



Figure S1 Boxplot of AUC with different restart probability r. AUC, area under curve.

Table S1 The AUC values for 56 drugs

Drug name	AUC
5-fluorouracil	0.895401
Arsenic trioxide	0.954807
Bortezomib	0.910698
Camptothecin	0.998841
Carboplatin	0.925854
Carmustine	0.992604
Celastrol	0.975066
Cisplatin	0.899972
Crizotinib	0.880352
Cyclopamine	0.979817
Cyclophosphamide	0.917642
Cytarabine	0.972832
Dasatinib	0.907179
Daunorubicin	0.960053
Decitabine	0.993539
Dexamethasone	0.969055
Docetaxel	0.940776
Doxorubicin	0.897135
Epirubicin	0.96032
Erlotinib	0.950577
Etoposide	0.948093
Fludarabine	0.994175
Fulvestrant	0.99276
Gefitinib	0.929079
Gemcitabine	0.883788
Herceptin	0.943137
Hydroxyurea	0.920964
Imatinib	0.939539
Irinotecan	0.816221
Lapatinib	0.935094
Letrozole	0.933701
Melphalan	0.998998
Methotrexate	0.927484
Mitomycin C	0.931888
Mitoxantrone	0.956754
Olaparib	0.962921
Oxaliplatin	0.902214
Paclitaxel	0.906851
PD-0325901	0.989943
Pemetrexed	0.984658
PLX4720	0.920567
Prednisolone	0.957559
Ribavirin	0.973524
Sunitinib	0.987083
Sorafenib	0.880669
Sunitinib	0.93242
Tamoxifen	0.928211
Temozolomide	0.938996
Teniposide	0.994462
Topotecan	0.925976
Vemurafenib	0.9186
Verapamil	0.911376
Vinblastine	0.94019
Vincristine	0.932329
Vinorelbine	0.896929
Vorinostat	0.926175

AUC, area under curve.

Table S2 Candidate ncRNA signatures of drug resistance

Drug name	Candidate ncRNAs (top 50)
5-fluorouracil	miR-335-5p, miR-16-5p, miR-124-3p, NEAT1, let-7a-5p, MALAT1, miR-519d-3p, miR-186-5p, miR-30c-5p, miR-19a-3p, miR-9-5p, let-7f-5p, miR-8485, miR-485-5p, miR-6499-3p, miR-149-3p, miR-455-3p, miR-4728-5p, miR-877-3p, miR-6883-5p, miR-6785-5p, miR-1827, miR-7106-5p, miR-30b-3p, LINC00657, miR-526b-3p, miR-362-3p, miR-6849-3p, miR-6778-3p, miR-1277-5p, miR-30c-1-3p, miR-30c-2-3p, miR-150-5p, miR-375, miR-181b-5p, miR-7977, miR-4459, miR-6808-5p, miR-6893-5p, OIP5-AS1, KCNQ1OT1, miR-302c-3p, miR-5011-5p, miR-6799-5p, miR-190a-3p, miR-6516-5p, miR-10a-5p, miR-1304-3p, miR-574-5p, miR-4768-3p
Cisplatin	miR-124-3p, NEAT1, miR-1-3p, LINC00657, miR-8485, miR-6499-3p, miR-877-3p, miR-455-3p, miR-149-3p, miR-1277-5p, miR-1827, miR-4728-5p, miR-362-3p, miR-6883-5p, miR-6785-5p, miR-30b-3p, miR-301a-3p, miR-7106-5p, miR-5011-5p, miR-665, miR-190a-3p, OIP5-AS1, miR-574-5p, miR-539-5p, miR-30c-1-3p, miR-30c-2-3p, miR-6849-3p, miR-454-3p, KCNQ1OT1, miR-6778-3p, CTB-89H12, miR-7977, miR-423-5p, miR-4459, miR-185-3p, miR-1304-3p, miR-6808-5p, miR-520b, miR-6893-5p, miR-520e, miR-186-3p, miR-590-3p, miR-302e, miR-6516-5p, miR-6799-5p, miR-3613-3p, miR-142-3p, miR-130b-5p, miR-137, miR-6779-5p
Gemcitabine	miR-335-5p, miR-26b-5p, miR-124-3p, miR-92a-3p, miR-93-5p, NEAT1, miR-106b-5p, miR-24-3p, miR-1-3p, MALAT1, miR-186-5p, XIST, miR-320a, miR-103a-3p, miR-30c-5p, miR-26a-5p, miR-8485, miR-6499-3p, miR-485-5p, miR-149-3p, miR-4728-5p, miR-6883-5p, miR-6785-5p, miR-877-3p, miR-1827, miR-107, let-7g-5p, miR-30b-5p, miR-7106-5p, miR-30b-3p, miR-215-5p, LINC00657, miR-6849-3p, miR-362-3p, miR-23b-3p, miR-6778-3p, miR-1277-5p, miR-4459, miR-526b-3p, miR-122-5p, OIP5-AS1, miR-7977, miR-150-5p, miR-375, miR-6808-5p, miR-6516-5p, miR-6893-5p, miR-6799-5p, miR-5011-5p, miR-4768-3p
Imatinib	miR-26b-5p, miR-93-5p, miR-92a-3p, NEAT1, miR-204-5p, miR-27a-3p, miR-497-5p, miR-106b-5p, miR-34a-5p, miR-20a-5p, miR-24-3p, miR-218-5p, miR-20b-5p, miR-19b-3p, miR-484, MALAT1, miR-192-5p, let-7g-5p, XIST, miR-19a-3p, miR-7-5p, miR-320a, miR-186-5p, miR-615-3p, miR-519d-3p, miR-106a-5p, miR-98-5p, miR-125b-5p, miR-92b-3p, miR-23b-3p, miR-29a-3p, miR-129-5p, miR-766-3p, miR-185-5p, miR-149-5p, miR-30d-5p, miR-485-5p, miR-23a-3p, KCNQ1OT1, miR-32-5p, miR-8485, LINC00657, miR-877-3p, miR-940, miR-215-5p, miR-145-5p, miR-375, miR-454-3p, miR-455-3p
Docetaxel	miR-335-5p, miR-124-3p, let-7b-5p, miR-92a-3p, miR-93-5p, miR-15b-5p, NEAT1, miR-106b-5p, miR-218-5p, miR-1-3p, miR-497-5p, miR-484, MALAT1, miR-192-5p, miR-19b-3p, let-7a-5p, miR-30c-5p, miR-320a, XIST, miR-103a-3p, miR-186-5p, miR-132-3p, miR-519d-3p, miR-615-3p, miR-19a-3p, let-7e-5p, miR-30b-5p, miR-106a-5p, miR-148b-3p, miR-130b-3p, miR-98-5p, miR-107, miR-92b-3p, let-7f-5p, miR-18a-5p, miR-23b-3p, miR-29b-3p, miR-32-5p, miR-8485, miR-766-3p, miR-485-5p, miR-215-5p, let-7g-5p, miR-185-5p, LINC00657, let-7i-5p, miR-877-3p, miR-455-3p, miR-23a-3p, miR-181c-5p
Doxorubicin	MALAT1, miR-24-3p, XIST, miR-519d-3p, miR-8485, LINC00657, miR-148b-3p, miR-940, miR-877-3p, miR-455-3p, miR-6499-3p, miR-1277-5p, miR-362-3p, miR-1827, miR-149-3p, miR-526b-3p, miR-5008-3p, miR-4728-5p, miR-5011-5p, miR-30b-3p, miR-190a-3p, miR-6883-5p, miR-6785-5p, miR-665, miR-7106-5p, miR-574-5p, miR-30c-1-3p, miR-6849-3p, miR-30c-2-3p, KCNQ1OT1, OIP5-AS1, miR-6778-3p, miR-1304-3p, miR-4459, miR-7977, miR-3613-3p, miR-6808-5p, miR-590-3p, miR-6893-5p, miR-302d-3p, miR-142-3p, miR-6516-5p, miR-186-3p, miR-6799-5p, miR-423-5p, miR-3653-5p, miR-4768-3p, miR-603, miR-520b, miR-520e
Erlotinib	miR-335-5p, miR-16-5p, miR-26b-5p, miR-93-5p, let-7b-5p, miR-124-3p, miR-15a-5p, miR-15b-5p, NEAT1, miR-92a-3p, miR-195-5p, miR-20a-5p, miR-106b-5p, miR-218-5p, miR-20b-5p, miR-24-3p, miR-30c-5p, miR-424-5p, miR-27b-3p, miR-27a-3p, miR-1-3p, let-7a-5p, XIST, miR-181a-5p, miR-19b-3p, MALAT1, miR-30a-5p, miR-484, miR-192-5p, miR-103a-3p, miR-7-5p, miR-193b-3p, miR-320a, miR-519d-3p, miR-26a-5p, let-7e-5p, miR-186-5p, miR-106a-5p, LINC00657, miR-19a-3p, CTB-89H12, miR-107, miR-9-5p, miR-98-5p, miR-130b-3p, let-7f-5p, miR-615-3p, miR-148b-3p, miR-101-3p, miR-129-5p
Tamoxifen	hsa-miR-335-5p, hsa-miR-26b-5p, hsa-miR-93-5p, hsa-miR-124-3p, hsa-miR-92a-3p, hsa-miR-15b-5p, hsa-miR-106b-5p, NEAT1, hsa-miR-195-5p, hsa-miR-484, hsa-miR-218-5p, hsa-miR-204-5p, hsa-miR-27a-3p, hsa-miR-1-3p, hsa-let-7a-5p, hsa-miR-497-5p, MALAT1, XIST, hsa-miR-186-5p, hsa-miR-424-5p, hsa-miR-320a, hsa-let-7e-5p, hsa-miR-26a-5p, LINC00657, hsa-miR-30a-5p, hsa-miR-9-5p, hsa-miR-30c-5p, hsa-miR-98-5p, hsa-let-7f-5p, hsa-miR-92b-3p, hsa-miR-215-5p, hsa-miR-129-5p, hsa-miR-766-3p, hsa-miR-130b-3p, hsa-miR-8485, hsa-let-7g-5p, hsa-miR-485-5p, hsa-miR-30b-5p, hsa-miR-23a-3p, hsa-miR-877-3p, hsa-miR-101-3p, hsa-miR-940, hsa-miR-25-3p, hsa-miR-455-3p, hsa-miR-526b-3p, hsa-let-7d-5p, hsa-miR-6499-3p, KCNQ1OT1, hsa-miR-29a-3p, CTB-89H12
Paclitaxel	miR-26b-5p, miR-185-5p, miR-92a-3p, miR-93-5p, MALAT1, miR-103a-3p, miR-519d-3p, let-7f-5p, miR-92b-3p, miR-98-5p, miR-766-3p, LINC00657, miR-148b-3p, miR-8485, miR-485-5p, miR-23a-3p, miR-940, miR-455-3p, miR-877-3p, miR-6499-3p, miR-149-3p, miR-1827, miR-4728-5p, miR-526b-3p, miR-362-3p, miR-1277-5p, miR-30b-3p, miR-6785-5p, miR-6883-5p, miR-665, miR-7106-5p, miR-122-5p, miR-30c-1-3p, miR-30c-2-3p, OIP5-AS1, miR-6849-3p, miR-5011-5p, miR-190a-3p, miR-520a-3p, miR-574-5p, miR-454-3p, let-7c-5p, miR-30d-5p, miR-302c-3p, miR-30e-5p, miR-302a-3p, miR-6778-3p, miR-7977, miR-4459, miR-520c-3p
Sorafenib	miR-335-5p, miR-16-5p, miR-26b-5p, miR-124-3p, let-7b-5p, miR-93-5p, miR-17-5p, miR-92a-3p, NEAT1, miR-1-3p, miR-15b-5p, miR-15a-5p, miR-27a-3p, miR-20b-5p, miR-218-5p, miR-24-3p, miR-484, miR-195-5p, miR-19b-3p, XIST, MALAT1, miR-155-5p, miR-497-5p, let-7a-5p, miR-186-5p, miR-519d-3p, miR-615-3p, miR-215-5p, miR-30c-5p, miR-19a-3p, miR-106a-5p, miR-26a-5p, miR-320a, let-7e-5p, miR-9-5p, miR-103a-3p, miR-424-5p, miR-30b-5p, miR-98-5p, miR-129-5p, miR-8485, miR-766-3p, miR-125b-5p, miR-92b-3p, miR-877-3p, miR-21-5p, OIP5-AS1, let-7f-5p, miR-101-3p, miR-455-3p

Table S3 candidate ncRNAs involved in multiple drugs resistance and enriched pathways

miRNA	Drug name	Pathway ID
miR-92a-3p	Paclitaxel, sorafenib, gemcitabine, imatinib, Docetaxel, tamoxifen, erlotinib	hsa04110, hsa03010, hsa03013, hsa05200, hsa04919, hsa05169, hsa03018, hsa05130, hsa05205, hsa04068, hsa05161, hsa03040, hsa04115, hsa05166, hsa03050, hsa04144, hsa04152, hsa04390, hsa01230, hsa04114
miR-124-3p	Cisplatin, gemcitabine, erlotinib, docetaxel, sorafenib, tamoxifen, 5-fluorouracil	hsa05200, hsa05100, hsa05205, hsa04933, hsa05166, hsa04072, hsa04611, hsa04360, hsa04370, hsa04071, hsa05132, hsa04550, hsa04530, hsa05161, hsa05130, hsa05202, M00087, hsa04730, hsa04520, hsa04912
miR-335-5p	Gemcitabine, docetaxel, erlotinib, tamoxifen, sorafenib, 5-fluorouracil	hsa00100, hsa04060, hsa04151, hsa04014, hsa05224, hsa04915, hsa04010, hsa04970, hsa04020, hsa04610, hsa04550, hsa05202, hsa04933, hsa04670, hsa04072, hsa04640, hsa04657, hsa04931, M00098, hsa04972
miR-8485	Cisplatin, paclitaxel, gemcitabine, imatinib, docetaxel, tamoxifen, sorafenib, doxorubicin, 5-fluorouracil	hsa05200, hsa05203, hsa05217, hsa04360, hsa05215, hsa04931, hsa05211, hsa04144, hsa04392, hsa04630, hsa05202, hsa04340
miR-877-3p	Cisplatin, paclitaxel, gemcitabine, imatinib, docetaxel, tamoxifen, sorafenib, doxorubicin, 5-fluorouracil	hsa03040, hsa05130, hsa03013, hsa04213, hsa04915, hsa05169, hsa05110, hsa04810, hsa04070, hsa04722, hsa05223, M00001, hsa05164, hsa04721, hsa00650, hsa04144, hsa03015
miR-455-3p	Cisplatin, paclitaxel, imatinib, docetaxel, tamoxifen, sorafenib, doxorubicin, 5-fluorouracil	hsa04142, hsa04141, hsa05202, hsa00270, hsa04130, hsa05200, hsa01040, hsa04115, hsa04110
miR-6499-3p	Cisplatin, paclitaxel, gemcitabine, tamoxifen, doxorubicin, 5-fluorouracil	M00034, hsa04141, hsa00512, hsa04142, hsa00130, hsa04062, hsa04064, hsa05230, hsa04915, hsa05162
miR-30c-5p	Gemcitabine, docetaxel, erlotinib, tamoxifen, sorafenib, 5-fluorouracil	hsa05211, hsa05212, hsa05200, hsa05169, hsa05206, hsa04120, hsa04380, hsa05168, hsa04310, hsa04141, hsa04932, hsa05166, hsa04371, hsa04115, hsa04390, hsa04320, hsa04520, hsa03040
miR-93-5p	Paclitaxel, erlotinib, gemcitabine, imatinib, docetaxel, tamoxifen, sorafenib	hsa05200, hsa05166, hsa04144, hsa05212, hsa04390, hsa05205, hsa04140, hsa05164, hsa04137, hsa04919, hsa04115, hsa04962, hsa04010, hsa04810, hsa04120, hsa04210, hsa04910, hsa04152, hsa03013, hsa04668
miR-519d-3p	Paclitaxel, imatinib, docetaxel, erlotinib, sorafenib, doxorubicin, 5-fluorouracil	hsa05200, hsa04144, hsa04350, hsa04140, hsa04115, hsa05205, hsa05164, hsa04810, hsa04962, hsa05211, hsa01524, hsa03018, hsa04360, hsa04137, hsa05203, hsa04151, hsa00240, hsa04611, hsa04931, hsa04010
miR-98-5p	Paclitaxel, imatinib, docetaxel, sorafenib, tamoxifen, erlotinib	hsa05203, hsa05200, hsa04066, hsa04068, hsa05206, hsa04630, hsa05205, hsa04211, hsa04550, hsa05202, hsa05169, hsa04668, hsa04115, hsa05120, hsa04350, hsa04666, hsa00230, hsa05162, hsa04010, hsa04977
miR-186-5p	Gemcitabine, imatinib, docetaxel, tamoxifen, erlotinib, sorafenib, 5-fluorouracil	hsa03010, hsa03013, hsa03040, hsa04550, hsa03050, hsa00310, hsa04014, hsa05230, hsa00190, M00135, hsa04710, hsa04390, hsa04137, hsa05205, hsa04540, hsa05220, hsa00620, hsa05412, hsa04360, hsa05100
let-7f-5p	Paclitaxel, docetaxel, tamoxifen, erlotinib, sorafenib, 5-fluorouracil	hsa04115, hsa04630, hsa04110, hsa05169, hsa04068, hsa05214, hsa05224, hsa05130, hsa04657, hsa05120, hsa04380, hsa00240
miR-1-3p	Cisplatin, docetaxel, gemcitabine, tamoxifen, erlotinib, sorafenib	hsa05200, hsa05205, hsa05034, hsa05410, hsa04261, hsa03030, hsa05132, hsa04933, hsa04062, hsa04530, hsa05214, hsa05100, hsa05206, hsa05323, hsa04320, hsa04520, hsa03015, hsa03040, hsa01212, hsa05418
miR-320a	Gemcitabine, imatinib, docetaxel, tamoxifen, erlotinib, sorafenib	hsa05131, hsa05202, hsa05203, hsa05200, hsa03010, hsa05012, hsa05211, hsa05166, hsa04919, hsa04114, hsa05206, hsa03013, hsa04722, hsa04141, hsa00230, hsa05130, hsa04390, hsa04550, hsa04022, hsa05110
miR-485-5p	Paclitaxel, tamoxifen, gemcitabine, imatinib, docetaxel, 5-fluorouracil	hsa04210, hsa03030, hsa04064, hsa00240, hsa04962, hsa05168, hsa05215, hsa05164, hsa00250, hsa05202
miR-26b-5p	Paclitaxel, gemcitabine, imatinib, tamoxifen, erlotinib, sorafenib	hsa04115, hsa05222, hsa05010, hsa05134, hsa05203, hsa01524, hsa04210, hsa04657, hsa05418, hsa04010, hsa04933, hsa04974, hsa05161, hsa05218, hsa04371, hsa04144, hsa04978, hsa04060, hsa04066, hsa04072
LINC00657	Cisplatin, paclitaxel, gemcitabine, imatinib, docetaxel, tamoxifen, erlotinib, doxorubicin, 5-fluorouracil	M00052, hsa04070, hsa04114