

Figure 2. Chemical structures of the isolated compounds from the seeds of *S. obassia*.

Table 1. 1D^a and 2D NMR data in CDCl₃ for compound **1**

C/H	DEPT	δ_C	δ_H	J (Hz)	COSY	HMBC (H → C)
2	C	156.1	—	—	—	—
3	CH	100.3	6.78, <i>s</i>	—	—	C-2/C-8/C-9
4	CH	112.3	6.95, <i>s</i>	—	—	C-3/C-6/C-8
5	C	136.9	—	—	—	—
6	CH	107.4	6.60, <i>s</i>	—	—	C-7/C-8
7	C	144.7	—	—	—	—
8	C	142.5	—	—	—	—
9	C	131.0	—	—	—	—
1'	C	124.6	—	—	—	—
2'	CH	105.5	7.31, <i>d</i>	1.5	—	C-2/C-3'/C-4'
3'	C	148.0	—	—	—	—
4'	C	147.9	—	—	—	—
5'	CH	108.5	6.87, <i>d</i>	8.5	H-6'	C-1'/C-3'/C-4'
6'	CH	119.2	7.40, <i>dd</i>	1.5, 8.5	H-5'	C-2/C-4'
OCH ₂ O	CH ₂	101.2	6.00, <i>s</i>	—	—	C-3'/C-4'
1''	CH ₂	32.4	2.74, <i>t</i>	7.5	H-2''	C-4/C-5/C-6/C-2''/C-3''
2''	CH ₂	30.7	2.00, <i>m</i>	—	H-1'', H-3''	C-5/C-1''/C-3''
3''	CH ₂	63.6	4.13, <i>t</i>	6.5	H-2''	C-1''/C-1a
OMe	CH ₃	56.1	4.03, <i>s</i>	—	—	C-7
1a	C	174.5	—	—	—	—
2a	CH ₂	27.6	2.34, <i>q</i>	7.5	H-3a	C-1a/C-3a
3a	CH ₃	9.2	1.15, <i>t</i>	7.5	H-2a	C-1a/C-2a

^a1H and ¹³C NMR recorded at 500 and 125 MHz, respectively.

elucidated as egonol propanoate.

Known compounds (**2–5**) (Figure 2) were identified by comparison of their spectral data with literature values as follow: egonol^{6,8,9} (**2**), egonolacetate^{6,8,9} (**3**), egonol-2-methylbutanoate^{6,8,9} (**4**) and 7-demethoxyegonol-2-methylbutanoate^{6,8} (**5**).

Experimental Section

General Methods. Melting points were determined on an Electrothermal IA-9200 melting point apparatus (Electrothermal Engg. Ltd. U.K.) and are uncorrected. Optical rotations were taken on a Jasco P1020 polarimeter. UV spectra were recorded on a Hewlett Packard 8452A Diode Array Spectrophotometer. IR spectra were recorded in KBr with a NEXUS FT-IR spectrophotometer. EIMS and HREIMS were obtained with a JEOL JMS-SX102A spectrophotometer. ¹H NMR (500 MHz), ¹³C NMR (125 MHz), DEPT, COSY, HMQC, and HMBC spectra were obtained with a Varian Unity-Inova 500 spectrophotometer. The NMR samples were prepared in CDCl₃/DMSO with tetramethylsilane (TMS) as an internal standard. The chemical shifts and coupling constants (J) were expressed in δ and Hz, respectively. Thin layer chromatography (TLC) was carried out on pre-coated Silica gel 60 F₂₅₄ (0.2 mm, Merck, Germany) plates. Preparative thin layer chromatography was carried out on pre-coated Silica gel 60 F₂₅₄ (20 × 20 cm², 2.0 mm, Merck, Germany) plates. TLC plates were developed with solvent system A (toluene/ethyl formate/formic acid = 20:2:1, v/v/v) and B (*n*-hexane/ethyl acetate/

toluene = 8:1:1, v/v/v). Developed TLC plates were visualized under UV light at 254 and 365 nm. Silica gel 60 (40–100 μ m, Kanto Chemical Co. Japan) was used for the column chromatography. An ADVENTEC SF-1600 was used as the automated fraction collector in the column chromatography.

Plant Material. The fruits of *S. obassia* were collected from Jiri mountain (Hadong-kun) in Kyungnam, Korea in September, 2004 and identified by Dr. Y. H. Kwon (Korea National Arboretum, Pocheon, Korea). A voucher specimen has deposited at the Korea Forest Research Institute, Seoul, Korea.

Extraction and Isolation. 8.0 Kg of air-dried and powdered seeds of *S. obassia* were extracted three times with MeOH at room temperature for 72 hrs each. The combined MeOH extracts were concentrated under vacuum at 40 °C until MeOH was completely removed. The concentrated MeOH extract was dissolved in distilled water and successively partitioned with *n*-hexane, dichloromethane and ethyl acetate.

Column chromatography of an oily mass from *n*-hexane soluble fraction on silica column gave 93 fractions (250 mL each) in benzene:ethyl acetate (20:1, v/v). On the basis of TLC profiles, these fractions are divided into four groups. Group one (46.6 g) was chromatographed on silica gel column using *n*-hexane:ethyl acetate (17:1, v/v) as an eluent to collect nine fractions (100 mL each), and then column was washed with MeOH to give an oily mass (43.7 g). Fraction 2 formed some precipitate which was washed with MeOH to give a pure compound **3** (3.7 g). At the same time, fraction 7 was purified by preparative TLC in *n*-hexane:

ethyl acetate (5:1, v/v) to give a pure compound **4** (40 mg). The oily mass (43.7 g) upon silica gel column chromatography in *n*-hexane:ethyl acetate (15:1, v/v) gave 85 fractions (250 mL each). TLC profiles of these fractions led them to divide into four groups. Group one (10.0 g) was chromatographed on silica column in *n*-hexane:chloroform:ethyl acetate (23:1:1, v/v/v) to give three fractions. Rechromatography of fraction 2 (3.5 g) on silica column in chloroform:toluene:ethyl acetate (17:1:1, v/v/v) gave pure compound **5** (88.8 mg). On the other hand, group four (1.36 g) was chromatographed on silica gel column using *n*-hexane:benzene:ethyl acetate (8:1:1, v/v/v) as an eluent to yield 80 fractions (4.0 g each by a fraction collector). On the basis of TLC profiles these fractions are divided into three parts. Part two (255 mg) was finally chromatographed using chloroform:toluene:ethyl acetate (8:1:1, v/v/v) as an eluent on silica to give a pure compound **1** (42.7 mg).

The ethyl acetate solubles (122.7 g) from MeOH extract was chromatographed on silica column with increasing polarity of *n*-hexane:ethyl acetate:acetone (9:2:1 → 5:2:1 → 3:2:1 → 1:2:2, v/v/v) to collect five fractions. Fraction 3 was concentrated to produce a powdery mass which was washed with toluene, benzene and finally with ethyl acetate. The ethyl acetate soluble part produced pure compound **2** (1.08 g).

5-(3''-Propanoyloxypropyl)-7-methoxy-2-(3',4'-methylenedioxyphenyl)-benzofuran (1): Colourless crystal. m.p. 86–87 °C. $[\alpha]_D^{20.4} +4.7^\circ$ (c = 0.22, CHCl₃). UV (CHCl₃) λ_{\max} nm (log ϵ): 242 (3.9), 318 (4.3). IR (KBr) ν_{\max} : 2954, 1738, 1601, 1481, 1371, 1232, 1190, 1038, 941 and 812 cm⁻¹. EIMS *m/z*: 382 ([M]⁺, base ion), 308, 282, 267 and 251. HREIMS *m/z*: 382.1416 ([M]⁺, calcd. for C₂₂H₂₂O₆, 382.1414). ¹H NMR (CDCl₃, 500 MHz), ¹³C NMR (CDCl₃, 125 MHz), COSY and HMBC see Table 1.

Egonol (2): White powder. m.p. 112–113 °C (lit.⁸ 113–115 °C). EIMS *m/z*: 326 ([M]⁺). UV, IR, ¹H and ¹³C NMR data are in agreement with literature.^{6,8,9}

Egonolacetate (3): Yellowish powder. m.p. 104–105 °C (lit.⁸ 103–105 °C). EIMS *m/z*: 368 ([M]⁺). UV, IR, ¹H and ¹³C NMR data are in agreement with literature.^{6,8,9}

Egonol-2-methylbutanoate (4): Pale yellow oil. EIMS

m/z: 410 ([M]⁺). UV, IR, ¹H and ¹³C NMR data are in agreement with literature.^{6,8,9}

7-Demethoxyegonol-2-methylbutanoate (5): Colourless needles. m.p. 54–55 °C (lit.⁶ 55.5–56 °C). EIMS *m/z*: 380 ([M]⁺). UV, IR, ¹H NMR data are in agreement with literature.^{6,8} ¹³C NMR (125 MHz, CDCl₃): δ 11.6*q* (C-4a), 16.6*q* (C-5a), 26.8*t* (C-3a), 30.9*t* (C-2''), 32.1*t* (C-1''), 41.1*d* (C-2a), 63.4*t* (C-3''), 100.0*d* (C-3), 101.3*t* (-O-CH₂-O-), 105.4*d* (C-2'), 108.6*d* (C-5'), 110.7*d* (C-7), 119.1*d* (C-6'), 120.0*d* (C-4), 124.5*d* (C-6), 124.8*s* (C-1'), 129.5*s* (C-9), 135.9*s* (C-5), 148.0*s* (C-4'), 148.1*s* (C-3'), 153.4*s* (C-8), 156.0*s* (C-2), 176.8*s*, (C-1a).

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