



Supplementary Material

# High-Resolution Magic Angle Spinning Nuclear Magnetic Resonance Spectroscopy of Paired Clinical Liver Tissue Samples from Hepatocellular Cancer and Surrounding Region

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Table S1. NMR Peak Assignments.

Peak assignment	Chemical shift/ppm	Upper bin limit /ppm	Lower bin limit /ppm
Lipid CH <sub>3</sub> (L1)	0.90	0.98	0.84
Lipid CH <sub>2</sub> (L2)	1.20	1.32	1.24
Lipid CH <sub>2</sub> CH <sub>2</sub> CO (L3)	1.60	1.62	1.55
Lipid CH=CHCH <sub>2</sub> CH <sub>2</sub> (L4)	2.04	2.10	1.98
Lipid CH <sub>2</sub> CH <sub>2</sub> CO (L5)	2.26	2.30	2.22
Lipid CH=CHCH <sub>2</sub> CH=CH (L6)	2.77	2.82	2.72
Lipid CH=CH (L7)	5.33	5.40	5.27
Valine doublet	1.04	1.06	1.02
Ethanol triplet	1.18	1.21	1.16
Lactate doublet	1.33	1.34	1.32
Alanine doublet	1.48	1.5	1.45
Acetate singlet	1.92	1.94	1.91
Choline	3.20	3.22	3.19
Phosphocholine	3.22	3.25	3.22
TMAO/glycerophosphocholine	3.26	3.29	3.25
Glucose doublet	5.22	5.26	5.21
Histidine	7.10	7.05	6.95
Histidine	7.75	7.80	7.70
Phenylalanine	7.32	7.33	7.28
Phenylalanine	7.34	7.38	7.33
Phenylalanine	7.42	7.44	7.38
Tyrosine	6.85	6.91	6.82
Tyrosine	7.17	7.20	7.13
Formate	8.46	8.48	8.43

**Table S2.** Summary of selected lipid and low molecular weight metabolite levels in surrounding tissue (sample IDs xxxA) and HCC (sample IDs xxxB) for each subject.

Sample details			Metabolite of interest, including spectral region used for binning definition								
ID	Aetiology on histology	Formate 8.48-8.42ppm	Glucose 5.26-5.21ppm	3.5-4.0 ppm region	Choline region 3.29-3.19ppm	Acetate 1.94-1.91ppm	Alanine 1.50-1.45ppm	L7 5.40-5.27ppm	L6 2.82-2.72ppm	Lipid- CH <sub>2</sub> 1.32-1.24ppm	Lipid-CH <sub>3</sub> 0.98-0.84ppm
039A	Alcohol	4.57E+05	4.19E+07	7.66E+08	1.08E+08	1.34E+07	4.47E+07	2.69E+08	9.38E+07	3.37E+09	1.47E+09
039B	Alcohol	5.12E+05	7.94E+06	2.29E+08	9.35E+07	4.55E+06	1.54E+07	2.24E+07	1.27E+07	1.22E+08	6.90E+07
141A	SLD+alcohol	3.63E+05	1.66E+07	1.07E+09	9.32E+07	7.93E+06	4.70E+07	1.33E+08	5.54E+07	1.41E+09	6.53E+08
141B	SLD+alcohol	9.48E+05	1.99E+07	1.37E+09	1.62E+08	1.28E+07	4.76E+07	1.96E+07	1.03E+07	2.29E+08	1.43E+08
116A	SLD	1.54E+06	6.22E+07	1.18E+09	3.60E+08	1.75E+07	8.37E+07	2.47E+08	1.02E+08	3.45E+09	1.55E+09
116B	SLD	1.11E+06	6.19E+07	1.42E+09	4.46E+08	1.24E+07	6.53E+07	6.61E+07	2.03E+07	1.10E+09	5.05E+08
134A	SLD	5.58E+05	6.03E+07	7.23E+08	2.70E+08	1.69E+07	7.86E+07	3.32E+08	1.27E+08	4.68E+09	2.03E+09
134B	SLD	6.01E+05	3.72E+07	1.26E+08	3.27E+07	1.39E+07	5.22E+07	3.63E+08	6.28E+07	6.03E+09	2.67E+09
168A	SLD	4.02E+05	1.73E+07	6.14E+08	2.00E+08	9.25E+06	4.13E+07	8.62E+07	4.01E+07	1.02E+09	4.23E+08
168B	SLD	1.18E+06	6.74E+06	3.22E+08	1.10E+08	1.12E+07	3.58E+07	9.52E+06	1.07E+07	7.42E+07	8.38E+07
117A	None→ SLD	4.08E+05	2.10E+07	5.34E+08	2.20E+08	8.62E+06	3.98E+07	5.04E+07	2.68E+07	5.71E+08	2.63E+08
117B	None→ SLD	5.87E+05	5.19E+07	5.86E+08	2.62E+08	1.56E+07	7.46E+07	3.11E+08	9.10E+07	4.32E+09	1.89E+09
107A	None	4.25E+05	1.41E+07	1.00E+09	2.22E+08	6.97E+06	1.77E+07	1.63E+07	9.38E+06	1.41E+08	8.08E+07
107B	None	7.19E+05	4.36E+07	1.67E+09	2.68E+08	8.79E+06	2.67E+07	2.10E+07	1.33E+07	1.38E+08	8.22E+07
235A	None	8.29E+05	2.18E+07	1.11E+09	2.47E+08	1.74E+07	6.75E+07	1.97E+07	1.41E+07	2.13E+08	1.54E+08
235B	None	6.36E+05	2.30E+07	9.66E+08	2.61E+08	1.23E+07	3.66E+07	1.61E+07	1.15E+07	2.29E+08	1.47E+08
268A	None	5.20E+05	2.43E+07	1.08E+09	2.29E+08	1.09E+07	4.39E+07	4.06E+07	2.42E+07	5.42E+08	2.76E+08
268B	None	1.70E+06	3.54E+07	1.29E+09	4.65E+08	7.04E+06	8.02E+07	2.73E+07	1.19E+07	4.42E+08	2.04E+08
099A	Treated HCV	6.17E+04	3.33E+07	1.30E+09	2.25E+08	1.23E+07	4.35E+07	3.85E+06	1.68E+07	1.28E+08	8.52E+07
099B	Treated HCV	5.98E+05	4.26E+06	1.35E+09	8.33E+07	7.52E+06	1.95E+07	1.47E+07	5.27E+06	1.71E+08	9.71E+07
Samples A	Median	4.41E+05	2.31E+07	1.04E+09	2.24E+08	1.16E+07	4.43E+07	6.83E+07	3.35E+07	7.96E+08	3.50E+08
Samples A	Q1	3.92E+05,	1.71E+07,	6.96E+08,	1.77E+07,	8.45E+06,	4.09E+07,	1.89E+07,	1.61E+07,	1.95E+08,	1.49E+08, 1.37E+09
Samples A	Q3	6.26E+05	4.65E+07	1.13E+09	2.53E+08	1.70E+07	7.03E+07	2.53E+08	9.59E+07	3.39E+09	
Samples B	Median	6.78E+05	2.92E+07	1.13E+09	2.12E+08	1.18E+07	4.21E+07	2.17E+07	1.23E+07	2.29E+08	1.43E+08
Samples B	Q1	5.95E+05,	7.64E+06,	2.99E+08,	9.10E+07,	7.40E+06,	2.49E+07,	1.58E+07,	1.06E+07,	1.34E+08,	8.30E+07,
Samples B	Q3	1.13E+06	4.75E+07	1.38E+09	3.13E+08	1.31E+07	6.76E+07	1.27E+08	3.09E+07	1.91E+09	1.20E+09