Synthesis of new 5-aryl-benzo[*f*][1,7]naphthyridines via a cascade process (Ugi-3CR / intramolecular aza Diels-Alder cycloaddition) / aromatization

Óscar Vázquez-Vera ¹, Daniel Segura-Olvera ², Mónica A. Rincón-Guevara ³, Atilano Gutiérrez-Carrillo ², Miguel A. García-Sánchez ², Ilich A. Ibarra ⁴, Leticia Lomas-Romero ^{2,*}, Alejandro Islas-Jácome ^{2,*}, and Eduardo González-Zamora ^{2,*}

- ¹ Unidad Profesional Interdisciplinaria de Biotecnología, Instituto Politécnico Nacional, Av. Acueducto de Guadalupe S/N, Barr. La Laguna Ticomán, C.P. 07340, Gustavo A Madero, Ciudad de México; vaveos@yahoo.com.mx (O.V.-V.)
- ² Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 186, Col. Vicentina, C.P. 09340, Iztapalapa, Ciudad de México; mudo-2@hotmail.com (D.S.-O.); agrmn@xanum.uam.mx (A.G.-C.); mags@xanum.uam.mx (M.A.G.-S.)
- ³ Departamento de Biotecnología, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 186, Col. Vicentina, C.P. 09340, Iztapalapa, Ciudad de México; monicarinconguevara@gmail.com (M.A.R.-G.)
- ⁴ Laboratorio de Fisicoquímica y Reactividad de Superficies, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito Exterior S/N, Ciudad Universitaria, C.P. 04510, Coyoacán, Ciudad de México; argel@unam.mx (I.A.I.)
- * Correspondence: llr@xanum.uam.mx (L.L.-R.); aij@xanum.uam.mx (A.I.-J.); egz@xanum.uam.mx (E.G.-Z.); Tel.: +52-55-5804-4913 (L.L.-R.; A.I.-J.; E.G.-Z.)

CONTENTS

1H and 13C NMR spectra of the products 3a-h	S1-S9
1H and 13C NMR spectra of the products 4a-h	S10-S17
2D-NMR spectra of the products 3a , 3c-h	S18-S28
2D-NMR spectra of the products 4a-h	S28-S40



Figure S1. ¹H NMR spectrum of the product 3a



Figure S2. ¹³C NMR spectrum of the product 3a



Figure S3. ¹H NMR spectrum of the product **3b** (mixture of inseparable diasteroisomers r = 4:3)



Figure S4. HRMS spectrum of the product 3b



Figure S5. ¹H NMR spectrum of the product **3**c (mixture of inseparable diasteroisomers r = 20:3)



Figure S6. 13 C NMR spectrum of the product 3c



Figure S7. ¹H NMR spectrum of the product 3d (mixture of inseparable diasteroisomers r = 5:1)



Figure S8. ¹³C NMR spectrum of the product 3d



Figure S9. ¹H NMR spectrum of the product 3e



Figure S10. ¹³C NMR spectrum of the product 3e



Figure S11. ¹H NMR spectrum of the product **3f** (mixture of inseparable diasteroisomers r = 10:3)



Figure S12. ¹³C NMR spectrum of the product 3f



Figure S13. ¹H NMR spectrum of the product **3g** (mixture of inseparable diasteroisomers r = 4:1)



Figure S14. ¹³C NMR spectrum of the product 3g



Figure S15. ¹H NMR spectrum of the product 3h



Figure S16. ¹³C NMR spectrum of the product 3h



Figure S17. ¹H NMR spectrum of the product 4a



Figure S18. ¹³C NMR spectrum of the product 4a



Figure S19. ¹H NMR spectrum of the product 4b



Figure S20. ¹³C NMR spectrum of the product 4b



Figure S21. ¹H NMR spectrum of the product 4c



Figure S22. ¹³C NMR spectrum of the product 4c



Figure S23. ¹H NMR spectrum of the product 4d



Figure S24. ¹³C NMR spectrum of the product 4d



Figure S25. ¹H NMR spectrum of the product 4e



Figure S26. ¹³C NMR spectrum of the product 4e



Figure S27. ¹H NMR spectrum of the product 4f



Figure S28. ¹³C NMR spectrum of the product 4f



Figure S29. ¹H NMR spectrum of the product 4g



Figure S30. ¹³C NMR spectrum of the product 4g



Figure S31. ¹H NMR spectrum of the product 4h







Figure S33. COSY spectrum of the product 3a



Figure S34. HSQC spectrum of the product 3a



Figure S35. HMBC spectrum of the product 3a



Figure S36. COSY spectrum of the product 3c



Figure S37. HSQC spectrum of the product 3c



Figure S38. HMBC spectrum of the product 3c



Figure S39. COSY spectrum of the product 3d







Figure S41. HMBC spectrum of the product 3d



Figure S42. COSY spectrum of the product 3e



Figure S43. HSQC spectrum of the product 3e



Figure S44. HMBC spectrum of the product 3e



Figure S45. COSY spectrum of the product 3f



Figure S46. HSQC spectrum of the product 3f



Figure S47. HMBC spectrum of the product 3f



Figure S48. COSY spectrum of the product 3g



Figure S49. HSQC spectrum of the product 3g



Figure S50. HMBC spectrum of the product 3g



Figure S51. COSY spectrum of the product 3h







Figure S53. HMBC spectrum of the product 3h

2D-NMR spectra for the products 4a-h















Figure S57. COSY spectrum of the product 4b







Figure S59. HMBC spectrum of the product 4b



Figure S60. COSY spectrum of the product 4c



Figure S61. HSQC spectrum of the product 4c



Figure S62. HMBC spectrum of the product 4c



Figure S63. COSY spectrum of the product 4d



Figure S64. HSQC spectrum of the product 4d



Figure S65. HMBC spectrum of the product 4d



Figure S66. COSY spectrum of the product 4e



Figure S67. HSQC spectrum of the product 4e



Figure S68. HMBC spectrum of the product 4e



Figure S69. COSY spectrum of the product 4f







Figure S71. HMBC spectrum of the product 4f







Figure S73. HSQC spectrum of the product 4g



Figure S74. HMBC spectrum of the product 4g



Figure S75. COSY spectrum of the product 4h







Figure S77. HMBC spectrum of the product 4h