Supporting Information

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Identification of Highly Potent and Selective α-Glucosidase Inhibitors with Antiglycation Potential, Isolated from *Rhododendron arboreum*.

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S1: General Considerations

The structures of the isolated compound was elucidated using different spectroscopic techniques including IH NMR, 13C-NMR, HMBC, HMQC, NOESY, COSY, HREI-MS and IR. UV-Visible spectra were recorded on a Perkins Elmer λ-EZ 201 spectrophotometer. Optical rotations were measured on a Jasco DIP-360 polarimeter. IR spectra were recorded in KBr disk on a Jasco 320-A spectrophotometer. The 1H, 13C NMR and related experiments such as COSY, NOESY, HSQC and HMBC were conducted on Bruker 400, 500 and 600 MHz spectrophotometers, respectively.

Mass spectrometry was performed using various ionization techniques like electron impact mass spectrum (EIMS), fast atom bombardment positive/negative spectrum (FAB +ve/FAB-ve), high resolution fast atom bombardment mass spectrum (HRFABMS) and GCMS spectrum measurements were performed on Varian Mat 312 and Jeol JMS -600H with GC and Jeol JMS HX 110 mass spectrometer. Melting points were determined in glass capillaries using Buchi 535 melting point apparatus. Optical rotations were measured on JASCO DIP-360 digital polarimeter.

S2: Spectroscopic Data of Compounds

(1) 3-*β*-acetoxyurs-11-en-13 *β*, 28-olide

White crystalline compound, Rf value = 0.5 (Acetone: n-hexane; 7:3), m.p = 250-251^{o}C, UV = 280 nm, HR-EIMS: m/z 496.7232 corresponds to the molecular formula $C_{32}H_{48}O_4$ (Calculated 496.7218). ^{1}H-NMR ($CDCl_3$, 600MHz) δ 5.92 (*d*, 1H, *J* = 10.2Hz, H-12), δ 5.5 (*dd*, 1H, *J* = 12Hz, H-11), δ 4.46 (*dd*, 1H, *J* = 12, 6Hz, H-3), δ 2.03 (s, 3H, H-2'), δ1.95 (s, 1H, H-9), δ1.94 (s, 1H, H-18), δ 1.75-1.77 (*m*, 2H, H-19, H-20), δ 1.14 (*s*, 6H, H-24 and H-26), δ 1.03 (*s*,3H, H-27), δ 0.84 (*s*, 6H, H-23 and H-25), δ 0.98 (*d*,3H, *J* = 6Hz, H-30) and δ 0.91 (*d*, 3H, *J* = 5.4 Hz, H-29). ^{13}C NMR (100 MHz, CDCl3) (Table S1) [1].

(2) 3-*O*-acetylbetulinic acid

White crystalline compound, m.p = 289^{o}C, UV (λ_{max}) 270 nm, IR (KBr) λ_{max} cm^{-1}: 2500-3500 (OH of COOH), 1729 (C=O of ester), (1698 C=O of acid), 1644 (C=C) and 1247 cm^{-1} (C-O). HR-EIMS: m/z 498.3710 correspond to the molecular formula $C_{32}H_{50}O_4$ (calculated 498.3768). ^{1}H-NMR ($CDCl_3$, 600MHz) δ 4.71 (*s*, 1H, Ha-29), δ 4.59 (*s*, 1H, Hb-29), δ 4.45

(*dd*, 1H, *J*=12, 6 Hz, H-3), δ 2.98 (*ddd*, 1H, *J*= 24, 12, 6 Hz, H-19), δ 2.2 (*s*, 3H, H-2'), 2.19 (*ddd*, 1H, *J*=24,18,6 Hz, H-18), δ 1.67 (s, 3H, H-30), δ 1.59 (*m*, 1H, H-13), δ 1.26 (*m*, 1H, H-9), δ 0.90- 0.91 (*s*, 9H, H-25, H-26, H-27), δ 0.77 (*d*, 1H, *J*= 12Hz, H-5), δ 0.7 (*s*, 1H, H-24) and 0.08 (*s*, 3H, H-23). ^{13}C NMR (150 MHz, CDCl3) (Table S1) [2]

(3) Betulin

White amorphous powder, Rf value = 0.54 (Ethyl acetate: Hexane; 8: 2), m.p. = 250-251^{o}C, UV (λ_{max}) 240 nm. IR (KBr) λ_{max} cm^{-1}: 3410 (for OH group) and 1635 cm^{-1}(C=C). HR-EIMS: m/z 442.3814 corresponding to the molecular formula $C_{30}H_{50}O_2$ (calculated 442.3810). ^{1}H-NMR ($CDCl_3$, 600MHz) δ 4.67 (s, 1H, Ha-29), δ 4.56 (s, 1H, Hb-29), 3.72 (d, 1H, *J*= 10.8Hz, Ha-28), δ 3.33 (d, 1H, *J*= 10.8 Hz, Hb-28), δ 3.1 (dd, 1H, *J*= 11.4, 4.8 Hz, H-3), δ 2.94 (m, 1H, H-19), δ 1.59 (t, 1H, *J* = 8 Hz, H-18), 1.59 (m, 1H, H-13), δ 0.96- 0.99 (s, 9H, H-23, H-26, H-27), δ 0.80 (s, 3H, H-25), 0.7 (d, 1H, *J* = 12Hz, H-5) and 0.7 (s, 3H, H-24). ^{13}C NMR (150 MHz, CDCl3) (Table S1) [3].

(4) Betulinic acid

White amorphous powder, Rf value = 0.55 (Methanol: Chloroform; 2: 8), m.p. = 278-280^{o}C, UV (λ_{max}) 284 nm. IR (KBr) λ_{max} cm^{-1}: 3456, 1686 and 1561 cm^{-1} indicating the presence of hydroxyl, carboxylic and olefinic groups respectively. HR-EIMS: m/z 456.7021 corresponds to the molecular formula $C_{30}H_{48}O_3$ (calculated 456.7003). ^{1}H-NMR ($CDCl_3$, 400MHz) δ 4.6 (*s*, 1H, Ha-29), δ 4.49 (*s*, 1H, Hb-29), δ 3.07 (*t*, 1H, *J* = 8Hz, H-3), δ 2.9 (*m*, 1H, H-19), δ 1.59 (*t*, 1H, *J* = 8Hz, H-18), δ 1.06 (*s*, 6H, H-23, H-27), δ 0.57 (*d*, 1H, *J* = 12Hz, H-5) and δ 0.7-0.63 (*s*, 12H, H-24, H-25, H-26, H-30).^{13}C NMR (100 MHz, CDCl3) (Table S1) [4].

(5) Ursolic acid

White amorphous powder, Rf = 0.31 (Methanol: Chloroform; 2: 8), m.p = 283ºC, UV (λ_{max}) = 270 nm. IR (KBr) λ_{max} cm^{-1}: 3510, 1697 and 1635 cm^{-1} indicating the presence of hydroxyl, carboxylic and olefinic groups respectively. HR-EIMS: m/z 456.3597 corresponds to the molecular formula $C_{30}H_{48}O_3$ (calculated 456.3622). ^{1}H-NMR ($CDCl_3$, 400MHz) δ 5.24 (*d*, 1H, *J* = 12 Hz, H-12), δ 3.19 (*dd*, 1H, *J* = 10.8, 4.4 Hz, H-3), δ 2.18 (*d*, 1H, *J* = 15 Hz, H-18), δ 1.06 (*s*, 3H, H-27), δ 0.91- 0.97 (*s*, 6H, H-23, H-24), δ 0.81 (*s*, 6H, H-25, H-26), δ 0.83 (*d*, 3H, *J* = 6.4Hz, H- 29) and δ 0.92 (*d*, 3H, *J* = 4.4Hz, H-30). ^{13}C NMR (100 MHz, CDCl3) (Table S1) [5].

(6) Lupeol

White amorphous powder, Rf = 0.72 (Ethyl acetate: Hexane; 3: 7), m.p = 213-214ºC, UV (λ_{max}) = 215 nm. IR (KBr) λ_{max} cm^{-1}: 3443, 3070, 1650 and 880 cm^{-1} for hydroxyl and C=CH_2 groups respectively. HR-EIMS: m/z 426.3835 corresponds to the molecular formula $C_{30}H_{50}O$ (calculated 426.3862). ^{1}H-NMR ($CDCl_3$, 500MHz) δ 4.63 (*m*, 2H, H-29), δ 3.64 (*dd*, 1H, *J* = 10.68, 4.27 Hz, H- 3), δ 2.8 (*m*, 1H, H-19), δ 1.64 (*s br*, 3H, H-30), δ 1.59 (*t*, 1H, *J* = 8Hz, H-18), δ 0.96 (*s*, 6H, H-25, H-27), δ 0.64-0.90 (*s*, 12H, H-23, H-24, H-26, H-28) and δ 0.57 (*d*, 1H, *J* = 12Hz, H-5). ^{13}C NMR (125 MHz, CDCl3) (Table S1) [6].

(7) 3-*O*-acetylursolic acid

White amorphous powder, Rf= 0.7(Chloroform: Hexane; 7: 3), m.p = 209 ºC, UV (λ_{max}) = 289 nm. IR (KBr) λ_{max} cm^{-1}: 2390 (C-H), 1710 (ester), 1680 (C=O) and 1561 cm^{-1} (C=C) groups respectively. HREI-MS: m/z 498.3710 corresponds to the molecular formula $C_{32}H_{50}O_4$ (calculated 498.3709). ^{1}H-NMR (600 MHz, CDCl3) δ 4.47 (*dd*, 1H, *J* = 4.4, 10.8 Hz, H- 3), δ 0.83 (*t*, 1H, *J* =12.0 Hz, H-5), δ 5.24 (*d*, 1H, *J* = 24 Hz, H-12), δ 2.15 (*d*,1H, *J* = 12 Hz, H-18), δ 1.33(*m*, 1H, H-19), δ 0.73 (*d*, 3H,*J* = 12 Hz, H-29), δ 0.93 (*d*,3H, *J* = 12 Hz, H-30), δ 0.81-1.06 (*s*, 15H, H-23, H-24, H-25, H-26, H-27) and δ 2.24 (*s*, 3H, H-2'). ^{13}C NMR ($CDCl_3$, 150 MHz) (Table S1) [7].

(8) *β*-sitosterol-3-*O*- *β*-D-glucosidose

Colorless amorphous powder, m.p = 281-283 ºC, IR (KBr) λ_{max} cm^{-1}: 3458 (OH), 1646 (C=C) groups respectively. HREI-MS: m/z 576.3041 corresponds to the molecular formula $C_{32}H_{50}O_4$ (calculated 576.3021). ^{1}H-NMR (300 MHz, CD_3OD) δ 5.29 (*d*, 1H, *J* = 7.18 Hz, H-1'), δ 5.29 (*d*, 1H, *J* = 5.4 Hz, H-6), δ 3.9 (*m*, 1H, H-3), δ 1.01 (*s*, 3H, H-19), δ 0.93 (*d*, 3H, *J* = 6.3 Hz, H-21), δ 0.84 (*t*, 3H, *J* = 6.99 Hz, H-29), δ 0.83 (*d*, 3H, *J* = 6.5 Hz, H-26), δ 0.80 (*d*, 3H, *J* = 6.5 Hz, H-27) and δ 0.67 (*s*, 3H, H-18). ^{13}C NMR (CD_3OD, 125 MHz) (Table S1) [8].

S3 : ^{13}C-NMR of compounds **1, 2, 3, 4, 5, 6, 7** and **8** (100 and 150 MHz, $CDCl_3$).

C.NO.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	37.91	38.34	40.03	38.68	38.63	38.78	38.16	38.71
2	27.69	23.66	27.90	27.77	28.04	27.3	28.0	29.92
3	80.59	80.91	79.63	78.75	79.06	78.75	80.89	80.94
4	41.64	37.76	38.86	38.71	38.77	38.81	39.19	43.92
5	54.79	55.38	55.64	55.30	55.25	55.30	55.20	143.0
6	17.52	18.13	18.6	18.2	18.3	18.3	18.08	122.10
7	31.28	34.20	35.09	34.25	30.62	34.25	32.72	33.03
8	41.87	40.64	42.12	40.59	39.53	40.87	39.40	31.99
9	52.89	50.32	51.86	50.48	47.56	50.48	47.36	50.42
10	36.23	37.07	37.5	37.5	37.03	37.4	37.64	37.17
11	128.88	20.82	21.80	20.80	23.6	20.80	23.95	21.51
12	133.28	25.40	26.57	26.91	125.89	25.91	125.65	40.83
13	89.66	49.21	49.15	49.14	137.9	39.14	137.88	43.01
14	41.87	42.37	43.17	42.35	42.0	42.65	41.78	56.93
15	25.48	30.49	30.42	30.5	28.04	27.5	27.90	25.84
16	23.28	32.10	28.14	32.18	27.25	35.18	23.95	29.72
17	45.05	56.26	47.89	56.13	47.93	42.93	47.90	56.55
18	52.89	38.34	38.68	38.68	52.7	48.18	52.38	12.21
19	38.07	46.88	48.9	46.9	38.84	46.9	38.75	19.52

20	37.22	150.36	151.87	150.67	39.06	150.67	38.94	37.24
21	30.76	29.65	30.34	29.5	24.17	29.8	30.53	19.71
22	31.11	36.99	35.37	37.2	32.96	39.87	37.98	39.56
23	27.69	27.91	29.63	29.58	28.15	28.58	28.03	29.51
24	16.06	15.99	15.18	15.96	15.58	15.46	15.50	50.5
25	17.52	16.44	16.13	15.76	16.47	15.76	16.67	26.10
26	18.90	15.16	16.21	15.21	17.08	15.9	17.04	18.21
27	19.15	14.62	14.53	14.53	23.6	14.53	23.56	20.14
28	179.97	180.59	60.31	178.98	181.4	18.18	184.21	23.73
29	17.86	109.75	110.27	109.33	17.08	109.33	17.0	11.90
30	17.96	19.31	19.34	19.16	21.16	19.16	21.17	-
1’	171.06	171.09	-	-	-	-	171.08	102.95
2’	21.33	21.32	-	-	-	-	21.33	74.21
	-	-	-	-	-	-	-	76.79
	-	-	-	-	-	-	-	71.2
	-	-	-	-	-	-	-	76.62
	-	-	-	-	-	-	-	62.3

S4 : References

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