Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

**Anti-Proliferative Activities of Flavone-Estradiol Stille-Coupling Adducts and of Indanone-Based Compounds Obtained by SnCl4/Zn-Catalysed McMurry Cross-Coupling Reactions**

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**1. Spectral data of indanofen derivatives and Flavone-Estradiol adducts**

**2. $^{1}H$ & $^{13}C$-NMR spectrum of indanofen derivatives and Flavone-Estradiol adducts**

**3. HRMS spectra of selected tamoxifen analogs**

**General procedure for determination of $IC_{50}$ value**

The half maximal inhibitory concentration ($IC_{50}$) value determination: The half maximal inhibitory concentration is a measure of the effectiveness of a compound in inhibiting biochemical processes and biological functions. According to the in vitro MTT assay, the $IC_{50}$ represents the concentration of the tested agent that is required for 50% inhibition of the cell viability. Based on the obtained data

using the in vitro MTT assay, the $IC_{50}$ values for tested compounds, calculated separately, most often at 48 h after cells exposure to these agents. To determine the IC50 values, the concentration range used of each agent should be determined properly.

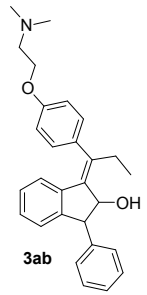
For this, first we have generate an equation Y = mx + C, and we can do this, one we have the % inhibition results at different concentration,
we will get and equation, which is based on Y = mx + C.
Here Y = % Inhibition
x= Concentration
C = Constant
m= Coefficient
Then simple mathematics we got the concentration which inhibit 50% of the cells/receptor etc.
Then put these values, in excel, and insert Scatter Graph, Then click on any data point on the graph, and click on add trendline, Then from there, we need to put the intercept at zero, and check display equation on the graph. Then select and kind of regression equation (linear, logarithmic etc). we got the $IC_{50}$ values.

**Antiproliferative (MTT assay):** MCF-7 and HeLa cells were seeded at a density of 4 x $10^4$ cells/mL and MDA-MB-231 cells were seeded at a density of 2 x $10^4$ cells/mL into 96-well plates and incubated for 24 h to allow attachment. After 24 h, the cells were treated with these synthesized derivatives at a range of concentrations (0 - 250 µM) or at single doses (10 µM against MCF-7 and MDA-MB-231 cells, and 50 µM against HeLa cells) for 67h. After 67 h, MTT assay was carried out by the addition of 20 µL of MTT (5mg/mL) solution in PBS into each well and the cells were incubated for 5 h. The purple crystals formed were dissolved in 100 µL of DMSO and the plates were read at 570 nm using a spectra max UV spectrometer (Bio-Rad). The data represented are the mean of the three individual experiments. The cell viability of the control is considered to be 100%.

**$IC_{50}$ determination:** MCF-7 and HeLa cells were seeded at a density of 1.5 x $10^5$ cells/mL into 96- well plates and incubated for 72 h. After 72 h, the medium was aspirated and the cells were washed twice with sterile PBS and then treated with a range of concentrations (0 - 1000 µM) of $H_2O_2$ in sterile PBS (with $Ca^{2+}$ and $Mg^{2+}$) for 1 h. After 1 h, $H_2O_2$ solution in the well is replaced with the warm medium and incubated for 17 h. After the 18 h exposure, the cell viability was determined using MTT assay (as described in the antiproliferative assay section). The data represented are the mean of the three individual experiments. The cell viability of the control is considered to be 100%.

**1. Spectral data of indanofen derivatives and Flavone-Estradiol adducts**

(E)-1-(1-(4-(2-(dimethylamino)ethoxy)phenyl)propylidene)-3-phenyl-2,3-dihydro-1H-inden-2-ol (**3ab**)



3ab

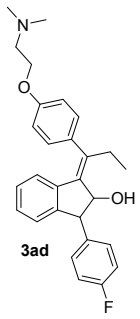
Light yellow semi solid; Yield: 66 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3452 (OH str), 2963 (aromatic C-H str), 1599 (aromatic, C=C str), 1451, 1419, 1262, 1021, 933, 868, 799 and 704; $^{1}$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.92 (d, *J* = 8 Hz, 2H), 7.83 (d, *J* = 7.5 Hz, 2H), 7.60 (d, *J* = 7 Hz, 1H), 7.49-7.45 (m, 2H), 7.41 (dd, *J* = 7.5, 2.5 Hz, 2H), 7.27-7.25 (m, 2H), 6.92 (d, J = 7.5 Hz, 2H) 4.73 (d, *J* = 3.5 Hz, 1H), 4.62 (d, *J* = 3.5 Hz, 1H), 4.15 (t, J = 1.5 Hz, 2H), 2.90 (s, 6H), 2.61 (t, J = 1.5 Hz, 2H), 2.25 (q, *J* = 7.0 Hz, 2H), 1.18 (t, *J* = 7.0 Hz, 3H) 3.60 (s, br, $D_2O$ exchangeable, 1 H); $^{13}$C-NMR ($CDCl_3$, 125 MHz) δ (ppm): 160.25, 157.05, 137.76, 132.57, 132.42, 131.77, 130.65, 130.49, 130.33, 129.65, 128.97, 128.68, 128.66, 127.05, 116.56, 116.32, 114.65, 71.65, 67.73, 61.35, 52.65, 48.35, 28.27, 14.03; MS (EI, 70eV): m/z = 413 [$M^{+\cdot}$, $C_{28}H_{31}NO_2$]; HRMS (ES-TOF) calcd for $C_{28}H_{31}NO_2$ 413.2355, found 413.2354.

(E)-1-(1-(4-(2-(dimethylamino)ethoxy)phenyl)propylidene)-5-fluoro-3-phenyl-2,3-dihydro-1H-inden-2-ol (**3ac**)

Light yellow semi solid; Yield: 60 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3408 (OH str), 2917 (aromatic C-H str), 1589 (aromatic, C=C str), 1489, 1415, 1288, 1177, 1091, 1014, 929 and 701; $^{1}$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.88 (t, *J* = 8 Hz, 2H), 7.86 (t, *J* = 8 Hz, 2H), 7.55-7.51 (m, 3H), 7.41-7.39 (m, 3H), 6.87 (t, *J* = 7.5 Hz, 2H), 4.58 (d, *J* = 4.0 Hz, 1H), 4.41 (d, *J* = 4.5 Hz, 1H), 4.15 (t, *J* = 3.0 Hz, 2H), 2.90 (s, 6H), 2.62 (t, *J* = 3.0 Hz, 2H), 2.25 (q, *J* = 7.0 Hz, 2H) 1.18 (t, *J* = 7.0 Hz, 3H), 3.42 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 159.68, 158.55, 157.11, 137.93, 132.55, 132.49, 131.65, 130.97, 130.77, 130.68, 129.65, 128.49,

128.47, 128.05, 127.66, 116.05, 114.11, 71.75, 67.72, 61.55, 52.11, 47.32, 26.05, 12.98; MS (EI, 70eV): m/z (%) = 431[$M^{+\cdot}$, $C_{28}H_{30}FNO_2$]; HRMS (ES-TOF) calcd for $C_{28}H_{30}FNO_2$ 431.2261, found 431.2259

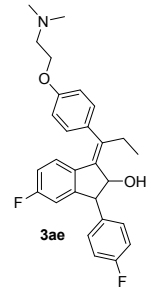
(E)-1-(1-(4-(2-(dimethylamino)ethoxy)phenyl)propylidene)-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-2-ol (**3ad**)



3ad

Light yellow semi solid; Yield: 64 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3391 (OH str), 2951 (aromatic C-H str), 1577 (aromatic, C=C str), 1468, 1401, 1271, 1152, 1084, 1002, 910 and 725; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.90 (t, *J* = 7.5 Hz, 2H) 7.82-7.71 (m, 2H), 7.70-7.42 (m, 2H), 6.96 (t, *J* = 8.5 Hz, 3H), 6.86 (t, *J* = 8.5 Hz, 3H), 4.50 (d, *J* = 2.0 Hz, 1H), 4.18 (d, *J* = 2.0 Hz, 1H), 4.03 (t, *J* = 2.5 Hz, 2H), 2.78 (s, 6H), 2.66 (t, *J* = 2.5 Hz, 2H), 1.78 (q, *J* = 7.0 Hz, 2H), 1.08 (t, *J* = 7.0 Hz, 3H), 3.39 (s, br, $D_2O$ exchangeable, 1 H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 159.54, 158.66, 137.95, 132.55, 132.49, 131.65, 130.49, 130.47, 130.05, 129.65, 128.97, 128.77, 128.68, 127.66, 116.03, 114.05, 71.73, 67.72, 61.05, 52.32, 47.11, 26.05, 12.95; MS (EI, 70eV): m/z (%) = 431[$M^{+\cdot}$, $C_{28}H_{30}FNO_2$]; HRMS (ES-TOF) calcd for $C_{28}H_{30}FNO_2$ 431.2261, found 431.2259.

(E)-1-(1-(4-(2-(dimethylamino)ethoxy)phenyl)propylidene)-5-fluoro-3-(4-fluorophenyl)-2,3-dihydro-1H-inden-2-ol (**3ae**)

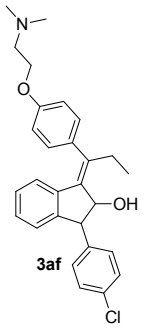


3ae

Light brown semi solid; Yield: 58 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3426 (OH str), 2923 (aromatic C-H str), 1591 (aromatic, C=C str), 1417, 1395, 1282, 1170, 1092; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.98 (t, *J* = 8.5 Hz, 2H), 7.79-7.76 (m, 2H), 7.70 (dd, *J* = 7.5, 1.5 Hz, 2H), 7.47 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.25-7.36 (m, 2 H), 6.86 (dd, *J* = 8.0, 3.0 Hz, 2H), 4.52 (d, *J* = 3.0, Hz, 1H), 4.44 (d, *J* = 3.0 Hz, 1H), 4.15 (t, *J* = 2.0 Hz, 2H), 2.98 (s, 6H), 2.72 (t, *J* = 2.0 Hz, 2H), 2.25 (q, *J* = 7.0 Hz, 2H), 1.19 (t, *J* = 7.0 Hz, 3H), 3.52 (s, br, $D_2O$ exchangeable, 1 H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 161.27, 160.55, 159.47, 158.77, 138.76, 138.54, 130.68, 130.49, 130.05, 129.65, 128.97, 128.65, 127.66, 117.97, 117.66, 114.76, 70.72, 66.73,

61.35, 52.32, 48.05, 26.95, 13.32; MS (EI, 70eV): m/z = 449 [$M^{+\cdot}$, $C_{28}H_{29}F_2NO_2$]; HRMS (ES-TOF) calcd for $C_{28}H_{29}F_2NO_2$ 449.2166, found 449.2168

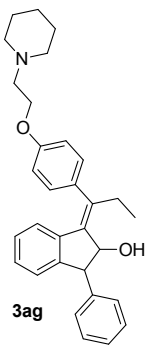
(E)-1-(4-chlorophenyl)-3-(1-(4-(2-(dimethylamino)ethoxy)phenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3af**)



3af

Light brown semi solid; Yield: 55 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3449 (OH str), 2950 (aromatic C-H str), 1582 (aromatic, C=C str), 1389, 1275, 1059, 854, 723 (C-Cl, str); $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.08 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.5, Hz, 1H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.47(d, *J* = 8.5 Hz, 1 H), 7.27 (t, *J* = 7.0 Hz, 2H), 7.16 (d, *J* = 8.5 Hz, 1H), 6.89 (dd, *J* = 8.0, 2.5 Hz, 2H), 4.67 (d, *J* = 3.0 Hz, 1H), 4.32 (d, *J* = 3.0 Hz, 1H), 3.94 (d, *J* = 2.5 Hz, 2H), 3.00 (s, 6H), 2.81(t, *J* = 3.0 Hz, 2H), 2.26 (q, *J* = 8.0 Hz, 2H,), 1.08 (t, *J* = 8.0 Hz, 3H), 3.41 (s, br, $D_2O$ exchangeable, 1 H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 159.55, 157.27, 137.76, 132.54, 132.47, 131.77, 130.65, 130.49, 130.05, 129.65, 128.97, 128.68, 128.66, 127.03, 117.95, 115.76, 71.72, 67.73, 61.35, 52.32, 48.97, 28.95, 14.05; MS (EI, 70eV): m/z (%) = 447[$M^{+\cdot}$, $C_{28}H_{30}ClNO_2$], 449[$M^{+2}$]; HRMS (ES-TOF) calcd for $C_{28}H_{30}ClNO_2$ 447.1965, found 447.1967.

(E)-1-phenyl-3-(1-(4-(2-(piperidin-1-yl)ethoxy)phenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3ag**)



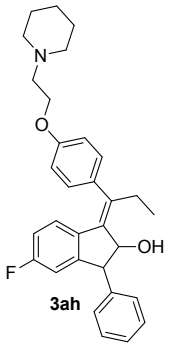
3ag

Light yellow semi solid; Yield: 58 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3420 (OH str), 2959, 2869 (aromatic C-H str), 1583 (aromatic, C=C str), 1253, 1063, 835; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.91(d, *J* = 8.0 Hz, 2H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.59 (t, *J* = 8.5 Hz, 1H), 7.48-7.45 (m, 2H), 7.42-7.39 (m, 2H), 7.27-7.25 (m, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 5.27 (d, *J* = 2.0 Hz, 1 H), 5.12 (d, *J* = 2.0 Hz, 1H), 4.14 (t, *J* = 2.5 Hz, 2H), 2.92 (m, 2H), 2.76 (t, *J* = 6.0 Hz, 2H), 2.49

(s, 4H), 1.59 (q, *J* = 8.0 Hz, 2H), 1.44 (t, *J* = 6.0 Hz, 2H), 1.18 (t, *J* = 8.0 Hz, 3H), 3.85 (s, br, $D_2O$ exchangeable, 1 H), $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 158.27, 153.65, 137.77, 132.54, 132.47, 131.77, 130.65, 130.49, 130.05, 129.65, 128.97, 128.68, 128.66, 127.03, 118.95, 117.66, 117.05, 115.65, 76.16, 74.32, 63.73, 58.79, 56.95, 28.15, 26.97, 25.04, 13.05; MS (EI, 70eV): m/z = 453[$M^{+\cdot}$, $C_{31}H_{35}NO_2$]; HRMS (ES-TOF) calcd for $C_{32}H_{35}NO_2$ 453.2668, found 453.2666.

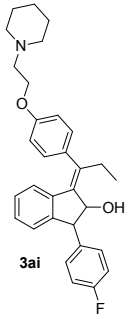
(E)-5-fluoro-3-phenyl-1-(1-(4-(2-(piperidin-1-yl)ethoxy)phenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3ah**)

Light brown semi solid; Yield: 59 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3415 (OH str), 2931, 2873 (aromatic C-H str), 1597 (aromatic, C=C str), 1263, 1081, 860, 737; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.88-7.84 (m, 4H), 7.55-7.49 (m, 4H), 7.42-7.26 (m, 2H), 6.87 (t, *J* = 7.5 Hz, 2H), 4.68 (d, *J* = 3.5 Hz, 1H), 4.51 (d, *J* = 3.0 Hz, 1H), 3.83 (d, *J* = 3.0 Hz, 2H), 3.84-3.80 (m, 2 H), 2.77 (t, *J* = 4.0 Hz, 2H), 2.39-2.36 (m, 4H), 1.49 (q, *J* = 7.5 Hz, 2H), 1.14 (t, *J* = 6 Hz, 4H ), 0.97 (t, *J* = 7.5 Hz, 3H), 3.83(s, br, $D_2O$ exchangeable, 1H), $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 161.15, 157.78, 153.62, 137.47, 132.74, 132.57, 131.65, 130.79, 130.45, 130.05, 129.79, 128.93, 128.68, 128.66, 127.05, 117.00, 116.65, 116.08, 76.32, 74.16, 64.75, 58.93, 56.70, 27.79, 26.95, 25.43, 14.55; MS (EI, 70eV): m/z (%) = 471[$M^{+\cdot}$, $C_{31}H_{34}FNO_2$]; HRMS (ES-TOF) calcd for $C_{31}H_{34}FNO_2$ 471.2574, found 471.2571.



3ah

(E)-1-(4-fluorophenyl)-3-(1-(4-(2-(piperidin-1-yl)ethoxy)phenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3ai**)

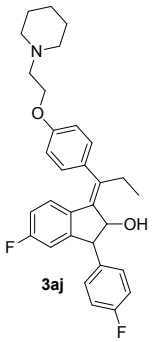


3ai

Light yellow semi solid; Yield: 58 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3429 (OH str), 2951, 2880 (aromatic C-H str), 1607 (aromatic, C=C str), 1271, 1107, 843, 729; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.89-7.85 (m, 4H), 7.56-7.50 (m, 4H), 7.41-7.39 (m, 2H), 6.87 (t, *J* = 7.5 Hz, 2H), 4.67 (d, *J* = 3.5 Hz, 1H), 4.50 (d, *J* = 4.0 Hz, H), 3.74 (t, *J* = 6.5 Hz, 2H), 3.85-3.80

(m, 2 H), 2.76 (t, $J$ = 6.0 Hz, 2H), 2.40-2.39 (m, 4H), 1.48 (q, $J$ = 8.0 Hz, 2H), 1.14(t, $J$ = 6.0 Hz, 4H), 0.97(t, $J$ = 8.0 Hz, 3H), 3.45 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 161.15, 157.62, 153.78,137.47, 132.74, 132.57, 131.65, 130.93, 130.68, 130.66, 129.79, 128.45, 128.16, 127.05, 117.00, 116.65, 116.05, 76.32, 74.08, 64.75, 58.93, 56.70, 27.87, 26.95, 25.79, 14.43; MS (EI, 70eV): m/z (%) = 471[$M^{+\cdot}$, $C_{31}H_{34}FNO_2$]; HRMS (ES-TOF) calcd for $C_{31}H_{34}FNO_2$ 471.2574, found 471.2571.

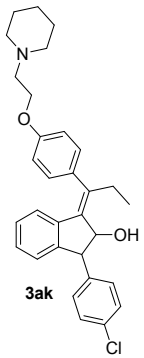
(E)-5-fluoro-3-(4-fluorophenyl)-1-(1-(4-(2-(piperidin-1-yl)ethoxy)phenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3aj**)



3aj

Light yellow semi solid; Yield: 55%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3382 (OH str), 2992, 2886 (aromatic C-H str), 1620 (aromatic, C=C str), 1262, 1095, 860, 743; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.05 (d, $J$ = 8.5 Hz, 2H), 7.94 (d, $J$ = 8.5 Hz, 1H), 7.83 (d, $J$ = 8.5 Hz, 1H), 7.53 (d, $J$ = 8.5 Hz, 2H), 7.47(d, $J$ = 8.5 Hz, 2H), 7.28 (t, $J$ = 8.5 Hz, 2H), 7.16 (d, $J$ = 8.5 Hz, 1H), 6.94 (d, $J$ = 8.5 Hz, 2H), 4.98 (d, $J$ = 3.5 Hz, 1H), 4.71 (d, $J$ = 4.0 Hz, 1H), 3.94 (t, $J$ = 6.0 Hz, 1H), 3.04-3.00 (m, 2H), 2.96 (t, $J$ = 6.0 Hz, 2H), 2.49-2.48 (m, 2H), 1.69 (q, $J$ = 7.5 Hz, 4H), 1.44 (t, $J$ = 7.5 Hz, 3H), 4.42 (s, br, $D_2O$ exchangeable, 1 H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):161.25, 160.57, 159.44, 158.76, 138.77, 138.57, 130.68, 130.49, 130.25, 129.65, 128.97, 128.65, 127.66, 117.97, 117.67, 114.76, 73.32, 70.72, 66.73, 61.35, 51.32, 30.09, 27.15, 26.09, 13.05; MS (EI, 70eV): m/z (%) = 489[$M^{+\cdot}$, $C_{31}H_{33}F_2NO_2$]; HRMS (ES-TOF) calcd for $C_{31}H_{33}F_2NO_2$ 489.2479, found 489.2477.

(E)-1-(4-chlorophenyl)-3-(1-(4-(2-(piperidin-1-yl)ethoxy)phenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3ak**)

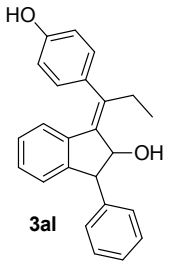


3ak

Light yellow semi solid; Yield: 52 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3440 (OH str), 2920 (aromatic C-H str), 1592 (aromatic, C=C str), 1406, 1336, 1233, 1125(C-O-C, str), 1091, 771 (C-Cl, str); $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.92 (d, $J$ = 7.0 Hz, 2H), 7.83 (d, $J$ = 7.5 Hz, 2H), 7.59 (d, $J$ = 7.0 Hz, 1H), 7.48-7.45 (m, 1H), 7.41(dd, $J$ = 7.0, 2.5 Hz, 1H), 7.27-7.25 (m,

2H), 6.91 (d, *J* = 7.5 Hz, 1H), 5.27 (d, *J* = 2.0 Hz, 1H), 5.12 (d, *J* = 3.0 Hz, 1H), 4.14 (t, *J* = 3.0 Hz, 2H), 2.94-2.90 (m, 2H), 2.77 (t, *J*=6.0 Hz, 2H), 2.49-2.47 (m, 4H), 1.59 (q, *J* = 7.0 Hz, 2H), 1.44 (t, *J* = 6.0 Hz, 4H), 1.19 (t, *J* = 7.0 Hz, 3H), 3.70 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 157.78, 153.62, 137.74, 132.57, 132.47, 131.79, 130.65, 130.45, 130.05, 129.63, 128.79, 128.68, 128.66, 127.05, 118.96, 117.65, 117.05, 115.66, 76.13, 74.32, 64.73, 58.90, 56.75, 27.95, 26.79, 25.45, 14.35; MS (EI, 70eV): m/z (%) = 487[$M^{+\cdot}$, $C_{31}H_{34}ClNO_2$], 489[$M^{+2}$]; HRMS (ES-TOF) calcd for $C_{24}H_{20}F_2O$ 487.2278, found 487.2276.

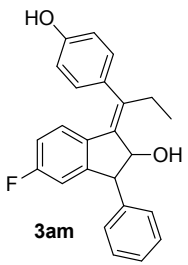
(E)-1-(1-(4-hydroxyphenyl) propylidene)-3-phenyl-2,3-dihydro-1H-inden-2-ol (**3al**)



**3al**

Light brown semi solid; Yield: 70%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3429 (OH str), 2951, 2880 (aromatic C-H str), 1607 (aromatic, C=C str), 1271, 1107, 843, 729; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.11(dd, *J* = 8.5, 2.0 Hz, 2H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.47(d, *J* = 8.5 Hz, 1H), 7.27 (t, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.5 Hz, 2H), 6.88 (dd, *J* = 8.0, 2.0 Hz, 2H), 4.67 (d, *J* = 4.0 Hz, 1H), 4.20 (d, *J* = 4.0 Hz, 1H), 2.19 (q, *J* = 8.0 Hz, 2H), 1.10 (t, *J* = 8.0 Hz, 3H), 3.68 (s, br, $D_2O$ exchangeable, 1H); 1.56 (s, br, $D_2O$ exchangeable, 1H) ; $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):159.60, 155.65, 142.65, 141.32, 138.52, 131.66, 130.97, 130.68, 129.97, 129.58, 128.68, 127.97, 126.68, 121.97, 121.68, 116.66, 115.32, 71.08, 51.68, 26.12, 13.03; MS (EI, 70eV): m/z (%) = 342[$M^{+\cdot}$, $C_{24}H_{22}O_2$]; HRMS (ES-TOF) calcd for $C_{24}H_{22}O_2$ 342.1620 $[M+H]^+$, found 342.1617.

(E)-5-fluoro-1-(1-(4-hydroxyphenyl)propylidene)-3-phenyl-2,3-dihydro-1H-inden-2-ol (**3am**)

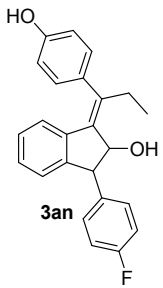


**3am**

Light brown semi solid; Yield: 72%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3415 (OH str), 2931, 2873 (aromatic C-H str), 1597 (aromatic, C=C str), 1263, 1081, 860, 737; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.99-7.86 (m, 2H), 7.79-7.76 (m,

2H), 7.71 (dd, *J* = 1.5, 8.0 Hz, 2H), 7.49-7.44 (m, 2H), 7.34(dd, *J* = 2.0, 8.0 Hz, 2H), 6.88 (dd, *J* = 2.0, 7.0 Hz, 2H), 4.49 (t, *J* = 3.0 Hz, 1H), 4.46 (d, *J* = 3.0 Hz, 1H), 2.29 (q, *J* = 8.0 Hz, 2H), 1.28 (t, *J* = 8.0 Hz, 3H), 6.17 (s, br, $D_2O$ exchangeable, 1H), 3.70 (s, br, $D_2O$ exchangeable, 1H); $^{13}C$- ($CDCl_3$, 125 MHz) δ (ppm):165.58, 158.32, 142.54, 141.47, 138.35, 130.97, 130.66, 129.97, 129.68, 128.97, 127.97, 126.95, 116.66, 115.05, 113.65, 73.05, 52.12, 28.03, 14.03; MS (EI, 70eV): m/z = 360[$M^{+\cdot}$, $C_{24}H_{21}FO_2$]; HRMS (ES-TOF) calcd for $C_{24}H_{21}FO_2$ 360.1526, found 360.1529.

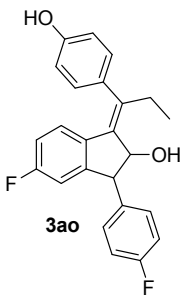
(E)-1-(4-fluorophenyl)-3-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3an**)



3an

Light yellow semi solid; Yield:70%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3382 (OH str), 2992, 2886 (aromatic C-H str), 1620 (aromatic, C=C str), 1262, 1095, 860, 743; $^1H$-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.88-7.84 (m, 4H), 7.55-7.50 (m, 4H), 7.42-7.39 (m, 2H), 6.87 (t, *J* = 8.0 Hz, 2H), 4.88 (d, *J* = 3.5 Hz, 1H), 4.61 (d, *J* = 3.5 Hz, 1H), 2.38 (q, *J* = 7.0 Hz, 2H), 1.37 (t, *J* = 7.0 Hz, 3H), 3.65 (s, br, $D_2O$ exchangeable, 1H), 1.62 (s, br, $D_2O$ exchangeable, 1H), $^{13}C$- ($CDCl_3$, 125 MHz) δ (ppm):162.32, 156.54, 142.47, 141.58, 138.65, 130.97, 130.68, 129.97, 129.68, 128.68, 127.96, 126.67, 116.65, 115.05, 113.66, 71.12, 55.08, 26.35, 14.35; MS (EI, 70eV): m/z (%) = 360[$M^{+\cdot}$, $C_{24}H_{21}FO_2$]; HRMS (ES-TOF) calcd for $C_{24}H_{21}FO_2$ 360.1526, found 360.1528.

(E)-5-fluoro-3-(4-fluorophenyl)-1-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3ao**)

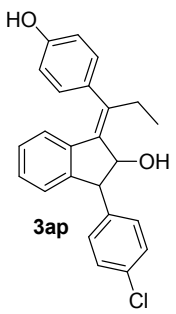


3ao

Light brown semi solid; Yield: 68%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3405 (OH str), 2922, 2875 (aromatic C-H str), 1595 (aromatic, C=C str), 1266, 1089, 858, 731; $^1H$-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.00-7.85 (m, 2H), 7.80-7.77 (m, 2H), 7.76-7.69 (m, 2H), 7.47 (dd, *J* = 2.0, 8.0 Hz, 1H), 7.36 (dd, *J* = 2.0, 7.0 Hz, 2H), 6.89 (dd, *J* = 2.0, 8.0 Hz, 2H),

4.50 (d, $J$ = 4.0 Hz, 1H), 4.46 (d, $J$ = 3.5 Hz, 1H), 2.29 (q, $J$ = 8.0 Hz, 2H), 1.28 (t, $J$ = 8.0 Hz, 3 H), 6.10 (s, br, $D_2O$ exchangeable, 1H), 1.72 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):163.58, 158.32, 142.65, 141.47, 138.54, 130.97, 130.68, 129.97, 129.68, 128.97, 127.68, 126.66, 116.65, 115.05, 113.66, 73.05, 52.12, 28.35, 14.59; MS (EI, 70eV): m/z (%) = 378[$M^{+\cdot}$, $C_{24}H_{20}F_2O_2$]; HRMS (ES-TOF) calcd for $C_{24}H_{20}F_2O_2$ 378.1431, found 378.1434.

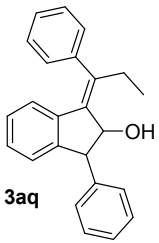
(E)-1-(4-chlorophenyl)-3-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**3ap**)



3ap

Light brown semi solid; Yield: 67%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3440 (OH str), 2920 (aromatic C-H str), 1592 (aromatic, C=C str), 1406, 1336, 1233, 1091, 771 (C-Cl, str); $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.09 (dd, $J$ = 2.0, 7.5 Hz, 2H), 7.94 (d, $J$ = 8.5 Hz, 1H), 7.83 (d, $J$ = 8.5 Hz, 1H), 7.53 (d, $J$ = 8.5 Hz, 2H), 7.47 (d, $J$ = 8.5 Hz, 1H), 7.27 (t, $J$ = 8.5 Hz, 1H), 7.16 (d, $J$ = 8.5Hz, 1H), 6.89 (dd, $J$ = 2.0, 8.0 Hz, 1H), 4.68 (d, $J$ = 3.5 Hz, 1H), 4.21 (d, $J$ = 4.5 Hz, 1H), 2.19(q, $J$ = 7.0 Hz, 2H), 1.19 (t, $J$ = 7.0 Hz, 3H), 3.67 (s, br, $D_2O$ exchangeable, 1H), 1.65 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):163.35, 142.68, 141.52, 138.75, 131.52, 130.97, 130.68, 129.98, 129.65, 128.68, 127.78, 126.36, 116.62115.35, 113.66, 70.13, 51.12, 26.66, 51.68, 15.68; MS (EI, 70eV): m/z (%) = 376[$M^{+\cdot}$, $C_{24}H_{21}ClO_2$], 378[$M^{+2}$]; HRMS (ES-TOF) calcd for $C_{24}H_{21}ClO_2$ 376.1230, found 376.1233.

(E)-1-phenyl-3-(1-phenylpropylidene)-2,3-dihydro-1H-inden-2-ol (**3aq**)

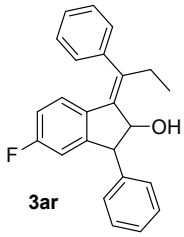


3aq

Light brown semi solid; Yield: 72%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3425 (OH str), 2935, 2877 (aromatic C-H str), 1585 (aromatic, C=C str), 1266, 1088, 862, 733 $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.91-7.66 (m, 4H), 7.6-7.54 (m, 1H), 7.54-7.50 (m, 4H), 7.37-7.34 (m, 2H ), 7.33-7.32 (m, 1H ), 7.31-23 (m, 2H), 4.72 (d, $J$ = 2.0 Hz, 1H), 4.18 (d, $J$ = 2.0

Hz, 1H), 2.31 (q, *J* = 7.0 Hz, 2H), 1.17 (t, *J* = 7.0 Hz, 3H ), 3.30 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):157.60, 142.65, 141.32, 138.58, 131.52, 130.97, 130.68, 129.97, 129.68, 128.68, 127.78, 126.35, 121.97, 121.68, 116.66, 115.32, 71.12, 51.03, 26.66, 13.68; MS (EI, 70eV): m/z (%) = 326[$M^{+\cdot}$, $C_{24}H_{22}O$]; HRMS (ES-TOF) calcd for $C_{24}H_{22}O$ 326.1671, found 326.1673.

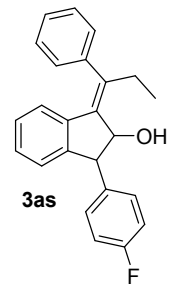
(E)-5-fluoro-3-phenyl-1-(1-phenylpropylidene)-2,3-dihydro-1H-inden-2-ol (**3ar**)



**3ar**

Light yellow semi solid; Yield: 74%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3449 (OH str), 2950 (aromatic C-H str), 1682 (C=O str), 1582 (aromatic, C=C str), 1389, 1275, 1059, 854; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.87-7.85 (m, 4H), 7.55-7.49 (m, 4H), 7.41-7.39 (m, 2H), 6.87 (t, *J* = 7.5 Hz, 2H), 4.58 (d, *J* = 3.5 Hz, 1H), 4.31 (d, *J* = 4.0 Hz, 1H), 2.37 (q, *J* = 7.5 Hz, 2H), 1.38 (t, *J* = 7.5 Hz, 3H), 1.88 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):160.54, 156.47, 142.32, 141.58, 138.65, 130.97, 130.68, 129.97, 129.68, 128.66, 127.97, 126.68, 116.06, 115.05, 113.65, 71.12, 51.08, 26.35, 13.95; MS (EI, 70eV): m/z (%) = 344[$M^{+\cdot}$, $C_{24}H_{21}FO$]; HRMS (ES-TOF) calcd for $C_{24}H_{21}F_2O$ 344.1576, found 344.1574

(E)-1-(4-fluorophenyl)-3-(1-phenylpropylidene)-2,3-dihydro-1H-inden-2-ol (**3as**)

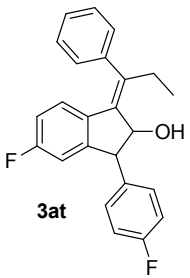


**3as**

Light yellow semi solid; Yield: 70 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3439 (OH str), 2922 (aromatic C-H str), 1670 (C=O str), 1594 (aromatic, C=C str), 1491, 1399, 1296, 1095; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.88-7.85 (m, 4H), 7.56-7.50 (m, 4H), 7.42-7.39 (m, 2H), 6.87 (t, *J* = 7.0 Hz, 2H), 4.88 (d, *J* = 3.5 Hz, 1H), 4.60 (d, *J* = 3.5 Hz, 1H), 2.38 (q, *J* = 7.5 Hz, 2H), 1.38 (t, *J* = 7.5 Hz, 3H), 1.70 (s, br, $D_2O$ exchangeable, 1 H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):160.52,

156.44, 142.32, 141.58, 138.65, 130.97, 130.68, 129.78, 129.68, 128.68, 127.97, 126.68, 116.66, 115.05, 113.65, 71.08, 51.12, 26.35, 13.66; MS (EI, 70eV): m/z (%) = 344[$M^{+\cdot}$, $C_{24}H_{21}FO$]; HRMS (ES-TOF) calcd for $C_{24}H_{21}F_2O$ 344.1576, found 344.1574.

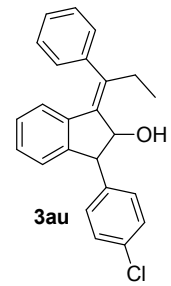
(E)-5-fluoro-3-(4-fluorophenyl)-1-(1-phenylpropylidene)-2,3-dihydro-1H-inden-2-ol (**3at**)



**3at**

Light yellow semi solid; Yield: 68 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3466 (OH str), 2920 (aromatic C-H str), 1593 (aromatic, C=C str), 1398, 1281, 1095, 843$^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.99-7.86 (m, 2H), 7.80-7.76 (m, 2H), 7.71 (dd, *J* = 2.5, 8.5 Hz, 2H), 7.47 (dd, *J* = 2, 7.5 Hz, 2H ), 7.37-7.34 (m, 2H), 6.89 (dd, J = 2.5, 7.5 Hz, 2H), 4.50 (d, *J* = 4.5 Hz, 1H), 4.46 (d, *J* = 4.5 Hz, 1 H), 2.29 (q, *J* = 8.0 Hz, 2H), 1.28(t, *J* = 8.0 Hz, 3H), 3.52 (s, br, $D_2O$ exchangeable, 1 H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):164.58, 160.32, 142.54, 141.47, 138.65, 130.97, 130.68, 129.97, 129.68, 128.66, 127.97, 126.95, 116.66, 115.05, 113.65, 73.12, 52.05, 28.35, 14.95; MS (EI, 70eV): m/z (%) = 362[$M^{+\cdot}$, $C_{24}H_{20}F_2O$]; HRMS (ES-TOF) calcd for $C_{24}H_{20}F_2O$ 362.1482, found 362.1482.

(E)-1-(4-chlorophenyl)-3-(1-phenylpropylidene)-2,3-dihydro-1H-inden-2-ol (**3au**)

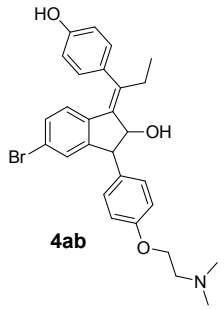


**3au**

Light brown semi solid; Yield: 65 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3426 (OH str), 2923 (aromatic C-H str), 1591 (aromatic, C=C str), 1417, 1395, 1282, 1170, 1092, 757 (C-Cl, str); $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.08 (dd, *J* = 2, 8 Hz, 2H), 7.94 (d, *J* = 7.5 Hz, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.53 (d, J = 7.5 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.27(t, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.87 (dd, *J* = 2.0, 7.5 Hz, 2H), 4.68 (d, *J* = 3.5 Hz, 1H), 4.21 (d, *J* = 3.5 Hz, 1H), 2.19 (q, *J* = 8.0 Hz, 2H), 1.10 (t, *J* = 8.0 Hz, 3H), 1.60 (s, br, $D_2O$ exchangeable, 1H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):156.60,

142.32, 141.58, 138.65, 131.52, 130.97, 130.68, 129.97, 129.68, 128.68, 127.7, 126.35, 116.66, 115.32, 113.65, 71.03, 51.12, 26.68, 13.66; MS (EI, 70eV): m/z = 360[$M^{+\cdot}$, $C_{24}H_{21}ClO$], 362[$M^{+2}$]; HRMS (ES-TOF) calcd for $C_{24}H_{21}ClO$ 360.1281, found 360.1283.

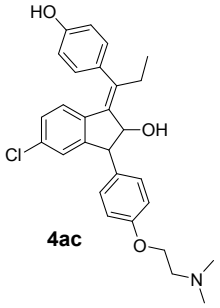
(E)-5-bromo-3-(4-(2-(dimethylamino)ethoxy)phenyl)-1-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**4ab**)



**4ab**

Yellow semi solid; Yield: 55%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3453 (OH str), 2957 (aromatic C-H str), 1587 (aromatic, C=C str), 1385, 1274, 1064, 851; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.88 (dd, *J* = 8.0, 2.5 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.69-7.59 (m, 4H), 7.35-7.32 (m, 1H), 6.95(d, *J* = 9 Hz, 3 H), 5.34 (s, 1H), 4.87 (d, *J* = 2.0 Hz, 1H), 4.48 (d, *J* = 2.0 Hz, 1H), 4.26 (t, *J* = 2.5 Hz, 2H), 3.52 (s, 1H), 2.74 (s, 6H), 2.58 (t, *J* = 2.5 Hz, 2H), 2.12 (q, *J* = 7.5, 1.5 Hz, 2H,), 1.04 (t, *J* = 7.0 Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 163.14, 161.127, 159.41, 157.88, 156.62, 140.112, 139.53, 136.28, 133.63, 131.54, 130.78, 129.62, 129.30, 124.37, 123.13, 116.12, 115.11, 73.13, 68.13, 62.15, 52.12, 47.45, 27.45, 14.10; HRMS (ES-TOF) calcd for $C_{28}H_{30}BrNO_3$ 507.1409, found 507.1407.

(E)-5-chloro-3-(4-(2-(dimethylamino)ethoxy)phenyl)-1-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**4ac**)

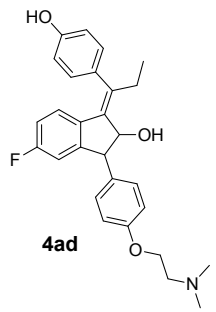


**4ac**

Yellow semi solid; Yield: 52%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3408 (OH str), 2917 (aromatic C-H str), 1589 (aromatic, C=C str), 1489, 1415, 1288, 1177, 1091, 1014, 929 and 701; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.88 (t, *J* = 8 Hz, 2H), 7.85 (t, *J* = 8 Hz, 2H), 7.88 -7.81 (m, 3H), 7.79 – 7.61 (m, 4H), 7.59 – 7.32 (m, 1H), 6.94 (d, *J* = 8.0 Hz, 3H), 5.34 (s, 1H), 4.87 (d, *J* = 2.0 Hz, 1H), 4.48 (d, *J* = 2.0 Hz, 1H), 4.26 (t, *J* = 2.5 Hz, 2H), 3.52 (s, 1H), 2.74 (s, 6H), 2.58 (t, *J* = 2.5 Hz, 2H), 2.12 (q, *J* = 7.5, 1.5 Hz, 1H), 1.04 (t, *J* = 7.0 Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ

(ppm): 160.07, 159.62, 144.00, 143.57, 137.30, 136.65, 133.00, 130.92, 129.62, 129.29, 128.66, 128.07, 122.30, 117.13, 116.93, 73.13, 66.26, 61.16, 51.79, 46.79, 31.19, 14.92; HRMS (ES-TOF) calcd for $C_{28}H_{30}ClNO_3$ 463.1914, found 463.1915.

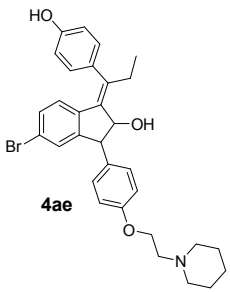
(E)-3-(4-(2-(dimethylamino)ethoxy)phenyl)-5-fluoro-1-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**4ad**)



**4ad**

Light yellow semi solid; Yield:52%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3393 (OH str), 2953 (aromatic C-H str), 1575 (aromatic, C=C str), 1464, 1403, 1275, 1152, 1081, 1002, 911 and 725; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.91 – 7.64 (m, 3H), 7.63 - 7.51 (m, 3H), 7.37 – 7.33 (m, 2H), 7.32 – 7.21 (m, 3H), 5.75 (s, 1H), 4.79 (d, *J* = 2.0 Hz, 1H), 4.18 (d, *J* = 2.0 Hz, 1H), 4.07 (d, *J* = 2.5 Hz, 2H), 3.6 (s, 1H), 3.12 (s, 6H), 2.50 (t, *J* = 2.5 Hz, 2H), 2.32(q, *J* = 8.5, 1.5 Hz, 2H), 1.17 (t, *J* = 7.0, Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 163.14, 161.12, 159.41, 157.87, 156.62, 140.11, 139.52, 136.27, 133.62, 131.54, 130.77, 129.62, 129.30, 124.36, 123.12, 116.12, 115.10, 73.13, 68.12, 62.14, 52.81, 47.45, 27.45, 14.10; HRMS (ES-TOF) calcd for $C_{28}H_{30}FNO_3$ 447.2210, found 447.2209.

(E)-5-bromo-1-(1-(4-hydroxyphenyl)propylidene)-3-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-2,3-dihydro-1H-inden-2-ol (**4ae**)

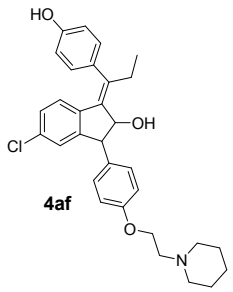


**4ae**

Yellow semi solid; Yield: 55%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3359 (OH str), 2957 (aromatic C-H str), 1572 (aromatic, C=C str), 1458, 1412, 1278, 1156, 1088, 1013, 915 and 732; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.03 (d, *J* = 8.0 Hz, 3H), 7.82 (d, *J* = 7.0 Hz, 2H), 7.76 (dd, *J* = 2.0, 7.0 Hz, 4H), 7.49 ( d, *J* = 9.0 Hz, 1H),7.12 (t, *J* = 7.5 Hz, 3H), 5.56 (s, 1H), 4.75 (d, *J* = 2.0 Hz, 1H), 4.36 (d, *J* = 2.0 Hz, 1H), 4.14 (t, *J* = 2.5 Hz, 2H), 3.75 (s, 1H), 3.05(t, *J* = 2.5, 2H), 2.65(t, *J* = 3.0 Hz, 4H), 2.33 (q, *J* = 1.5, 9.0 Hz, 2H), 1.64-1.61 (m, 2 H), 1.51 (t, , *J* = 2.5 Hz, 2H ),

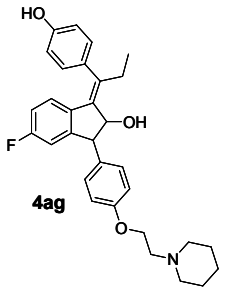
1.02 (t, , $J$ = 8.0 Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 161.13, 157.13, 156.41, 142.62, 140.10, 139.54, 136.27, 133.63, 131.54, 130.78, 129.62, 129.30, 122.37, 122.13, 116.19, 115.19, 73.13, 69.15, 58.10, 57.45, 52.81, 29.17, 25.14, 23.10, 12.56; HRMS (ES-TOF) calcd for $C_{31}H_{34}BrNO_3$ 547.1722, found 547.1724.

(E)-5-chloro-1-(1-(4-hydroxyphenyl)propylidene)-3-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-2,3-dihydro-1H-inden-2-ol (**4af**)




Brown semi solid; Yield: 55%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3419 (OH str), 2933, 2879 (aromatic C-H str), 1598 (aromatic, C=C str), 1262, 1083, 862, 739; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.96 (t, $J$ = 9.0 Hz, 2H), 7.55-7.47 (m, 4H), 7.45-7.39 (m, 3H), 6.99-6.97 (m, 2H), 5.77 (s, 1H), 4.64 (d, $J$ = 2.0 Hz, 1H), 4.21 (d, $J$ = 2.0 Hz, 1H), 4.04 (t, $J$ = 2.5 Hz, 2H), 3.75 (s, 1 H), 2.95 (t, $J$ = 2.5 Hz, 2H), 2.58 (t, $J$ = 2.5 Hz, 4H), 2.35 (q, $J$ = 7.0, 1.5 Hz, 2H), 1.48 (t, $J$ = 2.5 Hz, 4H ), 1.01 (t, $J$ = 7.5 Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 160.12, 158.41, 144.87, 144.62, 140.10, 139.54, 136.27, 133.63, 131.54, 130.78, 129.62, 124.37, 124.13, 117.69, 117.19, 73.15, 69.13, 58.10, 57.45, 52.81, 27.17, 25.14, 23.10, 13.13; HRMS (ES-TOF) calcd for $C_{31}H_{34}ClNO_3$ 503.2227, found 503.2227.

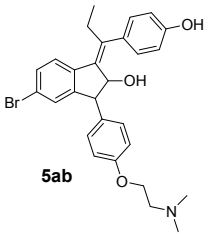
(E)-5-fluoro-1-(1-(4-hydroxyphenyl)propylidene)-3-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-2,3-dihydro-1H-inden-2-ol (**4ag**)




Yellow semi solid; Yield: 52%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3438 (OH str), 2953, 2882 (aromatic C-H str), 1609 (aromatic, C=C str), 1271, 1107, 846, 729; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 8.02 (d, $J$ = 8.0 Hz, 2H), 7.77 (t, $J$ = 7.0 Hz, 2H), 7.61 (t, $J$ = 7.0 Hz, 3H), 7.48 (d, $J$ = 8.0 Hz, 1H), 7.13 (t, $J$ = 8.0 Hz, 3H), 5.55 (s, 1H), 4.74 (d, $J$ = 2.0 Hz, 1H), 4.36 (d, $J$ = 2.0 Hz, 1H), 4.14 (t, $J$ = 2.5 Hz, 2H), 3.75 (s, 1H), 3.048 (t, $J$ = 2.5 Hz, 2H), 2.65 (t, $J$ = 2.5 Hz, 4H), 2.33 (q, $J$ = 2.5, 7.5 Hz, 2H), 1.65 – 161 (m, 2H), 1.51 (t, $J$ = 2.5 Hz, 4H), 1.02 (t, $J$ = 8.0 Hz, 3H); $^{13}$C-

($CDCl_3$, 125 MHz) δ (ppm): 161.12, 157.12, 156.41, 142.62, 140.10, 139.54, 136.27, 133.63, 131.54, 130.78, 129.62, 129.30, 122.37, 122.13, 116.19, 115.19, 73.13, 69.15, 58.10, 57.45, 52.81,27.17, 25.14, 23.10, 12.55; HRMS (ES-TOF) calcd for $C_{31}H_{34}FNO_3$ 487.2523, found 487.2524.

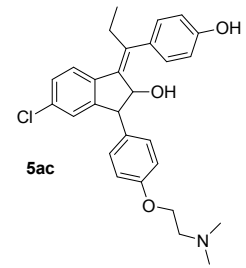
(Z)-5-bromo-3-(4-(2-(dimethylamino)ethoxy)phenyl)-1-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**5ab**)



**5ab**

Brown semi solid; Yield: 8%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3415 (OH str), 2934, 2875 (aromatic C-H str), 1599 (aromatic, C=C str), 1267, 1085, 865, 635; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.89-7.69 (m, 4H), 7.55-7.48 (m, 2H), 6.97-6.81(m, 5H), 4.69 (d, *J* = 2.5 Hz, 2H), 4.28 (d, *J* = 2.5 Hz, 2H), 4.27 (t, *J* = 2.5 Hz, 2H), 2.93 (s, 6H), 2.87 (t, *J* = 2.5 Hz, 2H), 1.78 (q, *J* = 8.0, 2.5 Hz, 2H), 0.67 (t, *J* = 7 Hz, 3H ); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 163.14, 161.22, 159.42, 157.87, 156.62, 140.12, 139.53, 136.27, 133.63, 132.54, 130.77, 129.62, 129.30, 124.37, 123.13, 116.12, 115.10, 71.14, 66.13, 60.13, 50.17, 46.45, 25.45, 12.20; HRMS (ES-TOF) calcd for $C_{28}H_{30}BrNO_3$ 507.1409, found 507.1407.

(Z)-5-chloro-3-(4-(2-(dimethylamino)ethoxy)phenyl)-1-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol **(5ac)**

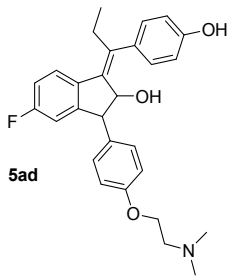


**5ac**

Brown semi solid; Yield: 10%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3451 (OH str), 2955 (aromatic C-H str), 1584 (aromatic, C=C str), 1387, 1275, 1062, 855, 725 (C-Cl, str); $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.90 -7.85 (m, 2H), 7.54 – 7.59 (m, 2H), 7.10 – 7.03 (m, 3H), 7.00- 6.93 (m, 4H), 5.52 (s, 1H), 4.52 (d, *J* = 2.0 Hz, 1H), 4.18 (d, *J* = 2.0 Hz, 1H), 4.06 (t, *J* = 2.5 Hz, 2H), 3.50 (s, 1H), 2.86 (s, 6H), 2.63 (t, *J* = 2.5 Hz, 2 H), 1.67 (q, *J* = 1.5, 7.5 Hz, 2H), 0.67 (t, *J* = 6.5 Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 160.12, 159.62, 159.29, 144.01, 143.62, 137.12, 136.65, 133.09,

130.92, 129.87, 129.29, 128.66, 128.07, 122.30, 117.29, 116.93, 72.33, 65.26, 61.17, 51.76, 45.69, 26.31, 11.92; HRMS (ES-TOF) calcd for $C_{28}H_{30}ClNO_3$ 463.1914, found 463.1912.

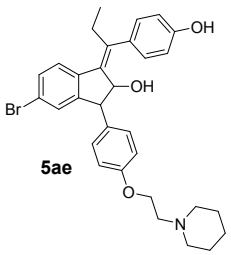
(Z)-3-(4-(2-(dimethylamino)ethoxy)phenyl)-5-fluoro-1-(1-(4-hydroxyphenyl)propylidene)-2,3-dihydro-1H-inden-2-ol (**5ad**)



**5ad**

Brown semi solid; Yield: 9%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3382 (OH str), 2992, 2886 (aromatic C-H str), 1620 (aromatic, C=C str), 1262, 1095, 860, 743; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.91 – 7.71 (m, 4H), 7.70-7.42 (m, 4H), 6.96 (t, *J* = 8.5 Hz, 1H), 6.86 (t, *J* = 8.5 Hz, 2H), 5.29 (s, 1H), 4.50 (d, *J* = 2.0 Hz, 1H), 4.18 (d, *J* = 2.0 Hz, 1H), 4.03 (t, *J* = 2.5 Hz, 2H), 3.39 (s, 1H), 2.78 (s, 6H), 2.66 (t, *J* = 2.5 Hz, 2H), 1.78 (q, *J* = 2.5, 6.0 Hz, 2H), 0.68 (t, *J* = 6.5 Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm):163.14, 161.12, 159.41, 157.87, 156.62, 140.11, 139.52, 136.27, 133.62, 131.54, 130.77, 129.62, 129.30, 124.36, 123.12, 116.17, 115.10, 71.13, 66.12, 60.13, 50.17, 46.45, 25.45, 12.10; HRMS (ES-TOF) calcd for $C_{28}H_{30}FNO_3$ 447.2210, found 447.2209..

(Z)-5-bromo-1-(1-(4-hydroxyphenyl)propylidene)-3-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-2,3-dihydro-1H-inden-2-ol (**5ae**)

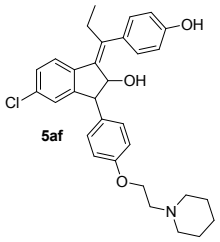


**5ae**

Light yellow semi solid; Yield:10 %; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3444 (OH str), 2922 (aromatic C-H str), 1595 (aromatic, C=C str), 1418, 1328, 1235, 1129(C-O-C, str), 1091; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.91-7.86 (m, 3H), 7.71-7.51 (m, 1H), 7.49-7.26 (t, *J* = 8.0 Hz, 4H), 7.12-6.85 (m, 4H), 5.59(s, 1H), 4.59 (d, *J* = 2.0 Hz, 1H), 4.18 (d, *J* = 2.0 Hz, 1H), 2.98 (t, *J* = 2.5 Hz, 2H), 2.87(t, *J* = 2.5 Hz, 4H), 4.02 (t, *J* = 2.5 Hz, 2H), 1.87 (q, *J* = 1.5, 8.0 Hz, 2H), 1.34 (t, *J* = 2.5 Hz, 2H), 1.26 (t, *J* = 2.5 Hz, 4H), 0.78 (t, *J* = 7.0 Hz, 3H)); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 161.124, 157.13,

156.41, 142.63, 140.10, 139.54, 136.27, 133.63, 131.54, 130.77, 129.62, 129.30, 122.36, 122.12, 116.19, 115.19, 73.11, 69.15, 58.48, 57.55, 52.81, 25.25, 23.14, 21.30, 10.77; HRMS (ES-TOF) calcd for $C_{31}H_{34}BrNO_3$ 547.1722, found 547.1724.

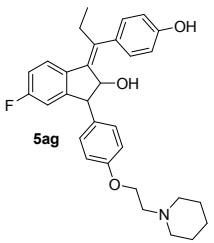
(Z)-5-chloro-1-(1-(4-hydroxyphenyl)propylidene)-3-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-2,3-dihydro-1H-inden-2-ol (**5af**)



5af

Light yellow semi solid; Yield: 8%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3431 (OH str), 2951, 2880 (aromatic C-H str), 1608 (aromatic, C=C str), 1271, 1109, 843, 729; $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.87 (t, *J* = 8.0 Hz, 3H), 7.52-7.11 (m, 3H), 7.01-6.92 (m, 5H), 5.61 (s, 1H), 4.67 (d, *J* = 2.0 Hz, 1H), 4.23 (d, *J* = 2.0 Hz, 1H), 4.11 (t, *J* = 2.5 Hz, 2H), 2.67-2.52 (m, 6 H), 1.86 (q, *J* = 8.5, 1.5 Hz, 2H), 1.49-1.25 (m, 6H), 0.68 (t, *J* = 7.0 Hz, 3H); $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 160.12, 158.41, 144.87, 144.67, 140.10, 139.54, 136.22, 133.62, 131.50, 130.77, 129.64, 129.32, 124.36, 123.12, 117.69, 117.10, 73.19, 69.13, 58.10, 57.44, 52.85, 25.67, 23.83, 21.14, 11.10; HRMS (ES-TOF) calcd for $C_{31}H_{34}ClNO_3$ 503.2227, found 503.2228.

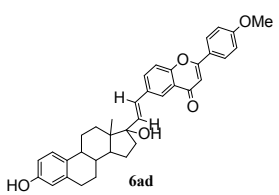
(Z)-5-fluoro-1-(1-(4-hydroxyphenyl)propylidene)-3-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-2,3-dihydro-1H-inden-2-ol (**5ag**)



5ag

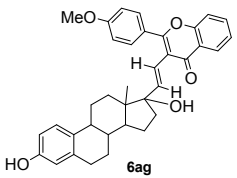
Light yellow semi solid; Yield: 10%; IR $\nu_{max}$ (KBr, $cm^{-1}$): 3440 (OH str), 2920 (aromatic C-H str), 1592 (aromatic, C=C str), 1408, 1338, 1231, 1125(C-O-C, str), 1091, 650 (C-F, str); $^1$H-NMR ($CDCl_3$, 500 MHz) δ (ppm): 7.91-7.18 (m, 3H), 7.70-7.42 (m, 4H), 6.96 (t, *J* = 8 Hz, 1H), 6.86 (t, *J* = 8.0 Hz, 3H), 5.59 (s, 1H), 4.59 (d, *J* = 2 Hz, 1H), 4.18 (d, *J* = 2.0 Hz, 1H), 4.03 (t, *J* = 2.5 Hz, 3H), 3.45 (s, 1H), 2.98 (t, *J*=2.5 Hz, 2H), 2.87 (t, *J* = 2.5 Hz , 4H), 1.87 (q, *J* = 8.0, 1.0 Hz, 2H), 1.34 (t, *J* = 2.5 Hz, 4H), 1.26 (t, *J* = 2.5 Hz, 4H), 0.78 (t, *J* = 7.0 Hz, 3H), $^{13}$C- ($CDCl_3$, 125 MHz) δ (ppm): 161.12, 157.13, 156.41, 142.62, 140.10, 139.54, 136.27, 133.62, 131.55, 130.77, 129.62, 129.30, 122.36, 122.12, 116.19,

115.19, 73.10, 69.14, 58.45, 57.55, 52.81, 25.25, 23.14, 21.30, 10.77; HRMS (ES-TOF) calcd for $C_{31}H_{34}FNO_3$ 487.2523, found 487.2525.



6ad

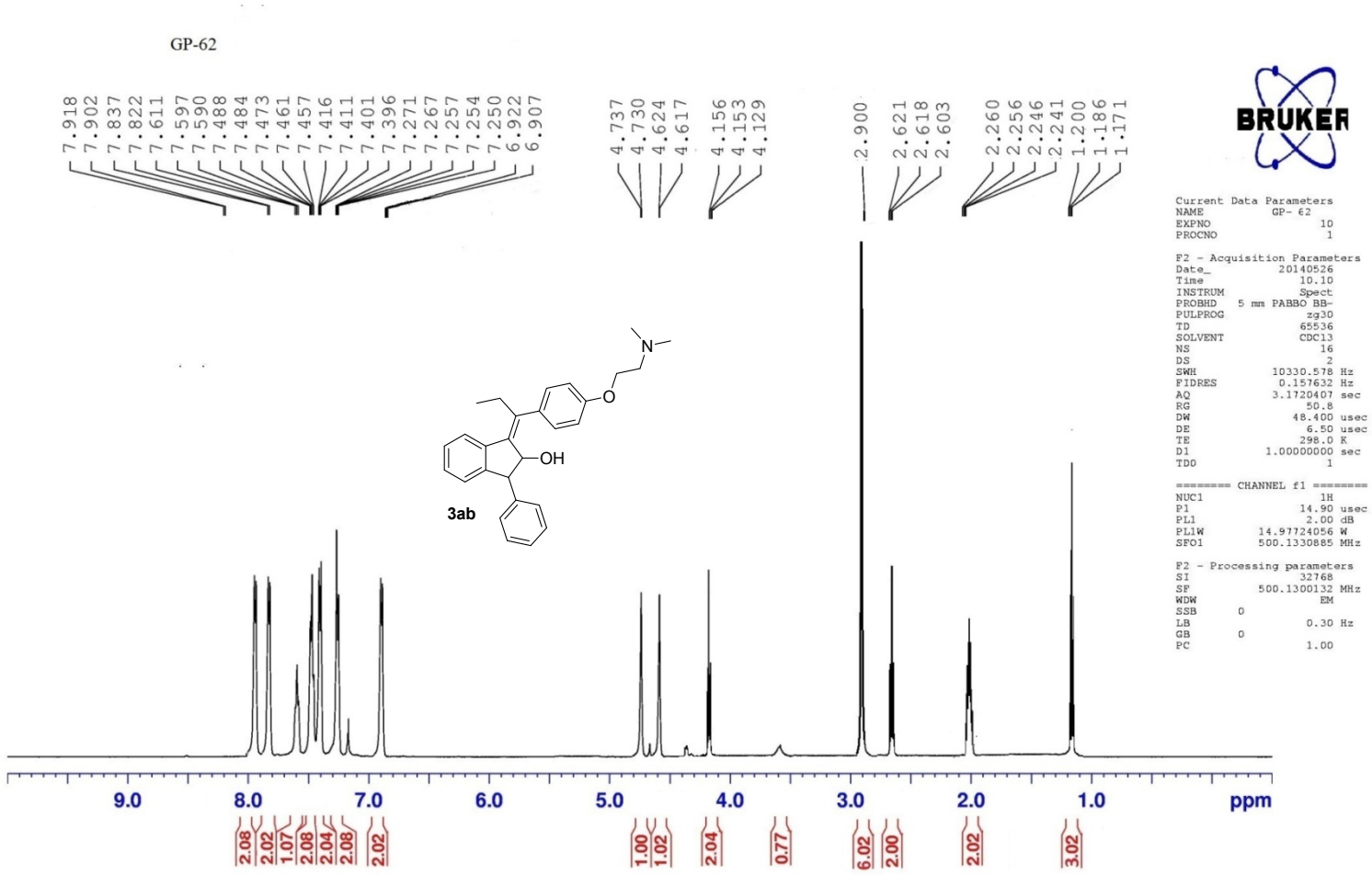
(E)-6-(2-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)vinyl)-2-(4-methoxyphenyl)-4H-chromen-4-one **(6ad):** Cream color solid, yield: 70%, $^1$H NMR($CDCl_3$, 500 MHz): 8.26 (s, 1H), 7.87 (d, J = 7Hz, 2H), 7.70 (d, J= 8.5Hz, 1H), 7.50 (d, J = 8.5Hz, 2H), 7.08 (d, J = 8.5Hz, 1H), 7.01 (d, J = 8.5Hz, 2H), 6.76 (s, 1H), 6.69-6.59 (m, 3H), 3.88 ( s, 3H), 3.70 (s, br, D2O exchangeable, 1H, OH ), 2.83-2.80 (m, 2H), 2.24-1.54 (m, 13H), 1.01 (s, 3H). HRMS: Anal calcd for $C_{36}H_{36}NaO_5$ (M+Na) 571.2460, found 571.2481.



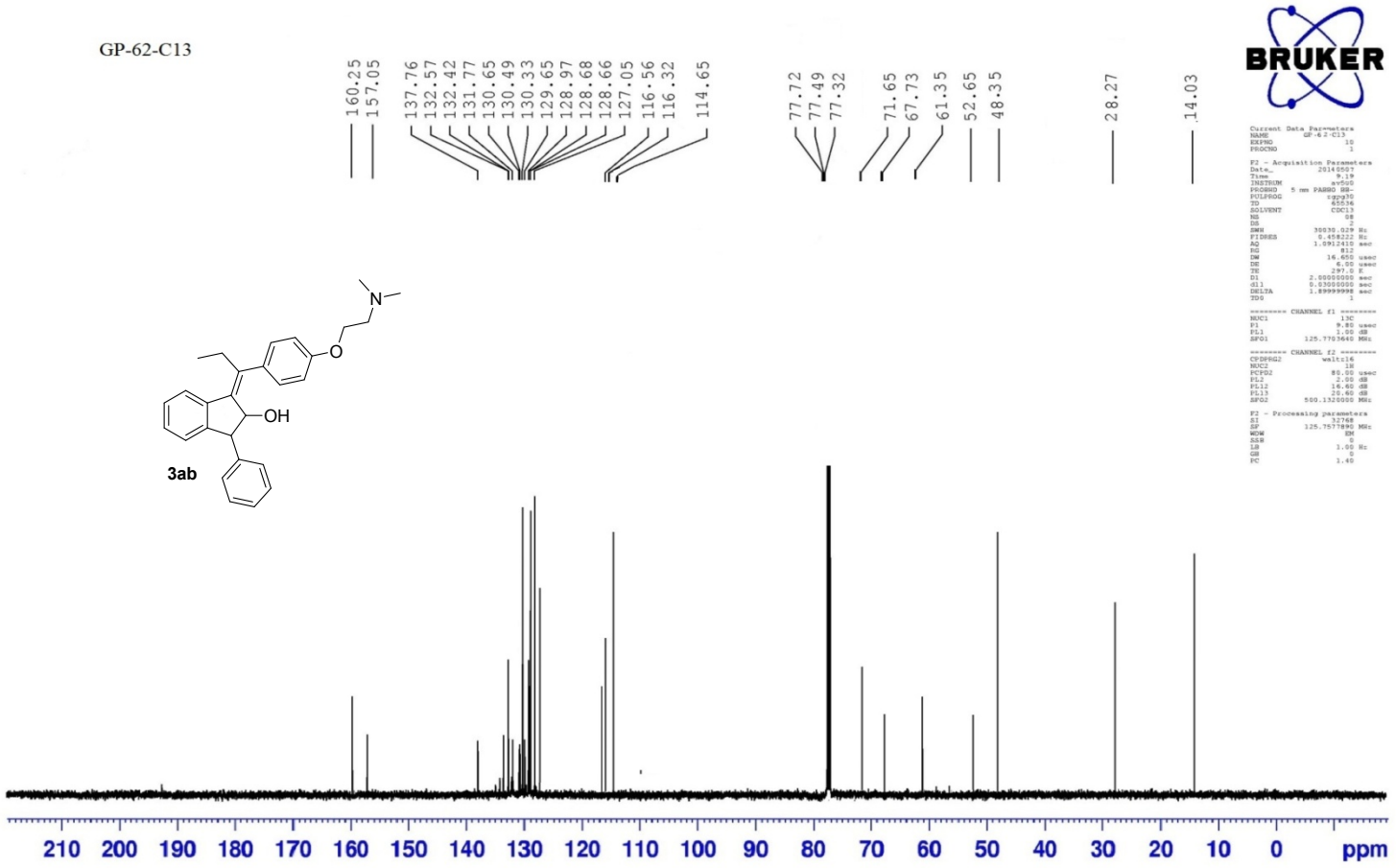
6ag

(E)-3-(2-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)vinyl)-2-(4-methoxyphenyl)-4H-chromen-4-one **(6ag):** Cream color solid, yield: 65%, $^1$H NMR($CDCl_3$, 500 MHz): 8.26 (s, 1H), 7.87 (d, J = 7Hz, 2H), 7.70 (d, J= 8.5Hz, 1H), 7.50 (d, J = 8.5Hz, 2H), 7.08 (d, J = 8.5Hz, 1H), 7.01 (d, J = 8.5Hz, 2H), 6.76 (s, 1H), 6.69-6.59 (m, 3H), 3.88 ( s, 3H), 3.70 (s, br, D2O exchangeable, 1H, OH ), 2.83-2.80 (m, 2H), 2.24-1.54 (m, 13H), 1.01 (s, 3H). IR (KBr): 3650, 3501, 1682, 1400, 1215, 1034 $cm^{-1}$. HRMS: Anal calcd for $C_{36}H_{36}NaO_5$ (M+Na) 571.2460, found 571.2481

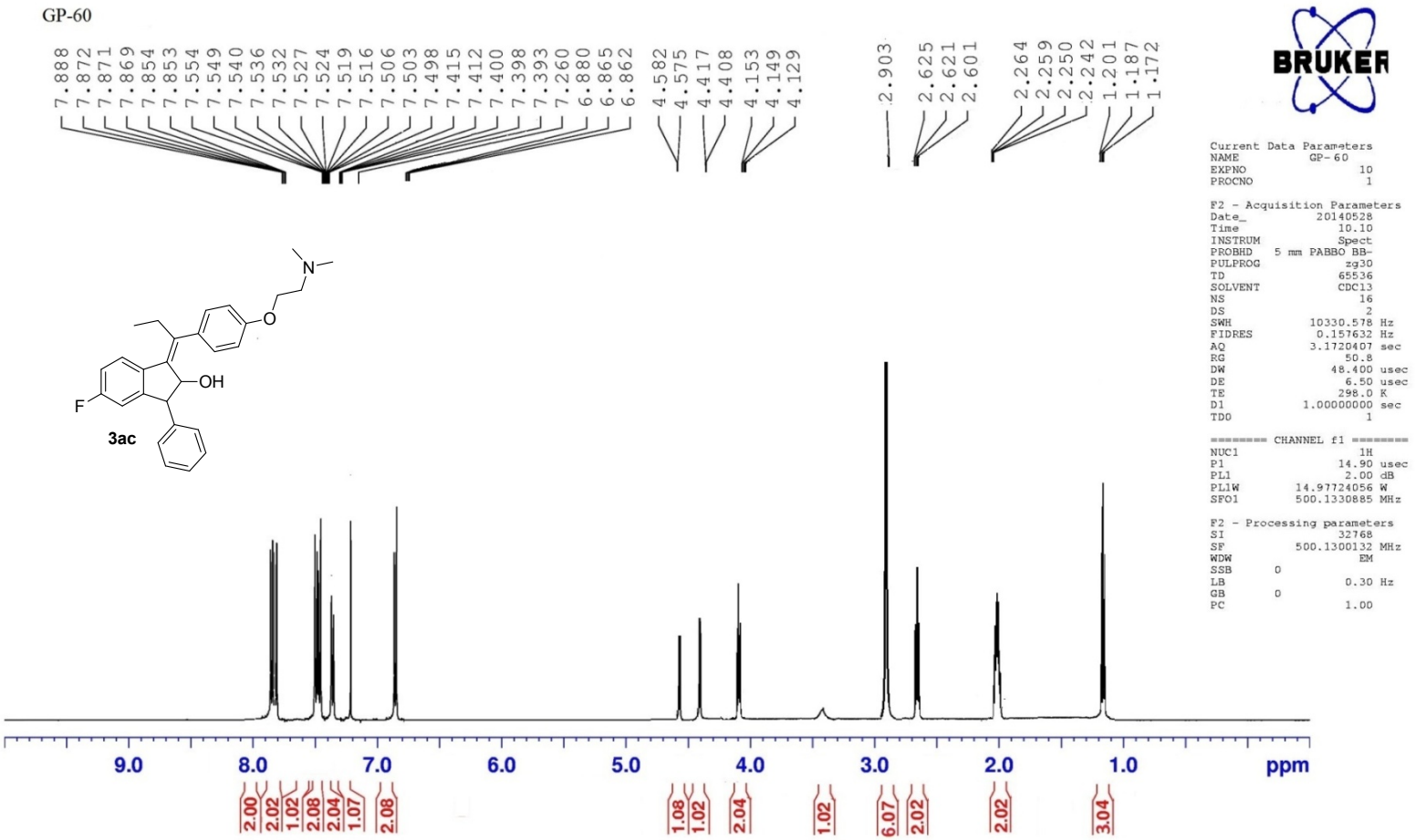
## 2. $^{1}H$ & $^{13}C$-NMR spectrum synthesized compounds



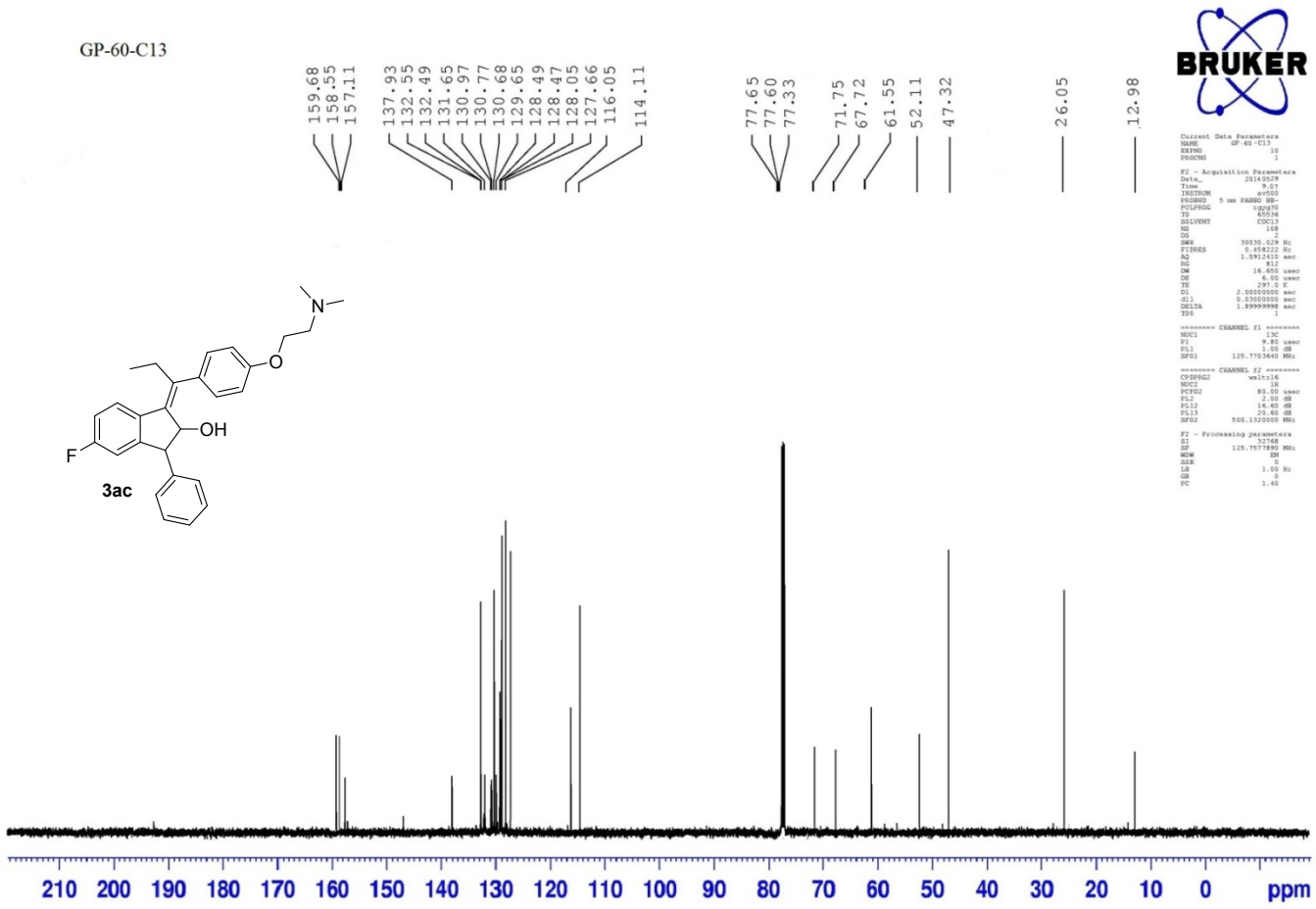
$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ab**



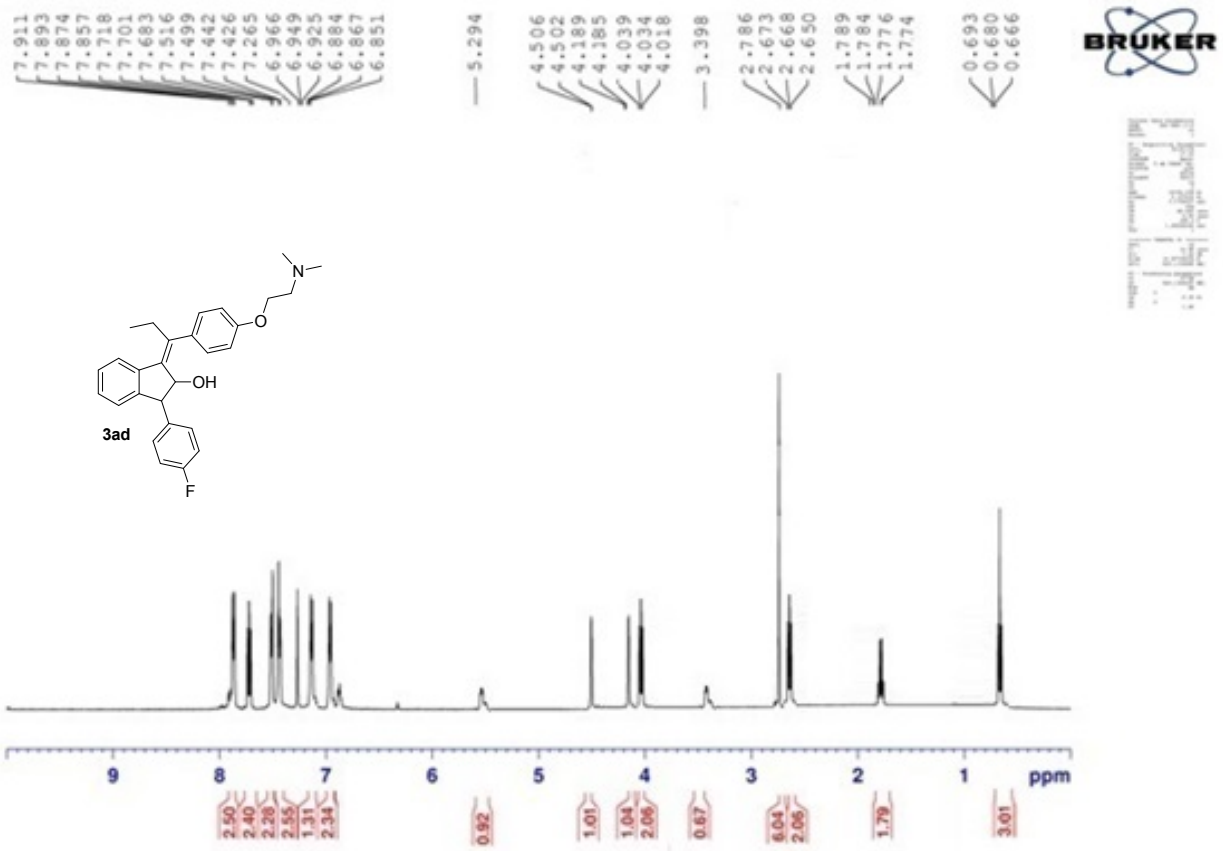

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ab**



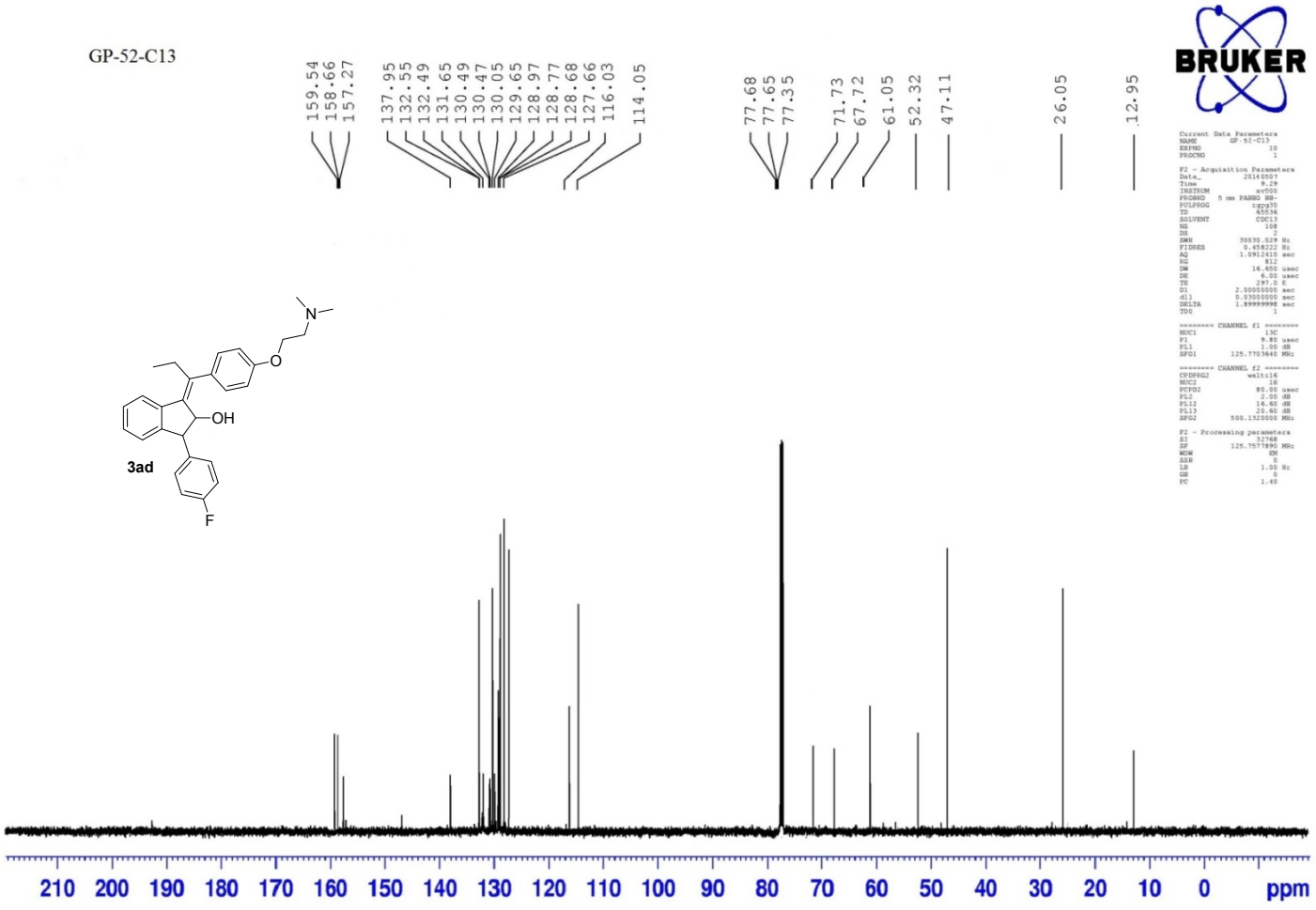

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ac**



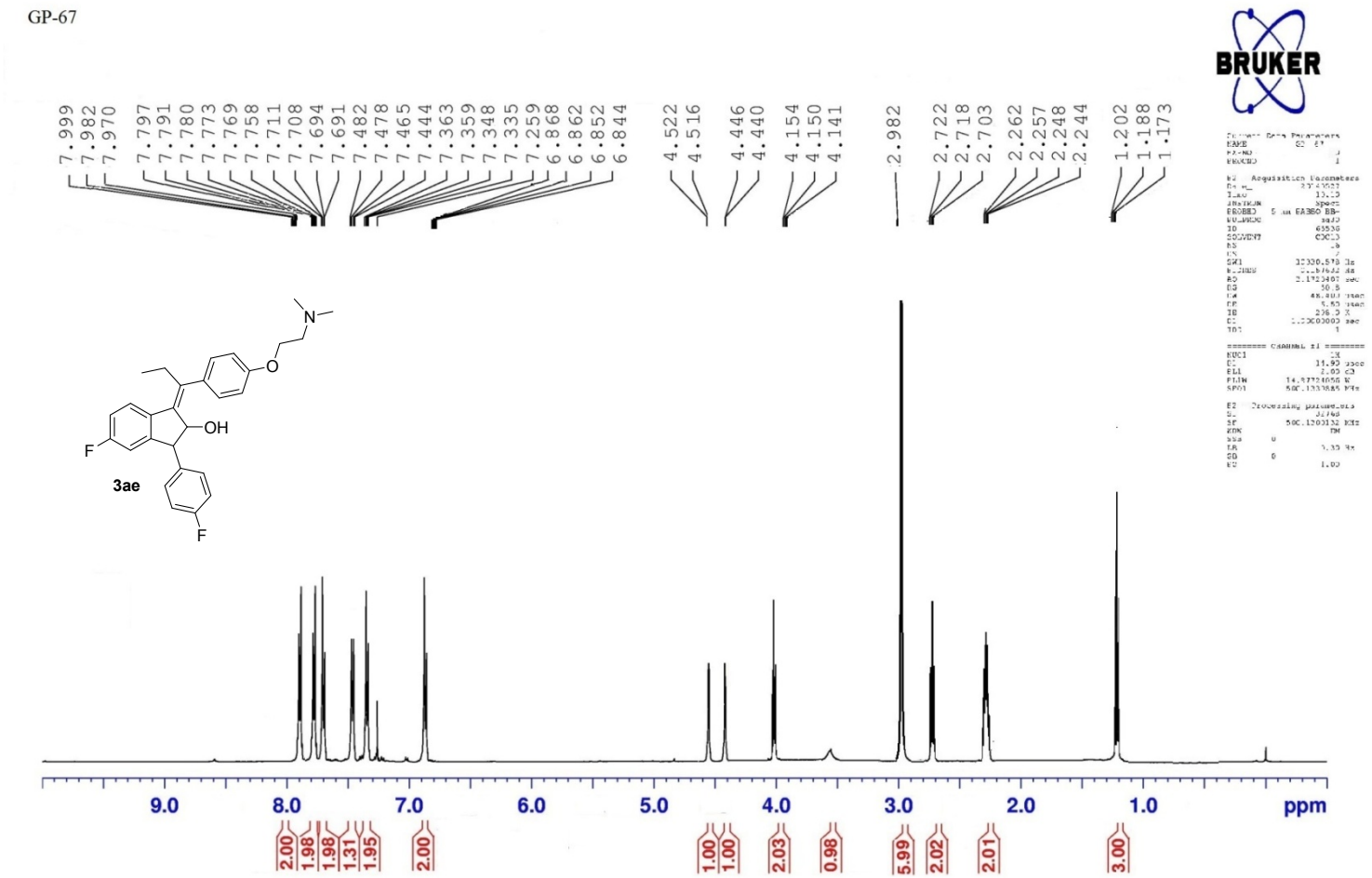

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ac**



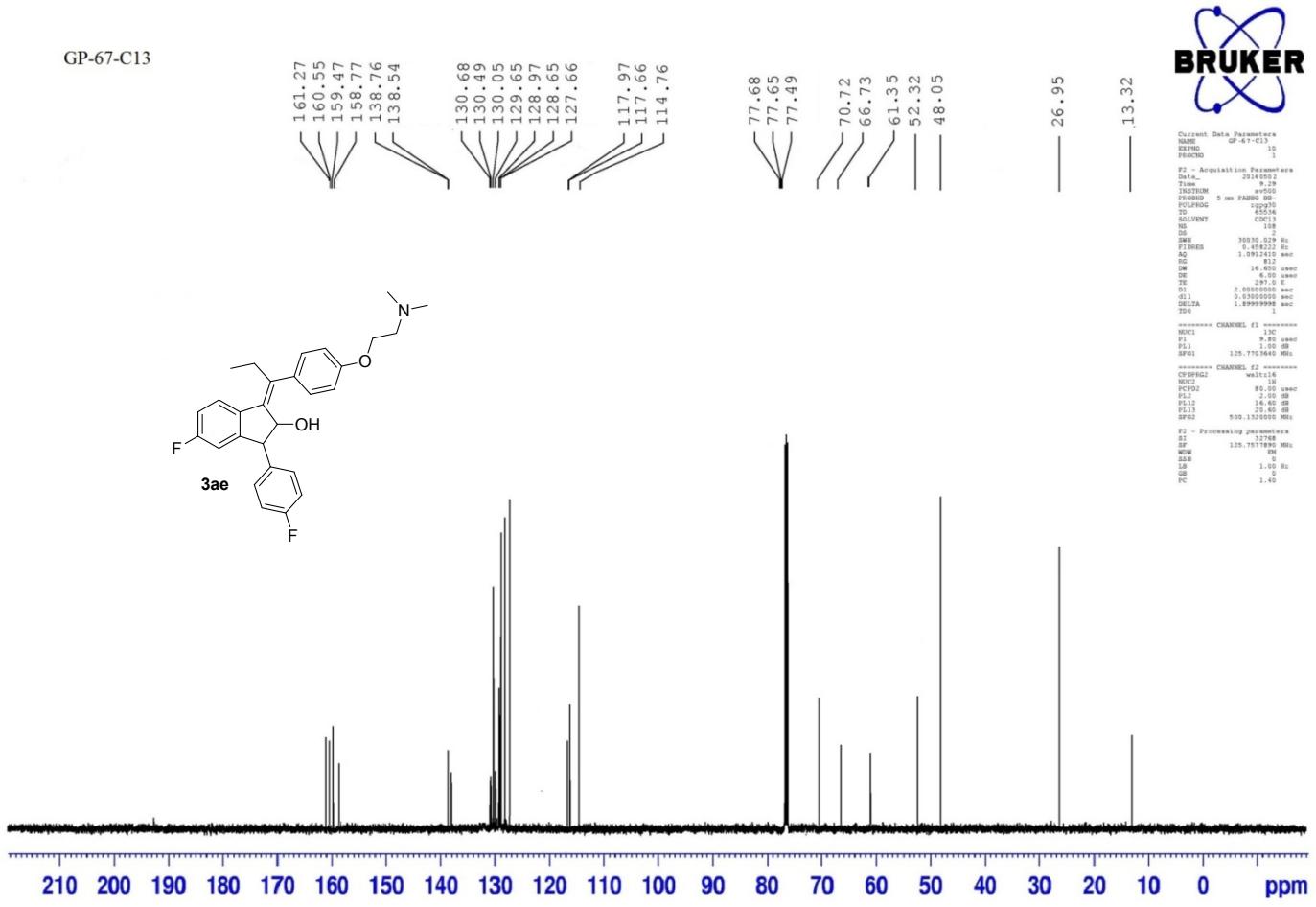

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ad**



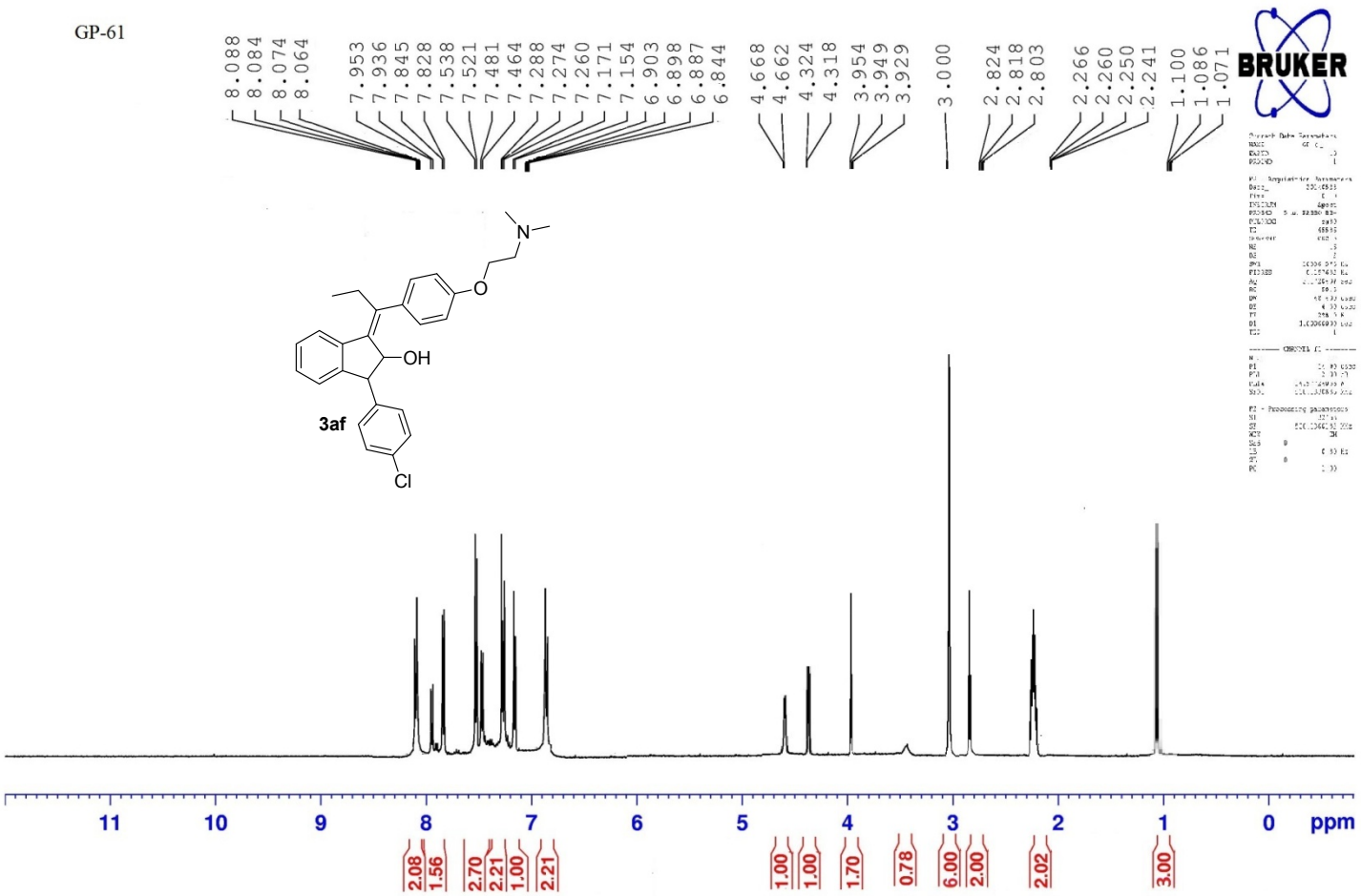

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ad**



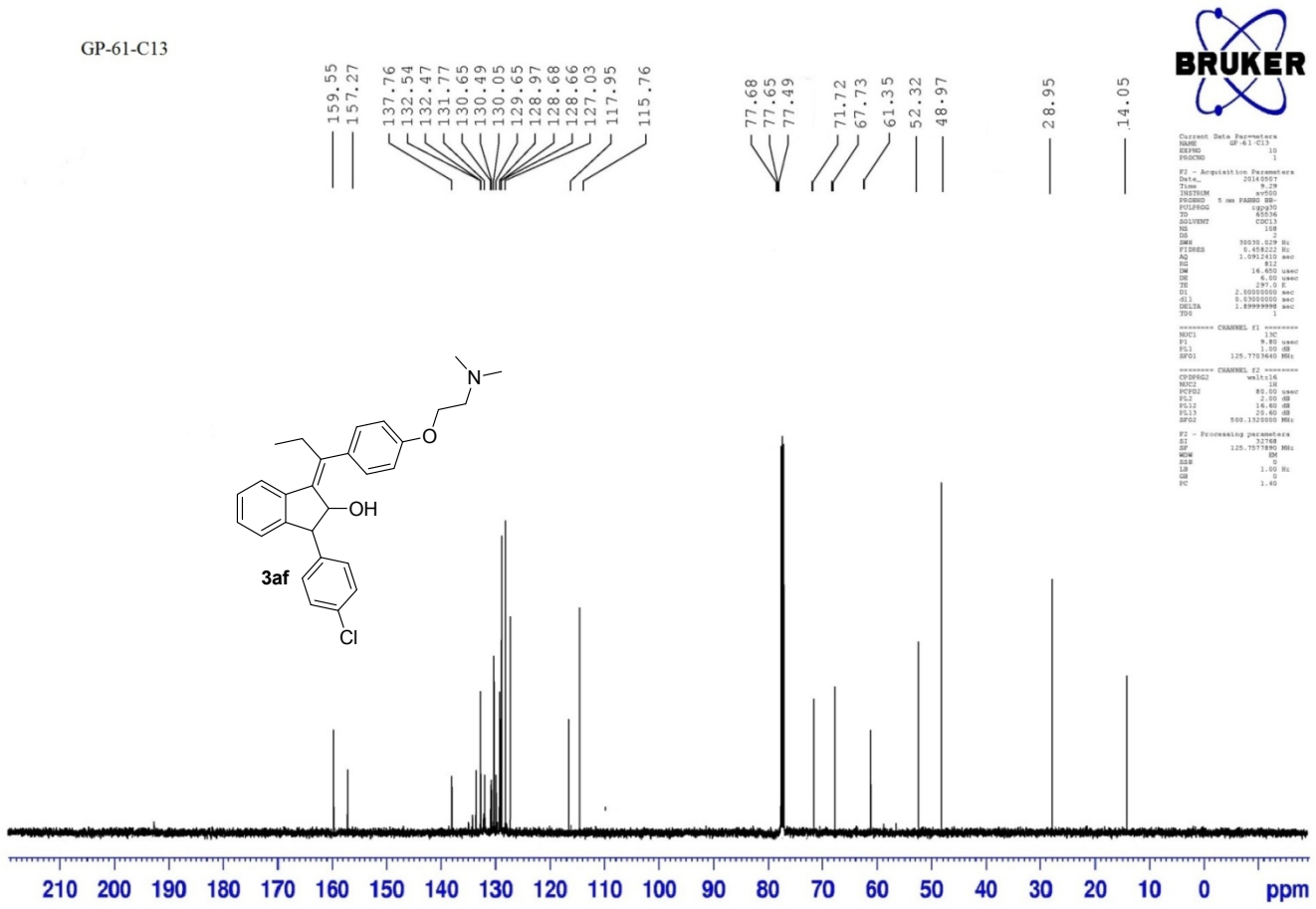

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ae**



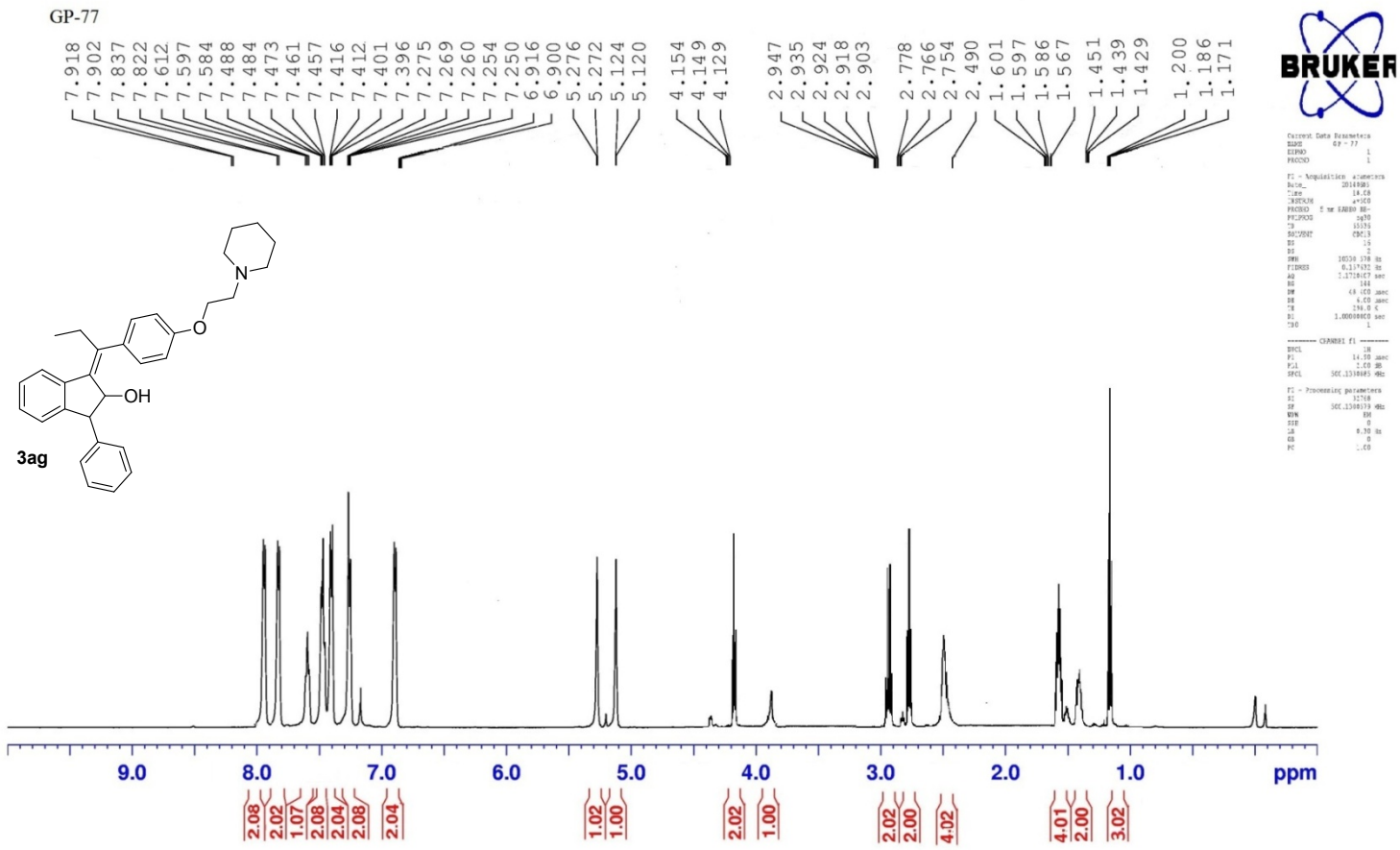

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ae**



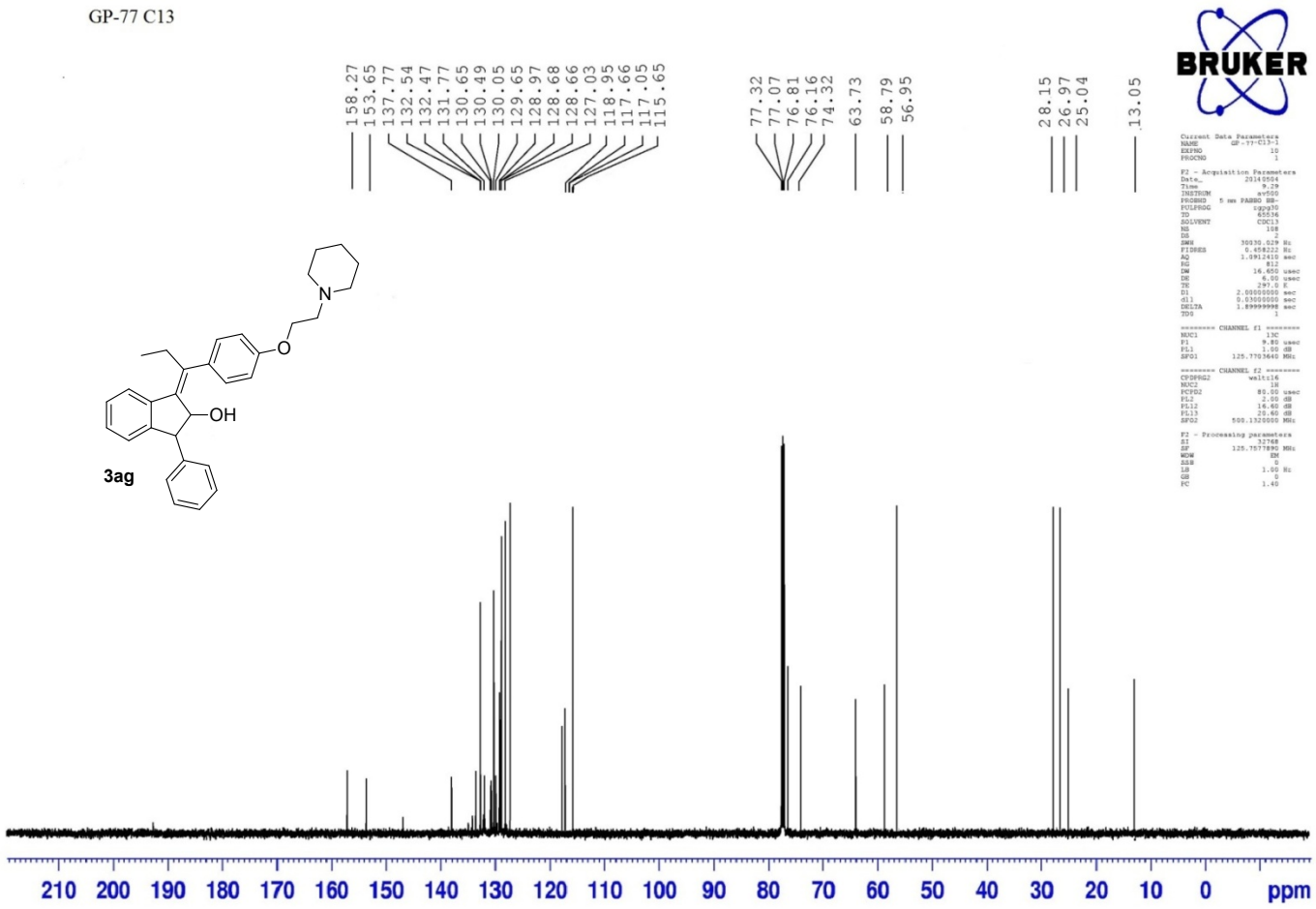

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3af**



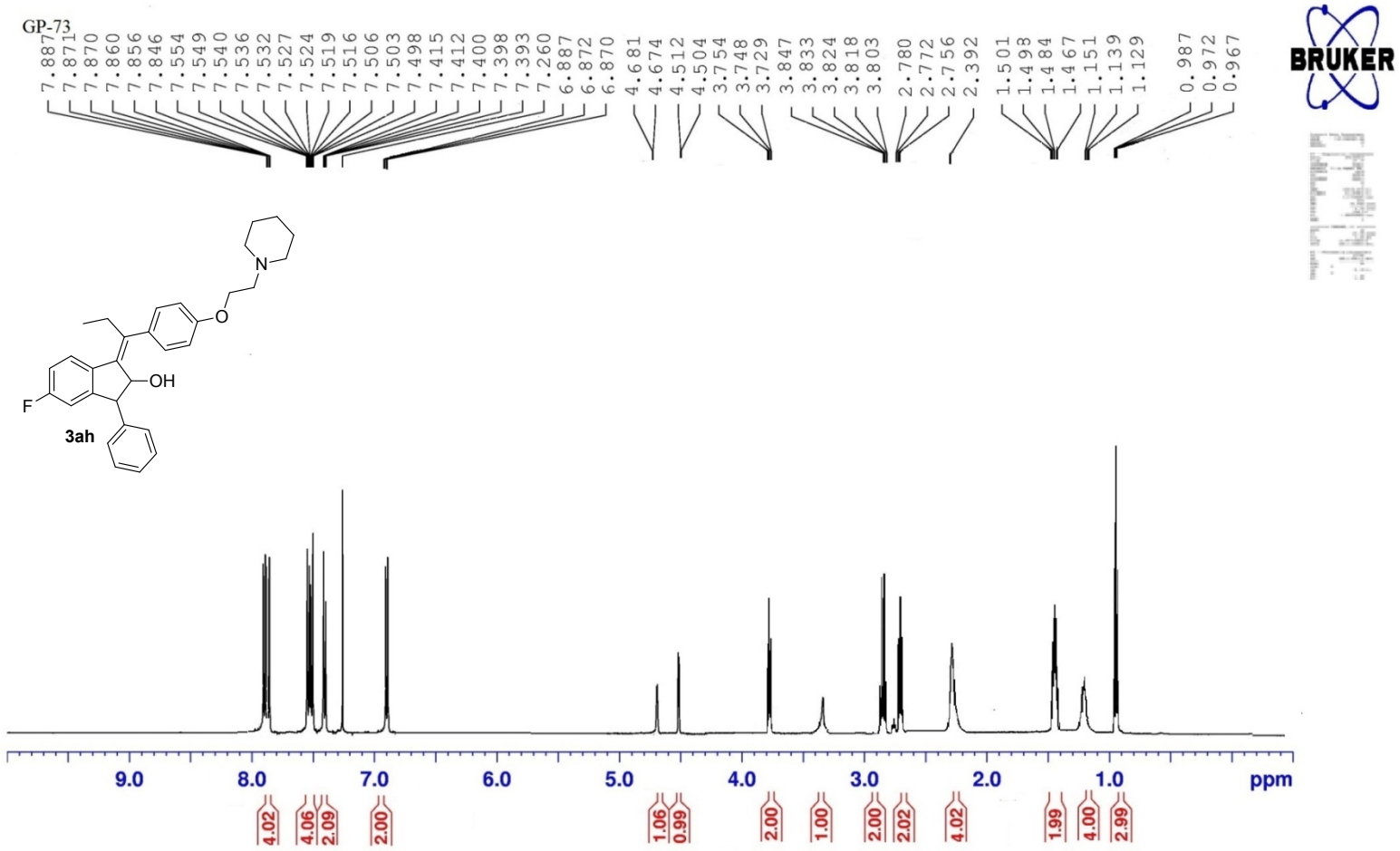

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3af**



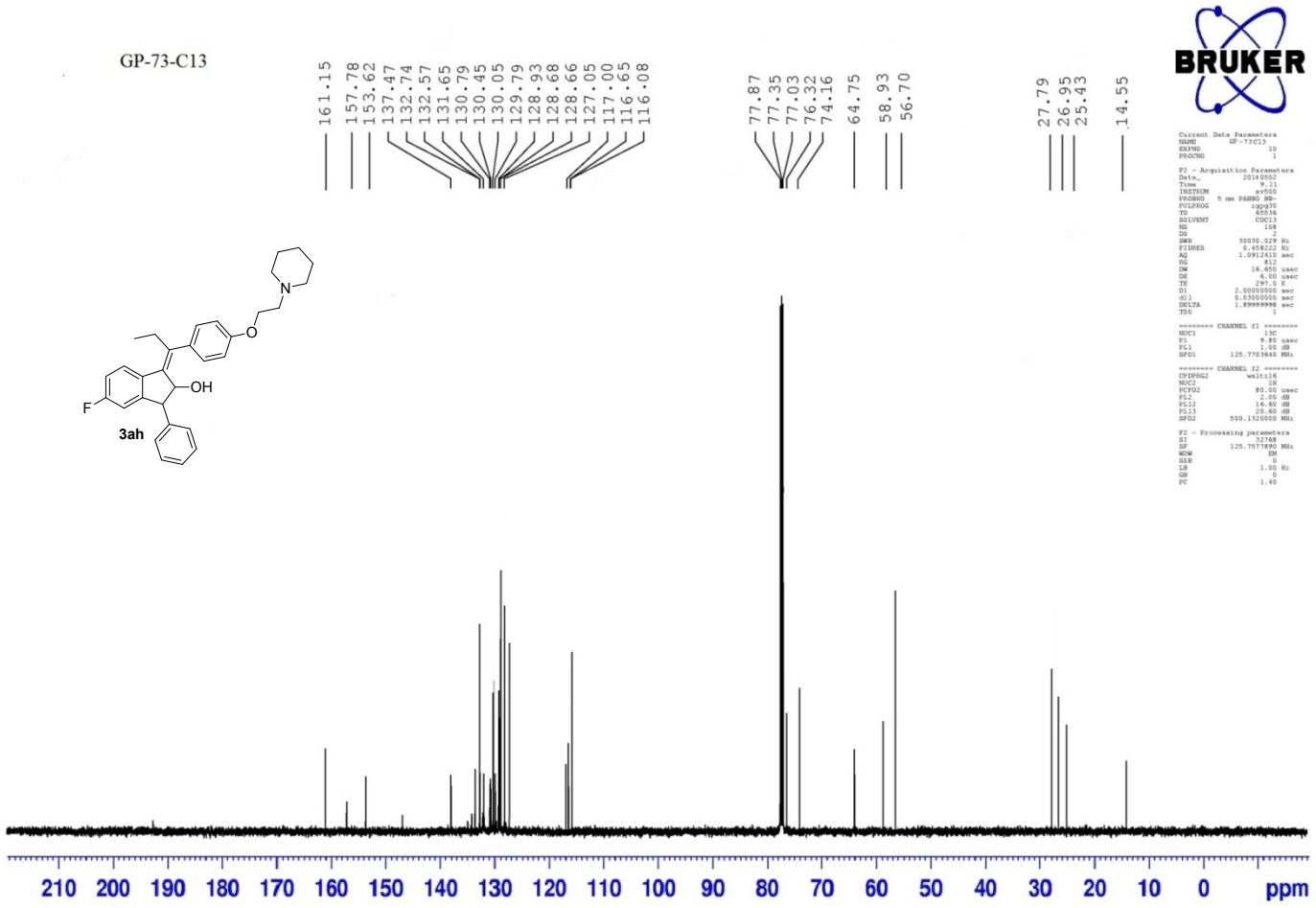

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ag**



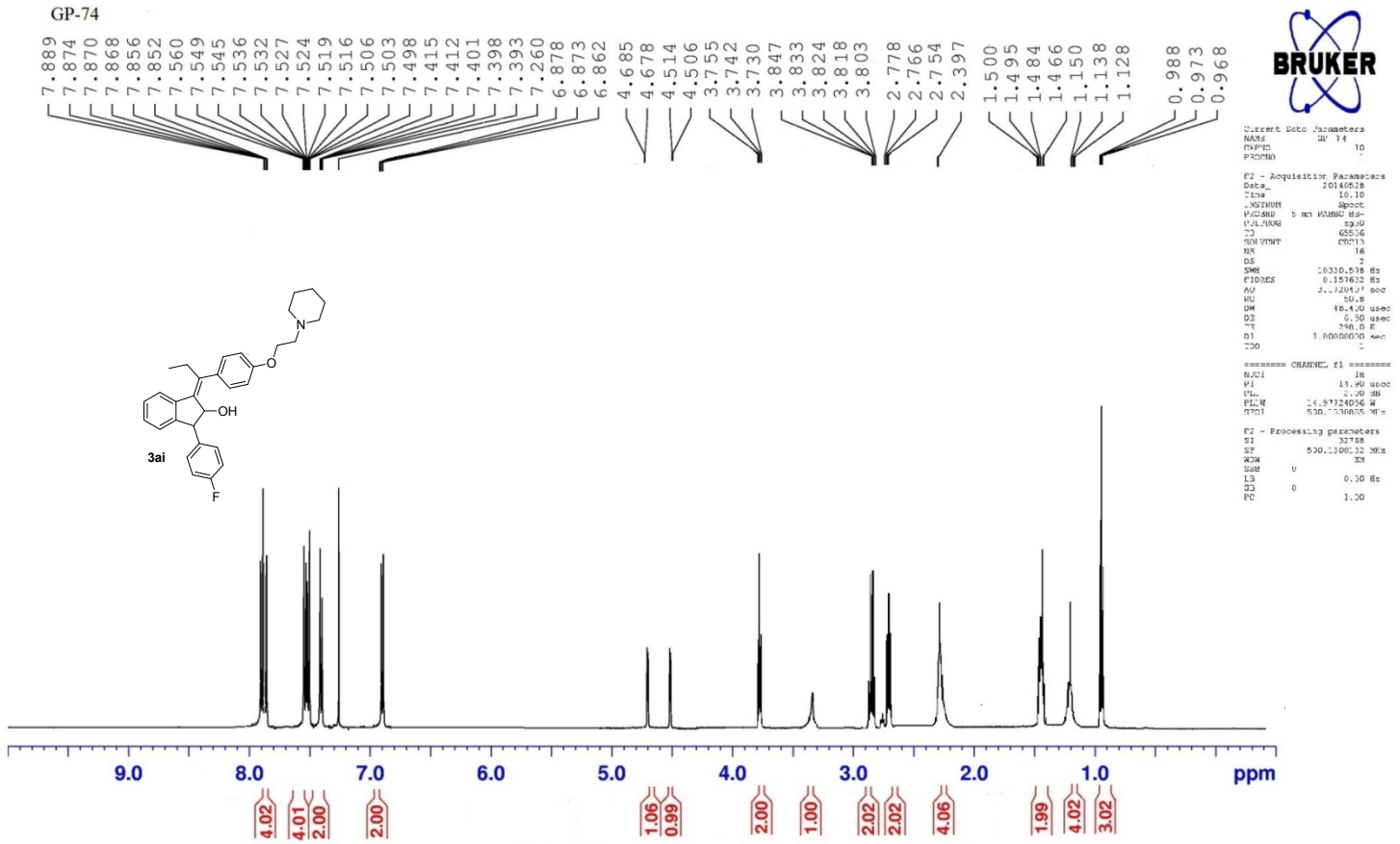

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ag**



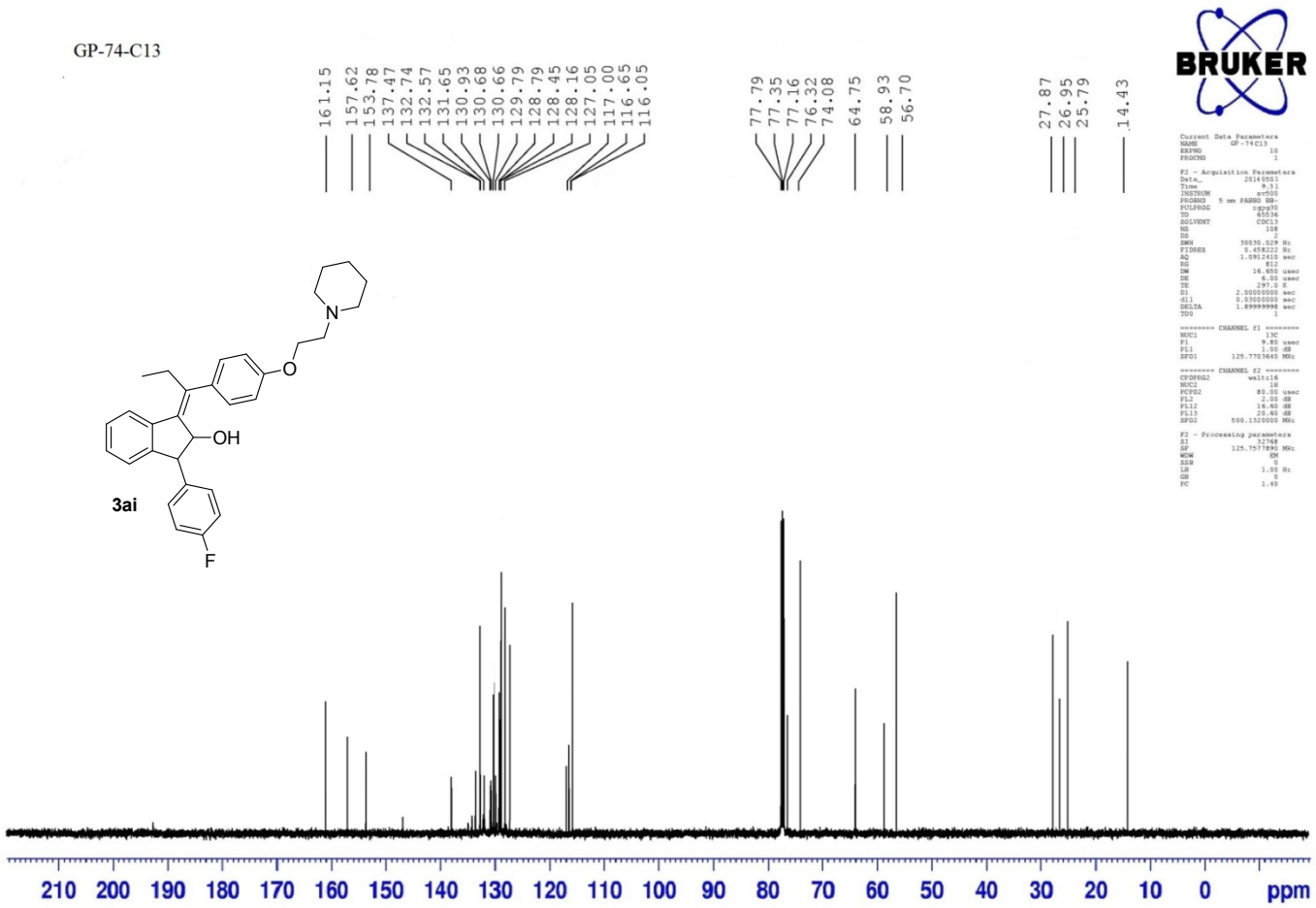

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ah**



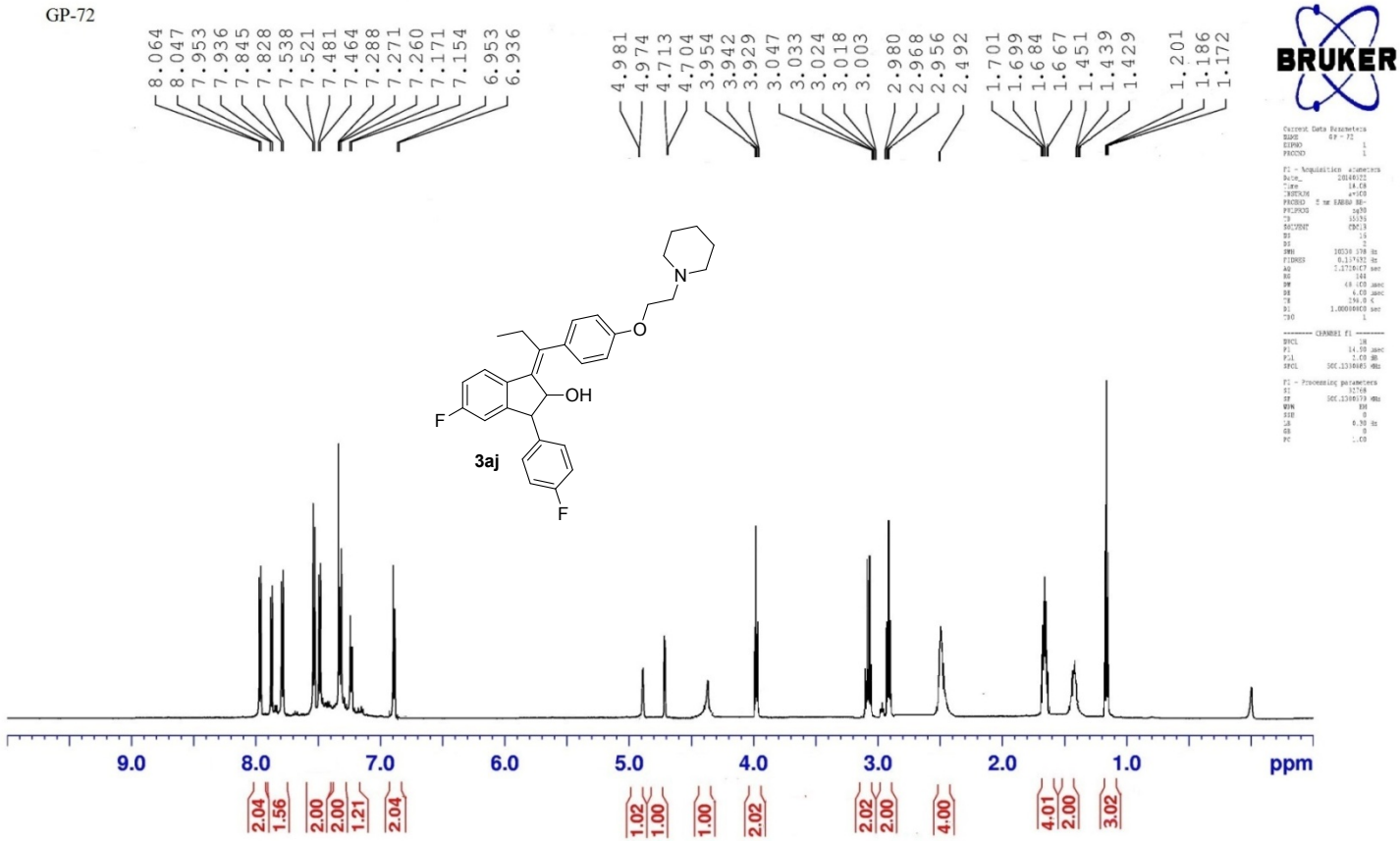

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ah**



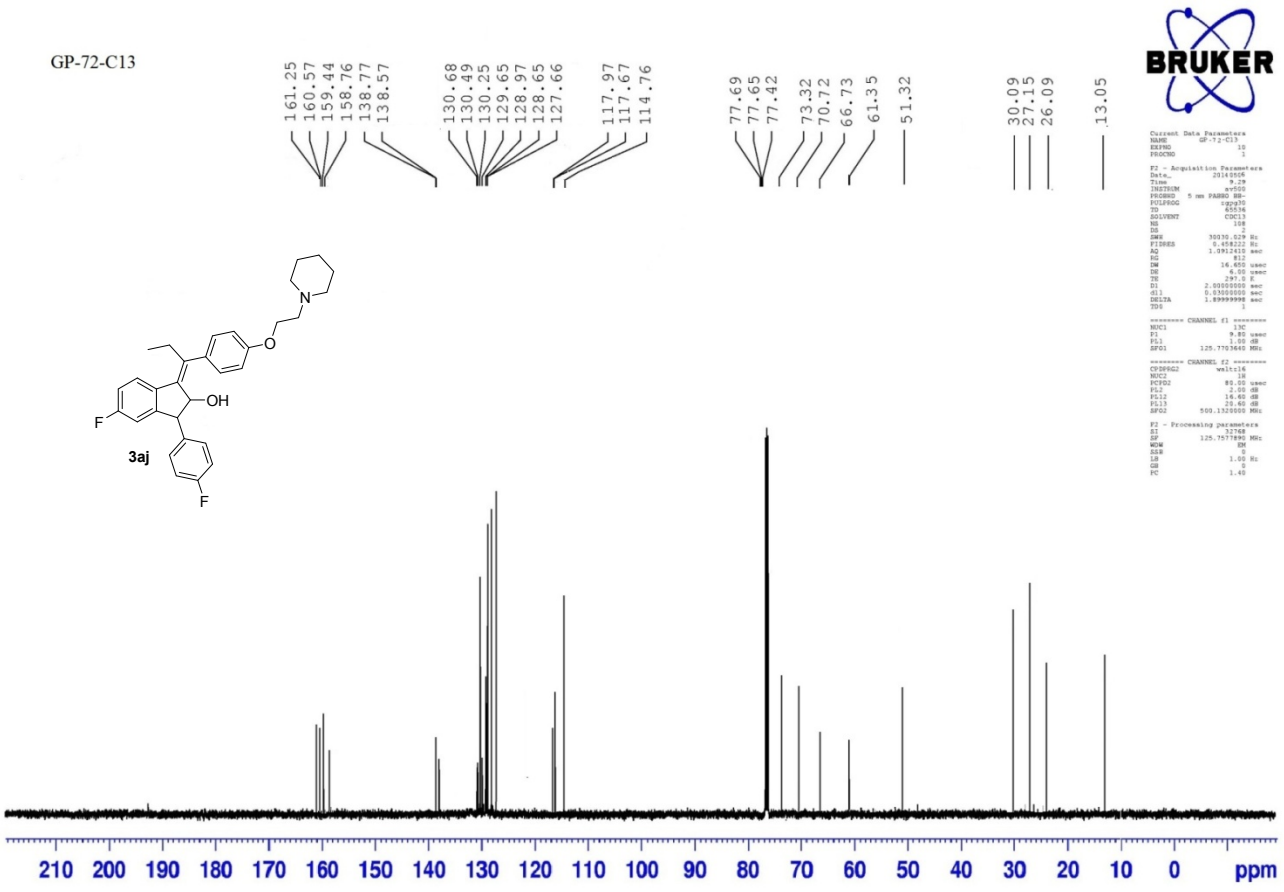

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ai**



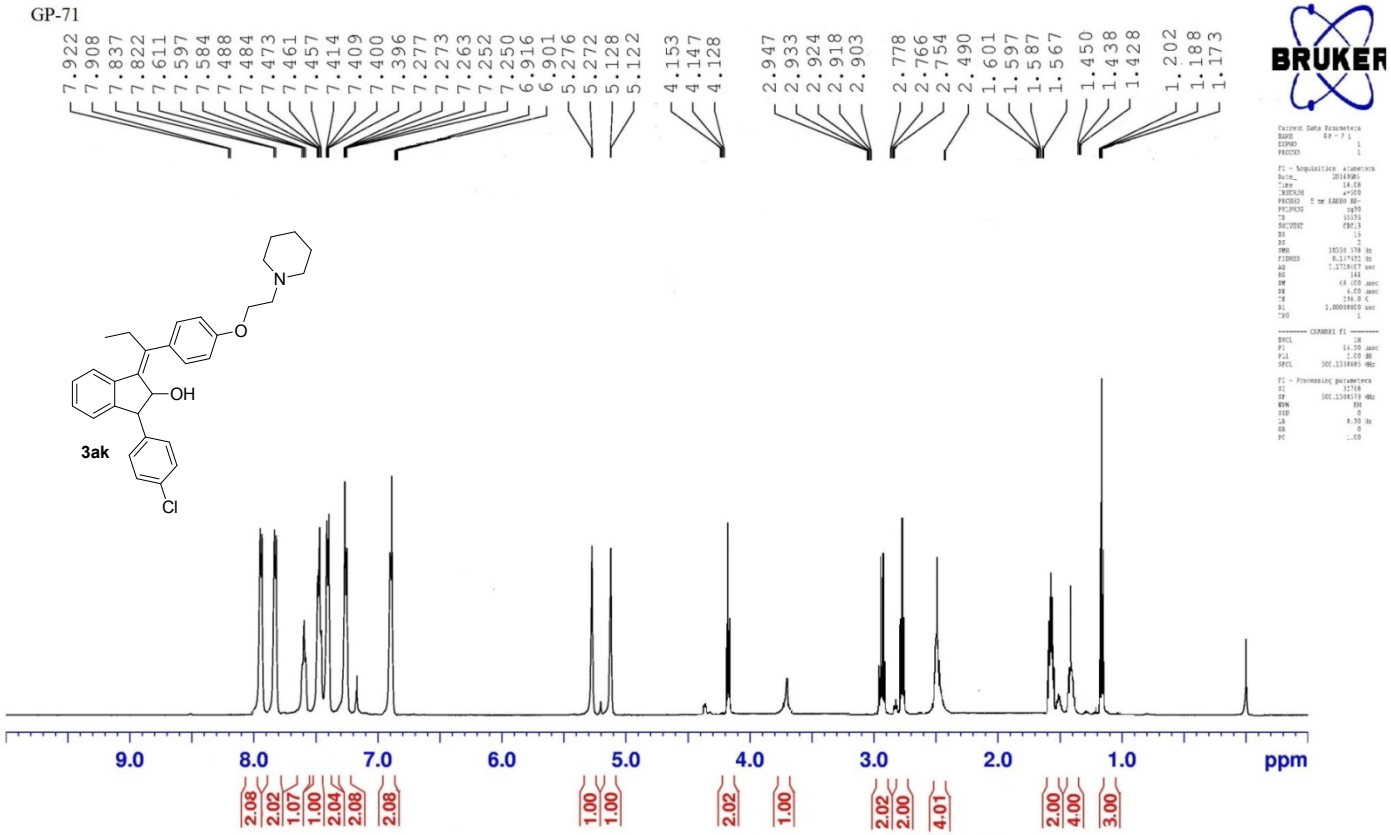

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ai**



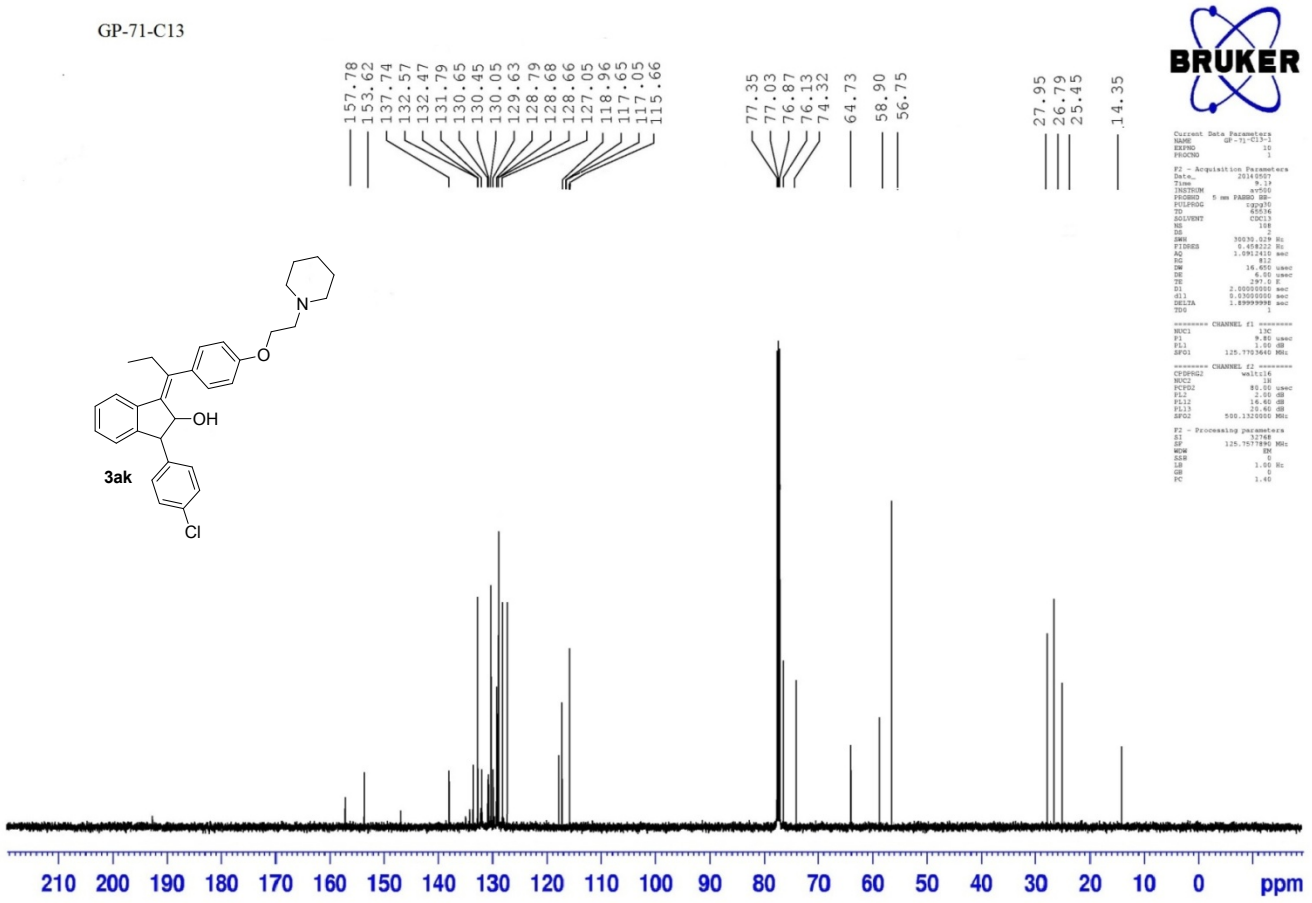

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3aj**



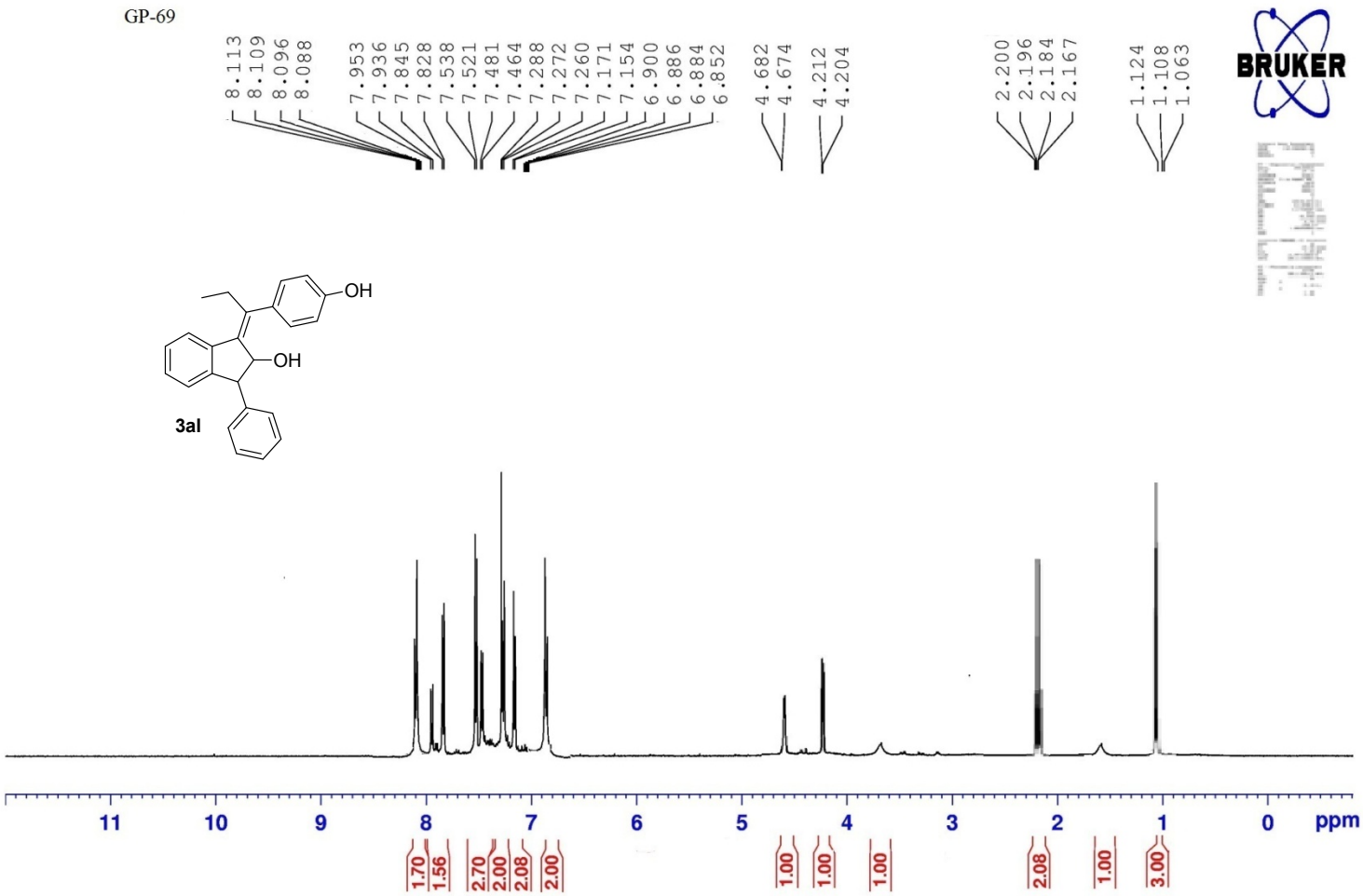

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3aj**



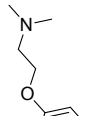

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ak**

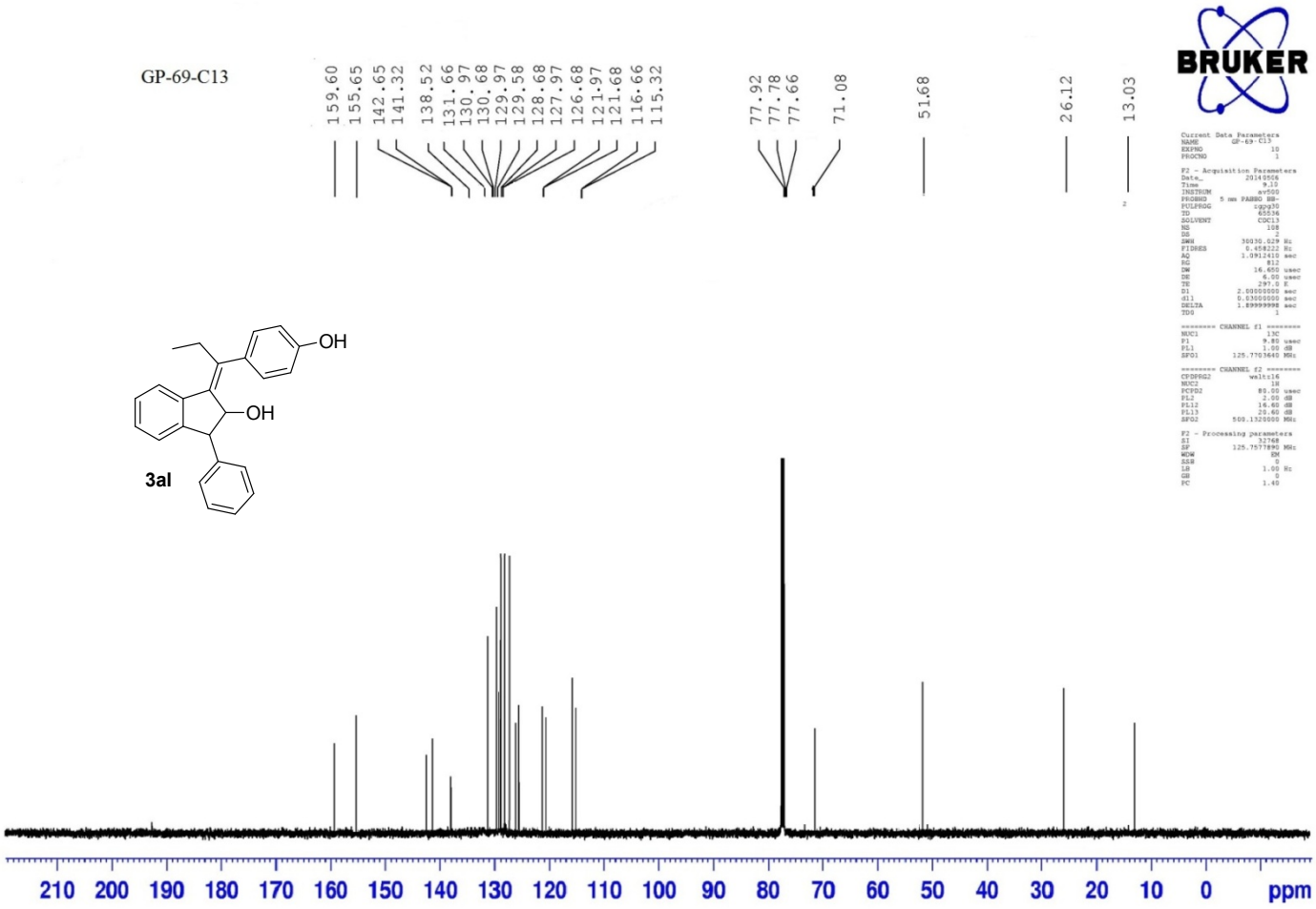



$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ak**

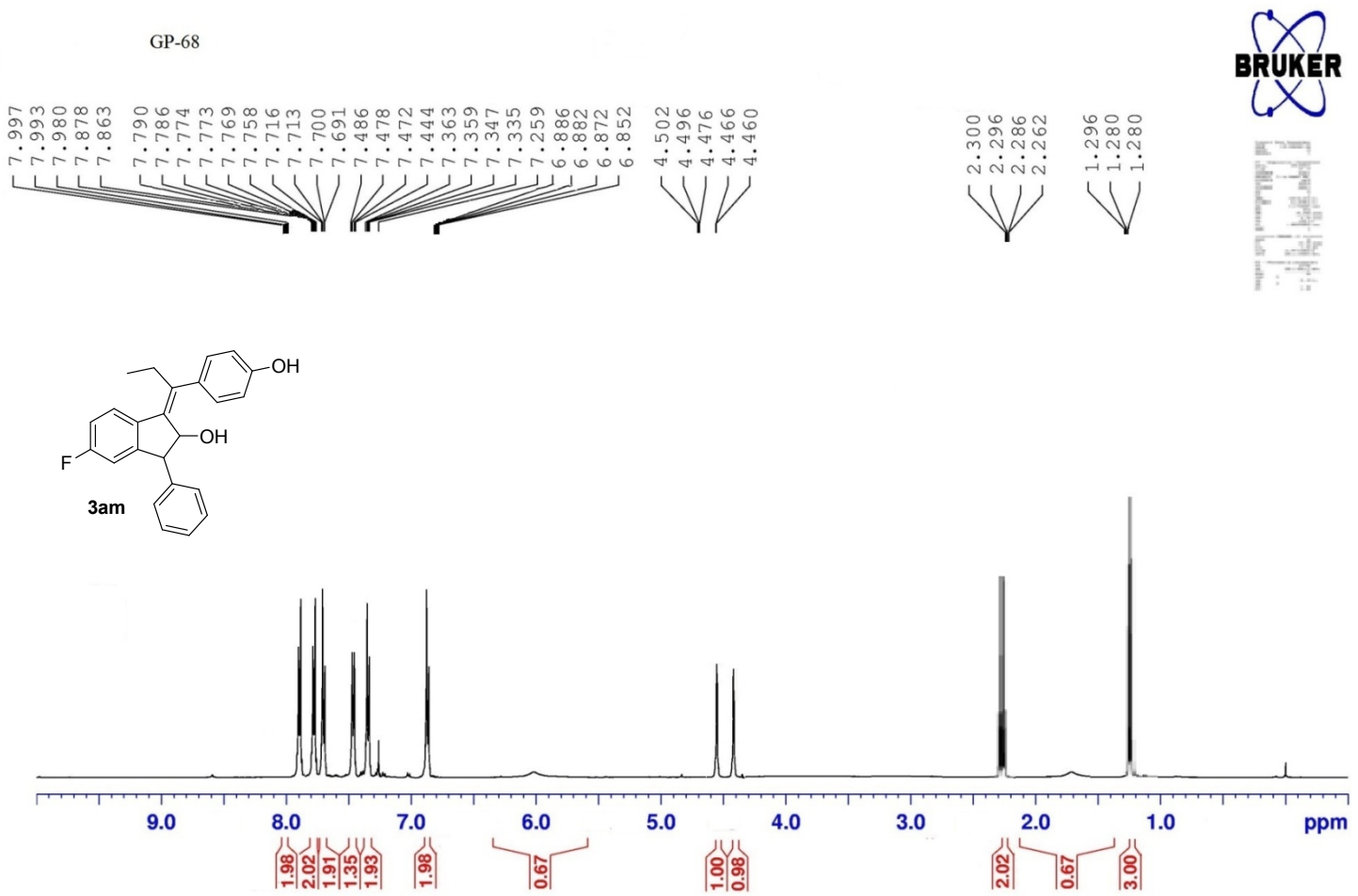



$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3al**

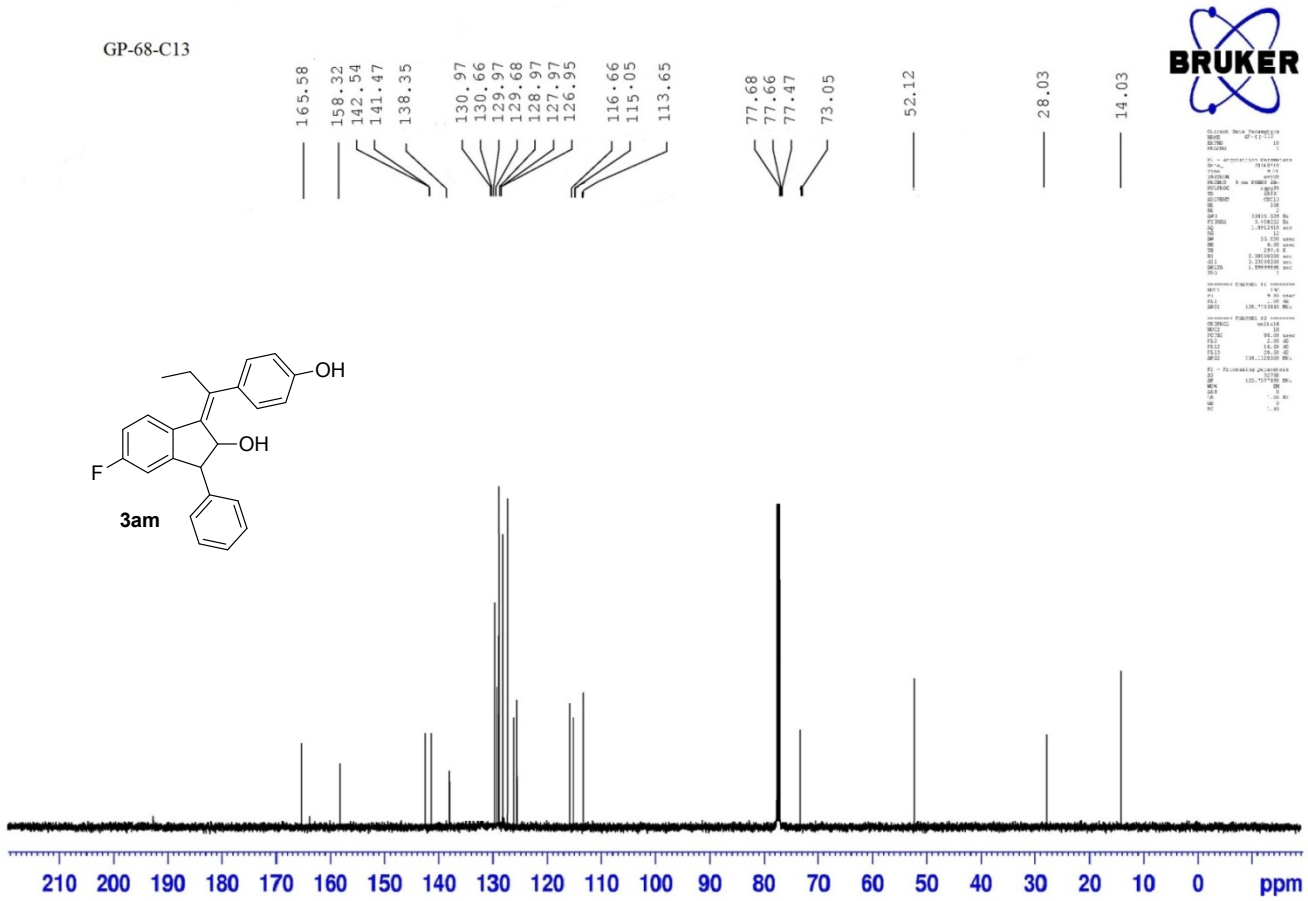




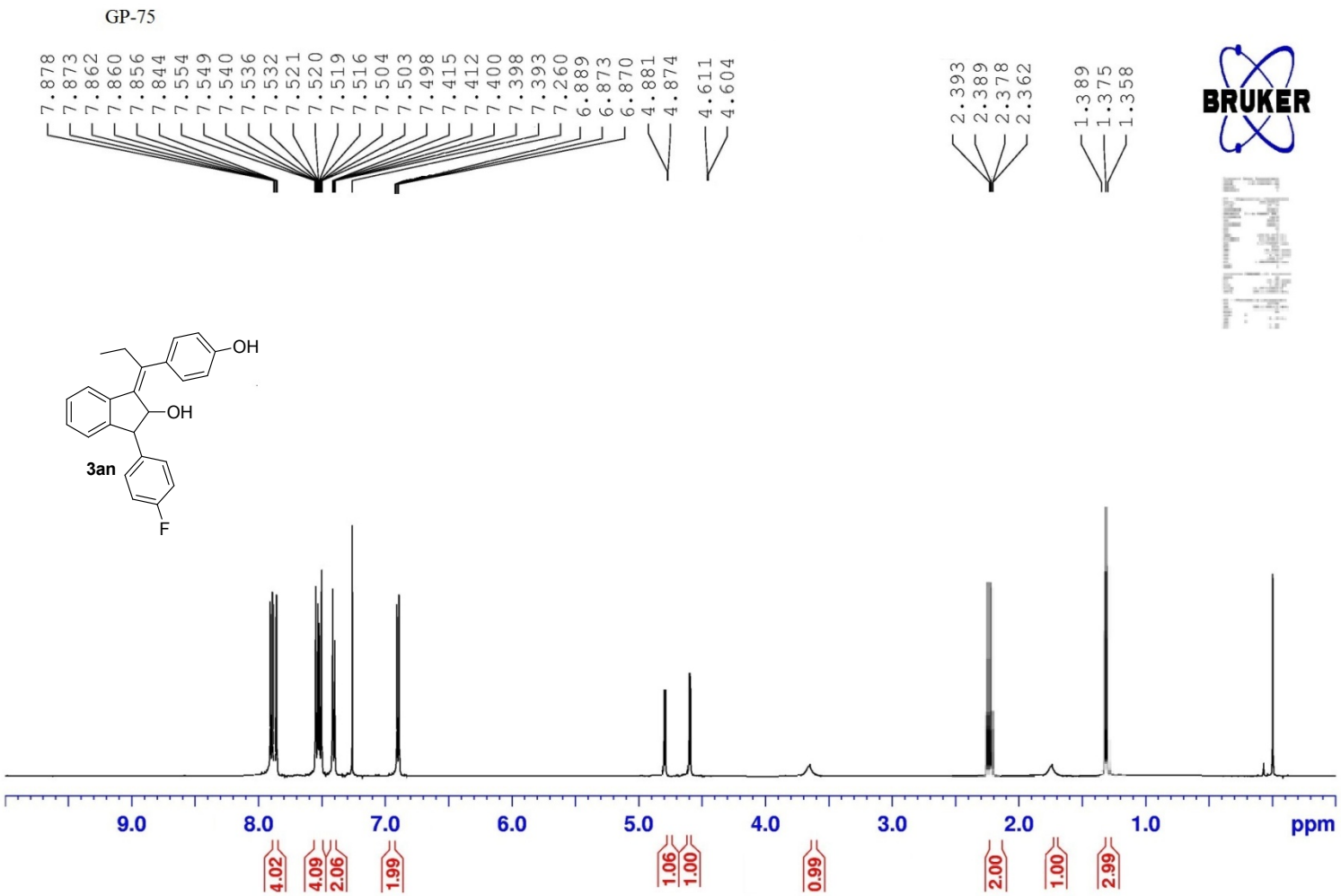

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3al**



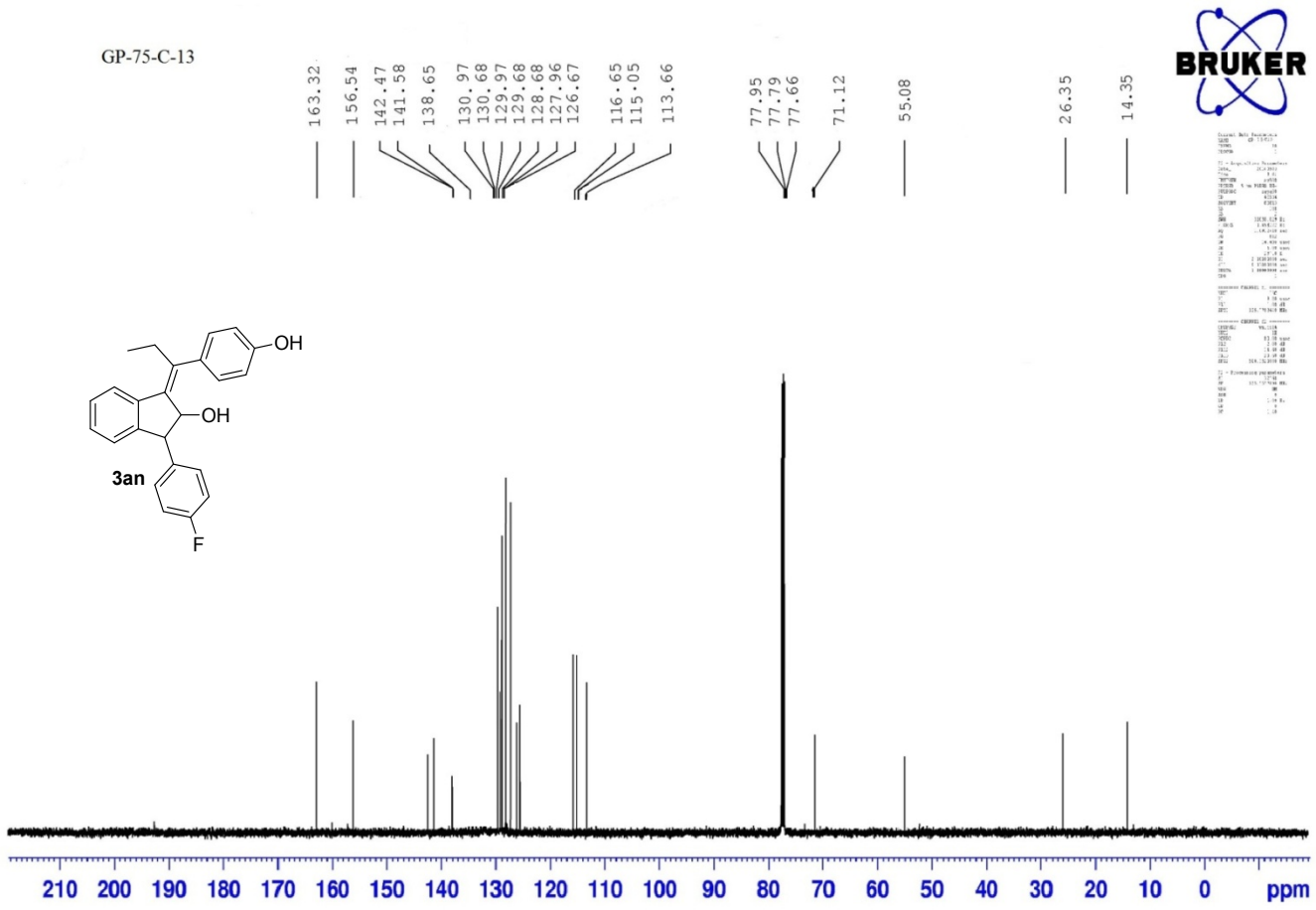

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3am**



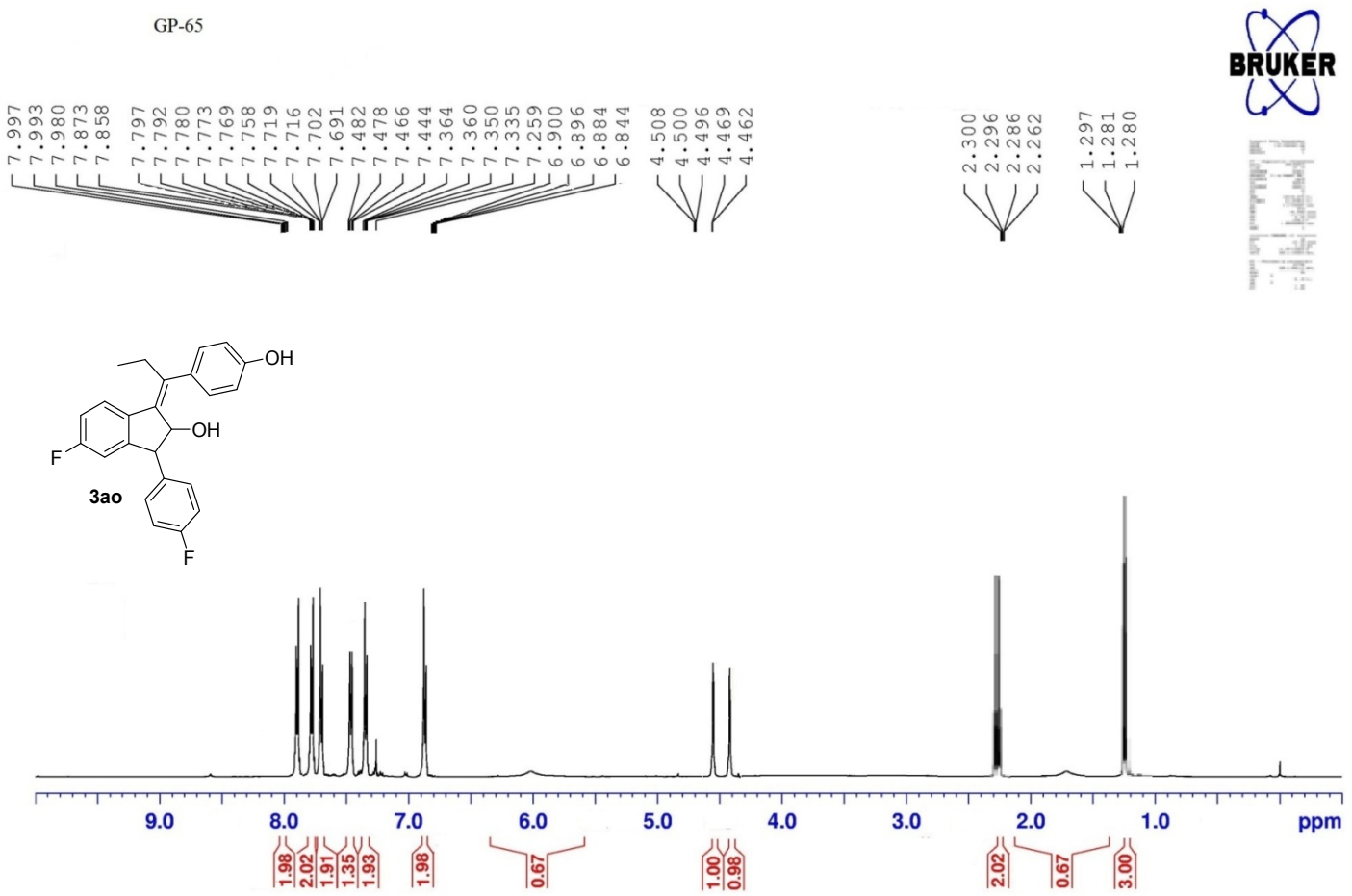

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3am**



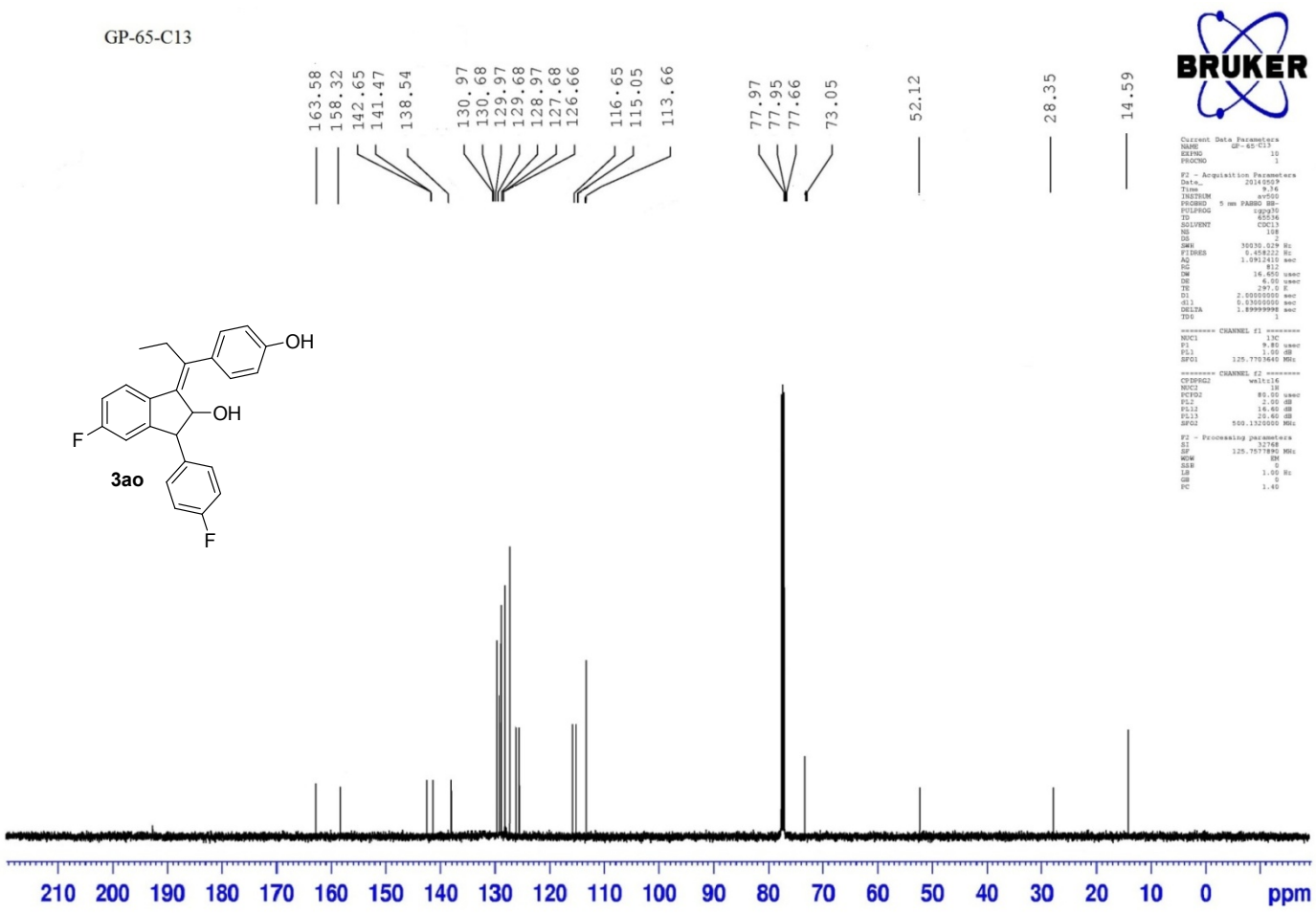

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3an**



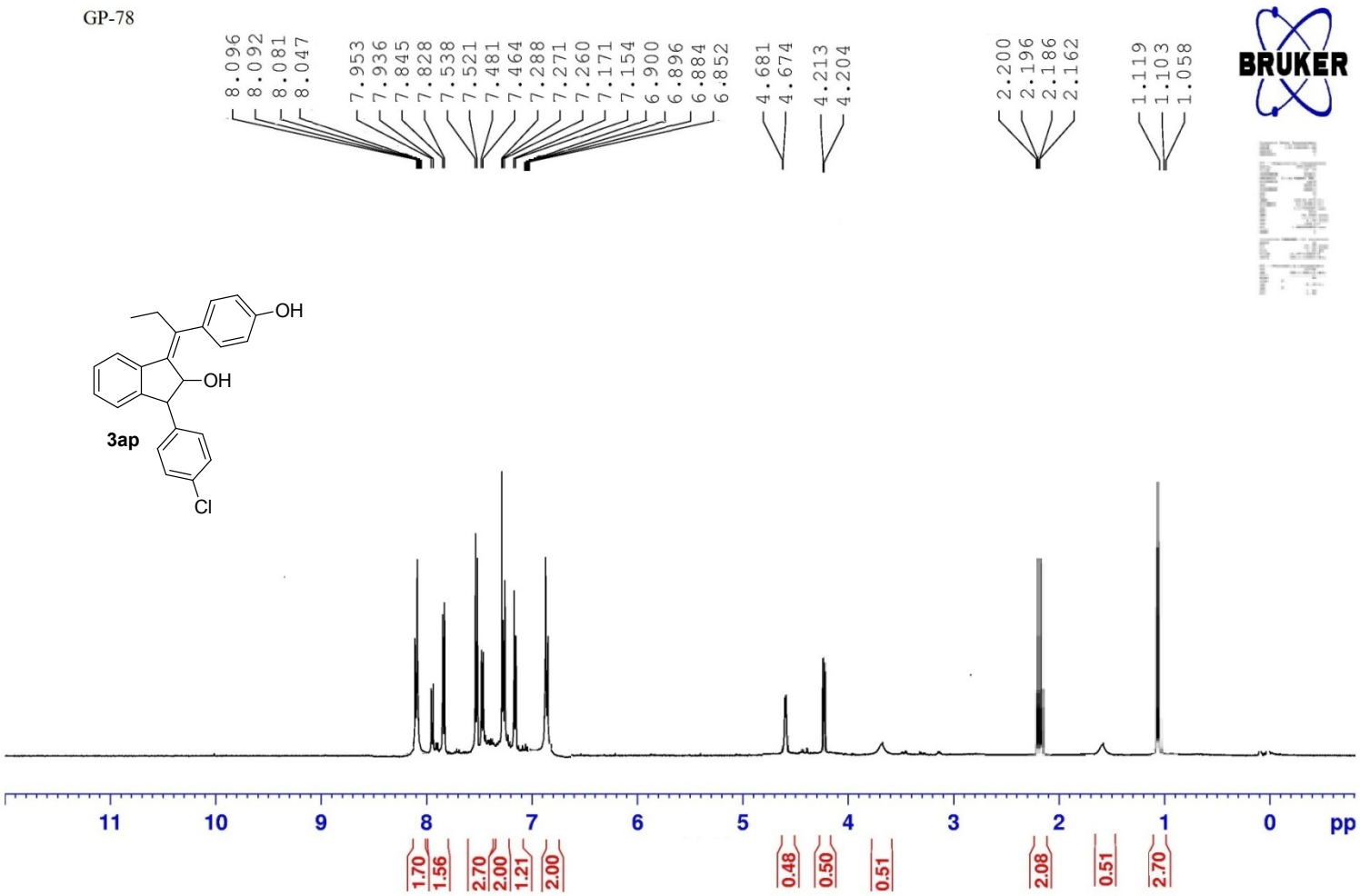

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3an**



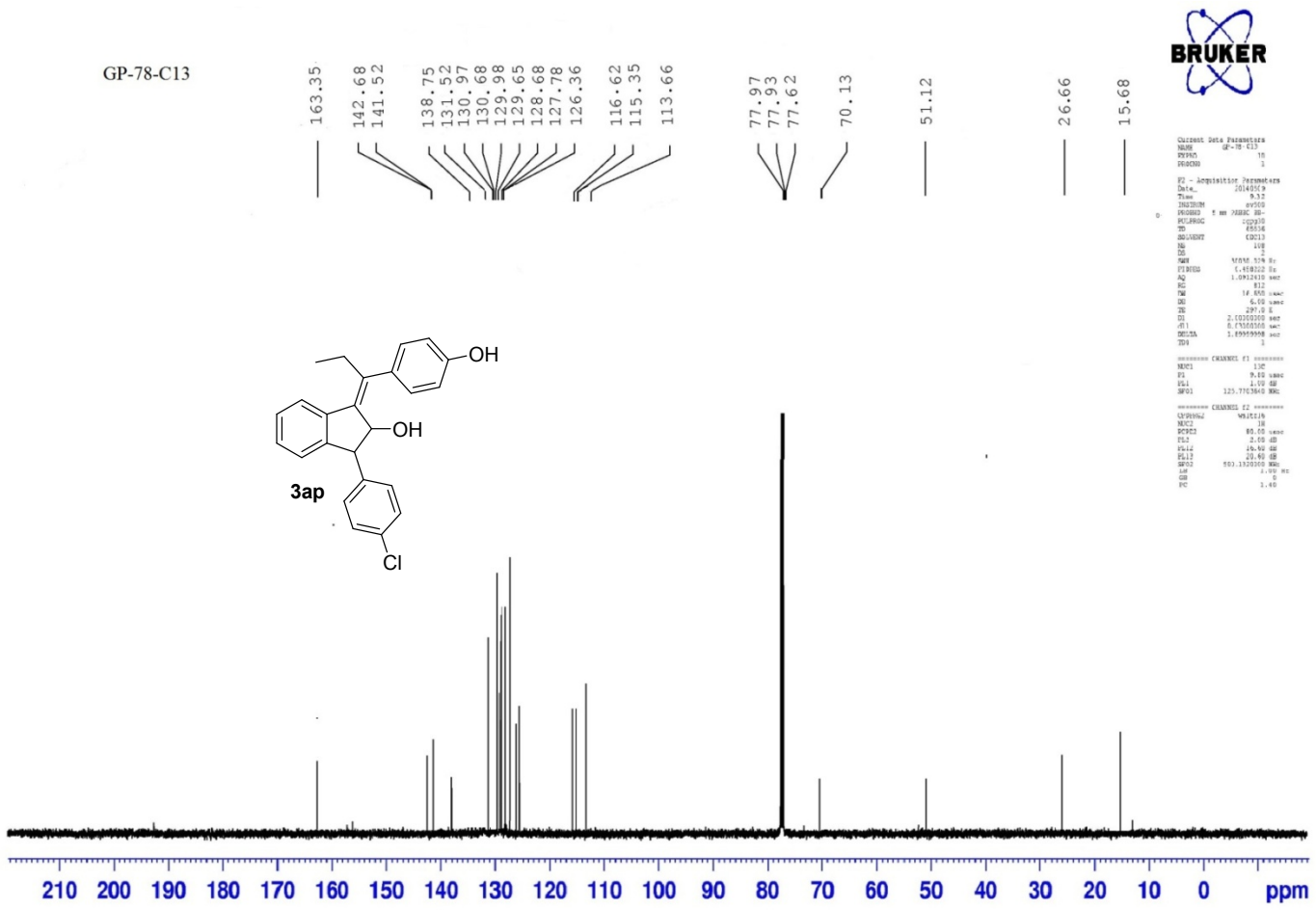

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ao**



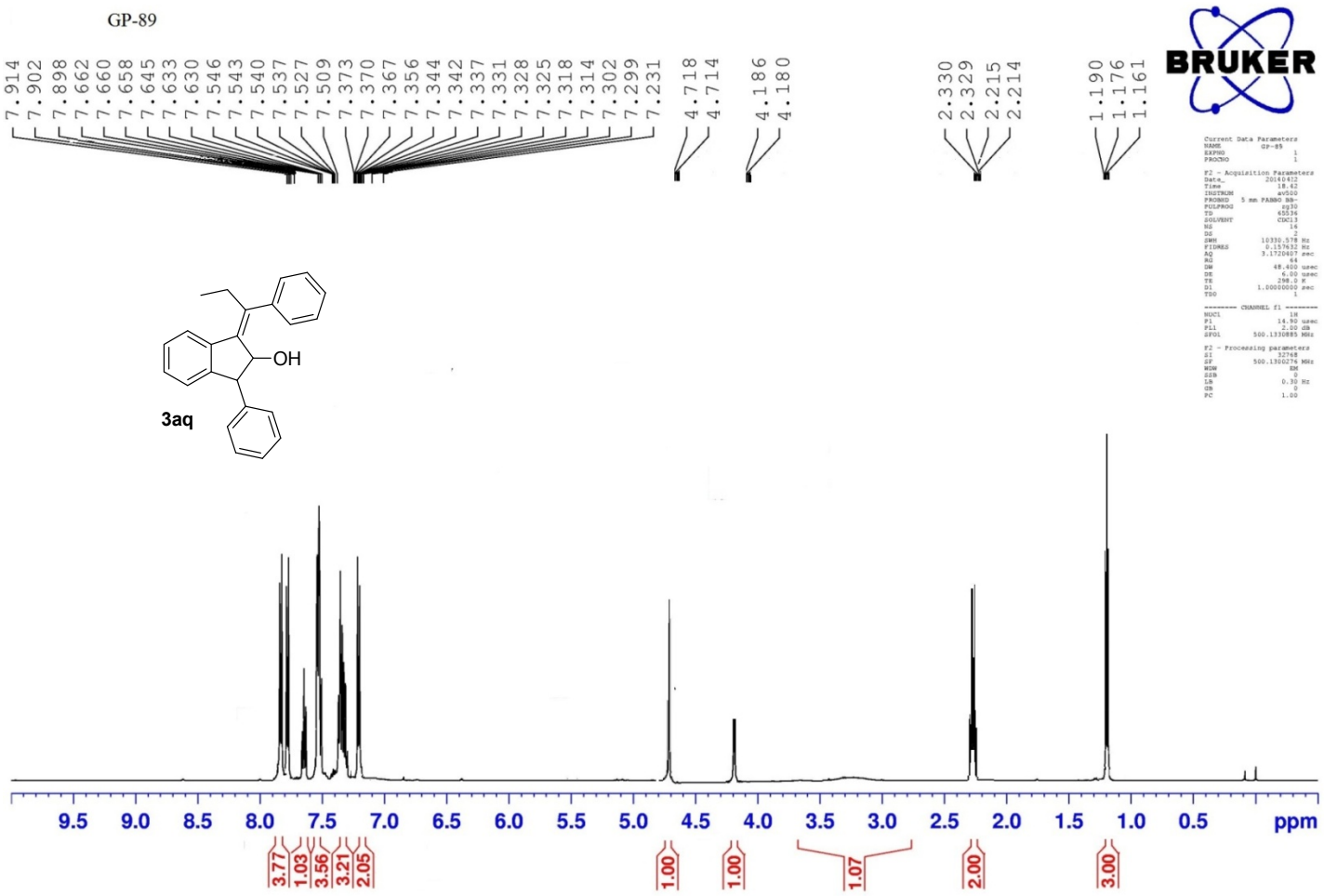

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ao**



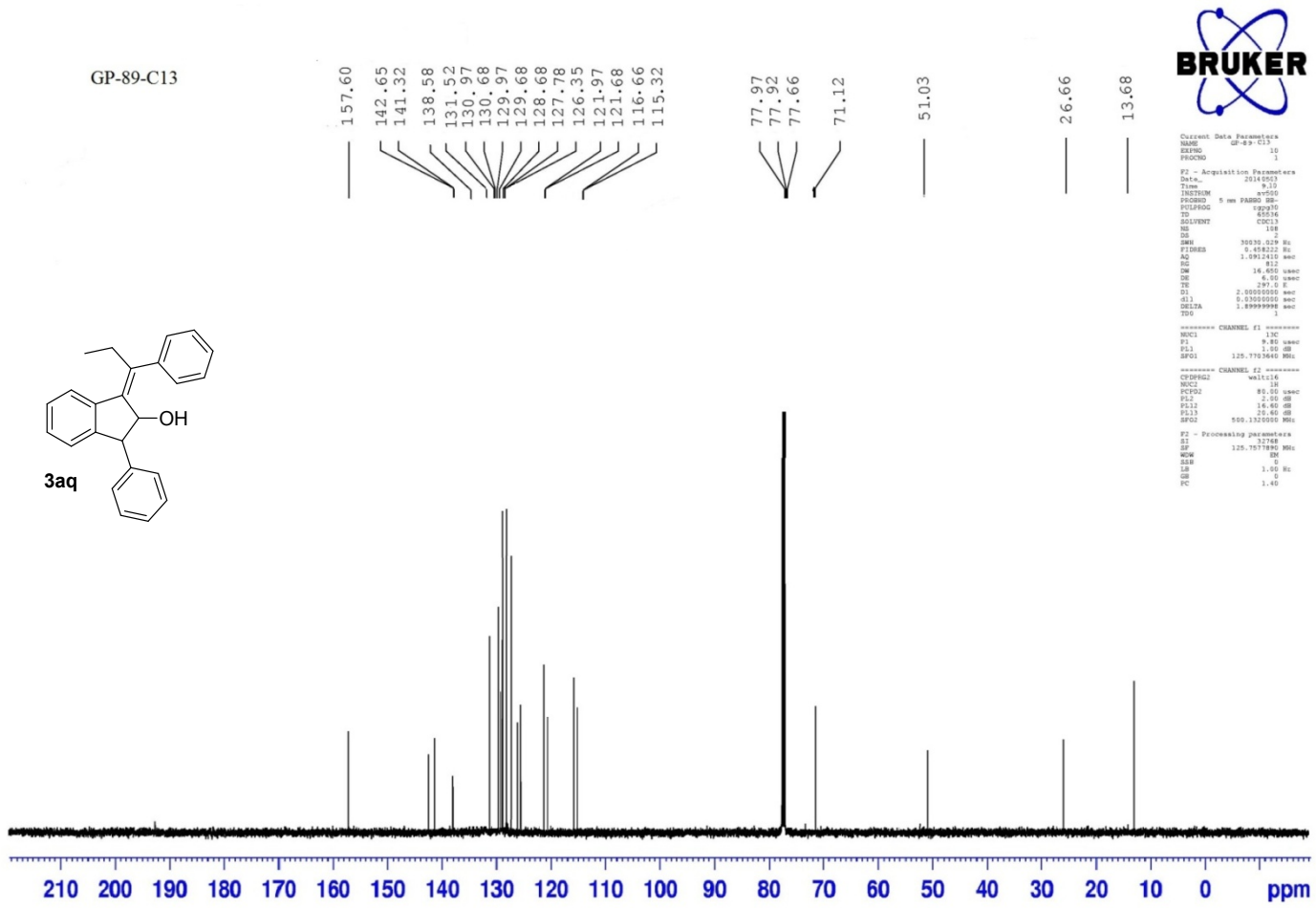

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ap**



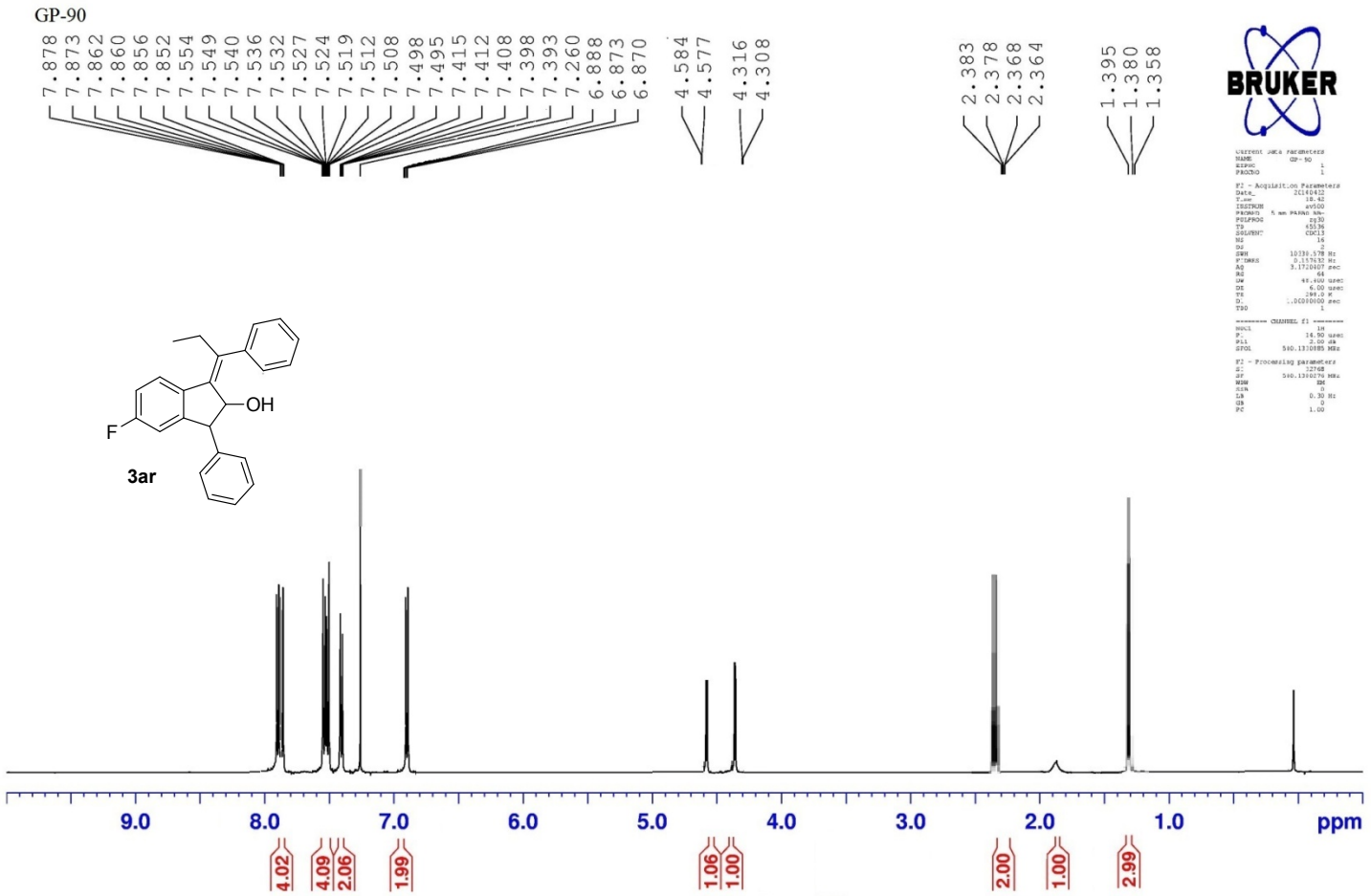

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ap**



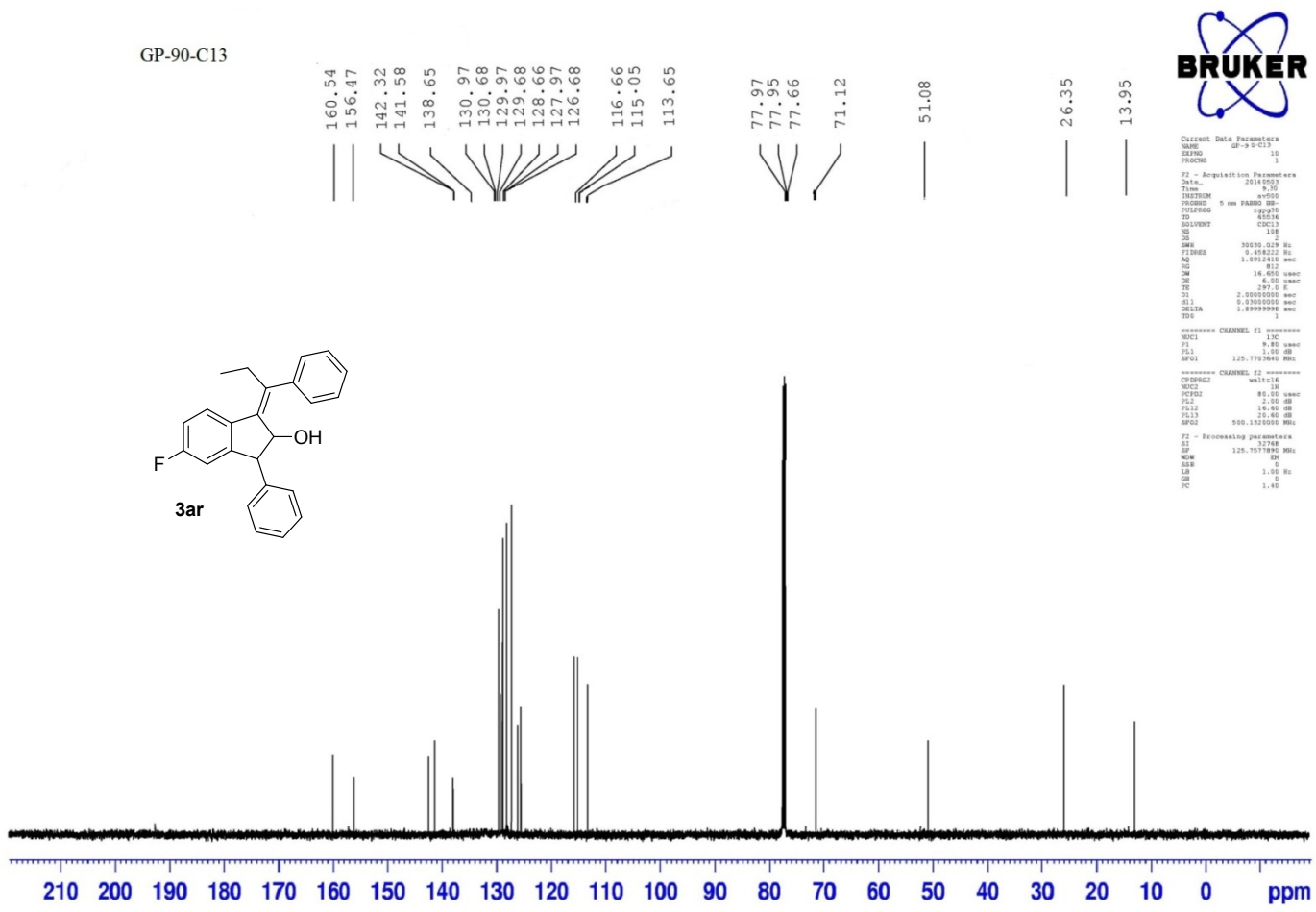

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3aq**



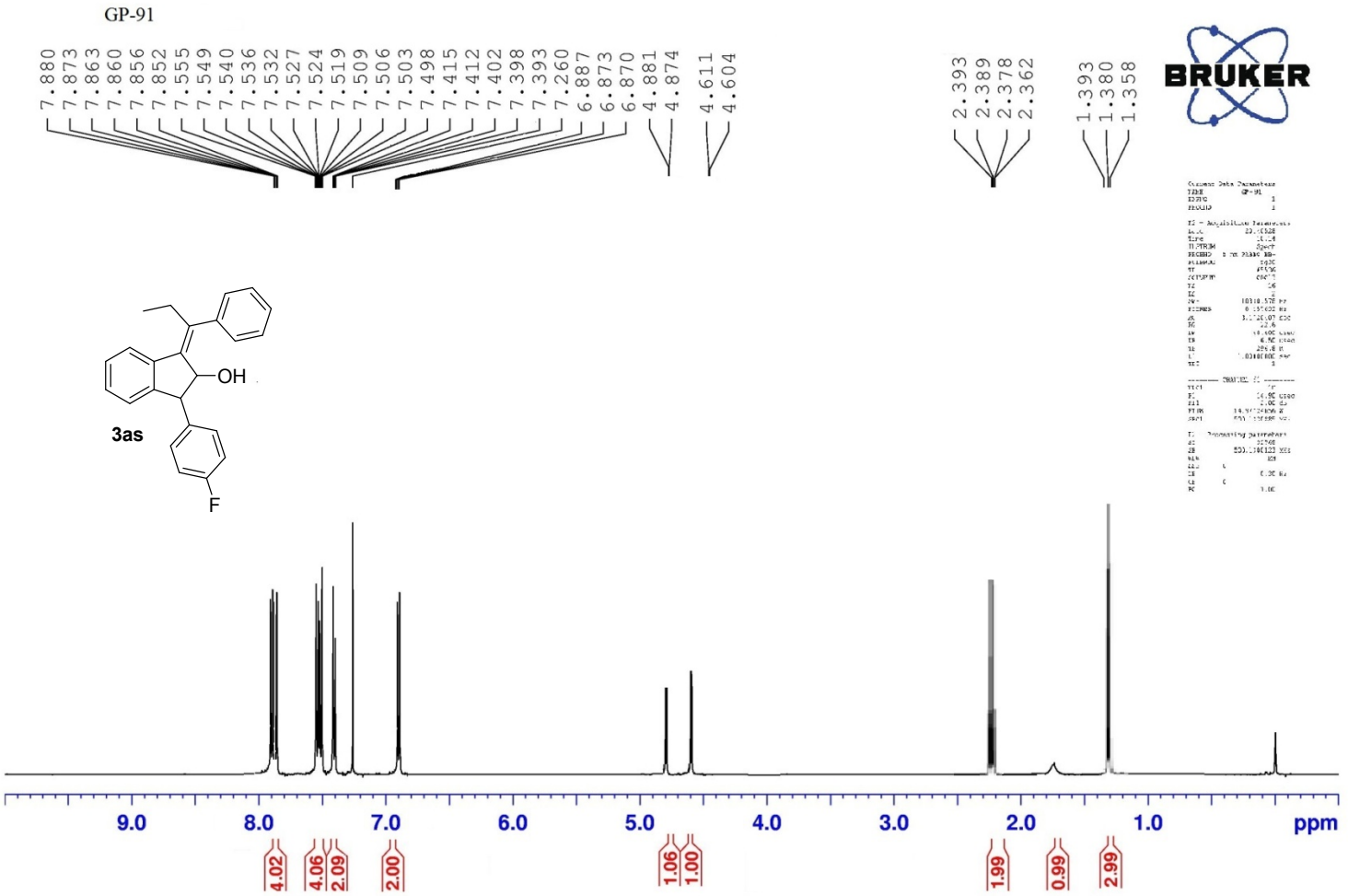

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3aq**



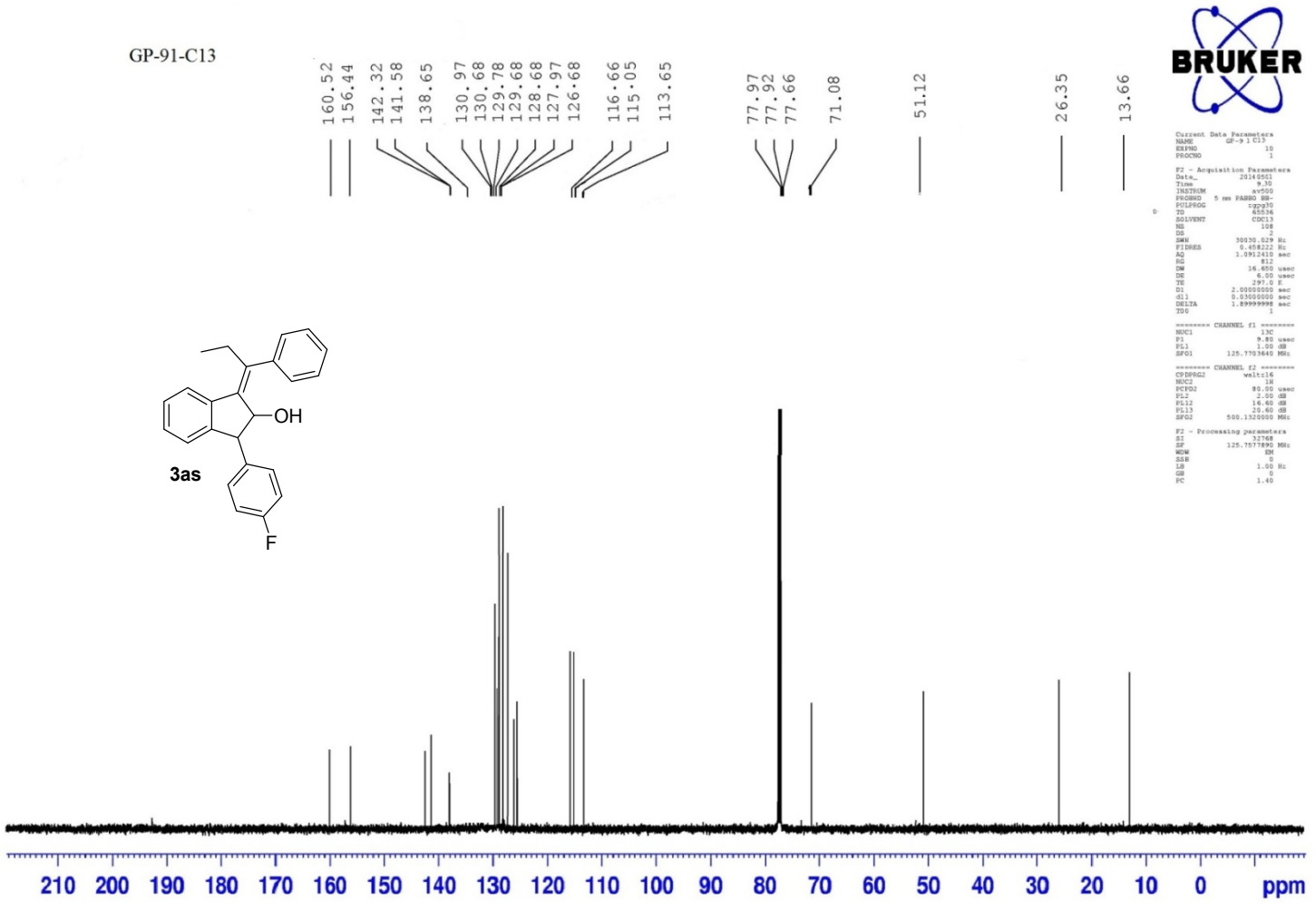

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3ar**



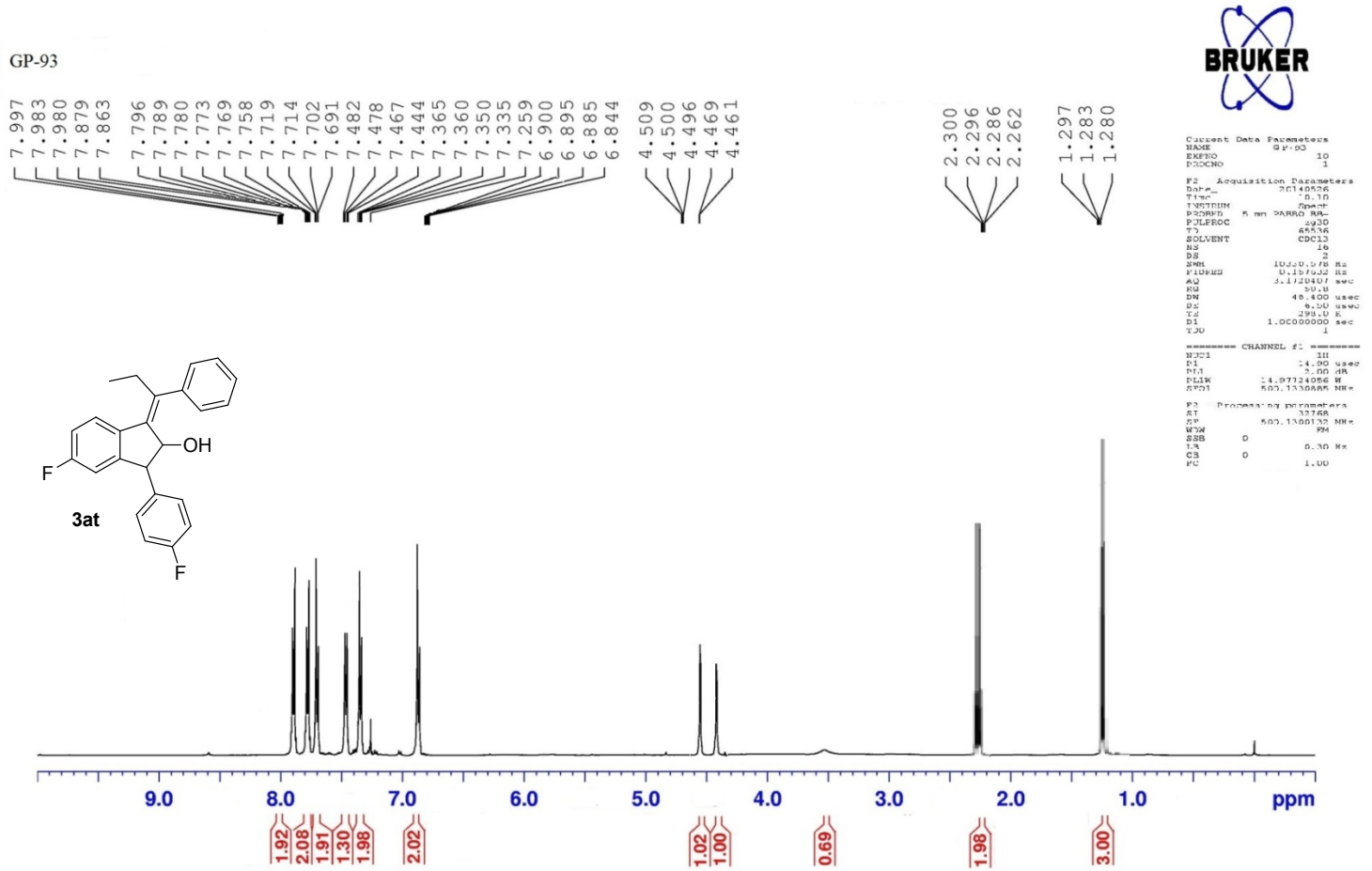

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3ar**



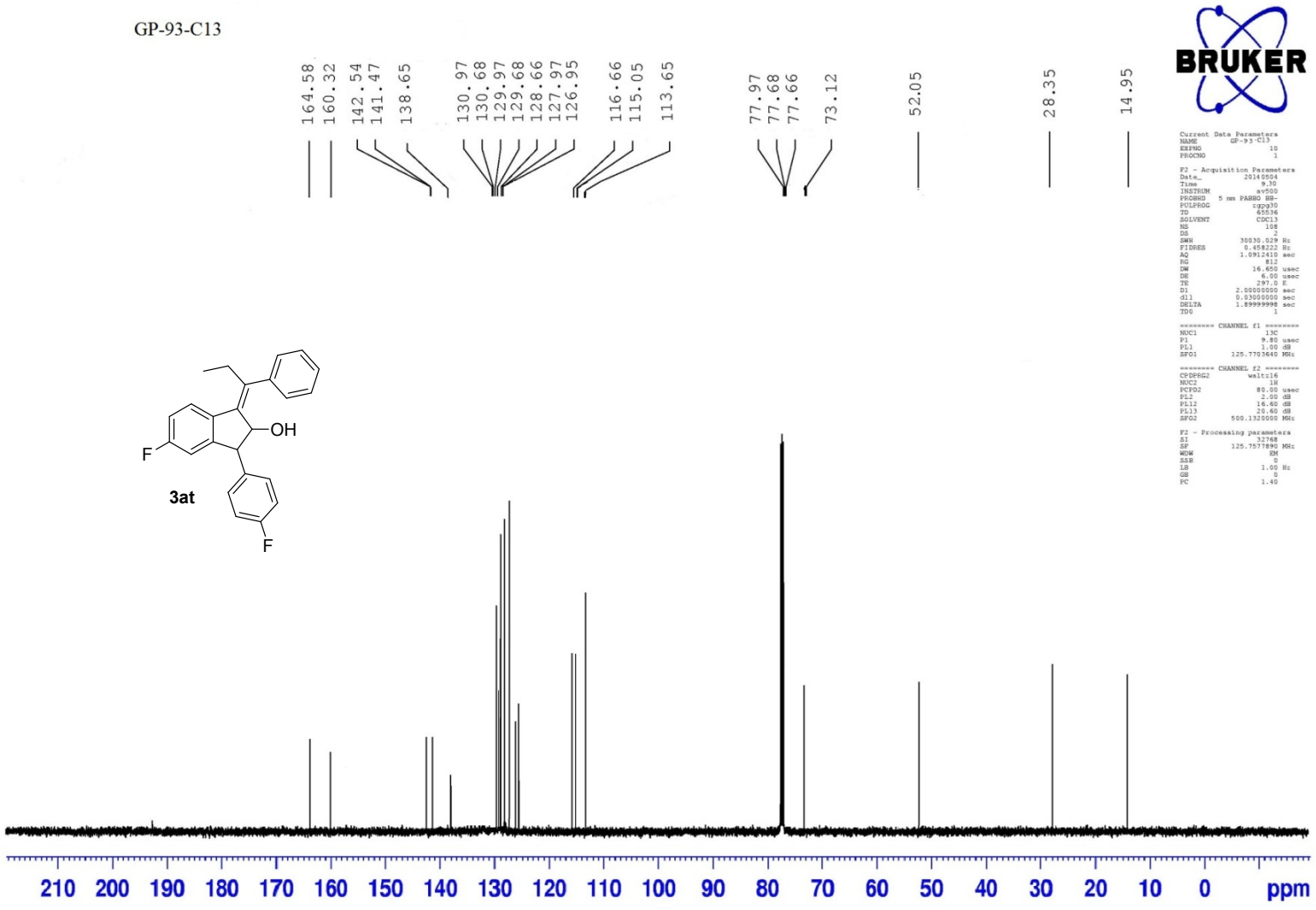

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3as**



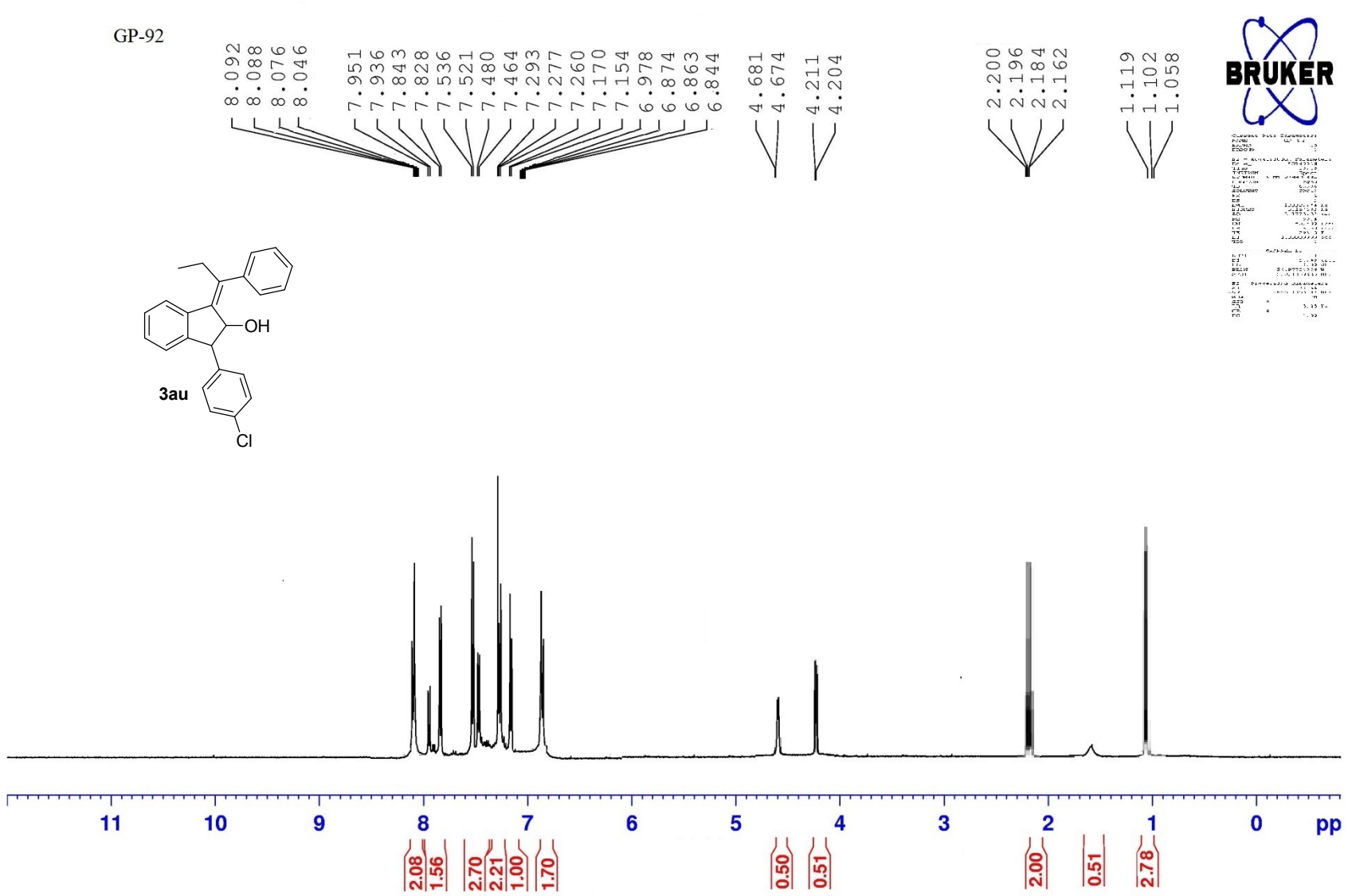

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3as**



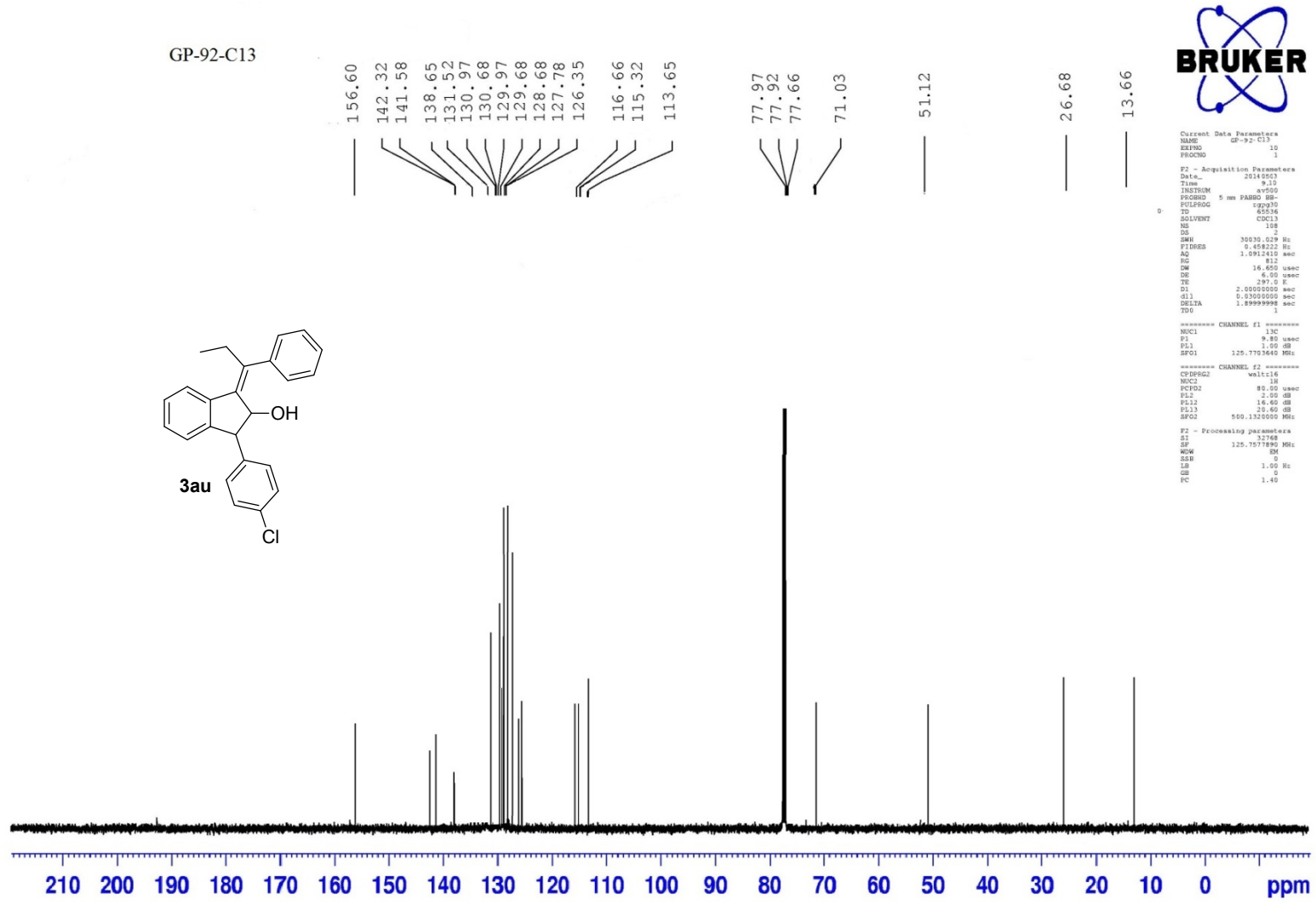

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3at**



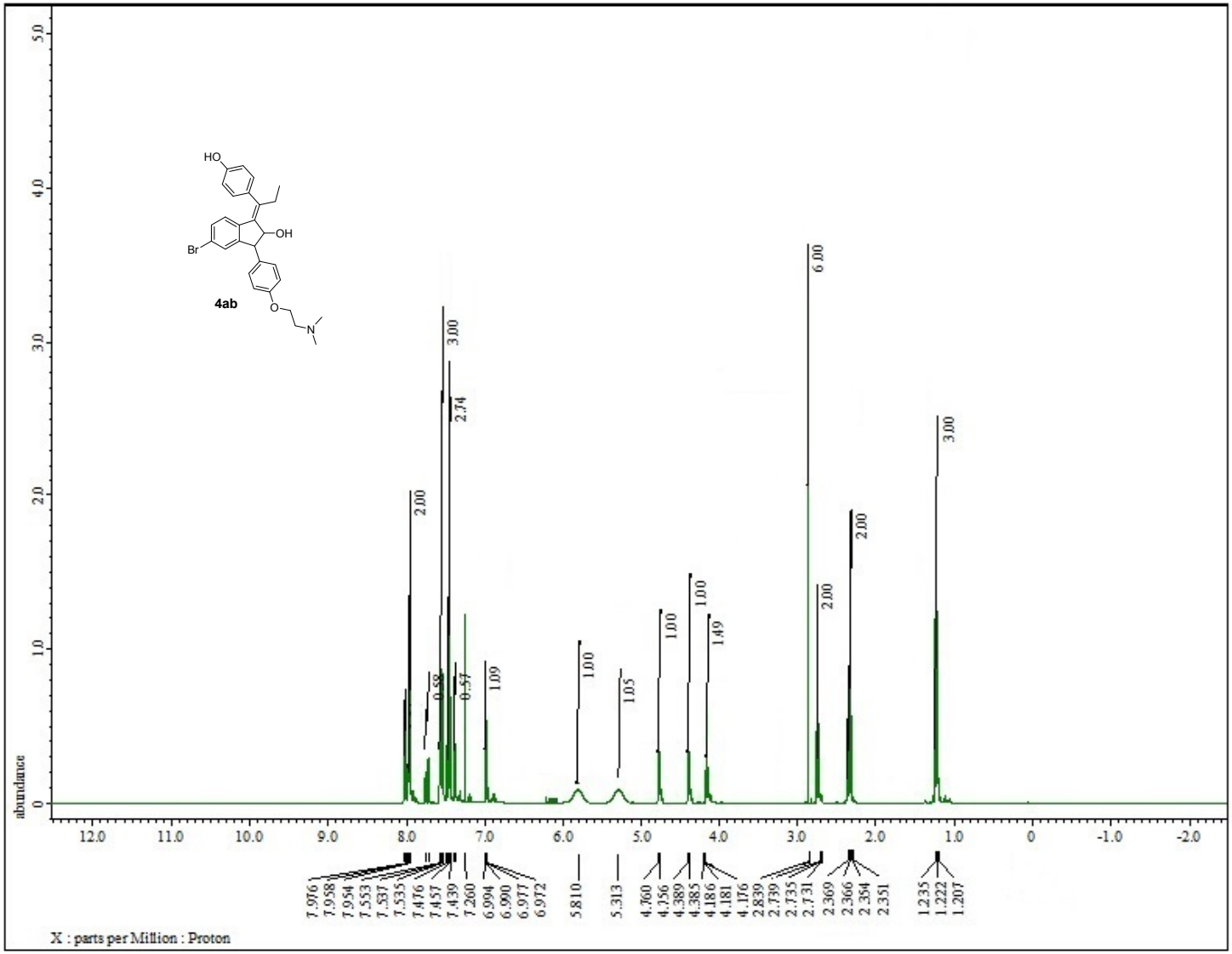

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3at**

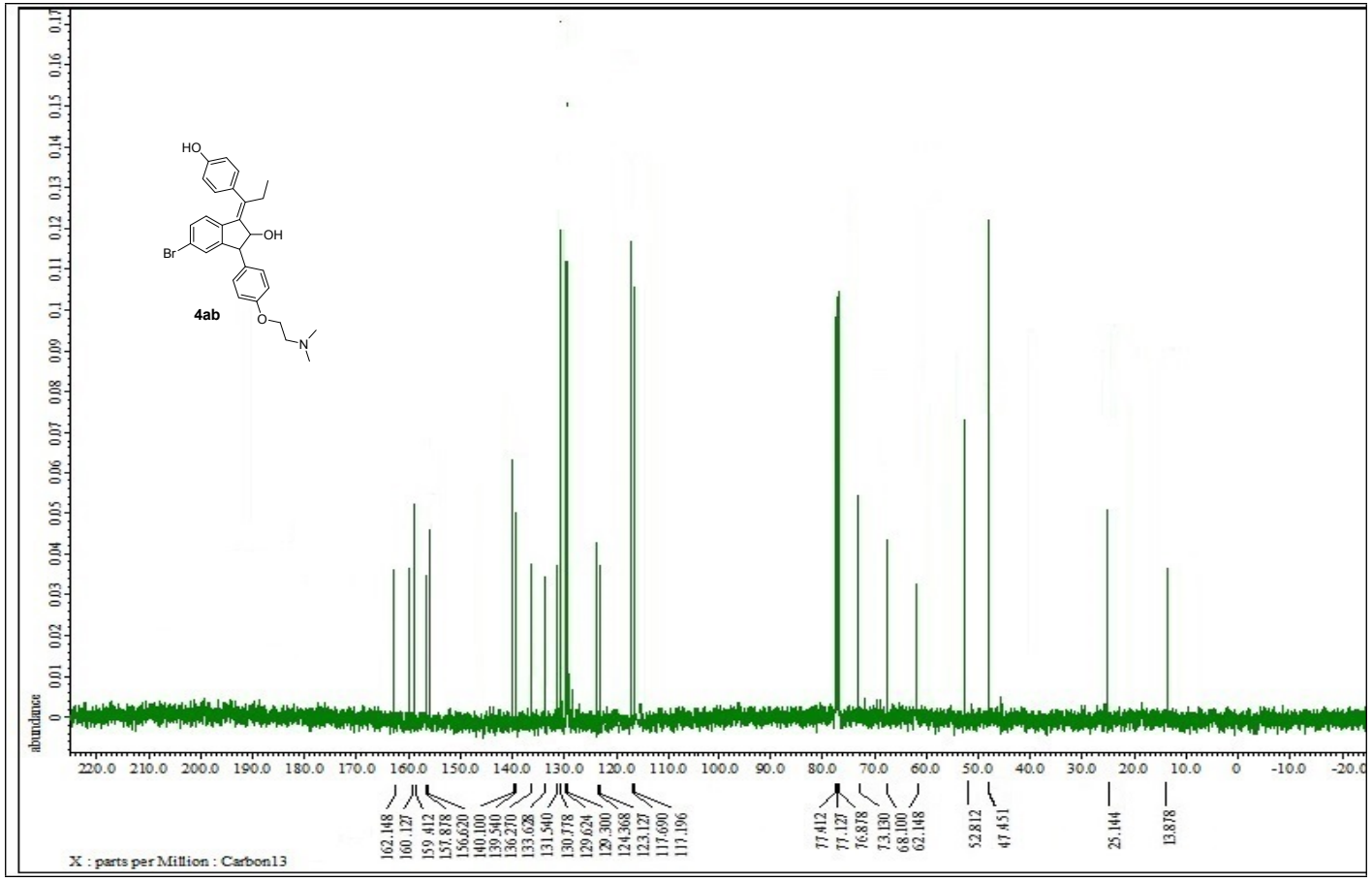


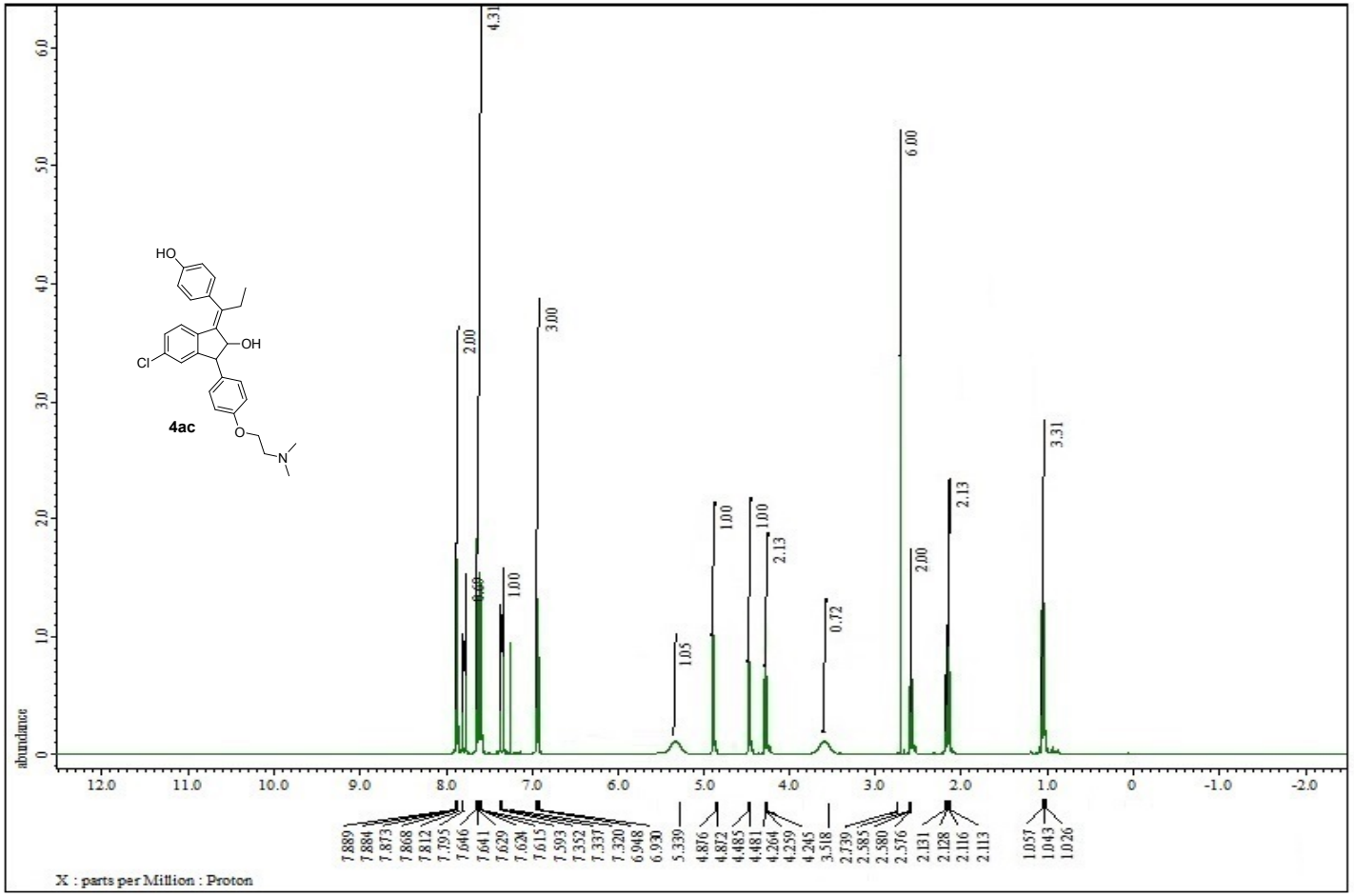

$^{1}$H-NMR (500 MHz, $CDCl_3$) Spectrum of **3au**

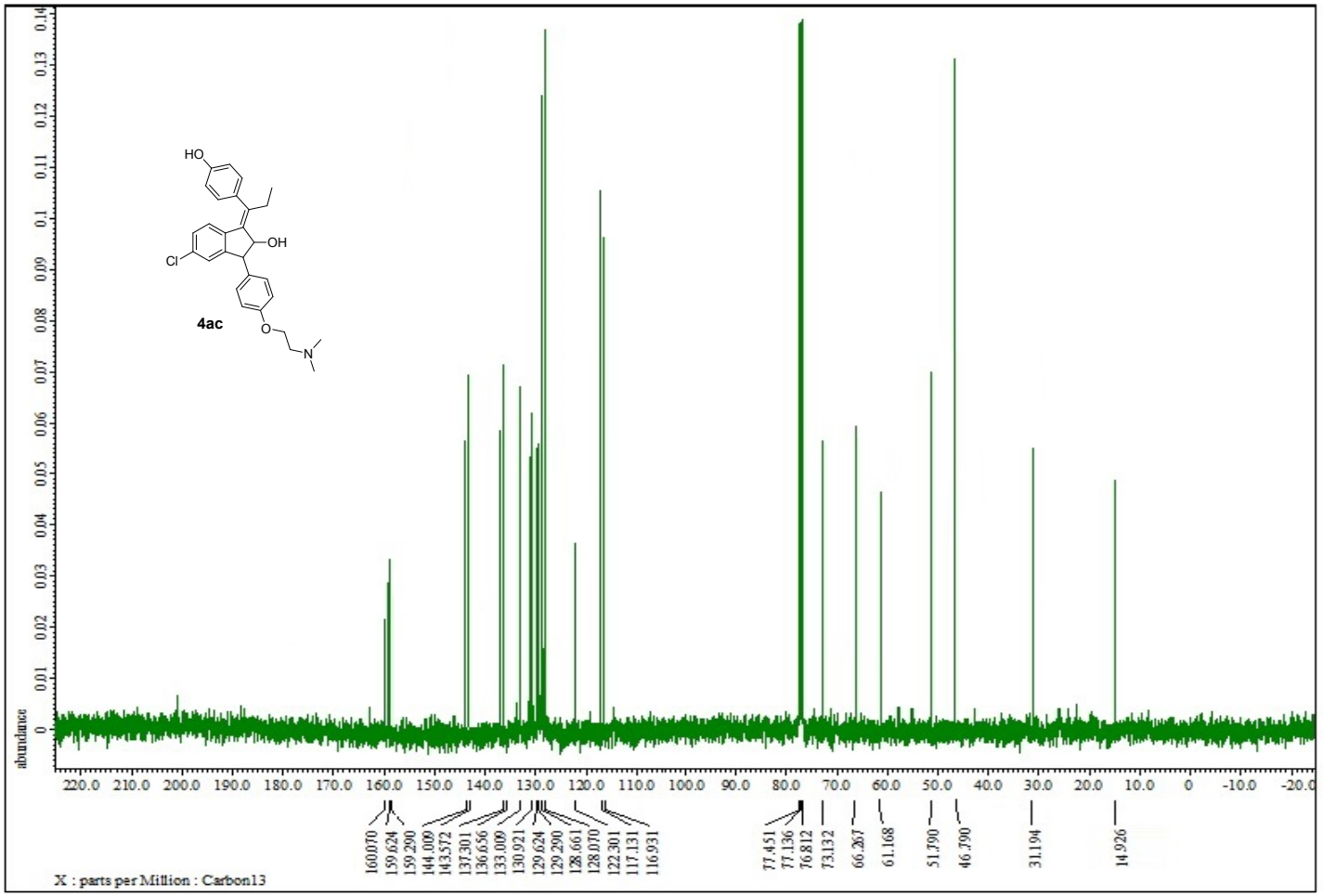


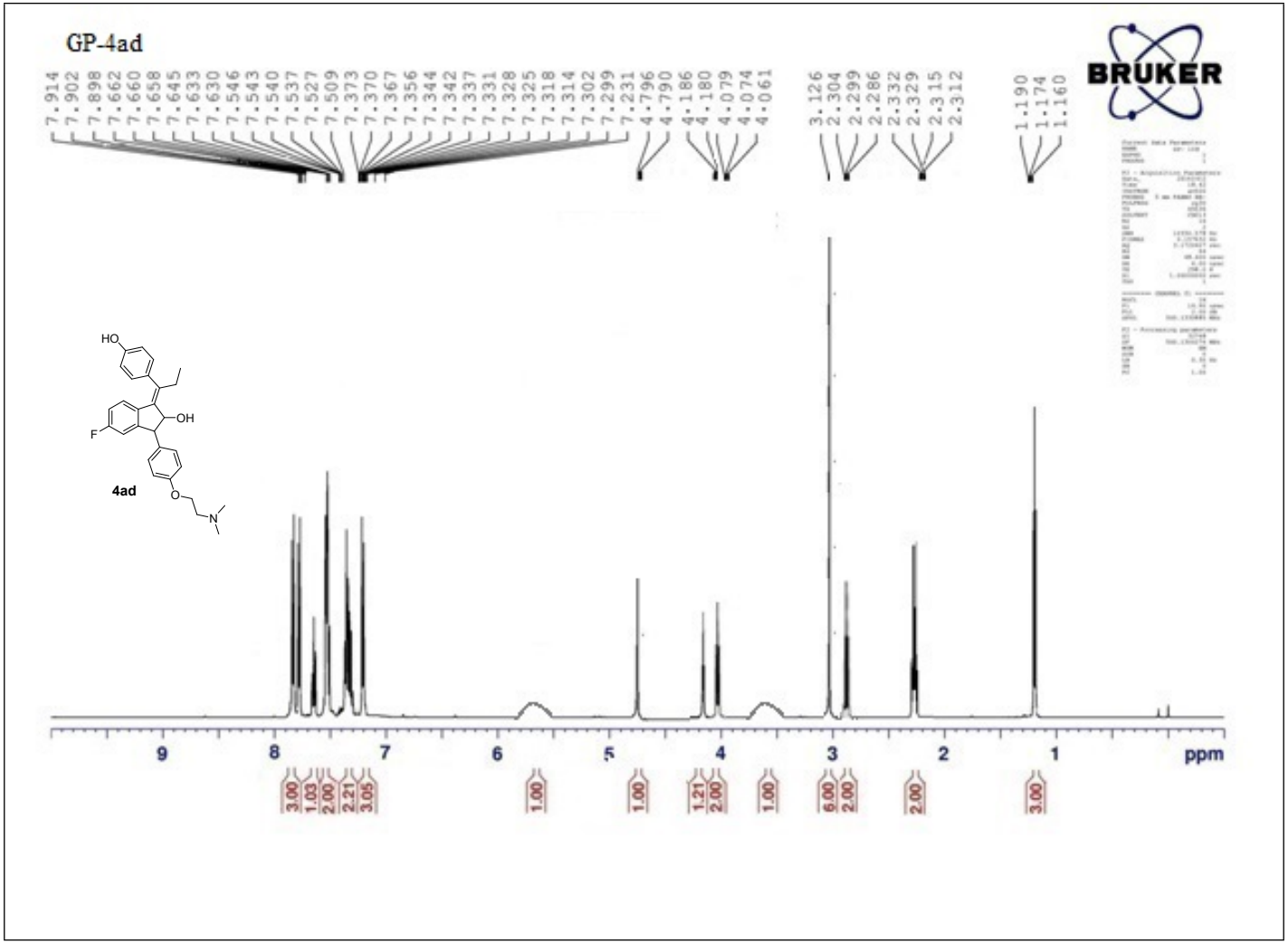

$^{13}$C-NMR (125 MHz, $CDCl_3$) Spectrum of **3au**


HO
OH
Br
O
N
4ab
abundance
2.00
3.00
2.74
0.58
0.57
1.09
1.00
1.05
1.00
1.00
1.49
6.00
2.00
2.00
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.976
7.958
7.954
7.553
7.537
7.535
7.476
7.457
7.439
7.260
6.994
6.990
6.977
6.972
5.810
5.313
4.760
4.156
4.389
4.385
4.186
4.181
4.176
2.839
2.739
2.735
2.731
2.369
2.366
2.354
2.351
1.235
1.222
1.207
X : parts per Million : Proton


HO
OH
Br
O
N
4ab
abundance
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
162.148
160.127
159.412
157.878
156.620
140.100
139.540
136.270
133.628
131.540
130.778
129.624
129.300
124.368
123.127
117.690
117.196
77.412
77.127
76.878
73.130
68.100
62.148
52.812
47.451
25.144
13.878
X : parts per Million : Carbon13


HO
OH
Cl
O
N
4ac
4.31
2.00
0.69
1.00
3.00
1.05
1.00
1.00
2.13
0.72
6.00
2.00
2.13
3.31
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.889
7.884
7.873
7.868
7.812
7.795
7.646
7.641
7.629
7.624
7.615
7.593
7.352
7.337
7.320
6.948
6.930
5.339
4.876
4.872
4.485
4.481
4.264
4.259
4.245
3.518
2.739
2.583
2.580
2.576
2.131
2.128
2.116
2.113
1.057
1.043
1.026
X : parts per Million : Proton


HO
OH
Cl
O
N
4ac
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
220.0
210.0
200.0
190.0
180.0
170.0
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
-10.0
-20.0
160.070
159.624
159.290
144.009
143.572
137.301
136.656
133.009
130.921
129.624
129.290
128.661
128.070
122.301
117.131
116.931
77.451
77.136
76.812
73.132
66.267
61.168
51.790
46.790
31.194
14.926
X : parts per Million : Carbon13


GP-4ad
7.914
7.902
7.898
7.662
7.660
7.658
7.645
7.633
7.630
7.546
7.543
7.540
7.537
7.527
7.509
7.373
7.370
7.367
7.356
7.344
7.342
7.337
7.331
7.328
7.325
7.318
7.314
7.302
7.299
7.231
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4.790
4.186
4.180
4.079
4.074
4.061
3.126
2.304
2.299
2.286
2.332
2.329
2.315
2.312
1.190
1.174
1.160
BRUKER
HO
OH
F
O
N
4ad
9
8
7
6
5
4
3
2
1
ppm
3.00
1.03
2.00
2.21
3.05
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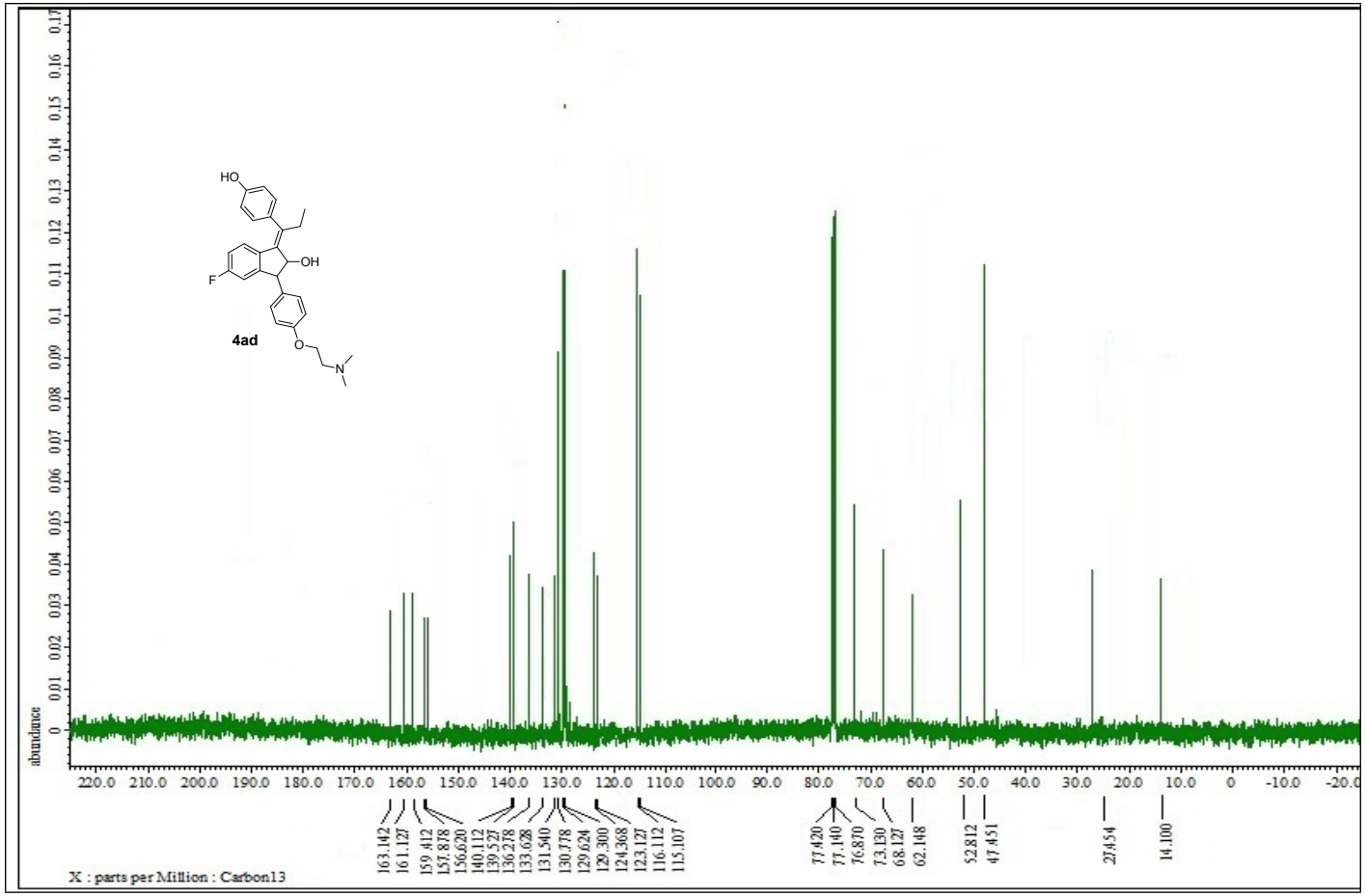
1.00
1.21
2.00
1.00
6.00
2.00
2.00
3.00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OH
F
O
N
4ad
abundance
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0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.142
161.127
159.412
157.878
156.620
140.112
139.527
136.278
133.628
131.540
130.778
129.624
129.300
124.368
123.127
116.112
115.107
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77.140
76.870
73.130
68.127
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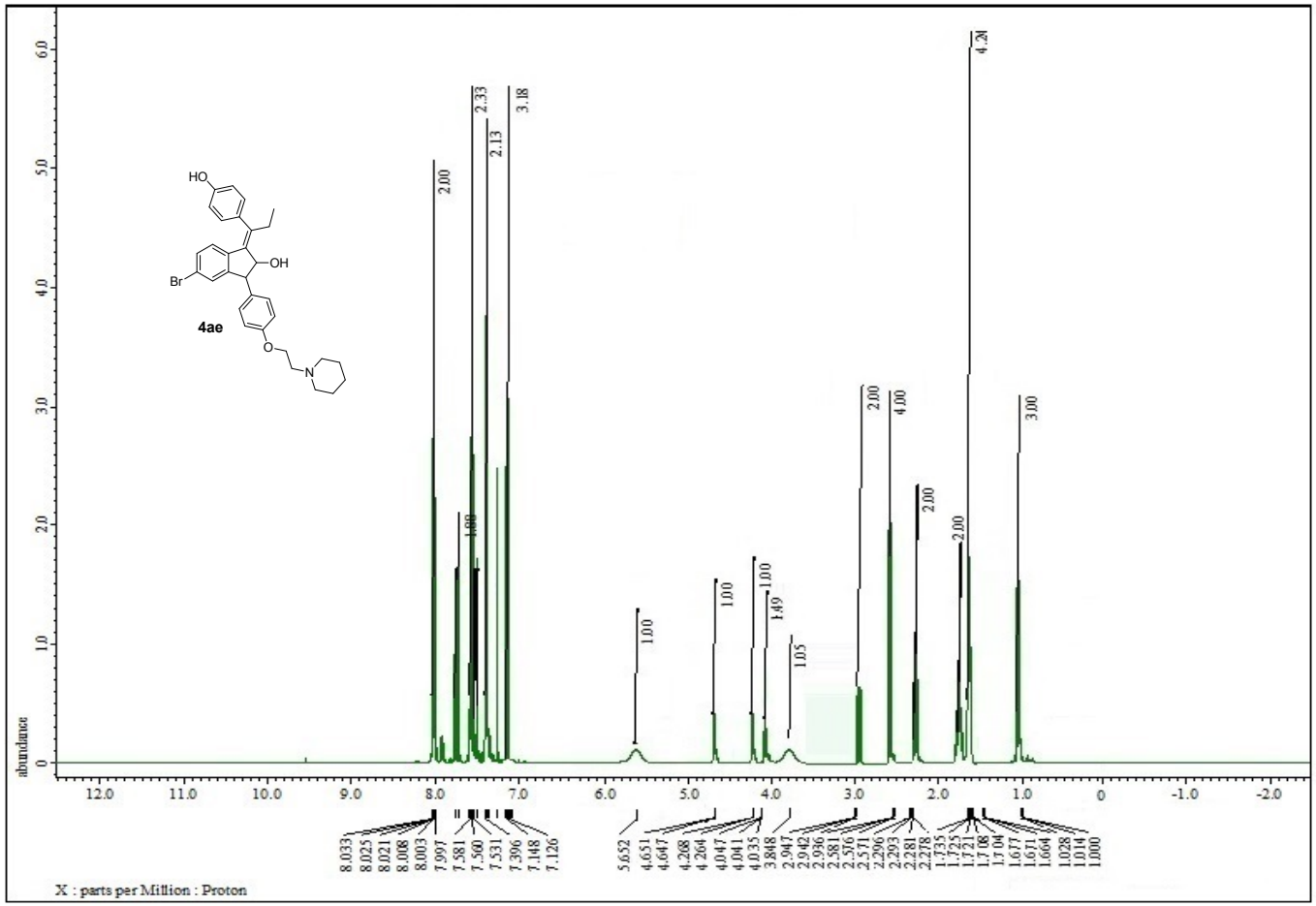
14.100
X : parts per Million : Carbon13


HO
OH
Br
O
N
4ae
abundance
X : parts per Million : Proton
2.00
1.08
2.33
2.13
3.18
1.00
1.00
1.00
1.49
1.05
2.00
4.00
2.00
2.00
4.20
3.00
8.033
8.025
8.021
8.008
8.003
7.997
7.581
7.560
7.531
7.396
7.148
7.126
5.652
4.651
4.647
4.268
4.264
4.047
4.041
4.035
3.848
2.947
2.942
2.996
2.581
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2.293
2.281
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1.704
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1.671
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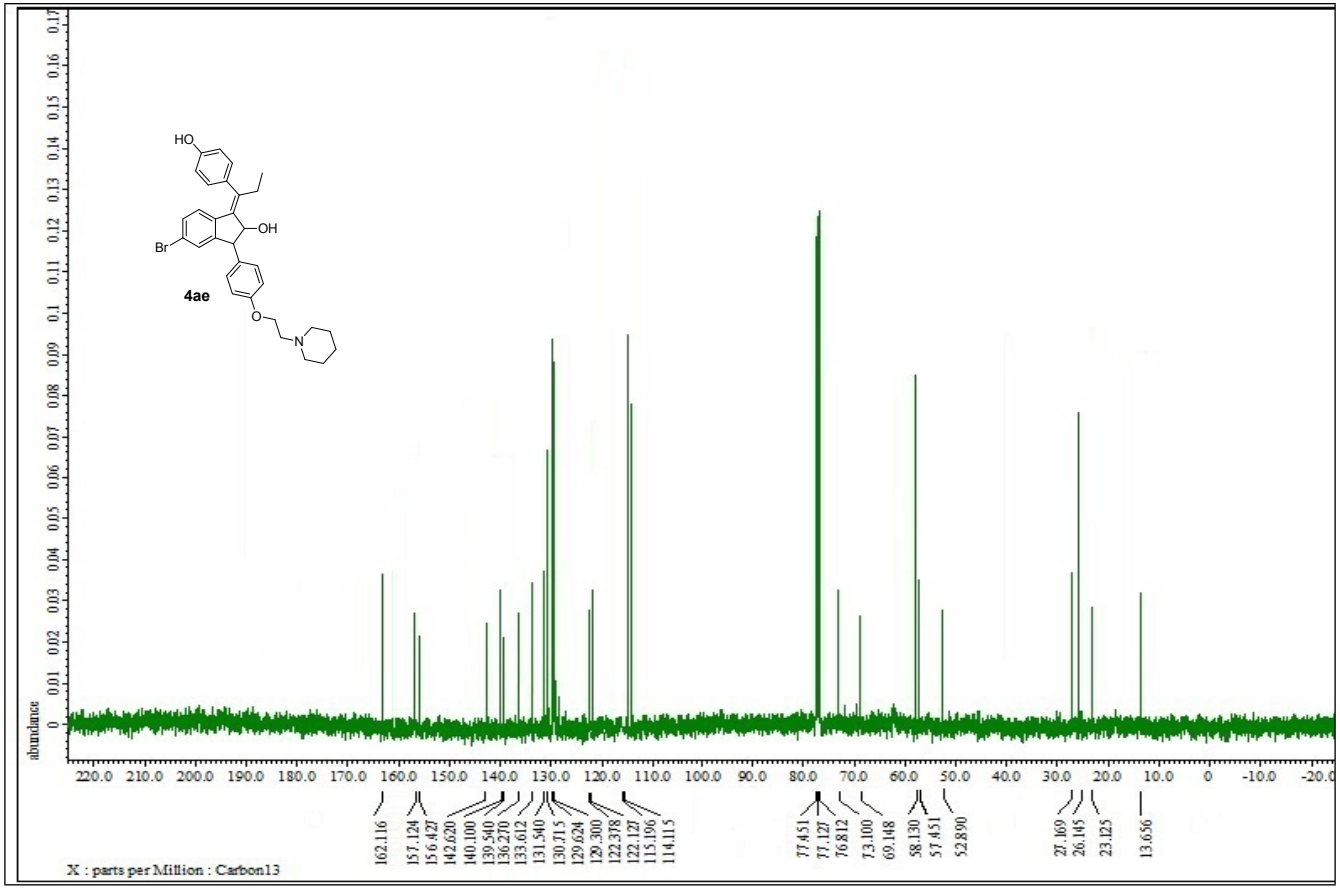
1.014
1.000


HO
OH
Br
4ae
O
N
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
0.16
0.17
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
162.116
157.124
156.427
142.620
140.100
139.540
136.270
133.612
131.540
130.715
129.624
129.300
122.378
122.127
115.196
114.115
77.451
77.127
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26.145
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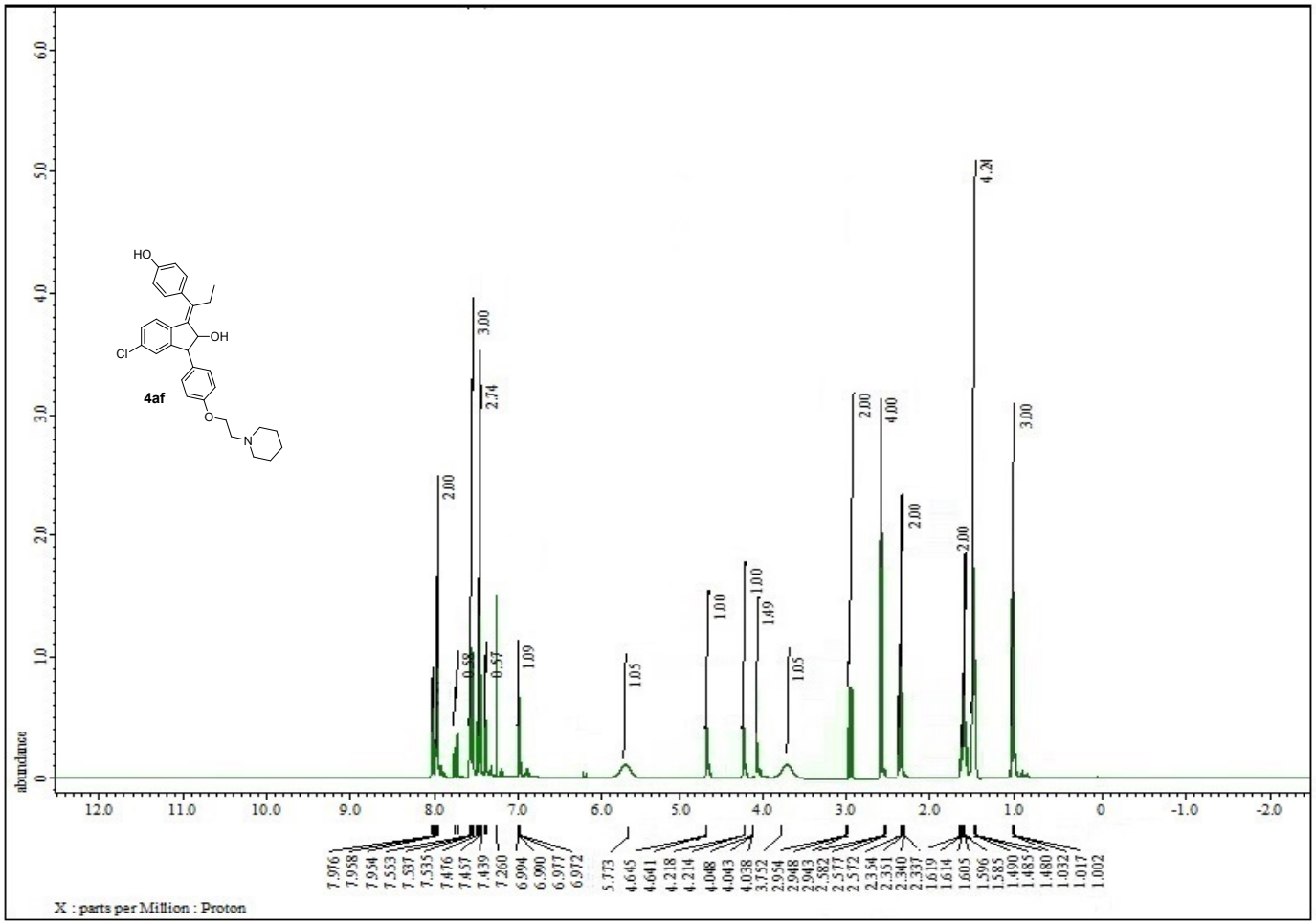
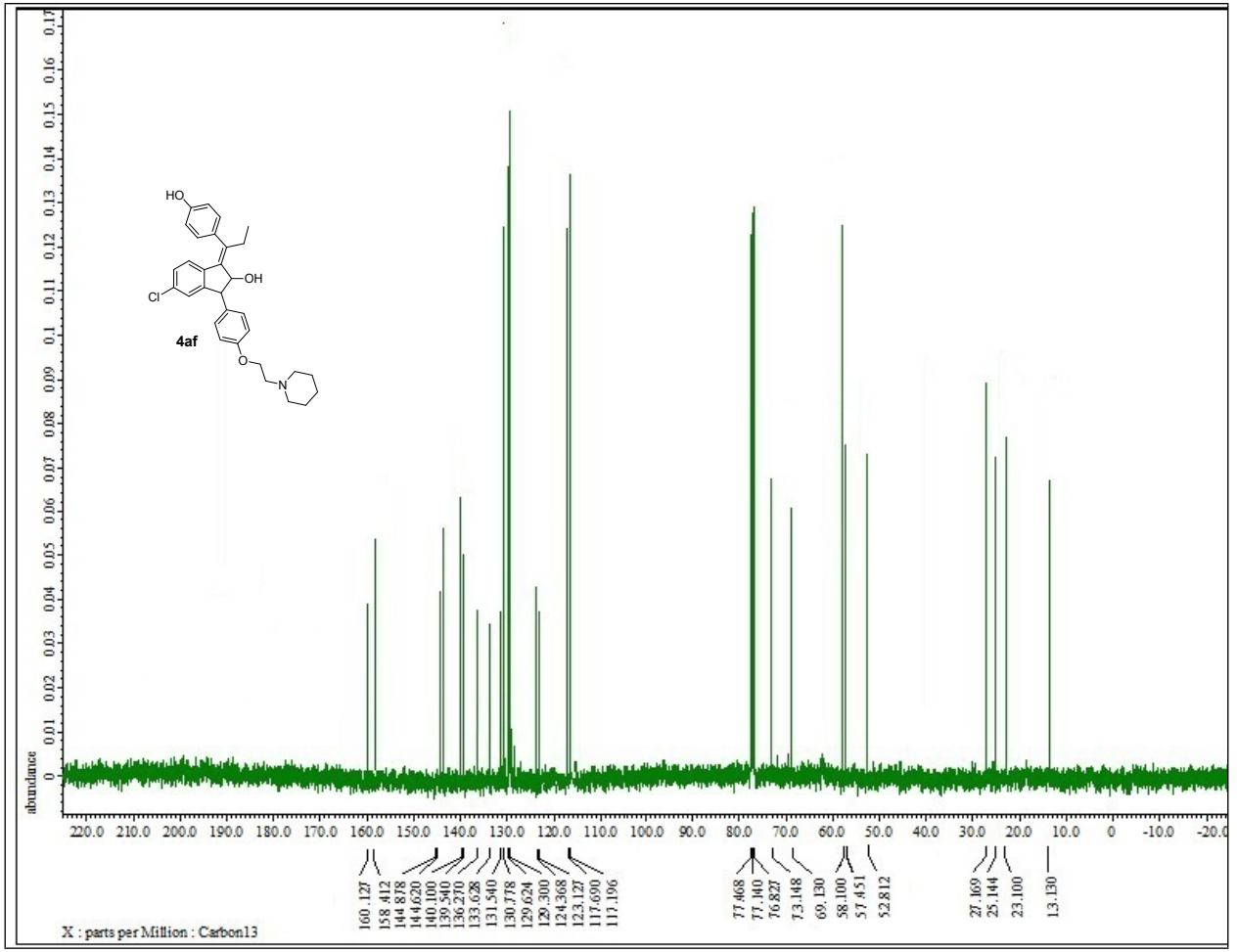
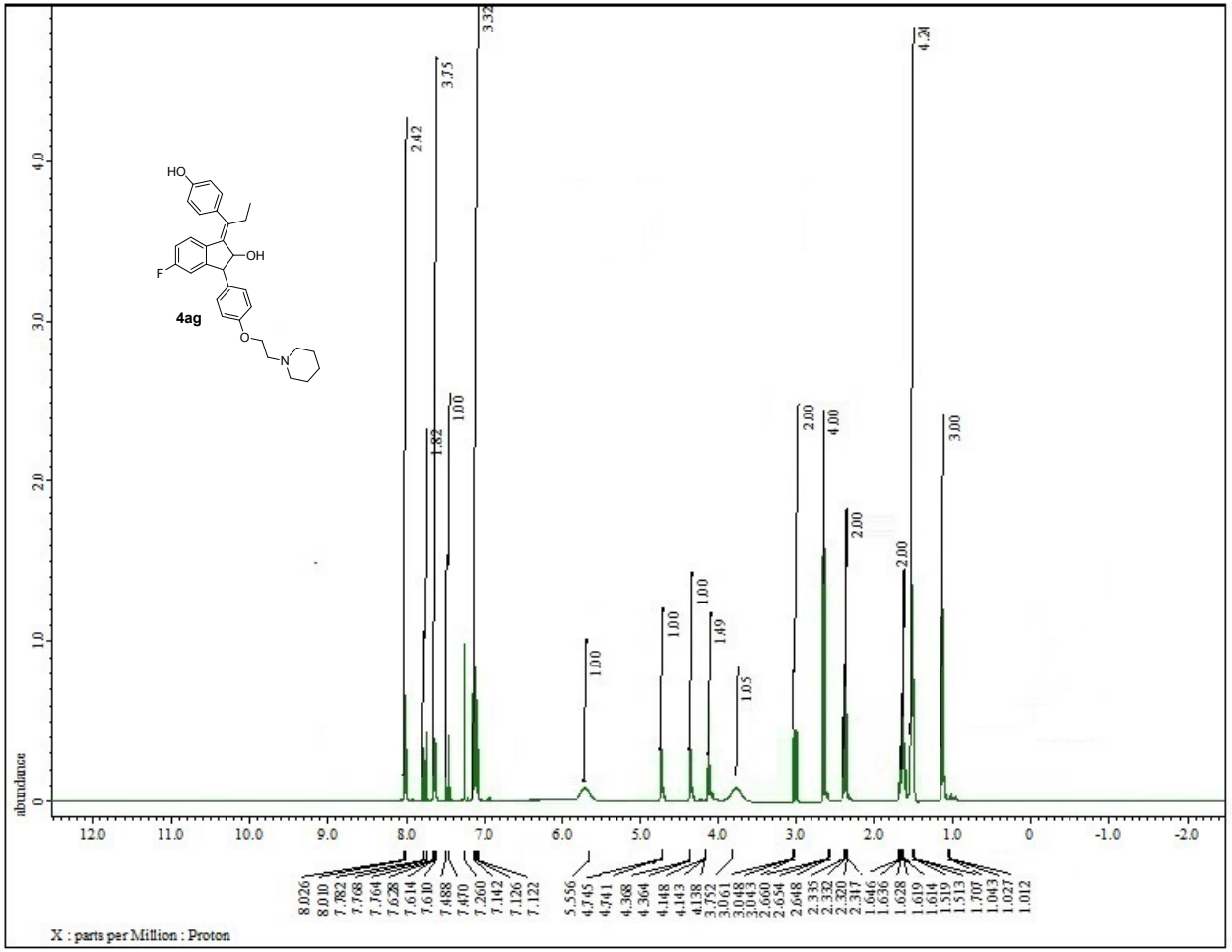
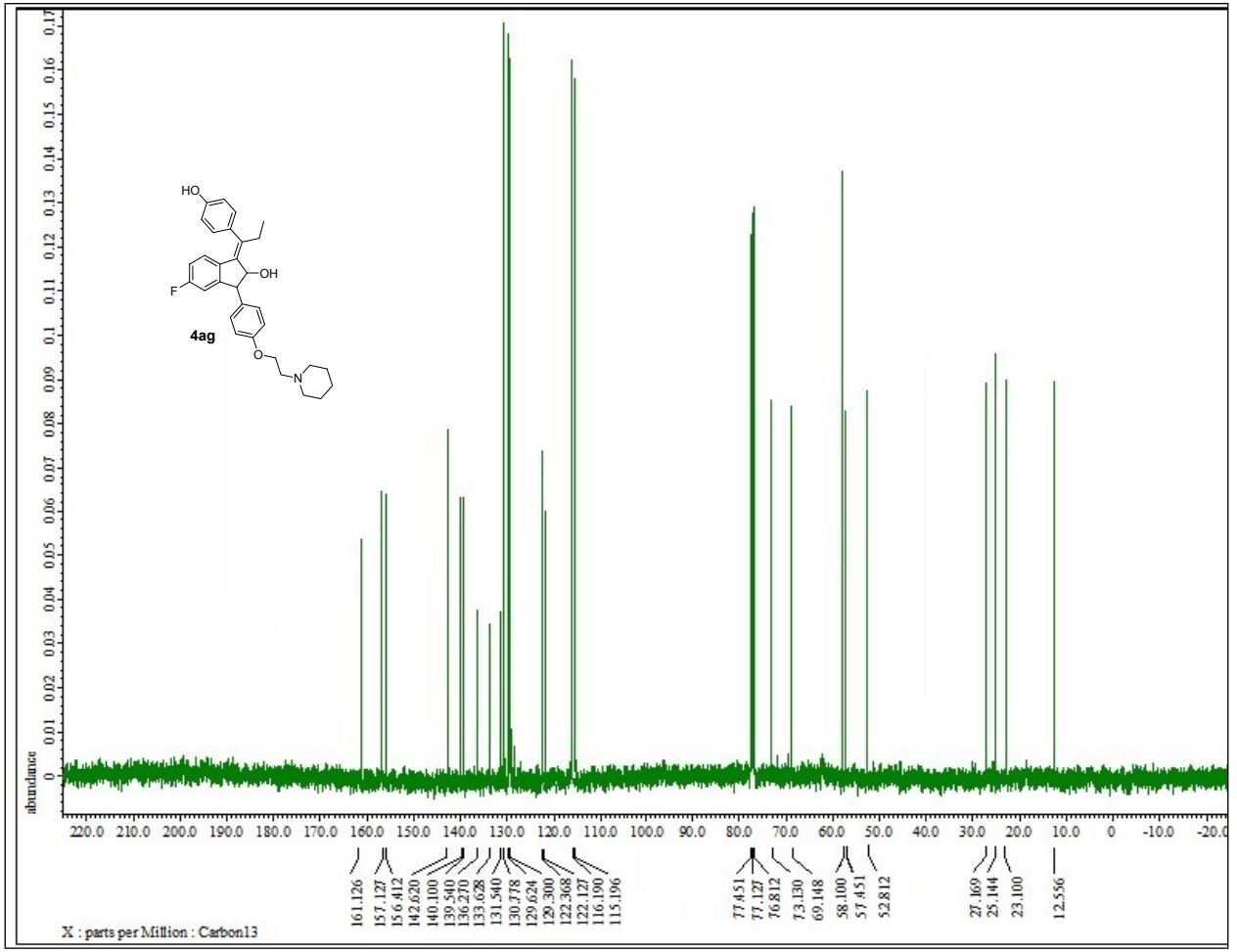
X : parts per Million : Carbon13

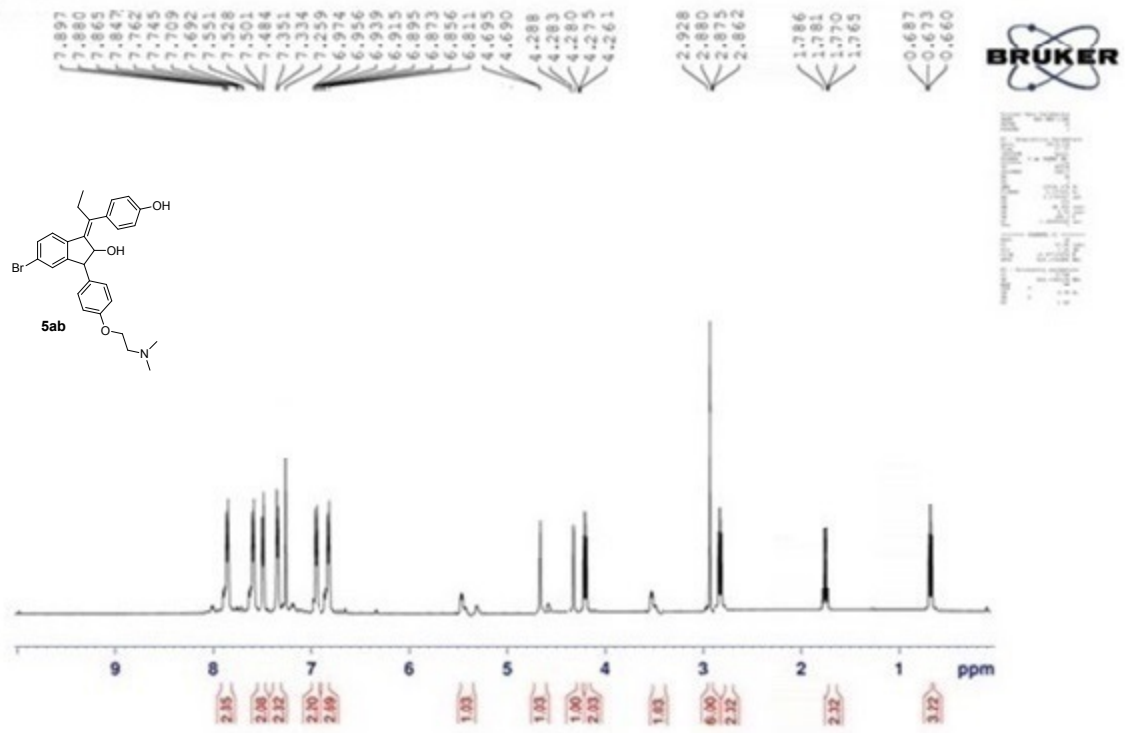

HO
OH
Cl
O
N
4af
abundance
X : parts per Million : Proton


HO
OH
Cl
O
N
4af
abundance
X : parts per Million : Carbon13
160.127
158.412
144.878
144.620
140.100
139.540
136.270
133.628
131.540
130.778
129.624
129.300
124.368
123.127
117.690
117.196
77.468
77.140
76.827
73.148
69.130
58.100
57.451
52.812
27.469
25.144
23.100
13.130


HO
OH
F
O
N
4ag
abundance
X : parts per Million : Proton


HO
OH
F
O
N
4ag
abundance
X : parts per Million : Carbon13
161.126
157.127
156.412
142.620
140.100
139.540
136.270
133.628
131.540
130.778
129.624
129.300
122.368
122.127
116.190
115.196
77.451
77.127
76.812
73.130
69.148
58.100
57.451
52.812
27.469
25.144
23.100
12.556

GP 5ab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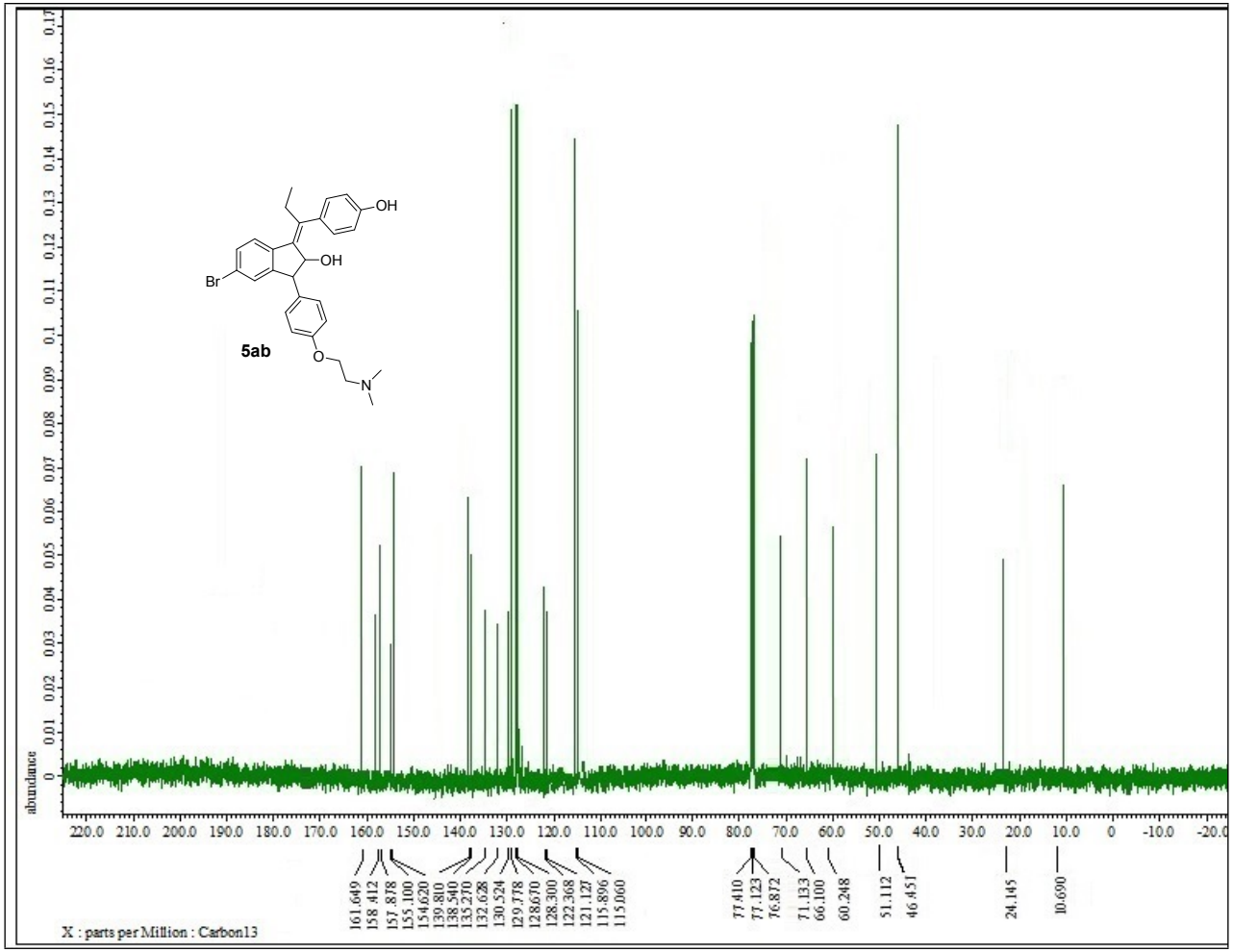
7.880
7.865
7.847
7.762
7.745
7.709
7.692
7.551
7.528
7.501
7.484
7.351
7.334
7.259
6.974
6.956
6.939
6.915
6.895
6.873
6.856
6.811
4.695
4.690
4.288
4.283
4.280
4.275
4.261
2.928
2.880
2.875
2.862
1.786
1.781
1.770
1.765
0.687
0.673
0.660
BRUKER
OH
OH
Br
O
N
5ab
9
8
7
6
5
4
3
2
1
ppm
2.15
2.08
2.12
2.00
2.09
1.03
1.03
1.00
2.03
1.83
6.00
2.12
2.12
3.22


OH
OH
Br
O
N
5ab
abundance
X : parts per Million : Carbon13
161.649
158.412
157.878
155.100
154.620
139.810
138.540
135.270
132.628
130.524
129.778
128.670
128.300
122.368
121.127
115.896
115.060
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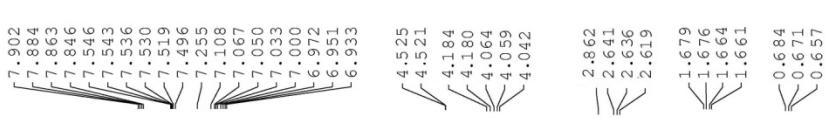
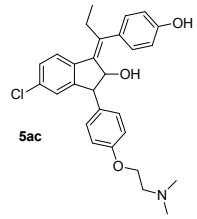
77.123
76.872
71.133
66.100
60.248
51.112
46.451
24.145
10.690

GP-5ac




5ac



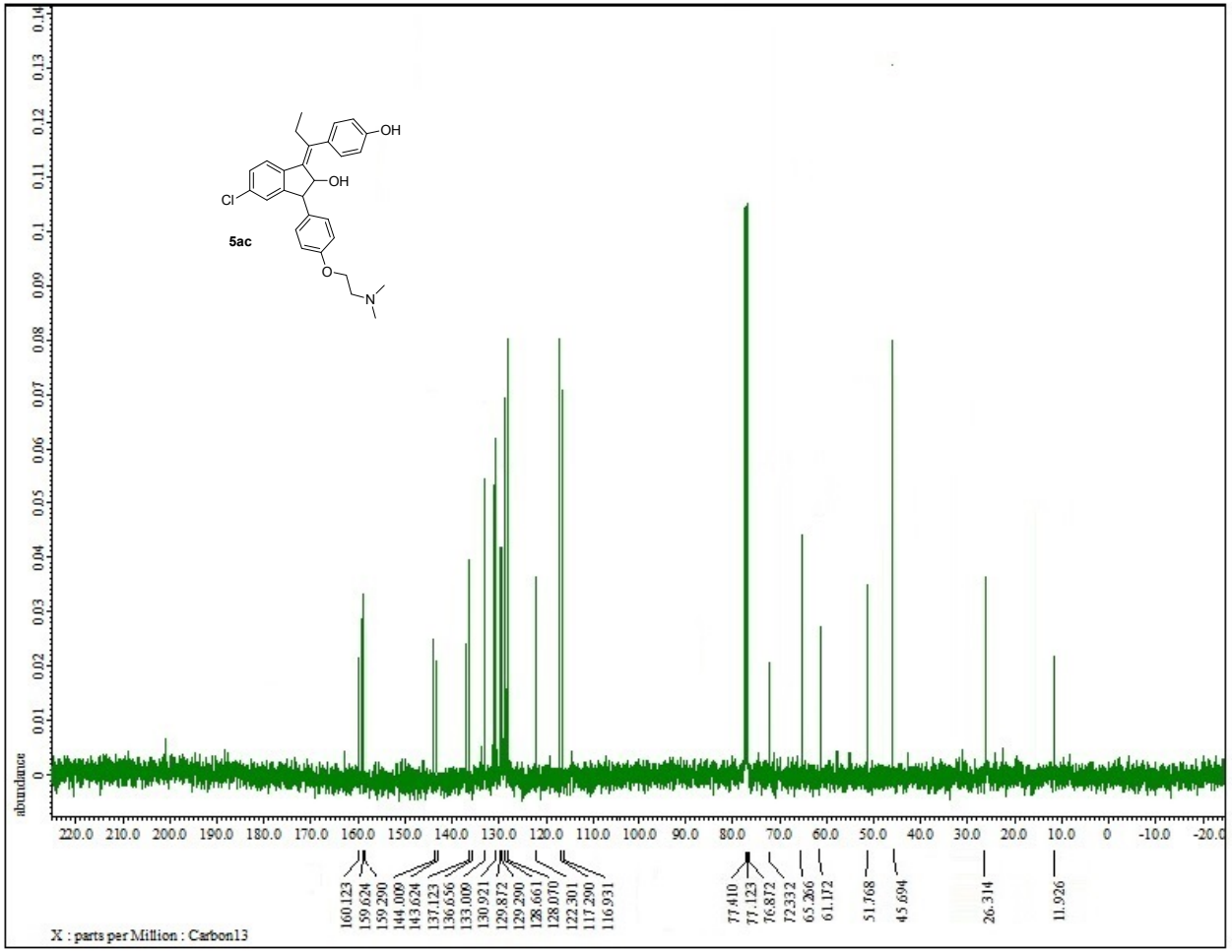


Current Data Parameters
NAME 5H-5ac
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141125
Time 11.25
INSTRUM Spect
PROBHD 5mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PLW1 14.97724854 W
SFO1 600.1330885 MHz

F2 - Processing parameters
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


OH
OH
Cl
5ac
O
N
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
160.123
159.624
159.290
144.009
143.624
137.123
136.656
133.009
130.921
129.872
129.290
128.661
128.070
122.301
117.290
116.931
77.410
77.123
76.872
72.332
65.266
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51.768
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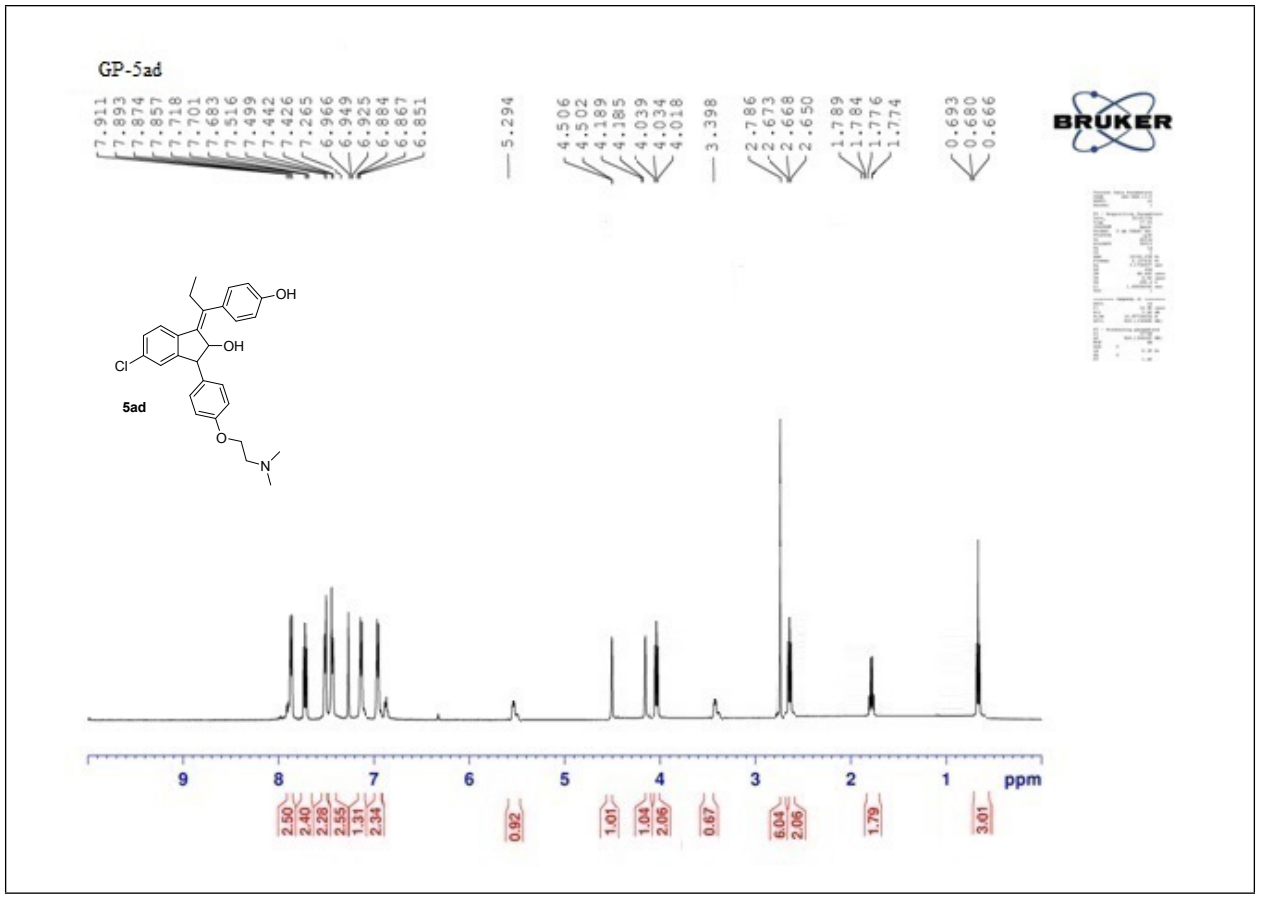
26.314
11.926
X : parts per Million : Carbon13


GP-5ad
7.911
7.893
7.874
7.857
7.718
7.701
7.683
7.516
7.499
7.442
7.426
7.265
6.966
6.949
6.925
6.884
6.867
6.851
5.294
4.506
4.502
4.189
4.185
4.039
4.034
4.018
3.398
2.786
2.673
2.668
2.650
1.789
1.784
1.776
1.774
0.693
0.680
0.666
BRUKER
OH
OH
Cl
O
N
5ad
9
8
7
6
5
4
3
2
1
ppm
2.50
2.40
2.28
2.55
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2.34
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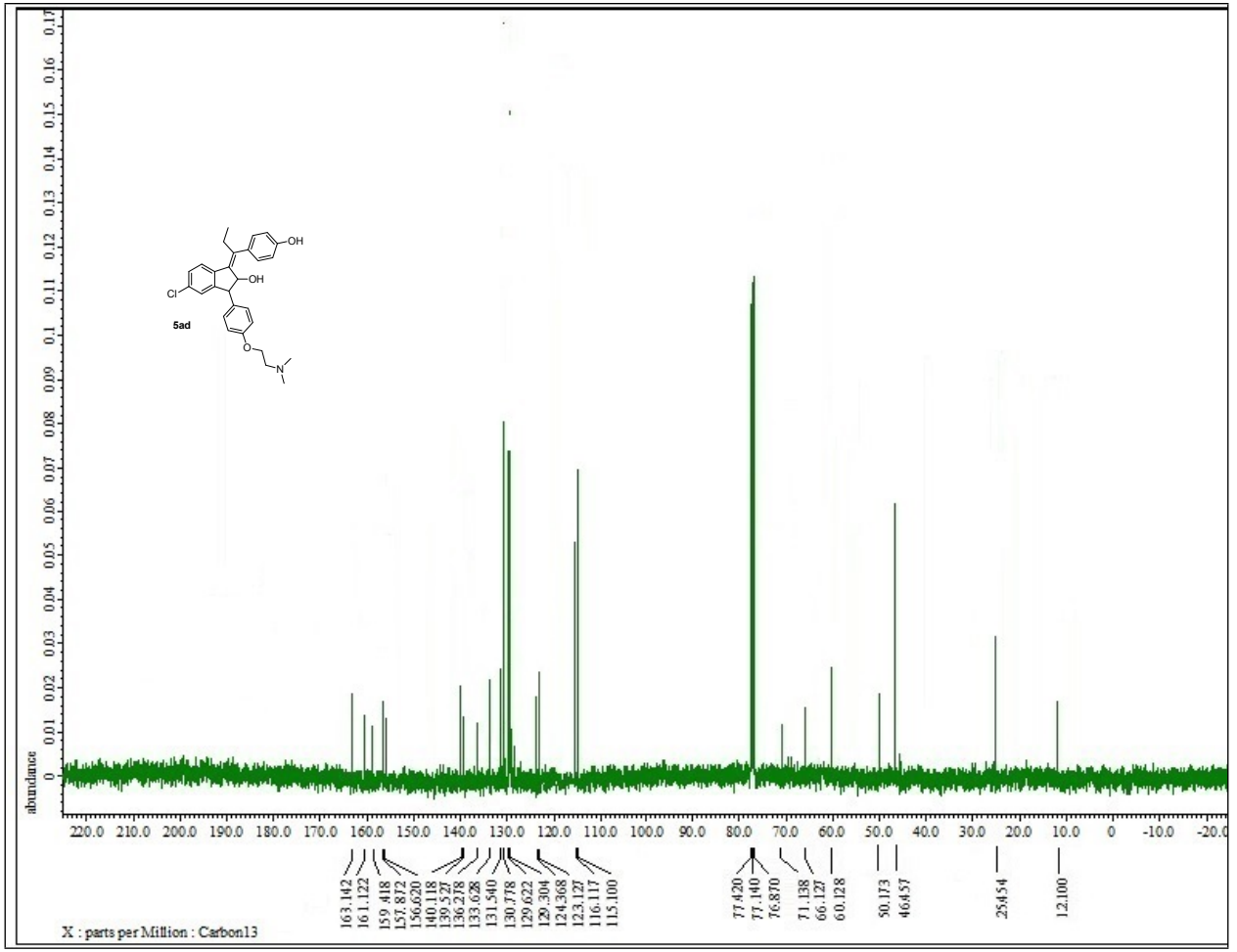
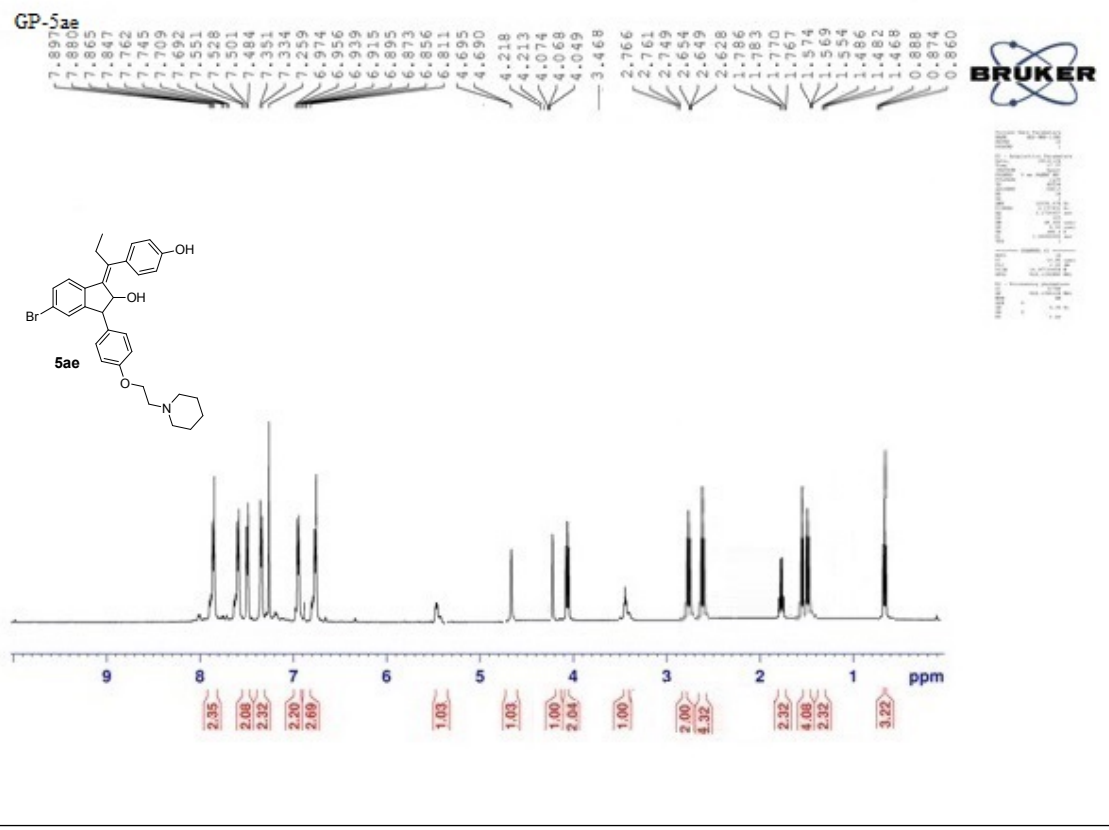
3.01


OH
OH
Cl
5ad
O
N
abundance
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.142
161.122
159.418
157.872
156.620
140.118
139.527
136.278
133.628
131.540
130.778
129.622
129.304
124.368
123.127
116.117
115.100
77.420
77.140
76.870
71.138
66.127
60.128
50.173
46.457
25.454
12.100
X : parts per Million : Carbon13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7.865
7.847
7.762
7.745
7.709
7.692
7.551
7.528
7.501
7.484
7.351
7.334
7.259
6.974
6.956
6.939
6.915
6.895
6.873
6.856
6.811
4.695
4.690
4.218
4.213
4.074
4.068
4.049
3.468
2.766
2.761
2.749
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1.574
1.569
1.554
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1.482
1.468
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0.874
0.860
BRUKER
OH
OH
Br
O
N
5ae
9
8
7
6
5
4
3
2
1
ppm
2.35
2.08
2.32
2.20
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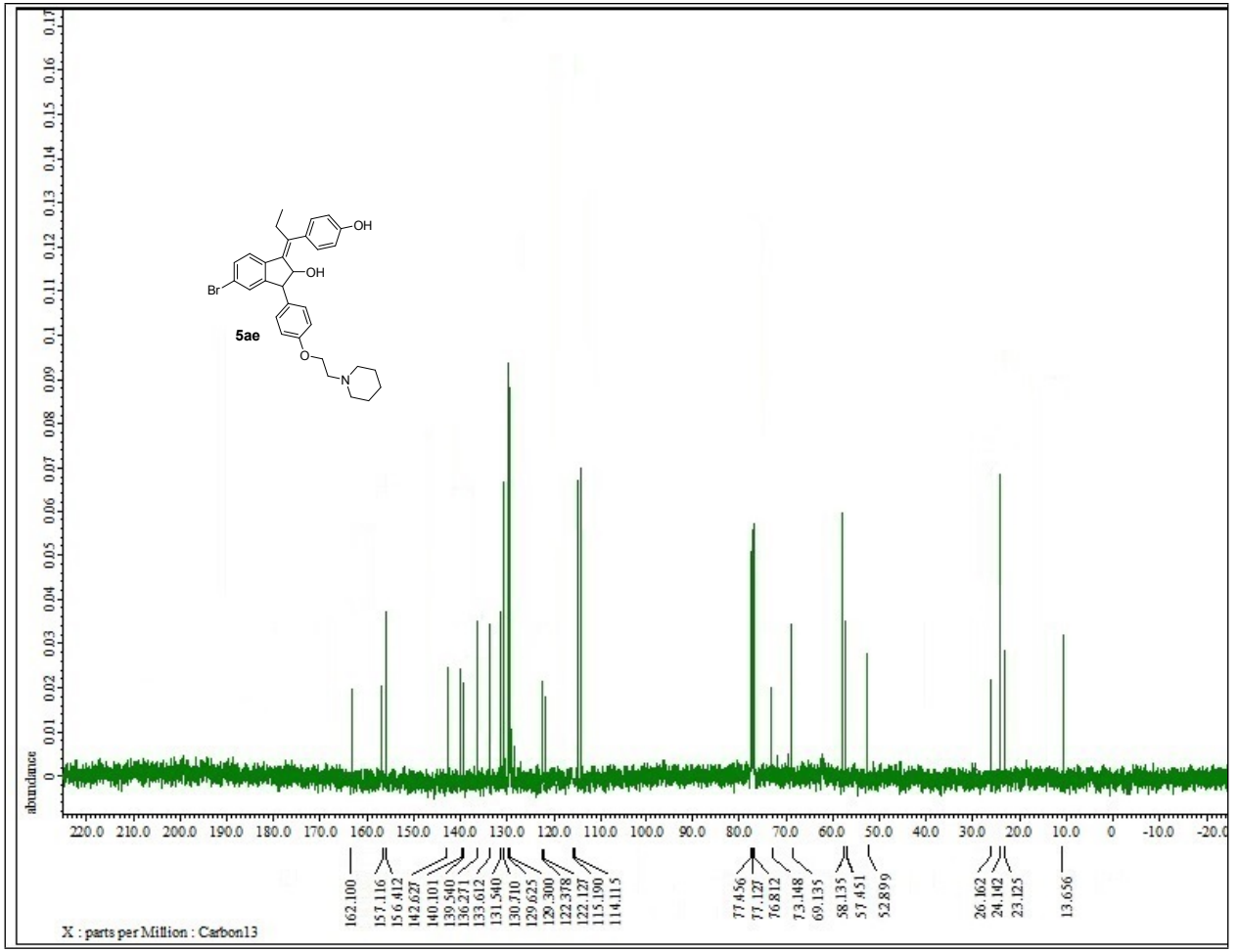
3.22


OH
OH
Br
5ae
O
N
abundance
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
162.100
157.116
156.412
142.627
140.101
139.540
136.271
133.612
131.540
130.710
129.625
129.300
122.378
122.127
115.190
114.115
77.456
77.127
76.812
73.148
69.135
58.135
57.451
52.899
26.162
24.142
23.125
13.656
X : parts per Million : Carbon13

GP-5af

7.887
7.871
7.854
7.530
7.514
7.497
7.443
7.426
7.269
7.022
6.985
6.961
6.944
6.922

4.680
4.676
4.242
4.238
4.117
4.112
4.102
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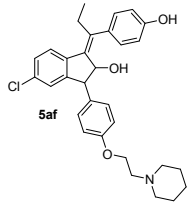
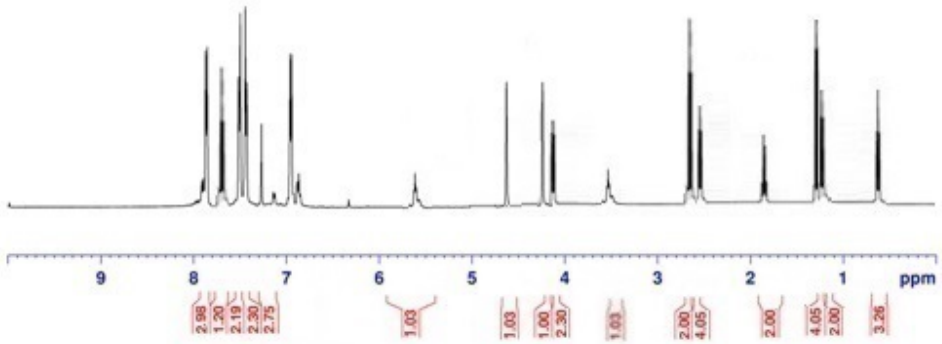
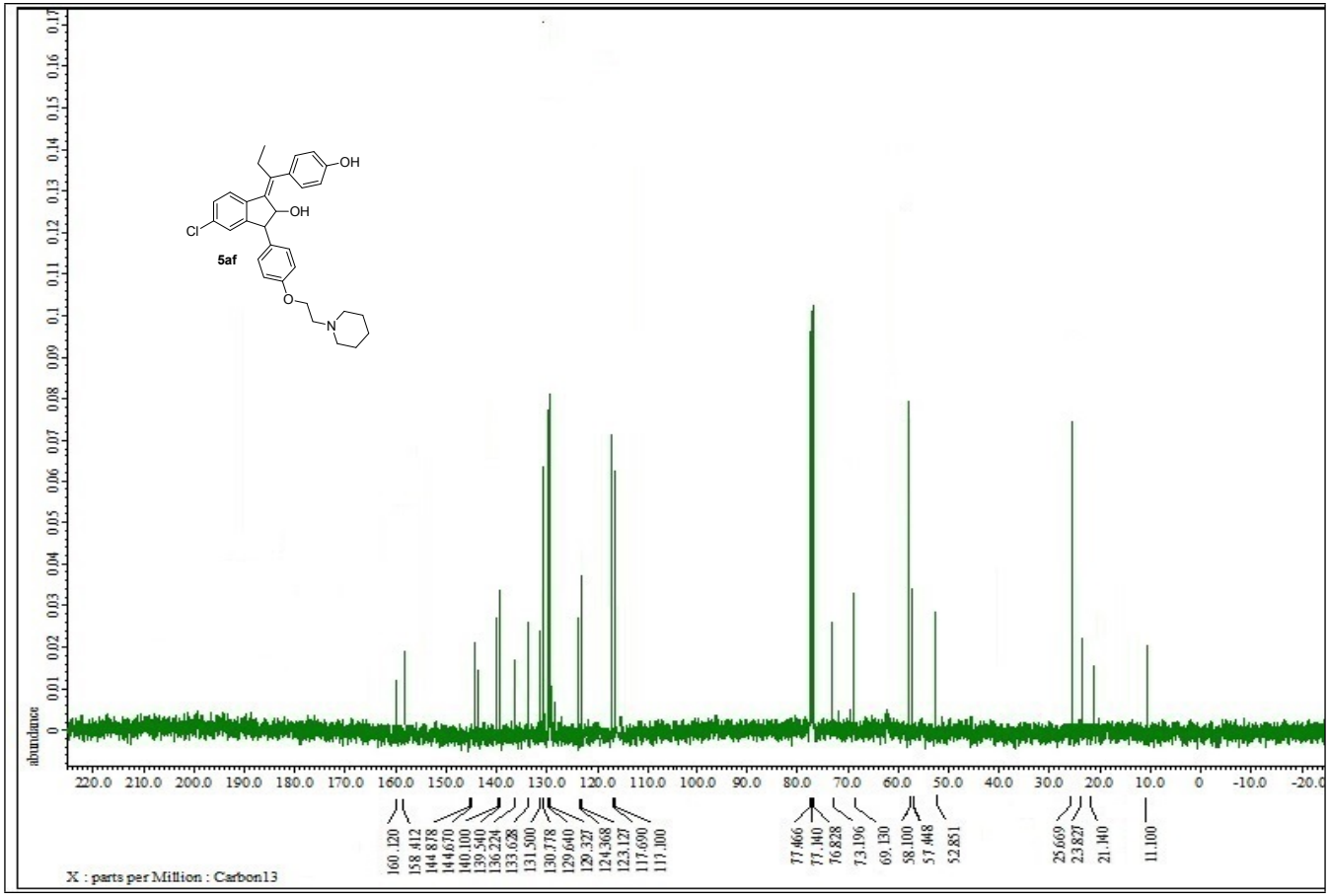
BRUKER




5af




OH
OH
Cl
5af
O
N
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
0.16
0.17
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
160.120
158.412
144.878
144.670
140.100
139.540
136.224
133.628
131.500
130.778
129.640
129.327
124.368
123.127
117.690
117.100
77.466
77.140
76.828
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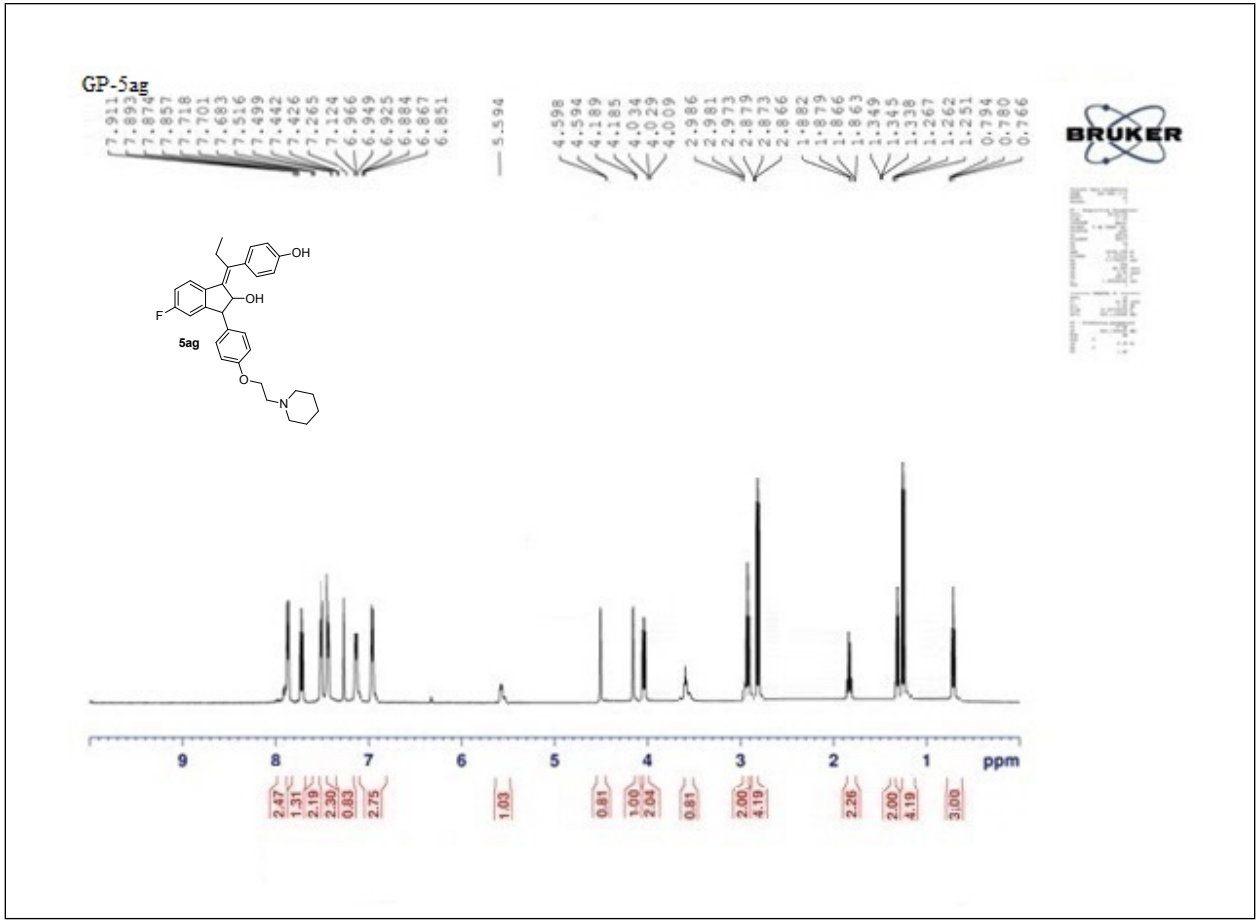
58.100
57.448
52.851
25.669
23.827
21.140
11.100
X : parts per Million : Carbon13


GP-5ag
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7.857
7.718
7.701
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7.516
7.499
7.442
7.426
7.265
7.124
6.966
6.949
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6.884
6.867
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4.598
4.594
4.189
4.185
4.034
4.029
4.009
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1.879
1.866
1.863
1.349
1.345
1.338
1.267
1.262
1.251
0.794
0.780
0.766
BRUKER
OH
OH
F
5ag
O
N
9
8
7
6
5
4
3
2
1
ppm
2.47
1.31
2.19
2.30
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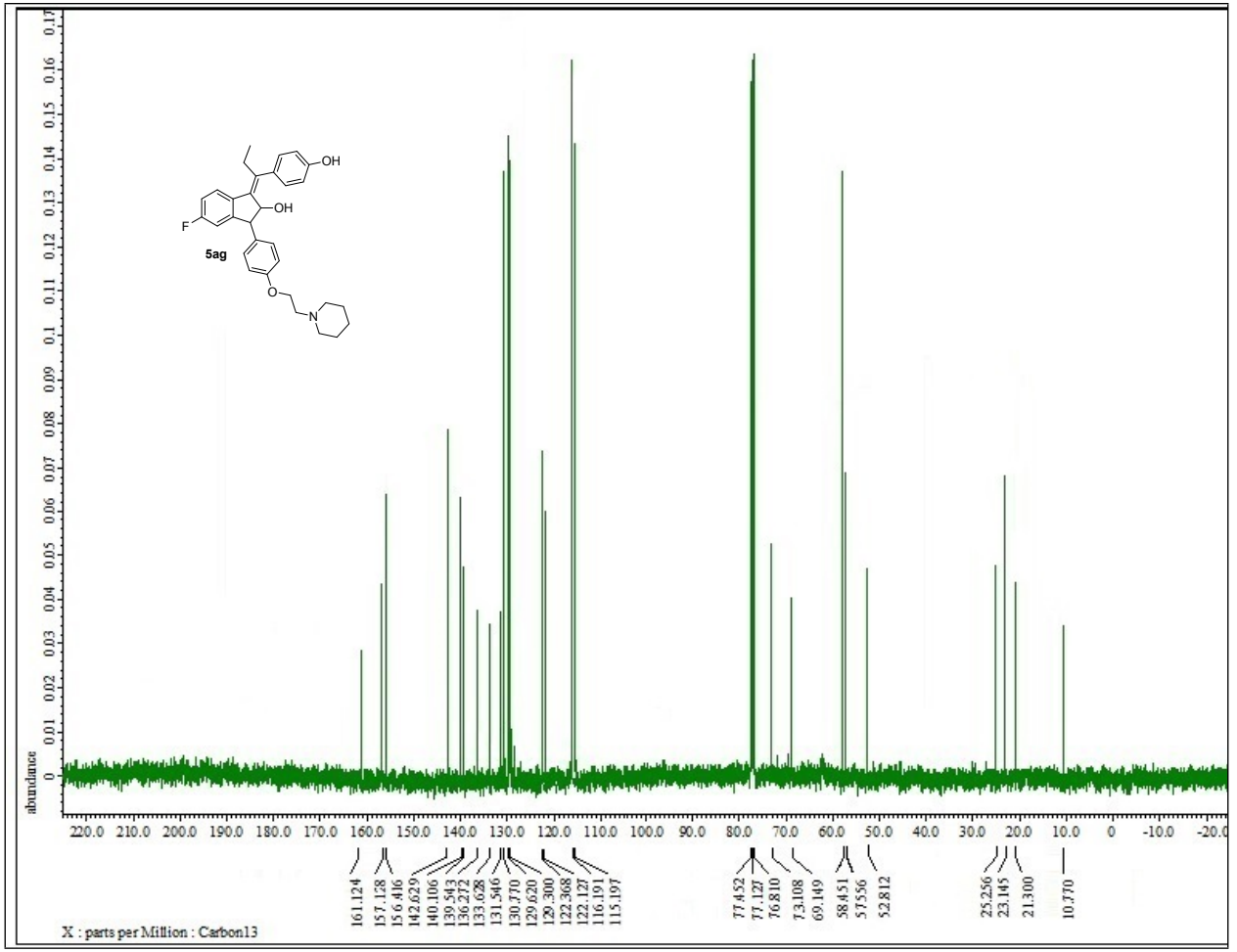
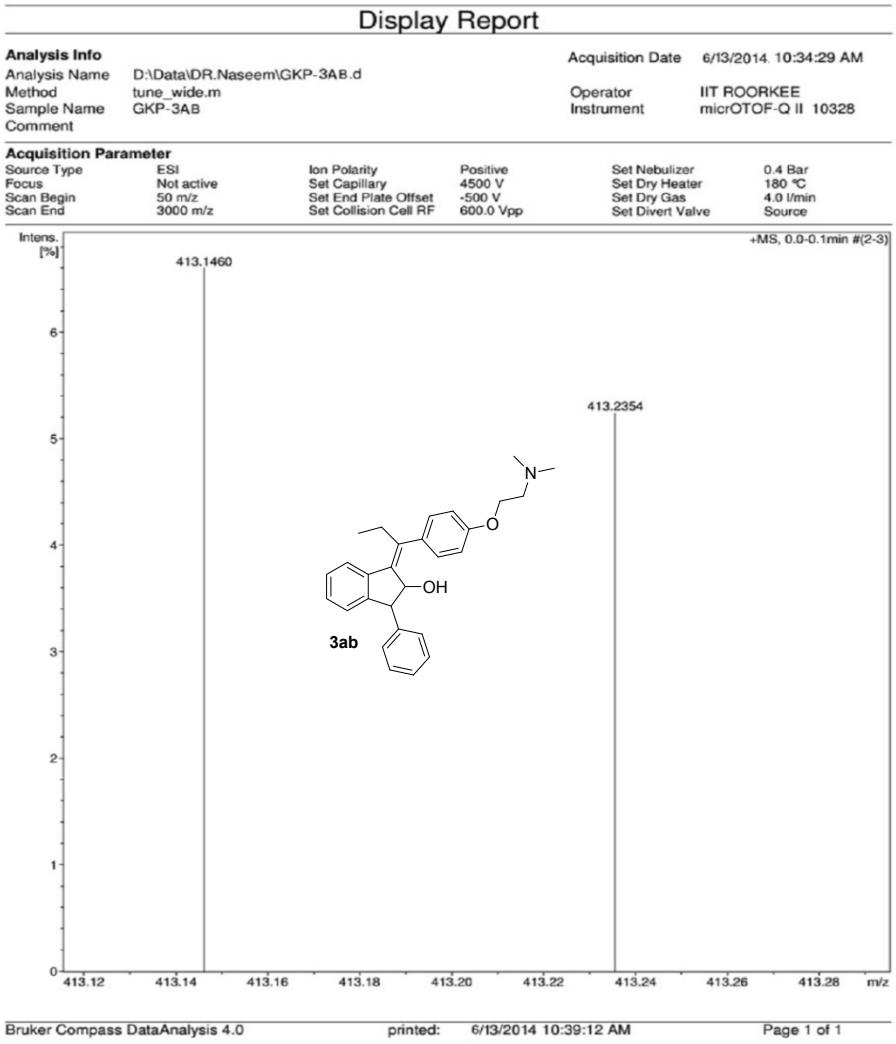
3.00


OH
OH
F
5ag
O
N
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
161.124
157.128
156.416
142.629
140.106
139.543
136.272
133.628
131.546
130.770
129.620
129.300
122.368
122.127
116.191
115.197
77.452
77.127
76.810
73.108
69.149
58.451
57.556
52.812
25.256
23.145
21.300
10.770
X : parts per Million : Carbon13

## 4. HRMS spectras of selected tamoxifen analogs



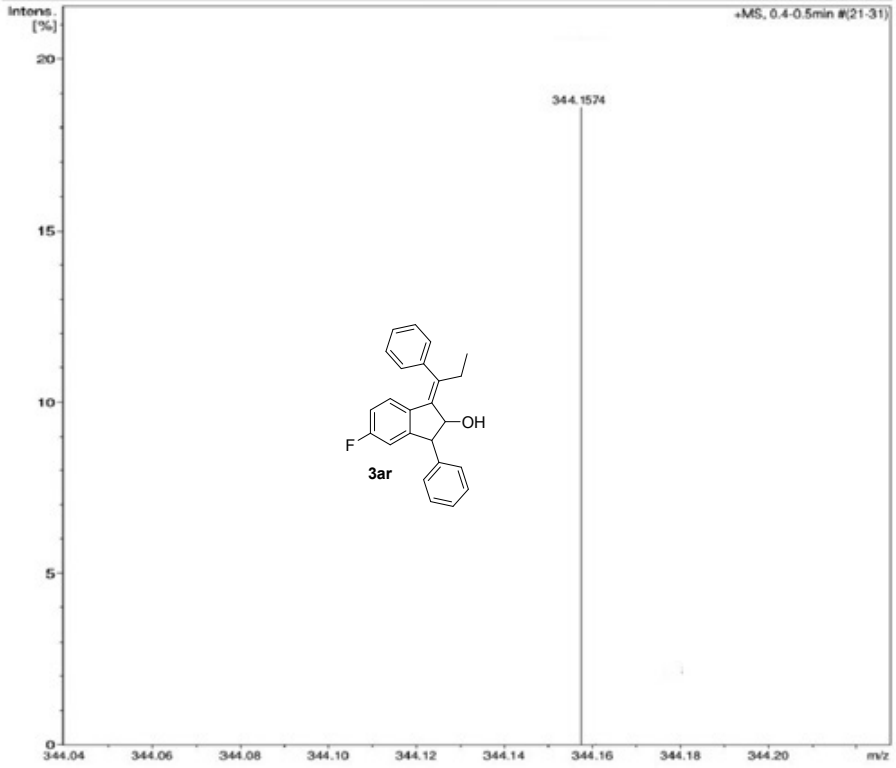
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\DR.Naseem\GKP3 AR.d | Acquisition Date | 6/23/2014 11:32:28 AM |
| Method | tune_wide.m | Operator | IIT ROORKEE |
| Sample Name | GKP3 AR | Instrument | micrOTOF-Q II 10328 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 600.0 Vpp | Set Divert Valve | Source |




**3ar**

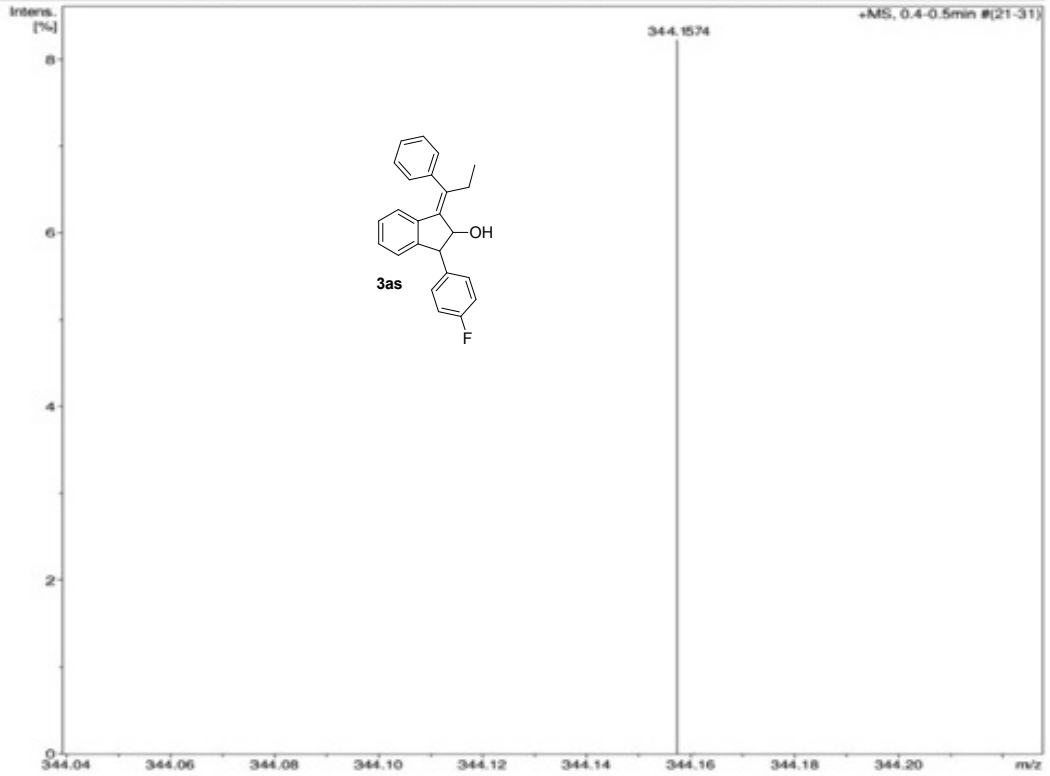
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\DR.Naseem\ GKP-3as .d | Acquisition Date | 6/23/2014 11:03:58 AM |
| Method | tune_wide.m | Operator | IIT ROORKEE |
| Sample Name | GKP-3as | Instrument | micrOTOF-Q II 10328 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 600.0 Vpp | Set Divert Valve | Source |




**3as**

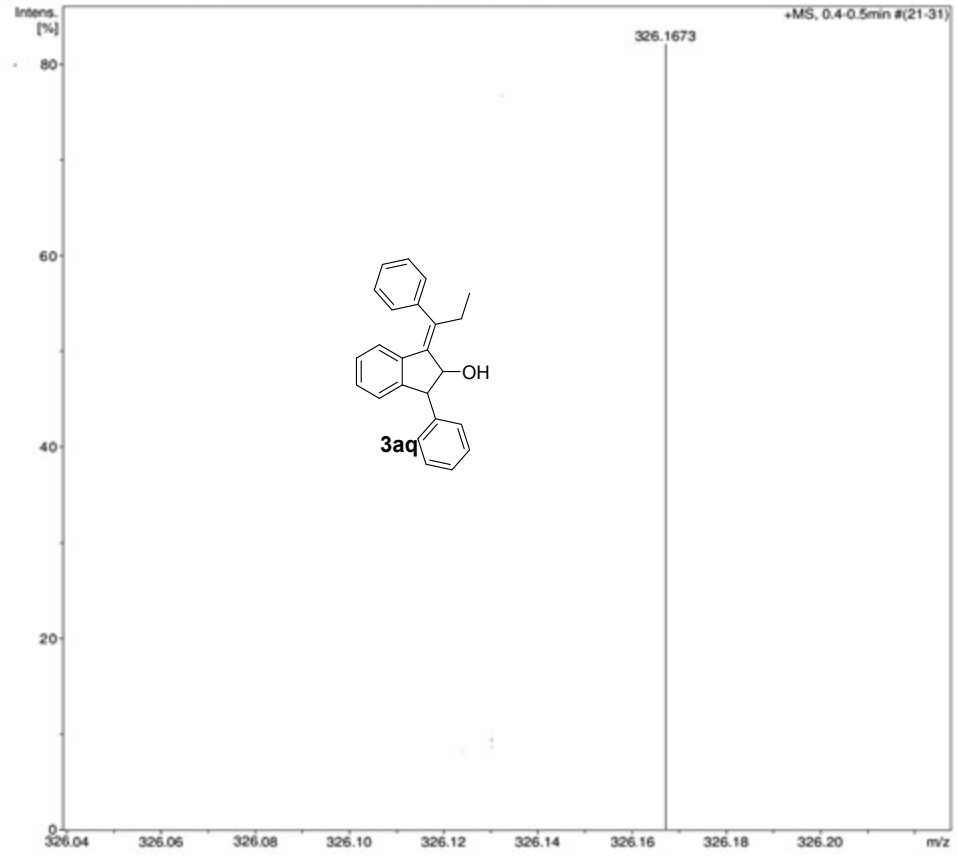
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\DR.Naseem\GKP-3aq d | Acquisition Date | 9/25/2014 10:03:28 AM |
| Method | tune_wide.m | Operator | IIT ROORKEE |
| Sample Name | GKP- 3aq | Instrument | micrOTOF-Q II 10328 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 600.0 Vpp | Set Divert Valve | Source |



# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\DR.Naseem\GKP-3AK.d | Acquisition Date | 9/21/2014 5:14:31 PM |
| Method | tune_wide.m | Operator | IIT ROORKEE |
| Sample Name | GKP-3AK | Instrument | micrOTOF-Q II 10328 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 600.0 Vpp | Set Divert Valve | Source |