

## Supplementary Data

# Facile Synthesis of Functionalized Phenoxy Quinolines: Antibacterial Activities against ESBL Producing *Escherichia coli* and MRSA, Docking Studies, and Structural Features Determination through Computational Approach

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**Table S1:** Experimental and Theoretical Calculated <sup>1</sup>H-NMR of compound **3b**.

Carbon No.	Carbon Type	Experimental <sup>1</sup> H-NMR (δ, ppm)	Calculated <sup>1</sup> H-NMR (δ, ppm)	Δδ, ppm
1	N	-	-	-
2	CH	8.44	9.32	-0.88
3	CH	6.79	6.02	0.77
4	C	-	-	-
5	CH	8.14	8.86	-0.72
6	C	-	-	-
7	CH	7.67	7.93	-0.26
8	CH	8.05	8.25	-0.20
1'	C	-	-	-
2'	CH	6.86	7.37	-0.51
3'	CH	6.73	7.59	-0.86
4'	C	-	-	-
5'	CH	6.86	7.59	-0.73
6'	CH	6.73	7.37	-0.64
Mean Absolute Error (MAE) = 0.23				
Root Mean Square Error (RMSE) = 0.40				

**Table S2:** Experimental and Theoretical Calculated <sup>1</sup>H-NMR of compound **3c**.

Carbon No.	Carbon Type	Experimental <sup>1</sup> H-NMR (δ, ppm)	Calculated <sup>1</sup> H-NMR (δ, ppm)	Δδ, ppm
1	N			
2	CH	<b>8.68</b>	8.74	-0.06
3	CH	7.49	7.16	0.33
4	C			
5	CH	8.57	8.62	-0.05
6	C			
7	CH	<b>7.81</b>	7.91	-0.10
8	CH	8.02	8.16	-0.14
1'	N			
2'	C			
3'	CH	<b>8.41</b>	7.46	0.95
4'	CH	7.07	8.16	-1.09
5'	CH	<b>7.07</b>	7.38	-0.31
6'	CH	6.89	8.24	-1.35
Mean Absolute Error (MAE) = 0.23				
Root Mean Square Error (RMSE) = 0.40				

**Table S3:** Experimental and Theoretical Calculated <sup>1</sup>H-NMR of compound **3d**.

Carbon No.	Carbon Type	Experimental <sup>1</sup> H-NMR (δ, ppm)	Calculated <sup>1</sup> H-NMR (δ, ppm)	Δδ, ppm
1	N			
2	CH	<b>8.21</b>	8.58	-0.37
3	CH	7.49	6.38	1.11
4	C			
5	CH	8.07	8.71	-0.64
6	C			
7	CH	<b>7.65</b>	7.91	-0.26
8	CH	8.02	8.12	-0.10
1'	S			
2'	CH	<b>7.95</b>	7.22	0.73
3'	C			
4'	CH	7.15	7.07	0.08
5'	CH	<b>7.35</b>	7.43	-0.08
1	N			
Mean Absolute Error (MAE) = 0.23				
Root Mean Square Error (RMSE) = 0.40				

**Table S4:** Experimental and Theoretical Calculated <sup>1</sup>H-NMR of compound **3e**.

Carbon No.	Carbon Type	Experimental <sup>1</sup> H-NMR (δ, ppm)	Calculated <sup>1</sup> H-NMR (δ, ppm)	Δδ, ppm
1	N			
2	CH	<b>8.45</b>	8.49	-0.04
3	CH	6.98	5.99	0.99
4	C			
5	CH	8.12	8.63	-0.51
6	C			
7	CH	<b>7.67</b>	7.83	-0.16
8	CH	8.05	8.09	-0.04
1'	C			
2'	CH	<b>6.82</b>	7.16	-0.34
3'	C			
4'	CH	6.82	7.39	-0.57
5'	C			
6'	CH	6.82	7.16	-0.34
Mean Absolute Error (MAE) = 0.10				
Root Mean Square Error (RMSE) = 0.25				

**Table S5:** Experimental and Theoretical Calculated <sup>1</sup>H-NMR of compound **3f**.

Carbon No.	Carbon Type	Experimental <sup>1</sup> H-NMR (δ, ppm)	Calculated <sup>1</sup> H-NMR (δ, ppm)	Δδ, ppm
1	N			
2	CH	<b>8.45</b>	8.48	-0.03
3	CH	6.98	6.00	0.98
4	C	-		
5	CH	8.13	8.64	-0.51
6	C			
7	CH	<b>7.67</b>	7.83	-0.16
8	CH	8.05	8.08	-0.03
1'	C			
2'	CH	<b>6.92</b>	7.42	-0.50
3'	C			
4'	C			
5'	CH	<b>6.82</b>	7.38	-0.56
6'	CH	6.7	7.23	-0.53
Mean Absolute Error (MAE) = 0.14				
Root Mean Square Error (RMSE) = 0.29				

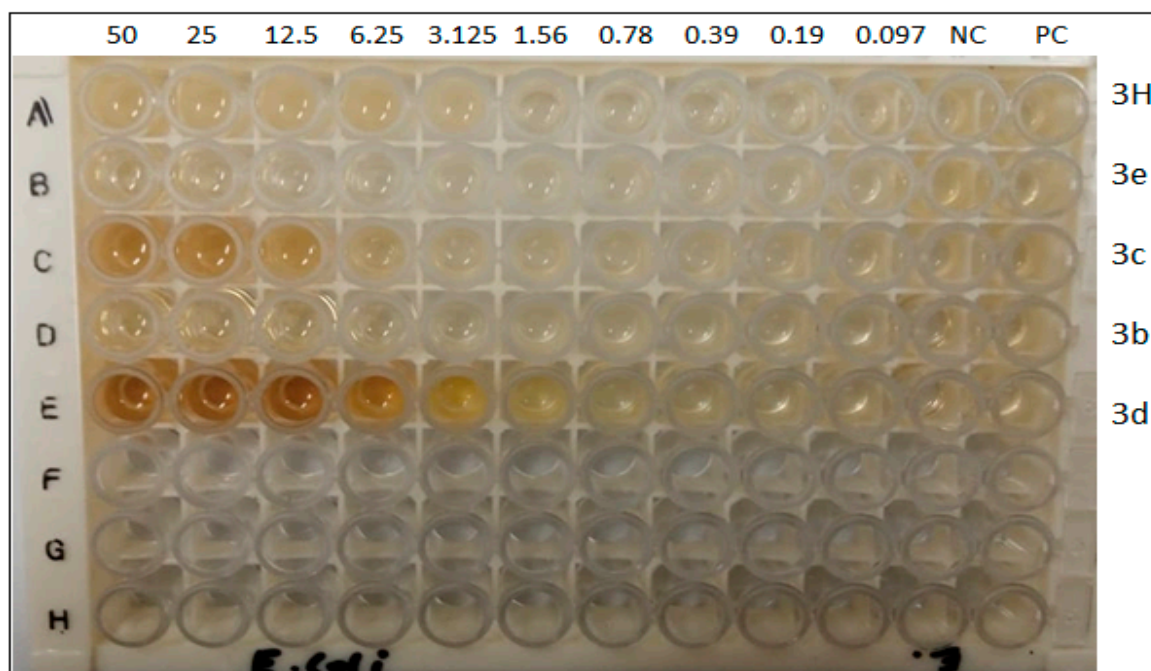
**Table S6:** Experimental and Theoretical Calculated <sup>1</sup>H-NMR of compound **3g**.

Carbon No.	Carbon Type	Experimental <sup>1</sup> H-NMR (δ, ppm)	Calculated <sup>1</sup> H-NMR (δ, ppm)	Δδ, ppm
1	N			
2	CH	<b>8.47</b>	8.44	0.03
3	CH	7.06	5.94	1.12
4	C			
5	CH	8.13	8.67	-0.54
6	C			
7	CH	<b>7.67</b>	7.82	-0.15
8	CH	8.05	8.07	-0.02
1'	C			
2'	CH	<b>6.86</b>	7.32	-0.46
3'	CH	<b>6.74</b>	7.90	-1.16
4'	C			
5'	CH	<b>6.74</b>	7.90	-1.16
6'	CH	6.86	7.32	-0.46
Mean Absolute Error (MAE) = 0.17				
Root Mean Square Error (RMSE) = 0.37				

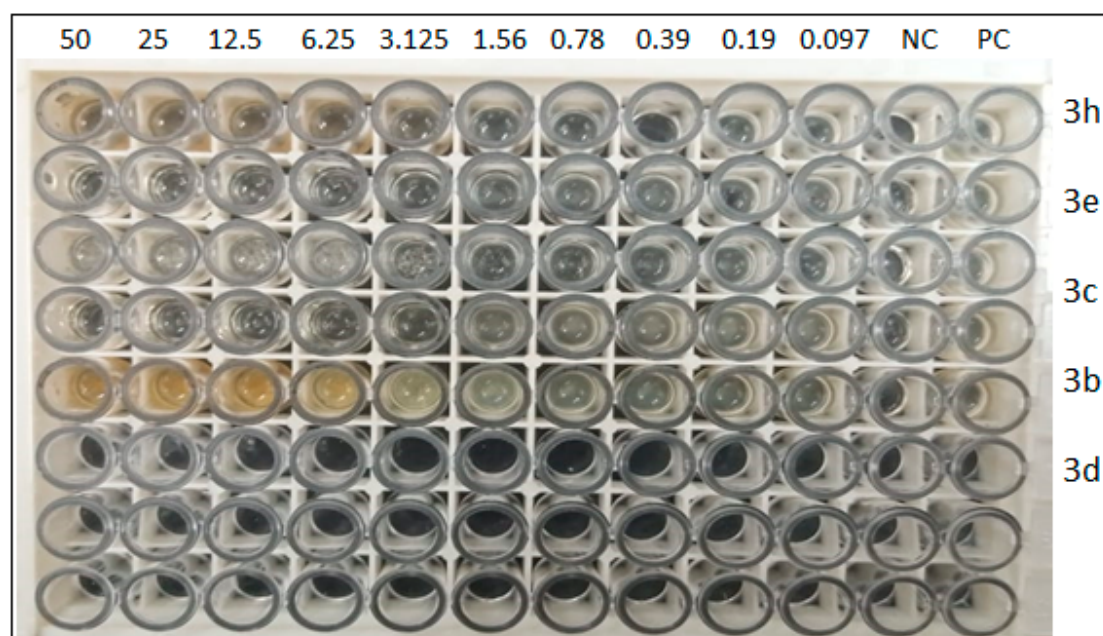


**Table S7:** Experimental and Theoretical Calculated  $^1\text{H}$ -NMR of compound **3h**.

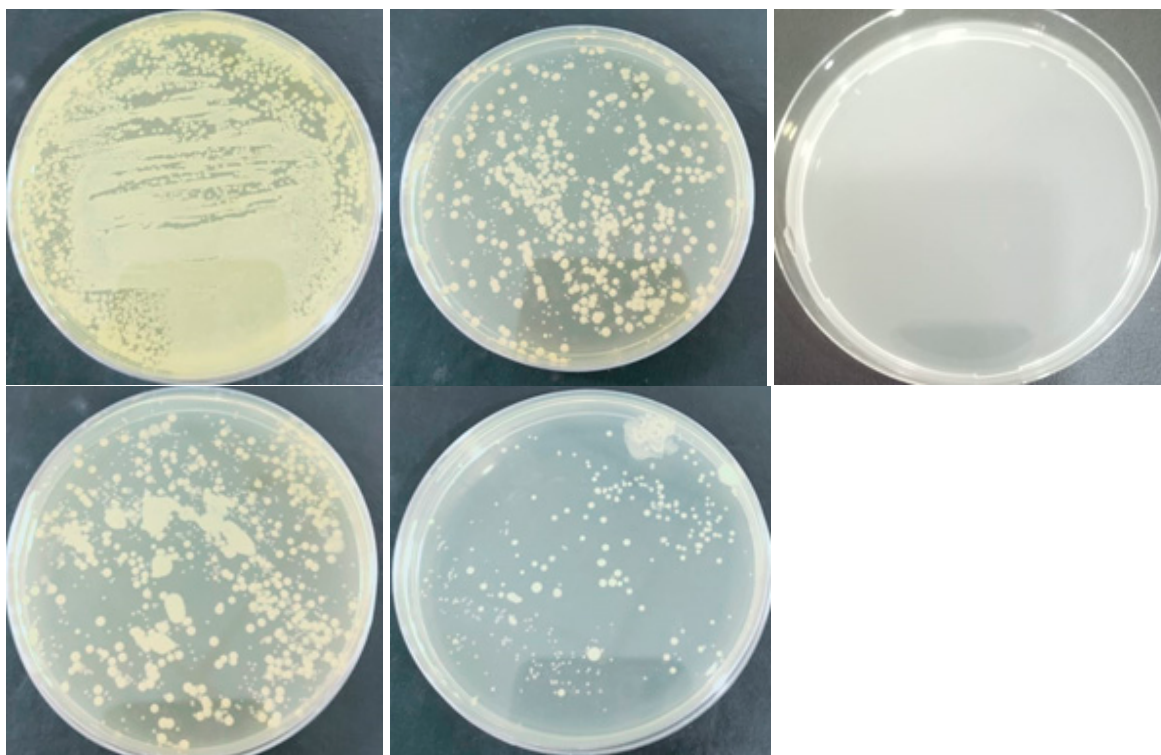
Carbon No.	Carbon Type	Experimental $^1\text{H}$ -NMR ( $\delta$ , ppm)	Calculated $^1\text{H}$ -NMR ( $\delta$ , ppm)	$\Delta\delta$ , ppm
1	N			
2	CH	<b>8.47</b>	8.45	0.02
3	CH	7.67	5.93	1.74
4	C			
5	CH	8.14	8.68	-0.54
6	C			
7	CH	<b>7.81</b>	7.83	-0.02
8	CH	8.05	8.08	-0.03
1'	C			
2'	CH	<b>6.85</b>	7.37	-0.52
3'	CH	<b>6.96</b>	8.34	-1.38
4'	C			
5'	CH	<b>6.85</b>	8.50	-1.65
6'	CH	6.96	7.46	-0.50
Mean Absolute Error (MAE) = 0.27				
Root Mean Square Error (RMSE) = 0.59				



**Figure S1:** MIC of different compounds against ESBL producing *E. coli*.



**Figure S2:** MIC of different compounds against MRSA.



**Figure S3:** MBC of ESBL producing *E. coli* and MRSA.