Development of selective steroid inhibitors for the glucose-6-phosphate dehydrogenase from *Trypanosoma cruzi*

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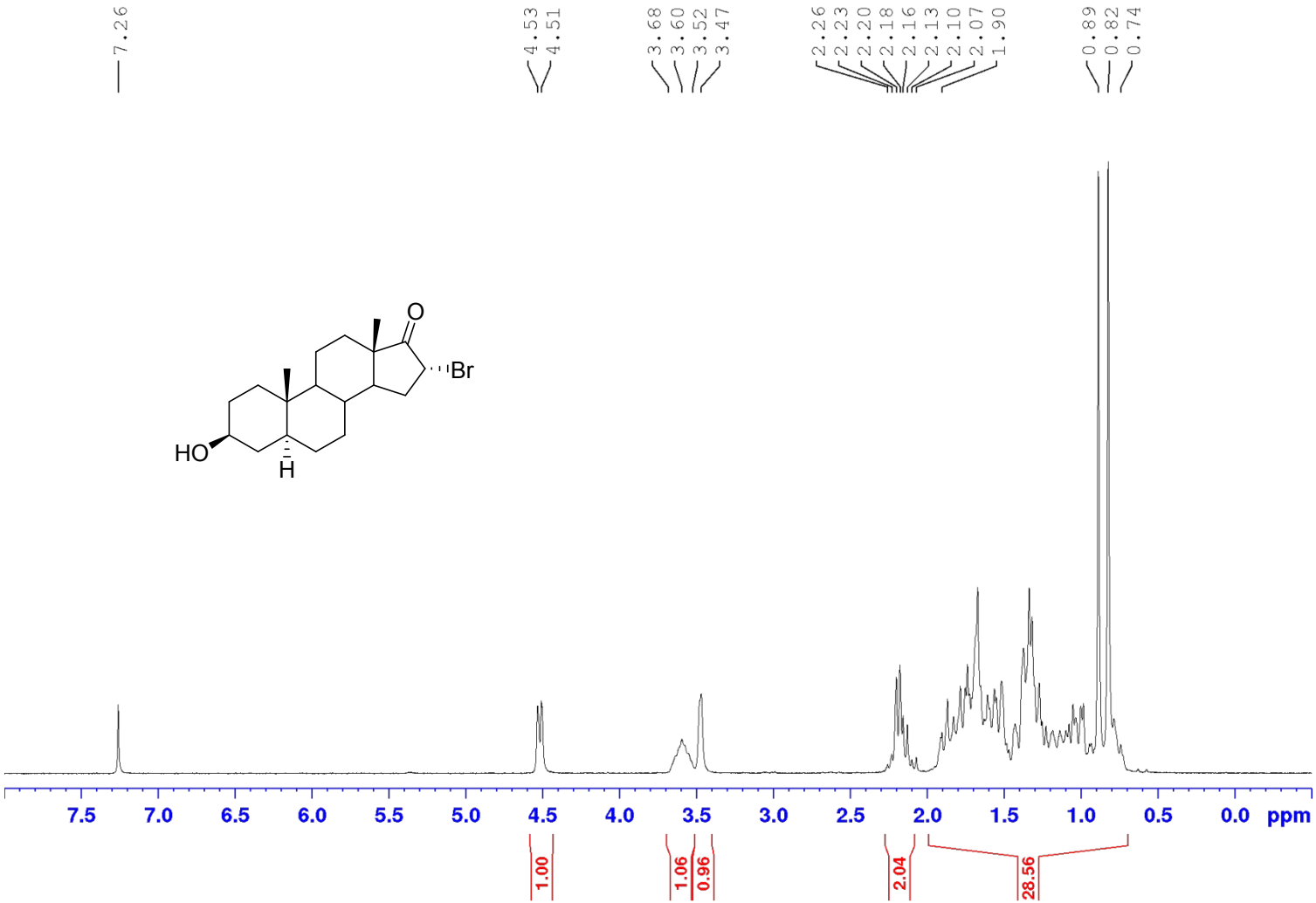
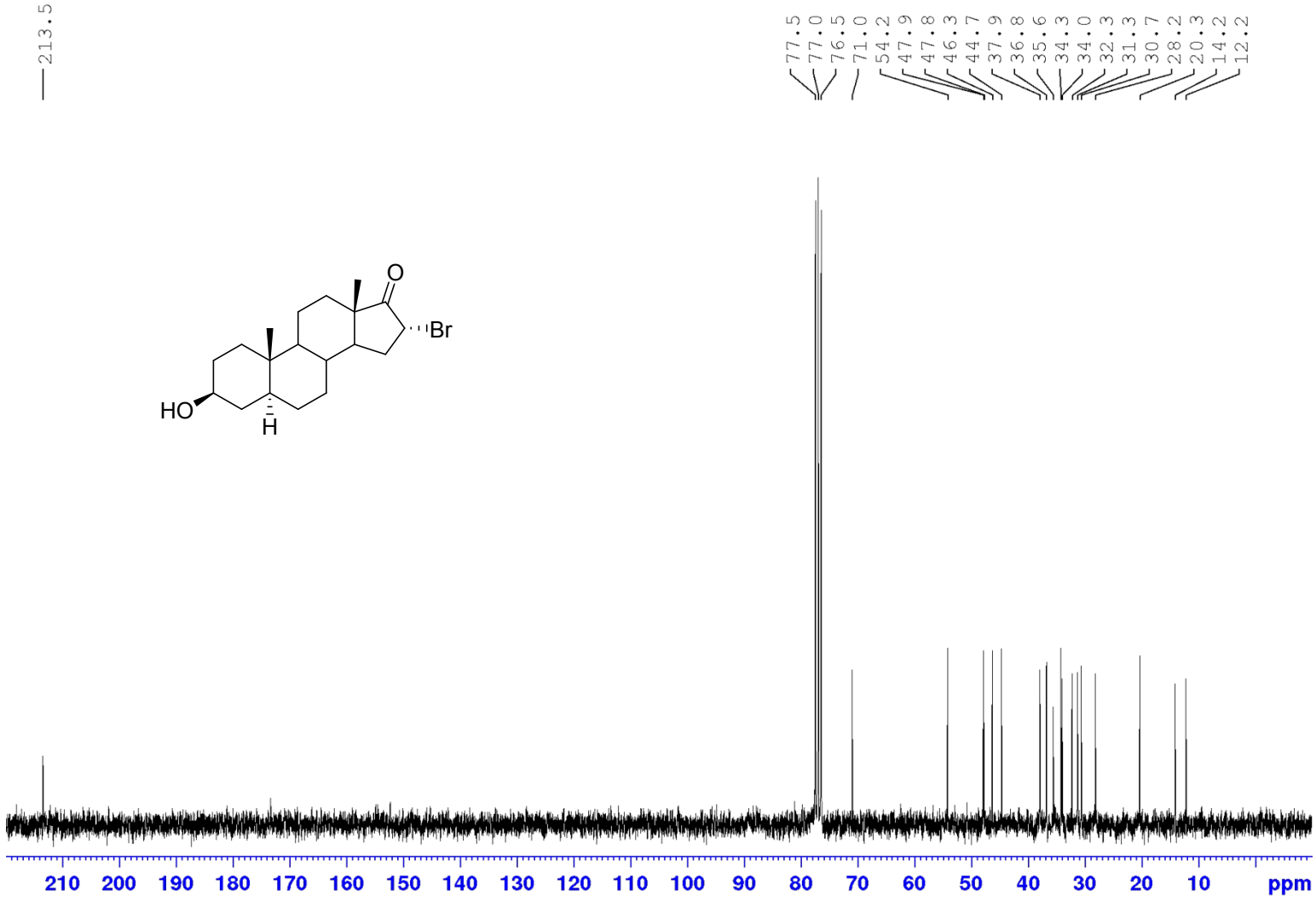
SUPPORTING INFORMATION - ANNEX

NMR spectra for compounds **3-42** and **45-50**

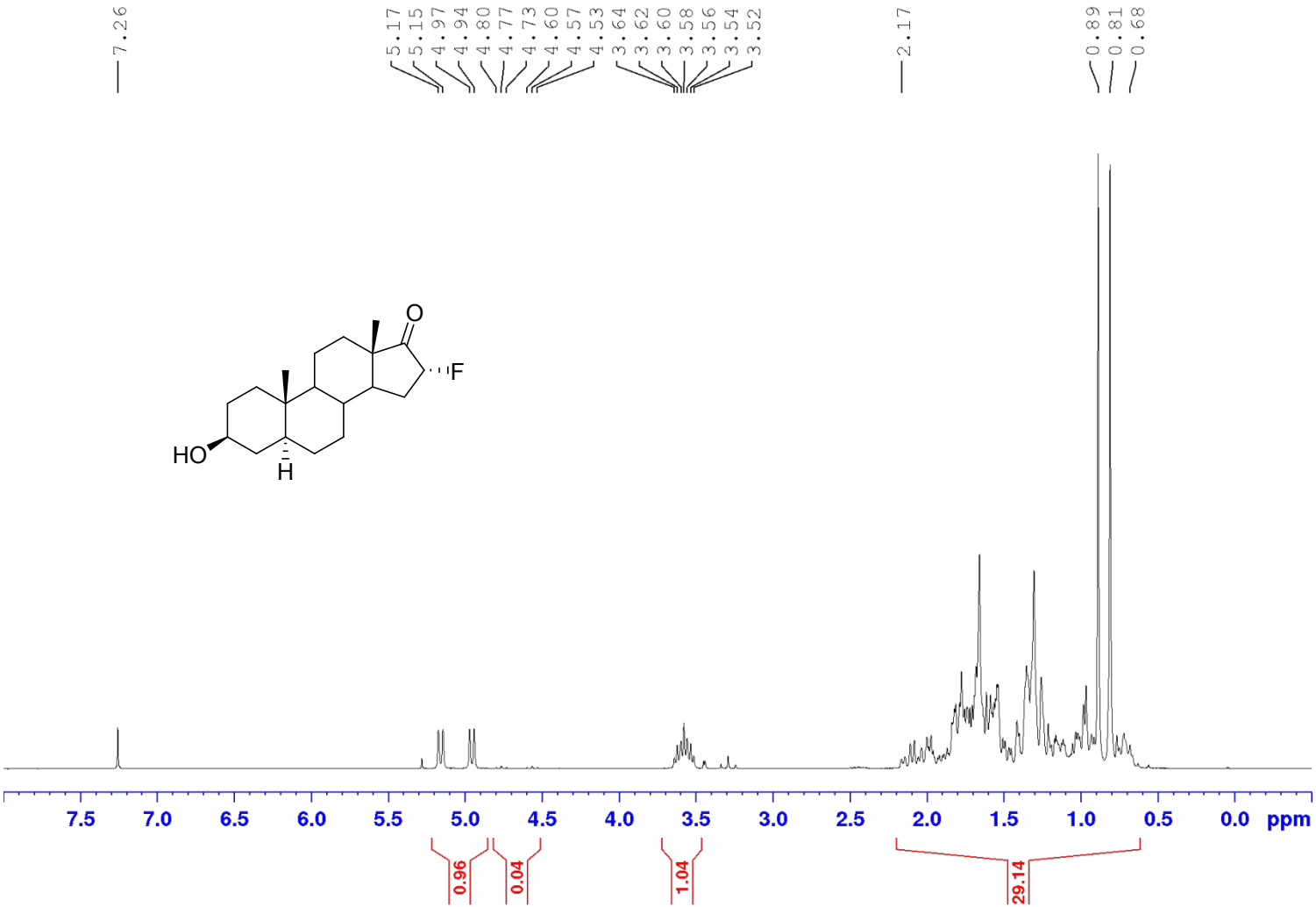
BrEA (3) – ^{1}H – $CDCl_3$ – 250 MHz



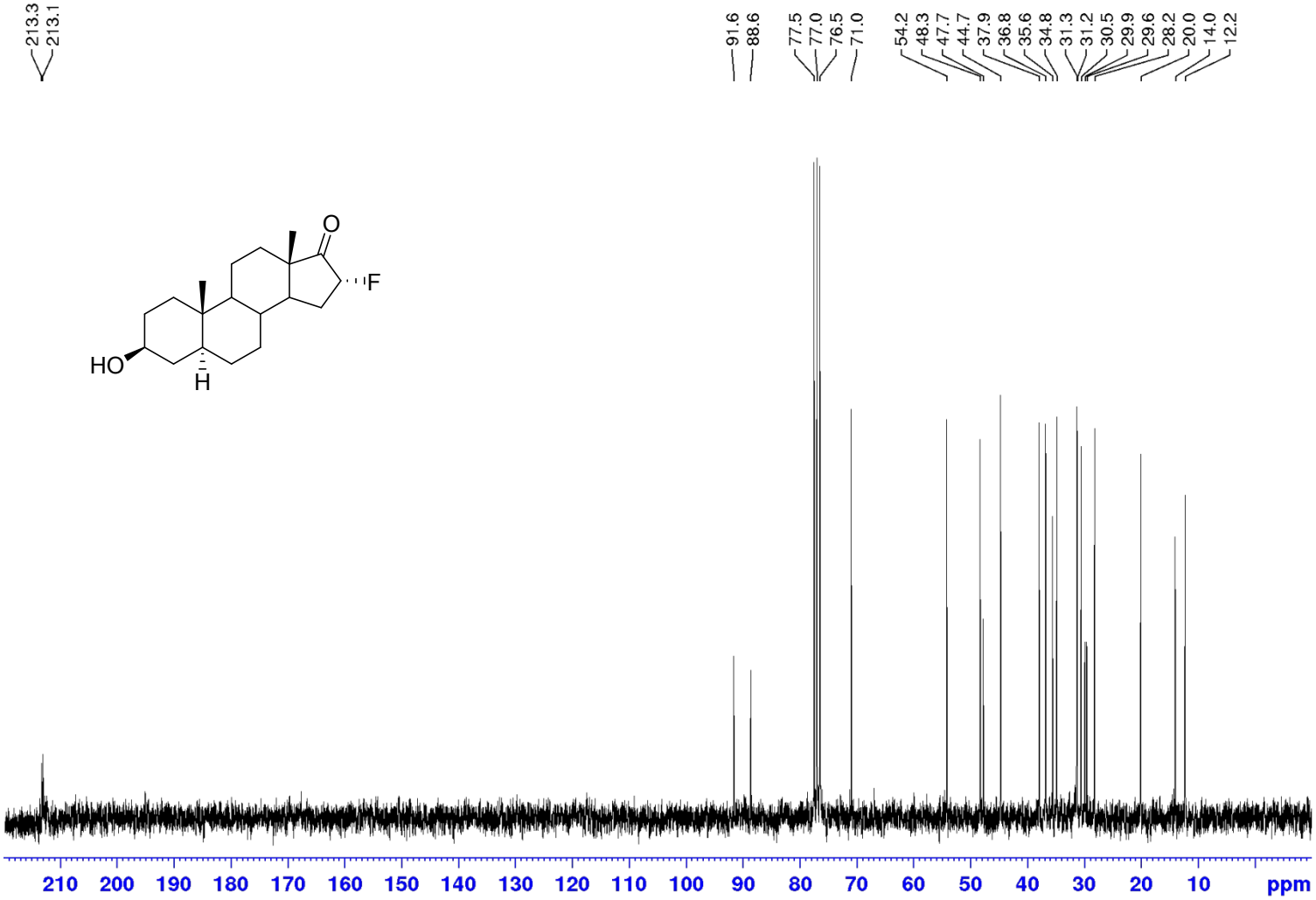
BrEA (3) – ^{13}C – $CDCl_3$ – 62.5 MHz



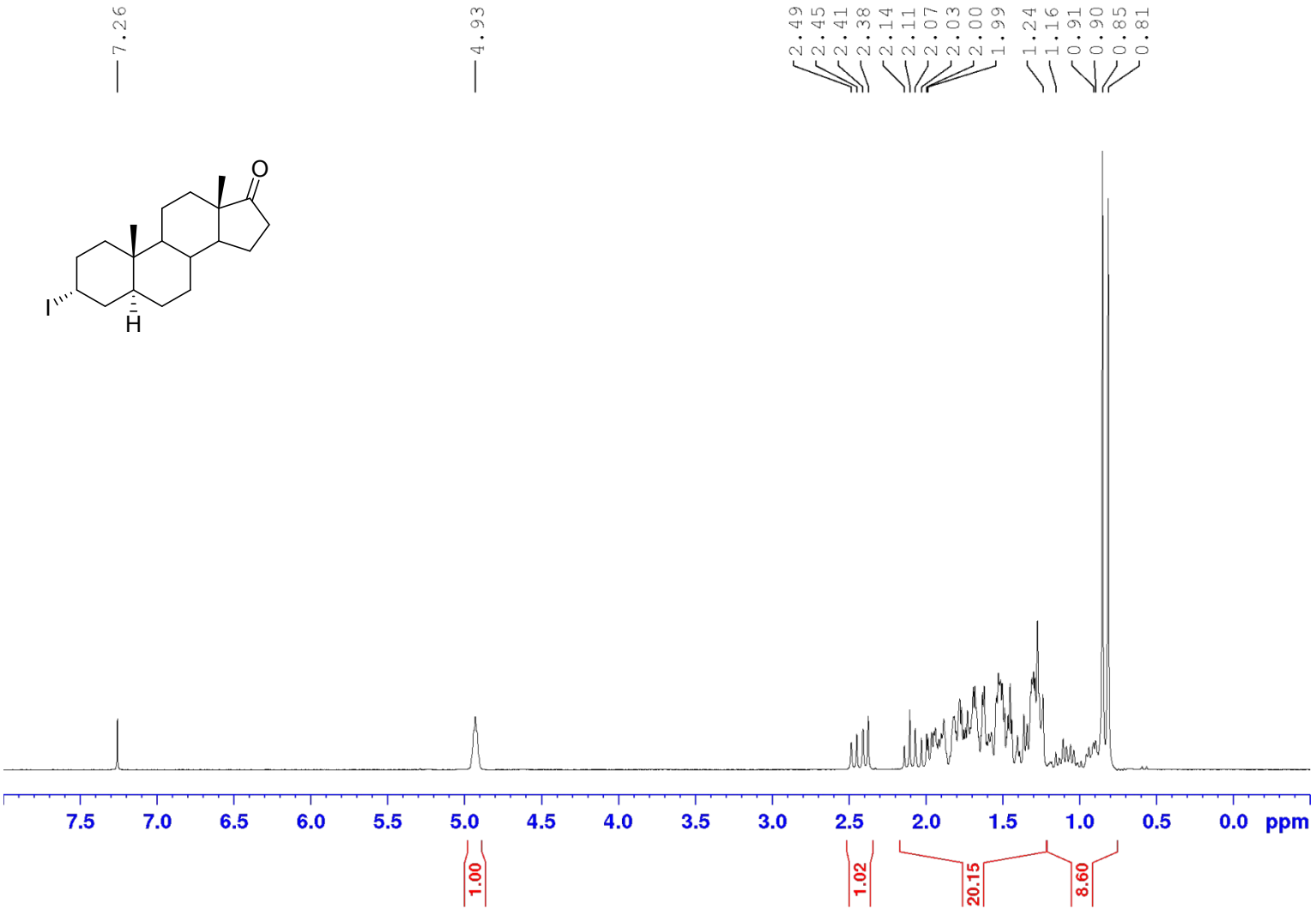
FEA (4) – ^{1}H – $CDCl_3$ – 250 MHz



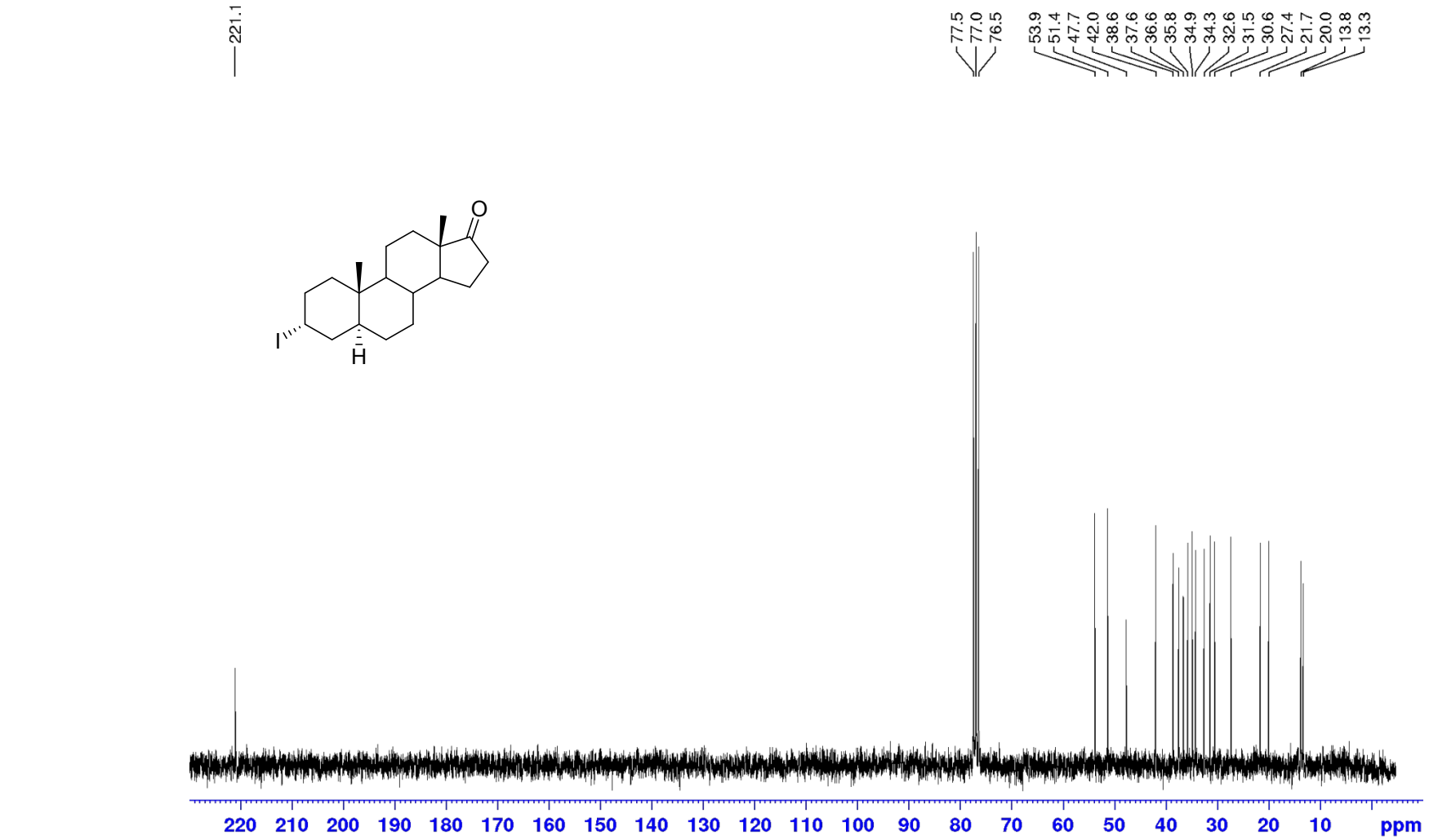
FEA (4) – ^{13}C – $CDCl_3$ – 62.5 MHz



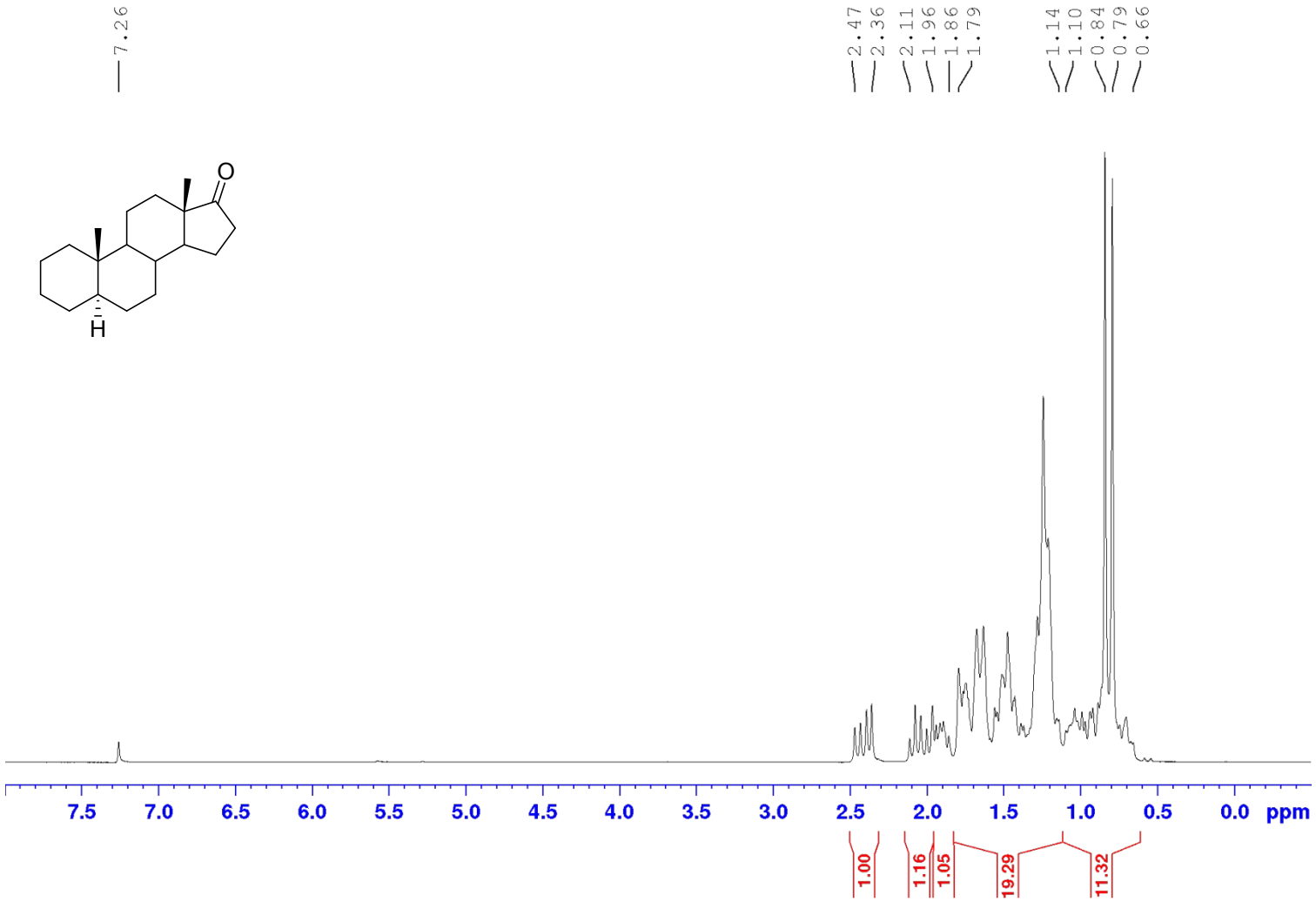
3-IEA – ^{1}H – $CDCl_3$ – 250 MHz



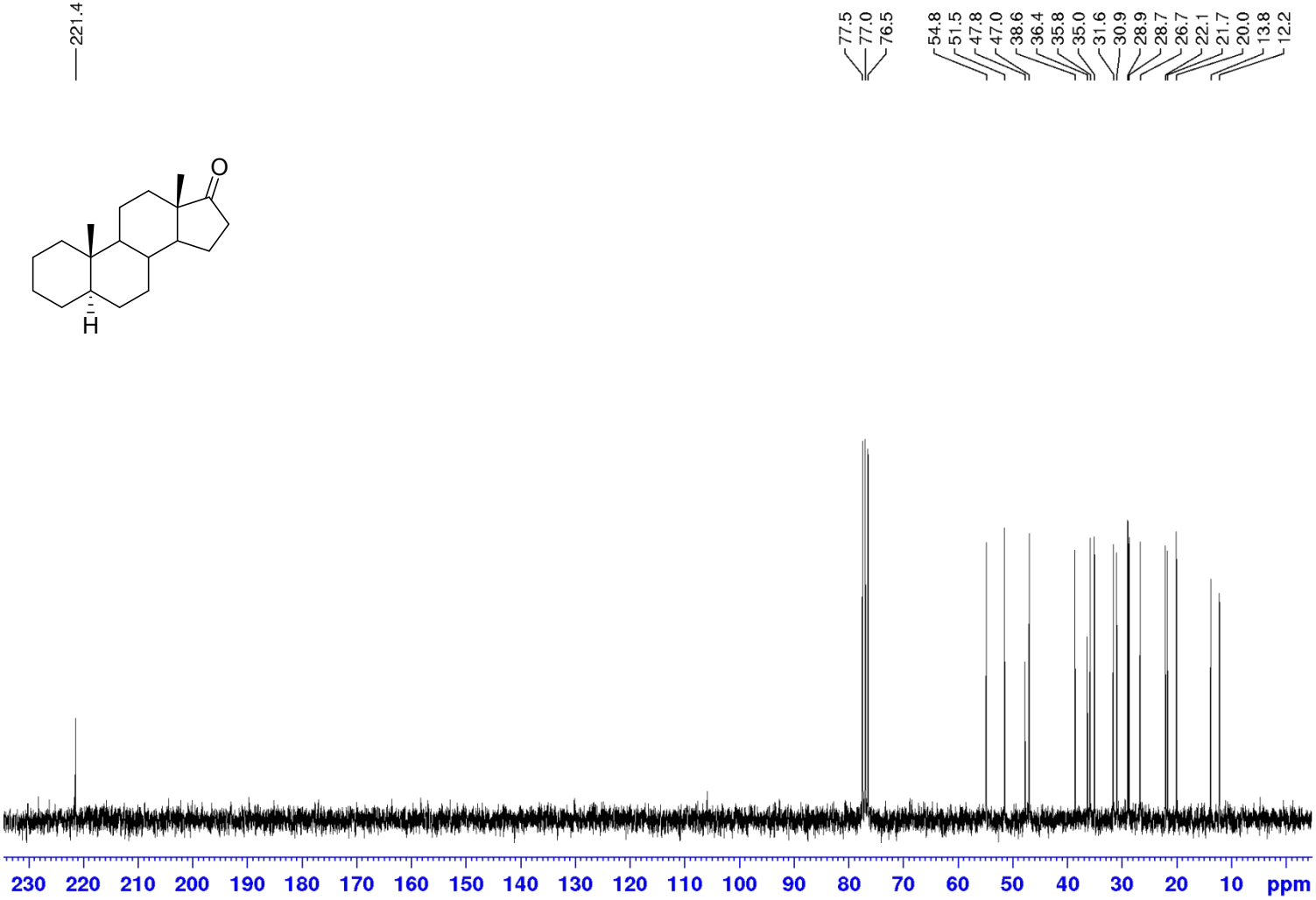
3-IEA – ^{13}C – $CDCl_3$ – 62.5 MHz



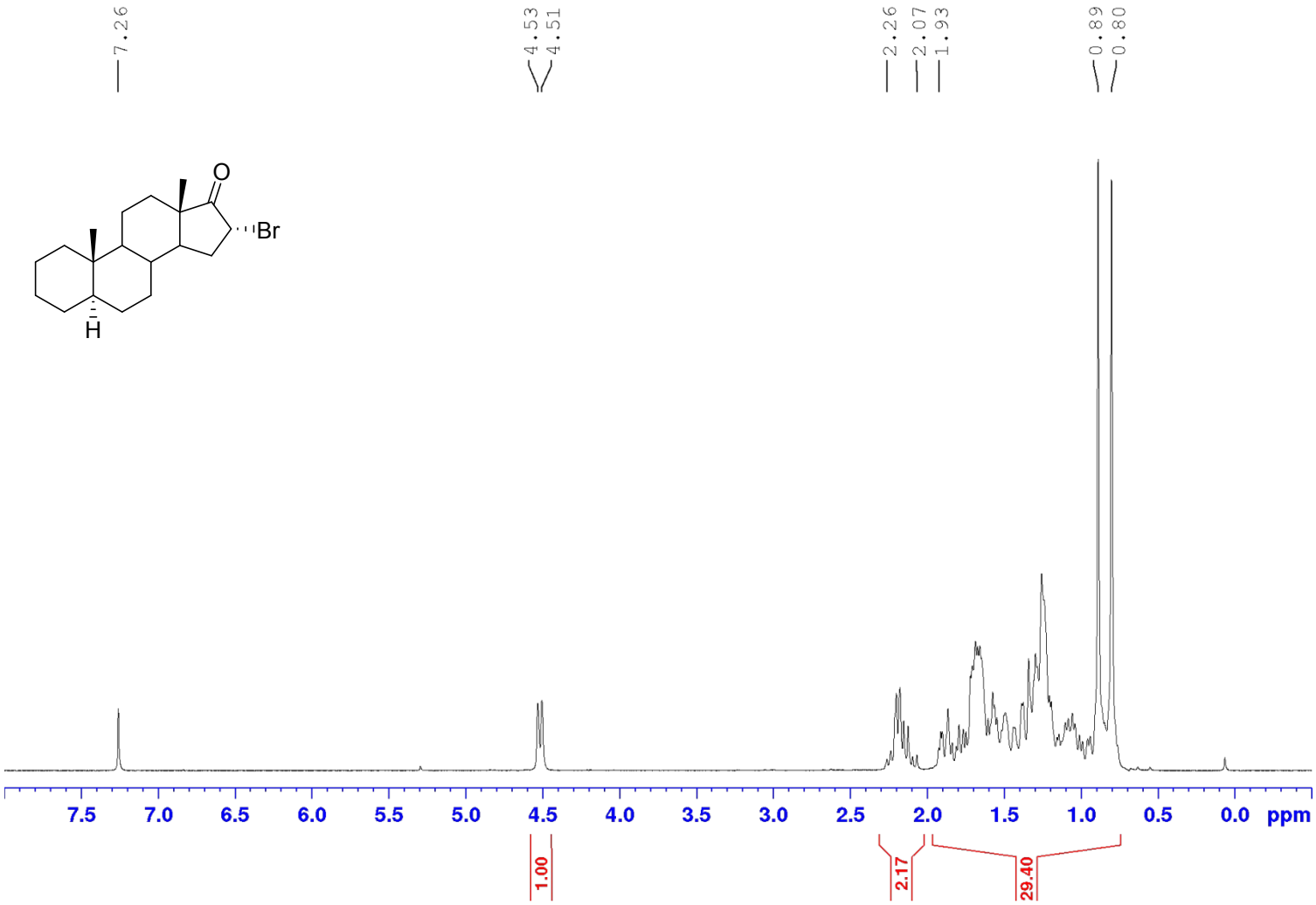
dEA (5) – ^{1}H – $CDCl_3$ – 250 MHz



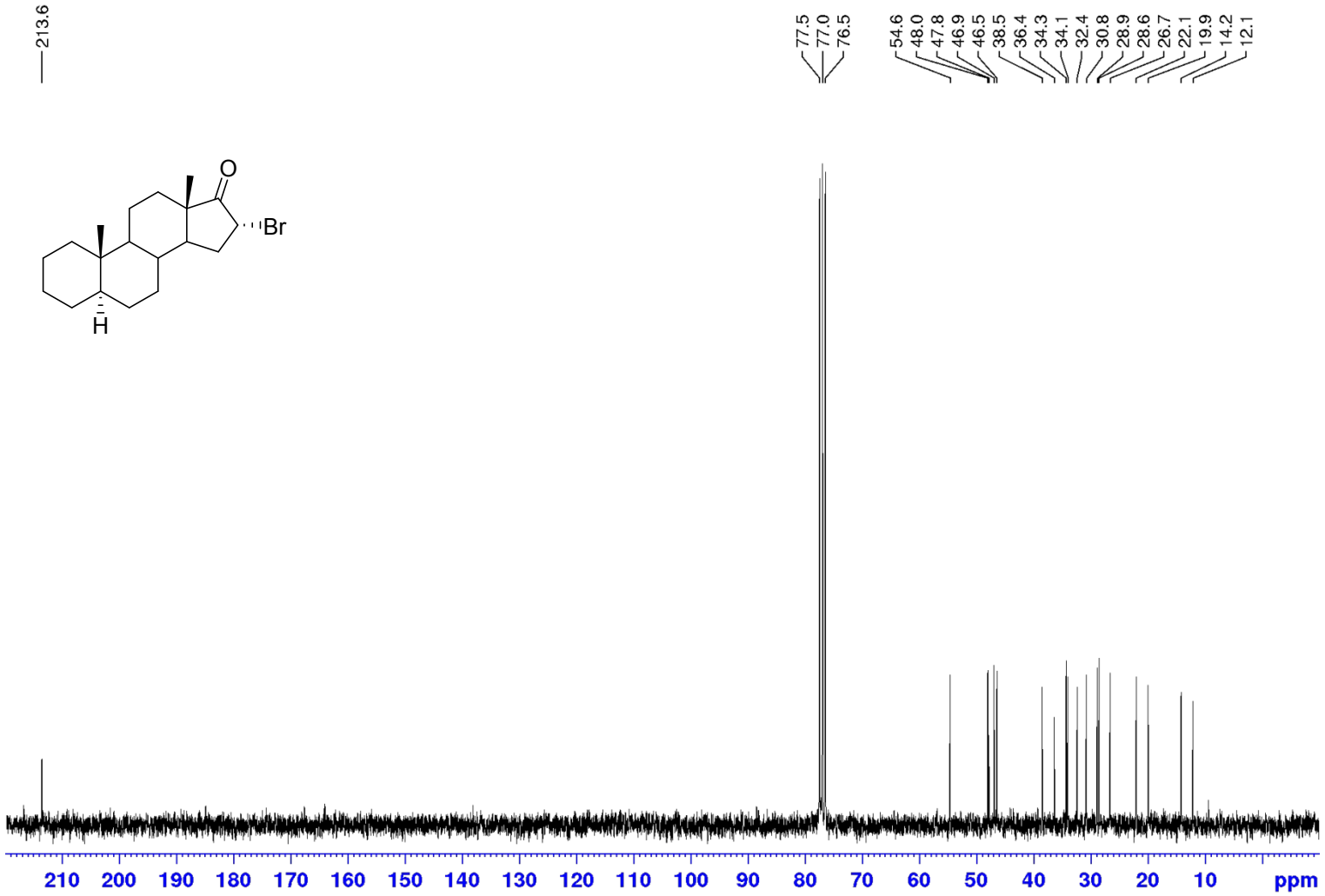
dEA (5) – ^{13}C – $CDCl_3$ – 62.5 MHz



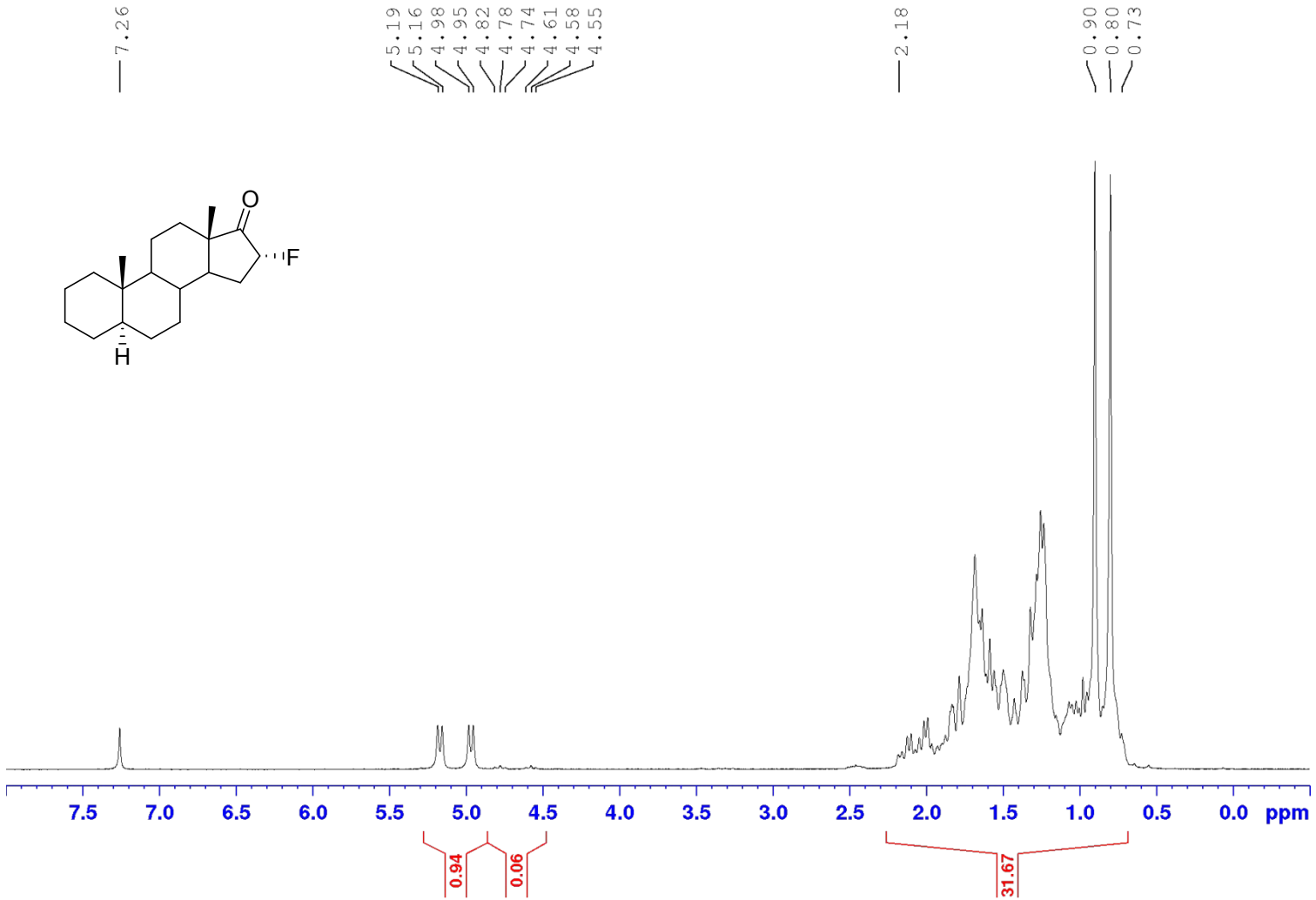
dBrEA (6) – ^{1}H – $CDCl_3$ – 250 MHz



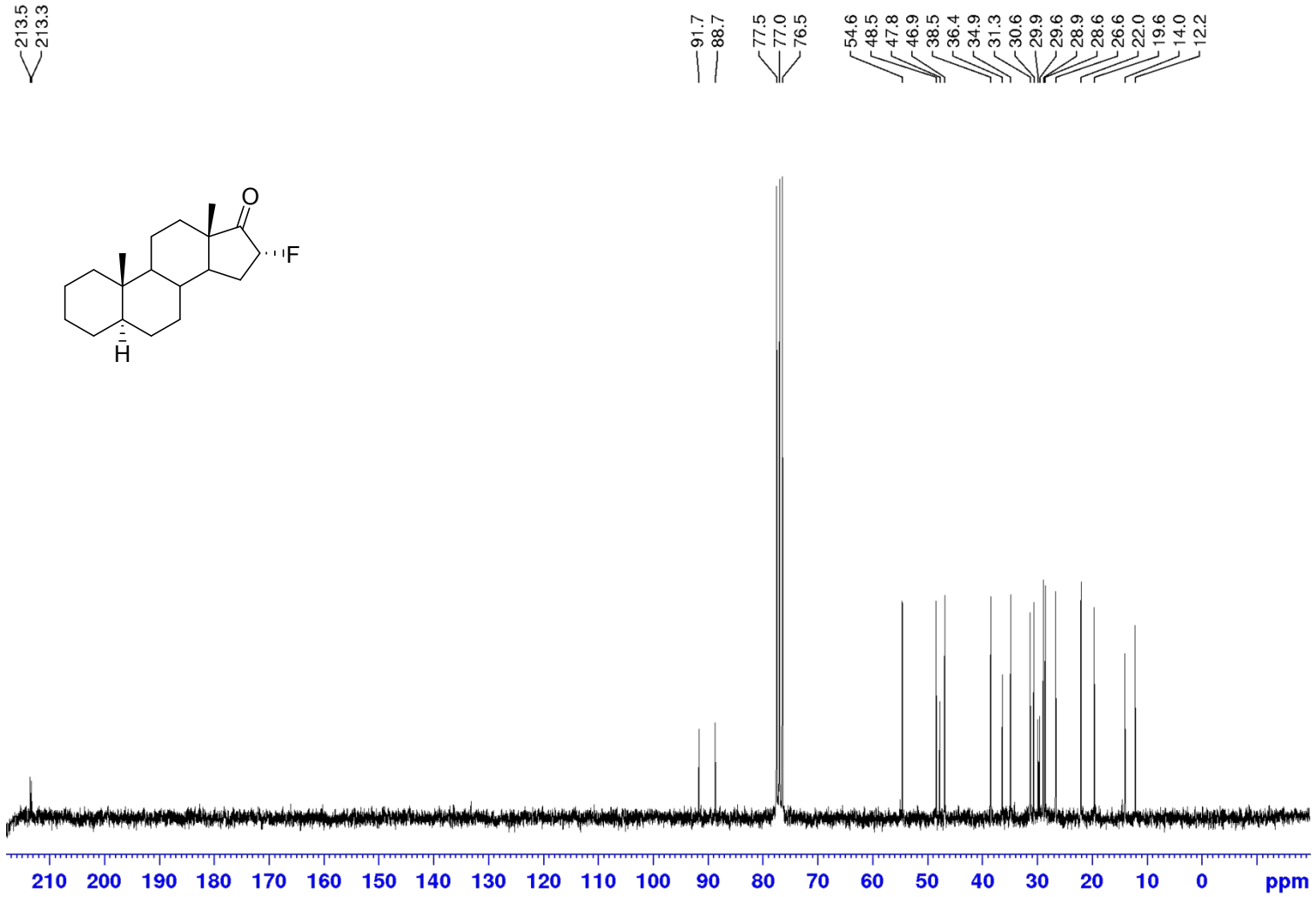
dBrEA (6) – ^{13}C – $CDCl_3$ – 62.5 MHz



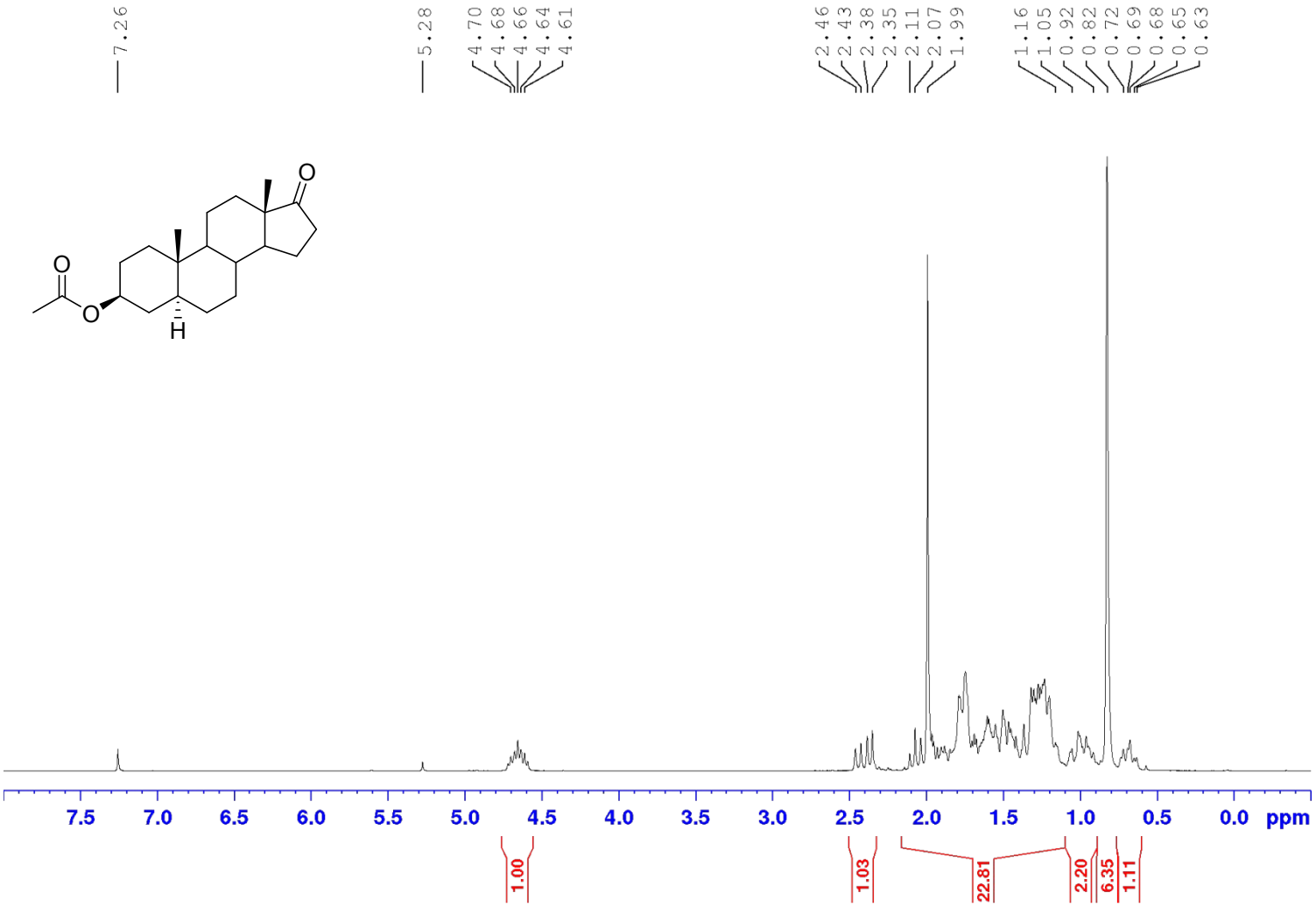
dFEA (7) – ^{1}H – $CDCl_3$ – 250 MHz



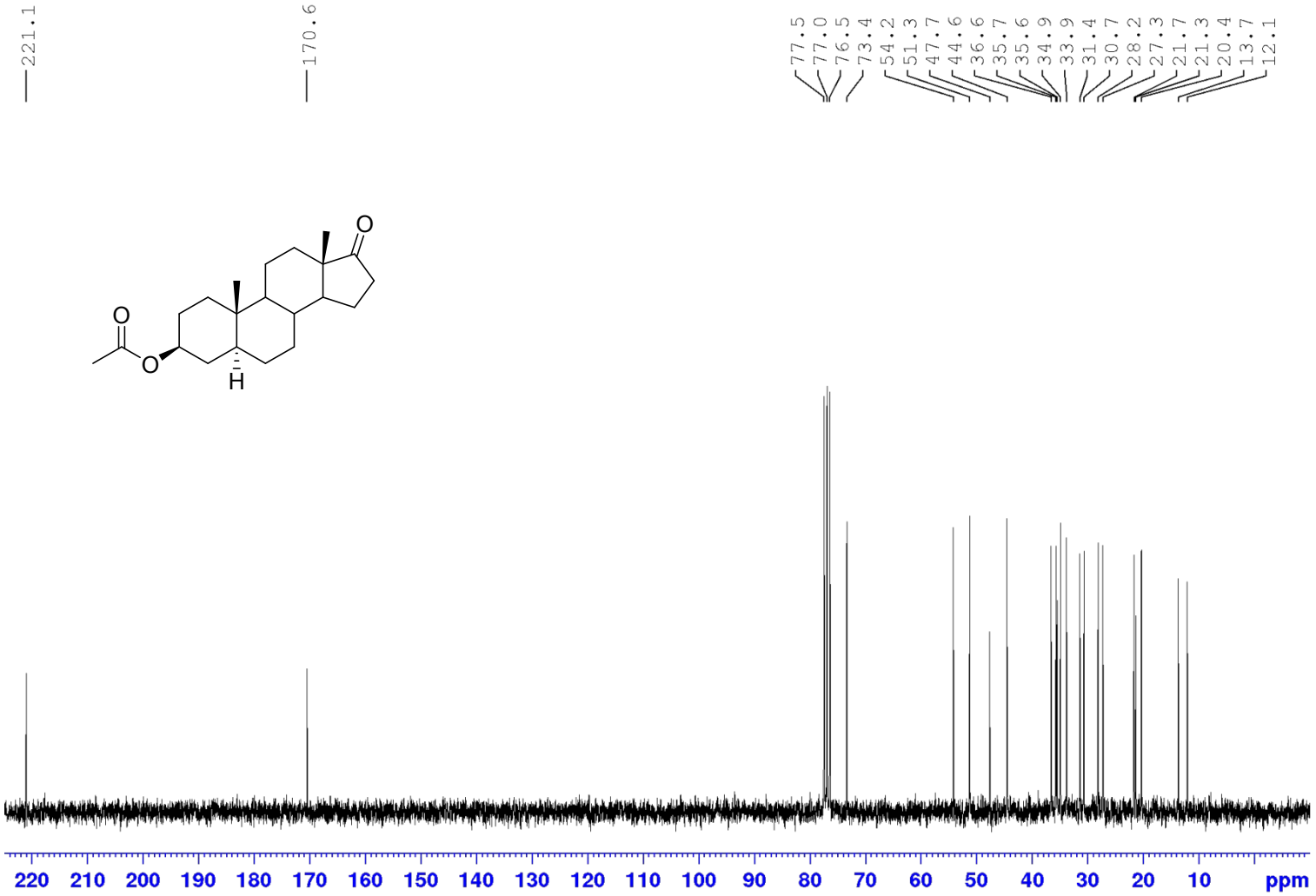
dFEA (7) – ^{13}C – $CDCl_3$ – 62.5 MHz



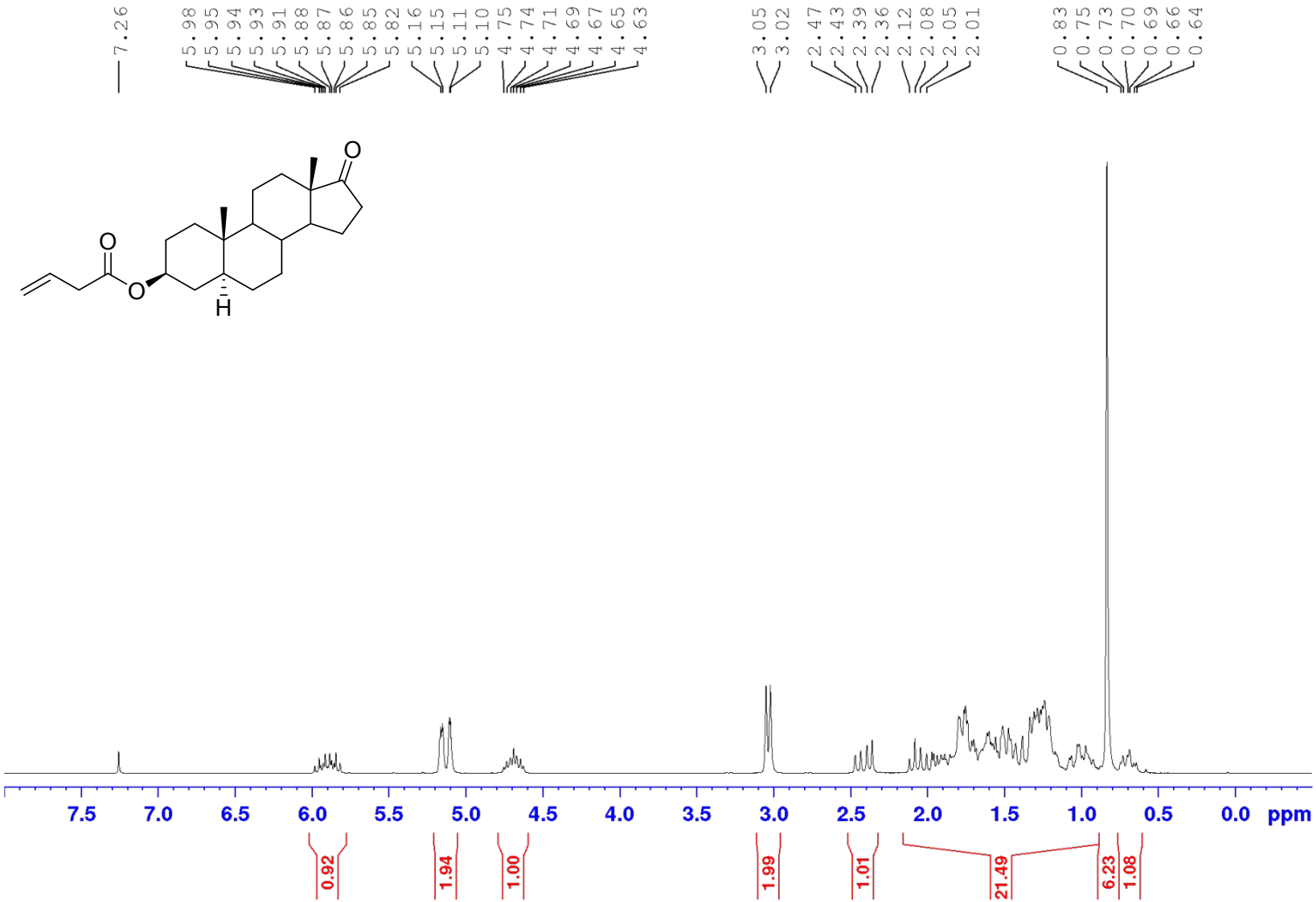
Epiandrosterone acetate (8) – ^{1}H – $CDCl_3$ – 250 MHz



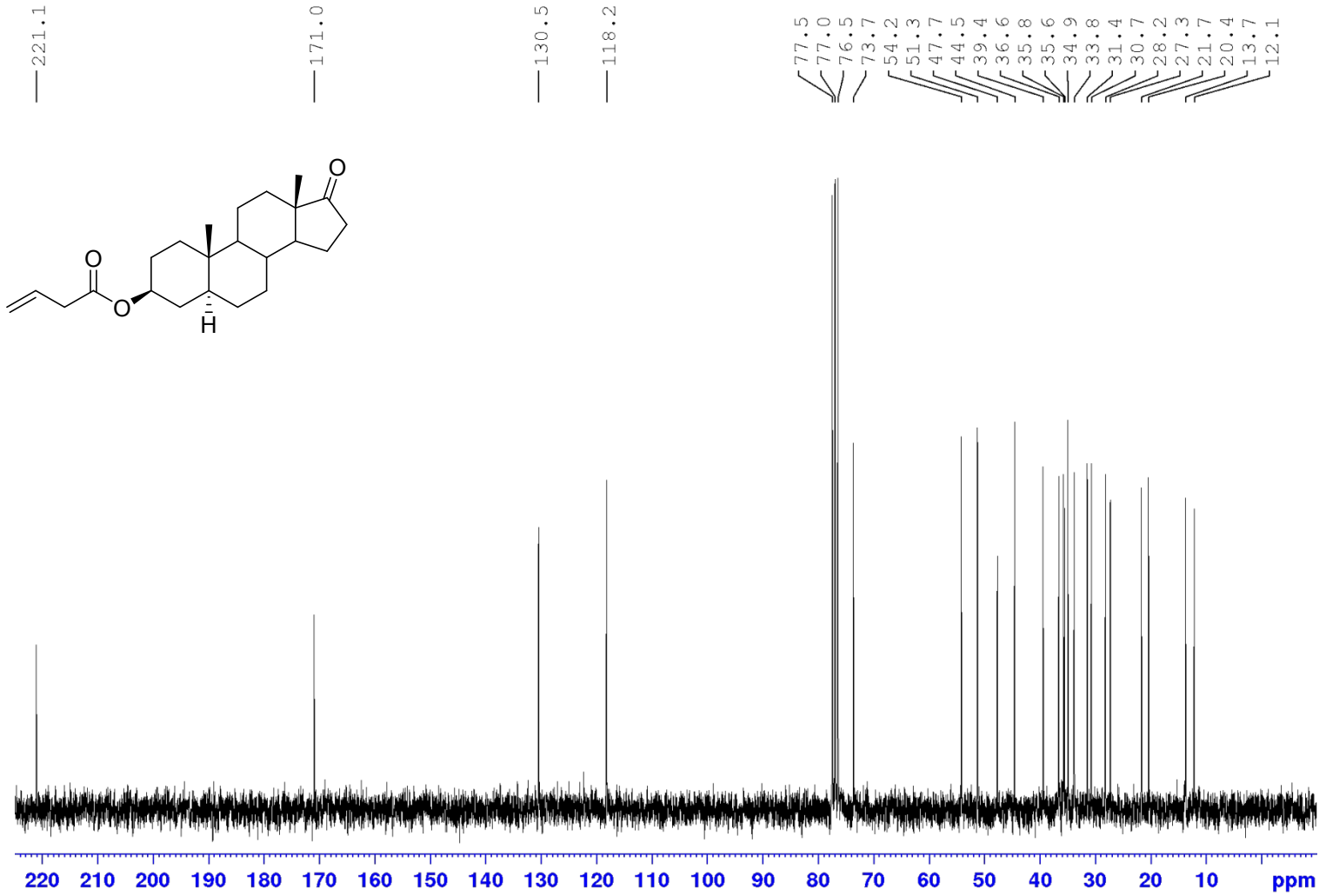
Epiandrosterone acetate (8) – ^{13}C – $CDCl_3$ – 62.5 MHz



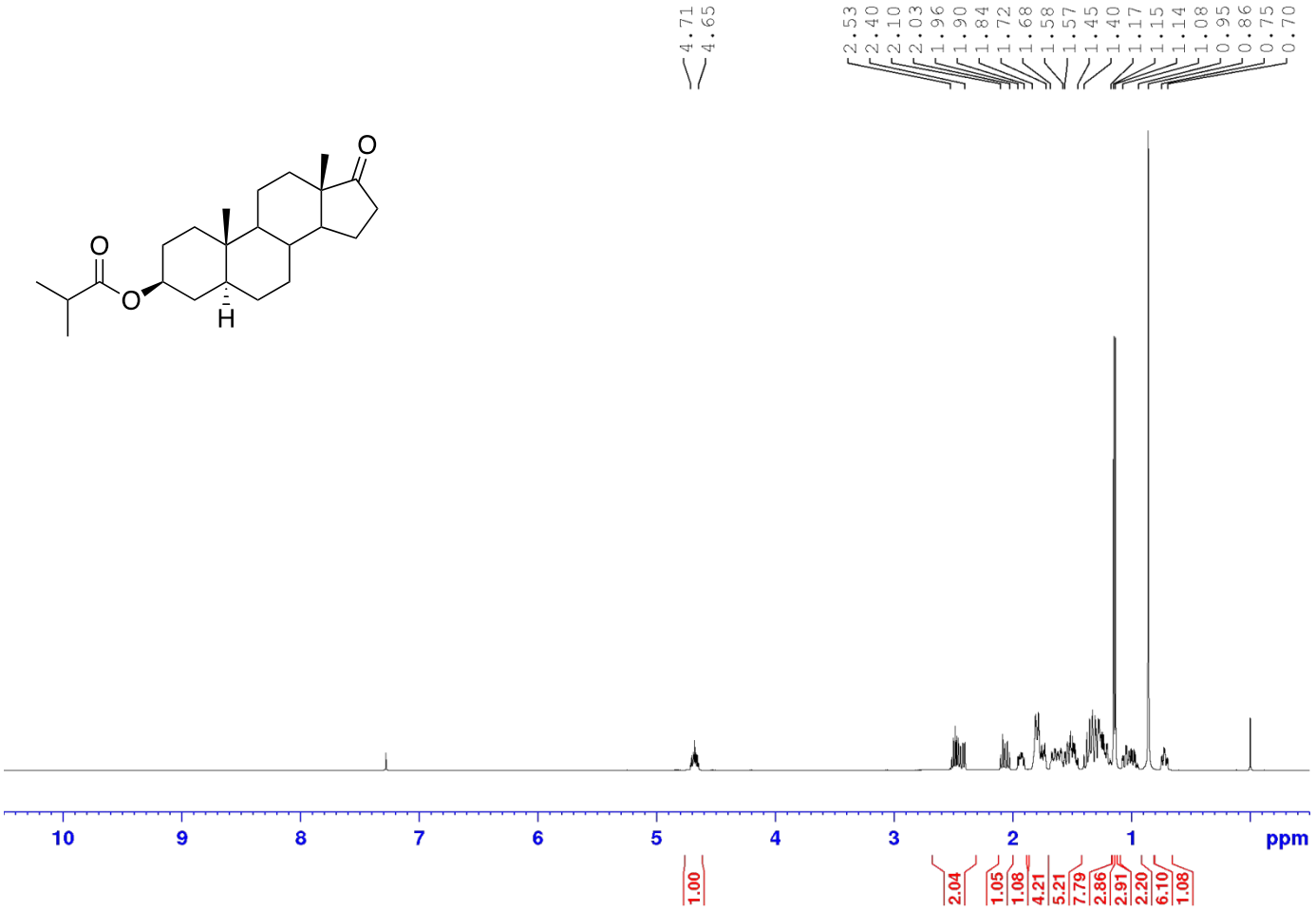
Epiandrosterone but-3-enoate (9) – ^{1}H – $CDCl_3$ – 250 MHz



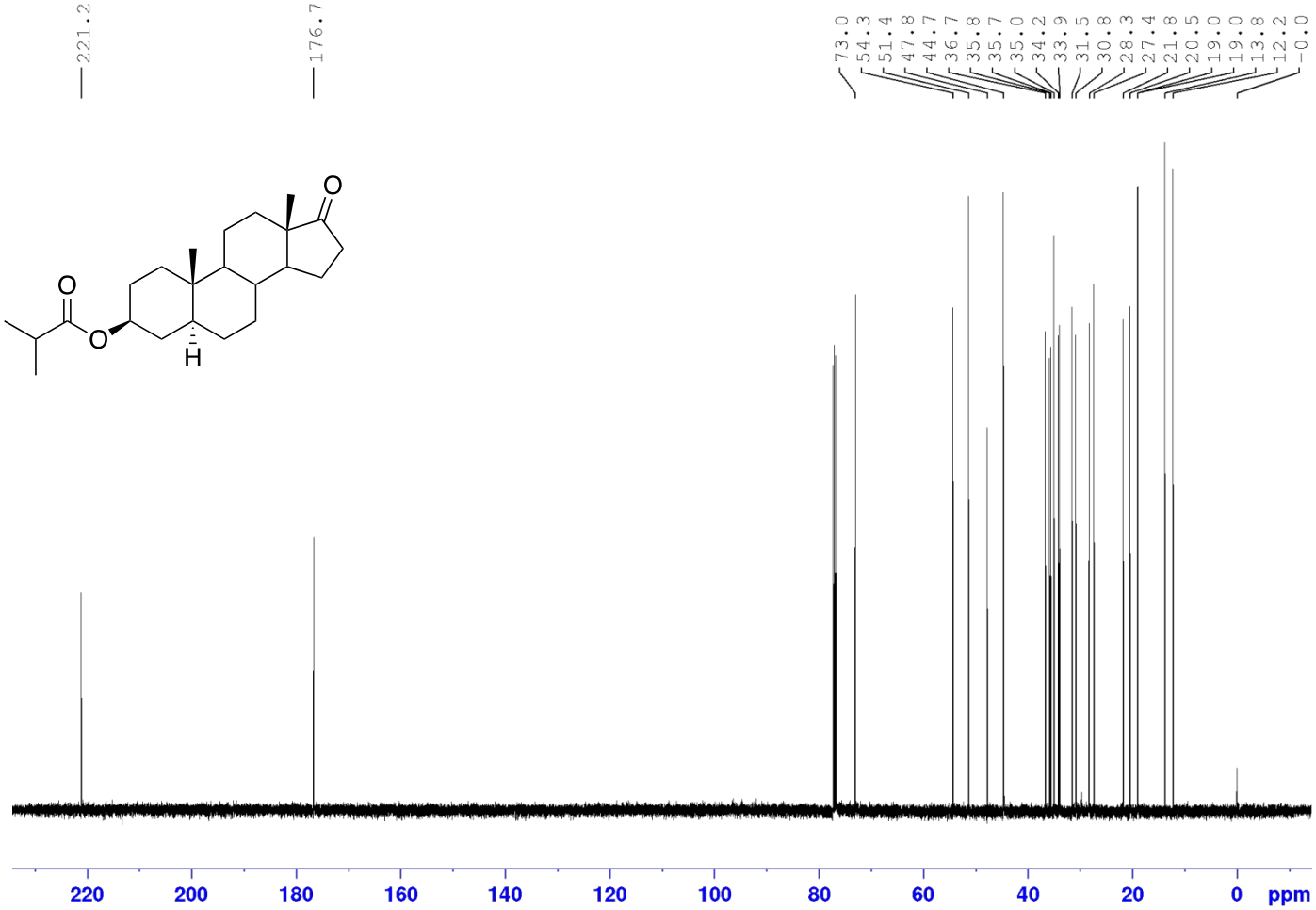
Epiandrosterone but-3-enoate (9) – ^{13}C – $CDCl_3$ – 62.5 MHz



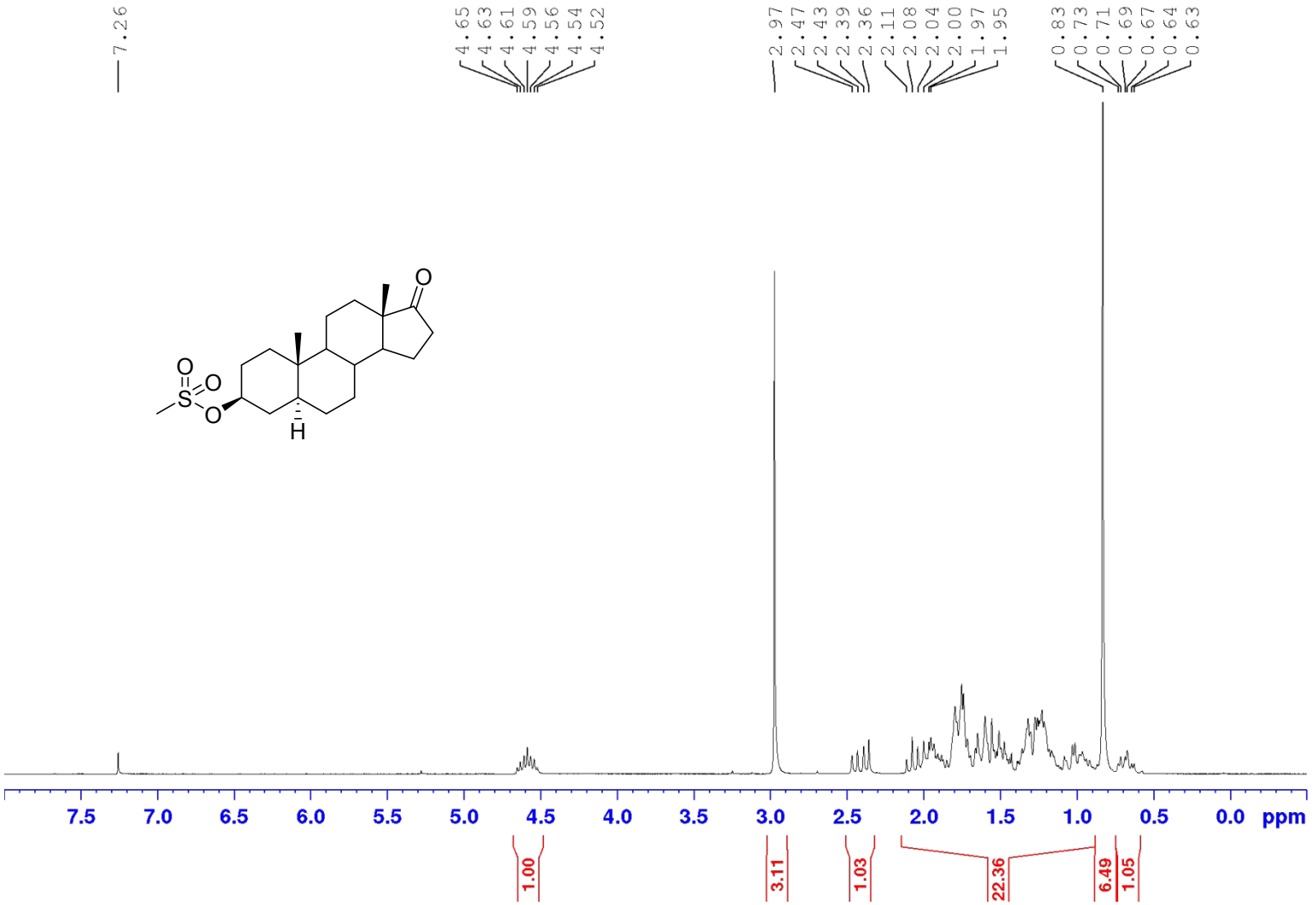
Epiandrosterone isobutyrate (10) – ^{1}H – $CDCl_3$ – 500 MHz



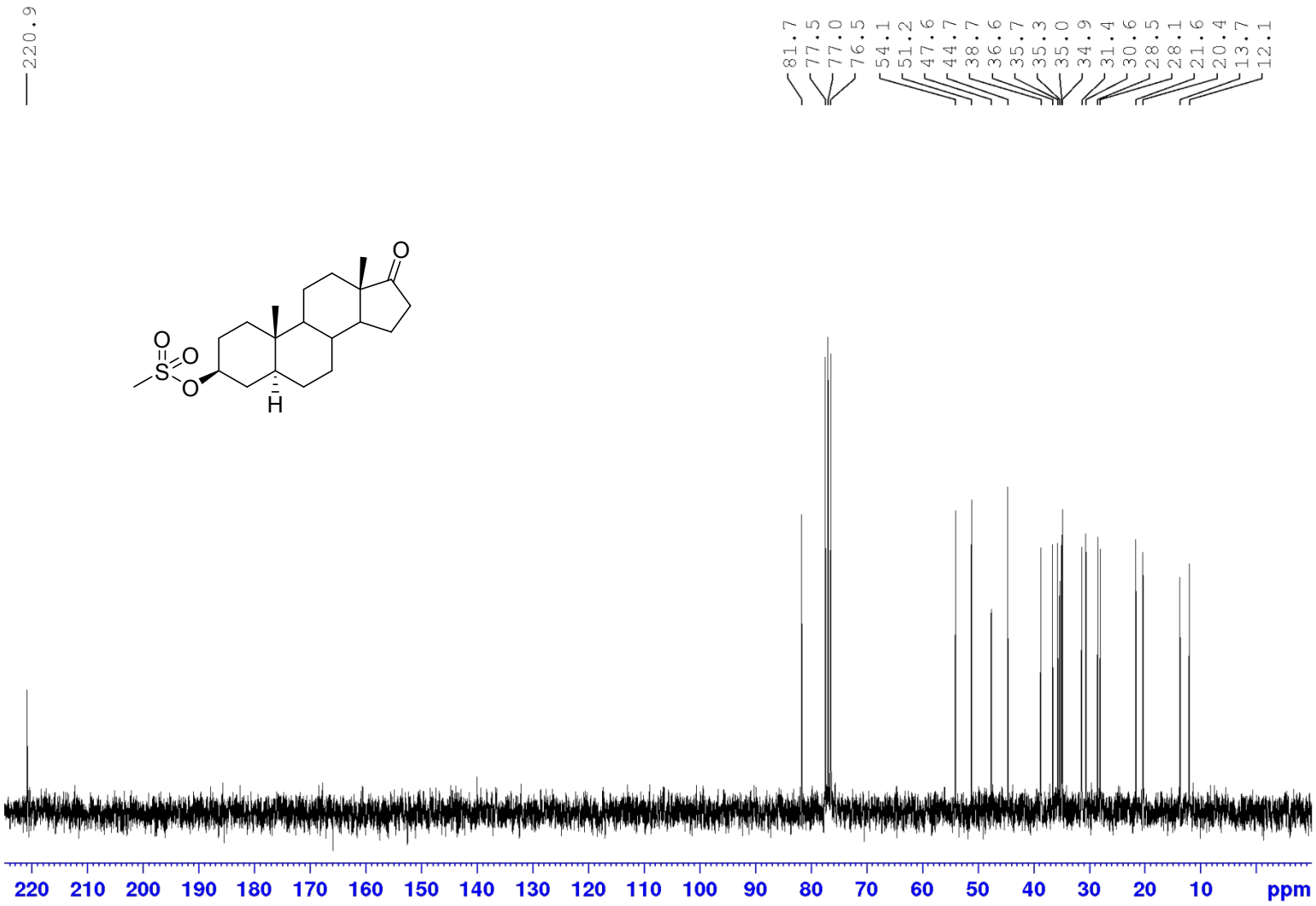
Epiandrosterone isobutyrate (10) – ^{13}C – $CDCl_3$ – 125 MHz



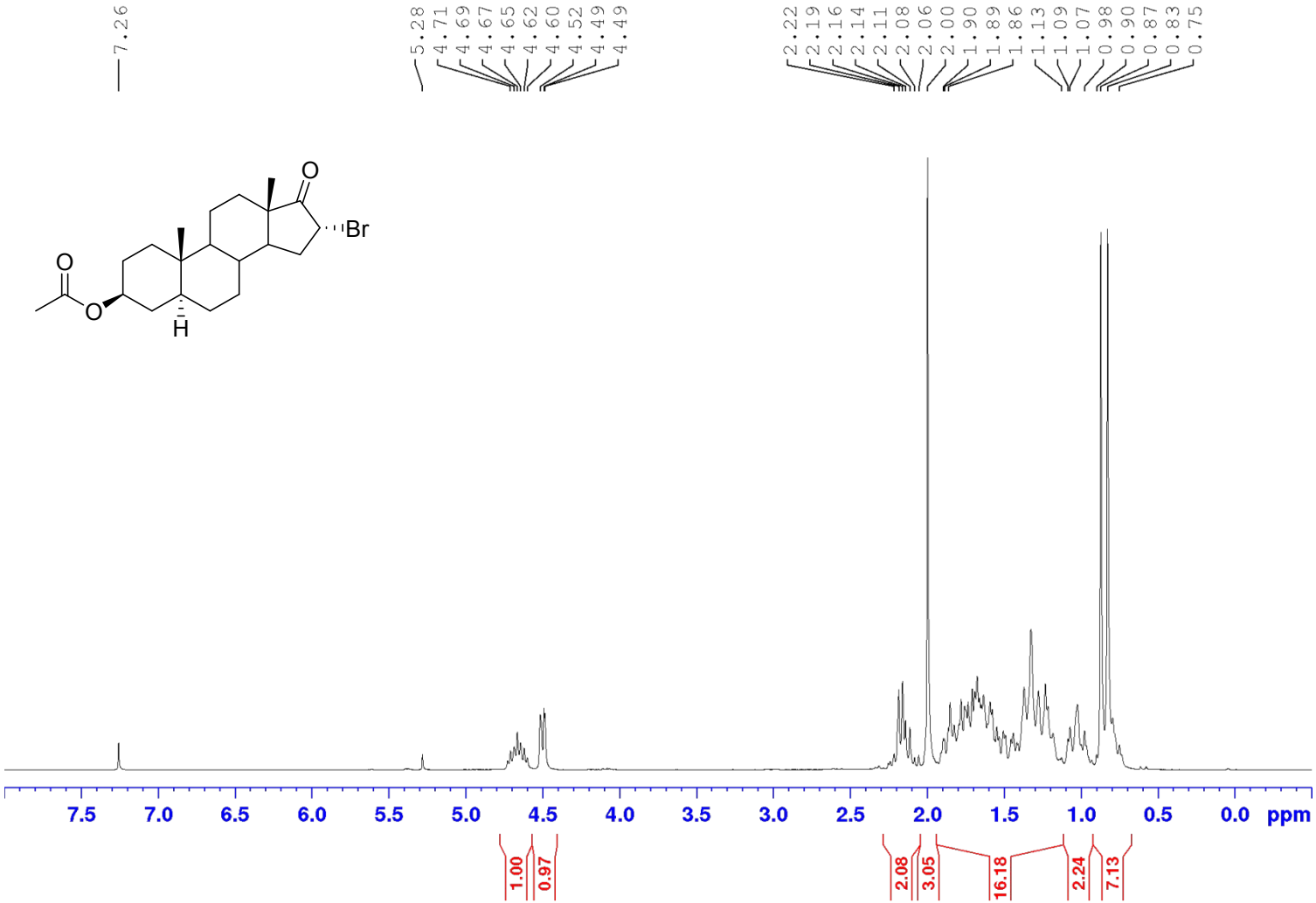
Epiandrosterone methanesulfonate (11) – ^{1}H – $CDCl_3$ – 250 MHz



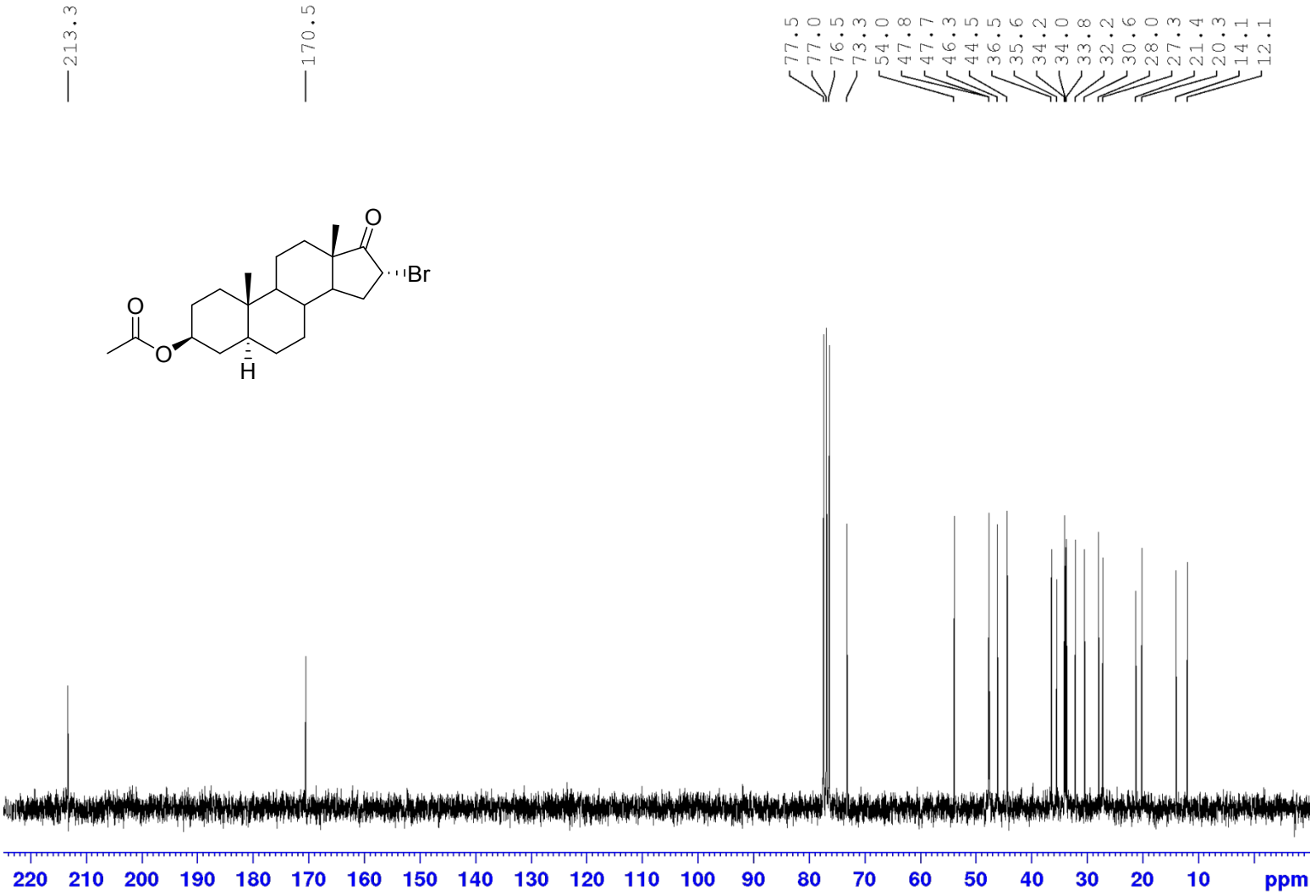
Epiandrosterone methanesulfonate (11) – ^{13}C – $CDCl_3$ – 62.5 MHz



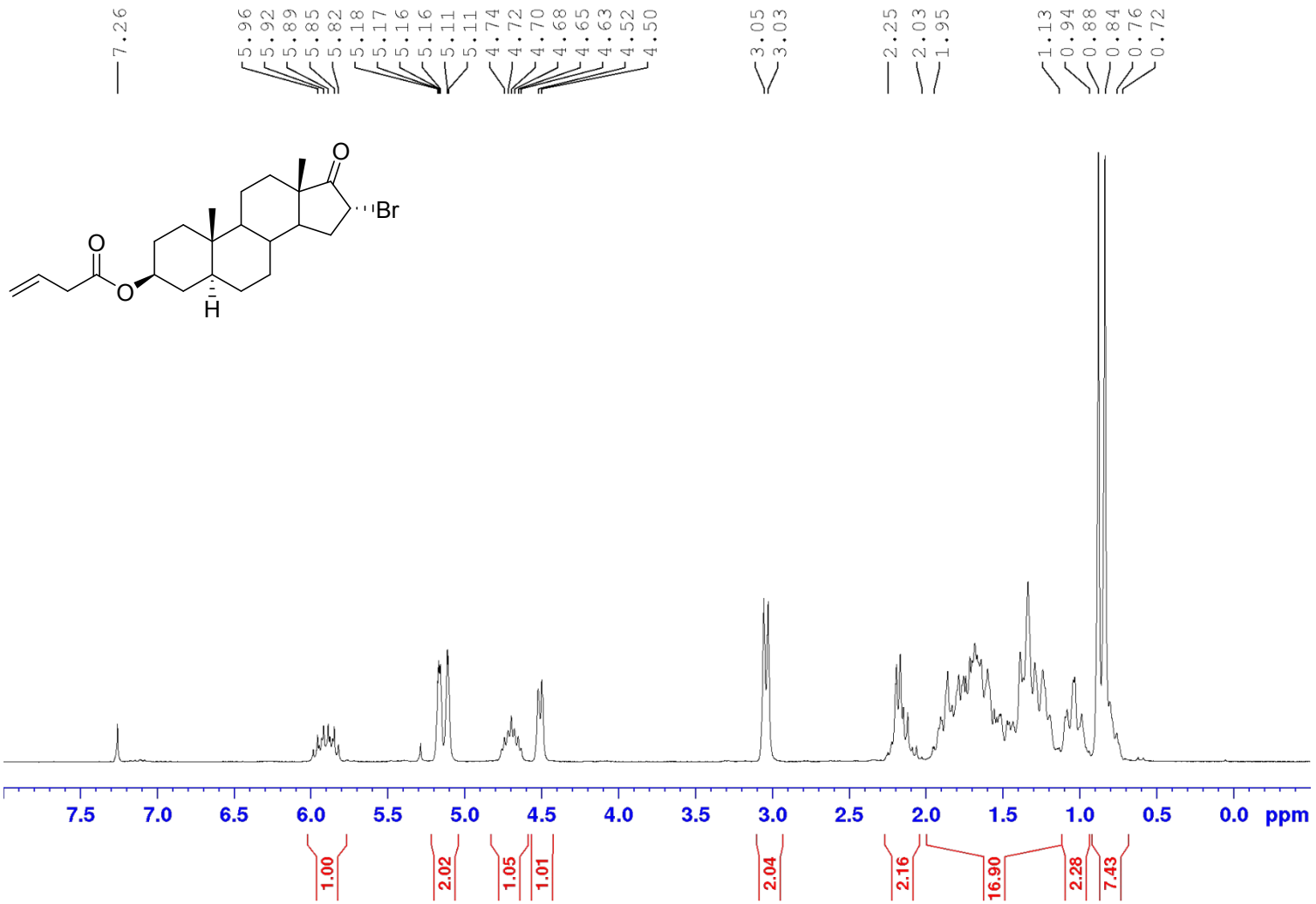
16α-Bromoepiandrosterone acetate (12) – ^{1}H – $CDCl_3$ – 250 MHz



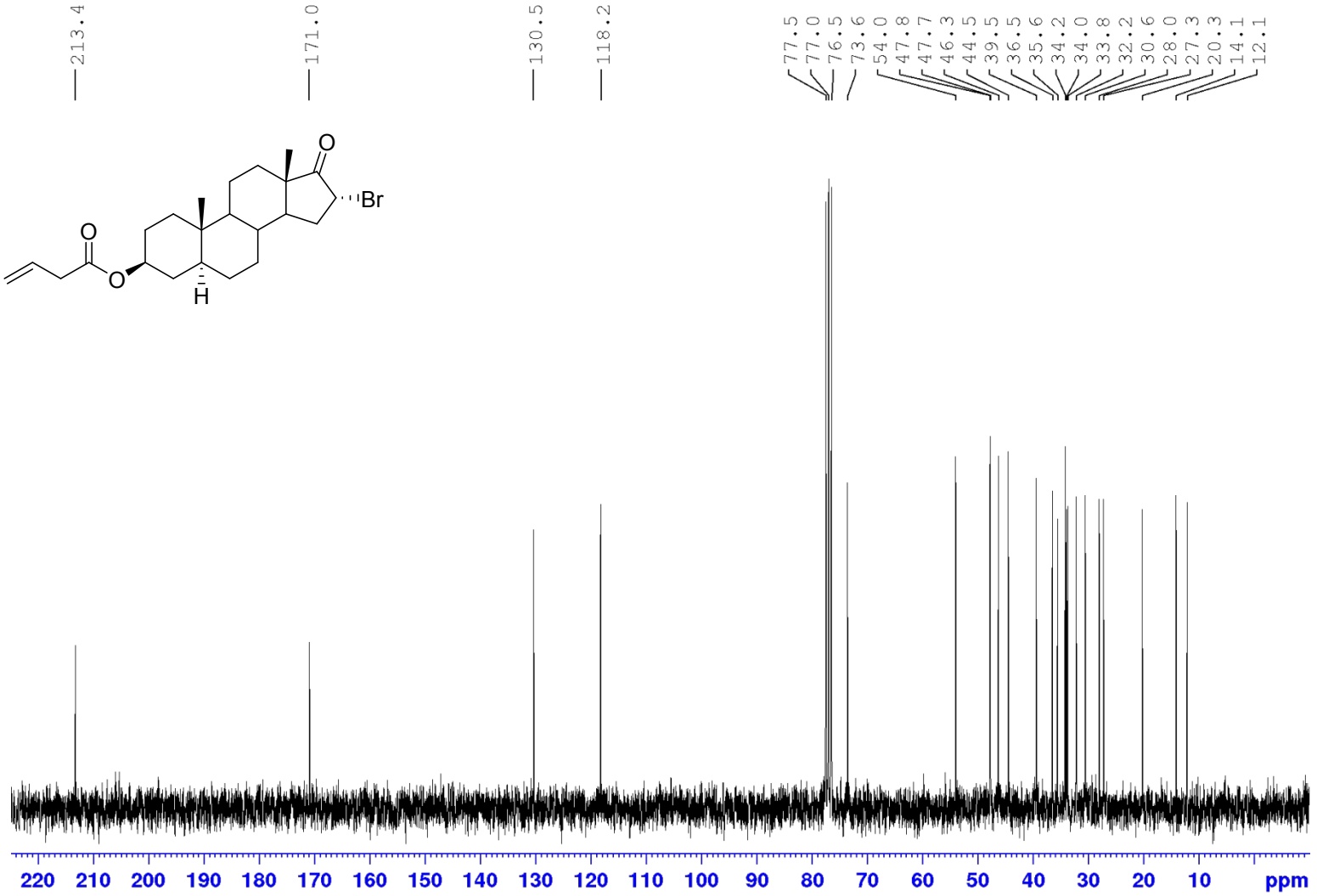
16α-Bromoepiandrosterone acetate (12) – ^{13}C – $CDCl_3$ – 62.5 MHz



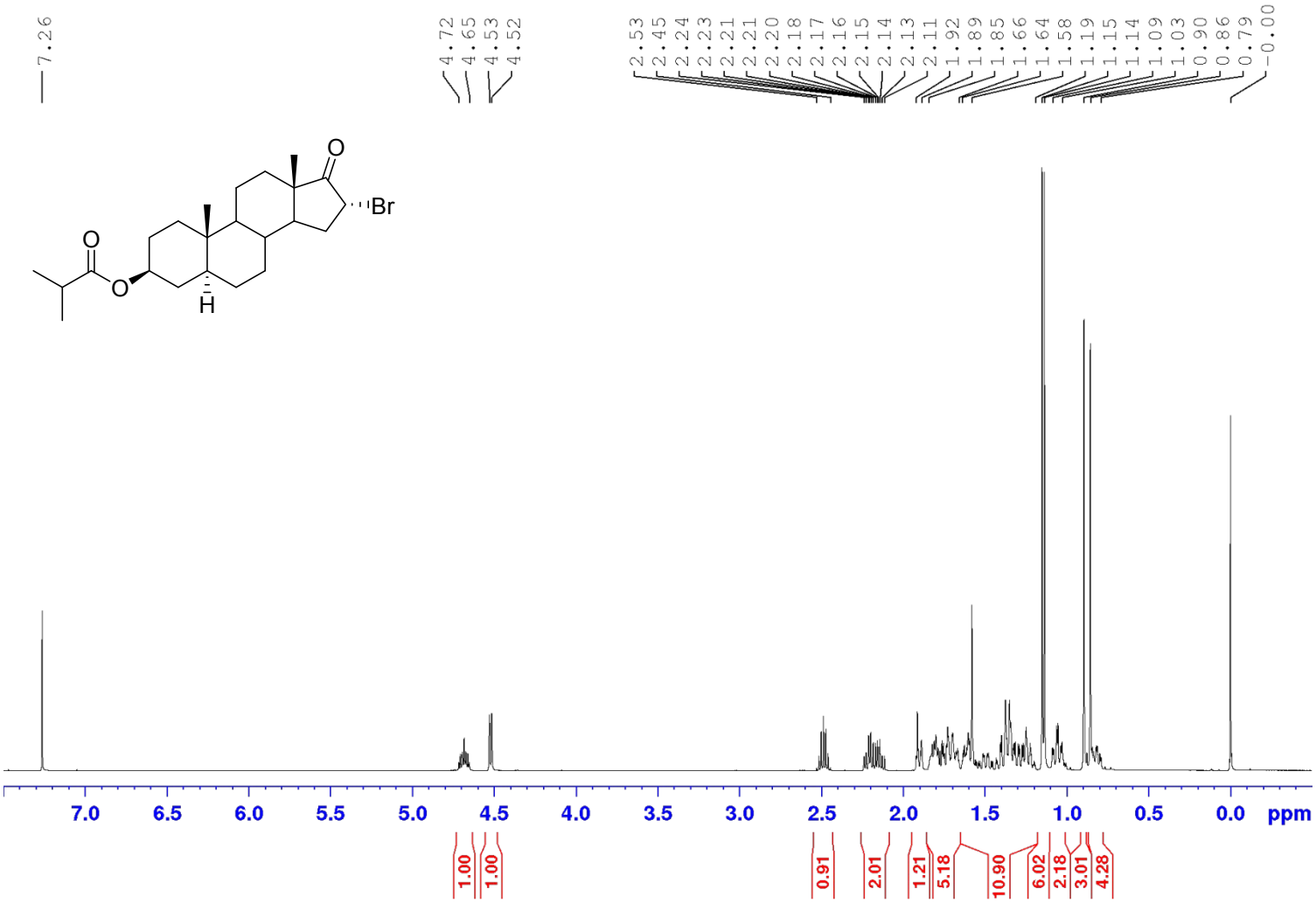
16α-Bromoepiandrosterone but-3-enoate (13) – ^{1}H – $CDCl_3$ – 250 MHz



16α-Bromoepiandrosterone but-3-enoate (13) – ^{13}C – $CDCl_3$ – 62.5 MHz

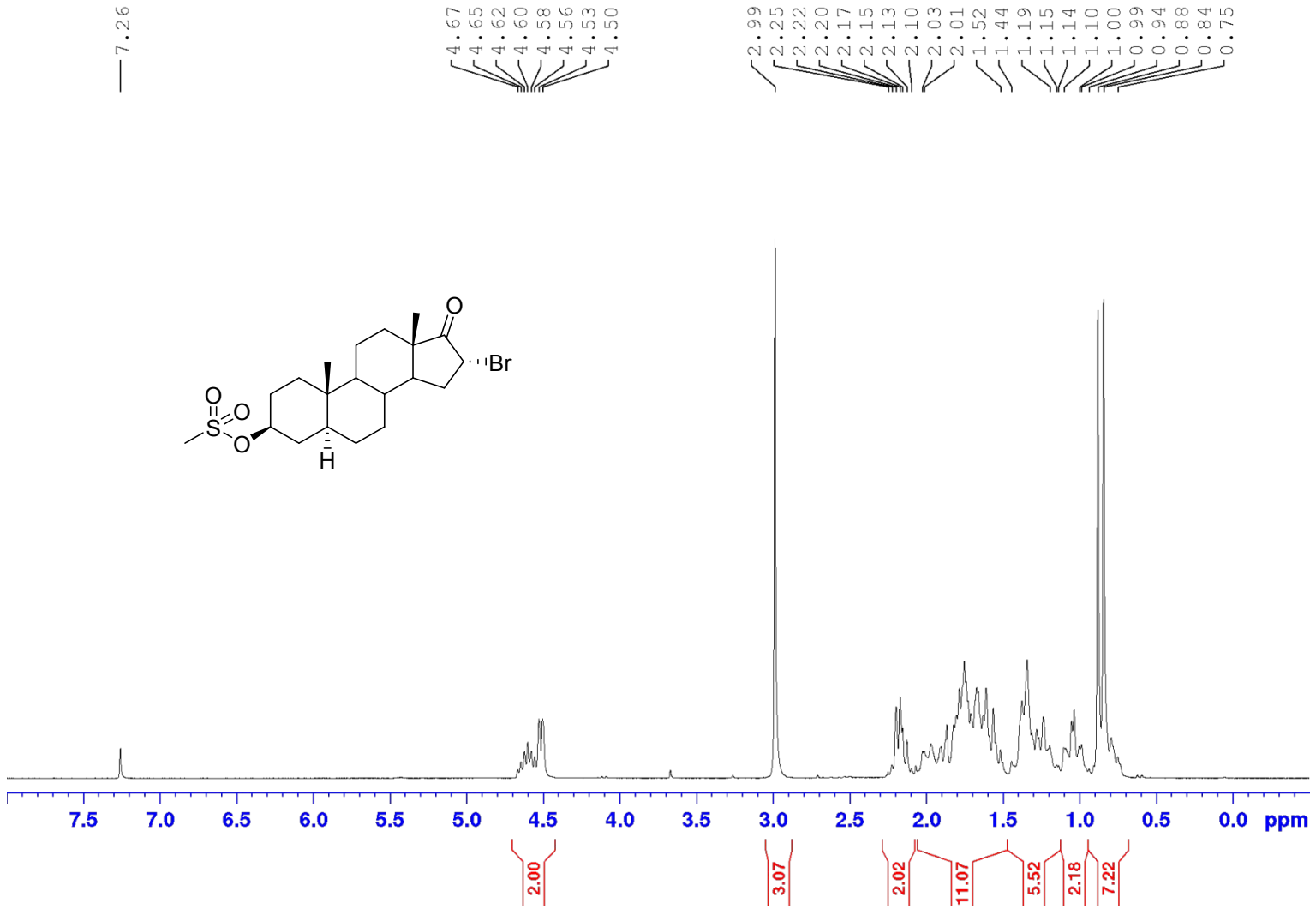


16α-Bromoepiandrosterone isobutyrate (14) – ^{1}H – $CDCl_3$ – 500 MHz

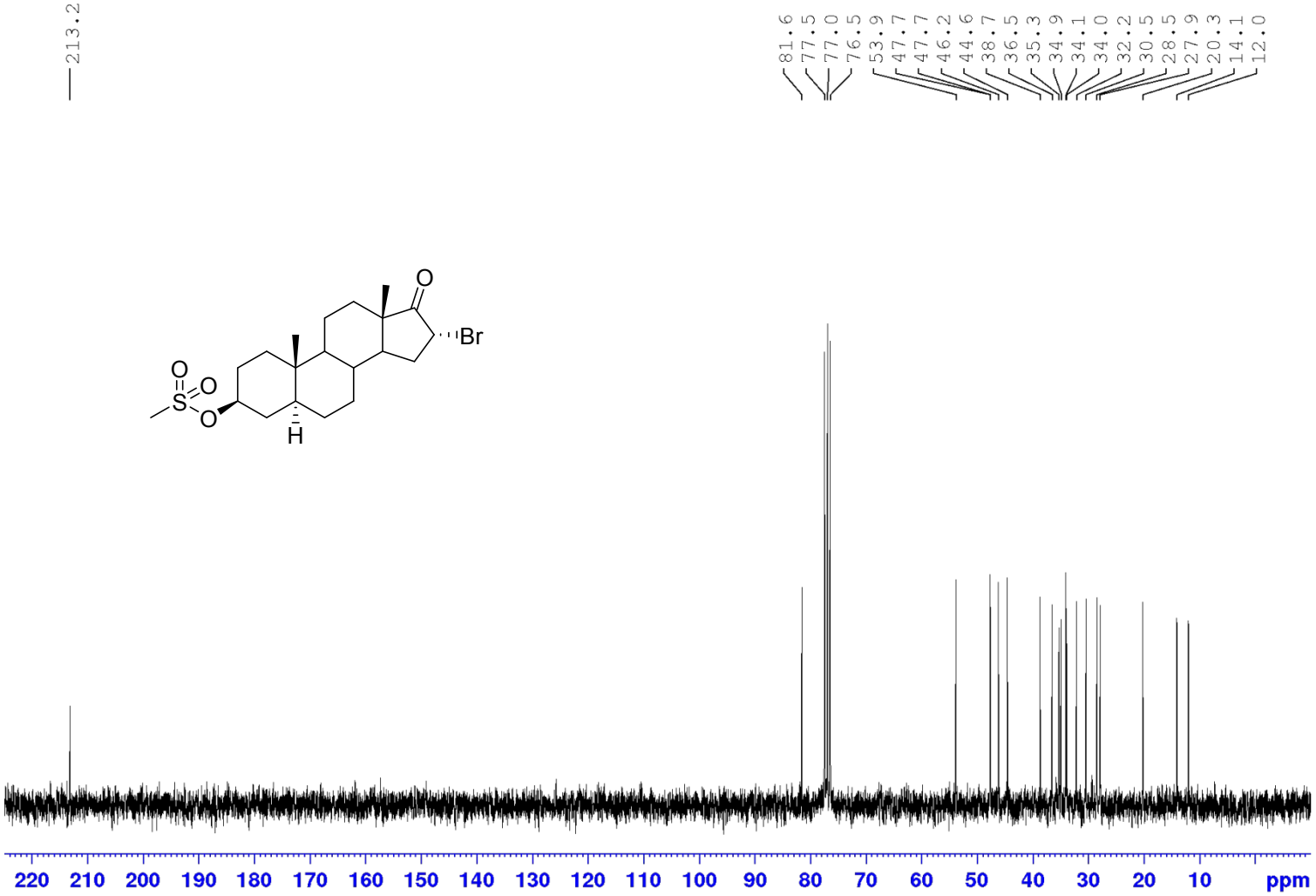


16α-Bromoepiandrosterone isobutyrate (14) – ^{13}C – $CDCl_3$ – 125 MHz

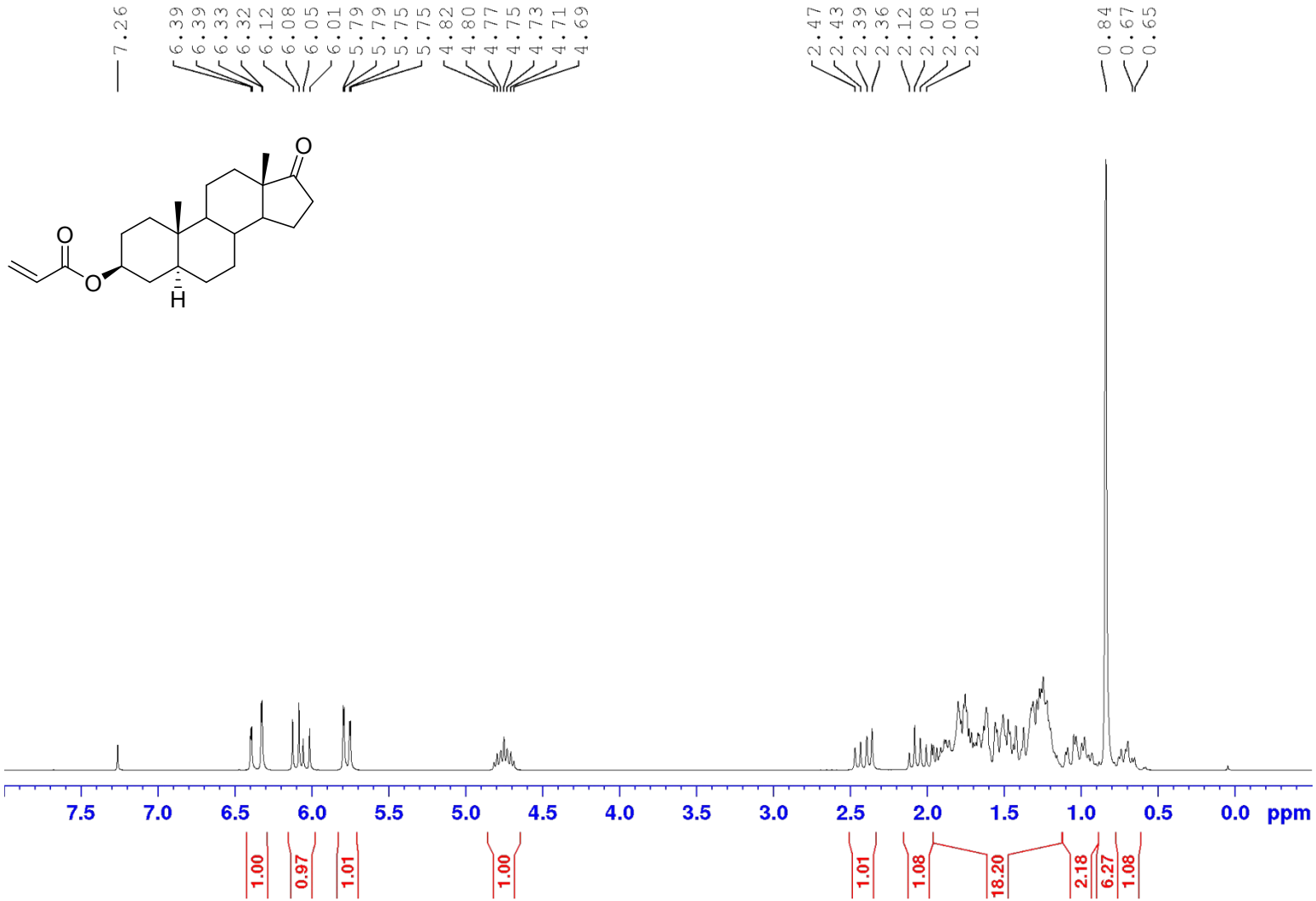
16α-Bromoepiandrosterone methanesulfonate (15) – ^{1}H – $CDCl_3$ – 250 MHz



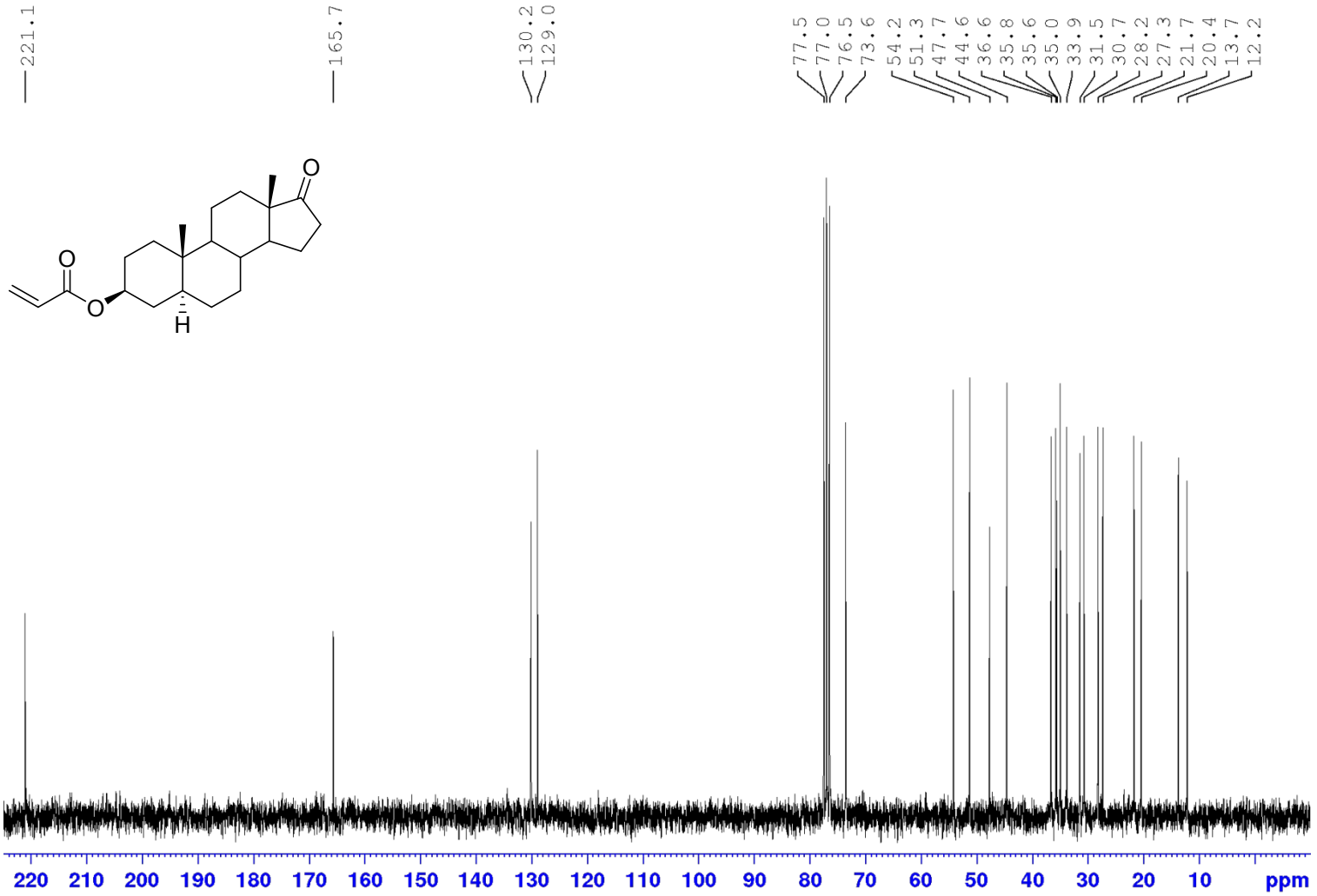
16α-Bromoepiandrosterone methanesulfonate (15) – ^{13}C – $CDCl_3$ – 62.5 MHz



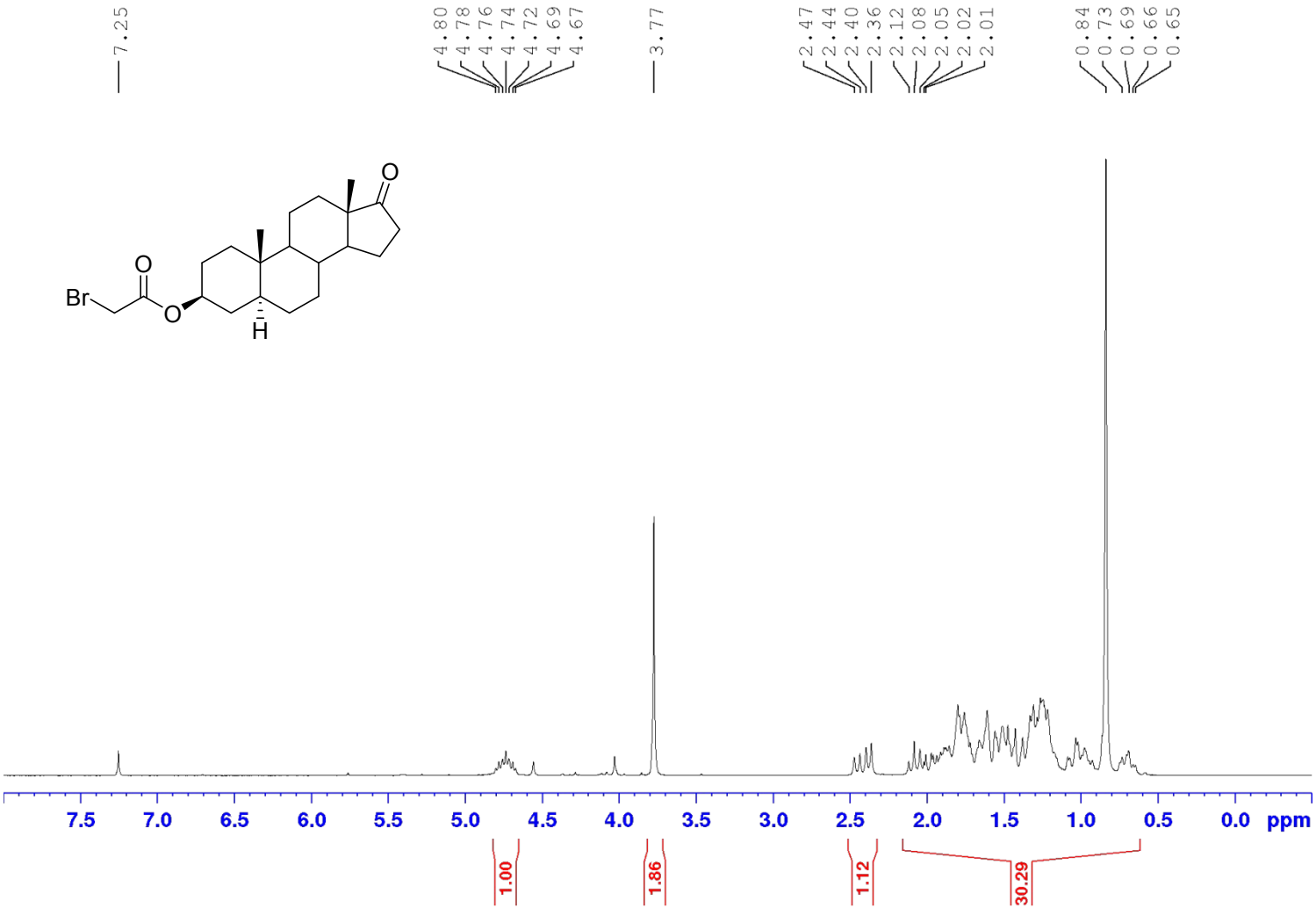
Epiandrosterone acrylate (16) – ^{1}H – $CDCl_3$ – 250 MHz



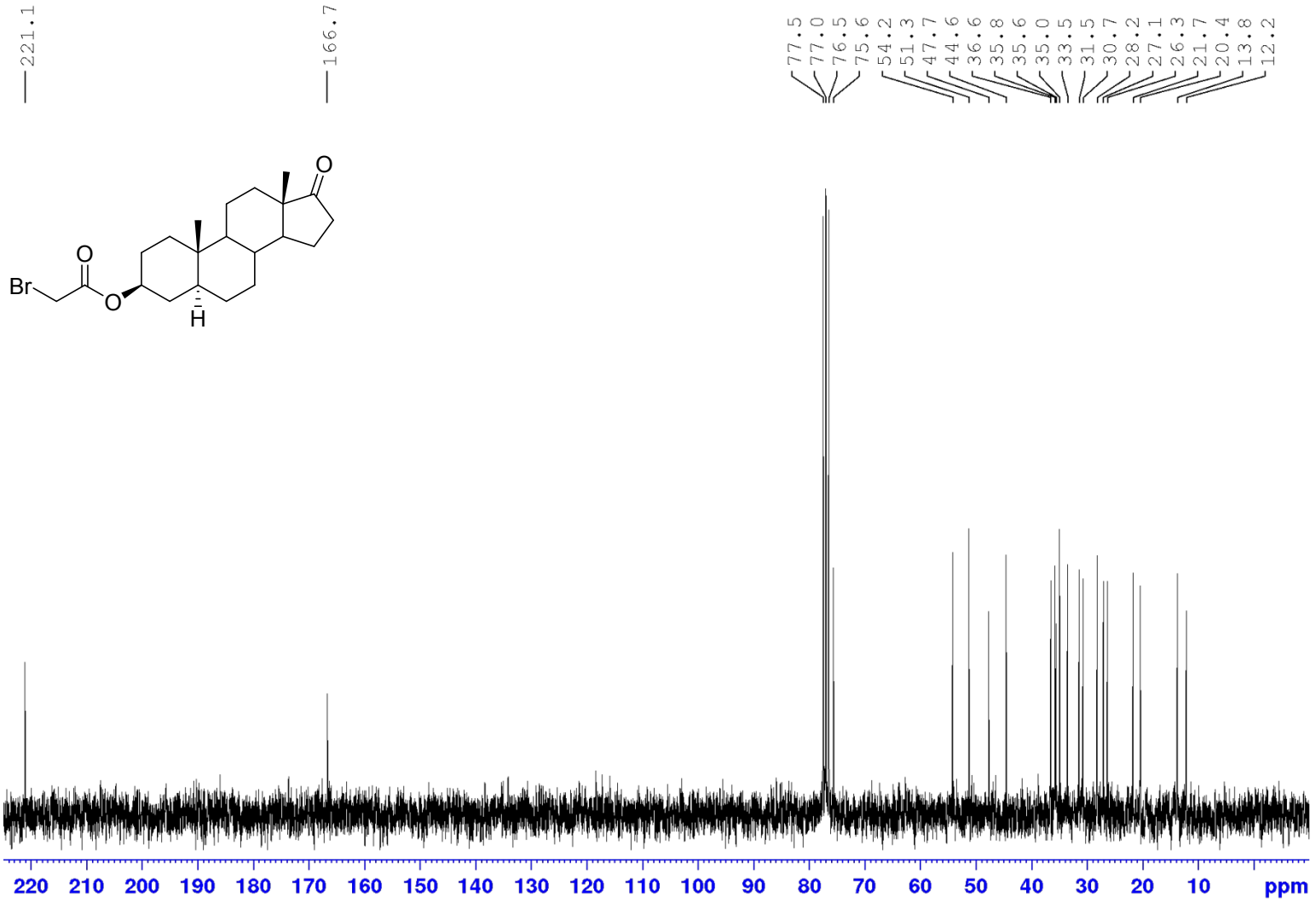
Epiandrosterone acrylate (16) – ^{13}C – $CDCl_3$ – 62.5 MHz



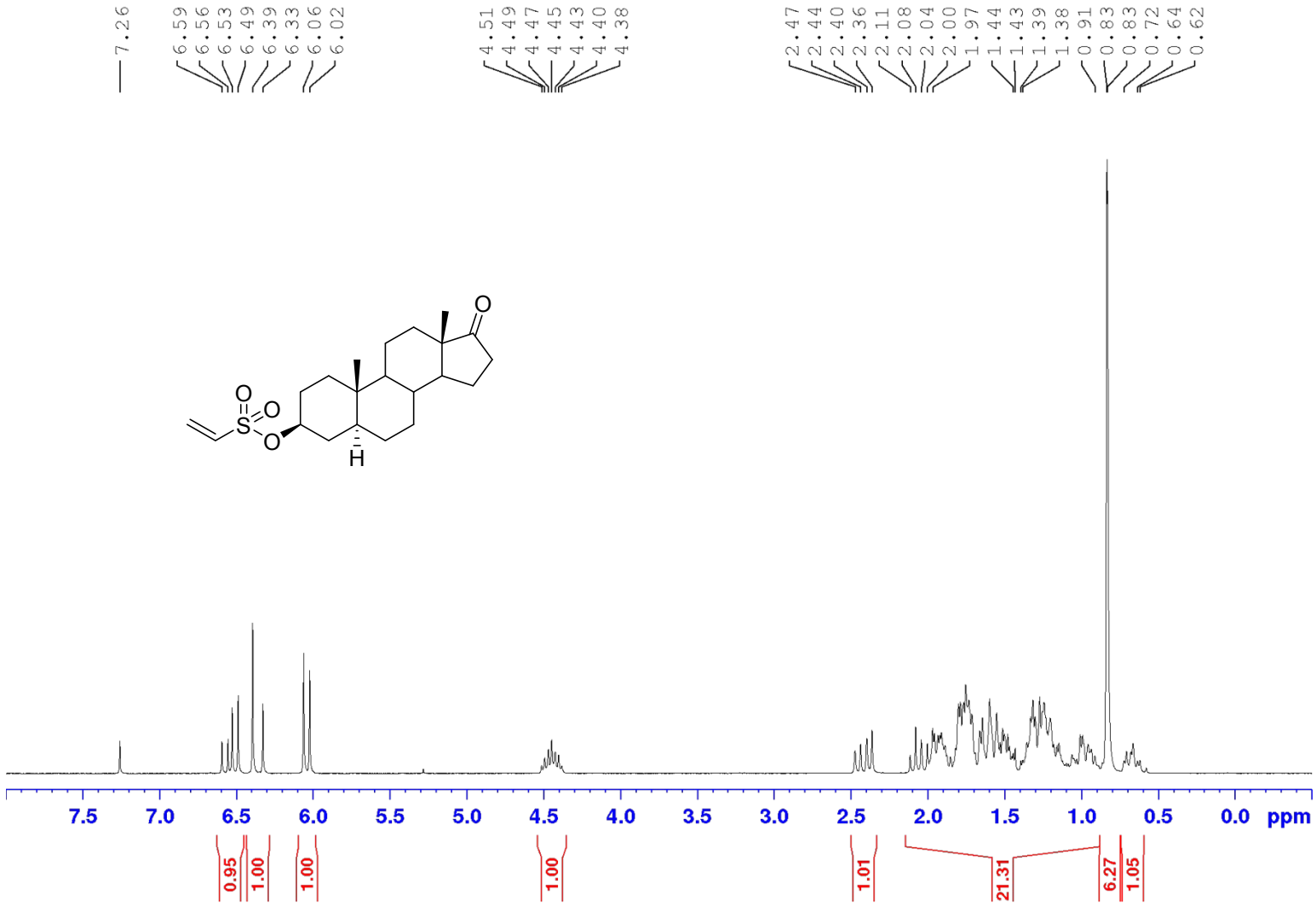
Epiandrosterone α-bromoacetate (17) – ^{1}H – $CDCl_3$ – 250 MHz



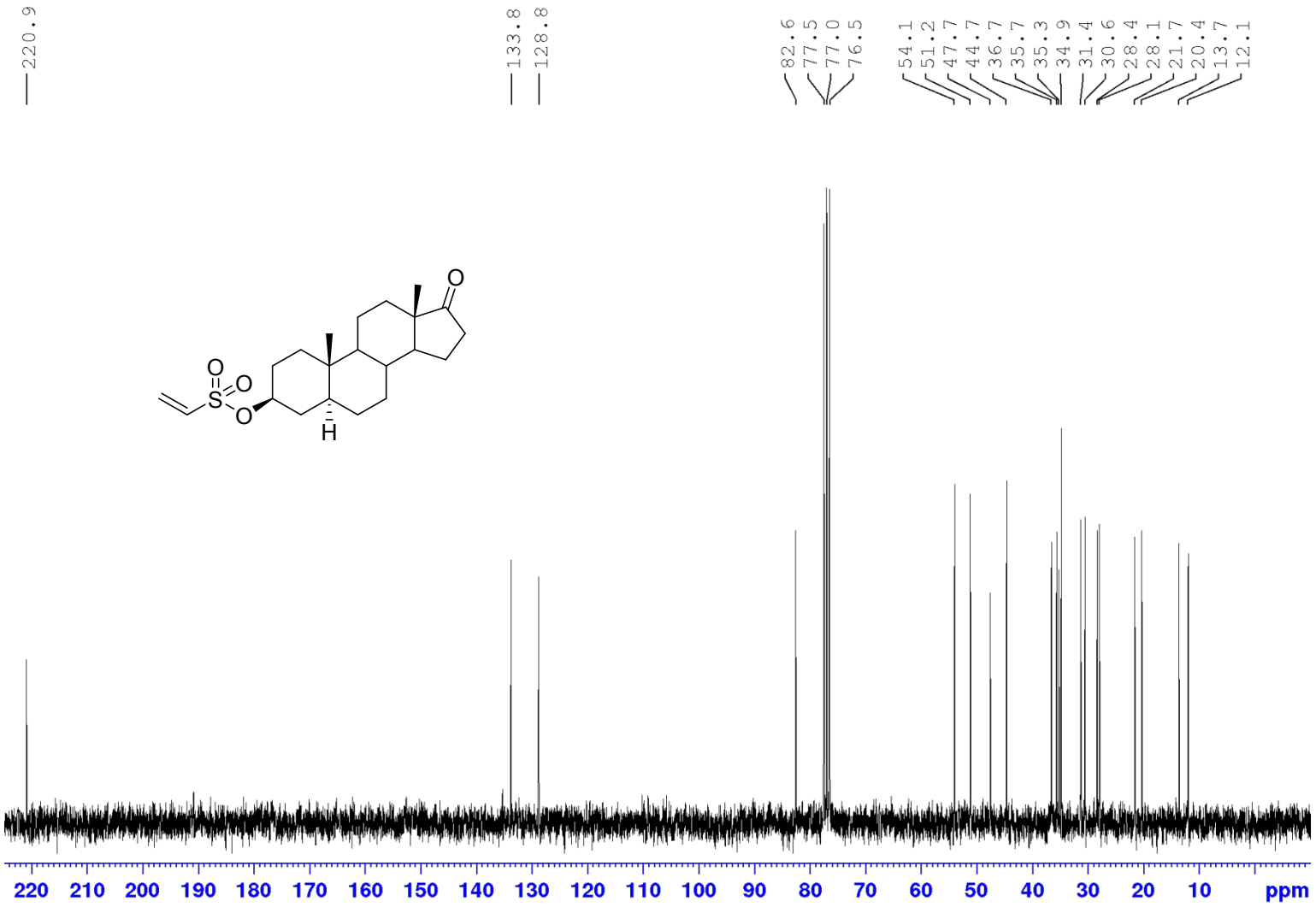
Epiandrosterone α-bromoacetate (17) – ^{13}C – $CDCl_3$ – 62.5 MHz



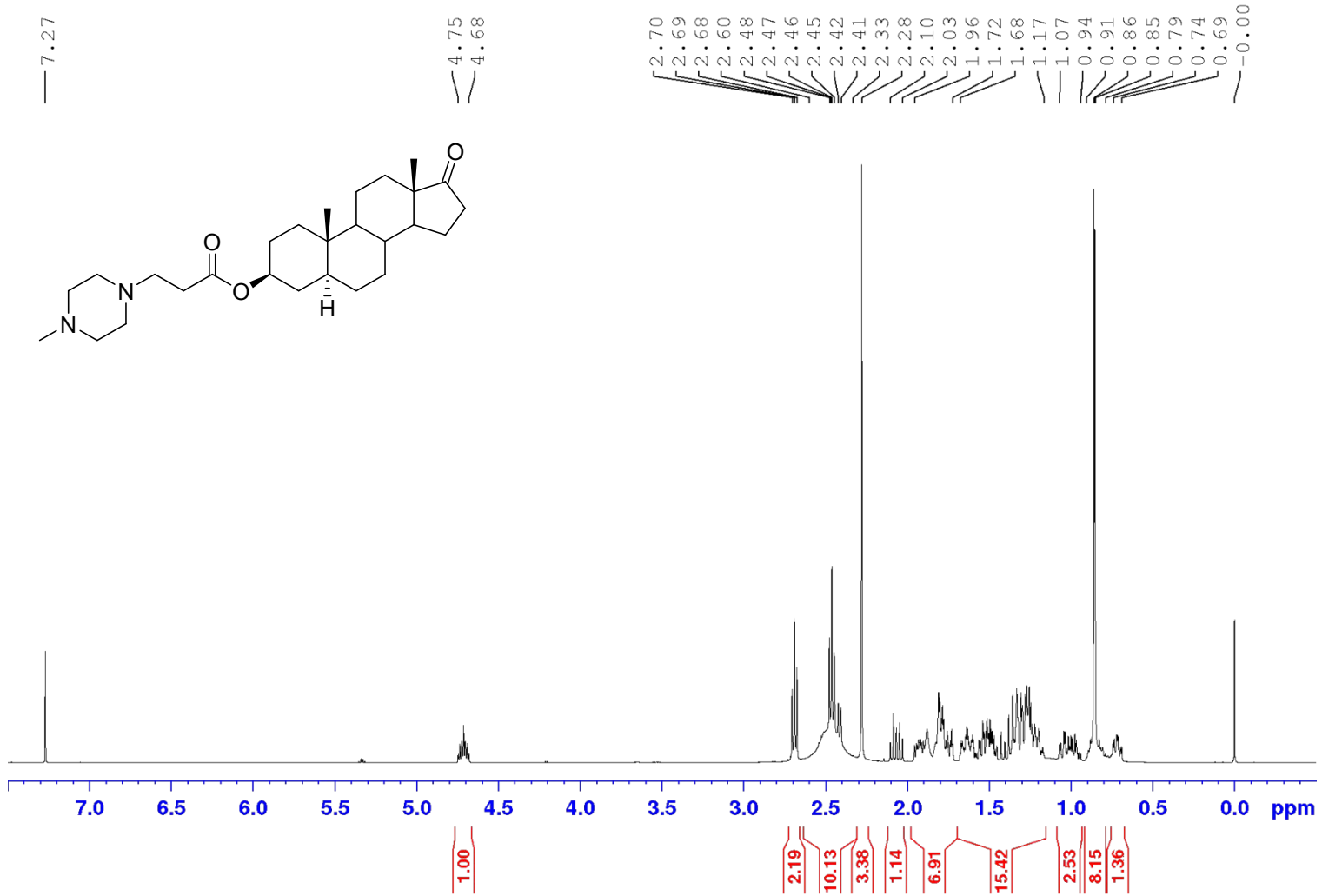
Epiandrosterone vinylsulfonate (18) – ^{1}H – $CDCl_3$ – 250 MHz



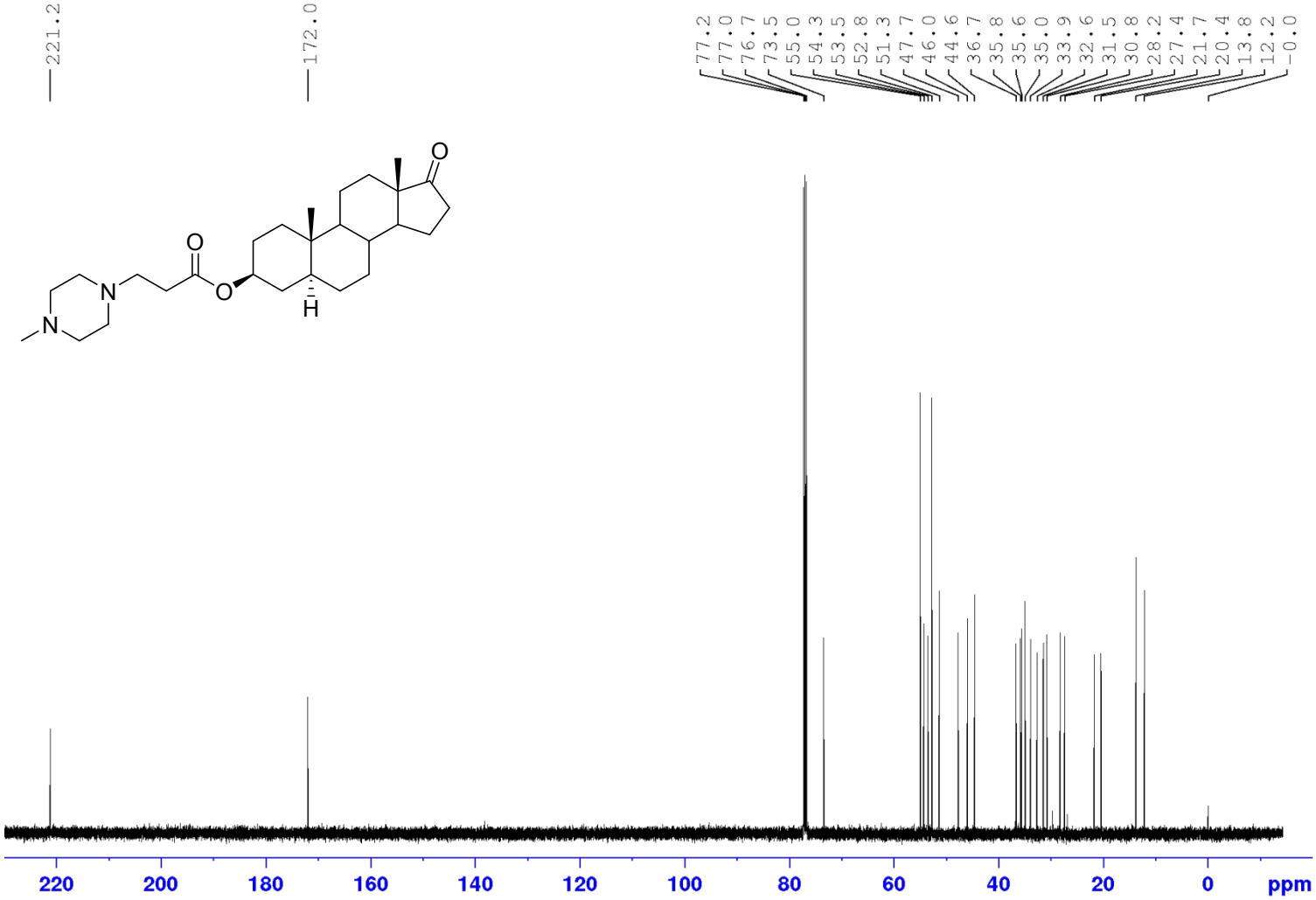
Epiandrosterone vinylsulfonate (18) – ^{13}C – $CDCl_3$ – 62.5 MHz



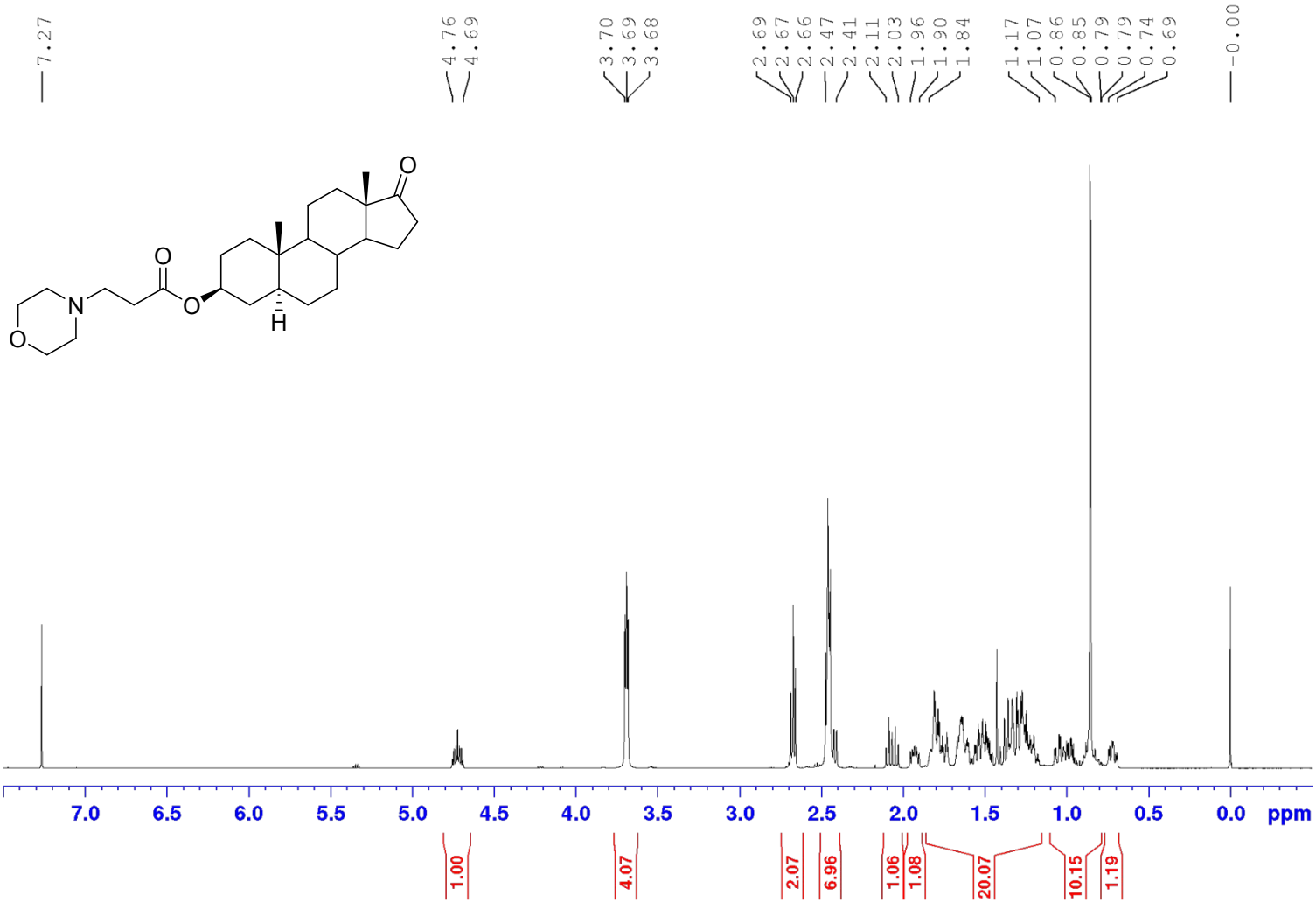
Epiandrosterone 3-(4-methylpiperazin-1-yl)propanoate (19) – ^{1}H – $CDCl_3$ – 500 MHz



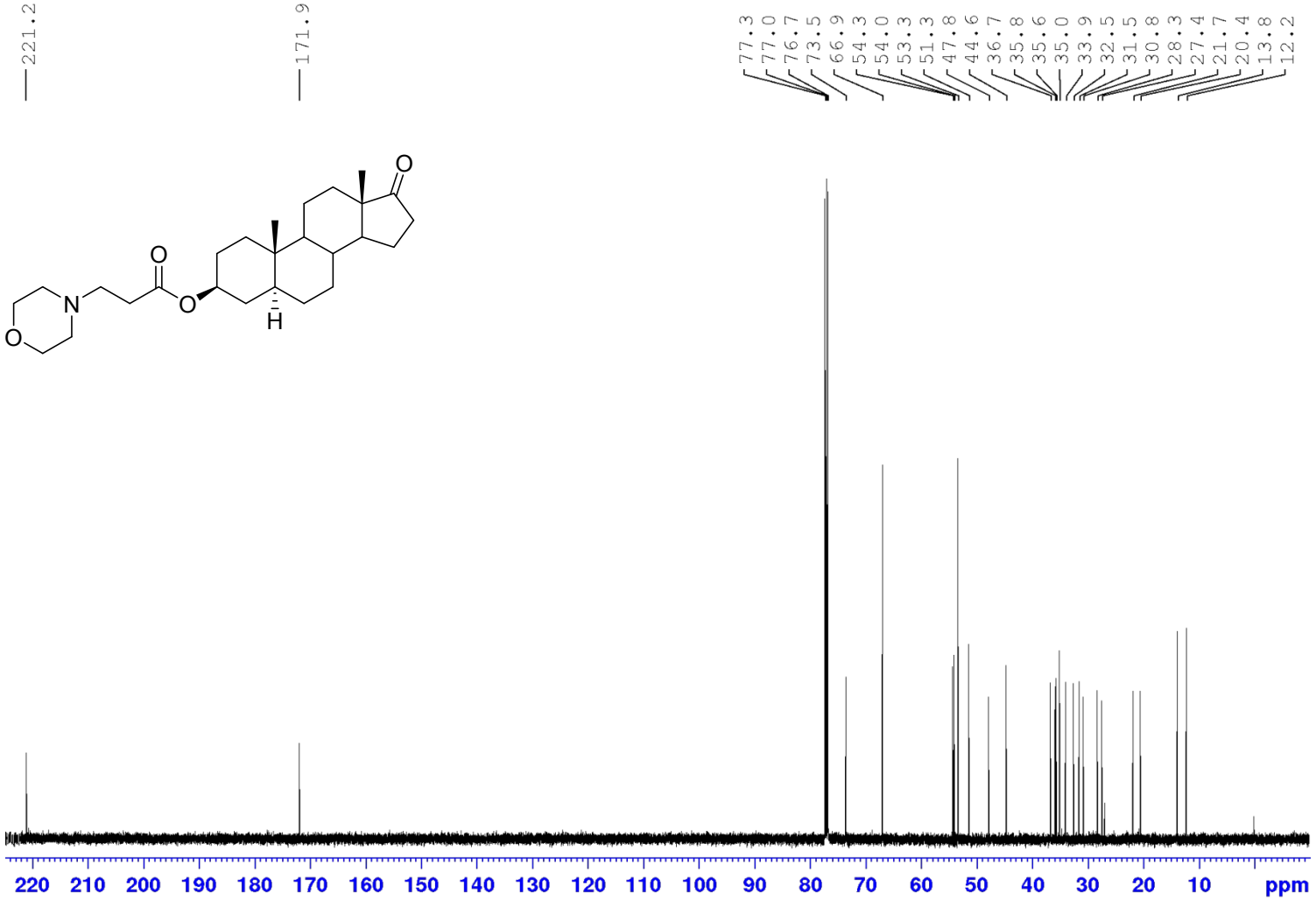
Epiandrosterone 3-(4-methylpiperazin-1-yl)propanoate (19) – ^{13}C – $CDCl_3$ – 125 MHz



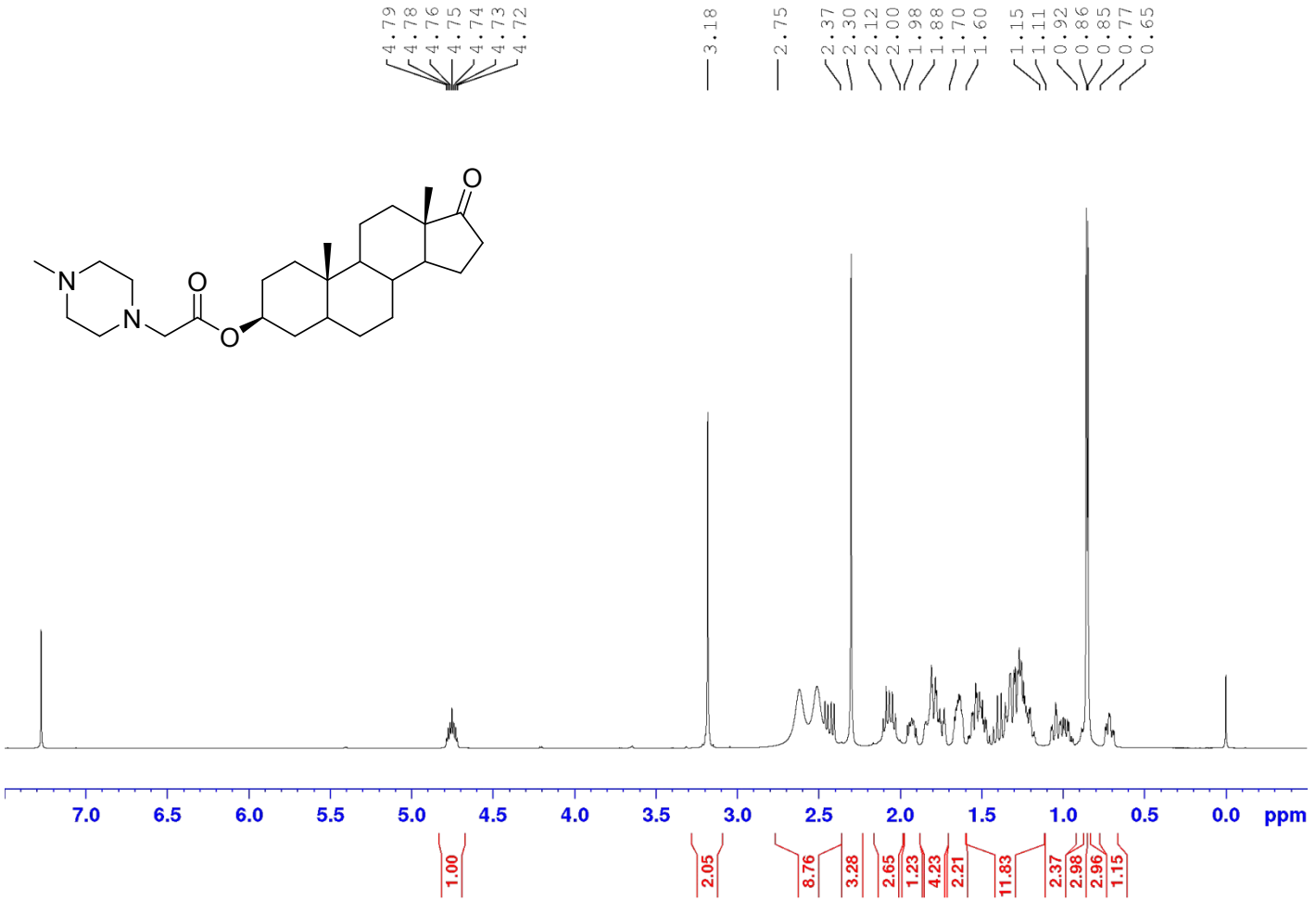
Epiandrosterone 3-morpholinopropanoate (20) – ^{1}H – $CDCl_3$ – 500 MHz



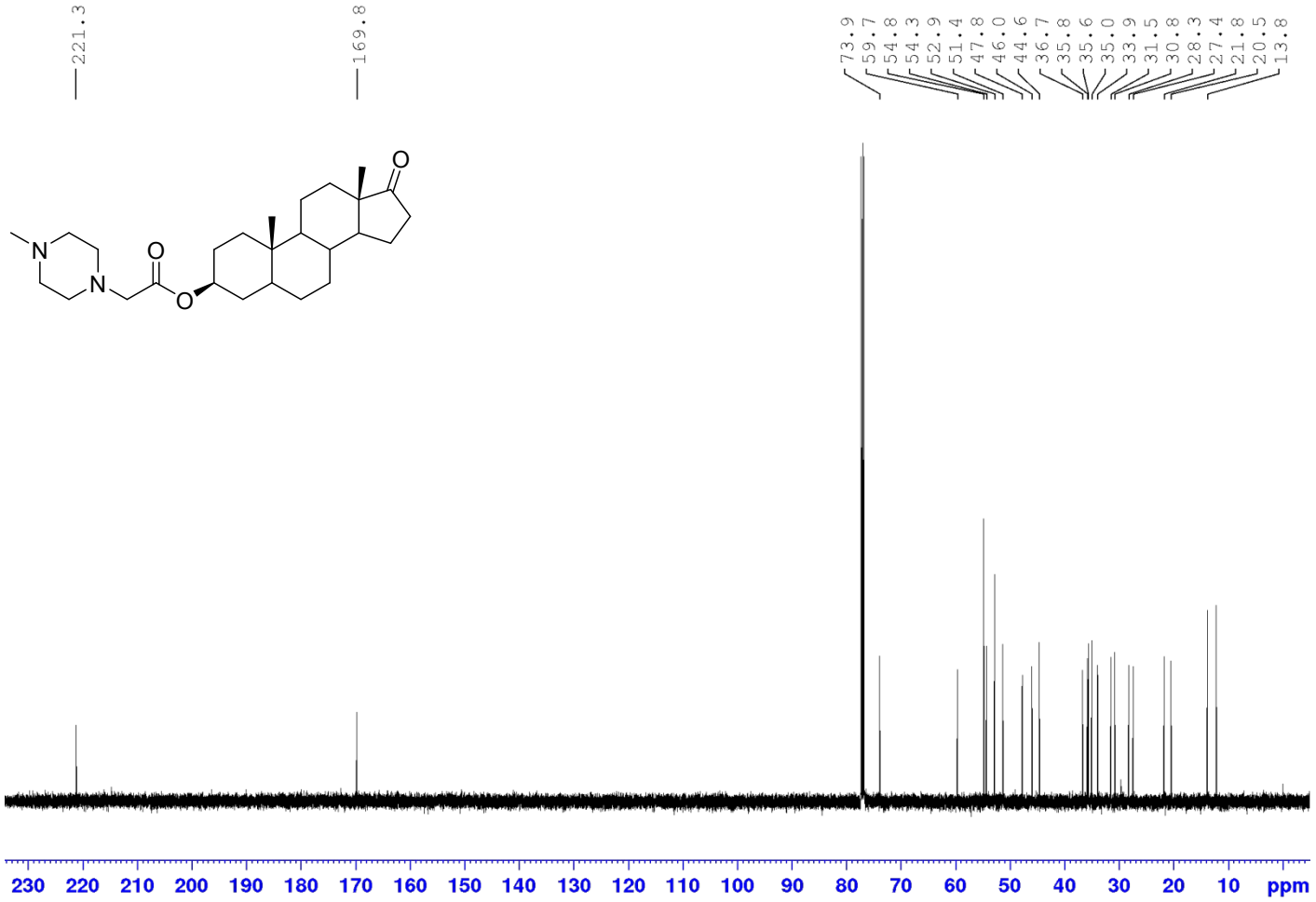
Epiandrosterone 3-morpholinopropanoate (20) – ^{13}C – $CDCl_3$ – 125 MHz



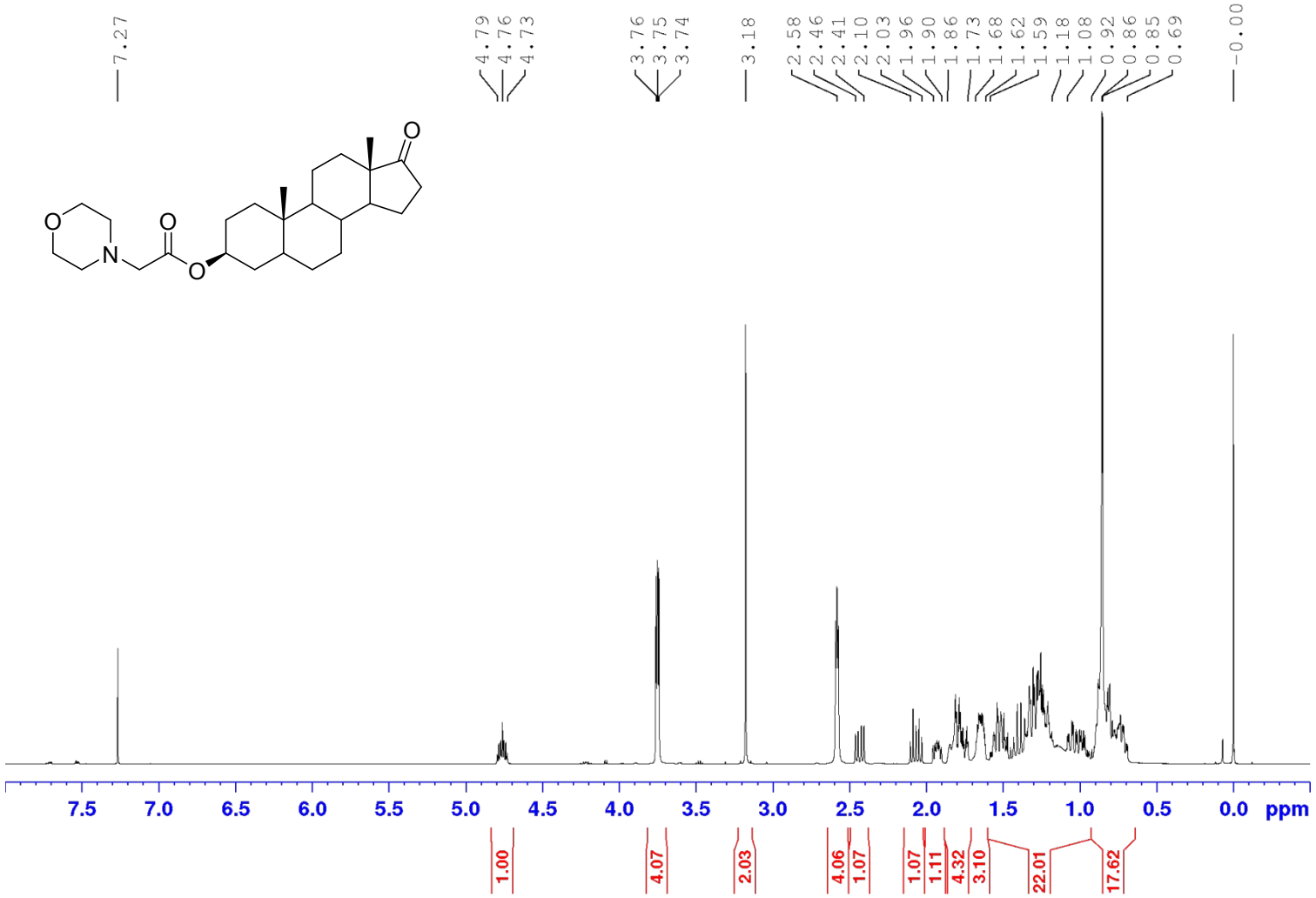
Epiandrosterone 2-(4-methylpiperazin-1-yl)acetate (21) – ^{1}H – $CDCl_3$ – 500 MHz



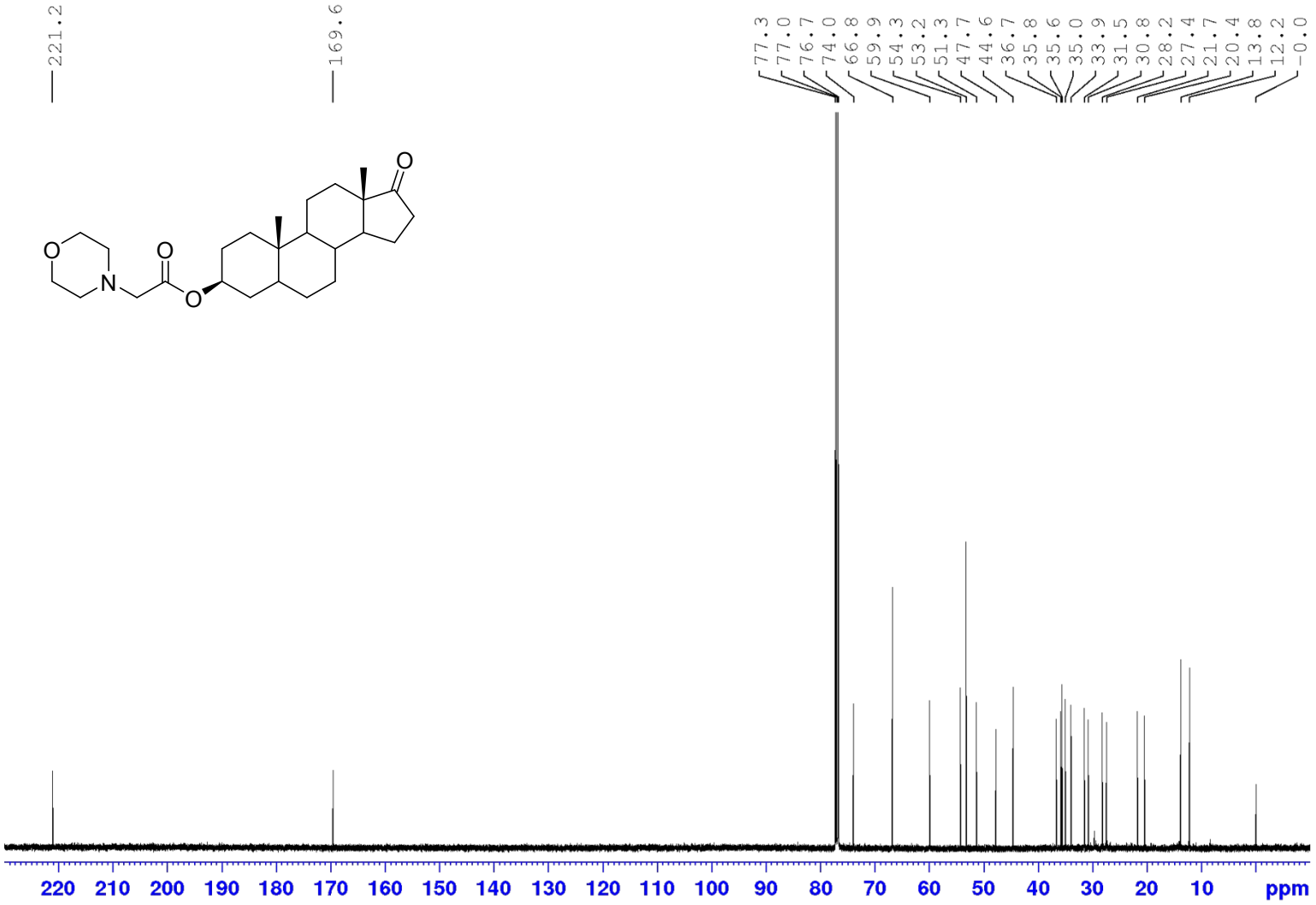
Epiandrosterone 2-(4-methylpiperazin-1-yl)acetate (21) – ^{13}C – $CDCl_3$ – 125 MHz



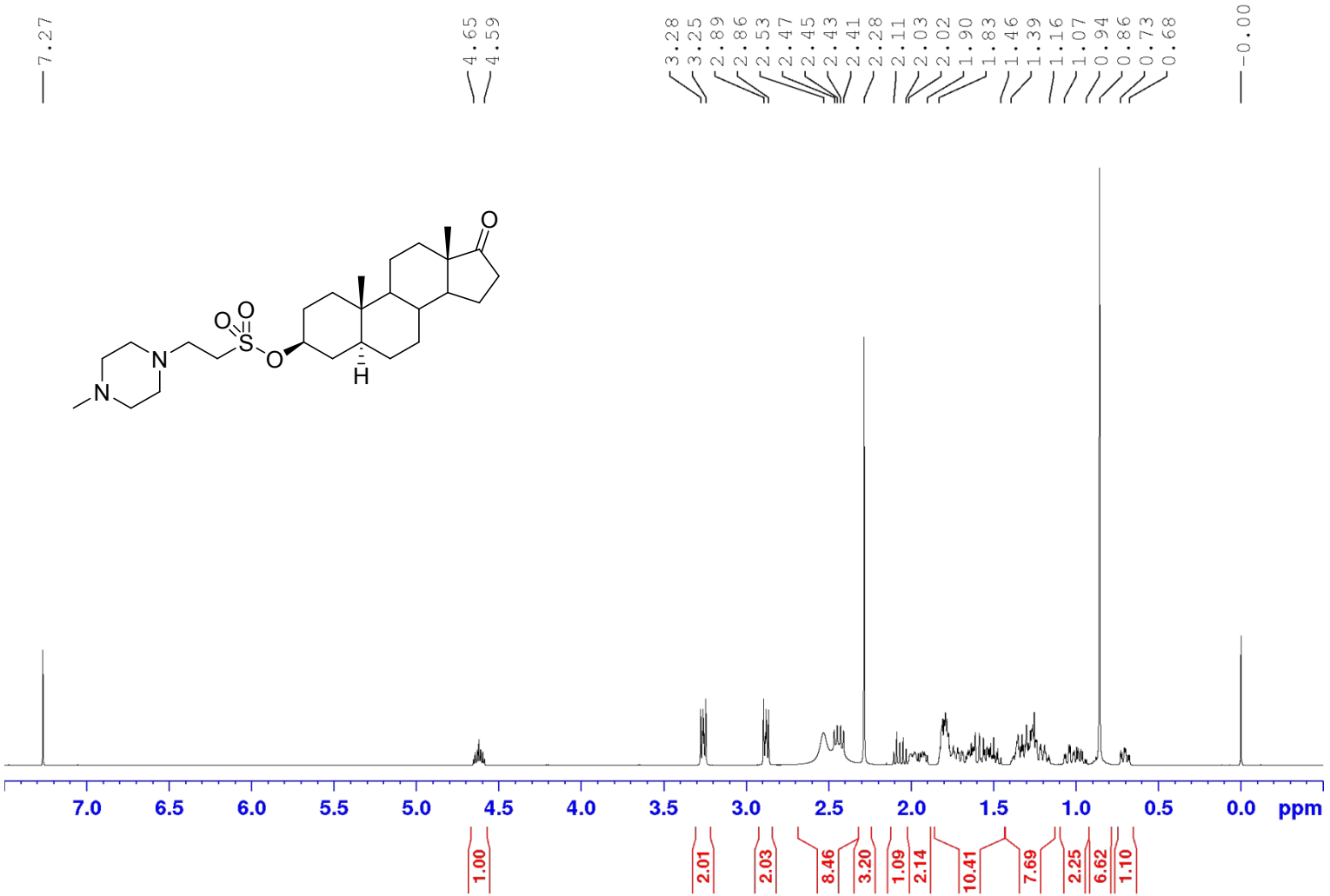
Epiandrosterone 2-morpholinoacetate (22) – ^{1}H – $CDCl_3$ – 500 MHz



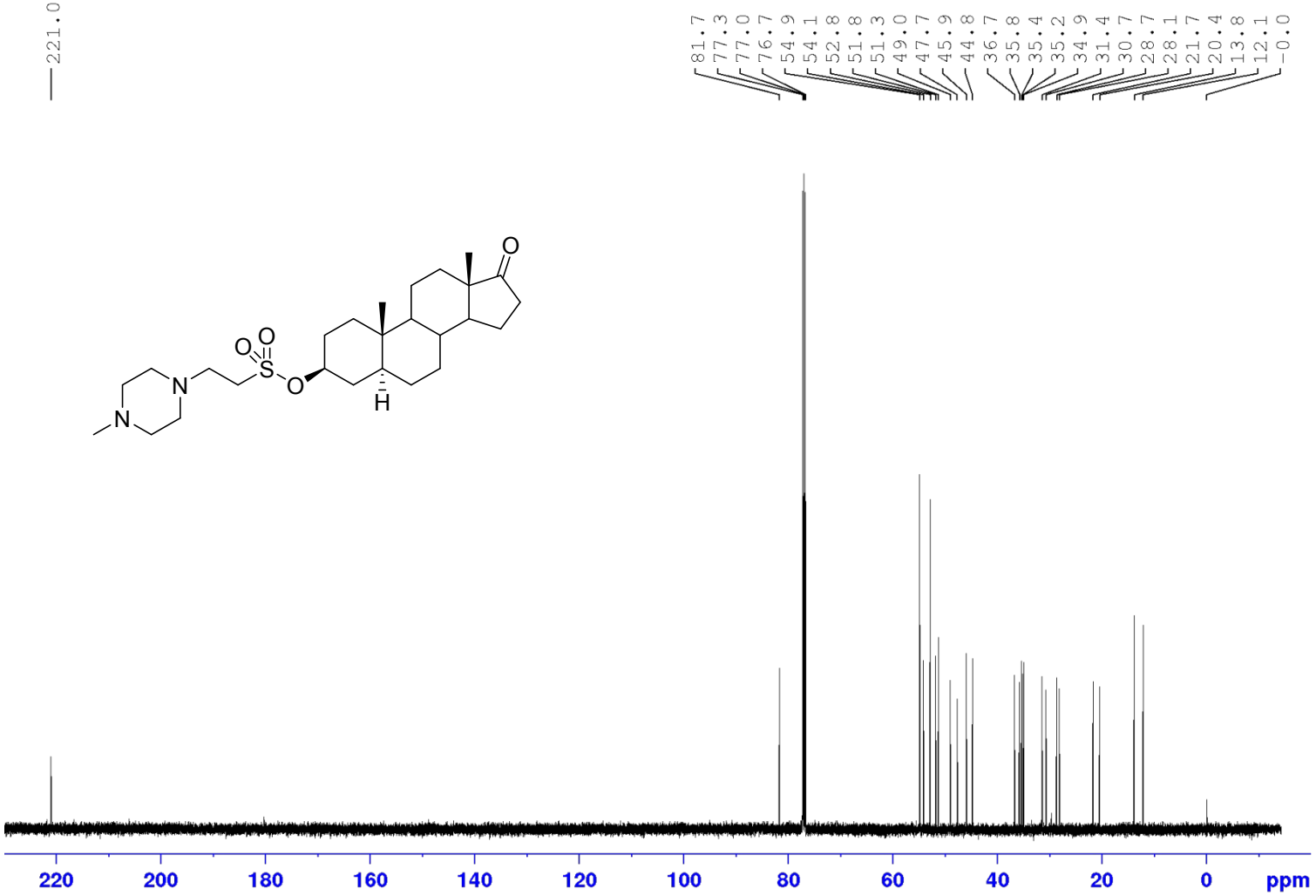
Epiandrosterone 2-morpholinoacetate (22) – ^{13}C – $CDCl_3$ – 125 MHz



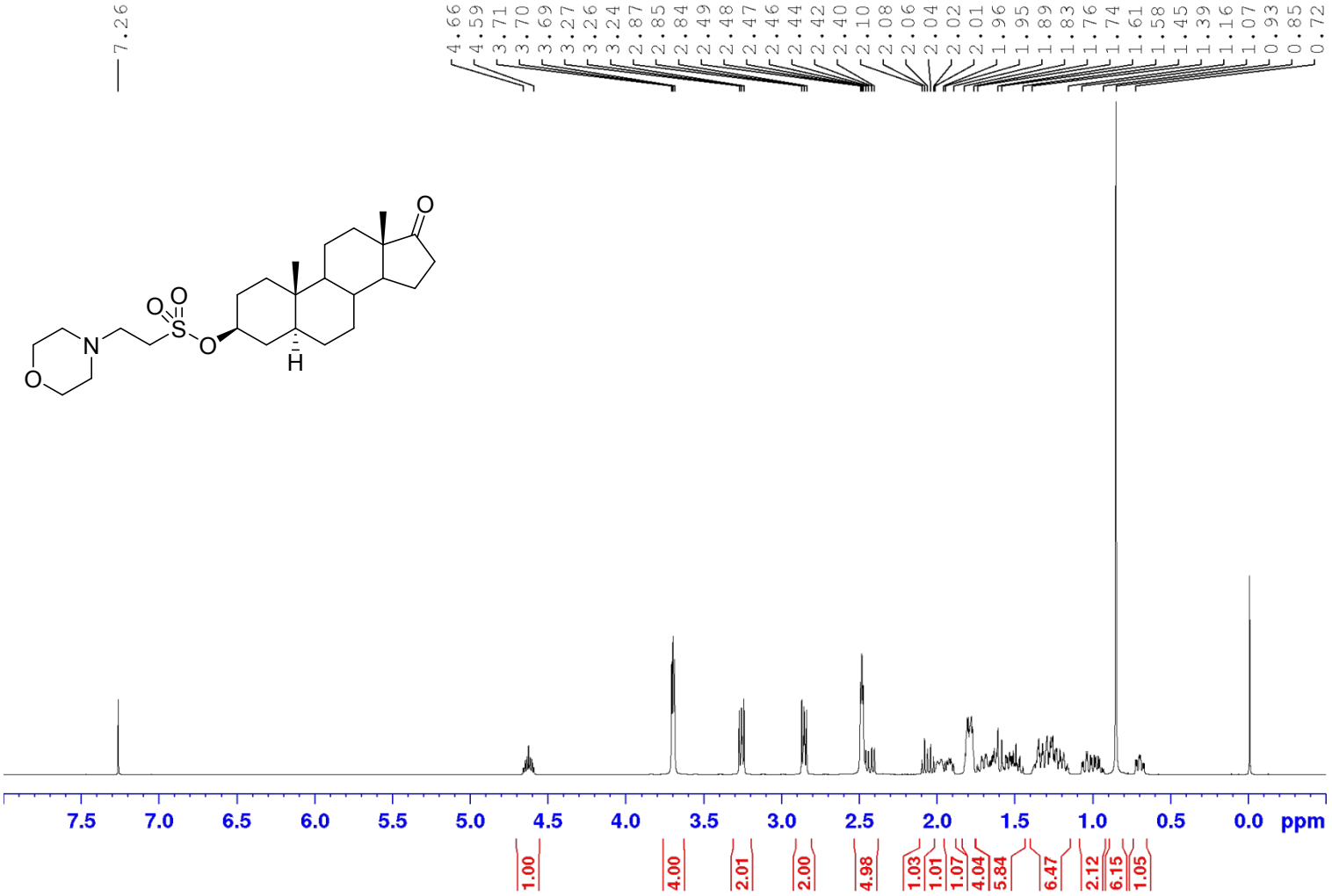
Epiandrosterone 2-(4-methylpiperazin-1-yl)ethane-1-sulfonate (23) – ^{1}H – $CDCl_3$ – 500 MHz



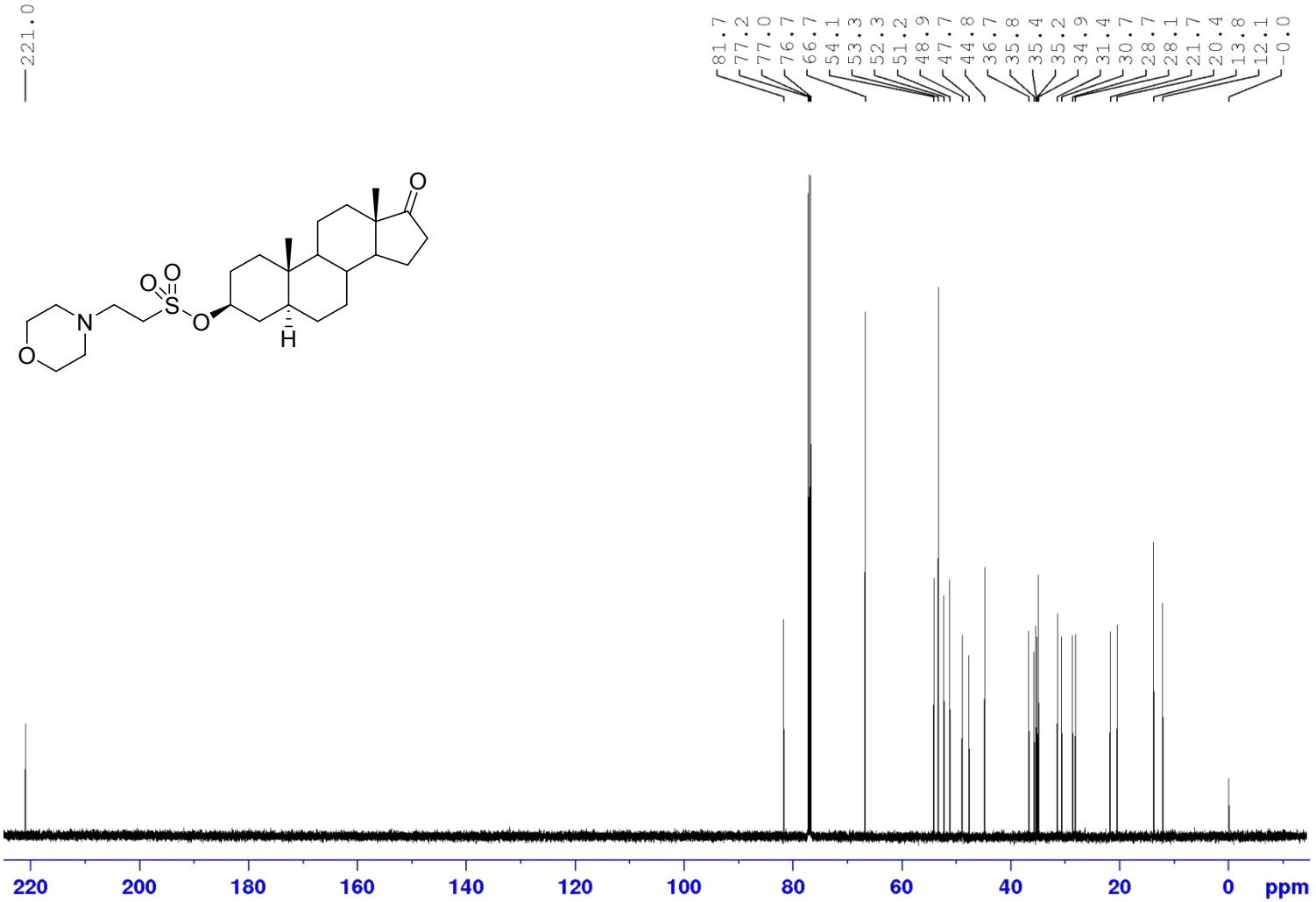
Epiandrosterone 2-(4-methylpiperazin-1-yl)ethane-1-sulfonate (23) – ^{13}C – $CDCl_3$ – 125 MHz



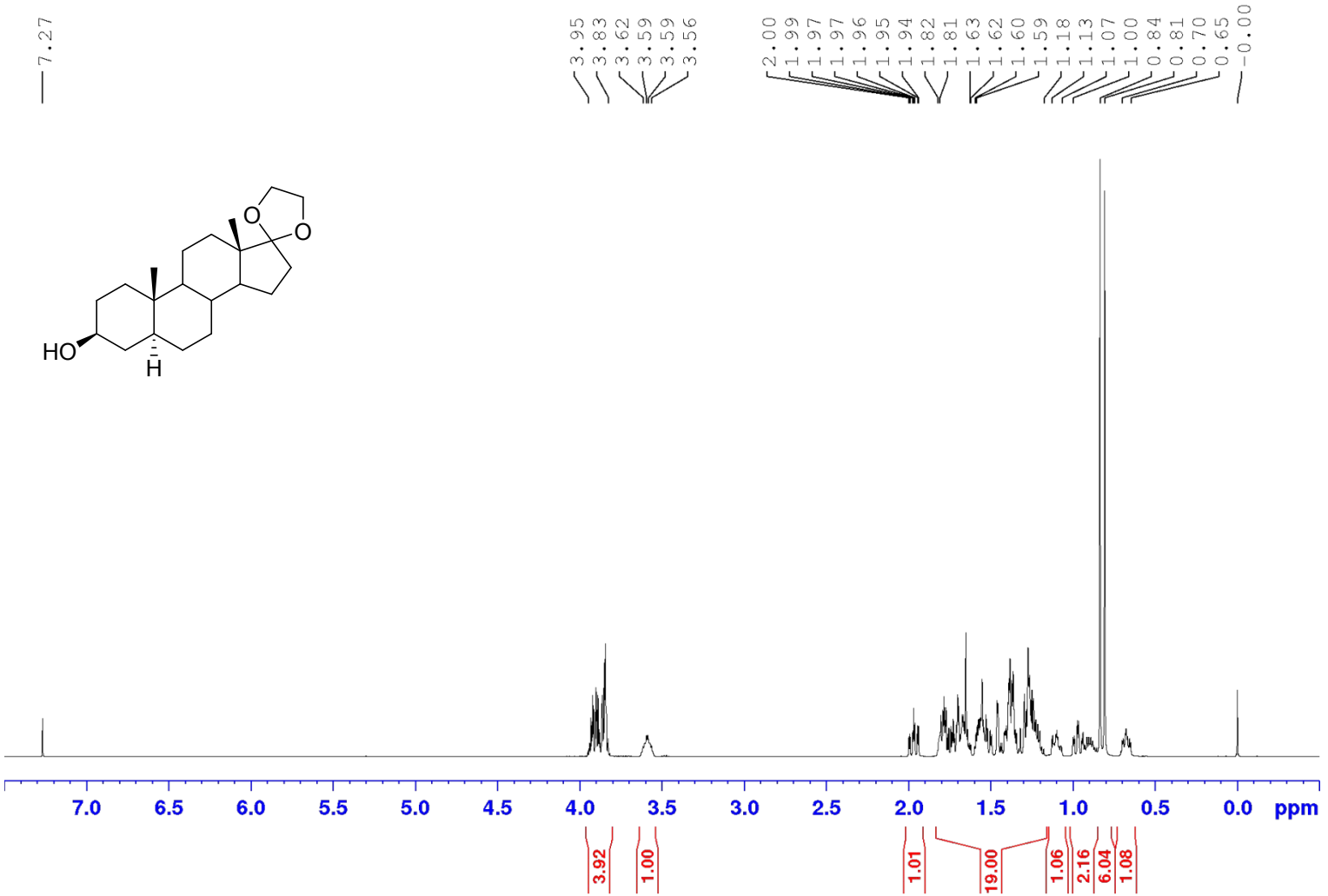
Epiandrosterone 2-morpholinoethanesulfonate (24) – ^{1}H – $CDCl_3$ – 500 MHz



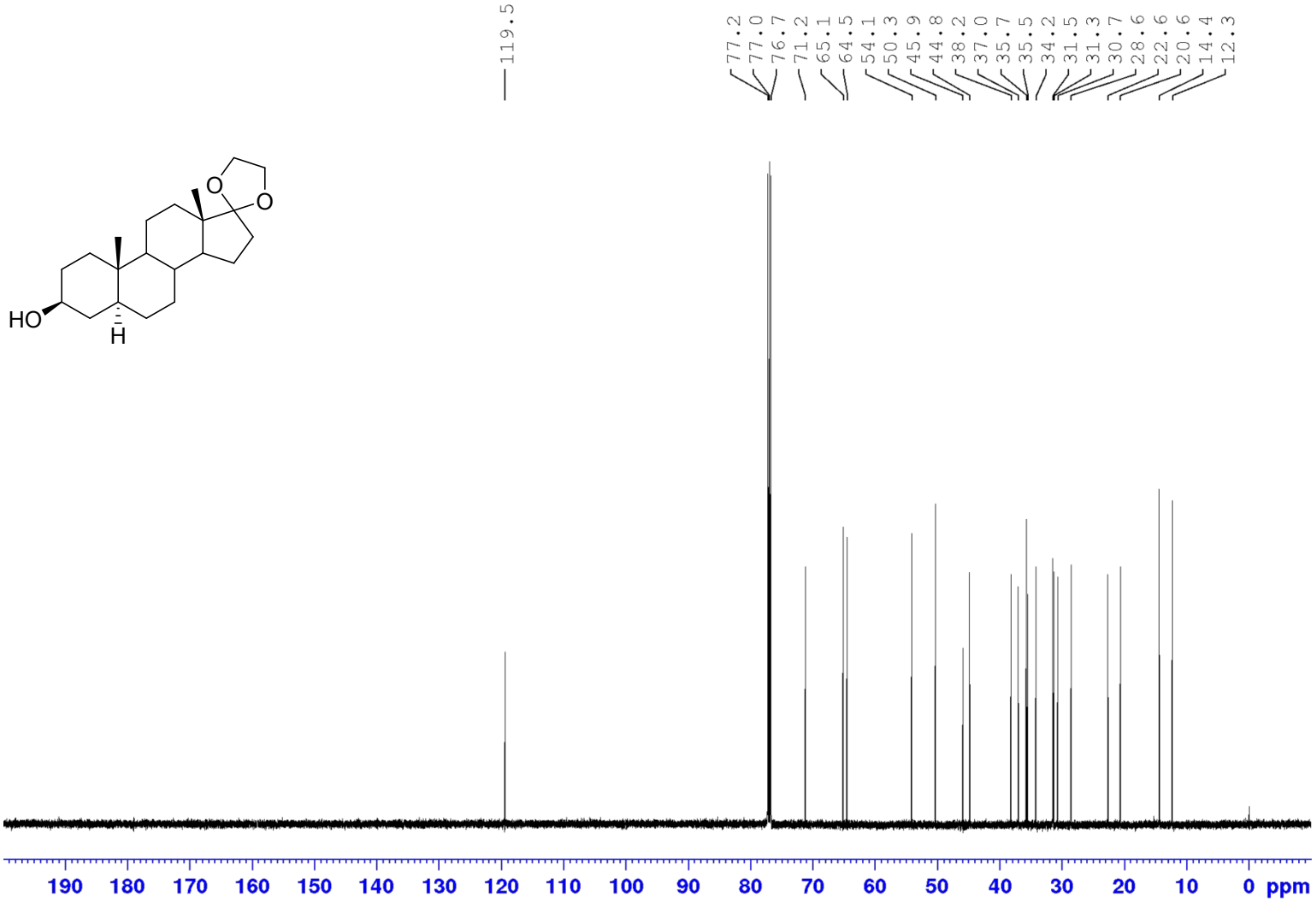
Epiandrosterone 2-morpholinoethanesulfonate (24) – ^{13}C – $CDCl_3$ – 125 MH



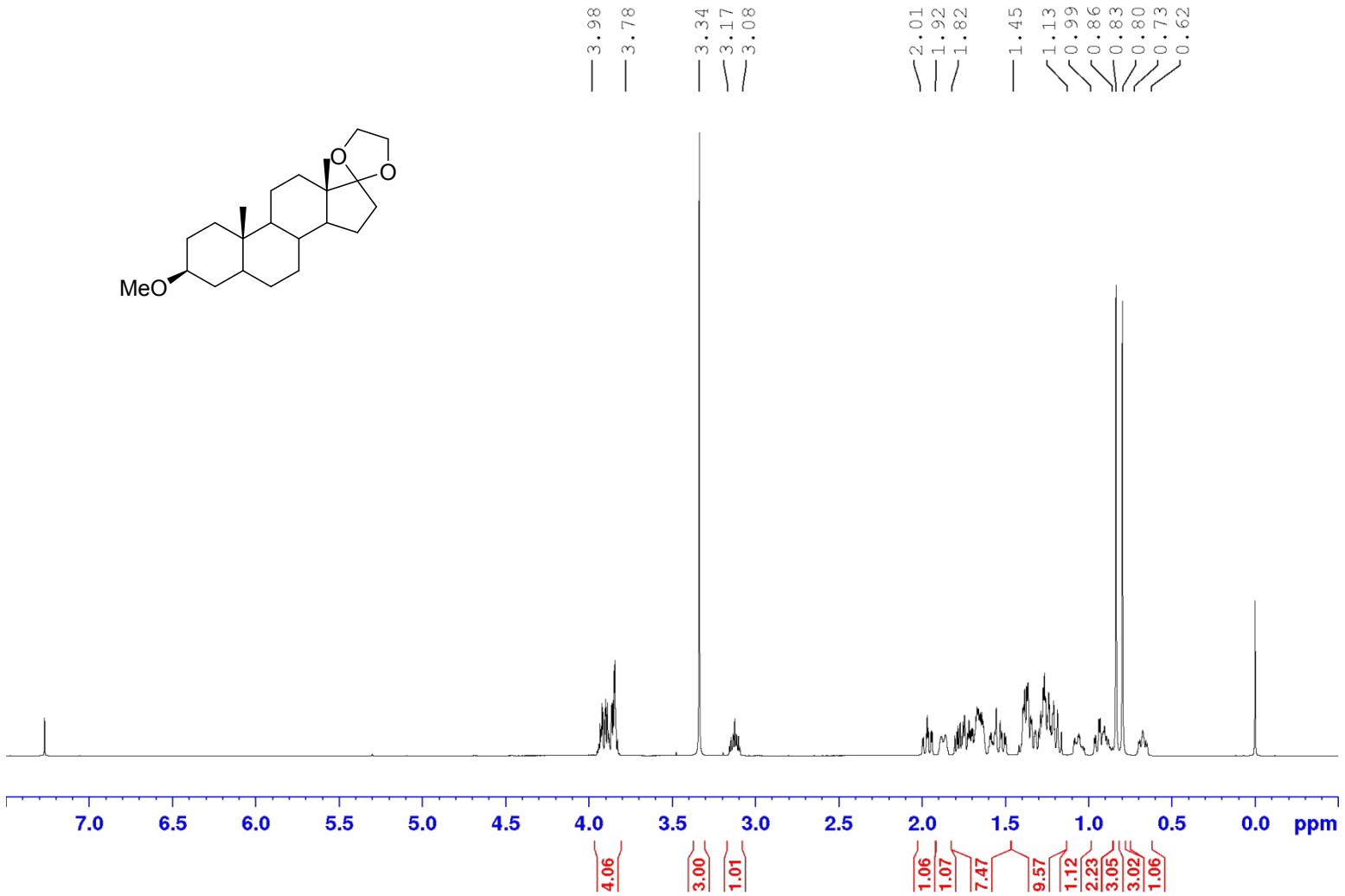
Epiandrosterone 17-acetal (25) – ^{1}H – $CDCl_3$ – 500 MHz



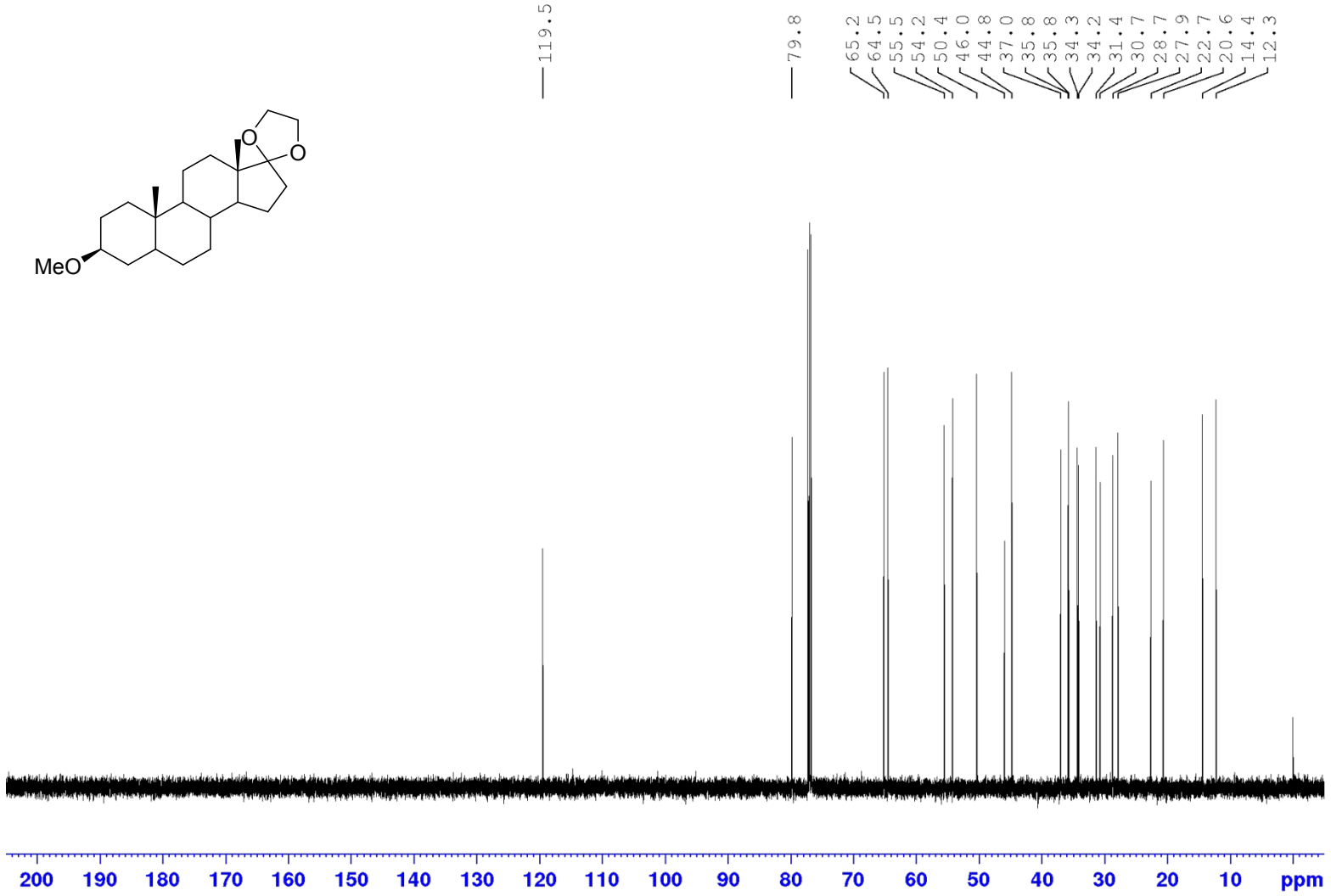
Epiandrosterone 17-acetal (25) – ^{13}C – $CDCl_3$ – 125 MHz



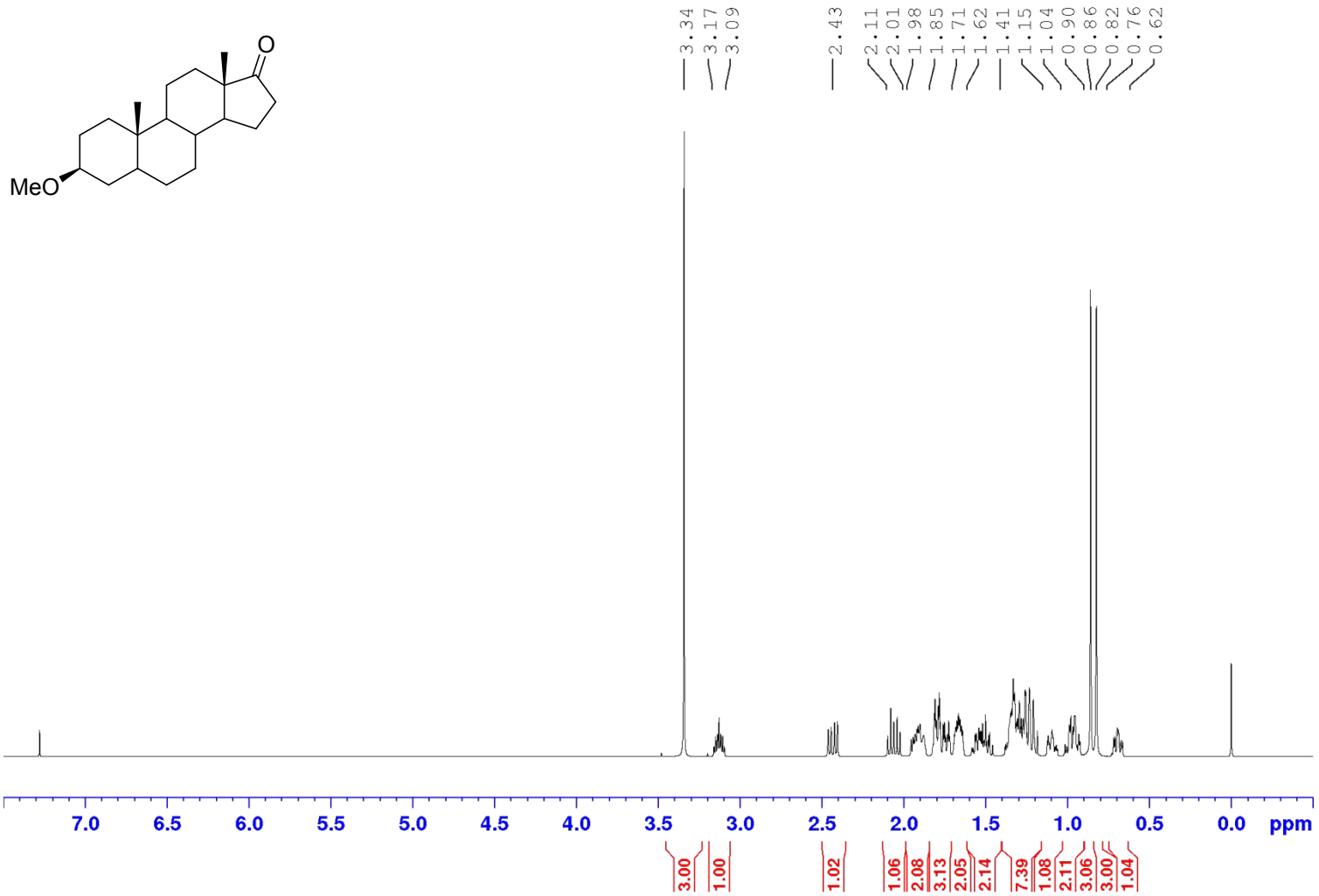
Epiandrosterone 17-acetal methyl ether (26) – ^{1}H – $CDCl_3$ – 500 MHz



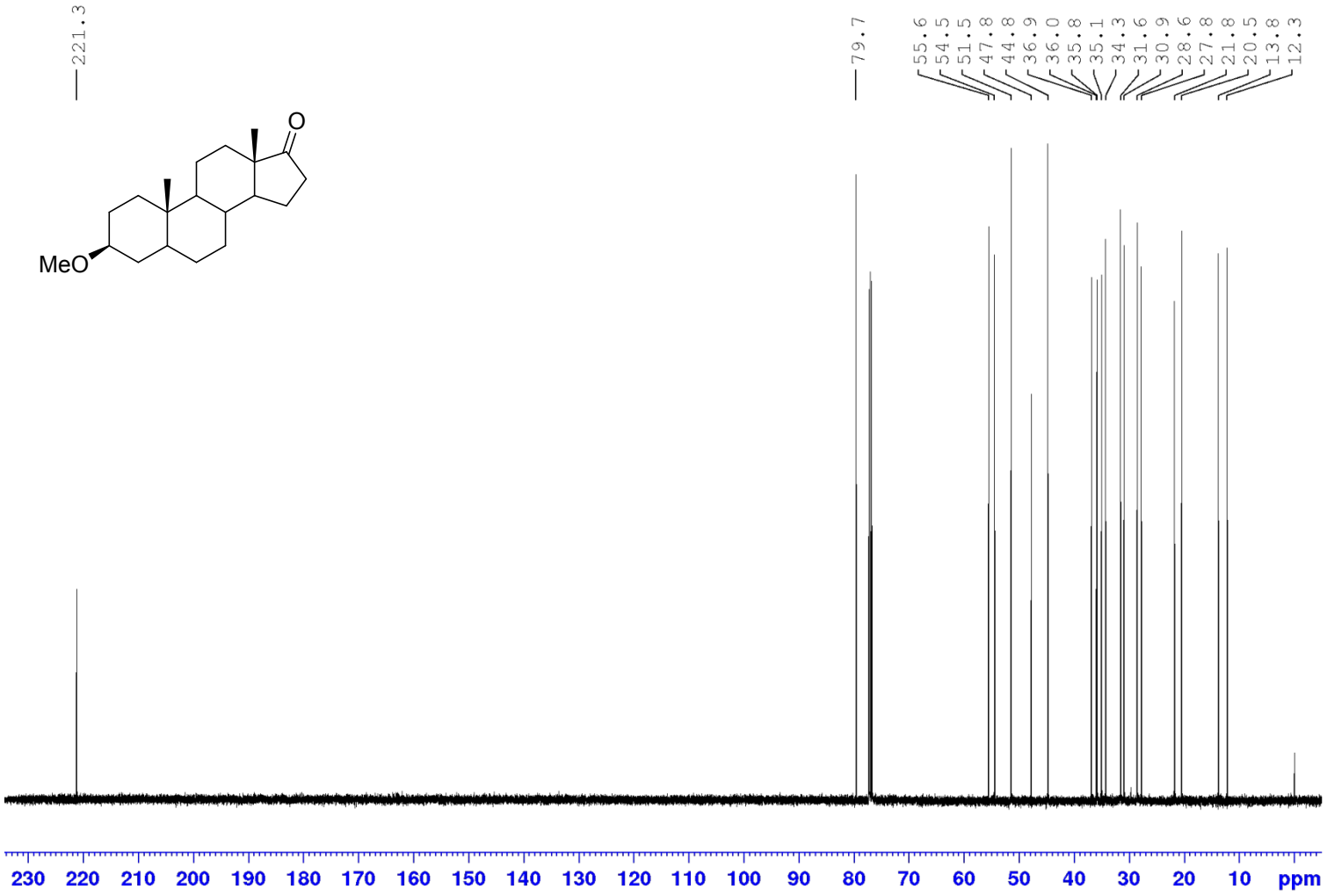
Epiandrosterone 17-acetal methyl ether (26) – ^{13}C – $CDCl_3$ – 125 MHz



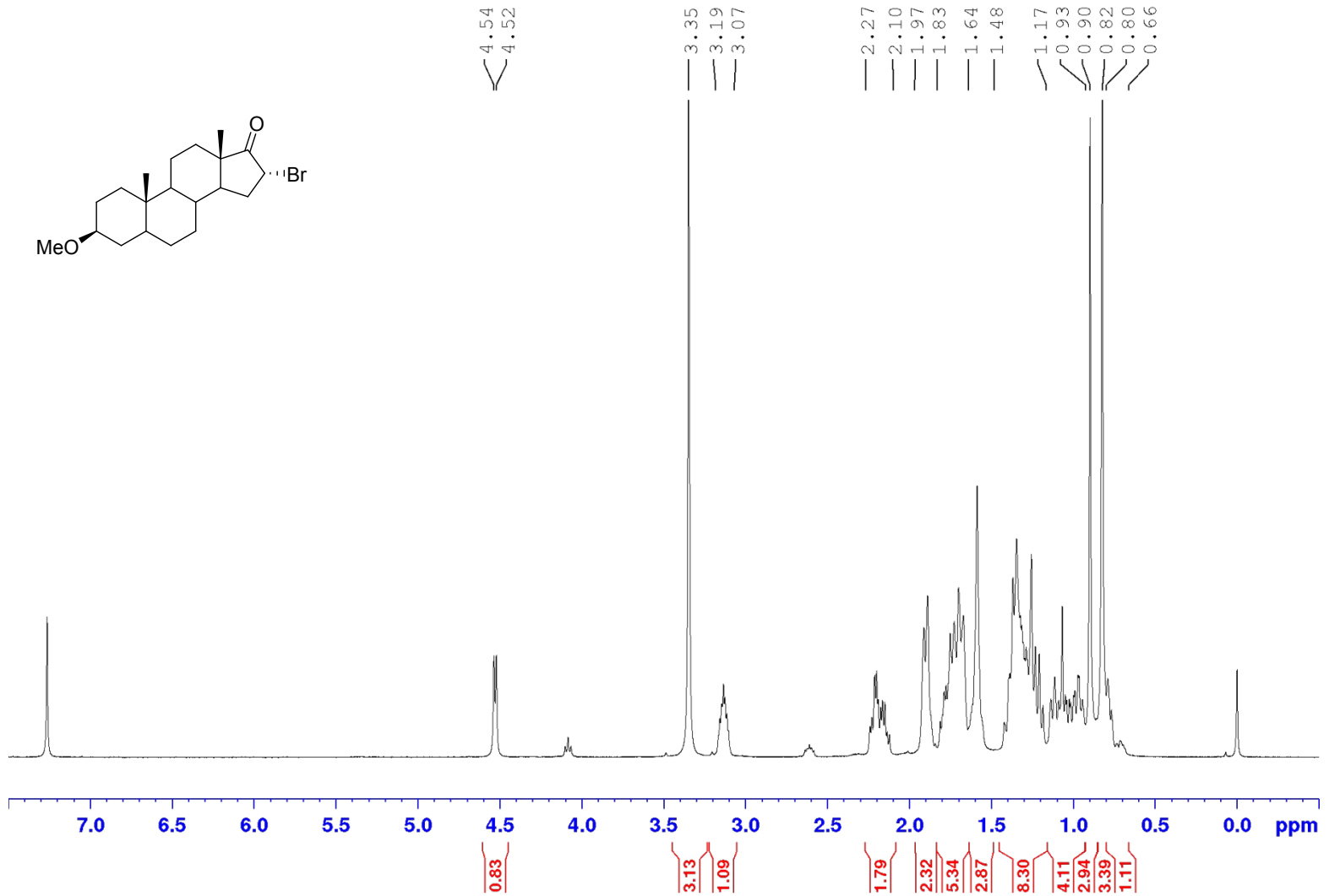
Epiandrosterone methyl ether (27) – ^{1}H – $CDCl_3$ – 500 MHz



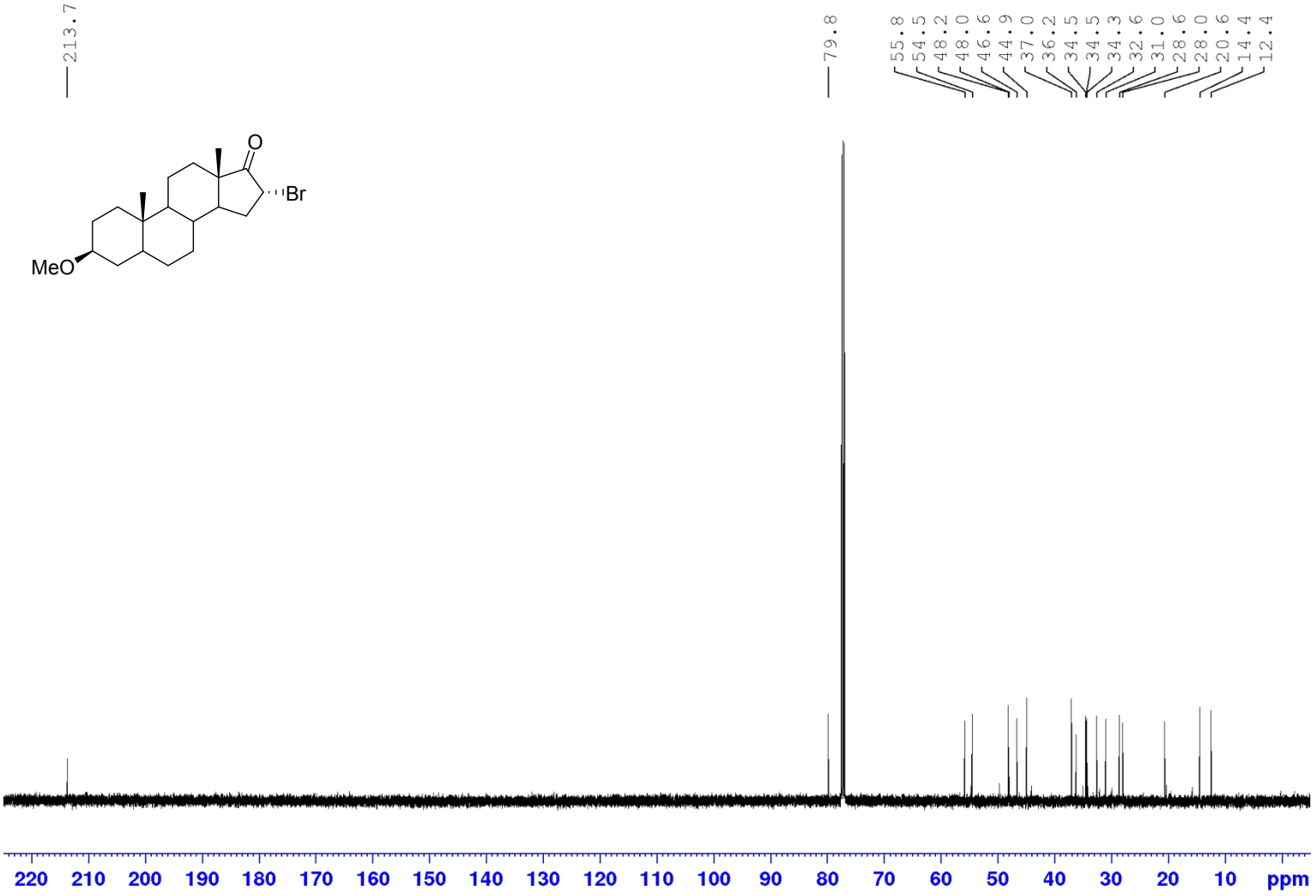
Epiandrosterone methyl ether (27) – ^{13}C – $CDCl_3$ – 125 MHz



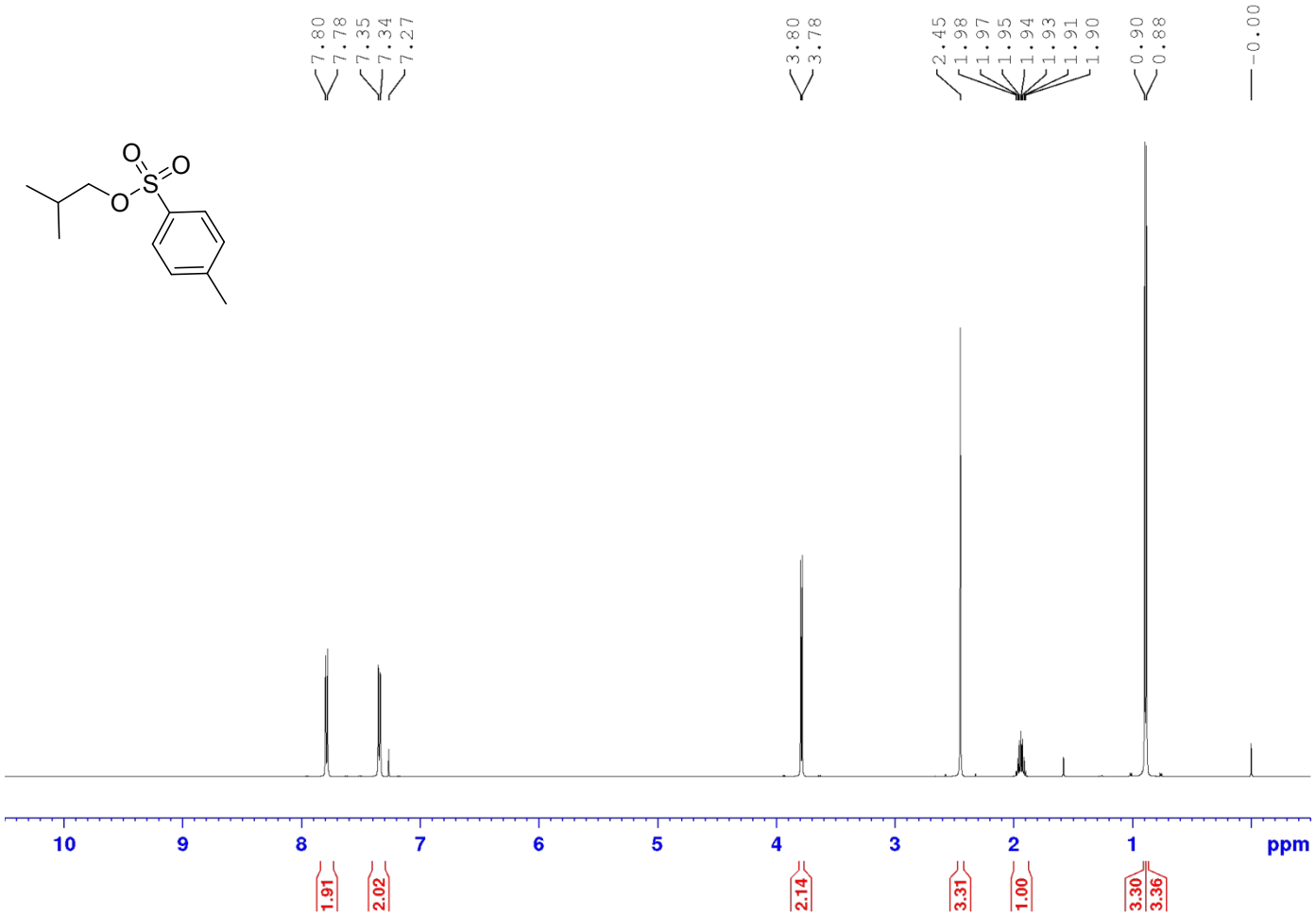
16α-Bromoepiandrosterone methyl ether (28) – ^{1}H – $CDCl_3$ – 500 MHz



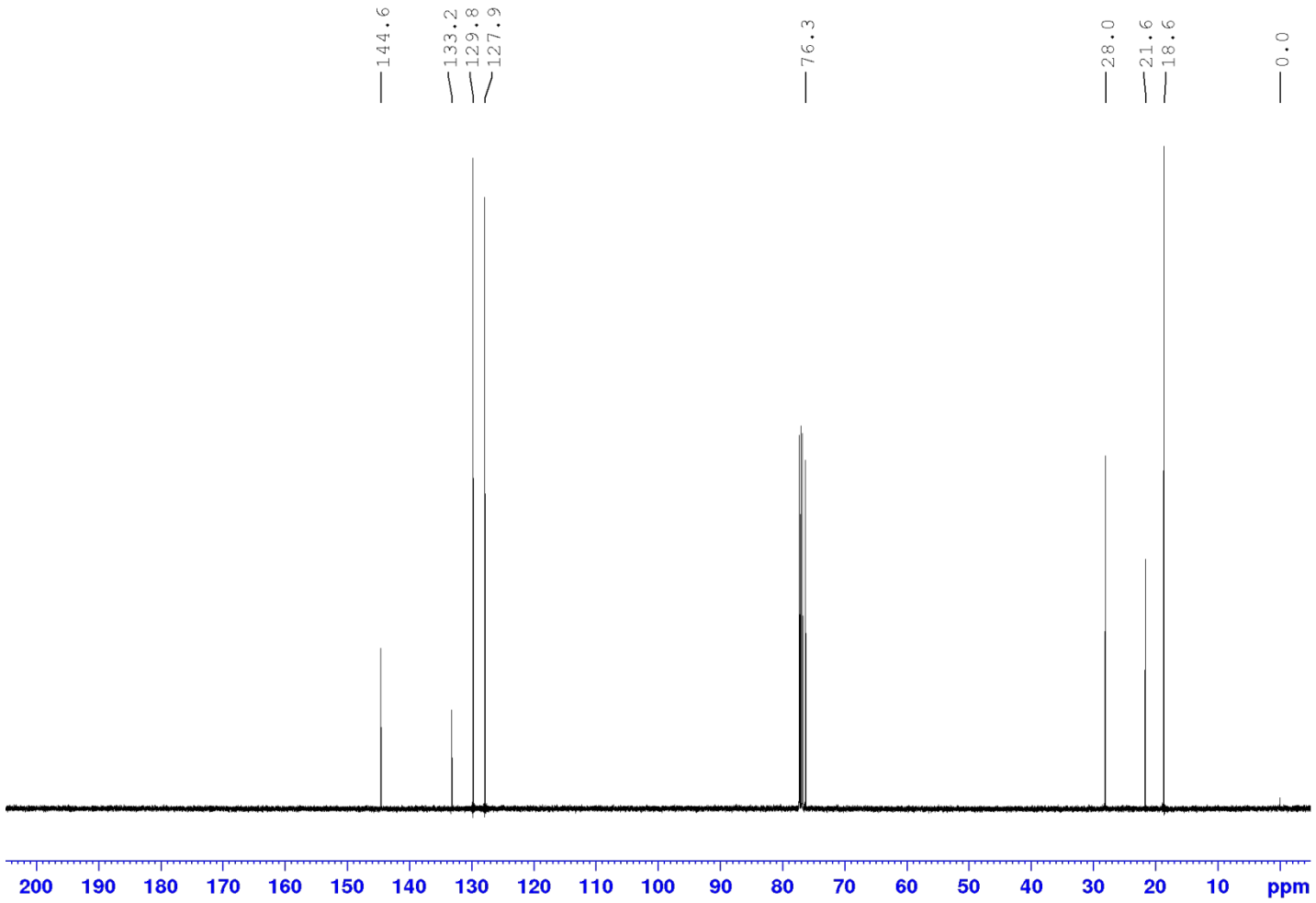
16α-Bromoepiandrosterone methyl ether (28) – ^{13}C – $CDCl_3$ – 125 MHz



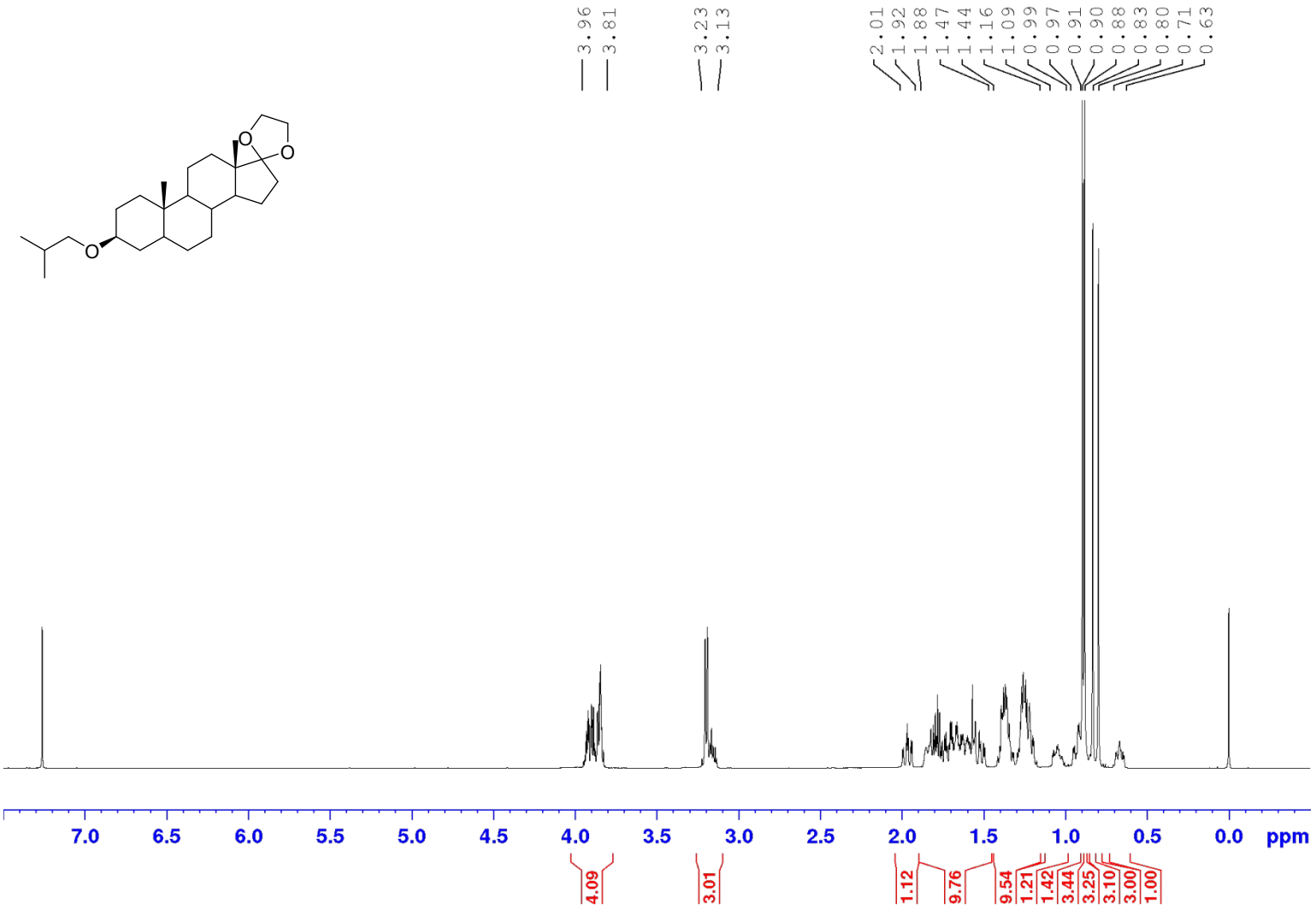
Isobutyl-4-toluenesulfonate (29) – ^{1}H – $CDCl_3$ – 500 MHz



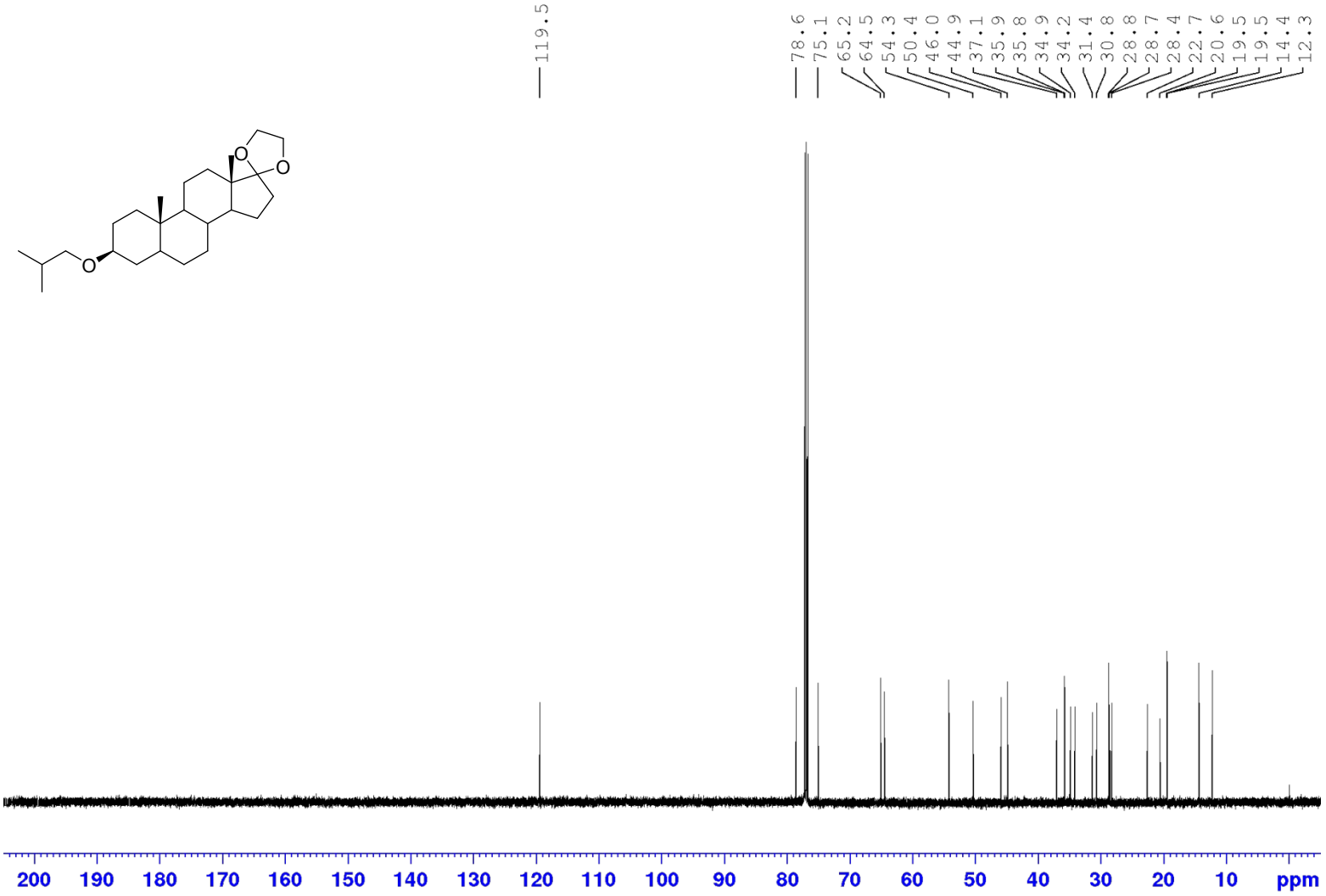
Isobutyl-4-toluenesulfonate (29) – ^{13}C – $CDCl_3$ – 125 MHz



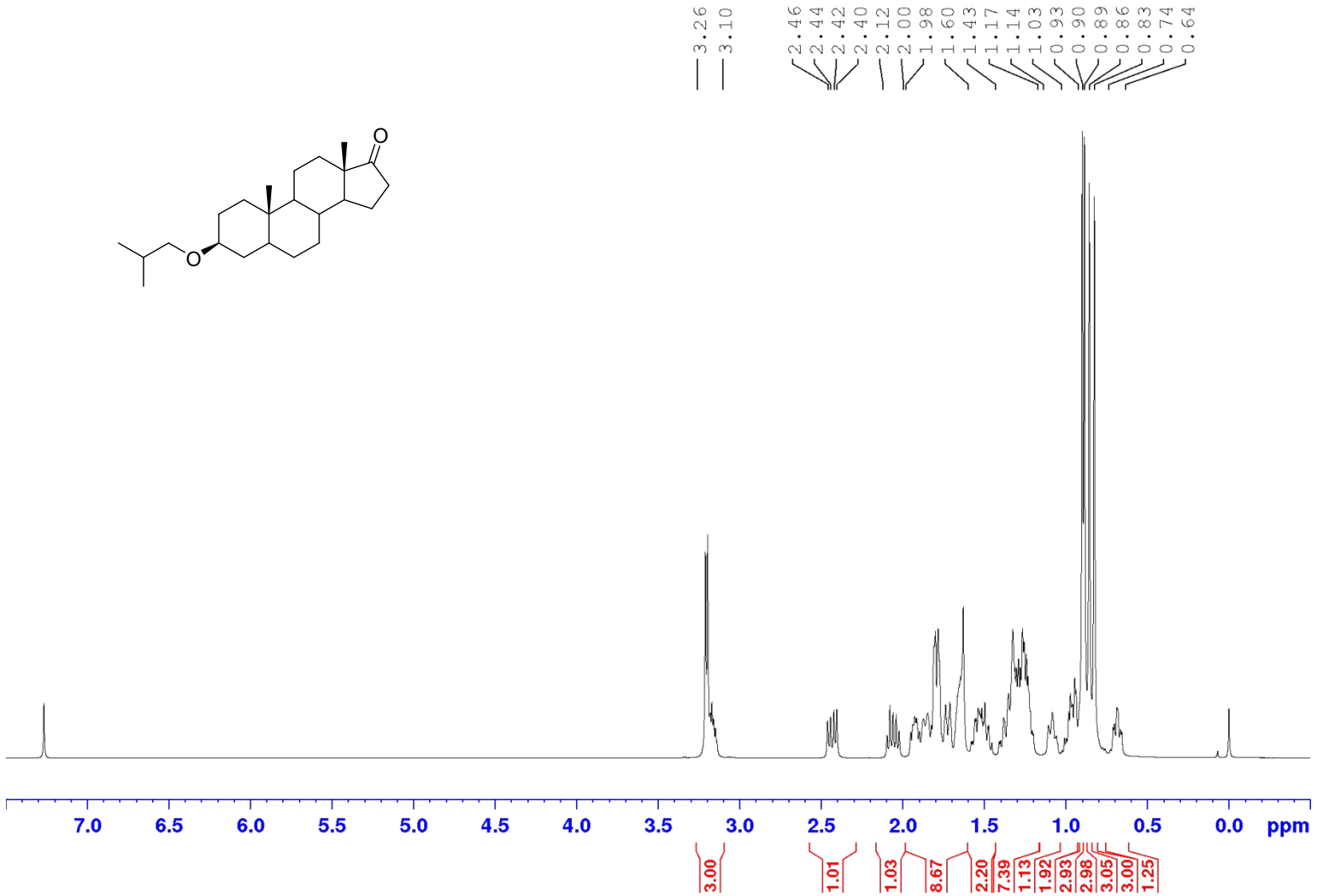
Epiandrosterone 17-acetal isobutyl ether (30) – ^{1}H – $CDCl_3$ – 500 MHz



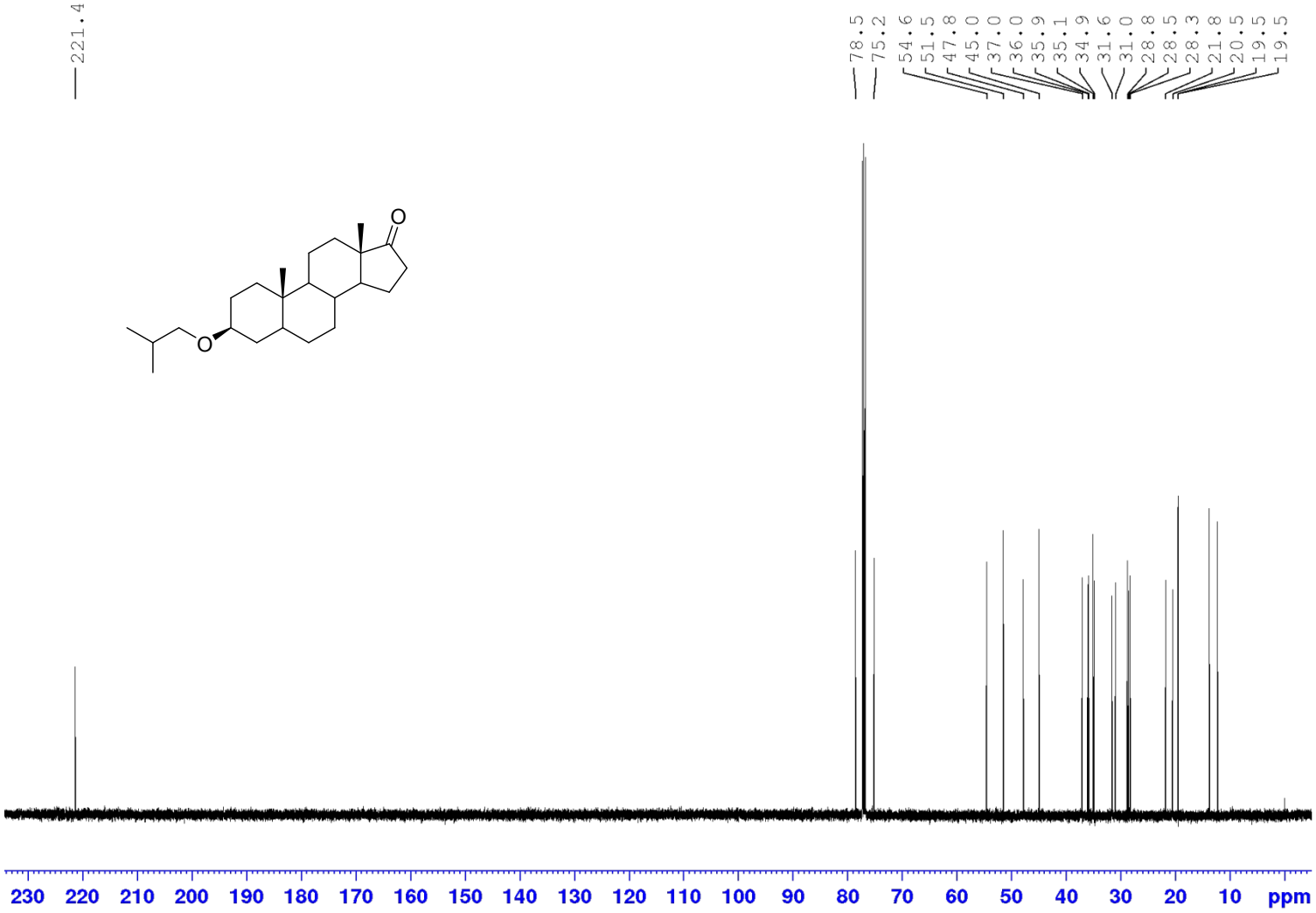
Epiandrosterone 17-acetal isobutyl ether (30) – ^{13}C – $CDCl_3$ – 125 MHz



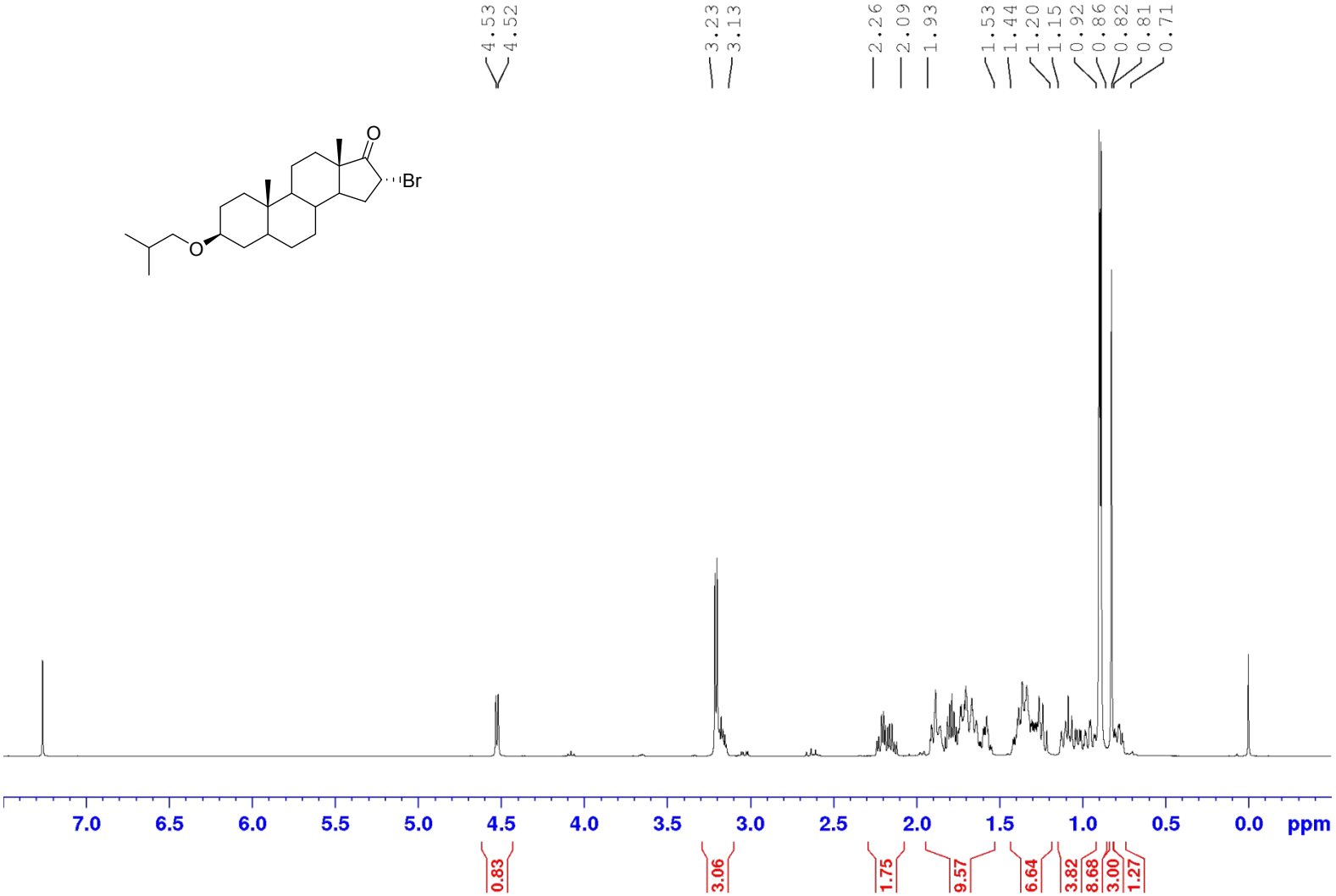
Epiandrosterone isobutyl ether (31) – ^{1}H – $CDCl_3$ – 500 MHz



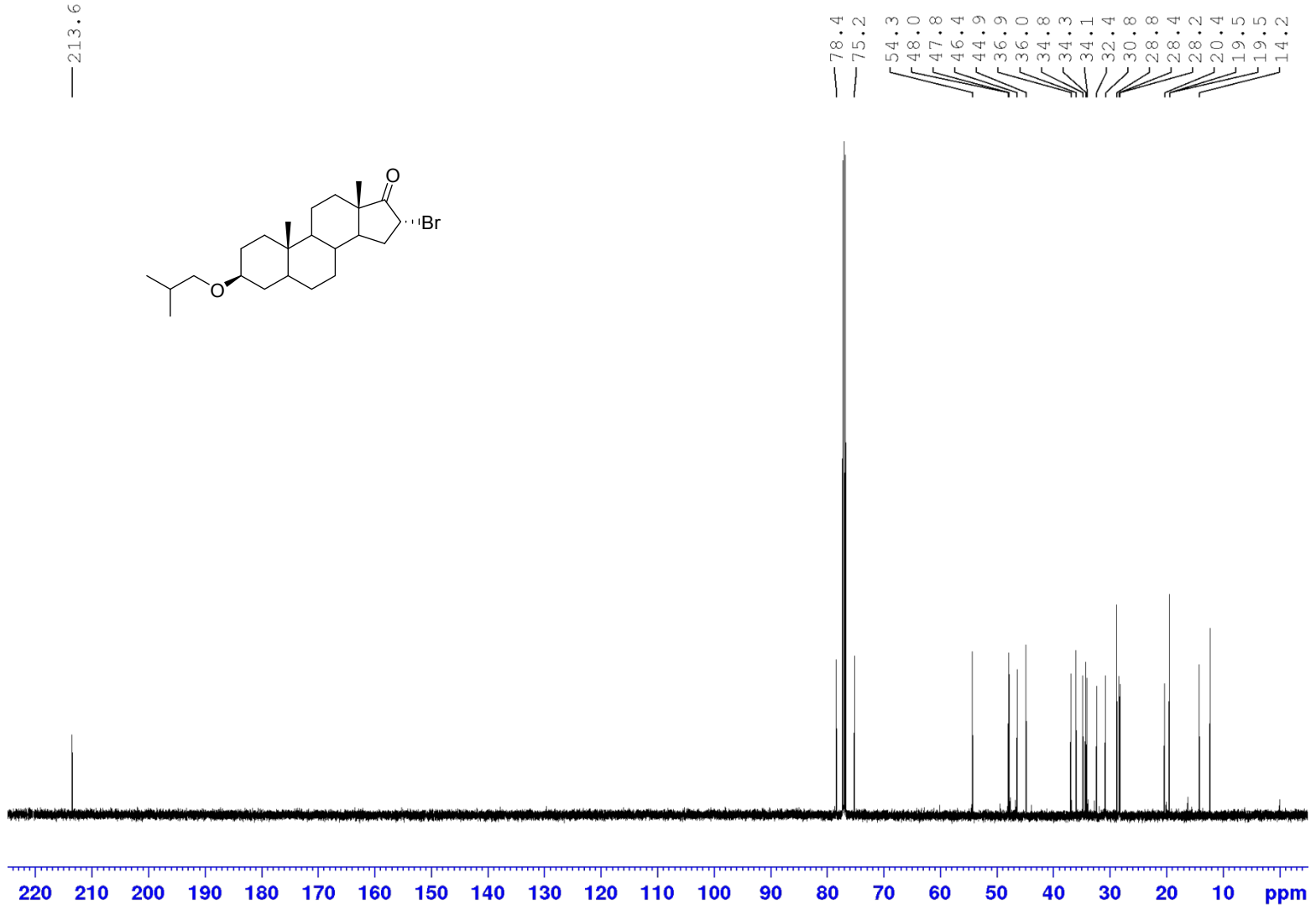
Epiandrosterone isobutyl ether (31) – ^{13}C – $CDCl_3$ – 125 MHz



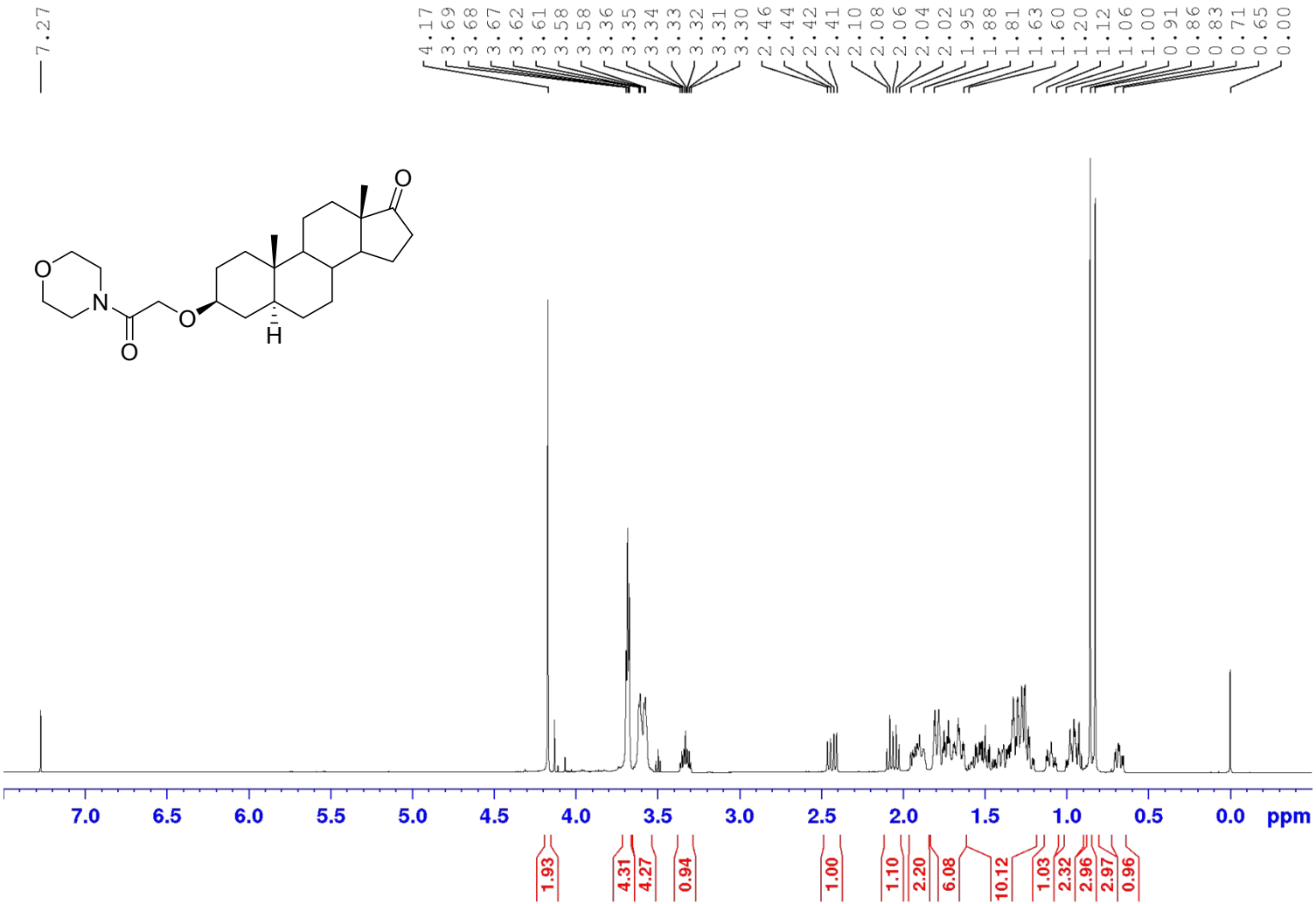
16α-Bromoepiandrosterone isobutyl ether (32) – ^{1}H – $CDCl_3$ – 500 MHz



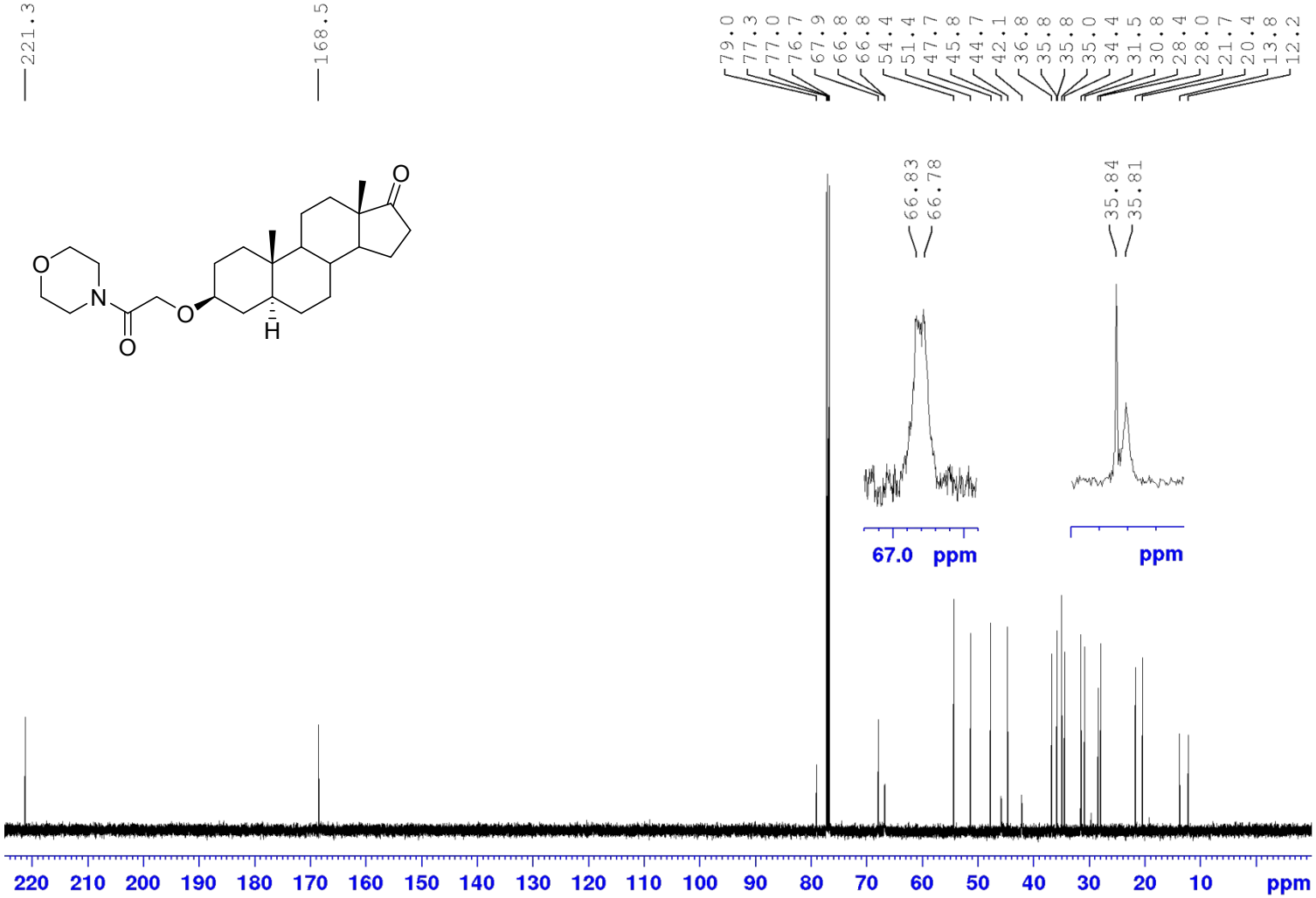
16α-Bromoepiandrosterone isobutyl ether (32) – ^{13}C – $CDCl_3$ – 125 MHz



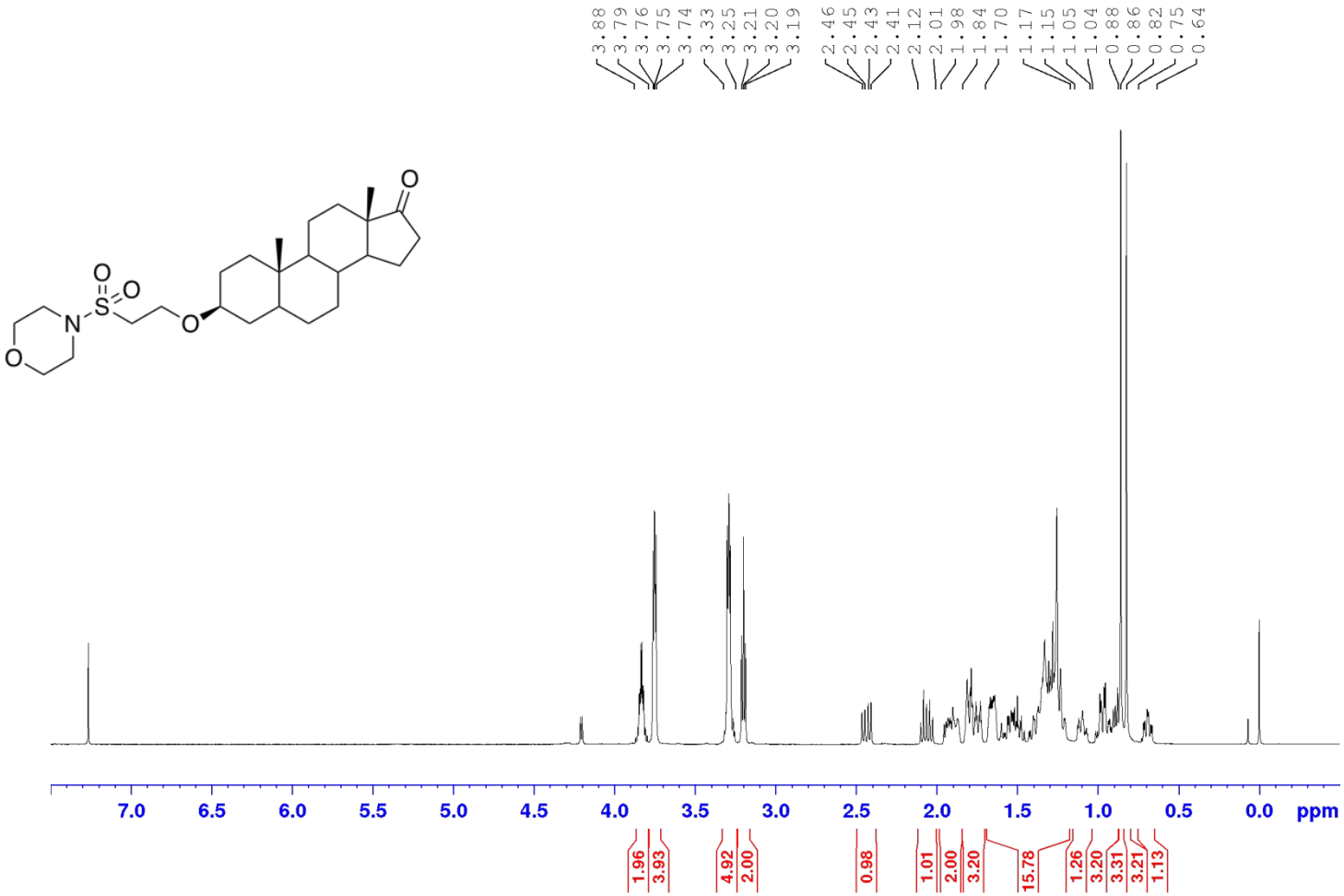
Epiandrosterone 2-morpholino-2-oxoethoxy ether (33) – ^{1}H – $CDCl_3$ – 500 MHz



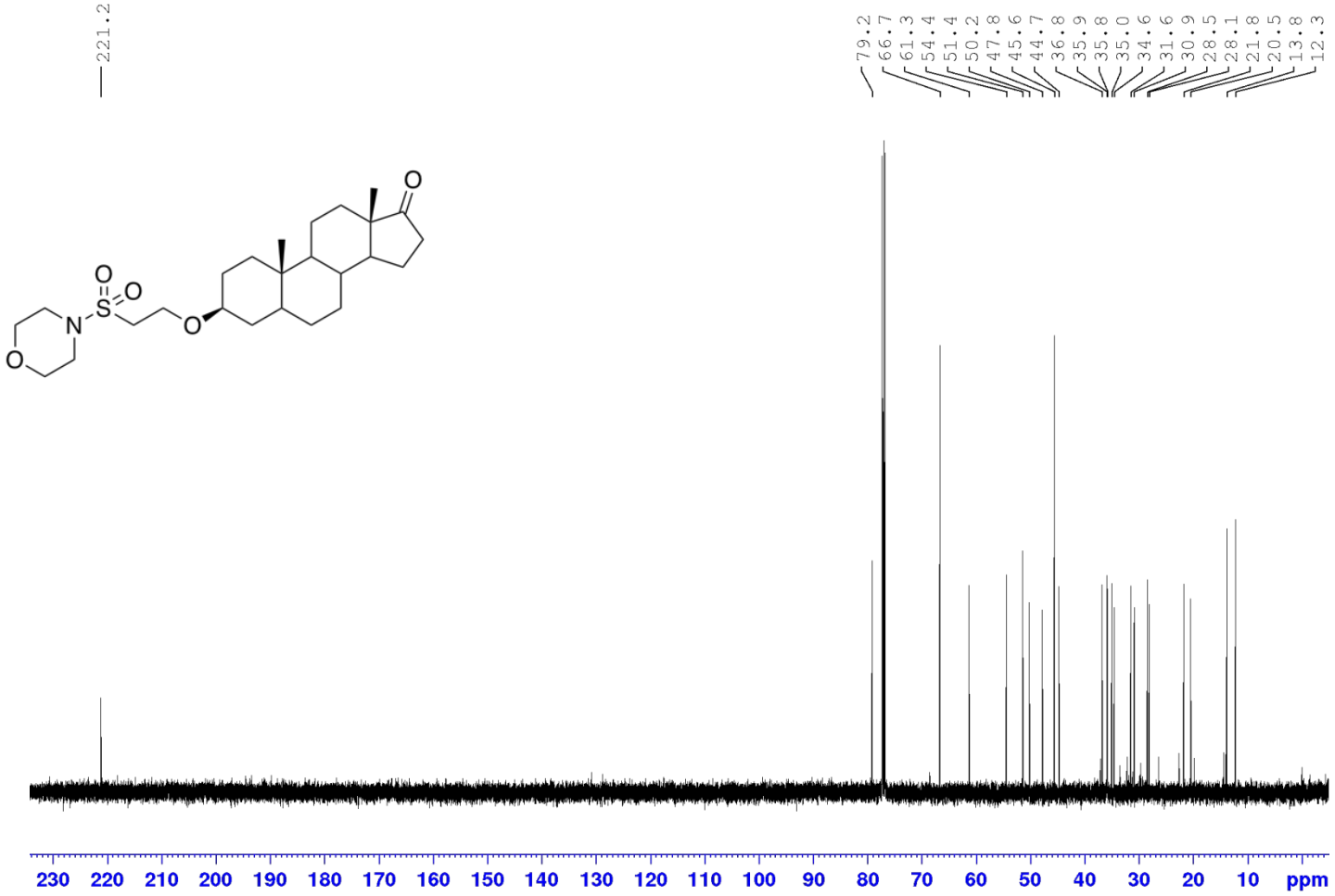
Epiandrosterone 2-morpholino-2-oxoethoxy ether (33) – ^{13}C – $CDCl_3$ – 125 MHz



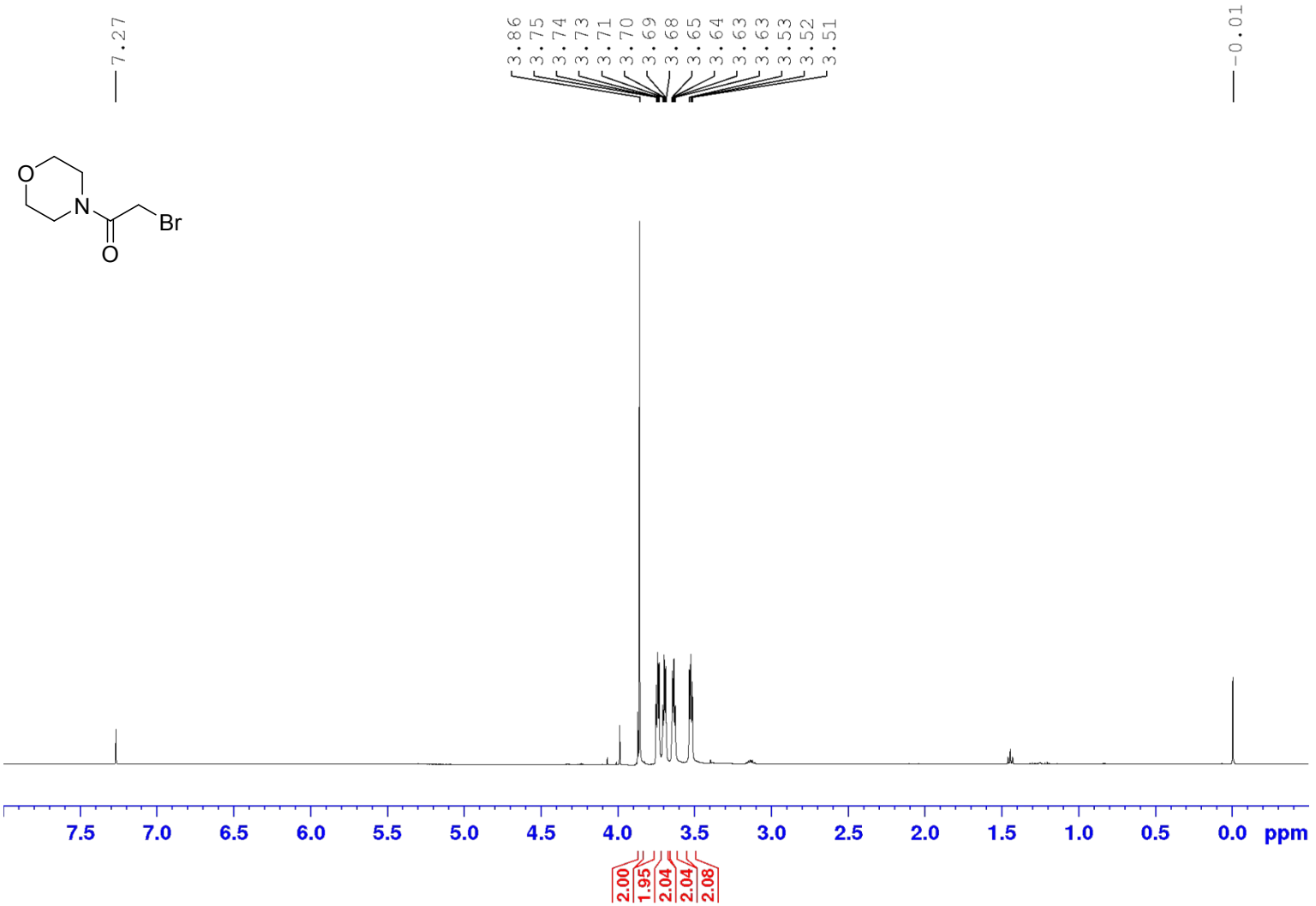
Epiandrosterone 2-(morpholinosulfonyl)ethyl ether (34) – ^{1}H – $CDCl_3$ – 500 MHz



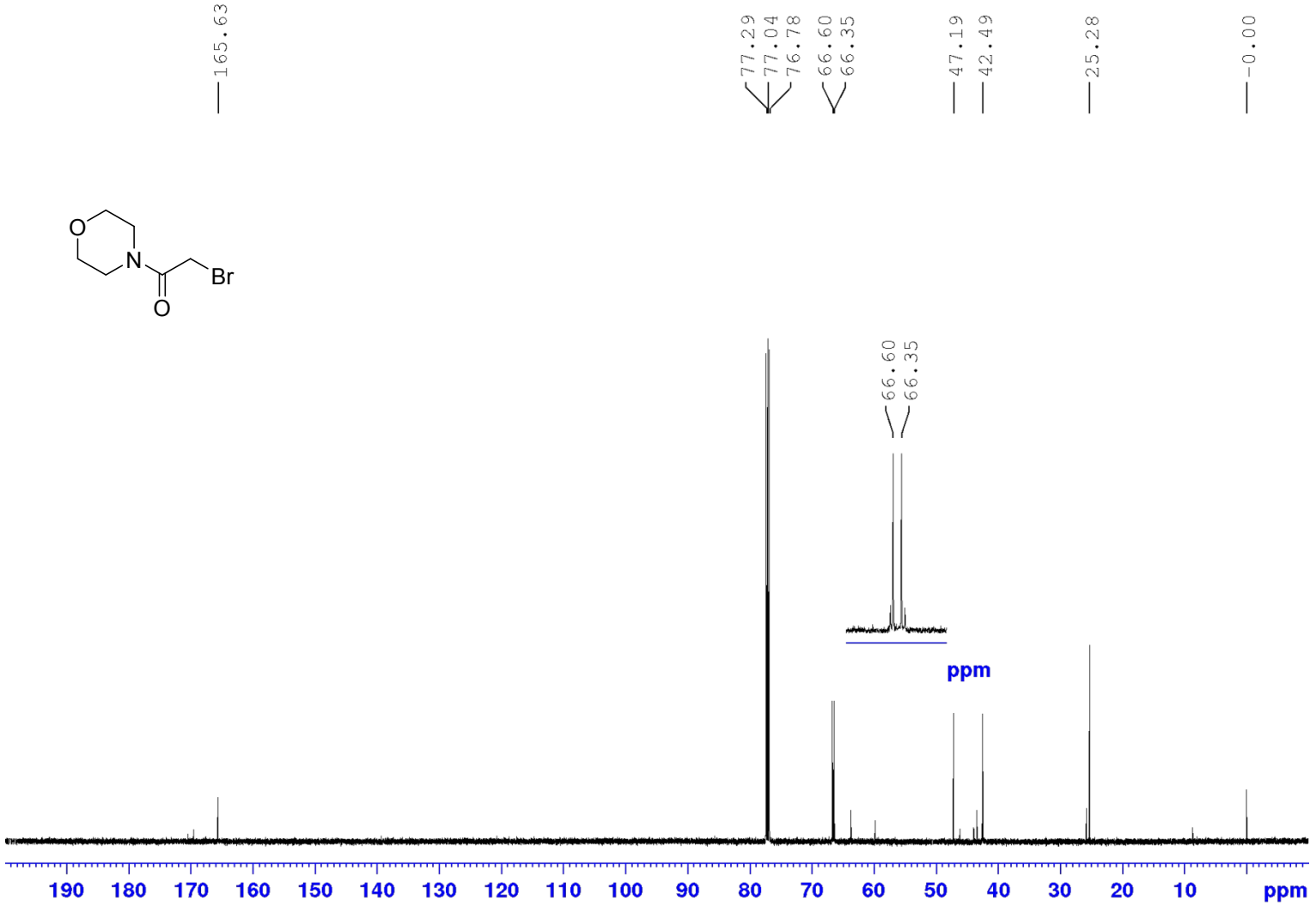
Epiandrosterone 2-(morpholinosulfonyl)ethyl ether (34) – ^{13}C – $CDCl_3$ – 125 MHz



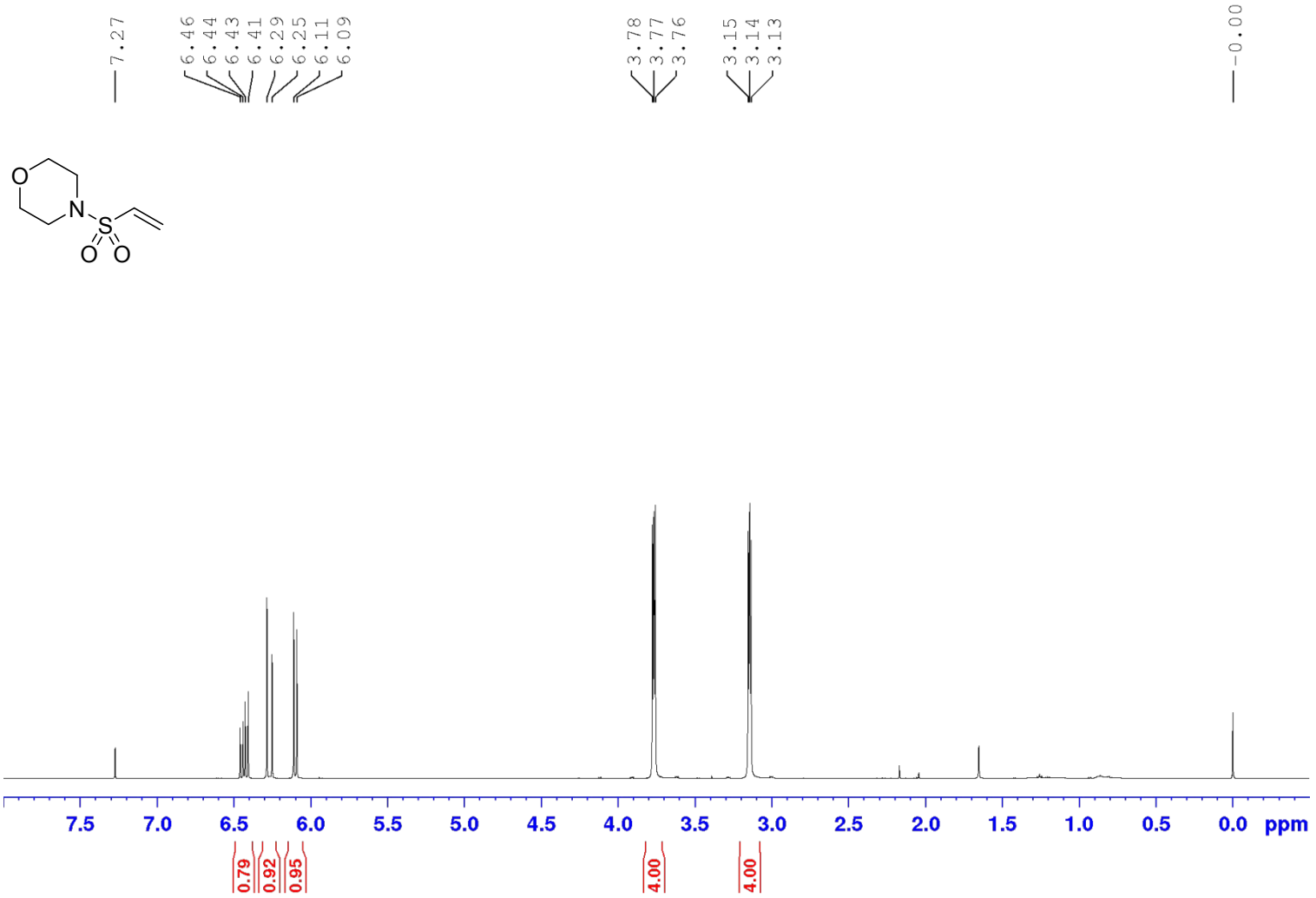
2-Bromo-1-morpholinoethan-1-one (35) – ^{1}H – $CDCl_3$ – 500 MHz



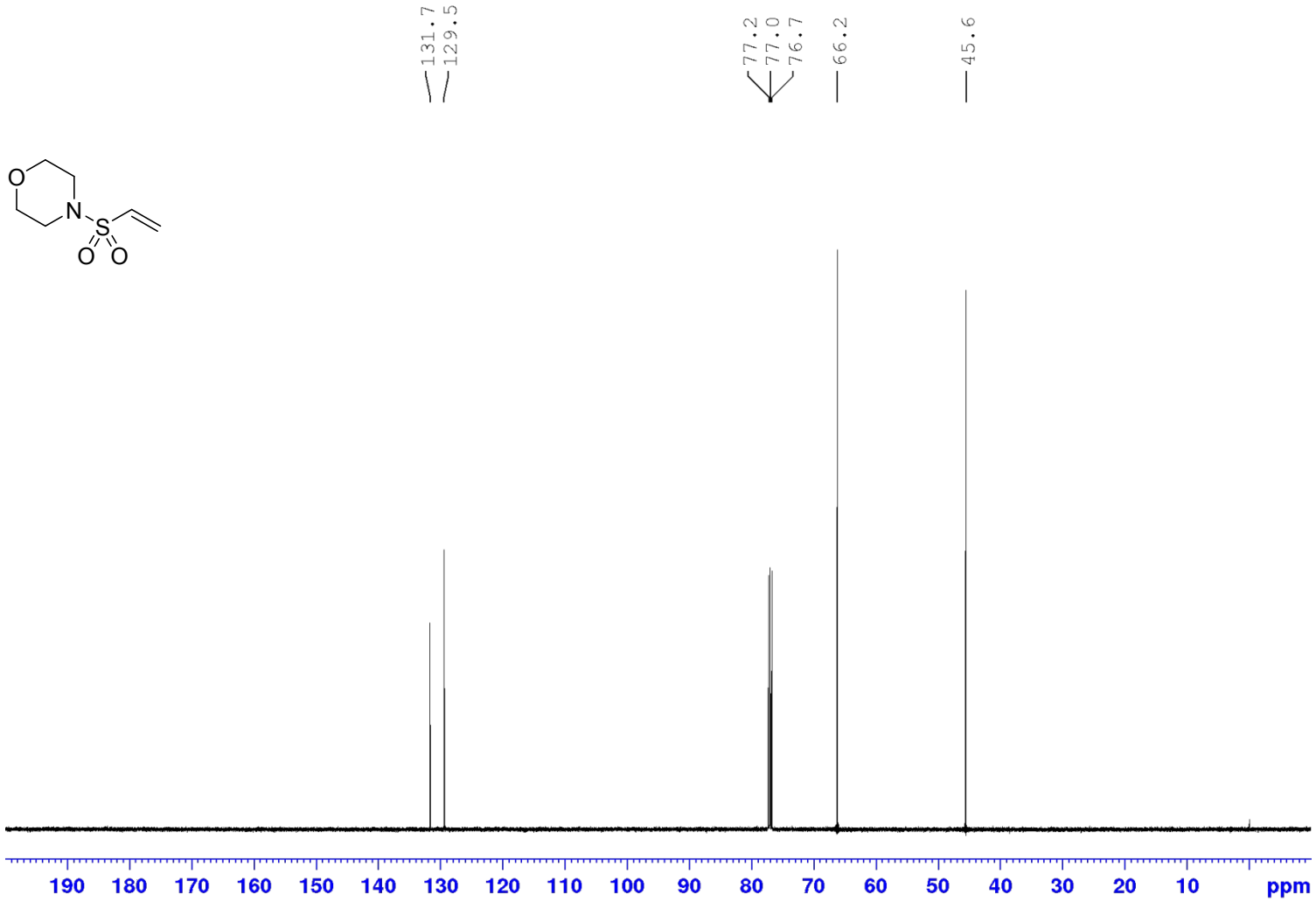
2-Bromo-1-morpholinoethan-1-one (35) – ^{13}C – $CDCl_3$ – 125 MHz



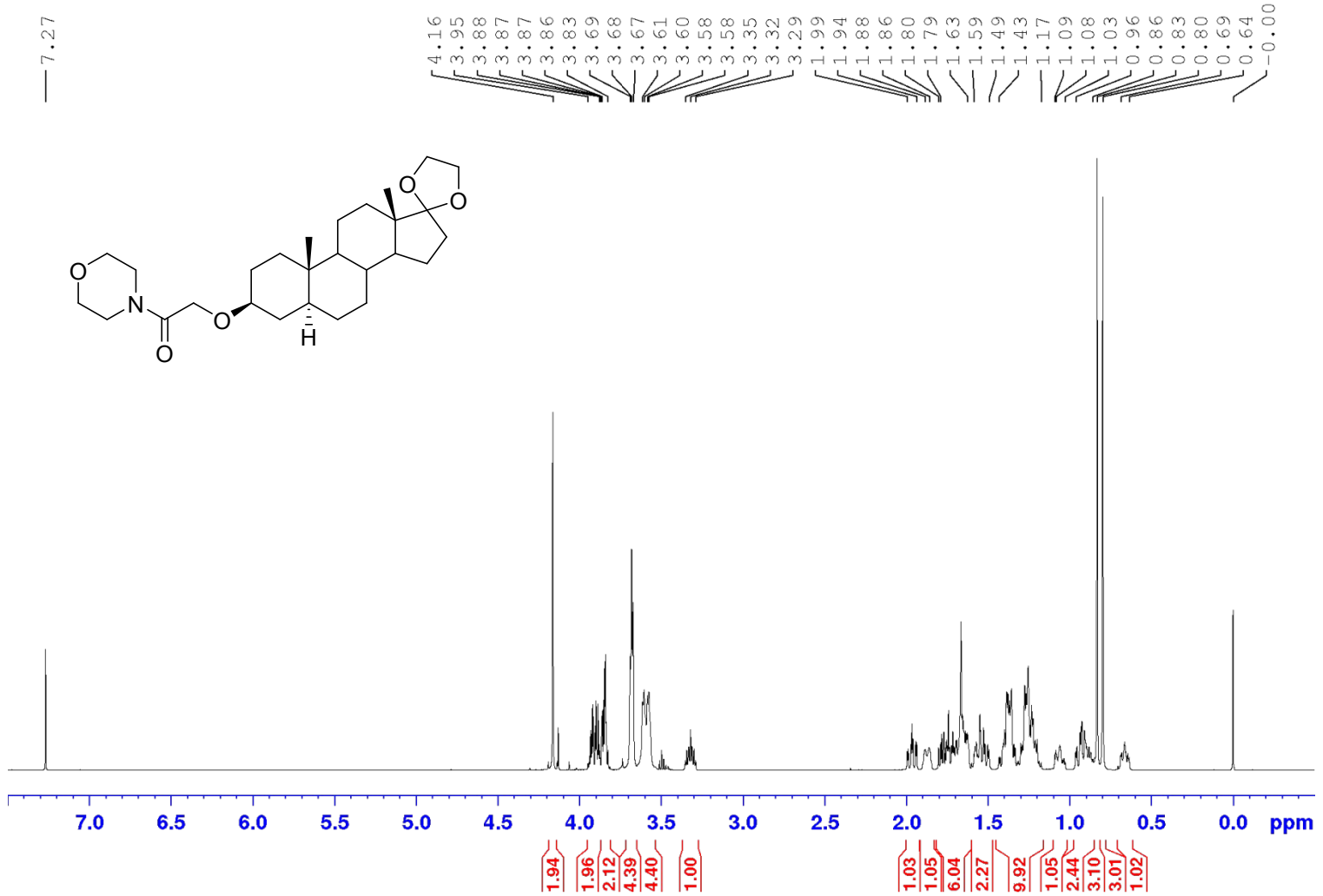
4-(Vinylsulfonyl)morpholine (36) – ^{1}H – $CDCl_3$ – 500 MHz



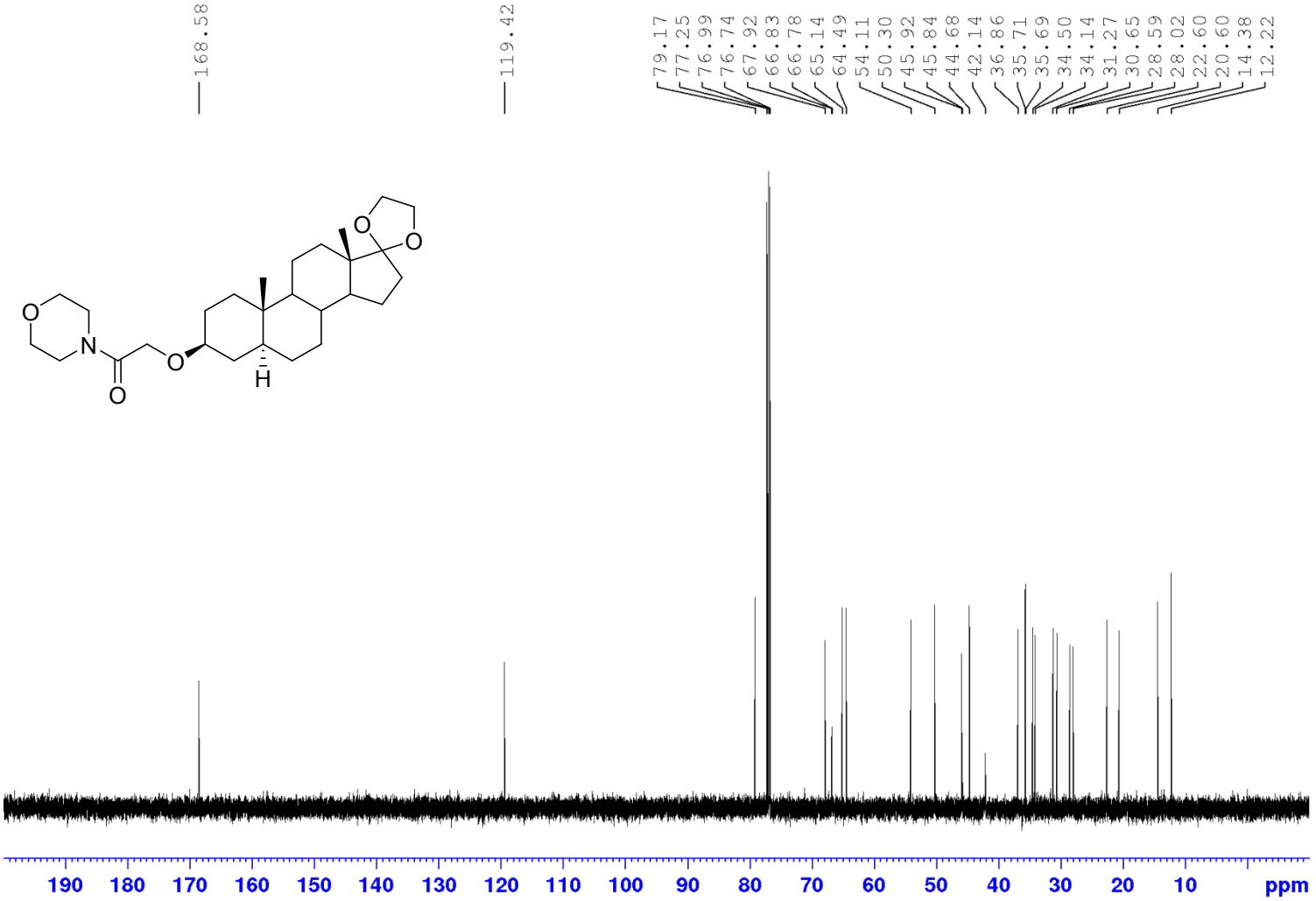
4-(Vinylsulfonyl)morpholine (36) – ^{13}C – $CDCl_3$ – 125 MHz



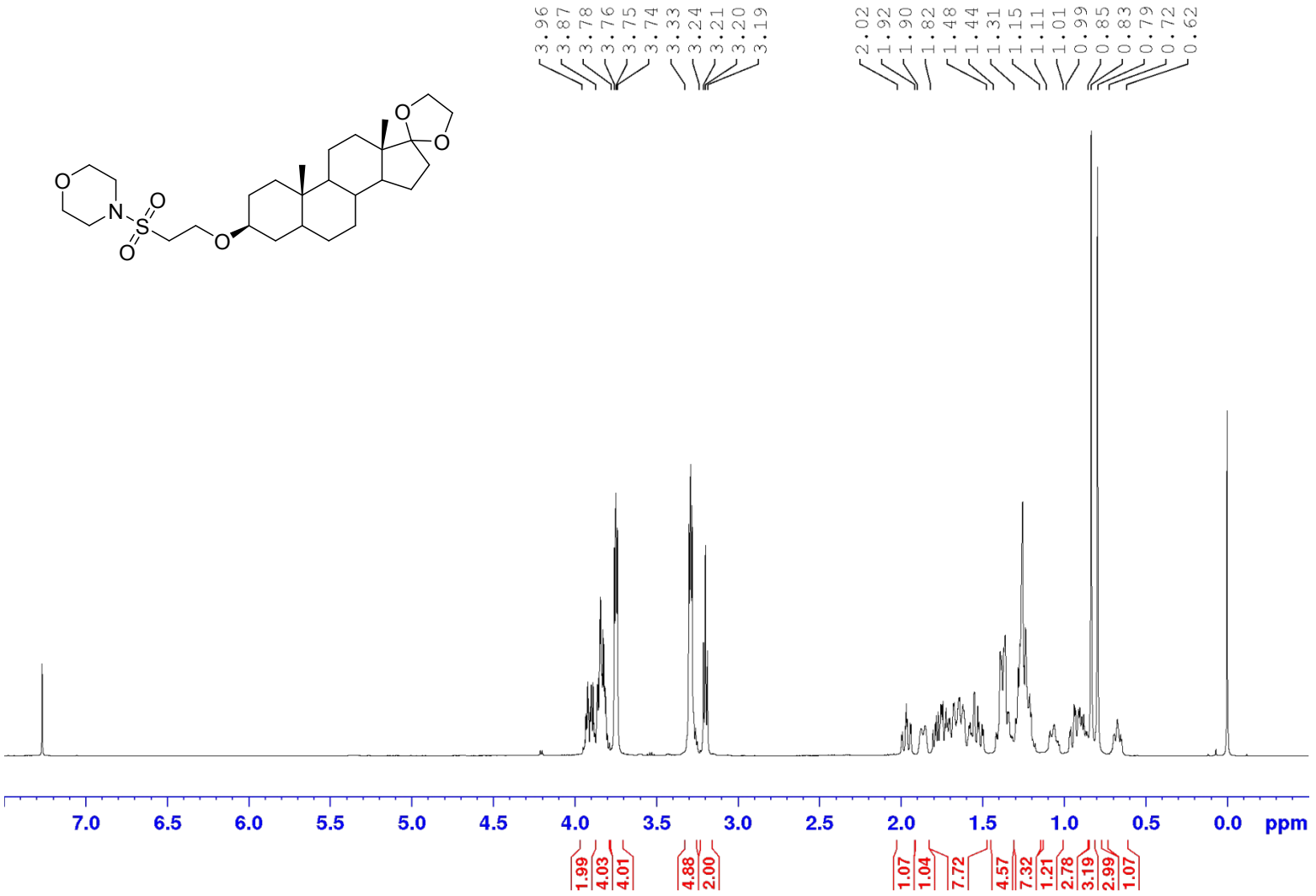
Epiandrosterone 17-acetal 2-morpholino-2-oxoethoxy ether (37) – ^{1}H – $CDCl_3$ – 500 MHz



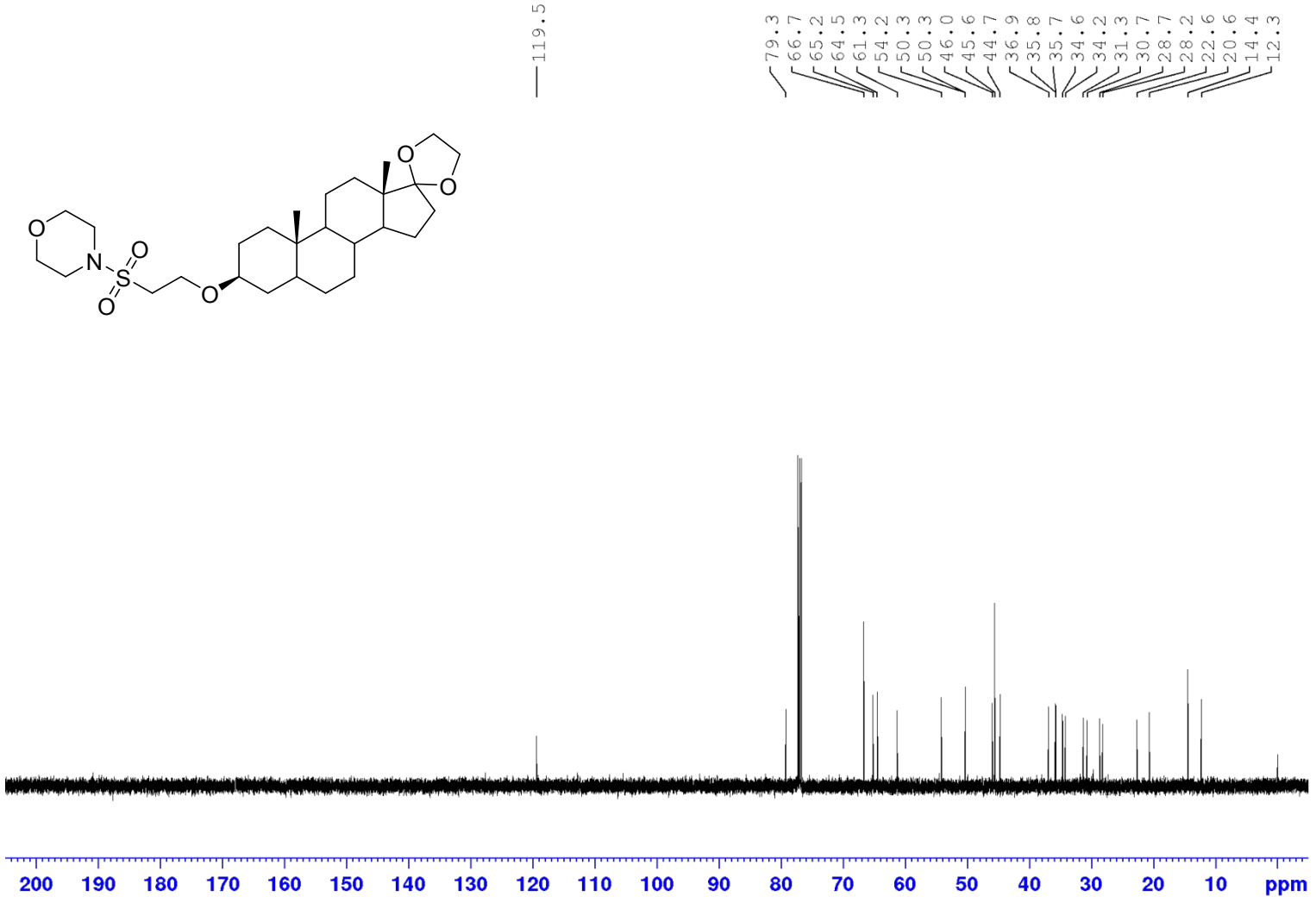
Epiandrosterone 17-acetal 2-morpholino-2-oxoethoxy ether (37) – ^{13}C – $CDCl_3$ – 125 MHz



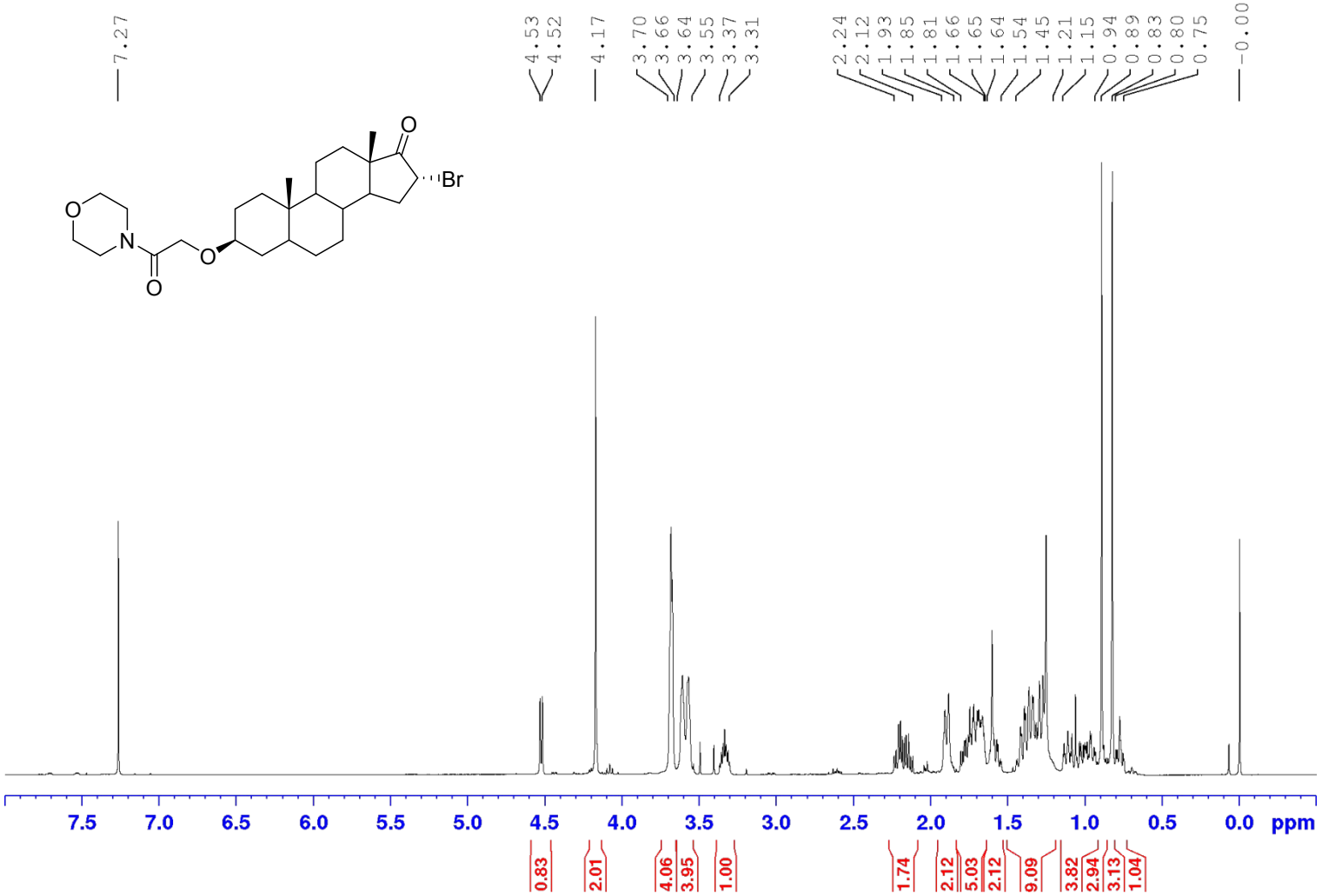
Epiandrosterone 17-acetal 2-(morpholinosulfonyl)ethyl ether (38) – ^{1}H – $CDCl_3$ – 500 MHz



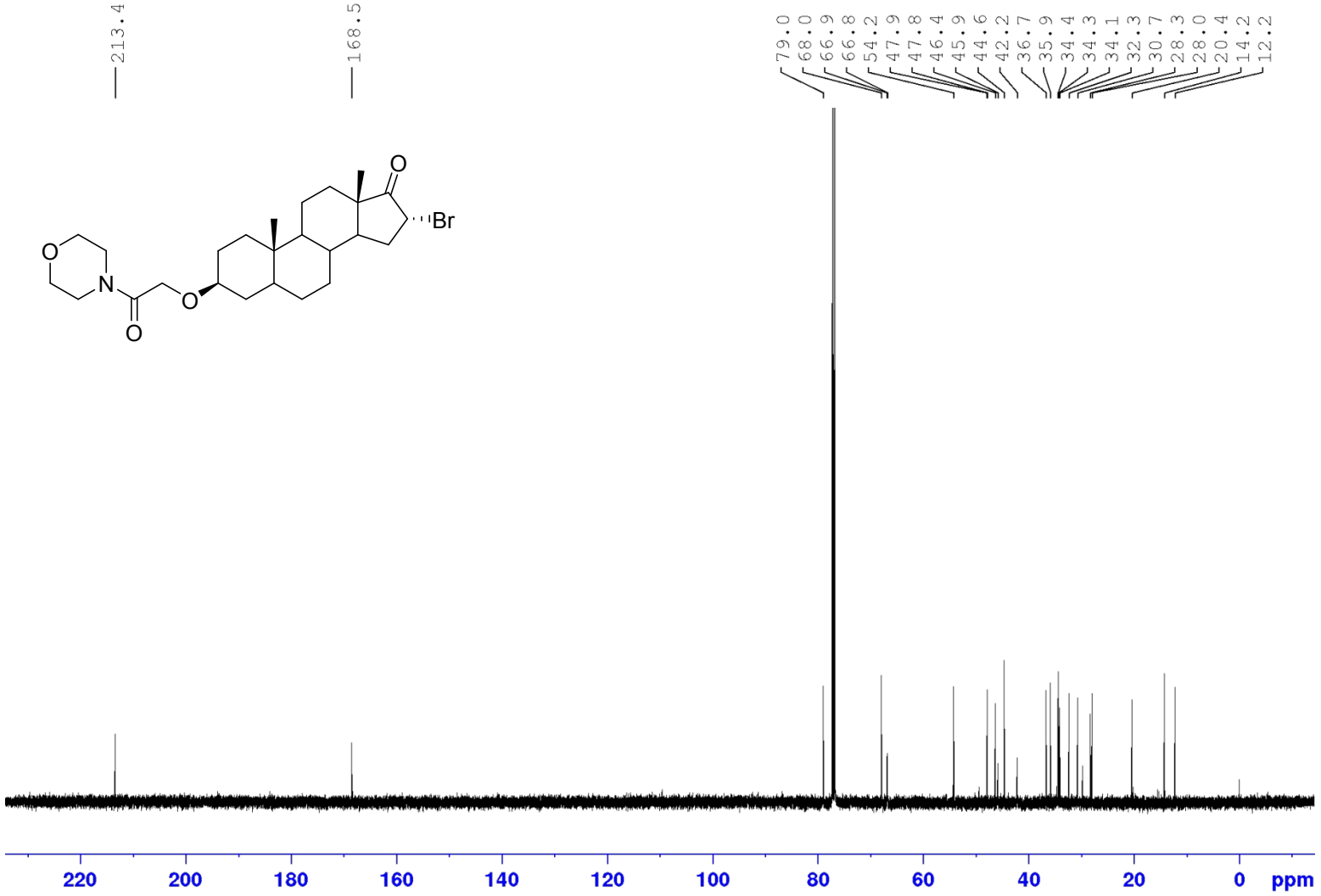
Epiandrosterone 17-acetal 2-(morpholinosulfonyl)ethyl ether (38) – ^{13}C – $CDCl_3$ – 125 MHz



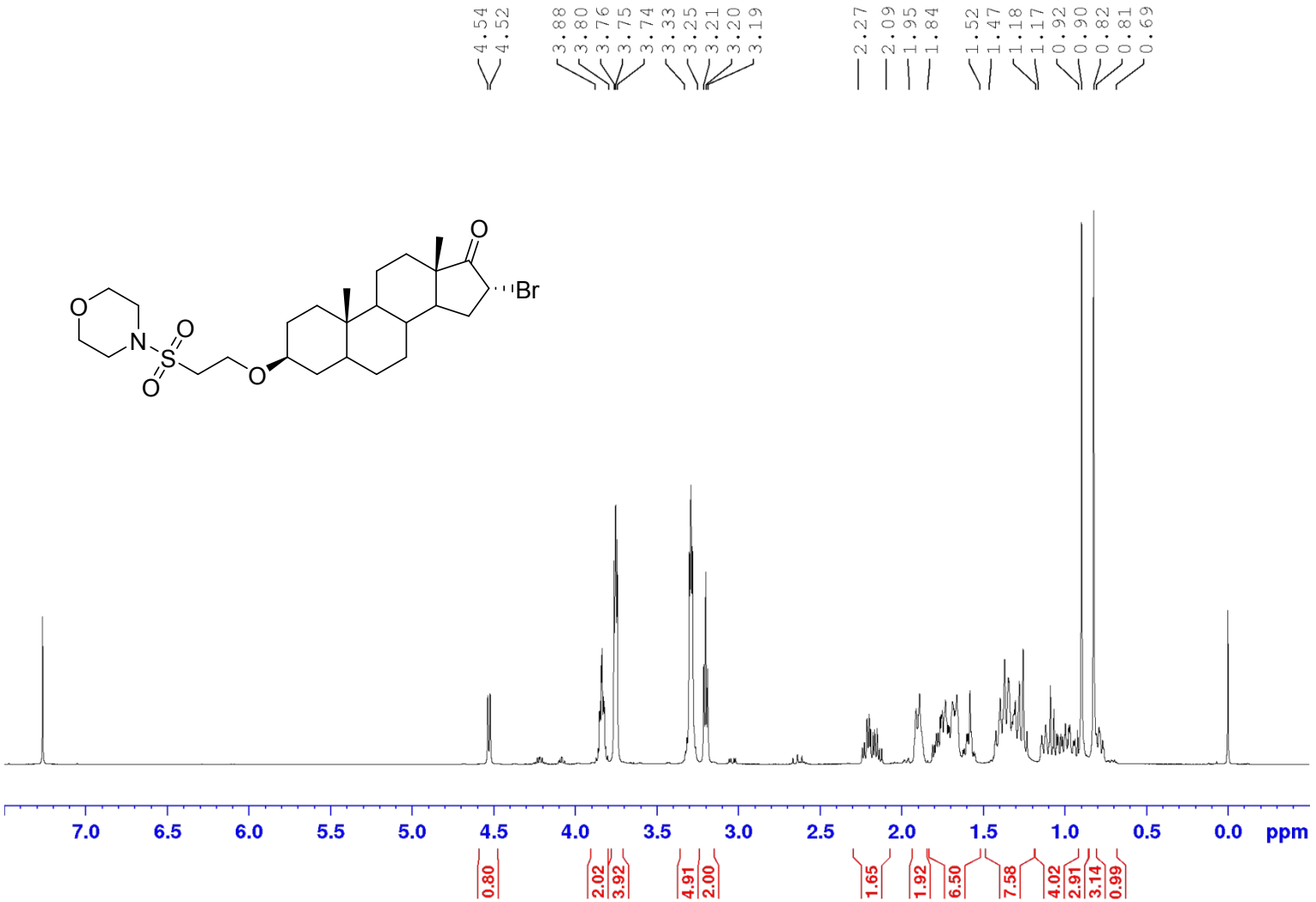
16α-Bromoepiandrosterone 2-morpholino-2-oxoethoxy ether (39) – ^{1}H – $CDCl_3$ – 500 MHz



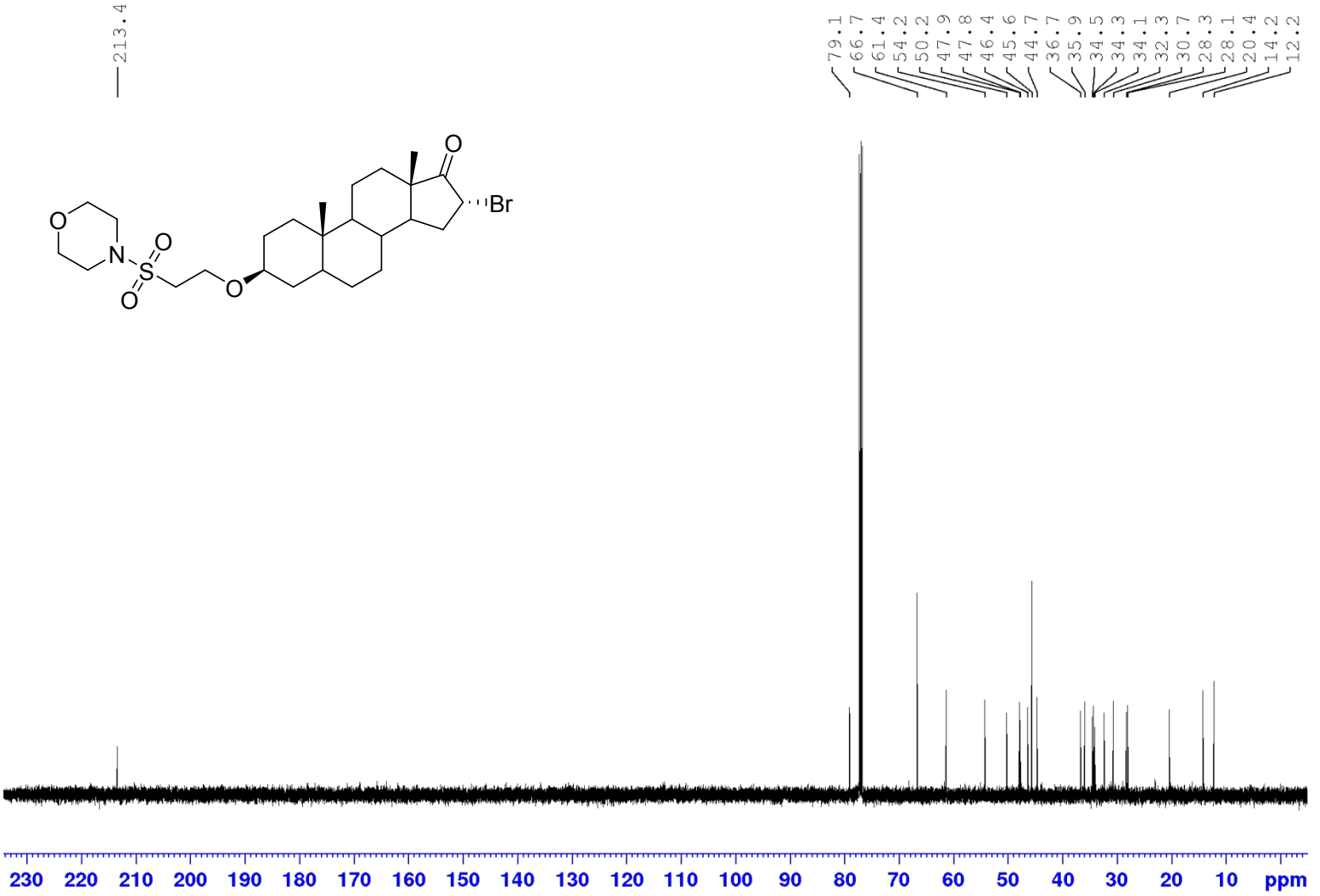
16α-Bromoepiandrosterone 2-morpholino-2-oxoethoxy ether (39) – ^{13}C – $CDCl_3$ – 125 MHz



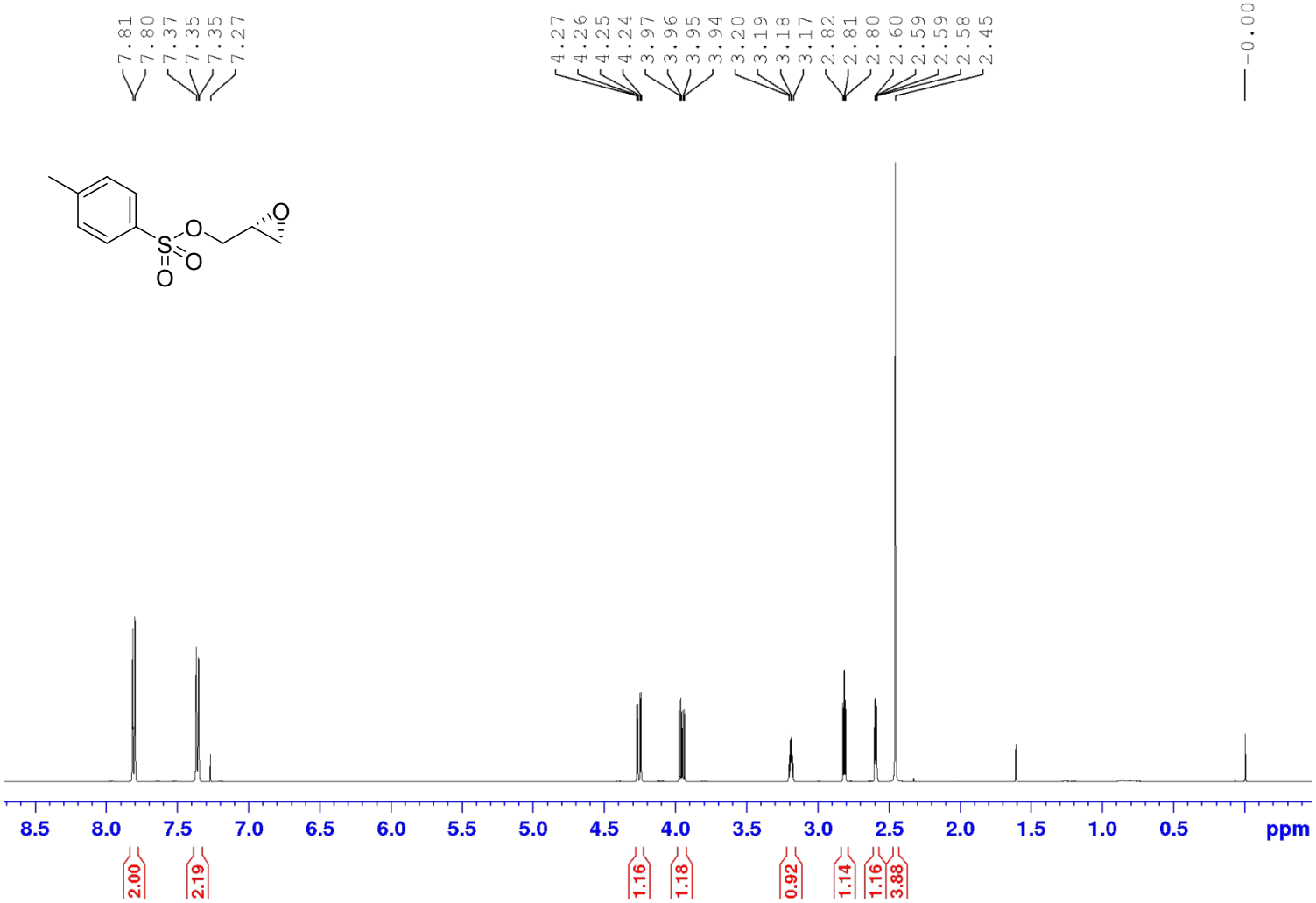
16α-Bromoepiandrosterone 2-(morpholinosulfonyl)ethyl ether (40) – ^{1}H – $CDCl_3$ – 500 MHz



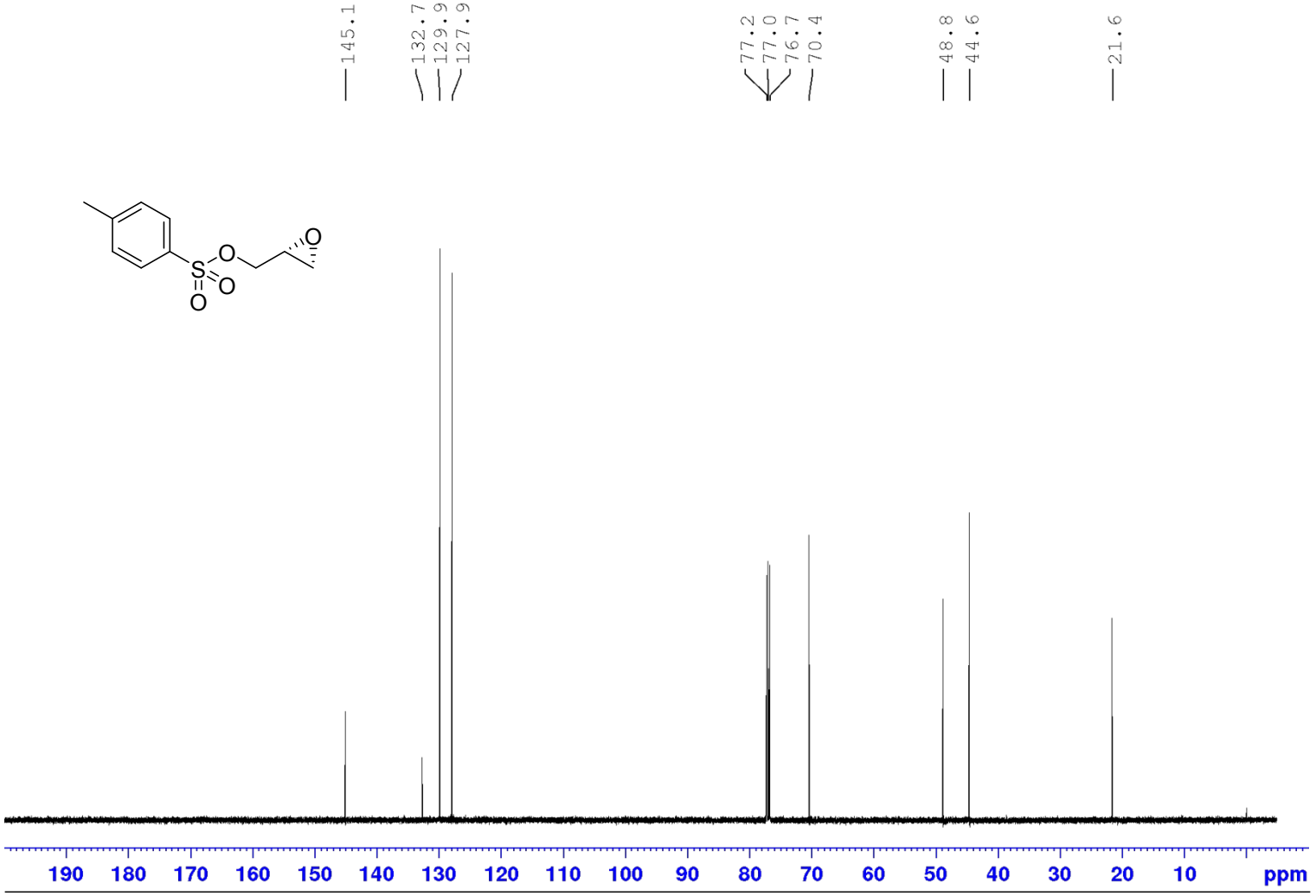
16α-Bromoepiandrosterone 2-(morpholinosulfonyl)ethyl ether (40) – ^{13}C – $CDCl_3$ – 125 MHz



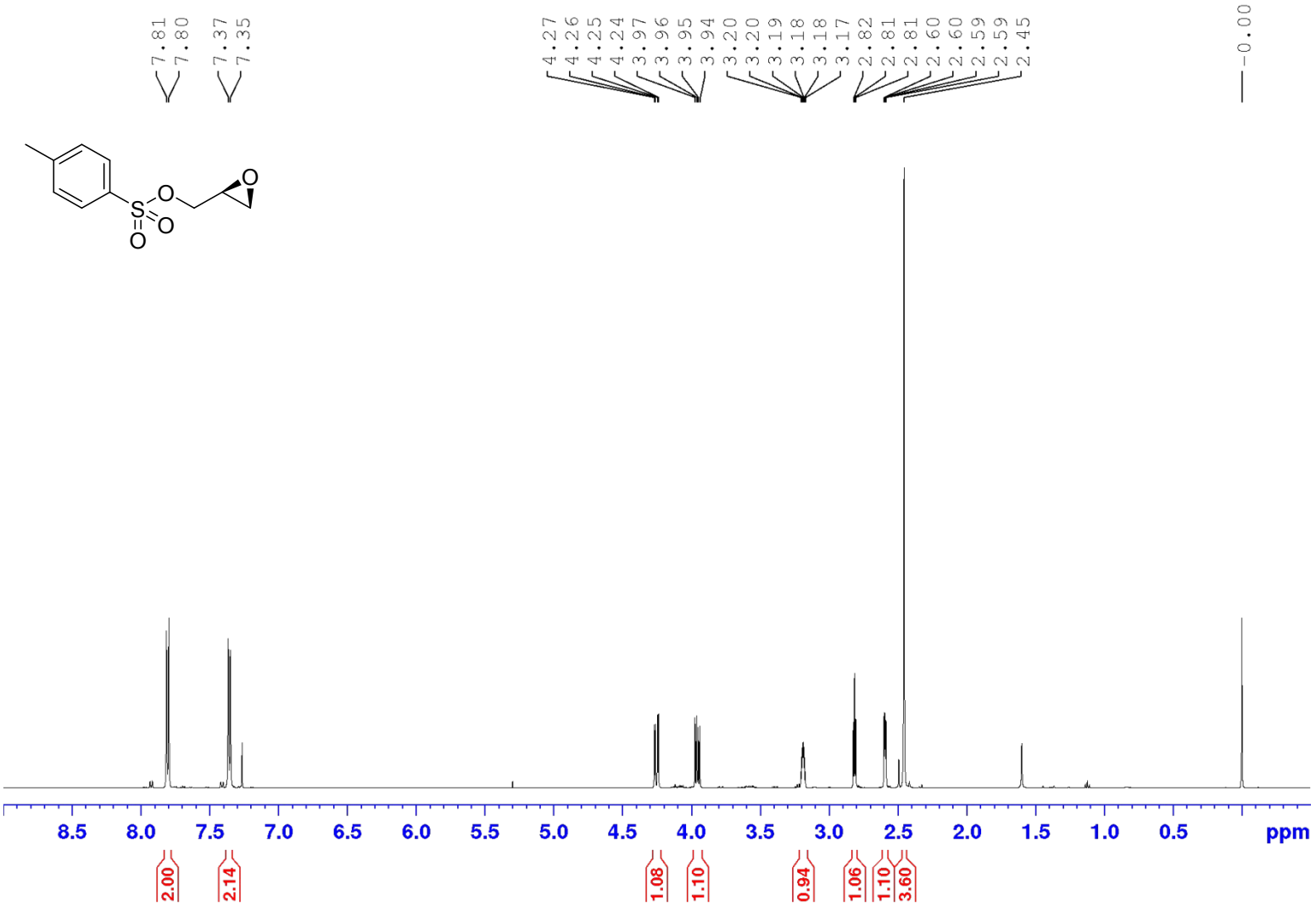
(*R*)-Oxiran-2-ylmethyl 4-methylbenzenesulfonate (41) – ^{1}H – $CDCl_3$ – 500 MHz



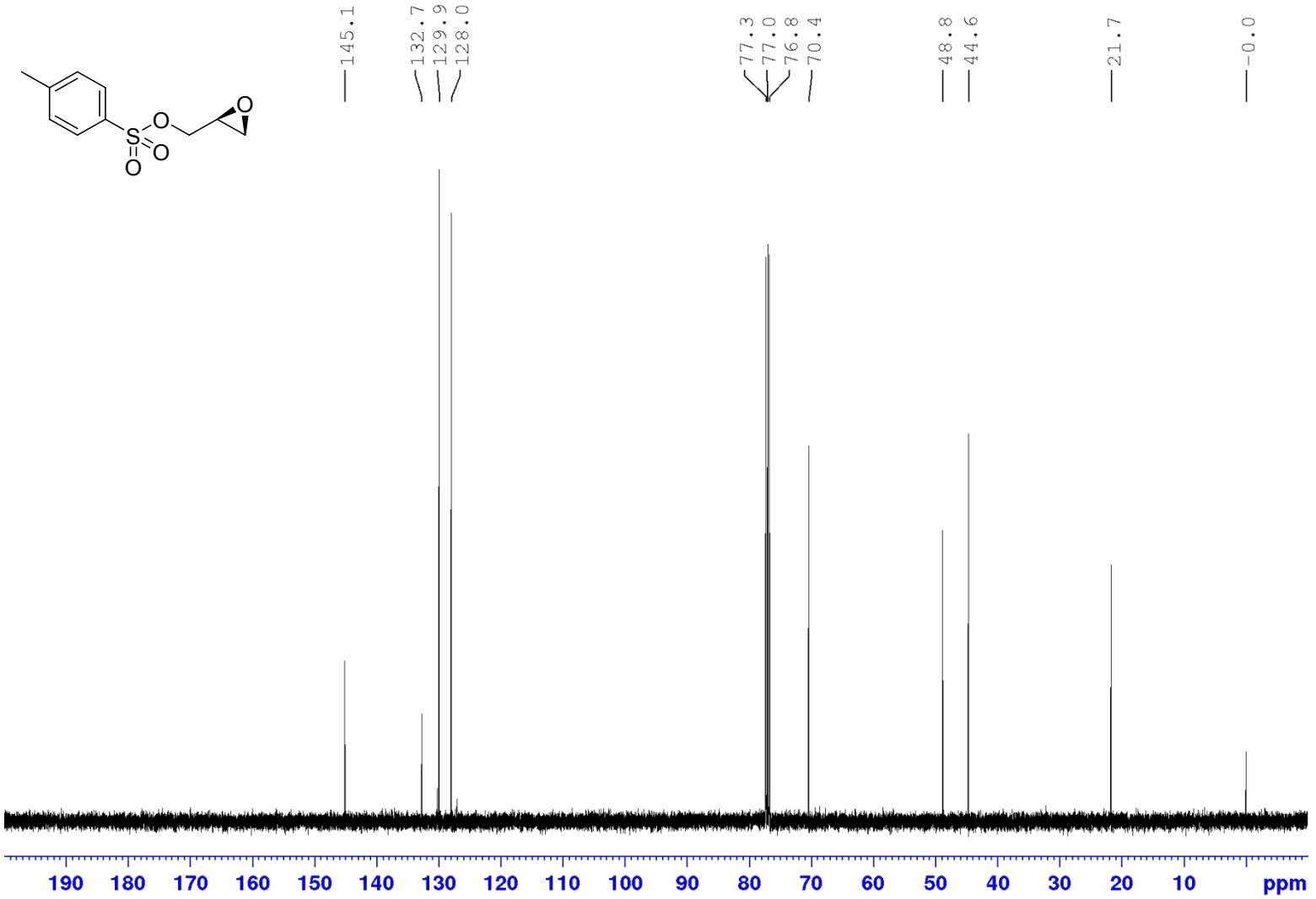
(*R*)-Oxiran-2-ylmethyl 4-methylbenzenesulfonate (41) – ^{13}C – $CDCl_3$ – 125 MHz



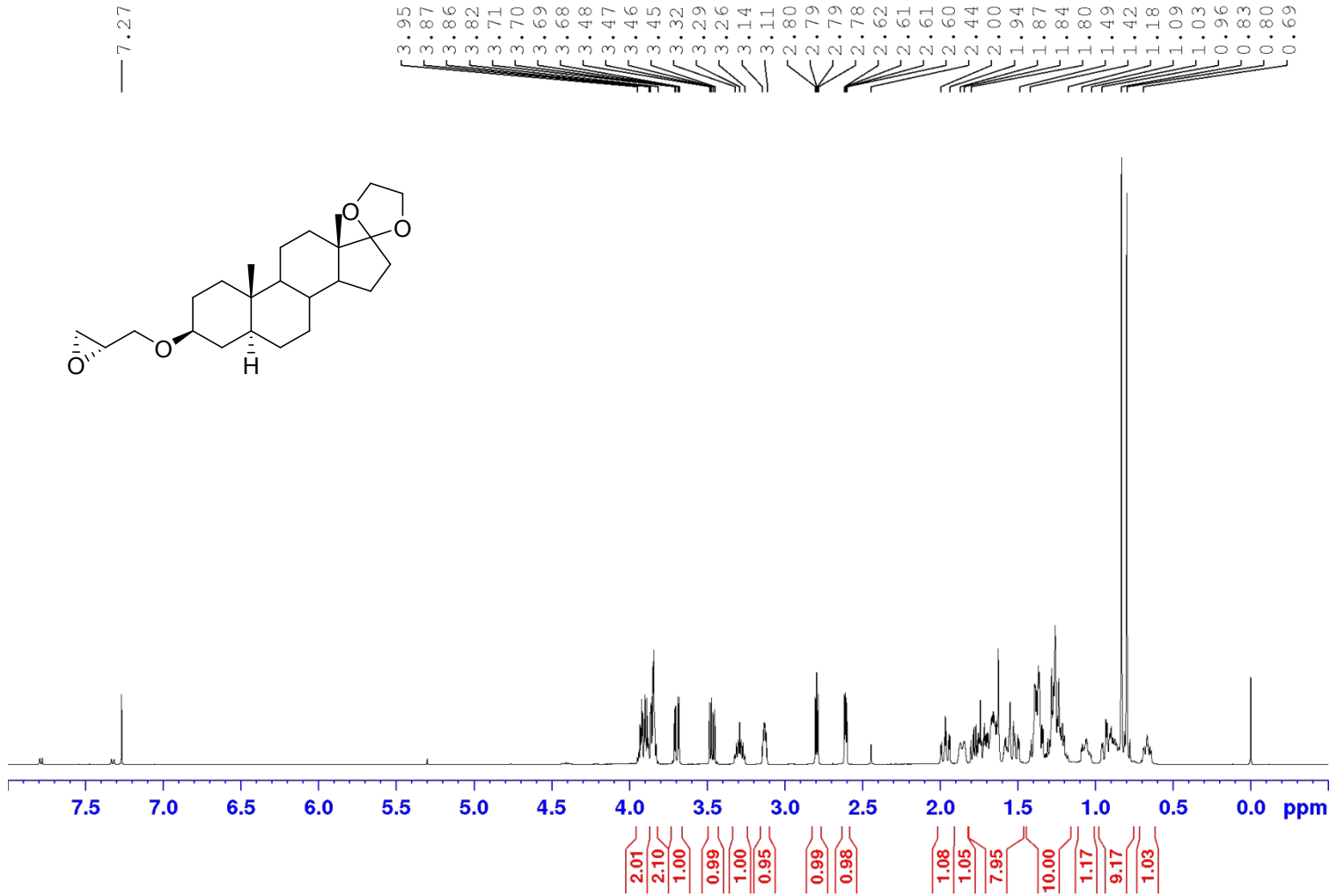
(*S*)-Oxiran-2-ylmethyl 4-methylbenzenesulfonate (42) – ^{1}H – $CDCl_3$ – 500 MHz



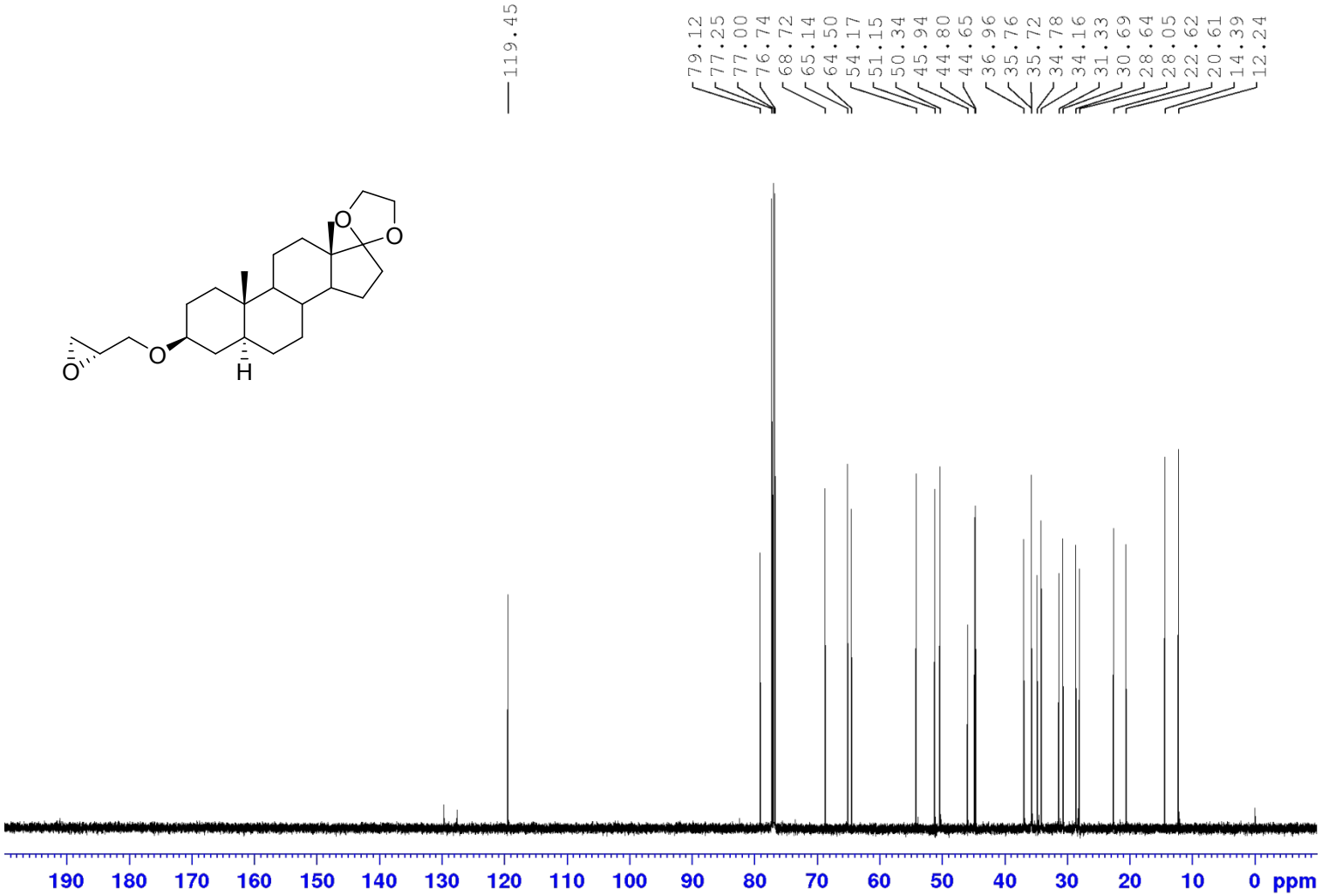
(*S*)-Oxiran-2-ylmethyl 4-methylbenzenesulfonate (42) – ^{13}C – $CDCl_3$ – 125 MHz



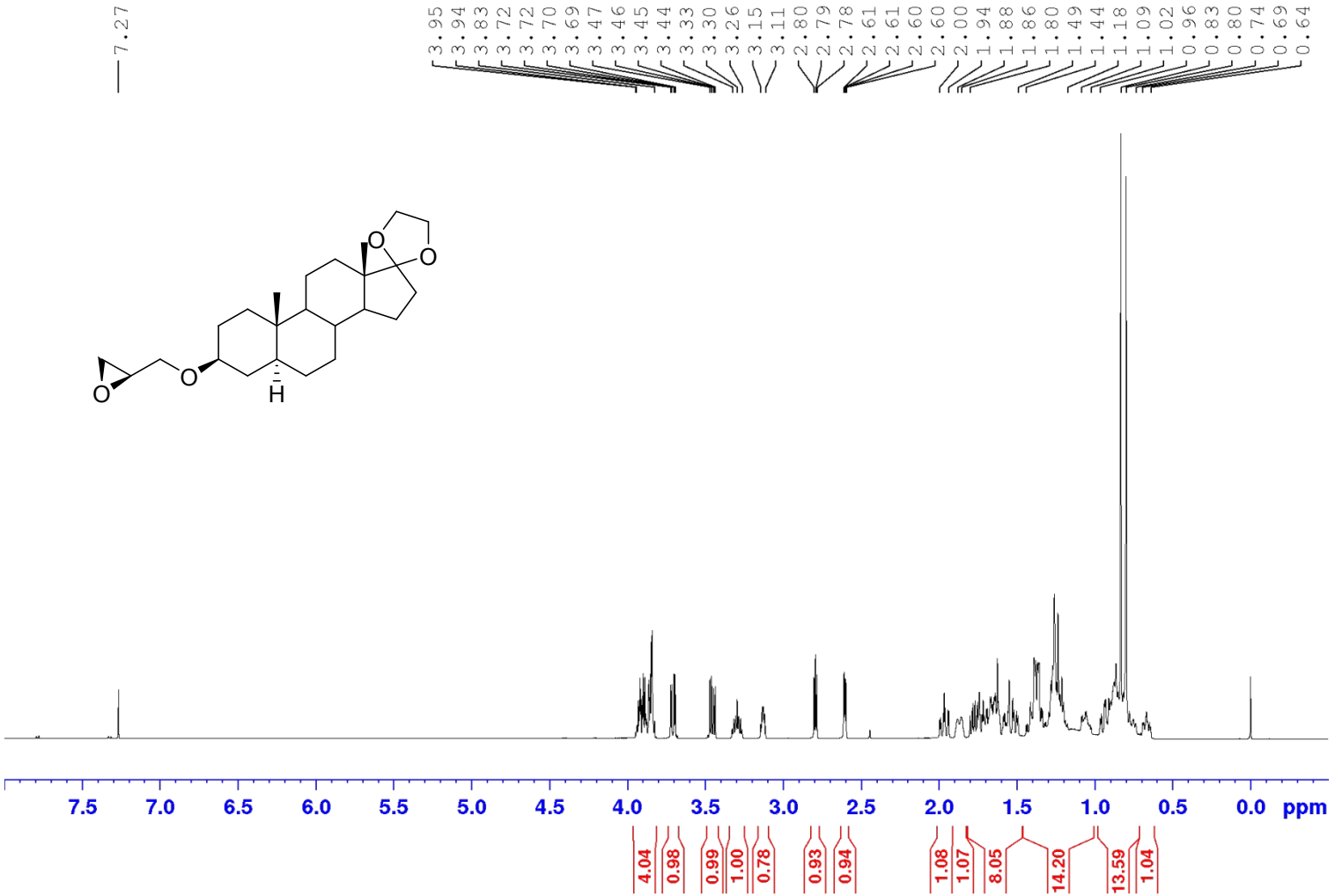
Epiandrosterone 17-acetal (*R*)-oxiran-2-yl)methyl ether (45) - ^{1}H – $CDCl_3$ – 500 MHz



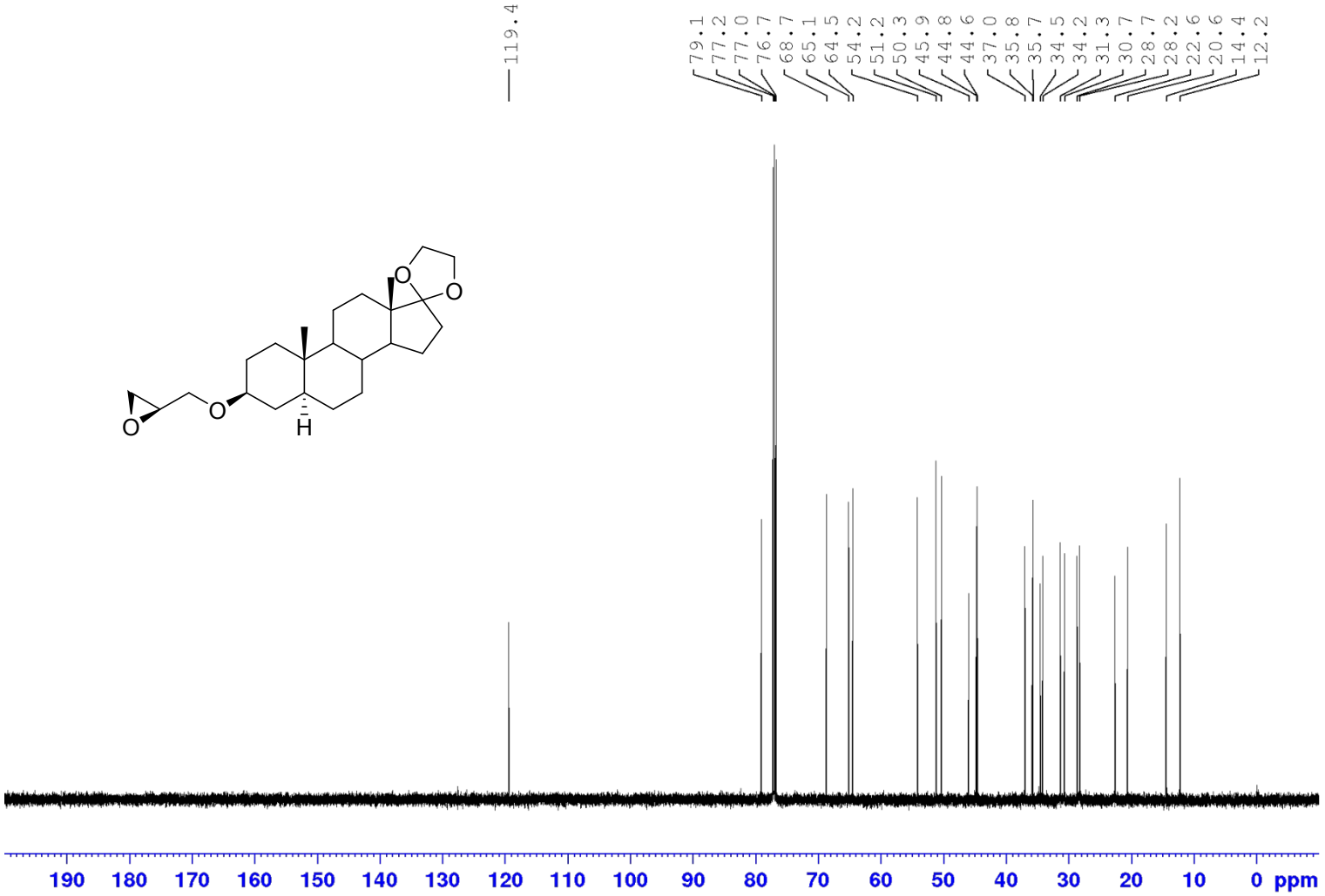
Epiandrosterone 17-acetal (*R*)-oxiran-2-yl)methyl ether (45) – ^{13}C – $CDCl_3$ – 125 MHz



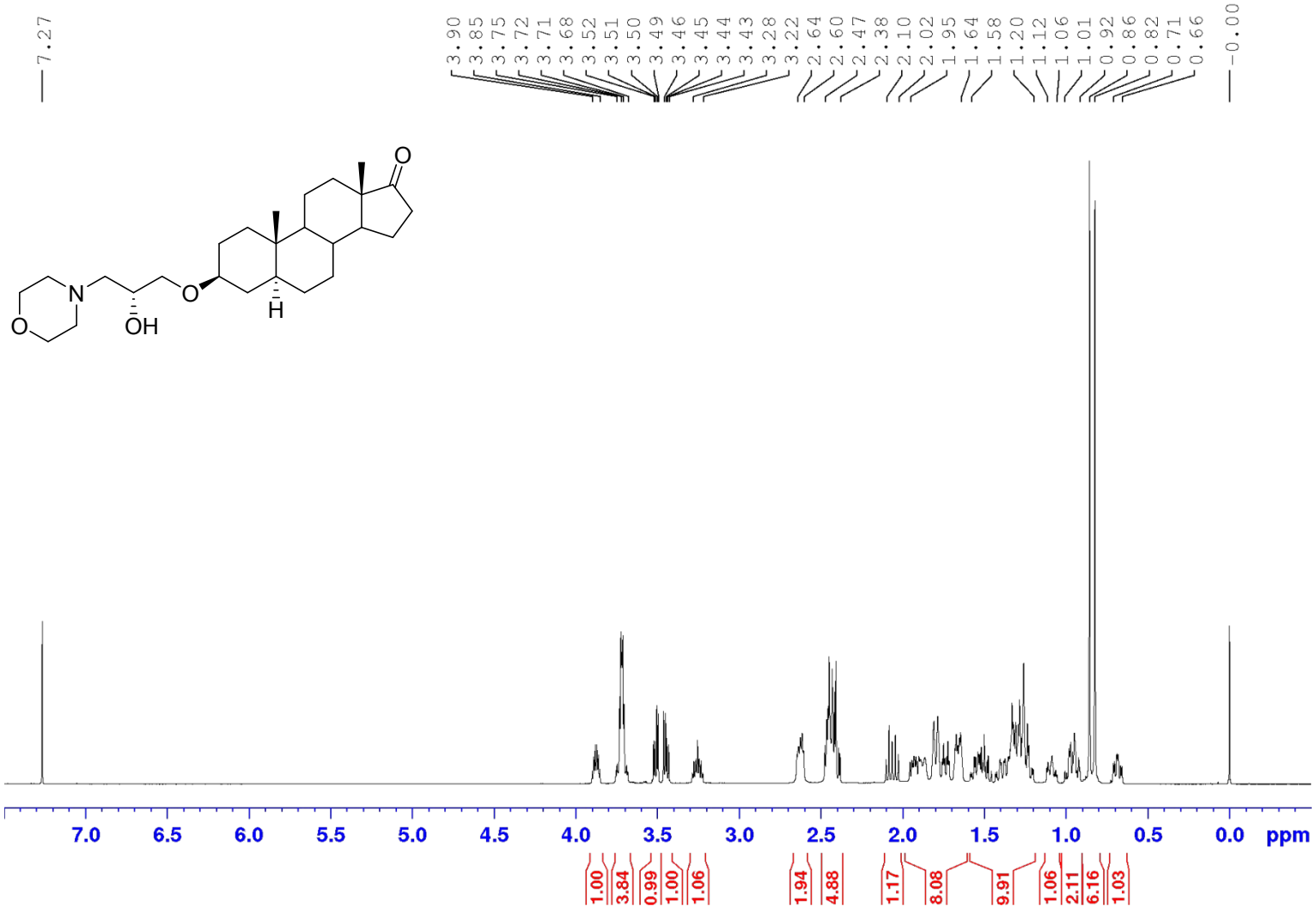
Epiandrosterone 17-acetal (*S*)-oxiran-2-yl)methyl ether (46) – ^{1}H – $CDCl_3$ – 500 MHz



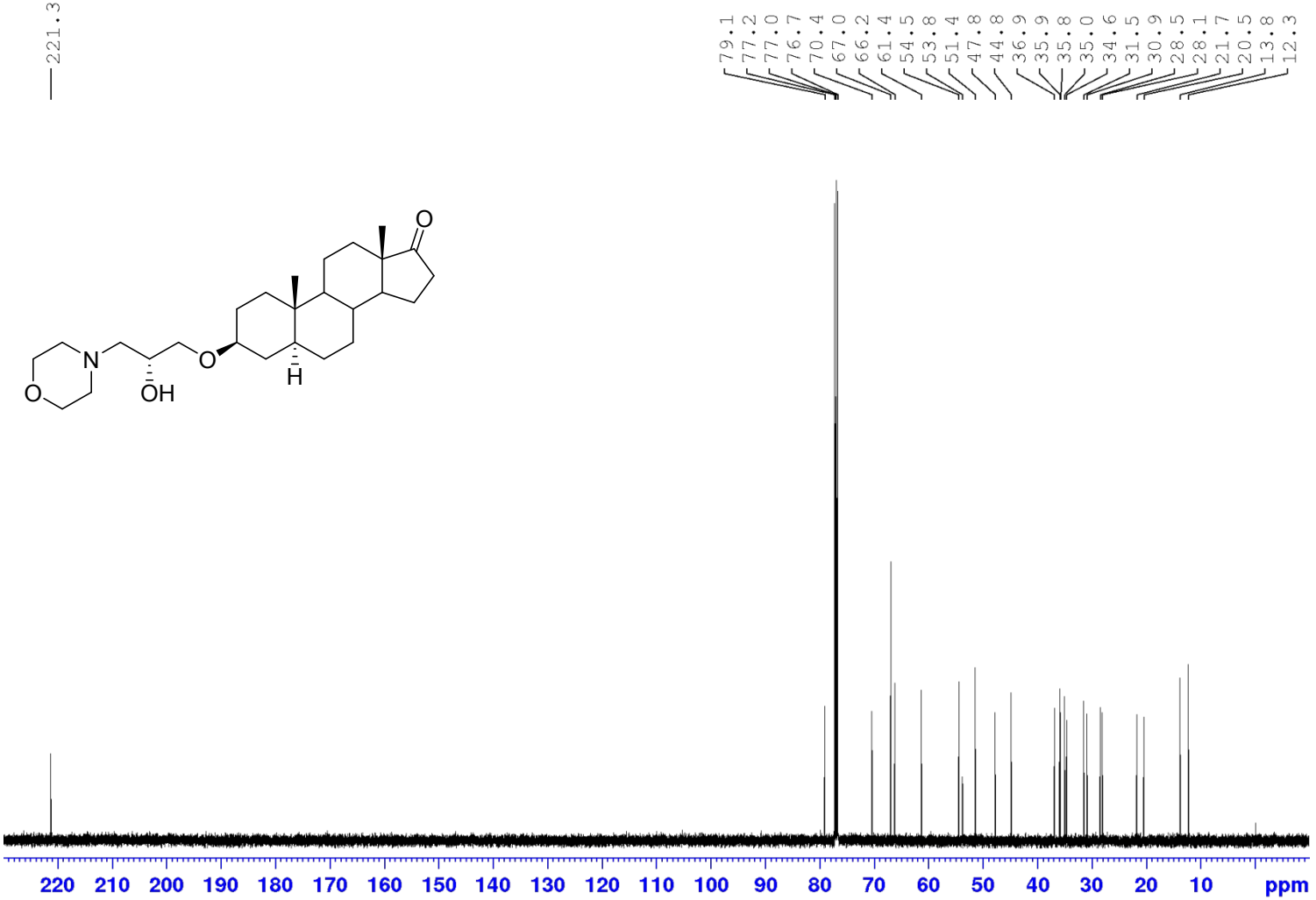
Epiandrosterone 17-acetal (*S*)-oxiran-2-yl)methyl ether (46) – ^{13}C – $CDCl_3$ – 125 MHz



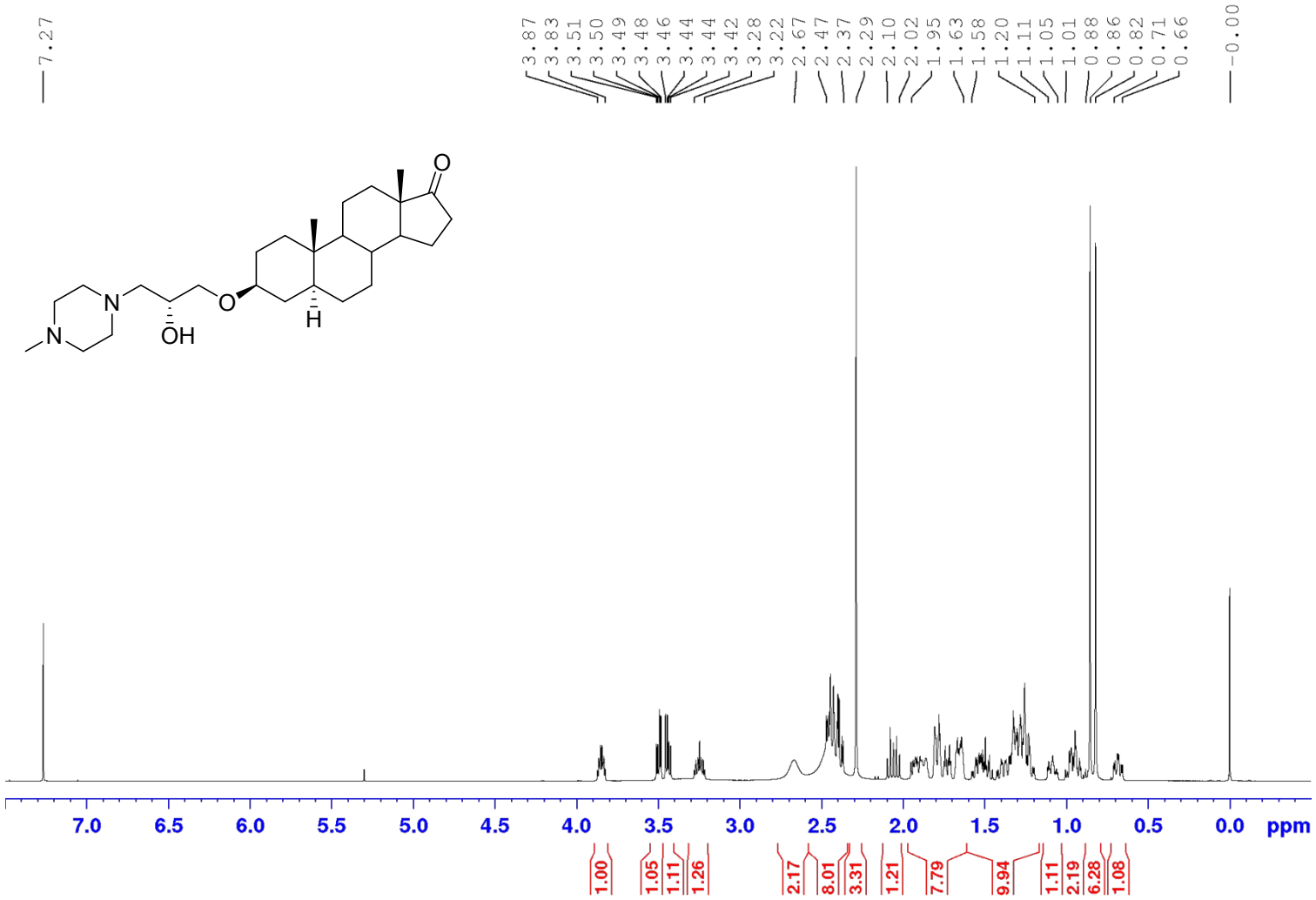
Epiandrosterone (*R*)-2-hydroxy-3-morpholinopropyl ether (47) – ^{1}H – $CDCl_3$ – 500 MHz



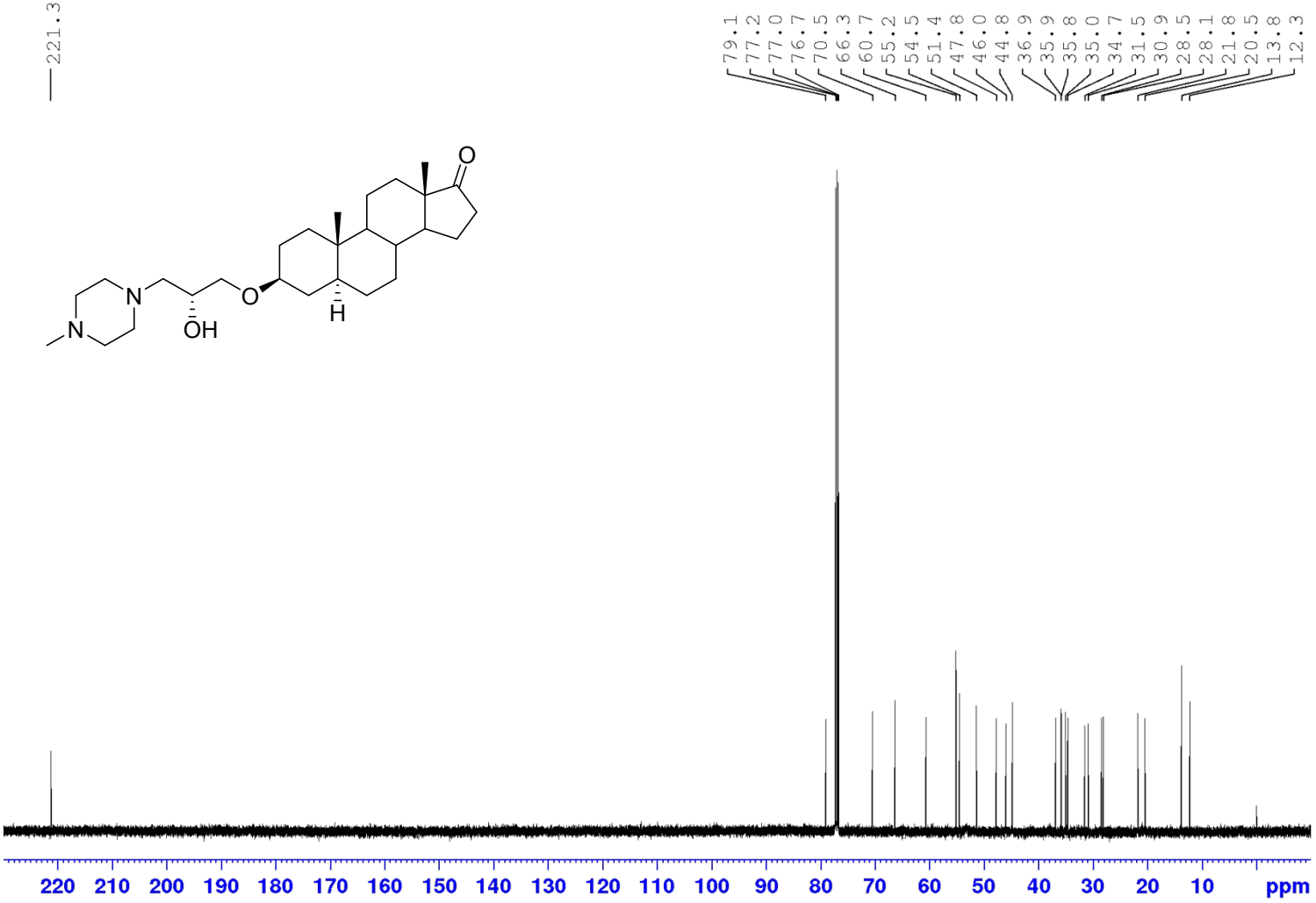
Epiandrosterone (*R*)-2-hydroxy-3-morpholinopropyl ether (47) – ^{13}C – $CDCl_3$ – 125 MHz



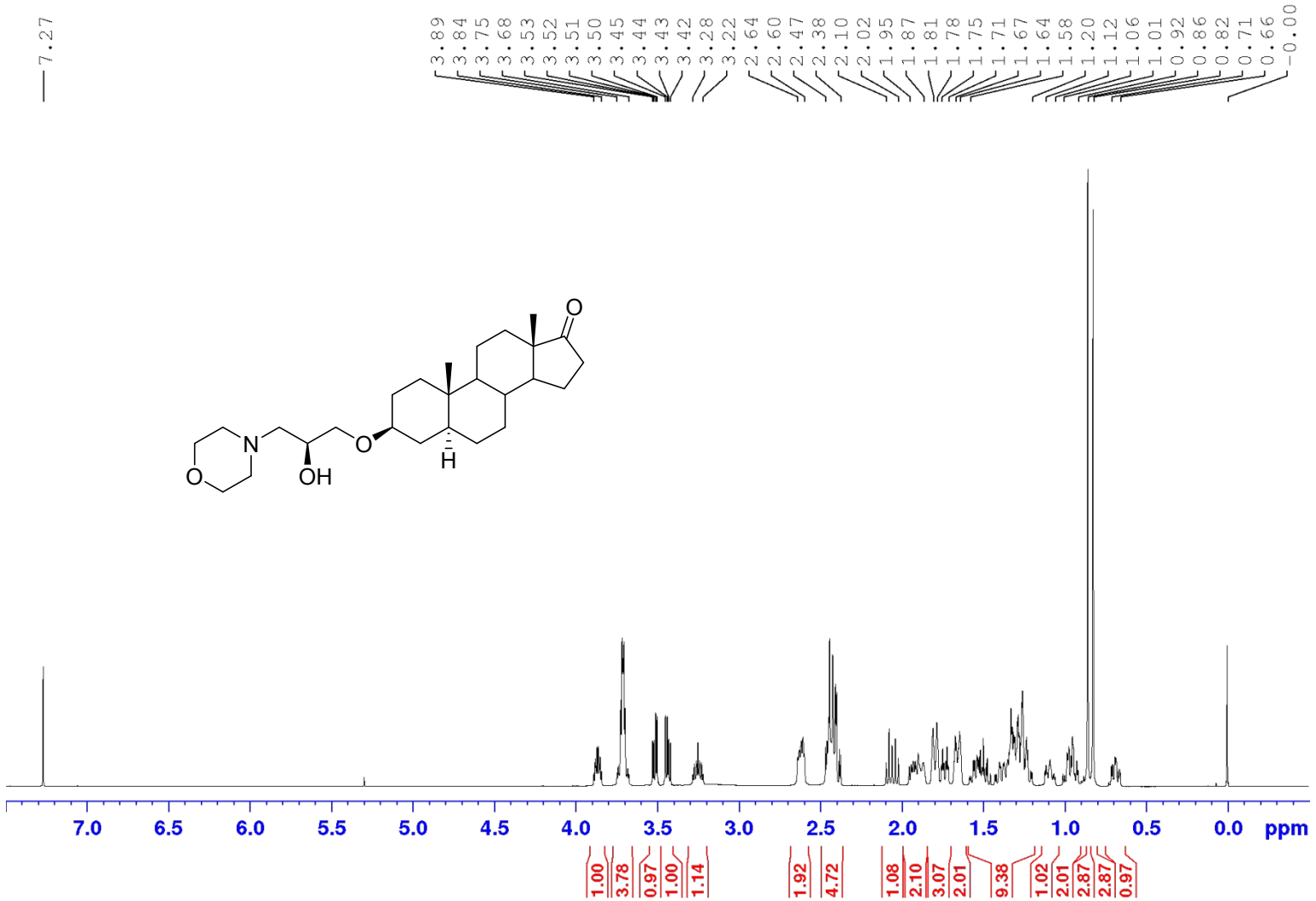
Epiandrosterone (*R*)-2-hydroxy-3-(4-methylpiperazin-1-yl)propyl ether (48) – ^{1}H – $CDCl_3$ – 500 MHz



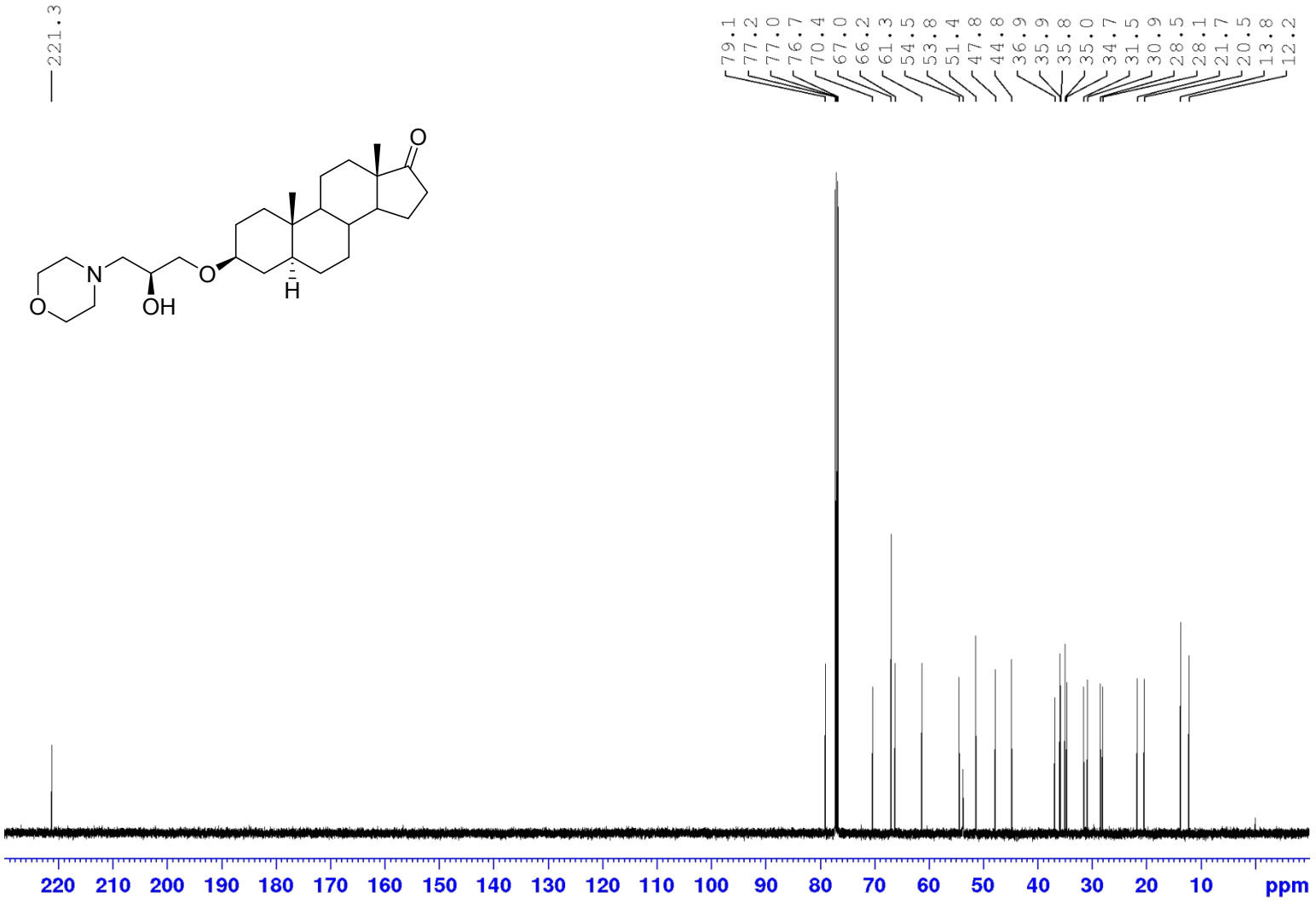
Epiandrosterone (*R*)-2-hydroxy-3-(4-methylpiperazin-1-yl)propyl ether (48) – ^{13}C – $CDCl_3$ – 125 MHz



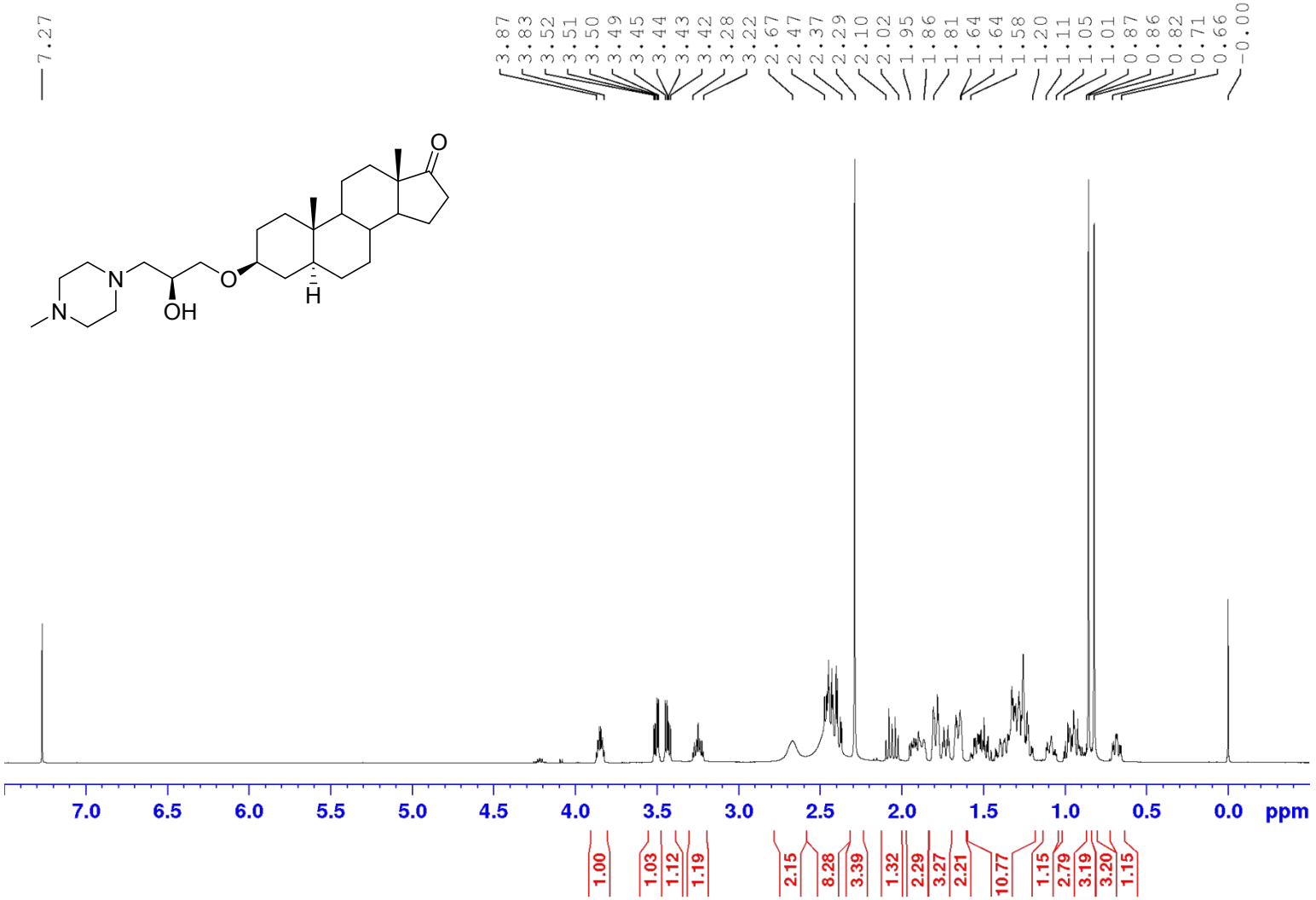
Epiandrosterone (*S*)-2-hydroxy-3-morpholinopropyl ether (49) – ^{1}H – $CDCl_3$ – 500 MHz



Epiandrosterone (*S*)-2-hydroxy-3-morpholinopropyl ether (49) – ^{13}C – $CDCl_3$ – 125 MHz



Epiandrosterone (*S*)-2-hydroxy-3-(4-methylpiperazin-1-yl)propyl ether (50) – ^{1}H – $CDCl_3$ – 500 MHz



Epiandrosterone (*S*)-2-hydroxy-3-(4-methylpiperazin-1-yl)propyl ether (50) – ^{13}C – $CDCl_3$ – 125 MHz