Supporting Information

Synthesis and evaluation of antiplasmodial efficacy of β-carboline derivatives against murine malaria

Varun Gorki,^{a,†} Rahul Singh,^{b,†} Neha Sylvia Walter,^a Upma Bagai,^{a,*} Deepak B. Salunke^{b,*}

^aParasitology Laboratory, Department of Zoology, Panjab University, Chandigarh 160014, India ^bDepartment of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh 160014, India.

*Corresponding Authors

Dr. Deepak B. Salunke, Assistant Professor, Department of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh-160014, India. Email: <u>salunke@pu.ac.in</u>

Prof. Upma Bagai, Professor, Department of Zoology, Panjab University, Chandigarh-160014, India. Email: <u>upmabagai@yahoo.co.in</u>

⁺Both the authors contributed equally to this work.

ghai29@yahoo.co.in singhrahul9041@gmail.com walterneha@gmail.com

Table of Content

Sr. No.	Contents	Page No.
1.	Analytical data for compound 8a	S3-S5
2.	Analytical data for compound 9a	S6-S8
3.	Analytical data for compound 8b	S9-S11
4.	Analytical data for compound 9b	S12-S14
5.	Analytical data for compound 8c	S15-S17
6.	Analytical data for compound 9c	S18-S20
7.	Analytical data for compound 8d	S21-S24
8.	Analytical data for compound 9d	S25-S28
9.	Analytical data for compound 10	S29-S30
10.	Pictet-Spengler Reaction Mechanism and Optimization of Reaction	S31-S32

Figure S1: ¹H NMR (400 MHz): 8a CDCl₃



Figure S2: FT-IR (Neat): 8a



Figure S3: LC-MS: 8a



Figure S4: ¹H NMR (400 MHz): 9a CDCl₃



Figure S5: FT-IR (Neat): 9a



Figure S6: LC-MS: 9a



Figure S7: ¹H NMR (400 MHz): 8b CDCl₃



Figure S8: FT-IR (Neat): 8b



Figure S9: LC-MS: 8b



Figure S10: ¹H NMR (400 MHz): 9b CDCl₃



Figure S11: FT-IR (Neat): 9b



Figure S12: LC-MS: 9b



Figure S13: ¹H NMR (400 MHz): 8c CDCl₃



Figure S14: FT-IR (Neat): 8c



Figure S15: LC-MS: 8c



Figure S16: ¹H NMR (400 MHz): 9c CDCl₃



Figure S17: FT-IR (Neat): 9c



Figure S18: LC-MS: 9c



Figure S19: ¹H NMR (400 MHz): 8d DMSO-d₆+CDCl₃



Figure S20: ¹³C (100 MHz): 8d DMSO-d₆+CDCl₃







Auto-Scaled Chromatogram

Figure S23: ¹H NMR (400 MHz): 9d DMSO-d₆+CDCl₃



Figure S24: ¹³C (100 MHz): 9d DMSO-d₆+CDCl₃





Figure S25: FT-IR (Neat): 9d



Name

1

3

4

÷ 0.40-Peak Results 290 Base RT Area Height Peak 0.30-(m/z) 2.658 6336 2854 301.54 0.20-2.790 2317197 464670 315.45 -3.941 - 311.5 -4.145 - 293.0 -2.658 - 301.5 3.941 28645 12340 311.45 4.145 13957 1339 292.96 0.10-0.00 4.00 成る 1.00 2.00 5.00 6.00 7.00 8.00 9.00 3.00 0.00 10.00 Minutes Ο Peak#2 - 2.790 - Q... Peak#3 - 3.941 - Q ... Peak#1 - 2.658 - Q ... Peak#4 - 4.145 - Q ... \sim ŇH H⁺ N H 315.5 311.5 304.5 M+1: 315.45

Apex

Apex

Apex

Auto-Scaled Chromatogram

Apex

Figure S27: ¹H NMR (400 MHz): 10 DMSO-d₆



Figure S28: FT-IR (Neat): 10

