Identification of 5-(2-Oxoalkyl)resorcinols and 5-(2-Oxoalkenyl)resorcinols in Wheat and Rye Grains

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Several homologs of 5-(2-oxoalkyl)- and 5-(2-oxoalkenyl)resorcinols were identified in extracts of wheat and rye grains. Homologs of the 5-(2-oxoalkyl)resorcinols included 5-(2-oxononadecyl)-, 5-(2-oxoheneicosanyl)-, 5-(2-oxotricosanyl)-, and 5-(2-oxopentacosanyl)resorcinol, with the heneicosanyl and tricosanyl homologs being predominant. The homologs of 5-(2-oxoalkenyl)resorcinols consisted of 5-(2-oxoheneicosenyl)- and 5-(2-oxotricosenyl)resorcinol. The major alkyl and alkenyl homologs were isolated by thin-layer (TLC) and high-performance liquid chromatography (HPLC) and then identified by TLC, HPLC, gas chromatography coupled with infrared and mass spectroscopy, and proton magnetic resonance spectroscopy. Abundances of the "oxo" components are minor compared to the 5-n-alkyl-resorcinols and, apparently, have been overlooked in previous studies of resorcinols in wheat and rye grains.

INTRODUCTION

Wheat, rye, and triticale grains contain a major group of 5-n-alkylresorcinols with odd-number side chains of C15–C25 (Wenkert et al., 1964; Wieringa, 1967; Verdeal and Lorenz, 1977; Gohil et al., 1988; Lorenz and Hengtrakul, 1990). A minor group of alkenylresorcinols has also been reported (Wieringa, 1967) with apparent side-chain lengths of C17–C25 (Gohil et al., 1988). In general, the alkenylresorcinols are not as well characterized as the alkylresorcinols, especially with regard to number and position(s) of double bonds in the side-chain group. Gohil et al. (1988) discussed mass spectral identification of two different alkenylresorcinols (apparently isomers) for each homolog, but the actual data supporting those identifications were not presented. Kozubek (1984) reported separations of 5-n-alk(en)ylresorcinol homologs from rye and wheat grains by using silica gel thin-layer chromatography plates impregnated with silver nitrate. Later, Kozubek (1985) described a preparative-scale isolation of 5-n-alkyl-, 5-n-alkenyl-, and 5-n-alkadienyl-resorcinol homologs from rye grain. The separations of saturated and unsaturated homologs were assumed to be caused by interactions of the double bonds with silver ions, but no spectroscopic or other evidence for unsaturation in the side-chain group was given. The presence of oxygen in the side chain had not been mentioned as a possible explanation for at least some of the minor components that were separated from the major saturated alkylresorcinols.

In this paper, I present evidence for minor resorcinol homologs in wheat and rye grains that have a ketone group at the second carbon of the side chain, i.e. 5-(2-oxoalkyl)-resorcinols with side chains containing 19, 21, 23, and 25 carbon atoms. Homologs with unsaturation in addition to the ketone group, i.e. 5-(2-oxoalkenyl)resorcinols, are also described. The identifications were based on results from several chromatographic and spectroscopic methods. Vapor-phase infrared spectra of 5-n-alkylresorcinols and 5-(2-oxoalkyl)resorcinols are shown for the first time.

Interest in alkylresorcinols and related compounds has been stimulated by various reports of antinutritional and other biological activity (Lorenz and Hengtrakul, 1990, and references therein; Sedlet et al., 1984). Kozubek and Demel (1980; 1981) reported that 5-n-alkylresorcinols from rye caused increased membrane permeability to small solutes (such as K⁺, glycerol, and erythritol), and that "unsaturated" resorcinols caused membrane lysis. Resorcinols with oxygenated side chains were probably present in some of the fractions previously tested for biological activity. Biological properties of the compounds reported in this paper are not known, and determination of such properties was beyond the scope of this paper.

EXPERIMENTAL PROCEDURES

Samples. Wheat and wheat bran represented mixtures of cultivars of hard-red winter wheat grown mostly in Kansas and adjoining states. Rye was a mixture of cultivars grown in the north-central United States.

Extraction and Base–Acid Cleanup Procedures. Ten-gram samples of ground whole kernels or bran were extracted with 50 mL of acetone by shaking the mixture for 60 min with a wrist shaker. After particulate material was allowed to settle, a 30-mL aliquot of supernatant was transferred with a syringe to a 25- × 150-mm screw-cap (Teflon-lined) culture tube. The solvent was evaporated under nitrogen and the residue dissolved in 30 mL of methanol. The methanol solution was made basic (pH ~10) by adding 10 mL of 0.6% KOH and partitioned with hexane (2 × 10 mL), and the hexane was discarded. The aqueous portion was then acidified (pH ~2) with 1 mL of 6 N HCl and partitioned again with hexane (3 × 5 mL). The final hexane extract was evaporated under nitrogen and the residue redissolved in methanol for analysis by HPLC or in chloroform for application to TLC plates. The procedure was scaled up proportionately when larger amounts of wheat or rye were extracted for isolation of compounds.

Chromatographic and Spectroscopic Analyses. Thin-layer chromatography (TLC) was performed by using glass-backed plates (20 × 20 cm, SIL-G coating; Brinkman Instruments, Waterbury, NY). Coating thickness was 0.25–2.0 mm, depending on the amount of material to be applied or the resolution required. Plates were developed in benzene–ethyl acetate (85/15, v/v). Resorcinol bands were identified by spraying a narrow strip along one edge of the plate with tetrazotized benzidene reagent (Randerath, 1964; Love, 1985). In this work, 3,3′,5,5′-tetramethyl-benzidine, a noncarcinogenic analog of benzidine (Aldrich Chemical Co., Milwaukee, WI), was used. Resorcinol bands in the nonsprayed area were scraped off, the silica gel was extracted with methanol, and the extract was evaporated on a steam bath with a gentle stream of nitrogen directed into the vial. The residue was dissolved in methanol and analyzed by high-performance liquid chromatography (HPLC) and/or by gas chromatography (GC) as described below.

Plates impregnated with silver were prepared by spraying each plate with AgNO₃ solution (1 g of AgNO₃ in 16 mL of methanol-water). The plates were dried for 30 min at 100 °C.

Resorcinol bands obtained by preparative TLC were further fractionated by preparative HPLC, generally using conditions as described below. Samples were repeatedly injected until enough component (or fraction) was collected for further chromatographic and spectroscopic analyses.

The HPLC instrument used in all analyses was a Hewlett-Packard Co. (Avondale, PA) Model 1084B equipped with a photodiode array detector, autosampler, autoinjector, integrator, column oven, and fraction collector. The detector, Model 1040A, records ultraviolet-visible (UV-vis) spectra (190-660 nm) without having to stop the flow of the mobile phase. Chromatograms are formed by monitoring the difference between absorbances of sample and reference wavelengths. For all analyses the reference wavelength was centered at 500 nm with a 100-nm bandwidth. Sample wavelengths were centered at 215 or 280 nm with a bandwidth of 8 nm.

The HPLC column (6.2 × 80 mm) contained C_{18} packing of 3-μm particle size (Golden Series Zorbax, DuPont, Wilmington, DE). An in-line filter was positioned between the column and the injector. Column temperature was 50 °C. The mobile phase was methanol or methanol-water mixtures as indicated below. The flow rate was 1.2 mL/min.

Most of the gas chromatographic-mass spectrometric (GC-MS) analyses were performed on a Hewlett-Packard system consisting of a Model 5790A GC containing a 30-m × 0.2-mm bonded-phase capillary column (DB-5, Supelco) connected to a Model 5970 mass-selective detector and Model 9816 data system. The temperature was programmed from 150 to 320 °C at 10 °C/min and then held at 320 °C for 15 min. Carrier gas was helium at about 1 mL/min. The ion source voltage was 70 eV, and the temperature was 250 °C.

Samples were also analyzed by a Hewlett-Packard GC-FTIR-MS system consisting of a gas chromatograph (Model 5890) coupled in series to a Fourier transform infrared detector (5965A) and a mass selective detector (5970). The column and other conditions were the same as given above. The transfer lines and sample cell in the infrared detector were held at 300 °C.

Proton spectra of samples dissolved in acetone-d_6 (100 atom % d, Gold Label; Aldrich Chemical Co., Milwaukee, WI) were obtained with a Bruker 400-MHz nuclear magnetic resonance spectrometer.

Reference Standard. 5-n-Pentadecylresorcinol was obtained from Sigma Chemical Co. (St. Louis, MO).

RESULTS AND DISCUSSION

Evidence for 5-(2-Oxoalkyl)resorcinols. Silica gel thin-layer chromatography (TLC) of base-acid-cleaned extracts from wheat (whole kernels or bran) and rye gave major (R_f 0.5) and minor (R_f 0.4) bands on plates with 0.25-mm coating thickness. The major band represented 5-n-alkylresorcinols as evidenced by its R_f being the same as for pentadecylresorcinol and by chromatographic and spectroscopic results discussed below. The minor band was a homologous series of 5-(2-oxoalkyl)resorcinols as indicated by evidence presented below, and its intensity was generally higher in rye than in wheat. Still other faint bands were observed at lower R_f's, which appear to represent other types of resorcinols since the benzidene spray produced a reddish-brown color similar to those for the bands at R_f 0.4 and 0.5. Further identification of these very minor components, which appear to be more prevalent in rye than in wheat, was not attempted. The TLC separations were not discernibly changed when plates impregnated with silver were used.

Results from HPLC analyses of the major and minor TLC bands from wheat are shown in Figure 1. The chromatogram for the major band indicated a homologous series of 5-n-alkylresorcinols as reported previously (Lorenz and Hengtrakul, 1990; Seitz and Love, 1987; Love, 1985). Each peak had the same UV spectrum with a shape
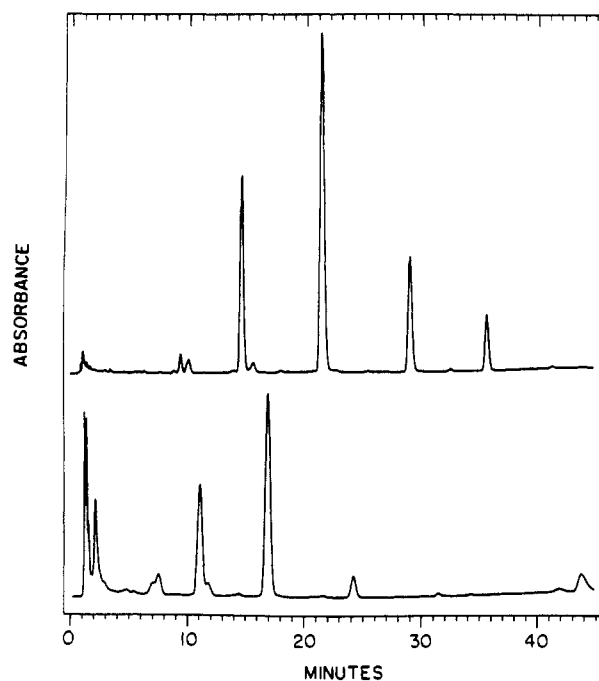

Figure 1. HPLC separations of components from the major TLC band at R_f 0.5 (upper chromatogram) and the minor TLC band at R_f 0.4 (lower chromatogram).
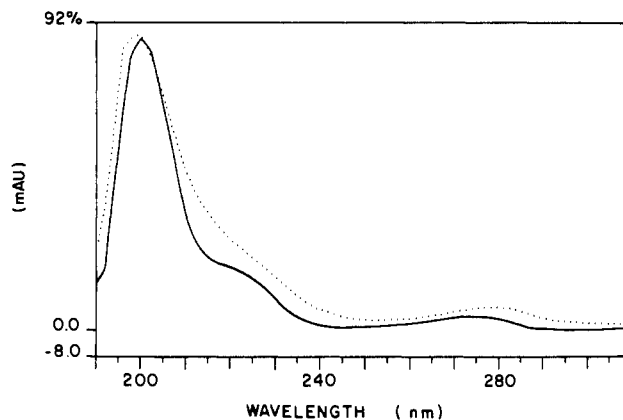

Figure 2. Ultraviolet spectra of peaks in Figure 1: (—) peak in upper chromatogram representing alkylresorcinol component at 21.5 min; (⋯) peak in lower chromatogram representing the 5-(2-oxoalkyl)resorcinol component at 17.0 min.

identical to that recorded for pentadecylresorcinol (Figure 2). The chromatogram for the minor TLC band (Figure 1) was consistent with a homologous series having a side-chain length distribution similar to that for the alkylresorcinols. Spectra of the two larger peaks at 11.1 and 17.0 min, and the smaller peaks at 7.5 and 24.2 min, were essentially the same. However, these spectra were slightly different from that of the alkylresorcinol (Figure 2), which was consistent with a ketone group located close, but not adjacent, to the aromatic ring.

Total ion chromatograms and mass spectra of individual components clearly showed that components in the major TLC band from wheat and rye were 5-n-alkylresorcinols, with homolog distribution differences between wheat and rye being similar to those reported previously (Lorenz and Hengtrakul, 1990; Gohil et al., 1988). In a comparison of components from rye, the elution positions of the two principle homologs from the minor TLC band, relative to the 5-n-alkylresorcinols in the major TLC band, are shown in Figure 3. The component eluting at 13.4 min gave the typical mass spectrum expected for a 5-n-alkylresorcinol with a molecular weight of 376 (Figure 4). The ions m/z
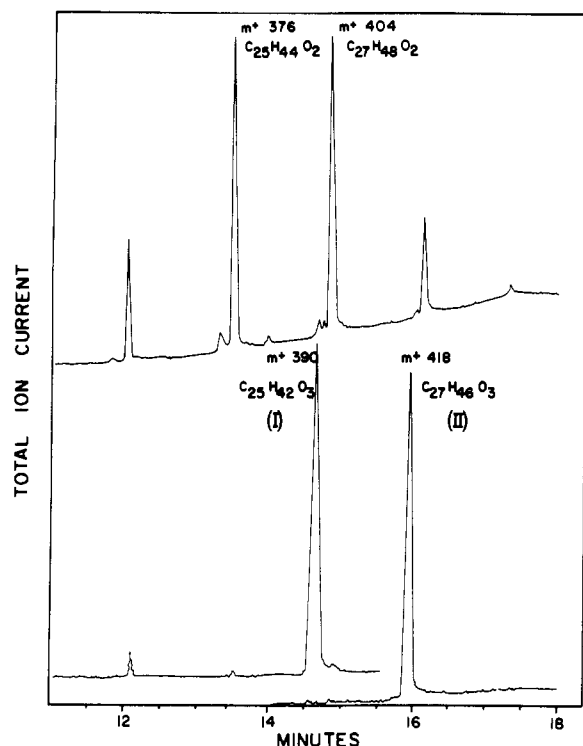
Figure 3. Total ion chromatograms of components from rye showing relative elution positions of 5-n-alkylresorcinols (upper curve) compared to the 5-(2-oxoalkyl)resorcinol components I and II (lower curves).
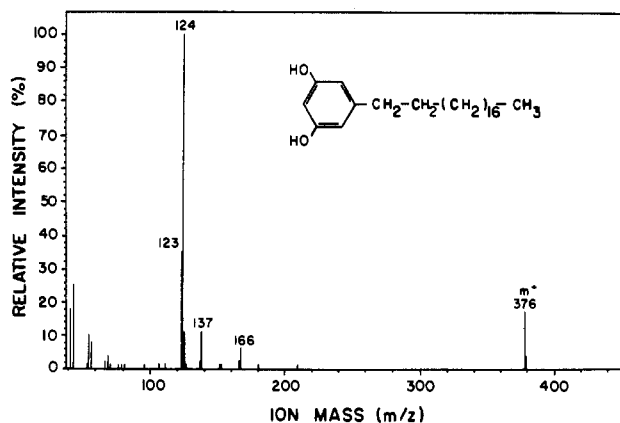

Figure 4. Mass spectrum of 5-n-nonadecanylresorcinol (MW 376).

123, 124 (base peak), 137, and 166 are characteristic of 5-n-alkylresorcinol homologs (Briggs, 1974). The minor TLC band components eluting from the GC column at 14.6 and 16.0 min gave mass spectra which were consistent with 5-(2-oxononadecanyl)resorcinol (I, MW 390) and 5-(2-oxoheneicosanyl)resorcinol (II, MW 418). Facile fragmentation in the side chain between the α-methylene group and the β-ketone group explained the observed ions m/z 123 and 267 for the former component (Figure 5) and 123 and 295 for the latter component. Also, this fragmentation process probably caused the greater m/z 123 ions intensity relative to ion m/z 124 in the spectra of the 5-(2-oxoalkyl) homologs than in the 5-n-alkyl homologs (compare Figures 4 and 5). An additional 5-(2-oxo-) homolog observed in samples of wheat and rye was 5-(2-oxotricosanyl)resorcinol (III), which gave ions m/z 446 (M⁺) and 323 plus lower mass ions as listed in Table I. Diagnostic ion masses for all three of the 5-(2-oxoalkyl)resorcinol homologs mentioned here are listed in Table I.

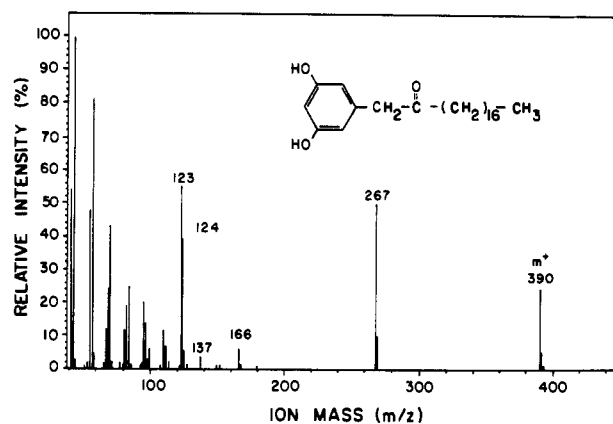Vapor-phase infrared spectra gave further evidence for

Figure 5. Mass spectrum of 5-(2-oxononadecanyl)resorcinol (I, MW 390).

Table I. Some Diagnostic Ion Masses (m/z) for 5-(2-Oxoalkyl)- and 5-(2-Oxoalkenyl)resorcinol Compounds[a]

	relatie intensity, %				
mass	I	II	III	IV	V
446			18		
444					14
418		22			
416				6	
390	24				
323			28		
322					23
321					94
296		8			
295		36			
294				16	
293				74	
268	10				
267	50				
166	6	5	8	5	7
137	4	4	5	5	5
124	40	32	41	54	48
123	55	50	57	57	55
111	7	6	13	13	13
109	12	9	17	17	16
99	5	5	10	2	1
97	14	13	27	40	25
95	19	16	27	35	30
85	25	22	32	8	7
83	19	13	22	44	42
81	12	9	17	31	23
71	43	36	49	13	12
69	23	25	25	65	53
67	12	10	13	35	21
57	81	69	86	41	38
55	48	50	52	100	100
43	100	100	100	70	57
41	54	45	48	68	49

[a] I = 5-(2-oxononadecanyl)resorcinol. II = 5-(2-oxoheneicosanyl)resorcinol. III = 5-(2-oxotricosanyl)resorcinol. IV = 5-(2-oxoheneicosenyl)resorcinol. V = 5-(2-oxotricosenyl)resorcinol.

the ketone group in the side chain of the minor group of resorcinols. A minor resorcinol component isolated by preparative TLC and HPLC was analyzed by the GC-FTIR-MS system. Both the total ion chromatogram from the MS and the total response chromatogram from the FTIR showed only one major peak. The component gave a mass spectrum having ions m/z 390 and 267 expected for I as discussed above. The IR spectrum showed an absorbance at 1725 cm⁻¹ (see spectrum C in Figure 6) which was consistent with a nonconjugated ketone group located at least on methylene group away from the benzene ring. The remainder of the infrared spectrum from I was similar to the spectra from the two alkylresorcinols, as expected for compounds of generally similar structure. The infrared
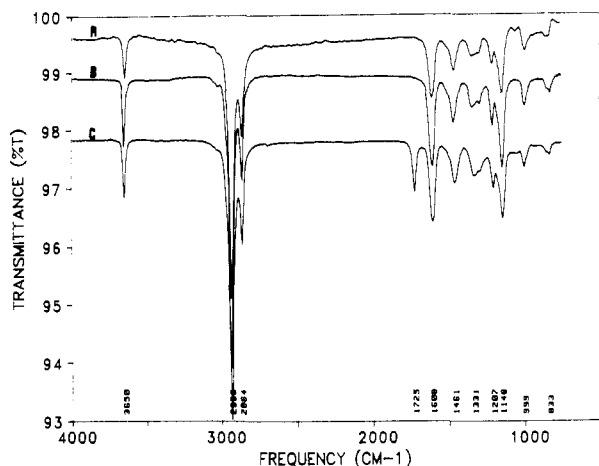
Figure 6. Vapor-phase infrared spectra of 5-*n*-alkyl- and 5-(2-oxoalkyl)resorcinols: A = 5-*n*-heneicosanylresorcinol from wheat; B = 5-*n*-pentadecanylresorcinol reference standard; C = 5-(2-oxononadecanyl)resorcinol (I) from wheat.

Table II. Proton Magnetic Resonance Data for the 5-(2-Oxoalkyl)resorcinols I and II in Acetone-d_6

protons		chemical		
type	no.	shift, ppm	coupling	J, Hz
aromatic	1	6.236	triplet	2.16
aromatic	2	6.208	doublet	2.16
ArCH$_2$CO	2	3.508	singlet	–
COCH$_2$R	2	2.442	triplet	7.32

spectra of the other 5-(2-oxoalkyl)resorcinol homologs mentioned above were very similar to spectrum C in Figure 6.

Proton magnetic resonance spectra provided conclusive evidence that the minor components were 5-(2-oxoalkyl)-resorcinols. The most informative chemical shifts and coupling constants for I and II are given in Table II. A singlet of intensity corresponding to 2 protons was observed at δ 3.508, which was consistent with a methylene group between a benzene ring and a ketone group (Silverstein et al., 1981). The chemical shifts and coupling constants for the aromatic protons were similar to those observed for 5-*n*-alkylresorcinols and, therefore, were consistent with the 2-oxoalkyl side chain being at the fifth position of the resorcinol group.

Evidence for 5-(2-Oxoalkenyl)resorcinols. During purification of I and II by HPLC, small peaks which eluted just after I and II, respectively, were collected. These secondary components had UV spectra that were essentially the same as those for I, II, and III. Ion masses observed in GC–MS analyses of these components, as shown in Table I, indicated that they were 5-(2-oxo-heneicosenyl)resorcinol (IV) and 5-(2-oxotricosenyl)-resorcinol (V). Infrared spectra from the GC–FTIR–MS system and NMR spectra of (IV, MW 416) and (V, MW 444) provided further evidence for unsaturation in the hydrocarbon side chain. Each infrared spectrum showed a weak absorbance at 3006 cm⁻¹, and each NMR spectrum had a triplet (J = 4.7 Hz) at 5.34 ppm. The NMR data was consistent with a cis double bond having several methylene groups on each side such that the two hydrogen atoms in the double bond were in nearly equivalent environments.

Furthermore, the GC–MS results for the HPLC fraction containing IV suggested the presence of at least three positional isomers because the total ion chromatogram (TIC) revealed three peaks about 0.06 min apart (Figure 7). Mass spectra were the same all across the three peaks;
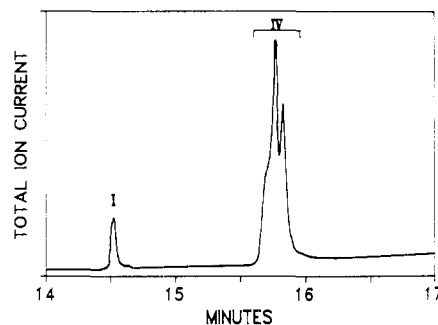

Figure 7. Portion of total ion chromatogram showing resolution of isomeric components near 15.8 min which had mass spectra expected for 5-(2-oxoheneicosenyl)resorcinol (IV). The minor peak at 14.6 min was I.
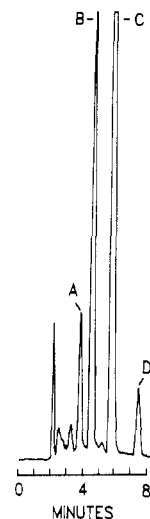

Figure 8. HPLC fractionation of resorcinols from wheat bran. The four peaks labeled with letters were collected and used for analyses of silylated derivatives.

the data shown in Table I represents the middle peak. The TIC for the fraction containing V had one major peak with two small shoulders, so the data in Table I is for the major peak.

Results from Silylated Derivatives. Work with tri-methylsilyl (TMS) derivatives gave further proof for 5-(2-oxoalkyl)resorcinols and 5-(2-oxoalkenyl)resorcinols and also provided evidence for traces of resorcinol components having a hydroxyl group and a double bond in the side chain. Samples for GC–MS analyses of silylated derivatives came from an extract (precleaned by the base–acid cleanup procedure followed by preparative TLC) of wheat bran that was separated into four fractions by HPLC (Figure 8). The results of the GC–MS analyses are summarized in Tables III and IV.

Silylated components with molecular ions m/z (M⁺) 534, 562, 590, and 618 (peaks A1, B1, C1, and D1) corresponded to 5-(2-oxoalkyl)resorcinols with both phenolic protons replaced with TMS groups. Thus, peaks A1, B1, and C1 are TMS derivatives of compounds I, II, and III described above. An additional homolog not observed in the analyses of the nonsilylanized derivatives was 5-(2-oxopentacosa-nyl)resorcinol (peak D1, Table III). Similarly, components with M⁺ 560 (peaks A3a, A3b, A3c) and 588 (B3a and B3b) corresponded to the 5-(2-oxoalkenyl)resorcinols IV and V. Mass spectra of the three A3 peaks were nearly identical to each other, and the spectra of the two B3 peaks were nearly identical to each other, which again suggests positional isomerization of the double bond in the side chain. Data for peaks A3a and B3a were selected for exhibit in Table IV.

Table III. GC-MS Results from Silylated Resorcinol Components in HPLC Fractions Shown in Figure 8

HPLC fraction	peak no.	retention time, min	relative amount[a]	molecular ion, m/z
A	A1	17.9	4.7	534
A	A2	19.0	2.7	606
A	A3a	20.7	1.7	560
A	A3b	20.9	2.9	560
A	A3c	21.1	3.3	560
A	A4a	22.1	0.9	632
A	A4b	22.3	1.2	632
A	A4c	22.6	1.6	632
B	B1	21.2	57.3	562
B	B2	22.6	9.1	634
B	B3a	25.1	2.6	588
B	B3b	25.6	2.2	588
C	C1	26.7	100.0	590
C	C2	28.3	6.9	662
D	D1	32.2	12.2	618
D	D2	34.2	0.7	690

[a] Calculated from HPLC peak areas from sample being fractionated (Figure 8) and areas of GC-MS peaks from each fraction.

Components listed in Tables III and IV with M[+] m/z 606, 634, 662, and 690 (peaks A2, B2, C2, and D2) contain three TMS groups: two replacing phenolic protons plus a third replacing a hydroxyl proton in the side chain. This means that molecular weights of the underivatized compounds were 390, 418, 446, and 474 (i.e. subtract 216 from the parent ions listed in Table III), which were the same as those for the 5-(2-oxoalkyl)resorcinols discussed above. A component with a hydroxyl group and a double bond in the side chain has the same molecular weight as a component having a side chain of the same length and containing only a ketone group. From this reasoning and further interpretation of MS data discussed below, it is possible that the components giving peaks A2, B2, C2, and D2 were resorcinols having side chains with a hydroxyl at the second carbon and a double bond either between the third and fourth carbon or further out in the side chain. Alternatively, however, these components could have been formed by enolization of the 5-(2-oxoalkyl)resorcinols during the silylation reaction. Ions m/z 339, 367, 395, and 423 for A2, B2, C2, and D2, respectively, listed in Table IV were consistent with cleavage between the first and second carbon on the side chain. Such intact side-chain ions were not observed in the silylated 5-(2-oxoalkyl)- or 5-(2-oxoalkenyl)resorcinol compounds. The presence of the silylated oxygen group apparently provided several fragmentation routes, as indicated by prevalence of ions at and near m/z 382, 306, and 292.

The component with M[+] 632 (peaks A4a, A4b, and A4c in Table III) and fragment ion mass m/z 265 appeared to have the same structure as B2, except with an additional double bond even further out in the side chain. All three peaks had nearly the same mass spectrum (data for A4a shown in Table IV), probably as a result of isomerism of the double bond(s) in the side chain. Again, an alternative explanation is that these components came from enolization of the 2-(oxoalkenyl)resorcinols represented by peaks A3a, A3b, and A3c. An attempt to isolate 2-hydroxyalkenyl resorcinols for spectroscopy study of nonderivatized compounds was beyond the scope of this project.

Other Observations. For determination of the side-chain structure in 5-(2-oxoalkyl)- and 5-(2-oxoalkenyl)resorcinols, MS data from nonderivatized components were more useful than that from silylated derivatives. With the nonsilylated derivatives, fragmentation between α-methylene and β-ketone groups was sufficiently facile that ions (m/z) representing COR fragments were observed, i.e. masses 267 for I and 295 for II, etc., as shown in Table

Table IV. Some Diagnostic Ion Masses (m/z) and Relative Intensities for Silylated Components (Peak Numbers) Listed in Table III

mass	relative intensity, %										
	A1	B1	C1	D1	A3a	B3a	A2	B2	C2	D2	A4a
690										11	
662									25		
634						38					
632											28
618			25								
606							47				
590		37									
588					19						
562		79									
560					21						
534	79										
423										9	
396							4	5	12		4
395							11	11	37	5	9
394							3	3	3		2
393								6	5		4
384							9	9	8		7
383							20	21	18	5	18
382							52	65	63	19	50
381							14	18	13	7	11
368							2	12	4		2
367							6	38	5	4	5
366							1	2			7
365		1	1				1	1			20
341				1				2	7	9	3
340							12	1			
339							37	1	2		1
323	5	5	5	5	5	5	1	1	2		3
311	7	7	6	5	5	6	1				
310	20	22	23	18	18	17	1	1			1
307		1	1	1	1	2	10	11	12	5	10
306						1	24	25	30	9	20
305		1	1		1		26	34	38	16	28
293	1	1	1	1	3	2	13	16	18	6	14
292					1		13	16	18	6	13
281	8	7	9	12	7	26	5	11	60	51	14
269	27	28	25	26	27	25	4	5	6	4	8
268	100	100	100	100	100	100	12	12	16	6	29
267	29	28	33	33	27	33	16	18	24	19	15
207	1	1	2	12	6	48	5	13	96	100	20
147	6	6	5	6	6	9	13	14	19	13	14
85	8	8	9	8	2	4	1	2	3		2
83	5	6	6	8	13	15	2	3	4		5
73	29	29	24	26	26	38	100	100	100	67	100
71	15	14	13	17	4	7	3	4	9	5	3
69	9	10	9	12	19	21	4	4	7	7	10
57	29	37	36	38	12	16	12	18	22	11	10
55	19	19	19	18	21	34	7	9	13	10	19

I. On the other hand, silylation (which is commonly done to aid GC analyses) apparently facilitated elimination of the CO and fragmentation of the remainder of the side chain in a manner similar to 5-n-alkylresorcinols, thus giving relatively little diagnostic information indicating a ketone group in the side chain.

Total concentrations of the 5-(2-oxoalkyl)resorcinols were estimated to be in the range of 5–50 μg/g. These estimates were made from relative peak heights in HPLC chromatograms of whole wheat and rye grain extracts by assuming that absorbancy constants for 5-(2-oxoalkyl)- and 5-n-alkylresorcinols were similar at 275 nm. From the data in Table III, it was estimated that total concentration of 5-(2-oxoalkenyl)resorcinols was about 11% of the total concentration of 5-(2-oxoalkyl)resorcinols.

During many previous analyses for alkylresorcinols in whole rye, whole wheat, and wheat milling fractions (Love, 1985; Seitz and Love, 1987), HPLC peaks and/or TLC bands corresponding to what we now know to be 5-(2-oxoalkyl)resorcinols were observed in all samples except for some flour fractions that contained little or no alk-

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ylresorcinols. More analyses are needed to determine how much the concentrations of these components are affected by type of cultivar and environmental conditions under which the grains are grown.

ACKNOWLEDGMENT

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