"*Infrared Metrics for Fixation-Free Liver Tumor Detection*", Zhaomin Chen, Ryan Butke, Barrie Miller, Charles L. Hitchcock, Heather C. Allen*, Stephen P. Povoski, Edward W. Martin Jr., and James V. Coe*, The Ohio State University

Supplementary Materials

Table 1s contains a combined set of IR biomarkers from the work of Fernandez et al[36] and ones that were added by us to help deal with lipids in liver tissue. The top 20 for identifying tumors in fixation free liver tissue were determined from this group.

Table 1s. IR Biomarkers considered for fixation-free liver tumor tissues. Each is a ratio of absorbance at the numerator (in cm^{-1}) to absorbance at denominator (in cm^{-1}). If a range is given, then the average absorbance over that range is used. Biomarkers *b1-b36* are from Fernandez et al[36], while biomarkers *b37-64* were added by us for fixation-free studies.

Name	Ratio	Name	Ratio
b1	966/1544	*b33*	(1478-1560)/1544
b2	1012/1256	*b34*	(1478-1578)/1544
b3	1034/1544	*b35*	(1572-1764)/1544
b4	1062/1544	*b36*	(3000-3682)/1544
b5	1080/1544	*b37*	1744/1244
b6	1114/1544	*b38*	1744/1162
b7	1158/1544	*b39*	1024/1080
b8	1170/1544	*b40*	1172/1154
b9	1206/1544	*b41*	2854/2962
b10	1236/1544	*b42*	1080/1244
b11	1278/1544	*b43*	1744/1548
b12	1502/1544	*b44*	2874/2854
b13	1516/1544	*b45*	1120/1020
b14	1536/1544	*b46*	2924/1544
b15	1588/1544	*b47*	1516/1582
b16	1654/1544	*b48*	1080/1548
b17	3290/1544	*b49*	964/1548
b18	3292/1544	*b50*	1030/1080
b19	1016/1080	*b51*	1588/1548
b20	1032/1080	*b52*	1520/1548
b21	1034/1062	*b53*	1160/1548

b22	1050/1034	*b54*	2916/1548
b23	1080/3290	*b55*	1600/1548
b24	1164/1080	*b56*	1100/1744
b25	1400/1390	*b57*	1632/1548
b26	1426/1450	*b58*	1556/1548
b27	1450/1544	*b59*	1252/1544
b28	1516/1236	*b60*	1100/1544
b29	(982-1144)/1544	*b61*	1556/1558
b30	(1144-1182)/1544	*b62*	858/1544
b31	(1184-1296)/1544	*b63*	1070/1544
b32	(1372-1420)/1544	*b64*	1742/1256

A k-means analysis with scaled biomarkers and 5 groups was performed to help in the process of identifying the top 20 IR biomarkers for tumors in fixation free liver tissue. The resulting image is shown in Figure 1s.

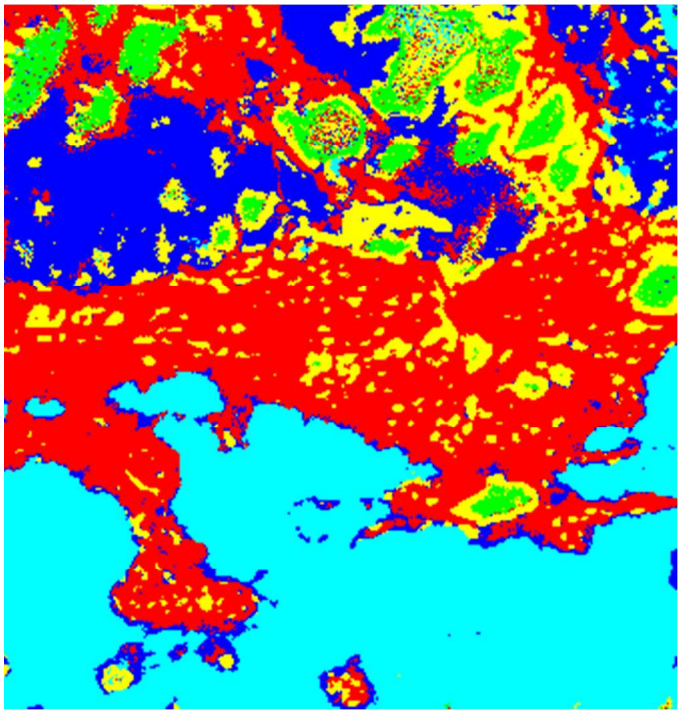

Figure 1s. K-means cluster analysis with 5 groups using scaled biomarkers. The nontumor portion is in cyan at the bottom half. The holes are in green. There are three tumor groups (red, blue, and yellow).

A 25 group k-means analysis was performed and the resulting 25 bitmaps for each group are given in Figure 2s. These images enable one to characterize the groups as associated with the

nontumor, tumor, or hole regions. The IR spectrum of each of these groups has also been added to the supplementary materials as an Excel file called "g25_spectra.xlsx".

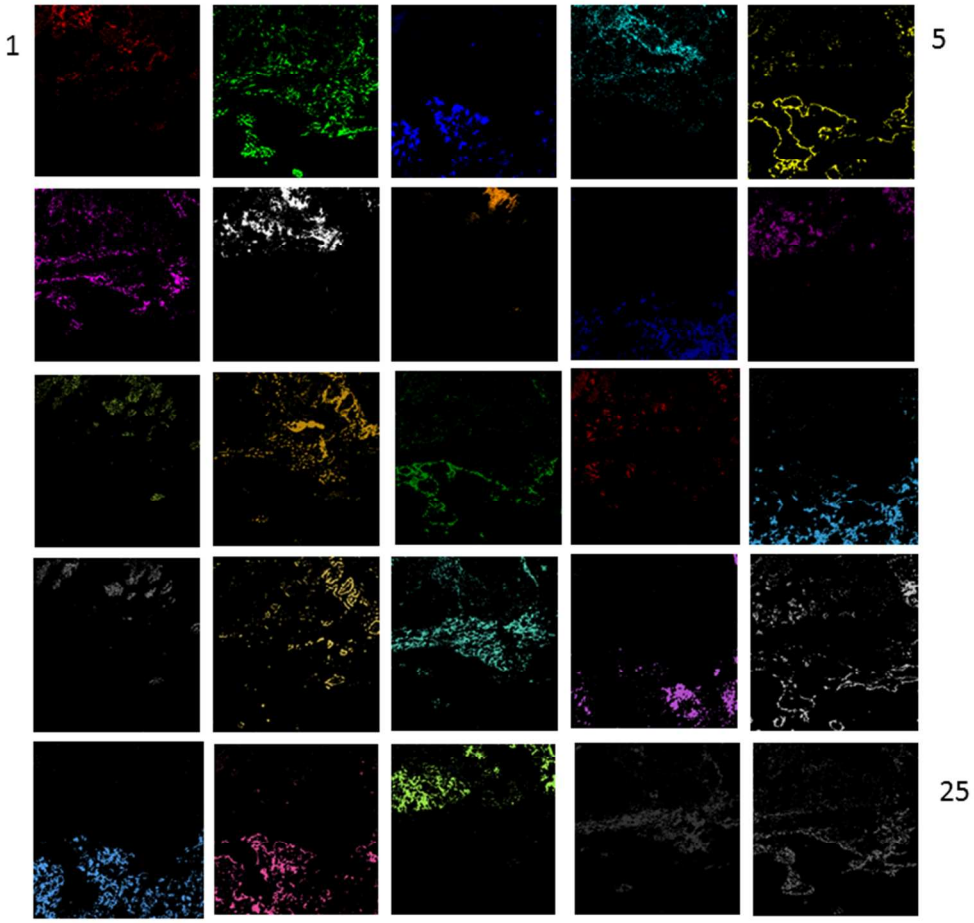

Figure 2s. Bitmap images of each group from a 25 group, k-means cluster analysis. One can determine whether the groups are from the nontumor, tumor, or hole regions. The groups are numbered from left-to-right, and top-to-bottom, from 1 to 25.