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Diversity Oriented Synthesis of Furan Epoxide

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Diversity Oriented Synthesis of Furan Epoxide

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Introduction

Diversity Oriented Synthesis (DOS) is a method to create a library of biological interesting small molecules that has similar structure. In our lab, we are focusing on epoxide as the basic structure. Epoxide is an important class in organic synthesis which the ring is a highly reactive nucleophile. Figure 1 shows the epoxide ring opening and the R substituent can also be modified to introduce more feature to the molecule.

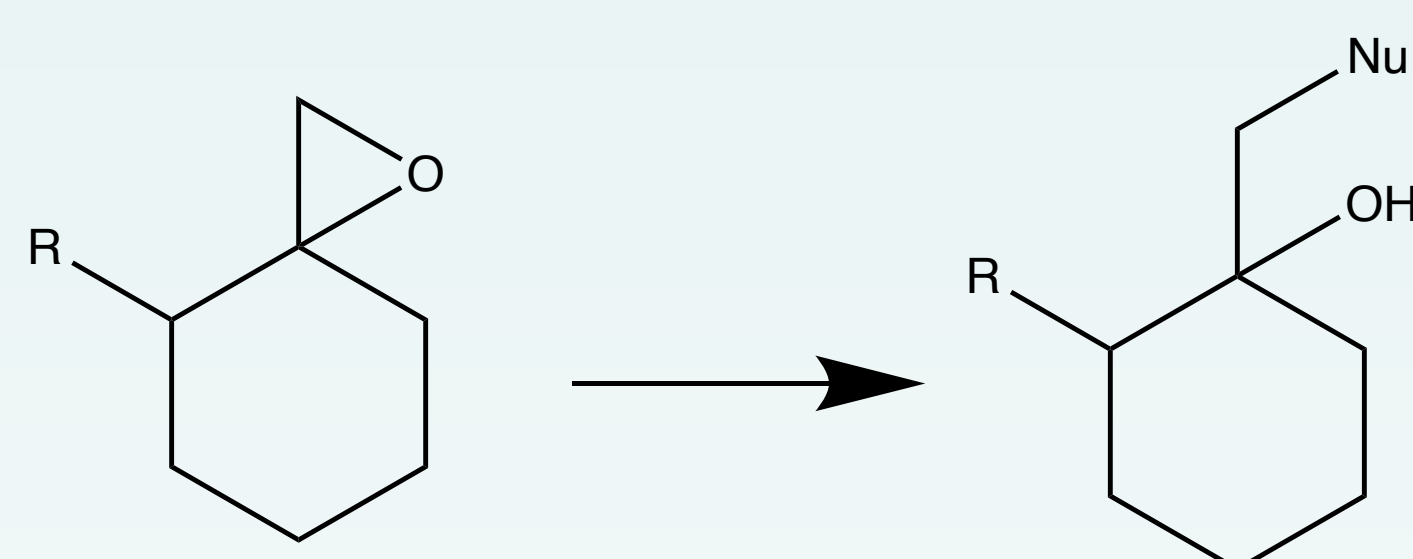


Figure 1: Epoxide ring opening reaction

Biological Result

We firstly tested our compound 3 that R group is a benzyl group with Brine Shrimp Lethality Assay and from the cross point in figure 3 got the LC₅₀ value 117.1 (ppm). We also did the Crystal Violet Assay data of MCF7 cell line treated by compound 3 over 96 hours to test its bioactivity.

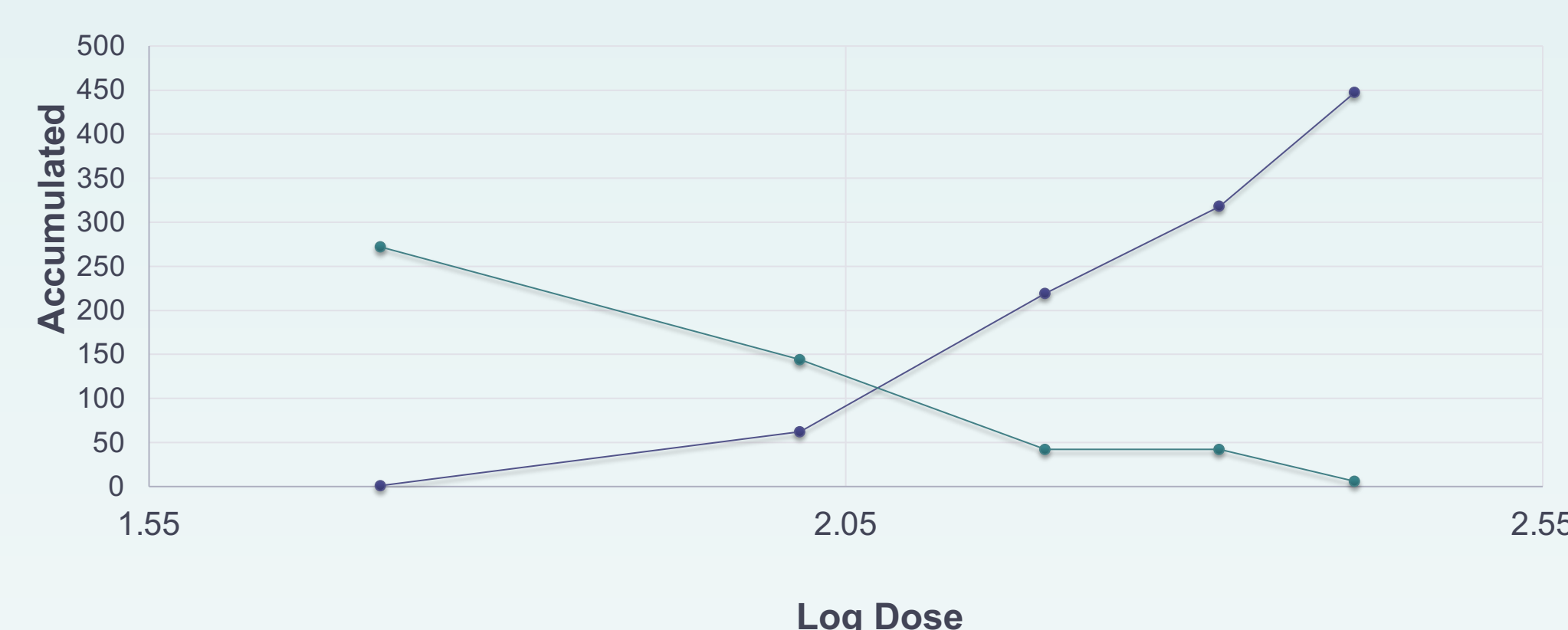


Figure 3: Reed-Muench Method LC50 plot

Experiment Set Up

Since the reaction that opens the epoxide ring with amine is a both water sensitive and air sensitive reaction, so we need to flame dry the reaction flask and flush nitrogen in to prevent air present. The condenser with water flow helps to condense solvent during heating.

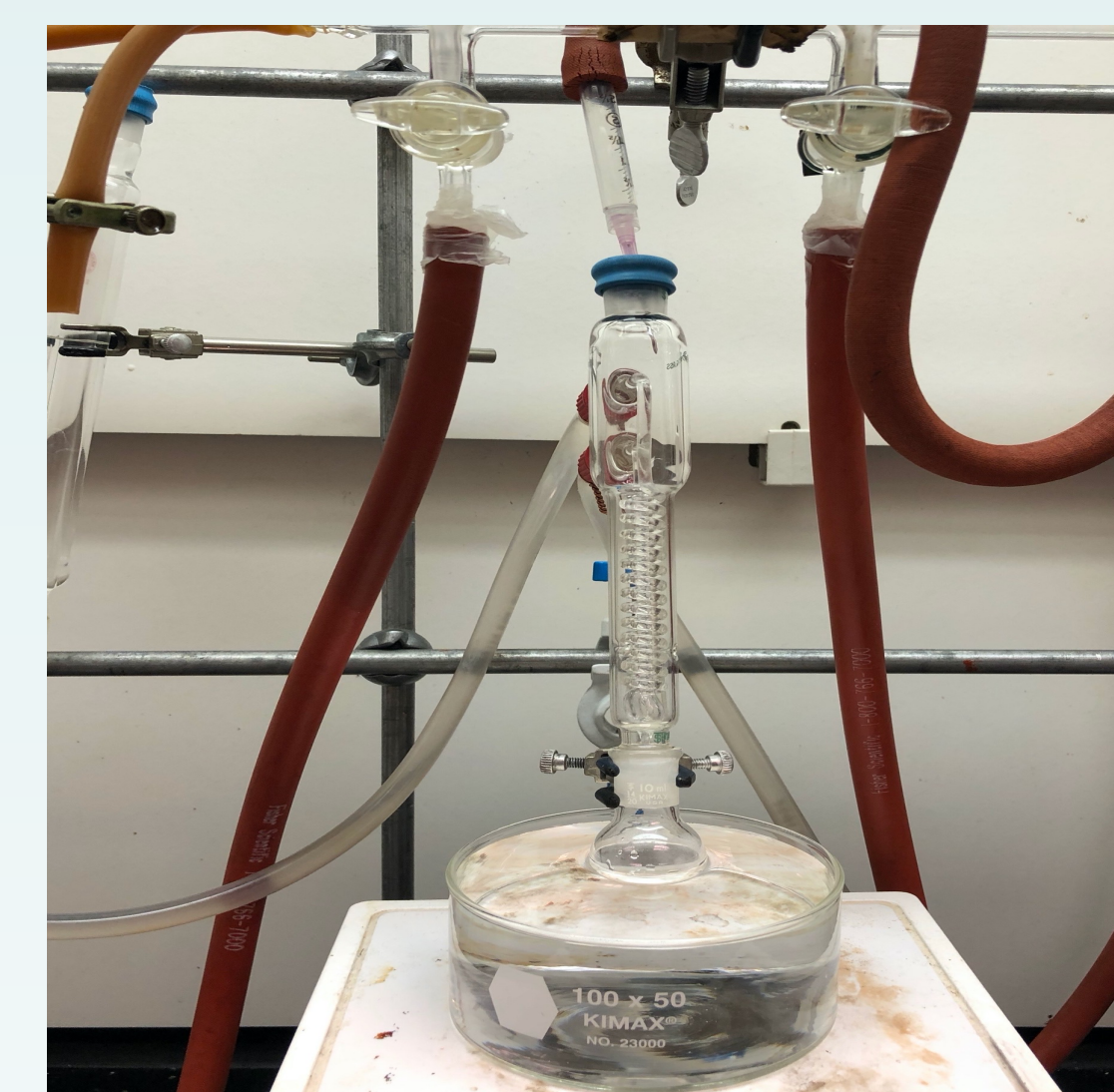


Figure 4: Epoxide ring opening reaction setup

Future Work

From the previous work, we are able to make compound 2 and 3, but not able to make either compound 4 or 7. Since we already know amino alcohol is a privileged (bioactive) structure in DOS, we are trying to add more structure complexity to the compound that could either increase or decrease the activity. Moreover, the results from this summer suggest that either compound 2 and 3 are having too much reacting point for the side reaction happens. For the further study, we are planning about adding a boc group to the amine while doing Achmatowicz reaction with compound 3.

Result and Discussion

Figure 2 shows for different reaction we did with furan epoxide. Primary amines with nonpolar substituent used in the reaction are represented by R that could be various.

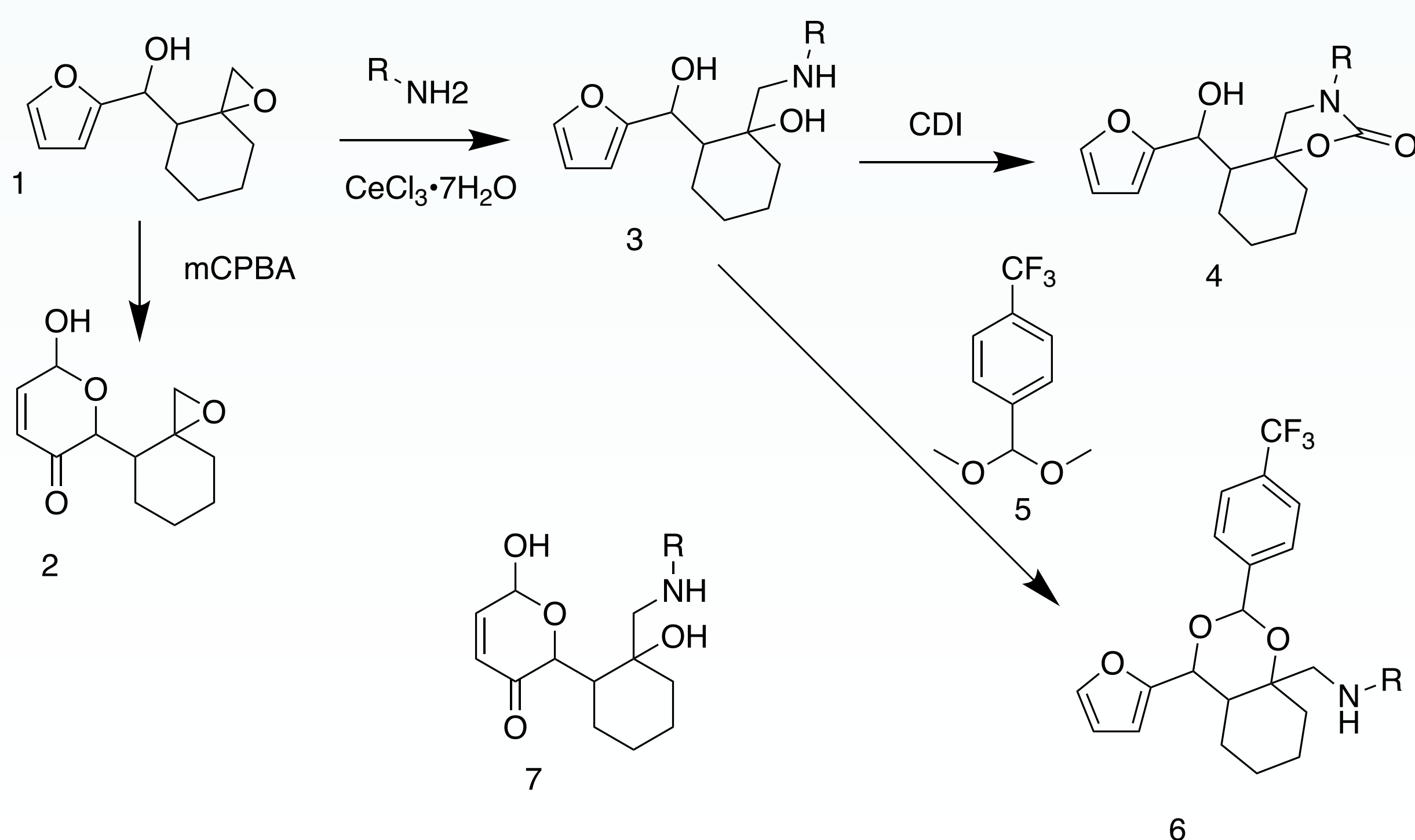


Figure 2: Strategy for the DOS using Furan Epoxide

Table 1 shows the the yield of each product. Product 4 and 7 haven't purified successfully to get a yield.

Table 1: Percentage yield of DOS products

Entry	Structure	Yield (%)
2		60
3		90
4		0
7		<20

2D Spectrum

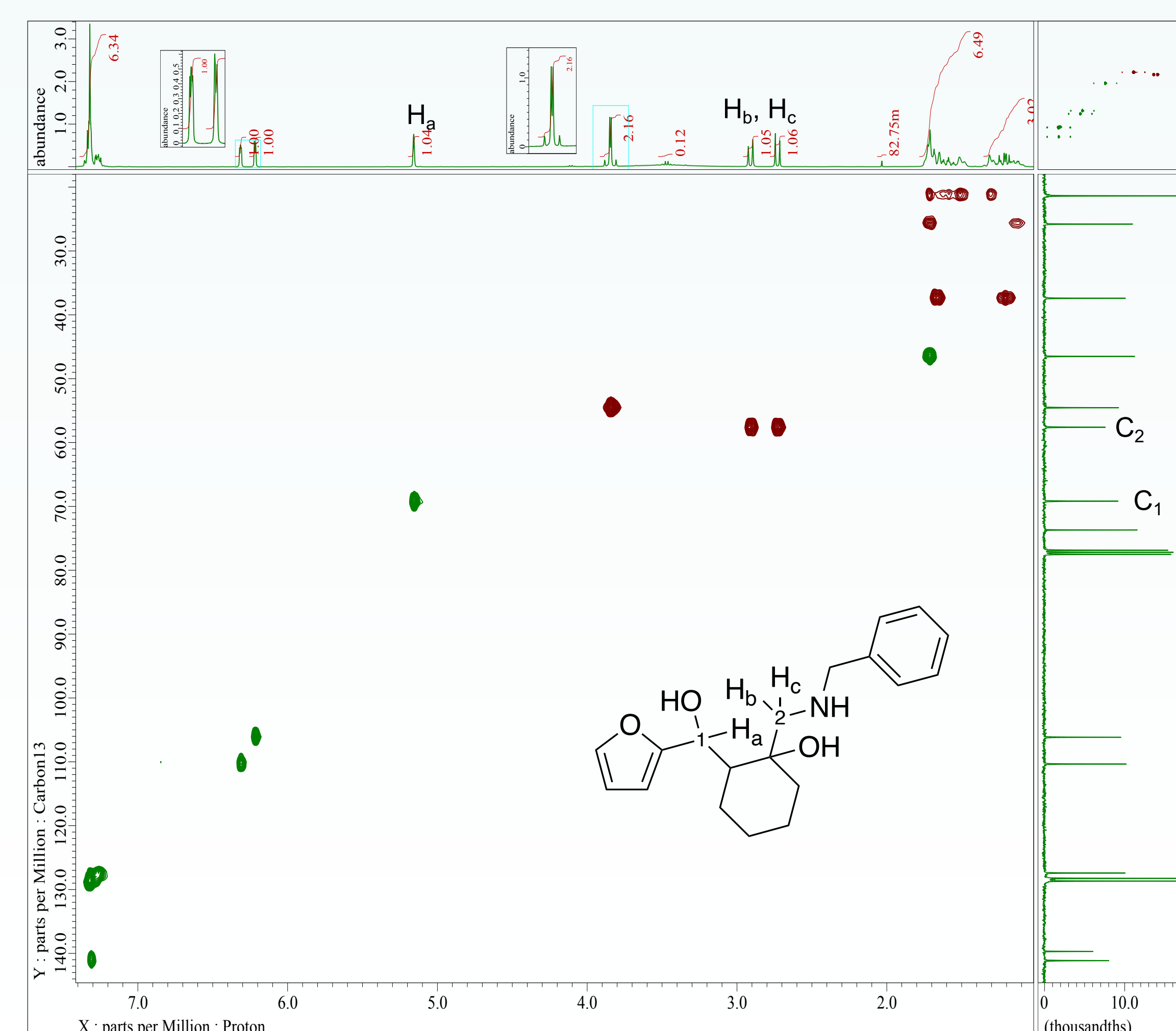


Figure 5: HSQC 2D Spectrum of Compound 3

Acknowledgements

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Reference

Epoxide. Epoxide - an overview | ScienceDirect Topics. (n.d.). Retrieved September 02, 2021, from <https://www.sciencedirect.com/topics/chemistry/epoxide>.
Lepovitz, L. T., & Martin, S. F. (2019). Diversity-Oriented synthesis of Bioactive Azaspirocycles. *Tetrahedron*, 75(47), 130637. <https://doi.org/10.1016/j.tet.2019.130637>