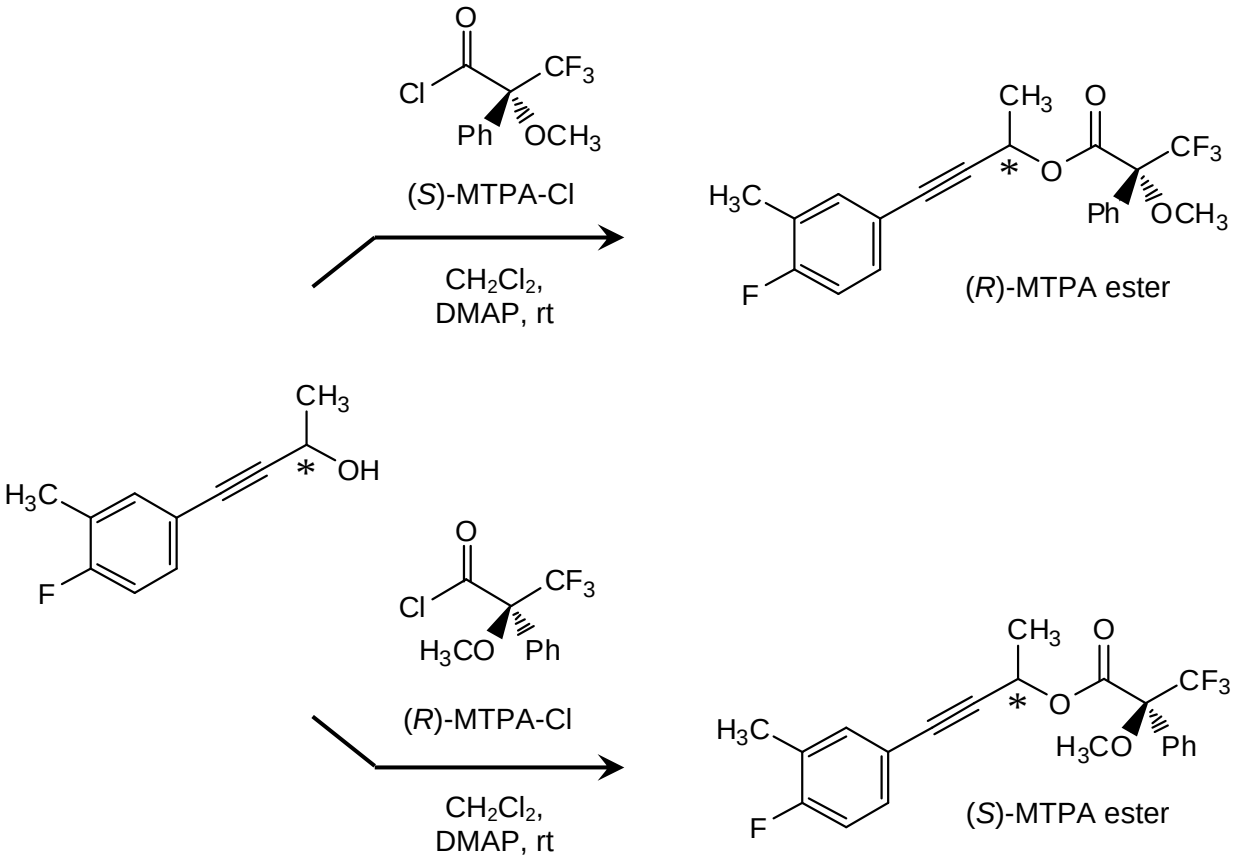
Chemistry 4361/8361 Friday, September 28

In-Class Exercise:
Resolving Stereochemistry with Mosher Esters

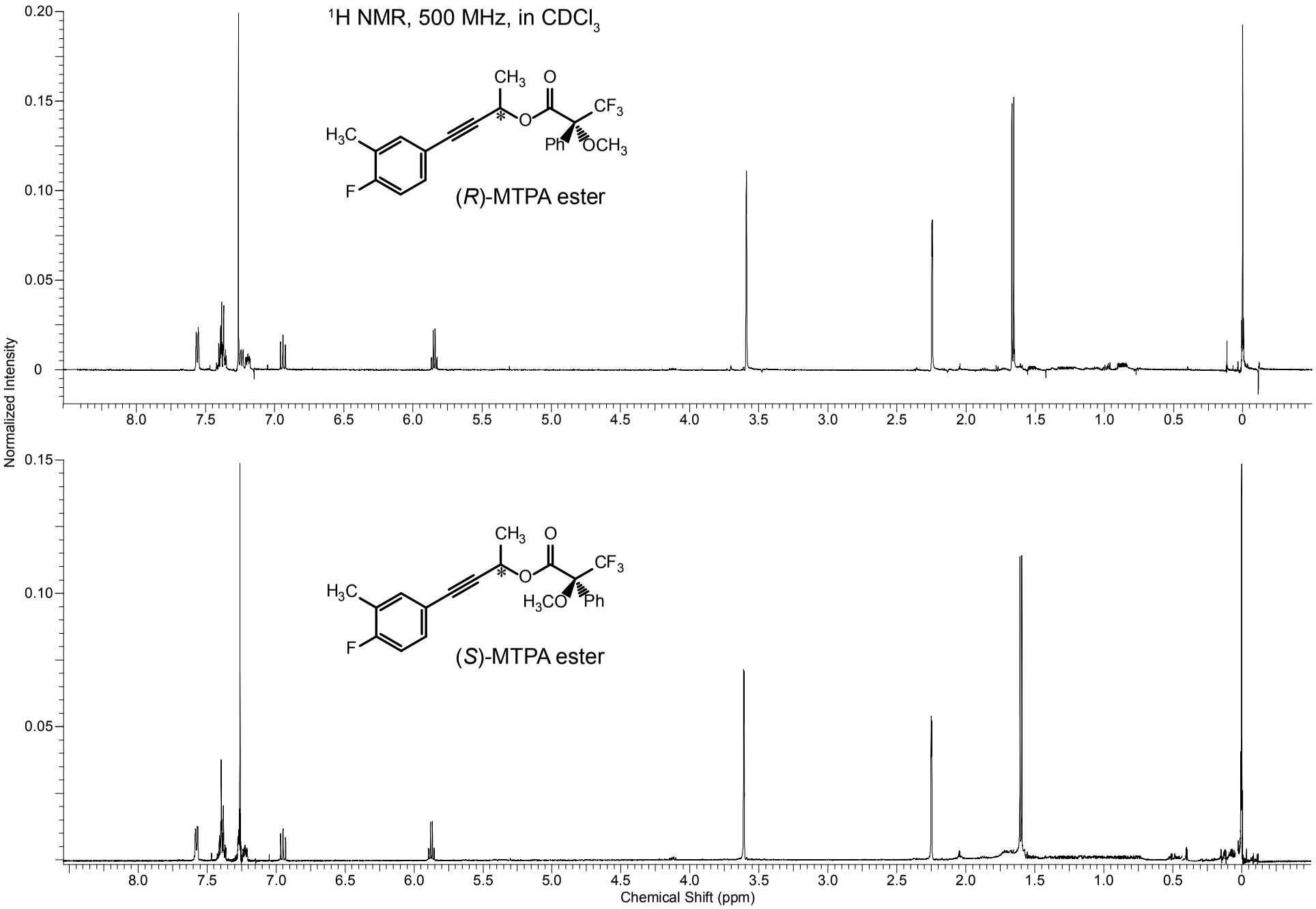
You have synthesized the phenylpropargyl alcohol shown below, and you know it to be enantiopure, but you don't know its absolute stereochemistry. In order to figure this out, you synthesize the (*R*)- and (*S*)-MTPA esters of your alcohol, and measure ^{1}H NMR spectra of those esters.

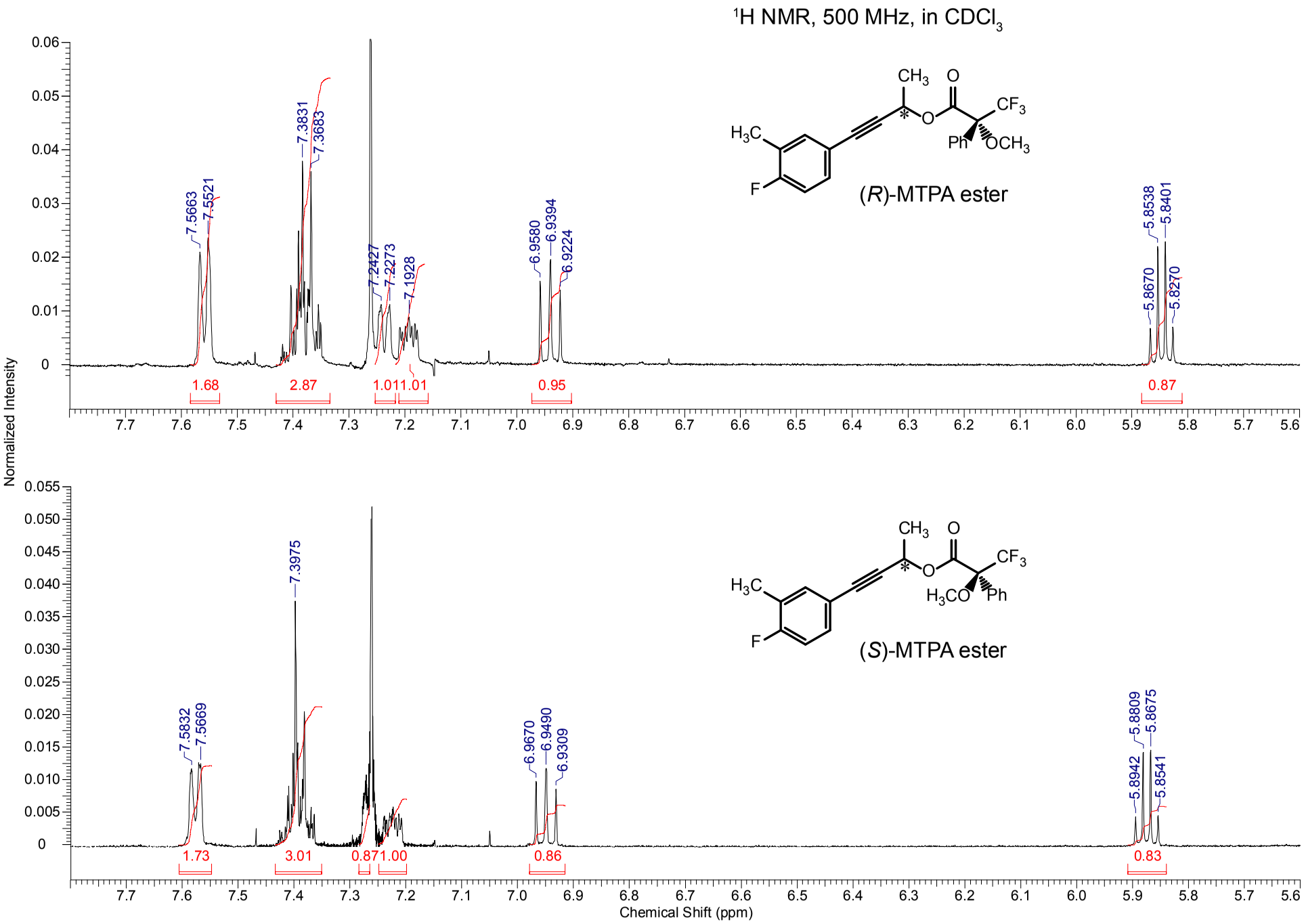


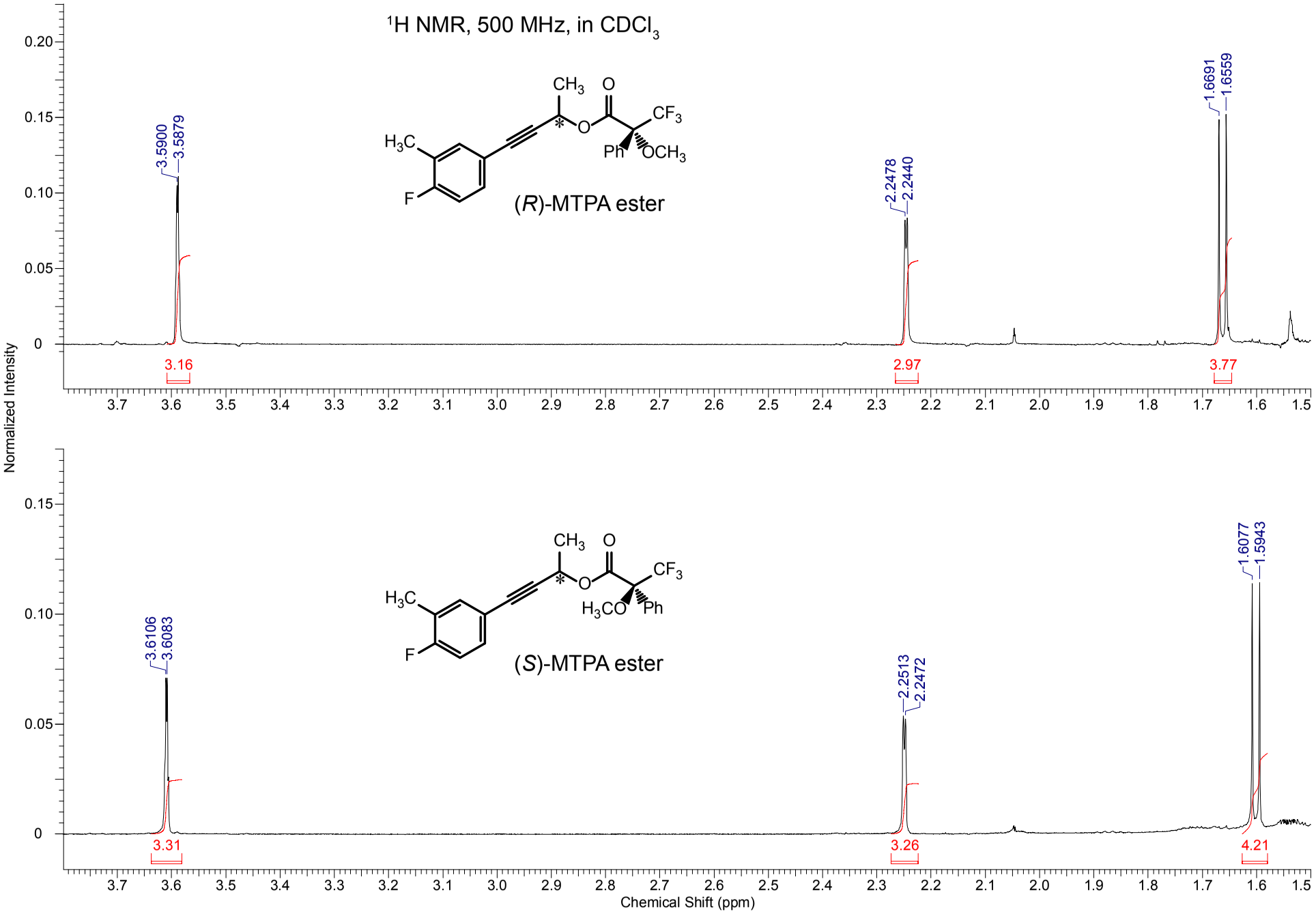
Those ^{1}H NMR spectra (500 MHz, in $CDCl_3$) and close-ups are shown on the following pages. On each page, the spectrum of the (*R*)-ester (synthesized from the (*S*)-MTPA chloride) is shown on top, and the (*S*)-ester (synthesized from the (*R*)-chloride) is on bottom.

a. What chemical shift differences $\Delta\delta = (\delta_S - \delta_R)$ do you observe in these spectra?

b. Assign stereochemistry to the chiral center in your molecule.


^{1}H NMR, 500 MHz, in $CDCl_3$
(*R*)-MTPA ester
(*S*)-MTPA ester
Normalized Intensity
Chemical Shift (ppm)


^{1}H NMR, 500 MHz, in $CDCl_3$
(*R*)-MTPA ester
(*S*)-MTPA ester
Normalized Intensity
Chemical Shift (ppm)
7.5663
7.5521
7.3831
7.3683
7.2427
7.2273
7.1928
6.9580
6.9394
6.9224
5.8538
5.8401
5.8670
5.8270
1.68
2.87
1.01
1.01
0.95
0.87
7.5832
7.5669
7.3975
6.9670
6.9490
6.9309
5.8809
5.8675
5.8942
5.8541
1.73
3.01
0.87
1.00
0.86
0.83


^{1}H NMR, 500 MHz, in $CDCl_3$
(*R*)-MTPA ester
(*S*)-MTPA ester
3.5900
3.5879
2.2478
2.2440
1.6691
1.6559
3.6106
3.6083
2.2513
2.2472
1.6077
1.5943
3.16
2.97
3.77
3.31
3.26
4.21
Normalized Intensity
Chemical Shift (ppm)