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Dr. T.A. Smith,
P.O. Box 6800,
Montreal, P.Q.,
CANADA.

12th April, 1978

Dear Tom,

I am very pleased that you found RD.1330 interesting and hope that it will be of some use to you in your studies concerning "off-taste".

With regard to Duolite ion exchange resin; I found an old O/WP trace of 100 mg of Duolite (GPA-327) and calculated the ratio of phenols:pyridines as 0.92. This compared well with the value of 0.68 given to Levatit resin. The smoke panel did not perceive an "off-taste" from this sample but the panel was specifically geared to detect carbon "off-taste" and as such would have concentrated on the first five puffs of the cigarette. The effect you describe does not sound like carbon "off-taste", especially since it occurred in the latter half of the cigarettes.

Your suggestion concerning low phenols:pyridines ratio indicating blended or air-cured character is certainly plausible and perhaps needs further investigation.

The O/WP data for various particulate filters is given below:

<u>Filter type</u>	<u>Pressure drop (cm W.G.)</u>	<u>Length (cm)</u>	<u>O/WP phenols:pyridines ratio</u>
Unplasticised CA.	10	20	0.02
Plasticised CA (7% Triacetin)	10	20	0.80
Soft polypropylene	10	20	0.69
Paper	10	20	0.69

(State Express tobacco rods were used for all above samples)

With reference to your second letter, there are a few points which I should make clear about the calculation of the phenols/pyridines ratio:

- 1) in the carbon "off-taste" report (RD 1330), a list of those peaks used to calculate the ratio is shown on page 7. The inclusion of peaks 30 and 31 in the pyridines group was unavoidable since any substantial amount of carbon reduces the intensity of the scan such that resolution peaks 29, 30 and 31 is lost. Peak 29 is pyridine itself, whilst 30 and 31 are both cyclopentanones. However, since the group was only

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representative of the semi-volatile portion of the scan, inclusion of non-pyridine type components does not detract from the validity of the ratio, provided the same peaks are used each time to calculate the ratio. In all other reports (e.g. RD.1320) the pyridines group does not contain peaks 30 and 31.

- 2) Triacetin and m & p cresol all co-elute and are labelled peak 84. Filters with TEGDA plasticiser (peak 98) were used for the carbon work, hence peak 84 could be included in the phenols group as m & p cresol. Normally triacetin is used as a filter plasticiser in commercial samples and therefore in most other reports peak 84 is not included as a phenol.

I have recalculated the ratios for the Canadian series (RD.1320) on the same basis as the groups in RD.1330 but as you will see (Table 2) the values are not very different.

In this case, the exclusion of peaks 30 and 31 from the pyridine group has almost balanced the exclusion of peak 84 from the phenols group. However, the use of previously published O/WP chemical group data could still be useful as a guide to smoke balance, provided the same peaks are used each time the calculation of group values. In view of the small difference between the two methods of group calculation, the normal chemical group data (as in RD.1320) will be adequate to monitor moderate changes in smoke balance.

The situation concerning the data in RD.1309 and RD.1263 is somewhat complicated. RD.1309 contains data collected by Dr. C.W. Ayers using her own O/WP set up and for this reason may not be strictly comparable with my own data. However, I doubt if this would change the dramatic imbalance seen for Cytrel and Tabrelle, although I wonder whether this is valid for non-tobacco materials, especially since they may contain only very small quantities of pyridines.

RD.1263 contains data from both Dr. Ayers and my own O/WP set-up. I have recalculated the ratios for three of the cigarettes using the peak numbers shown in the carbon "off-taste" report and these now seem similar to most other cigarettes (Table 3). The values in the table of chemical groups in RD.1263 were ratios to NB (taken as 100 for each chemical group) and as such only indicate the difference between the cigarettes and NB and not the distribution of components in the scan. I have now standardised the methods of analysis and any future reports containing chemical group data will be comparable with the data in RD.1320.

It is difficult to correlate the O/WP data from the carbon work with irritation because of the large reductions in almost all components in the first two thirds of the scan but I have enclosed the chemically grouped O/WP data for the carbon work as you requested (Table 4). Both peak area and percentage normalised data are included in the table. The peak area data indicates the actual levels of components whilst the percentage data shows the distribution of components in the scan. The cyclic ketones and pyridines group values are approximate since peaks 29, 30 and 31 had to be resolved by estimation. Peak 84 has been excluded

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from the phenol group so that the results are comparable with those in RD.1320. Figures in brackets (Table 1) are the ratios calculated using the groups as in RD.1320, i.e. excluding peaks 30 and 31 from the pyridines and excluding peak 84 from the phenols. As you can see the actual ratios have not changed very much.

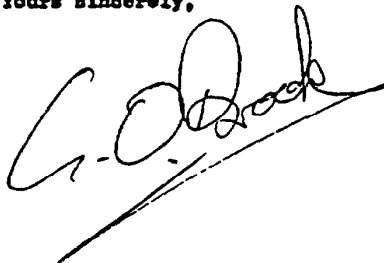
It would be difficult with 103 peaks per scan and many brands per report, to include all the O/WP data in every report. Without the full information at your disposal, your task of calculating ratios is of course made more difficult. If at any time you would like samples evaluated by O/WP, I would be happy to oblige. We have a current programme of work designed to attempt correlations between Woodrose characteristics and O/WP data. This work, which covers a very wide range of tobacco types, is currently being analysed.

Finally, I think I should emphasise that the phenols:pyridines ratio used in RD.1330 was specifically correlated with carbon off-taste and is also tobacco blend dependent. I do not know whether it has an understandable meaning with respect to cigarettes in general.

I thank you once again for your interest and hope that the explanations and data given here will help you. I would be very grateful if you would let me know whether you can find any interesting features in the data given here.

With best wishes,

Yours sincerely,



c.c. Dr. D.G. Felton

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O/WP Phenols:Pyridines Ratio; an Indicator of the Balance in Smoke?

TABLE 1

1. RD.1330 Relationship between O/WP scan and carbon "off-taste".

<u>Filter on State Express</u> <u>Flue-cured tobacco rod</u>	<u>Phenols</u> <u>Pyridines ratio</u>
Control acetate	0.62 (0.66)
<u>Carbons:</u> 50 mg BPL	1.49 (1.46)
100 mg BPL	2.56 (2.36)
150 mg BPL	4.49 (3.89)
100 mg MF3	2.79 (2.51)
100 mg MF3, puffs 1-4	3.62 (3.51)
100 mg MF3, puffs 7-10	2.22 (2.26)
100 mg coated carbon (Smith & Nephew)	1.19 (1.16)
<u>Non-Carbon</u>	
83 mg Lewatit	0.88 (1.01)
150 mg magnesium silicate (white) granules ex SEL-X-4 filter)	5.52 (5.26)
100 mg silica gel	4.38 (4.22)
100 mg spherical alumina	1.57 (1.56)
<u>Carbon on Primeros air-cured</u> <u>Fermented tobacco rod</u>	
Control acetate	0.50 (0.49)
50 mg BPL	1.08 (1.02)
100 mg BPL	1.83 (1.65)
150 mg BPL	2.60 (2.29)

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TABLE 2

2. RD.1320 O/WP Comparison of Canadian Brands

<u>Brands</u>	<u>Phenols Pyridines</u>	<u>ratio using peaks as in RD.1330</u>
Matinee K.S.	0.49	0.42
Craven A K.S.	0.62	0.59
Matinee Regular	0.48	0.41
Craven A Regular	0.52	0.43
du Maurier Regular	0.52	0.48
Belvedere Regular	0.49	0.44
du Maurier K.S.	0.52	0.49
Rothmans K.S.	0.59	0.56
Players Filter Regular	0.50	0.51
Export A Regular	0.52	0.50
<u>Grades</u>		
D	0.60	0.69
FS3	0.40	0.40
BFL	0.48	0.52
AFX	0.64	0.72
OF4	0.49	0.57
BF3	0.53	0.71

TABLE 3

3. RD.1263 O/WP Examination of low delivery West German brands

<u>Brand</u>	<u>Phenols Pyridines</u>	<u>ratio using peaks as in RD.1330</u>
Leichte Classe	1.02	
Peer Leicht	0.98	
California	1.29	0.55
R6	1.06	0.44
Auslese	1.00	0.39
Reynolds No. 1	0.62	
Krone	0.99	

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TABLE 4

Brand Name	Type of Data	Acyelic Aldehydes 4,12,27	Cyclic Aldehydes 52,57,60	Acyelic Ketones 11,14,15, 16,55	Cyclic Ketones 30,31,44,46, 50,56,65,82	Phenols 74,78,80, 89,90	Pyridines 29,32,34,37, 41,42,53	Pyrazines 36,43	Pyroles 24,37,56, 101	Micellins 20,22,62, 77,88
Control Acetate (State Express)	Norm	2.04	9.12	16.40	15.94	6.02	10.35	1.75	2.64	4.28
	Peak Area	4.81	21.50	38.67	37.58	16.08	24.40	4.13	6.22	10.33
50 mg BPL (State Express)	Norm	1.13	9.76	11.72	14.89	10.44	7.16	1.17	2.30	4.76
	Peak Area	1.52	13.09	15.72	19.98	14.03	9.61	1.57	3.09	6.39
100 mg BPL (State Express)	Norm	0.71	9.14	9.93	12.77	12.94	5.48	0.96	2.58	5.14
	Peak Area	0.77	9.90	10.75	13.83	14.03	5.93	0.93	2.79	5.36
150 mg BPL (State Express)	Norm	0.51	7.18	8.12	11.62	15.17	3.90	0.58	2.71	5.40
	Peak Area	0.43	6.07	6.87	9.83	12.83	3.30	0.49	2.29	4.74
100 mg MF3 (State Express)	Norm	0.92	8.50	9.88	12.96	13.08	5.21	0.86	2.51	5.55
	Peak Area	0.92	8.50	9.88	12.96	13.08	5.21	0.86	2.51	5.55
First Four 100 mg MF3 (State Express)	Norm	1.32	5.86	18.74	10.74	12.64	3.60	0.66	3.21	4.80
	Peak Area	0.46	2.03	6.48	3.71	4.37	1.24	0.23	1.11	1.66
100 mg MF3 (State Express)	Norm	1.39	6.20	13.32	11.03	10.97	4.86	0.81	2.68	4.76
	Peak Area	0.99	4.43	9.52	7.89	7.84	3.47	0.58	1.92	3.40
S & N Coated Carbon (7,11,75) 100 mg (State Express)	Norm	1.30	9.75	11.31	15.05	9.05	7.78	1.30	2.41	4.60
	Peak Area	2.06	15.43	17.90	23.82	14.32	12.31	2.06	3.81	7.28
Lumit Resin 83 mg (State Express)	Norm	1.48	6.44	14.65	15.34	7.96	7.86	1.76	2.61	4.21
	Peak Area	2.56	11.17	25.33	26.53	13.76	13.59	3.04	4.51	7.28
SEL-X-4 White Granules 150 mg (State Express)	Norm	1.66	4.07	10.63	7.94	15.58	2.96	0.55	4.07	5.91
	Peak Area	1.82	4.46	11.66	8.71	17.09	3.25	0.60	4.41	6.48
Spherical Alumina 100 mg (State Express)	Norm	2.73	6.43	15.88	10.14	8.25	5.28	0.86	3.16	5.32
	Peak Area	4.53	10.67	26.35	16.83	13.69	8.78	1.43	5.24	8.83
Silica Gel 100 mg (State Express)	Norm	2.37	5.99	12.62	10.13	14.19	3.36	0.56	3.78	5.36
	Peak Area	2.37	5.99	12.62	10.13	14.19	3.36	0.56	3.78	5.36
Control Acetate (Primero)	Norm	1.79	4.59	9.68	15.55	6.43	13.00	1.87	3.71	4.95
	Peak Area	3.27	8.38	17.68	28.40	11.74	23.74	3.42	6.78	9.04
50 mg BPL (Primero)	Norm	0.89	4.92	9.08	14.04	9.27	9.05	1.20	4.18	4.65
	Peak Area	0.95	5.24	9.67	14.96	9.67	9.64	1.28	4.45	4.95
100 mg BPL (Primero)	Norm	0.88	4.60	7.41	12.52	11.30	6.86	0.93	4.77	5.00
	Peak Area	0.57	3.83	6.18	10.44	9.62	5.72	0.78	3.98	4.17
150 mg BPL (Primero)	Norm	0.81	4.00	7.22	11.39	11.73	5.12	0.81	4.69	5.47
	Peak Area	0.67	3.31	5.97	9.42	9.70	4.23	0.67	3.88	4.52

NOTE: Norm. stands for percentage normalized data.

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