Supplementary Materials

Purine and Purine Isostere Derivatives of Ferrocene: An Evaluation of ADME, Antitumor and Electrochemical Properties

Valentina Rep ¹, Martina Piškor ¹, Helena Šimek ¹, Petra Mišetić ², Petra Grbčić ³, Jasna Padovan ², Vesna Gabelica Marković ⁴, Dijana Jadreško ⁵, Krešimir Pavelić ⁶, Sandra Kraljević Pavelić ³ and Silvana Raić-Malić ^{1,*}

- ¹ Department of Organic Chemistry, Faculty of Chemical Engineering and Technology, University of Zagreb, Zagreb 10000, Croatia; vrep@fkit.hr (V.R.); mpiskor@fkit.hr (M.P.); hsimek@fkit.hr (H.Š.)
- ² Fidelta d.o.o., Zagreb 10000, Croatia; Petra.Misetic@fidelta.eu (P.M.); Jasna.Padovan@fidelta.eu (J.P.)
- ³ Department of Biotechnology, Center for High-Throughput Technologies, University of Rijeka, Rijeka 51000, Croatia; petra.grbcic@biotech.uniri.hr (P.G.); sandrakp@biotech.uniri.hr (S.K.P.)
- ⁴ International Relations Office, Faculty of Chemical Engineering and Technology, University of Zagreb, Zagreb 10000, Croatia; vesnagm@fkit.hr
- ⁵ Division for Marine and Environmental Research, Ruder Bošković Institute, Zagreb 10000, Croatia; djadresko@irb.hr
- ⁶ Faculty of Medicine, Juraj Dobrila University of Pula, Pula 52100, Croatia; pavelic@unipu.hr
- * Correspondence: sraic@fkit.hr; Tel.: +385-1-4597213







Figure S4. a) 1 H i b) 13 C-NMR of **12a**





Figure S5. a) 1 H i b) 13 C-NMR of **12b**







Figure S7. a) 1 H i b) 13 C-NMR of **13a**



Figure S8. a) 1 H i b) 13 C-NMR of **13b**





Figure S9. a) $^1\mathrm{H}$ i b) $^{13}\mathrm{C}\text{-NMR}$ of 13c



Figure S10. a) 1 H i b) 13 C-NMR of **14a**



Figure S11. a) 1 H i b) 13 C-NMR of **14b**













Figure S14. a) 1 H i b) 13 C-NMR of **15b**







Figure S17. a) 1 H i b) 13 C-NMR of **23a**





Figure S18. a) 1 H i b) 13 C-NMR of **23b**

a)









Figure S20. a) 1 H i b) 13 C-NMR of **24a**





Figure S21. a) 1 H i b) 13 C-NMR of **24b**











^{150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0} f1 (ppm)

Figure S23. a) 1 H i b) 13 C-NMR of **25a**





Figure S24. a) 1 H i b) 13 C-NMR of **25b**

a)





Figure S25. a) 1 H i b) 13 C-NMR of **25c**

a)

Figure S26. a) 1 H i b) 13 C-NMR of **26**





Figure S27. a) 1 H i b) 13 C-NMR of **27**



Figure S28. a) 1 H i b) 13 C-NMR of **30b**



Figure S29. a) 1 H i b) 13 C-NMR of **30c**



Figure S30. a) 1 H i b) 13 C-NMR of **31a**



Figure S31. a) 1 H i b) 13 C-NMR of **31b**



Figure S32. a) 1 H i b) 13 C-NMR of **31c**





Figure S33. a) 1 H i b) 13 C-NMR of **34a**

Figure S34. a) 1 H i b) 13 C-NMR of **34b**





Figure S35. a) 1 H i b) 13 C-NMR of **34c**





Figure S36. a) 1 H i b) 13 C-NMR of **35a**



Figure S37. a) 1 H i b) 13 C-NMR of **35b**





Figure S38. a) 1 H i b) 13 C-NMR of **35c**



