

# Supporting Information for “The Objective Function Controversy for Group Testing: Much Ado About Nothing?”

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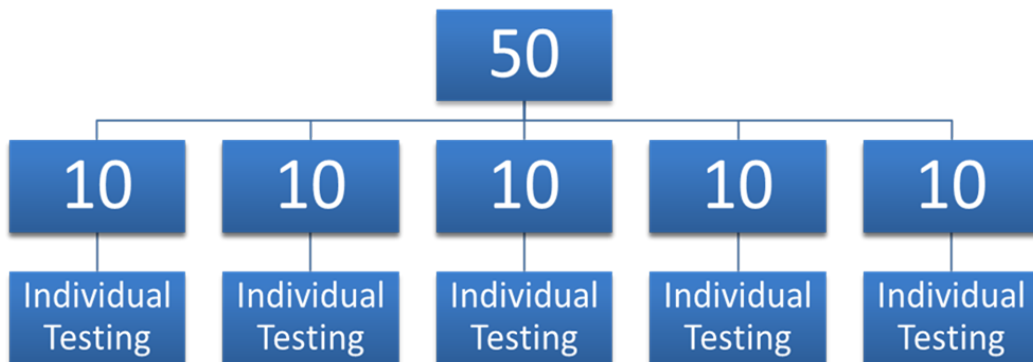


Figure S1: Diagram of the three-stage hierarchical testing algorithm used for HIV testing in San Francisco.

## S1. Notation for Section 2

In Section 2, we provided the following expression for the expected number of tests for three-stage hierarchical testing:

$$E(T) = 1 + m_{11}P(G_{11} = 1) + \sum_{j=1}^{c_2} m_{2j}P(G_{11} = 1, G_{2j} = 1).$$

To help explain the expression's notation, Figure S1 provides a visual representation of this type of algorithm as it is used for HIV testing in San Francisco[1]. The binary random variable  $G_{sj}$  indicates the positive (1) or negative (0) outcome for group  $j$  at stage  $s$ . For the initial group of 50 individuals in the first stage of Figure S1, there will be a single group testing result for  $G_{11}$ . When  $G_{11} = 1$ ,  $c_2 = 5$  subgroups of size  $m_{11} = 10$  are formed for a second stage of testing. These five subgroups have binary testing outcomes of  $G_{21}$ ,  $G_{22}$ ,  $G_{23}$ ,  $G_{24}$ , and  $G_{25}$ . If  $G_{2j} = 1$  for some subgroup  $j = 1, \dots, 5$ ,  $m_{2j} = 10$  individual tests are performed in the third and final stage of testing.

## S2. Additional results for Section 3.1

We provide additional results to coincide with our investigations in Section 3.1. Overall, these additional results continue to show that the OTCs have the same or very similar operating characteristics when using either objective function. We also include in our summaries the pooling positive predictive value,  $PPPV$ , and the pooling negative predictive value,  $PNPV$ , as additional accuracy measures. The pooling positive (negative) predictive value is the probability that an individual who is determined to be positive (negative) by the testing algorithm is truly positive (negative). Predictive values simply provide an alternative way of looking at accuracy in comparison to the pooling sensitivity and pooling specificity. Expressions for all accuracy measures are available in Kim et al[2], McMahan et al[3, 4], and Black et al[5].

Table 1 in the paper provides a summary of the optimal testing configurations (OTCs) and their operating characteristics when  $p = 0.01$ . This table is reproduced here as Table S1 with the addition of the predictive values. Similar tables for  $p = 0.05$  and  $p = 0.10$  are shown in Tables S2 and S3, respectively. The largest differences between operating characteristics for OTCs are shown in Table 2 of the main paper. Table S4 displays the same results with the addition of the predictive values.

## S3. Additional results for Section 3.2

### S3.1. Tables

We provide additional results to coincide with our investigations in Section 3.2. Once again, these additional results show that the same or very similar operating characteristics are obtained regardless of which objective function is used. Table S5 displays the same results as Table 3 in the paper but with the addition of the predictive values.

Similar tables for  $E(P_i) = 0.05$  and  $E(P_i) = 0.10$  are provided in Tables S6 and S7, respectively. Table S8 displays the same findings as Table 4 in the paper but with the addition of the predictive values.

Because informative group testing results in potentially different accuracy measures for each individual tested, we formed weighted averages across all individuals tested to present one overall value for each accuracy measure. These weighted averages are developed from accuracy definitions given by Altman and Bland[6, 7] and were used by Black et al[5]. The pooling sensitivity is defined as

$$PS_e^W = \frac{\sum_i p_i PS_{e,i}}{\sum_i p_i}, \quad (1)$$

and the pooling specificity is defined as

$$PS_p^W = \frac{\sum_i (1 - p_i) PS_{p,i}}{\sum_i (1 - p_i)}. \quad (2)$$

Similarly, the pooling positive predictive value is defined as

$$PPPV^W = \frac{\sum_i p_i PS_{e,i}}{\sum_i p_i PS_{e,i} + (1 - p_i)(1 - PS_{p,i})}, \quad (3)$$

and the pooling negative predictive value is defined as

$$PNPV^W = \frac{\sum_i (1 - p_i) PS_{p,i}}{\sum_i (1 - p_i) PS_{p,i} + p_i(1 - PS_{e,i})}. \quad (4)$$

Expressions (1) through (4) represent weighted averages over all  $I$  individuals within the initial group for a hierarchical algorithm or all  $I^2$  individuals within the array for an array testing algorithm.

### S3.2. OTCs for informative group testing

Due to the lack of available space, Tables S5, S6, and S7 display at most only the initial (stage 1) group size for the informative hierarchical algorithms. We display their full algorithms in Tables S9 - S14. Define  $I_{s,j}$  as the size of group  $j$  at stage  $s$ . For two-stage hierarchical testing, individuals are assembled into blocks[3], where we use a block size of 50. Thus, we have  $\sum_j I_{1j} = 50$  by design.

To better understand the displayed OTCs in the tables, consider the OTC given in the first row of results in Table S12. The algorithm is performed over  $S = 3$  stages with an initial group size of  $I_{11} = 10$  individuals. If this initial group tests positively, four new groups are formed for the second stage of testing with sizes  $I_{21} = 4$ ,  $I_{22} = 3$ ,  $I_{23} = 2$ , and  $I_{24} = 1$ . Informative group testing always orders individuals by their probabilities of positivity. Therefore, the first group consists of the individuals with the four smallest probabilities, and the last group consists of the individual with the largest probability. If any of these groups test positively and has a size greater than 1, individual testing is performed upon its group members. For the first group in stage 2, this means that individual tests would be performed on each of its members in stage 3 ( $I_{31} = I_{32} = I_{33} = I_{34} = 1$ ). For the last group in stage 2, no subsequent retesting would be performed. Figure S2 provides a pictorial representation of this group testing algorithm.

## S4. Additional results for Section 4

We provide additional results to coincide with our investigations in Section 4. Tables S15 and S16 display the same results as Tables 5 and 6 in the paper, respectively, but with the addition of the predictive values. Due to the lack of available space, Table S16 displays at most only the initial (stage 1) group size for the informative hierarchical algorithms. We display their full algorithms in Tables S17 and S18.

## S5. Additional results for Section 5

Graff and Roeloffs[8] proposed an objective function that is a linear combination of the expected number of tests, the number of misclassified negative individuals ( $FN_1$ ), and the number of misclassified positive individuals ( $FP_1$ ). This linear combination can be expressed as

$$E(T) + D_1 \times FN_1 + D_2 \times FP_1 = E(T) + \sum_{i=1}^I \{D_1(1 - PS_{p,i})(1 - p_i) + D_2(1 - PS_{e,i})p_i\},$$

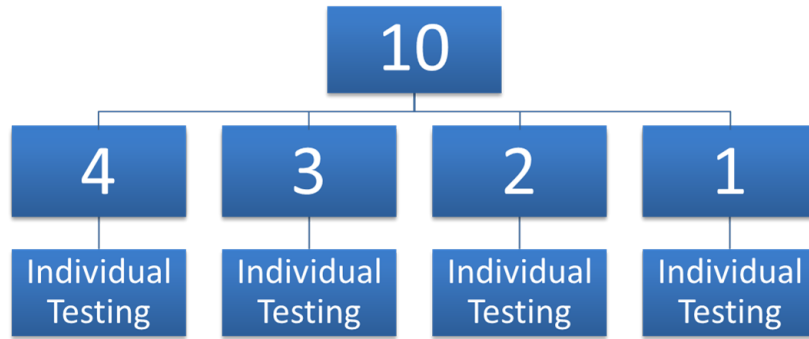


Figure S2: Diagram of the group testing algorithm described in Section S3.2. Group sizes are provided within nodes.

where  $D_1$  and  $D_2$  are subjectively chosen weights. The OTC is found by minimizing the value of this linear combination per individual, denoted by  $O_{GR}$ . Because weights are subjectively chosen, there will be weights that result in an OTC different than what is obtained by using  $O_{ET}$  or  $O_{MAR}$ . We provide results in Tables S19 and S20 to illustrate these differences. Overall, the value of  $D_1$  has a larger effect than the value of  $D_2$ , because there are many more individuals who are truly negative than positive due to the small probability of being positive.

## S6. R examples

To reproduce the research in this paper, we make available a set of R functions in the `binGroup` package that

- Calculate  $E(T)$  and associated accuracy measures for different objective functions, and
- Find the OTC over a wide variety of settings.

All calculations for the paper were performed in version 3.4.1 of R[9].

The examples provided next show how to use `binGroup` to reproduce results from Tables 1 and 3. Examples 1 and 2 use non-informative group testing with an overall disease prevalence of  $p = 0.01$ . Examples 3 and 4 use informative group testing with an overall disease prevalence of  $E(P_i) = 0.01$ . Estimated running times for each example were calculated using a computer with 16 GB of RAM and one core of an Intel i7-6500U processor.

```

> library(binGroup)
> #####
> # Example 1
> # Finding the OTC using non-informative
> # three-stage hierarchical testing, where
> # p denotes the overall prevalence of disease,
> # Se denotes the sensitivity of the diagnostic test,
> # Sp denotes the specificity of the diagnostic test,
> # group.sz denotes the range of initial pool sizes for consideration, and
> # obj.fn specifies the objective functions for which to find results.
> # This example takes approximately 2.5 minutes to run.
> results1 <- OTC(algorithm="D3", p=0.01, Se=0.99, Sp=0.99, group.sz=3:40,
+               obj.fn=c("ET", "MAR"))
You have specified an overall probability of disease.
A probability vector will be generated based on the algorithm specified.
Algorithm: Non-informative three-stage hierarchical testing
Initial Group Size = 3
Initial Group Size = 4
Initial Group Size = 5
<OUTPUT EDITED>
Initial Group Size = 38
Initial Group Size = 39
Initial Group Size = 40
Number of minutes running: 2.429667
> # Print the results.

```

```

> data.frame("Obj.Fn"=c("O_ET", "O_MAR"),
             "OTC"=c(paste(results1$opt.ET$OTC$Stage1,
                           results1$opt.ET$OTC$Stage2[1], 1, sep="-"),
                     paste(results1$opt.MAR$OTC$Stage1,
                           results1$opt.MAR$OTC$Stage2[1], 1, sep="-")),
             "ET.I"=c(round(results1$opt.ET$ET/results1$opt.ET$OTC$Stage1, 4),
                       round(results1$opt.MAR$ET/results1$opt.MAR$OTC$Stage1, 4)),
             "PSe"=c(round(results1$opt.ET$PSe, 4),
                     round(results1$opt.MAR$PSe, 4)),
             "PSp"=c(round(results1$opt.ET$PSp, 4),
                     round(results1$opt.MAR$PSp, 4)))
  Obj.Fn    OTC    ET.I    PSe    PSp
1  O_ET 25-5-1 0.1354 0.9703 0.9996
2  O_MAR 25-5-1 0.1354 0.9703 0.9996

> #####
> # Example 2
> # Finding the OTC using non-informative
> # array testing with master pooling.
> # The OTC differs for the ET and MAR objective functions in this example.

> # This example takes approximately 2 minutes to run.
> results2 <- OTC(algorithm="A2M", p=0.01, Se=0.90, Sp=0.90, group.sz=3:30,
                 obj.fn=c("ET", "MAR"))
You have specified an overall probability of disease.
A probability vector will be generated based on the algorithm specified.
Algorithm: Non-informative square array testing with master pooling
Row/Column Size = 3, Array Size = 9
Row/Column Size = 4, Array Size = 16
Row/Column Size = 5, Array Size = 25

<OUTPUT EDITED>

Row/Column Size = 28, Array Size = 784
Row/Column Size = 29, Array Size = 841
Row/Column Size = 30, Array Size = 900
Number of minutes running: 1.745667

> # Print the results.
> data.frame("Obj.Fn"=c("O_ET", "O_MAR"),
             "OTC"=c(paste(results2$opt.ET$OTC$Array.sz,
                           results2$opt.ET$OTC$Array.dim, 1, sep="-"),
                     paste(results2$opt.MAR$OTC$Array.sz,
                           results2$opt.MAR$OTC$Array.dim, 1, sep="-")),
             "ET.I"=c(round(results2$opt.ET$ET/results2$opt.ET$OTC$Array.sz, 4),
                       round(results2$opt.MAR$ET/results2$opt.MAR$OTC$Array.sz, 4)),
             "PSe"=c(round(results2$opt.ET$PSe, 4),
                     round(results2$opt.MAR$PSe, 4)),
             "PSp"=c(round(results2$opt.ET$PSp, 4),
                     round(results2$opt.MAR$PSp, 4)))
  Obj.Fn    OTC    ET.I    PSe    PSp
1  O_ET 625-25-1 0.145 0.6562 0.9934
2  O_MAR 576-24-1 0.145 0.6562 0.9937

> #####
> # Example 3
> # Finding the OTC using informative two-stage
> # hierarchical testing, implemented via the pool-specific optimal Dorfman
> # (PSOD) method described in McMahan et al. (2012), where
> # alpha denotes the level of heterogeneity in the beta distribution
> # used to generate the vector of individual probabilities.

> # Depending on the specified probability, level of heterogeneity,
> # and initial group size, simulation may be necessary in order
> # to generate an ordered vector of individual probabilities. This
> # is done with the beta.dist() function (see Black et al. 2015)
> # using 10,000 simulated data sets.
> # The user will need to set a seed in order to reproduce results.

> # This examples takes approximately 2.5 minutes to run.
> set.seed(1002)
> results3 <- OTC(algorithm="ID2", p=0.01, Se=0.95, Sp=0.95, group.sz=50,
                 obj.fn=c("ET", "MAR"), alpha=2)
You have specified an overall probability of disease.
A probability vector will be generated based on the algorithm specified.
A single group size was provided. The optimal testing configuration will be found
over all possible testing configurations for the specified group size.
NOTE: You have specified a maximum group size of 50 or larger.
This function may take a VERY long time to run.
Press 'ESC' if you wish to cancel the submitted statements.
Algorithm: Informative Dorfman testing

```

```

[1] "Using simulation"
Block Size = 50
[1] "Using simulation"
[1] "Using simulation"
Number of minutes running: 2.617833

> # Print the results.
> data.frame("Obj.Fn"=c("O_ET", "O_MAR"),
             "OTC"=c(results3$opt.ET$OTC$Block.sz,
                    results3$opt.MAR$OTC$Block.sz),
             "ET.I"=c(round(results3$opt.ET$ET/results3$opt.ET$OTC$Block.sz, 4),
                    round(results3$opt.MAR$ET/results3$opt.MAR$OTC$Block.sz, 4)),
             "PSe"=c(round(results3$opt.ET$PSe, 4),
                    round(results3$opt.MAR$PSe, 4)),
             "PSP"=c(round(results3$opt.ET$PSP, 4),
                    round(results3$opt.MAR$PSP, 4)))
  Obj.Fn OTC  ET.I  PSe  PSP
1  O_ET  50  0.2264  0.9025  0.9931
2  O_MAR  50  0.2264  0.9025  0.9931

> # Second-stage of OTCs
> results3$opt.ET$OTC$pool.szs
[1] 18 13 11 8
> results3$opt.MAR$OTC$pool.szs
[1] 18 13 11 8

> #####
> # Example 4
> # Finding the OTC using non-informative two-stage hierarchical testing

> # This example takes approximately 2.5 minutes to run.
> set.seed(1002)
> results4 <- OTC(algorithm="ID3", p=0.01, Se=0.95, Sp=0.95, group.sz=3:40,
                obj.fn=c("ET", "MAR"), alpha=0.5)
You have specified an overall probability of disease.
A probability vector will be generated based on the algorithm specified.
Algorithm: Informative three-stage hierarchical testing
Initial Group Size = 3
Initial Group Size = 4
Initial Group Size = 5
<OUTPUT EDITED>
Initial Group Size = 38
Initial Group Size = 39
Initial Group Size = 40
Number of minutes running: 2.614333

> # Print the results.
> data.frame("Obj.Fn"=c("O_ET", "O_MAR"),
             "OTC"=c(results4$opt.ET$OTC$Stage1,
                    results4$opt.MAR$OTC$Stage1),
             "ET.I"=c(round(results4$opt.ET$ET/results4$opt.ET$OTC$Stage1, 4),
                    round(results4$opt.MAR$ET/results4$opt.MAR$OTC$Stage1, 4)),
             "PSe"=c(round(results4$opt.ET$PSe, 4),
                    round(results4$opt.MAR$PSe, 4)),
             "PSP"=c(round(results4$opt.ET$PSP, 4),
                    round(results4$opt.MAR$PSP, 4)))
  Obj.Fn OTC  ET.I  PSe  PSP
1  O_ET  28  0.1291  0.8574  0.9977
2  O_MAR  28  0.1291  0.8574  0.9977

```

The next example shows how to use `binGroup` to reproduce results from Table S19.

```

> #####
> # Example 5
> # Finding the OTC using two-stage hierarchical testing with O_GR

> # This example takes less than 1 second to run.
> results5 <- OTC(algorithm="D2", p=0.01, Se=0.99, Sp=0.99, group.sz=3:40,
                obj.fn="GR", weights=matrix(data=c(1, 1, 1000, 1000), nrow=2, ncol=2,
                byrow=TRUE))
You have specified an overall probability of disease.
A probability vector will be generated based on the algorithm specified.
Algorithm: Non-informative two-stage hierarchical (Dorfman) testing

Initial Group Size = 3
Initial Group Size = 4
Initial Group Size = 5

```

```

<OUTPUT EDITED>
Initial Group Size = 38
Initial Group Size = 39
Initial Group Size = 40
Number of minutes running: 0.0001666667

> names(results5)
[1] "prob"      "Se"        "Sp"        "opt.ET"    "opt.GR1"   "opt.GR2"   "Configs"

> data.frame("Obj.Fn"=c("0_GR", "0_GR"),
  "OTC"=c(paste(results5$opt.GR1$OTC$Stage1, 1, sep="-"),
  paste(results5$opt.GR2$OTC$Stage1, 1, sep="-")),
  "ET.I"=c(round(results5$opt.GR1$ET / results5$opt.GR1$OTC$Stage1, 4),
  round(results5$opt.GR2$ET / results5$opt.GR2$OTC$Stage1, 4)),
  "PSe"=c(round(results5$opt.GR1$PSe, 4), round(results5$opt.GR2$PSe, 4)),
  "PSp"=c(round(results5$opt.GR1$PSp, 4), round(results5$opt.GR2$PSp, 4)))
  Obj.Fn OTC   ET.I   PSe   PSp
1  0_GR  11-1  0.2035  0.9801  0.9990
2  0_GR   3-1  0.3724  0.9801  0.9997

```

## References

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Table S1: OTC summary for  $p = 0.01$  under non-informative group testing. Equally sized groups are optimal at each stage; thus, an OTC of “24-6-1” means that stage 1 has a group of size 24, stage 2 has four groups of size 6, and stage 3 has twenty-four groups of size 1. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

Algorithm			Objective							
	$S_e$	$S_p$	function	OTC	$E(T)/I$	$PS_e$	$PS_p$	PPPV	PNPV	
Two-stage hierarchical	0.99	0.99	$O_{ET}$	11-1	0.2035	0.9801	0.9990	0.9052	0.9998	
			$O_{MAR}$	11-1	0.2035	0.9801	0.9990	0.9052	0.9998	
	0.95	0.95	$O_{ET}$	11-1	0.2351	0.9025	0.9932	0.5727	0.9990	
			$O_{MAR}$	11-1	0.2351	0.9025	0.9932	0.5727	0.9990	
	0.90	0.90	$O_{ET}$	12-1	0.2742	0.8100	0.9816	0.3081	0.9980	
			$O_{MAR}$	12-1	0.2742	0.8100	0.9816	0.3081	0.9980	
	0.99	0.90	$O_{ET}$	11-1	0.2841	0.9801	0.9815	0.3485	0.9998	
			$O_{MAR}$	11-1	0.2841	0.9801	0.9815	0.3485	0.9998	
	0.90	0.99	$O_{ET}$	11-1	0.1941	0.8100	0.9990	0.8959	0.9981	
			$O_{MAR}$	11-1	0.1941	0.8100	0.9990	0.8959	0.9981	
	Three-stage hierarchical	0.99	0.99	$O_{ET}$	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
				$O_{MAR}$	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
0.95		0.95	$O_{ET}$	24-6-1	0.1443	0.8574	0.9973	0.7634	0.9986	
			$O_{MAR}$	24-6-1	0.1443	0.8574	0.9973	0.7634	0.9986	
0.90		0.90	$O_{ET}$	24-6-1	0.1562	0.7290	0.9938	0.5437	0.9973	
			$O_{MAR}$	24-6-1	0.1562	0.7290	0.9938	0.5437	0.9973	
0.99		0.90	$O_{ET}$	24-6-1	0.1708	0.9703	0.9928	0.5780	0.9997	
			$O_{MAR}$	24-6-1	0.1708	0.9703	0.9928	0.5780	0.9997	
0.90		0.99	$O_{ET}$	25-5-1	0.1229	0.7290	0.9997	0.9564	0.9973	
			$O_{MAR}$	25-5-1	0.1229	0.7290	0.9997	0.9564	0.9973	
Array w/o master pooling		0.99	0.99	$O_{ET}$	25-1	0.1378	0.9703	0.9995	0.9529	0.9997
				$O_{MAR}$	25-1	0.1378	0.9703	0.9995	0.9529	0.9997
	0.95	0.95	$O_{ET}$	25-1	0.1475	0.8575	0.9970	0.7456	0.9986	
			$O_{MAR}$	24-1	0.1475	0.8575	0.9972	0.7566	0.9986	
	0.90	0.90	$O_{ET}$	25-1	0.1611	0.7291	0.9926	0.4996	0.9973	
			$O_{MAR}$	24-1	0.1611	0.7291	0.9930	0.5112	0.9973	
	0.99	0.90	$O_{ET}$	23-1	0.1726	0.9703	0.9923	0.5614	0.9997	
			$O_{MAR}$	23-1	0.1726	0.9703	0.9923	0.5614	0.9997	
	0.90	0.99	$O_{ET}$	27-1	0.1279	0.7292	0.9995	0.9410	0.9973	
			$O_{MAR}$	27-1	0.1279	0.7292	0/9995	0.9410	0.9973	
	Array w/ master pooling	0.99	0.99	$O_{ET}$	625-25-1	0.1364	0.9606	0.9995	0.9529	0.9996
				$O_{MAR}$	625-25-1	0.1364	0.9606	0.9995	0.9529	0.9996
0.95		0.95	$O_{ET}$	625-25-1	0.1402	0.8146	0.9972	0.7458	0.9981	
			$O_{MAR}$	576-24-1	0.1402	0.8146	0.9974	0.7569	0.9981	
0.90		0.90	$O_{ET}$	625-25-1	0.1450	0.6562	0.9934	0.4997	0.9965	
			$O_{MAR}$	576-24-1	0.1450	0.6562	0.9937	0.5115	0.9965	
0.99		0.90	$O_{ET}$	529-23-1	0.1708	0.9606	0.9924	0.5618	0.9996	
			$O_{MAR}$	529-23-1	0.1708	0.9606	0.9924	0.5618	0.9996	
0.90		0.99	$O_{ET}$	729-27-1	0.1151	0.6563	0.9996	0.9410	0.9965	
			$O_{MAR}$	729-27-1	0.1151	0.6563	0.9996	0.9410	0.9965	

Table S2: OTC summary for  $p = 0.05$  under non-informative group testing. Equally sized groups are optimal at each stage; thus, a “24-6-1” means that stage 1 has a group of size 24, stage 2 has four groups of size 6, and stage 3 has twenty-four groups of size 1. There are no differences between the OTCs.

Algorithm	$S_e$ $S_p$		Objective							
			function	OTC	$E(T)/I$	$PS_e$	$PS_p$	PPPV	PNPV	
Two-stage hierarchical	0.99	0.99	$O_{ET}$	5-1	0.4317	0.9801	0.9981	0.9642	0.9990	
			$O_{MAR}$	5-1	0.4317	0.9801	0.9981	0.9642	0.9990	
	0.95	0.95	$O_{ET}$	5-1	0.4536	0.9025	0.9892	0.8141	0.9948	
			$O_{MAR}$	5-1	0.4536	0.9025	0.9892	0.8141	0.9948	
	0.90	0.90	$O_{ET}$	6-1	0.4786	0.8100	0.9719	0.6027	0.9898	
			$O_{MAR}$	6-1	0.4786	0.8100	0.9719	0.6027	0.9898	
	0.99	0.90	$O_{ET}$	5-1	0.5013	0.9801	0.9735	0.6605	0.9989	
			$O_{MAR}$	5-1	0.5013	0.9801	0.9735	0.6605	0.9989	
	0.90	0.99	$O_{ET}$	5-1	0.4113	0.8100	0.9982	0.9605	0.9901	
			$O_{MAR}$	5-1	0.4113	0.8100	0.9982	0.9605	0.9901	
	Three-stage hierarchical	0.99	0.99	$O_{ET}$	9-3-1	0.3773	0.9703	0.9990	0.9812	0.9984
				$O_{MAR}$	9-3-1	0.3773	0.9703	0.9990	0.9812	0.9984
0.95		0.95	$O_{ET}$	9-3-1	0.3798	0.8574	0.9950	0.8993	0.9925	
			$O_{MAR}$	9-3-1	0.3798	0.8574	0.9950	0.8993	0.9925	
0.90		0.90	$O_{ET}$	12-4-1	0.3806	0.7290	0.9853	0.7227	0.9857	
			$O_{MAR}$	12-4-1	0.3806	0.7290	0.9853	0.7227	0.9857	
0.99		0.90	$O_{ET}$	9-3-1	0.4227	0.9703	0.9874	0.8023	0.9984	
			$O_{MAR}$	9-3-1	0.4227	0.9703	0.9874	0.8023	0.9984	
0.90		0.99	$O_{ET}$	12-4-1	0.3409	0.7290	0.9988	0.9701	0.9859	
			$O_{MAR}$	12-4-1	0.3409	0.7290	0.9988	0.9701	0.9859	
Array w/o master pooling		0.99	0.99	$O_{ET}$	10-1	0.3809	0.9705	0.9986	0.9735	0.9984
				$O_{MAR}$	10-1	0.3809	0.9705	0.9986	0.9735	0.9984
	0.95	0.95	$O_{ET}$	10-1	0.3852	0.8581	0.9926	0.8597	0.9925	
			$O_{MAR}$	10-1	0.3852	0.8581	0.9926	0.8597	0.9925	
	0.90	0.90	$O_{ET}$	10-1	0.3907	0.7302	0.9842	0.7086	0.9858	
			$O_{MAR}$	10-1	0.3907	0.7302	0.9842	0.7086	0.9858	
	0.99	0.90	$O_{ET}$	9-1	0.4243	0.9705	0.9839	0.7602	0.9984	
			$O_{MAR}$	9-1	0.4243	0.9705	0.9839	0.7602	0.9984	
	0.90	0.99	$O_{ET}$	11-1	0.3511	0.7301	0.9986	0.9659	0.9860	
			$O_{MAR}$	11-1	0.3511	0.7301	0.9986	0.9659	0.9860	
	Array w/ master pooling	0.99	0.99	$O_{ET}$	100-10-1	0.3772	0.9608	0.9986	0.9736	0.9979
				$O_{MAR}$	100-10-1	0.3772	0.9608	0.9986	0.9736	0.9979
0.95		0.95	$O_{ET}$	100-10-1	0.3660	0.8152	0.9930	0.8600	0.9903	
			$O_{MAR}$	100-10-1	0.3660	0.8152	0.9930	0.8600	0.9903	
0.90		0.90	$O_{ET}$	100-10-1	0.3517	0.6572	0.9858	0.7091	0.9820	
			$O_{MAR}$	100-10-1	0.3517	0.6572	0.9858	0.7091	0.9820	
0.99		0.90	$O_{ET}$	81-9-1	0.4201	0.9608	0.9842	0.7617	0.9979	
			$O_{MAR}$	81-9-1	0.4201	0.9608	0.9842	0.7617	0.9979	
0.90		0.99	$O_{ET}$	121-11-1	0.3160	0.6571	0.9988	0.9660	0.9823	
			$O_{MAR}$	121-11-1	0.3160	0.6571	0.9988	0.9660	0.9823	

Table S3: OTC summary for  $p = 0.10$  under non-informative group testing. Equally sized groups are optimal at each stage; thus, a “24-6-1” means that stage 1 has a group of size 24, stage 2 has four groups of size 6, and stage 3 has twenty-four groups of size 1. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

Algorithm	$S_e$	$S_p$	Objective		OTC	$E(T)/I$	$PS_e$	$PS_p$	PPPV	PNPV
			function							
Two-stage hierarchical	0.99	0.99	$O_{ET}$	4-1	0.5970	0.9801	0.9972	0.9753	0.9978	
			$O_{MAR}$	4-1	0.5970	0.9801	0.9972	0.9753	0.9978	
	0.95	0.95	$O_{ET}$	4-1	0.6095	0.9025	0.9853	0.8722	0.9891	
			$O_{MAR}$	4-1	0.6095	0.9025	0.9853	0.8722	0.9891	
	0.90	0.90	$O_{ET}$	4-1	0.6251	0.8100	0.9683	0.7396	0.9787	
			$O_{MAR}$	4-1	0.6251	0.8100	0.9683	0.7396	0.9787	
	0.99	0.90	$O_{ET}$	4-1	0.6561	0.9801	0.9659	0.7614	0.9977	
			$O_{MAR}$	4-1	0.6561	0.9801	0.9659	0.7614	0.9977	
	0.90	0.99	$O_{ET}$	4-1	0.5661	0.8100	0.9975	0.9728	0.9793	
			$O_{MAR}$	4-1	0.5661	0.8100	0.9975	0.9728	0.9793	
	Three-stage hierarchical	0.99	0.99	$O_{ET}$	9-3-1	0.5836	0.9703	0.9981	0.9827	0.9967
				$O_{MAR}$	9-3-1	0.5836	0.9703	0.9981	0.9827	0.9967
0.95		0.95	$O_{ET}$	9-3-1	0.5733	0.8574	0.9905	0.9091	0.9843	
			$O_{MAR}$	9-3-1	0.5733	0.8574	0.9905	0.9091	0.9843	
0.90		0.90	$O_{ET}$	9-3-1	0.5619	0.7290	0.9808	0.8081	0.9702	
			$O_{MAR}$	9-3-1	0.5619	0.7290	0.9808	0.8081	0.9702	
0.99		0.90	$O_{ET}$	9-3-1	0.6295	0.9703	0.9772	0.8254	0.9966	
			$O_{MAR}$	6-3-1	0.6295	0.9703	0.9786	0.8345	0.9966	
0.90		0.99	$O_{ET}$	9-3-1	0.5188	0.7290	0.9984	0.9809	0.9707	
			$O_{MAR}$	9-3-1	0.5188	0.7290	0.9984	0.9809	0.9707	
Array w/o master pooling		0.99	0.99	$O_{ET}$	7-1	0.5821	0.9705	0.9978	0.9800	0.9967
				$O_{MAR}$	7-1	0.5821	0.9705	0.9978	0.9800	0.9967
	0.95	0.95	$O_{ET}$	7-1	0.5776	0.8585	0.9888	0.8950	0.9843	
			$O_{MAR}$	7-1	0.5776	0.8585	0.9888	0.8950	0.9843	
	0.90	0.90	$O_{ET}$	7-1	0.5722	0.7310	0.9772	0.7808	0.9703	
			$O_{MAR}$	7-1	0.5722	0.7310	0.9772	0.7808	0.9703	
	0.99	0.90	$O_{ET}$	7-1	0.6250	0.9704	0.9732	0.8009	0.9966	
			$O_{MAR}$	7-1	0.6250	0.9704	0.9732	0.8009	0.9966	
	0.90	0.99	$O_{ET}$	7-1	0.5335	0.7324	0.9982	0.9778	0.9711	
			$O_{MAR}$	7-1	0.5335	0.7324	0.9982	0.9778	0.9711	
	Array w/ master pooling	0.99	0.99	$O_{ET}$	49-7-1	0.5767	0.9608	0.9978	0.9800	0.9957
				$O_{MAR}$	49-7-1	0.5767	0.9608	0.9978	0.9800	0.9957
0.95		0.95	$O_{ET}$	49-7-1	0.5491	0.8156	0.9894	0.8952	0.9797	
			$O_{MAR}$	49-7-1	0.5491	0.8156	0.9894	0.8952	0.9797	
0.90		0.90	$O_{ET}$	49-7-1	0.5154	0.6579	0.9795	0.7812	0.9626	
			$O_{MAR}$	49-7-1	0.5154	0.6579	0.9795	0.7812	0.9626	
0.99		0.90	$O_{ET}$	49-7-1	0.6191	0.9607	0.9735	0.8013	0.9955	
			$O_{MAR}$	49-7-1	0.6191	0.9607	0.9735	0.8013	0.9955	
0.90		0.99	$O_{ET}$	49-7-1	0.4806	0.6592	0.9983	0.9778	0.9635	
			$O_{MAR}$	49-7-1	0.4806	0.6592	0.9983	0.9778	0.9635	

Table S4: Largest differences between operating characteristics for OTCs under non-informative group testing. Values of  $p$  range from 0.005 to 0.150 by 0.005. The frequency column denotes the number of times a different OTC was found for  $O_{ET}$  and  $O_{MAR}$  among these values of  $p$ . Differences between operating characteristics are rounded to four decimal places. Note that the operating characteristic value for  $O_{ET}$  is always subtracted from the operating characteristic value for  $O_{MAR}$ . Thus, a negative value (indicated with parentheses) means that the value for  $O_{ET}$  was larger than the value for  $O_{MAR}$ .

Algorithm	$S_e$	$S_p$	Frequency	Largest difference				
				$E(T)/I$	$PS_e$	$PS_p$	$PPPV$	$PNPV$
Two-stage hierarchical	0.99	0.99	0	-	-	-	-	-
	0.95	0.95	3	0.0018	0.0000	0.0049	0.0262	0.0001
	0.90	0.90	4	0.0023	0.0000	0.0054	0.0345	0.0001
	0.99	0.90	7	0.0056	0.0000	0.0096	0.0382	0.0000
	0.90	0.99	0	-	-	-	-	-
Three-stage hierarchical	0.99	0.99	0	-	-	-	-	-
	0.95	0.95	1	0.0014	0.0000	0.0051	0.0296	0.0001
	0.90	0.90	3	0.0015	0.0000	0.0049	0.0575	0.0001
	0.99	0.90	7	0.0041	(0.0098)	0.0136	0.0580	(0.0015)
	0.90	0.99	1	0.0000	0.0000	0.0002	0.0097	0.0000
Array w/o master pooling	0.99	0.99	0	-	-	-	-	-
	0.95	0.95	5	0.0010	0.0018	0.0026	0.0195	0.0003
	0.90	0.90	8	0.0028	0.0022	0.0054	0.0305	0.0005
	0.99	0.90	5	0.0043	0.0005	0.0076	0.0317	0.0001
	0.90	0.99	1	0.0000	0.0006	0.0001	0.0042	0.0000
Array w/ master pooling	0.99	0.99	2	0.0005	0.0006	0.0008	0.0046	0.0001
	0.95	0.95	4	0.0012	0.0017	0.0026	0.0198	0.0003
	0.90	0.90	8	0.0015	0.0018	0.0051	0.0307	0.0005
	0.99	0.90	5	0.0048	0.0005	0.0077	0.0327	0.0001
	0.90	0.99	2	0.0003	0.0026	0.0005	0.0048	0.0004

Table S5: OTC summary for  $E(P_i) = 0.01$  under informative group testing. Multiple initial group sizes for two-stage hierarchical algorithms are found within a block size of 50, so they are not displayed here. The full OTCs are given in Tables S9 and S10. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

		$\alpha = 2$							$\alpha = 0.5$												
Algorithm	$S_e$	$S_p$	Objective function	Initial group size for OTC			$E(T)/I$	$PS_e^W$	$PS_p^W$	$PS_e^W$	$PS_p^W$	$PPP^W$	$PNPV^W$	Initial group size for OTC			$E(T)/I$	$PS_e^W$	$PS_p^W$	$PPP^W$	$PNPV^W$
				$O_{ET}$	$O_{MAR}$	$O_{MAR}$								$O_{ET}$	$O_{MAR}$	$O_{MAR}$					
Two-stage hierarchical	0.99	0.99	$O_{ET}$	-	0.1947	0.9801	0.9991	0.9204	0.9998	-	0.1683	0.9801	0.9992	0.9245	0.9998	-	0.1683	0.9801	0.9992	0.9245	0.9998
			$O_{MAR}$	-	0.1947	0.9801	0.9991	0.9204	0.9998	-	0.1683	0.9801	0.9992	0.9245	0.9998	-	0.1683	0.9801	0.9992	0.9245	0.9998
	0.95	0.95	$O_{ET}$	-	0.2264	0.9025	0.9931	0.5687	0.9990	-	0.2019	0.9025	0.9943	0.6115	0.9990	-	0.2019	0.9025	0.9943	0.6115	0.9990
			$O_{MAR}$	-	0.2264	0.9025	0.9931	0.5687	0.9990	-	0.2019	0.9025	0.9943	0.6115	0.9990	-	0.2019	0.9025	0.9943	0.6115	0.9990
	0.90	0.90	$O_{ET}$	-	0.2657	0.8100	0.9822	0.3143	0.9981	-	0.2439	0.8100	0.9843	0.3389	0.9981	-	0.2439	0.8100	0.9843	0.3389	0.9981
			$O_{MAR}$	-	0.2657	0.8100	0.9822	0.3143	0.9981	-	0.2439	0.8100	0.9843	0.3389	0.9981	-	0.2439	0.8100	0.9843	0.3389	0.9981
0.90	0.99	$O_{ET}$	-	0.2754	0.9801	0.9813	0.3459	0.9998	-	0.2511	0.9801	0.9837	0.3735	0.9998	-	0.2511	0.9801	0.9837	0.3735	0.9998	
		$O_{MAR}$	-	0.2754	0.9801	0.9813	0.3459	0.9998	-	0.2511	0.9801	0.9837	0.3735	0.9998	-	0.2511	0.9801	0.9837	0.3735	0.9998	
0.90	0.99	$O_{ET}$	-	0.1854	0.8100	0.9990	0.8937	0.9981	-	0.1611	0.8100	0.9993	0.9167	0.9981	-	0.1611	0.8100	0.9993	0.9167	0.9981	
		$O_{MAR}$	-	0.1854	0.8100	0.9990	0.8937	0.9981	-	0.1611	0.8100	0.9993	0.9167	0.9981	-	0.1611	0.8100	0.9993	0.9167	0.9981	
Three-stage hierarchical	0.99	0.99	$O_{ET}$	26	0.1285	0.9703	0.9996	0.9635	0.9997	33	0.1197	0.9703	0.9996	0.9637	0.9997	33	0.1197	0.9703	0.9996	0.9637	0.9997
			$O_{MAR}$	26	0.1285	0.9703	0.9996	0.9635	0.9997	28	0.1291	0.8574	0.9977	0.7883	0.9986	28	0.1291	0.8574	0.9977	0.7883	0.9986
	0.95	0.95	$O_{ET}$	26	0.1375	0.8574	0.9974	0.7655	0.9986	29	0.1422	0.7290	0.9942	0.5558	0.9973	29	0.1422	0.7290	0.9942	0.5558	0.9973
			$O_{MAR}$	26	0.1375	0.8574	0.9974	0.7655	0.9986	29	0.1422	0.7290	0.9942	0.5558	0.9973	29	0.1422	0.7290	0.9942	0.5558	0.9973
	0.90	0.99	$O_{ET}$	26	0.1638	0.9703	0.9930	0.5772	0.9997	28	0.1554	0.9703	0.9935	0.5990	0.9997	28	0.1554	0.9703	0.9935	0.5990	0.9997
			$O_{MAR}$	26	0.1638	0.9703	0.9930	0.5772	0.9997	37	0.1078	0.7290	0.9997	0.9548	0.9973	37	0.1078	0.7290	0.9997	0.9548	0.9973
0.90	0.99	$O_{ET}$	25	0.1349	0.9703	0.9995	0.9556	0.9997	28	0.1277	0.9703	0.9995	0.9542	0.9997	28	0.1277	0.9703	0.9995	0.9542	0.9997	
		$O_{MAR}$	25	0.1349	0.9703	0.9995	0.9556	0.9997	28	0.1277	0.9703	0.9995	0.9542	0.9997	28	0.1277	0.9703	0.9995	0.9542	0.9997	
Array w/o master pooling	0.95	0.95	$O_{ET}$	25	0.1448	0.8575	0.9972	0.7548	0.9986	27	0.1379	0.8574	0.9972	0.7581	0.9986	27	0.1379	0.8574	0.9972	0.7581	0.9986
			$O_{MAR}$	25	0.1448	0.8575	0.9972	0.7548	0.9986	28	0.1519	0.7290	0.9927	0.5017	0.9973	28	0.1519	0.7290	0.9927	0.5017	0.9973
	0.90	0.90	$O_{ET}$	25	0.1585	0.7291	0.9929	0.5089	0.9973	27	0.1519	0.7290	0.9930	0.5113	0.9972	27	0.1519	0.7290	0.9930	0.5113	0.9972
			$O_{MAR}$	23	0.1699	0.9703	0.9926	0.5702	0.9997	25	0.1631	0.9703	0.9926	0.5698	0.9997	25	0.1631	0.9703	0.9926	0.5698	0.9997
	0.90	0.99	$O_{ET}$	27	0.1251	0.7293	0.9996	0.9444	0.9973	30	0.1181	0.7291	0.9996	0.9439	0.9973	30	0.1181	0.7291	0.9996	0.9439	0.9973
			$O_{MAR}$	27	0.1251	0.7293	0.9996	0.9444	0.9973	30	0.1181	0.7291	0.9996	0.9439	0.9973	30	0.1181	0.7291	0.9996	0.9439	0.9973

Table S6: OTC summary for  $E(P_i) = 0.05$  under informative group testing. Multiple initial group sizes for two-stage hierarchical algorithms are found within a block size of 50, so they are not displayed here. The full OTCs are given in Tables S11 and S12. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

		$\alpha = 2$										$\alpha = 0.5$									
Algorithm	$S_e$	$S_p$	Objective function	Initial group size for OTC		$E(T)/I$	$PS_e^W$	$PS_p^W$	$PPPV^W$	$PNPV^W$	Initial group size for OTC		$E(T)/I$	$PS_e^W$	$PS_p^W$	$PPPV^W$	$PNPV^W$				
				$S_e$	$S_p$						$S_e$	$S_p$									
Two-stage hierarchical	0.99	0.99	$O_{ET}$	-	-	0.4101	0.9801	0.9981	0.9645	0.9990	-	-	0.3584	0.9801	0.9984	0.9705	0.9990				
			$O_{MAR}$	-	-	0.4101	0.9801	0.9981	0.9645	0.9990	-	-	0.3584	0.9801	0.9984	0.9705	0.9990				
	0.95	0.95	$O_{ET}$	-	-	0.4321	0.9025	0.9892	0.8152	0.9948	-	-	0.3830	0.9025	0.9908	0.8371	0.9948				
			$O_{MAR}$	-	-	0.4321	0.9025	0.9892	0.8152	0.9948	-	-	0.3830	0.9025	0.9908	0.8371	0.9948				
	0.90	0.90	$O_{ET}$	-	-	0.4586	0.8100	0.9733	0.6149	0.9898	-	-	0.4124	0.8100	0.9761	0.6403	0.9899				
			$O_{MAR}$	-	-	0.4586	0.8100	0.9733	0.6149	0.9898	-	-	0.4124	0.8100	0.9761	0.6403	0.9899				
Three-stage hierarchical	0.99	0.90	$O_{ET}$	-	-	0.4798	0.9801	0.9736	0.6619	0.9989	-	-	0.4308	0.9812	0.9746	0.6703	0.9990				
			$O_{MAR}$	-	-	0.4798	0.9801	0.9736	0.6619	0.9989	-	-	0.4311	0.9801	0.9767	0.6885	0.9989				
	0.90	0.99	$O_{ET}$	-	-	0.3898	0.8100	0.9983	0.9609	0.9901	-	-	0.3411	0.8100	0.9986	0.9675	0.9901				
			$O_{MAR}$	-	-	0.3898	0.8100	0.9983	0.9609	0.9901	-	-	0.3411	0.8100	0.9986	0.9675	0.9901				
	0.99	0.99	$O_{ET}$	10	10	0.3687	0.9725	0.9990	0.9803	0.9986	11	11	0.3365	0.9757	0.9988	0.9768	0.9987				
			$O_{MAR}$	10	10	0.3687	0.9725	0.9990	0.9803	0.9986	11	11	0.3365	0.9757	0.9988	0.9768	0.9987				
Array w/o master pooling	0.95	0.95	$O_{ET}$	11	11	0.3709	0.8574	0.9940	0.8821	0.9925	11	11	0.3433	0.8822	0.9934	0.8763	0.9938				
			$O_{MAR}$	11	11	0.3709	0.8574	0.9940	0.8821	0.9925	11	11	0.3433	0.8822	0.9934	0.8763	0.9938				
	0.90	0.90	$O_{ET}$	12	12	0.3724	0.7290	0.9862	0.7357	0.9857	10	10	0.3503	0.7582	0.9871	0.7560	0.9873				
			$O_{MAR}$	12	12	0.3724	0.7290	0.9862	0.7357	0.9857	10	10	0.3503	0.7582	0.9871	0.7560	0.9873				
	0.99	0.90	$O_{ET}$	9	8	0.4136	0.9727	0.9834	0.7554	0.9985	10	10	0.3833	0.9738	0.9852	0.7756	0.9986				
			$O_{MAR}$	8	8	0.4140	0.9729	0.9853	0.7772	0.9986	10	10	0.3833	0.9738	0.9852	0.7756	0.9986				
Two-stage hierarchical	0.90	0.99	$O_{ET}$	12	12	0.3315	0.7290	0.9989	0.9727	0.9859	15	15	0.3052	0.7515	0.9990	0.9749	0.9871				
			$O_{MAR}$	12	12	0.3336	0.7449	0.9989	0.9730	0.9867	11	11	0.3076	0.7735	0.9989	0.9747	0.9882				
	0.99	0.99	$O_{ET}$	10	10	0.3677	0.9705	0.9988	0.9761	0.9984	13	13	0.3372	0.9703	0.9986	0.9727	0.9985				
			$O_{MAR}$	10	10	0.3677	0.9705	0.9988	0.9761	0.9984	13	13	0.3372	0.9703	0.9986	0.9727	0.9985				
	0.95	0.95	$O_{ET}$	10	10	0.3731	0.8582	0.9933	0.8703	0.9925	13	13	0.3421	0.8575	0.9924	0.8551	0.9926				
			$O_{MAR}$	10	10	0.3731	0.8582	0.9933	0.8703	0.9925	13	13	0.3421	0.8575	0.9924	0.8551	0.9926				
Three-stage hierarchical	0.90	0.90	$O_{ET}$	11	11	0.3784	0.7295	0.9836	0.7004	0.9857	13	13	0.3484	0.7292	0.9837	0.7000	0.9859				
			$O_{MAR}$	11	11	0.3784	0.7295	0.9836	0.7004	0.9857	13	13	0.3484	0.7292	0.9837	0.7000	0.9859				
	0.99	0.90	$O_{ET}$	10	10	0.4113	0.9704	0.9829	0.7494	0.9984	11	11	0.3826	0.9703	0.9840	0.7610	0.9984				
			$O_{MAR}$	10	10	0.4113	0.9704	0.9829	0.7494	0.9984	11	11	0.3826	0.9703	0.9840	0.7610	0.9984				
	0.90	0.99	$O_{ET}$	11	11	0.3380	0.7303	0.9988	0.9693	0.9860	13	13	0.3060	0.7294	0.9988	0.9698	0.9861				
			$O_{MAR}$	11	11	0.3380	0.7303	0.9988	0.9693	0.9860	13	13	0.3060	0.7294	0.9988	0.9698	0.9861				

Table S7: OTC summary for  $E(P_i) = 0.10$  under informative group testing. Multiple initial group sizes for two-stage hierarchical algorithms are found within a block size of 50, so they are not displayed here. The full OTCs are given in Tables S13 and S14. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

		$\alpha = 2$										$\alpha = 0.5$																											
Algorithm	$S_e$	$S_p$	Objective function	Initial group size for OTC				$E(T)/I$				$PS_e^W$				$PS_p^W$				Initial group size for OTC				$E(T)/I$				$PS_e^W$				$PS_p^W$				$PNPV^W$			
				$O_{ET}$	$O_{MAR}$	$PPP^W$	$PPV^W$	$PNPV^W$	$O_{ET}$	$O_{MAR}$	$PPP^W$	$PPV^W$	$PNPV^W$	$O_{ET}$	$O_{MAR}$	$PPP^W$	$PPV^W$	$PNPV^W$	$O_{ET}$	$O_{MAR}$	$PPP^W$	$PPV^W$	$PNPV^W$	$O_{ET}$	$O_{MAR}$	$PPP^W$	$PPV^W$	$PNPV^W$	$O_{ET}$	$O_{MAR}$	$PPP^W$	$PPV^W$	$PNPV^W$	$O_{ET}$	$O_{MAR}$	$PPP^W$	$PPV^W$	$PNPV^W$	
Two-stage hierarchical	0.99	0.99	$O_{ET}$	-	-	0.5674	0.9801	0.9975	0.9772	0.9978	-	-	0.4868	0.9833	0.9977	0.9793	0.9981	-	-	0.4868	0.9833	0.9977	0.9793	0.9981	-	-	0.5054	0.9148	0.9873	0.8887	0.9905	-	-	0.5054	0.9148	0.9873	0.8887	0.9905	
	0.95	0.95	$O_{MAR}$	-	-	0.5815	0.9025	0.9863	0.8798	0.9891	-	-	0.5054	0.9148	0.9873	0.8887	0.9905	-	-	0.5054	0.9148	0.9873	0.8887	0.9905	-	-	0.5271	0.8333	0.9695	0.7522	0.9813	-	-	0.5271	0.8333	0.9695	0.7522	0.9813	
	0.90	0.90	$O_{MAR}$	-	-	0.5973	0.8100	0.9681	0.7382	0.9787	-	-	0.5271	0.8333	0.9695	0.7522	0.9813	-	-	0.5271	0.8333	0.9695	0.7522	0.9813	-	-	0.5491	0.9839	0.9678	0.7725	0.9982	-	-	0.5491	0.9839	0.9678	0.7725	0.9982	
	0.99	0.99	$O_{MAR}$	-	-	0.6277	0.9807	0.9657	0.7606	0.9978	-	-	0.5496	0.9833	0.9700	0.7844	0.9981	-	-	0.5496	0.9833	0.9700	0.7844	0.9981	-	-	0.4654	0.8333	0.9979	0.9774	0.9818	-	-	0.4654	0.8333	0.9979	0.9774	0.9818	
	0.90	0.99	$O_{MAR}$	-	-	0.5383	0.8100	0.9977	0.9749	0.9793	-	-	0.4654	0.8333	0.9979	0.9774	0.9818	-	-	0.4654	0.8333	0.9979	0.9774	0.9818	-	-	0.5074	0.9733	0.9976	0.9786	0.9970	-	-	0.5074	0.9733	0.9976	0.9786	0.9970	
	0.99	0.99	$O_{ET}$	5	5	0.5567	0.9764	0.9981	0.9824	0.9974	5	5	0.5074	0.9733	0.9976	0.9786	0.9970	-	-	0.5074	0.9733	0.9976	0.9786	0.9970	-	-	0.5050	0.8711	0.9876	0.8863	0.9857	-	-	0.5050	0.8711	0.9876	0.8863	0.9857	
	0.95	0.95	$O_{MAR}$	8	8	0.5550	0.8691	0.9891	0.8985	0.9855	8	8	0.5050	0.8711	0.9876	0.8863	0.9857	-	-	0.5050	0.8711	0.9876	0.8863	0.9857	-	-	0.4994	0.7469	0.9739	0.7604	0.9719	-	-	0.4994	0.7469	0.9739	0.7604	0.9719	
	0.90	0.90	$O_{ET}$	8	8	0.5461	0.7500	0.9781	0.7916	0.9724	8	8	0.4994	0.7469	0.9739	0.7604	0.9719	-	-	0.4994	0.7469	0.9739	0.7604	0.9719	-	-	0.5611	0.9774	0.9770	0.8254	0.9974	-	-	0.5611	0.9774	0.9770	0.8254	0.9974	
	0.99	0.90	$O_{MAR}$	5	5	0.6044	0.9764	0.9764	0.8216	0.9973	5	5	0.6044	0.9764	0.9764	0.8216	0.9973	-	-	0.6044	0.9764	0.9764	0.8216	0.9973	-	-	0.4442	0.7469	0.9980	0.9764	0.9726	-	-	0.4442	0.7469	0.9980	0.9764	0.9726	
	0.90	0.99	$O_{MAR}$	6	6	0.5203	0.7874	0.9978	0.9759	0.9769	6	6	0.4445	0.7537	0.9980	0.9767	0.9733	-	-	0.4445	0.7537	0.9980	0.9767	0.9733	-	-	0.5092	0.9704	0.9982	0.9837	0.9967	-	-	0.5092	0.9704	0.9982	0.9837	0.9967	
Array w/o master pooling	0.99	0.99	$O_{ET}$	7	7	0.5585	0.9706	0.9981	0.9823	0.9967	7	7	0.5092	0.9704	0.9982	0.9837	0.9967	-	-	0.5092	0.9704	0.9982	0.9837	0.9967	-	-	0.5076	0.8576	0.9892	0.8978	0.9843	-	-	0.5076	0.8576	0.9892	0.8978	0.9843	
	0.95	0.95	$O_{MAR}$	7	7	0.5563	0.8587	0.9900	0.9050	0.9844	7	7	0.5076	0.8576	0.9892	0.8978	0.9843	-	-	0.5076	0.8576	0.9892	0.8978	0.9843	-	-	0.5076	0.8576	0.9892	0.8978	0.9843	-	-	0.5076	0.8576	0.9892	0.8978	0.9843	
	0.90	0.90	$O_{ET}$	8	8	0.5494	0.7297	0.9757	0.7697	0.9701	8	8	0.5040	0.7294	0.9777	0.7842	0.9702	-	-	0.5040	0.7294	0.9777	0.7842	0.9702	-	-	0.5040	0.7294	0.9777	0.7842	0.9702	-	-	0.5040	0.7294	0.9777	0.7842	0.9702	
	0.90	0.90	$O_{MAR}$	8	8	0.5494	0.7297	0.9757	0.7697	0.9701	8	8	0.5040	0.7294	0.9777	0.7842	0.9702	-	-	0.5040	0.7294	0.9777	0.7842	0.9702	-	-	0.5558	0.9704	0.9769	0.8236	0.9966	-	-	0.5558	0.9704	0.9769	0.8236	0.9966	
	0.99	0.90	$O_{ET}$	7	7	0.6024	0.9705	0.9757	0.8161	0.9966	7	7	0.6024	0.9705	0.9757	0.8161	0.9966	-	-	0.6024	0.9705	0.9757	0.8161	0.9966	-	-	0.5558	0.9704	0.9769	0.8236	0.9966	-	-	0.5558	0.9704	0.9769	0.8236	0.9966	
	0.90	0.99	$O_{MAR}$	7	7	0.6024	0.9705	0.9757	0.8161	0.9966	7	7	0.6024	0.9705	0.9757	0.8161	0.9966	-	-	0.6024	0.9705	0.9757	0.8161	0.9966	-	-	0.5558	0.9704	0.9769	0.8236	0.9966	-	-	0.5558	0.9704	0.9769	0.8236	0.9966	
	0.90	0.99	$O_{ET}$	8	8	0.5099	0.7302	0.9980	0.9761	0.9708	8	8	0.5099	0.7302	0.9980	0.9761	0.9708	-	-	0.5099	0.7302	0.9980	0.9761	0.9708	-	-	0.4617	0.7298	0.9982	0.9788	0.9708	-	-	0.4617	0.7298	0.9982	0.9788	0.9708	
	0.90	0.99	$O_{MAR}$	8	8	0.5099	0.7302	0.9980	0.9761	0.9708	8	8	0.5099	0.7302	0.9980	0.9761	0.9708	-	-	0.5099	0.7302	0.9980	0.9761	0.9708	-	-	0.4617	0.7298	0.9982	0.9788	0.9708	-	-	0.4617	0.7298	0.9982	0.9788	0.9708	

Table S8: Largest differences between operating characteristics for OTCs under informative group testing. Values of  $E(P_i) = p$  range from 0.005 to 0.150 by 0.005. The frequency column denotes the number of times a different OTC was found among these values of  $p$ . Differences between operating characteristics are rounded to four decimal places. Note that the operating characteristic value for  $O_{ET}$  is always subtracted from the operating characteristic value for  $O_{MAR}$ . Thus, a negative value (indicated with parentheses) means that the value for  $O_{ET}$  was larger than the value for  $O_{MAR}$ .

Algorithm	$\alpha$	$S_e$	$S_p$	Frequency	Largest difference				
					$E(T)/I$	$PS_e^W$	$PS_p^W$	$PPPV^W$	$PNPV^W$
Two-stage hierarchical	2	0.99	0.99	0	-	-	-	-	-
		0.95	0.95	7	0.0006	(0.0023)	0.0011	0.0156	0.0004
		0.90	0.90	12	0.0010	(0.0052)	0.0023	0.0160	0.0007
		0.99	0.90	12	0.0011	(0.0008)	0.0022	0.0182	(0.0001)
		0.90	0.99	2	0.0003	0.0052	0.0000	0.0002	0.0007
	0.5	0.99	0.99	0	-	-	-	-	-
		0.95	0.95	3	0.0003	(0.0035)	0.0011	0.0102	0.0003
		0.90	0.90	15	0.0008	(0.0103)	0.0022	0.0277	0.0007
		0.99	0.90	16	0.0012	(0.0011)	0.0022	0.0194	(0.0001)
		0.90	0.99	11	0.0006	0.0078	(0.0002)	(0.0028)	0.0007
Three-stage hierarchical	2	0.99	0.99	1	0.0000	(0.0019)	0.0002	0.0057	(0.0001)
		0.95	0.95	2	0.0035	0.0219	0.0033	0.0270	0.0034
		0.90	0.90	6	0.0044	0.0152	0.0062	0.0409	0.0023
		0.99	0.90	4	0.0035	0.0006	0.0066	0.0445	0.0001
		0.90	0.99	14	0.0180	0.0500	0.0003	0.0046	0.0064
	0.5	0.99	0.99	1	0.0000	0.0001	0.0001	0.0018	0.0000
		0.95	0.95	0	-	-	-	-	-
		0.90	0.90	3	0.0010	0.0250	0.0033	0.0296	0.0025
		0.99	0.90	5	0.0022	0.0034	0.0070	0.0385	0.0005
		0.90	0.99	9	0.0057	0.0355	0.0003	0.0051	0.0030
Array w/o master pooling	2	0.99	0.99	1	0.0003	0.0004	0.0005	0.0039	0.0001
		0.95	0.95	2	0.0011	0.0012	0.0027	0.0169	0.0002
		0.90	0.90	5	0.0016	0.0012	0.0040	0.0265	0.0003
		0.99	0.90	4	0.0028	0.0003	0.0053	0.0277	0.0001
		0.90	0.99	0	-	-	-	-	-
	0.5	0.99	0.99	0	-	-	-	-	-
		0.95	0.95	4	0.0003	0.0004	0.0015	0.0129	0.0001
		0.90	0.90	14	0.0015	0.0004	0.0032	0.0194	0.0002
		0.99	0.90	8	0.0024	0.0001	0.0041	0.0211	0.0000
		0.90	0.99	1	0.0003	0.0005	0.0003	0.0027	0.0001



Table S9: Full OTCs for  $E(P_i) = 0.01$  under informative two-stage hierarchical group testing. There are no differences in the OTCs for  $O_{ET}$  and  $O_{MAR}$ .

$\alpha$	$S_e$	$S_p$	Objective function	Block size	$E(T)/I$	Group sizes					
						$I_{11}$	$I_{12}$	$I_{13}$	$I_{14}$	$I_{15}$	
2	0.99	0.99	$O_{ET}$	50	0.1947	16	11	9	8	6	
			$O_{MAR}$	50	0.1947	16	11	9	8	6	
	0.95	0.95	$O_{ET}$	50	0.2264	18	13	11	8		
			$O_{MAR}$	50	0.2264	18	13	11	8		
	0.90	0.90	$O_{ET}$	50	0.2657	18	13	11	8		
			$O_{MAR}$	50	0.2657	18	13	11	8		
	0.99	0.90	$O_{ET}$	50	0.2754	18	13	11	8		
			$O_{MAR}$	50	0.2754	18	13	11	8		
	0.90	0.99	$O_{ET}$	50	0.1854	18	13	11	8		
			$O_{MAR}$	50	0.1854	18	13	11	8		
	0.5	0.99	0.99	$O_{ET}$	50	0.1683	25	12	8	5	
				$O_{MAR}$	50	0.1683	25	12	8	5	
0.95		0.95	$O_{ET}$	50	0.2019	25	12	8	5		
			$O_{MAR}$	50	0.2019	25	12	8	5		
0.90		0.90	$O_{ET}$	50	0.2439	25	12	8	5		
			$O_{MAR}$	50	0.2439	25	12	8	5		
0.99		0.90	$O_{ET}$	50	0.2511	25	12	8	5		
			$O_{MAR}$	50	0.2511	25	12	8	5		
0.90		0.99	$O_{ET}$	50	0.1611	25	12	8	5		
			$O_{MAR}$	50	0.1611	25	12	8	5		

Table S10: Full OTCs for  $E(P_i) = 0.01$  under informative three-stage hierarchical group testing. There are no differences in the OTCs for  $O_{ET}$  and  $O_{MAR}$ .

$\alpha$	$S_e$	$S_p$	Objective function	Group sizes							
				$I_{11}$	$E(T)/I$	$I_{21}$	$I_{22}$	$I_{23}$	$I_{24}$	$I_{25}$	
2	0.99	0.99	$O_{ET}$	26	0.1285	9	5	5	4	3	
			$O_{MAR}$	26	0.1285	9	5	5	4	3	
	0.95	0.95	$O_{ET}$	26	0.1375	10	7	5	4		
			$O_{MAR}$	26	0.1375	10	7	5	4		
	0.90	0.90	$O_{ET}$	26	0.1497	10	7	5	4		
			$O_{MAR}$	26	0.1497	10	7	5	4		
	0.99	0.90	$O_{ET}$	26	0.1638	10	7	5	4		
			$O_{MAR}$	26	0.1638	10	7	5	4		
	0.90	0.99	$O_{ET}$	26	0.1168	9	5	5	4	3	
			$O_{MAR}$	26	0.1168	9	5	5	4	3	
	0.5	0.99	0.99	$O_{ET}$	33	0.1197	15	6	5	4	3
				$O_{MAR}$	33	0.1197	15	6	5	4	3
0.95		0.95	$O_{ET}$	28	0.1291	13	7	5	3		
			$O_{MAR}$	28	0.1291	13	7	5	3		
0.90		0.90	$O_{ET}$	29	0.1422	14	7	5	3		
			$O_{MAR}$	29	0.1422	14	7	5	3		
0.99		0.90	$O_{ET}$	28	0.1554	13	7	5	3		
			$O_{MAR}$	28	0.1554	13	7	5	3		
0.90		0.99	$O_{ET}$	37	0.1078	17	7	6	4	3	
			$O_{MAR}$	37	0.1078	17	7	6	4	3	

Table S11: Full OTCs for  $E(P_i) = 0.05$  under informative two-stage hierarchical group testing. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

$\alpha$	$S_e$	$S_p$	Objective function	Block size	$E(T)/I$	Group sizes								
						$I_{11}$	$I_{12}$	$I_{13}$	$I_{14}$	$I_{15}$	$I_{16}$	$I_{17}$	$I_{18}$	$I_{19}$
2	0.99	0.99	$O_{ET}$	50	0.4101	9	7	6	6	5	5	4	4	4
			$O_{MAR}$	50	0.4101	9	7	6	6	5	5	4	4	4
	0.95	0.95	$O_{ET}$	50	0.4321	9	7	6	6	5	5	4	4	4
			$O_{MAR}$	50	0.4321	9	7	6	6	5	5	4	4	4
	0.90	0.90	$O_{ET}$	50	0.4586	10	8	7	6	5	5	5	4	
			$O_{MAR}$	50	0.4586	10	8	7	6	5	5	5	4	
	0.99	0.90	$O_{ET}$	50	0.4798	9	7	6	6	5	5	4	4	4
			$O_{MAR}$	50	0.4798	9	7	6	6	5	5	4	4	4
	0.90	0.99	$O_{ET}$	50	0.3898	9	7	6	6	5	5	4	4	4
			$O_{MAR}$	50	0.3898	9	7	6	6	5	5	4	4	4
	0.5	0.99	0.99	$O_{ET}$	50	0.3584	16	9	6	5	4	4	3	3
				$O_{MAR}$	50	0.3584	16	9	6	5	4	4	3	3
0.95		0.95	$O_{ET}$	50	0.3830	16	9	6	5	4	4	3	3	
			$O_{MAR}$	50	0.3830	16	9	6	5	4	4	3	3	
0.90		0.90	$O_{ET}$	50	0.4124	17	9	7	5	5	4	3		
			$O_{MAR}$	50	0.4124	17	9	7	5	5	4	3		
0.99		0.90	$O_{ET}$	50	0.4308	17	9	6	5	5	4	3	1	
			$O_{MAR}$	50	0.4311	16	9	6	5	4	4	3	3	
0.90		0.99	$O_{ET}$	50	0.3411	16	9	6	5	4	4	3	3	
			$O_{MAR}$	50	0.3411	16	9	6	5	4	4	3	3	

Table S12: Full OTCs for  $E(P_i) = 0.05$  under informative three-stage hierarchical group testing. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

$\alpha$	$S_e$	$S_p$	Objective function	$I_{11}$	$E(T)/I$	Group sizes				
						$I_{21}$	$I_{22}$	$I_{23}$	$I_{24}$	
2	0.99	0.99	$O_{ET}$	10	0.3687	4	3	2	1	
			$O_{MAR}$	10	0.3687	4	3	2	1	
	0.95	0.95	$O_{ET}$	11	0.3709	5	3	3		
			$O_{MAR}$	11	0.3709	5	3	3		
	0.90	0.90	$O_{ET}$	12	0.3724	5	4	3		
			$O_{MAR}$	12	0.3724	5	4	3		
	0.99	0.90	$O_{ET}$	9	0.4136	5	3	1		
			$O_{MAR}$	8	0.4140	4	3	1		
	0.90	0.99	$O_{ET}$	12	0.3315	5	4	3		
			$O_{MAR}$	12	0.3336	5	3	3	1	
	0.5	0.99	0.99	$O_{ET}$	11	0.3365	6	3	1	1
				$O_{MAR}$	11	0.3365	6	3	1	1
0.95		0.95	$O_{ET}$	11	0.3433	6	3	1	1	
			$O_{MAR}$	11	0.3433	6	3	1	1	
0.90		0.90	$O_{ET}$	10	0.3503	6	3	1		
			$O_{MAR}$	10	0.3503	6	3	1		
0.99		0.90	$O_{ET}$	10	0.3833	6	3	1		
			$O_{MAR}$	10	0.3833	6	3	1		
0.90		0.99	$O_{ET}$	15	0.3052	7	4	3	1	
			$O_{MAR}$	11	0.3076	6	3	1	1	

Table S13: Full OTCs for  $E(P_i) = 0.10$  under informative two-stage hierarchical group testing. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

$\alpha$	$S_e$	$S_p$	Objective function	Block size	$E(T)/I$	Group sizes															
						$I_{11}$	$I_{12}$	$I_{13}$	$I_{14}$	$I_{15}$	$I_{16}$	$I_{17}$	$I_{18}$	$I_{19}$	$I_{1,10}$	$I_{1,11}$	$I_{1,12}$	$I_{1,13}$			
2	0.99	0.99	$O_{ET}$	50	0.5674	7	6	5	4	4	4	4	4	4	4	4	3	3	3	3	
			$O_{MAR}$	50	0.5674	7	6	5	4	4	4	4	4	4	4	4	4	3	3	3	3
	0.95	0.95	$O_{ET}$	50	0.5815	7	6	5	4	4	4	4	4	4	4	4	3	3	3	3	3
			$O_{MAR}$	50	0.5815	7	6	5	4	4	4	4	4	4	4	4	3	3	3	3	3
	0.90	0.90	$O_{ET}$	50	0.5973	8	6	5	5	4	4	4	4	4	4	4	4	3	3	3	3
			$O_{MAR}$	50	0.5973	8	6	5	5	4	4	4	4	4	4	4	4	3	3	3	3
0.5	0.99	0.90	$O_{ET}$	50	0.6277	7	6	5	5	4	4	4	4	4	4	4	3	3	3	1	
			$O_{MAR}$	50	0.6283	7	6	5	4	4	4	4	4	4	4	4	3	3	3	3	
	0.90	0.99	$O_{ET}$	50	0.5383	7	6	5	4	4	4	4	4	4	4	4	3	3	3	3	
			$O_{MAR}$	50	0.5383	7	6	5	4	4	4	4	4	4	4	4	3	3	3	3	
	0.99	0.99	$O_{ET}$	50	0.4868	13	7	5	4	4	4	4	3	3	3	3	1	1	1	1	
			$O_{MAR}$	50	0.4868	13	7	5	4	4	4	4	3	3	3	3	1	1	1	1	
0.95	0.95	$O_{ET}$	50	0.5054	13	7	5	5	4	4	4	3	3	3	3	1	1	1	1		
		$O_{MAR}$	50	0.5054	13	7	5	5	4	4	4	3	3	3	3	1	1	1	1		
0.90	0.90	$O_{ET}$	50	0.5271	14	7	6	5	4	4	4	4	3	3	1	1	1	1	1		
		$O_{MAR}$	50	0.5271	14	7	6	5	4	4	4	4	3	3	1	1	1	1	1		
0.99	0.90	$O_{ET}$	50	0.5491	13	7	6	5	4	4	4	3	3	3	1	1	1	1	1		
		$O_{MAR}$	50	0.5496	13	7	5	4	4	4	4	3	3	3	1	1	1	1	1		
0.90	0.99	$O_{ET}$	50	0.4654	13	7	5	5	4	4	4	3	3	3	1	1	1	1	1		
		$O_{MAR}$	50	0.4654	13	7	5	5	4	4	4	3	3	3	1	1	1	1	1		

Table S14: Full OTCs for  $E(P_i) = 0.10$  under informative three-stage hierarchical group testing. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

$\alpha$	$S_e$	$S_p$	Objective			Group sizes											
			function	$I_{11}$	$E(T)/I$	$I_{21}$	$I_{22}$	$I_{23}$	$I_{24}$	$I_{25}$	$I_{26}$	$I_{27}$	$I_{28}$	$I_{29}$	$I_{2,10}$		
2	0.99	0.99	$O_{ET}$	5	0.5567	3	1	1									
			$O_{MAR}$	5	0.5567	3	1	1									
	0.95	0.95	$O_{ET}$	8	0.5550	4	3	1									
			$O_{MAR}$	8	0.5550	4	3	1									
	0.90	0.90	$O_{ET}$	8	0.5461	4	3	1									
			$O_{MAR}$	8	0.5461	4	3	1									
	0.99	0.90	$O_{ET}$	5	0.6044	3	1	1									
			$O_{MAR}$	5	0.6044	3	1	1									
	0.90	0.99	$O_{ET}$	8	0.5055	4	3	1									
			$O_{MAR}$	6	0.5203	3	1	1	1								
	0.99	0.99	$O_{ET}$	40	0.5074	12	6	5	4	4	3	3	1	1	1		
			$O_{MAR}$	40	0.5074	12	6	5	4	4	3	3	1	1	1		
0.95	0.95	$O_{ET}$	40	0.5050	12	6	5	4	4	3	3	1	1	1			
		$O_{MAR}$	40	0.5050	12	6	5	4	4	3	3	1	1	1			
0.90	0.90	$O_{ET}$	40	0.4994	12	7	5	4	4	3	3	1	1				
		$O_{MAR}$	40	0.4994	12	7	5	4	4	3	3	1	1				
0.99	0.90	$O_{ET}$	6	0.5611	4	1	1										
		$O_{MAR}$	6	0.5611	4	1	1										
0.90	0.99	$O_{ET}$	40	0.4442	12	7	5	4	4	3	3	1	1				
		$O_{MAR}$	40	0.4445	12	6	5	4	4	3	3	1	1	1			

Table S15: OTC summary for HIV testing using  $S_e = 0.963$ ,  $S_p = 0.9903$ , and  $p = 0.004$  with non-informative group testing. Equally sized groups are optimal at each stage; thus, an OTC of “24-6-1” means that stage 1 has a group of size 24, stage 2 has four groups of size 6, and stage 3 has twenty-four groups of size 1. There are no differences in the OTCs for  $O_{ET}$  and  $O_{MAR}$ .

Algorithm	Objective						
	function	OTC	$E(T)/I$	$PS_e$	$PS_p$	$PPPV$	$PNPV$
Two-stage	$O_{ET}$	17-1	0.1313	0.9274	0.9993	0.8478	0.9997
hierarchical	$O_{MAR}$	17-1	0.1313	0.9274	0.9993	0.8478	0.9997
Three-stage	$O_{ET}$	49-7-1	0.0732	0.8931	0.9998	0.9402	0.9996
hierarchical	$O_{MAR}$	49-7-1	0.0732	0.8931	0.9998	0.9402	0.9996
Array w/o	$O_{ET}$	44-1	0.0749	0.8931	0.9997	0.9348	0.9996
master pooling	$O_{MAR}$	44-1	0.0749	0.8931	0.9997	0.9348	0.9996
Array w/	$O_{ET}$	1936-44-1	0.0721	0.8600	0.9998	0.9348	0.9994
master pooling	$O_{MAR}$	1936-44-1	0.0721	0.8600	0.9998	0.9348	0.9994

Table S16: OTC summary for chlamydia testing. The test accuracies are  $S_e = 0.805$  and  $S_p = 0.96$  for females and  $S_e = 0.93$  and  $S_p = 0.95$  for males. For non-informative group testing,  $p = 0.08$  for females,  $p = 0.081$  for males, and equally sized groups are optimal at each stage (see Table S1's caption for how group sizes are denoted). For informative group testing,  $P_i \sim \text{beta}(1.1, 11.54)$  for females,  $P_i \sim \text{beta}(1.8, 18.20)$  for males, and full OTCs are provided in Tables S17 and S18. Results are not displayed for informative array testing with master pooling because no group testing algorithms have been proposed for it. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

Algorithm	Objective function	Non-informative						Informative						
		OTC	$E(T)/I$	$PS_e$	$PS_p$	PPPV	PNPV	Stage 1 size	$E(T)/I$	$PS_e^W$	$PS_p^W$	PPPV <sup>W</sup>	PNPV <sup>W</sup>	
Female	Two-stage	5-1	0.5008	0.6480	0.9897	0.8457	0.9700	-	0.4757	0.6480	0.9901	0.8620	0.9672	
	hierarchical	5-1	0.5008	0.6480	0.9897	0.8457	0.9700	-	0.4761	0.6480	0.9910	0.8725	0.9673	
	Three-stage	12-4-1	0.4099	0.5217	0.9937	0.8789	0.9598	19	0.4102	0.5217	0.9930	0.8773	0.9561	
	hierarchical	12-4-1	0.4099	0.5217	0.9937	0.8789	0.9598	14	0.4113	0.5479	0.9933	0.8868	0.9584	
	Array w/o	$O_{ET}$	9-1	0.4327	0.5240	0.9931	0.8687	0.9600	10	0.4187	0.5226	0.9929	0.8742	0.9565
	master pooling	$O_{MAR}$	9-1	0.4327	0.5240	0.9931	0.8687	0.9600	10	0.4187	0.5226	0.9929	0.8742	0.9565
	Array w/	$O_{ET}$	81-9-1	0.3485	0.4218	0.9945	0.8687	0.9519	-	-	-	-	-	-
	master pooling	$O_{MAR}$	81-9-1	0.3485	0.4218	0.9945	0.8687	0.9519	-	-	-	-	-	-
	Two-stage	$O_{ET}$	4-1	0.5523	0.8649	0.9877	0.8606	0.9881	-	0.5462	0.8649	0.9867	0.8652	0.9866
	hierarchical	$O_{MAR}$	4-1	0.5523	0.8649	0.9877	0.8606	0.9881	-	0.5462	0.8649	0.9867	0.8652	0.9866
Male	Three-stage	9-3-1	0.4931	0.8044	0.9924	0.9036	0.9829	8	0.5081	0.8206	0.9905	0.8950	0.9824	
	hierarchical	9-3-1	0.4931	0.8044	0.9924	0.9036	0.9829	8	0.5081	0.8206	0.9905	0.8950	0.9824	
	Array w/o	$O_{ET}$	8-1	0.5015	0.8056	0.9901	0.8780	0.9830	8	0.5105	0.8053	0.9900	0.8882	0.9809
	master pooling	$O_{MAR}$	8-1	0.5015	0.8056	0.9901	0.8780	0.9830	8	0.5105	0.8053	0.9900	0.8882	0.9809
	Array w/	$O_{ET}$	64-8-1	0.4667	0.7492	0.9908	0.8781	0.9782	-	-	-	-	-	-
	master pooling	$O_{MAR}$	64-8-1	0.4667	0.7492	0.9908	0.8781	0.9782	-	-	-	-	-	-

Table S17: Full OTCs for informative, two-stage hierarchical testing summarized in Table S16. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

	Objective function	Block size	$E(T)/I$	Group sizes										
				$I_{11}$	$I_{12}$	$I_{13}$	$I_{14}$	$I_{15}$	$I_{16}$	$I_{17}$	$I_{18}$	$I_{19}$	$I_{1,10}$	$I_{1,11}$
Female	$O_{ET}$	50	0.4757	11	7	6	5	5	4	4	4	4		
	$O_{MAR}$	50	0.4761	10	7	6	5	4	4	4	4	4	3	3
Male	$O_{ET}$	50	0.5462	8	6	5	5	4	4	4	4	4	3	3
	$O_{MAR}$	50	0.5462	8	6	5	5	4	4	4	4	4	3	3

Table S18: Full OTCs for informative, three-stage hierarchical testing summarized in Table S16. Differences between  $O_{ET}$  and  $O_{MAR}$  are highlighted.

	Objective function	$I_{11}$	$E(T)/I$	Group sizes			
				$I_{21}$	$I_{22}$	$I_{23}$	$I_{24}$
Female	$O_{ET}$	19	0.4102	7	5	4	3
	$O_{MAR}$	14	0.4113	6	4	3	1
Male	$O_{ET}$	8	0.5081	4	3	1	
	$O_{MAR}$	8	0.5081	4	3	1	

Table S19: OTC summary for  $O_{GR}$  with  $p = 0.01$  under non-informative, two-stage hierarchical testing. An OTC of “11-1” means that stage 1 has a group of size 11 and stage 2 consists of individual testing.

$S_e$	$S_p$	$D_1$	$D_2$	OTC	$E(T)/I$	$PS_e$	$PS_p$	PPPV	PNPV
0.99	0.99	1	1	11-1	0.2035	0.9801	0.9990	0.9052	0.9998
		1000	1000	3-1	0.3724	0.9801	0.9997	0.9711	0.9998
		1	10	11-1	0.2035	0.9801	0.9990	0.9052	0.9998
		1	100	11-1	0.2035	0.9801	0.9990	0.9052	0.9998
		10	1	10-1	0.2037	0.9801	0.9991	0.9127	0.9998
		100	1	7-1	0.2194	0.9801	0.9993	0.9363	0.9998
0.95	0.95	1	1	11-1	0.2351	0.9025	0.9932	0.5727	0.9990
		1000	1000	3-1	0.4101	0.9025	0.9966	0.7286	0.9990
		1	10	11-1	0.2351	0.9025	0.9932	0.5727	0.9990
		1	100	11-1	0.2351	0.9025	0.9932	0.5727	0.9990
		10	1	9-1	0.2389	0.9025	0.9940	0.6040	0.9990
		100	1	4-1	0.3355	0.9025	0.9962	0.7038	0.9990
0.90	0.90	1	1	11-1	0.2746	0.8100	0.9824	0.3167	0.9981
		1000	1000	3-1	0.4571	0.8100	0.9884	0.4138	0.9981
		1	10	11-1	0.2746	0.8100	0.9824	0.3167	0.9981
		1	100	11-1	0.2746	0.8100	0.9824	0.3167	0.9981
		10	1	8-1	0.2868	0.8100	0.9846	0.3464	0.9981
		100	1	3-1	0.4571	0.8100	0.9884	0.4138	0.9981
0.99	0.90	1	1	11-1	0.2841	0.9801	0.9815	0.3485	0.9998
		1000	1000	3-1	0.4598	0.9801	0.9882	0.4568	0.9998
		1	10	11-1	0.2841	0.9801	0.9815	0.3485	0.9998
		1	100	11-1	0.2841	0.9801	0.9815	0.3485	0.9998
		10	1	8-1	0.2938	0.9801	0.9840	0.3816	0.9998
		100	1	3-1	0.4598	0.9801	0.9882	0.4568	0.9998
0.90	0.99	1	1	11-1	0.1941	0.8100	0.9990	0.8959	0.9981
		1000	1000	3-1	0.3698	0.8100	0.9997	0.9672	0.9981
		1	10	11-1	0.1941	0.8100	0.9990	0.8959	0.9981
		1	100	11-1	0.1941	0.8100	0.9990	0.8959	0.9981
		10	1	11-1	0.1941	0.8100	0.9990	0.8959	0.9981
		100	1	8-1	0.2038	0.8100	0.9993	0.9207	0.9981

Table S20: OTC summary for  $O_{GR}$  with  $p = 0.01$  under non-informative, three-stage hierarchical testing. When equally sized groups are optimal, we use the same notation as given in other tables (e.g., Table S1). When unequally sized groups are optimal, we write out each group size for its stage. For example, an OTC of “21-6,5,5,5-1” means that stage 1 has a group of size 21; stage 2 has groups of size 6, 5, 5, and 5; and stage 3 has groups of size 1.

$S_e$	$S_p$	$D_1$	$D_2$	OTC	$E(T)/I$	$PS_e$	$PS_p$	PPPV	PNPV
0.99	0.99	1	1	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
		1000	1000	14-2-1	0.1614	0.9703	0.9999	0.9889	0.9997
		1	10	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
		1	100	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
		10	1	25-5-1	0.1354	0.9703	0.9996	0.9604	0.9997
		100	1	18-3-1	0.1435	0.9703	0.9998	0.9791	0.9997
0.95	0.95	1	1	25-5-1	0.1444	0.8574	0.9977	0.7907	0.9986
		1000	1000	6-2-1	0.2401	0.8574	0.9993	0.9289	0.9986
		1	10	25-5-1	0.1444	0.8574	0.9977	0.7907	0.9986
		1	100	25-5-1	0.1444	0.8574	0.9977	0.7907	0.9986
		10	1	20-4-1	0.1479	0.8574	0.9982	0.8290	0.9986
		100	1	12-2-1	0.1841	0.8574	0.9992	0.9166	0.9986
0.90	0.90	1	1	24-6-1	0.1562	0.7290	0.9938	0.5437	0.9973
		1000	1000	4-2-1	0.3432	0.7290	0.9980	0.7900	0.9973
		1	10	24-6-1	0.1562	0.7290	0.9938	0.5437	0.9973
		1	100	24-6-1	0.1562	0.7290	0.9938	0.5437	0.9973
		10	1	20-4-1	0.1644	0.7290	0.9955	0.6192	0.9973
		100	1	10-2-1	0.2202	0.7290	0.9976	0.7533	0.9973
0.99	0.90	1	1	21-6,5,5,5-1	0.1714	0.9703	0.9937	0.6074	0.9997
		1000	1000	4-2-1	0.3486	0.9703	0.9979	0.8204	0.9997
		1	10	21-6,5,5,5-1	0.1714	0.9703	0.9937	0.6074	0.9997
		1	100	21-6,5,5,5-1	0.1714	0.9703	0.9937	0.6074	0.9997
		10	1	16-4-1	0.1785	0.9703	0.9951	0.6684	0.9997
		100	1	8-2-1	0.2438	0.9703	0.9975	0.7977	0.9997
0.90	0.99	1	1	25-5-1	0.1229	0.7290	0.9997	0.9564	0.9973
		1000	1000	3-1	0.3698	0.8100	0.9997	0.9672	0.9981
		1	10	25-5-1	0.1229	0.7290	0.9997	0.9564	0.9973
		1	100	11-1	0.1941	0.8100	0.9990	0.8959	0.9981
		10	1	25-5-1	0.1229	0.7290	0.9997	0.9564	0.9973
		100	1	21-3-1	0.1330	0.7290	0.9998	0.9766	0.9973