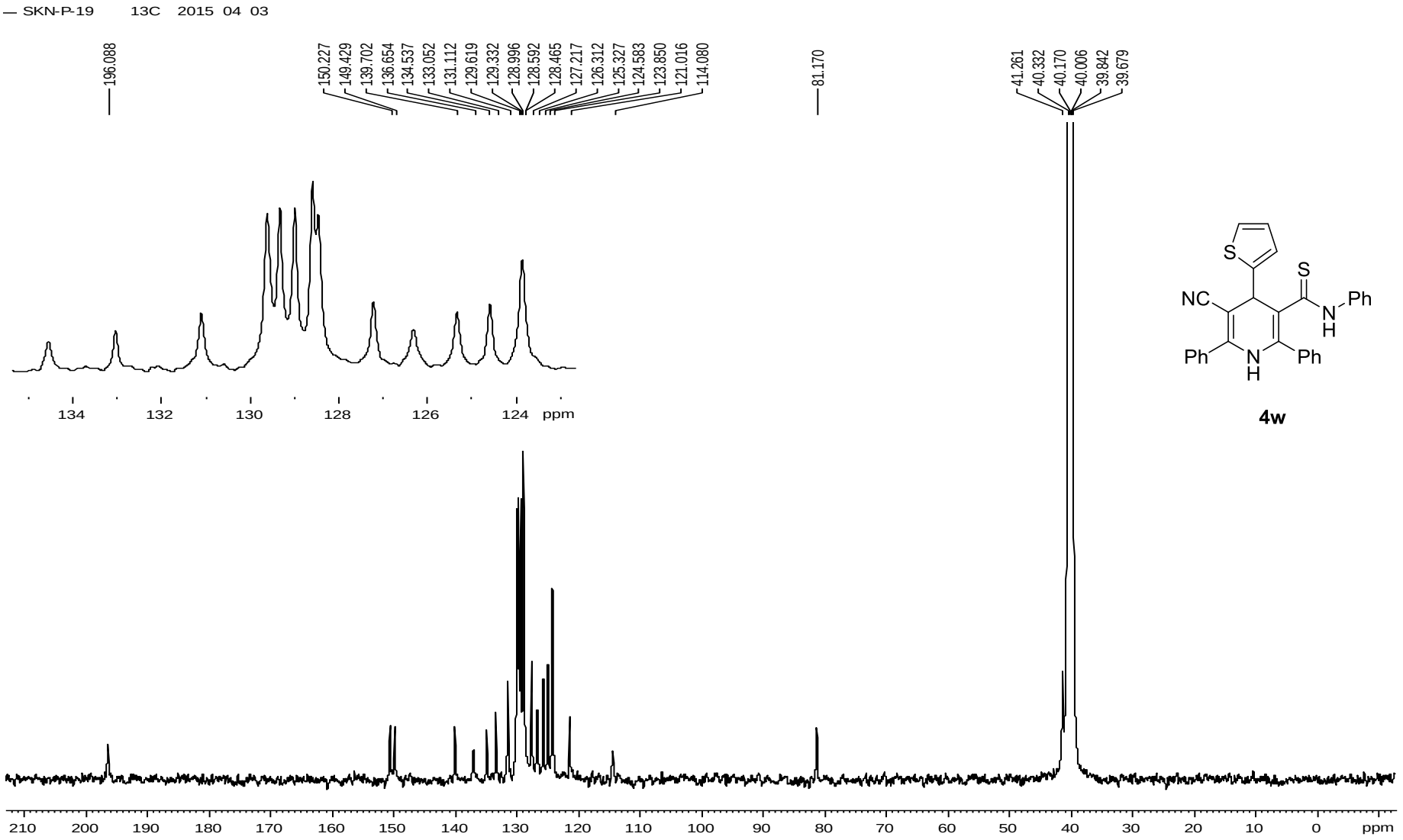

SKN-P-25 1H 2015 04 14
10.801
9.647
7.632
7.611
7.598
7.526
7.513
7.397
7.383
7.365
7.351
7.228
7.214
7.173
7.159
7.126
7.112
7.098
6.420
6.338
5.174
3.354
2.500
7.7 7.6 7.5 7.4 7.3 7.2 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.984
1.000
5.005
3.038
1.932
0.971
2.004
1.892
1.073
0.941
0.998
0.881
O
S
NC
N
H
Ph
Ph
N
H
Ph

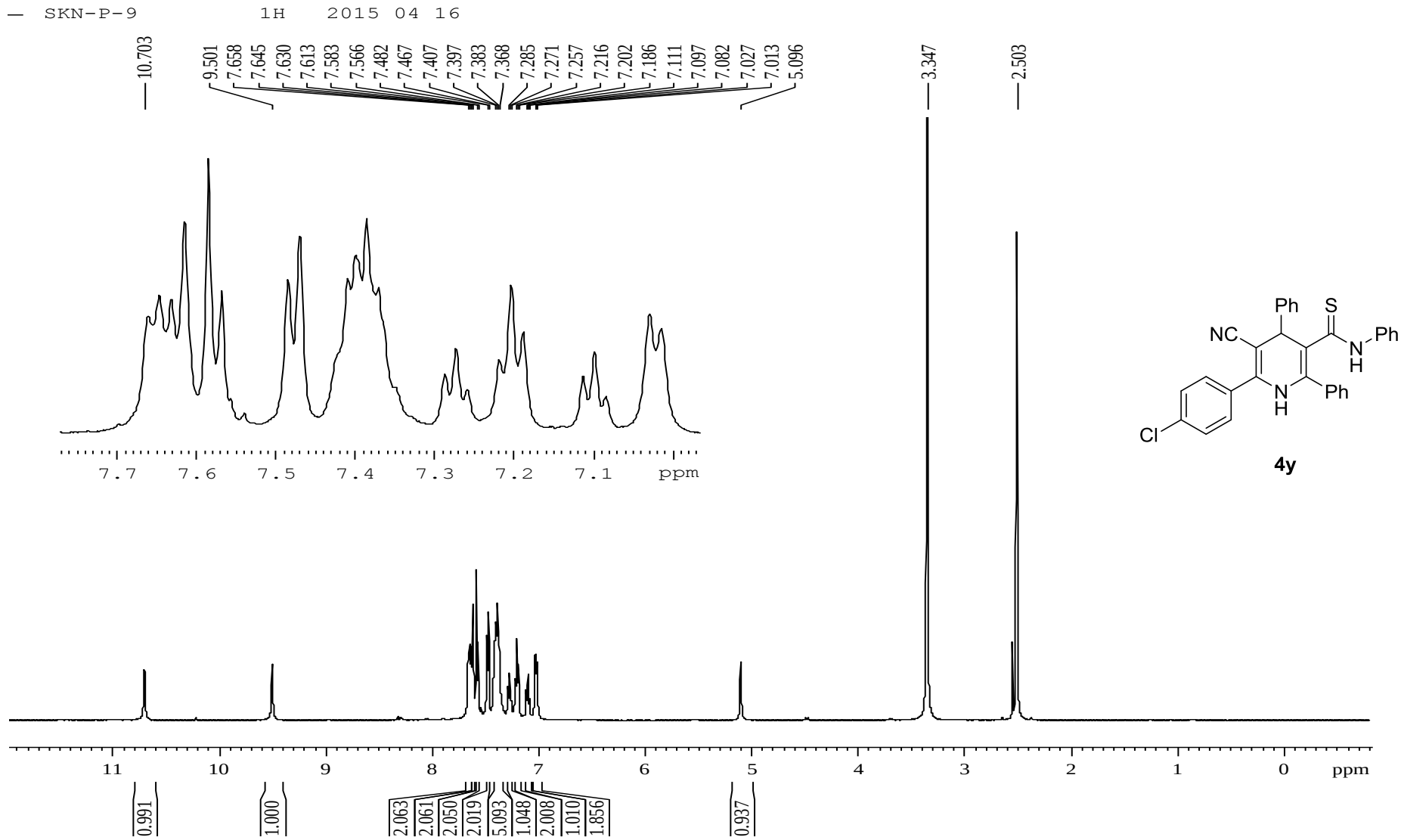
4v

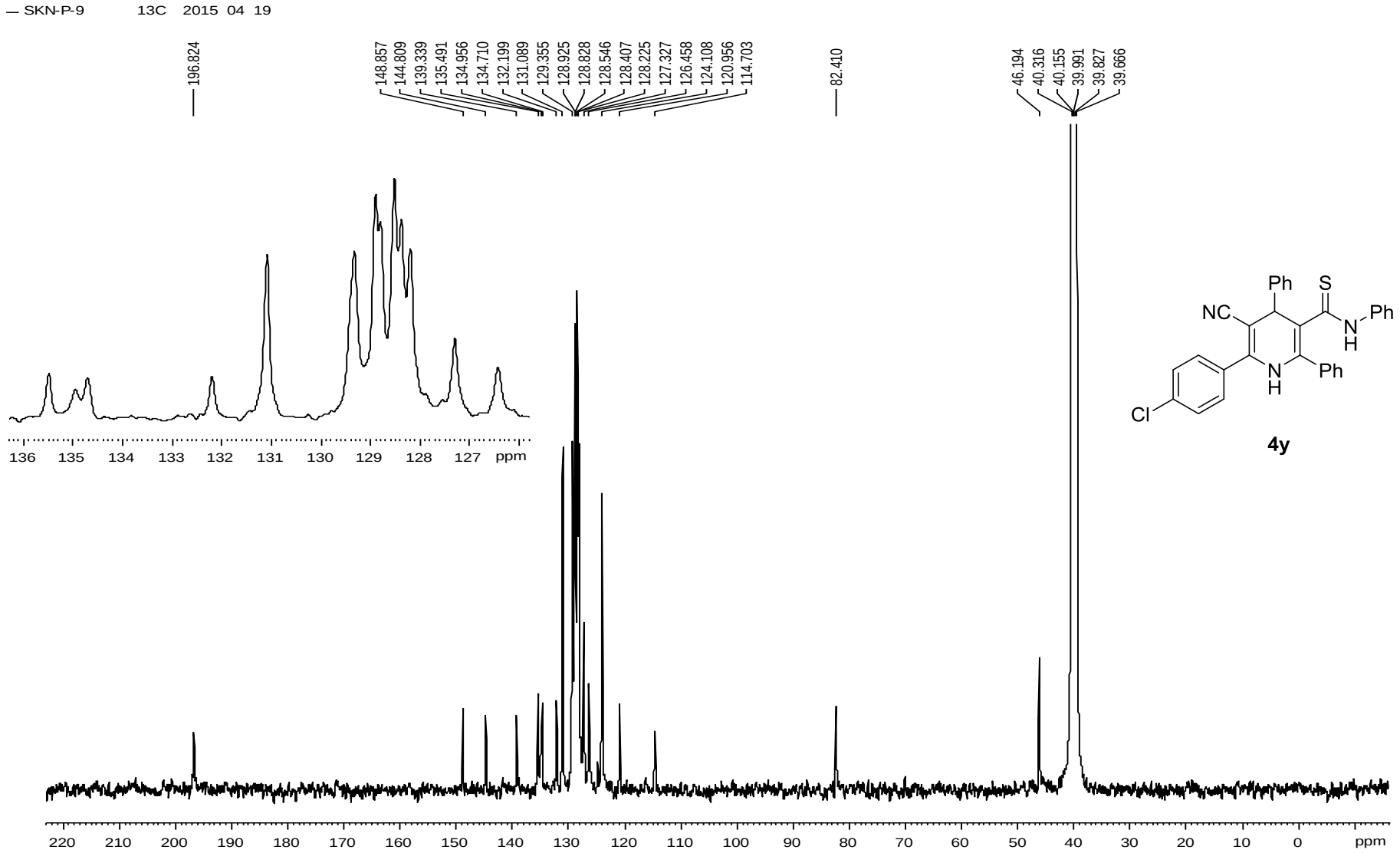

SKN-P-25 13C 2015 04 17
196.393
156.759
150.769
142.869
139.672
136.424
134.691
133.280
131.129
129.558
129.350
129.043
128.726
128.566
126.515
124.045
121.111
111.875
111.107
106.973
79.097
40.538
40.374
40.211
40.044
39.878
39.713
39.549
136
134
132
130
128
126
ppm
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
O
S
NC
Ph
N
H
Ph
N
H
Ph

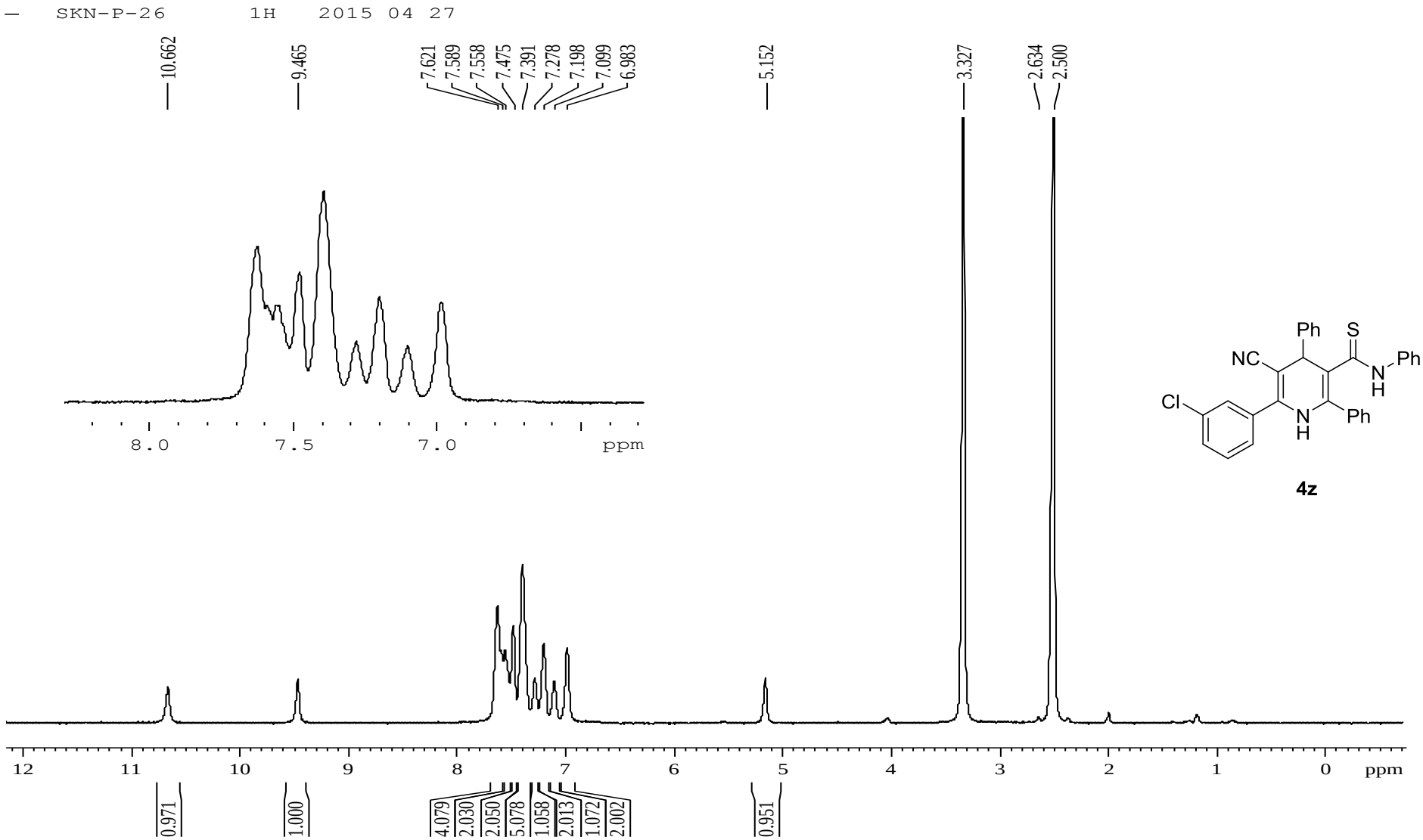
4v

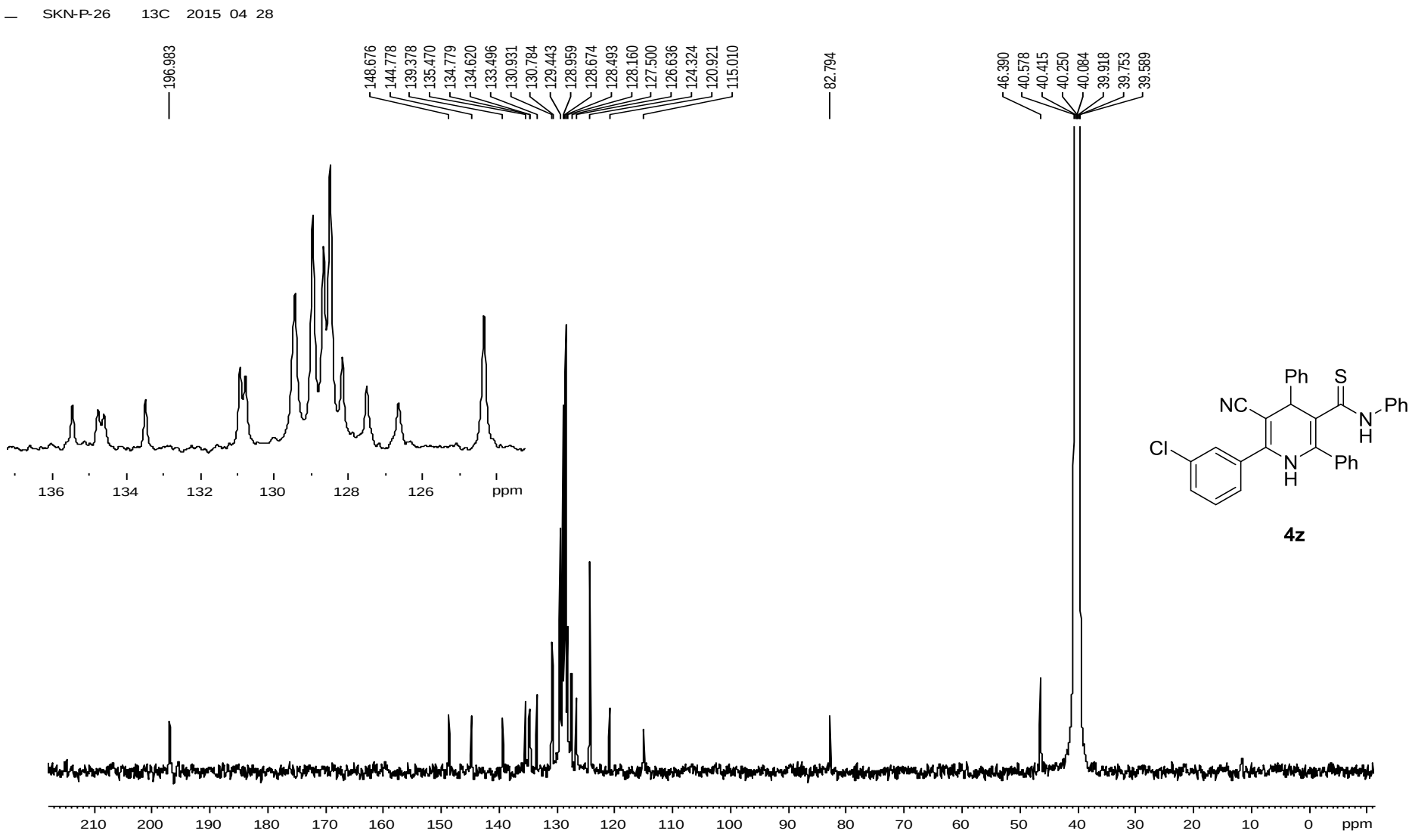

SKN-P-19 1H 2015 04 01
10.706
9.848
7.654
7.633
7.621
7.555
7.426
7.416
7.398
7.384
7.366
7.352
7.226
7.212
7.177
7.120
7.108
7.019
7.011
5.263
3.355
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.919
0.955
4.003
3.080
4.001
2.003
1.866
2.008
1.000
0.829
S
NC
S
N
H
Ph
Ph
N
H
Ph
4w


— SKN-P-19 13C 2015 04 03
196.088
150.227
149.429
139.702
136.654
134.537
133.052
131.112
129.619
129.332
128.996
128.592
128.465
127.217
126.312
125.327
124.583
123.850
121.016
114.080
81.170
41.261
40.332
40.170
40.006
39.842
39.679
134
132
130
128
126
124
ppm
S
S
NC
N
H
Ph
Ph
N
H
Ph
4w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

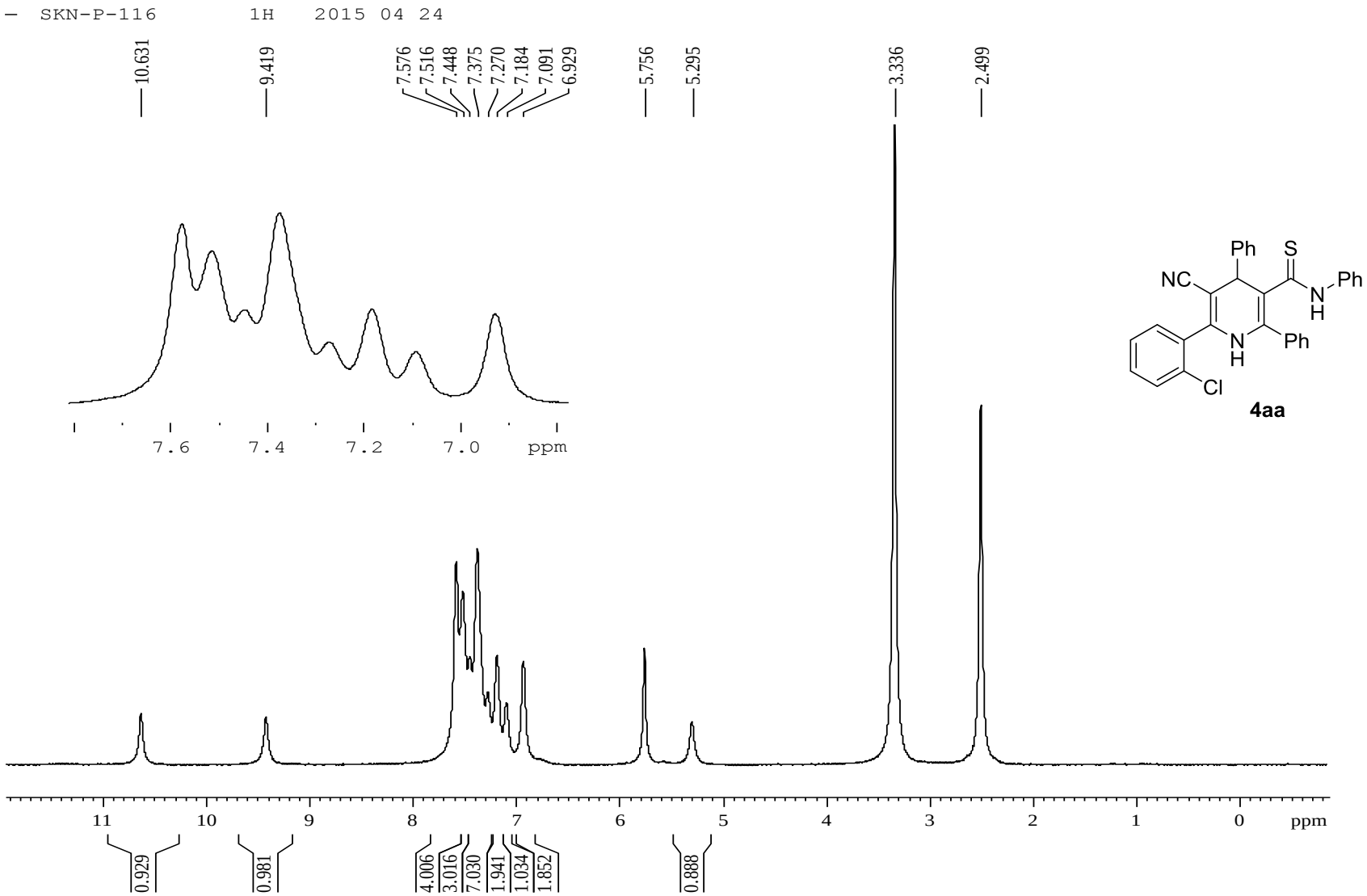

SKN-P-9 1H 2015 04 16
10.703
9.501
7.658
7.645
7.630
7.613
7.583
7.566
7.482
7.467
7.407
7.397
7.383
7.368
7.285
7.271
7.257
7.216
7.202
7.186
7.111
7.097
7.082
7.027
7.013
5.096
3.347
2.503
7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.991
1.000
2.063
2.061
2.050
2.019
5.093
1.048
2.008
1.010
1.856
0.937
Ph
S
NC
N
H
Ph
N
H
Ph
Cl
4y

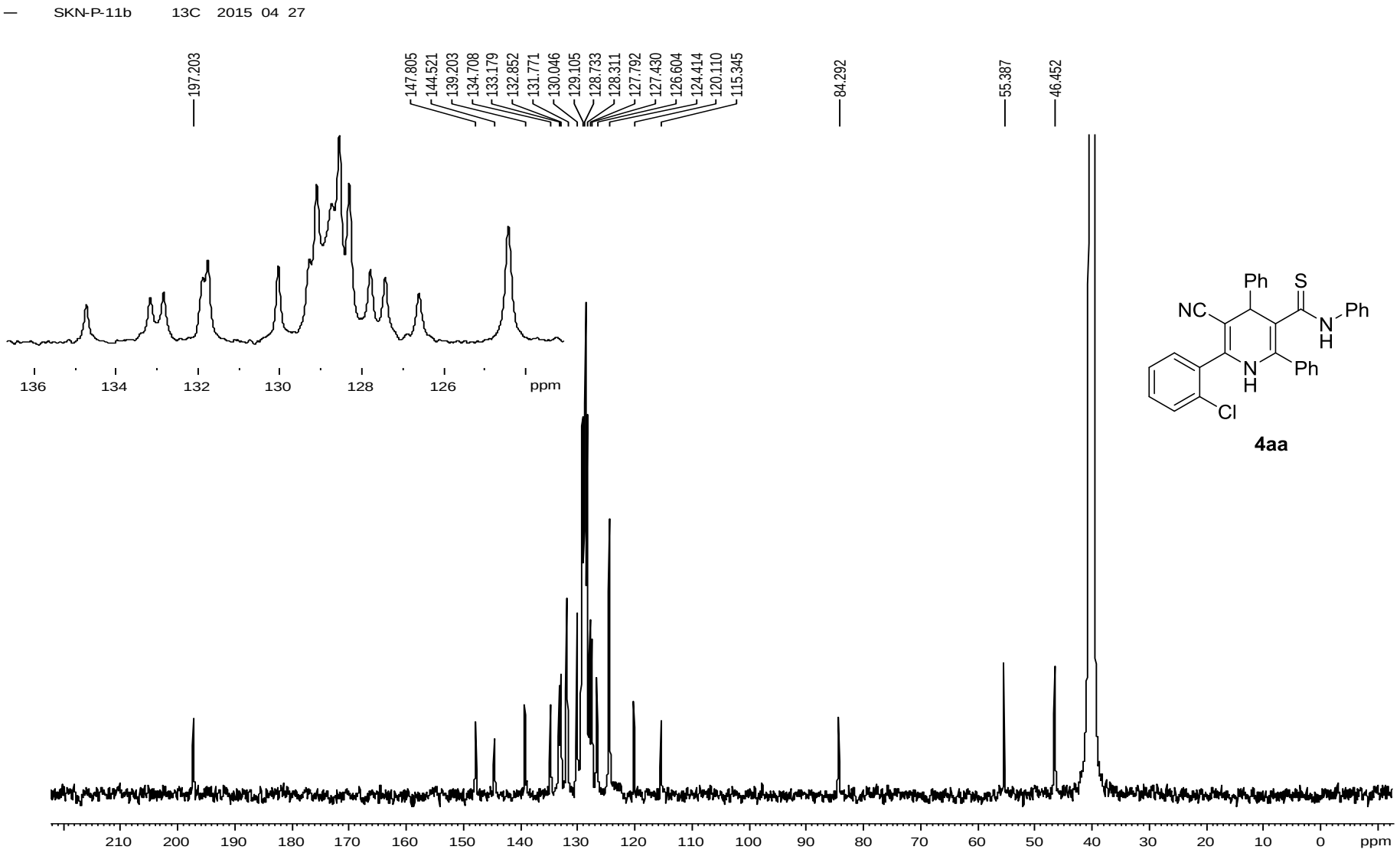

— SKN-P-9 13C 2015 04 19
196.824
148.857
144.809
139.339
135.491
134.956
134.710
132.199
131.089
129.355
128.925
128.828
128.546
128.407
128.225
127.327
126.458
124.108
120.956
114.703
82.410
46.194
40.316
40.155
39.991
39.827
39.666
136 135 134 133 132 131 130 129 128 127 ppm
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Ph
N
H
Ph
Cl
4y

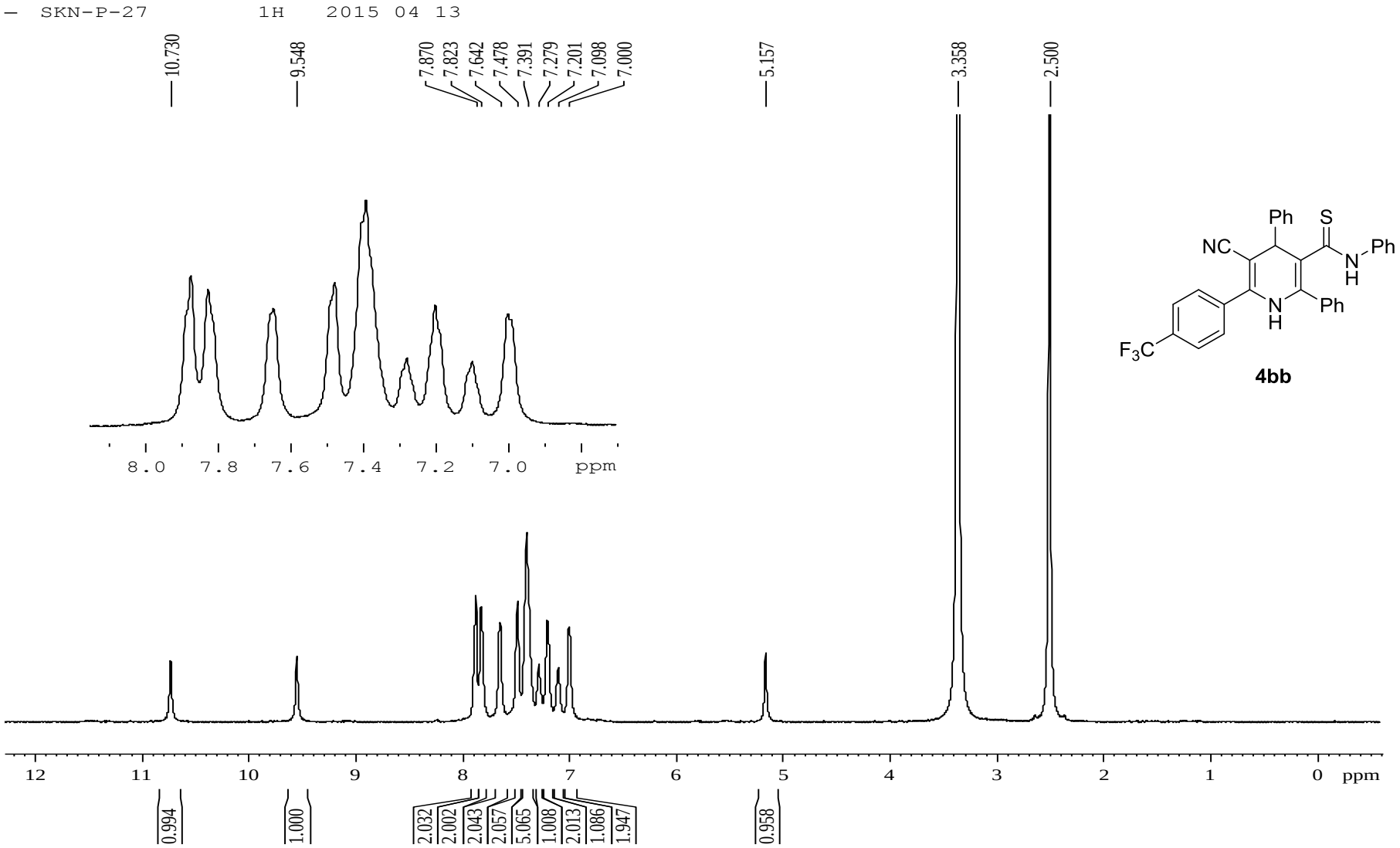

SKN-P-26 1H 2015 04 27
10.662
9.465
7.621
7.589
7.558
7.475
7.391
7.278
7.198
7.099
6.983
5.152
3.327
2.634
2.500
8.0
7.5
7.0
ppm
Ph
S
NC
N
H
Ph
Cl
N
H
Ph
4z
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.971
1.000
4.079
2.030
2.050
5.078
1.058
2.013
1.072
2.002
0.951

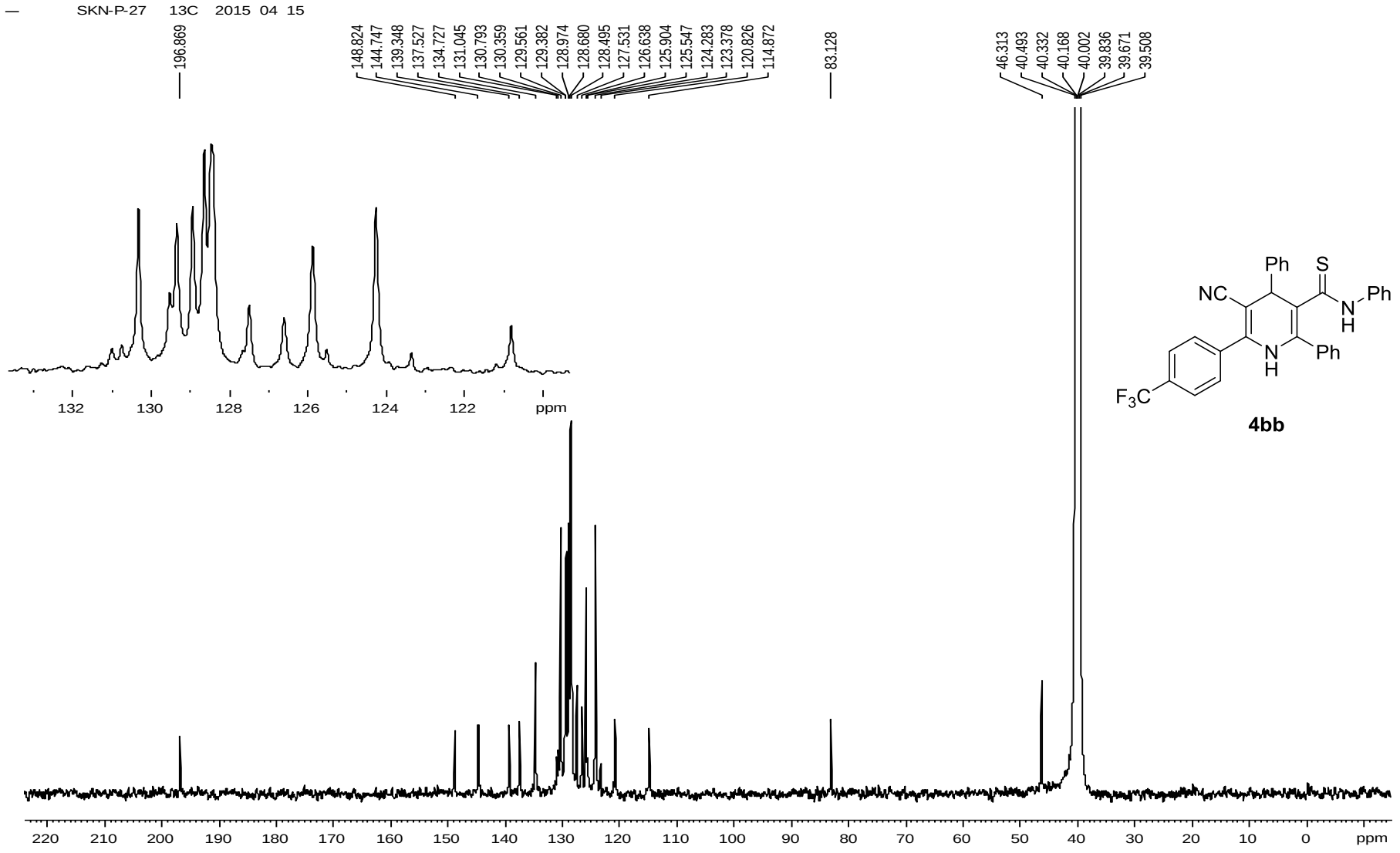

SKN-P-26 13C 2015 04 28
196.983
148.676
144.778
139.378
135.470
134.779
134.620
133.496
130.931
130.784
129.443
128.959
128.674
128.493
128.160
127.500
126.636
124.324
120.921
115.010
82.794
46.390
40.578
40.415
40.250
40.084
39.918
39.753
39.589
136
134
132
130
128
126
ppm
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
Ph
S
NC
N
H
Ph
Cl
N
H
Ph

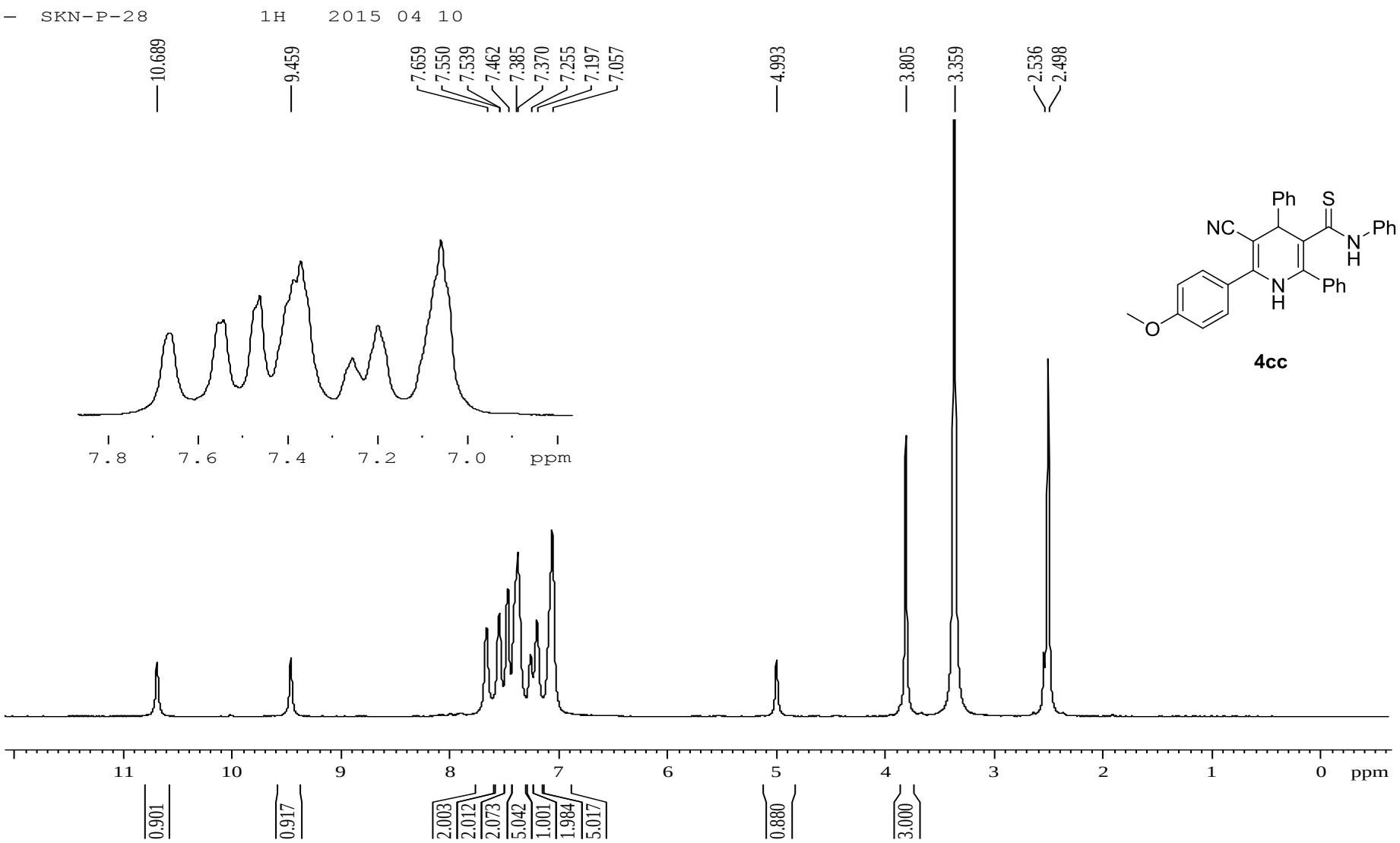
4z

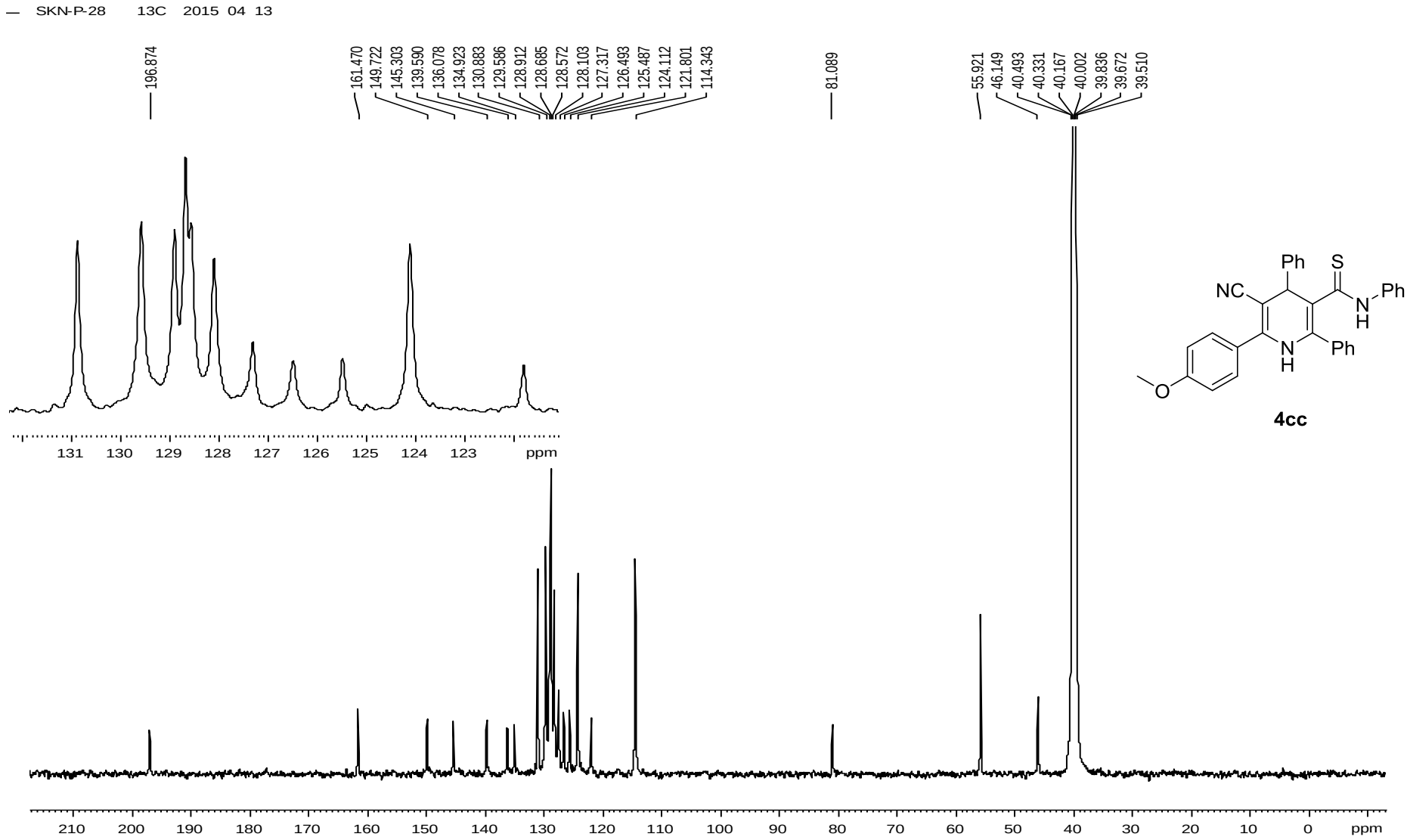

SKN-P-116 1H 2015 04 24
10.631
9.419
7.576
7.516
7.448
7.375
7.270
7.184
7.091
6.929
5.756
5.295
3.336
2.499
7.6
7.4
7.2
7.0
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.929
0.981
4.006
3.016
7.030
1.941
1.034
1.852
0.888
Ph
S
NC
N
H
Ph
N
H
Ph
Cl
4aa


SKN-P-11b 13C 2015 04 27
197.203
147.805
144.521
139.203
134.708
133.179
132.852
131.771
130.046
129.105
128.733
128.311
127.792
127.430
126.604
124.414
120.110
115.345
84.292
55.387
46.452
136
134
132
130
128
126
ppm
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
Ph
S
NC
N
H
Ph
N
H
Ph
Cl
4aa

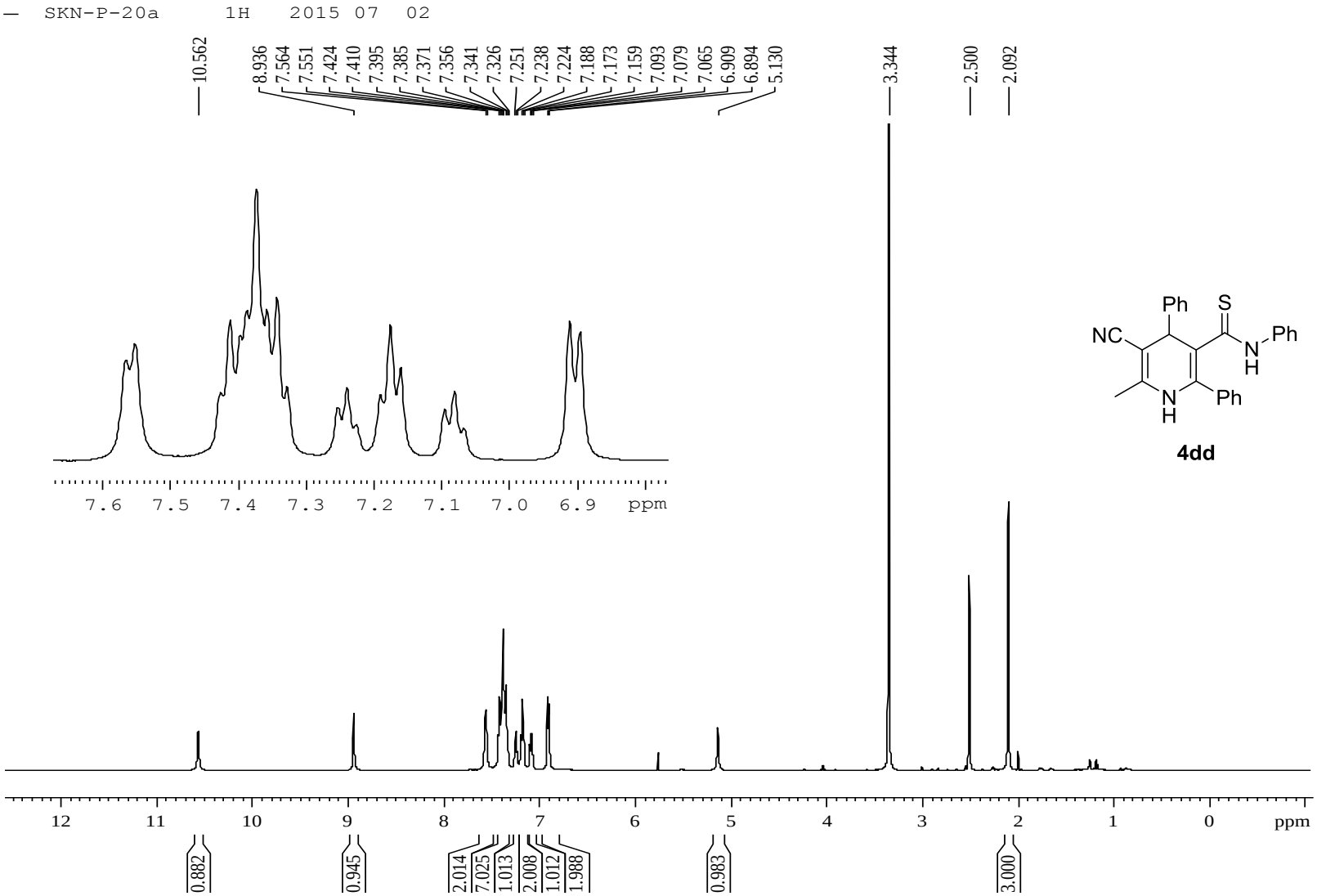

SKN-P-27 1H 2015 04 13
10.730
9.548
7.870
7.823
7.642
7.478
7.391
7.279
7.201
7.098
7.000
5.157
3.358
2.500
8.0 7.8 7.6 7.4 7.2 7.0 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.994
1.000
2.032
2.002
2.043
2.057
5.065
1.008
2.013
1.086
1.947
0.958
Ph
S
NC
N
H
Ph
N
H
Ph
F3C
4bb

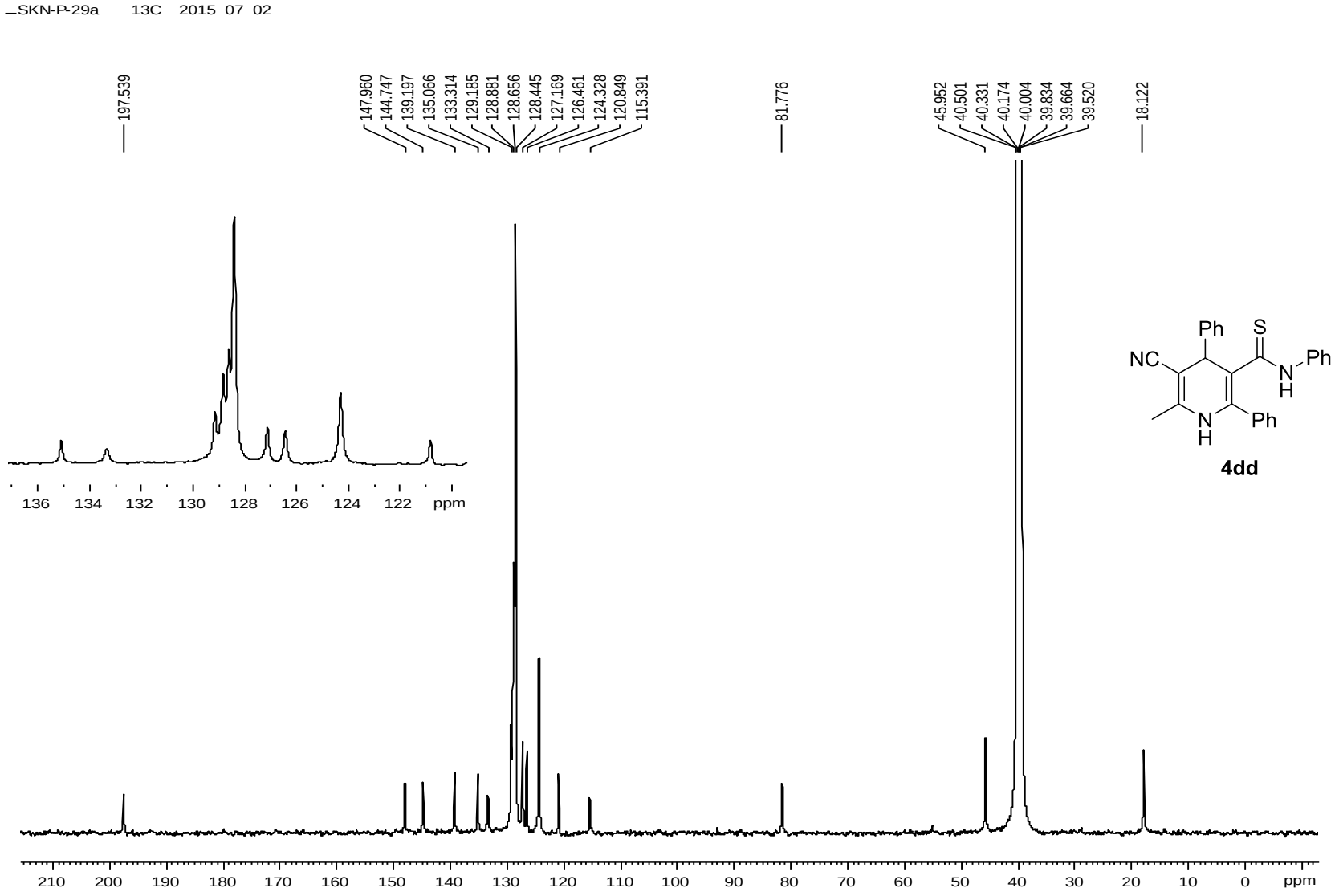

SKN-P-27 13C 2015 04 15
196.869
148.824
144.747
139.348
137.527
134.727
131.045
130.793
130.359
129.561
129.382
128.974
128.680
128.495
127.531
126.638
125.904
125.547
124.283
123.378
120.826
114.872
83.128
46.313
40.493
40.332
40.168
40.002
39.836
39.671
39.508
132
130
128
126
124
122
ppm
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
Ph
S
NC
N
H
Ph
N
H
Ph
F3C
4bb

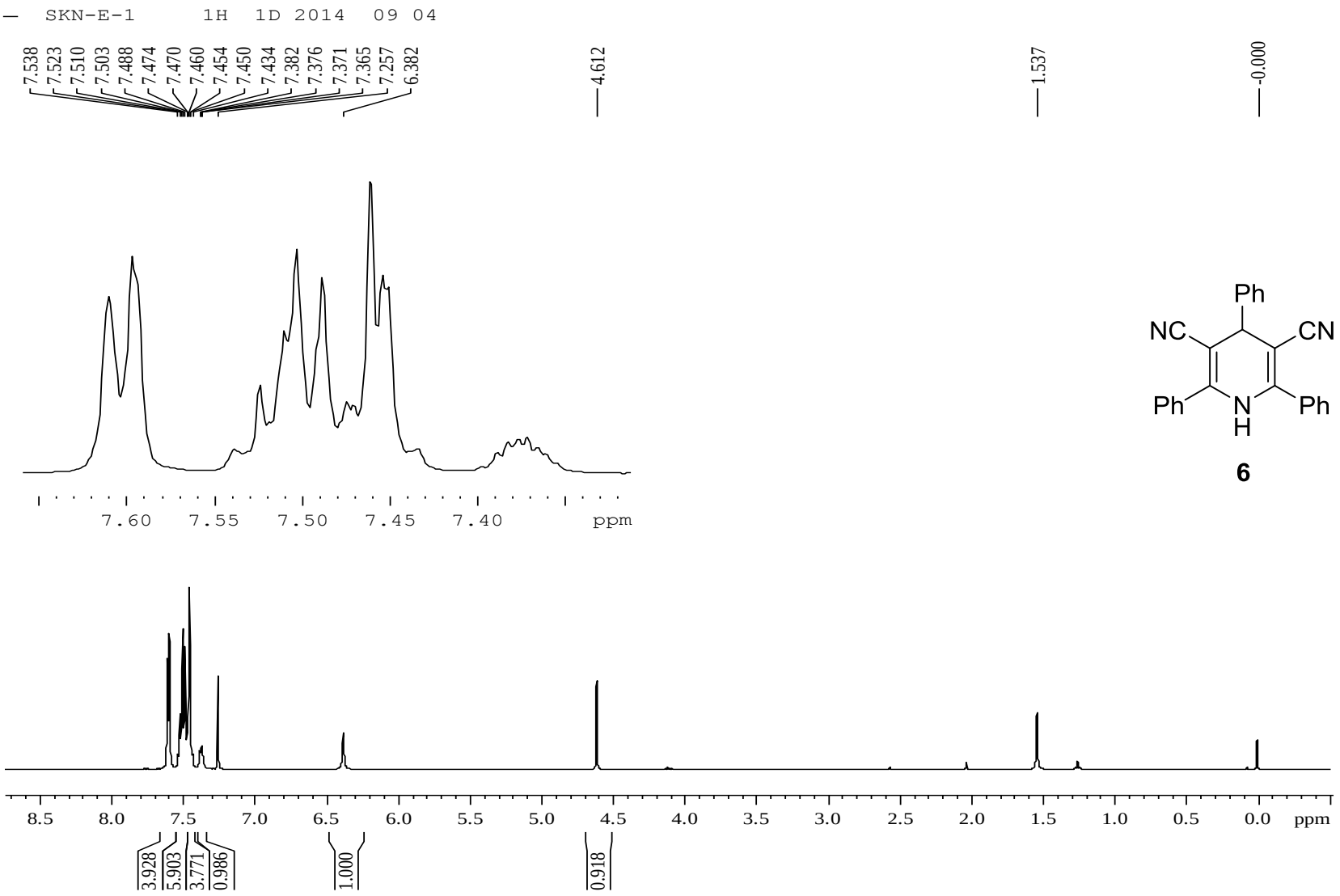

SKN-P-28 1H 2015 04 10
10.689
9.459
7.659
7.550
7.539
7.462
7.385
7.370
7.255
7.197
7.057
4.993
3.805
3.359
2.536
2.498
7.8
7.6
7.4
7.2
7.0
ppm
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.901
0.917
2.003
2.012
2.073
5.042
1.001
1.984
5.017
0.880
3.000
Ph
S
NC
N
H
Ph
N
H
Ph
O
4cc


SKN-P-28 13C 2015 04 13
196.874
161.470
149.722
145.303
139.590
136.078
134.923
130.883
129.586
128.912
128.685
128.572
128.103
127.317
126.493
125.487
124.112
121.801
114.343
81.089
55.921
46.149
40.493
40.331
40.167
40.002
39.836
39.672
39.510
131 130 129 128 127 126 125 124 123 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Ph
N
H
Ph
O

4cc


SKN-P-20a 1H 2015 07 02
10.562
8.936
7.564
7.551
7.424
7.410
7.395
7.385
7.371
7.356
7.341
7.326
7.251
7.238
7.224
7.188
7.173
7.159
7.093
7.079
7.065
6.909
6.894
5.130
3.344
2.500
2.092
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.882
0.945
2.014
7.025
1.013
2.008
1.012
1.988
0.983
3.000
Ph
S
NC
N
H
Ph
N
H
Ph
4dd


_SKN-P-29a 13C 2015 07 02
197.539
147.960
144.747
139.197
135.066
133.314
129.185
128.881
128.656
128.445
127.169
126.461
124.328
120.849
115.391
81.776
45.952
40.501
40.331
40.174
40.004
39.834
39.664
39.520
18.122
136 134 132 130 128 126 124 122 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Ph
S
NC
N
H
Ph
N
H
Ph
4dd


SKN-E-1 1H 1D 2014 09 04
7.538
7.523
7.510
7.503
7.488
7.474
7.470
7.460
7.454
7.450
7.434
7.382
7.376
7.371
7.365
7.257
6.382
4.612
1.537
-0.000
7.60
7.55
7.50
7.45
7.40
ppm
Ph
NC
CN
Ph
N
H
Ph
6
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
3.928
5.903
3.771
0.986
1.000
0.918