

BOX 3 | Analytical considerations

	Single metabolite tests		Unsupervised analyses			Supervised analyses		
	ANOVA	Linear models	PERMANOVA	WGCNA	ASCA	PLS-DA + VIP	SAM	ML
	DOODLES GO HERE							
How does concentration or composition change between treatments?	✓	✓						
How do compounds correlate with quantitative responses or time?			✓	✓	✓			✓
What compounds drive differences between treatments?						✓	✓	✓