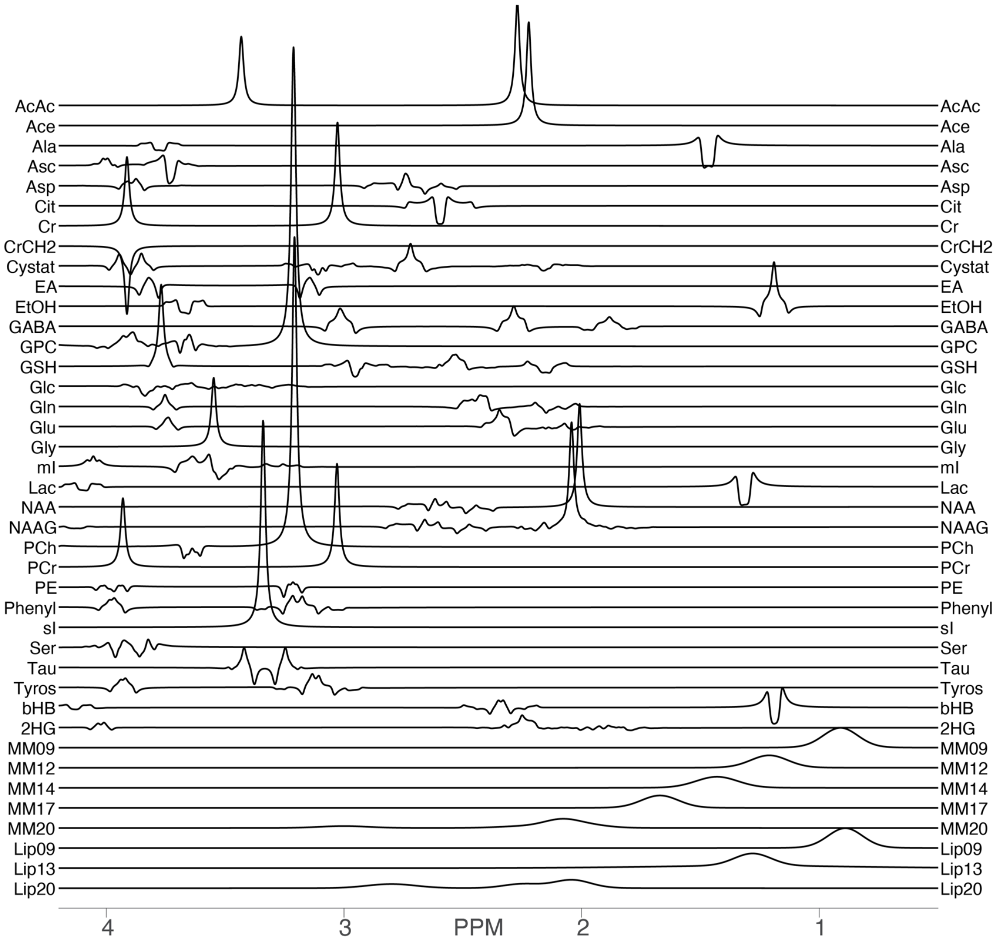
Basis function	linewidth [Hz]	Peak frequency [ppm]	Amplitude [1-proton area]
MM09	0.14	0.91	3
MM12	0.15	1.21	2
MM14	0.17	1.43	2
MM17	0.15	1.67	2
MM20	0.15	2.08	1.33
	0.2	2.25	0.33
	0.15	1.95	0.33
	0.2	3	0.4
Lip09	0.14	0.89	3
Lip13	0.15	1.28	2
	0.89	1.28	2
Lip20	0.15	2.04	1.33
	0.15	2.25	0.67
	0.2	2.8	0.87

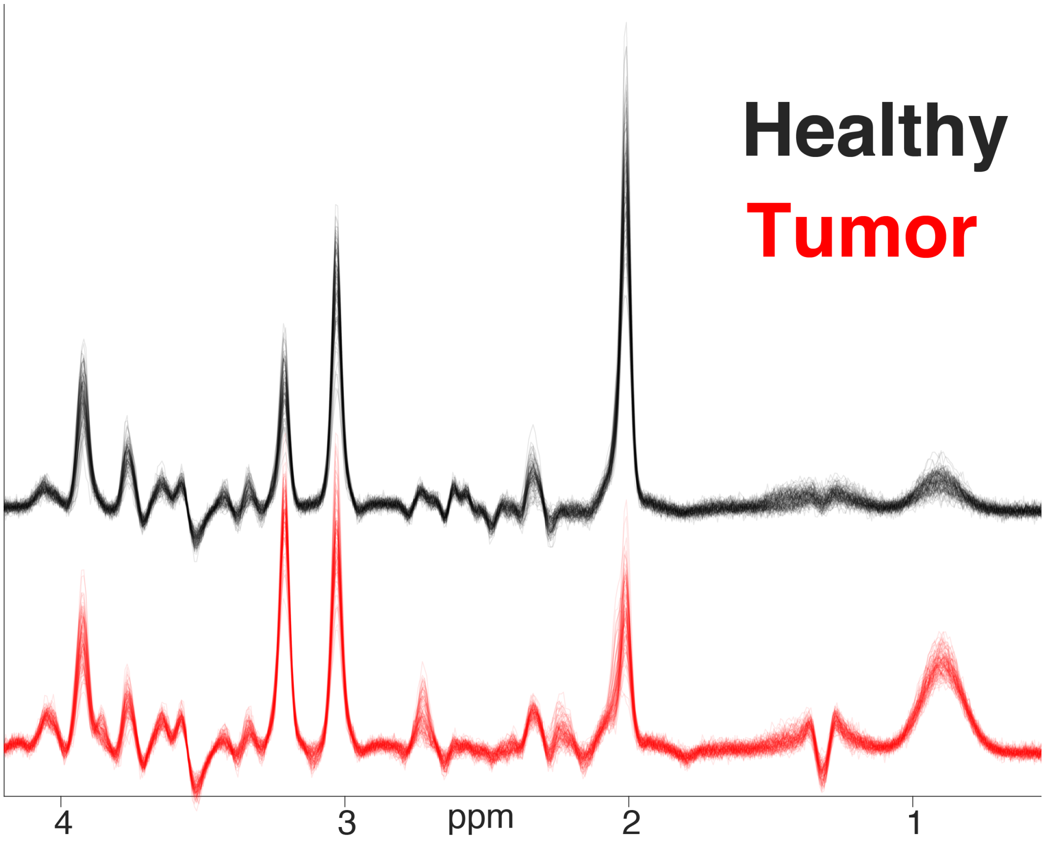
Supplementary Table 1. The width, center frequency, and relative amplitude of the parameterized lipid and MM resonances we included in the basis set. Specific values were based on the LCModel parameterizations of these signals.



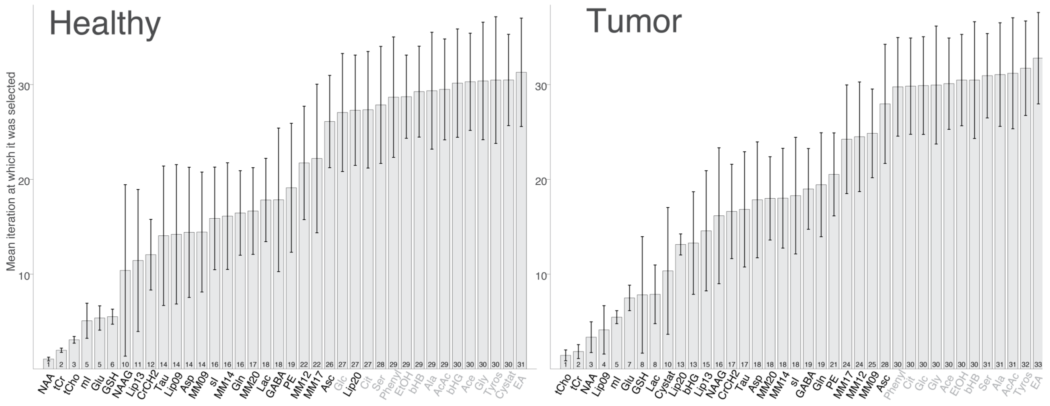
Supplementary figure 1. The full “library” basis set of metabolite basis functions with 1.3 Hz Lorentzian linebroadening.

		Healthy	**Tumor**
	Gaussian linebroadening [Hz]	7.44 ± 0.56	7.74 ± 0.62
	Lorentzian linebroadening [Hz]	2.36 ± 0.31	2.44 ± 0.36
	SNR	223.15 ± 67.06	229.75 ± 56.67
Amplitude	Asc	0.36 ± 0.28	0.42 ± 0.31
	Asp	1.46 ± 0.36	1.51 ± 0.36
	Cr	3.82 ± 1.01	4.02 ± 0.79
	CrCH2	0.91 ± 0.52	0.88 ± 0.56
	GABA	0.86 ± 0.43	0.87 ± 0.48
	GPC	0.59 ± 0.37	0.83 ± 0.24
	GSH	1.45 ± 0.45	1.33 ± 0.46
	Gln	1.44 ± 0.79	1.36 ± 0.91
	Glu	5.75 ± 1.88	5.72 ± 0.95
	Lac	0.50 ± 0.34	3.62 ± 0.50
	NAA	8.89 ± 1.42	3.50 ± 1.00
	NAAG	0.95 ± 0.42	0.78 ± 0.68
	PCh	0.47 ± 0.26	1.35 ± 0.22
	PCr	2.36 ± 1.26	1.99 ± 0.91
	PE	1.76 ± 0.65	1.82 ± 0.62
	Tau	1.31 ± 0.76	1.12 ± 0.81
	mI	5.28 ± 0.99	7.01 ± 1.10
	sI	0.18 ± 0.13	0.17 ± 0.12
	Cystat	0	3.22 ± 2.10
	2HG	0	3.55 ± 2.25
	Lip09	1.19 ± 0.51	7.61 ± 0.59
	Lip13	1.58 ± 0.60	1.56 ± 0.69
	Lip20	0.37 ± 0.18	2.59 ± 0.19
	MM09	1.99 ± 0.79	2.02 ± 0.97
	MM12	0.71 ± 0.58	0.64 ± 0.45
	MM14	1.76 ± 1.17	1.68 ± 1.10
	MM17	0.62 ± 0.43	0.67 ± 0.45
	MM20	2.14 ± 1.01	2.25 ± 0.99

Supplementary Table 2. Ground truth simulation parameters (mean ± standard deviation) used to derive the healthy-appearing spectra (left column) and low-grade glioma, “tumor” spectra (right column). The top three rows show the Gaussian and Lorentzian linebroadening terms and the SNR, with subsequent rows showing the metabolite-specific amplitudes.



Supplementary figure 2. The synthetic dataset used to test the algorithm. Healthy-appearing spectra (black) are plotted alongside the “tumor” spectra, representing low-grade glioma patients (red).



Supplementary Figure 3. Visualization of the mean (bar) and standard deviation (error bars) of the iterations at which each basis function was picked. Smaller bars, therefore, indicate a higher prioritization of a given basis function, whilst error bars indicate the inter-spectrum variability of the metabolite's prioritization. Basis functions are ordered based on their mean. The shade of the metabolite label indicates the presence (black) or absence (grey) of that particular metabolite in the ground truth simulation.