Supporting information

Design and synthesis of tricyclic terpenoid derivatives as novel PTP1B inhibitors with improved pharmacological property and in vivo antihyperglycemic efficacy

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Table of Contents

- 1. Cell viability in the MTT assay
- 2. The NMR spectra of compounds

Cell viability in the MTT assay

The toxicities of the compounds were evaluated by (3-(4, 5-dimethylthiazolyl-2)-2, 5-diphenyltetrazolium bromide) test. HepG2 cells were routinely grown in Dulbecco's Modified Eagle Medium (DMEM) supplemented with 10% (v/v) fetal bovine serum, streptomycin (100mg/mL), and penicillin (100U/mL), in a humidified atmosphere of 95% air, 5% CO₂ at 37°C. HepG2 cells were planked in a 96 well plate with a concentration of 1×10^4 cells/well and cultured in 37°C and 5%CO₂ for 24 h. Then HepG2 cells were treated with 40 µM of the synthetic compound. HepG2 cells untreated were used as control. HepG2 cells were cultured in 37°C and 5%CO₂ for 24 h, the old medium was carefully removed and were cultured for another 4 h in MTT (0.5%) containing DMEM, then the medium was carefully removed. 150 µL/well dimethyl sulfoxide was added and oscillated gently to make crystal dissolved. The absorbance at 560 nm was measured using a microplate reader. The cell viability was expressed as a percentage of OD560 (sample)/ OD560 (control) as shown in Fig.S1.



Fig. S1. Cell viability in the MTT assay.



The ¹H-NMR and ¹³C-NMR spectra of the compounds

¹H NMR (400 MHz, CDCl₃) spectrum of compound 3



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 3



¹H NMR (400 MHz, CDCl₃) spectrum of compound 4a



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 4a



¹H NMR (400 MHz, CDCl₃) spectrum of compound 4b



¹H NMR (400 MHz, DMSO) spectrum of compound 5



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 5



¹H NMR (400 MHz, CDCl₃) spectrum of compound 6a



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 6a



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 6b



¹H NMR (400 MHz, CDCl₃) spectrum of compound 7



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 7



¹H NMR (400 MHz, CDCl₃) spectrum of compound 11



¹H NMR (400 MHz, CDCl₃) spectrum of compound 13



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 13



¹H NMR (400 MHz, CDCl₃) spectrum of compound 14



 ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound 14



¹H NMR (400 MHz, CDCl₃) spectrum of compound 15



¹³C NMR ((300 MHz, CDCl₃) spectrum of compound 15



¹H NMR (400 MHz, CDCl₃) spectrum of compound 16



¹³C NMR ((300 MHz, CDCl₃) spectrum of compound 16



¹H NMR (400 MHz, CDCl₃) spectrum of compound 17



¹³C NMR ((300 MHz, CDCl₃) spectrum of compound 17



¹H NMR (400 MHz, CDCl3) spectrum of compound 18



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 18



¹H NMR (400 MHz, *d*₆-DMSO) spectrum of compound 19 ¹³C NMR (300 MHz, CDCl₃) spectrum of compound 19



¹H NMR (400 MHz, CDCl₃) spectrum of compound 20



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 20



¹H NMR (400 MHz, CDCl3) spectrum of compound 21 ¹³C NMR (300 MHz, CDCl₃) spectrum of compound 21



¹H NMR (400 MHz, CDCl₃) spectrum of compound 22



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 22



¹H NMR (400 MHz, CDCl₃) spectrum of compound 23



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 23



¹H NMR (400 MHz, CDCl₃) spectrum of compound 24



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 24



¹H NMR (400 MHz, CDCl₃) spectrum of compound 25



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 25



¹H NMR (400 MHz, CDCl₃) spectrum of compound 26



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 26



¹H NMR (400 MHz, CDCl₃) spectrum of compound 27 ¹³C NMR (300 MHz, CDCl₃) spectrum of compound 27



¹H NMR (400 MHz, CDCl₃) spectrum of compound 28



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 28



¹H NMR (400 MHz, CDCl₃) spectrum of compound 29



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 29



¹H NMR (400 MHz, CDCl₃) spectrum of compound 30



¹³C NMR (300 MHz, CDCl₃) spectrum of compound 30



¹H NMR (400 MHz, CDCl₃) spectrum of compound 31

¹³C NMR (300 MHz, CDCl₃) spectrum of compound 31

¹H NMR (400 MHz, CDCl₃) spectrum of compound 32

¹³C NMR (300 MHz, CDCl₃) spectrum of compound 32

¹H NMR (400 MHz, CDC₁₃) spectrum of compound 33

¹³C NMR (300 MHz, CDCl₃) spectrum of compound 33

¹H NMR (400 MHz, *d*₆-DMSO) spectrum of compound 34

¹³C NMR (300 MHz, *d*₆-DMSO) spectrum of compound 34