Appendix 1: Association of individual metabolite components of the urea cycle related factor* with CAD case status

Metabolite	Mean (SD)		Univariable analysis		Multivariable analysis**	
	Controls	Cases	OR (95% CI)	P	OR 95% CI	P
Citrulline	38.1 (14.5)	42.0 (14.9)	1.02 (1.01, 1.03)	0.0001	1.01 (1.00, 1.01)	0.18
Arginine	65.2 (19.6)	66.4 (20.4)	1.00 (1.00, 1.01)	0.26	1.00 (1.00, 1.01)	0.43
Histidine	58.9 (12.7)	59.7 (12.8)	1.01 (1.00, 1.01)	0.23	1.00 (0.99, 1.01)	0.88
Ci4-DC/C4-DC	0.07 (0.05)	0.08 (0.05)	63.51 (6.46, 624.66)	0.0001	7.79 (0.80, 75.63)	0.08

*Urea cycle factor from previous study by Shah et al.[29], with high factor loads for citrulline, arginine, histidine and Ci4-DC/C4-DC acylcarnitine.
**Adjusted for age, race, sex, diabetes, hypertension, smoking, dyslipidemia, family history of CAD, and BMI.

Appendix 2: Univariable and multivariable associations of PCA factors with number of diseased vessels

Factor	Name	Univariable		Multivariable*	
		β, SE	P value	β, SE	P value
1	Medium chain acylcarnitines	0.009, 0.02	0.67	-0.009, 0.02	0.70
2	Short chain dicarboxyl acylcarnitines	0.05, 0.02	0.01	0.02, 0.02	0.29
3	Long chain dicarboxyl acylcarnitines	0.07, 0.02	0.0005	0.03, 0.02	0.13
	Ketone related	0.03, 0.02	0.19	0.01, 0.02	0.53
5	Long chain acylcarnitines	0.03, 0.02	0.20	-0.005, 0.02	0.84
6	Branched chain amino acids & related metabolites	0.04, 0.02	0.05	-0.02, 0.02	0.39
7	**Short chain acylcarnitines**	**0.12, 0.02**	**<0.0001**	**0.08, 0.02**	**0.0003**
8	Amino acid factor	0.04, 0.02	0.05	0.03, 0.02	0.18
9	Medium chain acylcarnitines	0.06, 0.02	0.003	0.03, 0.02	0.15
10	**Branched chain amino acids & related metabolites**	**0.05, 0.02**	**0.02**	**0.05, 0.02**	**0.01**
11	Misc	-0.02, 0.02	0.24	0.005, 0.02	0.80
12	Non esterified fatty acids	0.03, 0.02	0.20	0.03, 0.02	0.25

*Adjusted for age, race, sex, diabetes, hypertension, smoking, dyslipidemia, family history of CAD, and BMI.