

CHAPTER V

DISCUSSION

Discussion on the Extraction Procedure

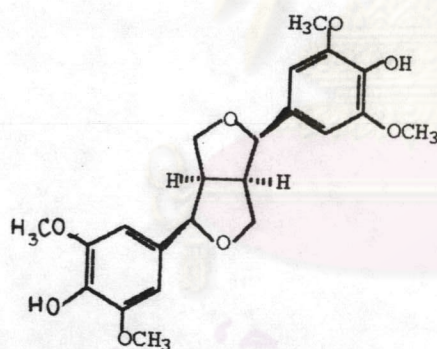
From the phytochemical information , the genus *Strychnos* is commonly a rich source of alkaloids , especially indole alkaloids as the main component. The screening test of the alcoholic extract from the stems of *Strychnos thorelii* Pierre ex Dop gave positive result with dragendorff's spraying reagent which is specific for alkaloids. Due to these reasons , the stems of *Strychnos thorelii* Pierre ex Dop were extracted by acid - base extraction , the specific extraction for alkaloids.

The crude chloroform extract of dried powdered stems of *Strychnos thorelii* Pierre ex Dop was separated by chromatographic techniques and afforded two isolated compounds , ST-1 , a tetralin lignan , and ST-2 , an unidentified alkaloid.

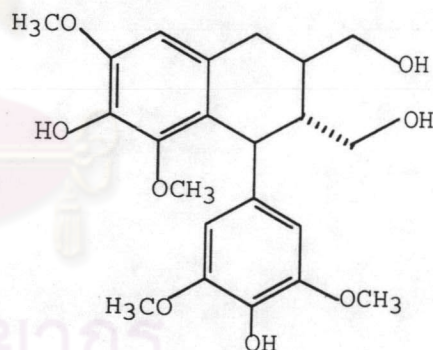
Discussion on Chemotaxonomy

Lignans are rarely found in the genus *Strychnos*. From the chemical constituents data of the *Strychnos* species, there is only one report about lignans. Lirioresinol A (48) and lirioresinol B (49) are the isolated lignans from the stem bark of the African *Strychnos*, *Strychnos dinklagei* Gilg.³¹ The result of this present study suggests the presence of lyoniresinol, the oxygenated tetralin lignan, from the stem of the Asian *Strychnos*, *Strychnos thorelii* Pierre ex Dop. It is remarkable example of chemotaxonomic relation that the two species which contain lignans are in the same section, Lanigeræ.

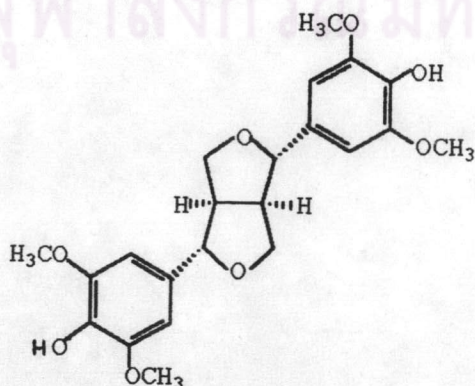
The main structure of lirioresinol A and B are furofurans, whereas lyoniresinol (50) is tetrahydronaphthalene.



(48) LIRIORESINOL A



(50) LYONIRESINOL



(49) LIRIORESINOL B

Discussion on Structure Elucidation

ST-1 was obtained as white amorphous compound. The structure elucidation was based on data from UV, IR, NMR, and Mass spectral interpretation, confirmed by comparison with those data reported in the literature.

Mass spectral study of ST-1 (Figure 26) shows molecular ion peak at m/z 420 (48.57%) which establishes the tentative molecular formula of $C_{22}H_{28}O_8$. The fragments at m/z 402 (31.89%) and m/z 371 (10.76) arise from loss of water and of the hydroxymethyl group, respectively. (Figure 4)

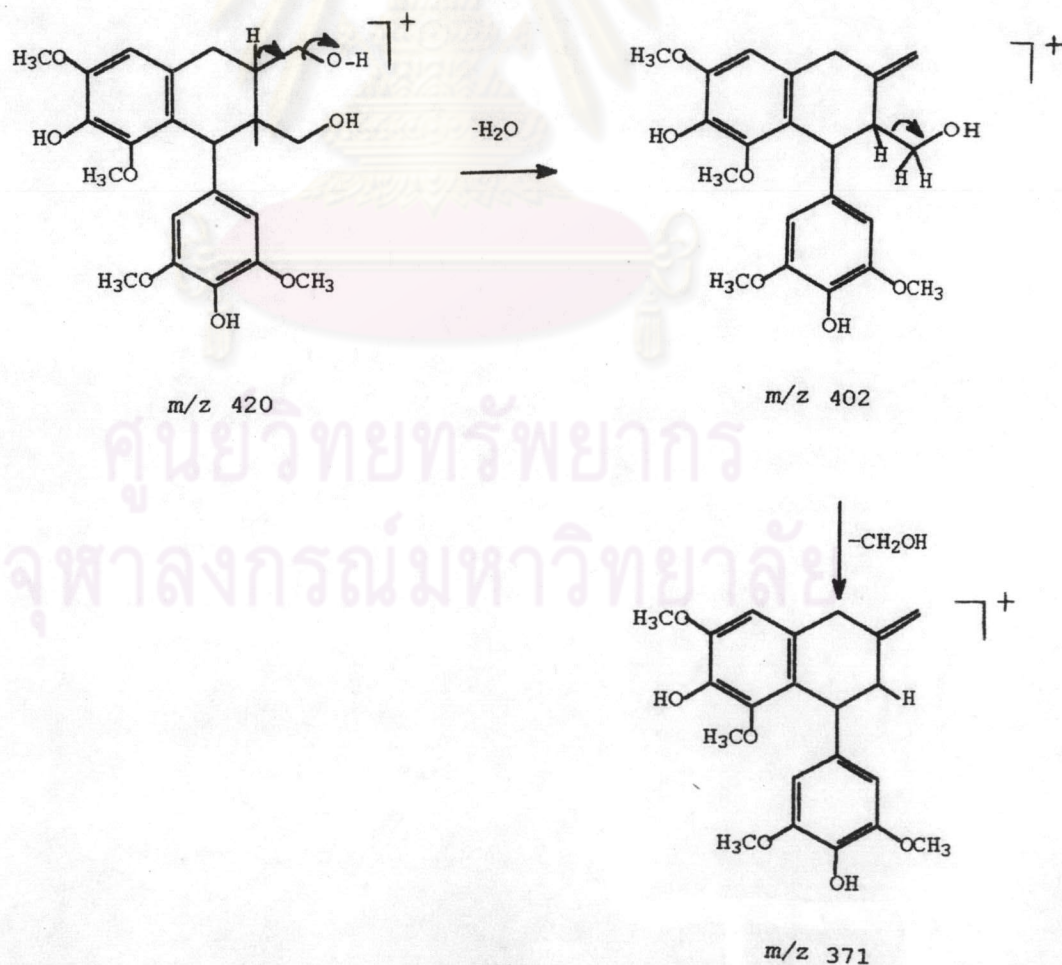


Figure 4 Mass Fragmentation of ST-1

Other features of mass fragmentation of ST-1 are those which follow hydrogen transfer from a hydroxyl group to an aromatic ring as shown in figure 5.¹³⁵ The loss of CH_2O causes the fragment at m/z 390 (2.56%). The rupture of the bond (a) causes the fragments at m/z 167 (28.95%) and m/z 205 (22.60%).

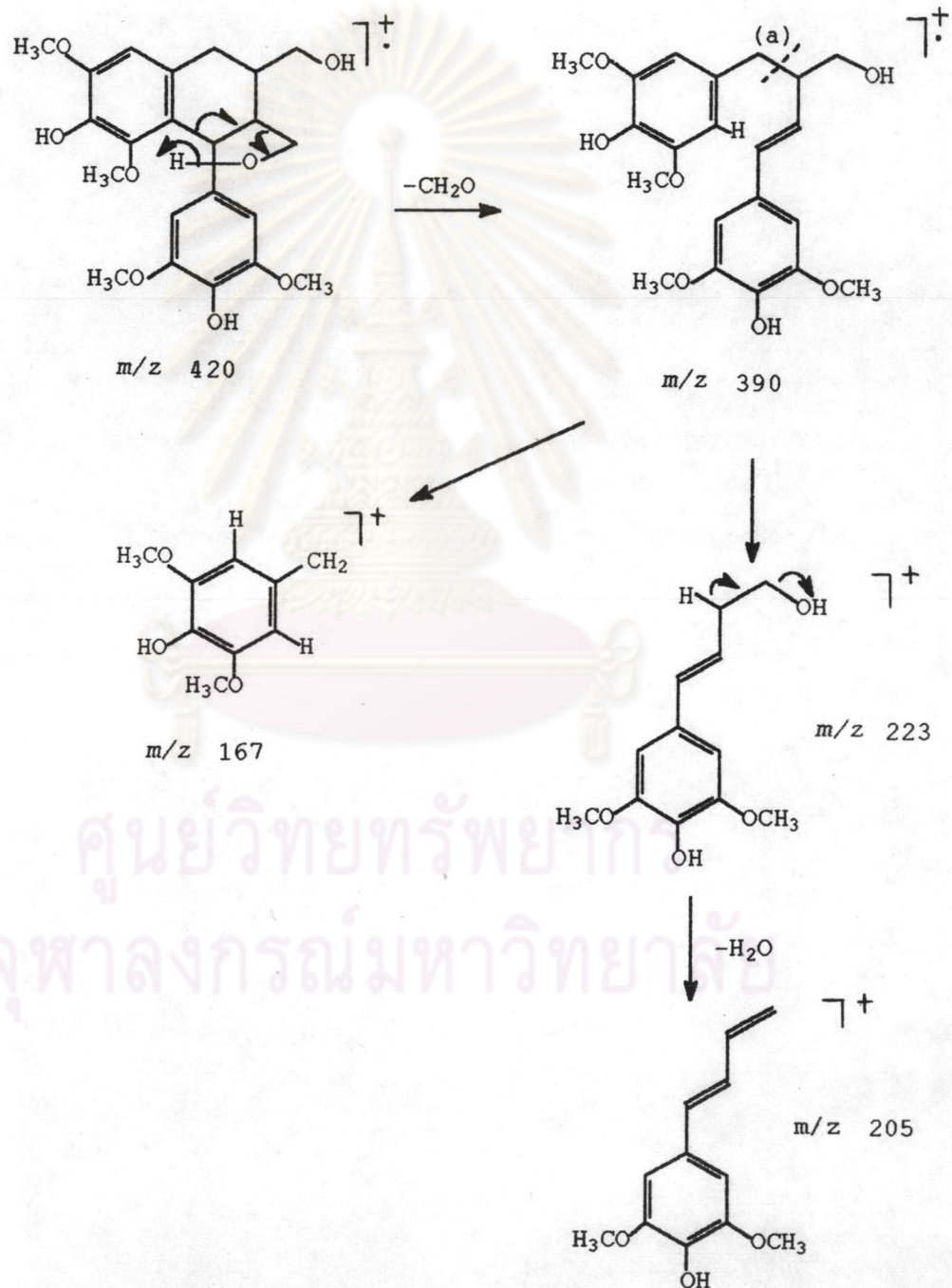
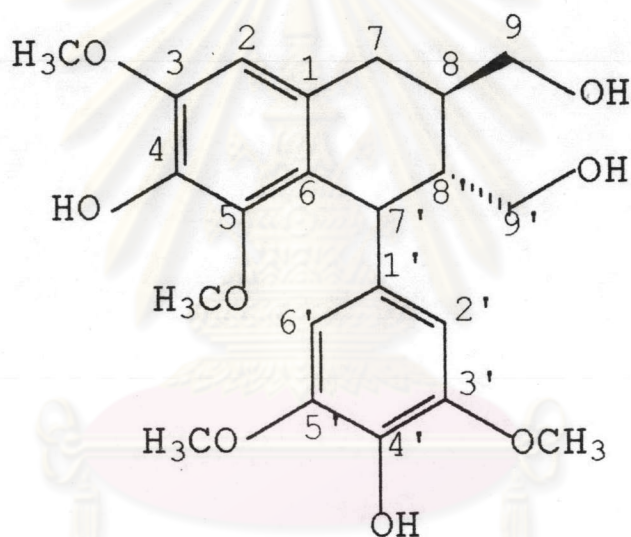


Figure 5 Mechanism of Hydrogen Transfer in the Mass Spectrum of ST-1

The IR spectrum of ST-1 (Figure 19) shows c-c vibrations of phenyl group at 1611 cm^{-1} . The vibration at 3443 cm^{-1} indicates hydroxyl functions in the molecule of ST-1. The O-H vibrations of phenolic function are shown at 2941 cm^{-1} .

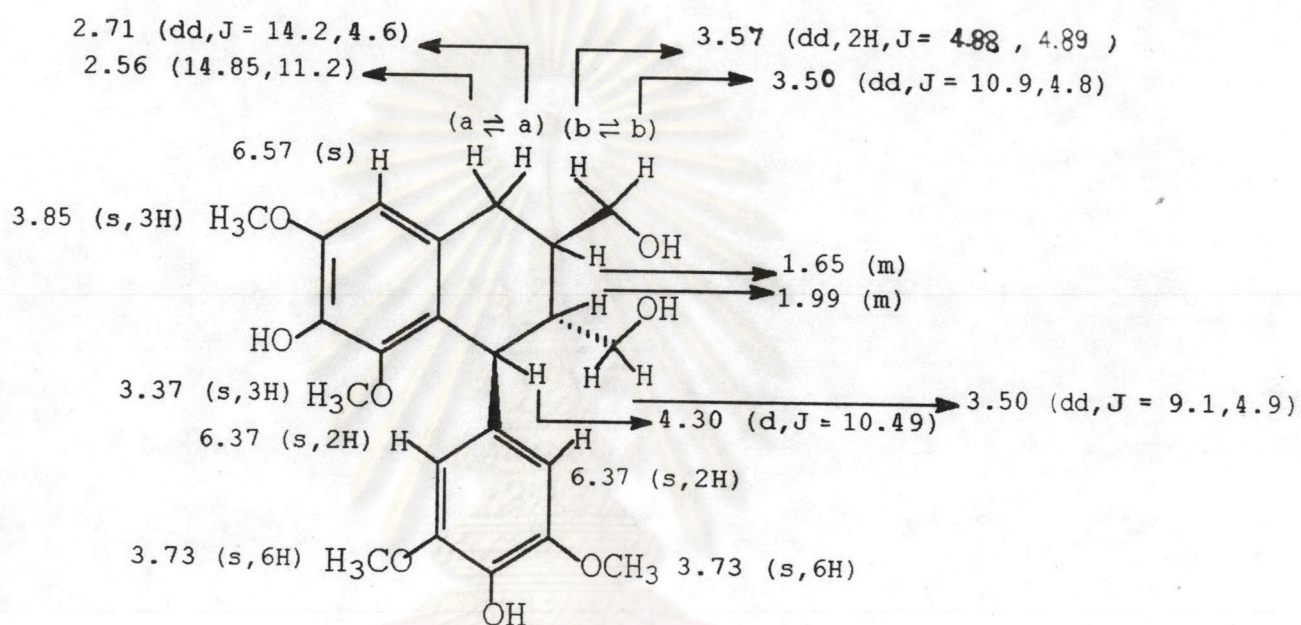
The UV absorption spectrum (Figure 18) shows $\lambda\text{ max}$ at 280 nm which indicates the characteristic of the substituted benzene in the molecule.



The ^1H - ^1H COSY NMR spectrum of ST-1 (Figure 22) shows two equivalent protons appears as singlet at $\delta\ 6.37\text{ ppm}$ which indicates the presence of a symmetrical substitution of aromatic proton in a part of ST-1 molecule. The remaining singlet signal at $\delta\ 6.57\text{ ppm}$ may be assigned to the position of the other part of the remaining benzene ring. The aromatic proton at $\delta\ 6.37\text{ ppm}$ correlates with a proton at $\delta\ 4.30\text{ ppm}$, so the latter proton can be assigned as a proton at C-7'. Consequently, the proton at $\delta\ 4.30\text{ ppm}$ showed

coupling effect with the proton at C-8' position of which shows a multiplet signal at δ 1.99 ppm. The proton at δ 1.99 ppm shows connection with the proton at C-8 position of which appears as a multiplet signal at δ 1.65 ppm. The aromatic proton at δ 6.57 ppm shows a long range correlation with a pair of geminal protons at δ 2.56 and 2.71 ppm, thus they could be assigned as protons at C-2 and C-7 position respectively. The multiplet proton at δ 1.65 ppm has coupling effect with two geminal proton ($J= 10.9$ Hz) at δ 3.50 and 3.57 ppm, so the latter two protons are assigned to be the protons at C-9 position. A group of singlets signals between 3 and 4 ppm indicates the presence of O-methyl protons integrated for four groups. The singlet signal at δ 3.73 ppm (6H,s) integrated to be two equivalent O-methyl groups at C-5' and C-3' position. The proton at δ 6.57 ppm correlates with three protons at δ 3.85 ppm which refers to the presence of O-methyl group at C-3 position. So the remaining O-methyl group is assigned by the singlet signal at δ 3.73 ppm.

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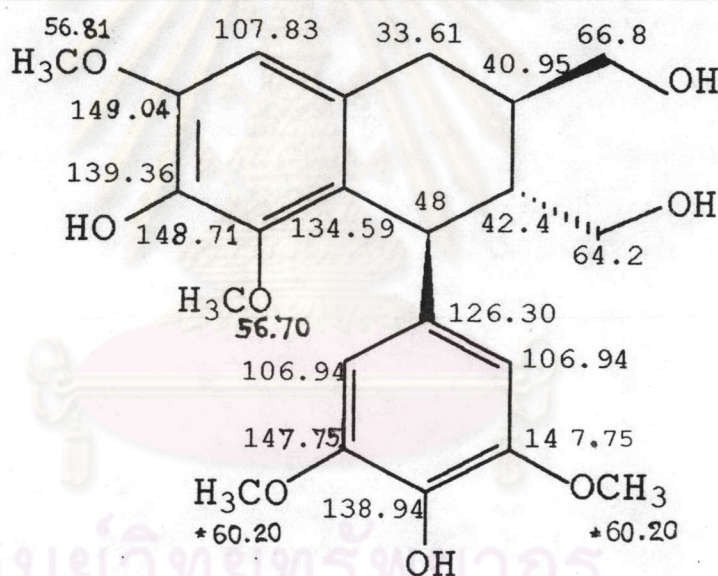


(a \rightleftharpoons a), (b \rightleftharpoons b) Values may be interchanged within parenthesis

Figure 6 ¹H-NMR Assignment of ST-1

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The ^{13}C -NMR spectrum of ST-1 (Figure 7) shows the aromatic carbon signals at δ 106.94, 107.83, 126.30, and 134.59 ppm. The signals at δ 149.04, 148.71, and 147.75 ppm are assigned as C-3, C-5, C-5', and C-3', respectively. The signals at δ 139.36 and 138.94 ppm are assigned as C-4, and C-4'. The four methoxy carbons are indicated by the signals at 56.70, 56.81, and 60.20 ppm. The remaining signals are the signals of C-7 (33.61 ppm), C-8 (40.95 ppm), C-9 (66.8 ppm), C-7' (48 ppm), C-8' (42.4 ppm), and C-9' (64.2 ppm).



* The assignment may be either one of these

Figure 7 ^{13}C -NMR Assignment of ST-1

From the above informations, ST-1 can be identified as lyoniresinol, the known lignan previously isolated from *Ulmus thomasi* Sarg. (Ulmaceae).¹⁴¹

The structure elucidation of the alkaloid "ST-2" has not been completely identified. Further investigations are needed to accomplish this study.



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