Sample Set 3

Files in this set were generated using the same retention times and peak areas; however different noise and baseline settings were used. The baseline used in generating drift is provided for potential baseline subtraction. Two files were generated using increased and decreased efficiency (N=100000 and N=5000). Details for each file are summarized in the tables below, and screen captures of program settings are provided on the following pages.

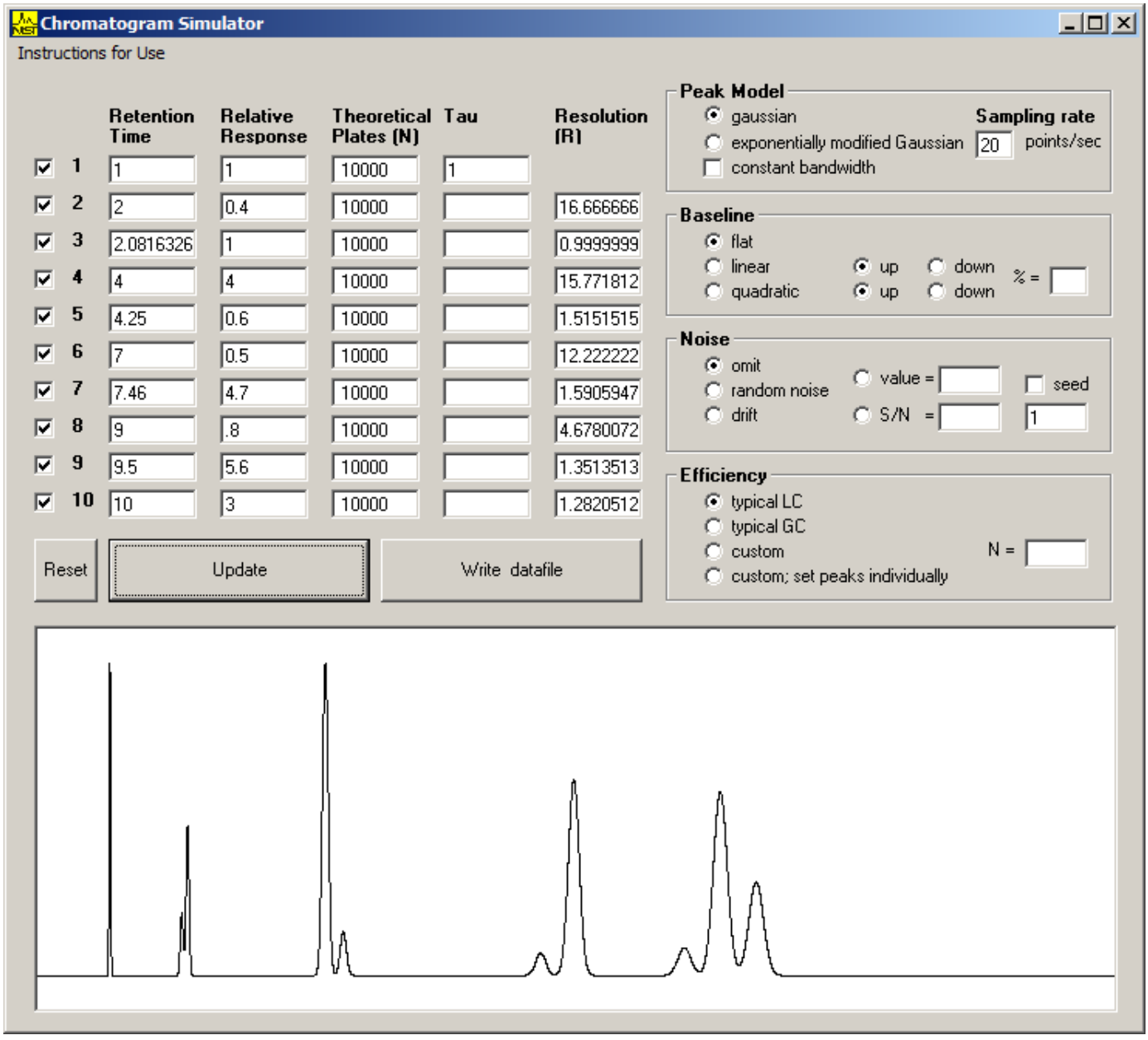
Component Identification

peak ID	retention (min)	response (area)
IS	1	1
peak 2	2	0.4
peak 2b	2.081	1
peak 4	4	4
peak 4a	4.25	0.6
peak 7	7	0.5
peak 7b	7.46	4.7
peak 9	9	0.8
peak 9a	9.5	5.6
peak 10	10	3

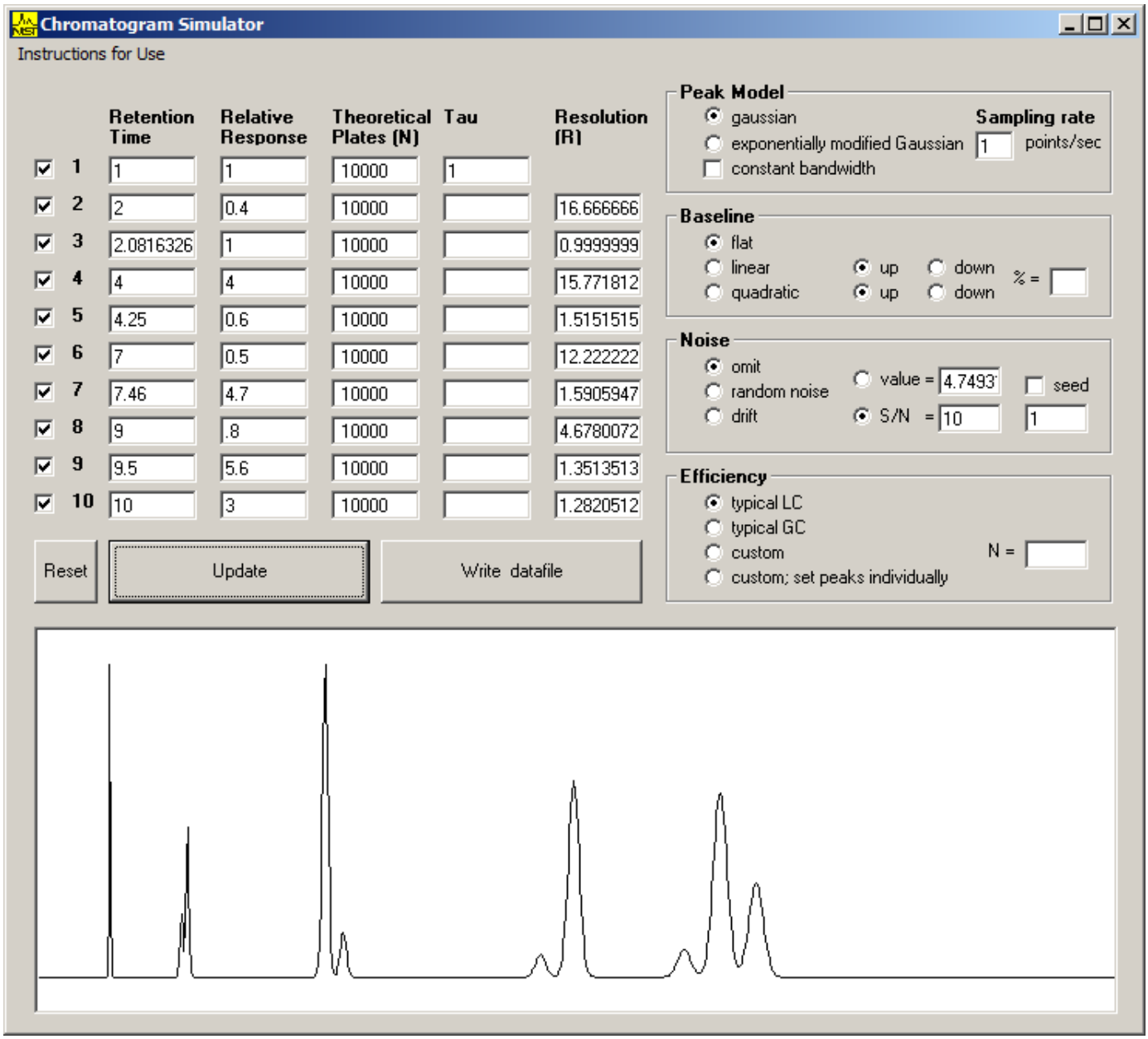
Sample Identification

Sample ID	**sampling rate**	**N**	**noise**
sample 21	20 points/sec	10000	
sample 22	1 point/sec	10000	
sample 23	100 point/sec	10000	
sample 24	20 points/sec	10000	random; S/N=10
sample 25	1 point/sec	10000	random; S/N=3
sample 26	20 points/sec	10000	drift; value=0.001
sample 27	20 points/sec	10000	sample 26 baseline only; drift; value=0.001
sample 28	20 points/sec	10000	drift; value=0.001; increasing baseline
sample 29	20 points/sec	100000	
sample 30	20 points/sec	5000	

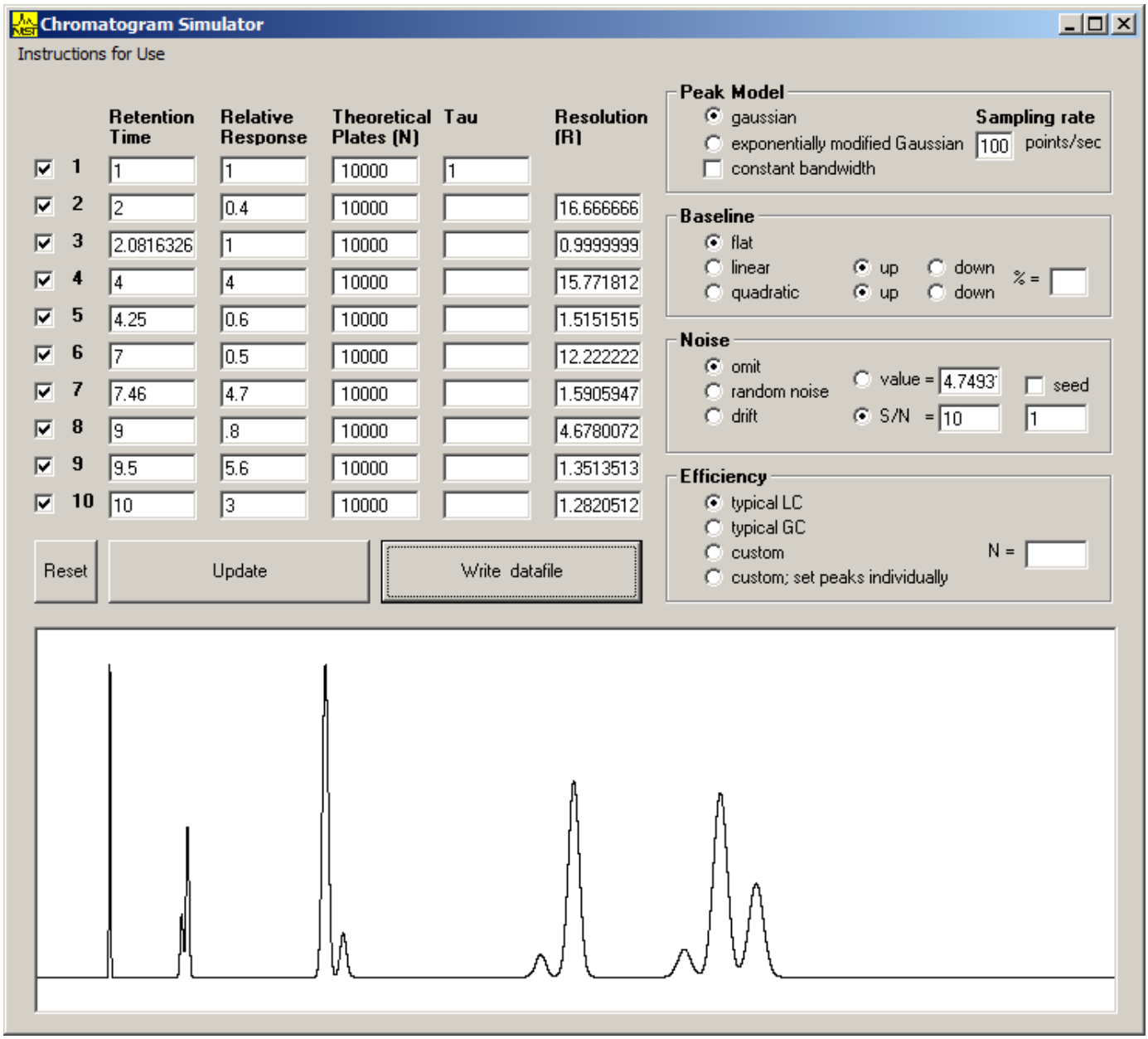
Sample 21


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
20
points/sec
Baseline
flat
linear
quadratic
up
down
up
down
% =
Noise
omit
random noise
drift
value =
S/N =
seed
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

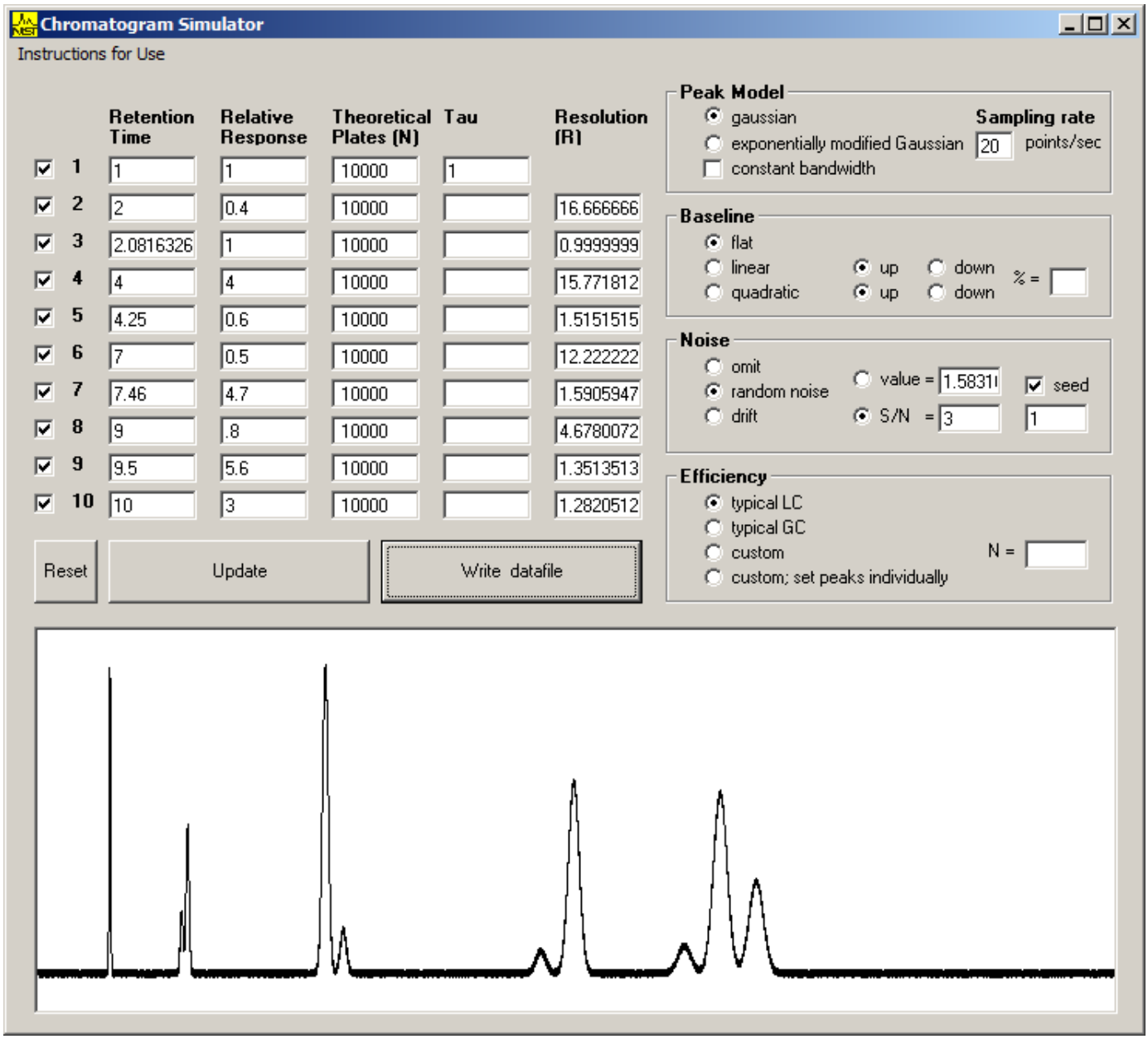
Sample 22


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
1
points/sec
Baseline
flat
linear
quadratic
up
down
up
down
% =
Noise
omit
random noise
drift
value = 4.7493
S/N = 10
seed
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

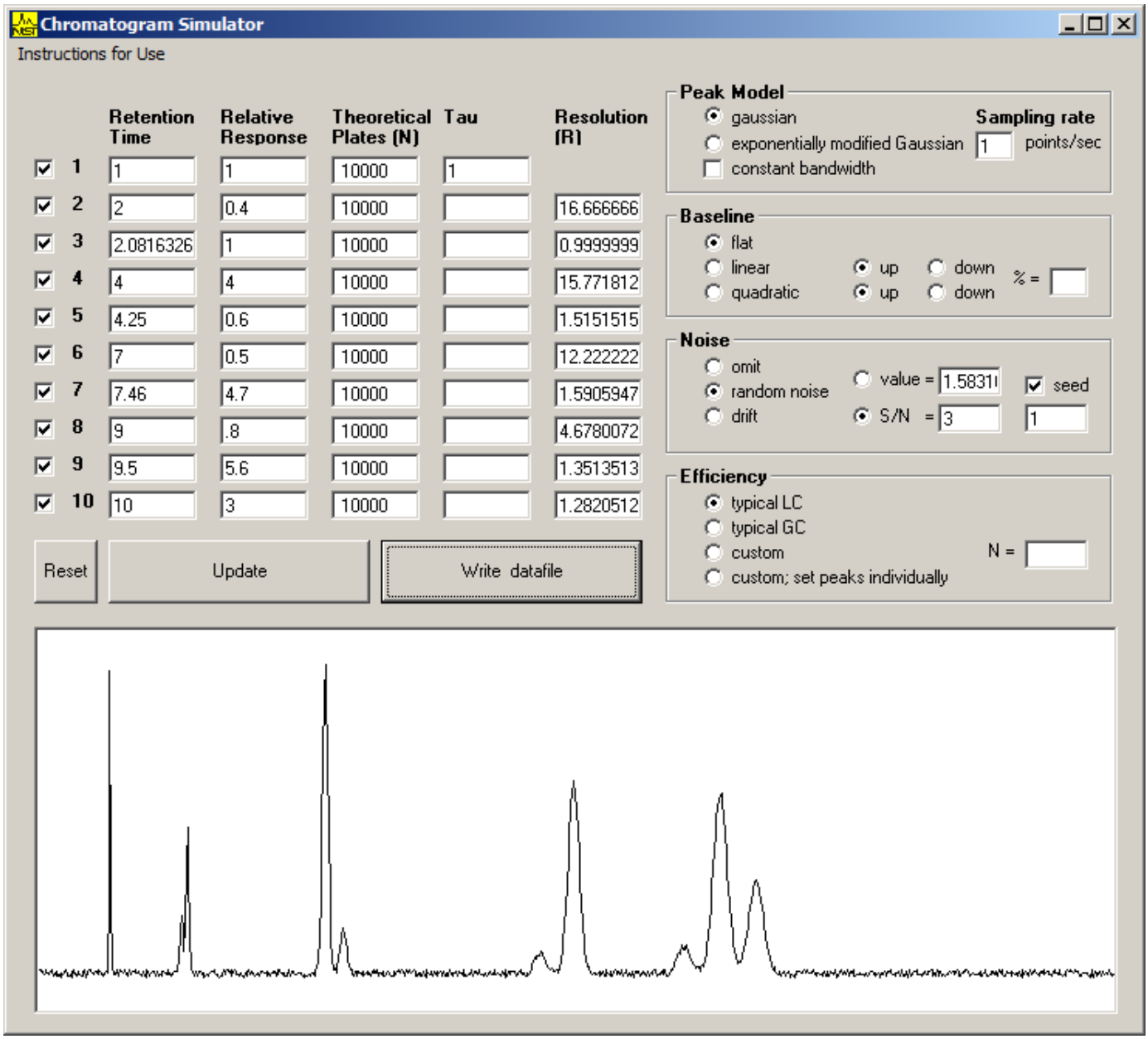
Sample 23


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
100 points/sec
Baseline
flat
linear up down
quadratic up down
% =
Noise
omit
random noise
drift
value = 4.7493
seed
S/N = 10 1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

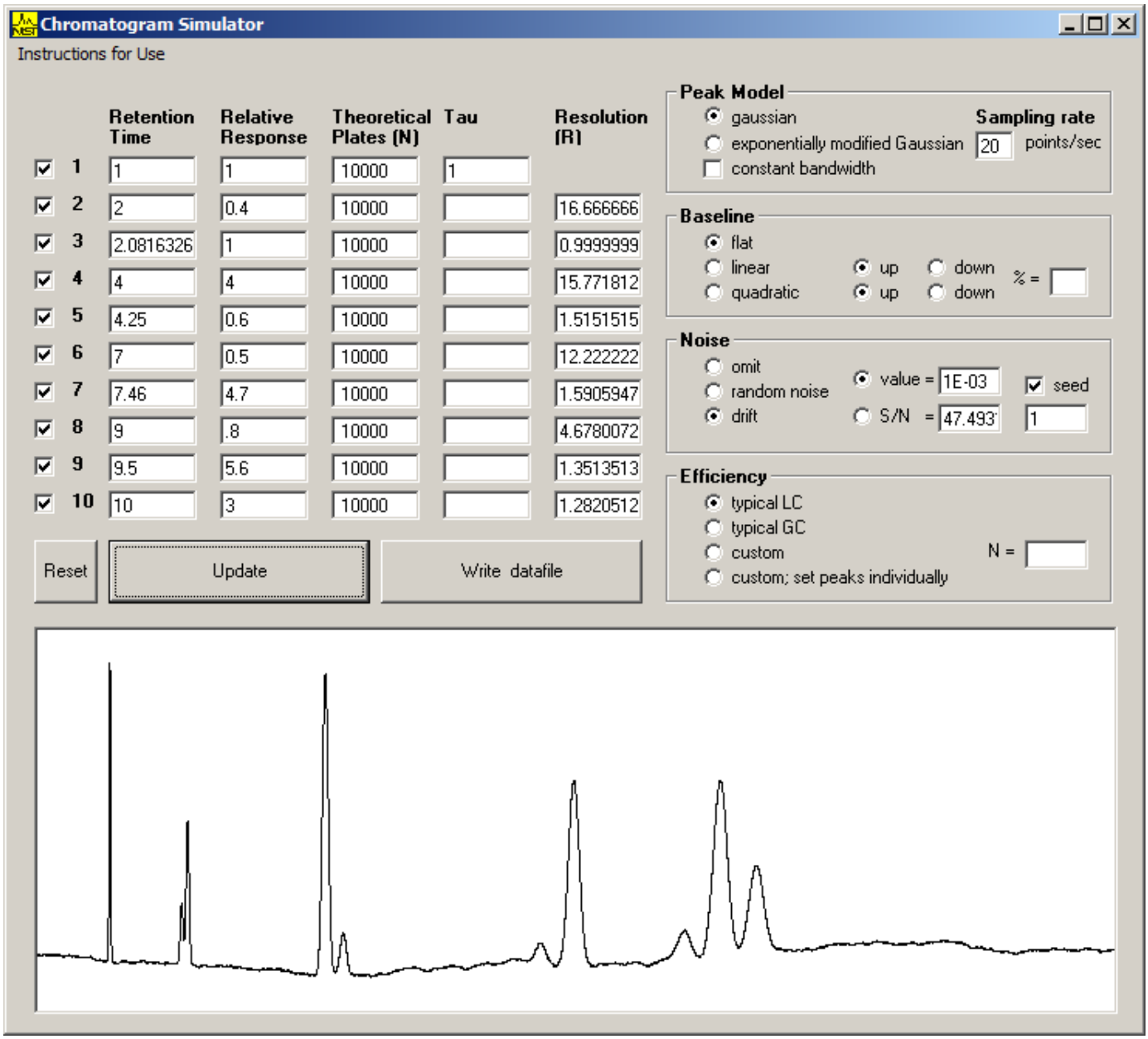
Sample 24


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
20
points/sec
Baseline
flat
linear
quadratic
up
down
up
down
% =
Noise
omit
random noise
drift
value = 1.58311
seed
S/N = 3
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

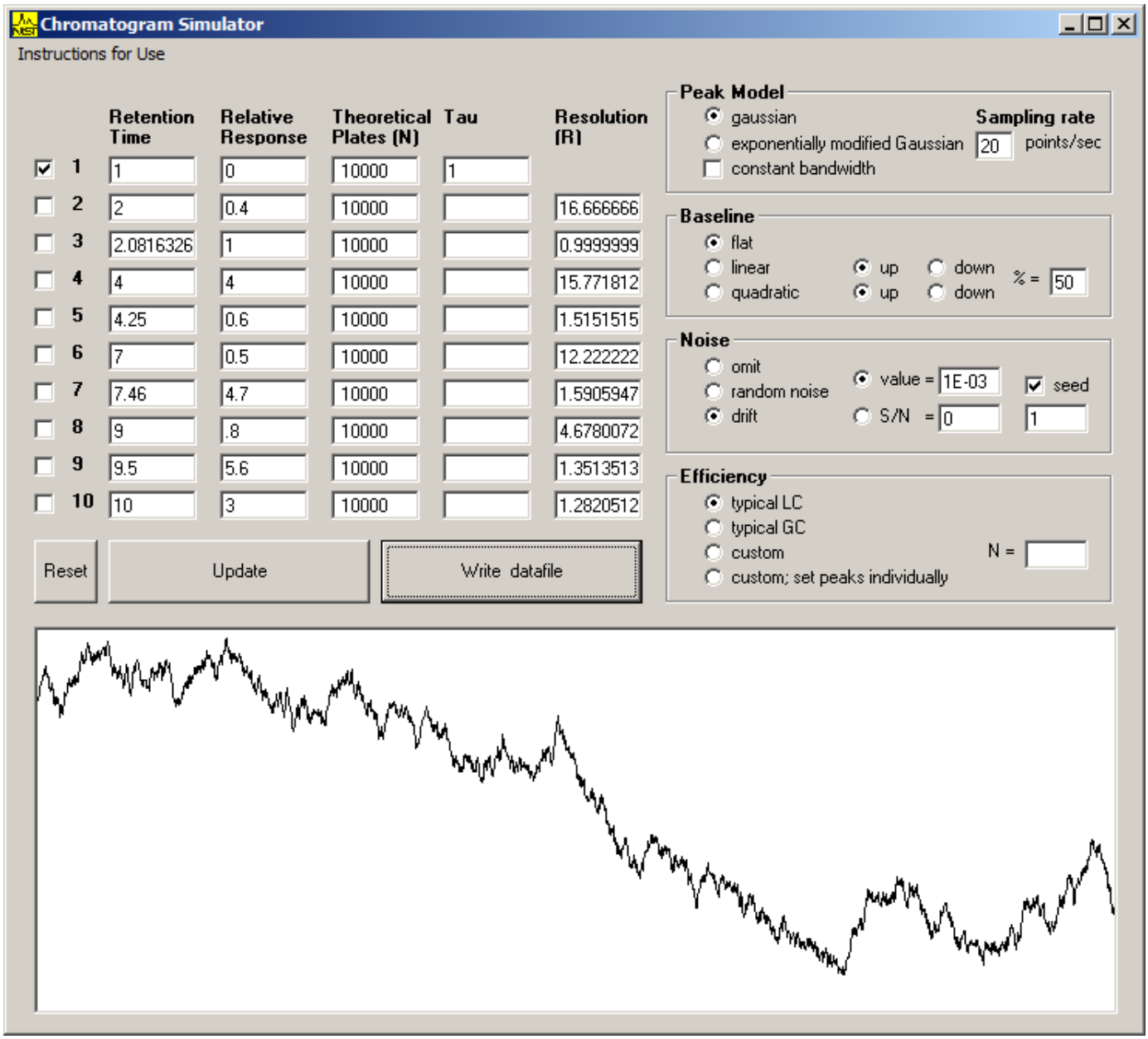
Sample 25


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
1
points/sec
Baseline
flat
linear
quadratic
up
down
up
down
% =
Noise
omit
random noise
drift
value = 1.58311
seed
S/N = 3
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

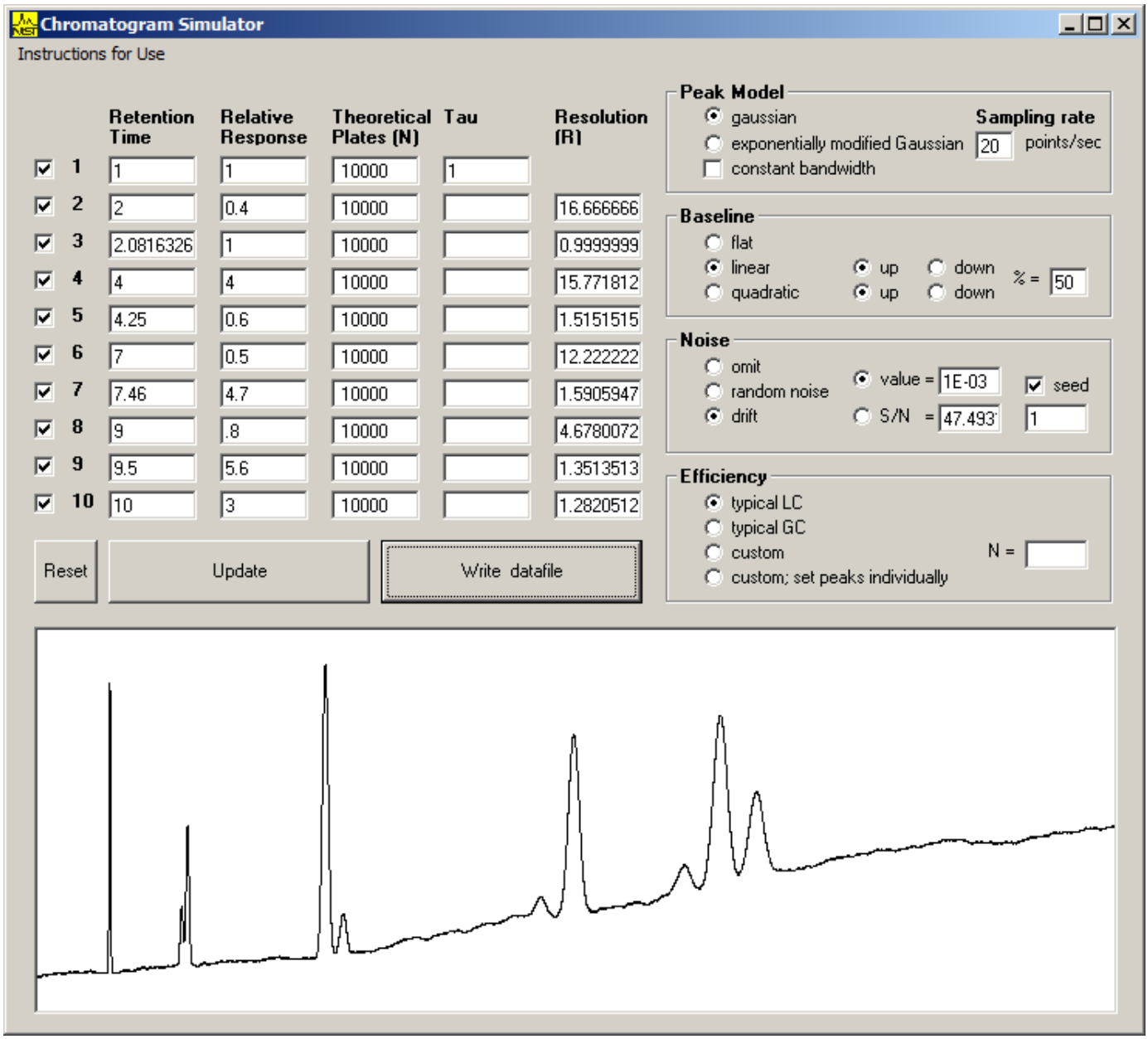
Sample 26


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
20
points/sec
Baseline
flat
linear
quadratic
up
down
up
down
% =
Noise
omit
random noise
drift
value = 1E-03
S/N = 47.493
seed
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

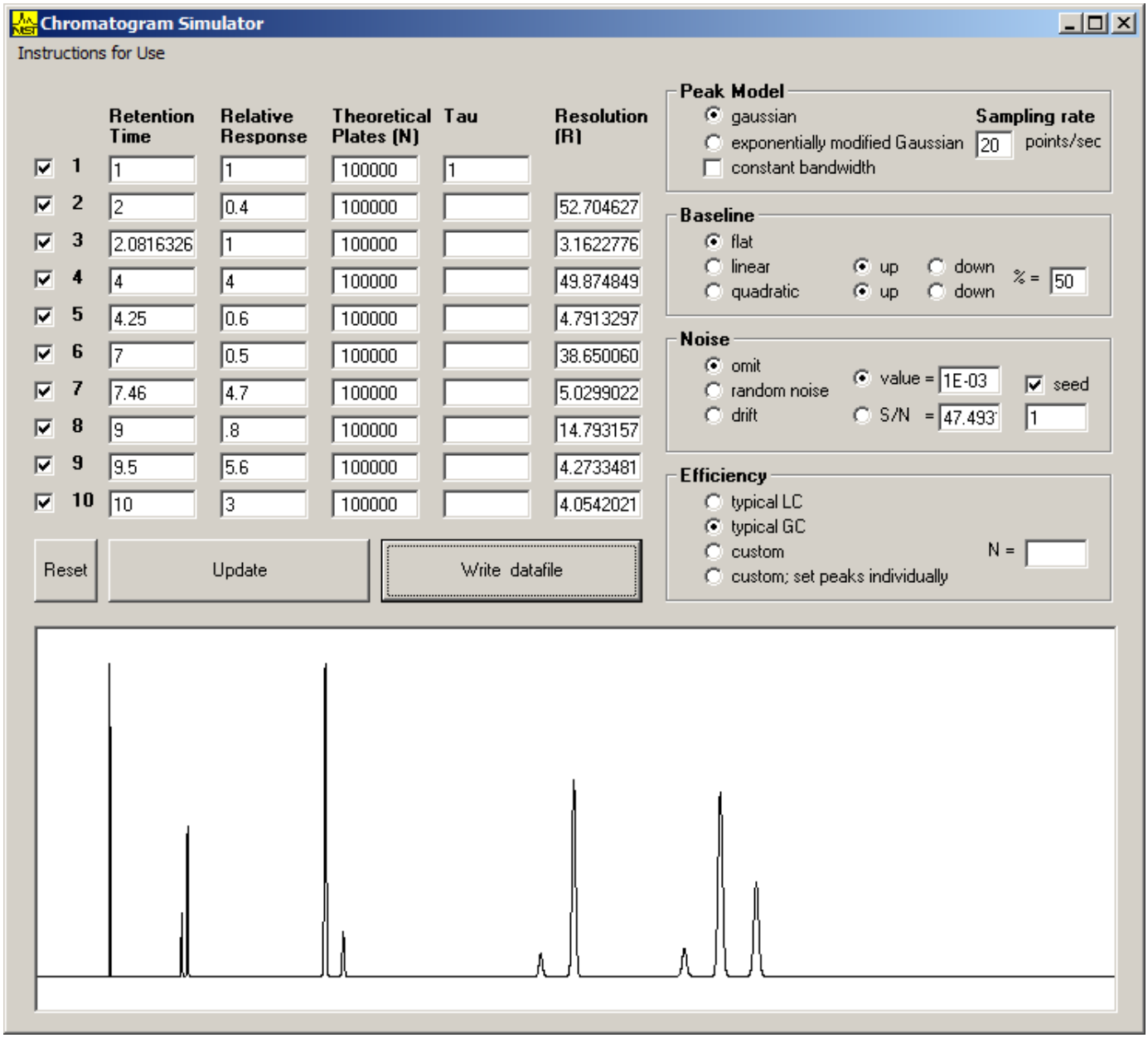
Sample 27


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 0 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
20 points/sec
Baseline
flat
linear up down
quadratic up down
% = 50
Noise
omit
random noise
drift
value = 1E-03
seed
S/N = 0 1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

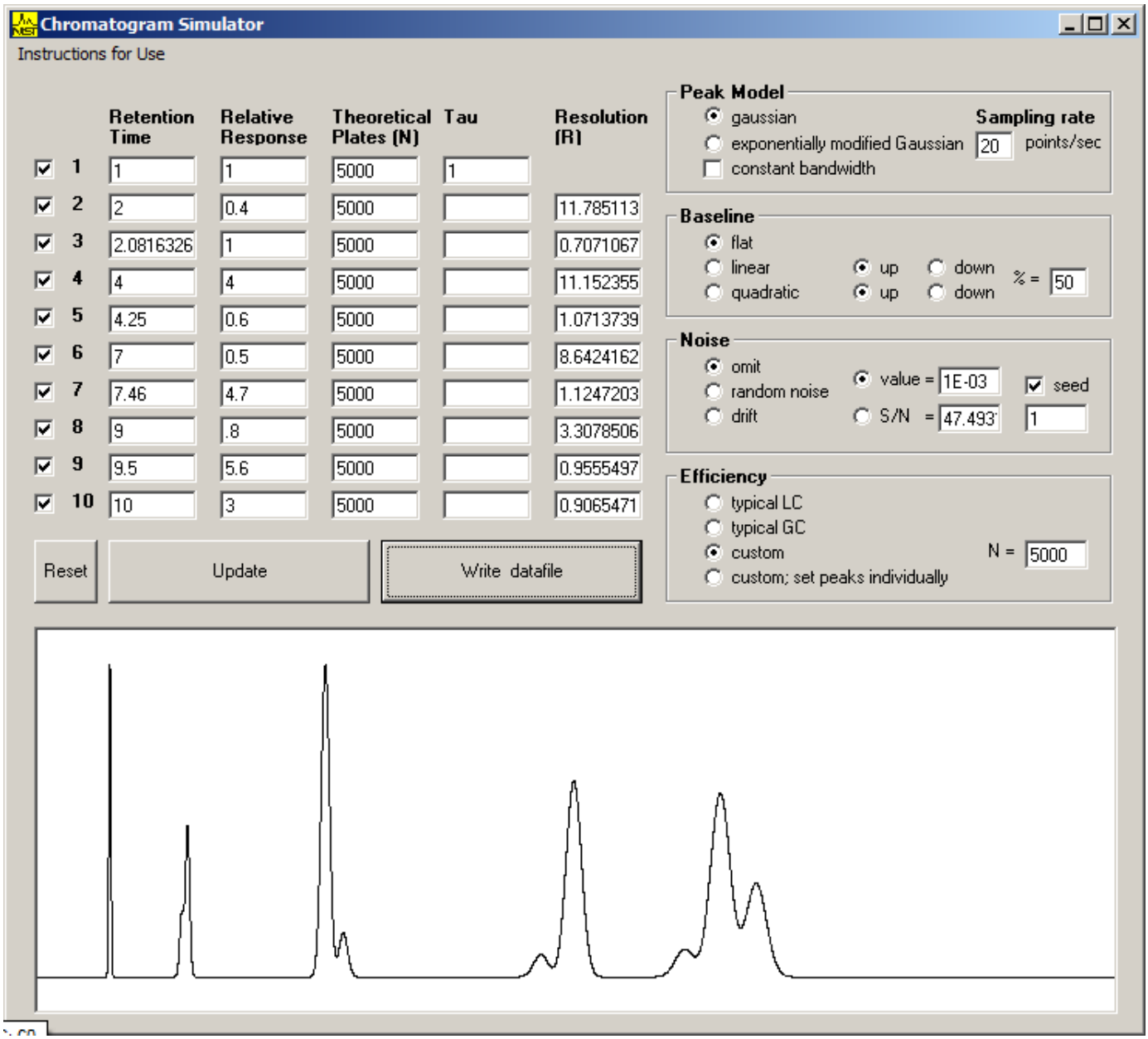
Sample 28


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 10000 1
2 2 0.4 10000 16.666666
3 2.0816326 1 10000 0.9999999
4 4 4 10000 15.771812
5 4.25 0.6 10000 1.5151515
6 7 0.5 10000 12.222222
7 7.46 4.7 10000 1.5905947
8 9 .8 10000 4.6780072
9 9.5 5.6 10000 1.3513513
10 10 3 10000 1.2820512
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
20 points/sec
Baseline
flat
linear up down
quadratic up down
% = 50
Noise
omit
random noise
drift
value = 1E-03
S/N = 47.493
seed
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

Sample 29


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 100000 1
2 2 0.4 100000 52.704627
3 2.0816326 1 100000 3.1622776
4 4 4 100000 49.874849
5 4.25 0.6 100000 4.7913297
6 7 0.5 100000 38.650060
7 7.46 4.7 100000 5.0299022
8 9 .8 100000 14.793157
9 9.5 5.6 100000 4.2733481
10 10 3 100000 4.0542021
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
20 points/sec
Baseline
flat
linear up down
quadratic up down
% = 50
Noise
omit
random noise
drift
value = 1E-03
S/N = 47.493
seed
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N =

Sample 30


Chromatogram Simulator
Instructions for Use
Retention Time
Relative Response
Theoretical Plates (N)
Tau
Resolution (R)
1 1 1 5000 1
2 2 0.4 5000 11.785113
3 2.0816326 1 5000 0.7071067
4 4 4 5000 11.152355
5 4.25 0.6 5000 1.0713739
6 7 0.5 5000 8.6424162
7 7.46 4.7 5000 1.1247203
8 9 .8 5000 3.3078506
9 9.5 5.6 5000 0.9555497
10 10 3 5000 0.9065471
Reset
Update
Write datafile
Peak Model
gaussian
exponentially modified Gaussian
constant bandwidth
Sampling rate
20 points/sec
Baseline
flat
linear up down
quadratic up down
% = 50
Noise
omit
random noise
drift
value = 1E-03
S/N = 47.493
seed
1
Efficiency
typical LC
typical GC
custom
custom; set peaks individually
N = 5000