Table S2 Comparison of plasma GCDCA-3G, GDCA-3G, CPI and CPIII performances in detecting different genetically-predicted OATP1B1 function groups versus normal function group (n=166)

OATP1B1 biomarker	Mean AUPRC (95% CI)	$F1_{max}$	Mean difference from GCDCA-3G (95% CI)	Mean AUROC (95% CI)	Difference from GCDCA-3G Mean (95% CI)	P value
Highly increased function (*n*=5), baseline AUPRC = 0.0292 and baseline AUROC = 0.5						
GCDCA-3G[*]	0.202 (0.0227, 0.692)	0.500	-	0.817 (0.751, 0.872)	-	-
GDCA-3G[*]	0.0526 (0.00109, 0.738)	0.162	-0.149 (-0.0251, -0.545)	0.641 (0.564, 0.713)	-0.177 (-0.0707, -0.282)	0.00110
CPI	0.210 (0.0300, 0.696)	0.545	0.00847 (-0.00951, 0.282)	0.720 (0.647, 0.786)	-0.0970 (0.128, -0.322)	0.398
CPIII	0.0509 (0.000995, 0.743)	0.200	-0.151 (-0.0288, -0.555)	0.564 (0.486, 0.639)	-0.254 (-0.0641, -0.443)	0.00870
Increased function (*n*=59), baseline AUPRC = 0.262 and baseline AUROC = 0.5						
GCDCA-3G[*]	0.351 (0.240, 0.480)	0.451	-	0.610 (0.543, 0.674)	-	-
GDCA-3G[*]	0.366 (0.253, 0.495)	0.473	0.0150 (-0.0440, 0.0411)	0.656 (0.590, 0.718)	0.0460 (0.0354, -0.128)	0.268
CPI	0.416 (0.298, 0.545)	0.428	0.0658 (0.0236, 0.124)	0.578 (0.511, 0.644)	-0.0317 (0.0637, -0.127)	0.515
CPIII	0.306 (0.203, 0.434)	0.417	-0.0443 (-0.00538, -0.0676)	0.531 (0.464, 0.598)	-0.0789 (0.0172, -0.175)	0.108
Decreased function (*n*=113), baseline AUPRC = 0.405 and baseline AUROC = 0.5						
GCDCA-3G[*]	0.568 (0.475, 0.656)	0.601	-	0.626 (0.567, 0.683)	-	-
GDCA-3G[*]	0.532 (0.440, 0.621)	0.593	-0.0361 (-0.0129, -0.0628)	0.627 (0.567, 0.684)	0.0004 (-0.0676, 0.0684)	0.991
CPI	0.489 (0.398, 0.581)	0.577	-0.0785 (-0.0564, -0.109)	0.560 (0.500, 0.619)	-0.0663 (0.00807, -0.141)	0.0806
CPIII	0.451 (0.362, 0.543)	0.579	-0.117 (0.00549, -0.244)	0.528 (0.467, 0.588)	-0.0986 (0.0138, -0.211)	0.0854
Poor function (*n*=13), baseline AUPRC = 0.0726 and baseline AUROC = 0.5						
GCDCA-3G[*]	0.961 (0.597, 0.998)	0.897	-	0.997 (0.973, 1.000)	-	-
GDCA-3G[*]	0.717 (0.431, 0.894)	0.720	-0.245 (-0.0753, -0.426)	0.878 (0.821, 0.922)	-0.119 (0.0224, -0.260)	0.0993
CPI	0.612 (0.341, 0.828)	0.571	-0.350 (-0.161, -0.555)	0.895 (0.841, 0.936)	-0.101 (0.00877, -0.212)	0.0712
CPIII	0.150 (0.0370, 0.447)	0.267	-0.812 (-0.678, -0.877)	0.718 (0.646, 0.783)	-0.279 (-0.148, -0.410)	<0.0001

CPI and CPIII data are adjusted for sex, body weight and clinical trial. GCDCA-3G and GDCA-3G data are adjusted for sex. Phenotypes classified by *SLCO1B1* allele pairs: highly increased function phenotype, two increased function (*14* or *20*) alleles; increased function phenotype, one normal function (*1* or *37*) allele with one increased function allele; normal function phenotype, two normal function alleles; decreased function phenotype, one normal function allele or one increased function allele with one decreased function (*5* or *15*) allele; poor function phenotype, two decreased function alleles; AUPRC, area under precision-recall curve; AUROC, area under receiver operating characteristic curve; CI, confidence interval; CPI, coproporphyrin I; CPIII, coproporphyrin III; GCDCA-3G, glycochenodeoxycholate 3-O-glucuronide; GDCA-3G, glycodeoxycholate 3-O-glucuronide; OATP1B1, organic anion transporting polypeptide 1B1. $F1_{max}$ represents the maximum harmonic mean of the precision and recall over all measurement levels.

[*]These data were reanalyzed from a previously published study (Neuvonen, M. *et al*. *Clin. Pharmacol. Ther.* **109**, 646-657 (2021).