Supporting Information to:

Apparently no Sedative Benzoflavone Moiety in Passiflorae Herba

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Extraction and Fractionation

In the pre-screening 20 g of the pulverized drug samples 1, 2 and 3 were successively pre-extracted at 60°C for 20 min. with petroleum ether (three times with 100 mL, each), chloroform (three times with 100 mL, each) and methanol (ten times with 100 mL, each). The extracts were evaporated under reduced pressure. The dried methanolic extract was further extracted with n-butanol, petroleum ether and chloroform (five times with 10 mL of each solvent). Each residue of the methanolic extracts (sample 1 = 3.52 g; sample 2 = 2.66 g; sample 3 = 4.50 g) was fractionated by vacuum liquid chromatography (VLC; column diameter 2 cm; length 45 cm) on ICN silica 60 using chloroform, chloroform-methanol mixtures of increasing polarity (95+5; 90+10; 85+15; 80+20; 70+30; 50+50; 20+80) and methanol as mobile phase. The elution was performed with three volumes of 80 mL of each solvent, resulting in 27 fractions.

For the isolation of the BZF-like compound 210 g of pulverized sample 2 from Italy were extracted 4 times with 1500 mL petroleum ether, 4 times with 1500 mL chloroform and finally three times 1500 mL n-butanol. Each extraction step was performed for 1 hour under reflux. The combined extracts of the same solvent were evaporated to dryness and resulted in 6.74 g of petroleum ether extract (F 3.1.), 4.25 g chloroform extract (F 3.2.) and 8.20 g n-butanol extract (F 3.3.). The compounds of interest (bands X) were enriched in F 3.1. and F3.3., which were further fractionated by VLC on ICN silica 60 A (column diameter 2.5 cm; length 85 cm) using petroleum ether-ethyl acetate-acetone (13+2+1) as mobile phase. 125 fractions of 10 mL/30 min were collected and combined to 12 fractions. Bands X were enriched in fractions 8 (61 mg) and 9 (118 mg). By extraction with petroleum ether polar accompanying substances were removed, finally resulting in 96 mg of the enriched fraction with bands X. By subsequent CC on Sephadex® LH 20 (column diameter 1.5 cm; length 55 cm) with ethyl acetate (15 fractions of 2 mL/30 min) the blue fluorescent BZF-like compound was enriched in fractions 6 to 9 (24 mg). By preparative TLC on silica plates using petroleum ether – toluol – ethyl acetate – acetone (13+4+2+1) as mobile phase 3.3 mg of this blue fluorescent compound were obtained.

Extraction of extract KY705P was performed by accelerated solvent extraction (ASE) on a ASE 200 instrument (Dionex) in 33 mL cartridges. The cartridges were preheated for 5 min.
to 40°C followed by three cycles of extraction for 4 min. at 150 bar and 40°C with petroleum ether. From 610 g of the extract 1.22 g of petroleum ether fraction were collected. CC on Sephadex® LH 20 (column diameter 2 cm; length 28 cm) with ethyl acetate (45 fractions of 3 mL/30 min) resulted in two collective fractions (A 190 mg and B 130 mg) showing two BZF-like blue fluorescent compounds besides high amounts of accompanying substances. CC of fraction A (column diameter 1 cm; length 60 cm) on silica 60 with petroleum ether-ethyl acetate-acetone (13+2+1) resulted in the isolation of the chromatographically homogenous compound A (1.3 mg). By CC of fraction B under the same conditions 5 mg of compound B were isolated.

**NMR Measurements**

NMR spectra were recorded on a Bruker Avance DRX 600 NMR spectrometer using a 5 mm switchable quadruple probe (QNP, $^1$H, $^{13}$C, $^{19}$F, $^{31}$P) with z axis gradients, automatic tuning and matching accessory. Resonance frequency for $^1$H NMR 600.13 MHz, for $^{13}$C NMR 150.92 MHz; solvent: deuterated chloroform at 298 K. Standard 1D and gradient-enhanced (ge) 2D experiments (double quantum filtered (DQF) COSY, TOCSY, NOESY, HSQC, and HMBC) were used as supplied by the manufacturer. Chemical shifts referenced internally to the residual, non-deuterated solvent signal for $^1$H ($\delta = 7.26$ ppm) or to the carbon signal of the solvent for $^{13}$C ($\delta = 77.00$ ppm).
**Fig. 1S** TLC of BZF-like compounds on silica plate; mobile phase: petroleum ether-toluene-ethyl acetate-acetone (13+4+2+1); detection under UV$_{366}$nm.

**Fig. 2S** Structure and $^{13}$C-NMR data of phytol isomer.

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Fig. 3S $^1$H-NMR of phytol isomer

Fig. 4S $^{13}$C-NMR of phytol isomer.
**Fig. 5S** HMBC of phytol isomer.

**Fig. 6S** HSQC of phytol isomer.