**SUPLEMENTAL DATA**

**Identification of a six‑gene signature predicting overall survival for Oxaliplatin and 5-Fluorouracil resistant Colon cancer and potential drug-repurposing**

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**Supplementary figures:**

地图上有字

描述已自动生成

**FIGURE S1**. The active site of ANO1 was found by Schrodinger maestro 2019-1

**Supplementary tables:**

**Table S1**. The clinical data of 22 patients treated by oxaliplatin and 5-fluorouracil.

|  |  |  |  |
| --- | --- | --- | --- |
| ID | Resistence | Time | Status |
| TCGA-A6-A566-01A | yes | 758 | dead |
| TCGA-AZ-6606-01A | yes | 357 | dead |
| TCGA-A6-A565-01A | yes | 494 | dead |
| TCGA-AA-3680-01A | yes | 335 | dead |
| TCGA-NH-A6GA-01A | yes | 302 | dead |
| TCGA-NH-A6GB-01A | yes | 476 | alive |
| TCGA-A6-A5ZU-01A | no | 293 | alive |
| TCGA-AA-A010-01A | no | 1064 | alive |
| TCGA-AA-3955-01A | no | 638 | alive |
| TCGA-AA-3678-01A | no | 1430 | alive |
| TCGA-D5-6533-01A | no | 775 | alive |
| TCGA-AA-3842-01A | no | 1126 | alive |
| TCGA-AA-3860-01A | no | 945 | alive |
| TCGA-AA-3841-01A | no | 1124 | alive |
| TCGA-AA-A00Q-01A | no | 1278 | alive |
| TCGA-AA-3542-01A | no | 395 | alive |
| TCGA-AA-3870-01A | no | 912 | alive |
| TCGA-AA-3971-01A | no | 489 | alive |
| TCGA-AA-A00U-01A | no | 518 | alive |
| TCGA-F4-6856-01A | no | 1074 | alive |
| TCGA-AA-A01K-01A | no | 943 | alive |
| TCGA-AA-3560-01A | no | 608 | alive |

**Table S2**. The person correlation value and p value between module and clinical traits.

|  |  |  |  |
| --- | --- | --- | --- |
| Module | Trait | PersonCorrelationValue | Pvalue |
| MEblack | Resistence | -0.13106 | 0.560999 |
| MEblue | Resistence | -0.50439 | 0.016675 |
| MEbrown | Resistence | 0.644388 | 0.001208 |
| MEcyan | Resistence | 0.287037 | 0.195253 |
| MEgreen | Resistence | -0.33627 | 0.125983 |
| MEgreenyellow | Resistence | -0.50265 | 0.017116 |
| MEgrey | Resistence | -0.1861 | 0.406995 |
| MEgrey60 | Resistence | 0.31042 | 0.159716 |
| MElightcyan | Resistence | 0.108489 | 0.630816 |
| MElightgreen | Resistence | -0.21536 | 0.335792 |
| MElightyellow | Resistence | 0.372112 | 0.08813 |
| MEmagenta | Resistence | -0.54501 | 0.008716 |
| MEmidnightblue | Resistence | -0.25813 | 0.246114 |
| MEpink | Resistence | 0.172444 | 0.442846 |
| MEpurple | Resistence | 0.054118 | 0.810955 |
| MEred | Resistence | -0.16253 | 0.469885 |
| MEsalmon | Resistence | -0.03181 | 0.888248 |
| MEtan | Resistence | -0.54416 | 0.008841 |
| MEturquoise | Resistence | 0.133516 | 0.553615 |
| MEyellow | Resistence | 0.150756 | 0.503064 |

**Table S3**. Genes related to chemotherapeutic resistance.

|  |  |  |  |
| --- | --- | --- | --- |
| ID | module | geneModuleMembership | geneTraitCor |
| GYG1 | brown | 0.5178589 | 0.5365771 |
| CREB3 | brown | 0.5562158 | 0.5694481 |
| LEF1 | brown | 0.5992042 | 0.6139571 |
| C1orf122 | brown | 0.6639202 | 0.5476656 |
| DDX5 | brown | 0.8353281 | 0.5959748 |
| CCDC14 | brown | 0.7899003 | 0.5903803 |
| PCBD1 | brown | 0.6305881 | 0.5644354 |
| SNX1 | brown | 0.5936754 | 0.507478 |
| AC006001.4 | brown | 0.783972 | 0.5737144 |
| TMOD3 | brown | 0.7890677 | 0.6090703 |
| FBL | brown | 0.5591397 | 0.5169086 |
| PTPN12 | brown | 0.7225549 | 0.5494986 |
| H3F3A | brown | 0.705656 | 0.5133633 |
| ZNF638 | brown | 0.8652467 | 0.5313881 |
| MSRB2 | brown | 0.7925326 | 0.5750424 |
| NUFIP2 | brown | 0.8514041 | 0.5174628 |
| HIF1A | brown | 0.8140778 | 0.6672621 |
| LEO1 | brown | 0.7491807 | 0.5233008 |
| SRRM1 | brown | 0.7753359 | 0.53653 |
| EBP | brown | 0.7016998 | 0.6876579 |
| DYNC1LI2 | brown | 0.8239872 | 0.5578475 |
| MRPS26 | brown | 0.7340279 | 0.5803238 |
| LRRFIP1 | brown | 0.846507 | 0.5170891 |
| ANP32E | brown | 0.7840135 | 0.5195379 |
| SIGMAR1 | brown | 0.7403242 | 0.5896433 |
| MPHOSPH8 | brown | 0.8463619 | 0.541986 |
| PRPF38B | brown | 0.8317914 | 0.5470773 |
| ARF5 | brown | 0.6478582 | 0.5300908 |
| BCKDK | brown | 0.8288216 | 0.6335221 |
| KLF6 | brown | 0.6287899 | 0.5967497 |
| AC018638.2 | brown | 0.7287019 | 0.5768522 |
| UXT | brown | 0.6134966 | 0.6550902 |
| RPP25L | brown | 0.5208211 | 0.5471701 |
| PQBP1 | brown | 0.6744895 | 0.7059518 |
| PXN | brown | 0.6032999 | 0.5464595 |
| GSDMB | brown | 0.7746207 | 0.6882127 |
| ATP2B1 | brown | 0.7962235 | 0.5640798 |
| P4HTM | brown | 0.7040473 | 0.5004624 |
| RALBP1 | brown | 0.6225117 | 0.5412556 |
| AL390728.4 | brown | 0.7854673 | 0.6786811 |
| XDH | brown | 0.6255241 | 0.6226171 |
| TUG1 | brown | 0.8997907 | 0.5940866 |
| AFG3L2 | brown | 0.6624678 | 0.5611163 |
| TIMM8B | brown | 0.6299326 | 0.5447221 |
| NEAT1 | brown | 0.7475089 | 0.5583649 |
| SRSF11 | brown | 0.8143873 | 0.5271474 |
| RPS4X | brown | 0.6411238 | 0.631444 |
| ATP6V0D1 | brown | 0.7508516 | 0.5662541 |
| DENND1C | brown | 0.7131856 | 0.5225651 |
| PRADC1 | brown | 0.8207566 | 0.5152641 |
| PNN | brown | 0.8743825 | 0.6311787 |
| SIAH2 | brown | 0.5347537 | 0.5325903 |
| MDH2 | brown | 0.6783194 | 0.5586183 |
| SLC46A3 | brown | 0.5935705 | 0.6286015 |
| HCCS | brown | 0.5322064 | 0.5372589 |
| NDUFB11 | brown | 0.8241342 | 0.6972095 |
| TRAPPC2L | brown | 0.6108201 | 0.5705638 |
| SF3B1 | brown | 0.6081929 | 0.5663218 |
| SRSF5 | brown | 0.6915807 | 0.5970587 |
| PLP2 | brown | 0.7717088 | 0.6735823 |
| KTN1 | brown | 0.8138769 | 0.5628331 |
| IVNS1ABP | brown | 0.8224797 | 0.7366342 |
| AC018638.4 | brown | 0.6534616 | 0.535919 |
| SRRM2 | brown | 0.8063306 | 0.5260271 |
| RNF181 | brown | 0.6691879 | 0.6794609 |
| MCM3AP | brown | 0.7044567 | 0.54617 |
| NAPG | brown | 0.6817643 | 0.6022187 |
| BNIP2 | brown | 0.7043112 | 0.580169 |
| SLC39A6 | brown | 0.6896912 | 0.5719741 |
| PPP4C | brown | 0.573086 | 0.5094455 |
| RPL41P5 | brown | 0.541858 | 0.5247372 |
| SON | brown | 0.8154629 | 0.5677361 |
| LUC7L3 | brown | 0.9123849 | 0.5359367 |
| B3GNT2 | brown | 0.7690962 | 0.6214297 |
| RBM25 | brown | 0.8583625 | 0.6173562 |
| ZMIZ1 | brown | 0.6842223 | 0.5157488 |
| ERBIN | brown | 0.8223052 | 0.5803237 |
| HNRNPH1 | brown | 0.8227069 | 0.5816868 |
| RNASEH2A | brown | 0.6955965 | 0.5138907 |
| MYO5B | brown | 0.6547318 | 0.5398368 |
| TPR | brown | 0.7930594 | 0.5217013 |
| MYDGF | brown | 0.7368319 | 0.5848503 |
| TRIP12 | brown | 0.7462394 | 0.633281 |
| KIAA0232 | brown | 0.8321099 | 0.5942574 |
| GTF3C5 | brown | 0.5110306 | 0.6191147 |
| UBA52 | brown | 0.7489584 | 0.5295833 |
| CIRBP | brown | 0.7269729 | 0.5041051 |
| GDA | brown | 0.5474326 | 0.5360806 |
| ANKRD10-IT1 | brown | 0.7350244 | 0.6274732 |
| HTATSF1 | brown | 0.647758 | 0.584981 |
| PSMB7 | brown | 0.5696597 | 0.5772626 |
| ALG3 | brown | 0.6205311 | 0.5190516 |
| SLC20A1 | brown | 0.7101389 | 0.5558465 |
| KLF13 | brown | 0.7448593 | 0.6991138 |
| CIAO2B | brown | 0.692004 | 0.5006767 |
| MBD2 | brown | 0.7802995 | 0.5251234 |
| RNF213 | brown | 0.7562443 | 0.5045423 |
| SLTM | brown | 0.8699194 | 0.624943 |
| DDX42 | brown | 0.8224444 | 0.5004885 |
| MYO1E | brown | 0.6396032 | 0.5354619 |
| RSRP1 | brown | 0.6562004 | 0.5073585 |
| STOML2 | brown | 0.529555 | 0.6427753 |
| TTC3 | brown | 0.860587 | 0.6066397 |
| ZC3H11A | brown | 0.8383756 | 0.6235163 |
| RBM6 | brown | 0.8113515 | 0.5102438 |
| VAPA | brown | 0.6894706 | 0.5719704 |
| CASP5 | brown | 0.5922258 | 0.5009686 |
| NUTF2 | brown | 0.8629291 | 0.5574305 |
| DCTN3 | brown | 0.8185219 | 0.6201347 |
| HSD17B10 | brown | 0.7874847 | 0.6392035 |
| AMFR | brown | 0.8313299 | 0.5752367 |
| AL390728.6 | brown | 0.6535359 | 0.6204363 |
| EIF4G3 | brown | 0.7842111 | 0.6037184 |
| CAB39 | brown | 0.7464842 | 0.5877418 |
| TIMM17B | brown | 0.6533133 | 0.6831848 |
| CCNQ | brown | 0.5337756 | 0.6218904 |
| HP1BP3 | brown | 0.8108076 | 0.6172935 |
| PRRC2C | brown | 0.752153 | 0.5855663 |
| MYO18A | brown | 0.7487021 | 0.5915392 |
| STX5 | brown | 0.7721661 | 0.522475 |
| AC016739.1 | tan | 0.8974802 | 0.5371492 |
| AL138785.1 | tan | 0.8359776 | 0.6109684 |
| AC098591.2 | tan | 0.8188628 | 0.5139336 |
| CDK11B | tan | 0.7201026 | 0.5268493 |
| AC010422.3 | tan | 0.8438135 | 0.5347749 |
| RPS6P25 | tan | 0.5663501 | 0.5123898 |
| RPL34P31 | tan | 0.8003914 | 0.5270947 |
| EP300 | tan | 0.7919426 | 0.5830773 |
| Z97353.1 | tan | 0.5467856 | 0.5299008 |
| AC010343.1 | tan | 0.7154218 | 0.5415777 |
| GPX4 | tan | 0.5194868 | 0.5860939 |
| RPL29 | tan | 0.7597837 | 0.5409486 |
| PDK3 | tan | 0.6180874 | 0.6148383 |
| AC074085.2 | tan | 0.7839488 | 0.5251882 |
| RPL18 | tan | 0.5519358 | 0.5491431 |
| ACTG1P20 | tan | 0.6340168 | 0.5348833 |
| AL136126.1 | tan | 0.8473739 | 0.5320071 |
| RPL35P2 | tan | 0.5791504 | 0.5011638 |
| ATP5F1EP2 | tan | 0.5442578 | 0.5149494 |
| RPL13P2 | tan | 0.9072357 | 0.5642533 |
| RPS19P1 | tan | 0.6200518 | 0.5318446 |
| RPS11P5 | tan | 0.8389272 | 0.5348692 |
| GAPDHP65 | tan | 0.8258156 | 0.5008682 |
| AC004453.1 | tan | 0.6794298 | 0.5349837 |
| AC009362.1 | tan | 0.6364131 | 0.5447112 |
| AP001024.1 | tan | 0.545145 | 0.5117969 |
| FTLP3 | tan | 0.8407688 | 0.5206571 |
| TRIR | tan | 0.8105401 | 0.5077397 |
| TMSB10P1 | tan | 0.7314032 | 0.5530075 |
| ACTBP2 | tan | 0.6883073 | 0.5048642 |
| FAUP1 | tan | 0.6346784 | 0.5454529 |
| AC012618.1 | tan | 0.5721091 | 0.5552621 |
| AC021074.1 | tan | 0.6231507 | 0.5460439 |
| RPS14P8 | tan | 0.7610742 | 0.6184912 |
| HNRNPUP1 | tan | 0.6254672 | 0.5236828 |
| DDX28 | magenta | 0.7104678 | 0.5607615 |
| PSPH | magenta | 0.5317773 | 0.5130231 |
| APEH | magenta | 0.831284 | 0.523702 |
| YIF1A | magenta | 0.644519 | 0.5251398 |
| TKT | magenta | 0.9174555 | 0.5956367 |
| POLR3GL | magenta | 0.69677 | 0.5139102 |
| MRPL2 | magenta | 0.6460433 | 0.5297557 |
| PAFAH1B3 | magenta | 0.6014352 | 0.6304785 |
| SF3B5 | magenta | 0.6725736 | 0.6408521 |
| PPP1CA | magenta | 0.6757808 | 0.5219818 |
| EMC8 | magenta | 0.8454915 | 0.512925 |
| UQCRC1 | magenta | 0.8348662 | 0.5504633 |
| THAP11 | magenta | 0.681396 | 0.5969116 |
| FOSL2 | magenta | 0.7082987 | 0.539329 |
| THOC6 | magenta | 0.6269068 | 0.5738859 |
| CYC1 | magenta | 0.6727234 | 0.5569632 |
| STAT2 | magenta | 0.7960569 | 0.5536658 |
| IFI16 | magenta | 0.7536577 | 0.539416 |
| RPUSD3 | magenta | 0.8619512 | 0.5204487 |
| GPT2 | magenta | 0.5814061 | 0.5049377 |
| TALDO1 | magenta | 0.8537162 | 0.5478926 |
| COX4I1 | magenta | 0.7662575 | 0.5991706 |
| ASB13 | magenta | 0.7460549 | 0.5686721 |
| FAM83D | magenta | 0.7960909 | 0.5197045 |
| EMP1 | magenta | 0.5480794 | 0.6198829 |
| PRDX2 | magenta | 0.8275419 | 0.5676988 |
| NDUFB10 | magenta | 0.7432139 | 0.5773132 |
| TUFM | magenta | 0.8547184 | 0.5036962 |
| CFAP20 | magenta | 0.7901928 | 0.6460393 |
| DHCR7 | magenta | 0.7030829 | 0.7093277 |
| MRPL49 | magenta | 0.5713481 | 0.5322071 |
| IDH2 | magenta | 0.5759917 | 0.6789729 |
| ZDHHC16 | magenta | 0.7741218 | 0.5250902 |
| PRDX4 | magenta | 0.5967272 | 0.6292627 |
| BHLHE41 | magenta | 0.614587 | 0.5163373 |
| PDHA1 | magenta | 0.6138084 | 0.5394806 |
| LCMT1 | magenta | 0.7445709 | 0.5370051 |
| MSRB1 | magenta | 0.5434692 | 0.5157193 |
| CYP3A5 | magenta | 0.5663921 | 0.5515166 |
| UTP4 | magenta | 0.7419648 | 0.5389865 |
| CCT7 | magenta | 0.8203931 | 0.6087546 |
| COG4 | magenta | 0.7976916 | 0.521841 |
| E2F4 | magenta | 0.6972734 | 0.5087448 |
| ALDOA | magenta | 0.5620797 | 0.5813814 |
| TLCD1 | magenta | 0.5759323 | 0.564295 |
| MZT2A | blue | 0.7375832 | 0.513653 |
| NMRAL1 | blue | 0.7458711 | 0.5198722 |
| SCAND1 | blue | 0.5789045 | 0.517618 |
| CARD19 | blue | 0.7760107 | 0.51633 |
| EEFSEC | blue | 0.676196 | 0.7040106 |
| ADGRL1 | blue | 0.6599077 | 0.5774077 |
| C8orf82 | blue | 0.5842951 | 0.5221764 |
| SSNA1 | blue | 0.5852878 | 0.5029773 |
| FGFR4 | blue | 0.685467 | 0.5145595 |
| SPATC1L | blue | 0.67612 | 0.5675065 |
| TECR | blue | 0.5338815 | 0.6283292 |
| RPLP2 | blue | 0.5652742 | 0.5113343 |
| SAC3D1 | blue | 0.6662254 | 0.5704605 |
| NPRL2 | blue | 0.7321541 | 0.5528247 |
| STX10 | blue | 0.6505042 | 0.590133 |
| SLC25A1 | blue | 0.6034127 | 0.6392781 |
| ACD | blue | 0.7005343 | 0.5059895 |
| RNF126 | blue | 0.7067549 | 0.5198444 |
| PDF | blue | 0.7191967 | 0.5098337 |
| PRMT1 | blue | 0.5504733 | 0.5420112 |
| RPL13 | blue | 0.6662069 | 0.5677343 |
| LRP3 | blue | 0.760877 | 0.5061644 |
| NOSIP | blue | 0.5339059 | 0.5657148 |
| SDHAF1 | blue | 0.5852257 | 0.5007377 |
| FBXL15 | blue | 0.5271935 | 0.5330257 |
| RPS2 | blue | 0.7805366 | 0.5482957 |
| H2AFX | blue | 0.6585589 | 0.5458206 |
| NUDT16L1 | blue | 0.5201973 | 0.6349257 |
| CPNE1 | greenyellow | 0.8568016 | 0.5343864 |
| ANO1 | greenyellow | 0.6288907 | 0.686598 |
| MANBAL | greenyellow | 0.7781175 | 0.5741766 |
| GSS | greenyellow | 0.8116473 | 0.5839538 |
| IL1R2 | greenyellow | 0.6207927 | 0.5022053 |
| PIGU | greenyellow | 0.9397002 | 0.516385 |
| MMP24OS | greenyellow | 0.6502046 | 0.5828545 |
| ACOT8 | greenyellow | 0.611957 | 0.5224105 |
| TP53RK | greenyellow | 0.7983067 | 0.5115327 |
| RALY | greenyellow | 0.7746395 | 0.5528844 |
| SLC37A4 | greenyellow | 0.713245 | 0.5828529 |
| TMEM208 | greenyellow | 0.6946304 | 0.5033341 |
| PXMP4 | greenyellow | 0.7739019 | 0.5150968 |
| EDEM2 | greenyellow | 0.8428982 | 0.5616338 |
| NFS1 | greenyellow | 0.8729552 | 0.5899614 |
| ROMO1 | greenyellow | 0.678191 | 0.5446571 |
| RASA3 | greenyellow | 0.7384369 | 0.6118842 |
| GJB5 | greenyellow | 0.5063983 | 0.5505016 |
| TCEAL9 | greenyellow | 0.7816408 | 0.5257371 |
| DYNLRB1 | greenyellow | 0.9283904 | 0.5912639 |
| ZSWIM3 | greenyellow | 0.8084657 | 0.5431095 |
| EIF6 | greenyellow | 0.8844135 | 0.5233076 |
| MBOAT2 | greenyellow | 0.5332738 | 0.5204409 |
| QPRT | greenyellow | 0.7514707 | 0.5166959 |
| GPR143 | greenyellow | 0.8282009 | 0.5304309 |
| RNF114 | greenyellow | 0.7574845 | 0.5706637 |
| CDC42BPB | greenyellow | 0.84185 | 0.5375382 |
| CTNNBL1 | greenyellow | 0.8129187 | 0.5141341 |
| ERGIC3 | greenyellow | 0.8372437 | 0.5669646 |
| SMYD5 | greenyellow | 0.5926631 | 0.516207 |
| COMMD7 | greenyellow | 0.7802872 | 0.5084335 |
| DUSP6 | greenyellow | 0.6869532 | 0.6101139 |
| TRPC4AP | greenyellow | 0.9012178 | 0.5154782 |
| AHCY | greenyellow | 0.7146494 | 0.5652989 |

**Table S4**. The results of GSEA. GSEA, Gene Set Enrichment Analysis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| GS follow link to MSigDB | SIZE | ES | NES | NOM p-val | FDR q-val |
| KEGG\_ECM\_RECEPTOR\_INTERACTION | 84 | 0.59 | 1.71 | 0 | 0.047 |
| KEGG\_HEMATOPOIETIC\_CELL\_LINEAGE | 85 | 0.57 | 1.67 | 0 | 0.047 |
| KEGG\_FOCAL\_ADHESION | 199 | 0.52 | 1.62 | 0 | 0.048 |
| KEGG\_RIBOSOME | 87 | -0.74 | -2.73 | 0 | 0 |
| KEGG\_PROTEASOME | 46 | -0.68 | -2.29 | 0 | 0 |
| KEGG\_PARKINSONS\_DISEASE | 127 | -0.57 | -2.28 | 0 | 0 |
| KEGG\_OXIDATIVE\_PHOSPHORYLATION | 131 | -0.56 | -2.22 | 0 | 0 |
| KEGG\_STEROID\_BIOSYNTHESIS | 17 | -0.82 | -2.17 | 0 | 0.001 |
| KEGG\_CITRATE\_CYCLE\_TCA\_CYCLE | 31 | -0.69 | -2.12 | 0 | 0.001 |
| KEGG\_PYRUVATE\_METABOLISM | 40 | -0.65 | -2.12 | 0 | 0.001 |
| KEGG\_PENTOSE\_PHOSPHATE\_PATHWAY | 27 | -0.72 | -2.06 | 0 | 0.001 |
| KEGG\_GLYCOLYSIS\_GLUCONEOGENESIS | 62 | -0.55 | -1.92 | 0 | 0.003 |
| KEGG\_HUNTINGTONS\_DISEASE | 180 | -0.44 | -1.84 | 0 | 0.006 |
| KEGG\_ALZHEIMERS\_DISEASE | 165 | -0.44 | -1.79 | 0 | 0.008 |
| KEGG\_PEROXISOME | 78 | -0.48 | -1.76 | 0 | 0.011 |
| KEGG\_PROPANOATE\_METABOLISM | 32 | -0.56 | -1.72 | 0.005 | 0.015 |
| KEGG\_DNA\_REPLICATION | 36 | -0.55 | -1.7 | 0.01 | 0.017 |
| KEGG\_BIOSYNTHESIS\_OF\_UNSATURATED\_FATTY\_ACIDS | 22 | -0.58 | -1.65 | 0.008 | 0.023 |
| KEGG\_ARGININE\_AND\_PROLINE\_METABOLISM | 54 | -0.49 | -1.64 | 0 | 0.024 |
| KEGG\_GLYOXYLATE\_AND\_DICARBOXYLATE\_METABOLISM | 16 | -0.61 | -1.6 | 0.029 | 0.029 |
| KEGG\_FRUCTOSE\_AND\_MANNOSE\_METABOLISM | 33 | -0.51 | -1.57 | 0.004 | 0.034 |
| KEGG\_SYSTEMIC\_LUPUS\_ERYTHEMATOSUS | 135 | -0.39 | -1.55 | 0 | 0.039 |

**Table S5**. The docking results of ANO1.

|  |  |  |
| --- | --- | --- |
| Title | docking score | glide gscore |
| ZINC000018043251 | -8.436 | -8.468 |
| ZINC000001997127 | -8.277 | -8.277 |
| ZINC000003871541 | -8.269 | -8.269 |
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