

Synthetic Efforts Towards Extending the Conjugation of Donor Acceptor Stenhouse Adducts

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Funding Sources



Real World Application

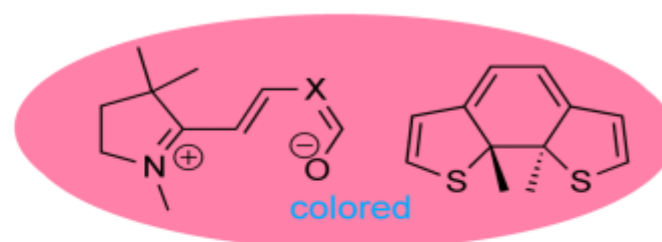
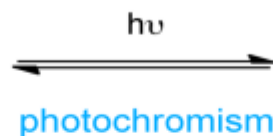
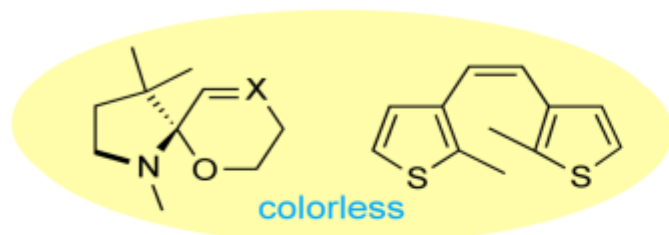


UV Protection

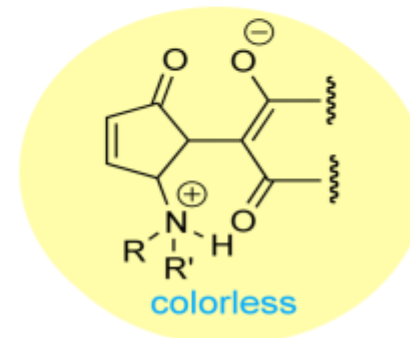
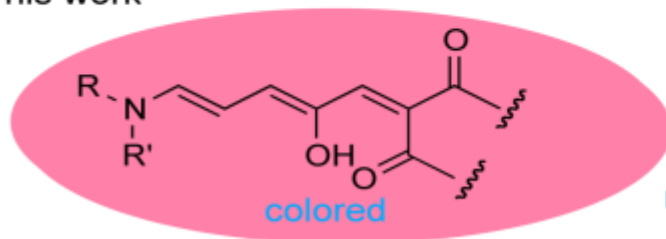


Entertainment

Previous photoswitches



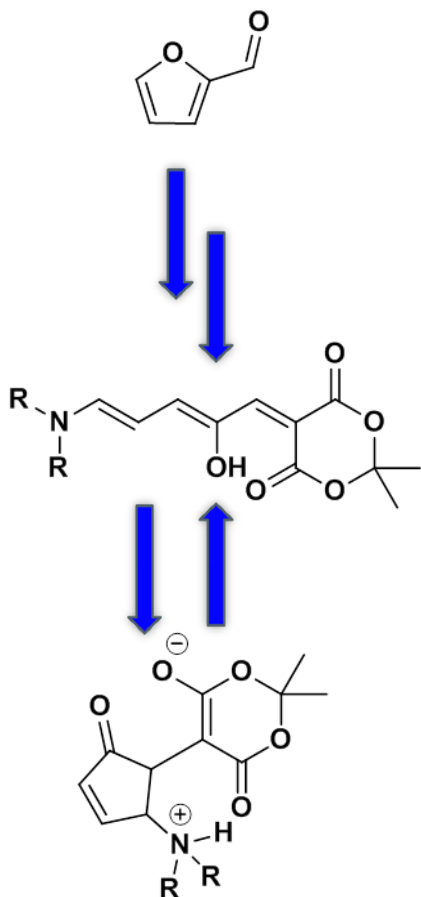
This work



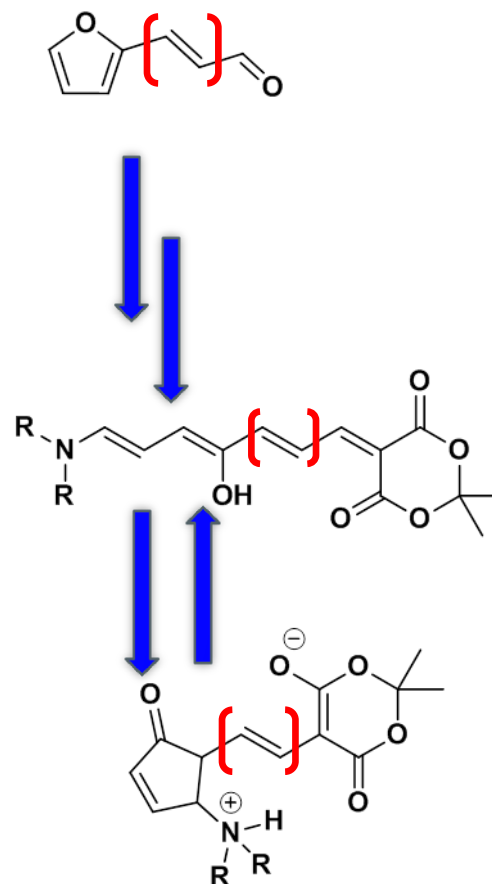
Research Objectives

Stenhouse adducts a *new class* of promising photochrome compounds exhibit unique properties

Past Research



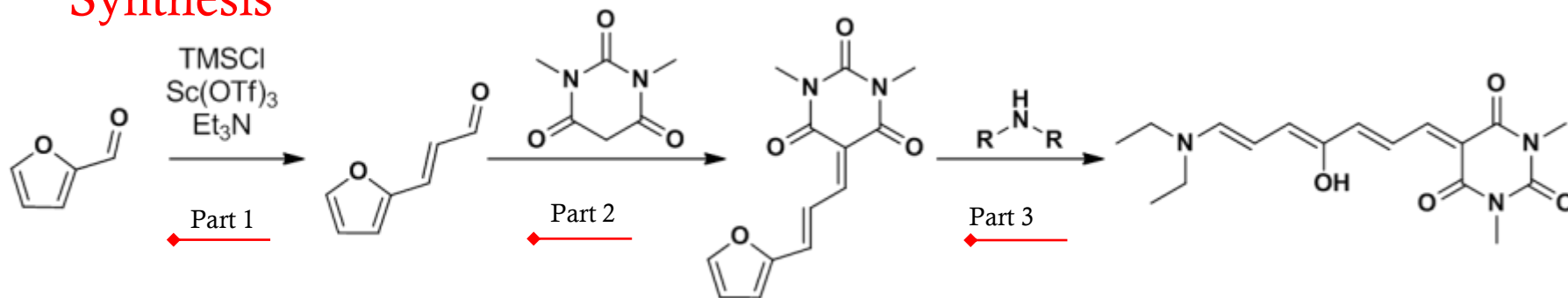
Research of focus



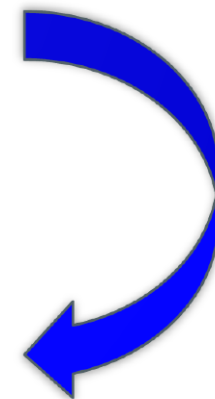
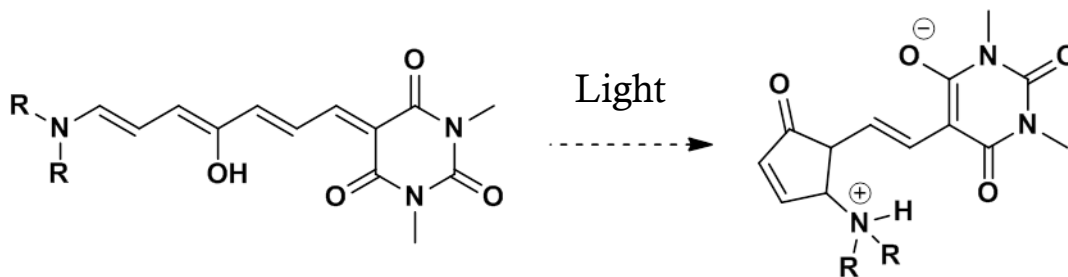
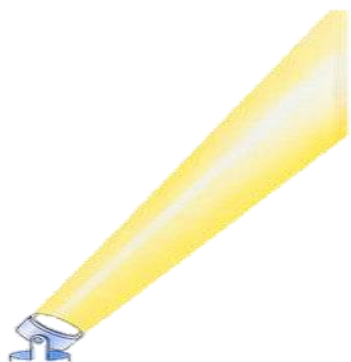
- Color
- Solubility
- Volume

Experimental Methods

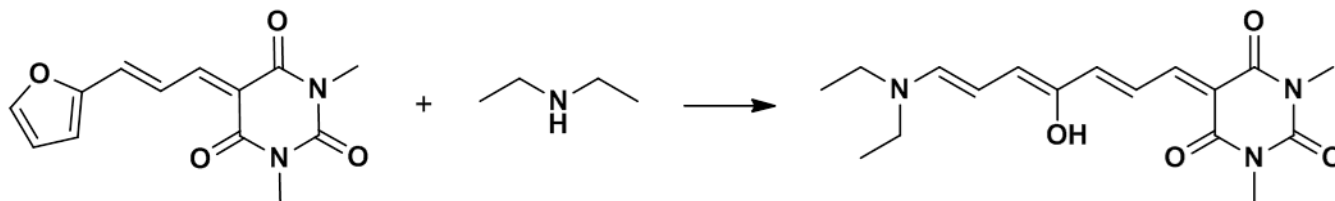
Synthesis



Explore Photo-dynamic Properties



Synthetic Progress



Equivalents	
Substrate	Nucleophile
1	2

Reaction Conditions

Solvent	Temperature	Reaction Time	Yield
THF	RT	15 min	56 % BRSM
	0 °C	3 hrs	
DCM			
EtOAc			
MeCN			
Benzene			
MeOH			
DMSO			
Anisole			
1,2-dichloroethane	RT	5 hrs	minimal product formation,
MeCN	RT	5 hrs	21% BRSM
MeCN	RT	3.5 hrs	9.40%
MeCN(dry)	RT	2.5 hrs	Minimal product formation
THF(dry)	60 °C	4 hrs	12.5%

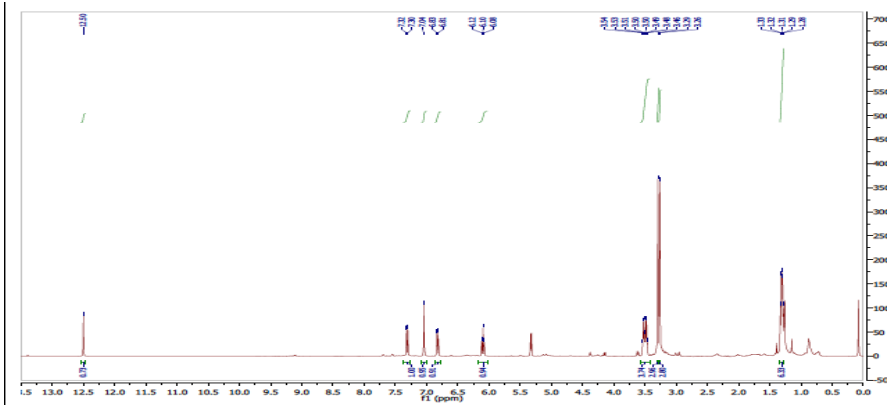
Optimal Reaction Conditions

Solvent	Temperature	Reaction Time
Anhydrous THF	60 °C	4 hrs.

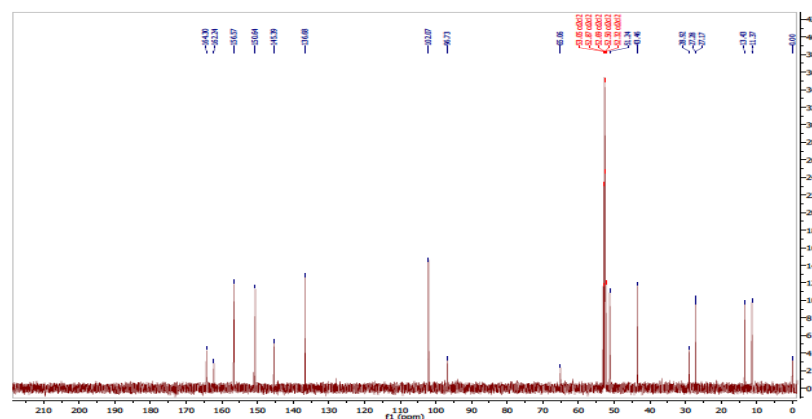


NMR Sample of Isolated Product

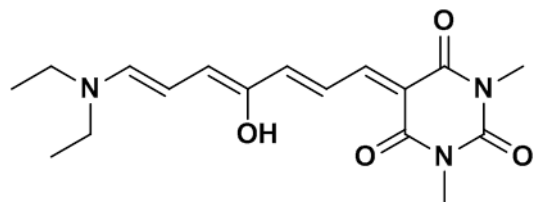
Instrumental Data



Proton NMR of isolated product



Carbon NMR of isolated product



Expected structure of isolated product

NMR

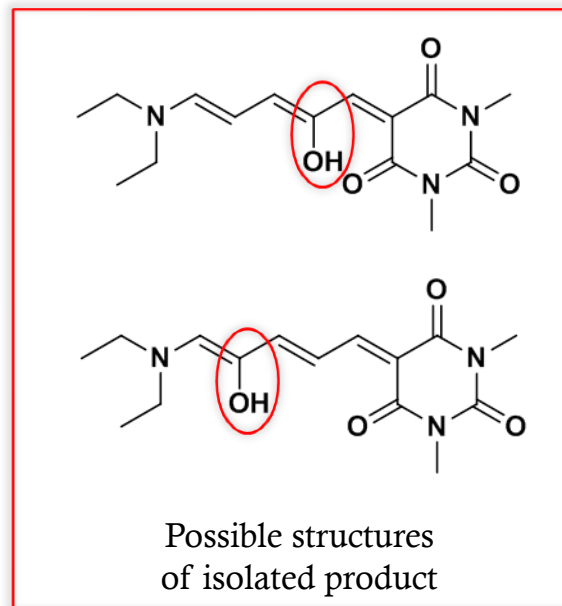
Expected: 10 ¹H, 17 ¹³C

Found: 8 ¹H, 15 ¹³C

Mass

Expected: 333.1689

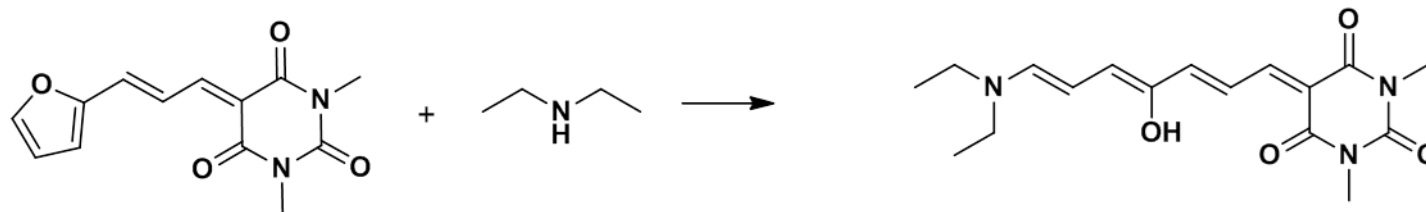
Found: 307.1532



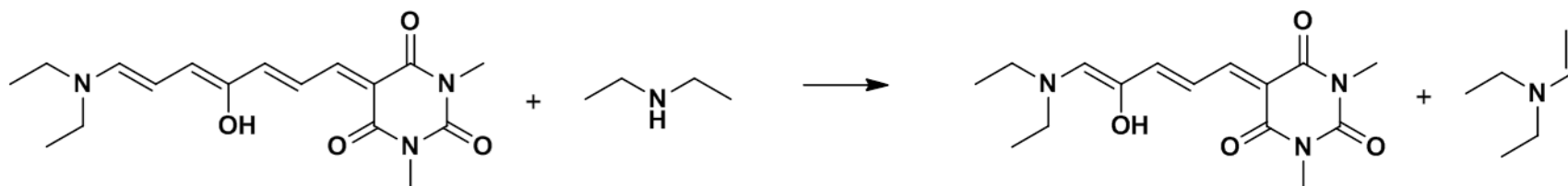
Possible structures of isolated product

Mechanistic Hypothesis

Ring Opening

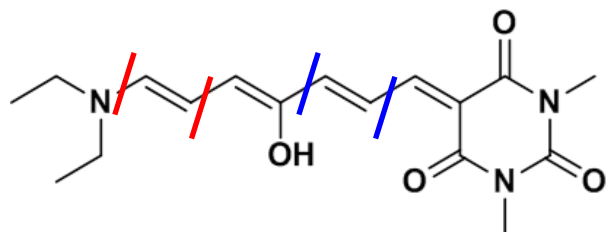


Retro Aldol

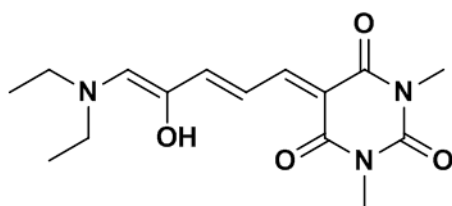


Matches Spectropic Data

Future Work

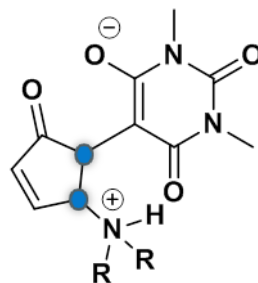
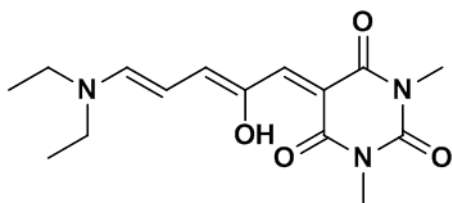


Expected Product



Structure supported by
mechanism/characterization

X-Ray-Crystallography of cyclized form
will confirm true structure of isolated
product



Structure supported by
characterization only

The opposite regio-chemistry may provide new synthetic possibilities

Acknowledgements

Read Group:

Dr. Javier Read de Alaniz

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Charles Frazier

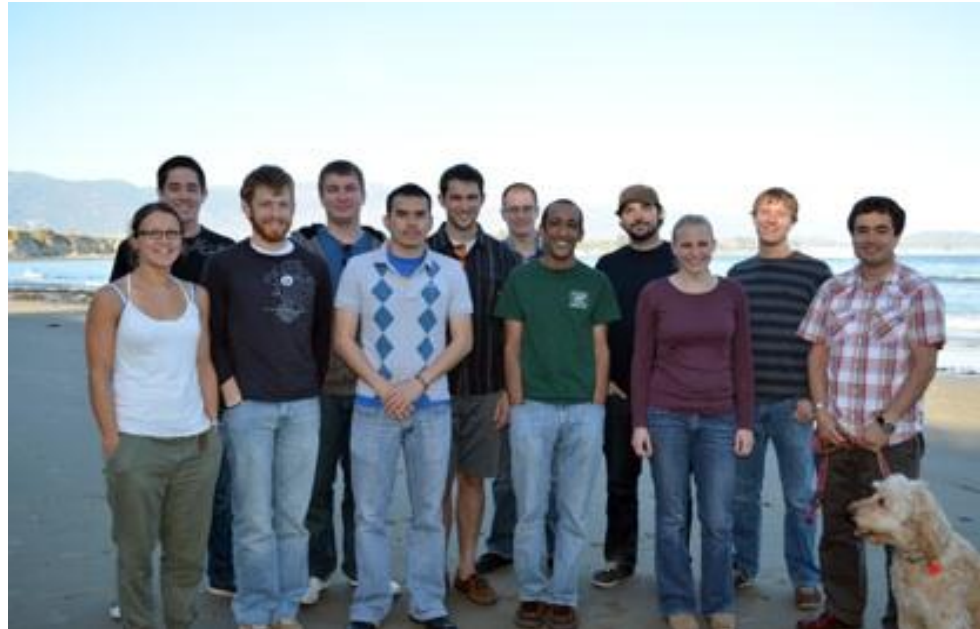
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