

PROTON MAGNETIC RESONANCE SPECTRA OF PTEROCARPAN AND RELATED PHYTOALEXINS

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Abstract - Proton magnetic resonance spectral data of pterocarpin and related phytoalexins are reviewed.

Many plants respond to invasion by both pathogenic and nonpathogenic microorganisms by producing low molecular weight antibiotics termed as phytoalexins¹⁻⁴. These antimicrobial compounds are also produced following an interaction between plants and various biotic⁵⁻¹⁰ and abiotic agents¹¹⁻⁵⁹, which act through the same mechanisms^{23, 60}. The genetic information for phytoalexin production is carried by the host and elicitors of such production, whether specific or nonspecific act through the host genome. Thus a given species may produce the same phytoalexins irrespective of the challenging agent.

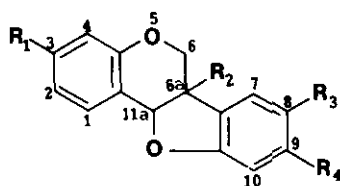
The accumulation of phytoalexins may be responsible for cessation of fungal development which has suggested that these compounds may have a role in disease resistance⁶¹⁻⁶⁶. Phytoalexins are mainly produced by members of the Leguminosae and Solanaceae family of plants during the first few hours of the penetration of the parasitic cells into the invaded tissue⁶⁷⁻⁶⁹. Oxygen heterocyclic phytoalexins having a 6a,11a-dihydro-6H-benzofurobenzopyran nucleus such as (1) called pterocarpan and other flavonoid and closely related C₆C₃ derived compounds are mainly elaborated by plants belonging to Leguminosae, while terpenoid phytoalexins are mainly produced by plants belonging to Solanaceae family.

Nuclear magnetic resonance (NMR) spectroscopy has played a major role in the structural elucidation of both benzenoid and terpenoid phytoalexins. The conformation of the 6a,11a-dihydro-6H-benzofuro[3,2-C]-(1)-benzopyran ring system (1) in pterocarpan by NMR spectroscopy has been reported by Pachler and Underwood¹⁰. The conformation of the heterocyclic rings has been mainly derived from the vicinal coupling constants and observation of the long range coupling.

These compounds have two asymmetric centres and relatively unstrained cis conjunction is considered more likely. Coupling constants helped Sugimoto⁷¹ and Underwood⁷⁰ to conclude

that the relative configuration of these centres in the stress metabolites homoptero-
carpin (1) is H,H cis. The absolute configuration⁷² of C_{11a} in trifolirhizin (2), a
phytoalexin elaborated by clover roots⁷³ and Ononis spinosa⁷⁴ has been established⁷⁵ as
R, and with cis relationship, the configuration of this compound will be 6a, R:11a, R.

The aromatic protons as in (4) at positions 1, 2 and 4 give rise to an ABC-type of
splitting pattern. On the other hand the protons of the second aromatic ring show either
a single resonance line due to the closely similar electronic environment of protons at
C₇ and C₁₀ or a second ABC pattern for compounds such as (2).



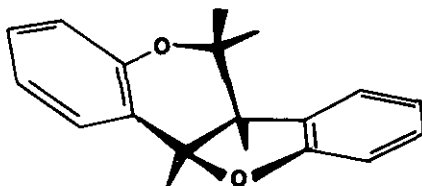
1. $R_1=R_2=R_3=R_4=H$
2. $R_1=R_4=OMe$; $R_2=R_3=H$
3. $R_1=O\text{-glucose}$; $R_2=H$; $R_3+R_4=O\text{-CH}_2\text{-O}$
4. $R_1=OMe$; $R_2=H$; $R_3+R_4=O\text{-CH}_2\text{-O}$

Thus protons from the two aromatic rings and from the heterocyclic system form three
isolated spin systems with very characteristic peak patterns. The first for proton at C₁
gives rise to a doublet ($J \sim 8.5 H_z$) coupled to the ortho proton at C₂, which because of
the additional meta coupling to a proton at C₄ ($J \sim 2.5 H_z$), shows a quartet. The reso-
nance from H-4 is expected to be a narrow doublet.

The second for protons at 6, 6a and 11a forms an ABMX system which gives a highly
characteristic spectral pattern which has been studied for many pterocarpan¹. While
the third common factor for pterocarpan is the AB-system for protons at C₇ and C₈ (2).
The quartet from these protons contains a typical aromatic ortho-coupling of $\sim 8.5 H_z$.
The deshielded doublet is assigned to the proton at C₈ because of the presence of an
adjacent oxygen atom at C₉. There are four possible arrangements of the oxygen and other
substituents on this aromatic ring which could produce an ortho AB-type system.

The heterocyclic ring protons gives rise to a highly complex four-spin due to strong
coupling between the two protons at C₆. The H_{11a} occurs at lowest field because of
diamagnetic aromatic ring currents as well deshielding by the oxygen atoms of the furan
ring. The proton at position 6a occurs at highest field and couples with the low field

proton at 11a. The magnitude of the vicinal coupling constants identify the protons on carbon atom 6, the axial one being nearer to the proton at H_{6a} than to its equatorial counterpart. The strong coupling between these two protons (axial on C_6 and on C_{6a}) is reported⁷⁰ to cause the complexity of the four spin spectrum. Spin coupling of the proton at C_{11a} renders the spectrum to a straightforward ABC-system. The resonance lines due to the proton on carbon 6a appears as broad, revealing a triplet fine structure at highest resolution. Double irradiation experiments have shown that the protons at C_{6a} and C_{11a} are coupled to aromatic protons across four and five bonds. The following coupling constants have been determined: $J_{6a,7} = 0.6H_z$; $J_{6a,10} = 0.5H_z$; $J_{a,11a} = 0.5H_z$; $J_{2,11a} \leq 0.1H_z$; $J_{4,11a} = 0.3H_z$. Pachler and Underwood⁷⁰, from coupling studies have concluded that the benzofuran ring system of pterocarpan exists in the following conformation (5).



5.

The isopentenyl side chain and dimethylchromene ring also produce characteristic NMR patterns. The two methyl groups of the dimethylchromene ring are non-equivalent and the ethylene protons give an AB quartet ($J = 10H_z$). In the isopentenyl chain, the methyl groups bring allylic, resonate at lower field than those of the dimethylchromene ring. The remaining protons $-CH_2-CH=$ form a typical ABX system, the methylene group appearing as a doublet and the methine proton as a broad singlet. ¹H-NMR data for more than one hundred pterocarpan and related phytoalexins, along with their sources is tabulated in the following Tables.

Stress Agents Referred in the Tables:

1. *Helminthosporium turcicum* 2. *Monilinia fructicola* 3. *Ascochyta pisi* Lib.
4. *Caldosporium* sp., *Phoma lingan* 5. *Spetoria apii* 6. *Peronospora tabacina* Adam
7. *Uromyces fabae* pers 8. *Sclerotinia fructicola* 9. *Aphanomyces euteiches*
10. *Fusarium solani* 11. *Rhizoctonia solani* 12. *Helminthosporium carbonum*

13. *Botrytis cinerea* 14. *Pseudomonas* spp. 15. *Colletotrichum lindemuthianum*
16. *Uromyces appendiculatus* 17. *E. Sandwicensis* 18. *Pseudomonas phaseolicola*
19. Inorganic materials 20. *Phytophthora megasperma* var *Sojae* 21. Ribonuclease-A
22. *Asc-ochytaimperfecta* 23. *Lathyrus* spp. 24. *Verticillium albo atrum*
25. *Phytophthora drechsleri* 26. *Botrytis fabae* 27. *Pithomyces chartarum*
28. *Phytophthora vignae* 29. Wound 30. *Fusarium oxyporum* 31. *Cladosporium herbarum*
32. *Phytophthora infestans* 33. *Ceratosystis fimbriata* 34. *Fusarium coeruleum*
35. *Phoma exigua* 36. *Thielaviopsis basicola* 37. *Alternaria brassicicola*
38. UV light 39. Actinomycin D 40. Temperature 41. *Sclerotinia trifoliorum*
42. *Cladosporium fulvum* 43. *Colletotrichum coffeanum*.

Solvents Referred in the Tables

1. Chloroform-d 2. Acetone-d₆
3. Methanol-d₄ 4. Carbon tetrachloride
5. Acetonitrile-d₃ 6. Dimethylformamide-d₇ + Chloroform-d
7. Dimethylsulfoxide-d₆ + Chloroform-d
8. Chloroform-d + Methanol-d₄
9. Dimethylformamide-d₇

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
<u>PTEROCARPANS</u>					
Pterocarpin (3-Methoxy-8,9-methylenedioxypterocarpin)	Pterocarpus santalinus, Pterocarpus dabergoides, Pterocarpus macrocarpus, Baphia nitida		1	7.4, H ₁ ; 6.67, H ₇ ; 6.61, H ₂ ; 6.45, H ₄ ; 6.41, H ₁₀ ; 5.87, -O.CH ₂ .O; 3.73, -OMe. J _{1,2} =8.4; J _{1,4} =0.3; J _{2,4} =2.4; J _{7,10} =0.3; J _{-O.CH₂.O} =1.3 Hz.	76
Homopterocarpin (3,9-Dimethoxypterocarpin)	Pterocarpus soyauxii, Pterocarpus santalinus	1	1	7.4, H ₁ ; 7.1, H ₇ ; 6.61, H ₂ ; 6.45, H ₄ ; 6.43, H ₁₀ ; 6.42, H ₈ ; 3.44, H _{6a} ; 4.2, 3.6, H ₆ ; 5.45, H _{11a} ; 3.74, -OMe; 3.72, -OMe. J _{1,2} =8.5; J _{1,4} =0.3; J _{2,4} =2.4; J _{7,8} =8.8; J _{7,10} =0.3; J _{9,10} =2.7 Hz.	70,77,78
Medicarpin (Demethylhomopterocarpin)	Melilotus alba, Medicago sativa, Canavalia ensiformis, Vigna unguiculata, Trifolium pratense, Trigonella foenum	1, 2, 12, 13, 15, 19, 20, 23, 24, 26, 27, 43	1	7.38, H ₁ ; 7.12, H ₇ ; 6.56, H ₂ ; 6.45, H ₁₀ ; 6.44, H ₈ ; 6.42, H ₄ ; 6.08, -OH; 5.48, H _{11a} ; 4.2, H _{6eq} ; 3.26, -OMe; 3.6, H _{6ax} ; 3.52, H _{6a} .	65,70,79, 81,87,88, 166,137-153
Isomedicarpin	Psophocarpus tetragonolobus, Medicago sativa	13, 19	1	7.45, H ₁ ; 6.66, H ₂ ; 7.1, H ₇ ; 6.4, H _{4,8,10} ; 5.52, H _{11a} ; 4.24, H _{6eq} ; 3.6, H _{6ax} ; 3.8, OMe. J _{7,8} =8; J _{2,4} =2.5 Hz.	155-160
Trifolirhizin (Maackiain β -D-Glucoside)	Trifolium pratense, Ononis spinosa	1	1	7.38, H ₁ ; 6.66, H ₇ ; 6.6, H ₂ ; 6.45, H ₄ ; 6.4, H ₁₀ ; 5.87, -O.CH ₂ .O-; 3.7, OMe. J _{1,2} =8.4; J _{1,4} =0.3; J _{2,4} =2.4; J _{7,10} =0.3; J _{-O.CH₂.O} =1.3 Hz	70,73-75, 80

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
Maackiain (Demethyl-pterocarpan)	Trifolium pratense, Maackia amurensis, Trigonella foenum	1	1	7.56, H ₁ ; 6.86, H ₂ ; 6.49, H ₄ ; 6.77, H ₇ ; 6.4, H ₁₀ ; 5.87, -O.CH ₂ .O-, 5.49, H _{11a} ; 4.31, H _{6eq} ; 6.17, H _{6ax} ; 6.42, H _{6a} . J _{1,2} =8.0; J _{6ax & eq} =11.0 Hz.	70, 73, 81-89
Inermin (6a-Hydroxy-maackiain)	Pisum sativum, Andira inermis, Trifolium pratense	2, 30, 3	1	7.37, H ₁ ; 6.56, H ₂ ; 6.43, H ₄ ; 6.42, H ₇ ; 6.82, H ₁₀ ; 5.96, 5.93, -O.CH ₂ .O-; 5.28, H _{11a} ; 4.18, H _{6eq} ; 4.00, H _{6ax} . J _{1,2} =8; J _{6ax & eq} =11.0 Hz.	73, 83, 90-94
Pisatin (6a-Hydroxy-pterocarpin)	Pisum sativum, Lathyrus odoratus	2-13	4	7.4, H ₁ ; 6.5, H ₂ ; 6.35, H ₄ ; 6.4, H ₁₀ ; 6.25, H ₇ ; 5.75, -O.CH ₂ .O-; 5.45, H _{11a} ; 4.1, H _{6eq} ; 3.47, H _{6ax} .	7, 45, 17, 76, 93, 95-115 286, 297, 298
Variabilin (6a-Hydroxyhomopterocarpan)	Lathyrus odoratus, Trifolium pratense	12, 13, 41	1	7.4, H ₁ ; 6.6, H ₂ ; 6.5, H ₁₀ ; 6.4, H ₄ ; 6.37, H ₇ ; 5.45, H _{11a} ; 3.86, -OMe; 3.76, -OMe; 3.65, H _{6ax} ; 5.85, H _{6eq} .	96, 116- 118, 157, 287, 288, 252
Dolichin-A (3,9-Dihydroxy-10-(2'-hydroxy-3'-methyl-3'-butenyl)-pterocarpan)	Dolichos biflorus	14	2	7.33, H ₁ ; 7.0, H ₇ ; 6.55, H ₂ ; 6.37, H ₈ ; 6.35, H ₄ ; 5.44, H _{11a} ; 4.88, H ₄ ; 4.32, H ₂ ; 4.25, H _{6eq} ; 3.55, H _{6a} & H _{6ax} ; 2.87, H ₁ ; 1.8, H ₅ .	119, 289
Dolichin-B (3,9-Dihydroxy-10-(2'-hydroxy-3'-methyl-3'-butyl)-pterocarpan)	Dolichos biflorus	14	2	7.2, H ₁ ; 7.02, H ₇ ; 6.55, H ₂ ; 6.38, H ₈ ; 6.37, H ₂ ; 6.35, H ₄ ; 5.46, H _{11a} ; 4.82, H ₄ ; 4.24, H _{6eq} ; 3.55, H _{6a} & H _{6ax} ; 2.81, H ₁ ; 1.76, H ₅ .	119, 289

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
Tuberosin	Neorautanenia edulis, Pueraria tuberosa		1	7.27, H ₁ ; 7.1, H ₇ ; 6.5, H ₂ ; 6.25, H ₄ ; 6.2, H ₁₂ ; 4.0, H ₆ ; 5.25, H _{13a} ; 1.3, 2 X Me.	120-123
Phaseollin	Phaseolus vulgaris, Vigna unguiculata	10,15,16, 13,2	1	7.37, H ₁ ; 6.92, H ₇ ; 6.54, H ₂ ; 6.41, H ₄ ; 6.32, H ₈ ; 5.55, H _{11a} ; 5.54, H ₁₃ ; 6.48, H ₁₂ ; 4.2 & 3.64, H ₆ ; 3.5, H _{6a} ; 1.49, (CH ₃) ₂ .	19,22,63 90,124- 135
Phaseollidin (3,9-Dihydroxy-10-isopentenylpterocarpan)	Phaseolus vulgaris, Vigna unguiculata Dolichos biflorus, Erythrina cristagali, Psophocarpus teragonolobus	12-15,2, 17,13,19	1	7.37, H ₁ ; 6.93, H ₇ ; 6.53, H ₂ ; 6.4, H ₄ ; 6.36, H ₈ ; 5.44, H _{11a} ; 5.28, H ₁₃ ; 4.21, 3.63, H ₆ ; 3.54, H _{6a} ; 3.36, H ₁₂ , 1.81, Me; 1.76, 2 X Me.	23,126, 130,136, 219
1-0-Methylphaseollidin	Psophocarpus tetragonolobus	13,19	1	6.98, H ₇ ; 6.37, H ₈ ; 6.08, H _{2,4} ; 5.6, H _{11a} ; 5.36, =CH; 4.2, H _{6eq} ; 3.85, H _{6ax} ; 3.87, OMe; 3.4, -CH ₂ ; 1.79, 1.75, 2 X Me.	158
Demethylmedicarpin	Erythrina cristagalli	12,17	1	7.58, H ₁ ; 7.1, H ₇ ; 6.88, H ₂ ; 6.7, H ₄ ; 6.4, H ₁₀ ; 6.37, H ₈ .	154
3,6a,9-Trihydroxypterocarpan	Medicago sativa	19	3	7.3, H ₁ ; 7.2, H ₇ ; 6.55, H ₂ ; 6.42, H ₈ ; 6.32, H ₄ ; 6.24, H ₁₀ ; 5.26, H _{11a} ; 4.16, 4.04, H ₆ . J _{1,2} =8.3; J _{2,4} =2.3; J _{7,8} =8.1 Hz	158,159
Cristacarpin (3,6a-Dihydroxy-9-methoxy-10-isopentenylpterocarpan)	Erythrina cristagalli, Psophocarpus tetragonolobus	12	2	7.33, H ₁ ; 7.18, H ₇ ; 6.56, H ₂ ; 6.54, H ₈ ; 6.31, H ₄ ; 5.27, H _{11a} ; 5.16, =CH; 4.16, 4.06, H ₆ & H _{6a} ; 3.25, -CH ₂ ; 3.83, -OMe, 1.76, Me; 1.65, -Me. J _{1,2} =8.5; J _{2,4} =2.3; J _{7,8} =8.0 Hz	154

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
3,6a-Dihydroxy-8,9-methylenedioxypterocarpan	Pisum sativum	10	2	7.3, H ₁ ; 7.18, H ₇ ; 6.5, H ₂ ; 6.3, H ₄ ; 6.16, H ₁₀ ; 5.25, H _{11a} ; 4.16, H _{6eq} ; 4.06, H _{6ax} .	90-94
Vesticarpan (3,10-Dihydroxy-9-methoxypterocarpan)	Lathyrus nissolia, Macharium vestitum, Platymiscium trinitatis	12	2	7.39, H ₁ ; 6.6, H ₂ ; 7.1, H ₇ ; 6.45, H ₈ ; 6.37, H ₄ ; 5.45, H _{11a} ; 4.2, H _{6eq} & H _{6a} ; 3.9, OMe; 3.6, H _{6ax} .	117
Methylnissolin (3-Hydroxy-9,10-dimethoxypterocarpan)	Lathyrus nissolia	12	2	7.37, H ₁ ; 6.6, H ₂ ; 7.08, H ₇ ; 6.45, H ₈ ; 6.35, H ₄ ; 5.46, H _{11a} ; 4.15, H _{6eq} & H _{6a} ; 3.6, H _{6ax} ; 3.87, -OMe.	117
2-Methoxymedicarpin (3-Hydroxy-2,9-dimethoxypterocarpan)	Pisum sativum	10	1	7.18, H ₁ ; 6.96, H ₇ ; 6.52, H ₄ ; 6.44, H ₁₀ ; 6.43, H ₈ ; 5.89, OH; 3.9, OMe; 3.77, OMe. J _{1,4} =2.3; J _{7,8} =8.8 Hz.	163
2,3,9-Trimethoxypterocarpan	Pisum sativum	10	1	7.12, H ₇ ; 6.97, H ₁ ; 6.47, H ₄ ; 6.45, H ₁₀ ; 6.44, H ₈ ; 3.91, 3.86, 3.78, 3 x OMe. J _{7,8} =8.8; J _{8,10} =2.5 Hz.	163, 164
4-Hydroxy-2,3,9-trimethoxypterocarpan	Pisum sativum	10	1	7.13, H ₇ ; 6.61, H ₁ ; 6.44, H ₁₀ ; 6.44, H ₈ ; 5.63, OH; 3.88, 3.84, 3.73, 3 x OMe. J _{7,8} =9; H _{8,10} =2.5 Hz.	163
3-Hydroxy-2,9-dimethoxypterocarpan	Pisum sativum	10	1	7.12, H ₇ ; 6.96, H ₁ ; 6.52, H ₄ ; 6.44, H ₁₀ ; 6.43, H ₈ ; 5.89, OH; 3.9, 3.77, 2 x OMe. J _{7,8} =8.8, J _{8,10} =1.3 Hz.	163

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	$^1\text{H-NMR}$ SHIFTS, δ	REF.
6a,7-Dihydroxy-phaseollin	Phaseolus vulgaris	15,18	1	7.1, H_1 ; 6.8-6.3, $\text{H}_{2,4,8}$; 6.36, =CH at C_{12} ; 5.4, =CH at C_{13} ; 5.26, H_{11a} ; 5.24, H_6 ; 4.77, H_{11a} ; 1.33, 1.3, 2 x Me. $J_{12,13}=10$; $J_{1,2}=8\text{H}_z$.	221-223, 182
6a-Hydroxyphaseollin	Phaseolus vulgaris	15,18	5	7.11, H_1 ; 7.32, H_7 ; 6.7-6.3, $\text{H}_{2,4,8}$; 6.41, =CH at C_{12} ; 5.64, =CH at C_{13} ; 5.3, H_{11a} ; 4.04, H_6 ; 1.37, 1.33, 2 x Me.	221-223, 182
1a-Hydroxyphaseollone	Phaseolus vulgaris	10	1	6.88, H_7 ; 6.69, H_1 ; 6.32, H_8 ; 6.22, H_{12} ; 6.09, H_2 ; 5.48, H_4 ; 5.48, H_{13} ; 5.14, H_{11a} ; 5.08, $\text{H}_{6\text{eq}}$; 4.33, $\text{H}_{6\text{ax}}$; 3.91, H_{6a} ; 1.37, 2 x Me. $J_{1,2}=10$; $J_{6\text{ax},\text{eq}}=10$; $J_{7,8}=8.5$; $J_{12,13}=10\text{H}_z$.	135
3-Hydroxy-4,9-dimethoxypterocarpan	Trifolium cherleri	12	2	7.13, H_7 ; 6.96, H_1 ; 6.6, H_2 ; 6.4, H_{10} ; 6.39, H_8 ; 3.95, 3.9, 2 x OMe.	165
Glyceollin-V (3,6a,9-Trihydroxypterocarpan)	Glycine max	14,19,20	2	7.3, H_1 ; 7.2, H_7 ; 6.55, H_2 ; 6.42, H_8 ; 6.32, H_4 ; 6.26, H_{10} ; 5.26, H_{11a} ; 4.16 & 4.04, H_6 ; $J_{1,2}=8.3$; $J_{2,4}=2.5$; $J_{7,8}=8.3$; $J_{6\text{ax},\text{eq}}=11.6\text{H}_z$.	167-176
Glyceollin-IV (3-Methoxy-6a,9-dihydroxy-2-isopen-tenylpterocarpan)	Glycine max	19,20	2	7.2, H_7 ; 7.18, H_1 ; 6.42, H_8 ; 6.4, H_4 ; 6.25, H_{10} ; 5.24, H_{13} ; 5.2, H_{11a} ; 4.13 & 4.01, H_6 ; 3.79, OMe; 1.72, 2 x Me. $J_{7,8}=8.6$; $J_{8,10}=2.1$, $J_{6a\&eq}=11.4$; $J_{12,13}=7.2\text{H}_z$.	159,174

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
Glyceollin-III	Glycine max	19,20	2	7.27, H ₁ ; 7.27, H ₇ ; 6.46, H ₈ ; 6.27, H ₄ ; 6.26, H ₁₀ ; 5.3, H _{11a} ; 4.15, & 4.05, H _{6ax} & eq. J _{7,8} =8; J _{8,10} =2; J _{6ax} & eq = 11.0 Hz.	169-174
Glyceollin-II	Glycine max	19,20	2	7.15, H ₁ ; 6.43, H ₈ ; 6.41, H ₁₂ ; 6.25, H ₁₀ ; 6.21, H _{4,7} ; 5.65, H ₁₃ ; 5.25, H _{11a} ; 4.13 & 4.04, H _{6ax} & eq; 1.4, 1.37, 2 x Me. J _{7,8} =8; J _{8,10} =2; J _{6ax} & eq = 12; J _{12,13} =10 Hz.	169-173
Glyceollin-I	Glycine max	14,19,20	2	7.2, H ₇ ; 7.16, H ₁ ; 6.6, H ₂ ; 6.42, H ₈ ; 6.41, H ₁₂ ; 6.25, H ₁₀ ; 5.44, H ₁₃ ; 5.15, H _{11a} ; 4.12 & 4.01, H ₆ ; 1.38 & 1.35, 2 x Me. J _{7,8} =10; J _{8,10} =2 Hz.	169-173
Glyceocarpin	Glycine max	14	2	7.19, H ₇ ; 7.16, H ₁ ; 6.41, H ₈ ; 6.36, H ₄ ; 6.24, H ₁₀ ; 5.4, H ₁₃ ; 5.27, H _{11a} ; 4.09 & 3.97, H ₆ ; 3.28, H ₁₂ ; 1.73, 2 x Me. J _{6ax,eq} =11; J _{7,8} =8; J _{12,13} = 7.5 Hz.	183-189, 124,172 156,170, 169,176, 39
Glyceofuran	Glycine max	14	2	7.7, H ₁ ; 7.24, H ₇ ; 6.95, H ₄ ; 6.63, H ₁₂ ; 6.44, H ₈ ; 6.24, H ₁₀ ; 5.47, H _{11a} ; 4.24 & 4.2, H ₆ ; 1.68, 2 x Me. J _{6ax,eq} =11; J _{7,8} =8.0 Hz.	183-189
Glyceofuran-9-O-methylether	Glycine max	14	2	7.2, H ₇ ; 7.16, H ₁ ; 6.9, H ₄ ; 2.37, H ₁₂ ; 6.34, H ₈ ; 6.3, H ₁₀ ; 5.45, H _{11a} ; 4.23 & 2.17, H ₆ ;	183-189

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
<u>COUMESTANS</u>					
Coumestrol (3,9-Dihydroxycoumestan)	Ladino clover, phase-collus vulgaris	14,19,21	9	1.72, 2 x Me. 7.9, H ₅ ; 7.2-7.0 complex, H _{6,8,10} ; 7.2-7.0 complex, H _{11,13} .	8,22,177, 178
9-O-Methylcoumestrol	Medicago sativa	19	9	7.7, H ₅ ; 7.3-7.0 complex, H _{6,8,10} ; 7.2-7.0 complex, H _{11,13} ; 3.79, OMe.	178,140
3-Hydroxy-8,9-dimethoxycoumestan	Medicago sativa	19,22	9	7.26, H ₁ ; 7.2, H ₇ ; 6.6, H ₂ ; 6.4, H ₄ ; 6.28, H ₁₀ ; 3.79 & 3.78, 2 x OMe.	179,180
Wairol (3-Hydroxy-7,9-dimethoxycoumestan)	Medicago sativa	22	1	7.3, H ₈ ; 7.28, H ₁ ; 6.5, H ₂ ; 6.4, H ₄ ; 6.3, H ₁₀ ; 3.8 & 3.78, 2 x OMe.	179
Repensol (3,7,9-Trihydroxycoumestan)	Ladino clover	22	6	7.31, H ₈ ; 7.28, H ₁ ; 6.45, H ₂ ; 6.38, H ₄ ; 6.25, H ₁₀ .	18,182
Trifoliol (3,7-Dihydroxy-9-methoxycoumestan)	Ladino clover	22	9	7.83, H ₁ ; 7.03, H ₂ ; 6.97, H ₄ ; 6.42, H ₈ ; 6.8, H ₁₀ ; 3.82, OMe.	18,182
<u>ISOFLAVONES AND ISOFLAVANS</u>					
Daidzein (7,4'-Dihydroxyisoflavone)	Glycine max	14	2	8.2, H ₂ ; 8.08, H ₅ ; 7.97, H ₆ ; 7.0, H ₈ ; 7.47, H _{2',6'} ; 6.9, H _{3',5'} . J _{5',6'} =8.5; J _{5,6} =8.8 Hz.	8,171
Isoformononetin (7-Methoxy-4'-hydroxyisoflavone)	Glycine max	14	2	8.21, H ₂ ; 8.1, H ₅ ; 7.07, H ₆ ; 7.05, H ₈ ; 7.48, H _{2',6'} ; 6.88, H _{3',5'} ; 3.86, OMe. J _{2',3'} =8.5; J _{5,6} =9; J _{5',6'} =9 Hz.	8,171

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
Genistein (5,7,4'-Trihydroxyiso-flavone)	Phaseolus vulgaris	2	7	8.2, H ₂ ; 8.05, H ₆ ; 7.03, H ₈ ; 7.45, H _{2',6'} ; 6.8, H _{3',5'} . J _{6,8} =2.3; J _{2',3'} =9; J _{5',6'} =9 Hz.	190
7,2',4'-Trihydroxyisoflavanone	Phaseolus vulgaris	2	2	7.74, H ₅ ; 6.81, H ₆ ; 6.54, H ₆ ; 6.45, H ₃ ; 6.39, H ₈ ; 6.24, H ₅ ; 4.59, H _{2ax} ; 4.44, H _{2eq} ; 4.09, H ₃ . J _{5,6} =8.8; J _{6,8} =2.2; J _{5',6'} =8.3; J _{2ax,eq} =10.7 Hz.	287
7,2',4'-Trihydroxyisoflavone	Phaseolus vulgaris	2	2	8.14, H ₂ ; 7.93, H ₅ ; 6.98, H ₆ ; 6.93, H ₆ ; 6.86, H ₈ ; 6.36, H ₃ ; 6.27, H ₅ . H _{5,6} =8.8, H _{6,8} =2.2; H _{5',6'} =8.3; H _{3',5'} =2.4 Hz.	287
2'-Hydroxygenisten (2',4',5,7-Tetrahydroxyisoflavone)	Phaseolus vulgaris	2	7	8.07, H ₈ ; 7.77, H ₆ ; 6.36, H ₃ ; 6.25, H ₅ ; 6.12, H ₆ . J _{5',6'} =8; J _{3',5'} =2.4 Hz.	136, 191-195
Luteone (2',4',5,7-Tetrahydroxy-6(3,3-dimethylallyl)-isoflavone)	Lupinus albus	3	2	7.98, H ₈ ; 7.75, H ₆ ; 6.35, H ₃ ; 6.2, H ₅ ; 5.18, =CH; 3.19, -CH ₂ ; 1.75 & 1.65, 2 x Me. J _{5,6} =8; J _{3',5'} =2 Hz.	241
Isoferreirin (5,7,4'-Trihydroxy-2'-methoxyflavone)	Dolichos biflorus	14		8.05, H ₈ ; 7.75, H ₆ ; 6.4, H ₃ ; 6.25, H ₅ ; 6.12, H ₆ . J _{5',6'} =8; J _{3',5'} =2.4 Hz.	289
Kievitone (2',4',5,7-Tetrahydroxy-8-isopentenyliso-flavone)	Phaseolus vulgaris, Dolichos biflorus, Ougeinia dalbergioides, Lablab niger	2, 10, 11 13-15, 19	7	6.91, H ₂ ; 6.45, H ₅ ; 6.04, H ₆ ; 6.32, H ₃ ; 5.18, -CH ₂ ; 4.6, 4.16, H ₂ & 3; 3.21, -CH ₂ ; 1.74 & 1.66, 2 x Me; 9.2, 8.78, 8.59, OH. J _{2',3'} =8; J _{3',5'} =2 Hz.	23, 190, 195-206, 290

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	$^1\text{H-NMR}$ SHIFTS, δ	REF.
Kievitone hydrate	Phaseolus vulgaris	10	3	6.97, $\text{H}_{2,7}$; 6.31, $\text{H}_{5,6}$; 6.25, $\text{H}_{3,4}$; 5.95, H_6 ; 4.5, H_{2a} & b; 4.15, H_3 ; 2.8, $\text{H}_{1,11}$; 1.6, $\text{H}_{2,11}$; 1.25, 2 x Me	135
Phaseoluteone [2', 4', 5, 7-Tetrahydroxy-3'-(3,3-dimethylallyl) isoflavone]	Phaseolus vulgaris	2	2	13.11, 5-OH; 8.12, H_2 ; 6.9, H_6 ; 6.55, H_5 ; 6.46, H_8 ; 6.33, H_6 ; 5.33, =CH; 3.44, -CH ₂ ; 1.78 & 1.64, 2 x Me. $J_{5,6}=8.6$; $J_{6,8}=2\text{H}_2$.	122, 220
7-Hydroxyflavan	Narcissus pseudo-narcissus	13	1	7.37, $\text{H}_{1,5}$; 6.94, H_5 ; 6.4, H_6 & 8; 5.05, H_2 ; 2.7, H_4 ; 2.1, H_3 . $J_{5,6}=8.5$; $J_{6,8}=4\text{H}_2$.	207
4', 7-Dihydroxyflavan	Narcissus pseudo-narcissus	13	8	7.24, $\text{H}_{1,6}$; 6.83, $\text{H}_{3,5}$; 6.35, H_8 ; 6.39, H_6 ; 6.89, H_5 ; 4.81, H_2 ; 2.8, H_4 ; 2.1, H_3 . $J_{5,6}=8.5$; $J_{6,8}=2.5\text{H}_2$.	207
4', 7-Dihydroxy-8-methylflavan	Narcissus pseudo-narcissus	13	3	7.26, $\text{H}_{1,6}$; 6.8, $\text{H}_{3,5}$; 6.7, H_5 ; 6.34, H_6 ; 4.95, H_2 ; 2.3, H_4 ; 2.11, Me; 2.0, H_3 .	207
Broussin (4'-Methoxy-7-hydroxyisoflavan)	Broussonetia papyrifera	29	1	4.98, dd, 1H, 2.12, m, 2H; 2.77, m, 2H, -CH ₂ .	208, 209
Demethylvestitol (2', 4', 7-Trihydroxyisoflavan)	Lotus corniculatus, Lotus hispidus, Lotus uliginosus, Tetragonolobus maritimus	12	2	7.12, H_6 ; 6.87, H_8 ; 6.5, H_3 ; 6.6, H_5 ; 6.39, H_6 ; 6.35, H_5 ; 3.77, H_2 ; 2.5, H_3 ; 2.8, H_4 .	79, 140, 142, 165, 210-212

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
Vestitol (2',7-Dihydroxy-4'-methoxyisoflavan)	Medicago sativa, Lotus corniculatus, Lotus hispidus, Lotus uliginosus	12,19	1	7.3, H ₆ ; 6.87, H ₈ ; 6.58, H ₅ ; 6.5, H ₃ , ₅ ; 6.41, H ₆ ; 6.34, H ₅ ; 3.9, OMe; 3.77, H ₂ ; 2.47, H ₃ ; 2.75, H ₄ .	165,210-212
Isovestitol (4',7-Dihydroxy-2'-methoxyisoflavan)	Tetragonolobus maritimus	12	1	7.12, H ₆ ; 6.8, H ₈ ; 6.5, H ₃ , ₅ ; 6.38, H ₆ ; 6.35, H ₅ ; 3.98, OMe; 3.77, H ₂ ; 2.47, H ₃ ; 2.8, H ₄ .	211,213
2'-Methoxyvestitol	Medicago sativa, Lotus corniculatus, Lotus hispidus	1,12,19 24	1	7.15, H ₆ ; 6.9, H ₈ ; 6.45, H ₃ , ₅ ; 7.38, H ₆ ; 7.35, H ₅ ; 3.98, 2 x OMe; 3.68, H ₂ ; 2.45, H ₃ ; 2.75, H ₄ .	165,140, 142,144, 214
5-Methoxyvestitol	Lotus hispidus	12	1	7.48, H ₆ ; 7.15, H ₆ ; 6.78, H ₈ ; 6.65, H ₃ , ₅ ; 3.9, 2 x OMe; 3.7, H ₂ ; 2.55, H ₃ ; 2.75, H ₄ .	165,211
Lotisoflavan (2',4'-Dihydroxy-5,7-dimethoxyisoflavan)	Lotus angustis-simus, Lotus edulis	12	7	8.96, 8.78, OH; 6.86, H ₆ ; 6.42, H ₃ ; 6.27, H ₅ ; 6.03, H ₆ &8; 4.28, H _{2eq} ; 3.92, H _{2ax} ; 3.75, 3.78, 2 x OMe; 3.5-3.1, H ₃ ; 2.7, H ₄ .	215
Mucronulatol (2',4'-Dimethoxy-3',7-dihydroxyisoflavan)	Astragalus cicer, Astragalus gummifer, Astragalus Pyrenai-cus	12		7.05, H ₆ ; 6.88, H ₆ ; 6.55, H ₅ ; 6.48, H ₅ ; 6.48, H ₈ ; 4.27, H _{2eq} ; 4.1, H _{2ax} ; 3.79, 2 x OMe; 3.67, H ₂ ; 2.55, H ₃ ; 2.65, H ₄ .	216
Astraciceran (7-Hydroxy-2'-methoxy-4',5'-methylenedioxyisoflavan)	Astragalus cicer, Astragalus Pyrenai-cus	12		7.11, H ₆ ; 6.9, H ₆ ; 6.45, H ₃ ; 6.15, H ₅ ; 6.21, H ₈ ; 4.3, H _{2eq} ; 4.05, H ₂ ; 3.8, OMe; 4.25, methylenedioxy; 3.5-3.3, H ₃ ; 2.5, H ₄ .	216,217

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	$^1\text{H-NMR}$ SHIFTS, δ	REF.
Phaseollin isoflavan (2',3,7-Trihydroxy- 4',5'-methylenedi- oxyisoflavan)	Phaseolus vulgaris, Pisum sativum	15,30,3	1	6.91 & 6.71, H_5 & 6,; 6.57, H_8 ; 6.5, 6.34, H_6 & 5,; 5.59, chromoene- βH ; 4.23, $\text{H}_{2\text{eq}}$; 3.91, $\text{H}_{2\text{ax}}$; 3.7-3.3, H_3 ; 2.89- 2.8, H_4 ; 1.38, 2 x Me.	92,137
2'-Methoxyphaseol- linisoflavan	Phaseollus vulgaris	10	1	6.9 & 6.7, H_5 & 6,; 6.56, H_8 ; 6.55, 6.35, $\text{H}_{6,5}$; 5.59, chromoene- βH ; 4.23, $\text{H}_{2\text{eq}}$; 3.91, $\text{H}_{2\text{ax}}$; 3.79, OMe; 3.8-3.4, H_3 ; 2.82, H_4 ; 1.38, 2 x Me.	138
2'-Methoxyphaseol- lidinisoflavan	Vigna unguiculata	15	1	6.91, H_6 ; 6.63, H_5 ; 5.27, =CH; 4.3, $\text{H}_{2\text{eq}}$; 3.93, $\text{H}_{2\text{ax}}$; 2.94 & 2.81, H_4 ; 3.45, -CH ₂ -; 1.8, 1.74; 2 x Me; 3.73, OMe.	218
<u>COUMARINS AND</u> <u>CHROMONES</u>					
Asculetin	Solanum tuberosum	32-35	3	7.85, H_5 ; 7.75, H_8 ; 5.4, H_4 ; 5.15, H_3 ; 3.85, OMe.	224-229
Scopoletin	Solanum tuberosum	32-35	3	7.82, H_5 ; 7.75, H_8 ; 5.35, H_4 ; 5.15, H_3 .	224-229
Isofraxidin-7- glucoside (7- Hydroxy-6,8-di- methoxycoumarin- 7-glucoside)	Solanum tuberosum	35	3	7.95, H_5 ; 6.41, H_4 ; 5.18, H_3 ; 3.9, OMe; 4.04, OMe.	224
6-Hydroxymellein (3-Methyl-6,8-di- hydroxy-3,4-di- hydroisocoumarin)	Carrots (Daucus carota)	33,36	1	6.3, H_7 ; 6.21, H_5 ; 4.61, H_3 ; 2.8, H_4 ; 1.41, Me; 11.3, OH at C_8 .	291-294

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
6-Methoxymellein	Carrots (Daucus Carota)	13,33,36	1	6.29, H ₇ ; 6.19, H ₅ ; 4.61, H ₃ ; 3.75, OMe; 2.79, H ₄ ; 1.43, Me $J_{5,7}=2$; $J_{3,Me}=6.5H_z$.	291-296
Lathodoratin (5,7-Dihydroxy-3-ethyl-chromone)	Lathyrus odoratus	3,12,13, 37-39	3	7.83, H ₂ ; 6.24, H ₆ ; 6.14, H ₈ ; 2.48, -CH ₂ ; 1.17, -Me.	96,230
<u>STILBENES AND DIPHENYLPROPANES</u>					
Resveratrol (Trans-3',4,5'-tri-hydroxystilbene)	Vitis vinifera	13,38	2	7.01, =CH-; 7.35, =CH-; 6.35, 6.39, 6.46-6.62, 6.65, 7.44, Ar-H. $J_{7.01,7.35}=16H_z$.	231-233
Oxyresveratrol	Morus alba	10	2	7.04, =CH; 7.4, =CH-; 6.39, 6.45-6.64, 6.7, 7.54, Ar-H $J_{7.4,7.04}=17H_z$.	234,236, 237
4'-(3-Methyl-2-butenyl)oxyresveratrol	Morus alba	10	2	7.39, =CH-; 7.03, =CH-; 7.58, H ₃ ; 6.8, H ₂ , ₆ ; 6.47-6.67, H ₅ , ₆ ; 5.16, =CH-; 3.31, -CH ₂ -; 1.75, 1.63, 2 x Me. $J_{7.39,7.03}=17$; $J_{CH=CH_2}=7H_z$.	234
4'-(3-Methyl-1-butenyl)resveratrol	Arachis hypogaea	40	2	7.38, H ₆ ; 7.38, H ₂ ; 6.82, H ₃ ; 6.82, H ₅ ; 6.91, CH=CH; 6.82, CH=CH; 6.58, H ₂ , ₁ ; 6.58, H ₆ , ₁ ; 5.3, =CH; 3.36, -CH ₂ -; 1.78, 1.65, 2 x Me. $J_{-CH=CH}=16$; $J_{5,6}=9$; $J_{2,3}=9$; $J_{=CH-CH_2}=6H_z$.	238,239

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	$^1\text{H-NMR}$ SHIFTS, δ	REF.
4-(3-Methylbut-1-enyl)oxyresveratrol	Arachis hypogaea	40	2	7.04, H_2 ; 6.89, H_6 ; 6.89, =CH-; 6.8, H_5 ; 6.76, =CH-; 6.68, =CH-; 6.68, =CH-; 6.57, H_2 ; 2.41, > CH_3 ; 1.09, 2 x Me. $J_{\text{=CH-CH}_2\text{-}}=6$; $J_{\text{CH=CH}}=16$; $J_{5,6}=9\text{H}_z$.	238
4-(3-Methylbut-1-enyl) resveratrol	Arachis hypogaea	40	2	7.39, H_2 ; 7.39, H_6 ; 7.82, H_3 ; 7.82, H_5 ; 6.94, -CH=CH-; 6.82, -CH=CH-; 6.6, H_2 ; 6.6, H_6 ; 6.68, =CH-; 2.4, >CH-; 1.1, 2 x Me. $J_{\text{CH-Me}}=7$; $J_{\text{-CH=CH-}}=16$; $J_{5,6}=8$; $J_{2,3}=8\text{H}_z$.	238
Resveratrol Dehydrodimer (ϵ -Vini-ferin)	Vitis vinifera	13,38	2	7.4, 5XOH; 6.73, =CH-; 6.93, =CH-; 7.22, (2H), 7.17, (2H), 6.86 (2H), 6.76 (2H), 6.75 (2H), 6.35 (1H), 6.27 (3H), Ar-H; 5.45, >CH-O; 4.5, Ar-CH<. $J_{\text{CH=CH}}=16$; $J_{\text{Ar-H}}=2.1, 8.5\text{H}_z$.	232
Broussonin-A (2,4'-Dihydroxy-4-methoxydiphenylpropane)	Broussonetia papyrifera, Morus alba	10,29	2	7.01, 6.96, 6.74, 6.41, 6.34, Ar-H; 3.68, OMe; 2.59, Ar- CH_2 -; 2.56, Ar- CH_2 ; 1.84, - CH_2 -, 8.1, OH. $J_{\text{-CH}_2\text{-CH}_2}=7.0$; $J_{\text{Ar-H}}=2.5 \text{ \& } 8\text{H}_z$	240
Broussonin-B (4,2'-Dihydroxy-2-methoxydiphenylpropane)	Broussonetia papyrifera, Morus alba	10,29	2	7.05, OH; 7.01, 6.73, 6.9, 6.34, 6.42, Ar-H; 3.75, OMe; 2.53, - CH_2 - CH_2 -; 1.78, - CH_2 -. $J_{\text{CH}_2\text{-CH}_2}=7$; $J_{\text{Ar-H}}=2.5, 8\text{H}_z$.	240

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
Broussonin-C (2,4,4'-Trihydroxy-5'-isopentenylidiphenyl propane)	Broussonetia papyrifera, Morus alba	29	2	5.34, =CH-; 3.3, Ar-CH ₂ -CH=; 2.55, Ar-CH ₂ ; 2.54, Ar-CH ₂ ; 1.85, CH ₂ ; 1.3, 2 x Me.	240
Morachalcone (2,2',4,4'-Tetrahydroxy-3'-isopentenyl-chalcone)	Broussonetia papyrifera, Morus alba	10	2	13.97, 9.26, 9.21, 8.9, 4 x OH; 8.23, =CH; 7.72, =CH; 7.89, 7.68, 6.51, 6.52, 6.46, 5Ar-H; 5.3, =CH; 3.18, -CH ₂ -; 1.75 & 1.63, 2 x Me. J _{CH=CH} = 15; J _{=CH-CH₂} = 7; J _{Ar-H} = 2 & 8 Hz.	242
<u>BENZOFURANS</u>					
Chalcomoracin	Broussonetia papyrifera, Morus alba	10	2	12.84, OH; 9-8, 6XOH; 8.4 (J9); 6.98 (J8); 6.49 (J2); 6.46 (J9), Ar-H; 6.31, (J2,8), 7.32 (J8), 6.89 (J2), 6.89, 6.75, 6.74, (J2,8), Ar-H; 5.17, =CH; 3.28, -CH ₂ (J7); 1.71, 1.5, 2 x Me.	242
Moracin-A	Morus alba	10	2	8.62, 2 x OH; 6.94 (J2), 6.82 (J2,8), 6.45 (J2), 6.44 (J2), 5 x Ar-H; 7.13, =CH-; 3.96, 3.88, 2 x OMe.	243
Moracin-B	Morus alba	10	2	8.5, 7.33, 2 x OH; 7.08 (J0.8); 7.04, 6.97, 6.5 (J2) 5 x Ar-H; 7.21, =CH; 3.94, 3.83, 2 x OMe.	243
Moracin-C	Morus alba	10	2	8.51, 8.35, 3 x OH; 7.43 (J8), H ₄ ; 7.01 (J2&0.8), H ₇ ; 6.97, H ₂ , 6; 6.85 (J8&2), H ₅ ; 6.95, (J0.8), H ₃ ; 5.38, =CH- (J7);	234

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	$^1\text{H-NMR}$ SHIFTS, δ	REF.
Moracin-D	Morus alba	10	2	3.45, $-\text{CH}_2$ (J7); 1.8, 1.7 2 x Me. 8.63, 2 x OH; 7.07 (J0.8), H_3 ; 7.01 (J2), H_7 ; 7.42 (J8) H_4 ; 6.86 (J1.6), H_6 ; 6.84 (J2&8), H_5 ; 6.82 (J1.6&8), H_8 ; 6.73 (J0.8 &10) H_4 ; 5.69 (J10), H_3 ; 1.42, 2 x Me.	234
Moracin-E	Morus alba	10	2	8.64, 2 x OH; 7.48 (J8), H_4 ; 7.04 (J2), H_5 ; 6.88 (J0.8), H_3 ; 6.85 (J0.8,10), H_4 ; 6.86 (J2,8), H_5 ; 6.83 (J2.4), H_6 ; 6.39 (J2.4,0.8), H_8 ; 5.68 (J10) H_3 ; 1.44, 2 x Me.	234,244
Moracin-F	Morus alba	10	2	8.37, 2 x OH; 7.16, H_7 ; 7.09, H_4 ; 7.01 (J0.8), H_3 ; 6.85 (J2), H_4 , 6, 6.36 (J2), H_4 ; 3.88, 3.83, 2 x OMe.	234,244
Moracin-G	Morus alba	10	2	8.57, 2 x OH; 7.38 (J8), H_4 ; 7.11, H_3 ; 6.95 (J8), H_5 ; 6.94 (J2), H_2 , 6, 6.43 (J2), H_4 ; 5.74, H_4 ; 4.47, H_2 ; 3.74, H_5 ; 1.58, Me.	234,244
Moracin-H	Morus alba	10	2	8.51, 2 x OH, 7.5, H_5 ; 6.93 (J2), H_2 , 6, 6.51, H_3 ; 6.41 (J2), H_4 ; 5.75, H_4 ; 4.48, H_2 ; 3.92, OMe; 3.67, H_5 ; 1.6, Me.	234,244

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	¹ H-NMR SHIFTS, δ	REF.
Vignafuran [2-(2'-Methoxy-4'-hydroxy-phenyl)-6-methoxy-benzofuran]	Vigna unguiculata	15	1	7.85, (J9.3), H ₆ ; 7.5 (J9), H ₄ ; 7.05, H _{3,7} ; 6.85 (J2.7&9), H ₅ ; 6.55, H _{3',5'} ; 3.9, OMe, 3.85, OMe.	265-271
6-Demethylvignafuran	Tetragonolobus maritimus	12	1	7.8 (J9), H ₆ ; 7.48 (J9), H ₄ ; 6.9, H _{3,7} ; 6.8 (J2.2&9), H ₅ ; 6.5, H _{3',5'} ; 3.9, OMe.	265, 213
<u>ACETYLENS AND PURANOACETYLEINS</u>					
Wyerone	Vicia fabae, Vicia narbonesis, Vicia galilea	13, 19	4	7.43, H ₁ ; 7.3, H ₈ ; 6.78, H ₈ ; 6.6, H ₂ ; 6.4, H ₅ ; 5.71, H ₄ ; 3.78, OMe; 2.56, H ₆ ; 1.25, H ₇ .	245, 246
Wyerone acid	Vicia fabae, Jack bean (canavalia ensiformis)	13, 26, 20	1	11.2, -COOH; 7.4, H ₁ ; 7.28, H ₈ ; 6.78, H ₈ ; 6.58, H ₂ ; 6.4, H ₅ ; 5.7, H ₄ ; 2.5, H ₆ ; 1.2, H ₇ .	247-254, 150
Wyerone epoxide	Vicia fabae	13, 26	1	7.48, H ₁ ; 6.37, (J3.7), H ₈ ; 6.75 (J3.7), H ₈ ; 6.4 (J16), H ₂ ; 3.83, OMe; 3.66 (J6.1), H ₄ ; 3.21 (J3.9&6), H ₅ ; 1.76, H ₆ ; 1.15 (J7.5), H ₇ .	254-256
Wyerol epoxide	Vicia fabae	26	1	6.4, H ₈ ; 6.53, H ₈ ; 5.53, H ₁ ; 3.54, H ₆ ; 3.09, H ₅ .	254
4,5-Dihydro-4,5-dihydroxywyerol	Vicia fabae	26	1	6.53, H ₈ ; 6.4, H ₈ ; 5.53, H ₁ ; 3.65, H ₅ ; 4.3, H ₄ .	254
Falcarindiol (Hep-tadeca-1,9-diene-4,6-diene-3,8-diol)	Lycopersicon esculentum, phaseolus vulgaris, Daucus carota, Aegopodium Podagraria	42	4	5.9 (J5,9,17), H ₁₋₁₃ ; 5.7-4.8, H ₈₋₁₀ ; 2.11, H _{11,12} ; 1.3, H ₁₃₋₁₆ ; 0.90, Me.	257-261

COMPOUND	PLANT SOURCE	STRESS AGENT	SOLVENT	$^1\text{H-NMR}$ SHIFTS, δ	REF.
Falcarinol (Hepta-deca-1,9-diene-4,6-diyne-3-ol)	Lycopersicon esculentum, phaseolus vulgaris, Daucus carota, Aegopodium Podagraria	42	4	5.3, H_1 ; 5.95 ($\text{J}_{4.5,9,16}$), H_2 ; 5.45, $\text{H}_{9,10}$; 4.8 ($\text{J}_{4.5}$), H_3 ; 2.1, H_{11} ; 3.0 (J_5), H_8 ; 1.3, H_{12-16} ; 0.90, Me.	257-261
Tetradeca-6-ene-1,3-diyne-5,8-diol	Lycopersicon esculentum		1	5.63, $\text{H}_{6,7}$; 5.3, H_5 ; 4.5, H_8 ; 2.85, 2 X OH; 2.2, H_1 ; 1.5, H_9 ; 1.3, H_{8-13} ; 0.90, Me.	260
Safynol (3,11-Tri-decadiene-5,7,9-triyne-1,2-diol)	Carthamus tinctorius	25,29	1	5.5, $\text{H}_{3,12}$; 4.7, $\text{H}_{2,4,11}$; 3.7, H_1 ; 1.8, Me.	262-264
Dehydrosafynol (11-Tridecene-3,5,7,9-tetrayne-1,2-diol)	Carthamus tinctorius	29	1	5.45, H_{12} ; 4.7, $\text{H}_{2,11}$; 3.75, H_1 ; 1.5, Me.	262-264
Gossypol	Gossypium hirsutum, Gossypium barbadense	24, 19	1	15.2, 2 X OH; 11.3, CHO; 7.8, 2 X Ar-H; 6.4, 2 X OH; 5.9, 2 X OH; 3.75, >CH-; 2.2, 2 X Ar-Me; 1.55, 4 X Me.	272-281
Hemigossypol	Gossypium hirsutum	24	1	7.3, -CHO; 6.5, Ar-H; 5.8, Ar-H; 3.7, >CH; 3.5, OH; 2.4, Ar-Me; 1.45, 2 X Me.	282,283
Vergosin (Deoxy-6-methoxyhemigossypol)	Gossypium hirsutum	24,11	1	7.28, CHO; 6.54, Ar-H; 5.75, Ar-H; 3.9, OMe; 3.65, >CH-; 3.5, OH; 2.3, Ar-Me; 1.45, 2 X Me.	282,283

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