

Table S3. Annotated metabolites associated with prediabetes risk in 143 overweight and obese adolescents from the SOLAR (discovery) cohort and 56 young adults from the CHS (validation) cohort. Metabolites were identified in the SOLAR cohort using LASSO regression and were independently validated in the CHS cohort. Annotation confidence is defined using the criteria of Schymanski et al. 2014 (40), where level 1 represents the confirmed structure and level 2 represents the probable structure based on diagnostic evidence.

Metabolite Name	m/z	Metabolite Class	Annotation Confidence	Direction of Association	
				SOLAR	CHS
Caprylic acid	125.0974	Medium-chain fatty acid	Level 1	+	+
Allylphenol sulfate	214.0261	Phenylsulfate/polyphenol	Level 2	-	-
Taurocholic acid	515.2873	Bile acid	Level 1	+	-