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Sythesis and Characterization of a Model Multicopper Oxidase

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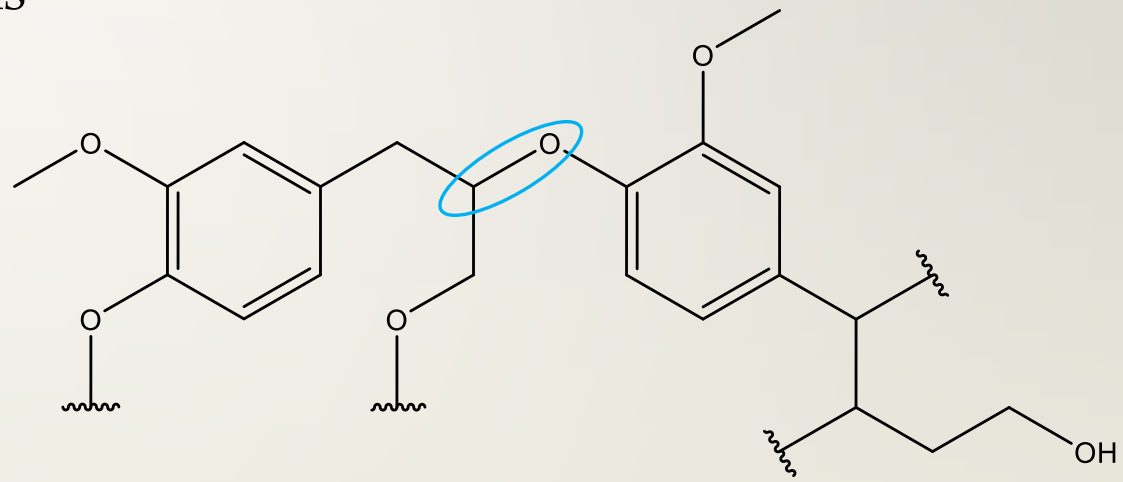
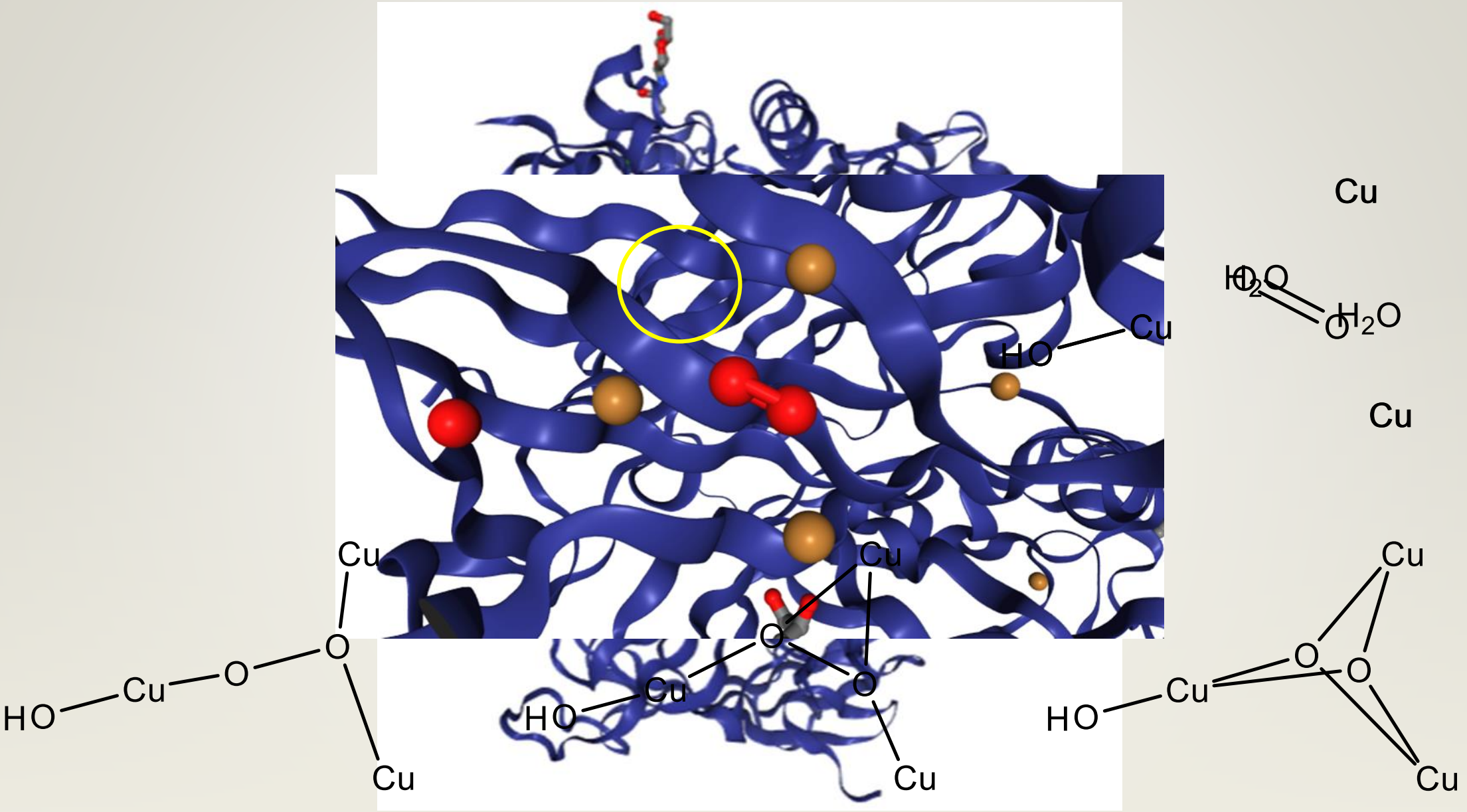
Multicopper Oxidases (MCO's)

$Fe^{2+} \longrightarrow Fe^{3+} + e^-$

- MCO's are class of enzymes
- Enzymes: BIG molecules with cool reactions
- $O_2 + 4\ H^+ + 4\ e^- \rightarrow 2\ H_2O$
  - Common reaction
  - Tricopper cluster
- Ceruloplasmin, laccase





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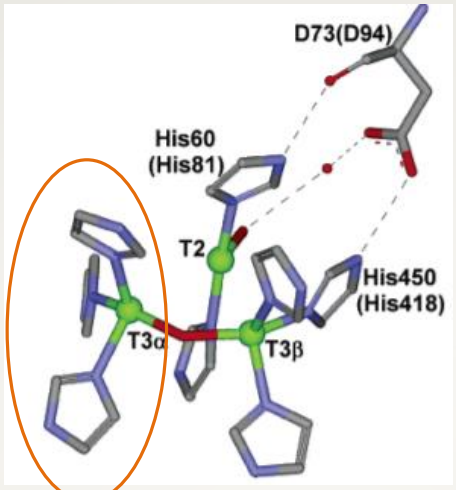
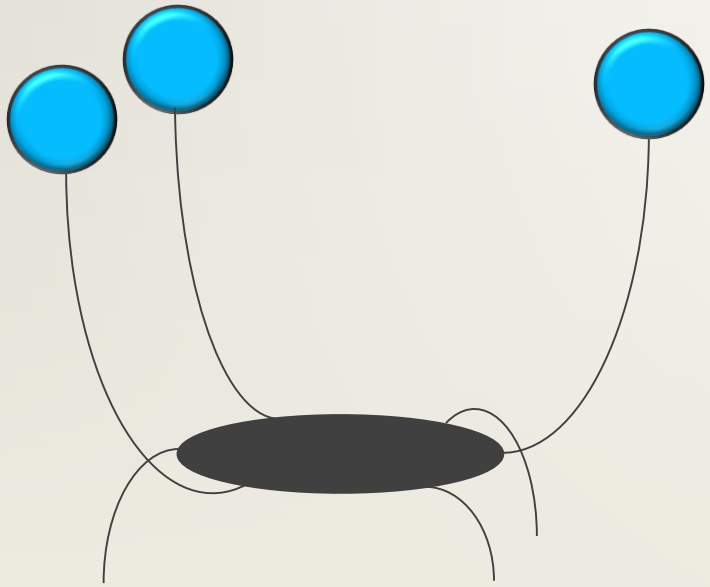
Biomimetic Chemistry

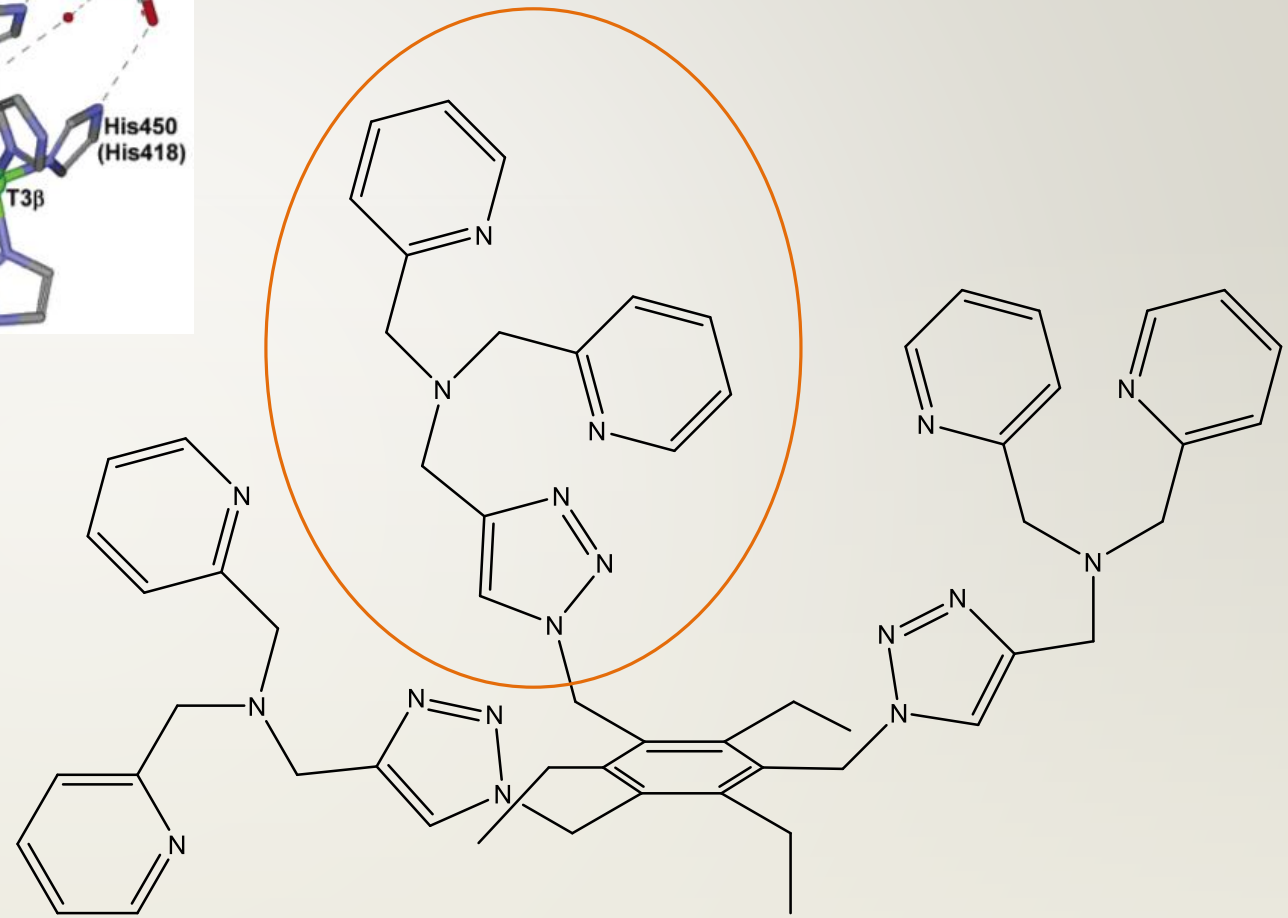
- Enzymes are BIG
- Build smaller model
  - Modifiable
  - Easier to study
  - Cost-effective
- Drawbacks
  - May not give accurate insight

Ligand Design

- Close proximity
- N-donor ligands







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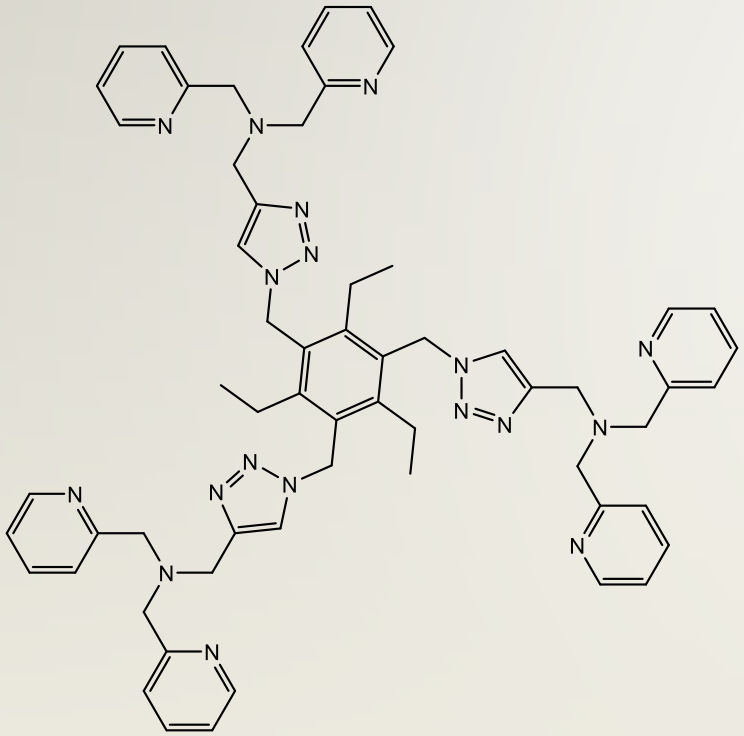
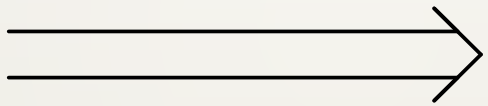
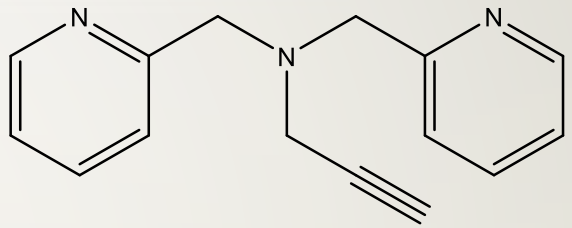
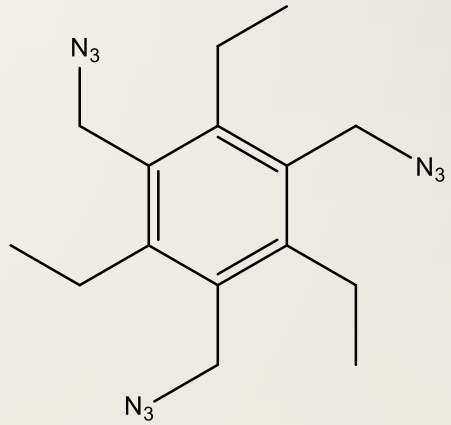
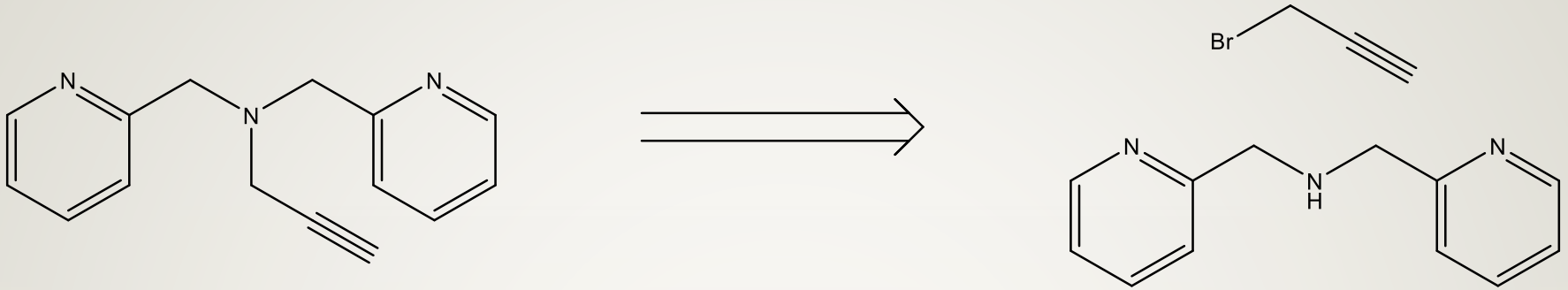
Retrosynthetic Analysis

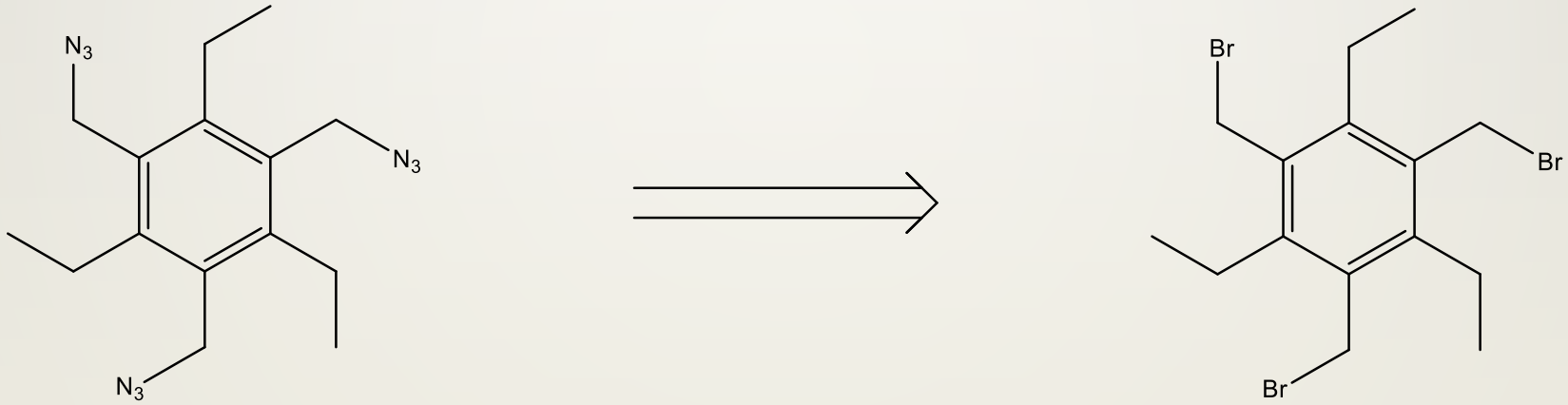






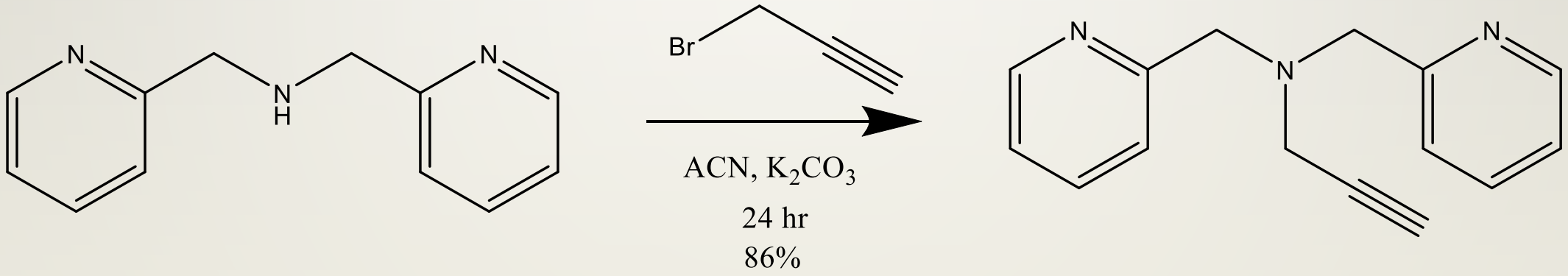



N
N
N
Br
N
N
N
H


N3
N3
N3
Br
Br
Br

Results and Discussion: Step 1

- Difficult to purify
- Changed conditions



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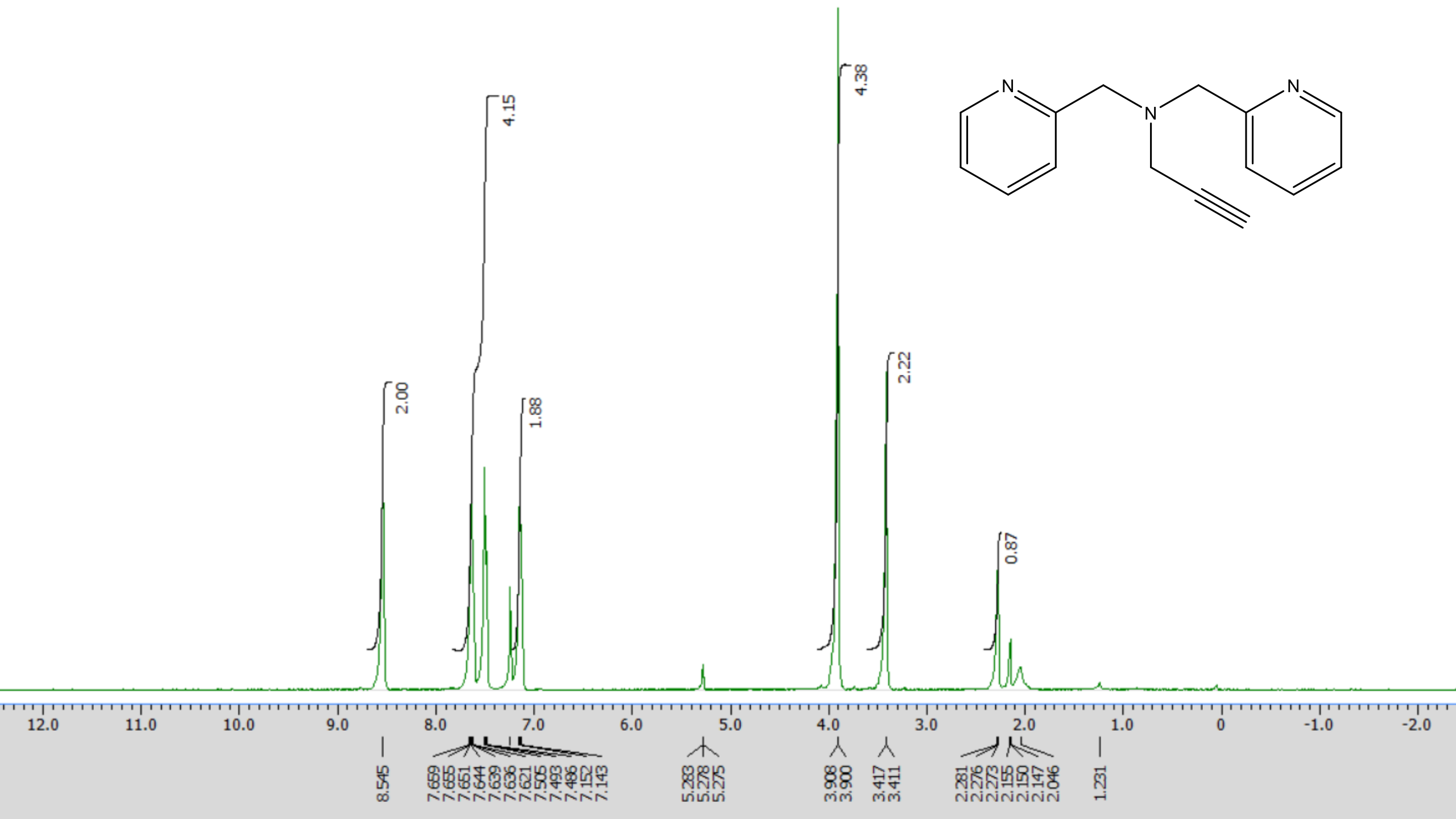
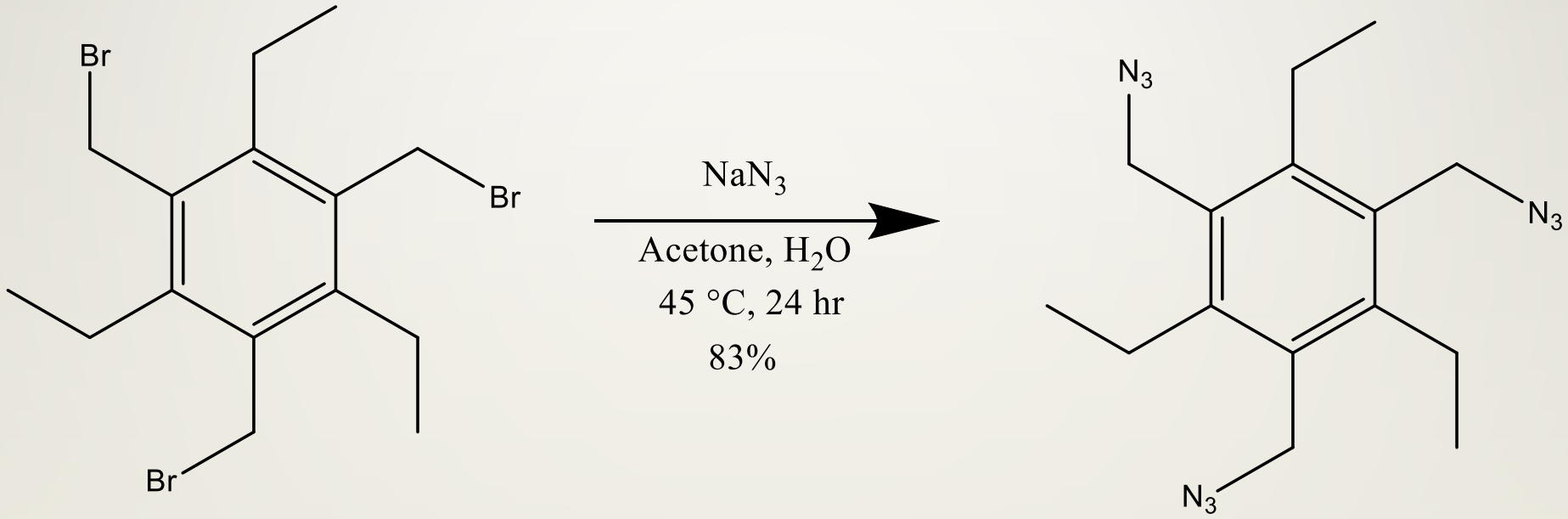

N
N
N
4.38
4.15
2.22
2.00
1.88
0.87
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.545
7.659
7.655
7.651
7.644
7.639
7.636
7.621
7.505
7.493
7.486
7.152
7.143
5.283
5.278
5.275
3.908
3.900
3.417
3.411
2.281
2.276
2.273
2.155
2.150
2.147
2.046
1.231

Step 2



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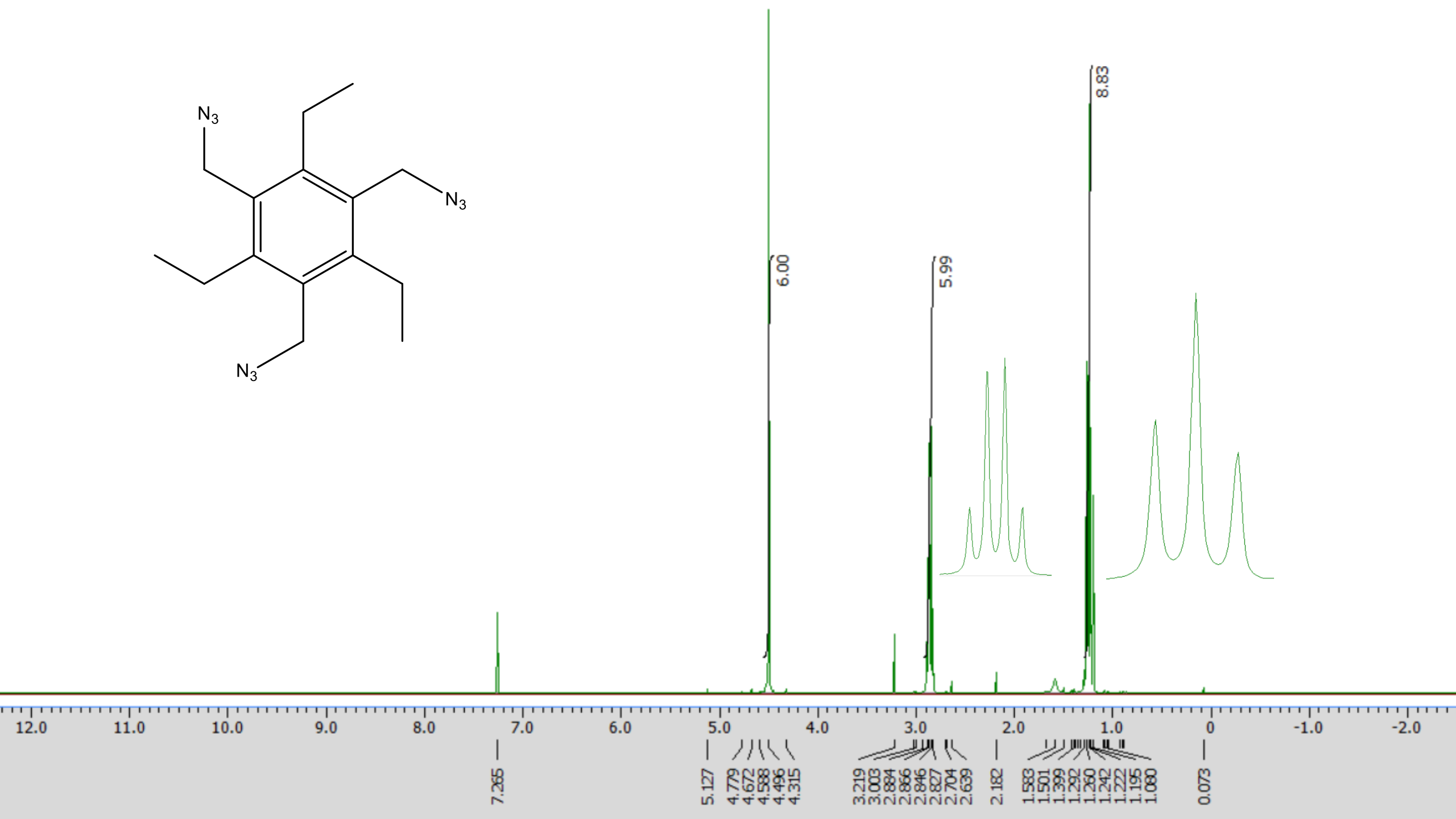
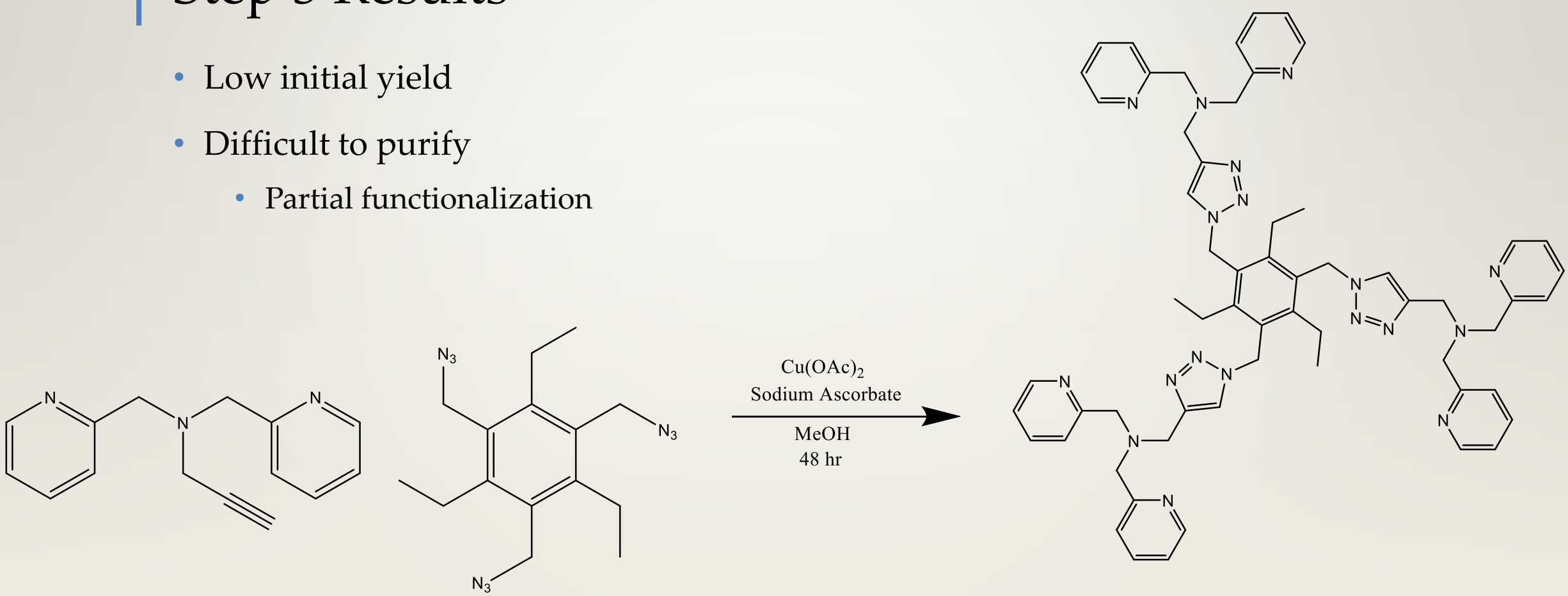

N3
N3
N3
6.00
5.99
8.83
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.265
5.127
4.779
4.672
4.588
4.496
4.315
3.219
3.003
2.894
2.866
2.846
2.827
2.704
2.639
2.182
1.583
1.501
1.399
1.292
1.260
1.242
1.222
1.195
1.080
0.073

Step 3 Results

- Low initial yield
- Difficult to purify
  - Partial functionalization



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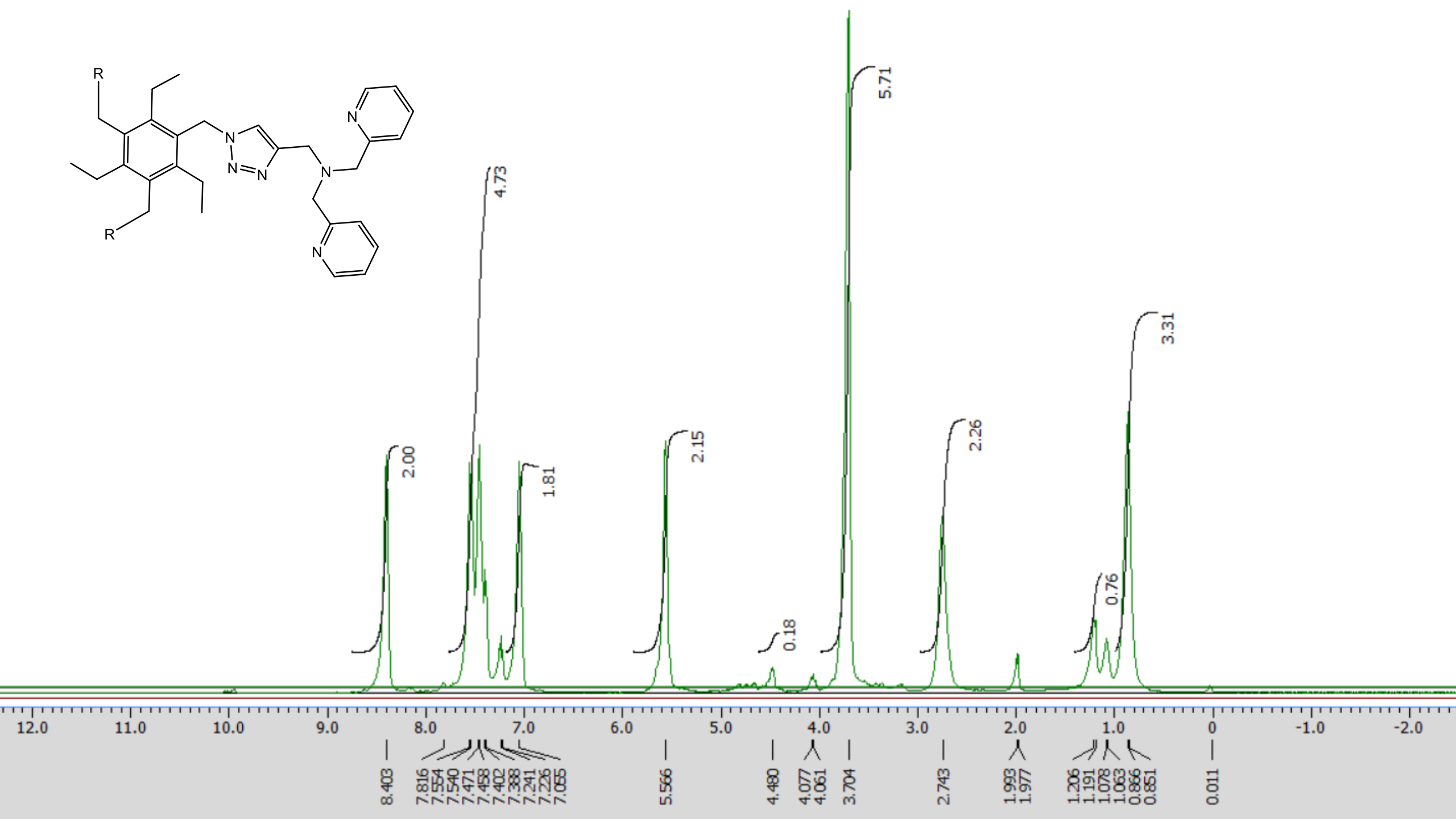
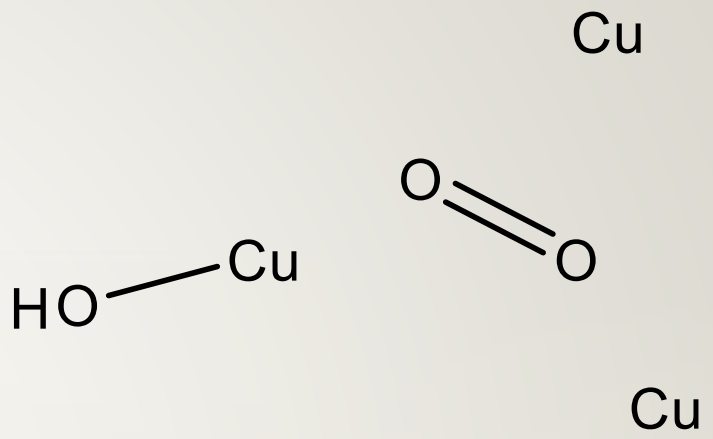

R
R
N
N
N
N
N
N
2.00
4.73
1.81
2.15
0.18
5.71
2.26
0.76
3.31
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.403
7.816
7.554
7.540
7.471
7.458
7.402
7.388
7.241
7.226
7.055
5.566
4.490
4.077
4.061
3.704
2.743
1.993
1.977
1.206
1.191
1.078
1.063
0.866
0.851
0.011

Conclusion

- Step one and two were successful
- Step three was unsuccessful
  - Progress made

Future Work

- Synthesize and purify ligand
- Bind copper
- Characterize
  - NMR
  - Crystals!!
- Studies with O_2



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Questions?