AMORPHAQUINONE, A NEW ISOFLAVANQUINONE FROM AMORPHA FRUTICOSA L.

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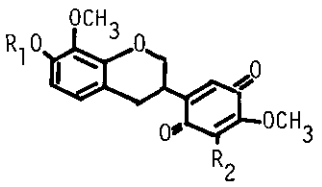
From the root of Amorpha fruticosa L.(Leguminosae), a novel isoflavanquinone, amorphaquinone, was isolated whose structure was shown to be I on the basis of spectral data.

In the course of our investigation of the constituents of the root of Amorpha fruticosa L., four isoflavonoids and a rotenoid have been isolated. Four known compounds, formononetin, ononin, wistin and amorphigenin were identified by direct comparison with the authentic samples respectively.

The fifth compound has been isolated by repeating the silica gel chromatography of the ether extractives of the root of A. fruticosa, as orange amorphous solid, $C_{18}H_{18}O_7$ (M^+ 346), $[\alpha]_D$ -92.9°. The orange color, UV [λ_{max}^{MeOH} nm (ε) 266 (12600), 385 (1150)] and IR (ν_{max}^{KBr} 1655 cm^{-1}) spectra suggested a typical quinonoid structure for this new isoflavonoid named amorphaquinone(I).

The nmr spectrum shows signals assignable to the CH_2-CH-CH_2 group of an isoflavan skelton.[1),2)] [δ 3.90-4.40 (2H,m, H-2), 3.20-2.70 (1H,m, H-3), 2.70-3.05 (2H,m, H-4)]. Additional signals are assignable to three methoxyl groups, one exchangeable hydroxyl proton and two ortho related aromatic protons. [δ 6.74 (1H,d, J= 8.5 Hz, H-5), 6.53 (1H,d, J= 8.5 Hz, H-6)]. The low field quinonoid

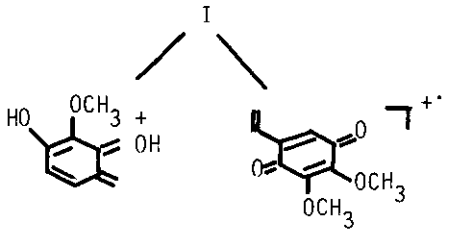
proton (H-6') at 6.33 ppm, shows long range coupling (J= 1.5 Hz) to a methine hydrogen at C-3. The existence of the quinonyl moiety was further confirmed by the MS of I which showed prominent peaks at m/e 153 (IIIa) and 194 (IIIb).



I : R_1= H; R_2= OCH_3

Ia : R_1= OAc, R_2= OCH_3

II : R_1= R_2= H



IIIa IIIb

Amorphaquinone on acetylation afforded a monoacetate(Ia) of orange needles, mp 125-125.5°C. [Found: C, 61.97; H, 5.14; M^+ 388(MS). $C_{20}H_{20}O_8$ requires: C, 61.85; H, 5.19; M^+ 388]. Deacetylation of Ia in acid media (0.14 N-HCl/MeOH, 50°C, 1 hr.) regenerated the original compound I in good yield (TLC & IR).

The location of substituents (7-hydroxy-8-methoxy-) on the ring A was favoured on the biogenetic ground, i.e. all isoflavonoids isolated from A. fruticosa had the C-7-oxygenated structure; and the shift to low field of two aromatic proton signals of Ia, relative to those of I, indicated that the hydroxyl group is associated with each proton on the ring A. Furthermore, I is similar to mucroquinone (II)[2] except that it contains an extra methoxyl group in the nmr data. On the basis of above data and comparison of these data with those reported from II[2], the structure I was accordingly assignable to amorphaquinone.

REFERENCES

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