

|        | Crossdock Default | Crossdock Default2018 | General Default | Redock Default | Redock Default2018 | All Ensemble | Vina |  |
|--------|-------------------|-----------------------|-----------------|----------------|--------------------|--------------|------|--|
|        | Default Ensemble  | Dense Ensemble        | 2018 Ensemble   | 2018 Ensemble  | 2018 Ensemble      |              |      |  |
| AA2AR  | 0                 | 0                     | 0               | 0              | 0                  | 0            | 0    |  |
| ABL1   | 21                | 19                    | 20              | 20             | 16                 | 21           | 18   |  |
| ACE    | 43                | 39                    | 43              | 34             | 45                 | 45           | 29   |  |
| ACES   | 12                | 11                    | 14              | 16             | 9                  | 13           | 8    |  |
| ADA    | 41                | 35                    | 34              | 36             | 34                 | 39           | 22   |  |
| ADA17  | 41                | 34                    | 38              | 43             | 34                 | 39           | 33   |  |
| ADRB1  | 65                | 55                    | 56              | 55             | 54                 | 64           | 42   |  |
| ADRB2  | 59                | 59                    | 47              | 56             | 59                 | 61           | 56   |  |
| AKT1   | 46                | 44                    | 45              | 41             | 43                 | 46           | 36   |  |
| AKT2   | 40                | 35                    | 37              | 33             | 32                 | 37           | 16   |  |
| ALDR   | 17                | 17                    | 17              | 17             | 17                 | 17           | 17   |  |
| AMPC   | 16                | 8                     | 11              | 18             | 10                 | 14           | 5    |  |
| ANDR   | 46                | 47                    | 35              | 43             | 38                 | 48           | 46   |  |
| AOFB   | 33                | 33                    | 33              | 33             | 33                 | 33           | 0    |  |
| BACE1  | 19                | 17                    | 17              | 18             | 13                 | 19           | 16   |  |
| BRAF   | 37                | 35                    | 36              | 37             | 33                 | 37           | 27   |  |
| CAH2   | 41                | 37                    | 37              | 50             | 38                 | 41           | 21   |  |
| CASP3  | 2                 | 1                     | 2               | 2              | 0                  | 3            | 1    |  |
| CDK2   | 35                | 32                    | 26              | 32             | 31                 | 34           | 10   |  |
| CP2C9  | 4                 | 4                     | 4               | 0              | 4                  | 0            | 0    |  |
| CP3A4  | 0                 | 0                     | 0               | 0              | 0                  | 0            | 0    |  |
| CSF1R  | 24                | 26                    | 23              | 26             | 23                 | 24           | 14   |  |
| DEF    | 50                | 54                    | 46              | 42             | 44                 | 52           | 40   |  |
| DPP4   | 23                | 21                    | 24              | 21             | 21                 | 24           | 14   |  |
| DYR    | 20                | 15                    | 26              | 19             | 13                 | 20           | 6    |  |
| EGFR   | 19                | 21                    | 17              | 17             | 15                 | 18           | 12   |  |
| ESR1   | 47                | 36                    | 37              | 39             | 36                 | 49           | 42   |  |
| ESR2   | 52                | 36                    | 31              | 46             | 43                 | 50           | 50   |  |
| FA10   | 68                | 62                    | 70              | 65             | 62                 | 68           | 50   |  |
| FA7    | 32                | 29                    | 36              | 30             | 29                 | 35           | 20   |  |
| FABP4  | 30                | 20                    | 34              | 21             | 21                 | 26           | 11   |  |
| FAK1   | 38                | 37                    | 38              | 37             | 34                 | 38           | 16   |  |
| FKB1A  | 47                | 49                    | 32              | 42             | 41                 | 49           | 36   |  |
| FNTA   | 14                | 8                     | 17              | 9              | 7                  | 13           | 4    |  |
| FPPS   | 37                | 21                    | 41              | 41             | 19                 | 33           | 7    |  |
| GCR    | 34                | 28                    | 28              | 47             | 17                 | 40           | 43   |  |
| GLCM   | 57                | 54                    | 50              | 38             | 54                 | 57           | 47   |  |
| GRIA2  | 52                | 47                    | 49              | 48             | 39                 | 50           | 27   |  |
| GRIK1  | 36                | 30                    | 41              | 36             | 28                 | 37           | 30   |  |
| HDAC2  | 65                | 60                    | 55              | 65             | 55                 | 60           | 60   |  |
| HDAC8  | 10                | 10                    | 5               | 2              | 5                  | 12           | 8    |  |
| HIVINT | 15                | 12                    | 10              | 12             | 18                 | 18           | 5    |  |
| HIVPR  | 26                | 18                    | 26              | 27             | 14                 | 22           | 13   |  |
| HIVRT  | 36                | 26                    | 30              | 23             | 25                 | 31           | 27   |  |
| HMDH   | 78                | 61                    | 79              | 69             | 68                 | 75           | 80   |  |
| HS90A  | 32                | 27                    | 37              | 31             | 17                 | 30           | 26   |  |
| HXK4   | 34                | 30                    | 25              | 27             | 29                 | 32           | 17   |  |
| IGF1R  | 14                | 14                    | 15              | 13             | 12                 | 15           | 7    |  |
| ITAL   | 14                | 17                    | 13              | 12             | 12                 | 14           | 10   |  |
| JAK2   | 31                | 34                    | 26              | 29             | 26                 | 33           | 19   |  |
| KIF11  | 62                | 60                    | 52              | 54             | 52                 | 60           | 55   |  |
| KIT    | 21                | 21                    | 21              | 17             | 17                 | 17           | 17   |  |
| KITH   | 50                | 50                    | 50              | 50             | 50                 | 50           | 50   |  |
| LCK    | 33                | 34                    | 34              | 31             | 32                 | 34           | 21   |  |
| LKHA4  | 32                | 27                    | 21              | 33             | 23                 | 32           | 18   |  |
| MAPK2  | 44                | 42                    | 36              | 46             | 31                 | 44           | 35   |  |
| MCR    | 58                | 60                    | 46              | 64             | 46                 | 66           | 73   |  |
| MET    | 34                | 30                    | 33              | 32             | 33                 | 34           | 34   |  |
| MK01   | 28                | 22                    | 25              | 25             | 23                 | 27           | 14   |  |
| MK10   | 25                | 24                    | 24              | 25             | 20                 | 26           | 15   |  |
| MK14   | 25                | 22                    | 25              | 22             | 22                 | 26           | 19   |  |
| MMP13  | 25                | 22                    | 21              | 21             | 20                 | 29           | 19   |  |
| MP2K1  | 28                | 23                    | 23              | 29             | 14                 | 29           | 17   |  |
| NRAM   | 61                | 43                    | 68              | 66             | 40                 | 55           | 17   |  |
| PA2GA  | 56                | 44                    | 53              | 57             | 40                 | 58           | 57   |  |
| PARP1  | 58                | 49                    | 54              | 52             | 52                 | 57           | 40   |  |
| PDE5A  | 20                | 19                    | 23              | 16             | 16                 | 17           | 5    |  |
| PGH1   | 48                | 34                    | 32              | 43             | 34                 | 46           | 25   |  |
| PGH2   | 21                | 23                    | 15              | 17             | 20                 | 24           | 17   |  |
| PLK1   | 54                | 52                    | 53              | 55             | 39                 | 55           | 36   |  |
| PNPH   | 29                | 34                    | 34              | 40             | 29                 | 37           | 14   |  |
| PPARA  | 29                | 20                    | 29              | 25             | 23                 | 27           | 19   |  |
| PPARD  | 22                | 18                    | 22              | 20             | 20                 | 20           | 20   |  |
| PPARG  | 5                 | 2                     | 7               | 11             | 5                  | 6            | 3    |  |
| PRGR   | 62                | 57                    | 51              | 52             | 51                 | 63           | 59   |  |
| PTN1   | 28                | 29                    | 30              | 32             | 27                 | 31           | 28   |  |
| PUR2   | 32                | 32                    | 27              | 33             | 32                 | 35           | 17   |  |
| PYGM   | 8                 | 4                     | 8               | 4              | 6                  | 10           | 0    |  |
| PYRD   | 41                | 38                    | 24              | 36             | 35                 | 41           | 20   |  |
| RENI   | 44                | 38                    | 43              | 40             | 33                 | 44           | 37   |  |
| ROCK1  | 36                | 28                    | 33              | 35             | 29                 | 34           | 16   |  |
| RXRA   | 40                | 30                    | 32              | 45             | 31                 | 39           | 47   |  |
| SAHH   | 0                 | 0                     | 0               | 0              | 0                  | 0            | 0    |  |
| SRC    | 28                | 26                    | 30              | 28             | 19                 | 29           | 12   |  |
| TGFR1  | 46                | 36                    | 44              | 47             | 32                 | 45           | 21   |  |
| THB    | 82                | 80                    | 72              | 81             | 77                 | 83           | 78   |  |
| THRB   | 62                | 53                    | 62              | 58             | 51                 | 61           | 46   |  |
| TRY1   | 33                | 35                    | 33              | 32             | 30                 | 33           | 30   |  |
| TRYB1  | 15                | 13                    | 18              | 23             | 14                 | 16           | 13   |  |
| TYSY   | 25                | 22                    | 25              | 19             | 20                 | 23           | 11   |  |
| UROK   | 25                | 16                    | 23              | 19             | 22                 | 23           | 14   |  |
| VGFR2  | 62                | 53                    | 55              | 58             | 45                 | 62           | 44   |  |
| WEE1   | 69                | 71                    | 61              | 71             | 65                 | 71           | 57   |  |
| XIAP   | 38                | 40                    | 44              | 39             | 38                 | 40           | 32   |  |