

Designing a Photoredox Approach to Target Identification Using an Intramolecular Substrate

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VBRN Career Day

Middlebury College

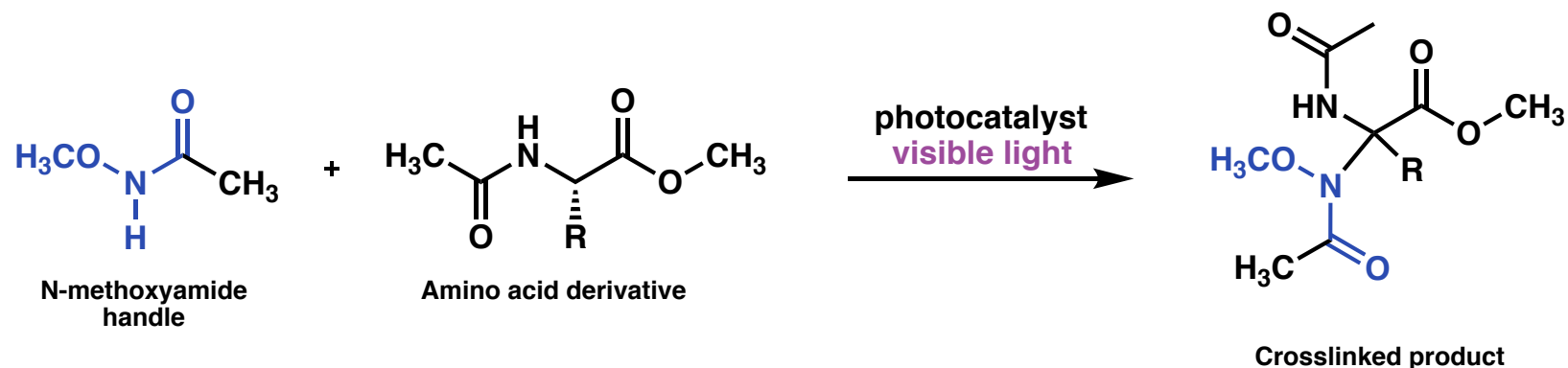
April, 2021

Our Small Molecule Approach

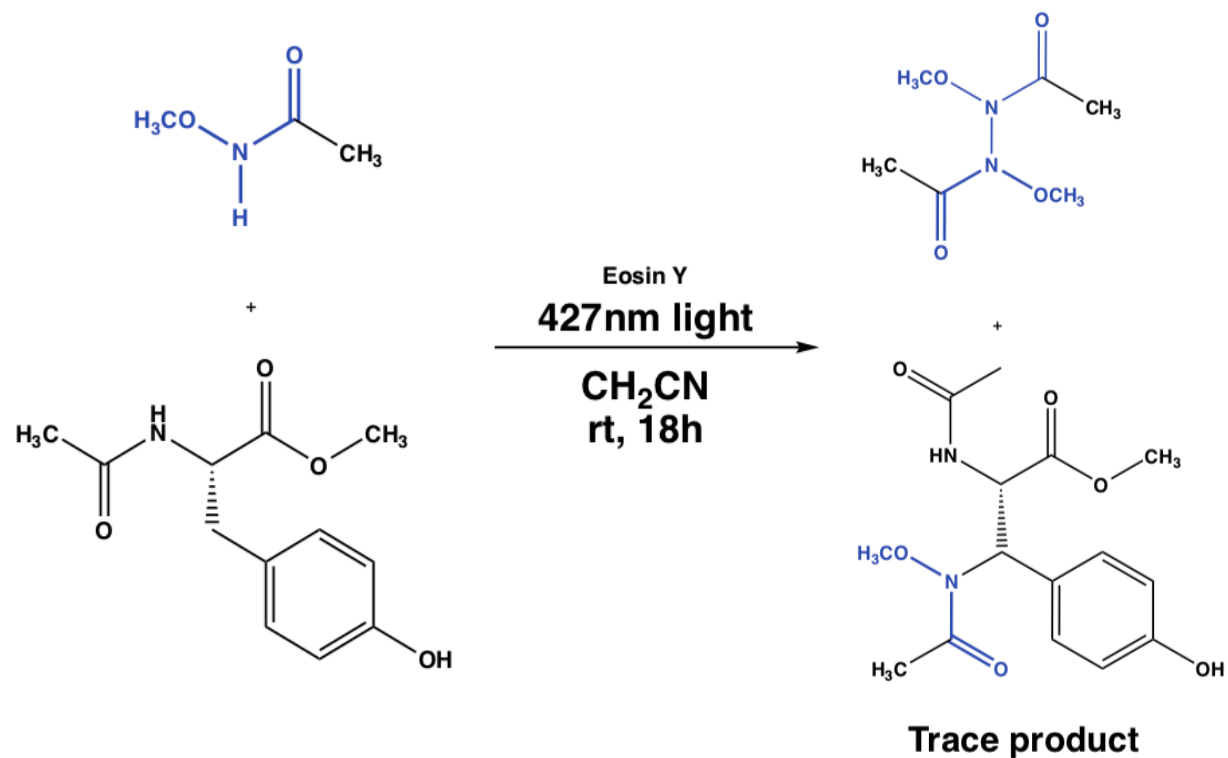
Existing Approach:



Our Approach:

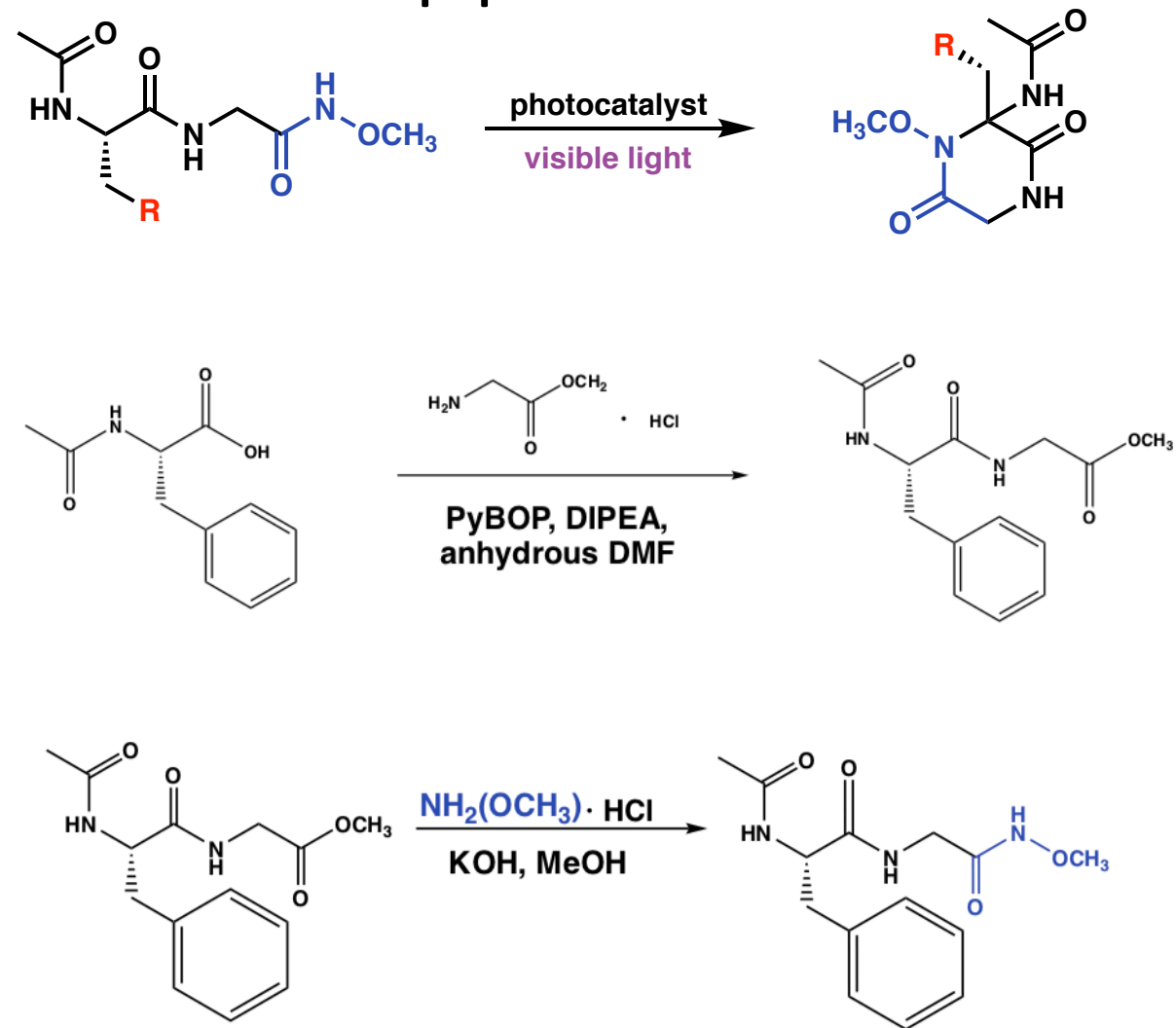


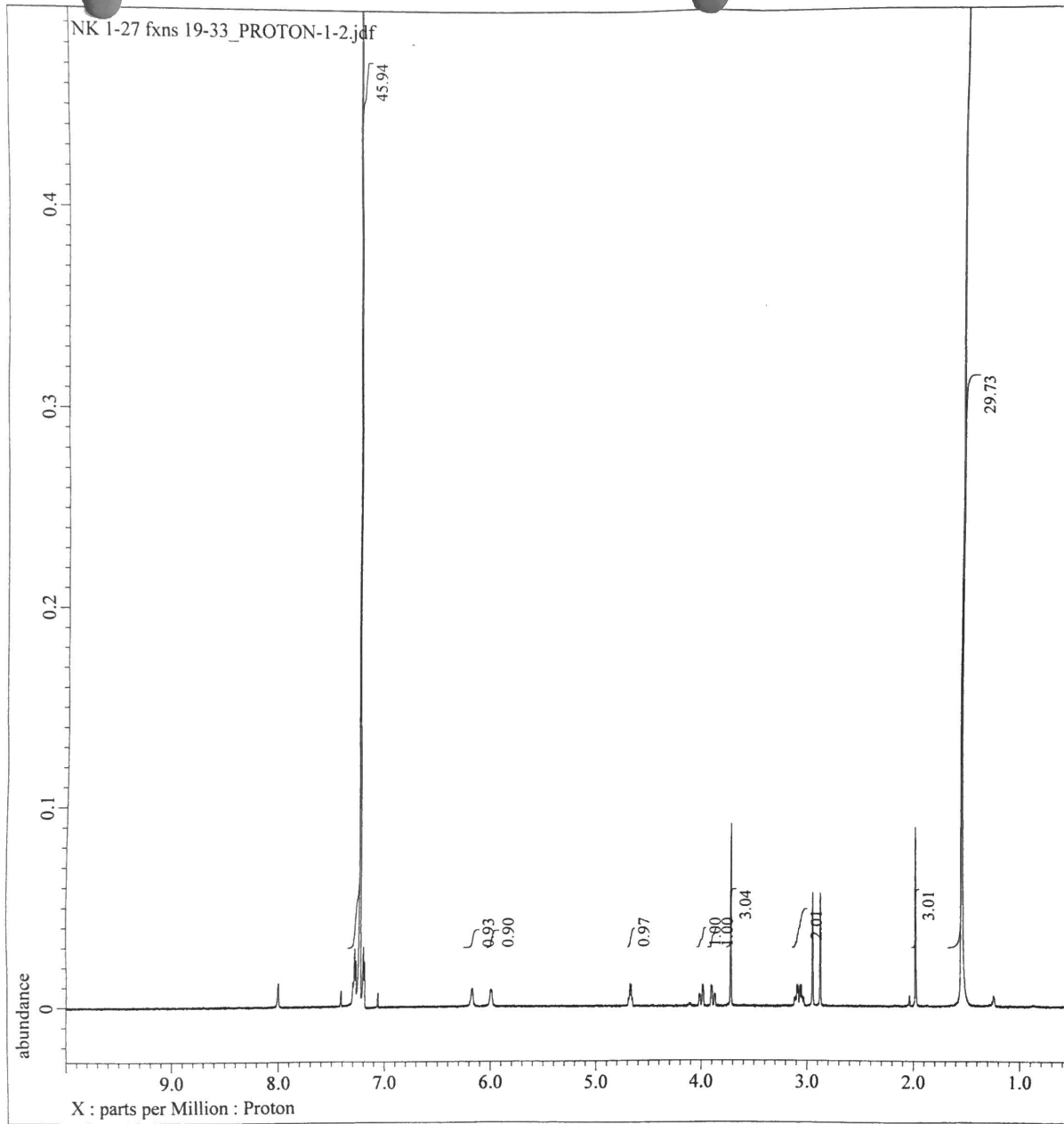
Dimerization



How do we increase product?

Intramolecular Approach





---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm

Derived from: NK 1-27 fxns 19-33_PROTON-1-1

Filename = NK 1-27 fxns 19-33_
 Author = Lindsay
 Experiment = proton.jxp
 Sample_Id = NK 1-27 fxns 19-33
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 1-OCT-2020 16:09:2
 Revision_Time = 1-OCT-2020 16:24:0

Data_Format = 1D COMPLEX
 Dim_Size = 26214
 X_Domain = Proton
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Site = Middlebury ECZ600R
 Spectrometer = JNM-ECZ600R/S1

Field_Strength = 14.09636928 [T] (600
 X_Acq_Duration = 2.90455552 [s]
 X_Domain = Proton
 X_Freq = 600.1723046 [MHz]
 X_Offset = 5 [ppm]
 X_Points = 32768
 X_Prescans = 0
 X_Resolution = 0.34428676 [Hz]
 X_Sweep = 11.28158845 [kHz]
 X_Sweep_Clippped = 9.02527076 [kHz]
 Irr_Domain = Proton
 Irr_Freq = 600.1723046 [MHz]
 Irr_Offset = 5 [ppm]
 Tri_Domain = Proton
 Tri_Freq = 600.1723046 [MHz]
 Tri_Offset = 5 [ppm]
 Blanking = 2 [us]
 Clipped = FALSE
 Scans = 32
 Total_Scans = 32

Relaxation_Delay = 4 [s]
 Recvr_Gain = 72
 Temp_Get = 21.6 [dC]
 X_90_Width = 8.96 [us]
 X_Acq_Time = 2.90455552 [s]
 X_Angle = 45 [deg]
 X_Atn = 9.9 [dB]
 X_Pulse = 4.48 [us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Loop = 400

Acknowledgements

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- Jody Smith, Lance Ritchie, and Caitlin Carr