Organocatalytic Asymmetric Intermolecular Dehydrogenative α-Alkylation of Aldehydes Using Molecular Oxygen as Oxidant

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Supporting Information

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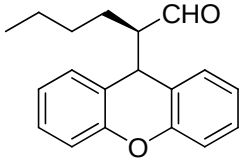
1. General Information

All manipulations were conducted with a standard Schlenk tube under dioxygen atmosphere, ^{1}H-NMR spectra were recorded on Bruker AVIII-400 spectrometer. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in $CDCl_3$ as an internal standard. ^{13}C-NMR spectra were obtained by the same NMR spectrometer and were calibrated with $CDCl_3$ (δ = 77.00 ppm). Mass spectra were obtained using electrospray ionization (ESI) mass spectrometer. Optical rotations were reported as follows: $[\alpha]_D^{rt}$ (*c* in g per 100 mL, solvent). HPLC analysis was performed on an Agilent 1200-series instrumentation using Daicel Chiralcel^{TM} AD-H columns or Daicel Chiralcel^{TM} OD-H columns. Unless otherwise noted, materials and solvents obtained from commercial suppliers were used without further purification. **2j, 2k** and **2l** were prepared according to literature methods.[1] **1c** were prepared according to literature methods.[2]

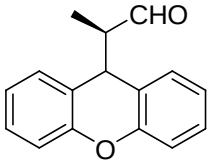
2. Experimental procedures and characterization of products

(*R*)-2-(9*H*-Xanthen-9-yl)hexanal (3aa)



Typical procedure: xanthene **1a** (36.4 mg, 0.2 mmol) and organocatalyst **B** (13.3 mg, 0.04 mmol) were placed in a 25 mL Schlenk tube，refilled with dioxygen for three times. The H_2O (10.0 eq.) and dry CH_3NO_2 1.0 mL was added at –5 °C, followed by the addition of hexanal **2a** (60.0 mg, 0.6 mmol). The reaction was stirred at -5 °C for four days as monitored by TLC. The crude reaction mixture was directly purified by flash chromatography column using hexane/DCM = 10/1 as the eluent to afforded 39.8 mg (71 % yield, 92% *ee*) of **3aa**. **3aa**: colorless oil. HPLC analysis (derivatized to alcohol) on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 19.3 min, t_R (minor) = 16.6 min; $[\alpha]_D^{rt}$ = -4.0 (*c* = 2.03, $CHCl_3$, 92 % *ee*); IR:(KBr) ν_{max} 2956, 2930, 2859, 1721, 1478, 1458, 1254, 755 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.63 (d, *J* = 2.4 Hz, 1H), 7.26-7.20 (m, 3H), 7.12-7.04 (m, 5H), 4.46 (d, *J* = 4.4 Hz, 1H), 2.54-2.49 (m, 1H), 1.57-1.47 (m, 1H), 1.42-1.04 (m, 5H), 0.78 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.6, 152.9, 152.9, 128.9, 128.7, 128.3, 128.2, 123.5, 123.3, 123.1, 122.1, 116.7, 116.6, 60.6, 40.0, 29.5, 25.0, 22.5, 13.7; HRMS m/z (ESI): Calcd. for $C_{19}H_{20}NaO_2$ $[M+Na]^+$ 303.1356, Found: 303.1355.

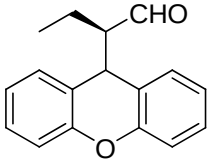
(*R*)-2-(9*H*-Xanthen-9-yl)propanal (3ab)[3]



The reaction of xanthene **1a** (36.9 mg, 0.2 mmol), organocatalyst **B** (13.3 mg, 0.04

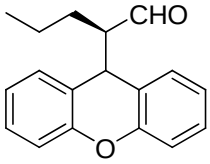
mmol), propanal **2b** (34.8 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at +5 °C under dioxygen afforded 29.2 mg (61 % yield, 81% *ee*) of **3ab**. **3ab**: colorless oil. HPLC analysis on a AD-H column at 25 °C: hexane/*i*-PrOH = 98/2, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 14.7 min., t_R (minor) = 16.6 min; $[\alpha]_D^{rt}$ = -1.6 (*c* = 2.50, $CHCl_3$, 81 % *ee*); IR:(KBr) ν_{max} 2961, 2925, 2853, 1721, 1479, 1458, 1255, 754 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.75 (d, *J* = 1.2 Hz, 1H), 7.27-7.22 (m, 3H), 7.12-7.02 (m, 5H), 4.62 (d, *J* = 4.4 Hz, 1H), 2.70-2.64 (m, 1H), 0.91 (d, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 203.7, 153.0, 152.8, 128.9, 128.5, 128.3, 128.1, 123.5, 123.4, 123.2, 121.4, 116.6, 55.7, 39.6, 9.3; MS m/z (ESI): $[M+Na]^+$ 261.1.

(*R*)-2-(9*H*-Xanthen-9-yl)butanal (3ac)[3]



The reaction of xanthene **1a** (36.8 mg, 0.2 mmol), organocatalyst **B** (13.7 mg, 0.04 mmol), butanal **2c** (43.2 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at +5 °C under dioxygen afforded 32.6 mg (65 % yield, 90% *ee*) of **3ac**. **3ac**: colorless oil. HPLC analysis (derivatized to alcohol) on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 23.6 min., t_R (minor) = 20.2 min; $[\alpha]_D^{rt}$ = -5.3 (*c* = 2.27, $CHCl_3$, 90 % *ee*); IR:(KBr) ν_{max} 2964, 2931, 2876, 1719, 1478, 1458, 1255, 754 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.64 (d, *J* = 2.4 Hz, 1H), 7.26-7.20 (m, 3H), 7.12-7.03 (m, 5H), 4.46 (d, *J* = 4.4 Hz, 1H), 2.47-2.42 (m, 1H), 1.57-1.39 (m, 2H), 0.82 (t, *J* = 7.4 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.5, 152.9, 152.9, 128.9, 128.6, 128.3, 128.2, 123.5, 123.3, 123.1, 122.1, 116.7, 116.6, 62.3, 39.9, 18.6, 12.0; MS m/z (ESI): $[M+Na]^+$ 275.1.

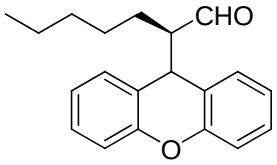
(*R*)-2-(9*H*-Xanthen-9-yl)pentanal (3ad)



The reaction of xanthene **1a** (36.8 mg, 0.2 mmol), organocatalyst **B** (13.8 mg, 0.04 mmol), pentanal **2d** (51.6 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at -5 °C under dioxygen afforded 40.7 mg (77 % yield, 90% *ee*) of **3ad**. **3ad**: colorless oil. HPLC analysis (derivatized to alcohol) on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 21.6 min., t_R (minor) = 18.2 min; $[\alpha]_D^{rt}$ = -4.3 (*c* = 1.88, $CHCl_3$, 90 % *ee*); IR:(KBr) ν_{max} 2959, 2931, 2871, 1720, 1478, 1458, 1254, 754 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.63 (d, *J* = 2.4 Hz, 1H), 7.26-7.20 (m, 3H), 7.12-7.03 (m, 5H), 4.46 (d, *J* = 4.4 Hz, 1H), 2.55-2.50 (m, 1H), 1.55-1.04 (m, 4H), 0.78 (t, *J* = 7.2 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.6, 152.9, 152.8, 128.9, 128.6, 128.3, 128.2, 123.5, 123.3, 123.0, 122.0, 116.7, 116.6, 60.4, 40.0, 27.4, 20.6, 13.9; HRMS m/z (ESI): Calcd. for

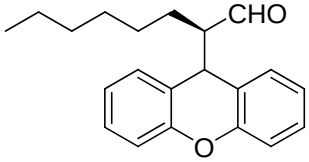
$C_{18}H_{18}NaO_2$ $[M+Na]^+$ 289.1199, Found: 289.1201.

(*R*)-2-(9*H*-Xanthen-9-yl)heptanal (3ae)



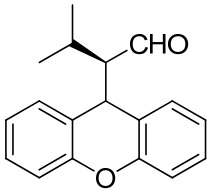
The reaction of xanthene **1a** (36.8 mg, 0.2 mmol), organocatalyst **B** (13.4 mg, 0.04 mmol), heptanal **2e** (68.4 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at +5 °C under dioxygen afforded 28.4 mg (48 % yield, 89% *ee*) of **3ae**. **3ae**: colorless oil. HPLC analysis (derivatized to alcohol) on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 18.1 min., t_R (minor) = 15.3 min; $[\alpha]_D^{rt}$ = -5.5 (*c* = 2.17, $CHCl_3$, 89 % *ee*); IR:(KBr) ν_{max} 2928, 2859, 1722, 1478, 1458, 1253, 754 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.63 (d, *J* = 2.8 Hz, 1H), 7.26-7.20 (m, 3H), 7.12-7.04 (m, 5H), 4.47 (d, *J* = 4.8 Hz, 1H), 2.54-2.49 (m, 1H), 1.54-1.46 (m, 1H), 1.39-1.11 (m, 7H), 0.80 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.6, 152.9, 152.9, 128.9, 128.7, 128.3, 128.2, 123.5, 123.3, 123.1, 122.1, 116.7, 116.6, 60.6, 40.0, 31.6, 27.1, 25.3, 22.3, 13.9; HRMS m/z (ESI): Calcd. for $C_{20}H_{22}NaO_2$ $[M+Na]^+$ 317.1512, Found: 317.1508.

(*R*)-2-(9*H*-Xanthen-9-yl)octanal (3af)[3]



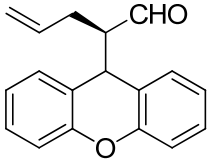
The reaction of xanthene **1a** (36.7 mg, 0.2 mmol), organocatalyst **B** (13.6 mg, 0.04 mmol), octanal **2f** (76.8 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at +5 °C under dioxygen afforded 40.0 mg (65 % yield, 83 % *ee*) of **3af**. **3af**: colorless oil. HPLC analysis (derivatized to alcohol) on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 16.7 min., t_R (minor) = 14.4 min; $[\alpha]_D^{rt}$ = -16.3 (*c* = 2.22, $CHCl_3$, 83 % *ee*); IR:(KBr) ν_{max} 2927, 2856, 1721, 1478, 1458, 1255, 755 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.63 (d, *J* = 2.4 Hz, 1H), 7.27-7.20 (m, 3H), 7.12-7.03 (m, 5H), 4.46 (d, *J* = 4.4 Hz, 1H), 2.54-2.49 (m, 1H), 1.54-1.11 (m, 10H), 0.82 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.6, 152.9, 152.9, 128.9, 128.7, 128.3, 128.2, 123.5, 123.3, 123.1, 122.1, 116.7, 116.6, 60.6, 40.0, 31.4, 29.0, 27.4, 25.3, 22.4, 13.9; MS m/z (ESI): $[M+Na]^+$ 331.2.

(*R*)-3-Methyl-2-(9*H*-xanthen-9-yl)butanal (3ag)[3]



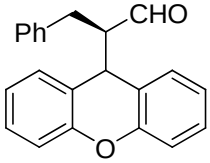
The rection of xanthene **1a** (36.8 mg, 0.2 mmol), organocatalyst **B** (13.7 mg, 0.04 mmol), isovaleraldehyde **2g** (51.6 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 at +5 °C (1.0 mL) under dioxygen afforded 21.1 mg (40 % yield, 69 % *ee*) of **3ag**. **3ag**: white solid. HPLC analysis (derivatized to alcohol) on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 20.8 min., t_R (minor) = 17.9 min; $[\alpha]_D^{rt}$ = -18.7 (*c* = 2.78, $CHCl_3$, 69 % *ee*); IR:(KBr) ν_{max} 2960, 1720, 1477, 1458, 1250, 752 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.51 (d, *J* = 4.0 Hz, 1H), 7.26-7.22 (m, 4H), 7.12-7.05 (m, 4H), 4.49 (d, *J* = 6.0 Hz, 1H), 2.32-2.28 (m, 1H), 2.04-1.92 (m, 1H), 1.11 (d, *J* = 7.2 Hz, 3H), 0.90 (d, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.5, 153.2, 152.9, 128.8, 128.7, 128.2, 128.2, 124.0, 123.5, 123.3, 123.1, 116.8, 116.8, 66.3, 38.2, 26.1, 21.7, 19.3; MS m/z (ESI): $[M+Na]^+$ 289.1.

(*R*)-2-(9*H*-Xanthen-9-yl)pent-enal (3ah)



The reaction of xanthene **1a** (36.8 mg, 0.2 mmol), organocatalyst **B** (13.6 mg, 0.04 mmol), 4-pentenal **2h** (50.4 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at +5 °C under dioxygen afforded 35.2 mg (67 % yield, 87% *ee*) of **3ah**. **3ah**: colorless oil. HPLC analysis (derivatized to alcohol) on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 23.9 min., t_R (minor) = 20.4 min; $[\alpha]_D^{rt}$ = -14.7 (*c* = 1.63, $CHCl_3$, 87 % *ee*); IR:(KBr) ν_{max} 3075, 3043, 2924, 2852, 1723, 1479, 1458, 1255, 756 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.63 (d, *J* = 2.0 Hz, 1H), 7.28-7.22 (m, 3H), 7.14-7.04 (m, 5H), 5.67-5.56 (m, 1H), 4.99-4.95 (m, 2H), 4.55 (d, *J* = 4.0 Hz, 1H), 2.70-2.64 (m, 1H), 2.30-2.12 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 203.9, 152.9, 152.9, 135.0, 128.9, 128.7, 128.4, 128.3, 123.6, 123.5, 122.7, 121.9, 117.3, 116.8, 116.7, 59.9, 39.3, 29.6; HRMS m/z (ESI): Calcd. for $C_{18}H_{16}NaO_2$ $[M+Na]^+$ 287.1038, Found: 287.1043.

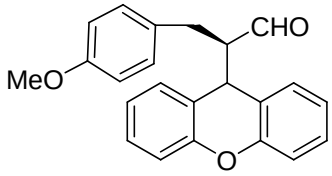
(*R*)-3-Phenyl-2-(9*H*-xanthen-9-yl)propanal (3ai)[3]



The reaction of xanthene **1a** (36.7 mg, 0.2 mmol), organocatalyst **B** (13.6 mg, 0.04 mmol)，3-Phenylpropionaldehyde **2i** (80.4 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at +5 °C under dioxygen afforded 40.0 mg (64 % yield, 92 % *ee*) of **3ai**. **3ai**: white solid. HPLC analysis on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 14.5 min., t_R (minor) = 16.4 min; $[\alpha]_D^{rt}$ = -25.3 (*c* = 1.90, $CHCl_3$, 92 % *ee*); IR:(KBr) ν_{max} 3062, 3028, 2925, 2853 2728, 1722, 1479, 1458, 1254, 756, 699 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.65 (d, *J* = 1.6 Hz, 1H), 7.29-7.06 (m, 11H), 6.96 (d, *J* = 7.2 Hz, 2H), 4.59 (d, *J* = 4.0

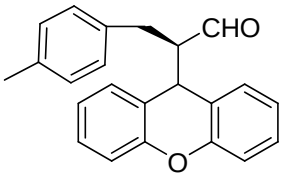
Hz, 1H), 3.01-2.96 (m, 1H), 2.83-2.67 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 203.5, 152.9, 152.9, 138.7, 129.0, 128.8, 128.6, 128.5, 128.4, 126.3, 123.7, 123.5, 122.6, 121.7, 116.8, 116.8, 62.4, 39.5, 31.2; MS m/z (ESI): $[M+Na]^+$ 337.1.

(*R*)-3-(4-Methoxyphenyl)-2-(9*H*-xanthen-9-yl)propanal (3aj)



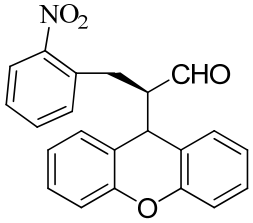
The reaction of xanthene **1a** (36.7 mg, 0.2 mmol), organocatalyst **B** (13.6 mg, 0.04 mmol) and 3-(4-methoxyphenyl)propanal **2j** (98.4 mg, 0.6 mmol) in commercial CH_3NO_2 (1.0 mL) at -5 °C under dioxygen for 7 days afforded 26 mg (79 % yield based on 48 % conversion of xanthene, 86 % *ee*) of **3aj**. **3aj**: white solid. HPLC analysis on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 22.1 min., t_R (minor) = 26.4 min; $[\alpha]_D^{rt}$ = -23.4 (*c* = 1.37, $CHCl_3$, 86 % *ee*); IR:(KBr) ν_{max} 2958, 2931, 2835, 1722, 1512, 1478, 1458, 1252, 1119, 1096, 827, 753 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.64 (d, *J* = 2.0 Hz, 1H), 7.29-7.25 (m, 3H), 7.15-7.06 (m, 5H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 2H), 4.58 (d, *J* = 4.0 Hz, 1H), 3.73 (s, 3H), 2.96-2.91 (m, 1H), 2.77-2.62 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 203.8, 158.1, 152.9, 152.9, 130.6, 129.8, 129.0, 128.6, 128.5, 128.4, 123.6, 123.5, 122.7, 121.8, 116.8, 116.8, 113.9, 62.6, 55.2, 39.5, 30.4; HRMS m/z (ESI): Calcd. for $C_{23}H_{20}NaO_3$ $[M+Na]^+$ 367.1305, Found: 367.1307.

(*R*)-3-*p*-Tolyl-2-(9*H*-xanthen-9-yl)propanal (3ak)



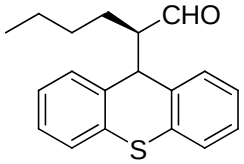
The reaction of xanthene **1a** (36.6 mg, 0.2 mmol), organocatalyst **B** (13.4 mg, 0.04 mmol) and 3-*p*-tolylpropanal **2k** (88.8 mg, 0.6 mmol) in commercial CH_3NO_2 (1.0 mL) at +5 °C under dioxygen for 7 days afforded 24.3 mg (82 % yield based on 45 % conversion of xanthene, 80% *ee*) of **3ak**. **3ak**: white solid. HPLC analysis on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 13.6 min., t_R (minor) = 16.7 min; $[\alpha]_D^{rt}$ = -14.0 (*c* = 2.29, $CHCl_3$, 80 % *ee*); IR:(KBr) ν_{max} 2960, 2920, 2881, 1724, 1477, 1456, 1253, 1078, 828, 753, 701 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.64 (d, *J* = 1.6 Hz, 1H), 7.29-7.25 (m, 3H), 7.14-7.05 (m, 5H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.88 (d, *J* = 8.0 Hz, 2H), 4.58 (d, *J* = 3.6 Hz, 1H), 2.98-2.93 (m, 1H), 2.79-2.64 (m, 2H), 2.26 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 203.7, 152.9, 152.9, 135.8, 135.5, 129.2, 129.0, 128.7, 128.5, 128.4, 123.6, 123.5, 122.7, 121.8, 116.8, 116.8, 62.4, 39.5, 30.8, 20.9; HRMS m/z (ESI): Calcd. for $C_{23}H_{20}NaO_2$ $[M+Na]^+$ 351.1356, Found: 351.1359.

(*R*)-3-(2-Nitrophenyl)-2-(9*H*-xanthen-9-yl)propanal (3al)



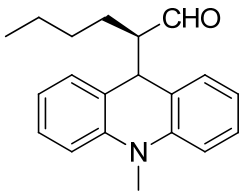
The reaction of xanthene **1a** (36.7 mg, 0.2 mmol), organocatalyst **B** (13.6 mg, 0.04 mmol), 3-(4-nitrophenyl)propanal **2l** (107.4 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry CH_3NO_2 (1.0 mL) at +5 °C under dioxygen for 7 days afforded 25.1 mg (81 % yield based on 43 % conversion of xanthene, 93 % *ee*) of **3al**. **3al**: light yellowish solid. HPLC analysis on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 31.4 min., t_R (minor) = 35.8 min; $[\alpha]_D^{rt}$ = -24.0 (*c* = 1.50, $CHCl_3$, 93 % *ee*); IR:(KBr) ν_{max} 2924, 2854, 1723, 1524, 1478, 1458, 1253, 1219, 772 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.60 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.27-7.22 (m, 5H), 7.15-7.07 (m, 5H), 4.64 (d, *J* = 2.8 Hz, 1H), 3.12-3.05 (m, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 202.3, 152.7, 152.6, 149.0, 134.3, 133.2, 133.0, 129.0, 128.7, 128.6, 127.6, 125.0, 123.7, 121.8, 121.7, 116.8, 116.8, 61.4, 40.5, 29.9; HRMS m/z (ESI): Calcd. for $C_{22}H_{17}NNaO_4$ $[M+Na]^+$ 382.1050, Found: 382.1059.

(*R*)-2-(9*H*-Thioxanthen-9-yl)hexanal (3ba)



The reaction of thioxanthene **1b** (40.1 mg, 0.2 mmol), organocatalyst **B** (13.7 mg, 0.04 mmol) and hexanal **2a** (60 mg, 0.6 mmol) in commercial CH_3NO_2 (1.0 mL) at -5 °C under dioxygen afforded 14.2 mg (24 % yield, 77 % *ee*) of **3ba**. **3ba**: colorless oil. HPLC analysis on a AD-H column at 0 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 19.3 min., t_R (minor) = 21.5 min; $[\alpha]_D^{rt}$ = -21.7 (*c* = 1.29, $CHCl_3$, 77 % *ee*); IR:(KBr) ν_{max} 2955, 2929, 2858, 1722, 1465, 1442, 913, 742 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.51 (d, *J* = 3.2 Hz, 1H), 7.45-7.41 (m, 2H), 7.29-7.17 (m, 6H), 4.30 (d, *J* = 9.6 Hz, 1H), 3.10-3.03 (m, 1H), 1.59-1.50 (m, 1H), 1.32-1.10 (m, 5H), 0.76 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.2, 135.7, 135.3, 133.2, 133.1, 130.0, 129.5, 127.5, 127.3, 127.0, 126.6, 126.3, 50.9, 49.8, 28.9, 27.9, 22.5, 13.6; HRMS m/z (ESI): Calcd. for $C_{19}H_{20}NaOS$ $[M+Na]^+$ 319.1127, Found: 319.1132.

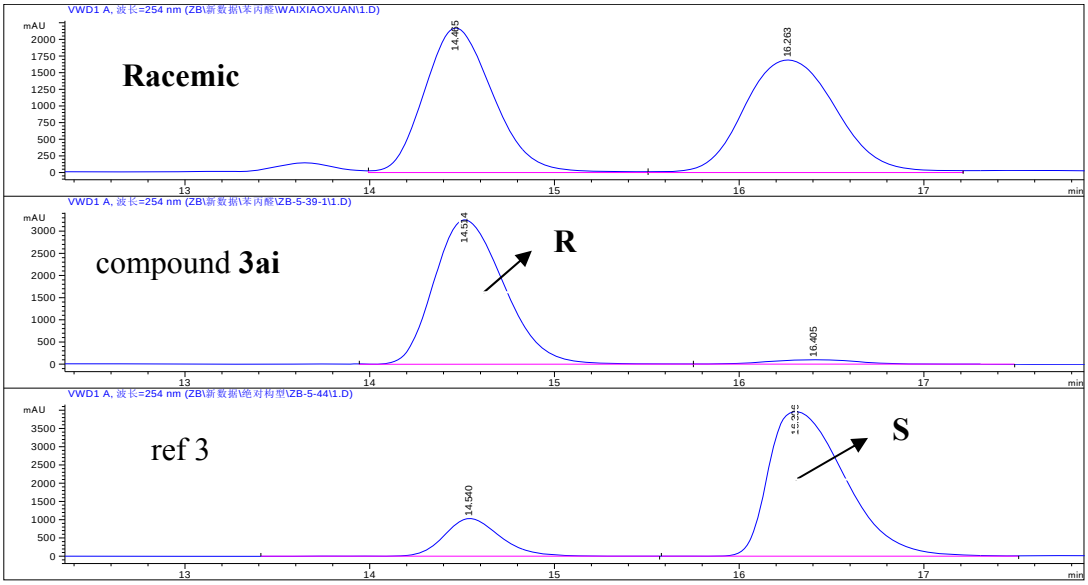
(*R*)-2-(10-Methyl-9,10-dihydroacridin-9-yl)hexanal (3ca)



The reaction of 10-methyl-9,10-dihydroacridine **1c** (39.5 mg, 0.2 mmol), organocatalyst **B** (13.4 mg, 0.04 mmol)，hexanal **2a** (60 mg, 0.6 mmol) and H_2O (10.0 eq.) in dry DCM (1.0 mL) at +5 °C under dioxygen afforded 30.5 mg (52 % yield, 45 % *ee*) of **3ca**. **3ca**: white solid. HPLC analysis on a OD-H column at 0 °C: hexane/*i*-PrOH = 98/2, flow rate 0.50 mL/min, λ = 254 nm: t_R (major) = 21.9 min., t_R (minor) = 19.3 min; $[\alpha]_D^{rt}$ = +2.1 (*c* = 1.91, $CHCl_3$, 45 % *ee*); IR:(KBr) ν_{max} 2956, 2930, 2858, 2826, 1715, 1592, 1474, 1341, 1269, 747 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$, ppm) δ 9.36 (d, *J* = 4.0 Hz, 1H), 7.26-7.21 (m, 2H), 7.18-7.13 (m, 2H), 6.99-6.92 (m, 4H), 4.21 (d, *J* = 6.8 Hz, 1H), 3.37 (s, 3H), 2.47-2.41 (m, 1H), 1.59-1.51 (m, 1H), 1.43-1.08 (m, 5H), 0.81 (t, *J* = 7.0 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 204.3, 143.1, 143.0, 128.6, 128.5, 127.6, 127.5, 124.8, 124.2, 120.9, 120.7, 112.5, 112.4, 57.7, 45.3, 32.9, 29.3, 26.7, 22.6, 13.7; HRMS m/z (ESI): Calcd. for $C_{20}H_{23}NNaO$ $[M+Na]^+$ 316.1672, Found: 316.1666.

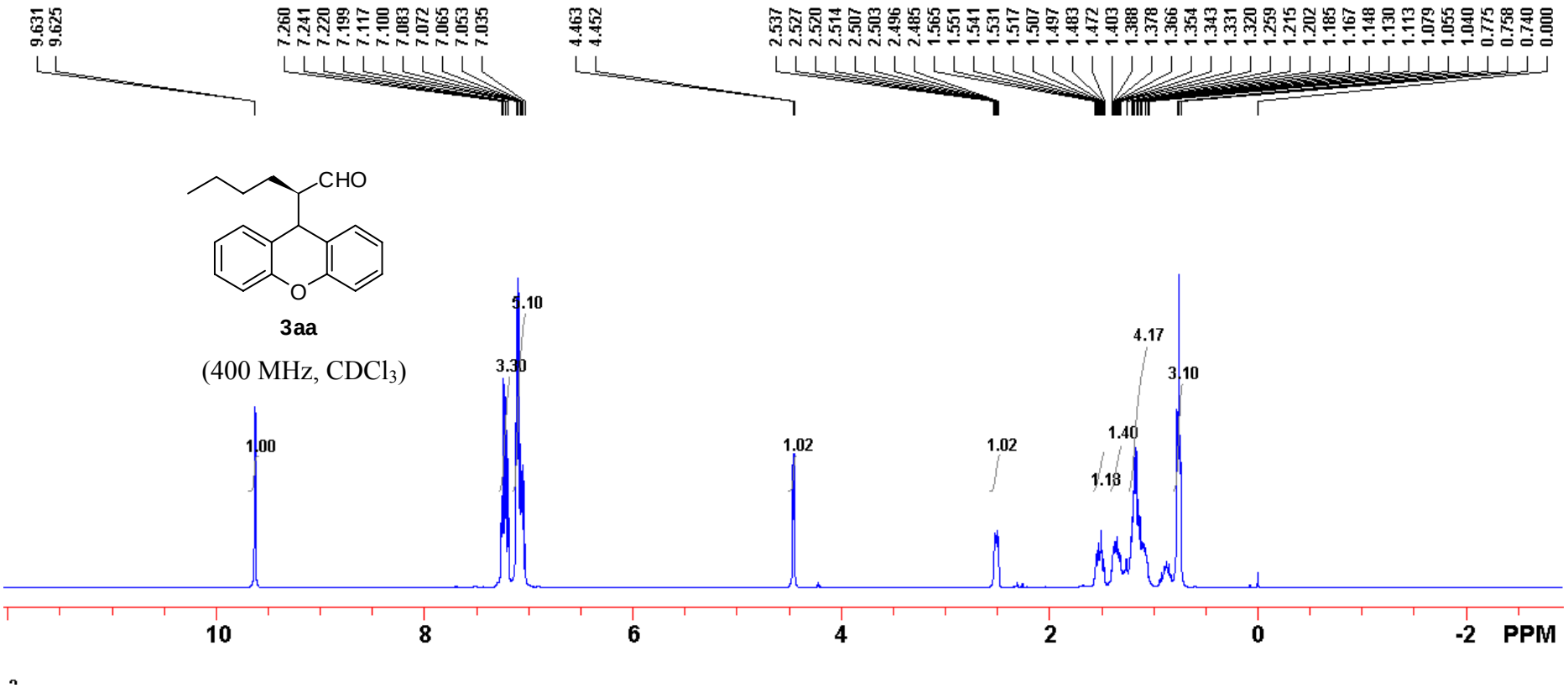
3. Determination of the absolute configuration.

The absolute configuration of compound **3ai** was determined to be *R* by comparison of the elution order of the products from a chiral phase HPLC column to the reported in the literature.[3] HPLC analysis on a AD-H column at 25 °C: hexane/*i*-PrOH = 95/5, flow rate 0.50 mL/min, λ = 254 nm.



Reference:

(1) Yang, J. W.; M. Fonseca, T. H.; List, B. *Angew. Chem. Int. Ed*. **2004**, *43*, 6660.
(2) Pintér, Á.; A. Sureshkumar, Sud, D.; Klussmann, M. *Angew. Chem. Int. Ed*. **2010**, *49*, 1.
(3) Benfatti, F.; Capdevila, M. G.; Zoli, L.; Benedetto, E.; Cozzi, P. G. *Chem. Common.* **2009**, 5919.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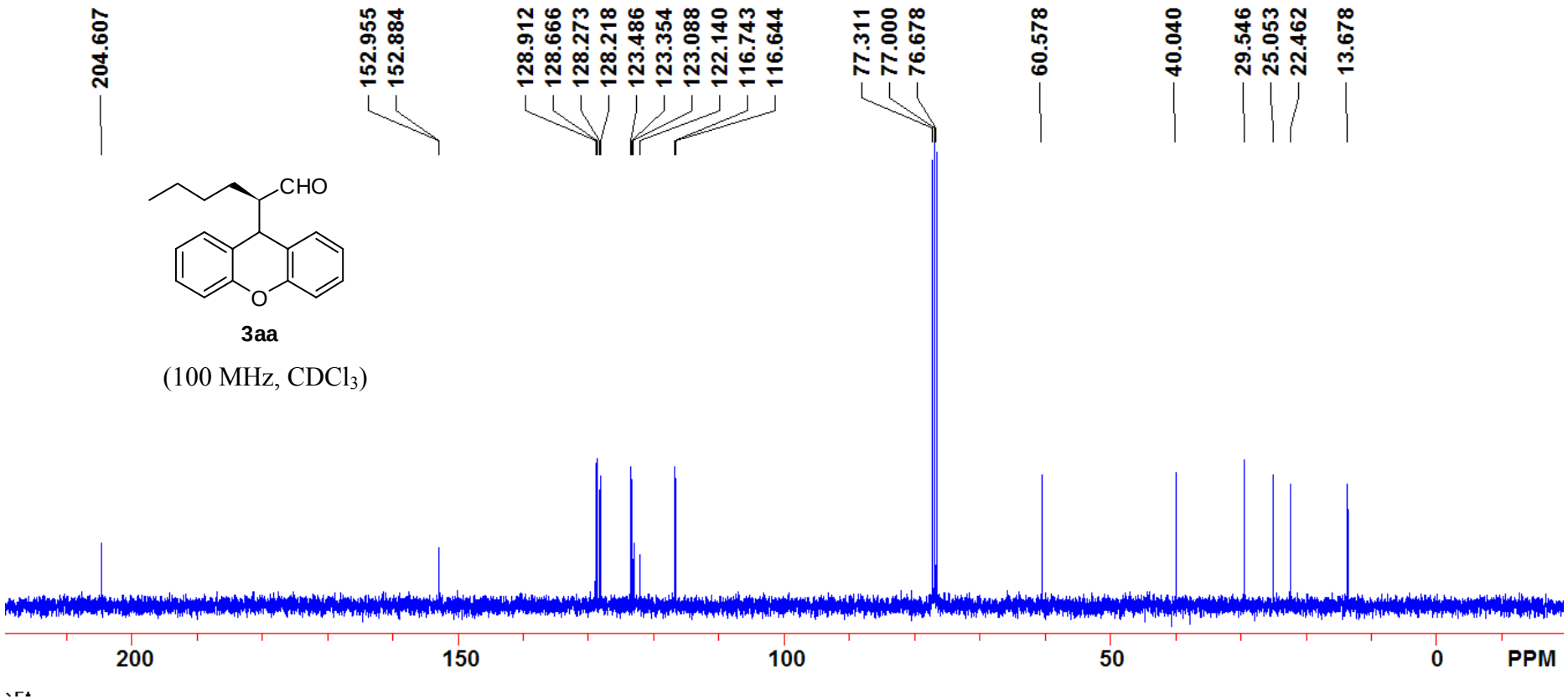
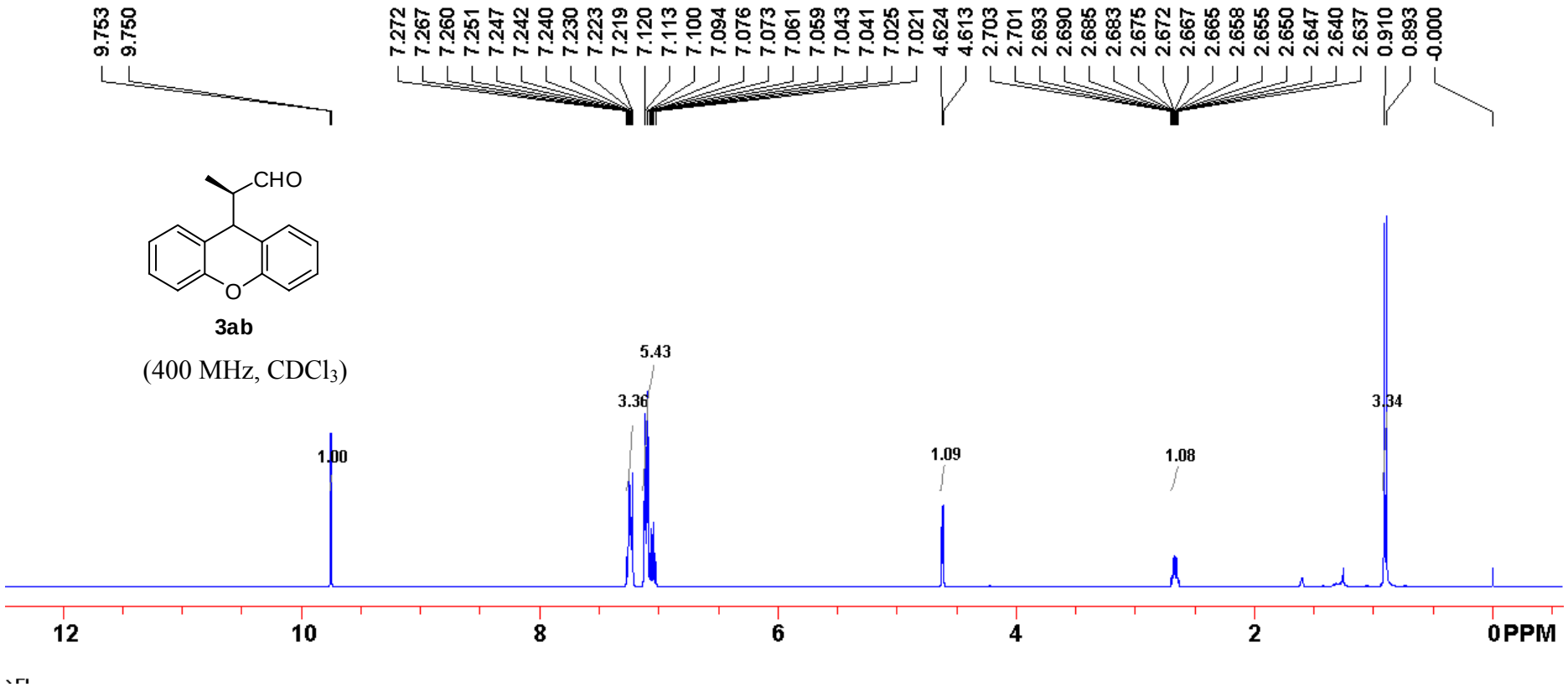
9.625
7.260
7.241
7.220
7.199
7.117
7.100
7.083
7.072
7.065
7.053
7.035
4.463
4.452
2.537
2.527
2.520
2.514
2.507
2.503
2.496
2.485
1.565
1.551
1.541
1.531
1.517
1.507
1.497
1.483
1.472
1.403
1.388
1.378
1.366
1.354
1.343
1.331
1.320
1.259
1.215
1.202
1.185
1.167
1.148
1.130
1.113
1.079
1.055
1.040
0.775
0.758
0.740
0.000
CHO
O
3aa
(400 MHz, CDCl3)
1.00
3.30
5.10
1.02
1.02
1.18
1.40
4.17
3.10
10
8
6
4
2
0
-2
PPM



3aa

(100 MHz, $CDCl_3$)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7.267
7.260
7.251
7.247
7.242
7.240
7.230
7.223
7.219
7.120
7.113
7.100
7.094
7.076
7.073
7.061
7.059
7.043
7.041
7.025
7.021
4.624
4.613
2.703
2.701
2.693
2.690
2.685
2.683
2.675
2.672
2.667
2.665
2.658
2.655
2.650
2.647
2.640
2.637
0.910
0.893
-0.000
CHO
O
3ab
(400 MHz, CDCl3)
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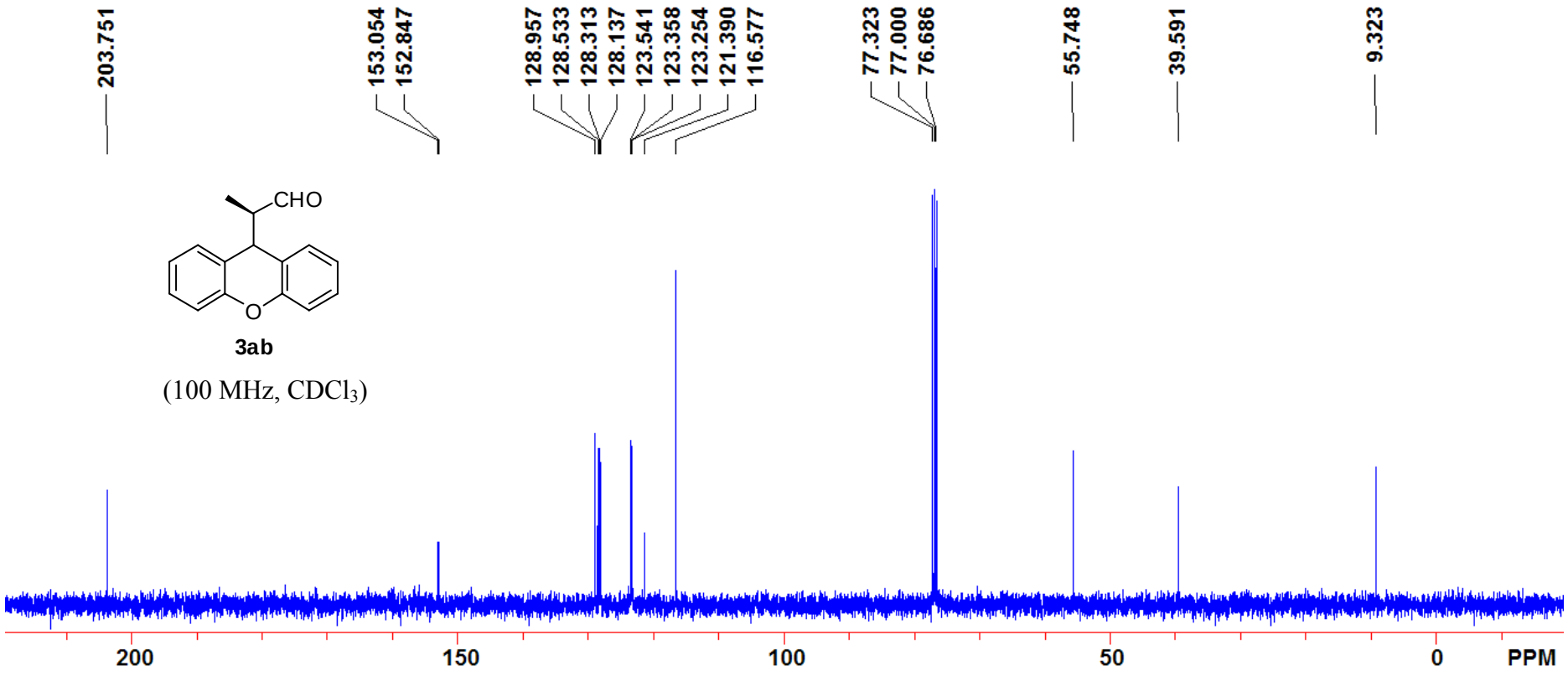
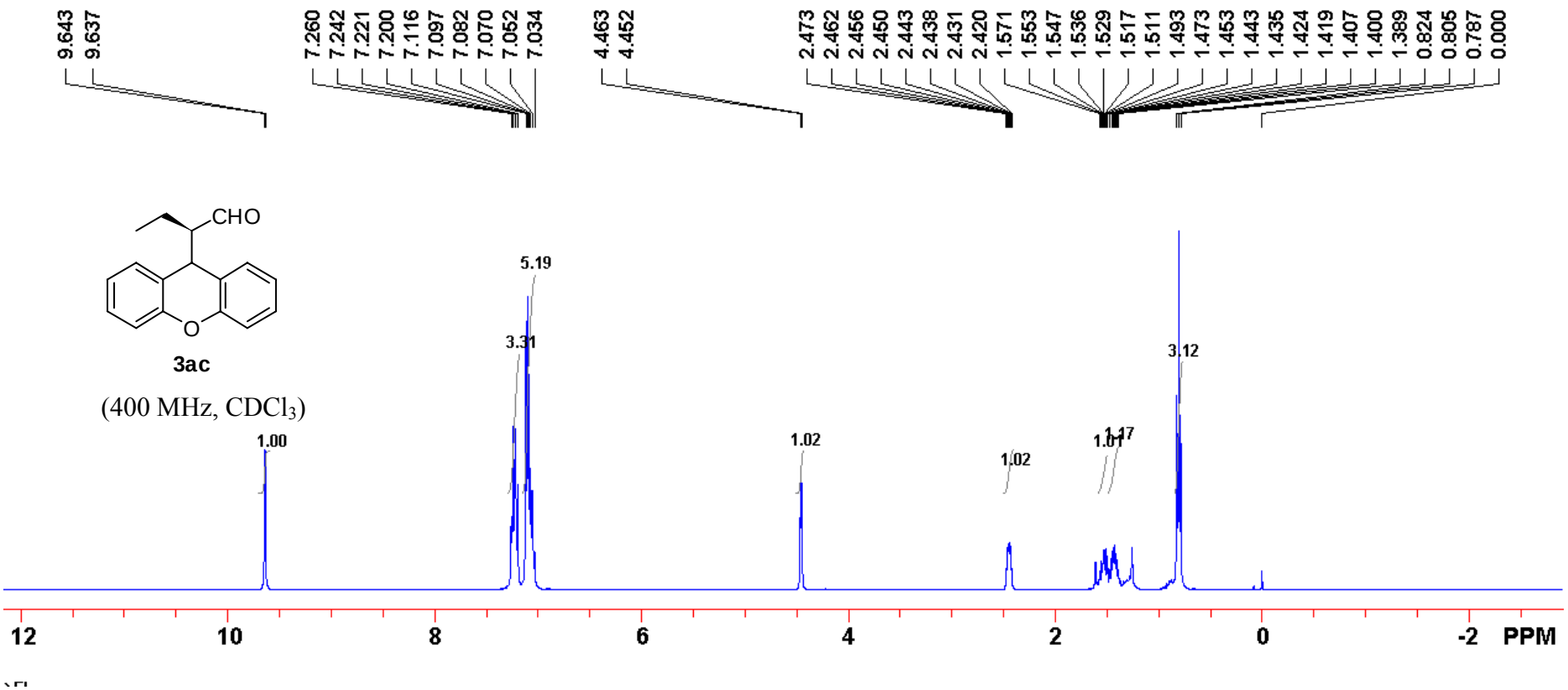
3.36
1.00
1.09
1.08
3.34
12
10
8
6
4
2
0 PPM



3ab

(100 MHz, $CDCl_3$)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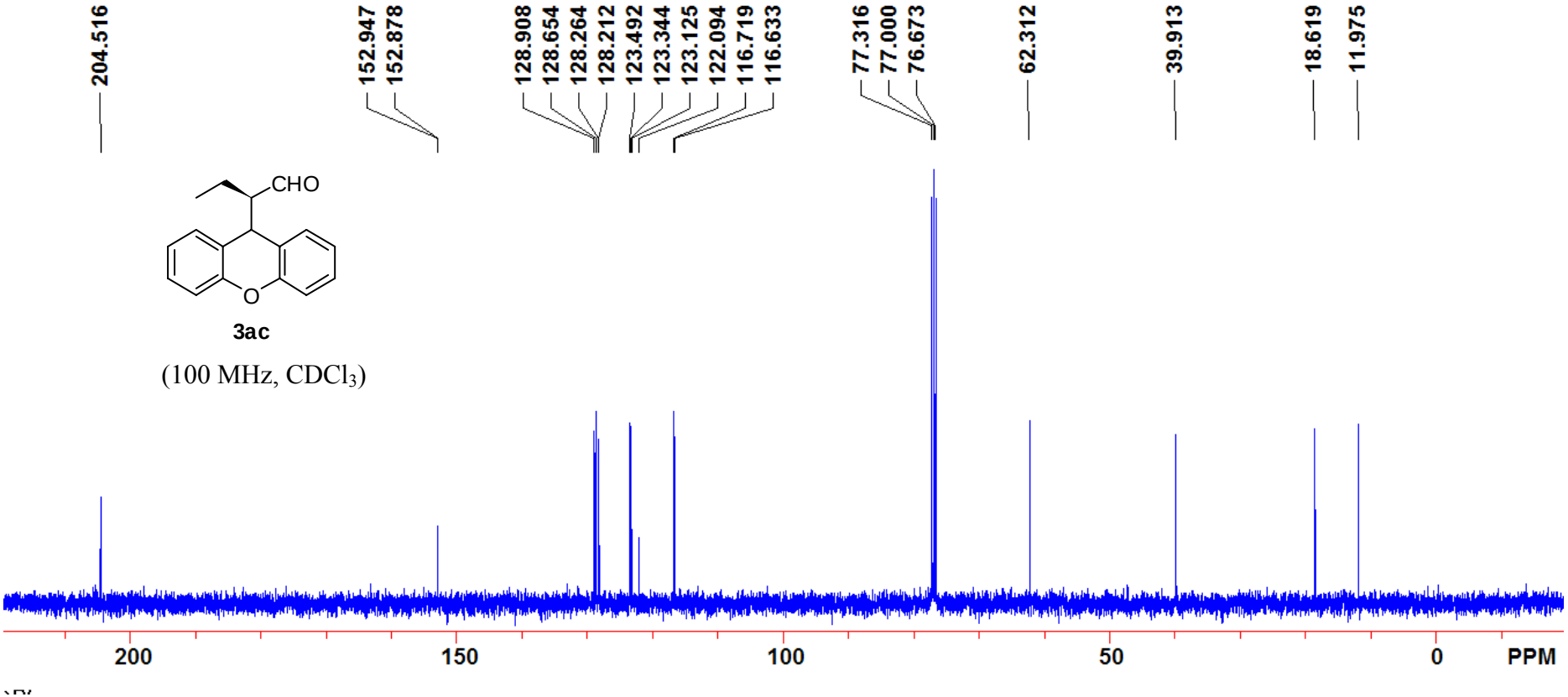
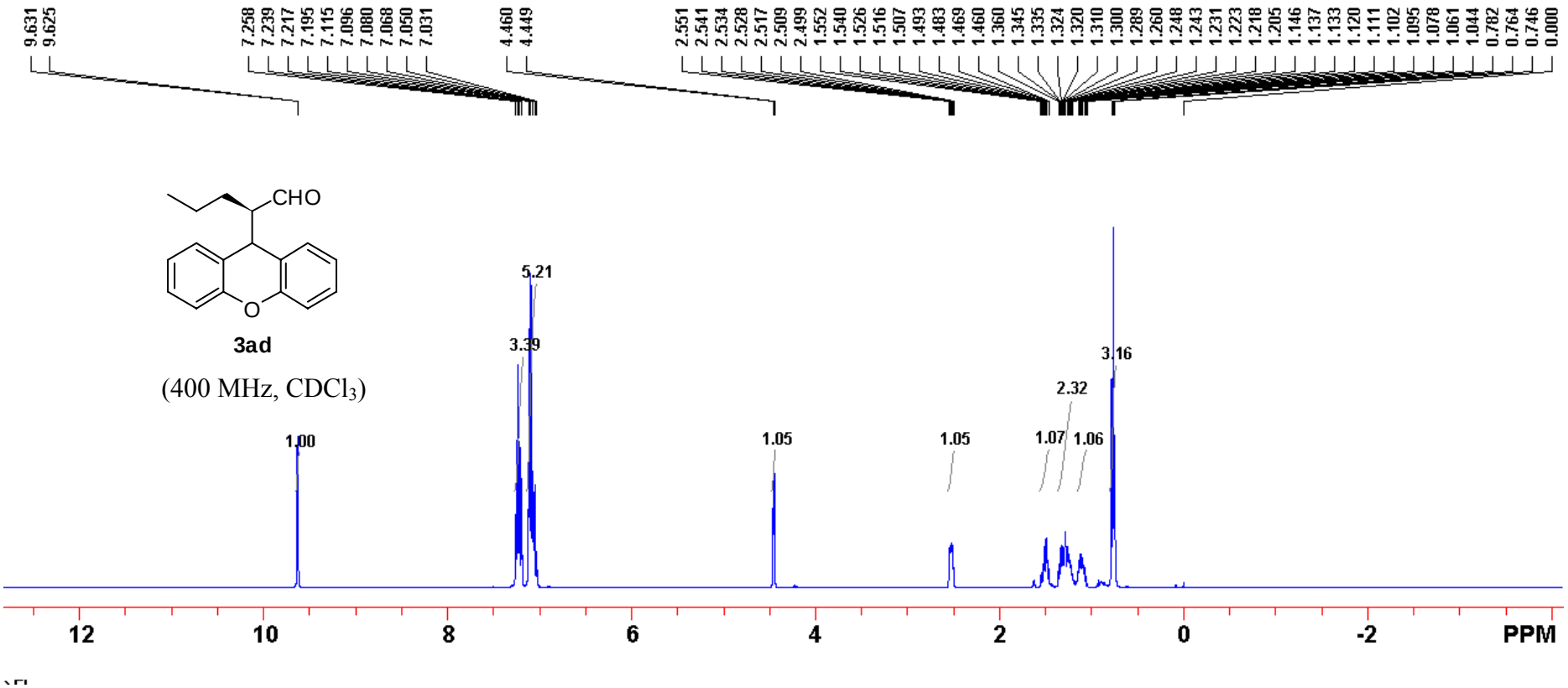
7.242
7.221
7.200
7.116
7.097
7.082
7.070
7.052
7.034
4.463
4.452
2.473
2.462
2.456
2.450
2.443
2.438
2.431
2.420
1.571
1.553
1.547
1.536
1.529
1.517
1.511
1.493
1.473
1.453
1.443
1.435
1.424
1.419
1.407
1.400
1.389
0.824
0.805
0.787
0.000
CHO
O
3ac
(400 MHz, CDCl3)
1.00
5.19
3.31
1.02
1.02
1.01
1.17
3.12
12
10
8
6
4
2
0
-2
PPM



3ac

(100 MHz, $CDCl_3$)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7.096
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7.068
7.050
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4.460
4.449
2.551
2.541
2.534
2.528
2.517
2.509
2.499
1.552
1.540
1.526
1.516
1.507
1.493
1.483
1.469
1.460
1.360
1.345
1.335
1.324
1.320
1.310
1.300
1.289
1.260
1.248
1.243
1.231
1.223
1.218
1.205
1.146
1.137
1.133
1.120
1.111
1.102
1.095
1.078
1.061
1.044
0.782
0.764
0.746
0.000
CHO
O
3ad
(400 MHz, CDCl3)
5.21
3.39
3.16
2.32
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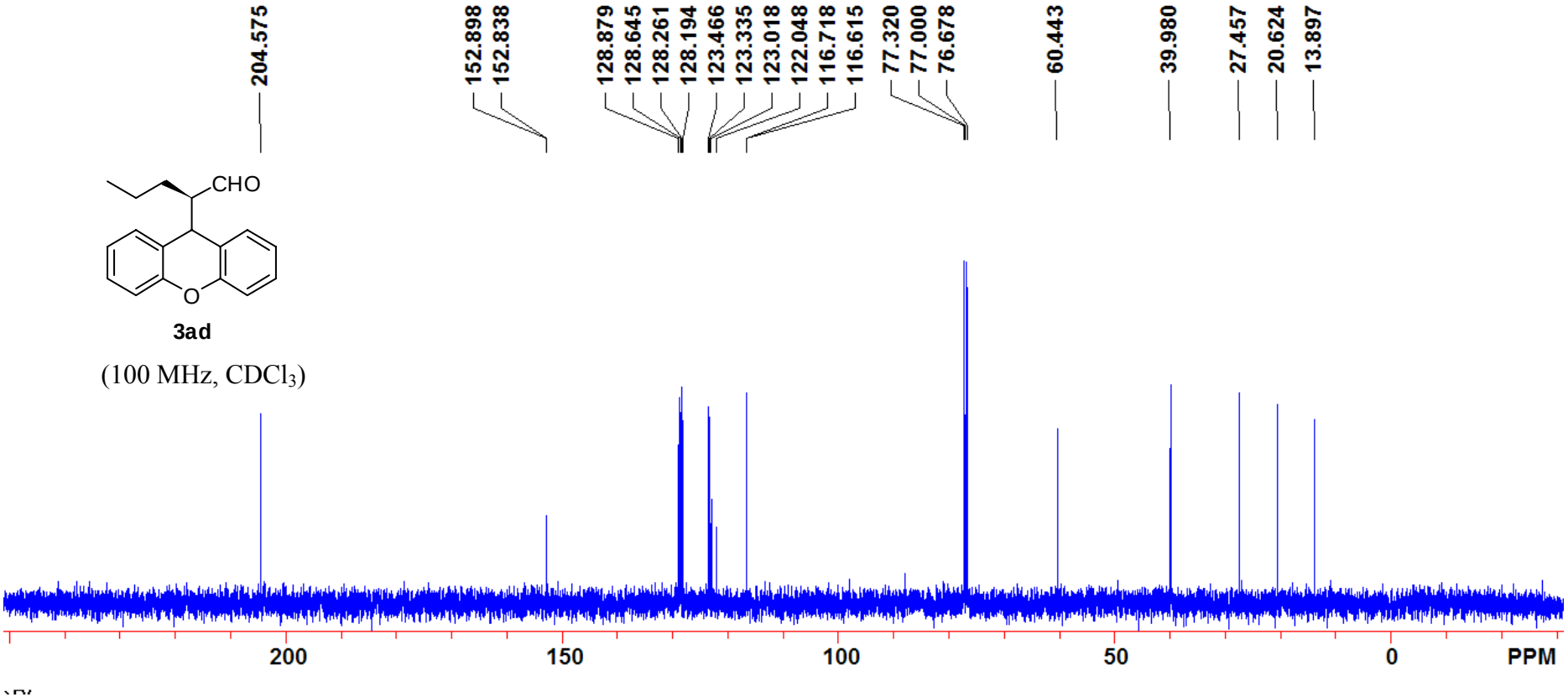
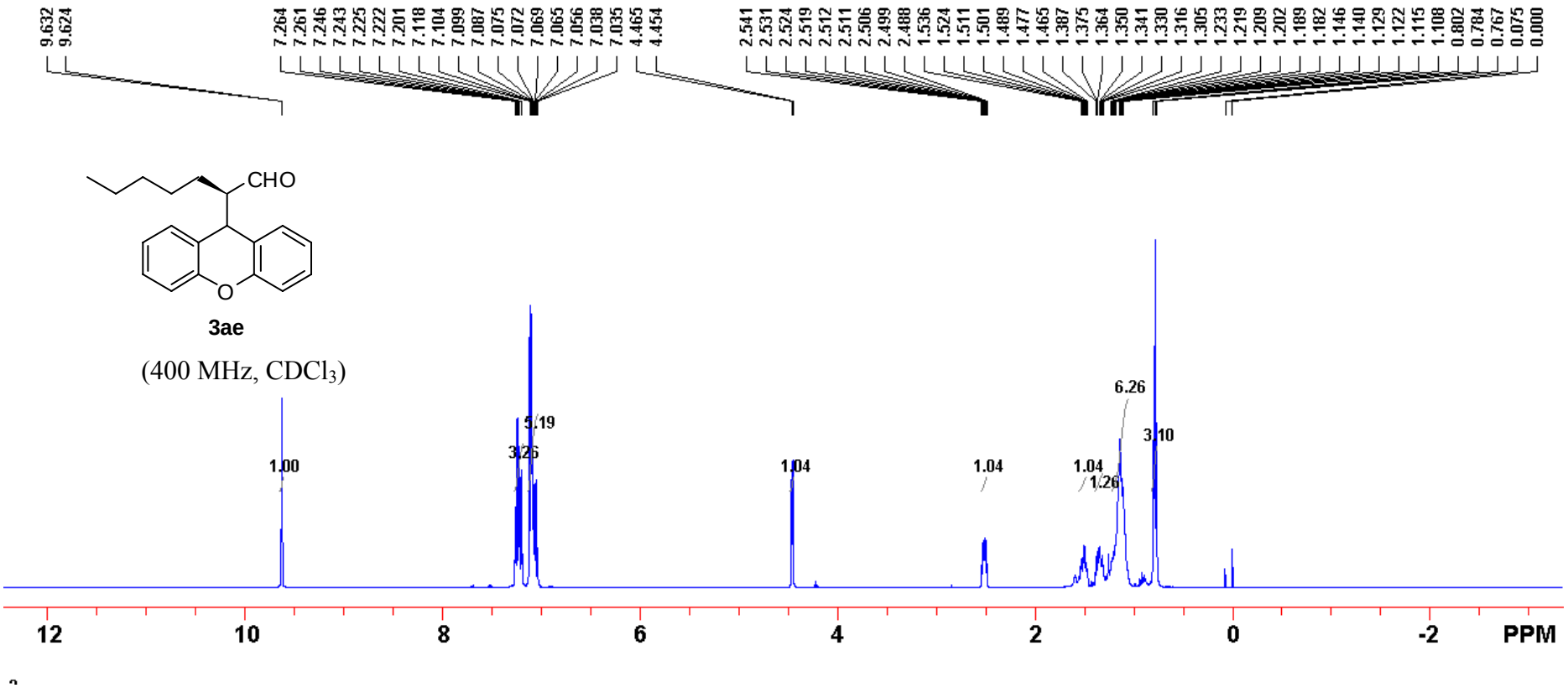
1.05
1.05
1.07
1.06
12
10
8
6
4
2
0
-2
PPM



3ad

(100 MHz, $CDCl_3$)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7.222
7.201
7.118
7.104
7.099
7.087
7.075
7.072
7.069
7.065
7.056
7.038
7.035
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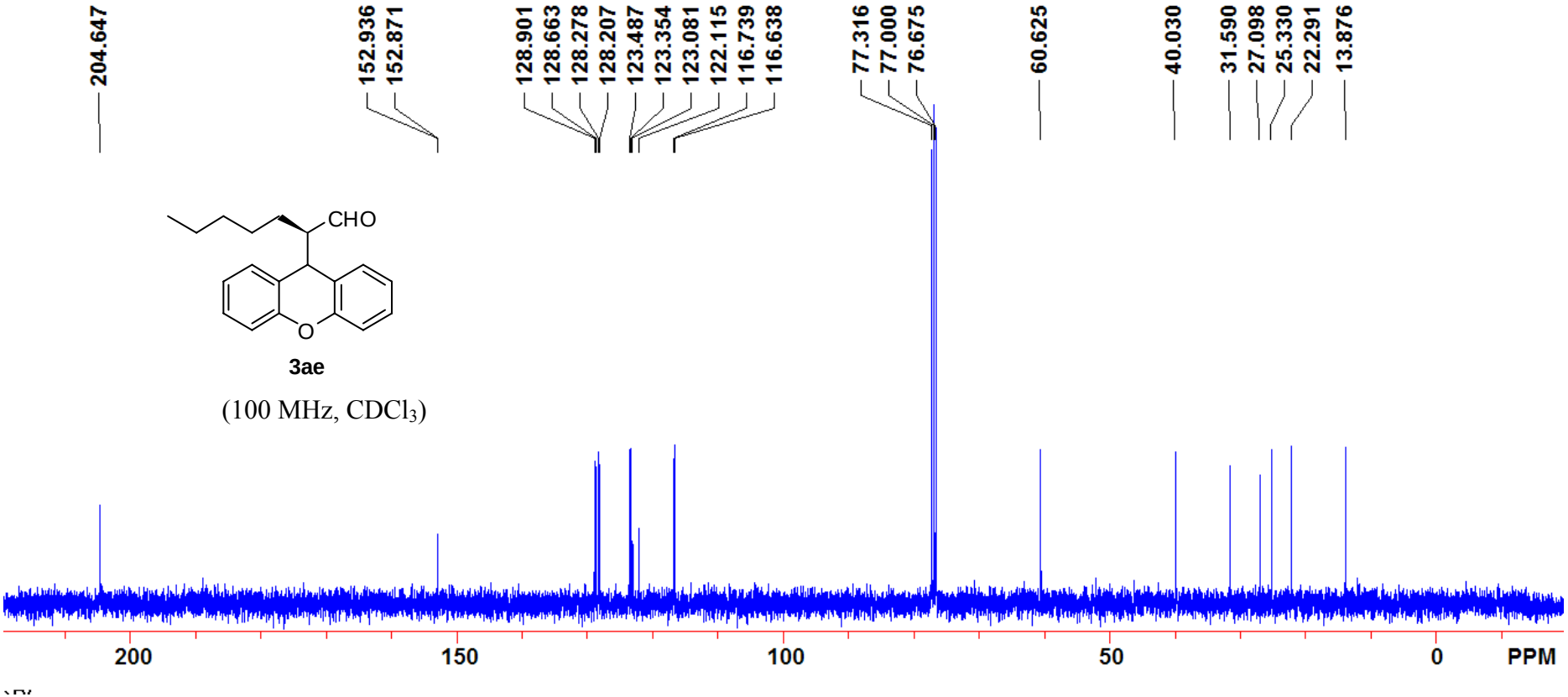
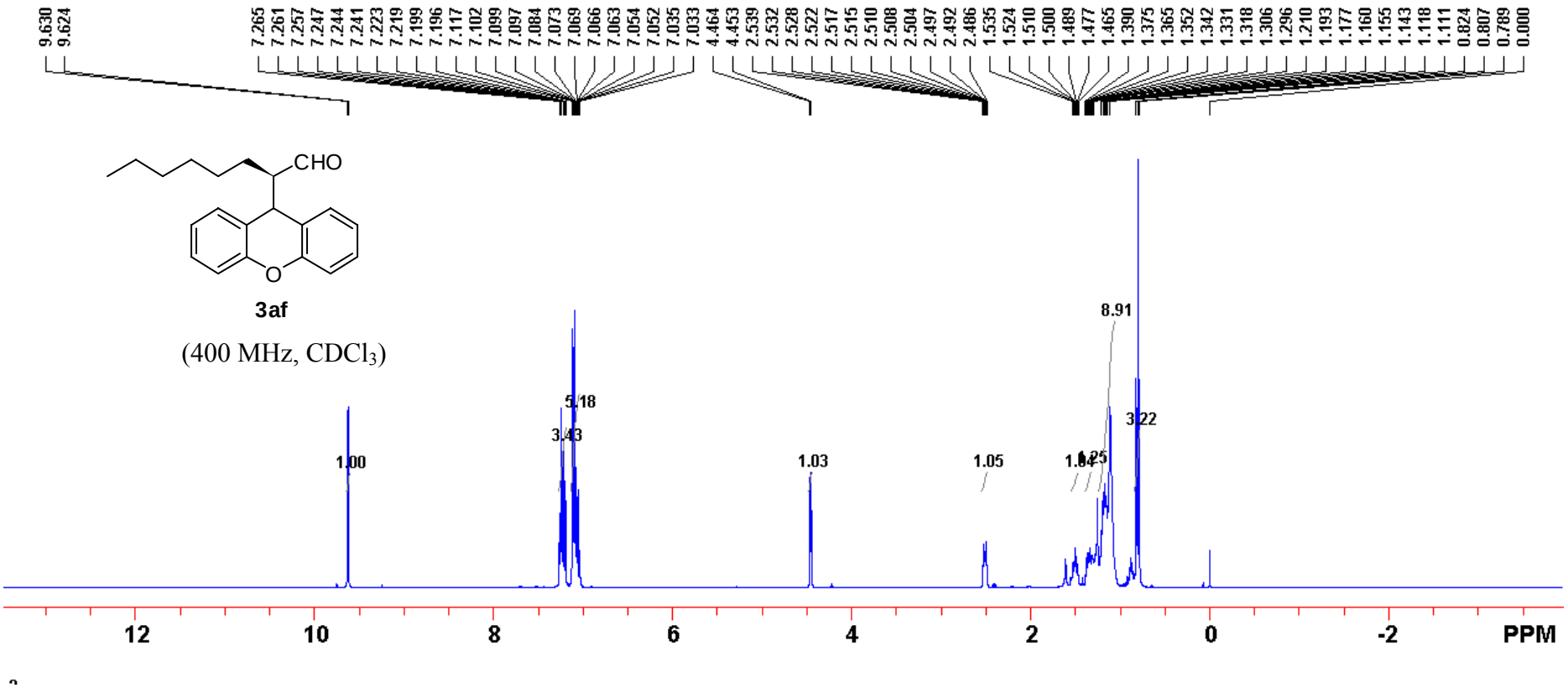
4.454
2.541
2.531
2.524
2.519
2.512
2.511
2.506
2.499
2.488
1.536
1.524
1.511
1.501
1.489
1.477
1.465
1.387
1.375
1.364
1.350
1.341
1.330
1.316
1.305
1.233
1.219
1.209
1.202
1.189
1.182
1.146
1.140
1.129
1.122
1.115
1.108
0.802
0.784
0.767
0.075
0.000
CHO
O
3ae
(400 MHz, CDCl3)
1.00
3.26
5.19
1.04
1.04
1.04
1.26
6.26
3.10
12
10
8
6
4
2
0
-2
PPM



3ae

(100 MHz, $CDCl_3$)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7.099
7.097
7.084
7.073
7.069
7.066
7.063
7.054
7.052
7.035
7.033
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4.453
2.539
2.532
2.528
2.522
2.517
2.515
2.510
2.508
2.504
2.497
2.492
2.486
1.535
1.524
1.510
1.500
1.489
1.477
1.465
1.390
1.375
1.365
1.352
1.342
1.331
1.318
1.306
1.296
1.210
1.193
1.177
1.160
1.155
1.143
1.118
1.111
0.824
0.807
0.789
0.000
CHO
O
3af
(400 MHz, CDCl3)
1.00
3.43
5.18
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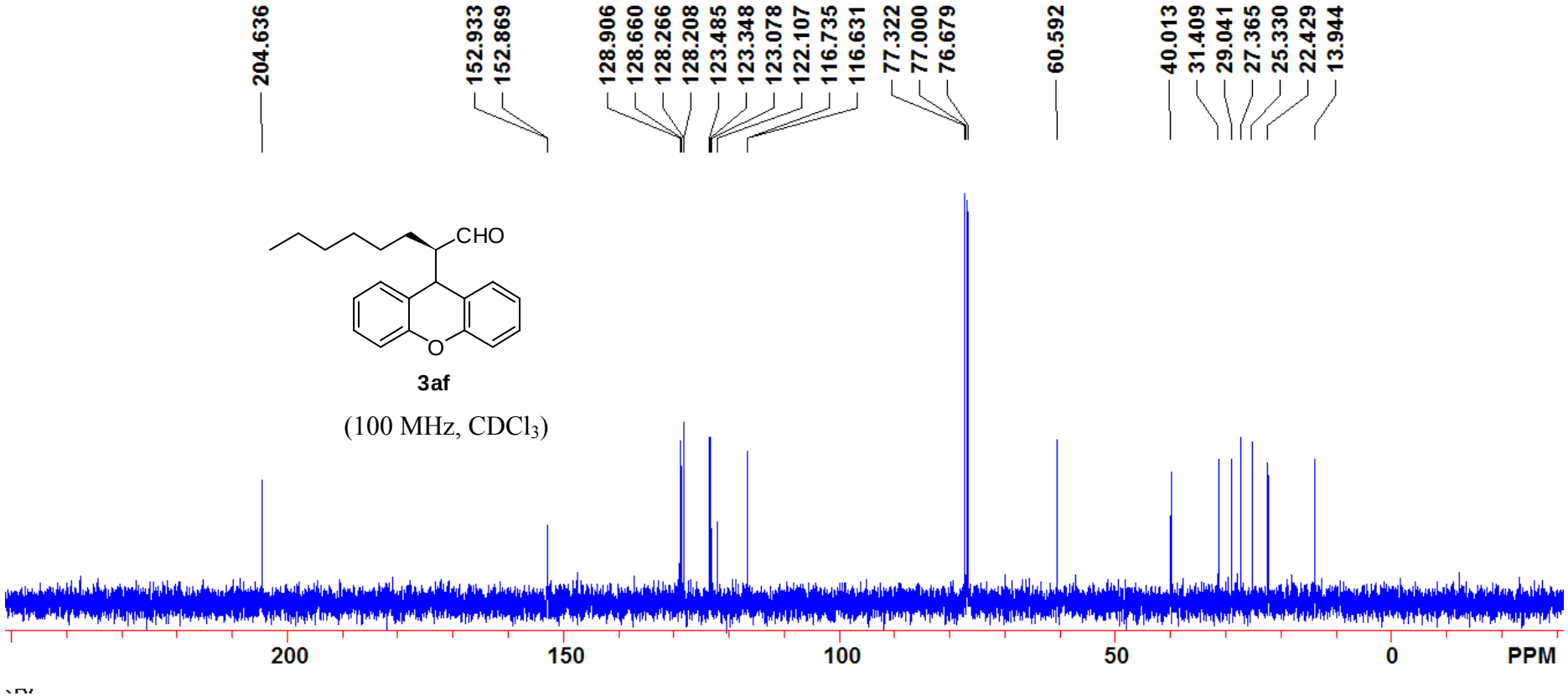
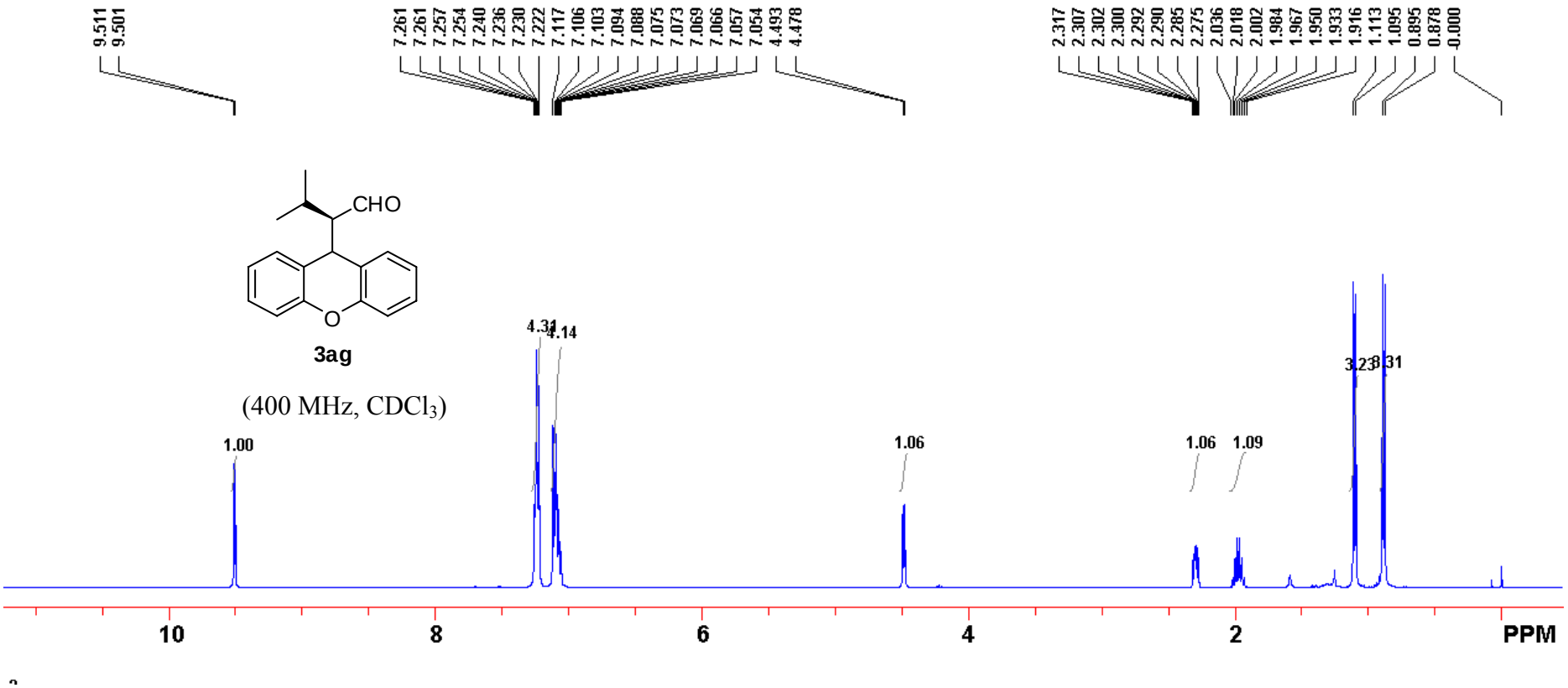
1.84
1.85
8.91
3.22
12
10
8
6
4
2
0
-2
PPM



3af

(100 MHz, $CDCl_3$)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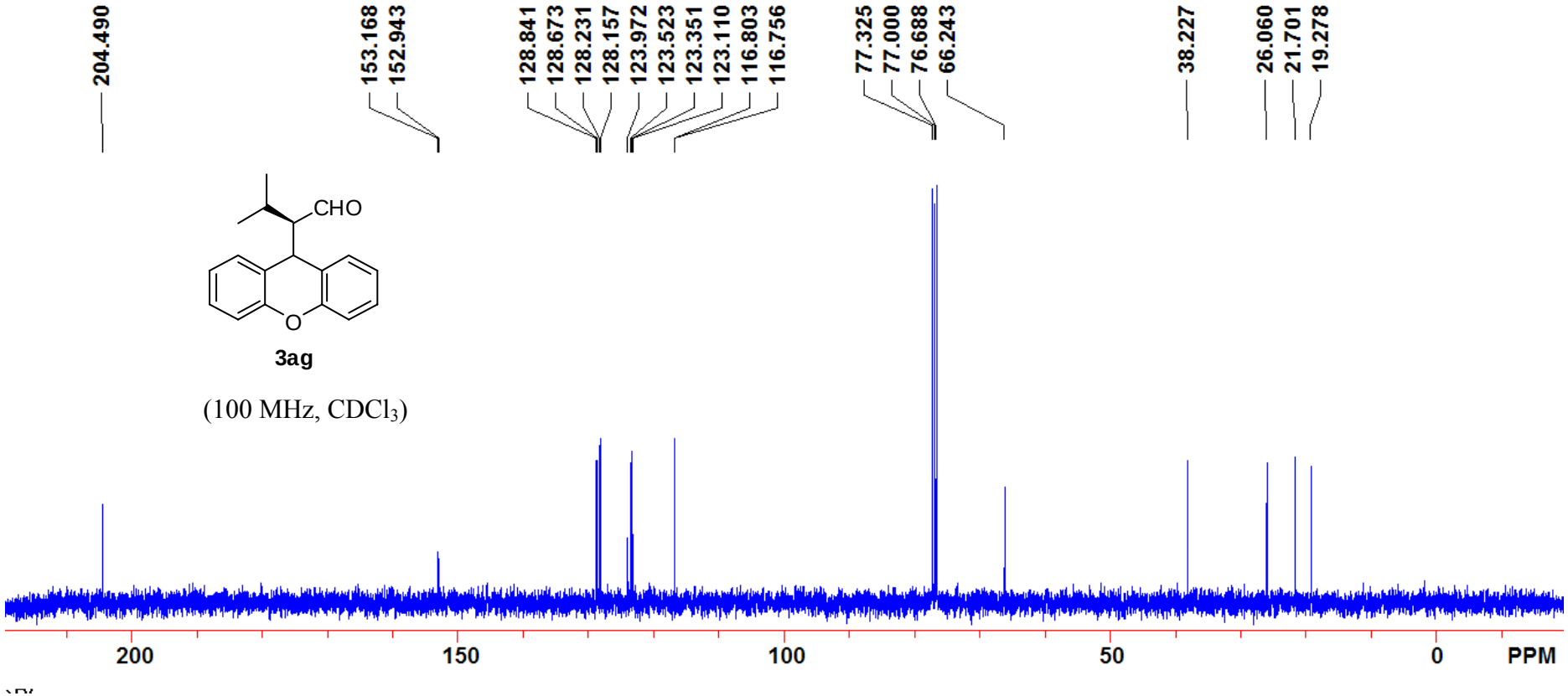
7.094
7.088
7.075
7.073
7.069
7.066
7.057
7.054
4.493
4.478
2.317
2.307
2.302
2.300
2.292
2.290
2.285
2.275
2.036
2.018
2.002
1.984
1.967
1.950
1.933
1.916
1.113
1.095
0.895
0.878
0.000
CHO
O
3ag
(400 MHz, CDCl3)
1.00
4.31
4.14
1.06
1.06
1.09
3.23
3.31
10
8
6
4
2
PPM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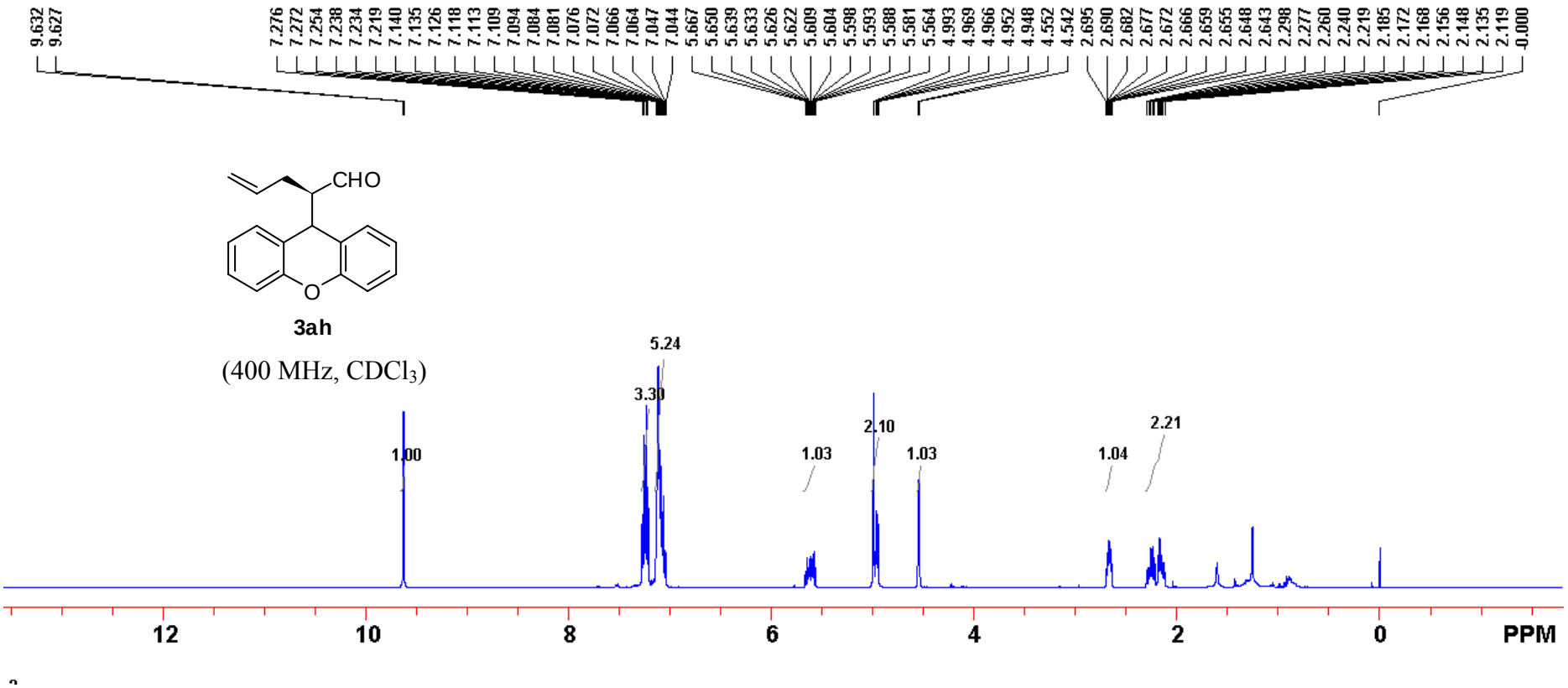
128.157
123.972
123.523
123.351
123.110
116.803
116.756
77.325
77.000
76.688
66.243
38.227
26.060
21.701
19.278
CHO
O
3ag
(100 MHz, CDCl3)
200
150
100
50
0
PPM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7.219
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7.126
7.118
7.113
7.109
7.094
7.084
7.081
7.076
7.072
7.066
7.064
7.047
7.044
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5.650
5.639
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5.604
5.598
5.593
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5.581
5.564
4.993
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4.966
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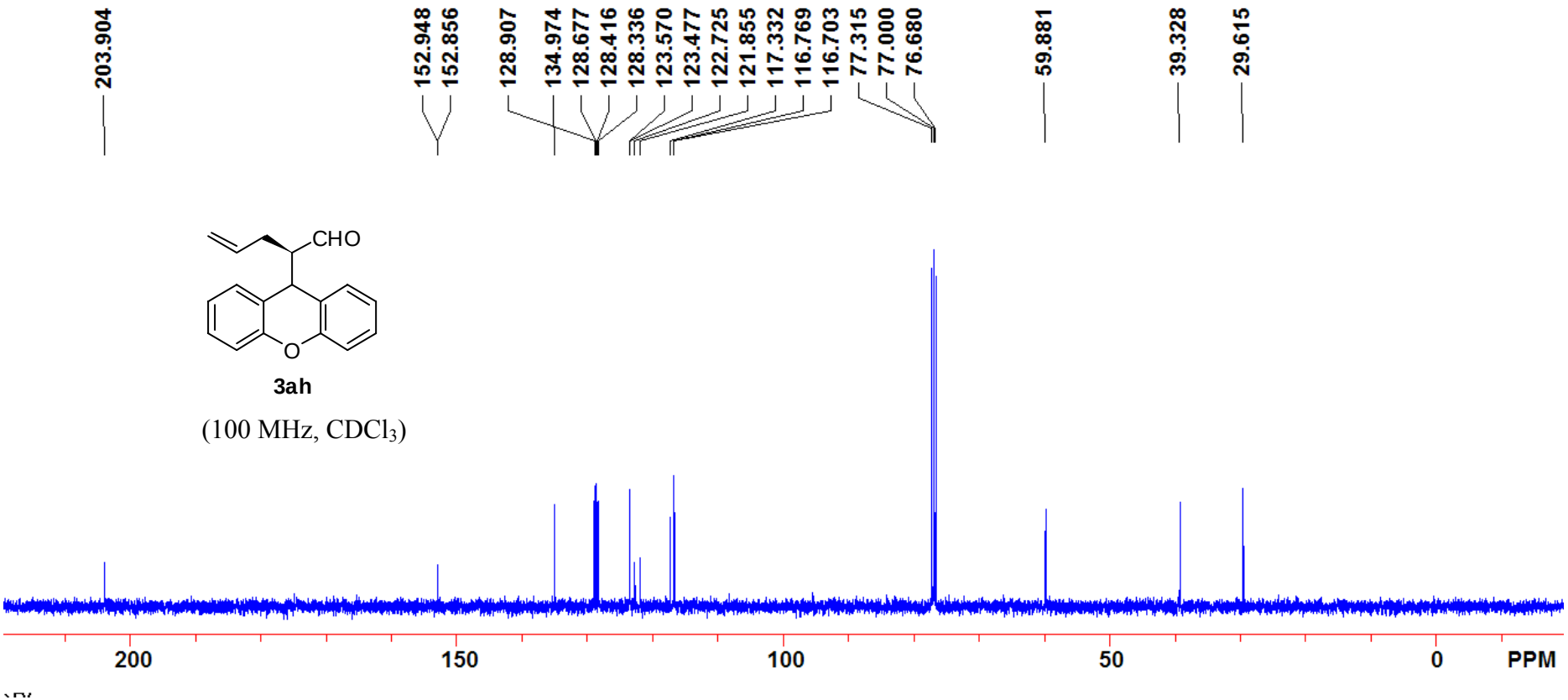
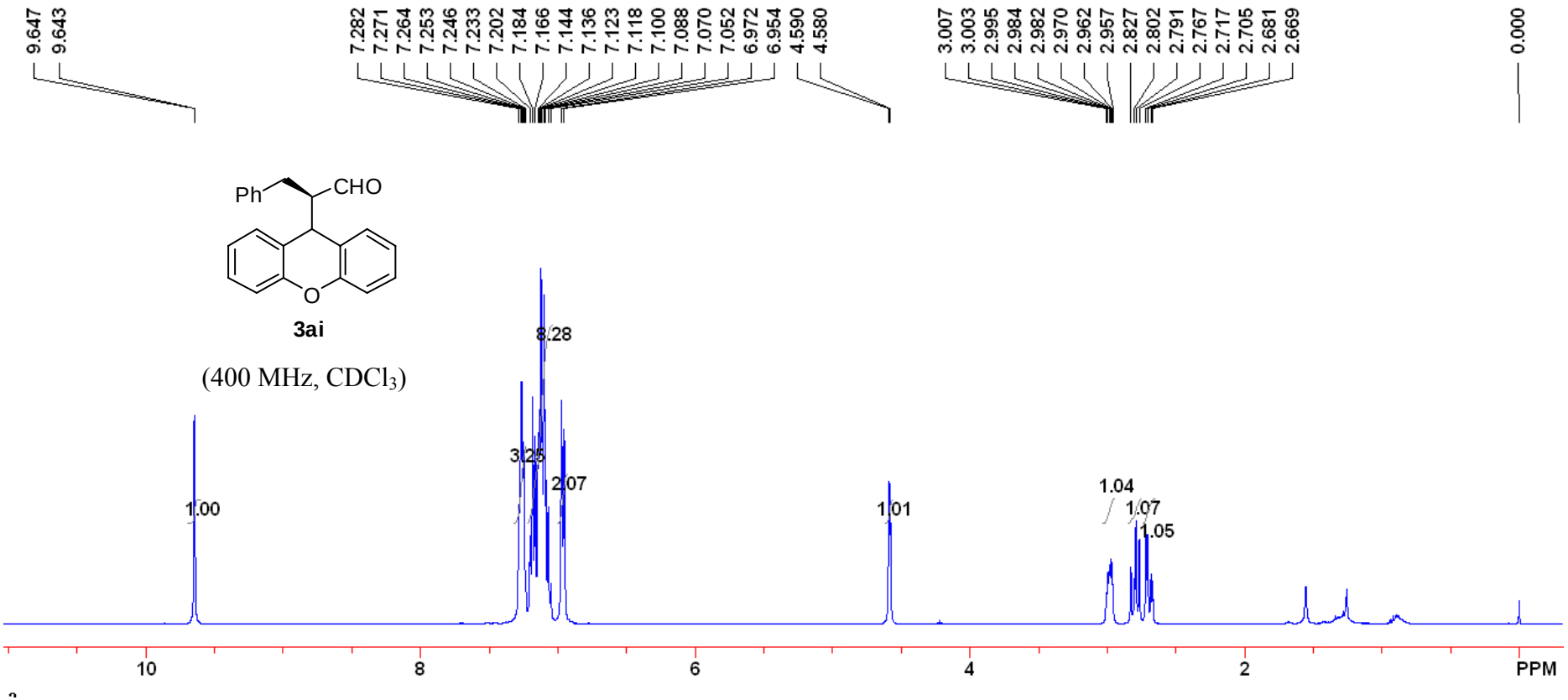
4.948
4.552
4.542
2.695
2.690
2.682
2.677
2.672
2.666
2.659
2.655
2.648
2.643
2.298
2.277
2.260
2.240
2.219
2.185
2.172
2.168
2.156
2.148
2.135
2.119
0.000
CHO
O
3ah
(400 MHz, CDCl3)
5.24
3.30
2.10
2.21
1.00
1.03
1.03
1.04
12
10
8
6
4
2
0
PPM



3ah

(100 MHz, $CDCl_3$)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7.264
7.253
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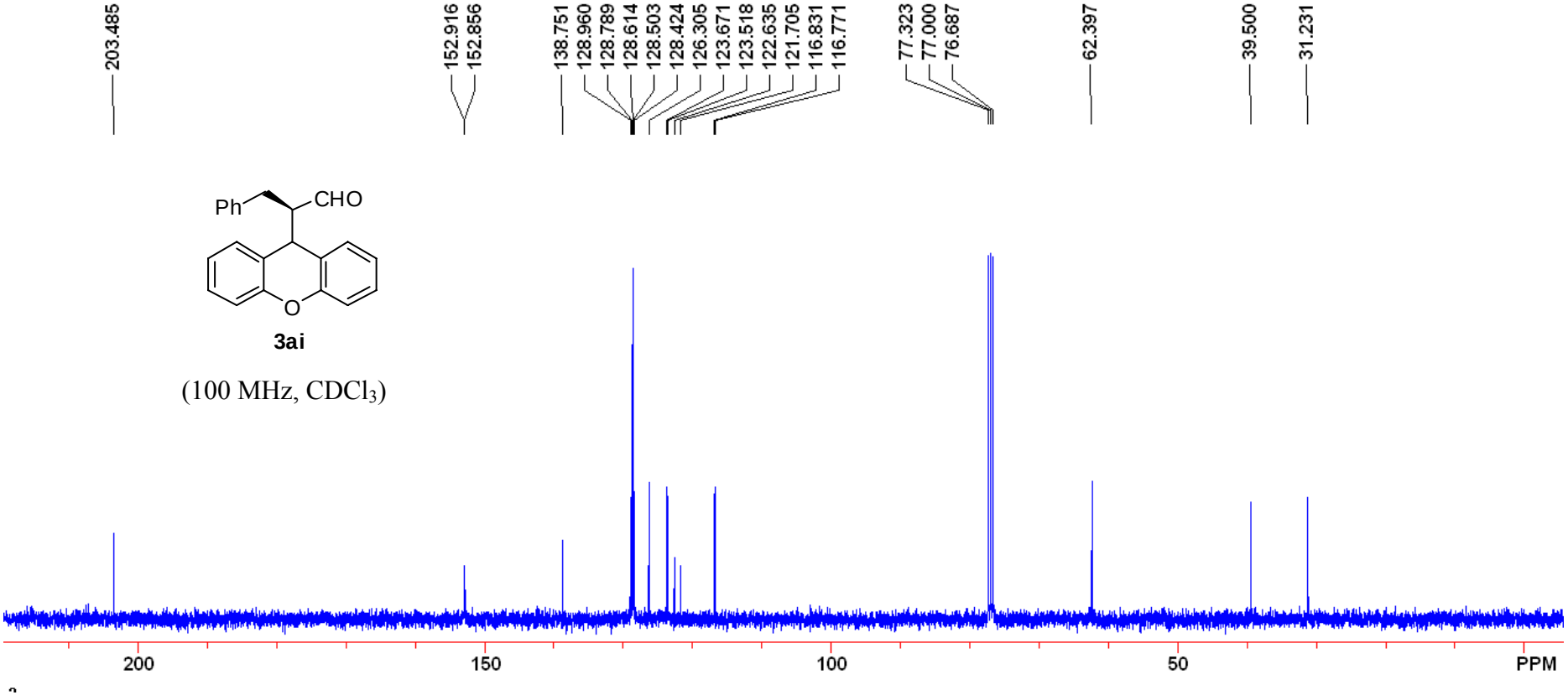
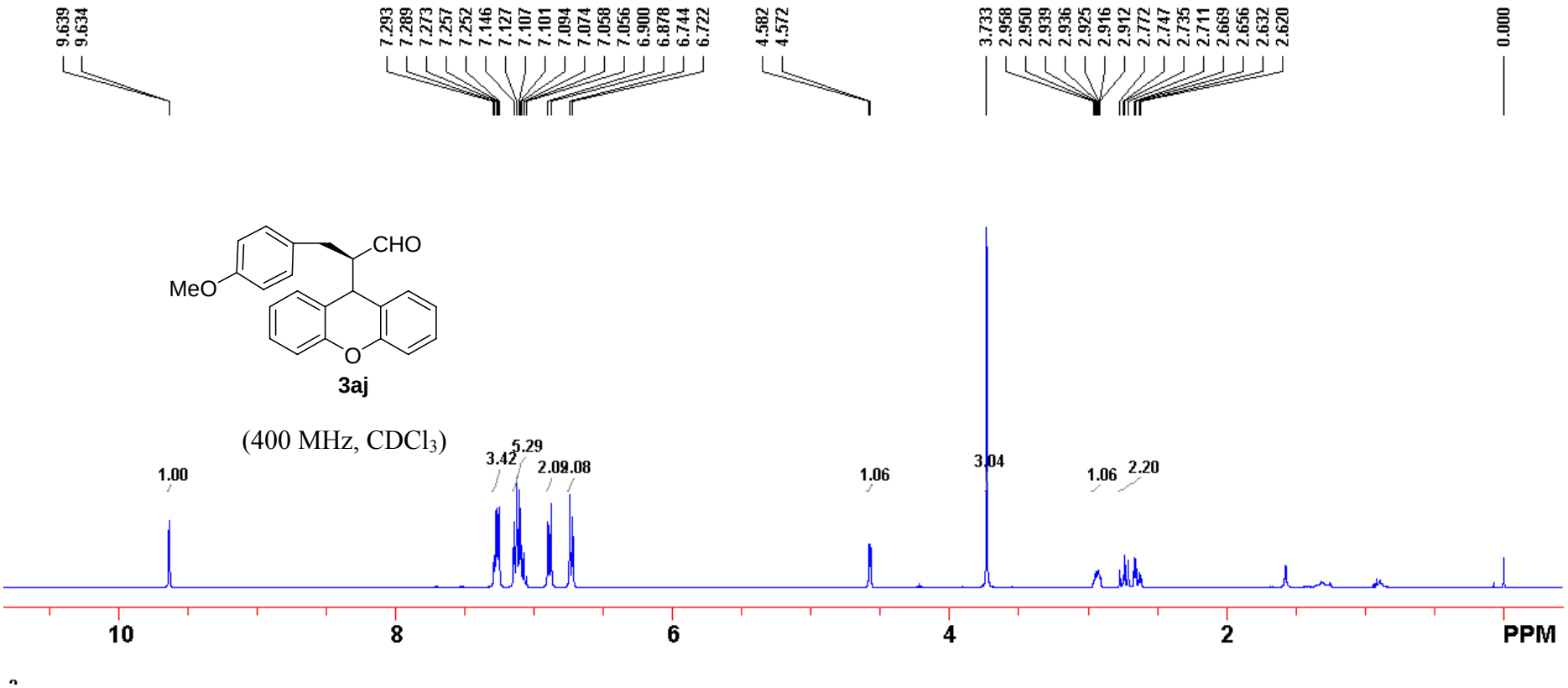
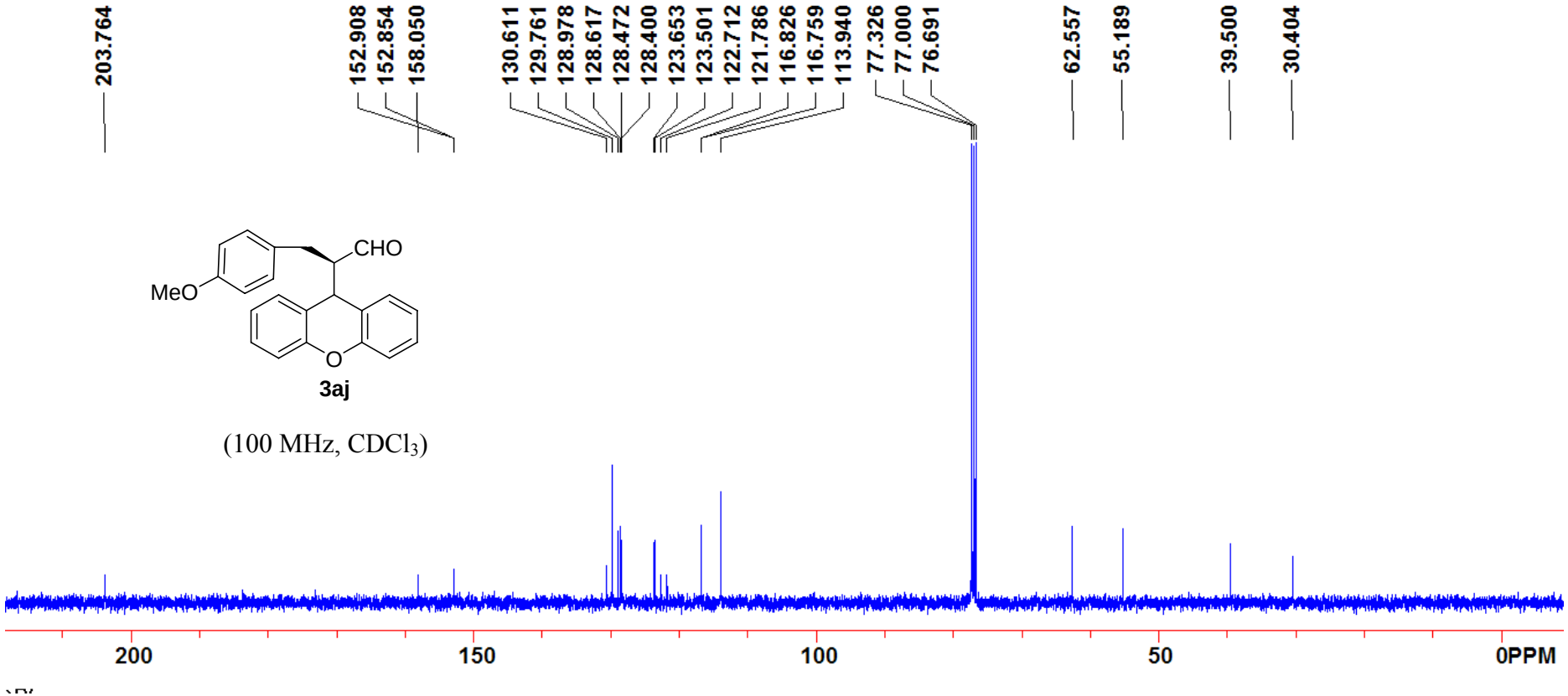
7.202
7.184
7.166
7.144
7.136
7.123
7.118
7.100
7.088
7.070
7.052
6.972
6.954
4.590
4.580
3.007
3.003
2.995
2.984
2.982
2.970
2.962
2.957
2.827
2.802
2.791
2.767
2.717
2.705
2.681
2.669
0.000
Ph
CHO
O
3ai
(400 MHz, CDCl3)
8.28
3.25
2.07
1.00
1.01
1.04
1.07
1.05
10
8
6
4
2
PPM



3ai

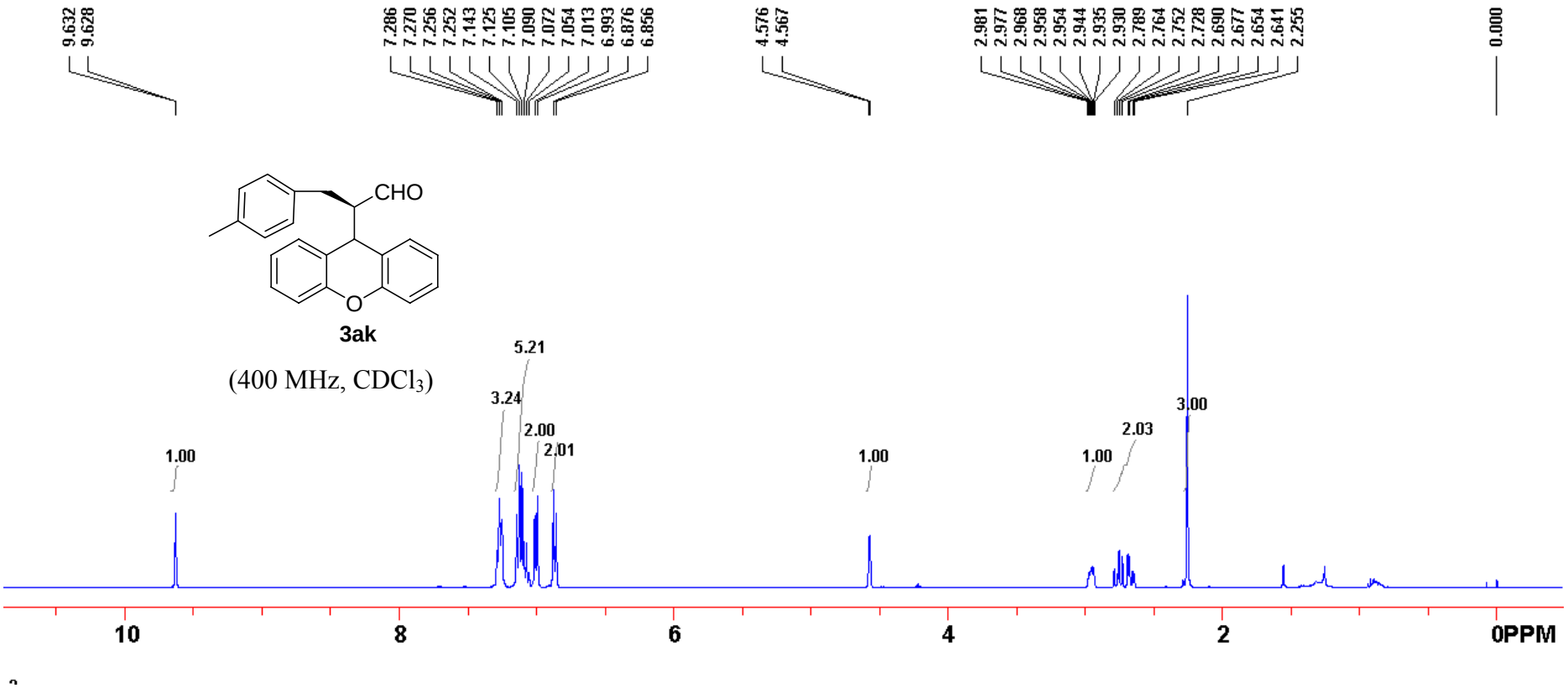
(100 MHz, $CDCl_3$)

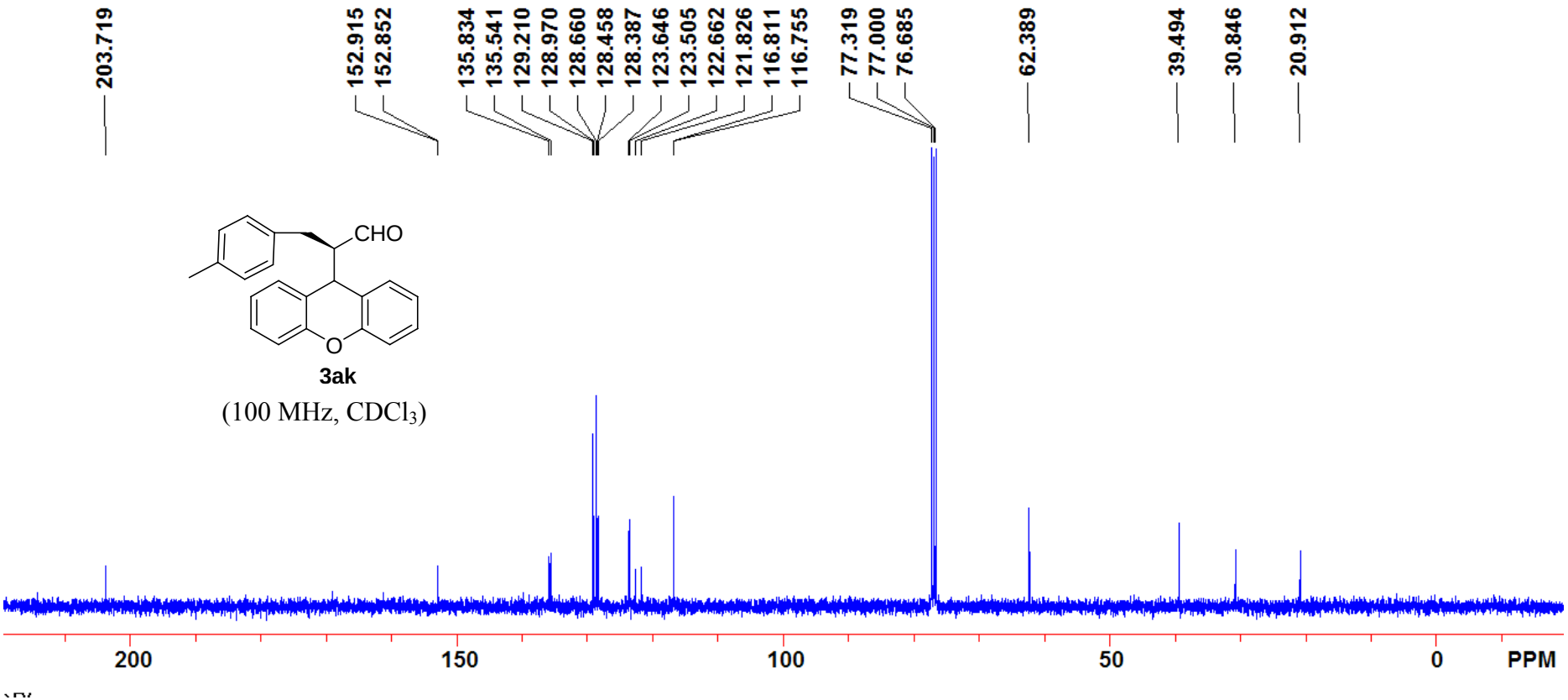

9.639
9.634
7.293
7.289
7.273
7.257
7.252
7.146
7.127
7.107
7.101
7.094
7.074
7.058
7.056
6.900
6.878
6.744
6.722
4.582
4.572
3.733
2.958
2.950
2.939
2.936
2.925
2.916
2.912
2.772
2.747
2.735
2.711
2.669
2.656
2.632
2.620
0.000
CHO
MeO
O
3aj
(400 MHz, CDCl3)
1.00
3.42
5.29
2.09
2.08
1.06
3.04
1.06
2.20
10
8
6
4
2
PPM



3aj

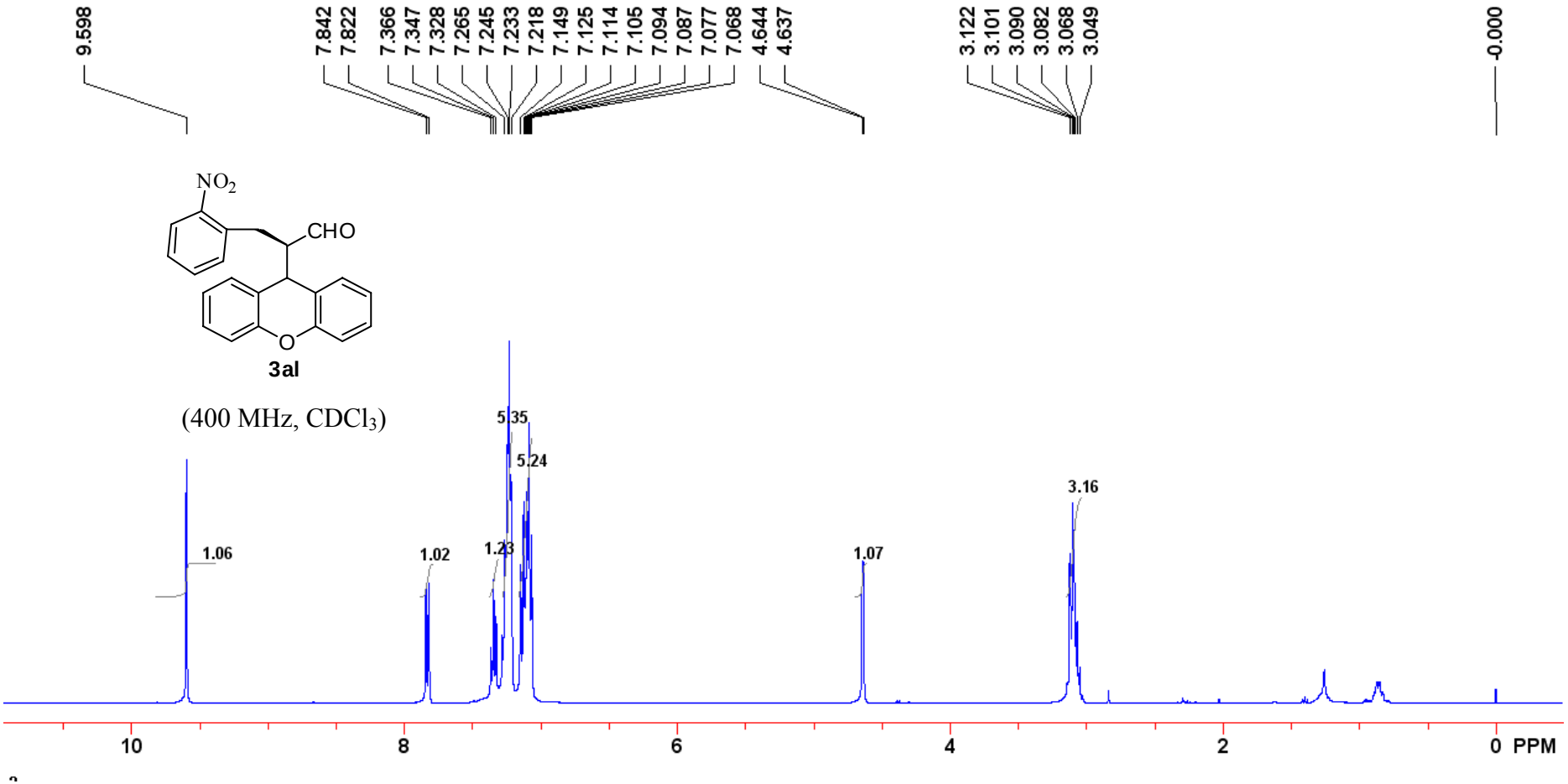
(100 MHz, $CDCl_3$)

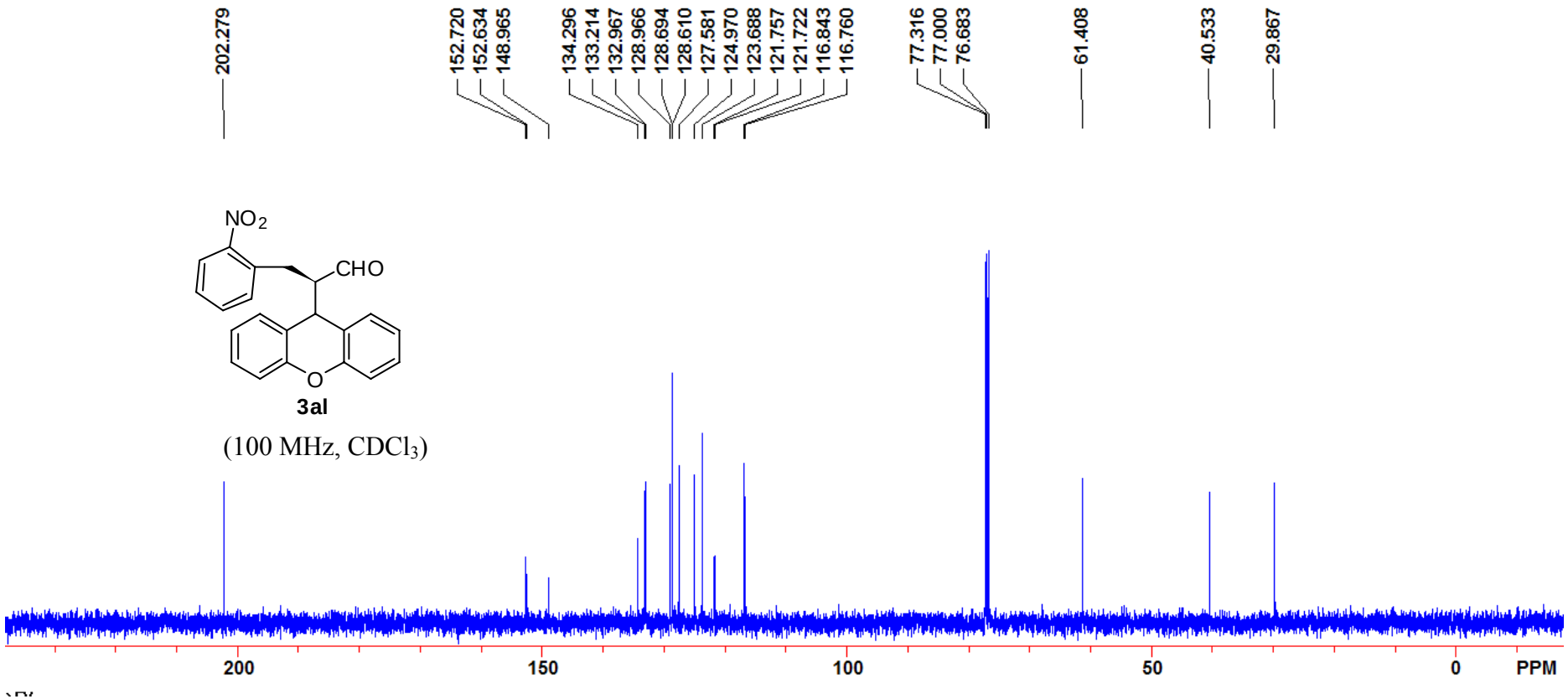

9.632
9.628
7.286
7.270
7.256
7.252
7.143
7.125
7.105
7.090
7.072
7.054
7.013
6.993
6.876
6.856
4.576
4.567
2.981
2.977
2.968
2.958
2.954
2.944
2.935
2.930
2.789
2.764
2.752
2.728
2.690
2.677
2.654
2.641
2.255
0.000
CHO
O
3ak
(400 MHz, CDCl3)
5.21
3.24
2.00
2.01
1.00
1.00
1.00
2.03
3.00
10
8
6
4
2
0PPM



3ak

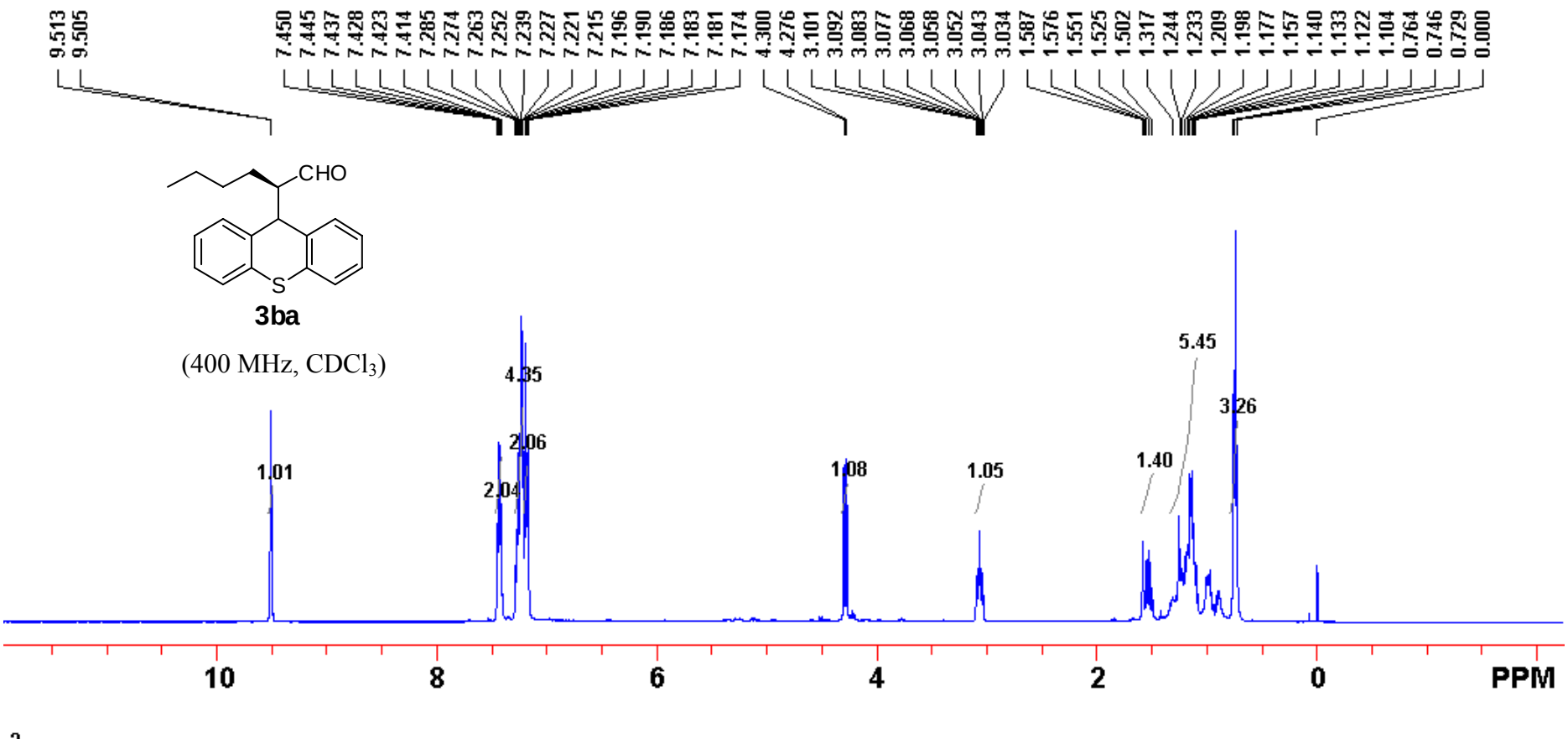
(100 MHz, $CDCl_3$)

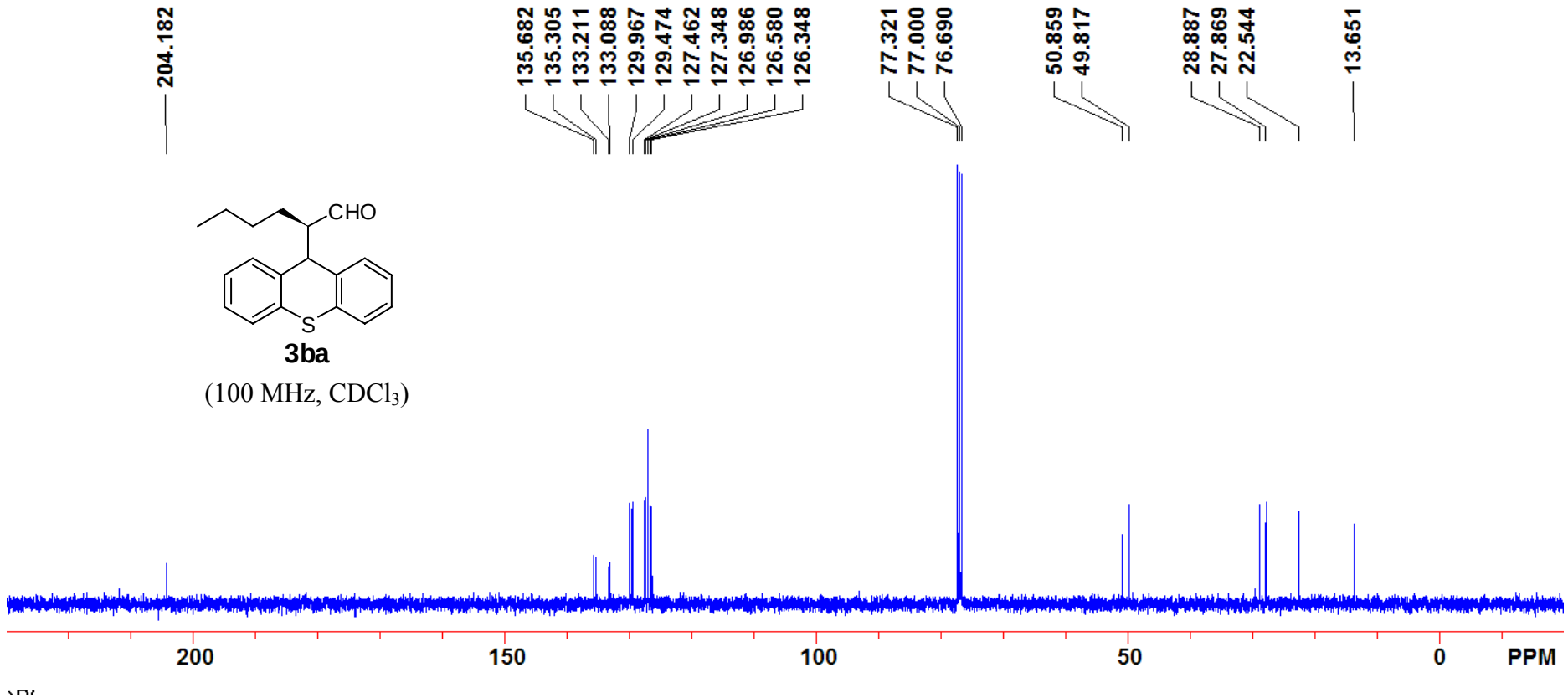

9.598
7.842
7.822
7.366
7.347
7.328
7.265
7.245
7.233
7.218
7.149
7.125
7.114
7.105
7.094
7.087
7.077
7.068
4.644
4.637
3.122
3.101
3.090
3.082
3.068
3.049
-0.000
NO2
CHO
O
3al
(400 MHz, CDCl3)
5.35
5.24
3.16
1.06
1.02
1.23
1.07
10
8
6
4
2
0 PPM



3al

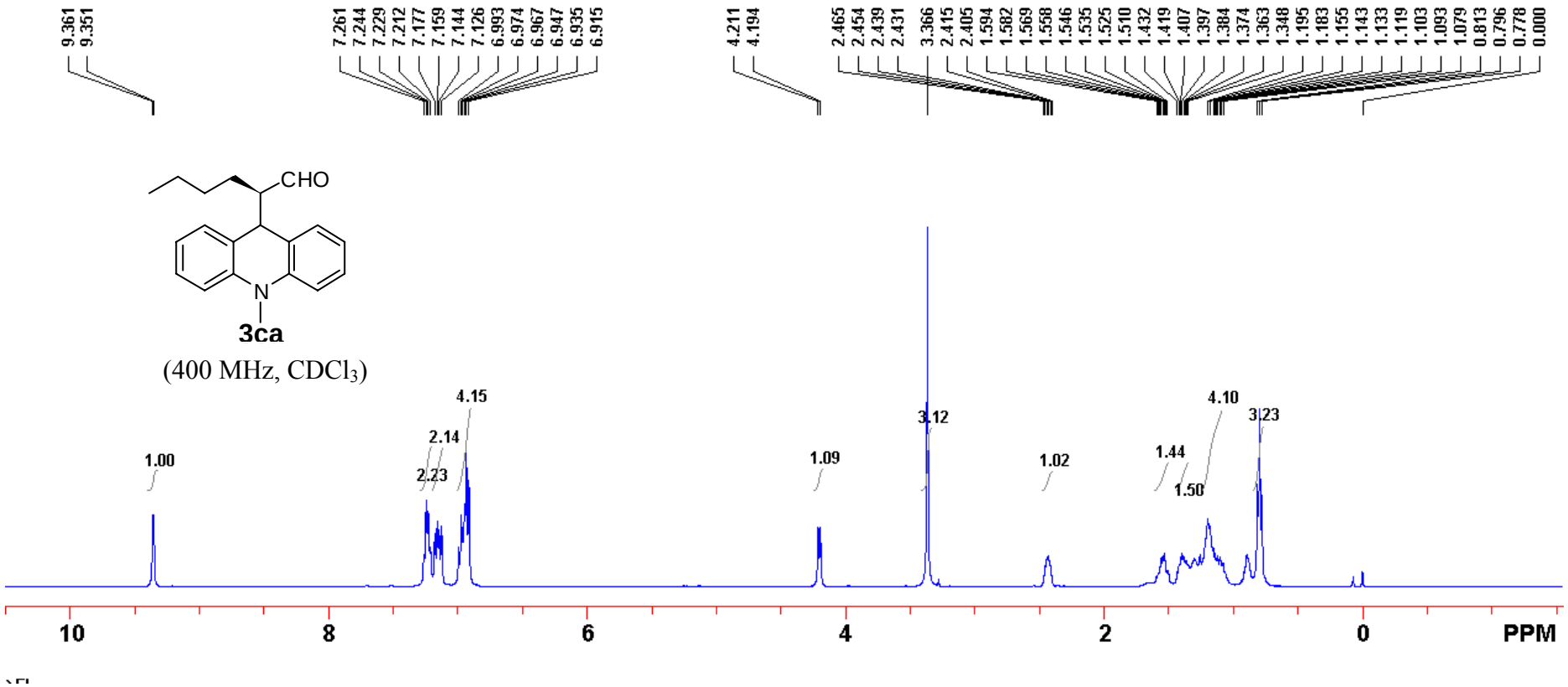
(100 MHz, $CDCl_3$)

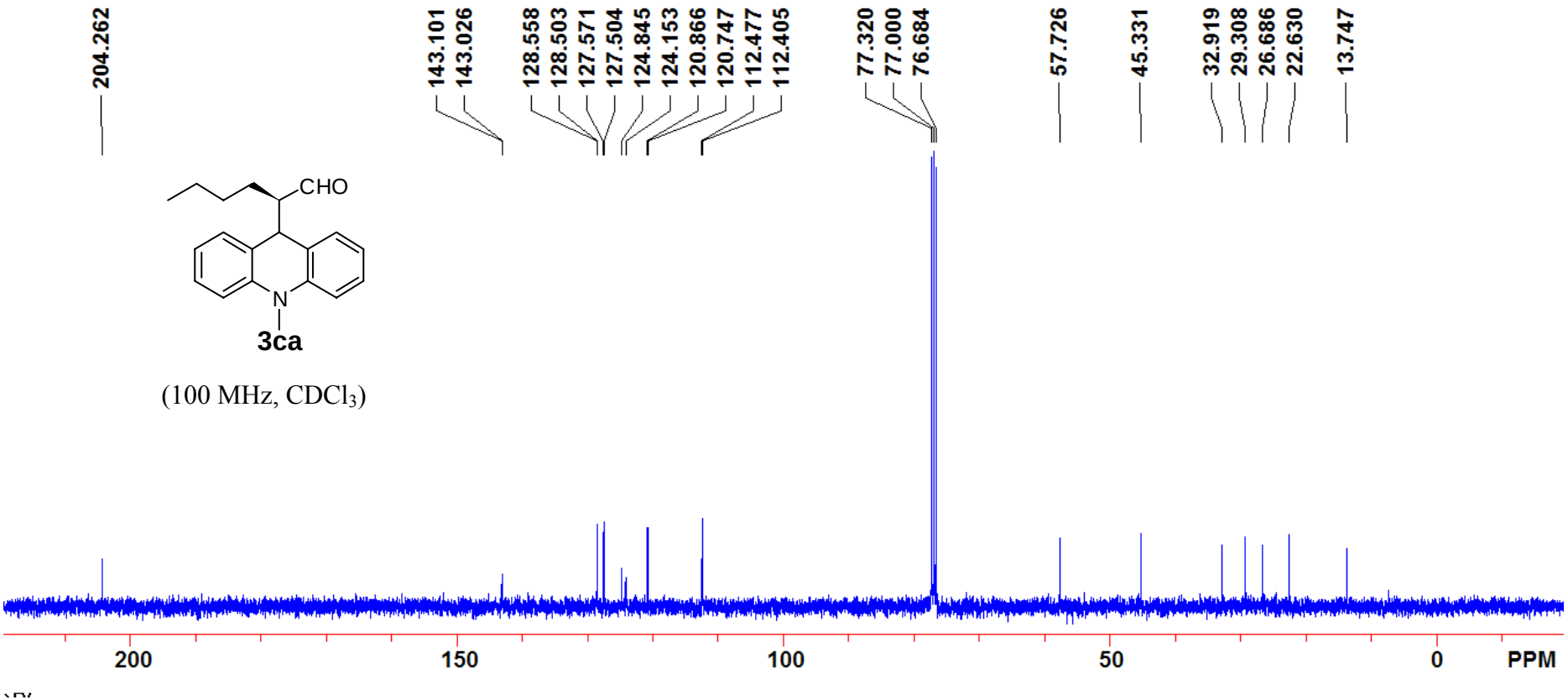

9.513
9.505
7.450
7.445
7.437
7.428
7.423
7.414
7.285
7.274
7.263
7.252
7.239
7.227
7.221
7.215
7.196
7.190
7.186
7.183
7.181
7.174
4.300
4.276
3.101
3.092
3.083
3.077
3.068
3.058
3.052
3.043
3.034
1.587
1.576
1.551
1.525
1.502
1.317
1.244
1.233
1.209
1.198
1.177
1.157
1.140
1.133
1.122
1.104
0.764
0.746
0.729
0.000
CHO
S
3ba
(400 MHz, CDCl3)
1.01
2.04
2.06
4.35
1.08
1.05
1.40
5.45
3.26
10
8
6
4
2
0
PPM



3ba

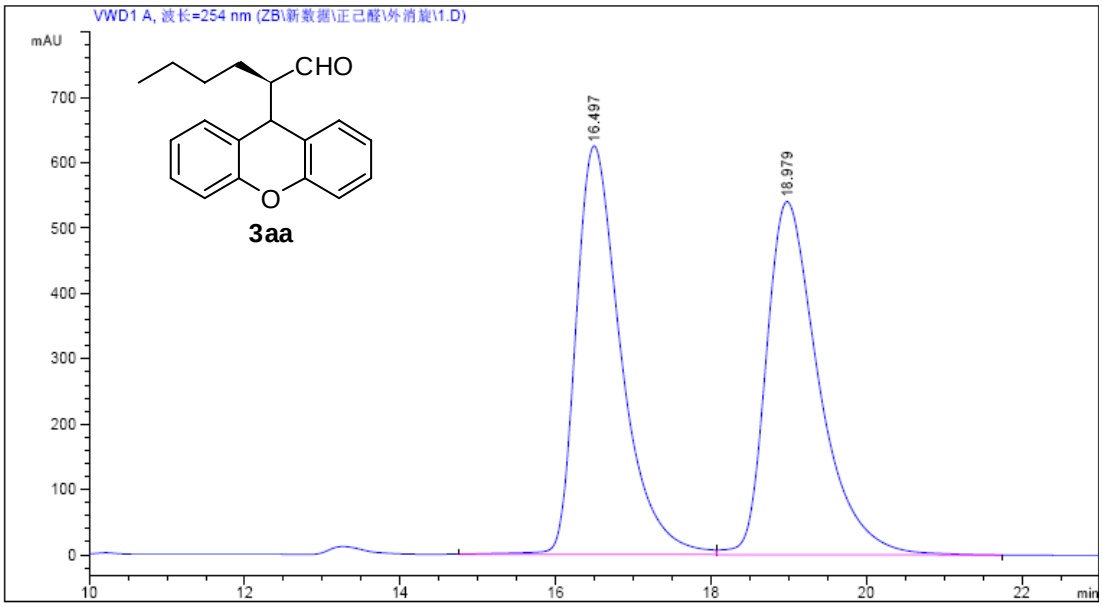
(100 MHz, $CDCl_3$)


9.361
9.351
7.261
7.244
7.229
7.212
7.177
7.159
7.144
7.126
6.993
6.974
6.967
6.947
6.935
6.915
4.211
4.194
2.465
2.454
2.439
2.431
3.366
2.415
2.405
1.594
1.582
1.569
1.558
1.546
1.535
1.525
1.510
1.432
1.419
1.407
1.397
1.384
1.374
1.363
1.348
1.195
1.183
1.155
1.143
1.133
1.119
1.103
1.093
1.079
0.813
0.796
0.778
0.000
CHO
N
3ca
(400 MHz, CDCl3)
1.00
2.14
2.23
4.15
1.09
3.12
1.02
1.44
1.50
4.10
3.23
10
8
6
4
2
0
PPM



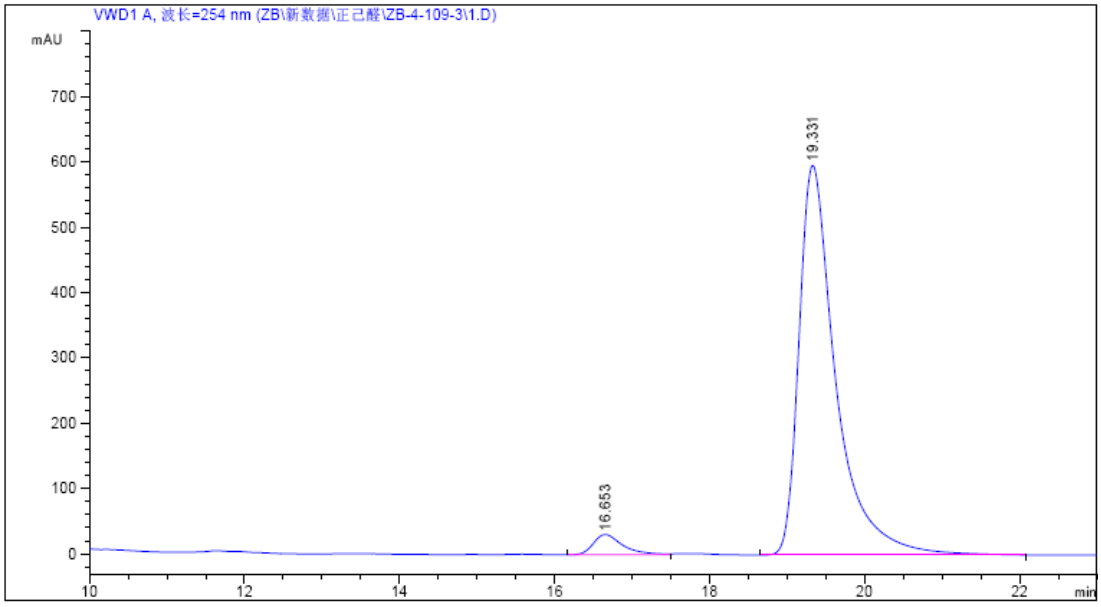
(100 MHz, $CDCl_3$)

Racemic



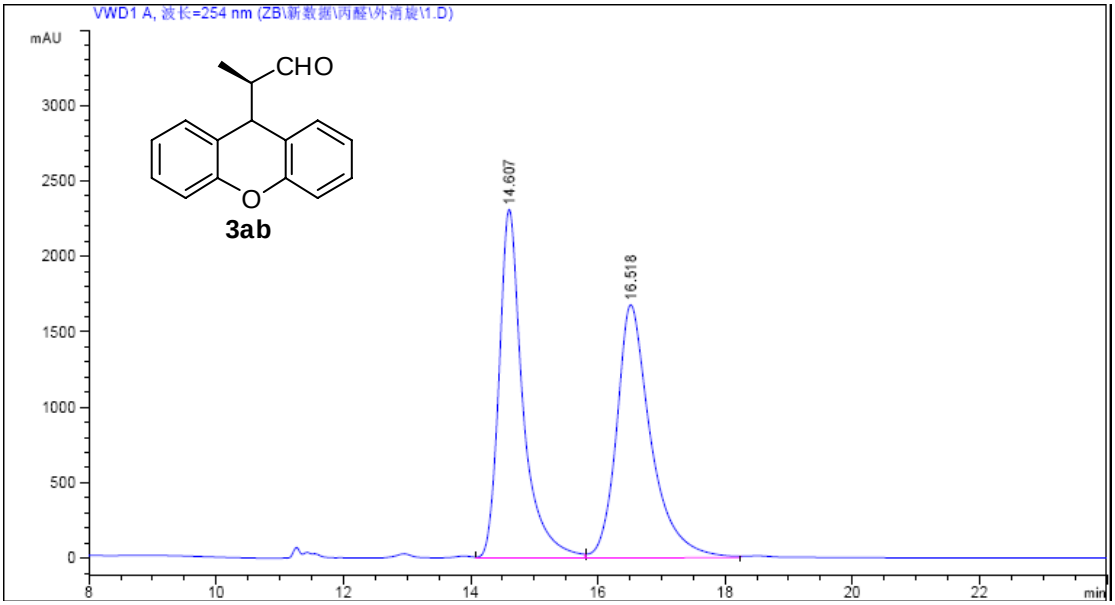
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	16.497	BV	0.6091	2.51525e4	625.27557	49.7979
2	18.979	VB	0.7175	2.53567e4	540.64624	50.2021

Sample



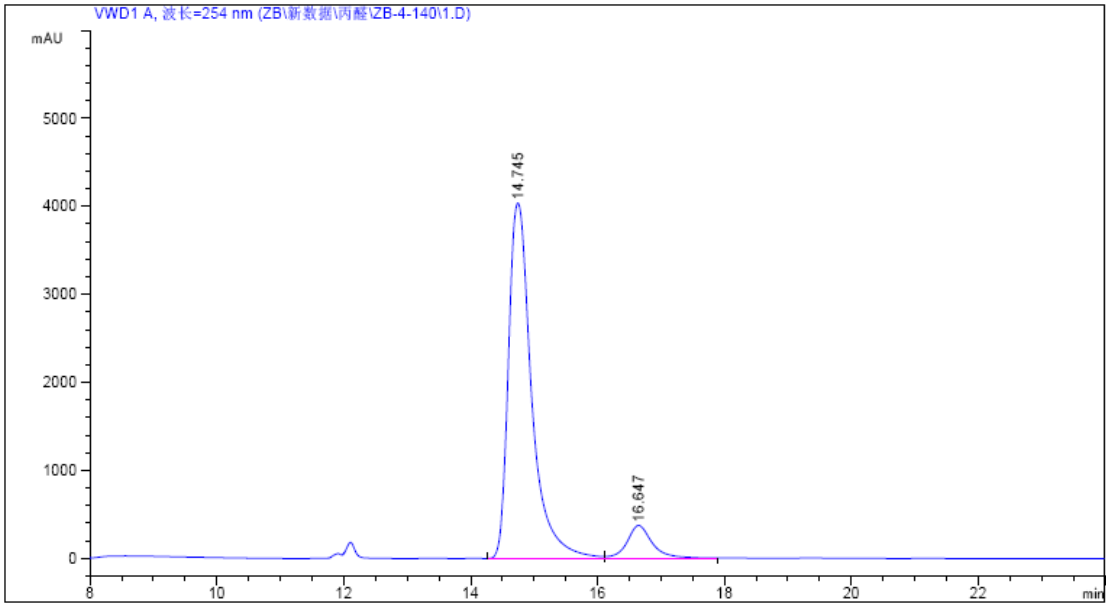
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	16.653	VB	0.4020	828.39160	31.00143	4.0352
2	19.331	VB	0.4932	1.97009e4	596.33691	95.9648

Racemic



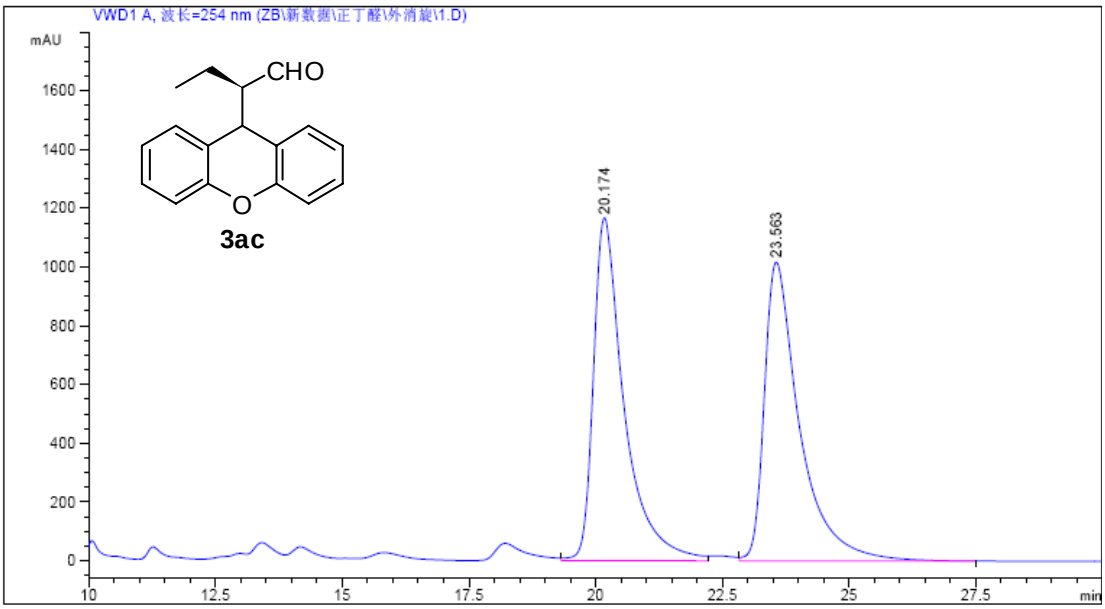
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	14.607	VV	0.3788	6.00236e4	2310.65454	48.9004
2	16.518	VV	0.5382	6.27231e4	1677.14429	51.0996

Sample



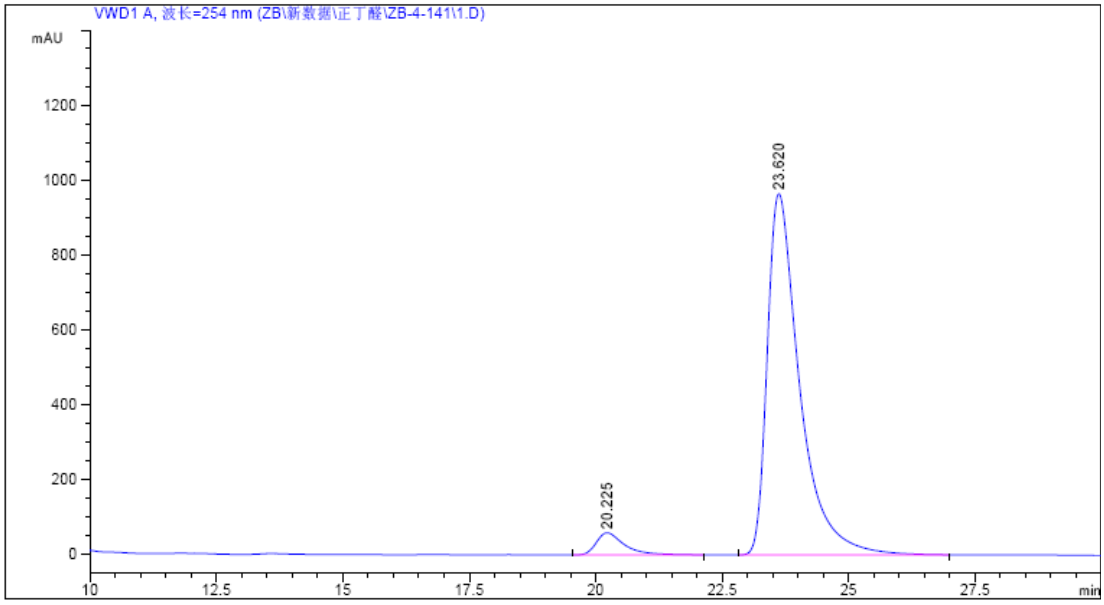
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	14.745	VV	0.3806	1.02499e5	4038.22046	90.4993
2	16.647	VV	0.4235	1.07605e4	376.71533	9.5007

Racemic



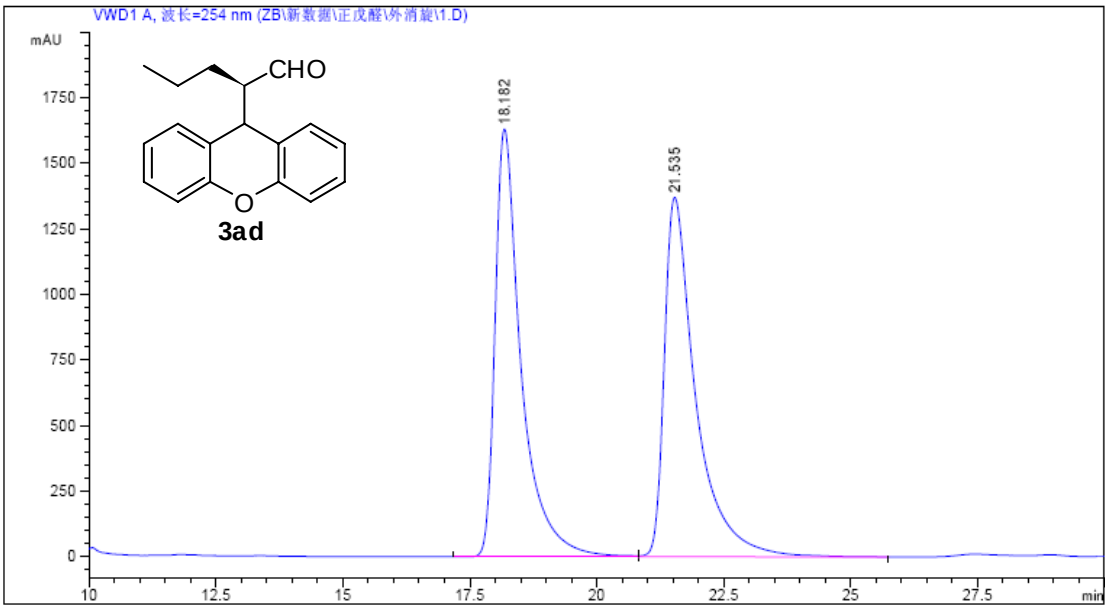
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	20.174	VV	0.6117	4.92288e4	1166.59521	50.0333
2	23.563	VB	0.7024	4.91631e4	1016.81671	49.9667

Sample



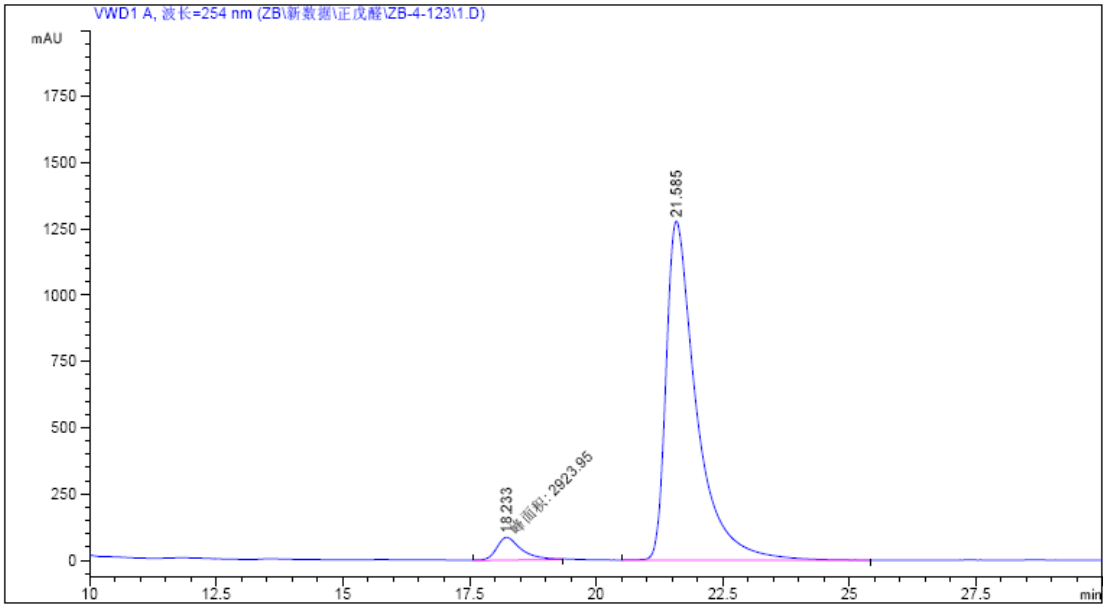
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	20.225	BB	0.5707	2291.27612	59.23592	5.0631
2	23.620	BB	0.6566	4.29634e4	964.32782	94.9369

Racemic



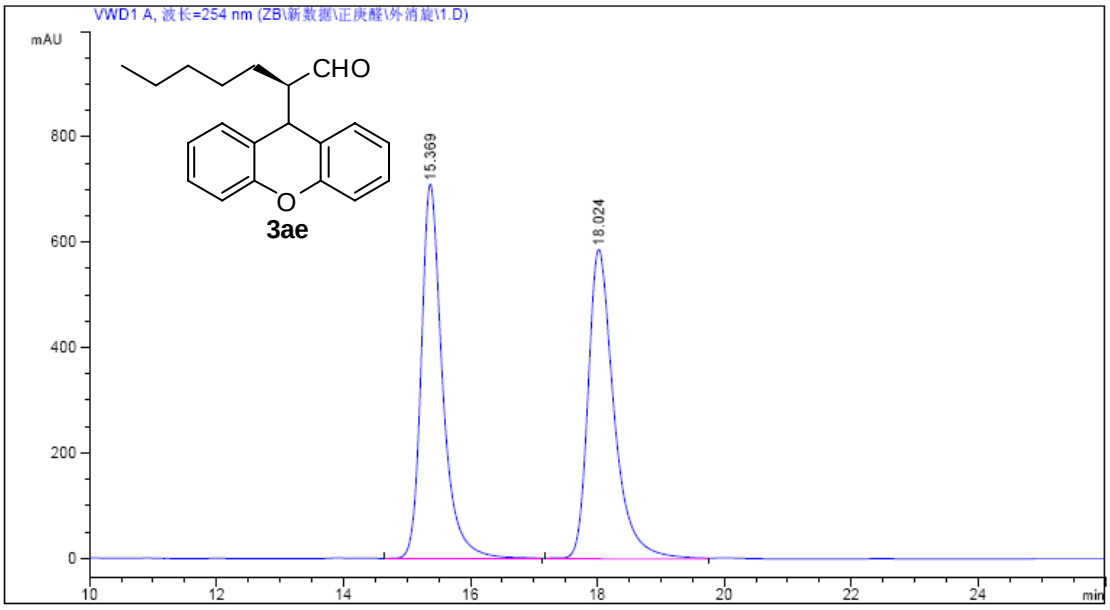
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	18.182	BV	0.5291	5.82277e4	1629.03247	49.7169
2	21.535	VB	0.6241	5.88908e4	1369.26050	50.2831

Sample



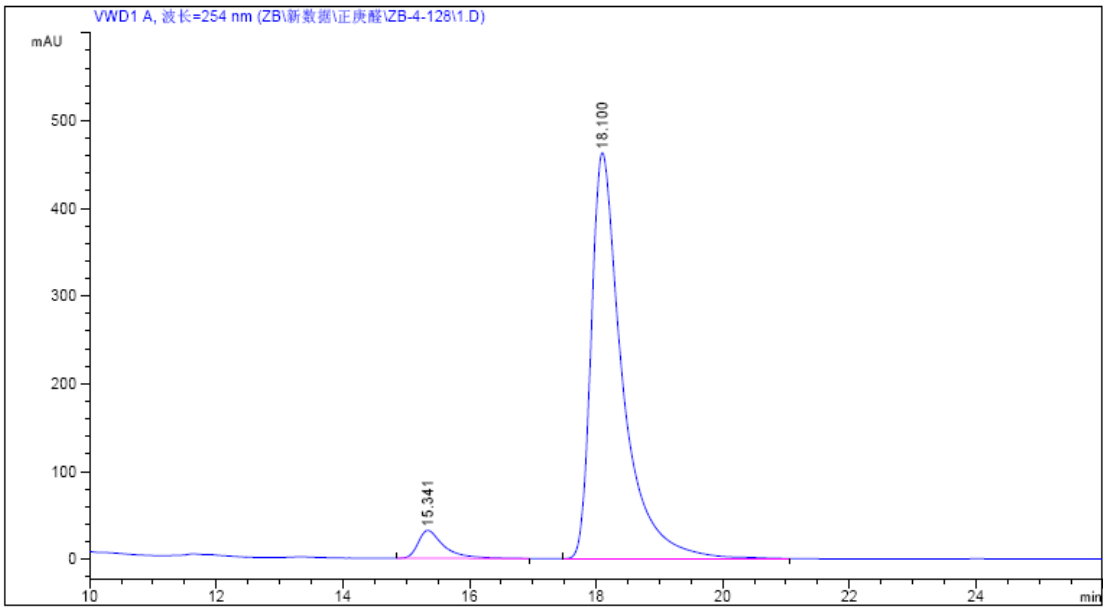
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	18.233	MM	0.5685	2923.95459	85.71626	5.2116
2	21.585	BB	0.6089	5.31809e4	1278.99048	94.7884

Racemic



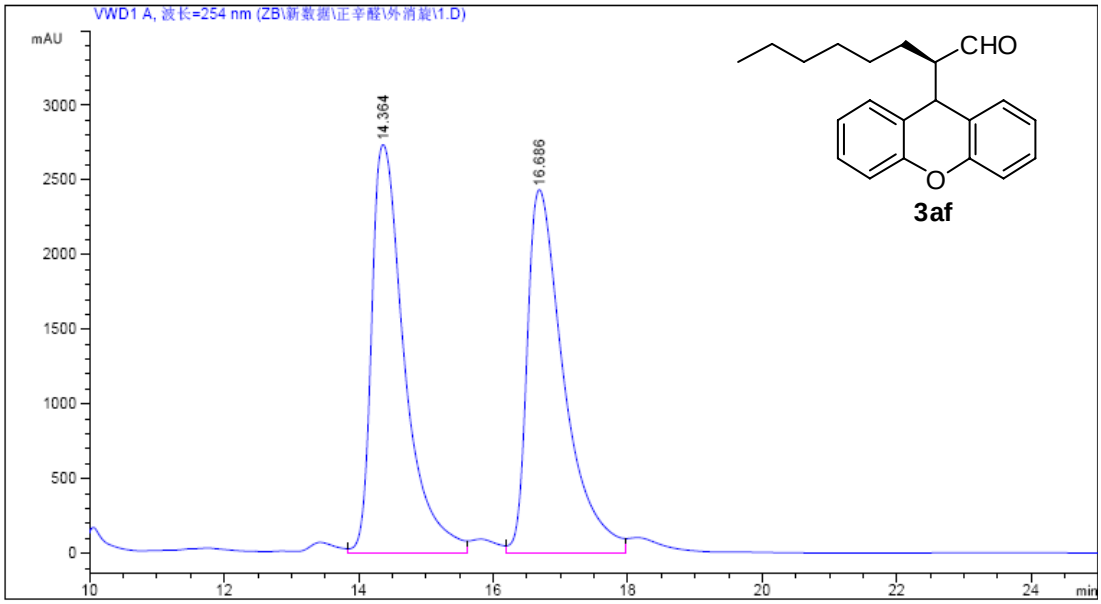
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	15.369	VB	0.3482	1.66016e4	710.90320	49.8949
2	18.024	BB	0.4288	1.66715e4	587.26544	50.1051

Sample



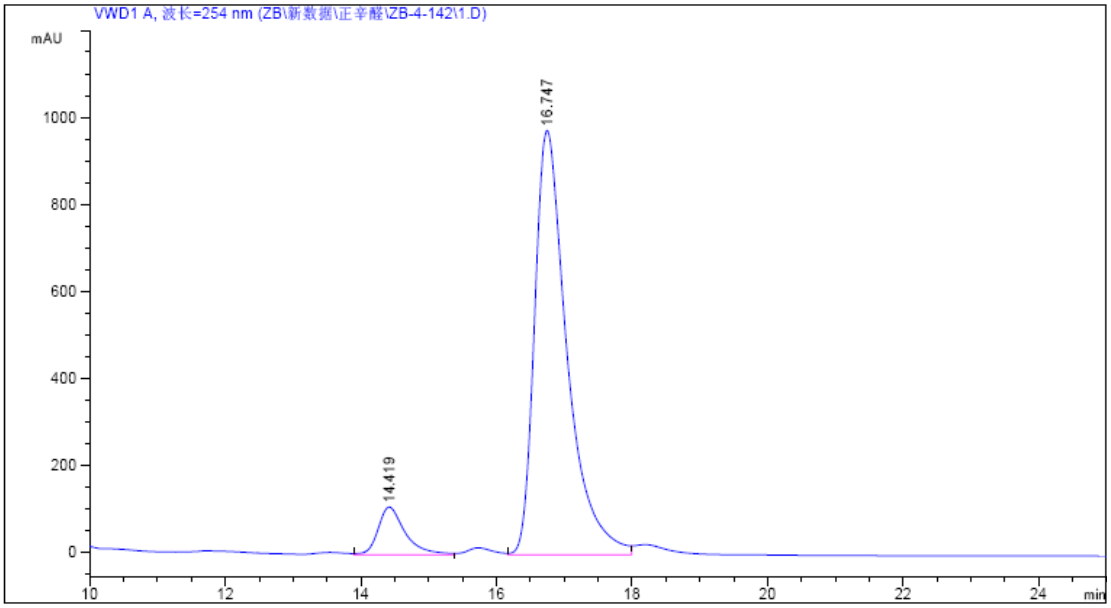
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	15.341	BB	0.4159	908.08026	31.82003	5.4183
2	18.100	BB	0.5000	1.58516e4	462.83591	94.5817

Racemic



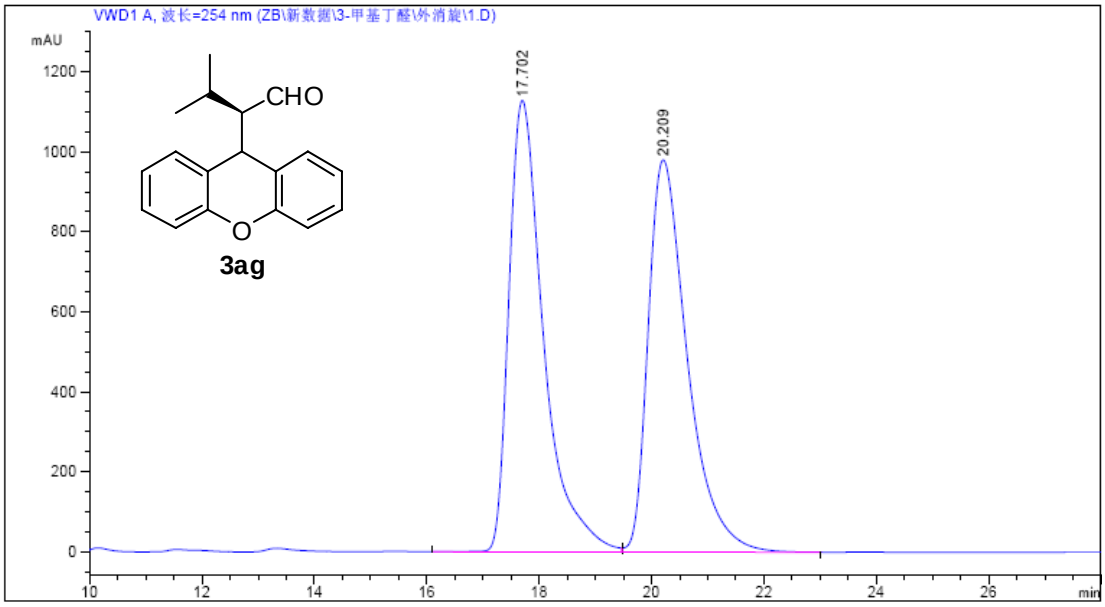
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	14.364	VV	0.5107	9.27730e4	2735.16772	50.1107
2	16.686	VV	0.5710	9.23630e4	2433.33691	49.8893

Sample



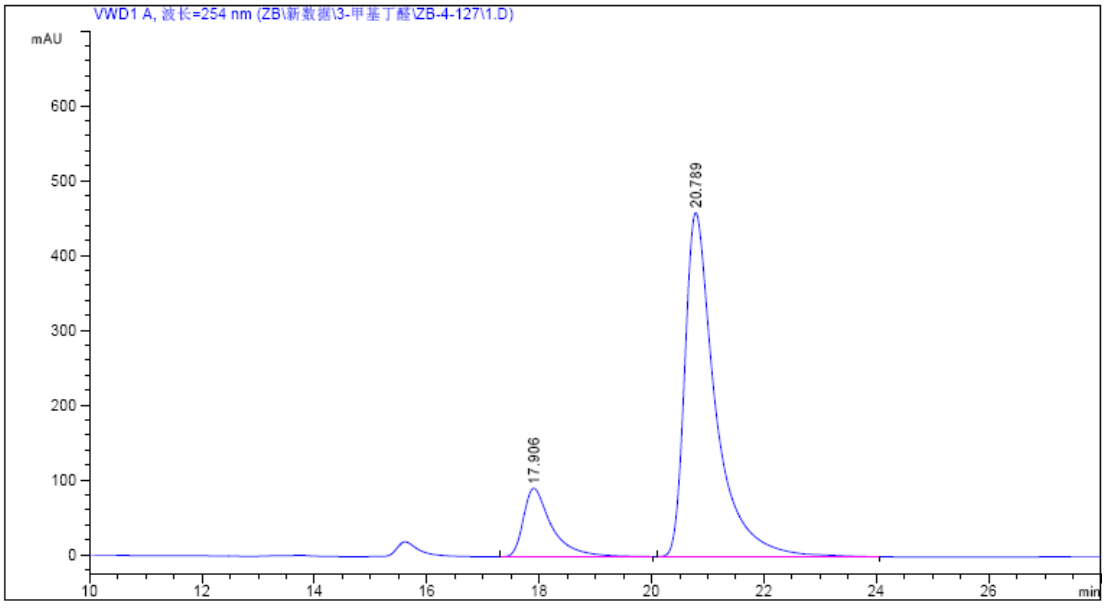
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	14.419	VV	0.4181	3088.79956	109.93024	8.6872
2	16.747	VV	0.5019	3.24671e4	975.52814	91.3128

Racemic



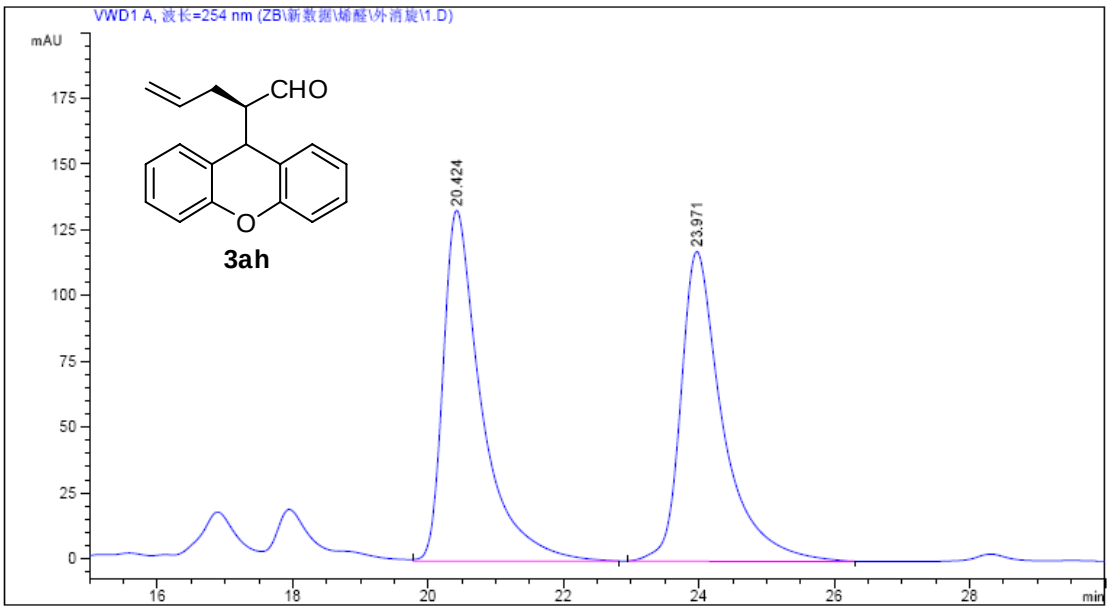
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	17.702	VV	0.6539	4.83125e4	1128.35437	50.4719
2	20.209	VB	0.7375	4.74091e4	980.35828	49.5281

Sample



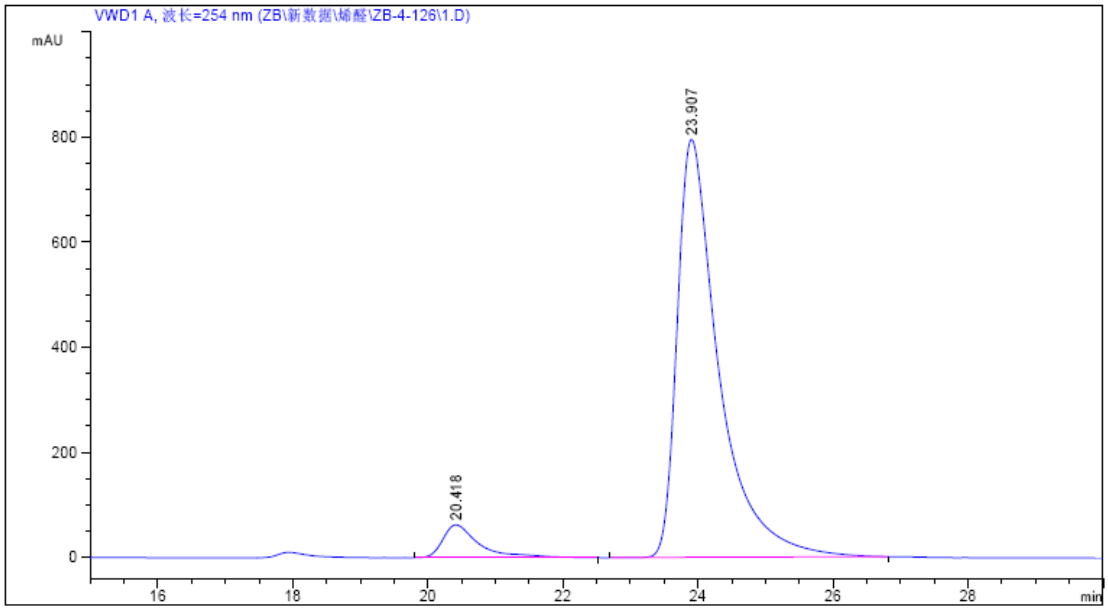
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	17.906	BB	0.5127	3225.05249	91.58625	15.6004
2	20.789	BB	0.5550	1.74478e4	459.62881	84.3996

Racemic



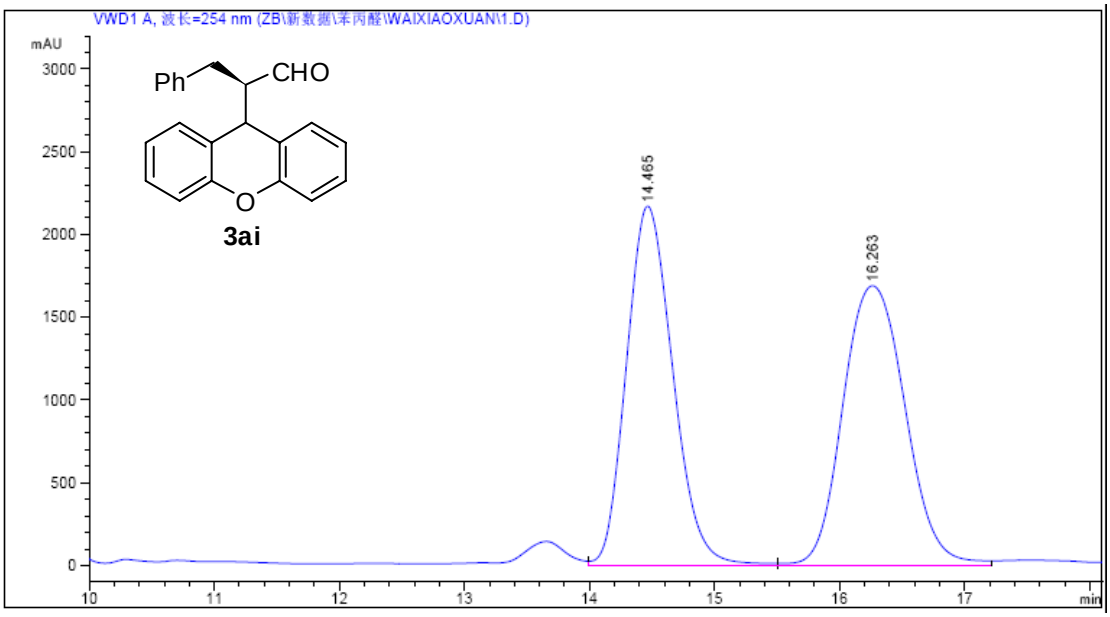
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	20.424	BB	0.5726	5227.12061	133.26588	50.8008
2	23.971	BB	0.6299	5062.32031	117.71165	49.1992

Sample



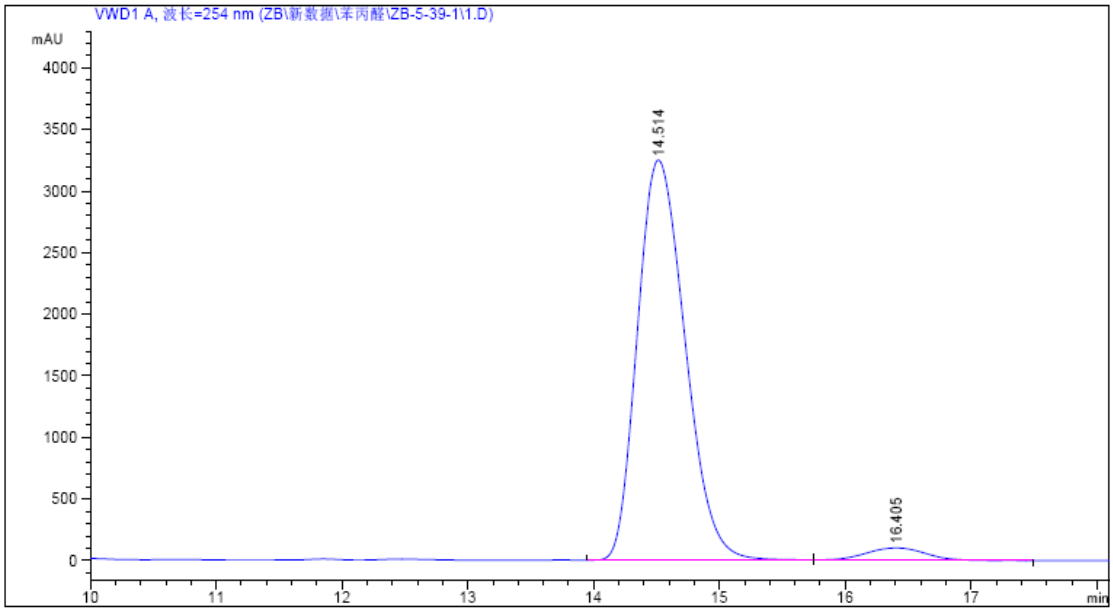
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	20.418	BB	0.5481	2342.61743	62.47823	6.4360
2	23.907	BB	0.6334	3.40560e4	795.53278	93.5640

Racemic



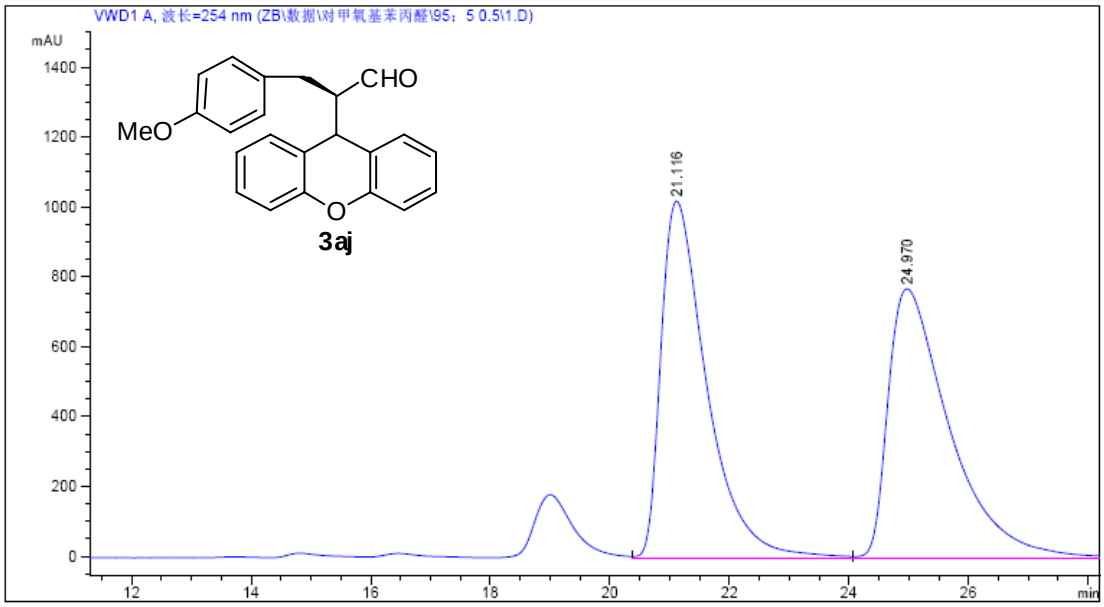
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	14.465	VV	0.4003	5.60807e4	2171.46875	48.8851
2	16.263	VV	0.5489	5.86387e4	1690.37292	51.1149

Sample



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	14.514	VV	0.4197	8.57467e4	3252.44189	96.1171
2	16.405	VB	0.5354	3463.91650	102.14732	3.8829

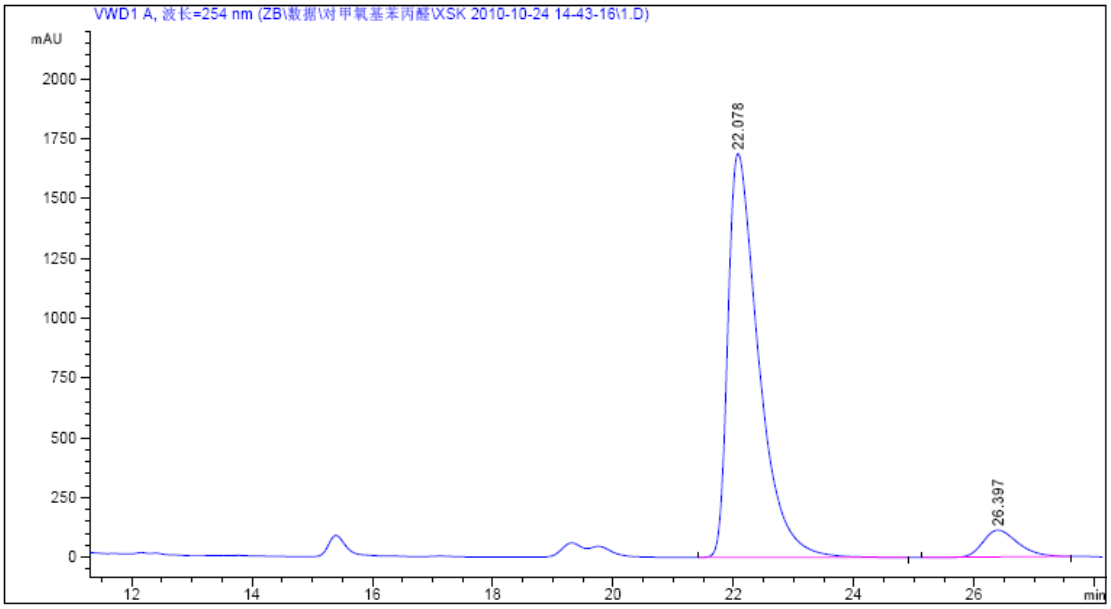
Racemic



信号 1: VWD1 A, 波长=254 nm

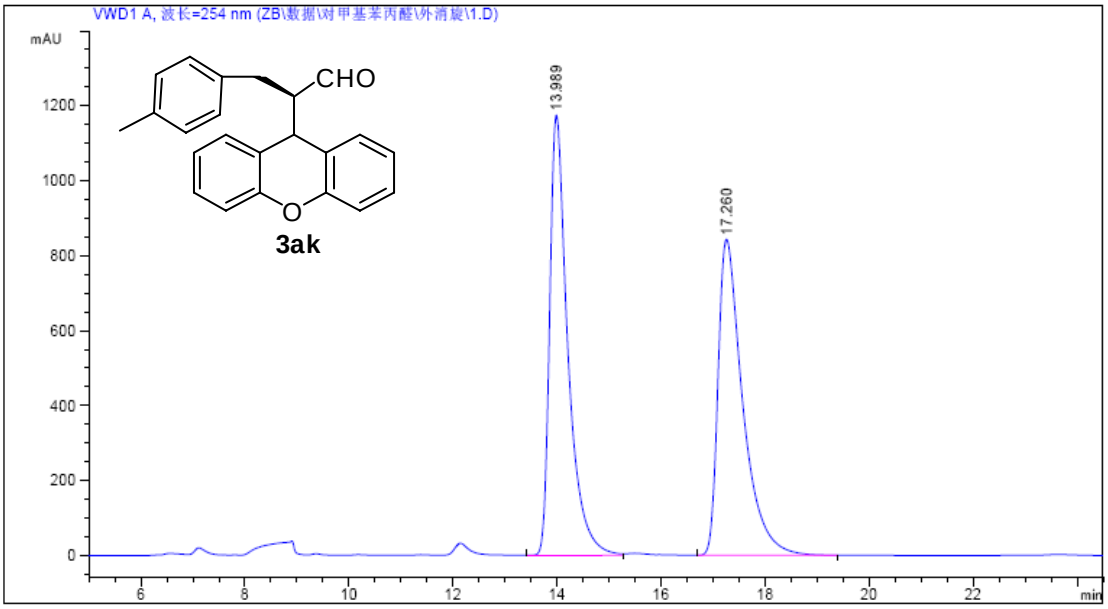
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	21.116	VV	0.7850	5.43311e4	1021.51495	49.7755
2	24.970	VV	1.0471	5.48211e4	770.44055	50.2245

Sample



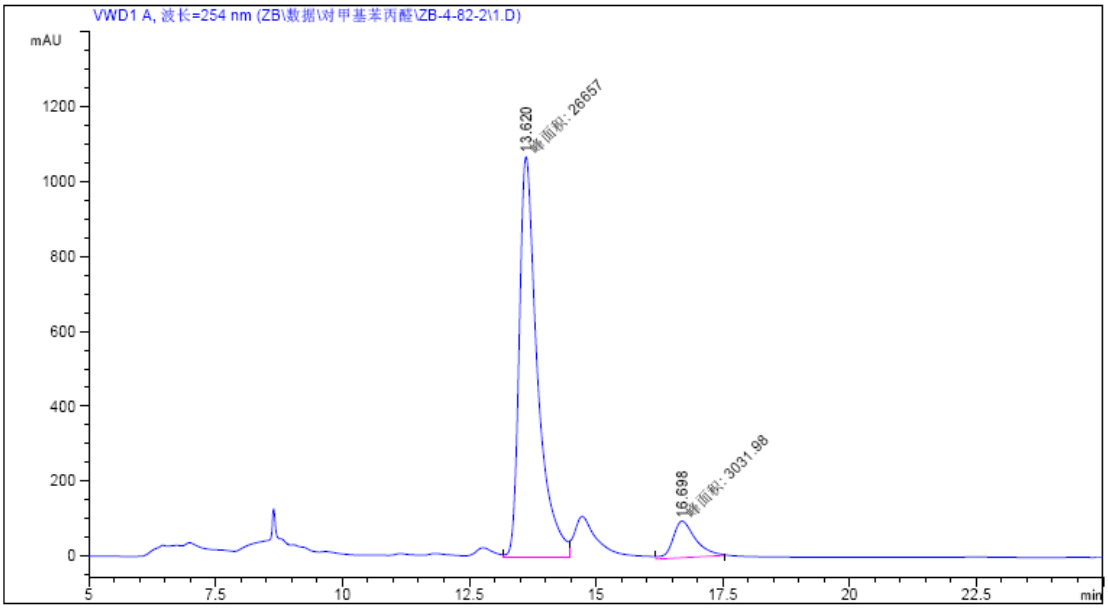
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	22.078	BB	0.5203	5.96754e4	1687.74084	93.0336
2	26.397	BB	0.6080	4468.54443	111.68652	6.9664

Racemic



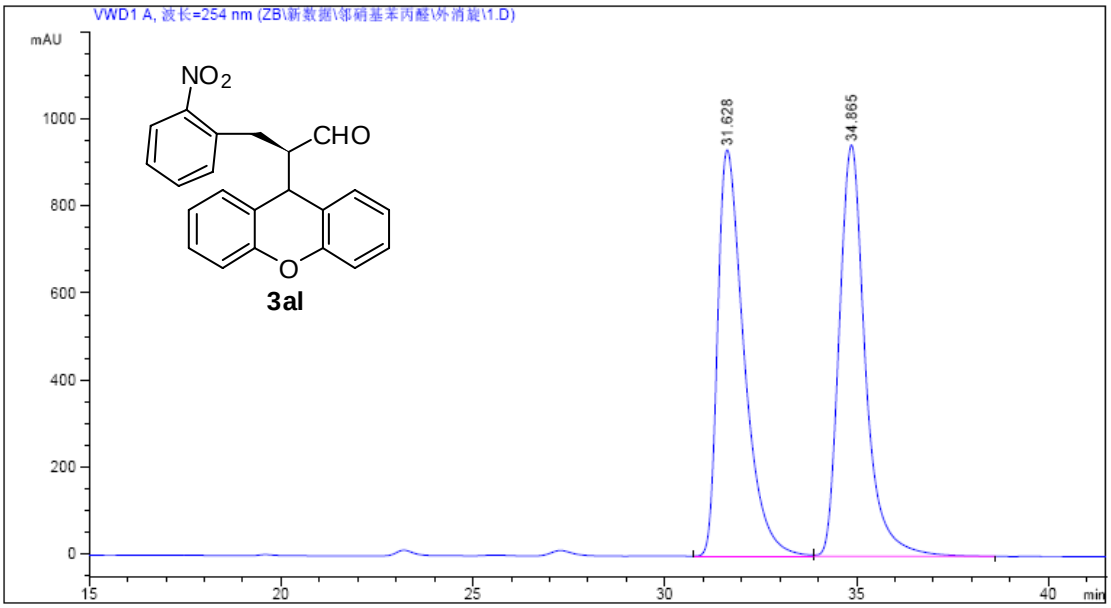
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	13.989	BV	0.3568	2.84497e4	1174.62988	50.6471
2	17.260	BB	0.4942	2.77227e4	843.35419	49.3529

Sample



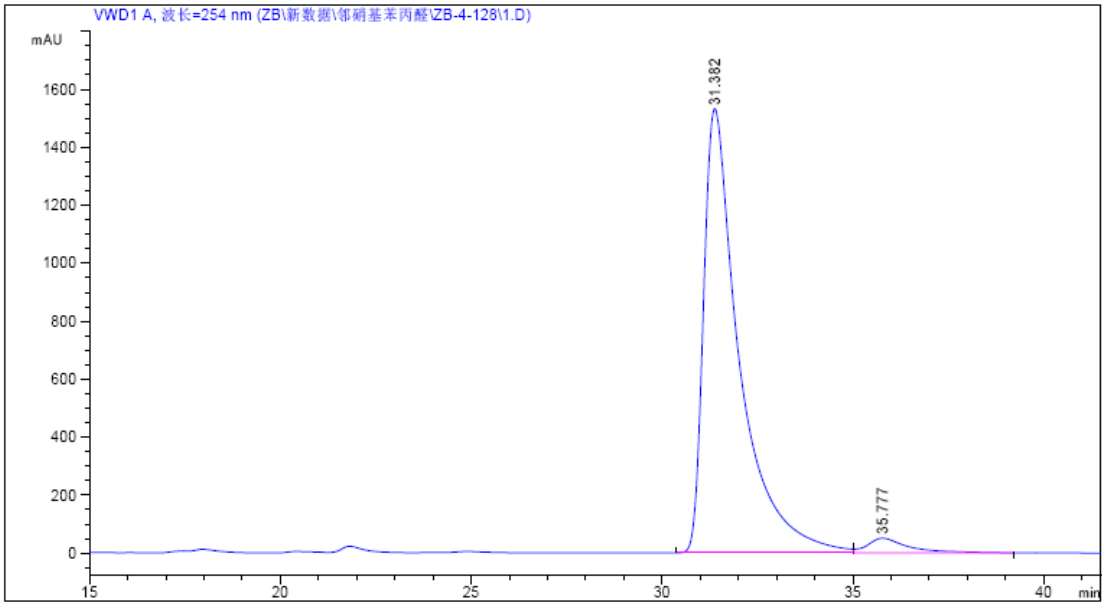
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	13.620	MM	0.4153	2.66570e4	1069.85132	89.7875
2	16.698	MM	0.5174	3031.97803	97.66032	10.2125

Racemic



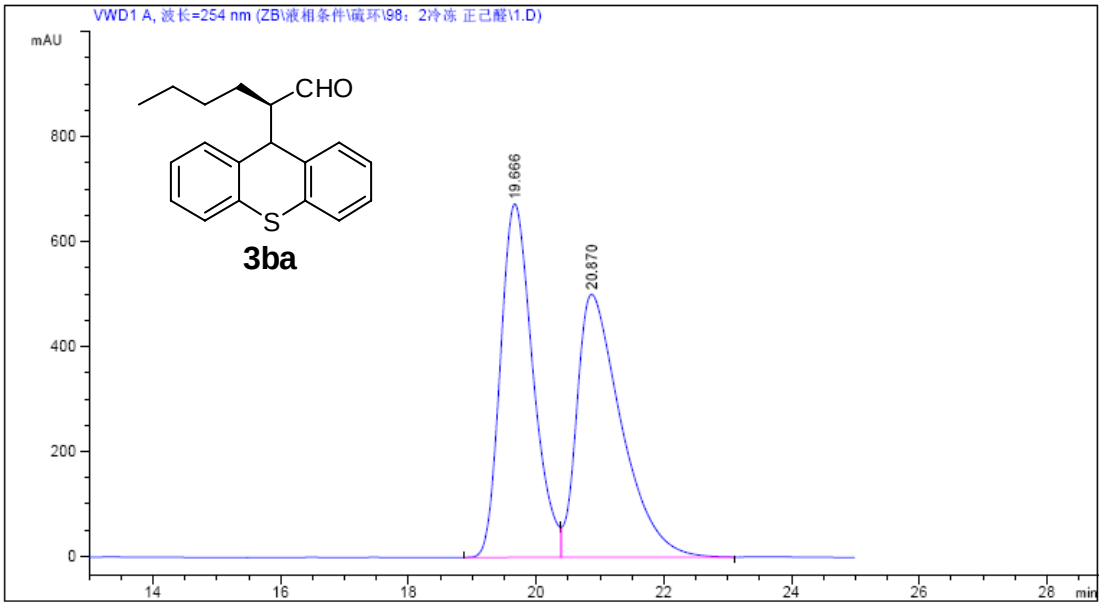
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	31.628	BV	0.7141	4.44958e4	932.29712	50.0085
2	34.865	VB	0.7100	4.44807e4	943.80048	49.9915

Sample



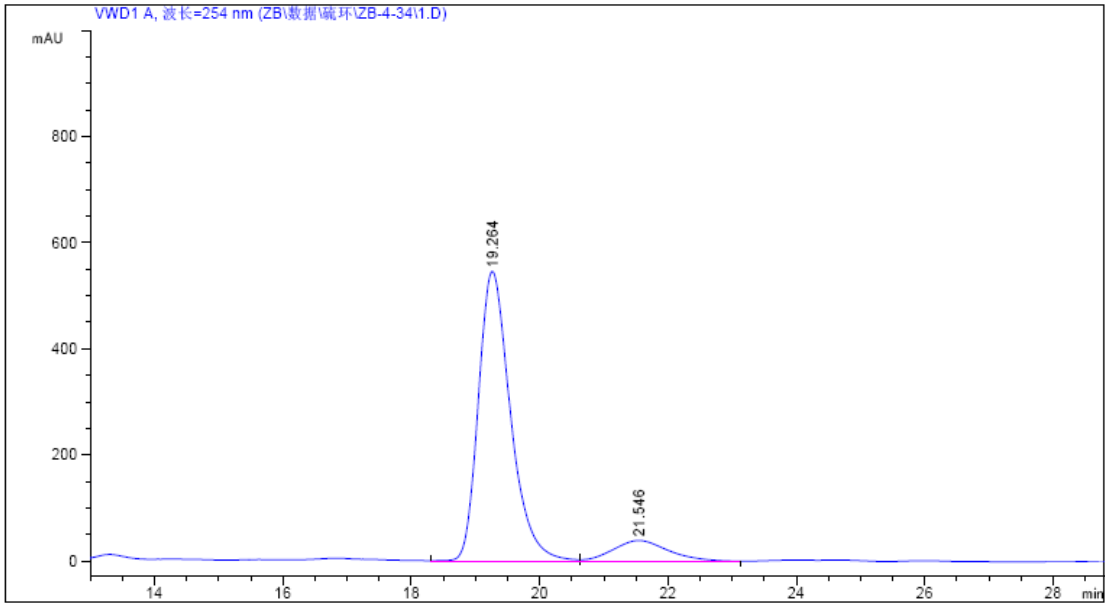
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	31.382	VV	0.9213	9.94038e4	1532.41296	96.3865
2	35.777	VB	1.0567	3726.57031	50.37516	3.6135

Racemic



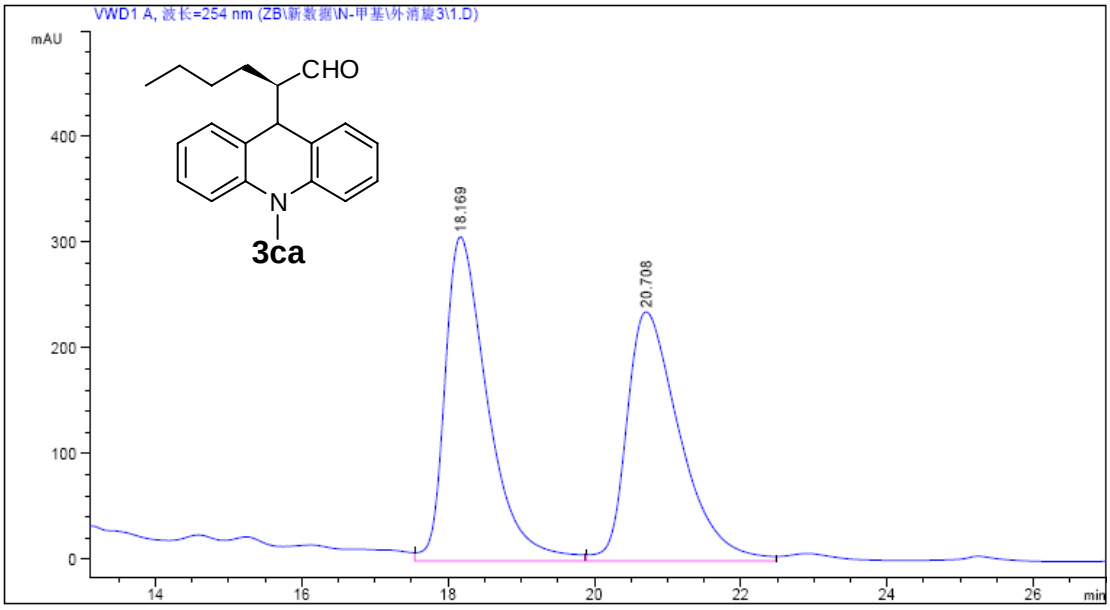
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	19.666	BV	0.5346	2.37199e4	673.63434	49.4959
2	20.870	VB	0.7192	2.42031e4	501.16092	50.5041

Sample



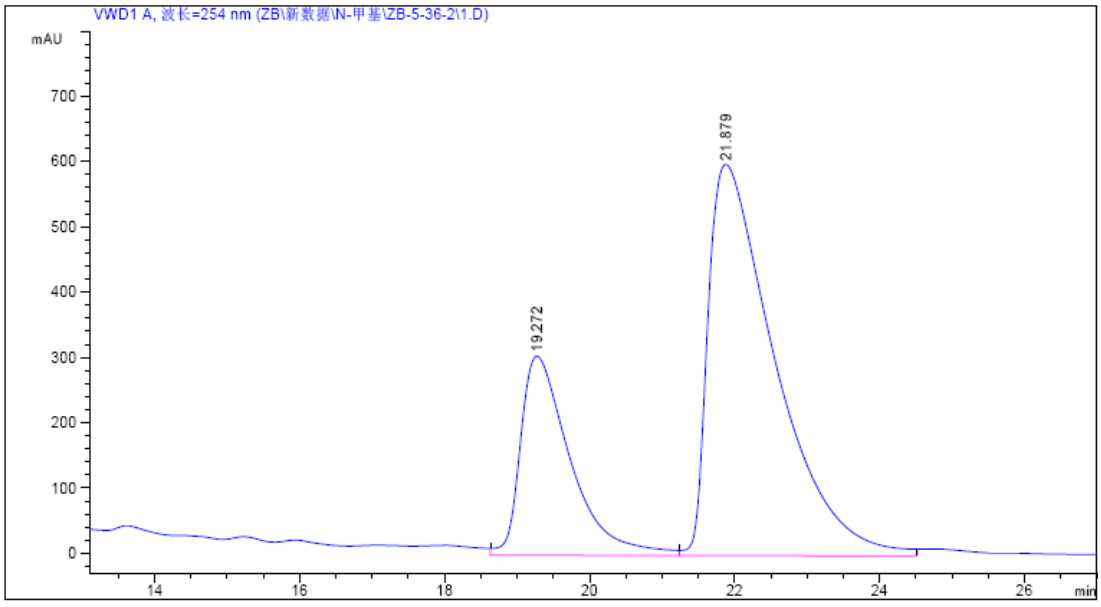
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	19.264	VV	0.5296	1.91693e4	547.09253	88.3856
2	21.546	VB	0.9090	2518.94727	40.26244	11.6144

Racemic



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	18.169	VB	0.6085	1.24336e4	306.65091	51.1718
2	20.708	BB	0.7595	1.18642e4	235.53751	48.8282

Sample



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 mAU *s	峰高 [mAU]	峰面积 %
1	19.272	VV	0.7086	1.46092e4	305.09473	27.5575
2	21.879	VB	0.9253	3.84044e4	599.27881	72.4425