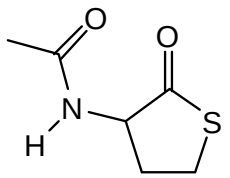
Chemistry 4361/8361 Tuesday, September 18

Discussion Section Exercise:
^{1}H NMR Multiplets with Different Coupling Constants

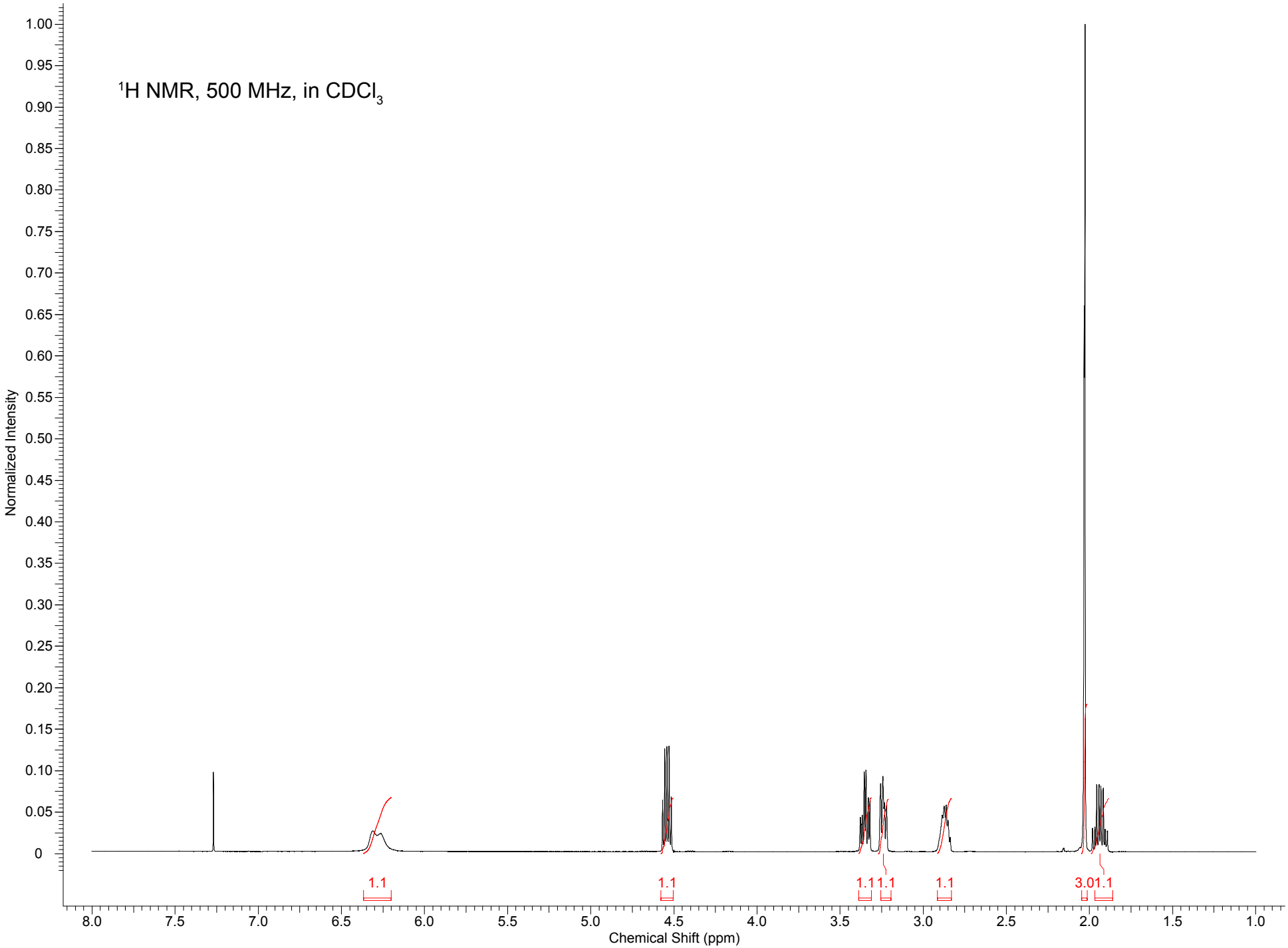
The NMR spectra of the thiolactone at right are shown on the following pages. Answer the following questions about these spectra:

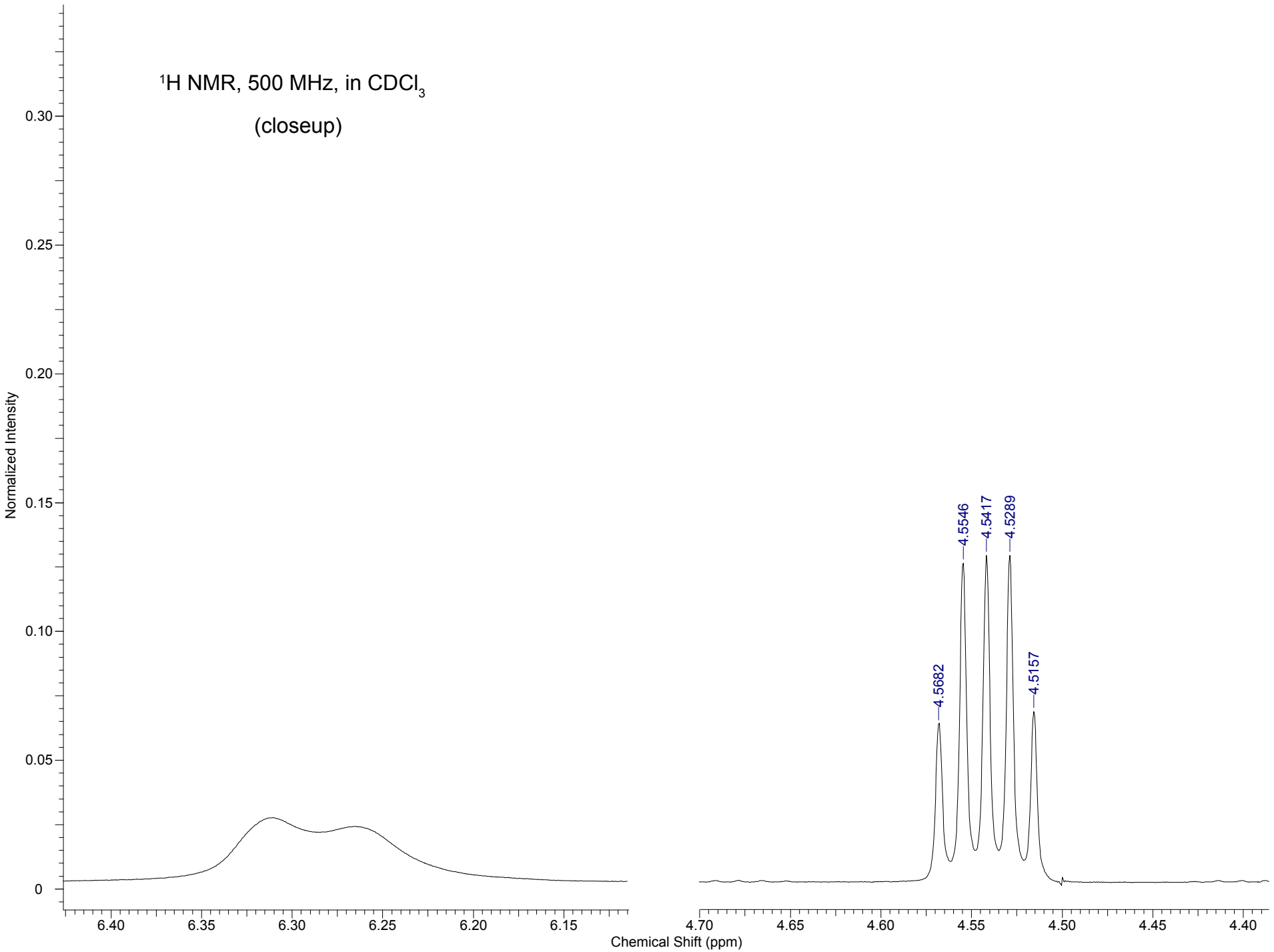


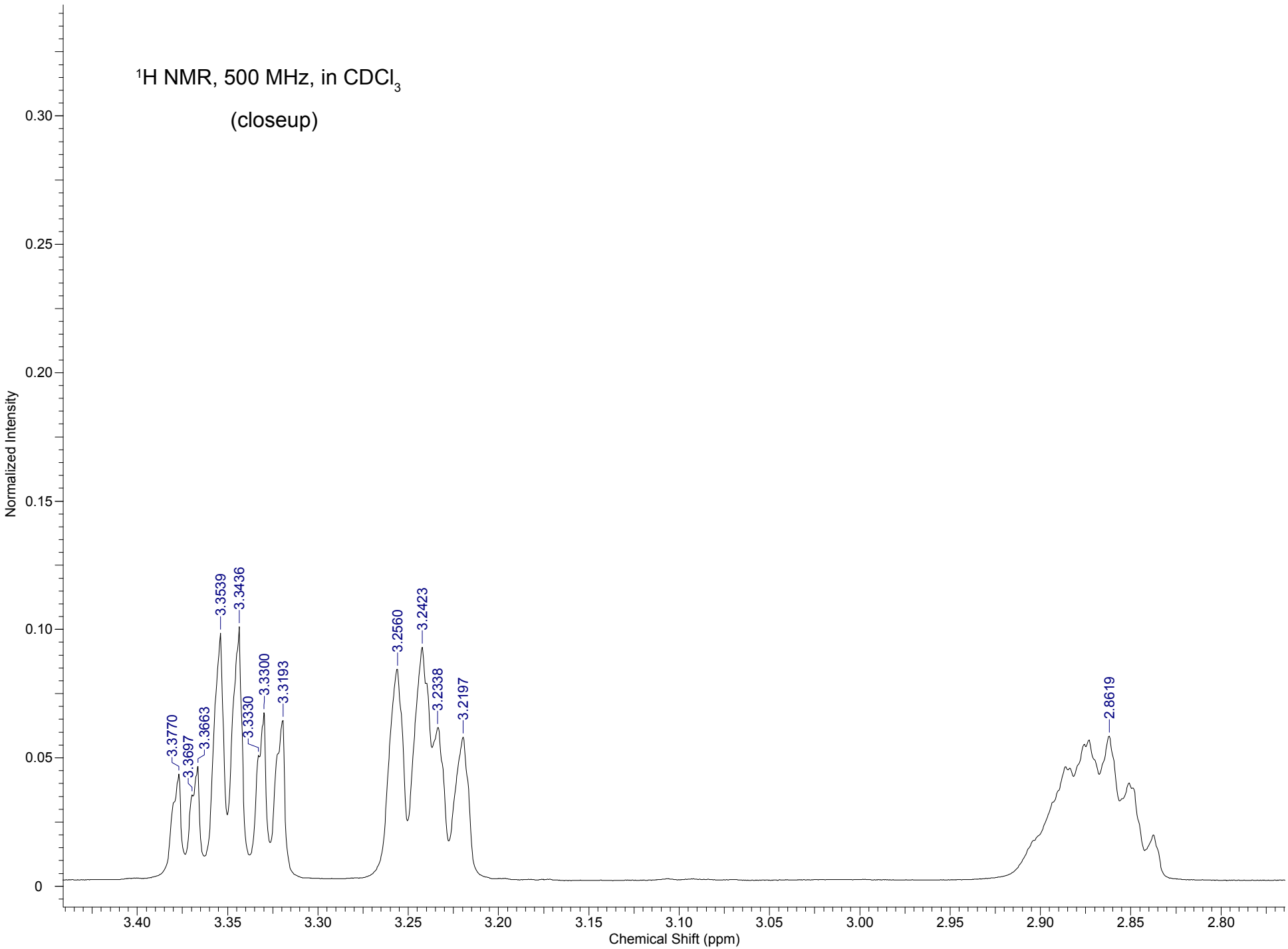
1. For each of the clearly split multiplets (i.e., not including the resonances at 6.3 and 2.9 ppm), what would you name the multiplet?

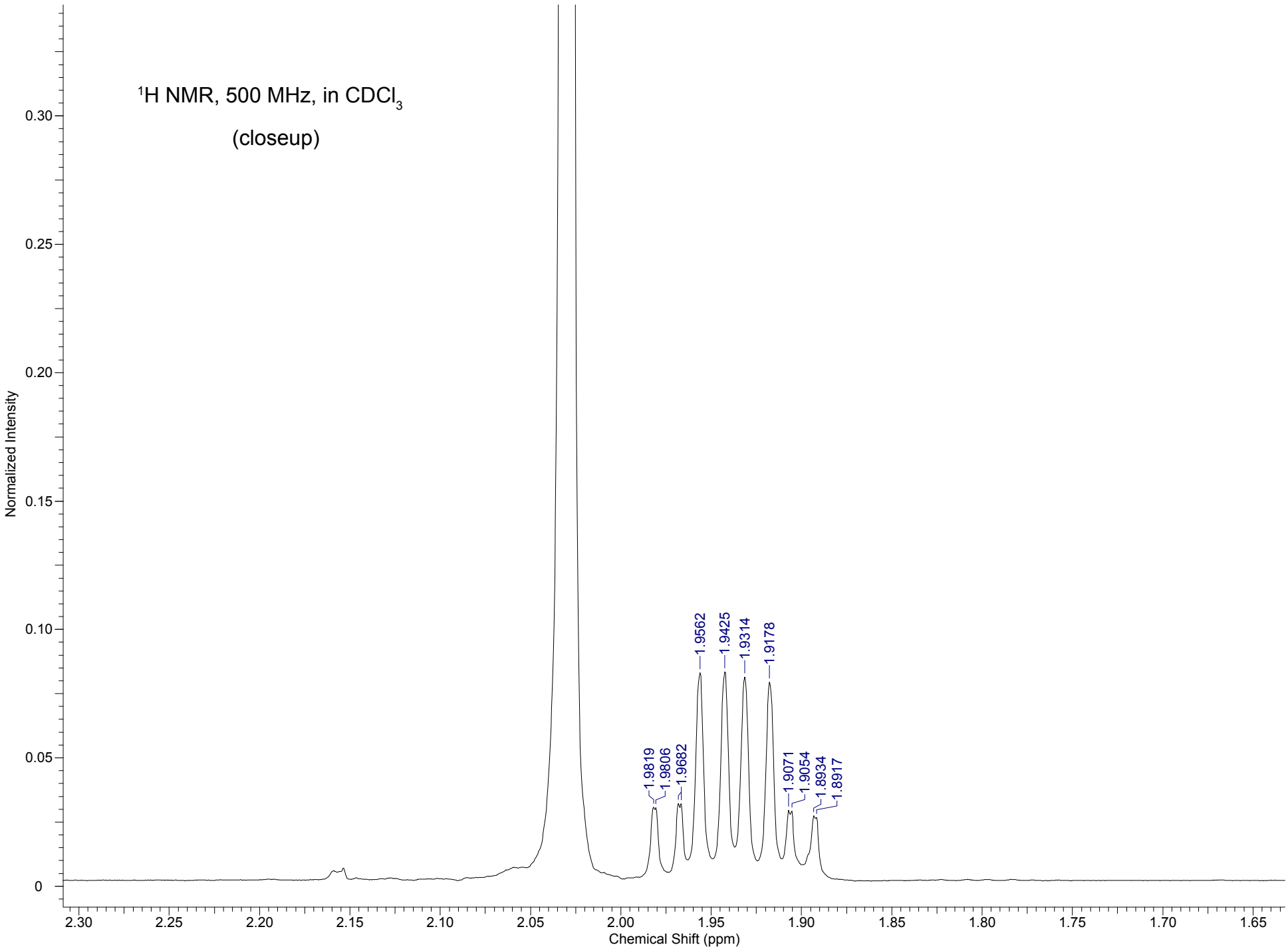
2. What coupling constants (*J*) do you calculate for each multiplet? How many coupling partners are responsible for these *J* values?

3. Considering chemical shift values, can you assign which protons in the thiolactone match each resonance in the spectra? Which protons are coupled to which, and by what *J* values?


^{1}H NMR, 500 MHz, in $CDCl_3$
Normalized Intensity
Chemical Shift (ppm)
1.1
1.1
1.1
1.1
1.1
3.0
1.1


^{1}H NMR, 500 MHz, in $CDCl_3$
(closeup)
Normalized Intensity
0.30
0.25
0.20
0.15
0.10
0.05
0
6.40
6.35
6.30
6.25
6.20
6.15
4.70
4.65
4.60
4.55
4.50
4.45
4.40
Chemical Shift (ppm)
4.5682
4.5546
4.5417
4.5289
4.5157


^{1}H NMR, 500 MHz, in $CDCl_3$
(closeup)
Normalized Intensity
0.30
0.25
0.20
0.15
0.10
0.05
0
3.40
3.35
3.30
3.25
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
Chemical Shift (ppm)
3.3770
3.3697
3.3663
3.3539
3.3436
3.3330
3.3300
3.3193
3.2560
3.2423
3.2338
3.2197
2.8619


^{1}H NMR, 500 MHz, in $CDCl_3$
(closeup)
Normalized Intensity
0.30
0.25
0.20
0.15
0.10
0.05
0
1.9819
1.9806
1.9682
1.9562
1.9425
1.9314
1.9178
1.9071
1.9054
1.8934
1.8917
2.30
2.25
2.20
2.15
2.10
2.05
2.00
1.95
1.90
1.85
1.80
1.75
1.70
1.65
Chemical Shift (ppm)