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Fast Cancer Imaging in Pancreatic Biopsies using Infrared Imaging

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no.	Band range [cm ⁻¹]			14	1190	1290
1	940	980		15	1270	1294
2	960	980		16	1292	1310
3	980	1004		17	1295	1320
4	1015	1040		18	1310	1324
5	1040	1070		19	1324	1356
6	1060	1100		20	1340	1360
7	1115	1138		21	1360	1390
8	1010	1155		22	1380	1400
9	1160	1180		23	1400	1420
10	1190	1210		24	1360	1425
11	1195	1212		25	1425	1480
12	1255	1270		26	1490	1590
13	1210	1280		27	1710	1760

Table 1. List of spectral regions used for QCL data. Additional region of 1600-1710 cm⁻¹(Amide I), was defined for normalization purpose.

Num.	Patient number	PA2081b	BIC14011a	
1	1	A1,A2	-	
2	2	A3,A4	-	
3	3	A5,A6	-	
4	4	A7,A8	-	
5	5	A9,A10,I5,I6	-	
6	6	A11,A12	-	
7	7	A13,A14	-	
8	8	A15,A16	-	
9	9	B1,B2	-	
10	10	B3,B4	-	
11	11	B5,B6	-	
12	12	B7,B8	-	
13	13	B9,B10	-	
14	14	B11,B12	-	
15	15	B13,B14	-	
16	16	B15,B16	-	
17	17	C1,C2	-	
18	18	C3,C4	-	
19	19	C5,C6	-	
20	20	C7,C8	-	
21	21	C9,C10	-	
22	22	C11,C12	-	
23	23	C13,C14	F1,F2	
24	24	C15,C16	-	
25	25	D1,D2	-	
26	26	D3,D4	-	
27	27	D5,D6	-	
28	28	D7,D8	-	
29	29	D9,D10	-	
30	30	D11,D12	-	
31	31	D13,D14	-	
32	32	D15,D16	-	
33	33	E1,E2	-	
34	34	E3,E4	-	
35	35	E5,E6	-	
36	36	E7,E8	-	
37	37	E9,E10	-	
38	38	E11,E12	-	
39	39	E13,E14	-	
40	40	E15,E16	-	
41	41	F1,F2	-	
42	42	F3,F4	-	

I	12	12	E5 E6	1
	43	43	Г 3, Г 0 Е 7 Е 9	-
	44	44	<u>г/,го</u> Е10	-
	43	43	F10 E11_E12	-
	40	40	F11, F12	
	4/	63	H13,H14	-
	48	64	H15,H16	-
	49	65	11,12	-
	50	66	13,14	-
	51	67	17,18	-
	52	68	19,110	-
	53	<u>69</u>		-
	54	70	113,114	-
	55	71	115,116	-
	56	72	J1,J2	-
	57	73	J3,J4	-
	58	74	J5,J6	-
	59	76	J9,J10	-
	60	77	J11,J12	-
	61	78	J13,J14	-
	62	79	J15,J16	-
	63	80	K1,K2	-
	64	81	K3,K4	-
	65	82	K5,K6	-
	66	83	K7,K8	-
	67	84	K9,K10	-
	68	85	K11,K12	-
	69	86	K13,K14	-
	70	87	K15,K16	-
	71	88	L1,L2	-
	72	89	L3,L4	-
	73	90	L5,L6	-
	74	91	L7,L8	-
	75	92	L9,L10	_
	76	93	L11,L12	-
	77	94	L13,L14	-
	78	95	L15,L15	-
	79	97	M3,M4	-
	80	98	M5,M6	-
	81	99	M7,M8	-
	82	100	M9.M10	-
	83	101	M11.M12	-
	84	102	M13.M14	_
	85	103	M15.M16	_
	86	119	-	F5.F6
	87	135	_	F3.F4
	88	142		F7.F8
I				,- ~

Table 2. Patients numeration

100	256	-	A7,A8			108	
99	255	-	A1,A2		To	tal patients nu	ımber
98	253	-	E7,E8		220		
97	252	-	C1,C2		Total cores number		
96	250	-	E3,E4	108	264	-	E5,E6
95	249	-	B5,B6	107	263	-	E1,E2
94	239	-	B3,B4	106	262	-	D7,D8
93	238	-	A5,A6	105	261	-	D5,D6
92	226	-	A3,A4	104	260	-	D3,D4
91	223	-	B1,B2	103	259	-	D1,D2
90	216	-	C3,C4	102	258	-	C7,C8
89	212	-	B7,B8	101	257	-	C5,C6

Table 3. QCL patient assigned to a test set, in each fold of Random Forst cross validation.

Fold number	Patients assigned to test set					
rola number	Cancer	Benign				
Fold no. 1	6, 14, 16, 19, 31, 39, 44, 135, 142	63, 68, 73, 78, 81, 90, 92, 102, 238,				
		239, 261				
Fold no. 2	2, 7, 8, 9, 12, 20, 27, 28, 42, 119	67, 77, 83, 85, 95, 97, 250, 252,				
		255, 257, 262, 263				
Fold no. 3	3, 17, 18, 23, 24, 25, 26, 30, 32, 34	65, 71, 72, 79, 80, 96, 98, 99, 101,				
		103, 216, 223, 256				
Fold no. 4	5, 10, 11, 15, 22, 29, 33, 38, 43, 46	64, 69, 84, 87, 91, 94, 100, 212,				
		249, 226, 253, 259				
Foldma 5	1, 4, 13, 21, 35, 36, 37, 40, 41, 45	66, 70, 74, 76, 82, 86, 88, 89, 93,				
Fold lio. 3		258, 264				



Figure S1. H&E images of PA2081b (A) and BIC14011a (C) Tissue Micro Arrays used for histopathological annotations, along with zoom-ins on single tissue cores (B).

Surgical margin - H&E image

2 mm



Figure S2. H&E image of resection material covering surgical margin (transition from cancerous to benign tissue).



Figure S3. The prediction image reveling surgical margins, based on Random Forest Model trained with full spectral information in the form of metrics.