CRC

Handbook of Chromatography

Volume I

Handbook

of

Chromatography

Volume I

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PREFACE

Volumes One and Two of the *Handbook of Chromatography* represent over three years of intensive labor by the editors and members of the Editorial Advisory Board. When the Publishers first suggested the production of a Handbook for Chromatographic Data, it seemed to the editors to be just a simple compilation of R_F-tables and retention times or volumes. However, a quick perusal of the literature of chromatography, accumulated during approximately twenty-five years of modern chromatography, revealed that the task would be a formidable one and could not be accomplished in one year, as was first estimated.

The Handbook, as it finally appears, should serve chemists in all fields as a working manual and reference book which should aid in their search for identification of unknowns as well as suggest quantitative methods of analysis.

Volume One of the Handbook contains over 549 tables of chromatographic data expressed in uniform terms of R_F values, retention times and retention volumes as well as other terms used in chromatography. Each table has literature citations which will refer to the primary and sometimes secondary sources. Over 12,000 compounds are cross-indexed to direct the reader to appropriate tables in this volume. Thus, for example, the amino acid alanine will have entries in tables under gas, liquid-column, paper, and thin-layer chromatography.

Volume Two of the Handbook has been designed to give the researcher, even the novice in chromatography, a working knowledge of the theory and practices of the various fields of chromatography—gas, liquid-column, paper, and thin-layer chromatography.

Volume Two also contains two useful sections. One is on detection reagents for paper and thin-layer chromatography, with an alphabetical index for chemical classes and "name" reagents. This section is very helpful for the interpretation of the tables in Volume One. The other section describes selected methods for sample preparations, which will be expanded in future editions of the Handbook. Subsequent sub-sections in **PRACTICAL APPLICATIONS** supply the researcher with useful information on commercial sources of all types of chromatographic supplies.

A Book Directory at the close of Volume Two should serve as a good source for more detailed reading in chromatography.

The editors would be ungrateful if they did not acknowledge the invaluable help and advice from the members of the Advisory Editorial Board.

Special thanks are due to the industrious group of compilers, especially Mrs. Ellen Burton, Miss Susan Rodems, Miss Irene Zweig, Mrs. Frances K. Zweig, and Dr. and Mrs. Coleman Hamel. Special thanks are also due to Dr. Irving Sunshine whose initiative and perseverance are in no small manner responsible for the writing and creation of this Handbook, and to Mrs. Florence Thomas and Mrs. Ruth Pokorney of The Chemical Rubber Co. for their unstinting effort in the production and final editing of the books.

The editors would greatly appreciate suggestions for improvements and additions in future editions from any interested persons.

Gunter Zweig

Joseph Sherma

November 1972

Advisory Board

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Column Packing	P1	P1	P1	P1	P1	P2	P3	P4
Temperature (°C)	150	170	180	200	220	150	150	175
Gas; Flow Rate (ml/min)	13,He	13,He	13,He	13,He	13,He	150,He	150,He	10.3,He
Column								
length, cm	190.5	190.5	190.5	190.5	190.5	228.6	228.6	150 ft
diameter, cm, I.D.[a]								
cm, O.D.[b]	0.8[a]	0.8[a]	0.8[a]	0.8[a]	0.8[a]	0.635[b]	0.635[b]	0.01 in.
form	U-tube	U-tube	U-tube	U-tube	U-tube	coiled	coiled	capillary
material	SS	SS	SS	SS	SS	copper	copper	na
Detector	TC	TC	TC	TC	TC	TC	TC	na
Literature	1	1	1	1	1	2	2	3

Compound	t_r							r*
Diethyl malonate	8.8	5.6	5.0	3.5	—	1.00	1.00	—
Diethyl succinate	13.4	8.6	7.5	5.4	—	1.48	1.30	—
Diethyl glutarate	20.7	12.1	10.0	—	—	—	—	—
Diethyl adipate	31.8	17.8	13.8	12.7	7.3	—	—	—
Diethyl pimelate	52.1	26.7	19.6	18.4	11.3	—	—	—
Diethyl suberate	—	—	—	24.5	14.8	—	—	—
Diethyl azelate	—	—	—	33.8	19.8	—	—	—
Diethyl fumarate	—	—	—	—	—	1.48	1.30	—
Diethyl maleate	—	—	—	—	—	2.06	2.04	—
Diethyl malate	—	—	—	—	—	—	6.81	—
Dimethyl oxalate	—	—	—	—	—	—	—	0.23
Dimethyl malonate	—	—	—	—	—	—	—	0.35
Dimethyl fumarate	—	—	—	—	—	—	—	0.38
Dimethyl succinate	—	—	—	—	—	—	—	0.47
Dimethyl itaconate	—	—	—	—	—	—	—	0.59
Dimethyl maleate	—	—	—	—	—	—	—	0.64
Dimethyl glutarate	—	—	—	—	—	—	—	0.70
Dimethyl adipate	—	—	—	—	—	—	—	1.00
Dimethyl pimelate	—	—	—	—	—	—	—	1.34
Dimethyl suberate	—	—	—	—	—	—	—	1.93
Dimethyl isosebacate	—	—	—	—	—	—	—	1.94
Dimethyl azelate	—	—	—	—	—	—	—	2.67
Dimethyl sebacate	—	—	—	—	—	—	—	3.44
Dimethyl orthophthalate	—	—	—	—	—	—	—	5.94
Dimethyl dodecanedioate	—	—	—	—	—	—	—	6.69

* Relative to dimethyl adipate.

Column Packing

P1 = 10% DC-550 on acid-washed, size-graded Celite 545 (40/120 mesh).
P2 = 25% Poly(1,4-butanediol succinate) on C-22 firebrick (60/80 mesh).
P3 = 25% Poly(diethylene glycol succinate) on C-22 firebrick (60/80 mesh).
P4 = Diethylene glycol succinate (coating).

Literature

1. Nowakowska, J., Melvin, E. H., and R. Wiebe, *J. Amer. Oil Chem. Soc.*, **34**, 411 (1957).
2. Mirocha, C. J. and J. E. DeVay, *Phytopathology*, **51**, 274 (1961).
3. Afremow, L. C., *J. Gas Chromatogr.*, **1**, (6), 29 (1963).

TABLE GC 2
ACIDS, ALIPHATIC; METHYL ESTERS

Column Packing	P1	P2	P3	P4
Temperature (°C)	150	150	150	150
Gas; Flow Rate (ml/min)	65,He	65,He	65,He	65,He
Column				
length, ft	12	12	12	12
diameter, in., O.D.	¼	¼	¼	¼
form	na	na	na	na
material	aluminum	aluminum	aluminum	aluminum
Detector	FI and TC	FI and TC	FI and TC	FI and TC
Compound	r*			
Methyl formate	0.075	0.123	0.170	0.350
Ethyl formate	0.129	0.220	0.260	0.560
Propyl formate	0.216	0.380	0.450	0.810
Isopropyl formate	0.162	0.125	0.250	0.560
Butyl formate	0.375	0.630	0.774	1.310
2-Methylpropyl formate	0.301	0.370	0.566	1.040
Pentyl formate	0.645	1.03	1.28	2.060
3-Methylbutyl formate	0.512	0.650	1.00	1.660
Hexyl formate	—	1.79	2.04	3.060
Octyl formate	—	4.93	5.50	7.310
Methyl acetate	0.140	0.260	0.330	0.500
Ethyl acetate	0.200	0.360	0.440	0.69
Propyl acetate	0.338	0.580	0.780	1.07
Isopropyl acetate	0.259	0.390	0.490	0.78
Butyl acetate	0.585	0.970	1.21	1.63
2-Methylpropyl acetate	0.468	0.800	0.490	1.32
Pentyl acetate	0.980	1.60	2.00	2.50
3-Methylbutyl acetate	0.798	1.30	1.56	2.10
Hexyl acetate	—	2.70	3.60	3.88
Octyl acetate	—	7.96	—	9.31
Methyl propionate	0.235	0.390	0.512	0.76
Ethyl propionate	0.335	0.550	0.700	1.00
Propyl propionate	0.570	0.950	1.18	1.55
Isopropyl propionate	0.405	0.700	0.770	1.19
Butyl propionate	0.955	1.53	1.95	2.44
2-Methylpropyl propionate	0.790	1.26	1.50	2.00
Pentyl propionate	1.602	2.56	3.14	3.75
3-Methylbutyl propionate	1.304	2.07	2.50	3.15
Hexyl propionate	—	4.16	5.05	5.82
Octyl propionate	—	—	12.95	14.50
Methyl butyrate	0.397	0.630	0.78	1.13
Ethyl butyrate	0.565	0.930	1.07	1.44
Propyl butyrate	0.920	1.57	1.80	2.25
Isopropyl butyrate	0.680	1.07	1.19	1.66
Butyl butyrate	1.48	2.47	2.93	3.35
2-Methylpropyl butyrate	1.18	1.97	2.35	2.72
Pentyl butyrate	2.35	4.11	4.78	5.12
3-Methylbutyl butyrate	1.97	3.32	3.80	4.28
Hexyl butyrate	—	6.704	7.58	7.80
Octyl butyrate	—	18.10	19.20	18.37
Methyl isobutyrate	0.319	—	—	—
Ethyl isobutyrate	0.445	0.710	0.83	1.19
Propyl isobutyrate	0.722	1.130	1.40	1.69
Isopropyl isobutyrate	0.565	0.770	0.86	1.23
Butyl isobutyrate	1.17	1.83	2.21	2.80
2-Methylpropyl isobutyrate	0.997	1.490	1.73	2.25
Pentyl isobutyrate	1.87	3.10	3.54	4.10
3-Methybutyl isobutyrate	1.59	2.46	2.86	3.44
Hexyl isobutyrate	—	4.94	5.70	6.57
Octyl isobutyrate	—	13.28	14.55	15.50
Methyl pentanoate	0.650	1.07	1.40	2.00
Ethyl pentanoate	0.900	1.50	1.90	2.31
Propyl pentanoate	1.480	2.46	3.00	3.63
Isopropyl pentanoate	1.110	1.68	2.00	2.50

TABLE GC 2—(Continued)
ACIDS, ALIPHATIC; METHYL ESTERS

Column Packing	P1	P2	P3	P4
Temperature (°C)	150	150	150	150
Gas; Flow Rate (ml/min)	65,He	65,He	65,He	65,He
Column				
length, ft	12	12	12	12
diameter, in., O.D.	¼	¼	¼	¼
form	na	na	na	na
material	aluminum	aluminum	aluminum	aluminum
Detector	FI and TC	FI and TC	FI and TC	FI and TC
Compound	r*			
Butyl pentanoate	2.34	4.01	4.86	5.67
2-Methylpropyl pentanoate	1.97	3.30	3.74	4.44
Pentyl pentanoate	3.72	6.40	7.50	8.40
3-Methylbutyl pentanoate	3.12	5.28	6.21	6.65
Hexyl pentanoate		10.20	12.0	12.46
Octyl pentanoate		—	29.8	28.15
Methyl 3-methylbutyrate	0.508	0.900	1.10	1.41
Ethyl 3-methylbutyrate	0.740	1.130	1.44	1.72
Propyl 3-methylbutyrate	1.19	1.900	2.25	2.62
Isopropyl 3-methylbutyrate	0.92	1.230	1.49	1.91
Butyl 3-methylbutyrate	1.89	3.06	3.58	4.05
2-Methylpropyl 3-methylbutyrate	1.58	2.43	2.86	3.25
Pentyl 3-methylbutyrate	2.99	5.30	5.45	6.12
3-Methylbutyl 3-methylbutyrate	2.52	3.95	4.70	4.96
Hexyl 3-methylbutyrate	—	8.35	9.14	9.16
Octyl 3-methylbutyrate	—	—	—	21.42
Methyl hexanoate	1.06	1.83	2.25	2.70
Ethyl hexanoate	1.47	2.68	3.08	3.26
Propyl hexanoate	2.36	4.35	4.90	5.19
Isopropyl hexanoate	1.78	3.07	3.30	3.63
Butyl hexanoate	3.75	7.30	7.64	7.88
2-Methylpropyl hexanoate	3.08	5.65	6.02	6.51
Pentyl hexanoate	5.96	11.72	12.12	12.20
3-Methylbutyl hexanoate	4.93	9.18	9.52	9.79
Hexyl hexanoate	—	—	19.68	18.09
Octyl hexanoate	—	—	—	41.40
Methyl 4-methylpentanoate	0.88	1.65	1.84	2.25
Ethyl 4-methylpentanoate	1.25	2.16	2.56	2.84
Propyl 4-methylpentanoate	1.96	3.50	3.96	4.38
Isopropyl 4-methylpentanoate	1.51	2.49	2.66	3.20
Butyl 4-methylpentanoate	3.20	5.52	6.37	6.63
2-Methylpropyl 4-methylpentanoate	2.65	4.70	4.80	5.35
Pentyl 4-methylpentanoate	5.02	9.45	10.00	10.10
3-Methylbutyl 4-methylpentanoate	4.25	7.70	7.79	8.03
Hexyl 4-methylpentanoate	—	13.25	15.80	15.30
Octyl 4-methylpentanoate	—	—	40.60	35.20

* Relative to nonane.

Column Packing
P1 = 10% SE-30 on acid-washed silanized Celite 560 (60/80 mesh).
P2 = 10% OV-17 on acid-washed silanized Celite 560 (60/80 mesh).
P3 = 10% OV-25 on acid-washed silanized Celite 560 (60/80 mesh).
P4 = 10% XE-60 on acid-washed silanized Celite 560 (60/80 mesh).

Literature
Allen, I. D. and J. K. Haken, *J. Chromatogr.*, **49**, 409 (1970).

TABLE GC 3
ACIDS, ALIPHATIC; METHYL ESTERS

Column Packing	P1	P2
Temperature (°C)	197	180
Gas; Flow Rate (ml/min)	Ar	Ar
Column		
length, ft	4	4
diameter, mm, I.D.	4 to 5	4 to 5
form	na	na
material	na	na
Detector	EC	EC

Compound	r*	
Methyl *n*-pentanoate	0.019	—
Methyl *n*-hexanoate	0.031	—
Methyl 4-methylhexanoate	0.041	—
Methyl *n*-heptanoate	0.046	—
Methyl 6-methylheptanoate	0.057	—
Methyl *n*-octanoate	0.071	0.141
Methyl 6-methyloctanoate	0.097	—
Methyl *n*-nonanoate	0.11	0.193
Methyl 8-methylnonanoate	0.144	—
Methyl *n*-decanoate	0.173	0.264
Methyl 8-methyldecanoate	0.235	—
Methyl *n*-undecanoate	0.274	0.360
Methyl 10-methylundecanoate	0.354	—
Methyl *n*-dodecanoate	0.426	0.510
Methyl 10-methyldodecanoate	0.567	—
Methyl *n*-tridecanoate	0.580	0.710
Methyl *cis*-Δ^9-tetradecenoate	0.92	1.2
Methyl *n*-tetradecanoate	1.0	1.0
Methyl 12-methyltetradecanoate	1.35	—
Methyl *n*-pentadecanoate	1.54	1.38
Methyl 14-methylpentadecanoate	2.04	—
Methyl *cis*-Δ^9-hexadecenoate	2.09	2.26
Methyl *trans*-Δ^9-hexadecenoate	2.16	2.26
Methyl *n*-hexadecanoate	2.34	1.96
Methyl 14-methylhexadecanoate	3.24	—
Methyl *n*-heptadecanoate	3.59	2.75
Methyl *cis*-$\Delta^{9,12}$-octadecadienoate	4.55	5.27
Methyl $\Delta^{9,12,15}$-octadecatrienoate	4.60	6.88
Methyl *cis*-Δ^9-octadecenoate	4.75	4.33
Methyl *trans*-Δ^9-octadecenoate	4.95	4.33
Methyl *cis*-Δ^6-octadecenoate	4.87	4.35
Methyl *cis*-Δ^4-octadecenoate	4.95	4.36
Methyl *trans*-Δ^4-octadecenoate	5.15	—
Methyl *n*-octadecanoate	5.5	3.86
Methyl $\Delta^{5,8,11,14}$-eicostatetraenoate	8.25	12.85
Methyl eicosapentaenoate	8.25	16.7
Methyl *n*-eicosanoate	12.1	7.54
Methyl docosahexaenoate	16.8	35.7
Methyl Δ^{13}-docosaenoate	25.6	16.0
Methyl *n*-docosanoate	26.3	—

* Relative to myristate.

Column Packing P1 — 20% Apiezon L grease on Celite (100/210 mesh).
P2 — 20% Polyethylene glycol adipate on Celite (100/210 mesh).

Literature James, A. T., *J. Chromatogr.*, 2, 552 (1959).

TABLE GC 4
ACIDS, AROMATIC, TRIMETHYLSILYL DERIVATIVES

Column Packing	P1
Temperature (°C)	T1
Gas; Flow Rate (ml/min)	170,N_2
Column	
length, ft	8
diameter, mm, I.D.	5.5
form	U-tube
material	—
Detector	FI

Compound	Methylene unit*
Benzoic acid	12.33
Phenylacetic acid	12.81
3-Phenylpropionic acid	13.98
***m*-Methoxyphenylacetic acid**	15.01
***p*-Methoxyphenylacetic acid**	15.17
Cinnamic acid	15.27
***o*-Hydroxyphenylacetic acid**	15.60
***m*-Hydroxybenzoic acid**	15.60
β-Phenyllactic acid	15.85
3-(*o*-Methoxyphenyl)propionic acid	15.90
***m*-Hydroxyphenylacetic acid**	15.98
***p*-Hydroxybenzoic acid**	16.21
***p*-Hydroxyphenylacetic acid**	16.28
3-(*p*-Methoxyphenyl)propionic acid	16.37
2,5-Dimethoxyphenylacetic acid	16.77
3,4-Dimethoxyphenylacetic acid	16.92
Phenylpyruvic acid	17.05
3-(*p*-Hydroxyphenyl)propionic acid	17.51
***o*-Methoxycinnamic acid**	17.54
***m*-Methoxycinnamic acid**	17.66
β-(*p*-Methoxyphenyl)lactic acid	17.97
***p*-Methoxycinnamic acid**	18.03
3,4,5-Trimethoxyphenylacetic acid	18.12
***o*-Methoxyphenylpyruvic acid**	18.60
β-(*p*-Hydroxyphenyl)lactic acid	19.06
3-(3,4-Dihydroxyphenyl)propionic acid	19.46
***p*-Methoxyphenylpyruvic acid**	19.50
3,5-Dimethoxycinnamic acid	19.94
3,4-Dimethoxycinnamic acid	19.98
***m*-Hydroxyphenylpyruvic acid**	20.00
2,4-Dimethoxycinnamic acid	20.12
***p*-Hydroxyphenylpyruvic acid**	20.51
4-Hydroxy-3-methoxycinnamic acid	20.80
3,4,5-Trimethoxycinnamic acid	21.19
3,4-Dimethoxyphenylpyruvic acid	21.30
3,4-Dihydroxycinnamic acid	21.36
3,4-Dihydroxyphenylpyruvic acid	22.09
3,5-Dimethoxy-4-hydroxycinnamic acid	22.12

* 1 methylene unit = retention time difference between an *n*-alkane with *m* and one with *m* + 1 carbons.

Column Packing P1 = 13% SE-30 on acid-washed Chromosorb W (silanized glass wool used at exit end of column).

Temperature T1 = programmed; held at 100 °C for 5 minutes after sample injection, then to 300 °C at 5°/minute.

Literature Hoffman, E., Milling, Jr., A., and D. Parmelee, *Anal. Biochem.*, **32**, 386 (1969).

TABLE GC 5
ACIDS, AROMATIC, TRIMETHYLSILYL DERIVATIVES

Column Packing	P1	P2	P1	P2
Temperature (°C)	T1	T1	T2	T2
Gas; Flow Rate (ml/min)	50,Ar	50,Ar	50,Ar	50,Ar
Column				
length, m	1.5	1.5	4	4
diameter, mm, I.D.	4	4	4	4
form	coiled	coiled	coiled	coiled
material	—	—	—	—
Detector	FI	FI	FI	FI
Compound	Methylene units			
Benzoic	13.65	12.26	13.96	12.31
Hippuric	21.05	18.02	21.13	18.04
Phenylacetic	14.40	12.64	14.40	12.72
Phenaceturic	21.67	18.47	21.77	18.43
	—	18.62	—	18.57
Phenylacetylglutamic	24.68	20.67	24.91	20.68
	26.06	22.39	26.00	22.35
	—	22.96	—	22.95
Phenylacetylglutamine	24.67	20.68	24.93	20.68
	24.97	20.80	25.21	20.82
	27.96	21.95	*ca.* 28.4	22.00
	—	—	*ca.* 28.5	—
β-Phenylpropionic	15.52	14.05	15.65	14.06
Cinnamic	17.04	14.97	17.17	15.21
Mandelic	15.91	14.69	15.90	14.57
β-Phenyllactic	16.88	15.87	16.83	15.82
Phenylpyruvic	18.28	17.02	18.32	16.99
***N*-Acetylphenylalanine**	19.39	17.88	19.31	17.90
	20.54	—	20.65	—
***o*-Hydroxybenzoic**	16.26	15.01	16.30	15.00
***o*-Hydroxyhippuric**	22.92	20.41	23.02	20.51
***o*-Hydroxyphenylacetic**	16.92	15.56	16.85	15.53
***o*-Hydroxyphenylpyruvic, lactone**	18.95	16.50	19.32	16.74
***o*-Hydroxycinnamic**	19.57	18.00	19.62	18.03
***m*-Hydroxybenzoic**	16.66	15.57	16.76	15.51
***m*-Hydroxyhippuric**	23.80	21.20	23.78	21.20
***m*-Hydroxyphenylacetic**	17.36	15.97	17.25	15.97
β-(*m*-Hydroxyphenyl)propionic	18.52	17.17	18.48	17.13
***m*-Hydroxycinnamic**	20.05	18.63	20.00	18.57
β-(*m*-Hydroxyphenyl)hydracrylic	19.41	18.63	19.22	18.50
***p*-Hydroxybenzoic**	17.32	16.20	17.25	16.20
***p*-Hydroxyphenylacetic**	17.65	16.29	17.59	16.25
β-(*p*-Hydroxyphenyl)propionic	18.88	17.53	18.83	17.48
***p*-Hydroxycinnamic**	20.84	19.28	20.84	19.30
***p*-Hydroxymandelic**	18.88	17.94	18.65	17.74
β-(*p*-Hydroxyphenyl)lactic	20.00	19.13	19.86	19.05
***p*-Hydroxyphenylpyruvic**	21.59	20.61	21.49	20.54
***N*-Acetyltyrosine**	24.86	21.29	24.90	21.24
***p*-Methoxybenzoic**	16.96	14.95	17.01	15.04
***p*-Methoxyhippuric**	24.47	20.79	24.58	20.83
***p*-Methoxyphenylacetic**	17.28	15.13	17.33	15.10
***p*-Methoxyphenaceturic**	24.75	20.82	24.82	20.85
***p*-Methoxyphenylacetylglutamic**	27.80	23.19	*ca.* 28.1	23.16
	ca. 28.8	24.44	*ca.* 28.8	24.42
β-(*p*-Methoxyphenyl)propionic	18.46	16.30	18.54	16.36
***p*-Methoxycinnamic**	20.58	17.96	20.69	18.08
***p*-Methoxymandelic**	18.75	16.91	18.64	16.81
β-(*p*-Methoxyphenyl)lactic	19.62	17.95	19.60	18.01
***p*-Methoxyphenylpyruvic**	21.42	19.54	21.46	19.54
***N*-Acetyl-*p*-methoxyphenylalanine**	23.51	20.09	23.56	20.13
2,3-Dihydroxybenzoic	18.48	17.49	18.45	17.51
2,4-Dihydroxybenzoic	19.20	18.23	19.07	18.18
2,5-Dihydroxybenzoic	18.78	17.85	18.60	17.74

TABLE GC 5—(Continued)
ACIDS, AROMATIC, TRIMETHYLSILYL DERIVATIVES

Column Packing	P1	P2	P1	P2
Temperature (°C)	T1	T1	T2	T2
Gas; Flow Rate (ml/min)	50,Ar	50,Ar	50,Ar	50,Ar
Column				
length, m	1.5	1.5	4	4
diameter, mm, I.D.	4	4	4	4
form	coiled	coiled	coiled	coiled
material	—	—	—	—
Detector	FI	FI	FI	FI

Compound		Methylene units			
2,5-Dihydroxyphenylacetic		19.40	18.45	19.27	18.32
2,5-Dihydroxyphenylacetic, lactone		18.70	17.30	18.71	17.30
2,5-Dihydroxyphenylpyruvic, lactone		22.03	20.21	22.27	20.35
2,6-Dihydroxybenzoic		18.86	17.68	18.81	17.64
3,4-Dihydroxybenzoic		19.17	18.25	19.05	18.21
3,4-Dihydroxyphenylacetic		19.39	18.35	19.31	18.30
3,4-Dihydroxyphenylcinnamic		22.48	21.49	22.43	21.40
3,4-Dihydroxymandelic		20.19	19.48	20.02	19.33
3,5-Dihydroxybenzoic		19.28	18.28	18.99	18.11
3-Hydroxy-4-methoxybenzoic		19.33	17.60	19.23	17.52
3-Hydroxy-4-methoxyhippuric		26.34	23.26	26.31	23.18
3-Hydroxy-4-methoxyphenylacetic		19.39	17.58	19.30	17.48
β-(3-Hydroxy-4-methoxyphenyl)propionic		20.45	18.71	20.42	18.68
3-Hydroxy-4-methoxycinnamic		22.57	20.54	22.55	20.59
β-(3-Hydroxy-4-methoxyphenyl)hydracrylic		21.18	20.04	21.06	19.88
4-Hydroxy-3-methoxybenzoic		19.11	17.53	19.05	17.49
4-Hydroxy-3-methoxyhippuric		24.88	23.27	24.71	23.32
4-Hydroxy-3-methoxyphenylacetic		19.38	17.61	19.33	17.54
β-(4-Hydroxy-3-methoxyphenyl)propionic		20.53	18.84	20.57	18.83
4-Hydroxy-3-methoxycinnamic		22.76	20.78	22.75	20.78
4-Hydroxy-3-methoxymandelic		20.20	18.92	20.06	18.74
β-(4-Hydroxy-3-methoxyphenyl)lactic		21.45	20.27	21.36	20.23
4-Hydroxy-3-methoxyphenylpyruvic		23.34	21.67	23.29	21.76
4-Hydroxy-3-ethoxybenzoic		19.55	18.04	19.46	18.02
3,4-Dimethoxybenzoic		19.47	16.84	19.44	16.76
3,4-Dimethoxyphenylacetic		19.61	16.87	19.56	16.78
4-Hydroxy-3,5-dimethoxybenzoic		20.90	18.89	20.83	18.80
3-Indolylcarboxylic		22.60	19.95	22.78	20.01
3-Indolylacetic	(i)	21.82	18.65	22.44	18.74
	(ii)	21.71	19.34	22.00	19.41
β-(3-Indolyl)propionic	(i)	23.15	19.71	23.55	19.86
	(ii)	22.76	20.53	23.07	20.81
β-(3-Indolyl)lactic	(i)	23.92	21.07	24.17	21.18
	(ii)	23.34	21.68	23.55	21.79
3-Indolylpyruvic		26.33	24.30	26.41	24.34
N-Acetyltryptophan		25.65	24.00	25.82	24.11
		27.60	—	27.62	—
3-(5-Hydroxyindolyl)acetic		24.31	22.06	24.29	22.03

Column Packing P1 = 10% OV-17 on Diatoport S (80/100 mesh).
P2 = 10% OV-1 on Diatoport S (80/100 mesh).

Temperature T1 = initial temperature 100 °C, 2°/minute.
T2 = initial temperature 170 °C, 1°/minute.

Literature Coward, R. F. and P. Smith, *J. Chromatogr.*, **45**, 230 (1969).

TABLE GC 6
ALDEHYDES, DIMETHYL ACETALS

Column Packing	P1	P2	P3
Temperature (°C)	190	150	150
Gas; Flow Rate (ml/min)	100,Ar	50,N_2	50,N_2
Column			
length, cm	120	150	150
diameter, mm	4	4	4
form	na	coiled	coiled
material	glass	glass	glass
Detector	na	na	na
Compound	r (hexadecanal acetal derivative)		
Dodecanal	0.170	0.214	0.251
11-Methyldodecanal	0.221	0.265	0.298
10-Methyldodecanal	0.229	0.279	0.324
Tridecanal	0.267	0.314	0.353
12-Methyltridecanal	0.345	0.392	0.417
11-Methyltridecanal	0.363	0.412	0.450
Tetradecanal (myristaldehyde)	0.412	0.460	0.500
13-Methyltetradecanal	0.541	0.570	0.593
12-Methyltetradecanal	0.563	0.596	0.628
Pentadecanal	0.645	0.68	0.705
14-Methylpentadecanal	0.840	0.846	0.84
13-Methylpentadecanal	0.895	0.890	0.90
Hexadecanal (palmitaldehyde)	1.00	1.00	1.00
Hexadecenal (palmitoleic aldehyde)	0.840	1.13	1.15
15-Methylhexadecanal	1.30	1.25	1.18
14-Methylhexadecanal	1.36	1.32	1.28
Heptadecanal	1.55	1.47	1.43
Octadecanal (stearaldehyde)	2.39	2.16	2.01
***cis*-Octadeca-9-Dienol (oleylaldehyde)**	2.02	2.43	2.33
Octadecenal	2.14	—	—
***cis,cis*-Octadeca-9,12-Dienol (linoleylaldehyde)**	1.89	2.92	—
Octadeca-9,12,15-enal (linolenylaldehyde)	1.89	3.67	—
Methyl hexadecanoate (palmitate)	0.775	1.16	1.25

Column Packing
P1 = 12.5% Apiezon L on "Alkaline" Gas Chrom P (80/100 mesh).
P2 = 10% EGA on Gas Chrom CLH (80/100 mesh).
P3 = 15% EGSSX on Gas Chrom CLH (80/100 mesh).

Literature
Gray, G. M., *J. Chromatogr.*, 6, 236 (1961).

TABLE GC 7
ALDEHYDES AND KETONES

Column Packing	P1	P2	P3	P4	P5	P6	P7	P7
Temperature (°C)	100	100	100	70	100	70	90	150
Gas; Flow Rate (ml/min.)	—	—	—	—	—	—	32,He	32,He
Column								
length, ft	—	—	—	—	—	—	10	10
diameter, in., O.D.	—	—	—	—	—	—	¼	¼
form	—	—	—	—	—	—	na	na
material	—	—	—	—	—	—	SS	SS
Detector	—	—	—	—	—	—	TC	TC
Literature	1	1	1	1	1	2	3	3

Compound	$r_{(pentane\ or\ benzene)}$					t_r		
Acetaldehyde	—	—	—	0.16	—	0.43	4.5	—
Propionaldehyde	0.80	1.36	1.70	0.34	10.5	0.72	6.8	—
Acrolein	0.74	1.49	1.96	0.46	13.9	0.96	9.2	—
Isobutyraldehyde	1.48	2.26	2.82	0.46	12.2	0.78	7.7	—
n-Butyraldehyde	1.97	3.12	4.06	0.69	19.3	1.2	10.4	—
Crotonaldehyde	3.22	6.00	8.43	1.9	58.4	4.0	—	6.9
Paraldehyde	12.8	26.8	13.2	—	61.7	—	—	—
Isovaleraldehyde	—	—	—	—	—	—	13.1	—
n-Valeraldehyde	—	—	—	—	—	—	17.0	—
2-Methyl-1-butanal	—	—	—	—	—	—	12.0	—
Crotonaldehyde	—	—	—	—	—	—	26.9	—
2,4-Pentadienal	—	—	—	—	—	—	—	12.2
2-Hexenal	—	—	—	—	—	—	—	12.7
Benzaldehyde	—	—	—	—	—	—	—	>32
Acetone	0.96	1.34	1.92	0.41	13.7	1.1	7.6	—
Methyl ethyl ketone	2.07	3.21	4.44	0.79	22.7	1.7	11.7	—
Diethyl ketone	4.29	6.68	9.01	1.5	37.9	2.4	—	—
Acetylacetone	8.10	17.5	22.9	—	159	—	—	—
Ethanol	0.69	1.49	1.68	0.73	31.5	1.1	—	—
2-Pentanone	—	—	—	—	—	—	17.8	4.6
3-Pentanone	—	—	—	—	—	—	19.1	5.3
3-Methyl-2-butanone	—	—	—	—	—	—	14.0	—
2-Hexanone	—	—	—	—	—	—	30.0	6.6
4-Methyl-3-penten-2-one	—	—	—	—	—	—	—	12.3
Cyclohexanone	—	—	—	—	—	—	—	24.6
Diacetyl (bis)	—	—	—	—	—	—	>25	—
n-Pentane	1.00	1.00	1.00	—	1.00	—	—	—
Benzene	—	—	—	1.00	—	1.00	—	—

Column Packing

P1 = Silicone.
P2 = Dioctyl sebacate.
P3 = Didecyl phthalate.
P4 = Hexamethylene glycol dimethyl ether.
P5 = Polyethylene glycol.
P6 = β,β′-Oxydipropionitrile.
P7 = 30% Carbowax 1540 on firebrick.

Literature

1. Raupp, G., *Z. Anal. Chemie.*, **164**, 135 (1958).
2. Kelker, H., *Angew. Chemie.*, **71**, 218 (1959).
3. Ralls, J. W., *Anal. Chem.*, **32**, 332 (1960).