Supporting information file for manuscript

Design, Synthesis and Structural Characterization of Thioflavones and Thioflavonols as Potential Tyrosinase Inhibitors: In Vitro and In Silico Studies

Ehsan Ullah Mughal^{*a}, Jamshaid Ashraf^a, Essam M. Hussein^{b,c}, Yasir Nazir^{d,e}, Abdulaziz S. Alwuthaynani^b, Nafeesa Naeem^a, Amina Sadiq^{*f}, Reem I. Alsantali^g, Saleh A. Ahmed^{*b,c}

^aDepartment of Chemistry, University of Gujrat, Gujrat-50700, Pakistan ^bDepartment of Chemistry, Faculty of Applied Sciences, Umm Al-Qura University, Makkah 21955, Saudi Arabia

^cDepartment of Chemistry, Faculty of Science, Assiut University, 71516 Assiut, Egypt ^dDepartment of Chemistry, Allama Iqbal Open University, Islamabad-44000 Pakistan ^eDepartment of Chemistry, University of Sialkot, Sialkot-51300, Pakistan ^fDepartment of Chemistry, Govt. College Women University, Sialkot-51300, Pakistan ^gDepartment of Pharmaceutical Chemistry, College of Pharmacy, Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia

^{*}Correspondence may be addressed to: Ehsan Ullah Mughal, Amina Sadiq and Saleh A. Ahmed; E-mail address: <u>ehsan.ullah@uog.edu.pk</u>, <u>amina.sadiq@gcwus.edu.pk</u>, <u>saahmed@uqu.edu.sa</u>



Figure S1. FTIR Spectrum of Compound 2a



Figure S2. FTIR Spectrum of Compound 2b



Figure S3. FTIR Spectrum of Compound 2c



Figure S4. FTIR Spectrum of Compound 2d



Figure S5. FTIR Spectrum of Compound 2e



Figure S6. FTIR Spectrum of Compound 2f



Figure S7. FTIR Spectrum of Compound 2g



Figure S8. FTIR Spectrum of Compound 2h



Figure S9. FTIR Spectrum of Compound 2i



Figure S10. FTIR Spectrum of Compound 2j



Figure S11. FTIR Spectrum of Compound 2k



Figure S12. FTIR Spectrum of Compound 21



Figure S13. FTIR Spectrum of Compound 2m



Figure S14. FTIR Spectrum of Compound 2n



Figure S15. FTIR Spectrum of Compound 20



Figure S16. FTIR Spectrum of Compound 2p



-600 -550 -500 -450 400 -350 -300 -250 -200 -150 -100 -50 -0 --50 190 180 170 160 150 140 130 120 110 100 f1 (ppm) 230 220 210 200 90 80 70 60 50 40 30 20 10 Ó -10

Figure S18. ¹³C NMR Spectrum (101 MHz, DMSO) (Compound 2a)



Figure S19. ¹H NMR Spectrum (400 MHz, DMSO) (Compound 2c)



Figure S20. ¹³C NMR Spectrum (101 MHz, DMSO) (Compound 2c)



Figure S21. ¹H NMR Spectrum (400 MHz, DMSO) (Compound 2d)



Figure S22. ¹³C NMR Spectrum (101 MHz, DMSO) (Compound 2d)



Figure S23. ¹H NMR Spectrum (400 MHz, DMSO) (Compound 2f)



Figure S24. ¹³C NMR Spectrum (101 MHz, DMSO) (Compound 2f)



Figure S25. ¹H NMR Spectrum (400 MHz, DMSO) (Compound 2h)



Figure S26. ¹³C NMR Spectrum (101 MHz, DMSO) (Compound 2h)



Figure S28. ¹³C NMR Spectrum (101 MHz, DMSO) (Compound 2i)



Figure S29. ¹H NMR Spectrum (400 MHz, DMSO) (Compound 2k)



Figure S30. ¹³C NMR Spectrum (101 MHz, DMSO) (Compound 2k)



Figure S31. DEPT NMR Spectrum (101 MHz, DMSO) (Compound 2k)



Figure S32. Docking Image of Compound 2a



Figure S33. Docking Image of Compound 2b



Figure S34. Docking Image of Compound 2c



Figure S35. Docking Image of Compound 2d



Figure S36. Docking Image of Compound 2e



Figure S37. Docking Image of Compound 2f



Figure S38. Docking Image of Compound 2g



Figure S39. Docking Image of Compound 2h



Figure S40. Docking Image of Compound 2i



Figure S41. Docking Image of Compound 2j



Figure S42. Docking Image of Compound 2k



Figure S43. Docking Image of Compound 21



Figure S44. Docking Image of Compound 2p



Figure S45. Docking Image of Kojic Acid