Supplementary Information

New In/SiO₂ composite catalyst in the solvent-free multicomponent synthesis of Ca²⁺ channel blockers Nifedipine and Nemadipine B.

Ricardo Ferreira Affeldt,^a Edilson Valmir Benvenutti^b and Dennis Russowsky^{*a}

^a Laboratório de Sínteses Orgânicas, Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves 9500, 91501-970, Porto Alegre, RS, Brasil.

^b Laboratório de Sólidos e Superfícies, Instituto de Química, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves 9500, 91501-970, Porto Alegre, RS, Brasil.

1. Caracterization of the In/SiO₂ Composite



Figure S1. Comparison of pore size distribution curves of of In/SiO₂ composite, obtained from BJH(Barret, Joyner and Halenda) method and from HK (Horvath Kawazoe) method.



Figure S2. EDS (Energy Dispersive Spectroscopy) of a In/SiO₂ sample.



Figure S3. SEM (Scanning Electron Microscopy) image of In/SiO2 composite, obtained with 1000x of magnification.



Figure S4. Pictures of In/SiO₂ composite as xerogel monolith and powder forms.



Figure S5. ¹H NMR (300 MHz, CDCl₃) - Compound 12a



Figura S6. ¹³C NMR (75 MHz, CDCl₃) – Compound 12a



Figure S7. IR (KBr, cm⁻¹) – Compound 12a



Figure S8. ¹H NMR (300 MHz, CDCl₃) - Compound 12b



Figura S9. ¹³C NMR (75 MHz, CDCl₃) – Compound 12b



Figure S10. IR (KBr, cm^{-1}) – Compound 12b



Figure S11. ¹H NMR (300 MHz, CDCl₃) - Compound 12c



Figura S12. ¹³C NMR (75 MHz, CDCl₃) – Compound 12c



Figure S13. IR (KBr, cm^{-1}) – Compound 12c



Figure S14. ¹H NMR (300 MHz, CDCl₃) - Compound 12d



Figura S15. ¹³C NMR (75 MHz, CDCl₃) – Compound 12d



Figure S16. IR (KBr, cm⁻¹) – Compound 12d



Figure S17. ¹H NMR (300 MHz, CDCl₃) - Compound 12e



Figura S18. ¹³C NMR (75 MHz, CDCl₃) – Compound 12e



Figure S19. IR (KBr, cm^{-1}) – Compound 12e



Figure S20. ¹H NMR (300 MHz, CDCl₃) - Compound 12f



Figura S21. ¹³C NMR (75 MHz, CDCl₃) – Compound 12f



Figure S22. IR (KBr, cm^{-1}) – Compound 12f



Figure S23. ¹H NMR (300 MHz, CDCl₃) - Compound 12g



Figura S24. ¹³C NMR (75 MHz, CDCl₃) – Compound 12g



Figure S25. IR (KBr, cm⁻¹) – Compound 12g



Figure S26. ¹H NMR (300 MHz, CDCl₃) - Compound 12h



Figura S27. ¹³C NMR (75 MHz, CDCl₃) – Compound 12h



Figure S28. IR (KBr, cm⁻¹) – Compound 12h



Figure S29. ¹H NMR (300 MHz, CDCl₃) - Compound 12i



Figura S30. ¹³C NMR (75 MHz, CDCl₃) – Compound 12i



Figure S31. IR (KBr, cm⁻¹) – Compound 12i



Figure S32. ¹H NMR (300 MHz, CDCl₃) - Compound 12j



Figura S33. ¹³C NMR (75 MHz, CDCl₃) – Compound 12j



Figure S34. IR (KBr, cm⁻¹) – Compound 12j



Figure S35. ¹H NMR (300 MHz, CDCl₃) - Compound 12k



Figura S36. ¹³C NMR (75 MHz, CDCl₃) – Compound 12k



Figure S37. IR (KBr, cm^{-1}) – Compound 12k



Figure S38. ¹H NMR (300 MHz, CDCl₃) - Compound 12l



Figura S39. ¹³C NMR (75 MHz, CDCl₃) – Compound 12l



Figure S40. IR (KBr, cm⁻¹) – Compound 12l



Figure S41. ¹H NMR (300 MHz, CDCl₃) - Compound 12m



Figura S42. ¹³C NMR (75 MHz, CDCl₃) – Compound 12m



Figure S43. IR (KBr, cm⁻¹) – Compound 12m



Figure S44. ¹H NMR (300 MHz, CDCl₃) - Compound 7 (Nifedipine)



Figura S45. ¹³C NMR (75 MHz, CDCl₃) – Compound 7 (Nifedipine)



Figure S46. IR (KBr, cm⁻¹) – Compound 7 (Nifedipine)



Figure S47. ¹H NMR (300 MHz, CDCl₃) - Compound 8 (Nemadipine B)



Figura S48. ¹³C NMR (75 MHz, CDCl₃) – Compound 8 (Niemadipine B)



Figure S49. IR (KBr, cm⁻¹) – Compound 8 (Nemadipene B)



Figura S50. ¹H NMR (300 MHz, CDCl₃) – Compound 14a



Figura S51. ¹³C NMR (75 MHz, CDCl₃) – Compound 14a



% sionstimenenT

Figure S52. IR (KBr, cm⁻¹) – Compound 14a



Figure S53. ¹H NMR (300 MHz, CDCl₃) - Compound 14b



Figura S54. ¹³C NMR (75 MHz, CDCl₃) – Compound 14b



Figure S55. IR (KBr, cm⁻¹) – Compound 14b



Figure S56. ¹H NMR (300 MHz, CDCl₃) - Compound 14c



Figura S57. ¹³C NMR (75 MHz, CDCl₃) – Compound 14c



7 Transmitancia %

Figure S58. IR (KBr, cm^{-1}) – Compound 14c



Figure S59. HRMS – Compound 14c



Figure S60. ¹H NMR (300 MHz, CDCl₃) - Compound 14d



Figura S61. ¹³C NMR (75 MHz, CDCl₃) – Compound 14d



Figure S62. IR (KBr, cm^{-1}) – Compound 14d



Figure S63. ¹H NMR (300 MHz, CDCl₃) - Compound 14e



Figura S64. ¹³C NMR (75 MHz, CDCl₃) – Compound 14e



Figure S65. IR (KBr, cm⁻¹) – Compound 14e



Figure S66. ¹H NMR (300 MHz, CDCl₃) - Compound 14f



Figure S67. ¹³C NMR (75 MHz, CDCl₃) - Compound 14f



Figure S68. IR (KBr, cm⁻¹) – Compound **14f**



Figure S69. ¹H NMR (300 MHz, CDCl₃) – Cmpound 15 (*E*,*Z* isomeric mixture)



Figure S70. ¹³C NMR (75 MHz, CDCl₃) – Compound 15 (E,Z isomeric mixture)