Supporting Information to Manuscript

Magic Angle Spinning NMR Based Metabolic Profiling of Head and Neck Squamous Cell Carcinoma Tissues

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Table S1: ^{1}H chemical shift of metabolites detected in the head and neck tissues.

Metabolite	Moiety	^{1}H Chemical Shift (ppm)
Acetate	CH_3	1.92
Alanine	αCH; βCH_3	3.77; 1.48
Aspartate	αCH; βCH_2	3.90; 2.82, 2.67
Choline	$N(CH_3)_3$; αCH_2; βCH_2	3.19; 4.05, 3.51
Creatine	$N\text{-}CH_3$; CH_2	3.04; 3.93
Glutamate	αCH; βCH_2; γCH_2	3.75; 2.09; 2.35
Glutamine	αCH; βCH_2; γCH_2	3.78; 2.14; 2.44
Glutathione	Glu (CH; CH_2; CH_2) Cys (CH; CH_2) Gly (CH_2)	3.76; 2.16; 2.54 4.51; 3.01 3.77
Glycerophosphocholine	$N(CH_3)_3$; OCH_2; NCH_2	3.22; 4.32; 3.68
Glycine	CH_2	3.57
Isoleucine	αCH; βCH; γCH_2;	3.65; 1.97; 1.26/1.47
	γCH_3; δCH_3	1.02; 0.94
Lactate	αCH; βCH_3	4.11; 1.33
Leucine	αCH; βCH_2; γCH;	3.73; 1.72; 1.70;
	δCH_3; δCH_3	0.97; 0.95
Phenylalanine	αCH; βCH_2;	3.99; 3.11/3.28;
	2,6-H; 3,5-H, 4H	7.34; 7.44; 7.37
Phosphocholine	$N(CH_3)_3$; OCH_2; NCH_2	3.20; 4.16; 3.58
Taurine	$S\text{-}CH_2$; $N\text{-}CH_2$	3.26; 3.42
Tyrosine	αCH; βCH_2;	3.93; 3.06/3.20
	2,6-H; 3,5-H	7.23; 6.89
Valine	αCH; βCH;	3.61; 2.25;
	γCH_3; γCH_3	1.04; 0.99

Figure S1. A comparison of NMR spectra of a tumor tissue with that of standard compounds to support the chemical shift assignments of isoleucine, leucine, valine, lactate, alanine, glutamate, glutamine and glutathione.

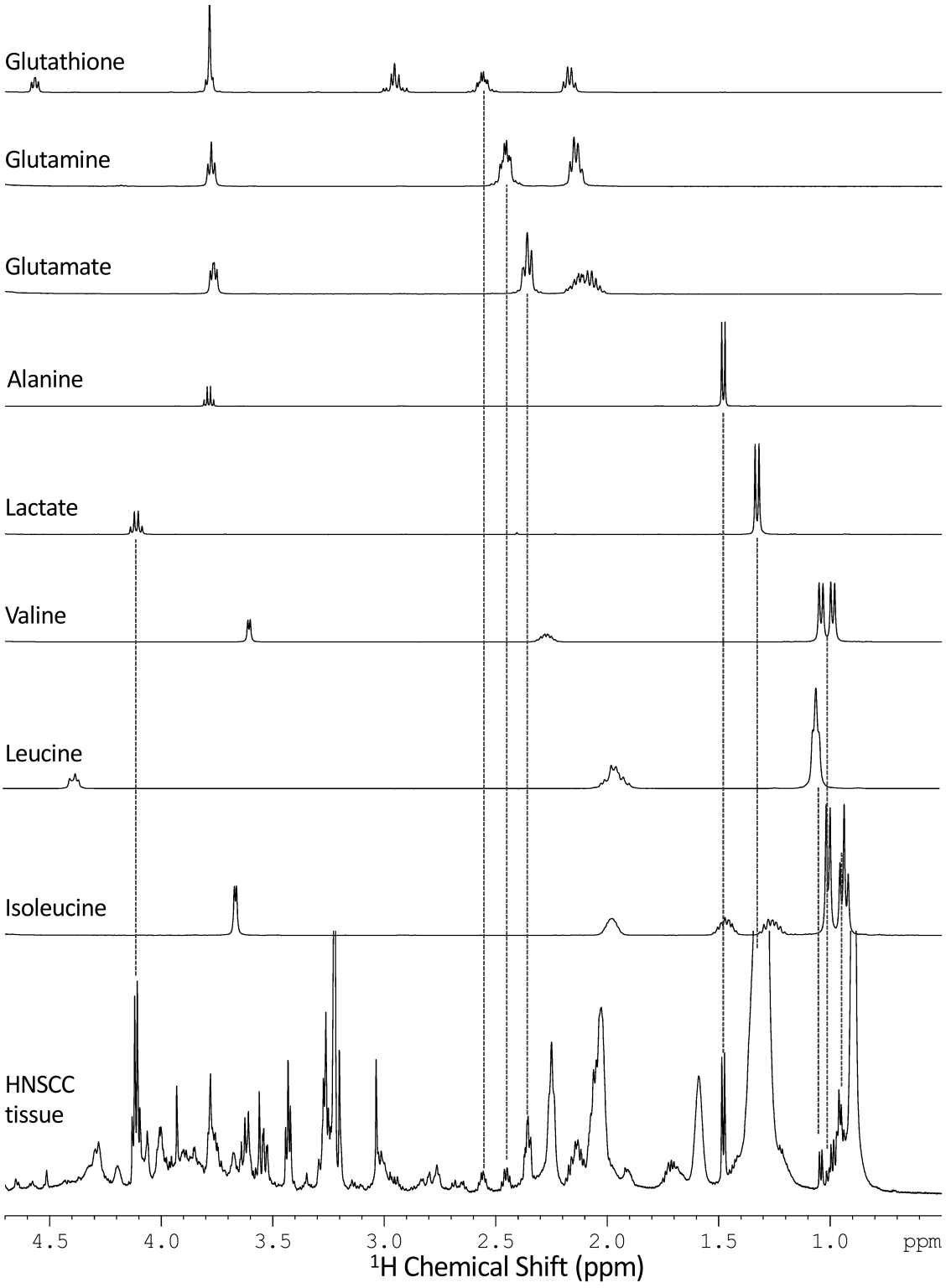

Figure S2. A comparison of NMR spectra of a tumor tissue with that of standard compounds to support the chemical shift assignments of aspartate, creatine, taurine, tyrosine and phenylalanine.

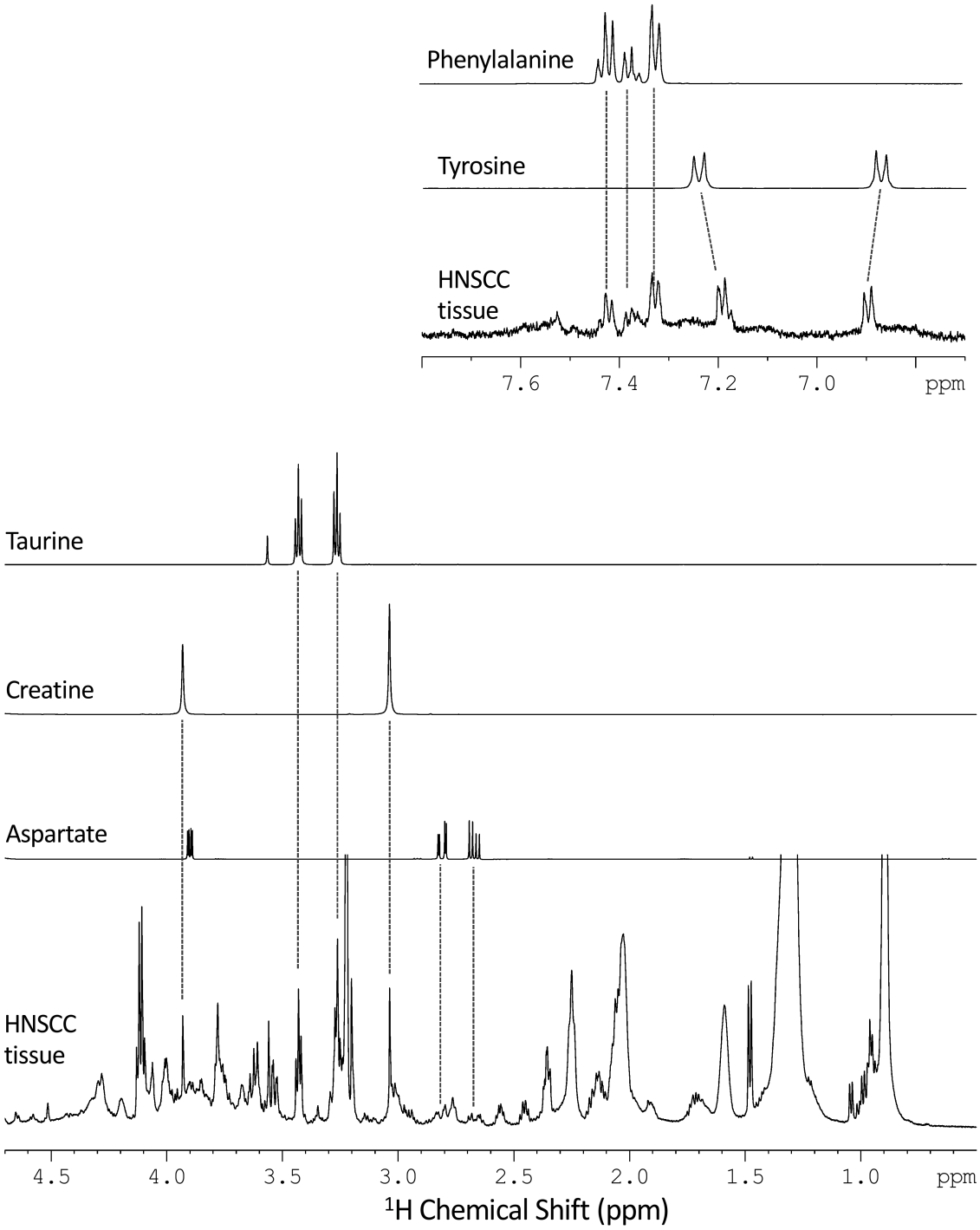

Figure S3. Average ^{1}H HR-MAS CPMG spectra obtained from area normalized spectra of (A) normal adjacent tissues (15 tissues), (B) tumor (18 tissues) and (C) lymph-node metastatic (7 tissues) tissues. The intensity of peaks in the chemical shift region 6.7 – 8.5 ppm was increased equally in all spectra to show the low-abundant taurine and phenylalanine. Triglyceride signals are marked as 'TG'.