Electronic Supplementary Material (ESI) for Chemical Communications

Generation of cyclopenta[c]chromenes via a palladium-catalyzed reaction of 2-alkynylphenol with 2-alkynylvinyl bromide

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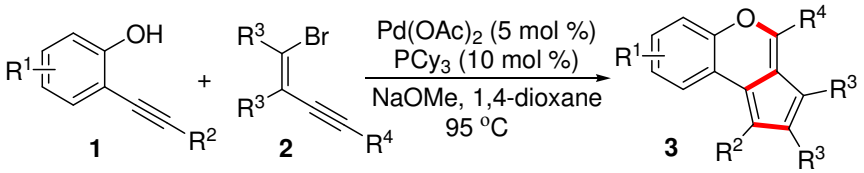
Supporting Information

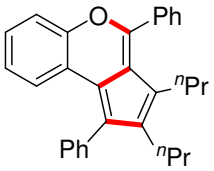
General Materials and Methods:

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

General procedure of the synthesis of cyclopenta[c]chromenes ***3*** *via a palladium-catalyzed reaction of 2-alkynylphenol* ***1*** *with 2-alkynylvinyl bromide* ***2***

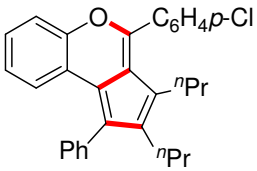


2-Alkynylhalobenzene **1** (0.20 mmol) was added to a mixture of $Pd(OAc)_2$ (5 mol %), tricyclohexylphosphine (10 mol %), CH_3ONa (0.40 mmol), and 2-alkynylvinyl bromide **2** (0.24 mmol) in 1,4-dioxane (2.0 mL). The mixture was stirred at 95 °C. After completion of the reaction as indicated by TLC, the mixture was cooled and diluted by EtOAc (10 mL), washed with saturated brine (2 × 10 mL), and dried by anhydrous Na_2SO_4. Evaporation of the solvent followed by purification on silica gel provided the product **3**.



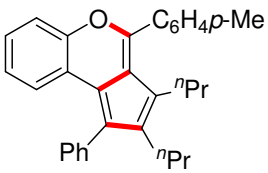
1,4-Diphenyl-2,3-dipropylcyclopenta[*c*]chromene (**3a**)

Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.48 (t, *J* = 7.1 Hz, 3H), 0.74 (t, *J* = 7.1 Hz, 3H), 1.04-1.10 (m, 2H), 1.23-1.30 (m, 2H), 2.29 (t, *J* = 7.8 Hz, 2H), 2.39 (t, *J* = 7.8 Hz, 2H), 6.96 (t, *J* = 7.6 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.38-7.41 (m, 4H), 7.45 (d, *J* = 6.4 Hz, 2H), 7.48-7.53 (m, 2H), 7.68 (d, *J* = 5.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.9, 23.5, 24.7, 25.5, 28.6, 117.0, 117.6, 120.8, 121.3, 123.7, 124.4, 124.6, 124.7, 128.2, 129.7, 129.8, 130.2, 135.7, 148.6, 153.0; HRMS (ESI) calcd for $C_{30}H_{28}O$: 405.2213 ($M + H^+$), found: 405.2190.



4-(4-Chlorophenyl)-1-phenyl-2,3-dipropylcyclopenta[*c*]chromene (**3b**)

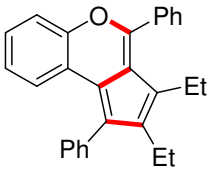
Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.56 (t, *J* = 7.1 Hz, 3H), 0.77 (t, *J* = 7.1 Hz, 3H), 1.08-1.13 (m, 2H), 1.26-1.31 (m, 2H), 2.32 (t, *J* = 7.8, 2H), 2.41 (t, *J* = 7.6 Hz, 2H), 6.98 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.38-7.42 (m, 4H), 7.47-7.53 (m, 4H), 7.65 (d, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.6, 24.0, 25.4, 28.6, 28.7, 117.5, 118.6, 120.4, 121.1, 123.6, 123.7, 124.5, 125.4, 127.0, 128.6, 128.7, 130.1, 130.2, 131.1, 133.0, 136.3, 138.7, 146.3, 148.6, 152.8; HRMS (ESI) calcd for $C_{30}H_{27}ClO$: 439.1823 ($M + H^+$), found: 439.1804.



1-Phenyl-2,3-dipropyl-4-(*p*-tolyl)cyclopenta[*c*]chromene (**3c**)

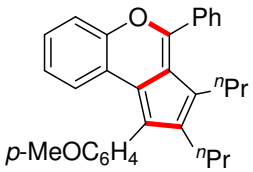
Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.58 (t, *J* = 7.3 Hz, 3H), 0.81 (t, *J* = 7.4 Hz, 3H), 1.13-1.19 (m, 2H), 1.31-1.37 (m, 2H), 2.39 (t, *J* = 7.6, 2H), 2.47 (t, *J* = 7.8 Hz,

2H), 2.51 (s, 3H), 7.01 (t, *J* = 7.6 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.37-7.39 (m, 3H), 7.43-7.54 (m, 6H), 7.64 (d, *J* = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.6, 21.7, 24.1, 25.5, 28.6, 28.7, 117.6, 118.6, 120.5, 120.8, 123.6, 124.2, 124.3, 125.2, 127.0, 128.7, 128.9, 129.7, 129.9, 130.2, 131.8, 139.0, 140.2, 145.6, 148.8, 154.7; HRMS (ESI) calcd for $C_{31}H_{30}O$: 419.2369 ($M + H^+$), found: 419.2370.



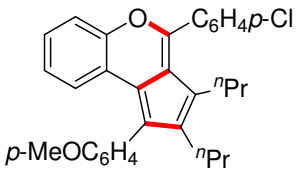
2,3-Diethyl-1,4-diphenylcyclopenta[*c*]chromene (**3d**)

Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.73 (t, *J* = 6.9 Hz, 3H), 0.92 (t, *J* = 6.9 Hz, 3H), 2.40 (q, *J* = 6.9 Hz, 2H), 2.47 (q, *J* = 6.9 Hz, 2H), 6.98 (t, *J* = 8.6 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.40-7.49 (m, 5H), 7.51-7.55 (m, 3H), 7.72 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.5, 16.4, 19.3, 19.5, 117.6, 118.7, 120.5, 120.6, 123.7, 124.4, 125.0, 125.3, 127.0, 128.3, 128.8, 129.7, 129.8, 130.2, 134.6, 138.9, 147.1, 148.7, 154.5; HRMS (ESI) calcd for $C_{28}H_{24}O$: 377.1900 ($M + H^+$), found: 377.1907.



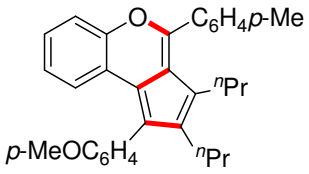
1-(4-Methoxyphenyl)-4-phenyl-2,3-dipropylcyclopenta[*c*]chromene (**3e**)

Red solid (plate), mp: 118.2-119.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.51 (t, *J* = 7.4 Hz, 3H), 0.80 (t, *J* = 7.4 Hz, 3H), 1.07-1.13 (m, 2H), 1.29-1.34 (m, 2H), 2.31 (t, *J* = 8.0 Hz, 2H), 2.42 (t, *J* = 7.8 Hz, 2H), 3.9 (s, 3H), 7.1 (t, *J* = 7.2 Hz, 1H), 7.05 (d, *J* = 8.8 Hz, 2H), 7.18 (t, *J* = 7.0 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.55-7.57 (m, 3H), 7.71 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.6, 24.1, 25.5, 28.6, 28.7, 55.3, 114.2, 114.3, 117.6, 120.8, 123.6, 124.0, 124.4, 125.2, 126.5, 128.3, 129.6, 129.7, 130.0, 130.9, 131.1, 134.6, 146.0, 148.7, 154.2, 158.6; HRMS (ESI) calcd for $C_{31}H_{30}O_2$: 435.2319 ($M + H^+$), found:435.2342.



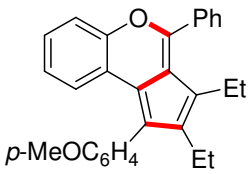
4-(4-Chlorophenyl)-1-(4-methoxyphenyl)-2,3-dipropylcyclopenta[*c*]chromene (**3f**)

Red solid (plate), mp: 113.5-114.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.56 (t, *J* = 7.0 Hz, 3H), 0.79 (t, *J* = 7.4 Hz, 3H), 1.08-1.13 (m, 2H), 1.26-1.31 (m, 2H), 2.32 (t, *J* = 8.0 Hz, 2H), 2.42 (t, *J* = 7.8 Hz, 2H), 3.86 (s, 3H), 7.04 (d, *J* = 7.6 Hz, 2H), 7.18-7.22 (m, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.49-7.52 (m, 2H), 7.65 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.6, 24.0, 25.5, 28.6, 28.7, 55.4, 114.3, 117.5, 120.5, 120.7, 122.9, 123.7, 123.8, 124.5, 125.1, 126.5, 128.6, 130.7, 131.1, 131.2, 146.6, 148.6, 154.8, 158.7; HRMS (ESI) calcd for $C_{31}H_{29}ClO_2$: 469.1929 ($M + H^+$), found: 469.1909.



1-(4-Methoxyphenyl)-2,3-dipropyl-4-(*p*-tolyl)cyclopenta[*c*]chromene (**3g**)

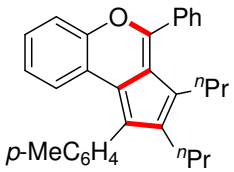
Red solid (plate), mp: 118.0-119.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.53 (t, *J* = 6.9 Hz, 3H), 0.79 (t, *J* = 6.9 Hz, 3H), 1.09-1.23 (m, 2H), 1.29-1.32 (m, 2H), 2.34 (t, *J* = 7.3 Hz, 2H), 2.42 (t, *J* = 7.8 Hz, 2H), 2.49 (s, 3H), 3.92 (s, 3H), 6.97-7.00 (m, 1H), 7.04 (d, *J* = 7.8 Hz, 2H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.34- 7.36 (m, 4H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.60 (d, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.7, 21.7, 24.1, 25.5, 28.6, 28.7, 55.3, 114.1, 117.6, 120.6, 120.7, 123.6, 124.0, 124.3, 125.1, 126.5, 128.9, 129.5, 129.6, 131.0, 131.2, 131.7, 140.2, 145.8, 148.7, 154.5, 158.6; HRMS (ESI) calcd for $C_{32}H_{33}O_2$: 449.2475 ($M + H^+$), found: 449.2471.



2,3-Diethyl-1-(4-methoxyphenyl)-4-phenylcyclopenta[*c*]chromene (**3h**)

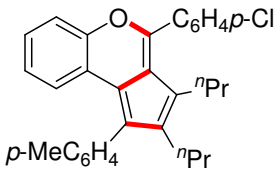
Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.75 (t, *J* = 7.1 Hz, 3H), 0.96 (t, *J* = 7.1 Hz,

3H), 2.41 (q, J = 7.1 Hz, 2H), 2.49 (q, J = 7.1 Hz, 2H), 3.92 (s, 3H), 7.01 (t, J = 7.4 Hz, 1H), 7.06 (d, J = 8.7 Hz, 2H), 7.19 (t, J = 7.6 Hz, 1H),7.38 (d, J = 7.3 Hz, 2H), 7.43 (d, J = 7.8 Hz, 2H), 7.55-7.57 (m, 3H), 7.74 (d, J = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.5, 16.4, 19.4, 19.5, 55.4, 114.2, 117.6, 120.5, 120.6, 123.7, 124.4, 124.9, 125.2, 126.5, 128.2, 129.5, 129.7, 130.1, 130.9, 131.2, 134.6, 147.4, 148.7, 154.3, 158.7; HRMS (ESI) calcd for $C_{29}H_{26}O_2$: 407.2006 ($M + H^+$), found: 407.2027.



4-Phenyl-2,3-dipropyl-1-(*p*-tolyl)cyclopenta[*c*]chromene (**3i**)

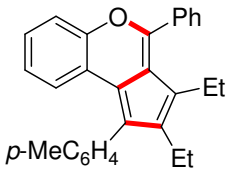
Red solid (plate), mp: 125.2-126.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.50 (t, J = 6.9 Hz, 3H), 0.78 (t, J = 6.9 Hz, 3H), 1.06-1.11 (m, 2H), 1.26-1.33 (m, 2H), 2.30 (t, J = 7.8 Hz, 2H), 2.41 (t, J = 7.6 Hz, 2H), 2.47 (s, 3H), 6.99 (t, J = 7.6 Hz, 1H), 7.16 (t, J = 7.6 Hz, 1H), 7.30-7.32 (m, 4H), 7.40 (d, J = 7.8 Hz, 2H), 7.53-7.55 (m, 3H), 7.70 (d, J = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.6, 21.5, 24.1, 25.5, 28.7, 117.6, 118.5, 120.6, 120.8, 123.7, 124.1, 124.3, 125.2, 128.3, 129.5, 129.7, 129.9, 130.0, 134.6, 135.7, 136.5, 145.9, 148.7, 154.2; HRMS (ESI) calcd for $C_{31}H_{30}O$: 419.2369 ($M + H^+$), found: 419.2399.



4-(4-Chlorophenyl)-2,3-dipropyl-1-(*p*-tolyl)cyclopenta[*c*]chromene (**3j**)

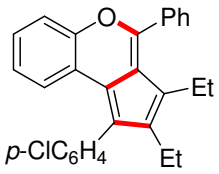
Red solid (plate), mp: 96.9-97.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.56 (t, J = 6.9 Hz, 3H), 0.78 (t, J = 7.1 Hz, 3H), 1.07-1.12 (m, 2H), 1.27-1.32 (m, 2H), 2.32 (t, J = 7.6 Hz, 2H), 2.41 (t, J = 7.6 Hz, 2H), 2.46 (s, 3H), 6.99 (t, J = 7.3 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 7.29-7.32 (m, 4H), 7.38 (d, J = 8.2 Hz, 2H), 7.51 (d, J = 7.4 Hz, 2H), 7.64 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.6, 21.5, 24.0, 25.5, 28.7, 117.5, 118.5, 120.5, 121.1, 123.7, 124.5, 125.3, 128.6, 129.5, 129.9, 130.3, 131.2, 133.1, 135.5, 136.3, 136.6, 146.5, 148.6, 152.7; HRMS (ESI) calcd for $C_{31}H_{29}ClO$:

453.1980 (M + H^+), found: 453.1964.



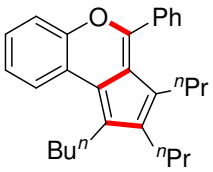
2,3-Diethyl-4-phenyl-1-(*p*-tolyl)cyclopenta[*c*]chromene (**3k**)

Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.74 (t, *J* = 6.9 Hz, 3H), 0.94 (t, *J* = 6.9 Hz, 3H), 2.40 (q, *J* = 6.9 Hz, 2H), 2.44-2.50 (m, 5H), 7.01 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.8 Hz, 1H), 7.30-7.35 (m, 4H), 7.40-7.43 (m, 2H), 7.54-7.56 (m, 3H), 7.73 (d, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.5, 16.4, 19.3, 19.5, 21.5, 117.6, 120.6, 123.7, 124.3, 125.0, 125.2, 128.2, 129.5, 129.7, 129.8, 129.9, 130.1, 134.6, 135.6, 136.5, 147.3, 148.7, 154.3; HRMS (ESI) calcd for $C_{29}H_{27}O$: 391.2056 (M + H^+), found: 391.2080.



1-(4-Chlorophenyl)-2,3-diethyl-4-phenylcyclopenta[*c*]chromene (**3l**)

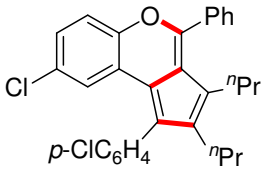
Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.72 (t, *J* = 7.3 Hz, 3H), 0.91 (t, *J* = 7.3 Hz, 3H), 2.38 (q, *J* = 7.3 Hz, 2H), 2.45 (q, *J* = 7.3 Hz, 2H), 7.12 (d, *J* = 8.7 Hz, 1H), 7.30-7.37 (m, 4H), 7.49-7.59 (m, 6H), 7.70 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.4, 16.3, 19.3, 19.4, 117.9, 119.1, 120.4, 121.5, 122.7, 125.5, 126.1, 128.3, 129.2, 129.4, 129.6, 129.7, 130.4, 131.3, 133.3, 134.1, 136.6, 147.0, 154.8; HRMS (ESI) calcd for $C_{28}H_{23}ClO$: 411.1510 (M + H^+), found: 411.1512.



1-Butyl-4-phenyl-2,3-dipropylcyclopenta[*c*]chromene (**3m**)

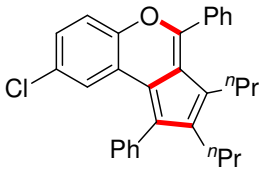
Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.47 (t, *J* = 6.9 Hz, 3H), 1.01-1.05 (m, 8H), 1.55-1.60 (m, 4H), 1.66-1.68 (m, 2H), 2.23 (t, *J* = 7.6 Hz, 2H), 2.53 (t, *J* = 7.4 Hz, 2H), 2.90 (t, *J* = 7.3 Hz, 2H), 7.23 (t, *J* = 5.0 Hz, 1H), 7.33 (t, *J* = 7.1 Hz, 1H), 7.43 (d,

J = 7.8 Hz, 1H), 7.50-7.52 (m, 3H), 7.65 (d, *J* = 6.8 Hz, 2H), 8.02 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.1, 14.2, 14.9, 23.5, 24.8, 25.6, 27.1, 28.6, 28.7, 31.9, 116.9, 117.7, 120.8, 121.3, 123.7, 124.4, 124.6, 124.7, 128.2, 129.7, 129.9, 130.2, 134.7, 145.7, 148.6, 153.0; HRMS (ESI) calcd for $C_{28}H_{32}O$: 385.2526 (M + H^+), found: 385.2536.



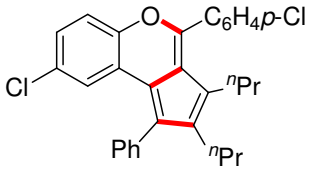
8-Chloro-1-(4-chlorophenyl)-4-phenyl-2,3-dipropylcyclopenta[*c*]chromene (**3n**)

Red solid (plate), mp: 117.8-118.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.50 (t, *J* = 7.1 Hz, 3H), 0.78 (t, *J* = 7.1 Hz, 3H), 1.04-1.10 (m, 2H), 1.23-1.27 (m, 2H), 2.29 (t, *J* = 8.02 Hz, 2H), 2.39 (t, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 8.7 Hz, 1H), 7.29 (s, 1H), 7.34-7.36 (m, 3H), 7.49 (d, *J* = 8.3, 2H), 7.54-7.56 (m, 3H), 7.68 (d, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.5, 24.0, 25.4, 28.6, 117.8, 119.1, 120.6, 121.5, 122.7, 125.1, 125.5, 128.3, 129.1, 129.5, 129.6, 130.3, 131.3, 133.2, 134.1, 136.6, 145.7, 147.0, 154.7; HRMS (ESI) calcd for $C_{30}H_{26}Cl_2O$: 473.1433 (M + H^+), found: 473.1469.



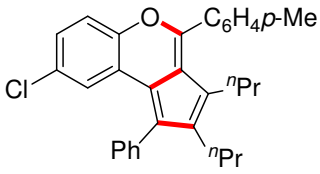
8-Chloro-1,4-diphenyl-2,3-dipropylcyclopenta[*c*]chromene (**3o**)

Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.51 (t, *J* = 7.1 Hz, 3H), 0.77 (t, *J* = 7.1 Hz, 3H), 1.06-1.12 (m, 2H), 1.26-1.32 (m, 2H), 2.31 (t, *J* = 7.8 Hz, 2H), 2.42 (t, *J* = 7.6 Hz, 2H), 7.09 (d, *J* = 8.7 Hz, 1H), 7.24 (s, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 6.4, Hz, 1H), 7.50 (d, *J* = 6.9 Hz, 2H), 7.52-7.56 (m, 3H), 7.69 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.6, 24.0, 25.5, 27.8, 28.6, 117.5, 118.9, 120.6, 121.7, 122.9, 124.9, 125.2, 127.4, 128.3, 128.9, 129.5, 129.7, 129.8, 130.2, 131.2, 134.2, 138.1, 146.1, 147.1, 154.4; HRMS (ESI) calcd for $C_{30}H_{27}ClO$: 439.1823 (M + H^+), found: 439.1803.



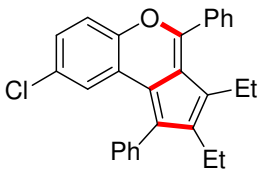
8-Chloro-4-(4-chlorophenyl)-1-phenyl-2,3-dipropylcyclopenta[*c*]chromene (**3p**)

Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.57 (t, *J* = 7.2 Hz, 3H), 0.78 (t, *J* = 7.4 Hz, 3H), 1.08-1.13 (m, 2H), 1.26-1.32 (m, 2H), 2.32 (t, *J* = 7.8 Hz, 2H), 2.42 (t, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 1H), 7.25 (s, 1H), 7.32 (d, *J* = 8.8 Hz, 1H), 7.39 (d, *J* = 6.8Hz, 2H), 7.45 (d, *J* = 7.2 Hz, 2H), 7.50-7.56 (m, 4H), 7.64 (d, *J* = 8.4, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.5, 24.0, 25.4, 28.5, 28.6, 117.6, 118.9, 120.9, 121.6, 122.9, 124.5, 125.3, 127.5, 128.6, 128.9, 129.6, 129.7, 131.1, 131.5, 132.6, 136.5, 137.9, 146.6, 147.0, 152.8; HRMS (ESI) calcd for $C_{30}H_{26}Cl_2O$: 473.1433 (M + H^+), found: 473.1421.



8-Chloro-1-phenyl-2,3-dipropyl-4-(*p*-tolyl)cyclopenta[*c*]chromene (**3q**)

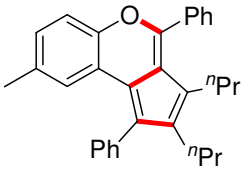
Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.53 (t, *J* = 7.1 Hz, 3H), 0.77 (t, *J* = 7.1 Hz, 3H), 1.08-1.12 (m, 2H), 1.27-1.30 (m, 2H), 2.34 (t, *J* = 7.8 Hz, 2H), 2.42 (t, *J* = 7.8 Hz, 2H), 2.48 (s, 3H), 7.08 (d, *J* = 8.7 Hz, 1H), 7.25 (s, 1H), 7.31-7.36 (m, 3H), 7.39-7.45 (m, 3H), 7.49-7.52 (m, 2H), 7.58 (d, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.6, 21.7, 24.0, 25.4, 28.6, 28.7, 117.5, 118.9, 120.5, 121.7, 122.9, 125.0, 125.1, 127.3, 128.9, 129.0, 129.4, 129.6, 129.8, 131.1, 131.3, 138.1, 140.4, 145.9, 147.1, 154.7; HRMS (ESI) calcd for $C_{31}H_{29}ClO$: 453.1980 (M + H^+), found: 453.1978.



8-Chloro-2,3-diethyl-1,4-diphenylcyclopenta[*c*]chromene (**3r**)

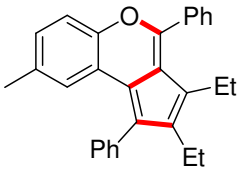
Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.74 (t, *J* = 7.3 Hz, 3H), 0.93 (t, *J* = 7.6 Hz,

3H), 2.40 (q, *J* = 7.6 Hz, 2H), 2.48 (q, *J* = 7.3 Hz, 2H), 7.10 (d, *J* = 8.7Hz, 1H), 7.25 (s, 1H), 7.34 (d, *J* = 9.2 Hz, 1H), 7.42-7.47 (m, 3H), 7.51-7.56 (m, 5H), 7.71 (d, *J* = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.4, 16.3, 19.3, 19.5, 117.6, 118.9, 120.4, 121.7, 122.9, 125.2, 125.8, 127.4, 128.3, 129.0, 129.5, 129.7, 129.8, 130.3, 131.0, 134.2, 138.0, 147.0, 147.4, 154.5; HRMS (ESI) calcd for $C_{28}H_{23}ClO$: 411.1510 ($M + H^+$), found: 411.1526.



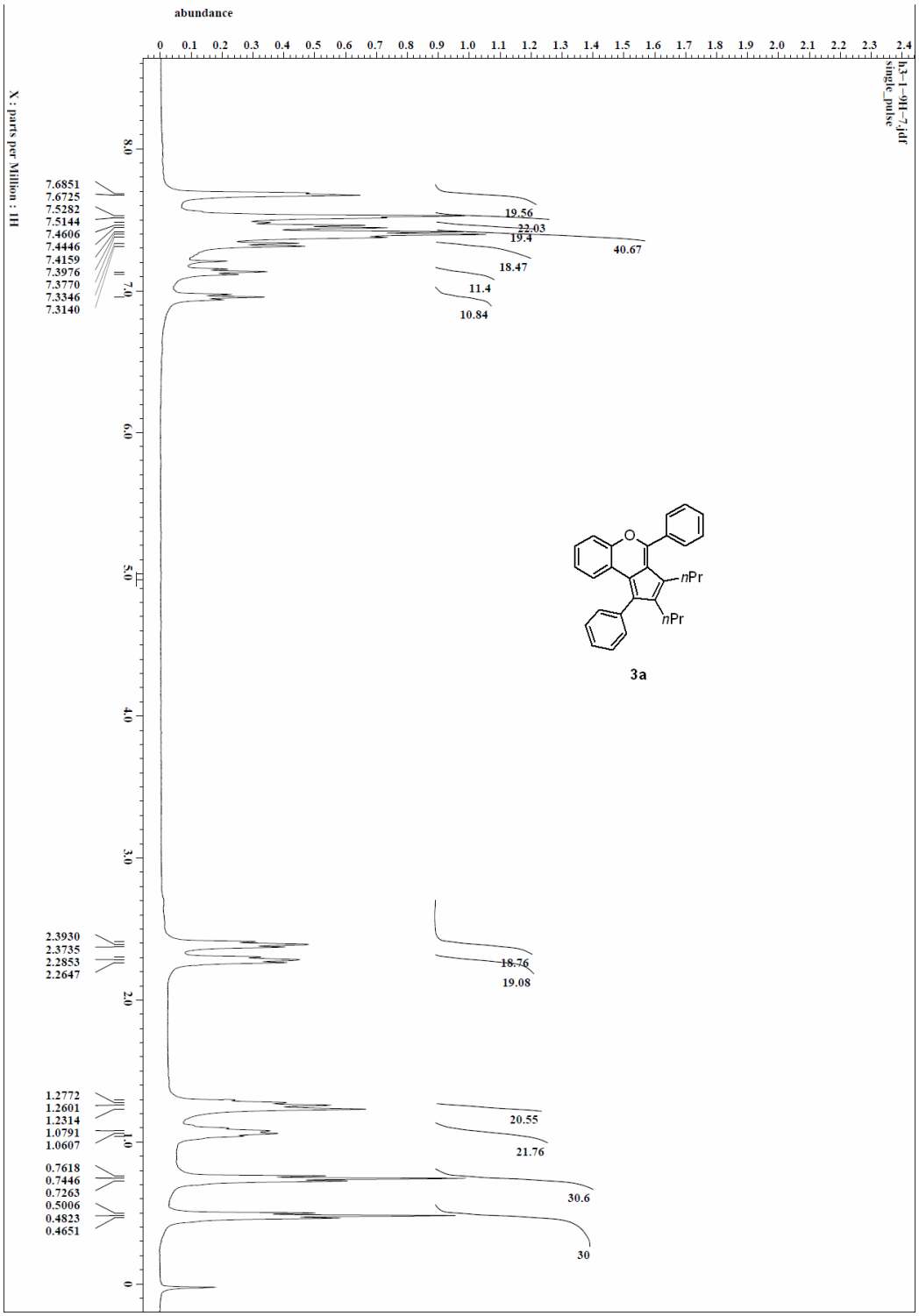
8-Methyl-1,4-diphenyl-2,3-dipropylcyclopenta[*c*]chromene (**3s**)

Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.50 (t, *J* = 7.3 Hz, 3H), 0.77 (t, *J* = 7.3 Hz, 3H), 1.06-1.10 (m, 2H), 1.25-1.31 (m, 2H), 2.13 (s, 3H), 2.30 (t, *J* = 8.2 Hz, 2H), 2.42 (t, *J* = 8.0 Hz, 2H), 6.97 (dd, *J* = 1.8, 8,2 Hz, 1H), 7.09-7.10 (m, 1H), 7.30 (d, *J* = 8.7, 2H), 7.39-7.54 (m, 7H), 7.70 (dd, *J* = 1.8, 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 14.6, 21.4, 24.1, 25.5, 28.7, 117.3, 118.7, 120.2, 120.7, 123.5, 123.9, 126.4, 126.9, 128.2, 128.6, 129.7, 130.0, 130.1, 133.7, 134.7, 139.0, 145.5, 147.0, 154.4; HRMS (ESI) calcd for $C_{31}H_{30}O$: 419.2369 ($M + H^+$), found: 419.2389.



2,3-Diethyl-8-methyl-1,4-diphenylcyclopenta[*c*]chromene (**3t**)

Red oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.74 (t, *J* = 7.3 Hz, 3H), 0.93 (t, *J* = 7.6 Hz, 3H), 2.14 (s, 3H), 2.39 (q, *J* = 7.6 Hz, 2H), 2.48 (q, *J* = 7.3 Hz, 2H), 6.98 (d, *J* = 8.2 Hz, 1H), 7.10 (s, 1H), 7.31 (d, *J* = 8.2 Hz, 2H), 7.42-7.55 (m, 7H), 7.72 (d, *J* = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.4, 16.4, 19.3, 19.5, 21.4, 117.3, 118.8, 120.1, 120.4, 123.5, 124.8, 126.4, 127.0, 128.2, 128.6, 129.5, 129.7, 130.1, 130.2, 133.7, 134.7, 138.9, 146.9, 147.0, 154.5; HRMS (ESI) calcd for $C_{29}H_{26}O$: 391.2056 ($M + H^+$), found: 391.2083.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7.4606
7.4446
7.4159
7.3976
7.3770
7.3346
7.3140
2.3930
2.3735
2.2853
2.2647
1.2772
1.2601
1.2314
1.0791
1.0607
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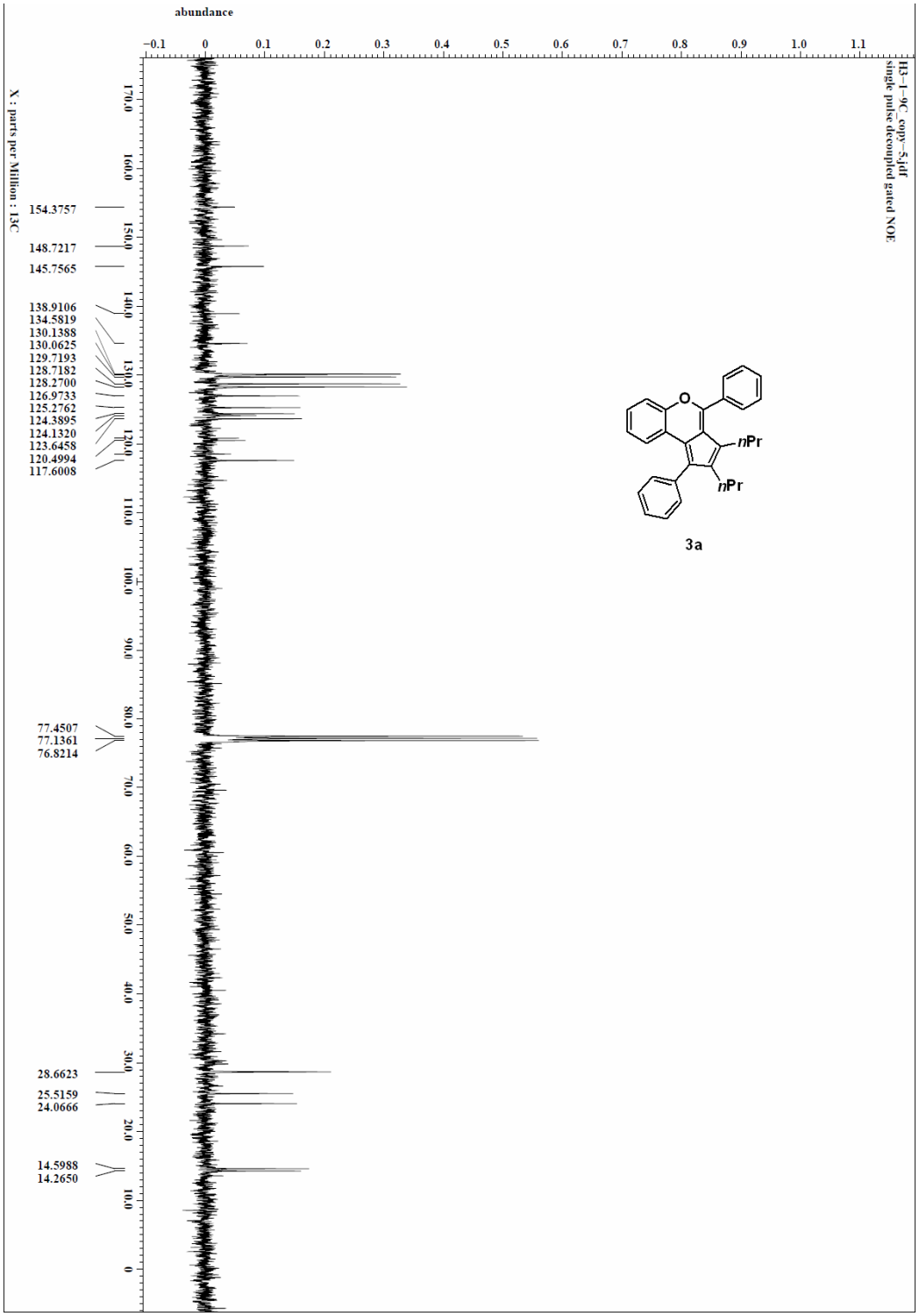
0.7446
0.7263
0.5006
0.4823
0.4651
19.56
22.03
19.4
40.67
18.47
11.4
10.84
18.76
19.08
20.55
21.76
30.6
30
nPr
nPr
3a


abundance
X : parts per Million : 13C
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single pulse decoupled gated NOE
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145.7565
138.9106
134.5819
130.1388
130.0625
129.7193
128.7182
128.2700
126.9733
125.2762
124.3895
124.1320
123.6458
120.4994
117.6008
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76.8214
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25.5159
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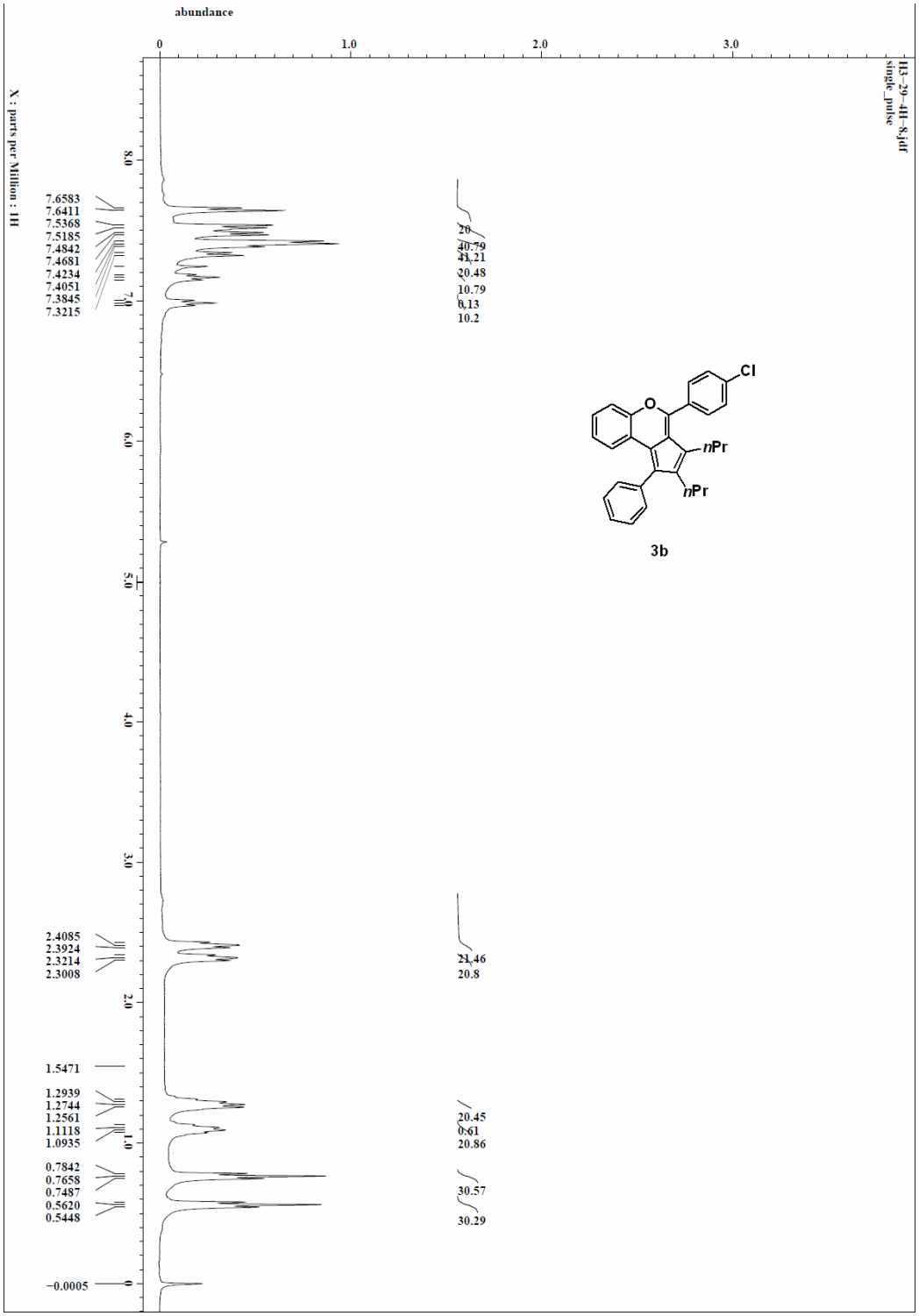
14.5988
14.2650
nPr
nPr
3a


abundance
X : parts per Million : 1H
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7.5368
7.5185
7.4842
7.4681
7.4234
7.4051
7.3845
7.3215
2.4085
2.3924
2.3214
2.3008
1.5471
1.2939
1.2744
1.2561
1.1118
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Cl
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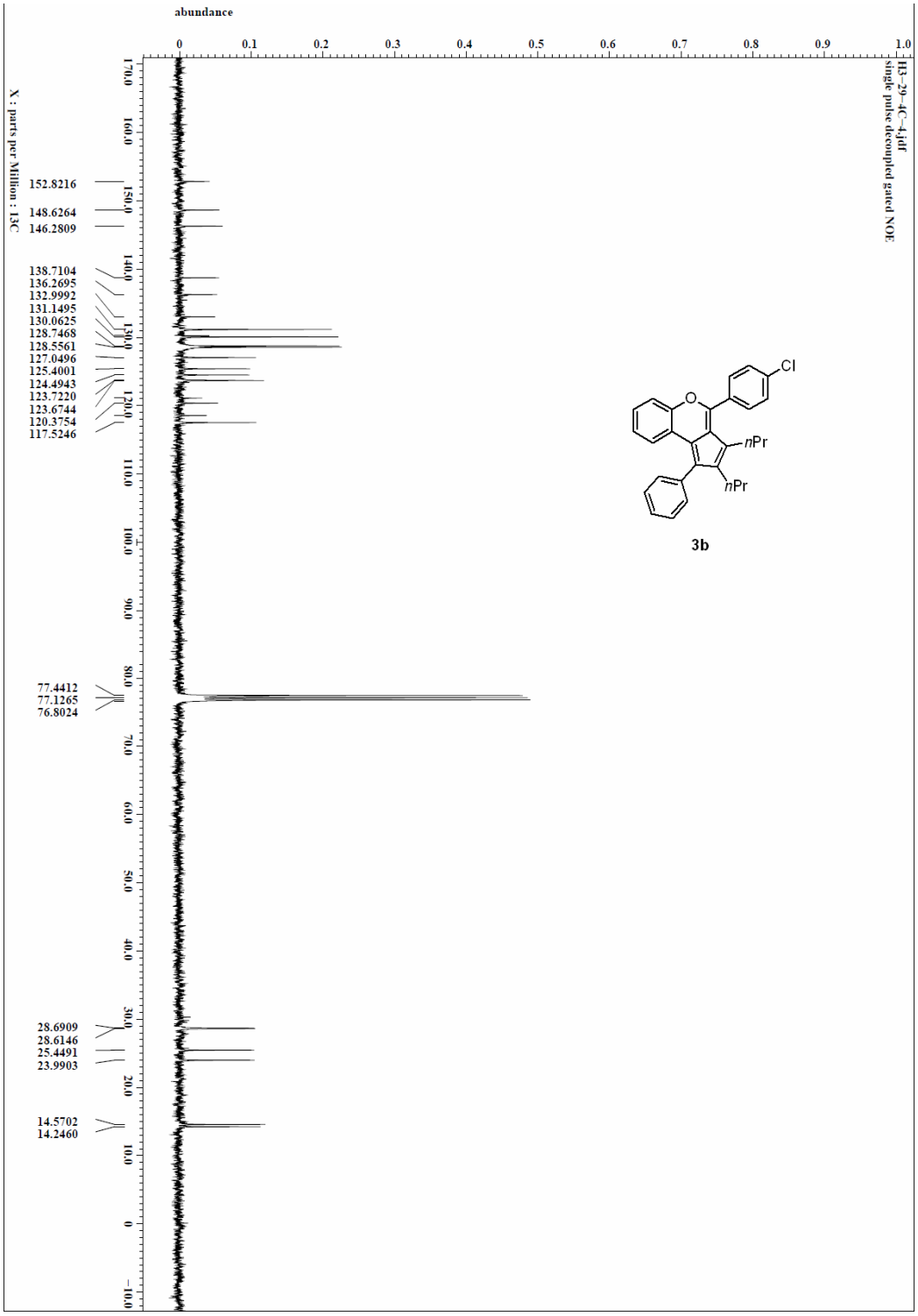
nPr
nPr
3b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0.8
0.9
1.0
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single pulse decoupled gated NOE
X : parts per Million : 13C
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150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
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152.8216
148.6264
146.2809
138.7104
136.2695
132.9992
131.1495
130.0625
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128.5561
127.0496
125.4001
124.4943
123.7220
123.6744
120.3754
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77.4412
77.1265
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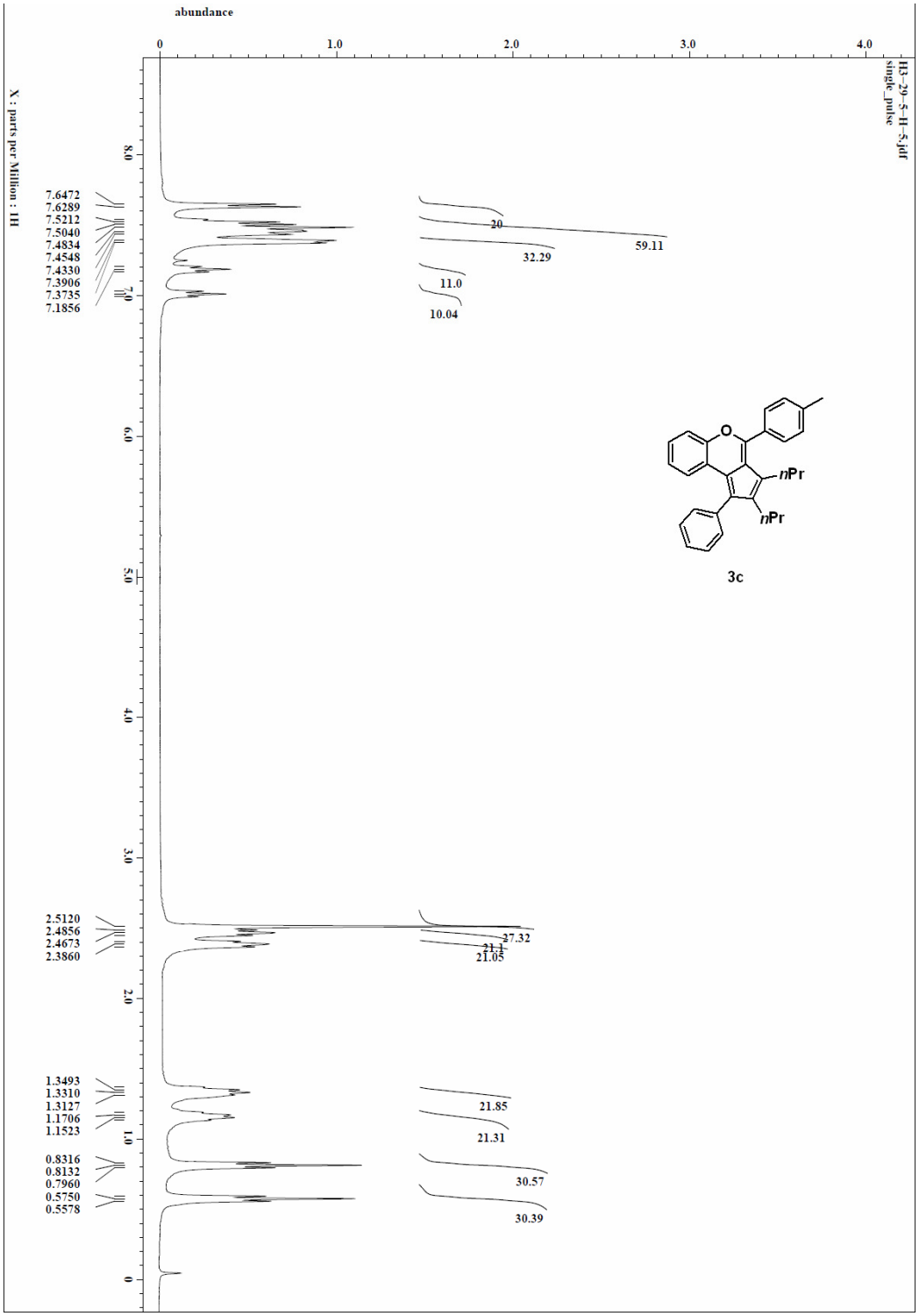
23.9903
14.5702
14.2460
Cl
O
nPr
nPr

3b


abundance
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7.4834
7.4548
7.4330
7.3906
7.3735
7.1856
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2.4856
2.4673
2.3860
1.3493
1.3310
1.3127
1.1706
1.1523
0.8316
0.8132
0.7960
0.5750
0.5578
20
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10.04
27.32
21.05
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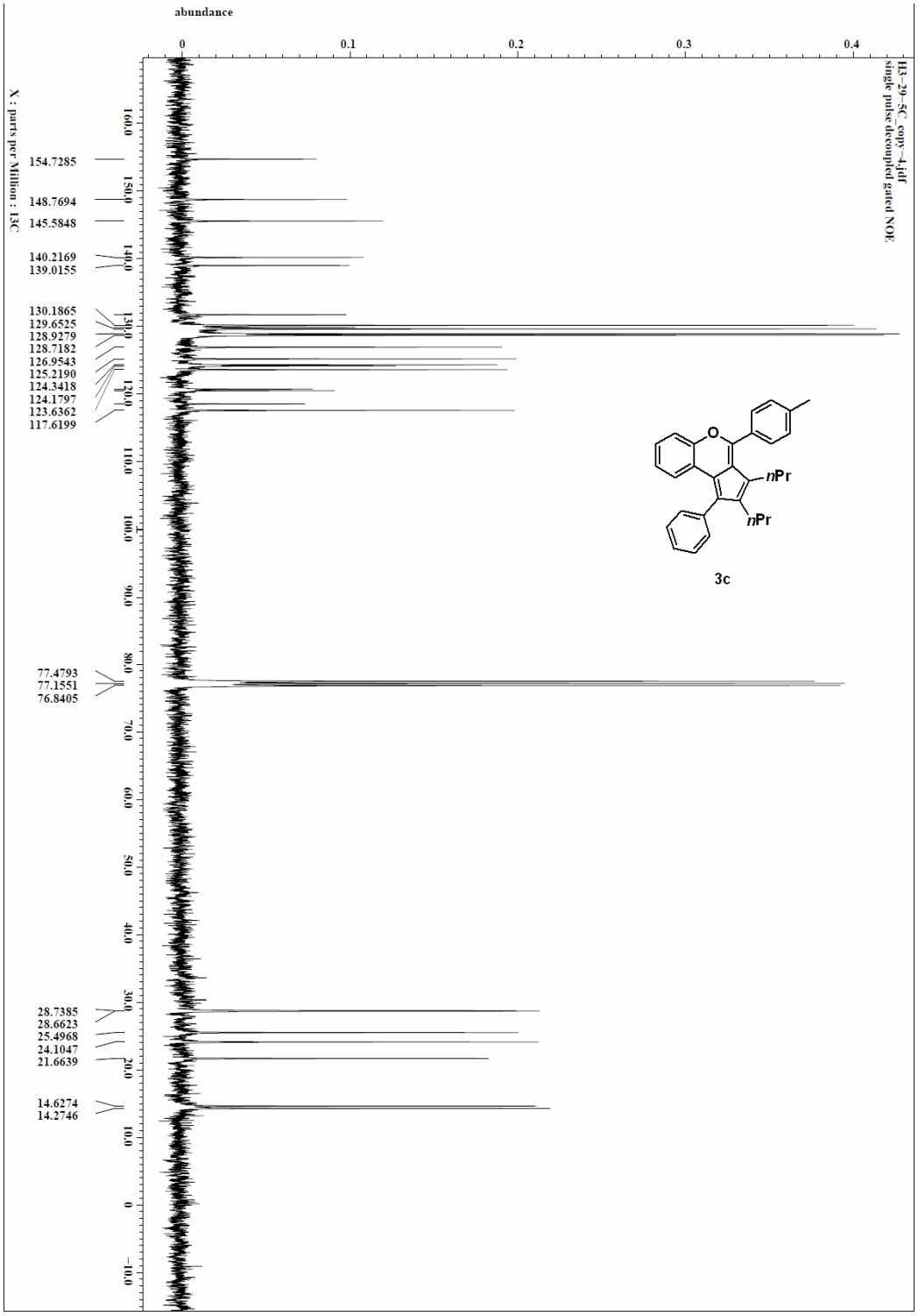
30.57
30.39
nPr
nPr
3c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0.4
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single pulse decoupled gated NOE
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139.0155
130.1865
129.6525
128.9279
128.7182
126.9543
125.2190
124.3418
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117.6199
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77.1551
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21.6639
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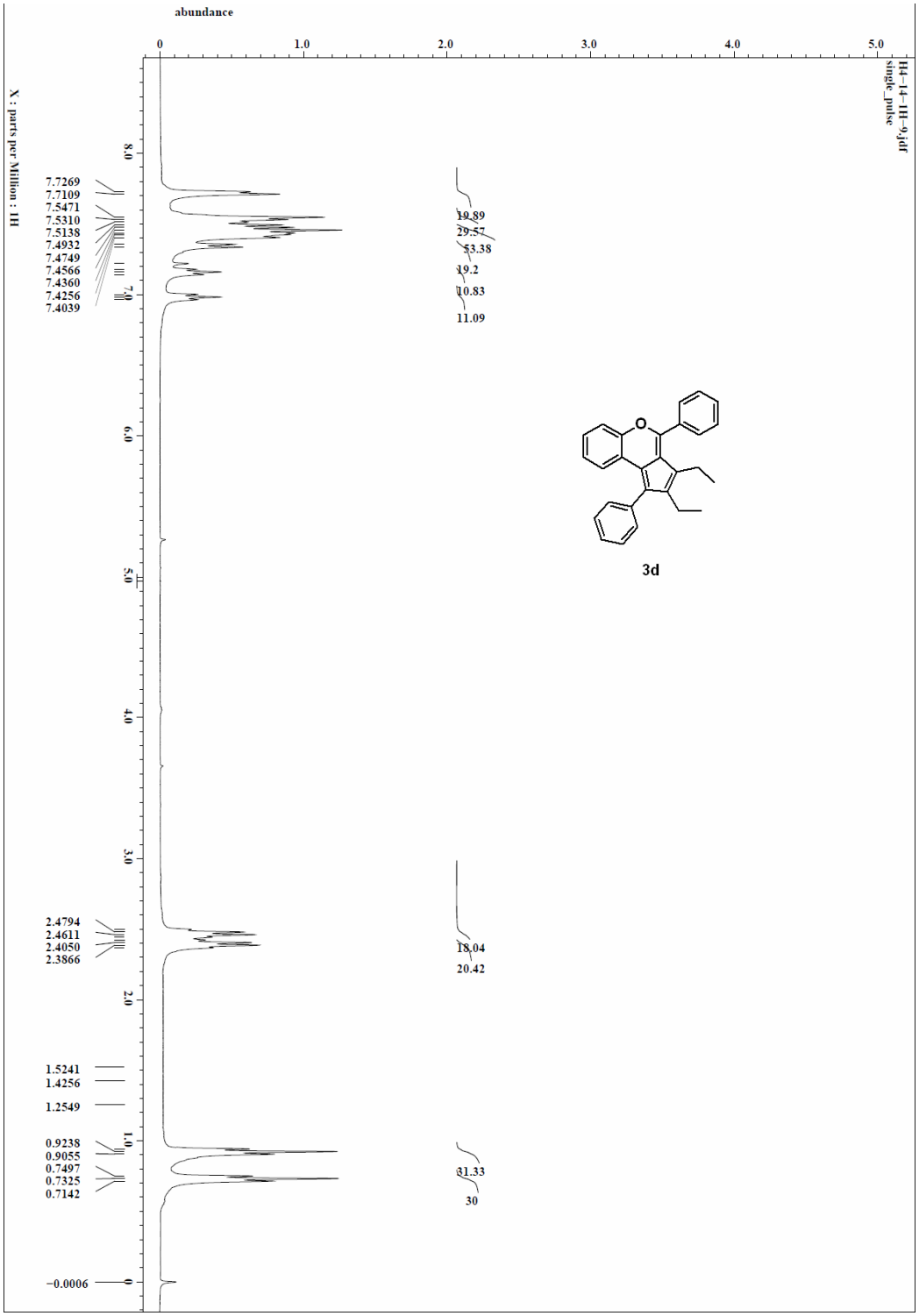
14.2746
nPr
nPr
3c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7.5138
7.4932
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7.4566
7.4360
7.4256
7.4039
2.4794
2.4611
2.4050
2.3866
1.5241
1.4256
1.2549
0.9238
0.9055
0.7497
0.7325
0.7142
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19.2
10.83
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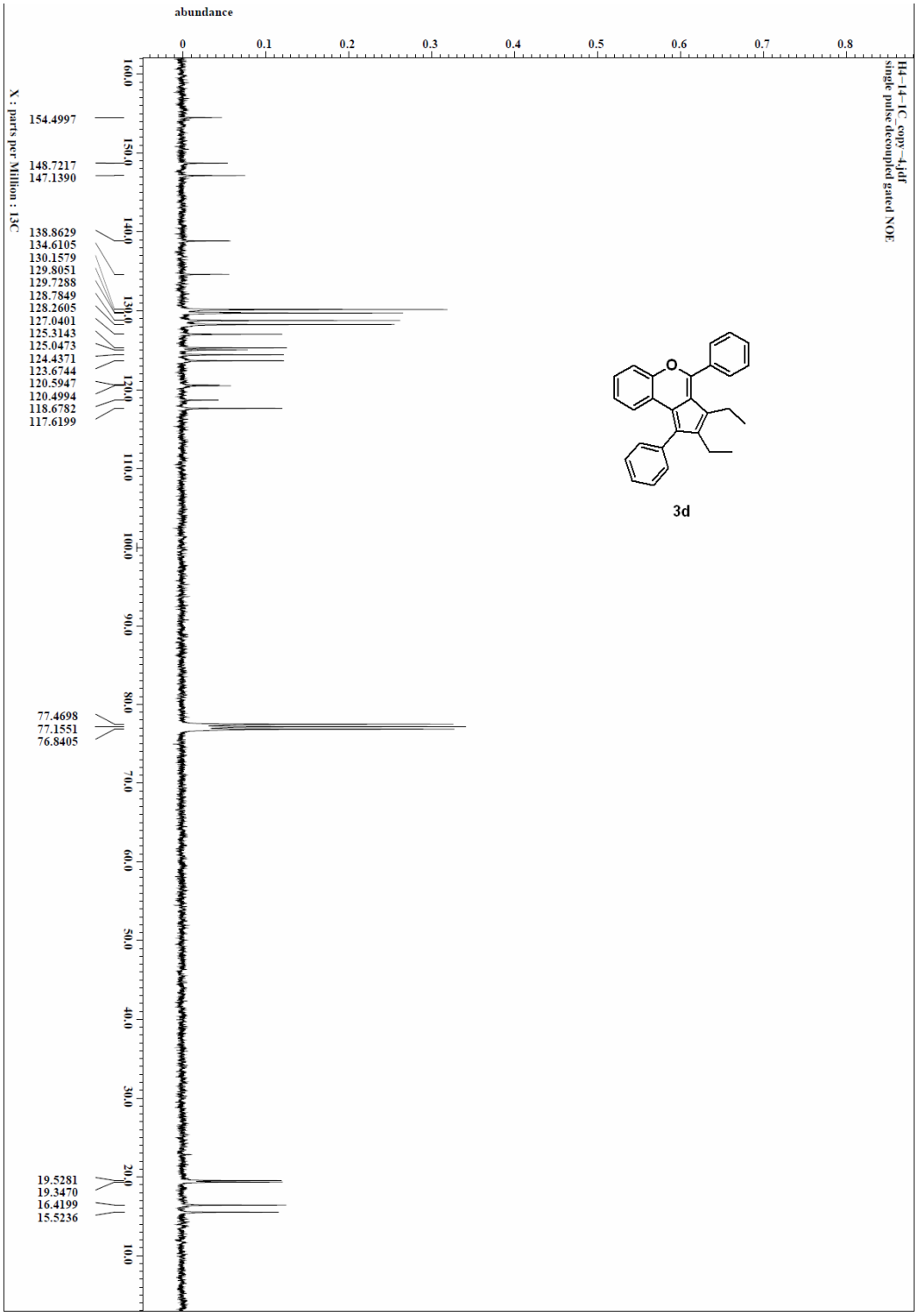
18.04
20.42
31.33
30
O
3d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147.1390
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123.6744
120.5947
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118.6782
117.6199
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77.1551
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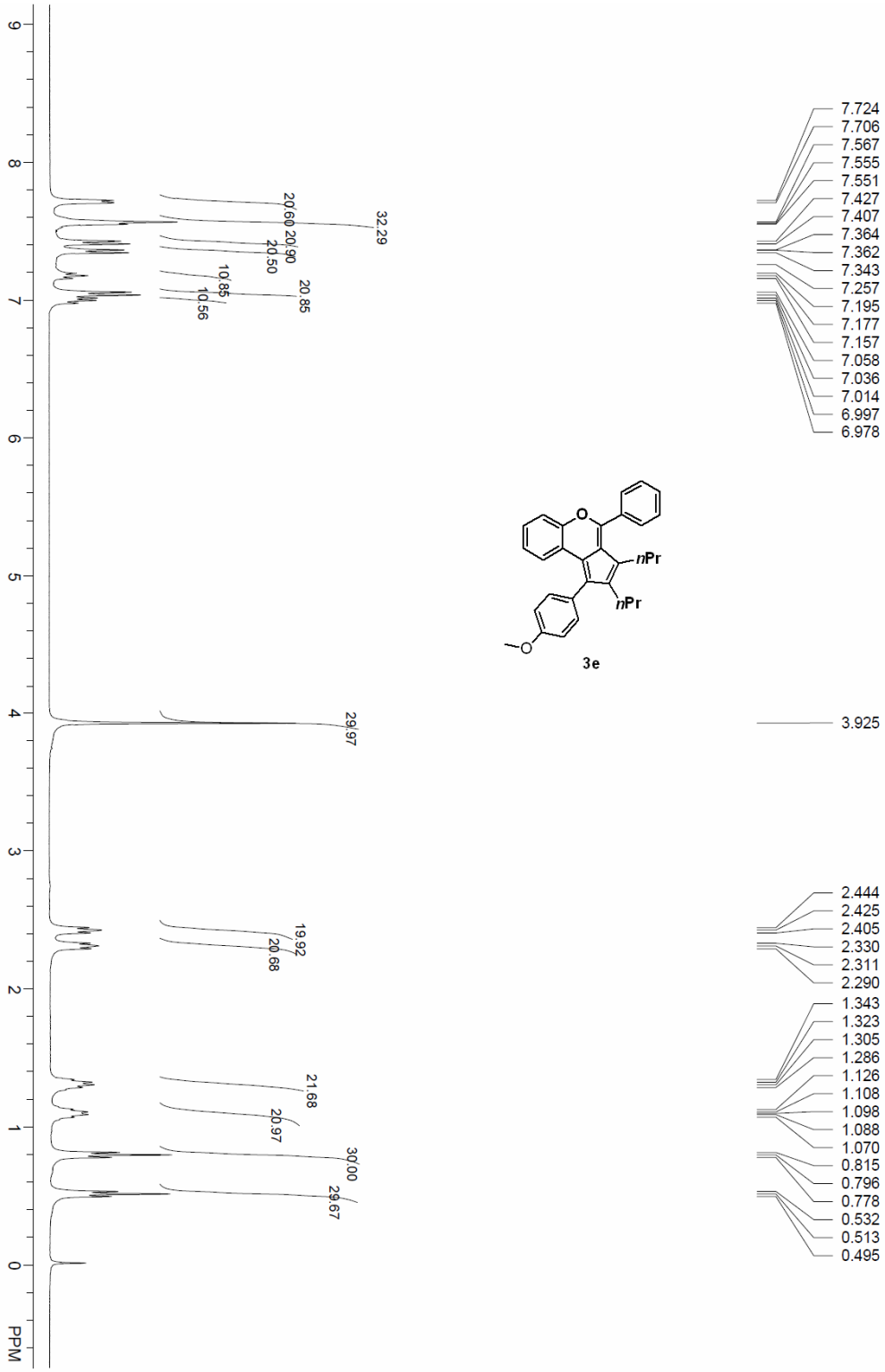
H4-14-1C copy-4.jdf
single pulse decoupled gated NOE
3d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19.92
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21.68
20.97
30.00
29.67
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7.427
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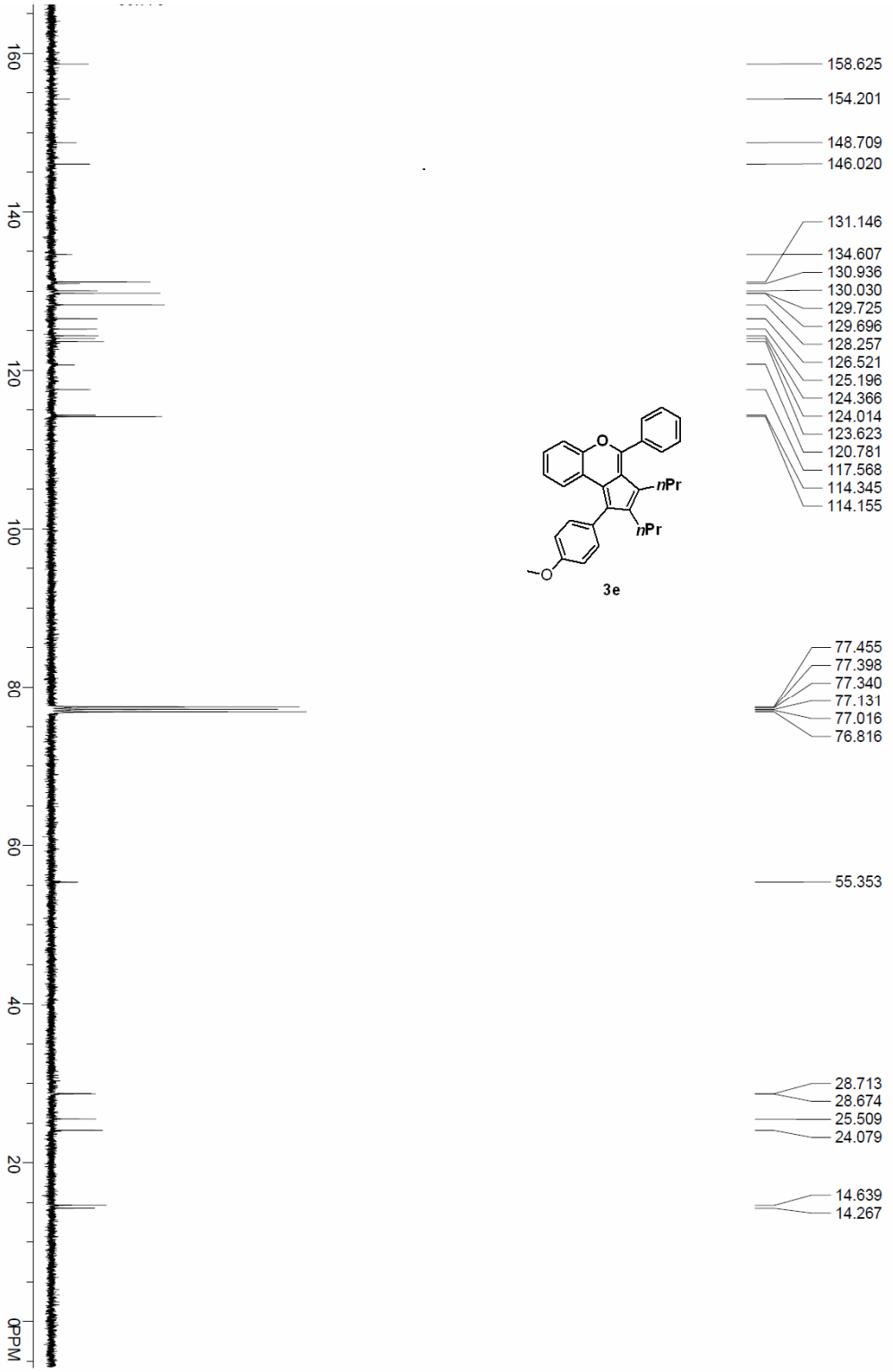
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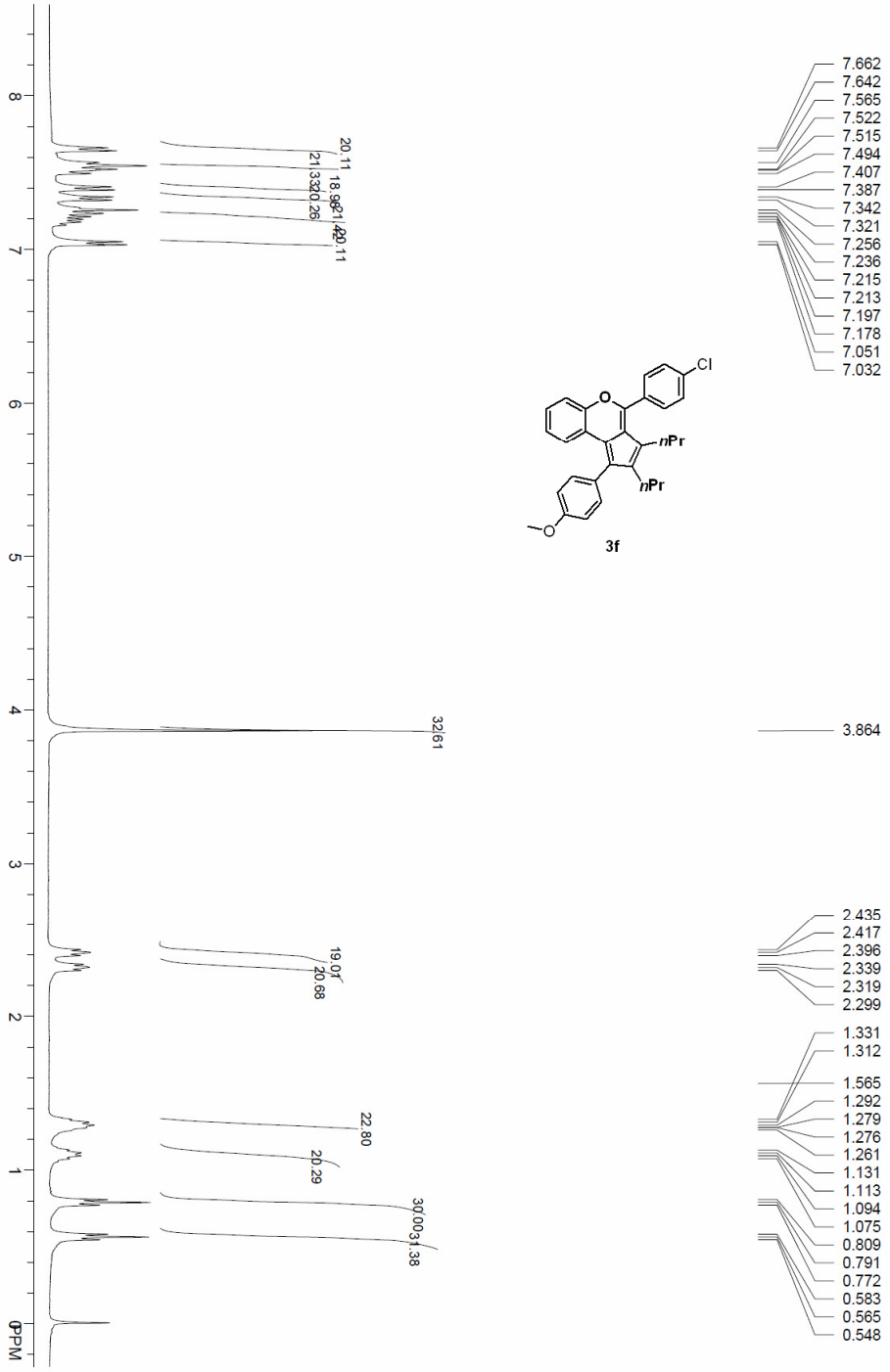
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7.213
7.197
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2.319
2.299
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21.42
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32.61
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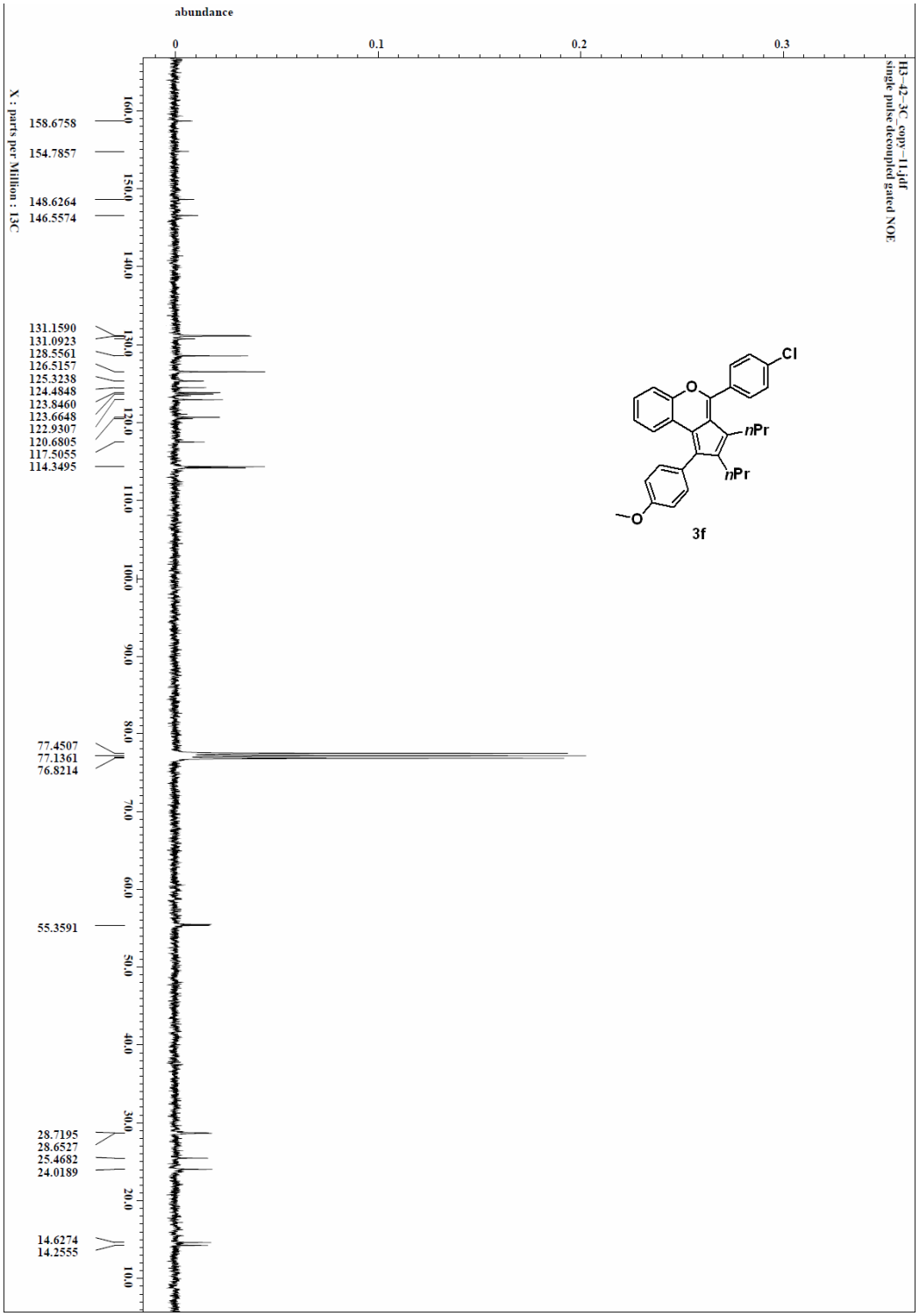
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0.1
0.2
0.3
X : parts per Million : 13C
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131.0923
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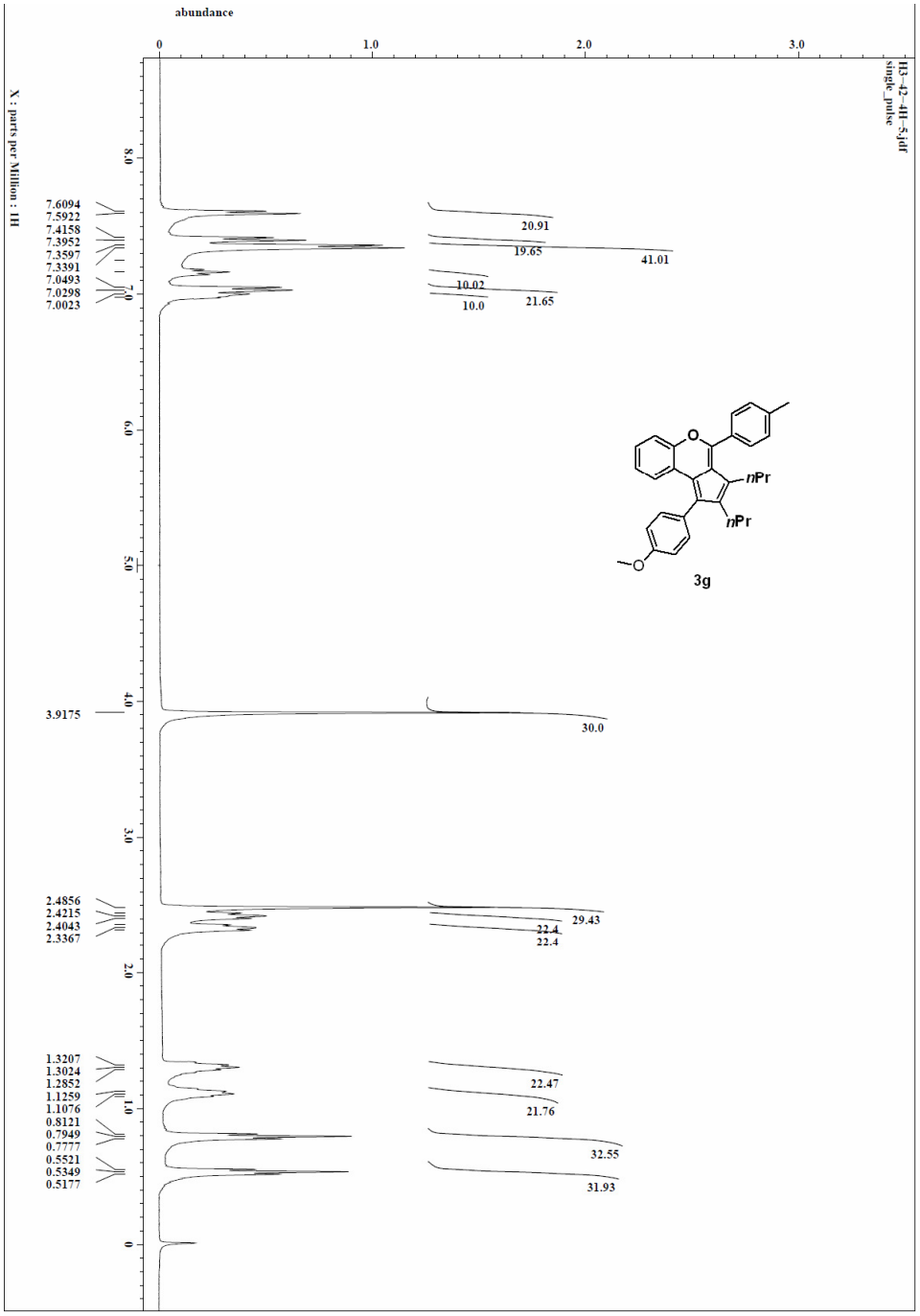
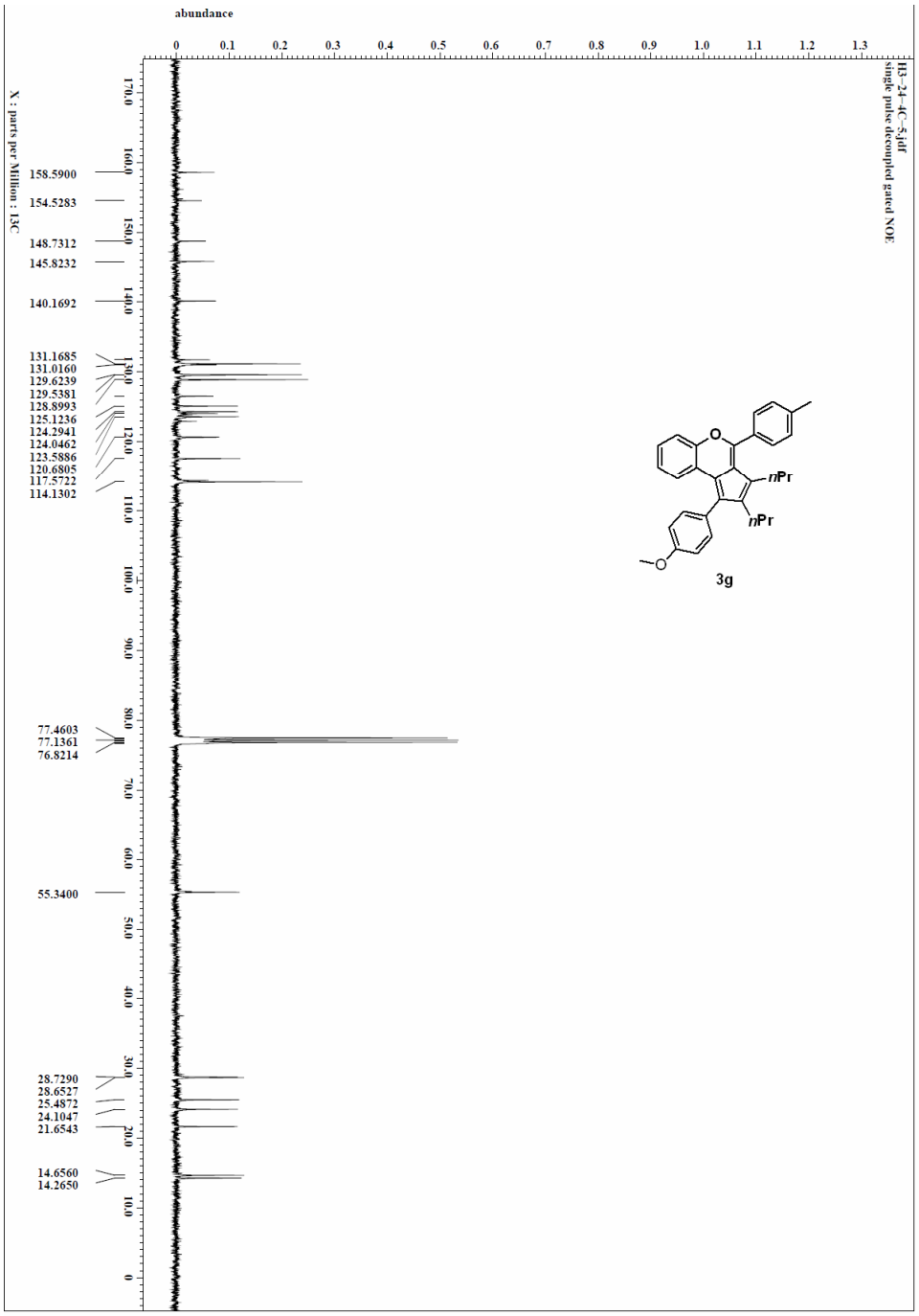
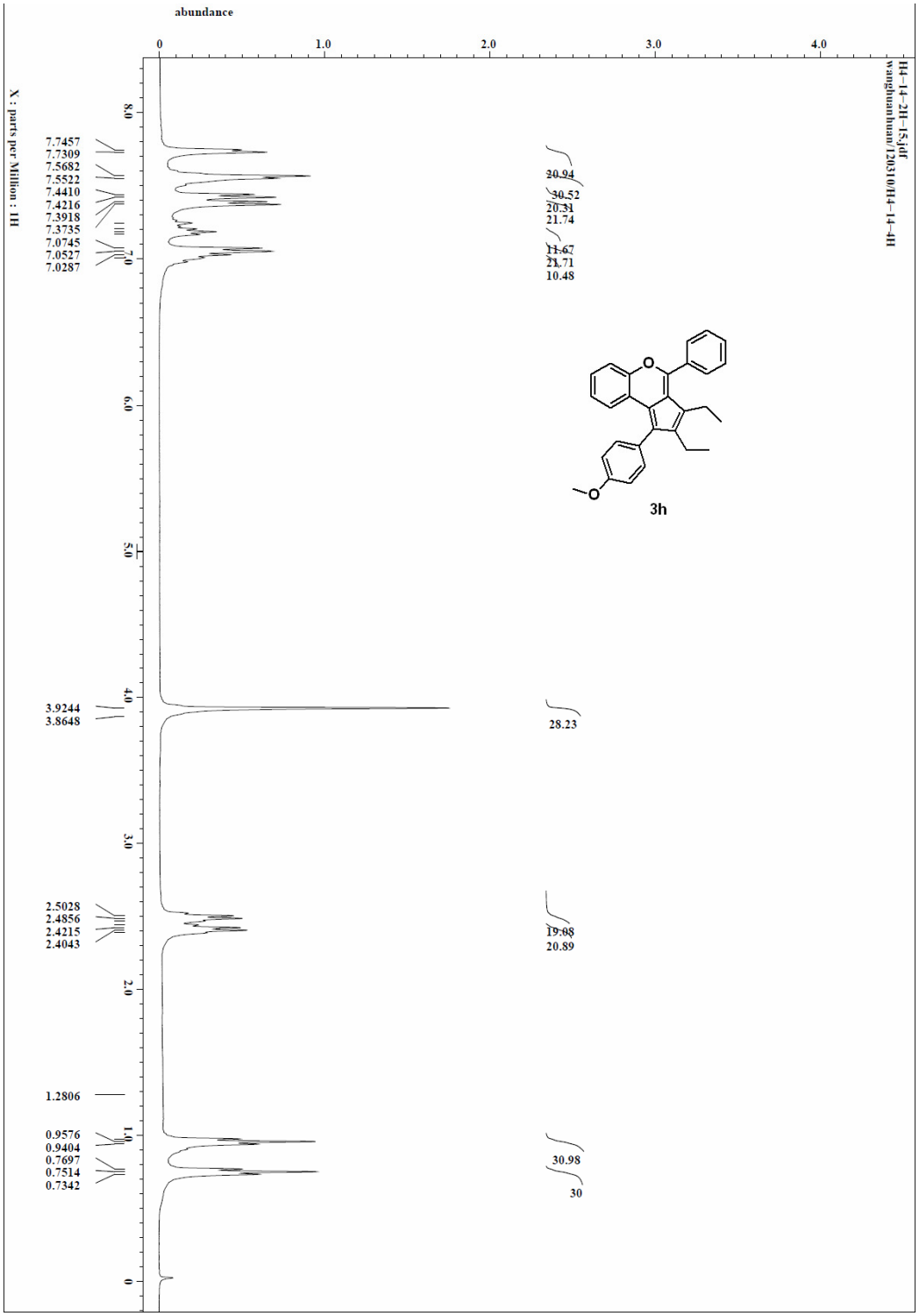
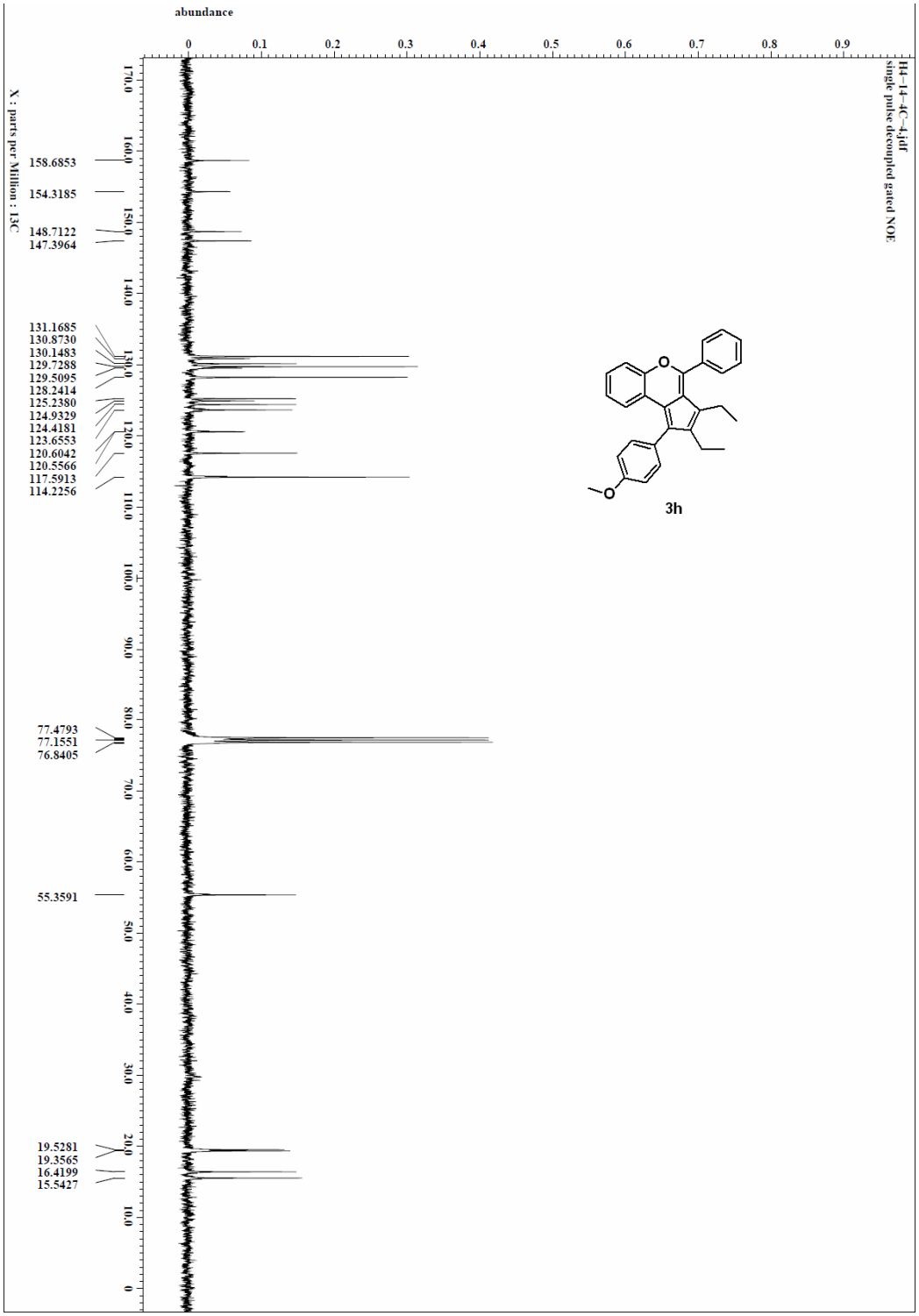
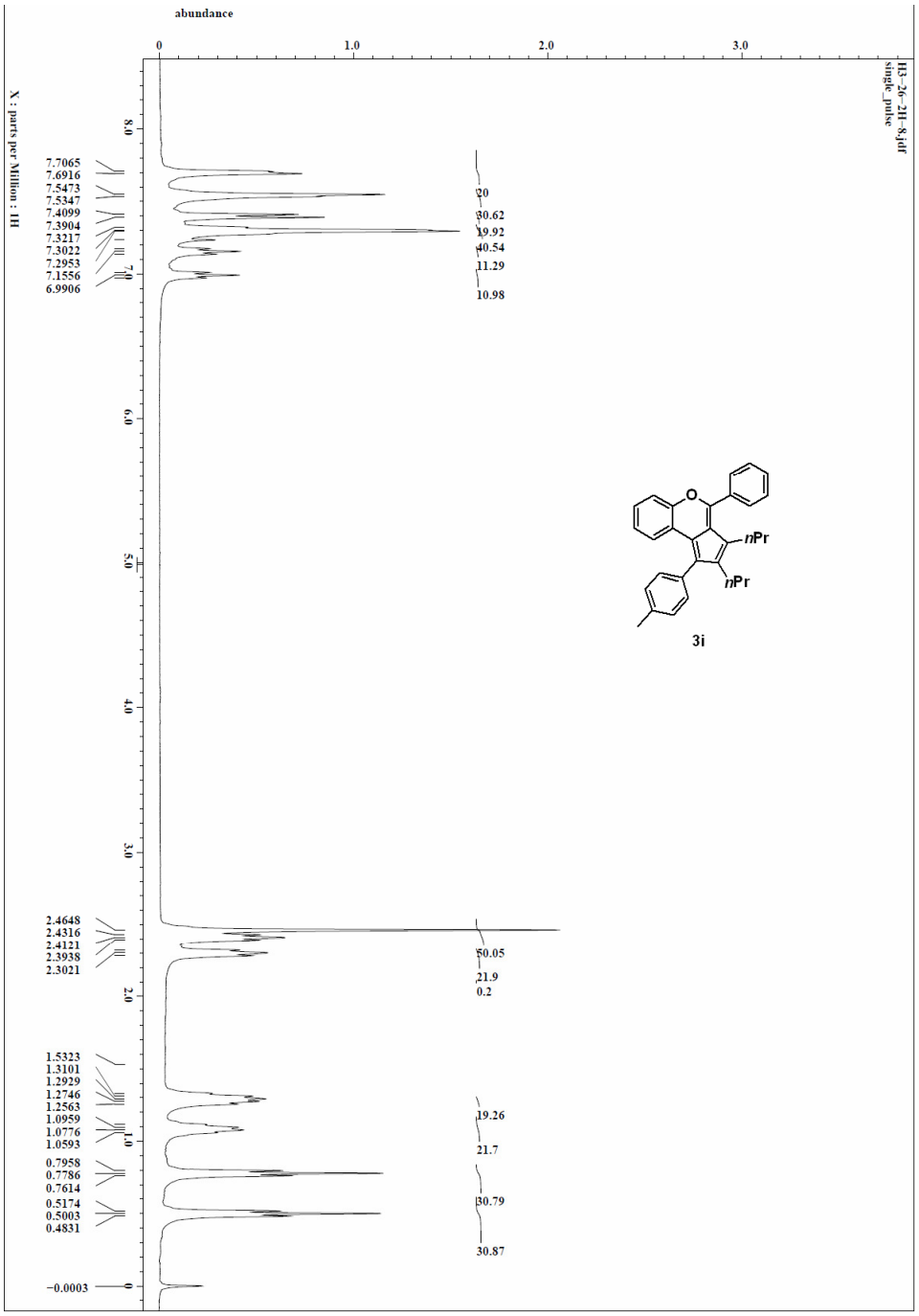
125.3238
124.4848
123.8460
123.6648
122.9307
120.6805
117.5055
114.3495
77.4507
77.1361
76.8214
55.3591
28.7195
28.6527
25.4682
24.0189
14.6274
14.2555
Cl
O
nPr
nPr
O
3f

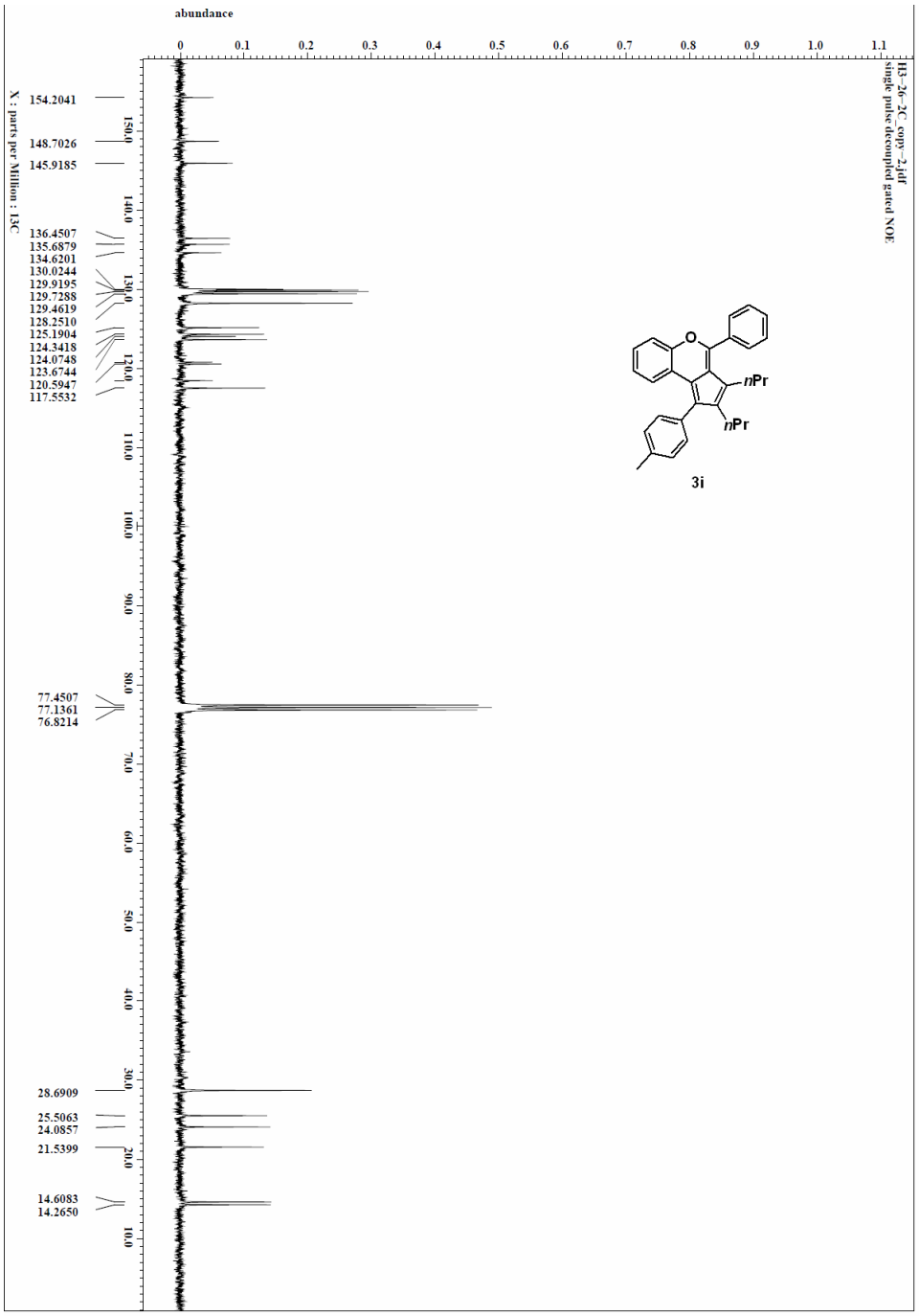

abundance
X : parts per Million : 1H
H3-42-4H-5.jdf
single_pulse
7.6094
7.5922
7.4158
7.3952
7.3597
7.3391
7.0493
7.0298
7.0023
3.9175
2.4856
2.4215
2.4043
2.3367
1.3207
1.3024
1.2852
1.1259
1.1076
0.8121
0.7949
0.7777
0.5521
0.5349
0.5177
20.91
19.65
41.01
10.02
10.0
21.65
30.0
29.43
22.4
22.4
22.47
21.76
32.55
31.93
nPr
nPr
3g

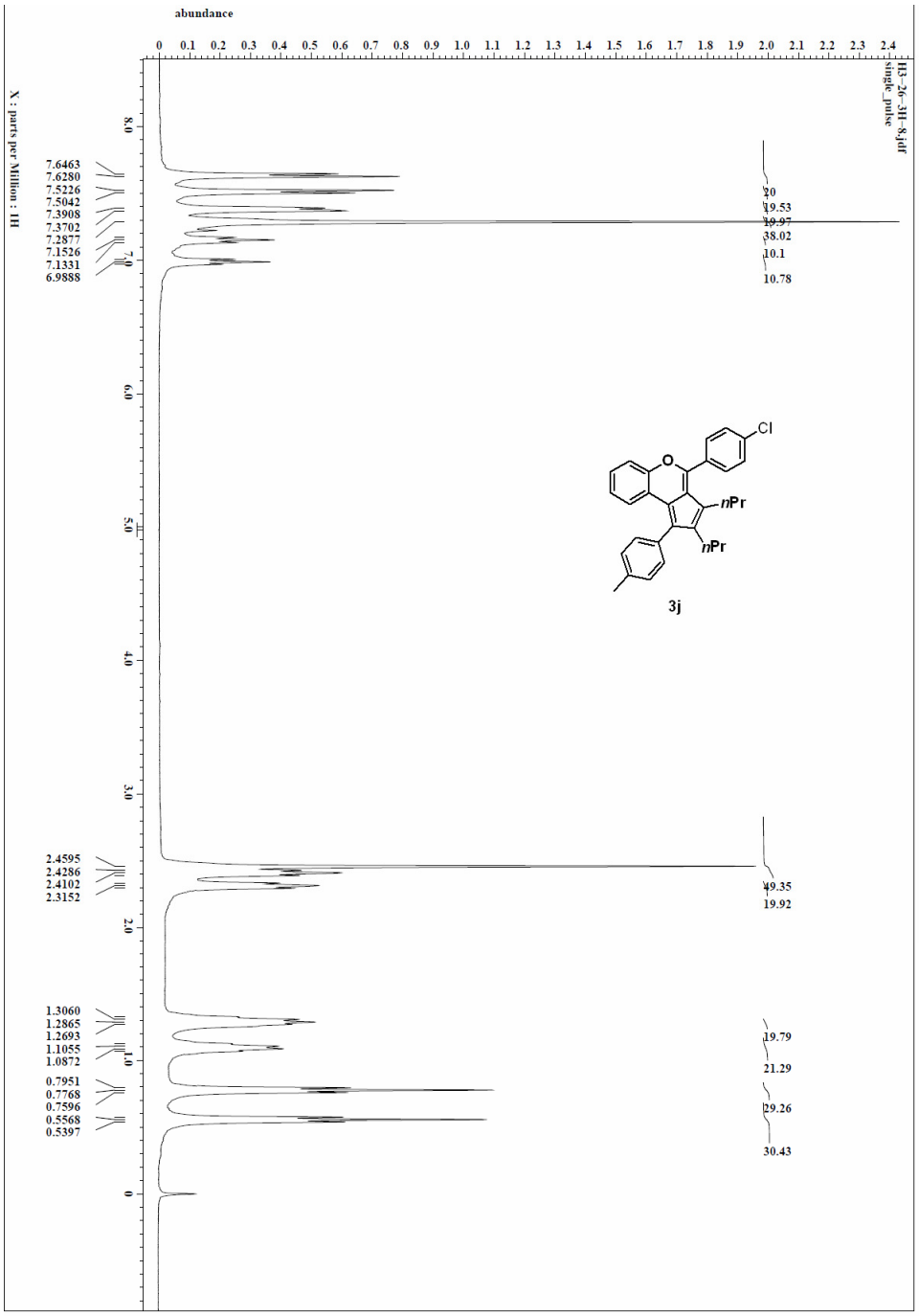

abundance
X : parts per Million : 13C
158.5900
154.5283
148.7312
145.8232
140.1692
131.1685
131.0160
129.6239
129.5381
128.8993
125.1236
124.2941
124.0462
123.5886
120.6805
117.5722
114.1302
77.4603
77.1361
76.8214
55.3400
28.7290
28.6527
25.4872
24.1047
21.6543
14.6560
14.2650
nPr
nPr
3g

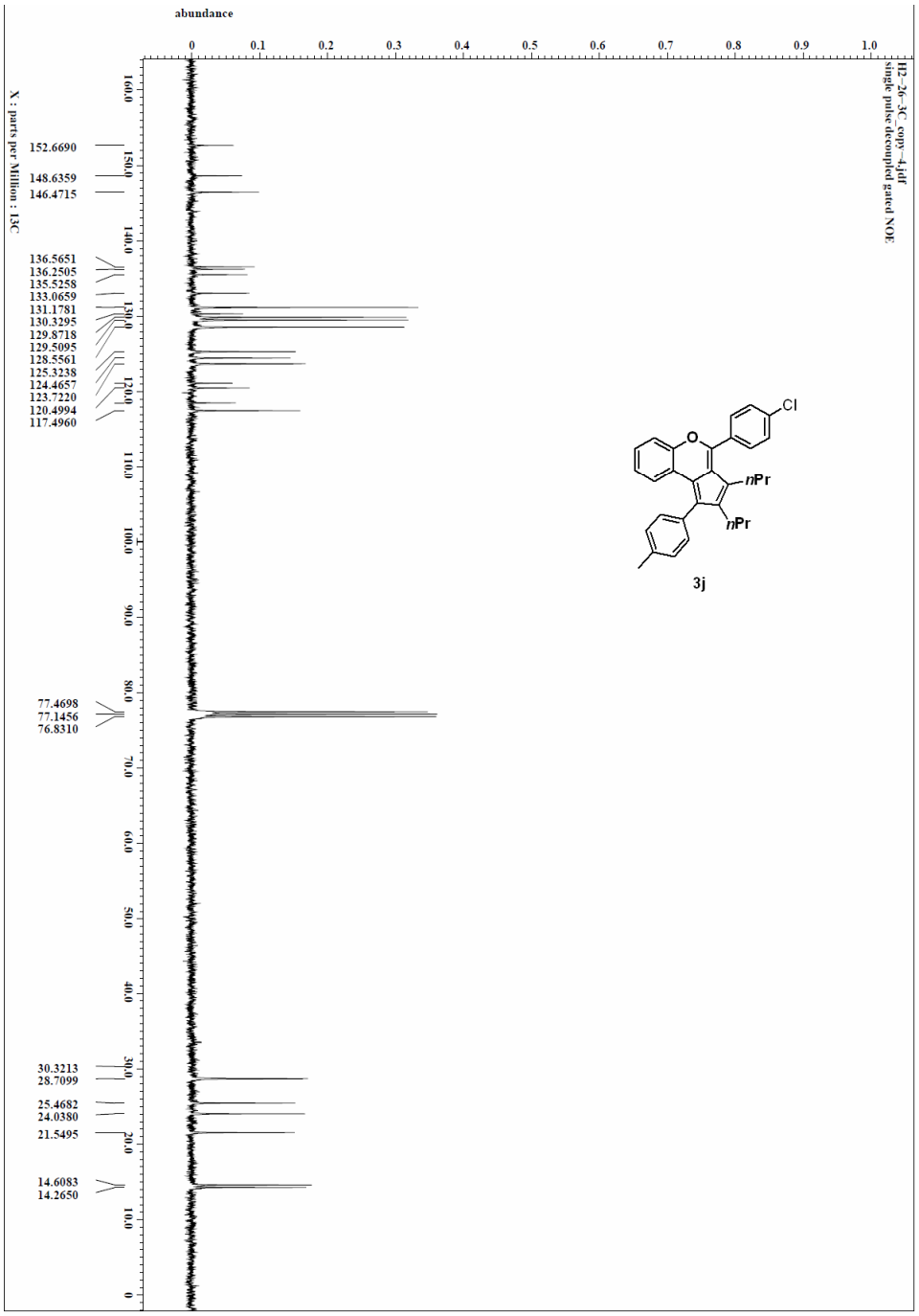

abundance
X : parts per Million : 1H
H4-14-2H-15.jdf
wanghuanhuan 120310 H4-14-4H
7.7457
7.7309
7.5682
7.5522
7.4410
7.4216
7.3918
7.3735
7.0745
7.0527
7.0287
3.9244
3.8648
2.5028
2.4856
2.4215
2.4043
1.2806
0.9576
0.9404
0.7697
0.7514
0.7342
20.94
30.52
20.31
21.74
11.67
21.71
10.48
28.23
19.98
20.89
30.98
30
3h

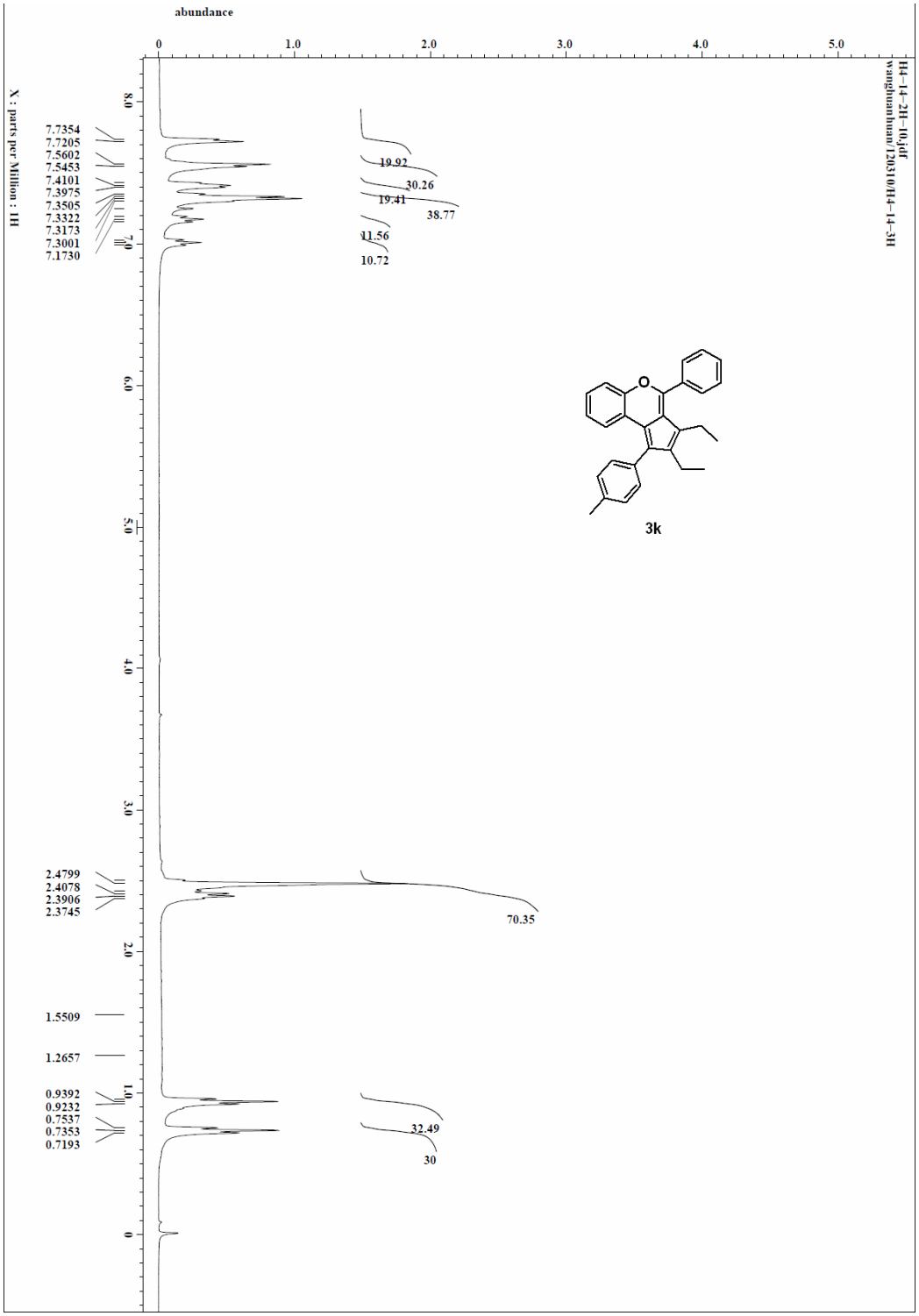

abundance
X : parts per Million : 13C
158.6853
154.3185
148.7122
147.3964
131.1685
130.8730
130.1483
129.7288
129.5095
128.2414
125.2380
124.9329
124.4181
123.6553
120.6042
120.5566
117.5913
114.2256
77.4793
77.1551
76.8405
55.3591
19.5281
19.3565
16.4199
15.5427
H4-14-4C-4.jdf
Single pulse decoupled gated NOE
3h

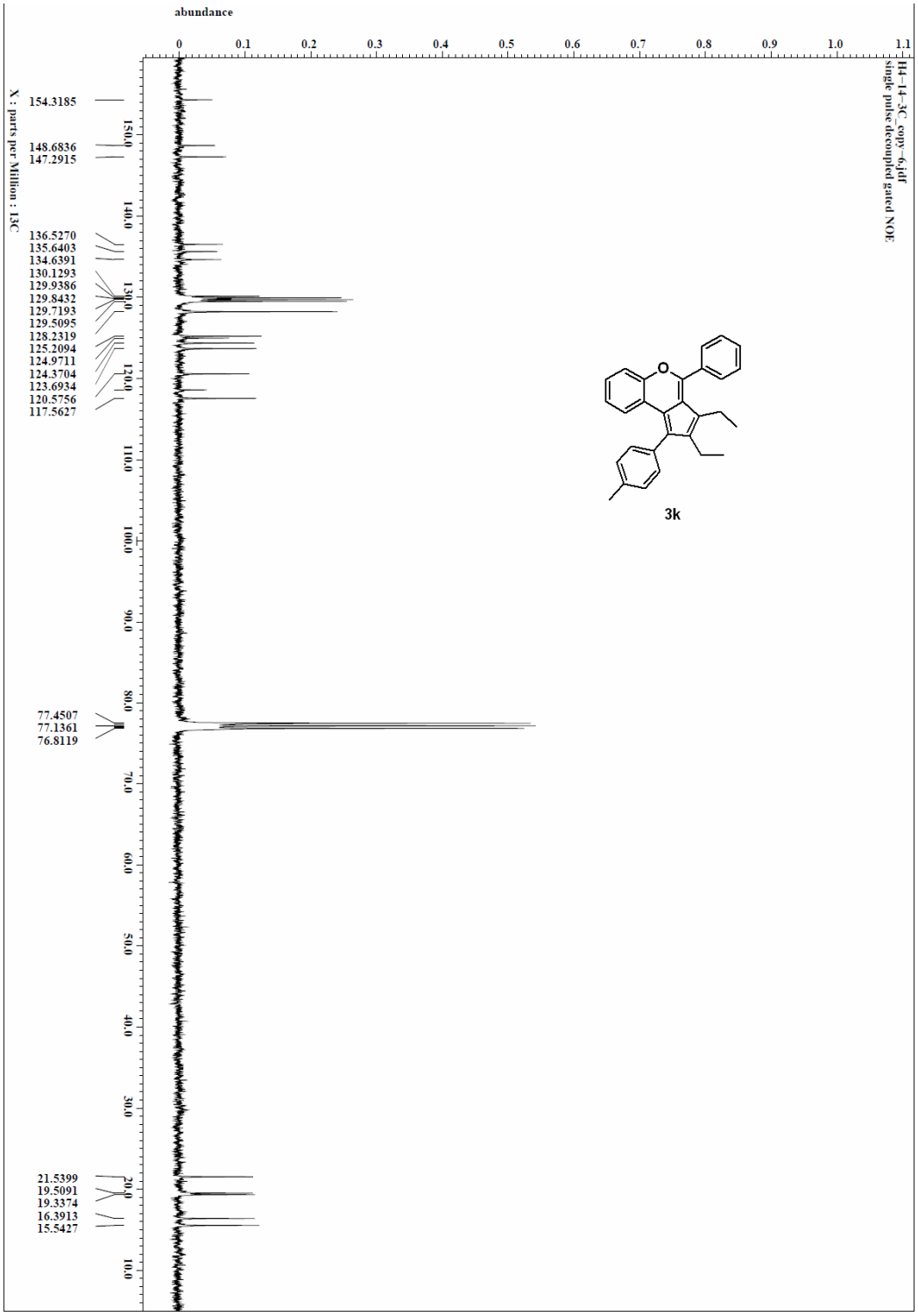

abundance
X : parts per Million : 1H
H3-26-2H-8.jdf
single_pulse
7.7065
7.6916
7.5473
7.5347
7.4099
7.3904
7.3217
7.3022
7.2953
7.1556
6.9906
2.4648
2.4316
2.4121
2.3938
2.3021
1.5323
1.3101
1.2929
1.2746
1.2563
1.0959
1.0776
1.0593
0.7958
0.7786
0.7614
0.5174
0.5003
0.4831
−0.0003
20
30.62
19.92
40.54
11.29
10.98
50.05
21.9
0.2
19.26
21.7
30.79
30.87
nPr
nPr
3i

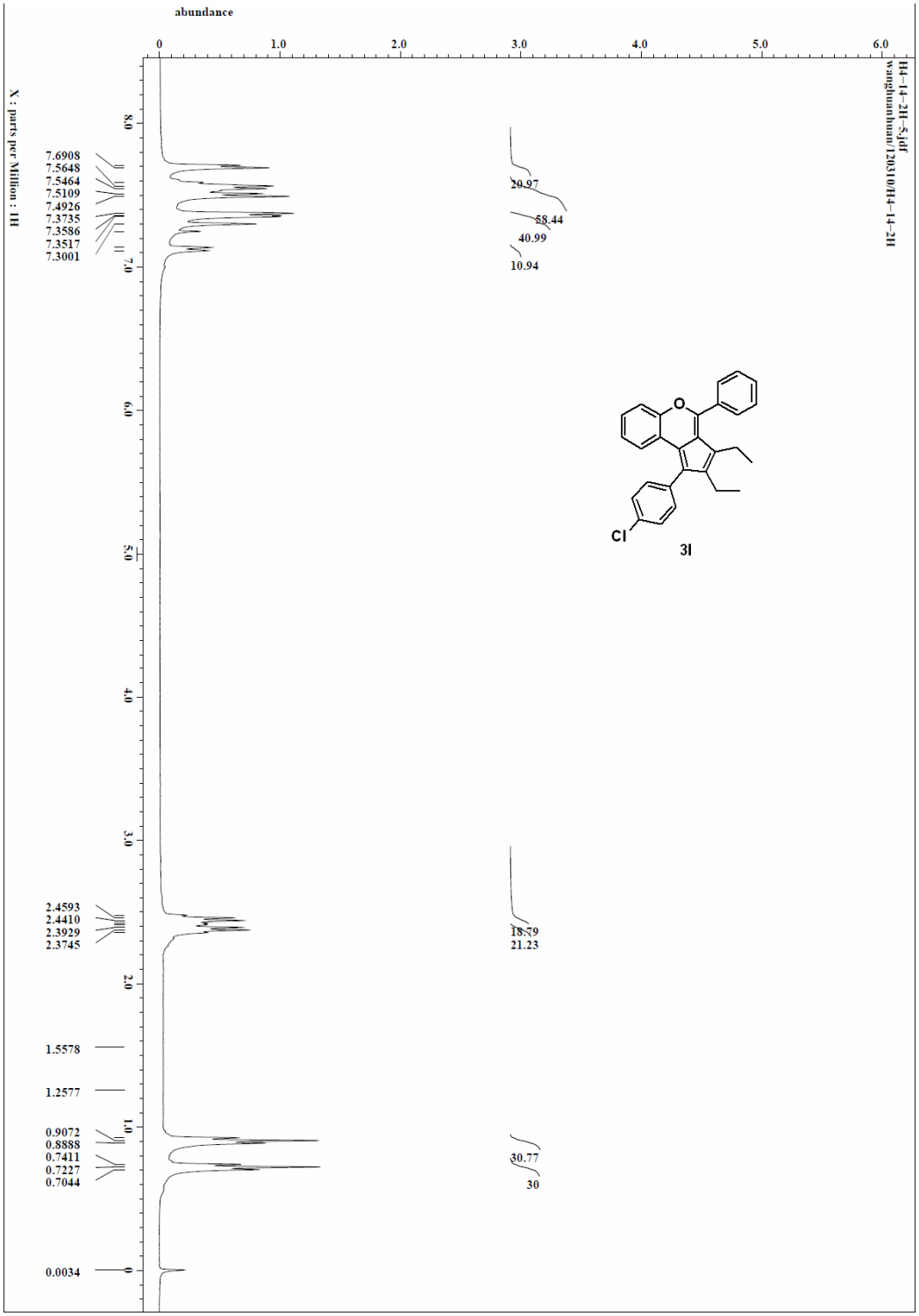

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
X : parts per Million : 13C
154.2041
148.7026
145.9185
136.4507
135.6879
134.6201
130.0244
129.9195
129.7288
129.4619
128.2510
125.1904
124.3418
124.0748
123.6744
120.5947
117.5532
77.4507
77.1361
76.8214
28.6909
25.5063
24.0857
21.5399
14.6083
14.2650
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
nPr
nPr
3i

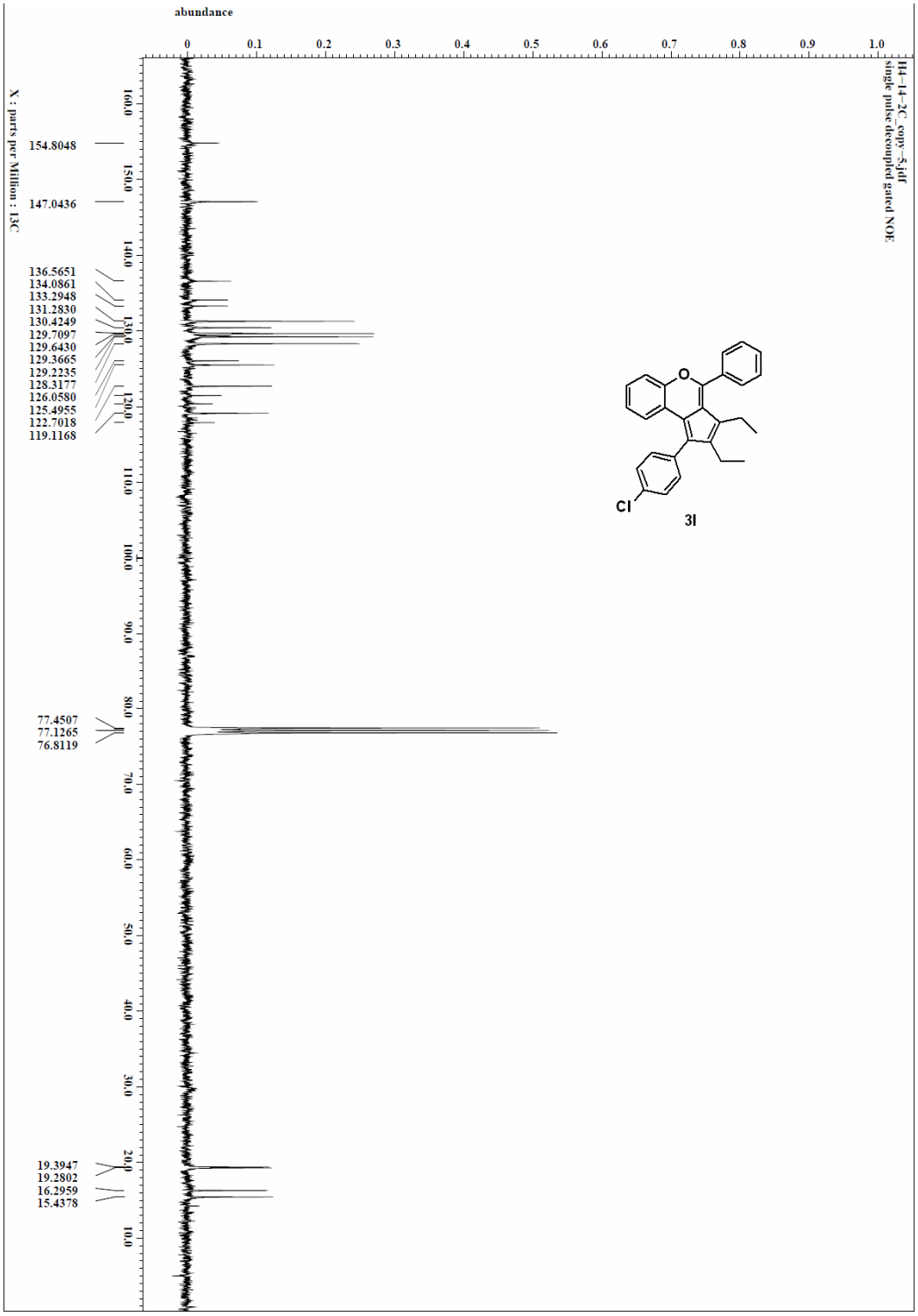

abundance
X : parts per Million : 1H
H3-26-3H-8.jdf
single_pulse
7.6463
7.6280
7.5226
7.5042
7.3908
7.3702
7.2877
7.1526
7.1331
6.9888
2.4595
2.4286
2.4102
2.3152
1.3060
1.2865
1.2693
1.1055
1.0872
0.7951
0.7768
0.7596
0.5568
0.5397
20
19.53
19.97
38.02
10.1
10.78
49.35
19.92
19.79
21.29
29.26
30.43
Cl
O
nPr
nPr
3j

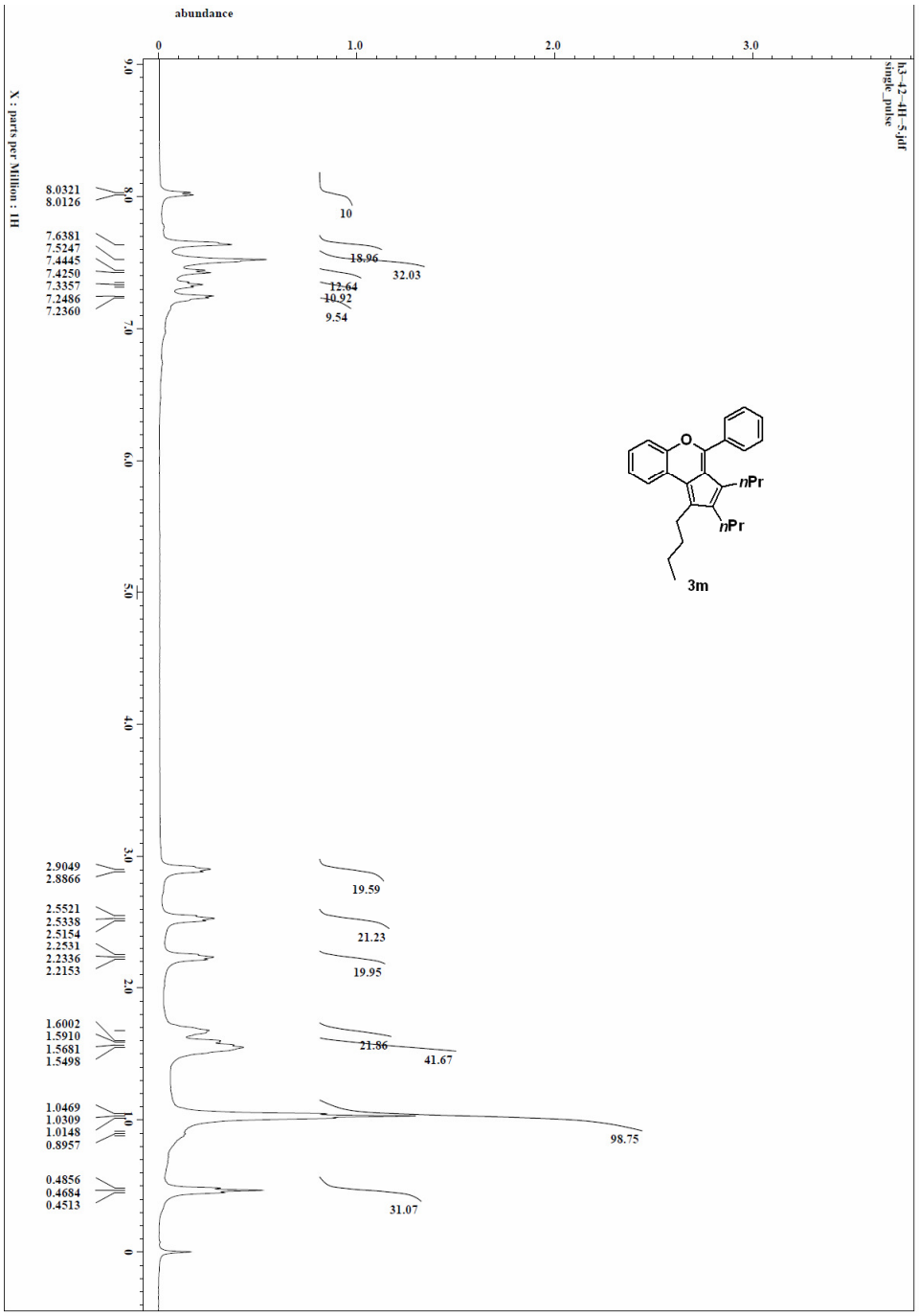

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
112-26-3C_oop-4.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
152.6690
148.6359
146.4715
136.5651
136.2505
135.5258
133.0659
131.1781
130.3295
129.8718
129.5095
128.5561
125.3238
124.4657
123.7220
120.4994
117.4960
77.4698
77.1456
76.8310
30.3213
28.7099
25.4682
24.0380
21.5495
14.6083
14.2650
O
Cl
nPr
nPr
3j

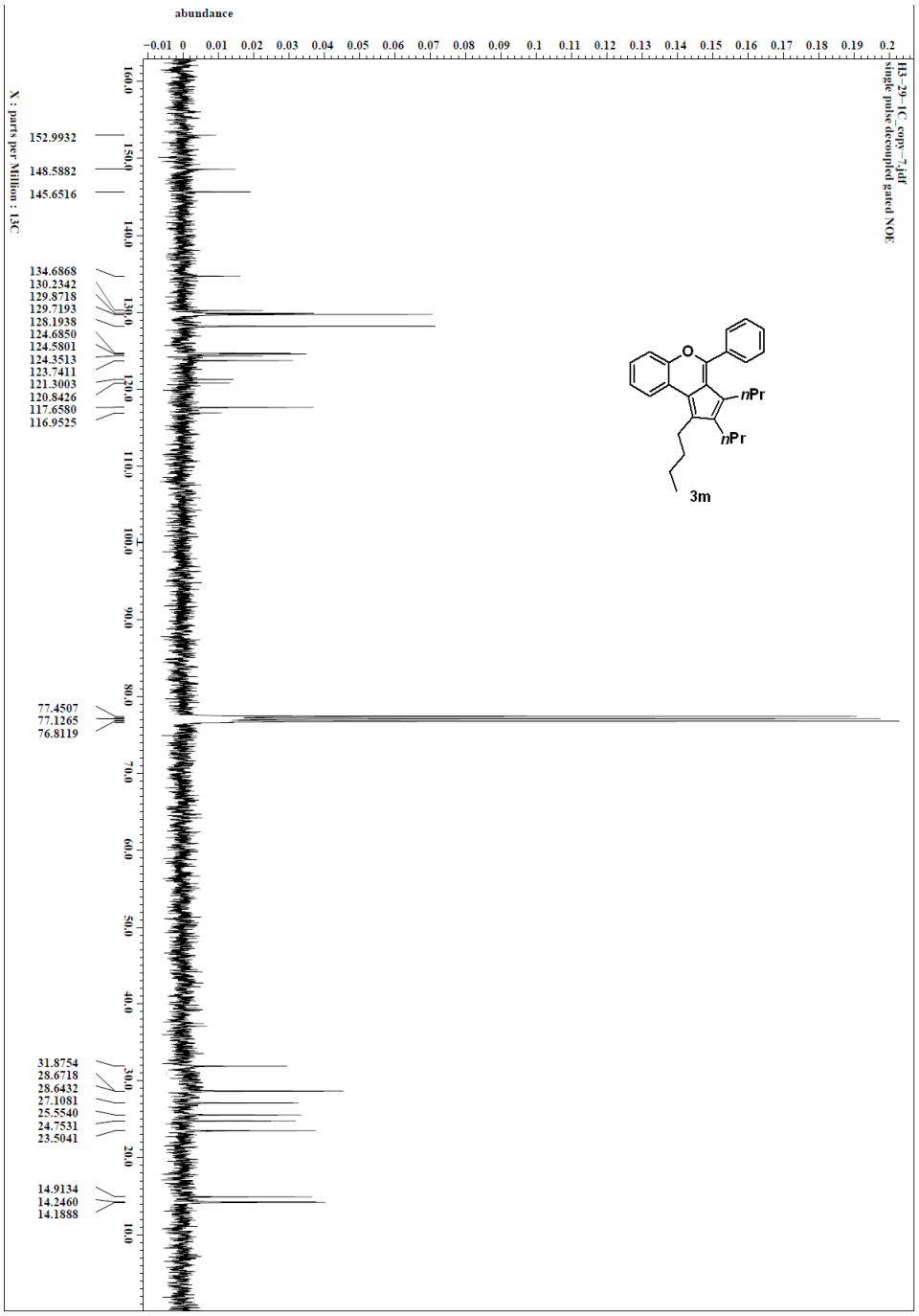

abundance
0
1.0
2.0
3.0
4.0
5.0
X : parts per Million : 1H
7.7354
7.7205
7.5602
7.5453
7.4101
7.3975
7.3505
7.3322
7.3173
7.3001
7.1730
19.92
30.26
19.41
38.77
11.56
10.72
2.4799
2.4078
2.3906
2.3745
70.35
1.5509
1.2657
0.9392
0.9232
0.7537
0.7353
0.7193
32.49
30
3k

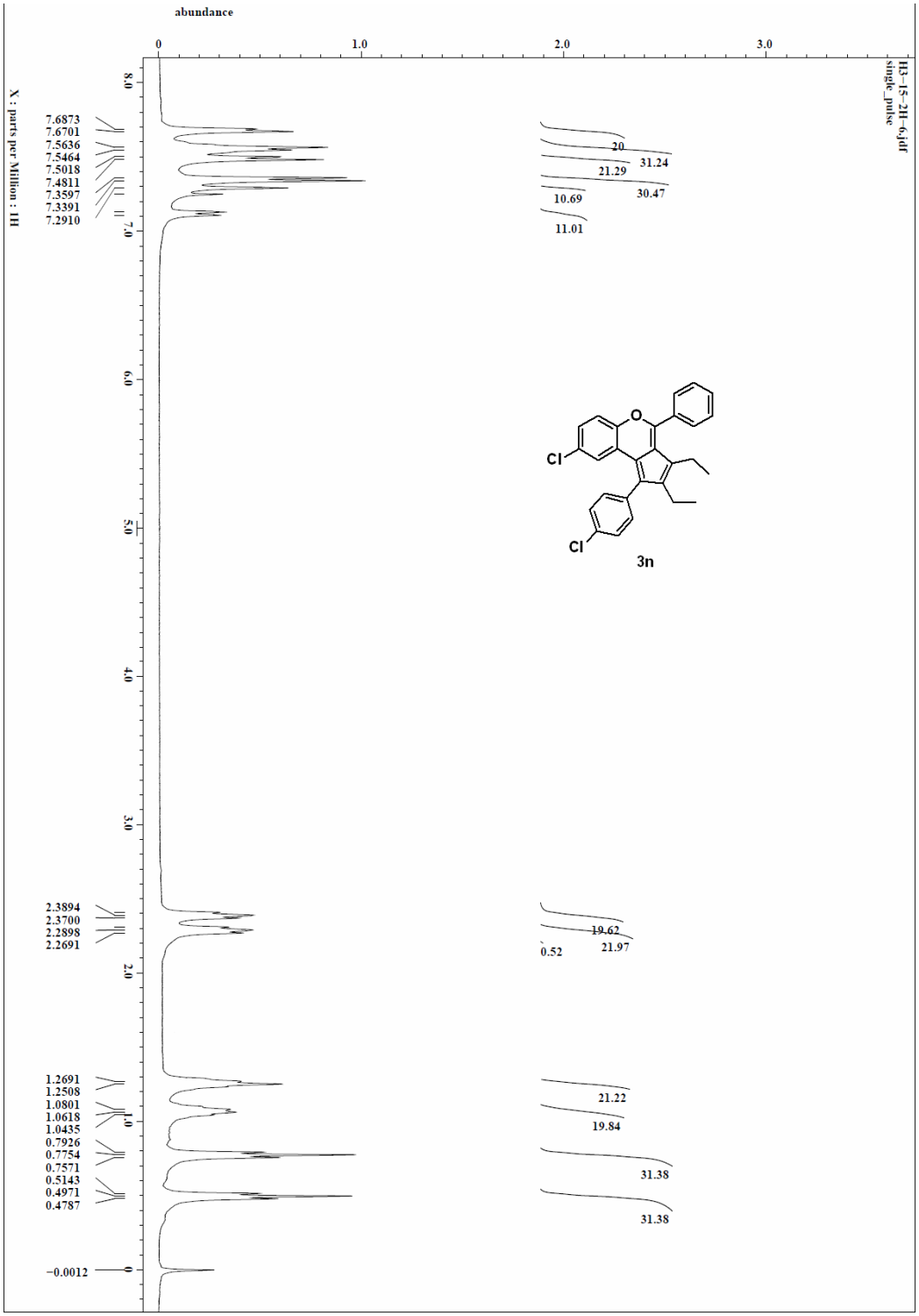

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
H4-14-3C_copy-6.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
154.3185
148.6836
147.2915
136.5270
135.6403
134.6391
130.1293
129.9386
129.8432
129.7193
129.5095
128.2319
125.2094
124.9711
124.3704
123.6934
120.5756
117.5627
77.4507
77.1361
76.8119
21.5399
19.5091
19.3374
16.3913
15.5427
O
3k

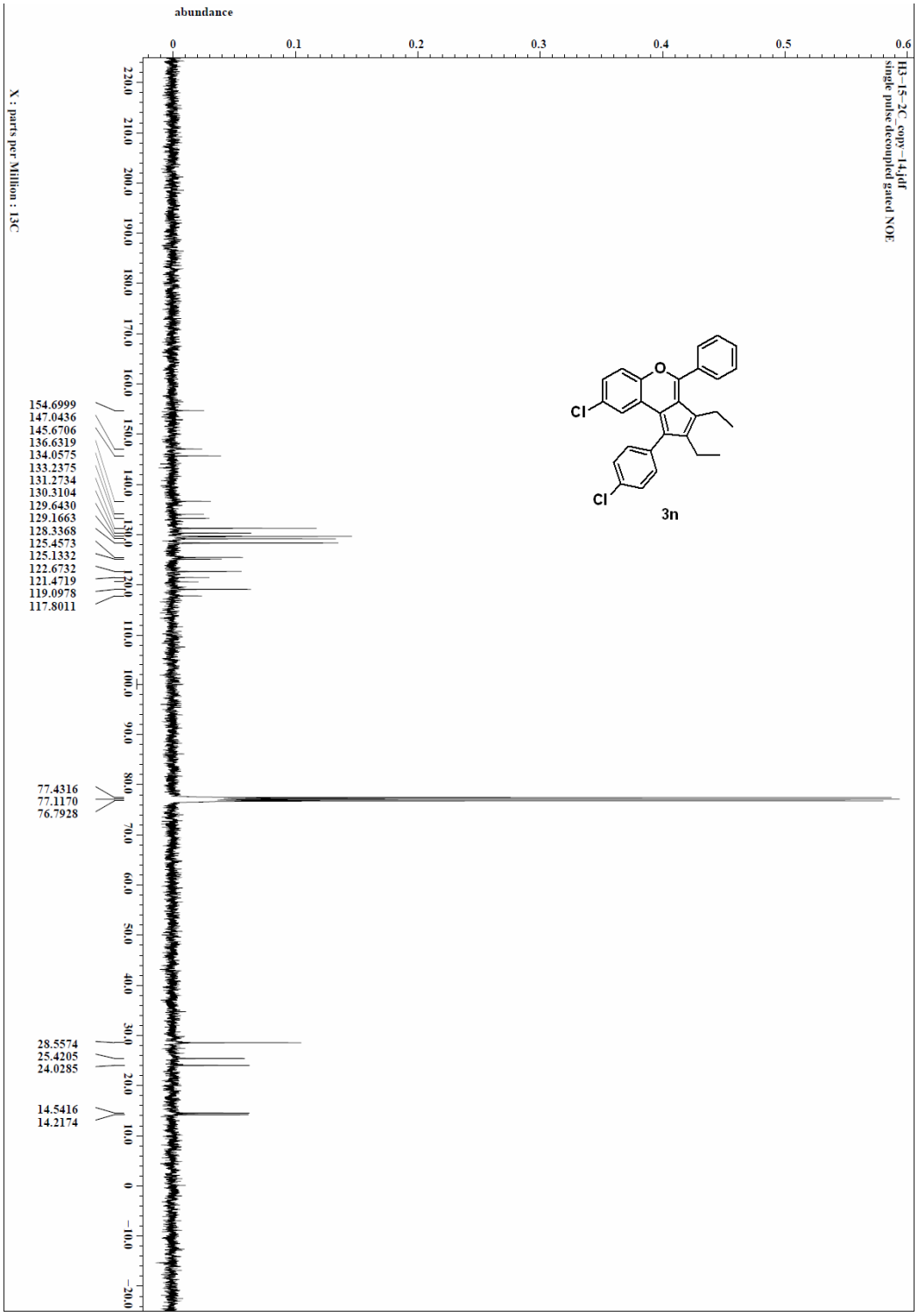

abundance
X : parts per Million : 1H
7.6908
7.5648
7.5464
7.5109
7.4926
7.3735
7.3586
7.3517
7.3001
2.4593
2.4410
2.3929
2.3745
1.5578
1.2577
0.9072
0.8888
0.7411
0.7227
0.7044
0.0034
20.97
58.44
40.99
10.94
18.79
21.23
30.77
30
Cl
3l

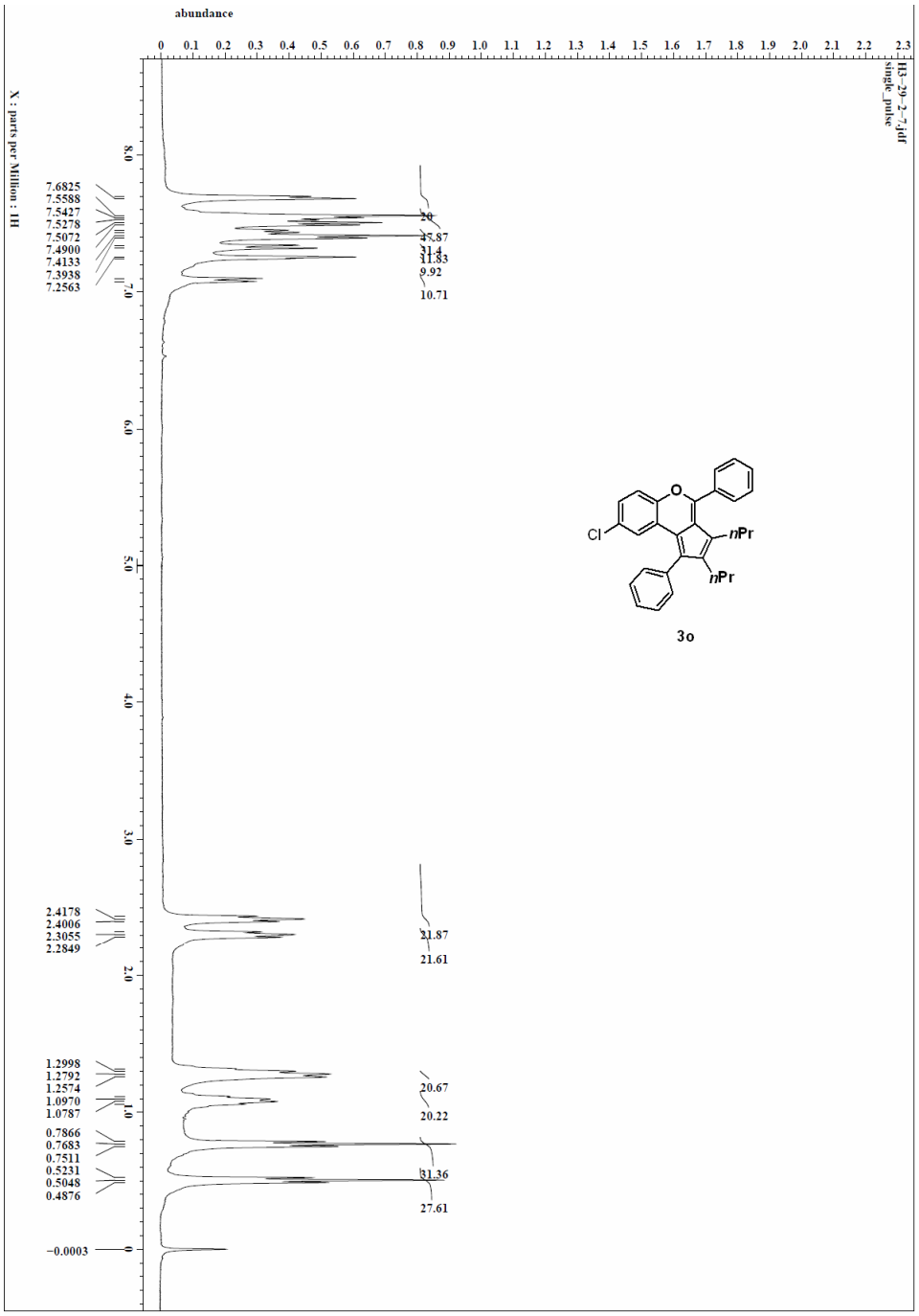

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
X : parts per Million : 13C
154.8048
147.0436
136.5651
134.0861
133.2948
131.2830
130.4249
129.7097
129.6430
129.3665
129.2235
128.3177
126.0580
125.4955
122.7018
119.1168
77.4507
77.1265
76.8119
19.3947
19.2802
16.2959
15.4378
H4-14-2C_copy-5.jdf
single pulse decoupled gated NOE
O
Cl
3l

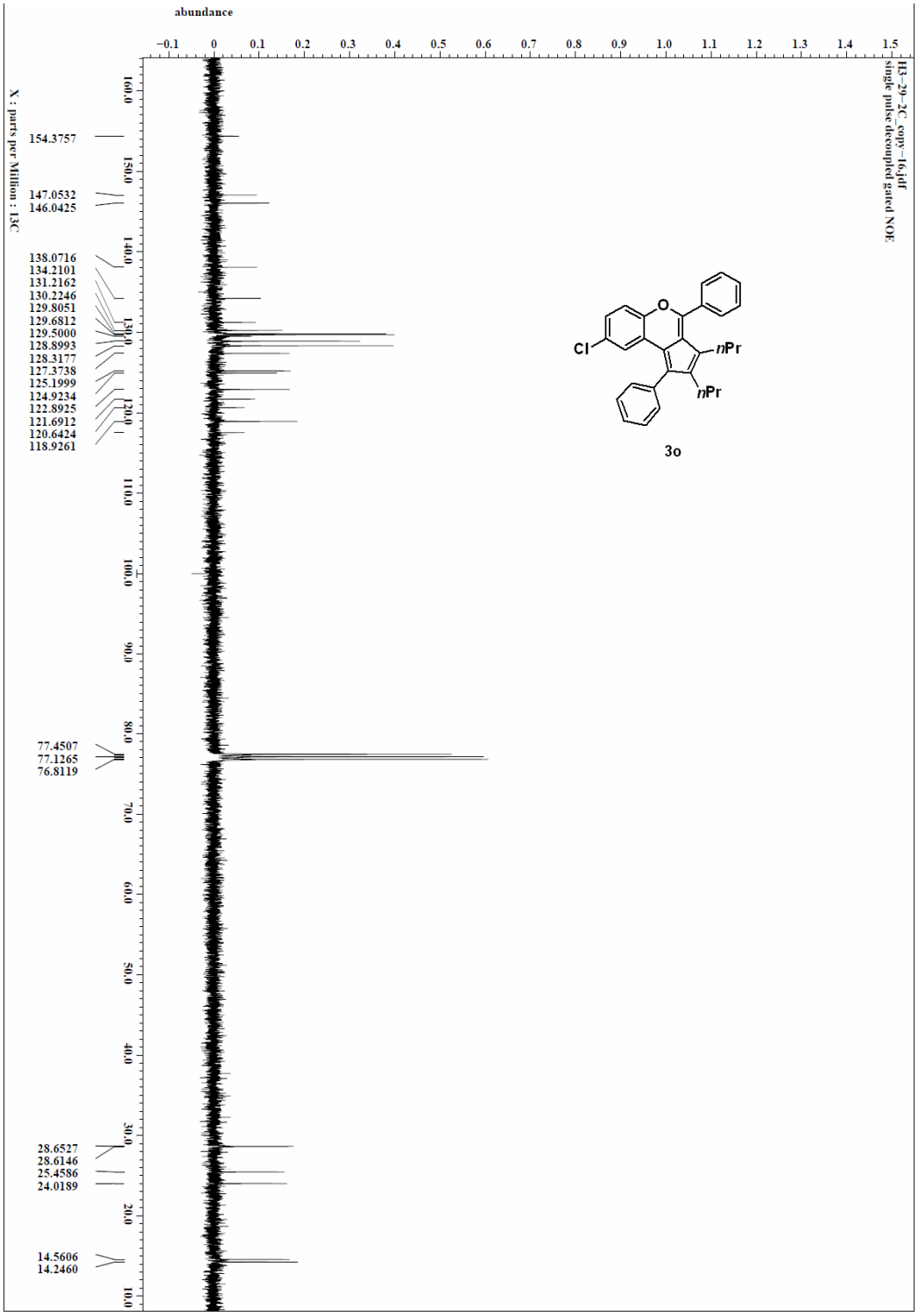

abundance
X : parts per Million : 1H
8.0321
8.0126
7.6381
7.5247
7.4445
7.4250
7.3357
7.2486
7.2360
2.9049
2.8866
2.5521
2.5338
2.5154
2.2531
2.2336
2.2153
1.6002
1.5910
1.5681
1.5498
1.0469
1.0309
1.0148
0.8957
0.4856
0.4684
0.4513
10
18.96
32.03
12.64
10.92
9.54
19.59
21.23
19.95
21.86
41.67
98.75
31.07
nPr
nPr
3m

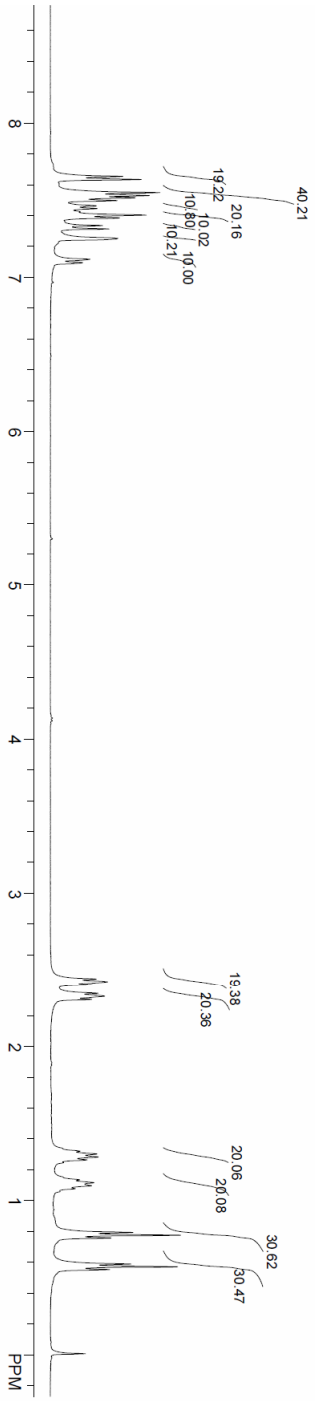

abundance
X : parts per Million : 13C
152.9932
148.5882
145.6516
134.6868
130.2342
129.8718
129.7193
128.1938
124.6850
124.5801
124.3513
123.7411
121.3003
120.8426
117.6580
116.9525
77.4507
77.1265
76.8119
31.8754
28.6718
28.6432
27.1081
25.5540
24.7531
23.5041
14.9134
14.2460
14.1888
nPr
nPr
3m

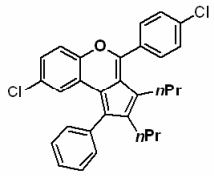

abundance
X : parts per Million : 1H
H3-15-2H-6.jdf
single_pulse
7.6873
7.6701
7.5636
7.5464
7.5018
7.4811
7.3597
7.3391
7.2910
2.3894
2.3700
2.2898
2.2691
1.2691
1.2508
1.0801
1.0618
1.0435
0.7926
0.7754
0.7571
0.5143
0.4971
0.4787
−0.0012
20
31.24
21.29
30.47
10.69
11.01
19.62
21.97
0.52
21.22
19.84
31.38
31.38
Cl
Cl
O
3n


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
H3-15-2C_copy-14.jdf
single pulse decoupled gated NOE
154.6999
147.0436
145.6706
136.6319
134.0575
133.2375
131.2734
130.3104
129.6430
129.1663
128.3368
125.4573
125.1332
122.6732
121.4719
119.0978
117.8011
77.4316
77.1170
76.7928
28.5574
25.4205
24.0285
14.5416
14.2174
Cl
Cl
O
3n

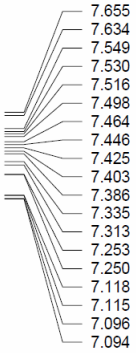

abundance
X : parts per Million : 1H
H3-29-2-7.jdf
single_pulse
7.6825
7.5588
7.5427
7.5278
7.5072
7.4900
7.4133
7.3938
7.2563
2.4178
2.4006
2.3055
2.2849
1.2998
1.2792
1.2574
1.0970
1.0787
0.7866
0.7683
0.7511
0.5231
0.5048
0.4876
−0.0003
20
17.87
31.4
31.83
9.92
10.71
31.87
21.61
20.67
20.22
31.36
27.61
Cl
nPr
nPr
3o

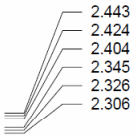

abundance
X : parts per Million : 13C
H3-29-2C_copy-16.jdf
single pulse decoupled gated NOE
154.3757
147.0532
146.0425
138.0716
134.2101
131.2162
130.2246
129.8051
129.6812
129.5000
128.8993
128.3177
127.3738
125.1999
124.9234
122.8925
121.6912
120.6424
118.9261
77.4507
77.1265
76.8119
28.6527
28.6146
25.4586
24.0189
14.5606
14.2460
Cl
O
nPr
nPr
3o

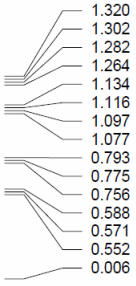

8
7
6
5
4
3
2
1
PPM
40.21
19.22
20.16
10.02
10.80
10.21
10.00
19.38
20.36
20.06
20.08
30.62
30.47

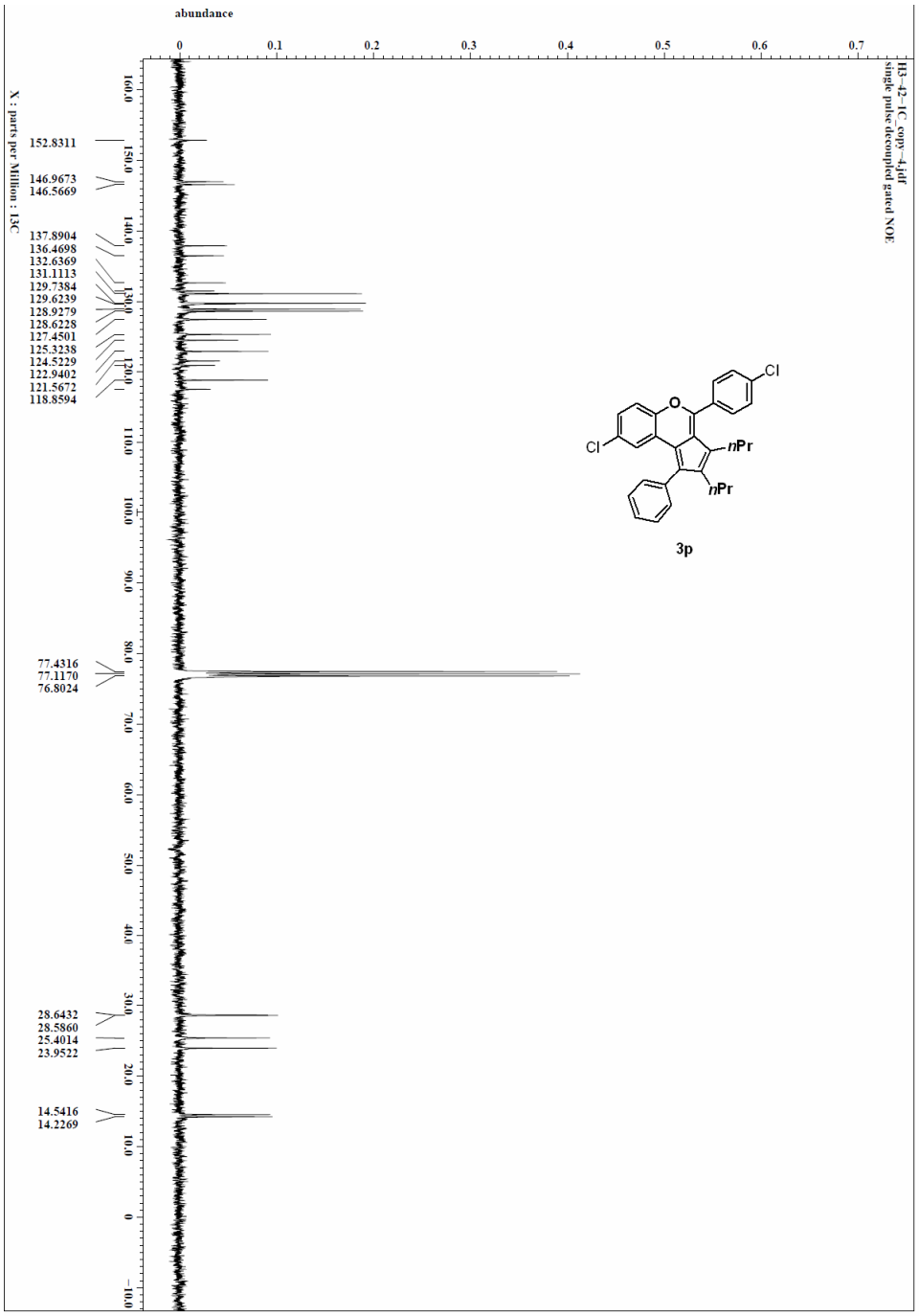

Cl
O
Cl
nPr
nPr

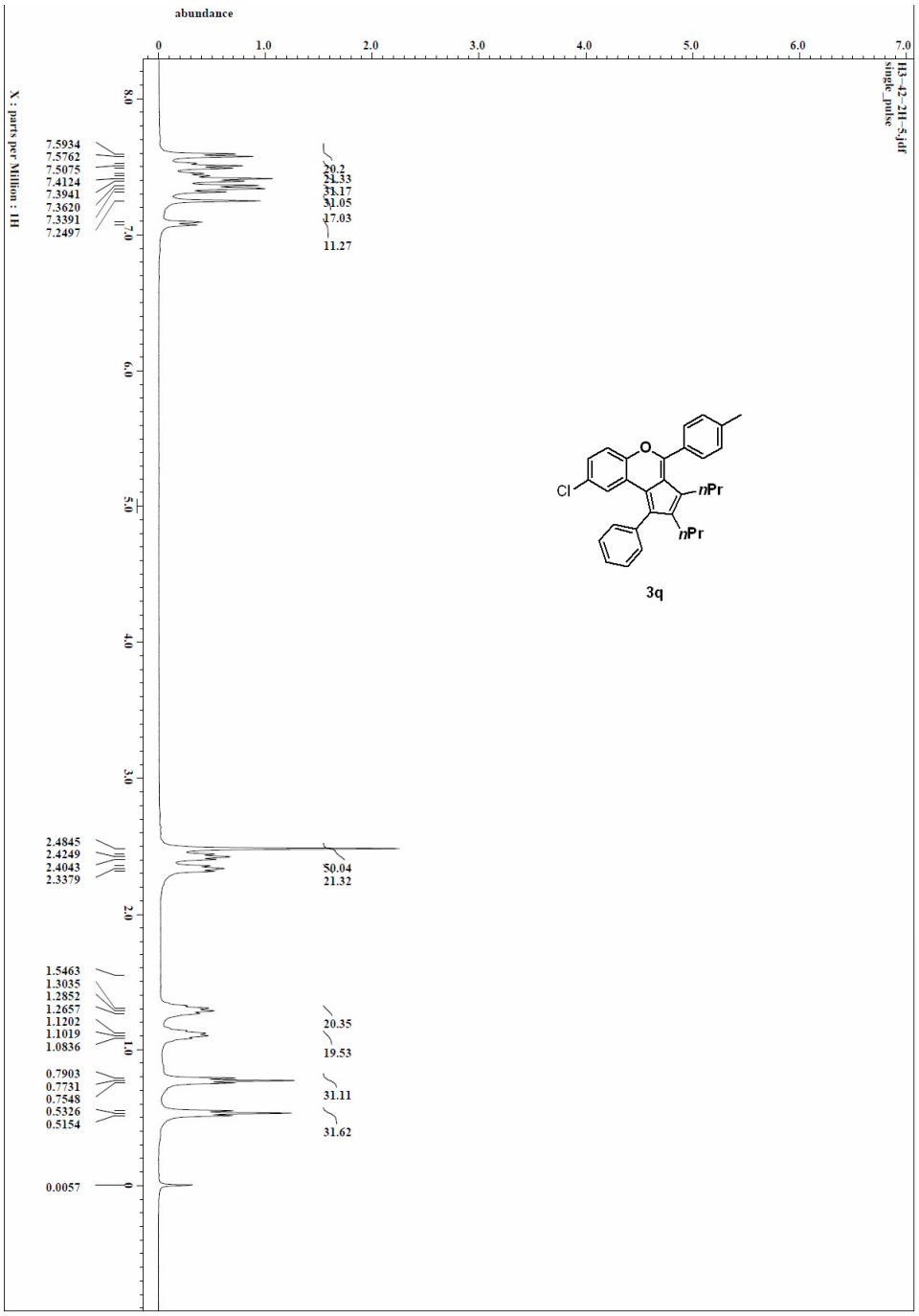
3p

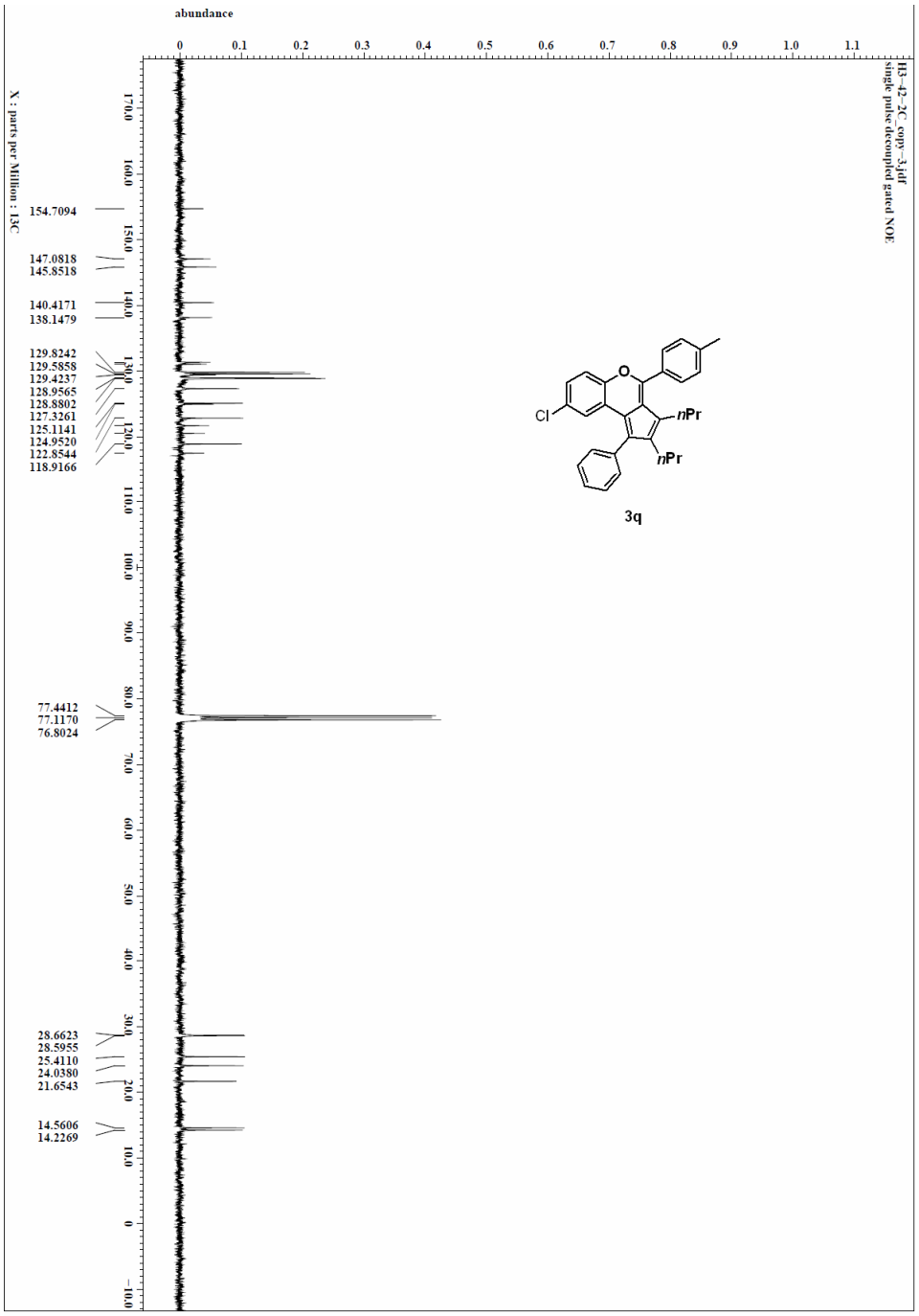

7.655
7.634
7.549
7.530
7.516
7.498
7.464
7.446
7.425
7.403
7.386
7.335
7.313
7.253
7.250
7.118
7.115
7.096
7.094

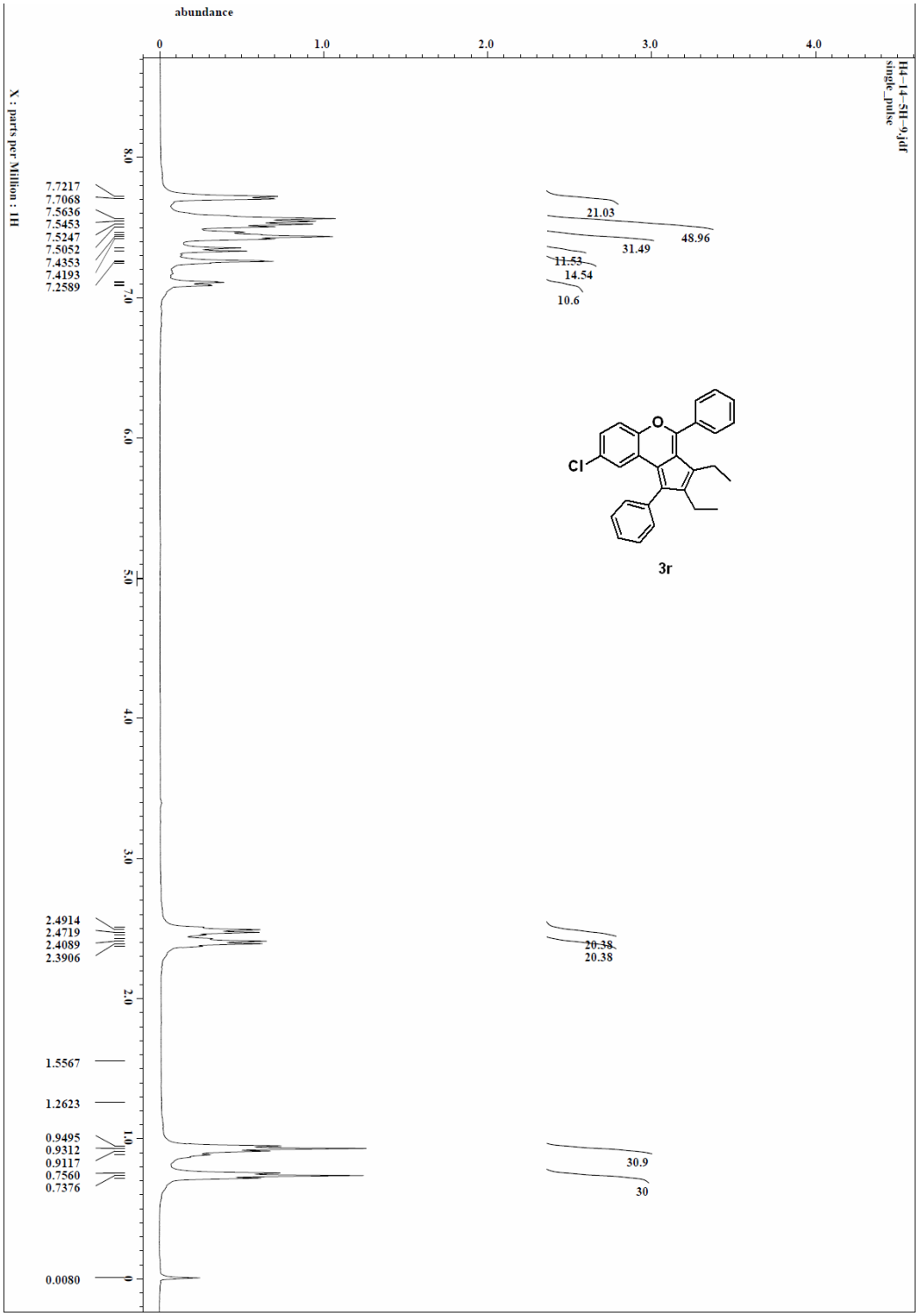

2.443
2.424
2.404
2.345
2.326
2.306

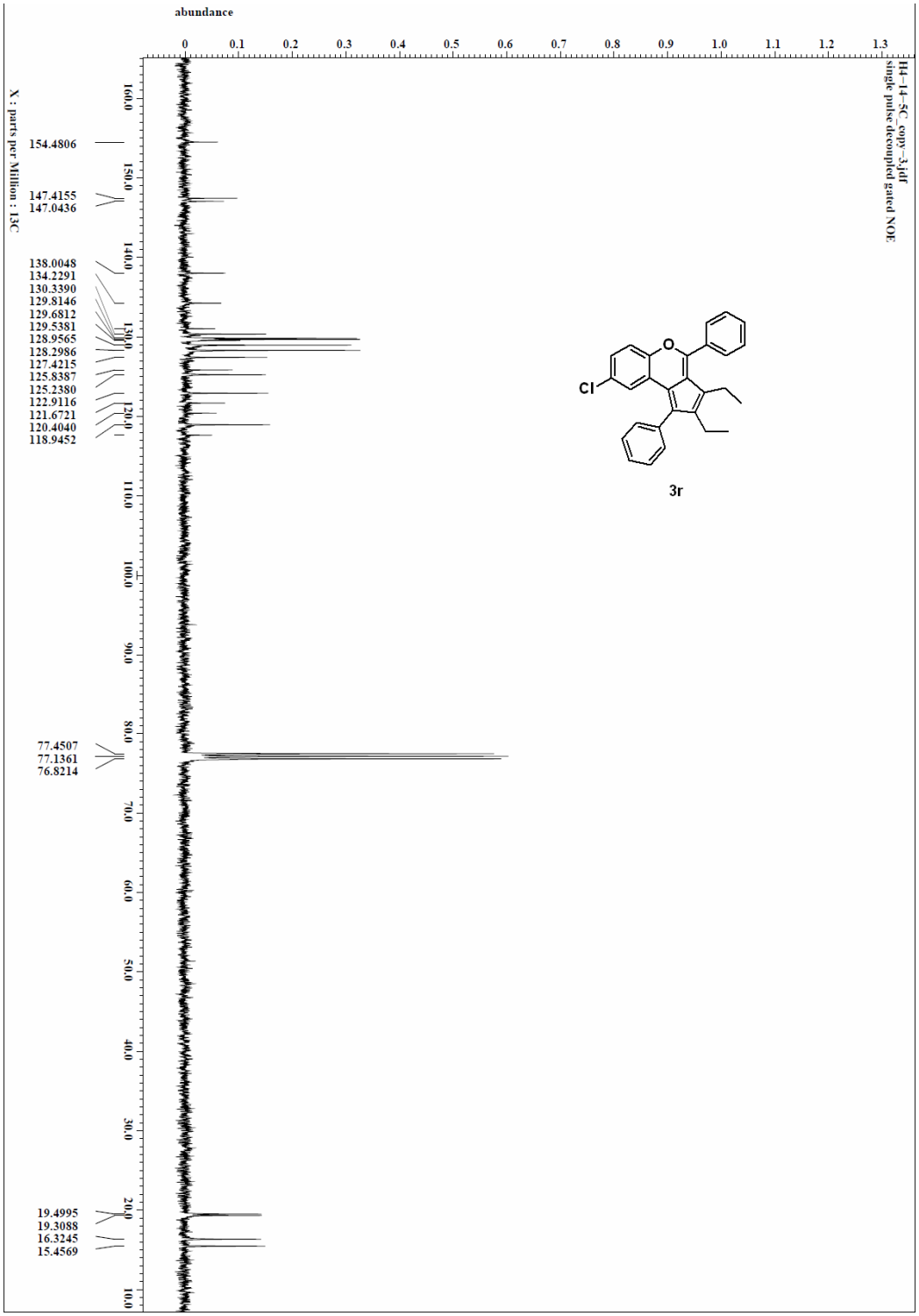

1.320
1.302
1.282
1.264
1.134
1.116
1.097
1.077
0.793
0.775
0.756
0.588
0.571
0.552
0.006

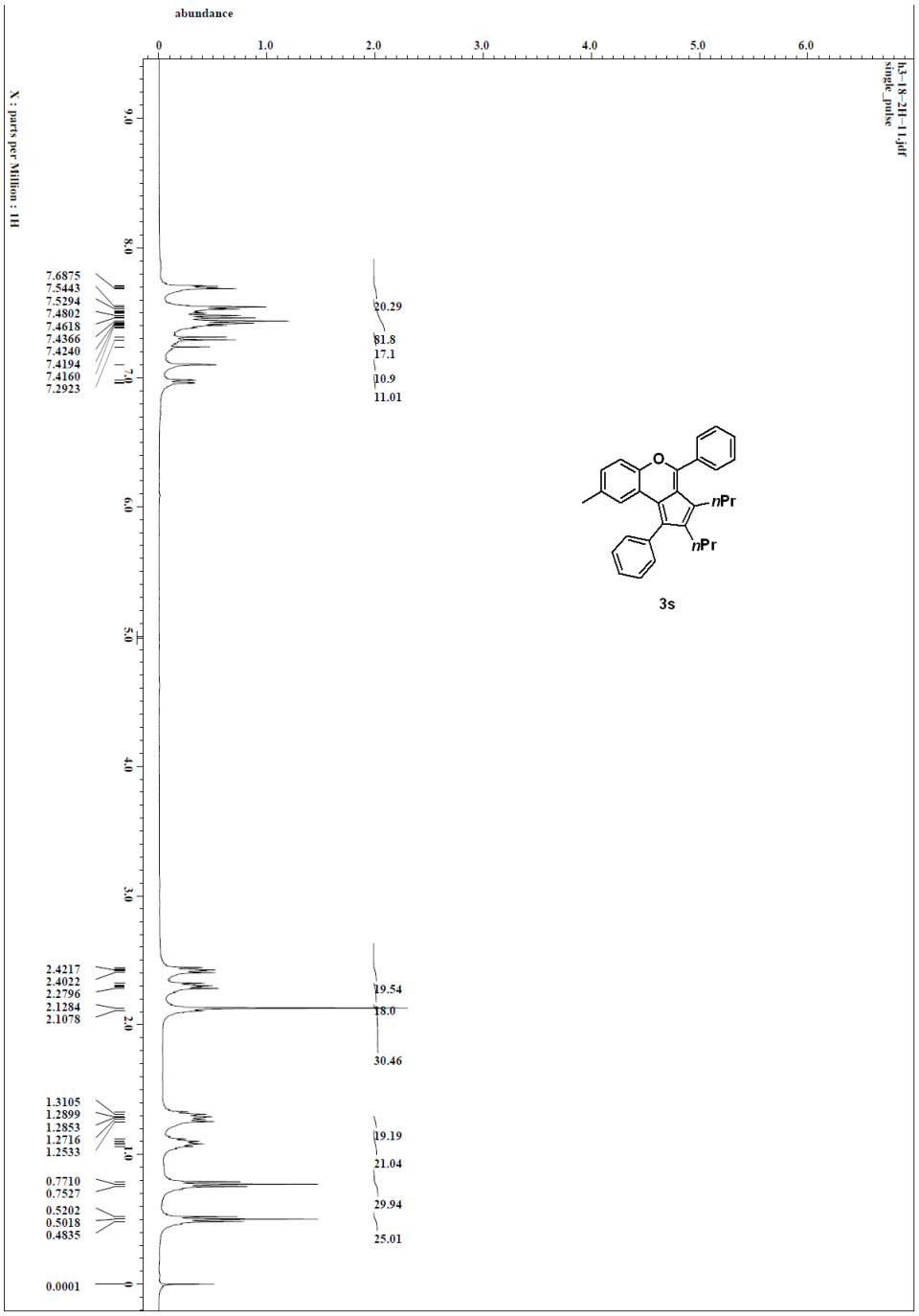

abundance
X : parts per Million : 13C
H3-42-1C_opp-4.jdf
single pulse decoupled gated NOE
152.8311
146.9673
146.5669
137.8904
136.4698
132.6369
131.1113
129.7384
129.6239
128.9279
128.6228
127.4501
125.3238
124.5229
122.9402
121.5672
118.8594
77.4316
77.1170
76.8024
28.6432
28.5860
25.4014
23.9522
14.5416
14.2269
Cl
Cl
nPr
nPr
3p

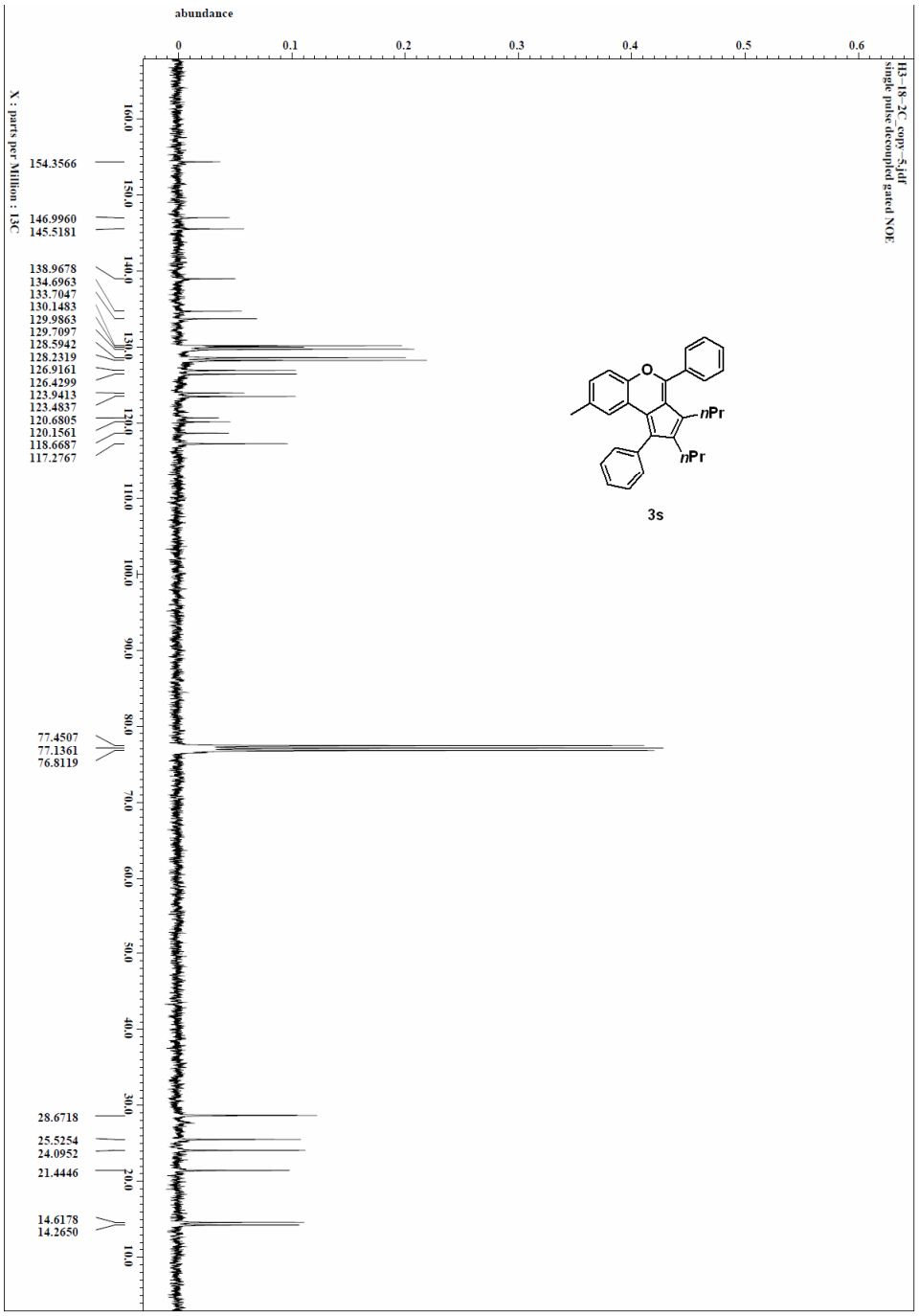

abundance
X : parts per Million : 1H
H3-42-2H-5.jdf
single_pulse
7.5934
7.5762
7.5075
7.4124
7.3941
7.3620
7.3391
7.2497
2.4845
2.4249
2.4043
2.3379
1.5463
1.3035
1.2852
1.2657
1.1202
1.1019
1.0836
0.7903
0.7731
0.7548
0.5326
0.5154
0.0057
20.2
31.33
31.17
31.05
17.03
11.27
50.04
21.32
20.35
19.53
31.11
31.62
Cl
nPr
nPr
3q

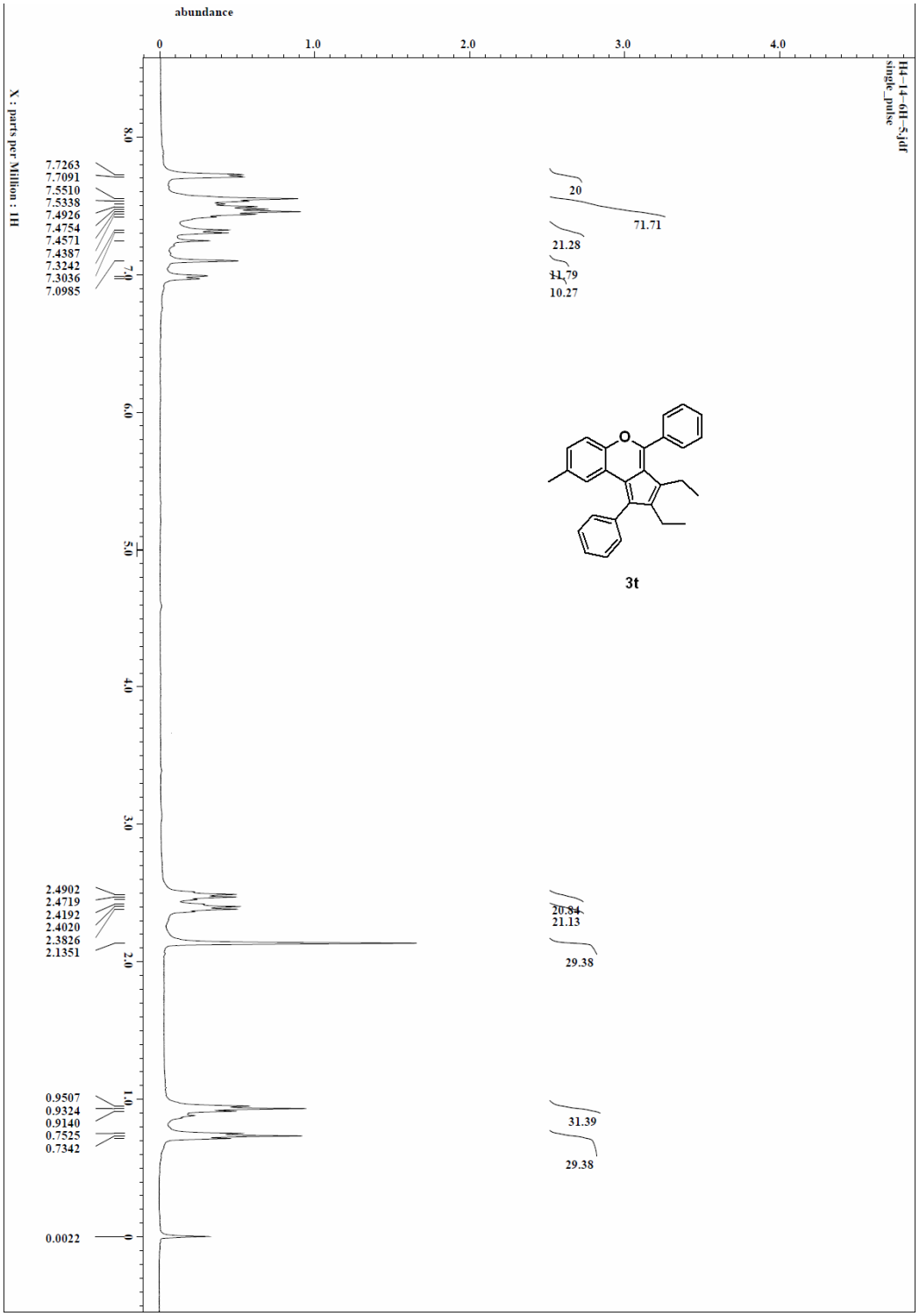

abundance
X : parts per Million : 13C
154.7094
147.0818
145.8518
140.4171
138.1479
129.8242
129.5858
129.4237
128.9565
128.8802
127.3261
125.1141
124.9520
122.8544
118.9166
77.4412
77.1170
76.8024
28.6623
28.5955
25.4110
24.0380
21.6543
14.5606
14.2269
Cl
nPr
nPr
3q

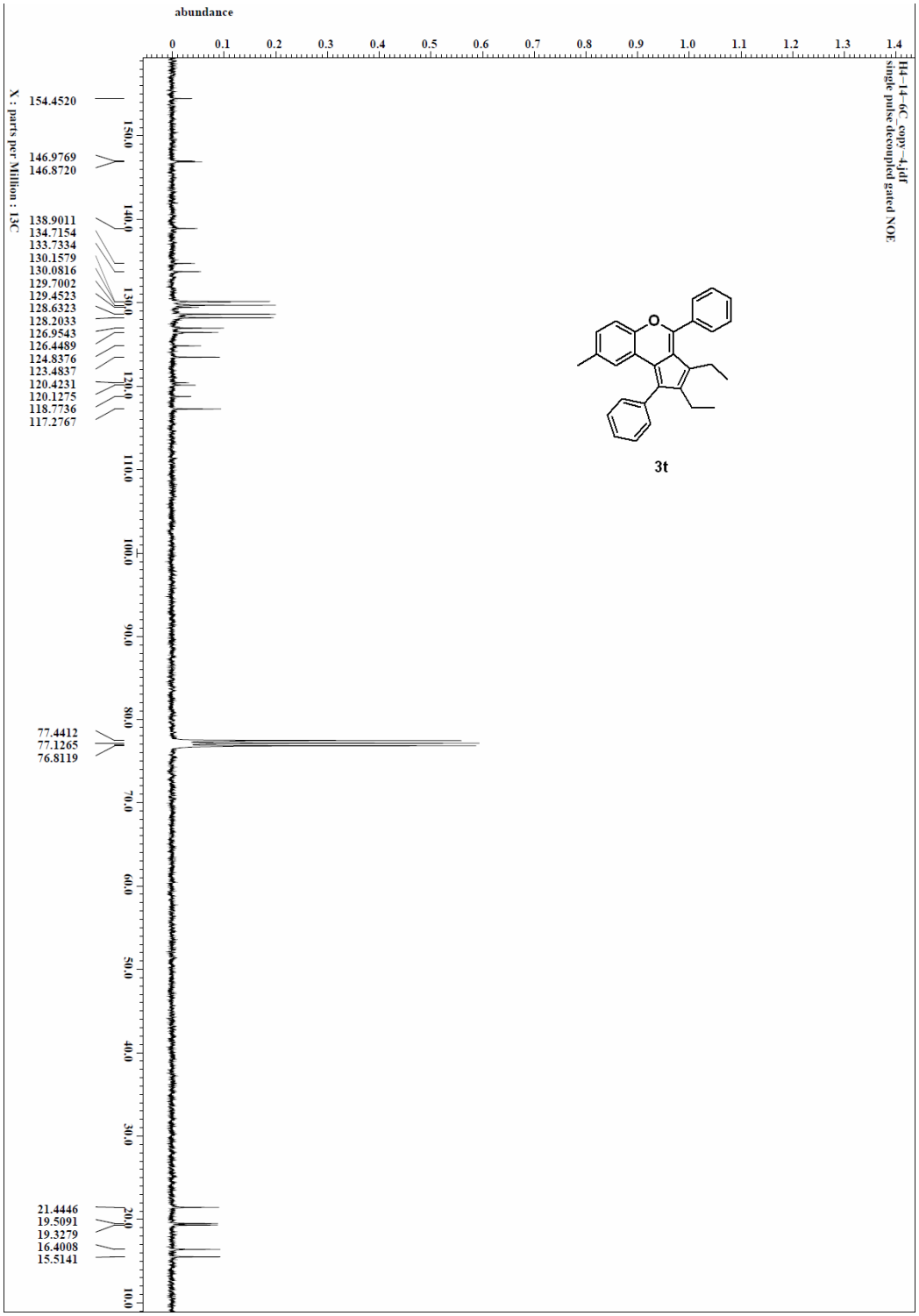

abundance
0
1.0
2.0
3.0
4.0
H4-14-5H-9.jdf
single_pulse
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.7217
7.7068
7.5636
7.5453
7.5247
7.5052
7.4353
7.4193
7.2589
2.4914
2.4719
2.4089
2.3906
1.5567
1.2623
0.9495
0.9312
0.9117
0.7560
0.7376
0.0080
21.03
48.96
31.49
11.53
14.54
10.6
20.38
20.38
30.9
30
O
Cl
3r


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
H4-14-5C_copy-3.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
154.4806
147.4155
147.0436
138.0048
134.2291
130.3390
129.8146
129.6812
129.5381
128.9565
128.2986
127.4215
125.8387
125.2380
122.9116
121.6721
120.4040
118.9452
77.4507
77.1361
76.8214
19.4995
19.3088
16.3245
15.4569
Cl
O
3r


abundance
X : parts per Million : 1H
h3-18-2H-11.jdf
single_pulse
7.6875
7.5443
7.5294
7.4802
7.4618
7.4366
7.4240
7.4194
7.4160
7.2923
20.29
81.8
17.1
10.9
11.01
2.4217
2.4022
2.2796
2.1284
2.1078
19.54
18.0
30.46
1.3105
1.2899
1.2853
1.2716
1.2533
19.19
21.04
0.7710
0.7527
29.94
0.5202
0.5018
0.4835
25.01
0.0001
nPr
nPr
3s


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 13C
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
154.3566
146.9960
145.5181
138.9678
134.6963
133.7047
130.1483
129.9863
129.7097
128.5942
128.2319
126.9161
126.4299
123.9413
123.4837
120.6805
120.1561
118.6687
117.2767
77.4507
77.1361
76.8119
28.6718
25.5254
24.0952
21.4446
14.6178
14.2650
O
nPr
nPr
3s
H3-18-2C_copy-5.jdf
single pulse decoupled gated NOE


abundance
0
1.0
2.0
3.0
4.0
H4-14-6H-5.jdf
single_pulse
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.7263
7.7091
7.5510
7.5338
7.4926
7.4754
7.4571
7.4387
7.3242
7.3036
7.0985
2.4902
2.4719
2.4192
2.4020
2.3826
2.1351
0.9507
0.9324
0.9140
0.7525
0.7342
0.0022
20
71.71
21.28
11.79
10.27
20.84
21.13
29.38
31.39
29.38
O
3t


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
H4-14-6C_copy-4.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C
154.4520
146.9769
146.8720
138.9011
134.7154
133.7334
130.1579
130.0816
129.7002
129.4523
128.6323
128.2033
126.9543
126.4489
124.8376
123.4837
120.4231
120.1275
118.7736
117.2767
77.4412
77.1265
76.8119
21.4446
19.5091
19.3279
16.4008
15.5141
O
3t