Supporting Information

Profiling of the Resin Glycoside Content of Mexican Jalap Roots with Purgative Activity

Rogelio Pereda-Miranda,[*,‡] Mabel Fragoso-Serrano,[‡] Edgar Escalante-Sánchez,[‡] Beatriz Hernández-Carlos,[‡] Edelmira Linares[§] and Robert Bye[§]

[‡]*Departamento de Farmacia, Facultad de Química, Universidad Nacional Autónoma de México, Ciudad Universitaria, Mexico City 04510 DF, and* [§]*Jardín Botánico, Instituto de Biología, Universidad Nacional Autónoma de México, Ciudad Universitaria, Mexico City 04510 DF, Mexico*

pereda@servidor.unam.mx

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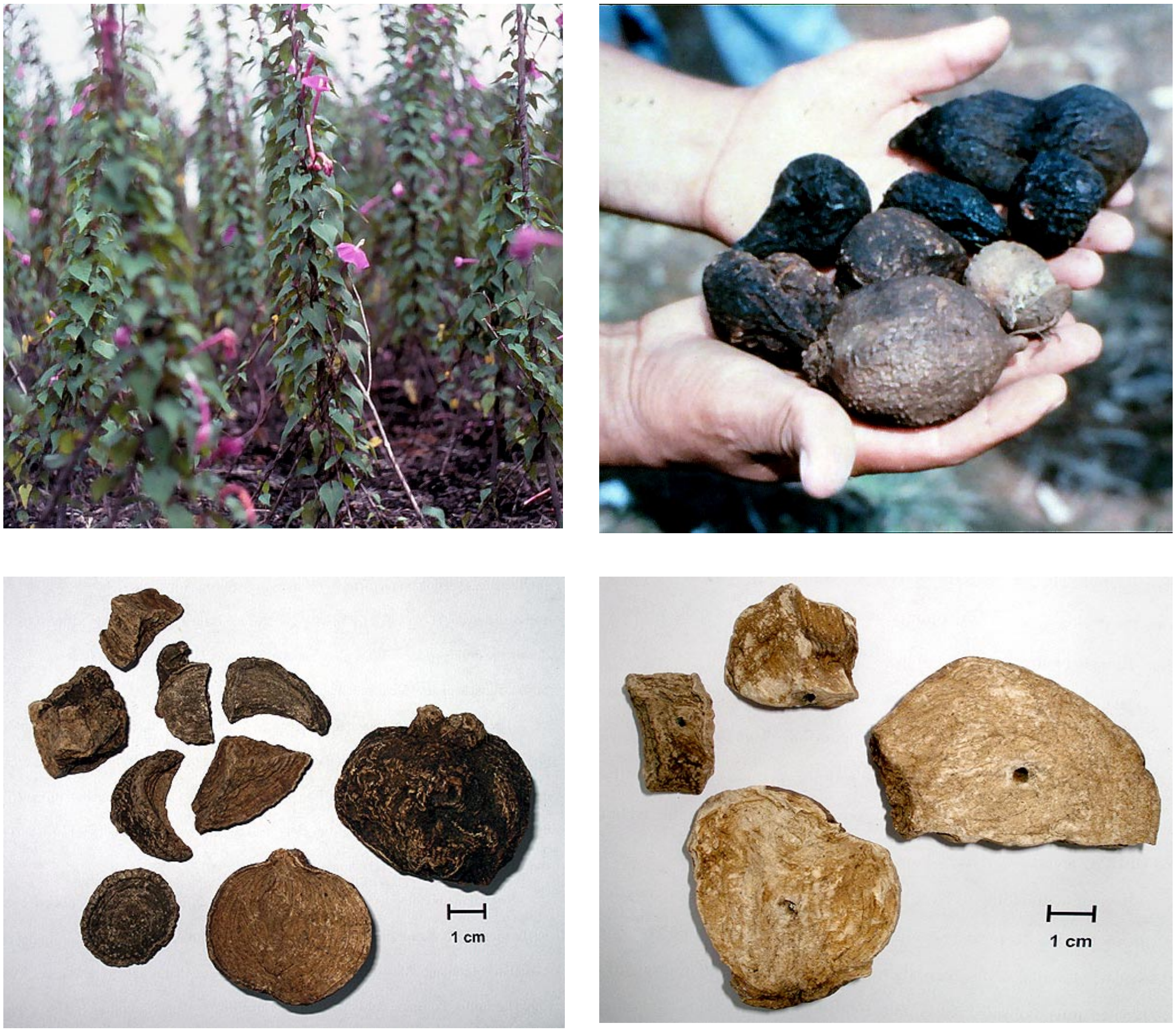

Figure S1. Jalap ("Rhizoma Jalapae"), the root of *Ipomoea purga*. The root of this evergreen vine has been used as a laxative or purgative since prehispanic times in Mexico. It is one of several distantly related tuberous New World *Ipomoea* species, including, *I. orizabensis*, *I. stans*, *I. jalapa*, and *I. simulans*, that are the source of a group of valued purgative remedies known as "jalaps". *Upper left*: Traditional production system of the jalap root in Central Veracruz, Mexico; *Upper right*: Fresh and smoke-dried roots; sample code: IP (Photographs courtesy of Biologist Alberto Linajes). *Above*: "Rhizoma Jalapae": The drug actually consists of the dried, usually fragmented, rhizomes. The ochre-yellow to dark brownish pieces often have a powdery surface and a characteristically faint smoky odor and a somewhat acrid, sweetish taste (authenticated commercial drug, *left*: sample code, IP-1; *right*: sample code, IP-2. Photographs by Dr. Rogelio Pereda-Miranda).

Figure S2. Mexican scammony or false jalap, the root of *Ipomoea orizabensis*. The Orizaba jalap is considered to be a less drastic purgative, hence its common name of “light jalap”. It is also known as woody or “male jalap” (“purga macho”). As a replacement for *I. purga* (“female jalap”: “purga hembra”), Mexican scammony root has been employed as a purgative, a vermifuge as well as a remedy for the treatment of abdominal inflammation, dysentery, epilepsy, hydrocephaly, meningitis, and tumors. *Above*: This root is fusiform and very large, being from 2 to 4 feet in length, and from 2 to 6 inches in diameter. In commercial form, this drug is sold in transverse slices, rectangular blocks or powder (Photographs by Dr. Rogelio Pereda-Miranda).

Figure S3. "Tumbavaquero", the root of *Ipomoea stans*. "Tumbavaquero", a Spanish composite word, literally means "knock the cowboy over" or "cowboy stunner". As an infusion it is used to treat convulsions, hypertension, epilepsy, Saint Vitus' dance and other nervous afflictions. *Upper left*: This perennial plant grows from a large woody root, often the size of a man's leg, with several protruding erect stems (0.3 to 1.2 m). *Upper right*: Purple flowers, large campanulate corolla, with white toward the base, 2 or 3 inches long (Photographs by Dr. Robert Bye). *Above*: Dried fragmented roots of the commercial crude drug which is easily found in herbal markets and health food stores in Mexico (Photograph by Dr. Rogelio Pereda-Miranda).

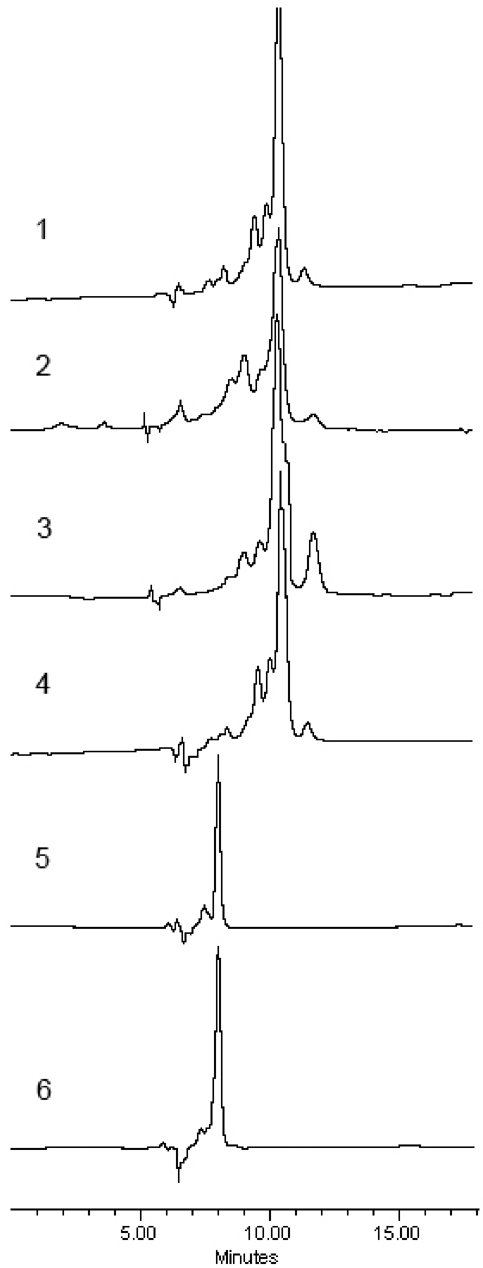

Figure S4. HPLC profiles of crude drug extracts from Mexican jalap samples. Instrumental conditions: stationary phase, standard column for carbohydrate analysis (3.9 × 300 mm, 10 μm; Waters); mobile phase, CH_3CN-H_2O (4:1); flow rate, 0.5 mL/min; sample injection, 10 μL (concentration: 10 mg/mL); detection: refractive index. Sample code assigments: **1**, IP (*Ipomoea purga*); **2**, IP-1; **3**, IP-2; **4**, IP-3; **5**, IO-1 (*Ipomoea orizabensis*); and **6**, IO-2. Saponified extracts were alkylated with CH_2N_2 and directly analyzed by HPLC.

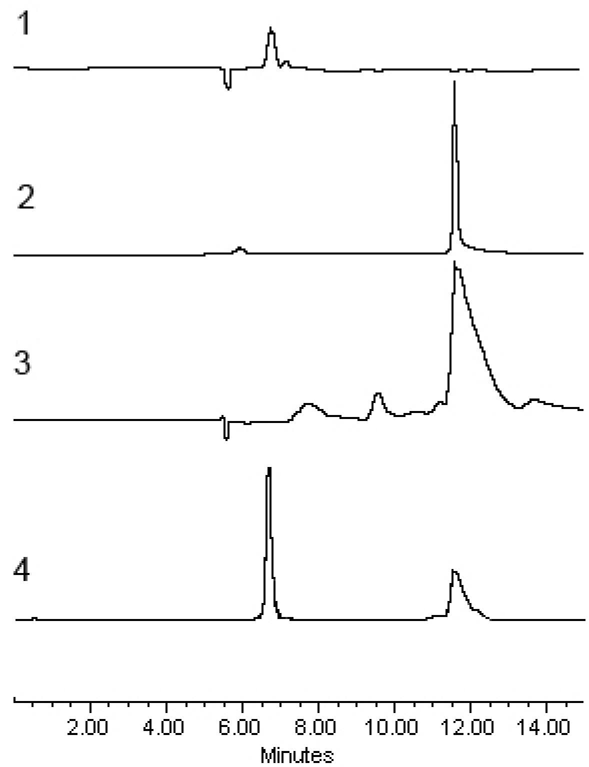

Figure S5. HPLC profiles of crude drug extracts from different root samples of "tumbavaquero". Instrumental conditions: standard column for carbohydrate analysis (3.9 × 300 mm, 10 μm; Waters); mobile phase, CH_3CN-H_2O (3:2); flow rate, 0.5 mL/min; sample injection, 10 μL (concentration: 10 mg/mL); detection: refractive index or UV. Sample code assigments: **1**, IO (*Ipomoea orizabensis*); **2**, IS (*Ipomoea stans*), UV detection (210 nm); **3**, IS-1; and **4**, IS-2.

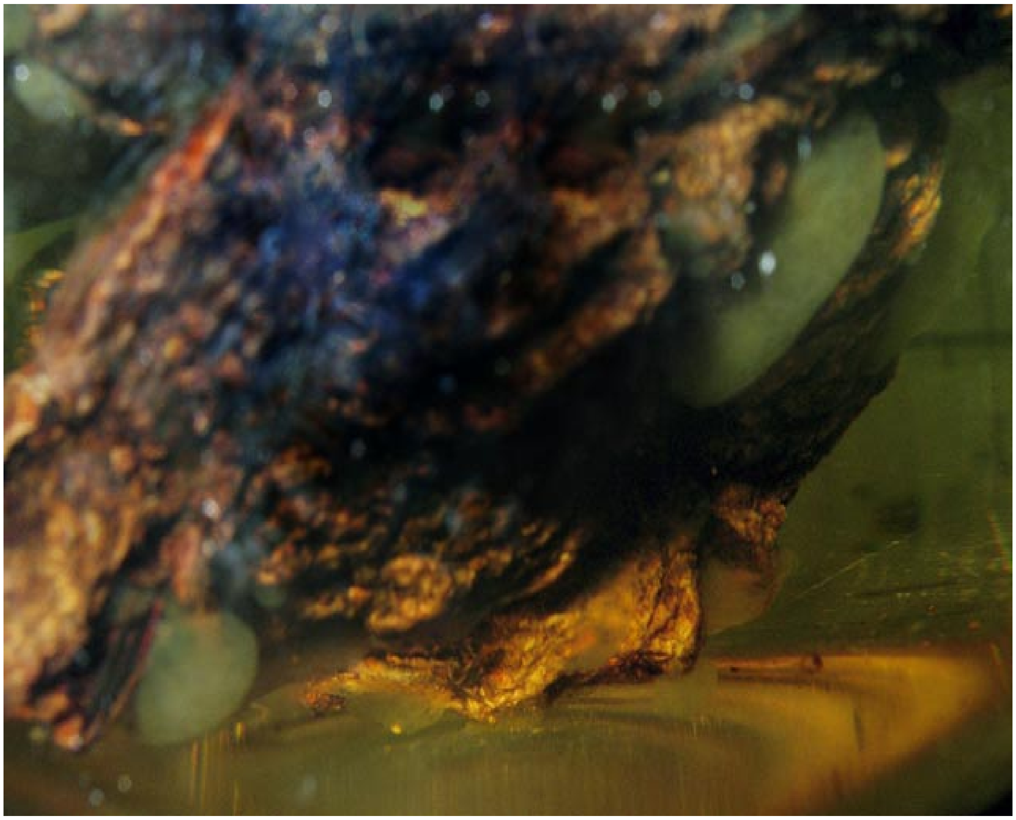

Figure S6. Extraction of polar resin glycosides from an authenticated commercial jalap root. Drops of translucent greenish-yellow MeOH-soluble resins in the process of being exuded from smoked-dried jalap root soaked in $CHCl_3$. The ratio of “jalapin” (ether soluble) to “convolvulin” (alcohol soluble) portion is used to distinguish each member of the medicinal plant complex of Mexican jalaps: jalap root (*Ipomoea purga*) yields the highest amount of MeOH-soluble resin glycosides (15-20 % dried weigth), Mexican scammony or false jalap (*Ipomoea orizabensis*) 10-18 % of “jalapin”, and the root of “tumbavaquero” (*Ipomoea stans*) < 1% of total resin glycoside content (Photograph by Dr. Rogelio Pereda-Miranda).

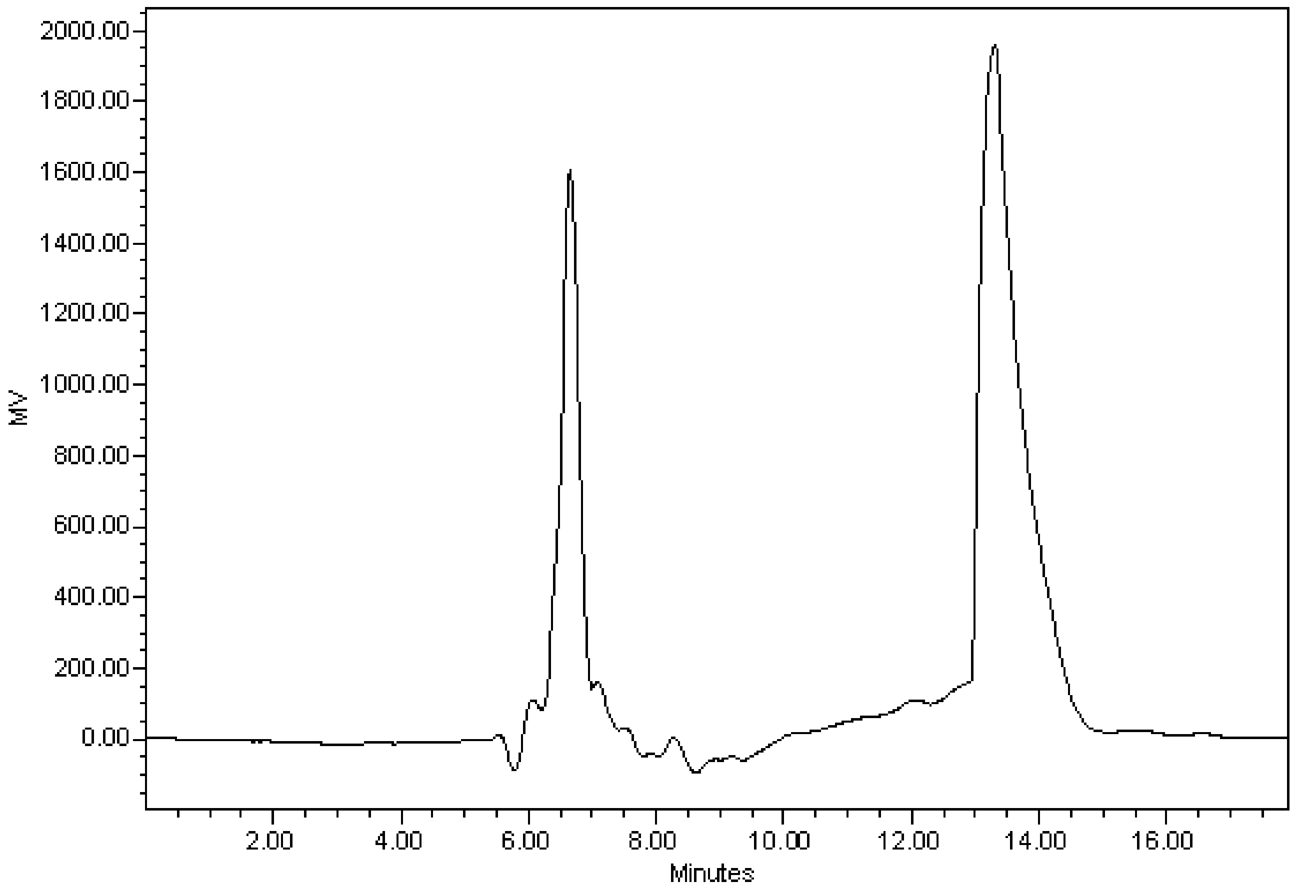

Figure S7. Semi-preparative HPLC purification of purgic acids A (1) and B (2). Instrumental conditions: column, μBondapak NH_2 (7.8 × 300 mm, 10 μm; Waters); mobile phase, CH_3CN-H_2O (4:1); flow rate, 3 mL/min; sample injection, 500 μL (concentration: 20-100 mg/mL); detection: refractive index. Retention time assigments: 13.9 min, purgic acid A (**1**); 6.6 min, purgic acid B (**2**).

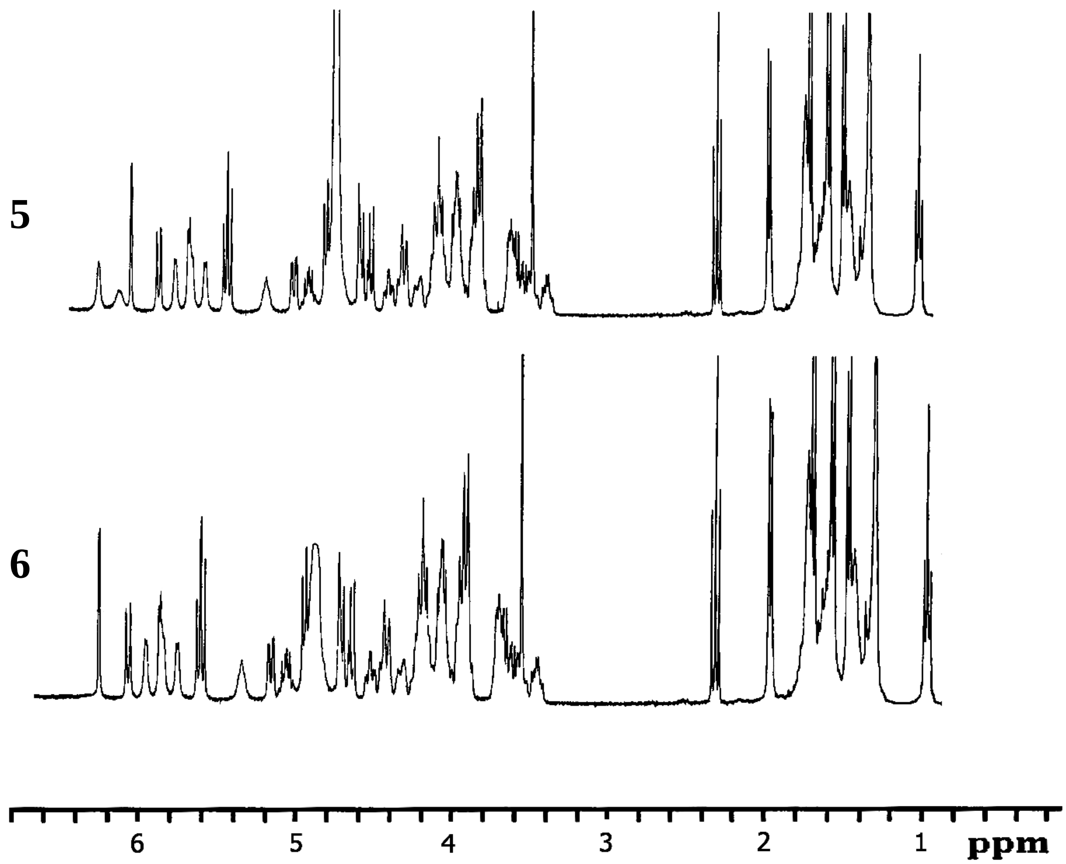

Figure S8. ^{1}H NMR spectra of purgic acid A methyl ester (5) and purgic acid B methyl ester (6). High field (500 MHz) ^{1}H NMR spectra of compounds (**5**) and (**6**) at 25 °C in pyridine-d_5.

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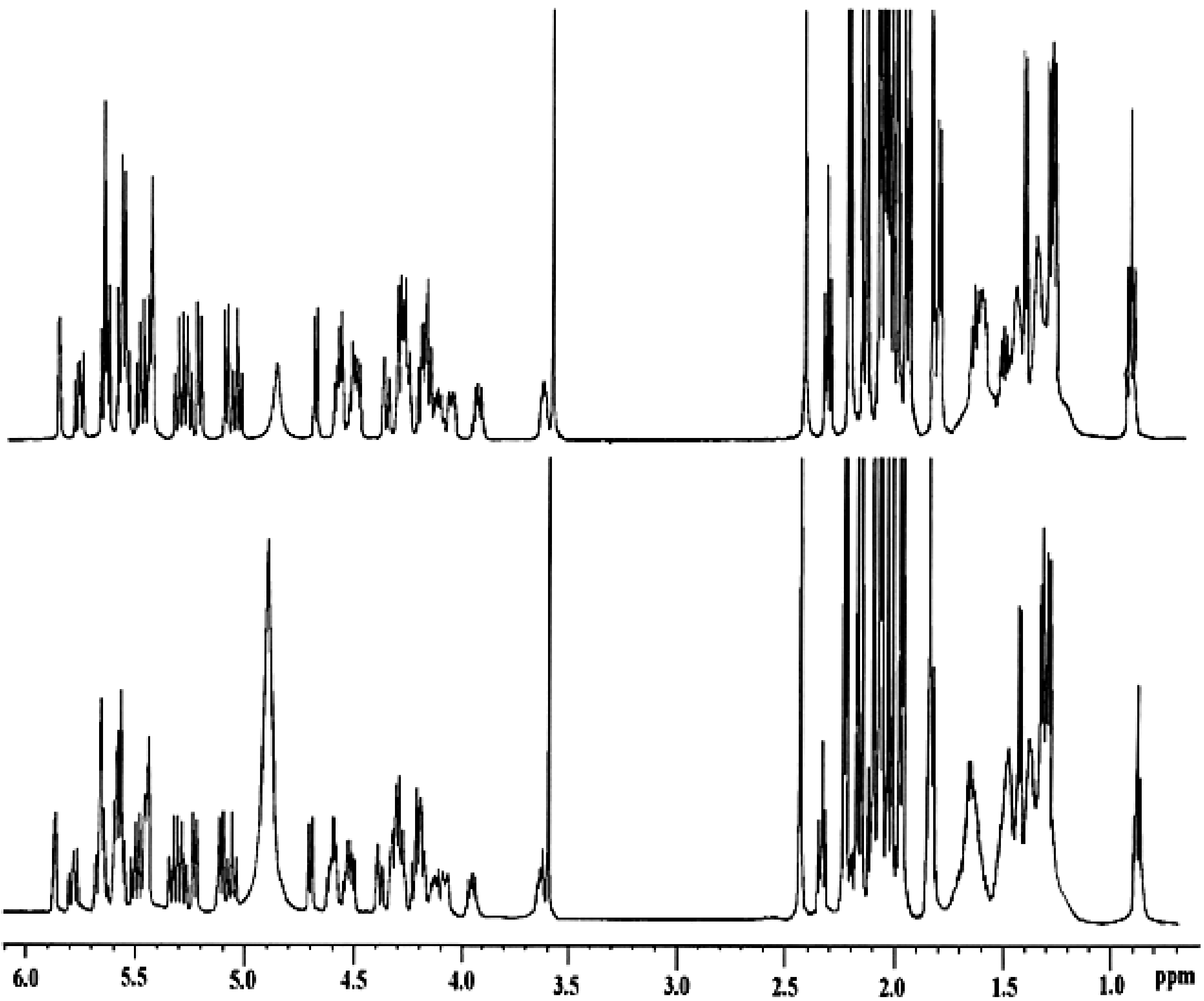

Figure S9. [1]H NMR spectra of peracetylated derivatives 7 and 8. High field (500 MHz) ^{1}H NMR spectra of peracetylated purgic acid A methyl ester (**7**) and peracetylated purgic acid B methyl ester (**8**) at 25 °C in pyridine-d_5.

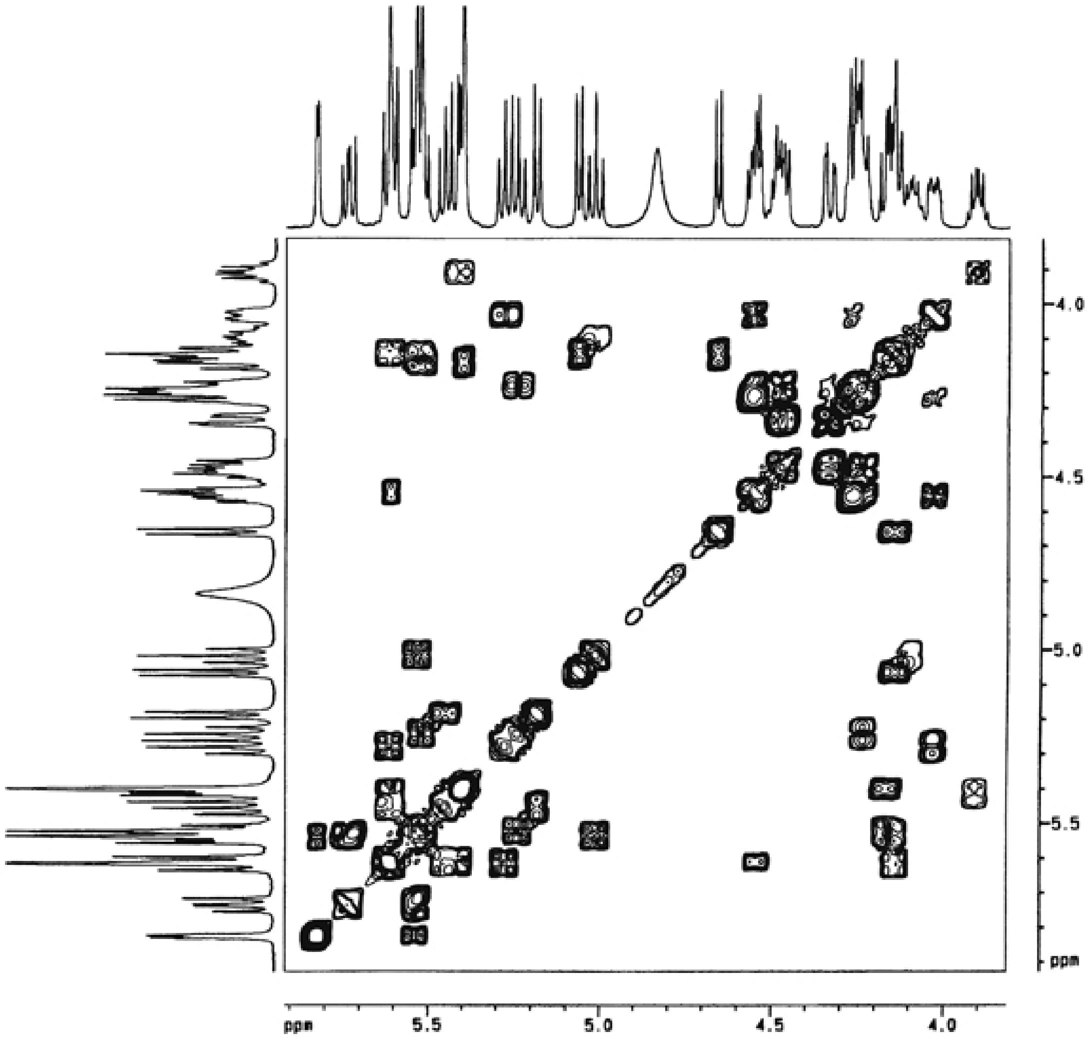

Figure S10. COSY spectrum of derivative 7. Expanded region of COSY NMR spectrum with high resolution 1-D projection for the oligosaccharide core of peracetylated purgic acid A methyl ester (**7**) at 25 °C in pyridine-d_5.

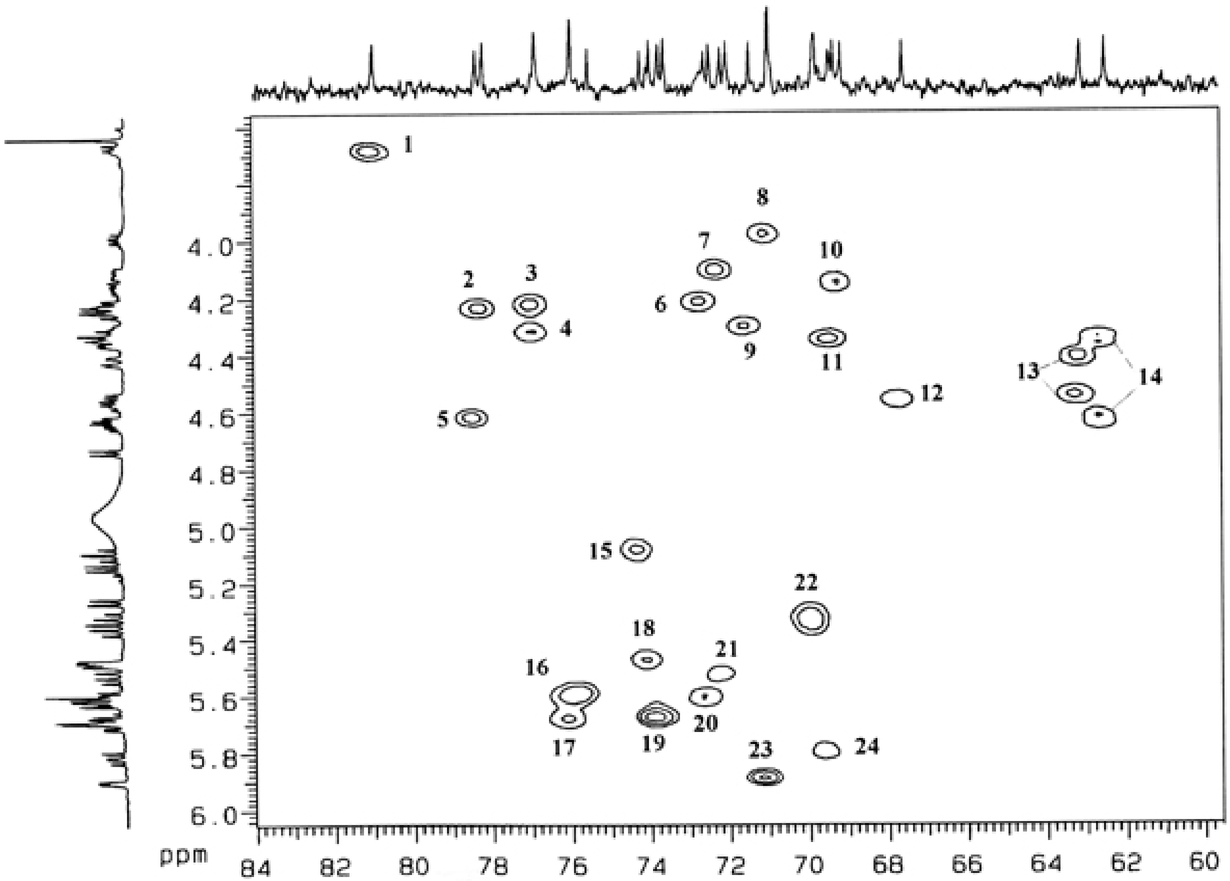

Figure 11. HMQC NMR spectrum of derivative 8. Expanded region ^{1}H-detected heteronuclear ($^{1}J_{CH}$) correlation spectrum for the oligosaccharide core of peracetylated purgic acid B methyl ester (**8**) with high resolution 1D ^{1}H and ^{13}C projection in pyridine-d_5. ^{13}C signal assigment: **1**, C_{11}-con; **2**, C_2-glc'; **3**, C_2-qui; **4**, C_4-rha; **5**, C_3-rha; **6**, C_2- glc; **7**, C_5-glc; **8**, C_5-qui; **9**, C_5- glc'; **10**, C_5-qui'; **11**, C_5-fuc; **12**, C_5-rha; **13**, C_6-glc'; **14**, C_6-glc; **15**, C_4-qui'; **16**, C_3-glc y C_3- glc'; **17**, C_3-qui; **18**, C_4-qui; **19**, C_2-rha; **20**, C_3-fuc; **21**, C_2-qui'; **22**, C_4-glc y C_4-glc'; **23**, C_4-fuc; **24**, C_2-fuc.

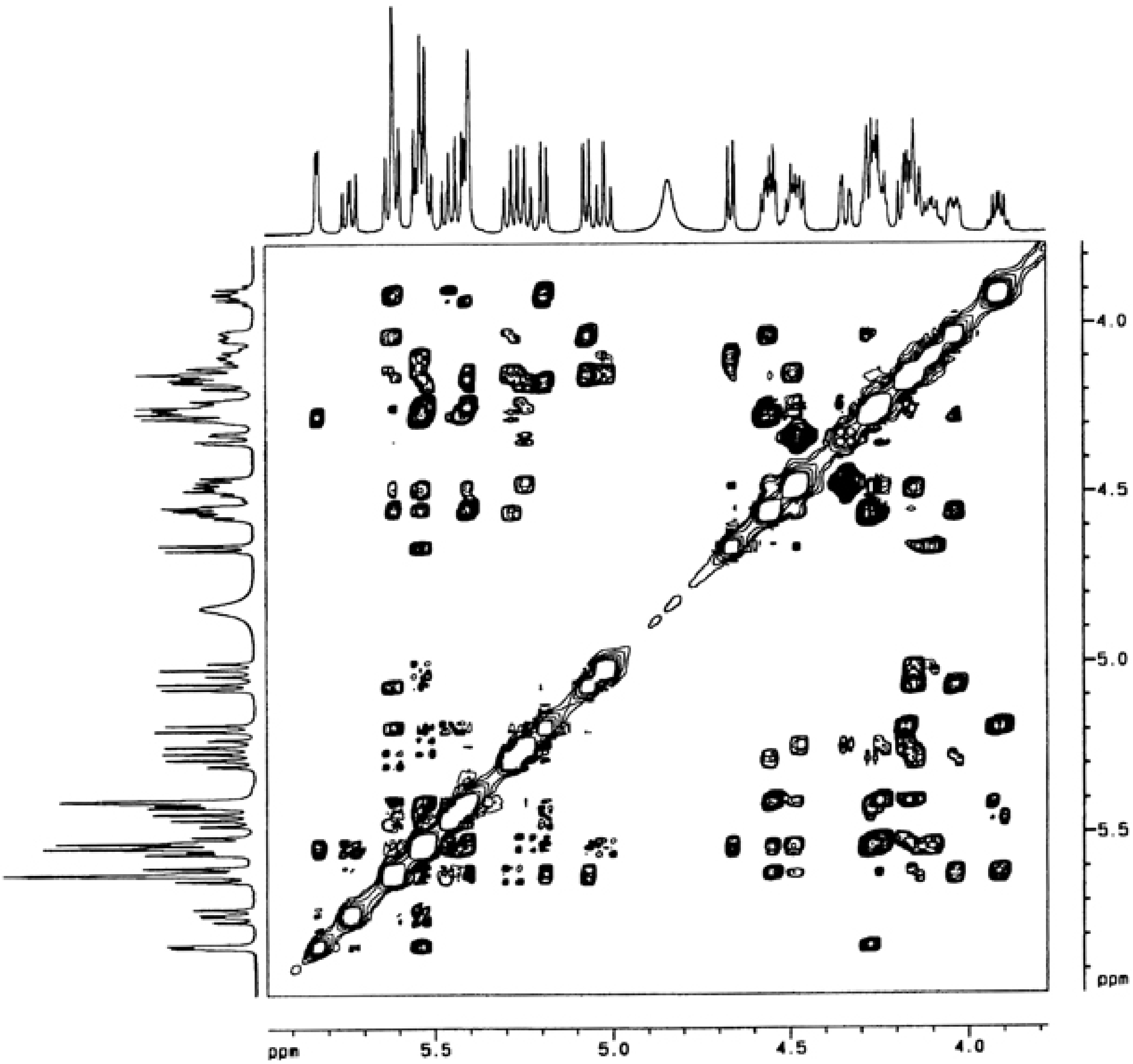

Figure S12. ROESY NMR spectrum of derivative 7. Expanded region with high resolution 1-D projection for the oligosaccharide core of peracetylated purgic acid A methyl ester (**7**) at 25 °C in pyridine-d_5.