**Predicting cell line-specific synergistic drug combinations through a relational graph convolutional network with attention mechanism**

Supplementary information

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Figure S1. The metrics ACC, F1, precision, and recall values of different methods in each cell line on the O’Neil dataset (Loewe). The mean values of different folds are shown as solid lines. Error bars in terms of one standard deviation are shown as shaded areas.



Figure S2. The metrics ACC, F1, precision, and recall values of SDCNet with and without the common features in each cell line on the O’Neil dataset (Loewe). The P-values are calculated by Wilcoxon signed-rank test. \* represents P-value < 0.05.



Figure S3. The distribution of the drug combinations who achieved the highest probability score predicted by SDCNet in each cell line on the O’Neil dataset (Loewe).

Table S1. The performances of SDCNet and state-of-the-art methods on the O’Neil dataset (Loewe) with threshold of 30 to label the combination as synergistic.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Methods** | **AUC** | **ACC** | **AUPR** | **F1** | **Precision** | **Recall** |
| DeepSynergy | 0.85 ± 0.03 | 0.82 ± 0.02 | 0.50 ± 0.06 | 0.10 ± 0.09 | 0.5 ± 0.5 | 0.09 ± 0.08 |
| Matchmaker | 0.86 ± 0.02 | **0.93 ± 0.01** | 0.52 ± 0.12 | 0.01 ± 0.02 | 0.10 ± 0.16 | 0.01 ± 0.01 |
| Jiang's method | 0.82 ± 0.02 | 0.69 ± 0.01 | 0.80 ± 0.02 | 0.60 ± 0.05 | 0.81 ± 0.01 | 0.48 ± 0.06 |
| DeepDDS | **0.89 ± 0.01** | 0.75 ± 0.01 | 0.86 ± 0.01 | 0.68 ± 0.02 | 0.94 ± 0.06 | 0.54 ± 0.04 |
| DTF | **0.89 ± 0.01** | 0.68 ± 0.01 | **0.89 ± 0.01** | 0.54 ± 0.02 | **0.97 ± 0.03** | 0.37 ± 0.13 |
| SDCNet | 0.88 ± 0.02 | 0.76 ± 0.02 | 0.88 ± 0.02 | **0.70 ± 0.03** | 0.92 ± 0.03 | **0.56 ± 0.04** |

Table S2. Summary of the drug combinations' synergy data in each cell line for the O’Neil dataset.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Cell line ID** | **Cell line** | **All DC** | **Loewe** | | **Bliss** | | **ZIP** | | **HSA** | |
| **Positive** | **Negative** | **Positive** | **Negative** | **Positive** | **Negative** | **Positive** | **Negative** |
| 0 | A2058 | 583 | 229 | 198 | 336 | 43 | 374 | 18 | 369 | 39 |
| 1 | A2780 | 583 | 211 | 185 | 415 | 10 | 470 | 10 | 498 | 10 |
| 2 | A375 | 583 | 270 | 171 | 315 | 78 | 338 | 36 | 355 | 68 |
| 3 | A427 | 583 | 195 | 222 | 121 | 162 | 176 | 89 | 290 | 52 |
| 4 | CAOV3 | 583 | 218 | 245 | 239 | 78 | 275 | 47 | 355 | 37 |
| 5 | ES2 | 583 | 181 | 232 | 240 | 70 | 297 | 29 | 280 | 65 |
| 6 | HCT116 | 583 | 174 | 235 | 163 | 115 | 216 | 54 | 259 | 81 |
| 7 | HT144 | 583 | 170 | 241 | 136 | 89 | 143 | 119 | 265 | 76 |
| 8 | HT29 | 583 | 222 | 211 | 288 | 51 | 302 | 21 | 367 | 38 |
| 9 | KPL1 | 583 | 234 | 181 | 167 | 158 | 161 | 166 | 275 | 54 |
| 10 | LNCAP | 583 | 204 | 277 | 74 | 309 | 136 | 202 | 231 | 144 |
| 11 | LOVO | 583 | 205 | 210 | 23 | 233 | 63 | 89 | 261 | 78 |
| 12 | MDAMB436 | 583 | 199 | 156 | 112 | 129 | 73 | 125 | 263 | 42 |
| 13 | MSTO | 583 | 220 | 259 | 304 | 134 | 375 | 92 | 386 | 104 |
| 14 | NCIH1650 | 583 | 187 | 241 | 101 | 151 | 103 | 148 | 230 | 77 |
| 15 | NCIH2122 | 583 | 164 | 271 | 247 | 85 | 298 | 47 | 338 | 62 |
| 16 | NCIH23 | 583 | 110 | 312 | 88 | 167 | 139 | 97 | 225 | 77 |
| 17 | NCIH460 | 583 | 184 | 245 | 150 | 113 | 172 | 84 | 276 | 55 |
| 18 | NCIH520 | 583 | 166 | 250 | 186 | 109 | 225 | 45 | 300 | 54 |
| 19 | OV90 | 583 | 158 | 264 | 70 | 142 | 96 | 131 | 234 | 51 |
| 20 | RKO | 583 | 224 | 193 | 199 | 117 | 228 | 55 | 326 | 65 |
| 21 | RPMI7951 | 583 | 146 | 289 | 191 | 74 | 236 | 42 | 318 | 52 |
| 22 | SKMEL30 | 583 | 223 | 182 | 363 | 51 | 369 | 31 | 346 | 50 |
| 23 | SKMES1 | 583 | 198 | 234 | 135 | 127 | 190 | 75 | 292 | 27 |
| 24 | SKOV3 | 583 | 240 | 166 | 342 | 28 | 339 | 18 | 371 | 21 |
| 25 | SW620 | 583 | 172 | 184 | 213 | 68 | 270 | 36 | 286 | 34 |
| 26 | SW837 | 583 | 205 | 241 | 115 | 197 | 174 | 131 | 251 | 112 |
| 27 | T47D | 583 | 195 | 286 | 257 | 106 | 256 | 90 | 321 | 63 |
| 28 | UACC62 | 583 | 231 | 197 | 181 | 114 | 159 | 91 | 308 | 58 |
| 29 | VCAP | 583 | 277 | 185 | 371 | 35 | 302 | 40 | 338 | 45 |
| 30 | ZR751 | 583 | 176 | 292 | 24 | 408 | 52 | 360 | 223 | 106 |
|  | Total | 18073 | 6188 | 7055 | 6166 | 3751 | 7007 | 2618 | 9437 | 1897 |

Table S3. Summary of the drug combinations' synergy data in each cell line for the ALMANAC dataset.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Cell line ID** | **Cell line** | **All DC** | **Loewe** | | **Bliss** | | **ZIP** | | **HSA** | |
| **Positive** | **Negative** | **Positive** | **Negative** | **Positive** | **Negative** | **Positive** | **Negative** |
| A0 | 786-0 | 2594 | 38 | 2052 | 443 | 370 | 393 | 595 | 365 | 557 |
| A1 | A498 | 2617 | 29 | 2101 | 374 | 476 | 276 | 810 | 303 | 610 |
| A2 | A549 | 2603 | 40 | 2016 | 519 | 367 | 549 | 495 | 475 | 549 |
| A3 | ACHN | 2648 | 19 | 2166 | 451 | 444 | 472 | 433 | 360 | 654 |
| A4 | BT-549 | 2629 | 44 | 2061 | 566 | 463 | 480 | 712 | 397 | 619 |
| A5 | CAKI-1 | 2608 | 32 | 2136 | 478 | 724 | 488 | 706 | 388 | 913 |
| A6 | CCRF-CEM | 2567 | 38 | 2091 | 624 | 550 | 762 | 345 | 441 | 773 |
| A7 | COLO 205 | 2593 | 28 | 2057 | 589 | 552 | 676 | 552 | 403 | 742 |
| A8 | DU-145 | 2618 | 35 | 2058 | 692 | 485 | 659 | 420 | 411 | 745 |
| A9 | EKVX | 2624 | 34 | 2025 | 424 | 461 | 322 | 451 | 257 | 726 |
| A10 | HCC-2998 | 2580 | 31 | 2089 | 622 | 752 | 613 | 637 | 369 | 941 |
| A11 | HCT-15 | 2639 | 23 | 2086 | 724 | 572 | 615 | 541 | 377 | 871 |
| A12 | HCT116 | 2604 | 35 | 2058 | 638 | 700 | 691 | 399 | 514 | 791 |
| A13 | HL-60(TB) | 2412 | 60 | 1827 | 694 | 531 | 886 | 329 | 475 | 864 |
| A14 | HOP-62 | 2540 | 23 | 2040 | 710 | 582 | 622 | 491 | 409 | 771 |
| A15 | HOP-92 | 2528 | 20 | 1983 | 433 | 573 | 317 | 869 | 273 | 674 |
| A16 | HS 578T | 2607 | 33 | 1994 | 643 | 499 | 554 | 565 | 430 | 603 |
| A17 | HT29 | 2624 | 33 | 2016 | 787 | 452 | 647 | 549 | 469 | 655 |
| A18 | IGROV1 | 2601 | 32 | 2017 | 432 | 319 | 366 | 599 | 422 | 516 |
| A19 | K-562 | 2578 | 64 | 1969 | 668 | 703 | 742 | 504 | 555 | 829 |
| A20 | KM12 | 2622 | 46 | 2064 | 532 | 846 | 555 | 893 | 334 | 927 |
| A21 | LOX IMVI | 2490 | 69 | 1936 | 498 | 663 | 557 | 604 | 420 | 754 |
| A22 | M14 | 2597 | 19 | 2182 | 591 | 431 | 595 | 483 | 274 | 717 |
| A23 | MALME-3M | 2617 | 32 | 2076 | 555 | 428 | 428 | 715 | 335 | 647 |
| A24 | MCF7 | 2650 | 26 | 2057 | 463 | 480 | 387 | 716 | 346 | 615 |
| A25 | MDA-MB-231 | 2636 | 24 | 2056 | 502 | 533 | 398 | 752 | 364 | 679 |
| A26 | MDA-MB-435 | 2582 | 17 | 2148 | 602 | 405 | 559 | 452 | 235 | 756 |
| A27 | MDA-MB-468 | 2607 | 51 | 2043 | 446 | 512 | 429 | 597 | 409 | 562 |
| A28 | MOLT-4 | 2535 | 70 | 1901 | 697 | 427 | 832 | 213 | 624 | 616 |
| A29 | NCI-H226 | 2638 | 24 | 2161 | 477 | 365 | 457 | 530 | 324 | 790 |
| A30 | NCI-H322M | 2609 | 23 | 2094 | 464 | 406 | 518 | 332 | 277 | 862 |
| A31 | NCI-H460 | 2589 | 75 | 1961 | 540 | 339 | 657 | 262 | 484 | 551 |
| A32 | NCI-H522 | 2579 | 38 | 2049 | 356 | 496 | 314 | 815 | 335 | 570 |
| A33 | NCIH23 | 2639 | 21 | 2138 | 522 | 588 | 426 | 624 | 371 | 733 |
| A34 | OVCAR-4 | 2611 | 13 | 2130 | 281 | 330 | 278 | 365 | 199 | 624 |
| A35 | OVCAR-5 | 2634 | 25 | 2129 | 433 | 436 | 378 | 726 | 321 | 589 |
| A36 | OVCAR-8 | 2615 | 31 | 2093 | 485 | 446 | 440 | 686 | 358 | 569 |
| A37 | OVCAR3 | 2553 | 33 | 2080 | 693 | 547 | 680 | 546 | 333 | 925 |
| A38 | PC-3 | 2614 | 34 | 1984 | 400 | 433 | 364 | 702 | 376 | 544 |
| A39 | RPMI-8226 | 2497 | 52 | 1956 | 684 | 603 | 739 | 516 | 470 | 810 |
| A40 | RXF 393 | 2557 | 25 | 2036 | 385 | 424 | 307 | 576 | 264 | 634 |
| A41 | SF-268 | 2641 | 23 | 2146 | 616 | 349 | 536 | 532 | 351 | 632 |
| A42 | SF-295 | 2480 | 33 | 1974 | 431 | 555 | 410 | 483 | 337 | 629 |
| A43 | SF-539 | 2596 | 22 | 2039 | 521 | 681 | 486 | 692 | 398 | 745 |
| A44 | SK-MEL-2 | 1392 | 30 | 1048 | 486 | 292 | 420 | 287 | 267 | 450 |
| A45 | SK-MEL-28 | 2643 | 28 | 2145 | 564 | 435 | 562 | 576 | 248 | 733 |
| A46 | SK-MEL-5 | 2630 | 27 | 2105 | 616 | 512 | 550 | 646 | 341 | 715 |
| A47 | SK-OV-3 | 2635 | 21 | 2179 | 473 | 406 | 393 | 692 | 293 | 657 |
| A48 | SN12C | 2621 | 31 | 2093 | 523 | 544 | 419 | 821 | 371 | 712 |
| A49 | SNB-19 | 2629 | 35 | 2123 | 549 | 449 | 555 | 546 | 373 | 649 |
| A50 | SNB-75 | 2463 | 21 | 1942 | 304 | 264 | 217 | 607 | 260 | 392 |
| A51 | SR | 2555 | 56 | 2051 | 548 | 670 | 700 | 322 | 462 | 776 |
| A52 | SW-620 | 2647 | 26 | 2187 | 465 | 419 | 550 | 567 | 375 | 676 |
| A53 | T-47D | 2589 | 22 | 1905 | 652 | 520 | 460 | 673 | 404 | 731 |
| A54 | TK-10 | 2637 | 20 | 2149 | 452 | 436 | 354 | 719 | 275 | 656 |
| A55 | U251 | 2622 | 33 | 2072 | 586 | 649 | 575 | 614 | 370 | 758 |
| A56 | UACC-257 | 2656 | 20 | 2167 | 358 | 296 | 325 | 405 | 197 | 571 |
| A57 | UACC62 | 2611 | 29 | 2017 | 352 | 446 | 313 | 692 | 356 | 442 |
| A58 | UO-31 | 2607 | 34 | 1942 | 360 | 325 | 286 | 794 | 290 | 498 |
|  | Total | 151939 | 1950 | 122574 | 30973 | 29541 | 29539 | 34330 | 21514 | 41161 |

Table S4. Summary of the drug combinations' synergy data in each cell line for the Transfer dataset.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Cell line ID** | **Cell line** | **All DC** | **Loewe** | | **Bliss** | | **ZIP** | | **HSA** | |
| **Positive** | **Negative** | **Positive** | **Negative** | **Positive** | **Negative** | **Positive** | **Negative** |
| 31 | COLO320DM | 583 | 189 | 139 | 362 | 40 | 354 | 28 | 402 | 28 |
| 32 | DLD1 | 583 | 220 | 134 | 232 | 67 | 226 | 61 | 310 | 35 |
| 33 | EFM192B | 583 | 175 | 242 | 144 | 84 | 179 | 67 | 279 | 63 |
| 34 | OCUBM | 583 | 220 | 191 | 258 | 40 | 302 | 30 | 383 | 20 |
| 35 | OVCAR3 | 583 | 238 | 251 | 188 | 106 | 189 | 98 | 231 | 75 |
| 36 | PA1 | 583 | 190 | 243 | 271 | 30 | 293 | 13 | 342 | 24 |
| 37 | UWB1289 | 583 | 206 | 226 | 85 | 188 | 128 | 127 | 288 | 34 |
| 38 | UWB1289BRCA1 | 583 | 196 | 196 | 123 | 120 | 128 | 92 | 286 | 43 |

Table S5. The performances of SDCNet and state-of-the-art methods on the CLOUD dataset with various synergy types.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Synergy type** | **Methods** | **AUC** | **ACC** | **AUPR** | **F1** | **Precision** | **Recall** |
|  | DeepSynergy | 0.62 ± 0.02 | 0.64 ± 0.02 | 0.56 ± 0.01 | 0.31 ± 0.02 | 0.72 ± 0.04 | 0.2 ± 0.02 |
|  | Matchmaker | 0.62 ± 0.01 | 0.63 ± 0.01 | 0.55 ± 0.01 | 0.22 ± 0.02 | **0.78 ± 0.04** | 0.13 ± 0.01 |
| **Loewe** | Jiang's method | 0.5 ± 0.02 | 0.5 ± 0.02 | 0.5 ± 0.0 | 0.21 ± 0.14 | 0.56 ± 0.11 | 0.15 ± 0.11 |
|  | DeepDDS | **0.67 ± 0.01** | 0.56 ± 0.01 | **0.67 ± 0.02** | 0.3 ± 0.04 | 0.75 ± 0.04 | 0.19 ± 0.03 |
|  | DTF | 0.65 ± 0.01 | **0.66 ± 0.01** | 0.5 ± 0.01 | 0.03 ± 0.05 | 0.26 ± 0.45 | 0.01 ± 0.02 |
|  | SDCNet | 0.51 ± 0.01 | 0.51 ± 0.0 | 0.5 ± 0.01 | **0.37 ± 0.08** | 0.5 ± 0.01 | **0.3 ± 0.1** |
|  | DeepSynergy | 0.68 ± 0.01 | 0.7 ± 0.01 | 0.6 ± 0.02 | 0.41 ± 0.04 | 0.81 ± 0.02 | 0.27 ± 0.03 |
|  | Matchmaker | 0.68 ± 0.01 | 0.7 ± 0.01 | 0.6 ± 0.01 | 0.39 ± 0.03 | **0.83 ± 0.02** | 0.25 ± 0.03 |
| **Bliss** | Jiang's method | 0.53 ± 0.01 | 0.53 ± 0.0 | 0.51 ± 0.01 | 0.21 ± 0.21 | 0.54 ± 0.05 | 0.17 ± 0.19 |
|  | DeepDDS | **0.76 ± 0.02** | 0.63 ± 0.01 | **0.74 ± 0.02** | 0.49 ± 0.02 | 0.8 ± 0.04 | 0.35 ± 0.02 |
|  | DTF | 0.75 ± 0.01 | **0.74 ± 0.03** | 0.51 ± 0.01 | 0.04 ± 0.05 | 0.5 ± 0.44 | 0.02 ± 0.02 |
|  | SDCNet | 0.52 ± 0.03 | 0.52 ± 0.03 | 0.51 ± 0.01 | **0.53 ± 0.01** | 0.51 ± 0.01 | **0.56 ± 0.04** |
|  | DeepSynergy | 0.67 ± 0.02 | 0.7 ± 0.02 | 0.63 ± 0.01 | 0.49 ± 0.03 | 0.8 ± 0.04 | 0.35 ± 0.03 |
|  | Matchmaker | 0.67 ± 0.02 | 0.7 ± 0.01 | 0.62 ± 0.02 | 0.45 ± 0.03 | **0.83 ± 0.04** | 0.31 ± 0.02 |
| **ZIP** | Jiang's method | 0.5 ± 0.03 | 0.51 ± 0.01 | 0.5 ± 0.01 | 0.39 ± 0.07 | 0.5 ± 0.01 | 0.33 ± 0.09 |
|  | DeepDDS | **0.77 ± 0.01** | 0.69 ± 0.02 | **0.78 ± 0.01** | **0.61 ± 0.02** | 0.82 ± 0.02 | **0.49 ± 0.02** |
|  | DTF | 0.76 ± 0.01 | **0.76 ± 0.02** | 0.6 ± 0.09 | 0.36 ± 0.32 | 0.54 ± 0.47 | 0.27 ± 0.24 |
|  | SDCNet | 0.51 ± 0.04 | 0.52 ± 0.03 | 0.51 ± 0.02 | 0.25 ± 0.25 | 0.58 ± 0.14 | 0.22 ± 0.27 |
|  | DeepSynergy | 0.6 ± 0.01 | 0.62 ± 0.01 | 0.57 ± 0.0 | 0.44 ± 0.01 | 0.63 ± 0.01 | 0.33 ± 0.01 |
|  | Matchmaker | 0.6 ± 0.0 | 0.62 ± 0.01 | 0.57 ± 0.01 | 0.37 ± 0.01 | 0.7 ± 0.02 | 0.25 ± 0.01 |
| **HSA** | Jiang's method | 0.51 ± 0.01 | 0.51 ± 0.0 | 0.51 ± 0.01 | 0.43 ± 0.28 | 0.52 ± 0.02 | **0.51 ± 0.39** |
|  | DeepDDS | **0.65 ± 0.01** | 0.61 ± 0.01 | **0.69 ± 0.01** | **0.51 ± 0.04** | 0.68 ± 0.02 | 0.42 ± 0.05 |
|  | DTF | 0.65 ± 0.02 | **0.66 ± 0.03** | 0.6 ± 0.01 | 0.45 ± 0.02 | **0.72 ± 0.04** | 0.32 ± 0.02 |
|  | SDCNet | 0.51 ± 0.01 | 0.5 ± 0.01 | 0.5 ± 0.01 | 0.3 ± 0.17 | 0.5 ± 0.03 | 0.24 ± 0.17 |

Table S6. The performances of SDCNet and state-of-the-art methods on the FORCINA dataset with various synergy types.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Synergy type** | **Methods** | **AUC** | **ACC** | **AUPR** | **F1** | **Precision** | **Recall** |
|  | DeepSynergy | 0.51 ± 0.03 | 0.66 ± 0.04 | 0.56 ± 0.08 | 0.68 ± 0.09 | 0.62 ± 0.04 | 0.77 ± 0.17 |
|  | Matchmaker | 0.51 ± 0.05 | 0.65 ± 0.03 | 0.6 ± 0.05 | **0.74 ± 0.06** | 0.62 ± 0.01 | **0.91 ± 0.15** |
| **Loewe** | Jiang's method | 0.61 ± 0.13 | **0.74 ± 0.08** | 0.49 ± 0.05 | 0.43 ± 0.17 | **0.74 ± 0.12** | 0.35 ± 0.2 |
|  | DeepDDS | **0.71 ± 0.06** | 0.64 ± 0.09 | **0.8 ± 0.05** | 0.72 ± 0.11 | 0.68 ± 0.03 | 0.78 ± 0.21 |
|  | DTF | 0.59 ± 0.14 | 0.68 ± 0.1 | 0.37 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 |
|  | SDCNet | 0.65 ± 0.04 | 0.68 ± 0.08 | 0.59 ± 0.01 | 0.55 ± 0.09 | 0.61 ± 0.03 | 0.53 ± 0.19 |
|  | DeepSynergy | 0.58 ± 0.03 | 0.88 ± 0.0 | 0.83 ± 0.01 | 0.91 ± 0.01 | 0.84 ± 0.0 | 0.99 ± 0.01 |
|  | Matchmaker | 0.5 ± 0.06 | 0.85 ± 0.03 | 0.84 ± 0.0 | 0.91 ± 0.0 | 0.84 ± 0.0 | **1.0 ± 0.0** |
| **Bliss** | Jiang's method | 0.59 ± 0.12 | **0.89 ± 0.04** | 0.52 ± 0.17 | 0.61 ± 0.19 | 0.87 ± 0.04 | 0.51 ± 0.28 |
|  | DeepDDS | **0.67 ± 0.05** | 0.82 ± 0.04 | **0.93 ± 0.01** | 0.9 ± 0.02 | 0.86 ± 0.02 | 0.94 ± 0.04 |
|  | DTF | 0.55 ± 0.03 | 0.87 ± 0.03 | 0.17 ± 0.02 | 0.03 ± 0.05 | 0.33 ± 0.58 | 0.01 ± 0.02 |
|  | SDCNet | 0.6 ± 0.07 | 0.86 ± 0.05 | 0.85 ± 0.04 | **0.92 ± 0.02** | **0.87 ± 0.02** | 0.97 ± 0.02 |
|  | DeepSynergy | 0.36 ± 0.14 | 0.76 ± 0.05 | 0.8 ± 0.04 | 0.89 ± 0.02 | 0.82 ± 0.01 | 0.97 ± 0.05 |
|  | Matchmaker | 0.39 ± 0.03 | 0.75 ± 0.01 | 0.82 ± 0.0 | 0.9 ± 0.0 | 0.82 ± 0.0 | **1.0 ± 0.0** |
| **ZIP** | Jiang's method | **0.64 ± 0.06** | 0.87 ± 0.04 | 0.29 ± 0.09 | 0.26 ± 0.16 | 0.83 ± 0.2 | 0.16 ± 0.11 |
|  | DeepDDS | 0.6 ± 0.19 | 0.82 ± 0.0 | **0.91 ± 0.0** | 0.9 ± 0.0 | 0.82 ± 0.01 | 0.99 ± 0.01 |
|  | DTF | 0.48 ± 0.03 | 0.81 ± 0.02 | 0.19 ± 0.01 | 0.04 ± 0.04 | 0.56 ± 0.51 | 0.02 ± 0.02 |
|  | SDCNet | 0.57 ± 0.06 | **0.9 ± 0.03** | 0.85 ± 0.03 | **0.92 ± 0.02** | **0.89 ± 0.01** | 0.94 ± 0.02 |
|  | DeepSynergy | 0.47 ± 0.08 | 0.77 ± 0.05 | 0.8 ± 0.01 | 0.89 ± 0.0 | 0.8 ± 0.01 | **1.0 ± 0.0** |
|  | Matchmaker | 0.49 ± 0.03 | 0.78 ± 0.01 | 0.8 ± 0.0 | 0.89 ± 0.0 | 0.8 ± 0.0 | **1.0 ± 0.0** |
| **HSA** | Jiang's method | 0.42 ± 0.07 | 0.77 ± 0.01 | 0.29 ± 0.09 | 0.29 ± 0.21 | 0.65 ± 0.13 | 0.21 ± 0.19 |
|  | DeepDDS | 0.63 ± 0.12 | 0.77 ± 0.04 | **0.9 ± 0.0** | 0.86 ± 0.03 | 0.81 ± 0.02 | 0.93 ± 0.09 |
|  | DTF | 0.52 ± 0.05 | 0.84 ± 0.04 | 0.21 ± 0.01 | 0.01 ± 0.02 | 0.33 ± 0.58 | 0.01 ± 0.01 |
|  | SDCNet | **0.64 ± 0.11** | **0.87 ± 0.06** | 0.83 ± 0.03 | **0.9 ± 0.01** | **0.86 ± 0.03** | 0.95 ± 0.03 |

Table S7. The performances of different methods on the merged dataset with Loewe score. The model is trained and tested on the merged dataset.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Datasets** | **Methods** | **AUC** | **ACC** | **AUPR** | **F1** | **Precision** | **Recall** |
|  | DeepSynergy | 0.63 ± 0.01 | 0.59 ± 0.01 | 0.62 ± 0.01 | 0.48 ± 0.02 | 0.64 ± 0.01 | 0.38 ± 0.02 |
|  | Matchmaker | 0.62 ± 0.01 | 0.57 ± 0.01 | 0.61 ± 0.01 | 0.47 ± 0.01 | 0.62 ± 0.02 | 0.38 ± 0.02 |
| **Merged** | Jiang's method | 0.70 ± 0.01 | 0.62 ± 0.01 | 0.7 ± 0.01 | 0.5 ± 0.04 | 0.75 ± 0.07 | 0.38 ± 0.06 |
|  | DeepDDS | 0.77 ± 0.01 | 0.65 ± 0.01 | 0.78 ± 0.01 | 0.58 ± 0.02 | **0.78 ± 0.02** | 0.46 ± 0.02 |
|  | DTF | 0.78 ± 0.01 | 0.64 ± 0.01 | 0.73 ± 0.01 | 0.52 ± 0.03 | 0.77 ± 0.03 | 0.45 ± 0.04 |
|  | SDCNet | **0.79 ± 0.01** | **0.68 ± 0.01** | **0.80 ± 0.01** | **0.70 ± 0.02** | 0.66 ± 0.02 | **0.75 ± 0.06** |

Table S8: The performances of SDCNet with different strategies on the O’Neil dataset (Loewe). For leave one drug out strategy, there are 38 drugs in this study, each drug is selected as the test drug in turn and the other drugs are the training drugs. Then, the drug combinations which contain the test drug are regarded as the test dataset, while the rest drug combinations are the training dataset. For leave one cell line out strategy, there are 31 cell lines in this study, the drug combination in each line are regarded as the test dataset in turn and the combinations in other 30 cell lines are the training dataset.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Strategy** | **Methods** | **AUC** | **ACC** | **AUPR** | **F1** | **Precision** | **Recall** |
|  | DeepSynergy | 0.80 ± 0.01 | 0.73 ± 0.01 | 0.78 ± 0.01 | 0.71 ± 0.01 | 0.71 ± 0.01 | 0.70 ± 0.02 |
|  | Matchmaker | 0.81 ± 0.01 | 0.73 ± 0.01 | 0.79 ± 0.01 | 0.71 ± 0.01 | 0.70 ± 0.01 | 0.73 ± 0.02 |
| **Our strategy** | Jiang's method | 0.86 ± 0.01 | 0.78 ± 0.01 | 0.86 ± 0.01 | 0.76 ± 0.01 | 0.80 ± 0.01 | 0.71 ± 0.02 |
|  | DeepDDS | 0.89 ± 0.01 | 0.83 ± 0.01 | 0.86 ± 0.01 | 0.81 ± 0.01 | 0.81 ± 0.02 | 0.81 ± 0.01 |
|  | DTF | 0.91 ± 0.01 | 0.82 ± 0.01 | 0.90 ± 0.01 | 0.81 ± 0.01 | 0.83 ± 0.03 | 0.81 ± 0.02 |
|  | SDCNet | **0.93 ± 0.01** | **0.85 ± 0.01** | **0.92 ± 0.01** | **0.83 ± 0.01** | **0.84 ± 0.01** | **0.82 ± 0.01** |
|  | DeepSynergy | 0.66 ± 0.07 | 0.57 ± 0.11 | 0.58 ± 0.2 | 0.5 ± 0.21 | 0.54 ± 0.2 | 0.6 ± 0.27 |
| **Leave one drug out** | Matchmaker | 0.58 ± 0.09 | 0.53 ± 0.14 | 0.54 ± 0.22 | 0.48 ± 0.25 | 0.47 ± 0.24 | **0.65 ± 0.34** |
| Jiang's method | 0.56 ± 0.08 | 0.52 ± 0.11 | 0.49 ± 0.19 | 0.32 ± 0.2 | 0.47 ± 0.27 | 0.33 ± 0.22 |
|  | DeepDDS | **0.73 ± 0.06** | 0.65 ± 0.09 | 0.71 ± 0.13 | **0.56 ± 0.19** | 0.6 ± 0.22 | 0.62 ± 0.23 |
|  | DTF | 0.69 ± 0.09 | 0.59 ± 0.15 | 0.64 ± 0.18 | 0.34 ± 0.16 | 0.66 ± 0.27 | 0.28 ± 0.2 |
|  | SDCNet | 0.68 ± 0.12 | **0.7 ± 0.1** | **0.73 ± 0.1** | 0.51 ± 0.22 | **0.77 ± 0.18** | 0.46 ± 0.32 |
|  | DeepSynergy | 0.67 ± 0.05 | 0.61 ± 0.04 | 0.64 ± 0.08 | 0.51 ± 0.06 | 0.63 ± 0.1 | 0.45 ± 0.1 |
| **Leave one cell line out** | Matchmaker | 0.66 ± 0.05 | 0.61 ± 0.05 | 0.62 ± 0.09 | 0.55 ± 0.09 | 0.6 ± 0.1 | 0.54 ± 0.13 |
| Jiang's method | 0.78 ± 0.06 | 0.66 ± 0.07 | 0.74 ± 0.09 | 0.49 ± 0.08 | 0.81 ± 0.1 | 0.36 ± 0.08 |
|  | DeepDDS | 0.83 ± 0.05 | 0.74 ± 0.05 | 0.79 ± 0.06 | 0.7 ± 0.07 | 0.76 ± 0.11 | 0.68 ± 0.13 |
|  | DTF | 0.86 ± 0.05 | 0.77 ± 0.05 | 0.84 ± 0.07 | 0.75 ± 0.06 | 0.77 ± 0.1 | **0.75 ± 0.08** |
|  | SDCNet | **0.91 ± 0.01** | **0.84 ± 0.03** | **0.9 ± 0.02** | **0.79 ± 0.06** | **0.93 ± 0.02** | 0.69 ± 0.08 |

Table S9. The performances of SDCNet without common features in each cell line on the O’Neil dataset (Loewe).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Cell line ID** | **Cell line** | **AUC** | **ACC** | **AUPR** | **F1** | **Precision** | **Recall** |
| 0 | A2058 | 0.72 ± 0.09 | 0.64 ± 0.03 | 0.69 ± 0.11 | 0.58 ± 0.12 | 0.74 ± 0.17 | 0.54 ± 0.21 |
| 1 | A2780 | 0.87 ± 0.05 | 0.74 ± 0.06 | 0.81 ± 0.07 | 0.69 ± 0.1 | 0.85 ± 0.08 | 0.6 ± 0.13 |
| 2 | A375 | 0.73 ± 0.06 | 0.57 ± 0.04 | 0.68 ± 0.06 | 0.38 ± 0.12 | 0.74 ± 0.17 | 0.27 ± 0.11 |
| 3 | A427 | 0.9 ± 0.02 | 0.73 ± 0.06 | 0.89 ± 0.05 | 0.65 ± 0.1 | 0.91 ± 0.08 | 0.52 ± 0.12 |
| 4 | CAOV3 | 0.74 ± 0.11 | 0.55 ± 0.1 | 0.68 ± 0.13 | 0.31 ± 0.21 | 0.6 ± 0.38 | 0.22 ± 0.17 |
| 5 | ES2 | 0.82 ± 0.04 | 0.64 ± 0.09 | 0.79 ± 0.06 | 0.44 ± 0.26 | 0.71 ± 0.4 | 0.32 ± 0.2 |
| 6 | HCT116 | 0.56 ± 0.15 | 0.49 ± 0.08 | 0.55 ± 0.1 | 0.38 ± 0.2 | 0.51 ± 0.14 | 0.39 ± 0.33 |
| 7 | HT144 | 0.77 ± 0.15 | 0.66 ± 0.04 | 0.74 ± 0.17 | 0.61 ± 0.04 | 0.8 ± 0.19 | 0.53 ± 0.14 |
| 8 | HT29 | 0.7 ± 0.16 | 0.58 ± 0.06 | 0.7 ± 0.18 | 0.4 ± 0.15 | 0.76 ± 0.22 | 0.3 ± 0.13 |
| 9 | KPL1 | 0.88 ± 0.05 | 0.74 ± 0.06 | 0.84 ± 0.06 | 0.69 ± 0.1 | 0.84 ± 0.06 | 0.58 ± 0.11 |
| 10 | LNCAP | 0.69 ± 0.22 | 0.62 ± 0.13 | 0.72 ± 0.21 | 0.48 ± 0.2 | 0.75 ± 0.3 | 0.36 ± 0.16 |
| 11 | LOVO | 0.89 ± 0.06 | 0.8 ± 0.08 | 0.87 ± 0.08 | 0.76 ± 0.11 | 0.9 ± 0.09 | 0.67 ± 0.14 |
| 12 | MDAMB436 | 0.81 ± 0.07 | 0.62 ± 0.05 | 0.78 ± 0.11 | 0.44 ± 0.12 | 0.84 ± 0.15 | 0.32 ± 0.13 |
| 13 | MSTO | 0.82 ± 0.11 | 0.65 ± 0.1 | 0.77 ± 0.15 | 0.5 ± 0.19 | 0.81 ± 0.15 | 0.37 ± 0.17 |
| 14 | NCIH1650 | 0.88 ± 0.12 | 0.71 ± 0.07 | 0.85 ± 0.14 | 0.61 ± 0.1 | 0.91 ± 0.14 | 0.47 ± 0.1 |
| 15 | NCIH2122 | 0.69 ± 0.2 | 0.57 ± 0.06 | 0.72 ± 0.19 | 0.38 ± 0.16 | 0.76 ± 0.23 | 0.29 ± 0.18 |
| 16 | NCIH23 | 0.59 ± 0.14 | 0.46 ± 0.08 | 0.57 ± 0.14 | 0.25 ± 0.16 | 0.38 ± 0.27 | 0.2 ± 0.13 |
| 17 | NCIH460 | 0.74 ± 0.2 | 0.6 ± 0.1 | 0.75 ± 0.19 | 0.43 ± 0.15 | 0.79 ± 0.25 | 0.31 ± 0.13 |
| 18 | NCIH520 | 0.9 ± 0.03 | 0.73 ± 0.08 | 0.91 ± 0.02 | 0.62 ± 0.16 | 1.0 ± 0.0 | 0.46 ± 0.17 |
| 19 | OV90 | 0.89 ± 0.04 | 0.82 ± 0.08 | 0.86 ± 0.09 | 0.79 ± 0.1 | 0.93 ± 0.07 | 0.69 ± 0.14 |
| 20 | RKO | 0.77 ± 0.05 | 0.64 ± 0.08 | 0.73 ± 0.08 | 0.5 ± 0.15 | 0.79 ± 0.11 | 0.38 ± 0.15 |
| 21 | RPMI7951 | 0.89 ± 0.07 | 0.71 ± 0.06 | 0.87 ± 0.1 | 0.64 ± 0.08 | 0.88 ± 0.11 | 0.5 ± 0.07 |
| 22 | SKMEL30 | 0.77 ± 0.14 | 0.65 ± 0.06 | 0.77 ± 0.15 | 0.55 ± 0.07 | 0.81 ± 0.19 | 0.43 ± 0.08 |
| 23 | SKMES1 | 0.88 ± 0.06 | 0.67 ± 0.04 | 0.86 ± 0.08 | 0.53 ± 0.08 | 0.94 ± 0.08 | 0.37 ± 0.06 |
| 24 | SKOV3 | 0.78 ± 0.13 | 0.62 ± 0.06 | 0.75 ± 0.15 | 0.45 ± 0.14 | 0.84 ± 0.17 | 0.33 ± 0.14 |
| 25 | SW620 | 0.82 ± 0.03 | 0.71 ± 0.13 | 0.78 ± 0.07 | 0.61 ± 0.25 | 0.82 ± 0.11 | 0.52 ± 0.26 |
| 26 | SW837 | 0.91 ± 0.04 | 0.81 ± 0.07 | 0.88 ± 0.09 | 0.78 ± 0.1 | 0.9 ± 0.04 | 0.7 ± 0.14 |
| 27 | T47D | 0.82 ± 0.05 | 0.66 ± 0.09 | 0.82 ± 0.09 | 0.52 ± 0.21 | 0.89 ± 0.15 | 0.4 ± 0.19 |
| 28 | UACC62 | 0.83 ± 0.03 | 0.71 ± 0.03 | 0.82 ± 0.07 | 0.61 ± 0.08 | 0.93 ± 0.07 | 0.46 ± 0.1 |
| 29 | VCAP | 0.74 ± 0.12 | 0.64 ± 0.07 | 0.71 ± 0.1 | 0.49 ± 0.17 | 0.79 ± 0.13 | 0.38 ± 0.18 |
| 30 | ZR751 | 0.81 ± 0.13 | 0.69 ± 0.08 | 0.79 ± 0.16 | 0.62 ± 0.1 | 0.84 ± 0.17 | 0.49 ± 0.1 |
|  | Mean | 0.79 ± 0.01 | 0.66 ± 0.01 | 0.77 ± 0.02 | 0.54 ± 0.03 | 0.8 ± 0.05 | 0.43 ± 0.02 |

Table S10. The performance of SDCNet in each cell line on the O’Neil dataset (Loewe).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Cell line ID** | **Cell line** | **AUC** | **ACC** | **AUPR** | **F1** | **Precision** | **Recall** |
| 0 | A2058 | 0.89 ± 0.02 | 0.82 ± 0.05 | 0.88 ± 0.04 | 0.82 ± 0.05 | 0.83 ± 0.06 | 0.81 ± 0.06 |
| 1 | A2780 | 0.95 ± 0.03 | 0.89 ± 0.04 | 0.96 ± 0.02 | 0.89 ± 0.04 | 0.89 ± 0.05 | 0.9 ± 0.05 |
| 2 | A375 | 0.89 ± 0.04 | 0.81 ± 0.07 | 0.9 ± 0.04 | 0.81 ± 0.05 | 0.81 ± 0.11 | 0.82 ± 0.07 |
| 3 | A427 | 0.91 ± 0.02 | 0.85 ± 0.03 | 0.92 ± 0.03 | 0.83 ± 0.04 | 0.92 ± 0.06 | 0.77 ± 0.07 |
| 4 | CAOV3 | 0.91 ± 0.04 | 0.83 ± 0.07 | 0.91 ± 0.03 | 0.82 ± 0.09 | 0.86 ± 0.07 | 0.79 ± 0.15 |
| 5 | ES2 | 0.86 ± 0.04 | 0.81 ± 0.05 | 0.87 ± 0.07 | 0.79 ± 0.04 | 0.87 ± 0.1 | 0.73 ± 0.02 |
| 6 | HCT116 | 0.86 ± 0.06 | 0.78 ± 0.06 | 0.87 ± 0.06 | 0.76 ± 0.09 | 0.83 ± 0.05 | 0.71 ± 0.12 |
| 7 | HT144 | 0.93 ± 0.03 | 0.86 ± 0.04 | 0.95 ± 0.02 | 0.85 ± 0.05 | 0.95 ± 0.06 | 0.78 ± 0.08 |
| 8 | HT29 | 0.92 ± 0.04 | 0.83 ± 0.03 | 0.92 ± 0.04 | 0.82 ± 0.03 | 0.86 ± 0.06 | 0.78 ± 0.04 |
| 9 | KPL1 | 0.93 ± 0.03 | 0.86 ± 0.06 | 0.94 ± 0.03 | 0.85 ± 0.07 | 0.87 ± 0.06 | 0.84 ± 0.11 |
| 10 | LNCAP | 0.86 ± 0.04 | 0.79 ± 0.03 | 0.85 ± 0.06 | 0.76 ± 0.04 | 0.86 ± 0.05 | 0.69 ± 0.07 |
| 11 | LOVO | 0.97 ± 0.03 | 0.94 ± 0.03 | 0.97 ± 0.02 | 0.94 ± 0.03 | 0.94 ± 0.05 | 0.94 ± 0.08 |
| 12 | MDAMB436 | 0.95 ± 0.02 | 0.83 ± 0.04 | 0.95 ± 0.02 | 0.81 ± 0.05 | 0.88 ± 0.09 | 0.77 ± 0.12 |
| 13 | MSTO | 0.84 ± 0.09 | 0.76 ± 0.05 | 0.84 ± 0.09 | 0.76 ± 0.06 | 0.78 ± 0.06 | 0.75 ± 0.09 |
| 14 | NCIH1650 | 0.94 ± 0.03 | 0.89 ± 0.07 | 0.95 ± 0.03 | 0.88 ± 0.07 | 0.93 ± 0.05 | 0.84 ± 0.11 |
| 15 | NCIH2122 | 0.89 ± 0.09 | 0.8 ± 0.08 | 0.89 ± 0.09 | 0.78 ± 0.09 | 0.87 ± 0.09 | 0.71 ± 0.12 |
| 16 | NCIH23 | 0.94 ± 0.03 | 0.84 ± 0.1 | 0.95 ± 0.03 | 0.81 ± 0.12 | 0.93 ± 0.11 | 0.73 ± 0.13 |
| 17 | NCIH460 | 0.92 ± 0.04 | 0.84 ± 0.02 | 0.93 ± 0.03 | 0.83 ± 0.03 | 0.87 ± 0.09 | 0.81 ± 0.12 |
| 18 | NCIH520 | 0.93 ± 0.05 | 0.86 ± 0.05 | 0.95 ± 0.04 | 0.85 ± 0.05 | 0.91 ± 0.06 | 0.79 ± 0.06 |
| 19 | OV90 | 0.95 ± 0.03 | 0.86 ± 0.04 | 0.95 ± 0.03 | 0.85 ± 0.05 | 0.91 ± 0.06 | 0.8 ± 0.09 |
| 20 | RKO | 0.87 ± 0.06 | 0.8 ± 0.06 | 0.89 ± 0.05 | 0.79 ± 0.06 | 0.83 ± 0.07 | 0.76 ± 0.05 |
| 21 | RPMI7951 | 0.94 ± 0.06 | 0.87 ± 0.06 | 0.94 ± 0.06 | 0.86 ± 0.06 | 0.93 ± 0.08 | 0.81 ± 0.08 |
| 22 | SKMEL30 | 0.87 ± 0.07 | 0.81 ± 0.08 | 0.87 ± 0.07 | 0.81 ± 0.08 | 0.81 ± 0.11 | 0.82 ± 0.06 |
| 23 | SKMES1 | 0.9 ± 0.04 | 0.84 ± 0.06 | 0.88 ± 0.08 | 0.84 ± 0.06 | 0.86 ± 0.06 | 0.82 ± 0.06 |
| 24 | SKOV3 | 0.89 ± 0.05 | 0.84 ± 0.05 | 0.86 ± 0.08 | 0.85 ± 0.04 | 0.83 ± 0.08 | 0.87 ± 0.07 |
| 25 | SW620 | 0.89 ± 0.04 | 0.79 ± 0.05 | 0.9 ± 0.02 | 0.77 ± 0.07 | 0.84 ± 0.05 | 0.72 ± 0.13 |
| 26 | SW837 | 0.94 ± 0.04 | 0.85 ± 0.07 | 0.92 ± 0.06 | 0.84 ± 0.07 | 0.91 ± 0.11 | 0.79 ± 0.04 |
| 27 | T47D | 0.9 ± 0.05 | 0.8 ± 0.06 | 0.9 ± 0.05 | 0.78 ± 0.06 | 0.89 ± 0.11 | 0.69 ± 0.07 |
| 28 | UACC62 | 0.94 ± 0.03 | 0.86 ± 0.04 | 0.95 ± 0.03 | 0.86 ± 0.04 | 0.87 ± 0.05 | 0.85 ± 0.07 |
| 29 | VCAP | 0.91 ± 0.03 | 0.84 ± 0.07 | 0.9 ± 0.03 | 0.84 ± 0.07 | 0.82 ± 0.06 | 0.87 ± 0.09 |
| 30 | ZR751 | 0.94 ± 0.05 | 0.84 ± 0.05 | 0.94 ± 0.04 | 0.82 ± 0.06 | 0.95 ± 0.04 | 0.72 ± 0.08 |
|  | Mean | 0.91 ± 0.01 | 0.83 ± 0.01 | 0.91 ± 0.01 | 0.83 ± 0.01 | 0.87 ± 0.01 | 0.79 ± 0.01 |

Table S11. The top 10 SDC predicted by SDCNet in each cell line on the O’Neil dataset (Loewe).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Cell line ID** | **Cell line** | **Tissue** | **Drug 1** | **Drug 2** | **Probability** |
| 0 | A2058 | Melanoma | SN-38 | TOPOTECAN | 0.97 |
| 0 | A2058 | Melanoma | SN-38 | VINBLASTINE | 0.96 |
| 0 | A2058 | Melanoma | METFORMIN | TOPOTECAN | 0.92 |
| 0 | A2058 | Melanoma | CYCLOPHOSPHAMIDE | VINBLASTINE | 0.91 |
| 0 | A2058 | Melanoma | 5-FU | METFORMIN | 0.91 |
| 0 | A2058 | Melanoma | CARBOPLATIN | TOPOTECAN | 0.85 |
| 0 | A2058 | Melanoma | METFORMIN | SN-38 | 0.83 |
| 0 | A2058 | Melanoma | METFORMIN | VINBLASTINE | 0.77 |
| 0 | A2058 | Melanoma | 5-FU | TOPOTECAN | 0.77 |
| 0 | A2058 | Melanoma | CYCLOPHOSPHAMIDE | METFORMIN | 0.76 |
| 1 | A2780 | Ovarian | CARBOPLATIN | ETOPOSIDE | 0.98 |
| 1 | A2780 | Ovarian | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.97 |
| 1 | A2780 | Ovarian | ETOPOSIDE | TOPOTECAN | 0.97 |
| 1 | A2780 | Ovarian | CYCLOPHOSPHAMIDE | TOPOTECAN | 0.96 |
| 1 | A2780 | Ovarian | 5-FU | ETOPOSIDE | 0.96 |
| 1 | A2780 | Ovarian | ETOPOSIDE | SN-38 | 0.95 |
| 1 | A2780 | Ovarian | CARBOPLATIN | SN-38 | 0.94 |
| 1 | A2780 | Ovarian | CYCLOPHOSPHAMIDE | SN-38 | 0.94 |
| 1 | A2780 | Ovarian | SN-38 | TOPOTECAN | 0.91 |
| 1 | A2780 | Ovarian | CARBOPLATIN | TOPOTECAN | 0.91 |
| 2 | A375 | Melanoma | 5-FU | ETOPOSIDE | 0.99 |
| 2 | A375 | Melanoma | PACLITAXEL | SN-38 | 0.97 |
| 2 | A375 | Melanoma | DEXAMETHASONE | SN-38 | 0.97 |
| 2 | A375 | Melanoma | SN-38 | VINBLASTINE | 0.96 |
| 2 | A375 | Melanoma | SN-38 | TOPOTECAN | 0.95 |
| 2 | A375 | Melanoma | CYCLOPHOSPHAMIDE | SN-38 | 0.91 |
| 2 | A375 | Melanoma | SN-38 | VINORELBINE | 0.9 |
| 2 | A375 | Melanoma | CYCLOPHOSPHAMIDE | PACLITAXEL | 0.9 |
| 2 | A375 | Melanoma | DEXAMETHASONE | PACLITAXEL | 0.84 |
| 2 | A375 | Melanoma | 5-FU | SN-38 | 0.81 |
| 3 | A427 | Lung | 5-FU | TOPOTECAN | 0.95 |
| 3 | A427 | Lung | PACLITAXEL | TOPOTECAN | 0.85 |
| 3 | A427 | Lung | 5-FU | PACLITAXEL | 0.82 |
| 3 | A427 | Lung | ETOPOSIDE | TOPOTECAN | 0.69 |
| 3 | A427 | Lung | GEMCITABINE | TOPOTECAN | 0.68 |
| 3 | A427 | Lung | SN-38 | TOPOTECAN | 0.66 |
| 3 | A427 | Lung | METFORMIN | TOPOTECAN | 0.52 |
| 3 | A427 | Lung | TOPOTECAN | VINBLASTINE | 0.5 |
| 3 | A427 | Lung | DOXORUBICIN | TOPOTECAN | 0.47 |
| 3 | A427 | Lung | MITOMYCINE | TOPOTECAN | 0.46 |
| 4 | CAOV3 | Ovarian | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.99 |
| 4 | CAOV3 | Ovarian | CARBOPLATIN | ETOPOSIDE | 0.99 |
| 4 | CAOV3 | Ovarian | ETOPOSIDE | SN-38 | 0.99 |
| 4 | CAOV3 | Ovarian | DEXAMETHASONE | ETOPOSIDE | 0.99 |
| 4 | CAOV3 | Ovarian | DEXAMETHASONE | SN-38 | 0.99 |
| 4 | CAOV3 | Ovarian | ETOPOSIDE | OXALIPLATIN | 0.99 |
| 4 | CAOV3 | Ovarian | 5-FU | ETOPOSIDE | 0.98 |
| 4 | CAOV3 | Ovarian | ETOPOSIDE | METFORMIN | 0.98 |
| 4 | CAOV3 | Ovarian | DOXORUBICIN | ETOPOSIDE | 0.97 |
| 4 | CAOV3 | Ovarian | ETOPOSIDE | TOPOTECAN | 0.97 |
| 5 | ES2 | Ovarian | PACLITAXEL | VINBLASTINE | 0.99 |
| 5 | ES2 | Ovarian | DOXORUBICIN | VINBLASTINE | 0.99 |
| 5 | ES2 | Ovarian | PACLITAXEL | SN-38 | 0.99 |
| 5 | ES2 | Ovarian | 5-FU | PACLITAXEL | 0.98 |
| 5 | ES2 | Ovarian | MITOMYCINE | VINBLASTINE | 0.98 |
| 5 | ES2 | Ovarian | SN-38 | VINBLASTINE | 0.97 |
| 5 | ES2 | Ovarian | CYCLOPHOSPHAMIDE | PACLITAXEL | 0.97 |
| 5 | ES2 | Ovarian | CARBOPLATIN | PACLITAXEL | 0.97 |
| 5 | ES2 | Ovarian | ETOPOSIDE | VINBLASTINE | 0.97 |
| 5 | ES2 | Ovarian | ETOPOSIDE | TOPOTECAN | 0.95 |
| 6 | HCT116 | Colon | SN-38 | TOPOTECAN | 0.96 |
| 6 | HCT116 | Colon | CYCLOPHOSPHAMIDE | SN-38 | 0.92 |
| 6 | HCT116 | Colon | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.91 |
| 6 | HCT116 | Colon | CARBOPLATIN | TOPOTECAN | 0.88 |
| 6 | HCT116 | Colon | CYCLOPHOSPHAMIDE | DOXORUBICIN | 0.87 |
| 6 | HCT116 | Colon | CARBOPLATIN | CYCLOPHOSPHAMIDE | 0.81 |
| 6 | HCT116 | Colon | 5-FU | CYCLOPHOSPHAMIDE | 0.76 |
| 6 | HCT116 | Colon | DEXAMETHASONE | ETOPOSIDE | 0.76 |
| 6 | HCT116 | Colon | ETOPOSIDE | VINBLASTINE | 0.7 |
| 6 | HCT116 | Colon | DEXAMETHASONE | TOPOTECAN | 0.63 |
| 7 | HT144 | Melanoma | PACLITAXEL | SN-38 | 0.99 |
| 7 | HT144 | Melanoma | ETOPOSIDE | PACLITAXEL | 0.99 |
| 7 | HT144 | Melanoma | PACLITAXEL | VINBLASTINE | 0.99 |
| 7 | HT144 | Melanoma | SN-38 | VINBLASTINE | 0.98 |
| 7 | HT144 | Melanoma | PACLITAXEL | TOPOTECAN | 0.97 |
| 7 | HT144 | Melanoma | ETOPOSIDE | VINBLASTINE | 0.97 |
| 7 | HT144 | Melanoma | SN-38 | TOPOTECAN | 0.92 |
| 7 | HT144 | Melanoma | ETOPOSIDE | SN-38 | 0.91 |
| 7 | HT144 | Melanoma | CARBOPLATIN | PACLITAXEL | 0.89 |
| 7 | HT144 | Melanoma | CYCLOPHOSPHAMIDE | PACLITAXEL | 0.86 |
| 8 | HT29 | Colon | CARBOPLATIN | ETOPOSIDE | 0.99 |
| 8 | HT29 | Colon | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.98 |
| 8 | HT29 | Colon | DEXAMETHASONE | ETOPOSIDE | 0.97 |
| 8 | HT29 | Colon | ETOPOSIDE | TOPOTECAN | 0.94 |
| 8 | HT29 | Colon | ETOPOSIDE | METFORMIN | 0.92 |
| 8 | HT29 | Colon | 5-FU | ETOPOSIDE | 0.9 |
| 8 | HT29 | Colon | DEXAMETHASONE | TOPOTECAN | 0.89 |
| 8 | HT29 | Colon | ETOPOSIDE | SN-38 | 0.87 |
| 8 | HT29 | Colon | DEXAMETHASONE | GEMCITABINE | 0.85 |
| 8 | HT29 | Colon | CYCLOPHOSPHAMIDE | GEMCITABINE | 0.82 |
| 9 | KPL1 | Breast | 5-FU | TOPOTECAN | 0.99 |
| 9 | KPL1 | Breast | SN-38 | TOPOTECAN | 0.99 |
| 9 | KPL1 | Breast | CARBOPLATIN | DEXAMETHASONE | 0.99 |
| 9 | KPL1 | Breast | DEXAMETHASONE | SN-38 | 0.99 |
| 9 | KPL1 | Breast | DEXAMETHASONE | ETOPOSIDE | 0.99 |
| 9 | KPL1 | Breast | DEXAMETHASONE | TOPOTECAN | 0.98 |
| 9 | KPL1 | Breast | CARBOPLATIN | TOPOTECAN | 0.98 |
| 9 | KPL1 | Breast | CARBOPLATIN | ETOPOSIDE | 0.98 |
| 9 | KPL1 | Breast | ETOPOSIDE | VINBLASTINE | 0.98 |
| 9 | KPL1 | Breast | ETOPOSIDE | SN-38 | 0.96 |
| 10 | LNCAP | Prostate | ETOPOSIDE | METFORMIN | 0.98 |
| 10 | LNCAP | Prostate | METFORMIN | SN-38 | 0.96 |
| 10 | LNCAP | Prostate | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.85 |
| 10 | LNCAP | Prostate | ETOPOSIDE | OXALIPLATIN | 0.69 |
| 10 | LNCAP | Prostate | CARBOPLATIN | ETOPOSIDE | 0.67 |
| 10 | LNCAP | Prostate | DEXAMETHASONE | ETOPOSIDE | 0.67 |
| 10 | LNCAP | Prostate | DEXAMETHASONE | METFORMIN | 0.67 |
| 10 | LNCAP | Prostate | ETOPOSIDE | MITOMYCINE | 0.61 |
| 10 | LNCAP | Prostate | DOXORUBICIN | ETOPOSIDE | 0.57 |
| 10 | LNCAP | Prostate | ETOPOSIDE | SN-38 | 0.51 |
| 11 | LOVO | Colon | DEXAMETHASONE | PACLITAXEL | 0.89 |
| 11 | LOVO | Colon | DEXAMETHASONE | MITOMYCINE | 0.76 |
| 11 | LOVO | Colon | DEXAMETHASONE | SN-38 | 0.71 |
| 11 | LOVO | Colon | DEXAMETHASONE | ETOPOSIDE | 0.66 |
| 11 | LOVO | Colon | DEXAMETHASONE | VINBLASTINE | 0.58 |
| 11 | LOVO | Colon | DEXAMETHASONE | VINORELBINE | 0.53 |
| 11 | LOVO | Colon | MITOMYCINE | SN-38 | 0.5 |
| 11 | LOVO | Colon | 5-FU | DEXAMETHASONE | 0.42 |
| 11 | LOVO | Colon | SN-38 | TOPOTECAN | 0.41 |
| 11 | LOVO | Colon | CARBOPLATIN | DEXAMETHASONE | 0.4 |
| 12 | MDAMB436 | Breast | ETOPOSIDE | SN-38 | 0.99 |
| 12 | MDAMB436 | Breast | 5-FU | ETOPOSIDE | 0.98 |
| 12 | MDAMB436 | Breast | ETOPOSIDE | METFORMIN | 0.97 |
| 12 | MDAMB436 | Breast | ETOPOSIDE | PACLITAXEL | 0.93 |
| 12 | MDAMB436 | Breast | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.89 |
| 12 | MDAMB436 | Breast | CARBOPLATIN | ETOPOSIDE | 0.88 |
| 12 | MDAMB436 | Breast | 5-FU | METFORMIN | 0.87 |
| 12 | MDAMB436 | Breast | DEXAMETHASONE | ETOPOSIDE | 0.85 |
| 12 | MDAMB436 | Breast | 5-FU | SN-38 | 0.82 |
| 12 | MDAMB436 | Breast | 5-FU | PACLITAXEL | 0.79 |
| 13 | MSTO | Lung | TOPOTECAN | VINORELBINE | 0.99 |
| 13 | MSTO | Lung | CYCLOPHOSPHAMIDE | VINORELBINE | 0.97 |
| 13 | MSTO | Lung | CYCLOPHOSPHAMIDE | PACLITAXEL | 0.94 |
| 13 | MSTO | Lung | CARBOPLATIN | VINORELBINE | 0.94 |
| 13 | MSTO | Lung | ETOPOSIDE | PACLITAXEL | 0.94 |
| 13 | MSTO | Lung | PACLITAXEL | TOPOTECAN | 0.93 |
| 13 | MSTO | Lung | SN-38 | VINORELBINE | 0.9 |
| 13 | MSTO | Lung | PACLITAXEL | VINORELBINE | 0.9 |
| 13 | MSTO | Lung | ETOPOSIDE | VINORELBINE | 0.87 |
| 13 | MSTO | Lung | MITOMYCINE | VINORELBINE | 0.86 |
| 14 | NCIH1650 | Lung | SN-38 | TOPOTECAN | 0.99 |
| 14 | NCIH1650 | Lung | DEXAMETHASONE | TOPOTECAN | 0.99 |
| 14 | NCIH1650 | Lung | DEXAMETHASONE | SN-38 | 0.99 |
| 14 | NCIH1650 | Lung | ETOPOSIDE | TOPOTECAN | 0.99 |
| 14 | NCIH1650 | Lung | PACLITAXEL | SN-38 | 0.99 |
| 14 | NCIH1650 | Lung | SN-38 | VINBLASTINE | 0.99 |
| 14 | NCIH1650 | Lung | DEXAMETHASONE | PACLITAXEL | 0.99 |
| 14 | NCIH1650 | Lung | DEXAMETHASONE | ETOPOSIDE | 0.99 |
| 14 | NCIH1650 | Lung | DEXAMETHASONE | VINBLASTINE | 0.99 |
| 14 | NCIH1650 | Lung | ETOPOSIDE | PACLITAXEL | 0.98 |
| 15 | NCIH2122 | Lung | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.98 |
| 15 | NCIH2122 | Lung | DEXAMETHASONE | ETOPOSIDE | 0.97 |
| 15 | NCIH2122 | Lung | CYCLOPHOSPHAMIDE | TOPOTECAN | 0.96 |
| 15 | NCIH2122 | Lung | DEXAMETHASONE | TOPOTECAN | 0.89 |
| 15 | NCIH2122 | Lung | DEXAMETHASONE | GEMCITABINE | 0.86 |
| 15 | NCIH2122 | Lung | DEXAMETHASONE | SN-38 | 0.85 |
| 15 | NCIH2122 | Lung | ETOPOSIDE | VINBLASTINE | 0.79 |
| 15 | NCIH2122 | Lung | CYCLOPHOSPHAMIDE | GEMCITABINE | 0.77 |
| 15 | NCIH2122 | Lung | CYCLOPHOSPHAMIDE | SN-38 | 0.76 |
| 15 | NCIH2122 | Lung | 5-FU | CYCLOPHOSPHAMIDE | 0.72 |
| 16 | NCIH23 | Lung | MITOMYCINE | SN-38 | 0.93 |
| 16 | NCIH23 | Lung | PACLITAXEL | SN-38 | 0.89 |
| 16 | NCIH23 | Lung | SN-38 | TOPOTECAN | 0.89 |
| 16 | NCIH23 | Lung | CYCLOPHOSPHAMIDE | SN-38 | 0.78 |
| 16 | NCIH23 | Lung | CYCLOPHOSPHAMIDE | TOPOTECAN | 0.74 |
| 16 | NCIH23 | Lung | DEXAMETHASONE | TOPOTECAN | 0.58 |
| 16 | NCIH23 | Lung | DEXAMETHASONE | SN-38 | 0.57 |
| 16 | NCIH23 | Lung | 5-FU | TOPOTECAN | 0.54 |
| 16 | NCIH23 | Lung | 5-FU | SN-38 | 0.49 |
| 16 | NCIH23 | Lung | ETOPOSIDE | SN-38 | 0.42 |
| 17 | NCIH460 | Lung | ETOPOSIDE | PACLITAXEL | 0.99 |
| 17 | NCIH460 | Lung | PACLITAXEL | SN-38 | 0.99 |
| 17 | NCIH460 | Lung | CYCLOPHOSPHAMIDE | PACLITAXEL | 0.99 |
| 17 | NCIH460 | Lung | SN-38 | TOPOTECAN | 0.99 |
| 17 | NCIH460 | Lung | DEXAMETHASONE | PACLITAXEL | 0.98 |
| 17 | NCIH460 | Lung | SN-38 | VINBLASTINE | 0.98 |
| 17 | NCIH460 | Lung | 5-FU | PACLITAXEL | 0.98 |
| 17 | NCIH460 | Lung | CYCLOPHOSPHAMIDE | DOXORUBICIN | 0.97 |
| 17 | NCIH460 | Lung | DEXAMETHASONE | SN-38 | 0.96 |
| 17 | NCIH460 | Lung | CYCLOPHOSPHAMIDE | VINORELBINE | 0.95 |
| 18 | NCIH520 | Lung | ETOPOSIDE | TOPOTECAN | 0.99 |
| 18 | NCIH520 | Lung | SN-38 | TOPOTECAN | 0.98 |
| 18 | NCIH520 | Lung | DEXAMETHASONE | TOPOTECAN | 0.93 |
| 18 | NCIH520 | Lung | 5-FU | TOPOTECAN | 0.85 |
| 18 | NCIH520 | Lung | 5-FU | SN-38 | 0.83 |
| 18 | NCIH520 | Lung | PACLITAXEL | SN-38 | 0.78 |
| 18 | NCIH520 | Lung | SN-38 | VINBLASTINE | 0.75 |
| 18 | NCIH520 | Lung | PACLITAXEL | TOPOTECAN | 0.7 |
| 18 | NCIH520 | Lung | ETOPOSIDE | PACLITAXEL | 0.68 |
| 18 | NCIH520 | Lung | DEXAMETHASONE | ETOPOSIDE | 0.64 |
| 19 | OV90 | Ovarian | 5-FU | VINORELBINE | 0.99 |
| 19 | OV90 | Ovarian | TOPOTECAN | VINORELBINE | 0.98 |
| 19 | OV90 | Ovarian | VINBLASTINE | VINORELBINE | 0.98 |
| 19 | OV90 | Ovarian | METFORMIN | VINORELBINE | 0.97 |
| 19 | OV90 | Ovarian | PACLITAXEL | VINORELBINE | 0.97 |
| 19 | OV90 | Ovarian | CYCLOPHOSPHAMIDE | VINORELBINE | 0.97 |
| 19 | OV90 | Ovarian | SN-38 | VINORELBINE | 0.96 |
| 19 | OV90 | Ovarian | ETOPOSIDE | VINORELBINE | 0.95 |
| 19 | OV90 | Ovarian | DEXAMETHASONE | VINORELBINE | 0.9 |
| 19 | OV90 | Ovarian | ETOPOSIDE | TOPOTECAN | 0.86 |
| 20 | RKO | Colon | SN-38 | TOPOTECAN | 0.99 |
| 20 | RKO | Colon | SN-38 | VINBLASTINE | 0.99 |
| 20 | RKO | Colon | PACLITAXEL | SN-38 | 0.99 |
| 20 | RKO | Colon | ETOPOSIDE | SN-38 | 0.97 |
| 20 | RKO | Colon | 5-FU | CARBOPLATIN | 0.96 |
| 20 | RKO | Colon | CARBOPLATIN | SN-38 | 0.96 |
| 20 | RKO | Colon | DEXAMETHASONE | SN-38 | 0.96 |
| 20 | RKO | Colon | DEXAMETHASONE | ETOPOSIDE | 0.93 |
| 20 | RKO | Colon | 5-FU | SN-38 | 0.93 |
| 20 | RKO | Colon | CARBOPLATIN | ETOPOSIDE | 0.87 |
| 21 | RPMI7951 | Melanoma | SN-38 | TOPOTECAN | 0.99 |
| 21 | RPMI7951 | Melanoma | CYCLOPHOSPHAMIDE | SN-38 | 0.98 |
| 21 | RPMI7951 | Melanoma | ETOPOSIDE | SN-38 | 0.89 |
| 21 | RPMI7951 | Melanoma | 5-FU | ETOPOSIDE | 0.88 |
| 21 | RPMI7951 | Melanoma | PACLITAXEL | SN-38 | 0.86 |
| 21 | RPMI7951 | Melanoma | MITOMYCINE | SN-38 | 0.85 |
| 21 | RPMI7951 | Melanoma | ETOPOSIDE | METFORMIN | 0.81 |
| 21 | RPMI7951 | Melanoma | 5-FU | TOPOTECAN | 0.79 |
| 21 | RPMI7951 | Melanoma | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.76 |
| 21 | RPMI7951 | Melanoma | METFORMIN | TOPOTECAN | 0.61 |
| 22 | SKMEL30 | Melanoma | ETOPOSIDE | PACLITAXEL | 0.99 |
| 22 | SKMEL30 | Melanoma | PACLITAXEL | SN-38 | 0.99 |
| 22 | SKMEL30 | Melanoma | ETOPOSIDE | TOPOTECAN | 0.98 |
| 22 | SKMEL30 | Melanoma | DEXAMETHASONE | ETOPOSIDE | 0.98 |
| 22 | SKMEL30 | Melanoma | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.98 |
| 22 | SKMEL30 | Melanoma | SN-38 | TOPOTECAN | 0.98 |
| 22 | SKMEL30 | Melanoma | PACLITAXEL | TOPOTECAN | 0.97 |
| 22 | SKMEL30 | Melanoma | ETOPOSIDE | VINBLASTINE | 0.96 |
| 22 | SKMEL30 | Melanoma | CYCLOPHOSPHAMIDE | SN-38 | 0.95 |
| 22 | SKMEL30 | Melanoma | 5-FU | ETOPOSIDE | 0.92 |
| 23 | SKMES1 | Lung | SN-38 | TOPOTECAN | 0.99 |
| 23 | SKMES1 | Lung | CYCLOPHOSPHAMIDE | PACLITAXEL | 0.99 |
| 23 | SKMES1 | Lung | DEXAMETHASONE | PACLITAXEL | 0.99 |
| 23 | SKMES1 | Lung | DEXAMETHASONE | TOPOTECAN | 0.99 |
| 23 | SKMES1 | Lung | PACLITAXEL | SN-38 | 0.99 |
| 23 | SKMES1 | Lung | 5-FU | PACLITAXEL | 0.99 |
| 23 | SKMES1 | Lung | CYCLOPHOSPHAMIDE | SN-38 | 0.98 |
| 23 | SKMES1 | Lung | CYCLOPHOSPHAMIDE | VINORELBINE | 0.97 |
| 23 | SKMES1 | Lung | METFORMIN | PACLITAXEL | 0.96 |
| 23 | SKMES1 | Lung | 5-FU | TOPOTECAN | 0.95 |
| 24 | SKOV3 | Ovarian | ETOPOSIDE | TOPOTECAN | 0.99 |
| 24 | SKOV3 | Ovarian | SN-38 | VINBLASTINE | 0.99 |
| 24 | SKOV3 | Ovarian | DEXAMETHASONE | SN-38 | 0.97 |
| 24 | SKOV3 | Ovarian | CYCLOPHOSPHAMIDE | SN-38 | 0.96 |
| 24 | SKOV3 | Ovarian | PACLITAXEL | VINBLASTINE | 0.96 |
| 24 | SKOV3 | Ovarian | DEXAMETHASONE | PACLITAXEL | 0.95 |
| 24 | SKOV3 | Ovarian | PACLITAXEL | SN-38 | 0.94 |
| 24 | SKOV3 | Ovarian | DEXAMETHASONE | VINBLASTINE | 0.92 |
| 24 | SKOV3 | Ovarian | DEXAMETHASONE | TOPOTECAN | 0.9 |
| 24 | SKOV3 | Ovarian | SN-38 | TOPOTECAN | 0.9 |
| 25 | SW620 | Colon | TOPOTECAN | VINBLASTINE | 0.99 |
| 25 | SW620 | Colon | MITOMYCINE | VINBLASTINE | 0.99 |
| 25 | SW620 | Colon | SN-38 | VINBLASTINE | 0.99 |
| 25 | SW620 | Colon | CARBOPLATIN | VINBLASTINE | 0.99 |
| 25 | SW620 | Colon | SN-38 | TOPOTECAN | 0.99 |
| 25 | SW620 | Colon | DOXORUBICIN | VINBLASTINE | 0.98 |
| 25 | SW620 | Colon | PACLITAXEL | VINBLASTINE | 0.98 |
| 25 | SW620 | Colon | DEXAMETHASONE | TOPOTECAN | 0.98 |
| 25 | SW620 | Colon | 5-FU | VINBLASTINE | 0.98 |
| 25 | SW620 | Colon | CYCLOPHOSPHAMIDE | TOPOTECAN | 0.98 |
| 26 | SW837 | Colon | SN-38 | TOPOTECAN | 0.9 |
| 26 | SW837 | Colon | ETOPOSIDE | SN-38 | 0.87 |
| 26 | SW837 | Colon | ETOPOSIDE | TOPOTECAN | 0.84 |
| 26 | SW837 | Colon | ETOPOSIDE | VINBLASTINE | 0.76 |
| 26 | SW837 | Colon | ETOPOSIDE | GEMCITABINE | 0.68 |
| 26 | SW837 | Colon | DEXAMETHASONE | ETOPOSIDE | 0.6 |
| 26 | SW837 | Colon | ETOPOSIDE | MITOMYCINE | 0.6 |
| 26 | SW837 | Colon | SN-38 | VINBLASTINE | 0.58 |
| 26 | SW837 | Colon | MITOMYCINE | VINBLASTINE | 0.57 |
| 26 | SW837 | Colon | GEMCITABINE | SN-38 | 0.5 |
| 27 | T47D | Breast | 5-FU | METFORMIN | 0.98 |
| 27 | T47D | Breast | METFORMIN | SN-38 | 0.91 |
| 27 | T47D | Breast | DOXORUBICIN | METFORMIN | 0.91 |
| 27 | T47D | Breast | 5-FU | SN-38 | 0.83 |
| 27 | T47D | Breast | GEMCITABINE | METFORMIN | 0.74 |
| 27 | T47D | Breast | CYCLOPHOSPHAMIDE | DOXORUBICIN | 0.64 |
| 27 | T47D | Breast | ETOPOSIDE | METFORMIN | 0.54 |
| 27 | T47D | Breast | SN-38 | VINBLASTINE | 0.48 |
| 27 | T47D | Breast | METFORMIN | MITOMYCINE | 0.45 |
| 27 | T47D | Breast | CYCLOPHOSPHAMIDE | METFORMIN | 0.44 |
| 28 | UACC62 | Melanoma | SN-38 | TOPOTECAN | 0.99 |
| 28 | UACC62 | Melanoma | 5-FU | TOPOTECAN | 0.95 |
| 28 | UACC62 | Melanoma | PACLITAXEL | SN-38 | 0.94 |
| 28 | UACC62 | Melanoma | SN-38 | VINBLASTINE | 0.89 |
| 28 | UACC62 | Melanoma | DEXAMETHASONE | SN-38 | 0.87 |
| 28 | UACC62 | Melanoma | MITOMYCINE | VINBLASTINE | 0.86 |
| 28 | UACC62 | Melanoma | 5-FU | ETOPOSIDE | 0.85 |
| 28 | UACC62 | Melanoma | 5-FU | PACLITAXEL | 0.74 |
| 28 | UACC62 | Melanoma | ETOPOSIDE | VINBLASTINE | 0.73 |
| 28 | UACC62 | Melanoma | ETOPOSIDE | SN-38 | 0.71 |
| 29 | VCAP | Prostate | DOXORUBICIN | TOPOTECAN | 0.98 |
| 29 | VCAP | Prostate | CYCLOPHOSPHAMIDE | DOXORUBICIN | 0.97 |
| 29 | VCAP | Prostate | ETOPOSIDE | VINBLASTINE | 0.96 |
| 29 | VCAP | Prostate | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.96 |
| 29 | VCAP | Prostate | CYCLOPHOSPHAMIDE | GEMCITABINE | 0.95 |
| 29 | VCAP | Prostate | CYCLOPHOSPHAMIDE | SN-38 | 0.95 |
| 29 | VCAP | Prostate | 5-FU | ETOPOSIDE | 0.94 |
| 29 | VCAP | Prostate | 5-FU | CYCLOPHOSPHAMIDE | 0.94 |
| 29 | VCAP | Prostate | ETOPOSIDE | SN-38 | 0.94 |
| 29 | VCAP | Prostate | TOPOTECAN | VINBLASTINE | 0.93 |
| 30 | ZR751 | Breast | DEXAMETHASONE | ETOPOSIDE | 0.98 |
| 30 | ZR751 | Breast | CYCLOPHOSPHAMIDE | GEMCITABINE | 0.98 |
| 30 | ZR751 | Breast | CYCLOPHOSPHAMIDE | DEXAMETHASONE | 0.98 |
| 30 | ZR751 | Breast | CYCLOPHOSPHAMIDE | ETOPOSIDE | 0.97 |
| 30 | ZR751 | Breast | CYCLOPHOSPHAMIDE | DOXORUBICIN | 0.96 |
| 30 | ZR751 | Breast | DEXAMETHASONE | SN-38 | 0.95 |
| 30 | ZR751 | Breast | CYCLOPHOSPHAMIDE | PACLITAXEL | 0.95 |
| 30 | ZR751 | Breast | ETOPOSIDE | SN-38 | 0.92 |
| 30 | ZR751 | Breast | DEXAMETHASONE | PACLITAXEL | 0.89 |
| 30 | ZR751 | Breast | CYCLOPHOSPHAMIDE | MITOMYCINE | 0.88 |