Simulated data

All drug response matrices we used have 100 drugs and 150 cell lines. We first embedded five true clusters in the response matrix *Rtrue* as follows: $Rtrue = UV^T$, where *U* and *V* are shown in Table S1, and their dimensions are 100×5 and 150×5, respectively. The (x, y)-element of *Rtrue* represents activity of drug *x* to cell line *y* such as activity area, and is 0 if drug *x* is the most resistant to cell line *y*; otherwise a higher value indicates a better sensitivity of cell line *y* to drug *x*. Then Gaussian noise *E* was added to *Rtrue* with *Rnoisy*=*Rtrue*-(noise_level)*E, where noise_level is a value being changed from 0 to 0.5 by the interval of 0.05. Furthermore, we masked 50% of the values of the cluster and 12.5% of the rest of values for *Rnoisy*, and the resulting matrix was used as input for the drug responses.

As to drug (cell line) similarity, we first generated a true similarity matrix *Strue* so that the (i, j)-element of *Strue* is 1 if d_i and d_j (or c_i and c_j) belong to the same true cluster; otherwise this value is 0. We then generated a random matrix *Srandom*, where each element of this matrix randomly takes a value between 0 and 1. We finally generated similarity matrices (for both drugs and cell lines) by *Snoisy*=*Strue*-(noise_level)*Srandom, where noise_level is a value being changed from 0 to 0.5 by the interval of 0.05, and the diagonal elements of *Snoisy* are forced to be 1. Figure 1S shows a simulated example with noise level = 0.2 to illustrate the efficiency of SRMF.

U

Row\Col	1st	2nd	3rd	4th	5th
u_1 ⋮ u_{20}	rand(20,1)	0	0	0	0
u_{21} ⋮ u_{40}	0	rand(20,1)	0	0	0
u_{41} ⋮ u_{60}	0	0	rand(20,1)	0	0
u_{61} ⋮ u_{80}	0	0	0	rand(20,1)	0
u_{81} ⋮ u_{100}	0	0	0	0	rand(20,1)

V

Row\Col	1st	2nd	3rd	4th	5th
v_1 ⋮ v_{50}	rand(50,1)	0	0	0	0
v_{51} ⋮ v_{90}	0	rand(40,1)	0	0	0
v_{91} ⋮ v_{120}	0	0	rand(30,1)	0	0
v_{121} ⋮ v_{140}	0	0	0	rand(20,1)	0
v_{141} ⋮ v_{150}	0	0	0	0	rand(10,1)

Table S1. Detailed *U and V* used to construct target drug response matrix *Strue*. The function rand(x, y) creates an $x \times y$ dimensional matrix with random elements in the range of (0.4, 1).

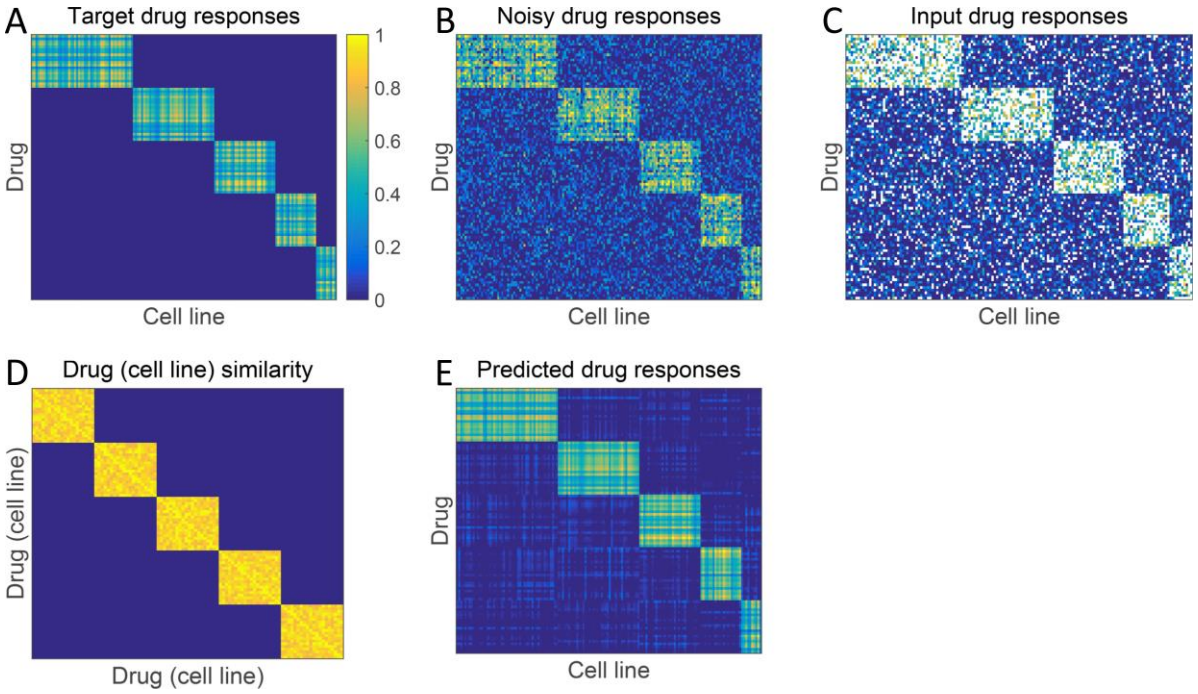

Figure S1. A simulated example illustrating the efficiency of SRMF. A) The target drug response matrix. B) The Gaussian noise with noise level = 0.2 is added to the target response matrix. C) For each drug cluster, 50% of values in the bicluster and 12.5% of the remaining cell lines were masked as missing data. D) The drug (cell line) similarity matrix. E) The predicted drug response matrix.