|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Descriptor ID | Fitness | Model | R2 | Q2 | R2Pred\_Validation | R2Pred\_Test | |
| [81L, 101L, 164L, 175L, 185L, 230L] | 0.44 | MLR | 0.34 | 0.08 | 0.08 | -0.33 |  |
| [4L, 132L, 174L, 264L, 382L] | 0.45 | MLR | 0.25 | 0.07 | 0.05 | -0.02 |  |
| [11L, 20L, 27L, 50L, 82L, 125L, 164L, 173L, 247L, 299L, 377L] | 0.45 | MLR | 0.46 | -0.2 | 0.48 | -0.44 |  |
| **[177L, 269L, 327L, 368L]** | **0.47** | **MLR** | **0.14** | **-0.04** | **0.12** | **0.32** | **row of best fitness** |
| [164L, 187L, 264L, 274L, 307L, 379L] | 0.48 | MLR | 0.28 | -0.13 | 0.24 | 0.46 |  |
| [57L, 181L, 197L, 276L, 306L, 318L, 321L, 337L] | 0.49 | MLR | 0.27 | -0.13 | 0.17 | 0.05 |  |
| [151L, 218L, 303L] | 0.49 | MLR | 0.09 | -0.08 | 0.07 | -0.14 |  |
| [83L, 112L, 157L, 161L, 170L, 232L, 296L, 316L] | 0.49 | MLR | 0.39 | 0.1 | -0.19 | -0.01 |  |
| [99L, 157L, 175L, 248L, 271L, 359L, 366L, 371L] | 0.49 | MLR | 0.39 | 0.09 | -0.18 | -0.27 |  |
| [85L, 100L, 103L, 105L, 175L, 307L, 356L] | 0.49 | MLR | 0.24 | 0 | -0.05 | -0.69 |  |
| [36L, 64L, 86L, 156L, 168L, 184L, 190L, 335L, 384L] | 0.5 | MLR | 0.44 | 0.07 | -0.24 | -0.15 |  |
| [80L, 131L, 182L, 194L, 294L, 300L, 370L] | 0.5 | MLR | 0.14 | -0.26 | 0.32 | -0.93 |  |
| [29L, 105L, 221L, 239L, 257L, 312L] | 0.5 | MLR | 0.24 | 0.02 | -0.15 | -0.61 |  |
| [77L, 215L, 239L] | 0.51 | MLR | 0.08 | -0.08 | -0.01 | -0.23 |  |
| [43L, 245L, 272L] | 0.52 | MLR | 0.01 | -0.15 | 0.07 | -0.08 |  |
| [59L, 128L, 140L, 286L] | 0.52 | MLR | 0.11 | -0.08 | -0.1 | -0.13 |  |
| [55L, 175L, 225L, 311L, 322L] | 0.53 | MLR | 0.11 | -0.16 | 0.02 | -0.32 |  |
| [3L, 87L, 110L, 136L, 163L, 174L, 314L] | 0.53 | MLR | 0.18 | -0.07 | -0.16 | -0.43 |  |
| [44L, 149L, 266L, 272L] | 0.53 | MLR | 0.09 | -0.21 | 0.1 | -0.22 |  |
| [11L, 113L, 151L, 384L] | 0.54 | MLR | 0.02 | -0.21 | 0.01 | -0.11 |  |
| [24L, 180L, 238L, 249L, 273L] | 0.56 | MLR | 0.18 | -0.12 | -0.24 | -0.47 |  |
| [107L, 169L, 296L, 310L, 314L, 316L, 367L] | 0.56 | MLR | 0.15 | -0.18 | -0.12 | -0.03 |  |
| [119L, 230L, 312L, 360L] | 0.56 | MLR | 0.07 | -0.14 | -0.21 | -0.43 |  |
| [2L, 106L, 200L, 301L, 383L] | 0.56 | MLR | 0.09 | -0.13 | -0.22 | -0.29 |  |
| [33L, 79L, 86L, 174L, 201L] | 0.56 | MLR | 0.24 | -0.24 | -0.03 | 0.08 |  |
| [46L, 69L, 159L] | 0.57 | MLR | 0.21 | 0.11 | -0.68 | -0.2 |  |
| [95L, 117L, 265L, 344L, 356L, 372L] | 0.57 | MLR | 0.21 | -0.03 | -0.46 | -0.42 |  |
| [0L, 113L, 174L, 175L, 195L, 212L] | 0.59 | MLR | 0.2 | -0.05 | -0.49 | -0.33 |  |
| [37L, 47L, 66L, 261L, 266L, 371L] | 0.59 | MLR | 0.26 | -0.21 | -0.25 | -0.12 |  |
| [101L, 104L, 209L, 213L, 288L] | 0.59 | MLR | 0.05 | -0.25 | -0.2 | -0.23 |  |
| [200L, 218L, 355L, 359L] | 0.59 | MLR | 0.22 | 0.05 | -0.67 | -0.55 |  |
| [21L, 111L, 153L, 213L, 235L, 305L] | 0.6 | MLR | 0.07 | -0.27 | -0.22 | -0.5 |  |
| [32L, 56L, 58L, 89L, 116L, 156L, 232L, 363L] | 0.6 | MLR | 0.34 | 0.02 | -0.67 | -0.51 |  |
| [4L, 39L, 142L, 236L, 282L, 302L, 321L, 363L, 373L] | 0.64 | MLR | 0.16 | -0.32 | -0.33 | -0.08 |  |
| [174L, 187L, 192L, 239L, 358L, 361L] | 0.65 | MLR | 0.12 | -0.16 | -0.65 | -0.65 |  |
| [62L, 135L, 272L, 279L, 292L] | 0.65 | MLR | 0.08 | -0.19 | -0.58 | -0.75 |  |
| [83L, 137L, 165L, 207L, 225L, 310L, 342L] | 0.66 | MLR | 0.16 | -0.13 | -0.79 | -0.83 |  |
| [5L, 308L, 335L, 364L, 367L] | 0.66 | MLR | 0.14 | -0.1 | -0.83 | -0.68 |  |
| [11L, 131L, 197L, 200L] | 0.68 | MLR | 0.12 | -0.08 | -0.97 | -0.7 |  |
| [5L, 30L, 123L] | 0.68 | MLR | 0.12 | -0.08 | -0.99 | -0.85 |  |
| [3L, 34L, 66L, 214L, 289L, 327L, 370L] | 0.74 | MLR | 0.29 | -0.04 | -1.36 | -1.72 |  |
| [4L, 14L, 109L, 130L, 180L, 227L, 293L, 306L, 346L, 366L] | 0.79 | MLR | 0.34 | 0.09 | -1.87 | -0.92 |  |
| [55L, 96L, 106L, 107L, 268L, 278L, 281L, 284L, 366L] | 0.82 | MLR | 0.24 | -0.07 | -1.78 | -1.45 |  |
| [32L, 42L, 102L, 181L, 191L, 198L, 212L, 345L, 380L] | 0.88 | MLR | 0.3 | -0.67 | -1.1 | -0.94 |  |
| [1L, 18L, 132L, 133L, 142L, 213L, 318L, 321L, 352L, 353L, 364L, 372L] | 0.91 | MLR | 0.19 | -0.52 | -1.51 | -1.18 |  |
| [59L, 138L, 189L, 195L, 279L, 310L] | 0.98 | MLR | 0.2 | -1.32 | -0.53 | -0.56 |  |