SUPPORTING INFORMATION

Iodine-Catalyzed Functionalization of Primary Aliphatic Amines to Oxazoles, 1,4-Oxazines, and Oxazinones

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Figure S3. ¹H and ¹³C NMR of 4c



Figure S4. ¹H and ¹³C NMR of 4d







Figure S6. ¹H and ¹³C NMR of 4f



Figure S7. ¹H and ¹³C NMR of 4g







Figure S9. ¹H and ¹³C NMR of 4i





Figure S11. ¹H and ¹³C NMR of 4k













Figure S15. ¹H and ¹³C NMR of 40







Figure S17. ¹H and ¹³C NMR of 4r







Figure S20. ¹H and ¹³C NMR of 6b



Figure S21. ¹H and ¹³C NMR of 6c



Figure S22. ¹H and ¹³C NMR of 6d



Figure S23. ¹H and ¹³C NMR of 6e





Figure S25. ¹H and ¹³C NMR of 6g



Figure S26. ¹H and ¹³C NMR of 6h



Figure S27. ¹H and ¹³C NMR of 6i



200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



Figure S29. ¹H and ¹³C NMR of 8b





X-ray diffraction data of 4j(CCDC 1551936)





Figure S31. Thermal ellipsoid plot of 4j with ellipsoids at 50% of probability.

Table S1.Crystal data and structure refinement for 4j

Bond precision:	C-C = 0.0067 A	Wavelength=0.71073	
Cell:	a=12.216(4)	b=5.1110(17)	c=21.371(8)
	alpha=90	beta=96.953(7)	gamma=90
Temperature:	296 K		
	Calculated	Reported	1
Volume	1324.5(8)	1324.5(8	3)
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C18 H15 N O	C18 H15	N O
Sum formula	C18 H15 N O	C18 H15	N O
Mr	261.31	261.32	
Dx,g cm-3	1.310	1.321	
Z	4	4	
Mu (mm-1)	0.081	0.083	
F000	552.0	588.0	
F000'	552.22		
h,k,lmax	14,6,25	11,4,20	
Nref	2409	1220	
Tmin, Tmax	0.934,0.960	0.945,0.	970
Tmin'	0.930		
Correction meth AbsCorr = MULTI	od= # Reported T -SCAN	Limits: Tmin=0.945	Tmax=0.970
Data completeness= 0.506		Theta(max) = 25.296	
R(reflections)=	0.0603(1043)	wR2(reflections)	= 0.1421(1220)
S = 1.113	Npar=	184	

X-ray diffraction data of 6a (CCDC 1551938)





Figure S32. Thermal ellipsoid plot of 6a with ellipsoids at 50% of probability.

Table S2.Crystal data and structure refinement for 6a

Bond precision:	C-C = 0.0051 A	Wavelength=0.71073	
Cell:	a=21.664(10)	b=5.207(2)	c=27.742(13)
	alpha=90	beta=106.51(2)	gamma=90
Temperature:	296 K		2 - 19-19-19-19-19-19-19-19-19-19-19-19-19-1
	Calculated	Reported	
Volume	3000(2)	3000(2)	
Space group	C 2/C	C 2/C	
Hall group	-C 2VC	-C 27C	
Moioty formula	C22 U15 N 0	C22 H15 N	I O
Sum formula	C22 H15 N 0	C22 H15 I	IO
Mr	200 25	200 26	
Dy a am 2	1 270	1 272	
DX, g CIII-3	1.370	1.373	
A Mar (mm 1)	8	8	
Mu (mm-1)	0.084	0.084	
FOOD	1296.0	1304.0	
F.000	1296.52		
h, k, 1max	26,6,33	23,5,29	
Nrei	2742	1720	
Tmin, Tmax	0.934,0.960	0.945,0.9	970
Tmin'	0.930		
Correction meth AbsCorr = MULTI	od= # Reported T 1 -SCAN	Limits: Tmin=0.945	Tmax=0.970
Data completene	aa 0 627	Thata (max) 25.2	10
Data completene	55= 0.021	11100a(max) = 25.34	to
R(reflections) =	0.0482(936)	wR2(reflections):	= 0.1270(1720)
S = 0.973 Npar= 218			

Crystal structure experimental protocol:

Single crystal of compound **4j** and **6a** were mounted on a Bruker-AXS SMART APEX II diffractometer equipped with a graphite monochromator and Mo K α ($\lambda = 0.71073$ Å) radiation. The crystal was placed 60 mm from the CCD, and frames (360) were measured with a counting time of 5s. The structures were solved using the Patterson method using the SHELXS 97 program. Non-hydrogen atoms were refined with independent anisotropic displacement parameters, while difference Fourier synthesis and least-squares refinement showed the positions of any remaining non-hydrogen atoms. The non-hydrogen atoms were refined with anisotropic thermal parameters. Successful convergence was indicated by the maximum shift/error of 0.001 for the last cycle of the least-squares refinement. All other crystallographic details such as h, k, l ranges, 20 ranges, and R-factors can be found above (Table S1 and S2).

Section III: Mass spectra data

Mass spectra were taken in infusion method.

Parameters

Source - capillary (kv): 3.06, Sampling cone: 85, source offset: 80

Temp(°C) - Source: 120, Desolvation: 300

Gas flows- Cone gas (L/h) 50, Desolvation gas (L/h) 600, Lock spray capillary (kv) 2.50

ESI-MS Study of the ongoing reaction

Herein, we have also carried out the HRMS study of the two reaction mixtures separately. In all cases a certain amount of aliquot was withdrawn from the reaction mixture which was subjected to mass analysis. The following spectra are the spectra of intermediates (IA-B and IIIA-B) and each of the spectrum is followed by their simulated pattern.





Figure S34. ESI-MS spectra of IB









Figure S36. ESI-MS spectra of IIIB

