

Table 2: Summary of significant metabolite features changed when comparing low and high dose chemical exposure and metabolite Identification challenges

Chemical	Metabolite Features Changed¹	Database hits within mass error²
Chlorpromazine	392	152
Rifampicin	1551	352
Tamoxifen	303	97
Ritonavir	635	215
Sucrose	120	37
Potassium Chloride	166	35

1. A change is considered significant if p-value ≤ 0.05 and fold-change ≥ 1.5
2. An acceptable mass error was considered to be ≤ 10 ppm