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### Supplementary Information for

# Late-Stage Diversification of Biologically Active Pyridazinones via Direct C-H Functionalization Strategy

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#### 1. Copies of NMR Data for All Compounds.

<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3a.** 

# 



1.18 1.17 1.15  $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3b.** 

7.71 7.75 7.75 7.75 7.48 7.48 7.48 7.48 7.48 7.38 7.38 7.33 7.33 7.33 7.33 7.33



4.43 4.44 4.39 4.38 1.19 1.17 1.15

-2.31

 $^{1}$ H and  $^{13}$ C NMR spectra of compound **3c.** 



1.22 1.18 <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3c'**.

# 7.56 7.55 7.55 7.55 7.56 7.72 8.80 8.90 6.91 6.95 6.96 6.96 6.97 6.96 6.97 6.98 6.99 6.99 6.90 6.90 6.91 </tr





 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3d'.** 



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3e.** 

4.43 4.41 4.37 -3.91 **1.20 1.18 1.16** 

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 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3f.** 



121 119 1.19  $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3g.** 



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3h.** 

 123 121 121



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3i.** 



1.20 1.18 1.16  $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3j.** 



-1.66



 $^{1}$ H and  $^{13}$ C NMR spectra of compound **3k**.







 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **31.** 





<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3m**.

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**1.18 1.18 1.18** 



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3n.** 





 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **30.** 

-7.70 -7.33 -7.23 -7.24 -7.23 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 -7.24 1.18 1.16 1.14

4.36



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3p**.



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **3q.** 



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **3r.** 



-2.42



f1 (ppm)  $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **5a.** 





<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **5b.** 



4.49 4.47 4.45 129 124



S24

<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **5c.** 



**1.35 1.35 1.30** 



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **5d.** 

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 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 5e.

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 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound **5f.** 



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 7a.

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 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 7b.

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√1.42 √1.39 √1.37  $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 7c.

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 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 8.

-7.73 -7.35 -7.35 -7.35 -7.33 -7.33 -7.33 -7.33 -7.33 -7.33 -7.33 -7.33 -7.33 -7.33 -7.33 -7.33 -7.35 -7.33 -7.35 -7.25 -7.55



4.68 4.68 4.66 1.41 1.39 1.36



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 9.



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 10.

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1.44 1.41 1.39



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **11**.



1.37 1.35 1.35  $^{1}\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **12**.





 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 14a.





<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **14b.** 

7.85 7.46 7.45 7.45 7.45 7.45 7.45 7.45 7.45 7.33 7.33 7.33 7.33 7.33 7.33 7.33 7.3	7.12 7.12 7.109 6.91 6.92 6.92 6.92 6.92 6.92 7.09 6.92 6.93 6.92 6.93
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1.14 1.12 1.09



 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 14c.

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 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 14d.



1.30 1.28 1.26 <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound **14e.** 





 $^1\mathrm{H}$  and  $^{13}\mathrm{C}$  NMR spectra of compound 14f.



**1.37 1.35 1.35 1.33** 



#### 2. X-ray Data of Compound 12.



**Table 1** Crystal data and structure refinement details for compound 12.

Identification code	2014283		
Chemical formula	$C_{39}H_{26}Cl_2N_2O$		
Formula weight	609.52		
Temperature	296(2) K		
Wavelength	0.71073 Å		
Crystal size	0.200 x 0.300 x 0.700 mm		
Crystal system	orthorhombic		
Space group	P 21 21 21		
Unit cell dimensions	a = 7.1928(3) Å	$\alpha = 90^{\circ}$	
	b = 13.3215(6) Å	$\beta = 90^{\circ}$	
	c = 32.7007(16)  Å	$\gamma = 90^{\circ}$	
Volume	3133.3(2) Å <sup>3</sup>		
Z	4		
Density (calculated)	1.292 Mg/cm <sup>3</sup>		
Absorption coefficient	0.242 mm <sup>-1</sup>		
F(000)	1264		
Theta range for data collection	1.65 to 27.65°		
Index ranges	-9<=h<=8, -17<=k<=16, -33<=l<=42		
Reflections collected	16279		
Independent reflections	7109 [R(int) = 0.0221]		
Coverage of independent reflections	99.6%		
Absorption correction	multi-scan		
Max. and min. transmission	0.9522 and 0.8459		
Structure solution technique	direct methods		

Structure solution program	SHELXS-97 (Sheldrick, 2008)		
Refinement method	Full-matrix least-squares on F <sup>2</sup>		
Refinement program	SHELXL-97 (Sheldrick, 2008)		
Function minimized	$\Sigma \mathrm{w}(\mathrm{F_o}^2 - \mathrm{F_c}^2)^2$		
Data / restraints / parameters	7109 / 0 / 399		
Goodness-of-fit on F <sup>2</sup>	1.023		
Final R indices	5579 data; I>2σ(I)	R1 = 0.0596, $wR2 = 0.1151$	
	all data	R1 = 0.0418, $wR2 = 0.1051$	
Weighting scheme	w=1/[ $\sigma^2(F_o^2)$ +(0.0600P) <sup>2</sup> +0.2800P] where P=( $F_o^2$ +2 $F_c^2$ )/3		
Extinction coefficient	0.0018(6)		
Largest diff. peak and hole	0.242 and -0.221 eÅ <sup>-3</sup>		
R.M.S. deviation from mean	0.037 eÅ <sup>-3</sup>		
CCDC	1023268		