Supplementary Data

Metabolite identification of ursolic acid in mouse plasma and urine after oral administration by ultra-high performance liquid chromatography/quadrupole time-of-flight mass spectrometry

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No.	¹ H NMR	¹³ C NMR	No.	¹ H NMR	¹³ C NMR
1	1.67 1.00, 2m	39.3	16	2.05 1.10, 2m	22.8
2	1.81, 2m	27.9	17		45.4
3	3.44, dd	77.8	18	2.73, d	52.3
4	—	39.1	19	1.87. m	38.6
5	0.82, m	55.5	20	0.87, m	39.8
6	1.56, 2m	18.0	21	1.90, 2m	32.1
7	1.50 1.31, 2m	34.2	22	1.66, 2m	29.1
8	—	42.7	23	0.96, s	29.8
9	1.44, m	49.8	24	0.93, s	16.0
10		37.0	25	0.86, s	16.6
11	2.15 2.00, 2m	30.9	26	1.16, s	18.7
12	4.29, dd	68.9	27	1.26, s	17.3
13		94.8	28		179.5
14	—	43.7	29	1.03, d	16.3
15	2.05 1.22, 2m	28.4	30	0.88, d	19.3

Table S1. ¹H NMR and ¹³C NMR spectral data of compound 1 (measured in C_5D_5N).







Fig. S2 ¹H spectrum of compound 1.



Fig. S3 ¹³C spectrum of compound 1.



Fig. S4 DEPT 135 spectrum of compound 1.



Fig. S5 ¹H-MQC spectrum of compound 1.



Fig. S6 ¹H-MBC spectrum of compound 1.







Fig. S8 NOESY spectrum of compound 1.



Fig. S9 MS spectrum of compound 1.