

Table S4: The study identifiers from the 38 studies of the MetaboLights repository that were used for processing and analysis.

Study identifier	Experiments chosen for PCA	Experiments chosen for Pearson
MTBLS28		
MTBLS87		
MTBLS88		
MTBLS103		
MTBLS127		
MTBLS140		
MTBLS198		
MTBLS213		
MTBLS233		
MTBLS234		
MTBLS263	x	
MTBLS264	x	
MTBLS265	x	x
MTBLS266	x	x
MTBLS267	x	x
MTBLS277		
MTBLS307	x	
MTBLS315		
MTBLS321		
MTBLS354		
MTBLS401		
MTBLS404		
MTBLS413		
MTBLS414		
MTBLS417		
MTBLS423		
MTBLS449		
MTBLS473		
MTBLS476		
MTBLS549		
MTBLS558		
MTBLS620		
MTBLS721		
MTBLS729		
MTBLS739		
MTBLS749		
MTBLS842		
MTBLS916		