Lipid derivatives from *Mucuna pruriens* seeds

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The seeds of *Mucuna pruriens* have afforded three new lipid derivatives from its *n*-hexane extract, namely: (Z)-Triacont-5,7,9-triene; (Z)-Docos-2,4,6-trien-1,8-diol and (Z)-Docos-5-en-1-oic acid. Their structures have been elucidated mainly by spectroscopic methods.

Keywords: *Mucuna pruriens* (L.) Papilionaceae, seeds, Lipid derivatives, L-DOPA, fatty acid

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*Mucuna pruriens* (L.) DC is a medicinal plant of India well known for its use as a remedy for male impotency, as an aphrodisiac as well as a cure for sexual debility and as a nervine tonic. The pods are known to have anthelmintic and the seeds anti-inflammatory and aphrodisiac properties. The seed powder has shown anti-Parkinson activity which is supposed to be due to the presence of L-DOPA in it. The presence of tetrahydroisoquinoline alkaloids from its seeds has recently been reported.

Work on the non-polar part of the extract has yielded some lipid derivatives whose structure elucidation by spectroscopic methods is being reported now.

### Results and Discussion

**Fatty acids.** The seeds were extracted with *n*-hexane, acetone and ethyl acetate. The yield of oil was: *n*-hexane (4.1%), acetone (4.5%) and ethyl acetate (3.8%). The main components of the oil were the palmitic, stearic, oleic and linoleic acids.

**Compounds 1-3.** From the *n*-propanol extract, three compounds were purified and their structure elucidated by spectroscopic methods. The IR of compound 1 showed bands at 2950, 1645, 1440, 1385 and 720 cm$^{-1}$ indicating that it was a hydrocarbon. The EIMS showed [M]$^+$ ion at *m/z* 416 and HRMS at *m/z* 416.7721 for C$_{30}$H$_{56}$. The 'H NMR spectrum showed typical signals for CH$_3$(CH$_2$)$_n$ at $\delta$ 0.89, 1.28 and 1.59. Additional signals (overlapping triple doublets, $J$ = 11.0, 5.5 Hz, 6H) at $\delta$ 5.33 followed by multiplets at $\delta$ 2.05 and 2.28 (each 2H) indicated that 1 contains three conjugated double bonds. The lower $J$ value (11.0 Hz) of double bond protons clearly indicated that they belong to the Z form. The presence of three conjugated double bonds was further supported by the typical signals in $^{13}$C NMR (Table II). The prominent fragments in MS of 1 at *m/z* 359 and 373 as well as 281 and 267 due to $\alpha$ and $\beta$ fission of double bonds, further established that double bonds were situated at C-5, C-7 and C-9. Thus the structure of compound 1 was given as (Z)-triacont-5,7,9-triene.

Similarly, compound 2 showed IR bands at 3400-3300, 2950, 1640, 1440, 1380 and 720 cm$^{-1}$ indicating the presence of OH functional group. Its EIMS showed [M]$^+$ at *m/z* 336 and HRMS at *m/z* 336.5562 for C$_{22}$H$_{46}$O$_2$. Its 'H NMR spectrum clearly indicated the presence of CH$_3$(CH$_2$)$_n$ by the typical signals at $\delta$ 0.88, 1.28 and 1.61. Additional signals (overlapping

<table>
<thead>
<tr>
<th>Extract No</th>
<th>Name of solvent</th>
<th>Solvent (mL)</th>
<th>Material (g)</th>
<th>Yield of oil (g)</th>
<th>% of oil</th>
<th>Main fatty acid</th>
</tr>
</thead>
<tbody>
<tr>
<td>MHX-1299</td>
<td><em>n</em>-Hexane</td>
<td>2×40</td>
<td>20</td>
<td>0.82</td>
<td>4.1</td>
<td>Palmitic, Stearic, oleic, linoleic</td>
</tr>
<tr>
<td>MAC-1299</td>
<td>Acetone</td>
<td>2×40</td>
<td>20</td>
<td>0.89</td>
<td>4.5</td>
<td>Palmitic, oleic, linoleic</td>
</tr>
<tr>
<td>METAC-0200</td>
<td>Ethyl acetate</td>
<td>2×40</td>
<td>20</td>
<td>0.76</td>
<td>3.8</td>
<td>Palmitic, oleic, linoleic</td>
</tr>
</tbody>
</table>

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**Note**

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Table I — Extraction and identification of fatty oil from *M. pruriens* seeds by GC-MS

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presence of two doublets for H-1 at unsaturation at C-2 was further supported by the double bonds were situated at C-2, C-4 and C-6. The lower protons clearly indicated that they belong to the chain hydrocarbon is quite unusual. The presence of three conjugated double bonds, further established that the double bond was situated at C-5 (Scheme 1). The presence of terminal carboxylic acid group at C-1 was supported by the signals at δ 179.47 and 37.93 (for C-2) in 13C NMR. The presence of the carboxylic acid group was again supported by the methylation of 3 into 3a giving supporting signals in 1H and 13C NMR spectra of 3a confirming the structure of 3 as (Z)-docos-5-en-1-oic acid.

The structures of lipid derivatives 1-3 show that besides normal fatty acids and unsaturated fatty acids, hydroxylated unsaturated lipids are also present in the extract which could be of biological significance. On the other hand, the isolation of the unsaturated straight chain hydrocarbon is quite unusual.

### Experimental Section

1H and 13C NMR, DEPT spectra were recorded on Jeol instrument at 400 MHz and 100 MHz, respectively. IR was recorded on a Perkin-Elmer 1710 instrument and HRMS as well as EIMS was recorded on Jeol JMS 700 at 70 eV. GC-MS of the esters were carried out on Perkin-Elmer, Turbo Mass Auto XL instrument.

**Extraction of lipid derivatives.** The residual part of the seeds (500 g), obtained after the extraction by acetone, was further extracted by n-propanol to ascertain the presence of polar fatty acid (lipid).
Scheme I

1 (MS fragments in m/z)

2, R= H  (MS fragments in m/z)
2a, R= Ac

3, R= H  (MS fragments in m/z)
3a, R= Me
derivatives. The seed powder was extracted by 1.25 L n-propanol (three times) by shaking overnight at rt to obtain 8.84 g extract. Out of this extract, 2.5 g was subjected to Medium Pressure Liquid Chromatography (Gilson instrument model 303) at a pressure of 500 psi and flow rate 2.5 mL/min over Buechi glass column on silica gel (230-400 mesh), with mobile phase as n-butanol-n-propanol-water, 6:6:1. The MPLC gave mainly 5 fractions of which the first two were a complex mixture of fatty acid derivatives and the third contained mainly sucrose (170 mg). The 4th fraction yielded some basic material while the 5th fraction yielded L-DOPA (10 mg). The first fraction on crystallization gave compound 1 (750 mg, Rf 0.90, TLC, n-butanol-n-propanol, 1:1) while the second fraction on crystallization gave compound 2 (40 mg, Rf 0.70, TLC, n-butanol-n-propanol-water, 4:4:1) and its mother liquor after centrifugation and TLC gave compound 3 (30 mg, Rf 0.60, TLC, n-butanol-n-propanol-water, 4:4:1) and a complex mixture of further neutral compounds.

(Z)-Triacont-5,7,9-triene 1: Viscous oil; IR (CHCl₃): 2950, 1645, 1440, 1385 and 720 cm⁻¹; HRMS (m/z): 416.7721 (calcd. for C₃₀H₅₆: 416.7724); EIMS (m/z, relative intensity): 416 (25) [M⁺], 373 (36) [M-43]⁺, 359 (51) [M-57]⁺, 333 (42) [M-83]⁺, 307 (58) [M-109]⁺, 281 (50) [M-135]⁺, 267 (60) [M-149]⁺, 199 (50), 135 (100), 117 (100), 113 (45), 87 (15); ¹H NMR (CD3OD): δ 0.89 (6H, overlapping t (J = 6.5 Hz), H-1 and H-30), 1.28 (36H, broad s, H-2 and H-13 to H-29), 1.59 (4H, m, H-3 and H-12), 2.05 and 2.28 (2H each, m, H-4 and H-11), 5.33 (6H, overlapping m, H-5 to H-10); ¹³C NMR (CD3OD): see Table II.

(Z)-Docos-5-en-1-oic acid 3: Viscous liquid; IR (CHCl₃): 3400-3100 (COOH), 2950, 1720 (COOH), 1640, 1440, 1380 and 720 cm⁻¹; HRMS (m/z): 338.5728 (calcd. for C₂₂H₄₂O₂: 338.5726); EIMS (m/z, relative intensity): 338 (18) [M⁺], 293 (20) [M-45]⁺, 279 (25) [M-CH₂COOH]⁺, 265 (22) [M-73]⁺, 251 (10) [M-87]⁺, 225 (8) [M-113]⁺, 211 (8) [M-127]⁺, 159 (33), 117 (100), 113 (45), 87 (15); ¹H NMR (CD3OD): δ 0.89 [3H, t (J= 6.5 Hz), H-22], 1.28 (24H, br s, H-9 to H-21), 1.61 (2H, m, H-8), 2.06 (2H, m, H-7), 2.19 (2H, m, H-4), 1.38 (2H, m, H-3), 2.77 (2H, m, H-2) 5.33 (2H, overlapping m, H-5 and H-6); ¹³C NMR (CD3OD): see Table II. Methyl ester 3a: 20 mg 3 was taken in a flask and 2 mL freshly prepared diazo methane was added to it. After usual work-up 3a was obtained (20 mg): ¹H NMR (CDCl₃): δ 3.66 (3H, s, OMe); ¹³C NMR (CD3OD): see Table II.

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References
2 Misra L N, Mishra H O & Wagner H, IUPAC International Conference on Biodiversity and Natural Products: Chemistry and Medicinal applications, 26-31 Jan, 2004, Delhi University, New Delhi, India.