

Supplemental Table 1. Canonical loadings of individual metabolites

Metabolite	Canonical Loading
Aspartate	-0.0813
Creatine	-0.629
Myo-inositol	-0.573
Lipid 13a	0.401
Taurine	-0.107

Canonical loadings, a measure of the importance of each metabolite in the classifier, reveals creatine, myo-inositol, and lipid 13a as the most influential metabolites in this classifier.

Supplemental Table 2. Comparing LOOCV classification to true molecular classification

		LOOCV Classification	
		Group 3 or Group 4	SHH
True Molecular Classification	Group 3 or Group 4	16	1
	SHH	2	10

Confusion matrix for the LDA classifier, based on LOOCV. The overall correct classification rate was $26/29 = 89.7\% \pm 5.6\%$, with sensitivity for identifying SHH tumors $10/11 = 90.9\% \pm 8.7\%$ and specificity $16/18 = 88.9\% \pm 7.4\%$.