## **RSC** Advances

### **Supplementary Information**

# Synthesis and bioevaluation of 2-phenyl-5-methyl-2*H*-1,2,3-triazole -4-carboxylic acid/carbohydrazide derivatives as potent xanthine

#### oxidase inhibitors

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Figure S1. <sup>1</sup>H NMR spectrum (600 MHz, DMSO) of compound 7a



Figure S2. <sup>13</sup>C NMR spectrum (100 MHz, DMSO) of compound 7a



Figure S3. HRESIMS spectrum of compound 7a



Figure S4. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 7b



Figure S5. <sup>13</sup>C NMR spectrum (100 MHz, CDCl3) of compound 7b



Figure S6. HRESIMS spectrum of compound 7b



Figure S7. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 7c



Figure S8. <sup>13</sup>C NMR spectrum (150 MHz, CDCl3) of compound 7c



Figure S9. HRESIMS spectrum of compound 7c



Figure S10. IR spectrum of compound 7c



Figure S11. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 7d



Figure S12. <sup>13</sup>C NMR spectrum (100 MHz, DMSO) of compound 7d



Figure S13. HRESIMS spectrum of compound 7d



Figure S14. IR spectrum of compound 7d



Figure S15. <sup>1</sup>H NMR spectrum (600 MHz, DMSO) of compound 7e



Figure S16. <sup>13</sup>C NMR spectrum (150 MHz, DMSO) of compound 7e



Figure S17. HRESIMS spectrum of compound 7e



Figure S18. IR spectrum of compound 7e



Figure S19. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 7f



Figure S20. <sup>13</sup>C NMR spectrum (100 MHz, DMSO) of compound 7f



Figure S21. HRESIMS spectrum of compound 7f



Figure S22. IR spectrum of compound 7f



Figure S23. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 7g



Figure S24. <sup>13</sup>C NMR spectrum (100 MHz, CDCl3) of compound 7g



Figure S25. HRESIMS spectrum of compound 7g



Figure S26.  $^{1}$ H NMR spectrum (400 MHz, CDCl3) of compound 7h



Figure S27. <sup>13</sup>C NMR spectrum (100 MHz, CDCl3) of compound 7h



Figure S28. HRESIMS spectrum of compound 7h



Figure S29. <sup>1</sup>H NMR spectrum (600 MHz, DMSO) of compound 8a



Figure S30. <sup>13</sup>C NMR spectrum (150 MHz, DMSO) of compound 8a



Figure S31. HRESIMS spectrum of compound 8a



Figure S32. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 8b



Figure S33. <sup>13</sup>C NMR spectrum (100 MHz, DMSO) of compound 8b



Figure S34. HRESIMS spectrum of compound 8b



Figure S35. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 8c



Figure S36. <sup>13</sup>C NMR spectrum (100 MHz, DMSO) of compound 8c



Figure S37. HRESIMS spectrum of compound 8c



Figure S38. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 8d



Figure S39. <sup>13</sup>C NMR spectrum (100 MHz, DMSO) of compound 8d



Figure S40. HRESIMS spectrum of compound 8d



Figure S41. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 8e



Figure S42. <sup>13</sup>C NMR spectrum (100 MHz, CDCl3) of compound 8e



Figure S43. HRESIMS spectrum of compound 8e



Figure S44. IR spectrum of compound 8e



Figure S45. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 8f



Figure S46. <sup>13</sup>C NMR spectrum (100 MHz, CDCl3) of compound 8f



Figure S47. HRESIMS spectrum of compound 8f



Figure S48. IR spectrum of compound 8f



Figure S49. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 8g



Figure S50. <sup>13</sup>C NMR spectrum (100 MHz, CDCl3) of compound 8g



Figure S51. HRESIMS spectrum of compound 8g



Figure S52. <sup>1</sup>H NMR spectrum (400 MHz, CDCl3) of compound 8h



Figure S53. <sup>13</sup>C NMR spectrum (100 MHz, DMSO) of compound 8h



Figure S54. HRESIMS spectrum of compound 8h



Figure S55. <sup>1</sup>H NMR spectrum (600 MHz, DMSO) of compound 9e



Figure S56. <sup>13</sup>C NMR spectrum (150 MHz, DMSO) of compound 9e



Figure S57. <sup>1</sup>H NMR spectrum (600 MHz, DMSO) of compound 9f



Figure S58. <sup>13</sup>C NMR spectrum (150 MHz, DMSO) of compound 9f



Figure S59. HRESIMS spectrum of compound 9f



Figure S60. IR spectrum of compound 9f



Figure S61. <sup>1</sup>H NMR spectrum (600 MHz, DMSO) of compound 10e



Figure S62. <sup>13</sup>C NMR spectrum (150 MHz, DMSO) of compound 10e



Figure S63. HRESIMS spectrum of compound 10e



Figure S64. <sup>1</sup>H NMR spectrum (600 MHz, DMSO) of compound 10f



Figure S65. <sup>13</sup>C NMR spectrum (150 MHz, DMSO) of compound 10f



Figure S66. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 13c



Figure S67. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 13d



Figure S68. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 13e



Figure S69. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 13f



Figure S70. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 14a



Figure S71. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14b



Figure S72. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14c



Figure S73. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14d



Figure S74. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14e



Figure S75. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14f



Figure S76. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14g



Figure S77. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 14h



Figure S78. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 17a



Figure S79. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 17b



Figure S80.  $^{1}$ H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 17c



Figure S81. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 17d



Figure S82. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 17e



Figure S83. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 17f



Figure S84. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 17g



Figure S85. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 17h



Figure S86 <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 22a



Figure S87. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 22b



Figure S88. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 22c



Figure S89. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 22d



Figure S90.  $^{1}$ H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 22e



Figure S91. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 22f



Figure S92. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 22g



Figure S93. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 22h



Figure S94. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23a



Figure S95. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23b



Figure S96. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23c



Figure S97. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23d



Figure S98. <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of compound 23e



Figure S99. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23f



Figure S100. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23g



Figure S101. <sup>1</sup>H NMR spectrum (400 MHz, CDCl<sub>3</sub>) of compound 23h