


Greener Synthesis of Substituted 1,2,3-Triazoles: Green Chemistry in the Teaching Laboratory

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The 12 Principles of Green Chemistry

- 1) Preventing waste is better than cleaning it up
- 2) Things in the flask should be in the product
- 3) Lower toxicity
- 4) Keep the molecule's function
- 5) No auxiliaries
- 6) Room Temp, ambient pressure
- 7) Recycle
- 8) No extra steps (protection / deprotection)
- 9) Catalytic is better than stoichiometric
- 10) Biodegradable products
- 11) Analysis in real-time, in-process
- 12) Minimize physical hazards (fires, etc.)

<http://www.chemistry.org/portal/ac/s/1/acsdisplay.html?DOC=greenchemistryinstitute/whatare.html>




How Can You be "Green"?

- No Solvent
- No Catalysts
- Short Reactions
- Simple Clean-ups




Why Use a Microwave?

- Speed
- Efficient heating of smaller samples
- "Microwave Effect"
- High temperatures (in sealed vials)



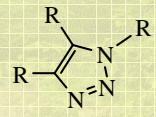
Advanced Organic Lab, Chem 125 . . .

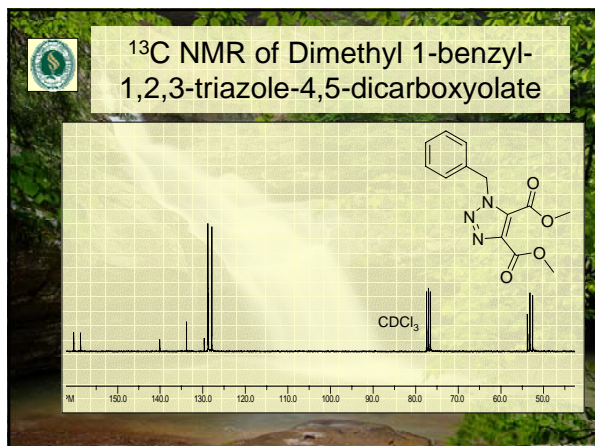
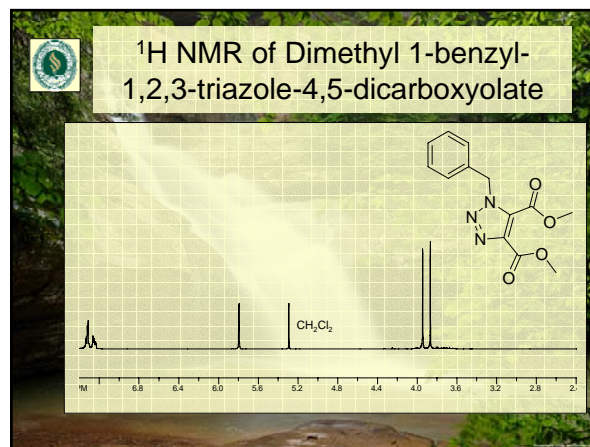
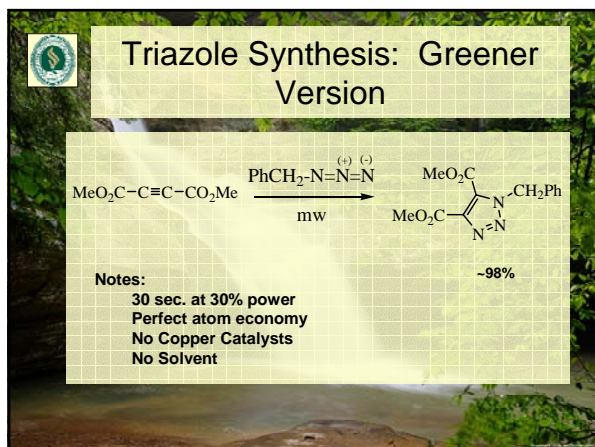
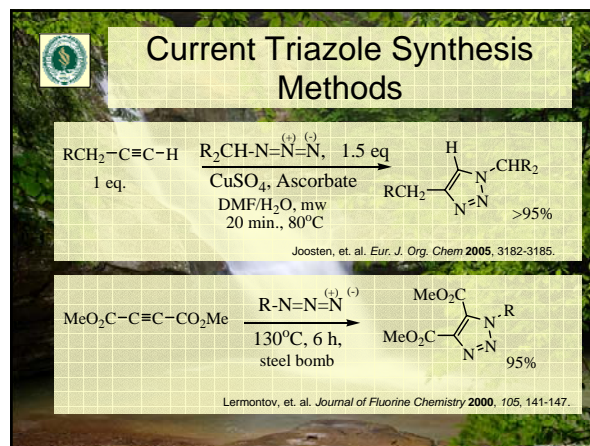
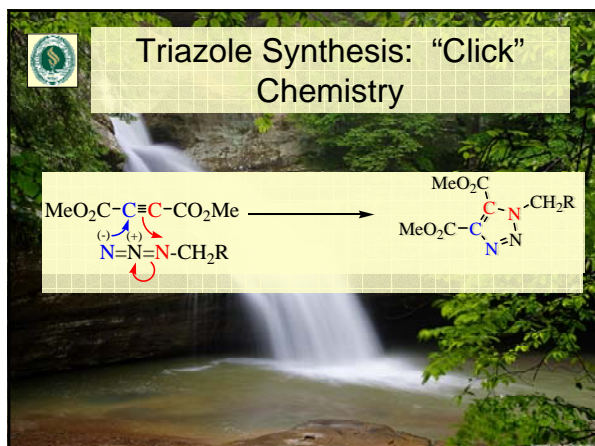
- Upper division Organic Laboratory
- All Chemistry majors (mostly BS, forensics)
- Students know all basic synthetic techniques
- Focus on advanced skills, analysis and spectroscopy

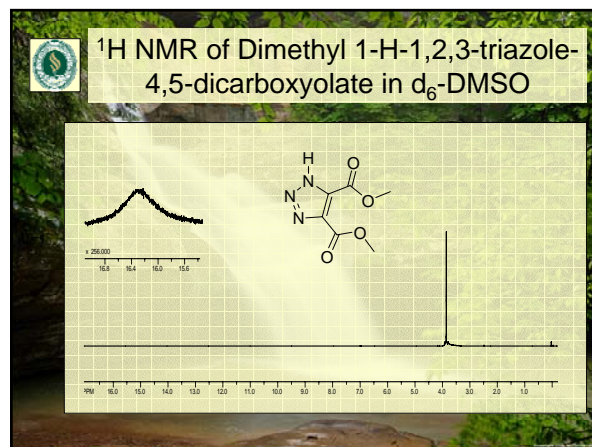
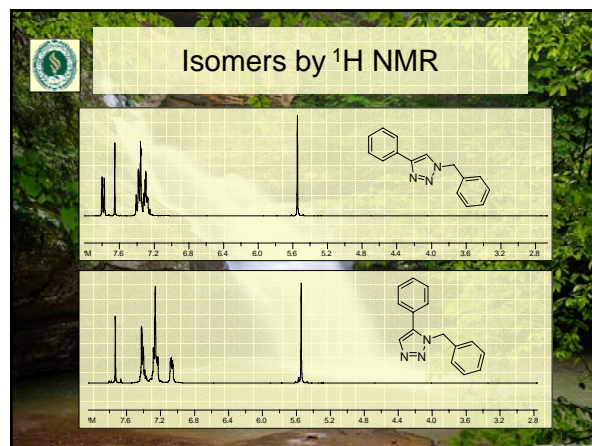
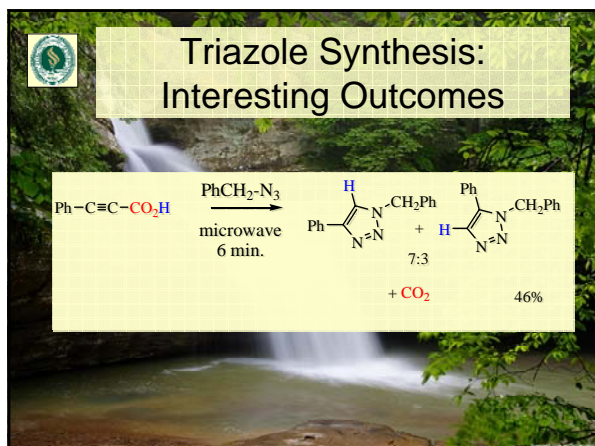


Why Triazoles?

- anti-allergenic
- anti-bacterial
- anti-microbial
- anti-HIV activities
- osteoarthritis
- obesity
- more likely to be water soluble than normal aromatic systems
- stable under biological conditions







More Results

Entry	Azide	Alkyne	Triazole Product(s)	Yield
1	$\text{Ph}-\text{CH}_2-\text{N}_3$	$\text{H}-\text{C}\equiv\text{C}-\text{N}(\text{py})$	$\text{Ph}-\text{C}(\text{H})=\text{N}(\text{N}=\text{N})-\text{CH}_2-\text{N}(\text{py}) + \text{Ph}-\text{C}(\text{H})=\text{N}(\text{N}=\text{N})-\text{CH}_2-\text{N}(\text{py})$	54%
2	$\text{Ph}-\text{CH}_2-\text{N}_3$	$\text{H}-\text{C}\equiv\text{C}-\text{CO}_2\text{H}$	$\text{Ph}-\text{C}(\text{H})=\text{N}(\text{N}=\text{N})-\text{CH}_2-\text{CO}_2\text{H}$	99%
3	$\text{Ph}-\text{CH}_2-\text{N}_3$	$\text{Ph}-\text{C}\equiv\text{C}-\text{Ph}$	$\text{Ph}-\text{C}(\text{H})=\text{N}(\text{N}=\text{N})-\text{CH}_2-\text{Ph}$	97%

- ### Learning Outcomes
- Green Chemistry
 - New Techniques — Small-Scale Microwave Synthesis
 - Old Techniques — Extraction, Recrystallization, Chromatography
 - Analysis — TLC, NMR, GC-MS, IR
 - Presentation skills (posters and lab reports)



Conclusions

- Easy reaction to perform
- Inexpensive glassware and equipment
- Good way to illustrate Atom Economy and Green Chemistry
- Novel outcomes to challenge more advanced students



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