Tables

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| --- | --- | --- | --- | --- | --- | --- |
| **𝜆** | SVM | | RFR | | XGBR | |
|  | Train R2 | Test Q2 | Train R2 | Test Q2 | Train R2 | Test Q2 |
| Morgan | 0.865 (421) | 0.897 | 0.816 (51). | 0.789 | 0.880 (490) | 0.898 |
| Morganfeatures | 0.874 (244) | 0.929 | 0.845 (249). | 0.830 | 0.891 (135) | 0.907 |
| Avalon | 0.879 (197) | 0.894 | 0.852 (165). | 0.867 | 0.883 (387). | 0.905 |
| Rdkfp | 0.846 (396) | 0.912 | 0.831 (55). | 0.824 | 0.813 (20) | 0.781 |
| Rdkfplinear | 0.839 (335) | 0.929 | 0.838 (461). | 0.867 | 0.858 (473) | 0.892 |
| Layered | 0.888 (497) | 0.924 | 0.839 (13). | 0.848 | 0.836(483) | 0.875 |
| Torsion | 0.869 (175) | 0.901 | 0.832 (73). | 0.875 | 0.851 (93). | 0.873 |
| atompairs | 0.854 (320) | 0.896 | 0.807 (383). | 0.810 | 0.865 (263) | 0.863 |
| Circus | 0.906 (126) | 0.904 | 0.787 (443). | 0.771 | 0.881 (487) | 0.902 |
| chyline | 0.896 (24) | 0.894 | 0.697 (47). | 0.691 | 0.848 (499) | 0.873 |
| Logt12 | SVM | | | RFR | | |
| Morgan | 0.537 (377) | | | 0.451 (120) | | |
| Morganfeatures | 0.547 (33) | | | 0.478 (374) | | |
| Avalon | 0.484 (323) | | | 0.500 (358) | | |
| Rdkfp | 0.544 (70) | | | 0.507 (347) | | |
| Rdkfplinear | 0.535 (361) | | | 0.492 (412) | | |
| Layered | 0.487 (214) | | | 0.504 (471) | | |
| Torsion | 0.437 (340) | | | 0.485 (327) | | |
| atompairs | 0.381 (136) | | | 0.429 (217) | | |
| Circus | 0,527 (311) | | | 0.498 (253) | | |
| chyline | 0.583 (57) | | | 0.545 (337) | | |