Supplementary Material

Synthesis of novel oxa-carbocycle annulated flavones and bis-flavones by ring closing/cross metathesis

Rachakonda Sydhulu, ^a Yerrabelly Hemasri, ^{*a} and Yerrabelly Jayaprakash Rao^b

^aDepartment of Chemistry, Nizam College, Osmania University, Hyderabad, Telangana-500001, India ^bDepartment of Chemistry, Osmania University, Hyderabad, Telangana-500007, India E-mail: <u>hemay2@yahoo.com</u>

Table of Contents

Figures ¹ H and ¹³ C NMR spectra of all synthesized compounds	S2
Figures ESI-HRMS spectra of all synthesized compounds	



Figure S1. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-1a



Figure S2. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-1a



Figure S4. ¹³C NMR Spectrum (101 MHz, DMSO) of compound-1b



Figure S6. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-2a



Figure S8. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-2b



Figure 9. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-3a



Figure S10. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-3a



Figure S11. ¹H NMR Spectrum (400 MHz, DMSO) of compound-3b







Figure S14. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-4a



Figure S15. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-4b



Figure S16. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-4b



Figure S17. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-**4**c



Figure S18. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-4c



Figure S19. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-4d



Figure S20. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-4d



Figure S21. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-4e



Figure S22. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-4e







Figure S24. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-5a



Figure S25. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-5b



Figure S26. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-5b



Figure S28. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-5c



Figure S30. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-5d







Figure S34. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-6a



Figure S36. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-6b



Figure S37. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-7a



Figure S38. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-7a



Figure S39. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-7b



Figure S40. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-7b



Figure S41. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-8a



Figure S42. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-8a



Figure S44. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-9a



Figure S45. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-2c







Figure S48. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-2d









Figure S52. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-2f



Figure S53. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-10a



Figure S54. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-10a



Figure S55. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-10b



Figure S56. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-10b



Figure S57. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-10c



Figure S58. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-10c



Figure S59. ¹H NMR Spectrum (400 MHz, CDCl₃) of compound-10d







Figure S62. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-10e



Figure S64. ¹³C NMR Spectrum (101 MHz, CDCl₃) of compound-10f







Figure S66. ESI-HRMS spectrum of 3-(4-chlorophenyl)-8,11-dihydro-1H-oxepino[3,2-f]chromen-

1-one (5b)



Figure S67. ESI-MS spectrum of (Z)-3-phenyl-9,12-dihydrooxocino [3,2-f]chromen-1(8H)-one

(5c)



Figure S68. ESI-HRMS spectrum (Z)-3-(4-chlorophenyl)-9,12-dihydrooxocino[3,2-f]chromen-1(8H)-one (5d)



Figure S69. ESI-MS spectrum of (Z)-3-phenyl-8,9,10,13-tetrahydro-1H-oxonino[3,2-f]chromen-1-



Figure S70. ESI-HRMS spectrum 3-phenyl-9-vinyl-8,11-dihydro-1H-oxepino [3,2-f]chromen-1-

one (7a)



Figure S71. ESI-HRMS spectrum 3-(4-chlorophenyl)-9-vinyl-8,11-dihydro-1H-oxepino[3,2-



Figure S72. ESI-HRMS spectrum (E)-5,5'-(but-2-ene-1,4-diyl)bis(6-methoxy-2-phenyl-4H-

chromen-4-one) (9a)



Figure S73. ESI-HRMS spectrum (E)-6,6'-(but-2-ene-1,4-diylbis(oxy))bis(2-phenyl-4H-chromen-4-



Figure S74. ESI-HRMS spectrum (E)-6,6'-(but-2-ene-1,4-diylbis(oxy))bis(2-(4-chlorophenyl)-4Hchromen-4-one) (10b)

Page S41



Figure S75. ESI-HRMS spectrum of (E)-6,6'-(hex-3-ene-1,6-diylbis(oxy))bis(2-phenyl-4H-

chromen-4-one) (10c)



Figure S76. ESI-HRMS spectrum of (E)-6,6'-(hex-3-ene-1,6-diylbis(oxy))bis(2-(4-chlorophenyl)-

4H-chromen-4-one) (**10d**)



Figure S77. ESI-HRMS spectrum (E)-6,6'-(dec-5-ene-1,10-diylbis(oxy))bis(2-phenyl-4H-chromen-

4-one) (**10e)**



Figure S78. ESI-HRMS spectrum (E)-6,6'-(dec-5-ene-1,10-diylbis(oxy))bis(2-(4-chlorophenyl)-4H-

chromen-4-one) (10f)