# **Supplementary Information**

Design and Synthesis of Imidazo/benzimidazo[1,2-*c*]quinazoline Derivatives and Evaluation of their Antimicrobial Activity

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- 1. Figure S1 S36: Copies of <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of 8aa-gd.
- 2. Figure S37 S54: Copies of HRMS data of 8aa-gd.
- 3. Figure S55 S72: HPLC Purity profile of 8aa-gd.





Figure S2. <sup>13</sup>C NMR spectrum of compound 8aa in CDCl<sub>3</sub>

80 70 f1 (ppm)

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145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 f1 (ppm) Figure S4. <sup>13</sup>C NMR spectrum of compound 8ab in CDCl<sub>3</sub>



Figure S6. <sup>13</sup>C NMR spectrum of compound 8ac in CDCl<sub>3</sub>



















Figure S16. <sup>13</sup>C NMR spectrum of compound 8cf in CDCl<sub>3</sub>



Figure S17. <sup>1</sup>H NMR spectrum of compound 8df in CDCl<sub>3</sub>



Figure S18. <sup>13</sup>C NMR spectrum of compound 8df in CDCl<sub>3</sub>









Figure S21. <sup>1</sup>H NMR spectrum of compound 8eg in CDCl<sub>3</sub>



Figure S22. <sup>13</sup>C NMR spectrum of compound 8eg in CDCl<sub>3</sub>



Figure S24. <sup>13</sup>C NMR spectrum of compound 8fb in CDCl<sub>3</sub>



Figure S26. <sup>13</sup>C NMR spectrum of compound 8gf in CDCl<sub>3</sub>



Figure S28. <sup>13</sup>C NMR spectrum of compound 8ga in CDCl<sub>3</sub>



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Figure S32. <sup>13</sup>C NMR spectrum of compound 8gc in CDCl<sub>3</sub>



Figure S34. <sup>13</sup>C NMR spectrum of compound 8gi in CDCl<sub>3</sub>



Figure S36. <sup>13</sup>C NMR spectrum of compound 8gd in CDCl<sub>3</sub>















Figure S40. ESI-HRMS spectrum of 8ad



Figure S41. ESI-HRMS spectrum of 8ae



















Figure S46. ESI-HRMS spectrum of 8ef















Figure S50. ESI-HRMS spectrum of 8ga



Figure S51. ESI-HRMS spectrum of 8gh







Figure S53. ESI-HRMS spectrum of 8gi









	Processed Channel Descr.	RT	Area	% Area	Height		
1	PDA 270.0 nm	4.032	198024	99.26	47411		
2	PDA 270.0 nm	4.192	1483	0.74	497		

Figure S55. HPLC analysis report of compound 8aa.

	SAMPLE	INFORMATIC	D N	
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 662A Unknow n 1 12 20.00 ul 20.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 662 270.0nm PDA 270.0 nm	
Date Acquired: Date Processed:	8/9/2018 12:37:46 PM IST 8/9/2018 12:53:26 PM IST			



	1111						
	Processed Channel Descr.	RT	Area	% Area	Height		
1	PDA 270.0 nm	7.669	711319	99.44	36024		
2	PDA 270.0 nm	8.846	3971	0.56	428		

Figure S56. HPLC analysis report of compound 8ab.

	SAMPLE	INFORMATIC	) N
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 641 Unknow n 1 19 20.00 ul 20.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 641 270.0nm PDA 270.0 nm
Date Acquired: Date Processed:	8/7/2018 3:53:59 PM IST 8/8/2018 6:42:23 PM IST		



Processed Channel D	Descr.: PDA 270.0
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nm						
	Processed Channel Descr.	RT	Area	% Area	Height	
1	PDA 270.0 nm	3.638	6987	1.06	1141	
2	PDA 270.0 nm	7.215	2888	0.44	418	
3	PDA 270.0 nm	7.902	650965	98.51	77050	

Figure S57. HPLC analysis report of compound 8ac.

	SAMPLE	INFORMATIC	N	
Sample Name: Sample Type: Vial: Injection #: Injection Volume:	NN 652 Unknow n 1 39 20.00 ul	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name:	System amol NN 648 F 270.0nm	
Run Time: Date Acquired: Date Processed:	12.0 Minutes 8/14/2018 8:54:46 PM IST 8/14/2018 9:14:55 PM IST	Proc. Chnl. Descr.:	PDA 270.0 nm	



	nm							
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 270.0 nm	2.606	1404172	99.53	72852			
2	PDA 270.0 nm	8.416	6674	0.47	824			

Figure S58. HPLC analysis report of compound 8ad.

	SAMPLE	INFORMATIC	N	
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 674 C Unknow n 1 38 20.00 ul 12.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 652 FINAL 270.0nm PDA 270.0 nm	
Date Acquired: Date Processed:	8/14/2018 8:37:35 PM IST 8/14/2018 8:52:19 PM IST			



Channel: 2998; Processed Channel: PDA 270.0 nm; Result Id: 3879; Processing Method: NN 652 FINAL

Processed	Channel	Descr.:	PDA 27	0.0
	10.10			

_	1101							
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 270.0 nm	3.773	1145744	98.75	62113			
2	PDA 270.0 nm	6.920	8221	0.71	1080			
3	PDA 270.0 nm	8.523	6310	0.54	812			

Figure S59. HPLC analysis report of compound 8ae





Processed	Channel	Descr · PDA 270.0
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	nm							
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 270.0 nm	4.310	11046	2.96	1344			
2	PDA 270.0 nm	5.035	361883	97.04	64561			

Figure S60. HPLC analysis report of compound 8bf

	SAMPLE	INFORMATIC	) N
Sample Name: Sample Type: Vial: Injection #: Injection Volume:	NN 673 Unknow n 1 24 20.00 ul	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name:	System amol NN 673 270.2nm
Run Time: Date Acquired: Date Processed:	20.0 Minutes 8/14/2018 5:59:32 PM IST 8/14/2018 6:22:28 PM IST	Proc. Chnl. Descr.:	PDA 270.2 nm



Processed	Channel	Descr.:	PDA 270.2
	0.00		

11111						
	Processed Channel Descr.	RT	Area	% Area	Height	
1	PDA 270.2 nm	6.185	50281	1.92	3756	
2	PDA 270.2 nm	9.162	2565644	98.08	113341	

Figure S61. HPLC analysis report of compound 8bb





Processed Channel Des	scr.: PDA 270.	.0
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	nm						
	Processed Channel Descr.	RT	Area	% Area	Height		
1	PDA 270.0 nm	3.849	205055	96.41	44693		
2	PDA 270.0 nm	4.229	7641	3.59	1405		

Figure S62. HPLC analysis report of compound 8cf

	SAMPLE	INFORMATIC	N	
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 565D Unknow n 1 19 20.00 ul 20.00 ul	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 565 270.0nm PDA 270.0 nm	
Date Acquired: Date Processed:	8/14/2018 1:42:23 PM IST 8/14/2018 1:57:53 PM IST			



- Channel: 2998; Processed Channel: PDA 270.0 nm; Result ld: 3799; Processing Method: NN 565

Processed Char	nnel Descr.:	PDA 270.0
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nm					
	Processed Channel Descr.	RT	Area	% Area	Height
1	PDA 270.0 nm	6.077	4036	2.20	604
2	PDA 270.0 nm	7.922	179809	97.80	17825

Figure S63. HPLC analysis report of compound 8df

	SAMPLE	INFORMATIC	) N
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 642 Unknow n 1 23 20.00 ul 10.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 642 270.0nm PDA 270.0 nm
Date Acquired: Date Processed:	8/7/2018 4:37:19 PM IST 8/8/2018 6:38:21 PM IST		



— Channel: 2998; Processed Channel: PDA 270.0 nm; Result ld: 3453; Processing Method: NN 642

Processed	Channel	Descr.:	PDA 270.0
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nm								
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 270.0 nm	5.019	6531	1.12	1081			
2	PDA 270.0 nm	5. <mark>60</mark> 7	57 <mark>418</mark> 6	98.88	92758			

Figure S64. HPLC analysis report of compound 8ef

	SAMPLE	INFORMATIC	N	
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN211 100 FINAL Unknow n 1 6 20.00 ul 10.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 211 270.0nm PDA 270.0 nm	
Date Acquired: Date Processed:	8/7/2018 11:35:11 AM IST 8/9/2018 11:02:53 AM IST			



Processed Channel Descr.: PDA 270.0

_	nm							
		Processed Channel Descr.	RT	Area	% Area	Height		
	1	PDA 270.0 nm	4.639	2442	0.44	293		
2	2	PDA 270.0 nm	5.220	553022	99.56	95328		

Figure S65. HPLC analysis report of compound 8eg

	SAMPLE	INFORMATIC	N
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 674 C Unknow n 1 36 20.00 ul 12.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 674 F 270.0nm PDA 270.0 nm
Date Acquired: Date Processed:	8/14/2018 8:23:59 PM IST 8/14/2018 8:42:53 PM IST		



#### - Channel: 2998; Processed Channel: PDA 270.0 nm; Result ld: 3876; Processing Method: NN 674 F

nm								
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 270.0 nm	6.679	5759	0.86	505			
2	PDA 270.0 nm	7.312	633798	95.03	34130			
3	PDA 270.0 nm	8.077	13287	1.99	1071			
4	PDA 270.0 nm	8.396	14106	2.12	1418			

Figure S66. HPLC analysis report of compound 8fb





#### - Channel: 2998; Processed Channel: PDA 272.0 nm; Result ld: 3541; Processing Method: NN 116

	1111							
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 272.0 nm	2.988	6433	5.26	659			
2	PDA 272.0 nm	3.837	115837	94.74	26874			

Figure S67. HPLC analysis report of compound 8gf

	SAMPLE	INFORMATIC	D N	
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN-115B Unknow n 1 5 20.00 ul 10.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 115 F 270.0nm PDA 270.0 nm	
Date Acquired: Date Processed:	8/8/2018 1:23:24 PM IST 8/8/2018 6:32:51 PM IST			



- Channel: 2998; Processed Channel: PDA 270.0 nm; Result ld: 3447; Processing Method: NN 115 F

	nm							
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 270.0 nm	3.768	217328	96.59	50365			
2	PDA 270.0 nm	4.023	7672	3.41	1133			

Figure S68. HPLC analysis report of compound 8ga

	SAMPLE	INFORMATIC	) N
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 562A Unknow n 1 10 20.00 ul 10.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 562 270.0nm PDA 270.0 nm
Date Acquired: Date Processed:	8/9/2018 12:15:48 PM IST 8/9/2018 12:30:05 PM IST		



Processed Channel Descr.: PDA 270.0

	nm							
	Processed Channel Descr.	RT	Area	% Area	Height			
1	PDA 270.0 nm	3.377	5704	3.33	1198			
2	PDA 270.0 nm	4.343	165832	96.67	30618			

Figure S69. HPLC analysis report of compound 8gh

	SAMPLE	INFORMATIC	D N
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 570 Unknow n 1 20 20.00 ul 10.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 570 270.0nm PDA 270.0 nm
Date Acquired: Date Processed:	8/8/2018 8:01:10 PM IST 8/13/2018 10:54:30 AM IST		



Processed Channel Descr.: PDA 270.0 nm

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		Processed Channel Descr.	RT	Area	% Area	Height			
	1	PDA 270.0 nm	4.003	199049	99.13	43494			
2	2	PDA 270.0 nm	4.202	1754	0.87	994			

Figure S70. HPLC analysis report of compound 8gc

	SAMPLE	INFORMATIC	D N
Sample Name: Sample Type: Vial: Injection #: Injection Volume: Run Time:	NN 642 Unknow n 1 23 20.00 ul 10.0 Minutes	Acquired By: Sample Set Name: Acq. Method Set: Processing Method: Channel Name: Proc. Chnl. Descr.:	System amol NN 642 270.0nm PDA 270.0 nm
Date Acquired: Date Processed:	8/7/2018 4:37:19 PM IST 8/8/2018 6:38:21 PM IST		



Processed Channel	Descr.: PDA 270.0

_	nm						
		Processed Channel Descr.	RT	Area	% Area	Height	
Γ	1	PDA 270.0 nm	5.019	6531	1.12	1081	
	2	PDA 270.0 nm	5.607	574186	98.88	92758	

Figure S71. HPLC analysis report of compound 8gi





Processed	Channel	Descr.:	PDA	270.0
	10 100			

	1111					
		Processed Channel Descr.	RT	Area	% Area	Height
	1	PDA 270.0 nm	7.196	934553	98.87	123536
	2	PDA 270.0 nm	7.706	10641	1.13	1218

Figure S72. HPLC analysis report of compound 8gd