**Table S1.** Structures and antidiabetic activity () of the dataset compounds

|  |  |  |
| --- | --- | --- |
| **No.** | **Compound structure** | **pIC50** |
| 1 |  | 5.842 |
| 2 |  | 6.292 |
| 3 |  | 5.469 |
| 4 |  | 6.310 |
| 5 |  | 6.387 |
| 6 |  | 6.310 |
| 7 |  | 5.856 |
| 8 |  | 5.824 |
| 9 |  | 6.456 |
| 10 |  | 5.509 |
| 11 |  | 6.393 |
| 12 |  | 6.412 |
| 13 |  | 5.194 |
| 14 |  | 6.224 |
| 15 |  | 6.374 |
| 16 |  | 6.652 |
| 17 |  | 6.622 |
| 18 |  | 6.103 |
| 19 |  | 6.745 |
| 20 |  | 6.541 |
| 21 |  | 6.824 |
| 22 |  | 7.301 |
| 23 |  | 7.174 |
| 24 |  | 6.585 |
| 25 |  | 8.456 |
| 26 |  | 8.398 |
| 27 |  | 8.495 |
| 28 |  | 8.201 |
| 29 |  | 7.824 |
| 30 |  | 8.268 |
| 31 |  | 8.149 |
| 32 |  | 8.409 |
| 33 |  | 8.699 |
| 34 |  | 8.638 |
| 35 |  | 8.215 |
| 36 |  | 8.000 |
| 37 |  | 8.569 |
| 38 |  | 8.886 |
| 39 |  | 8.658 |
| 40 |  | 8.319 |
| 41 |  | 8.432 |
| 42 |  | 8.201 |
| 43 |  | 8.229 |
| 44 |  | 8.456 |
| 45 |  | 8.959 |
| 46 |  | 8.167 |
| 47 |  | 8.108 |
| 48 |  | 7.569 |
| 49 |  | 7.921 |
| 50 |  | 8.252 |
| 51 |  | 8.824 |
| 52 |  | 8.569 |
| 53 |  | 5.009 |
| 54 |  | 6.066 |
| 55 |  | 6.238 |
| 56 |  | 5.921 |
| 57 |  | 5.602 |
| 58 |  | 5.538 |
| 59 |  | 6.167 |
| 60 |  | 6.215 |
| 61 |  | 5.745 |
| 62 |  | 6.155 |
| 63 |  | 6.397 |
| 64 |  | 6.228 |
| 65 |  | 6.821 |
| 66 |  | 5.347 |
| 67 |  | 5.481 |
| 68 |  | 5.796 |
| 69 |  | 6.180 |
| 70 |  | 6.069 |
| 71 |  | 6.358 |
| 72 |  | 6.666 |
| 73 |  | 6.672 |
| 74 |  | 7.009 |
| 75 |  | 5.854 |
| 76 |  | 6.149 |
| 77 |  | 5.569 |
| 78 |  | 5.658 |
| 79 |  | 5.796 |
| 80 |  | 5.721 |
| 81 |  | 5.252 |
| 82 |  | 5.796 |
| 83 |  | 5.523 |
| 84 |  | 5.796 |
| 85 |  | 6.114 |
| 86 |  | 5.886 |
| 87 |  | 5.509 |
| 88 |  | 5.678 |
| 89 |  | 5.699 |
| 90 |  | 5.796 |
| 91 |  | 5.041 |
| 92 |  | 5.051 |
| 93 |  | 6.161 |
| 94 |  | 5.721 |
| 95 |  | 5.319 |
| 96 |  | 5.585 |
| 97 |  | 5.131 |
| 98 |  | 5.432 |
| 99 |  | 5.444 |
| 100 |  | 5.854 |
| 101 |  | 5.229 |
| 102 |  | 5.602 |
| 103 |  | 5.553 |
| 104 |  | 6.292 |
| 105 |  | 5.367 |
| 106 |  | 5.071 |
| 107 |  | 5.569 |
| 108 |  | 5.658 |
| 109 |  | 6.244 |
| 110 |  | 7.081 |
| 111 |  | 7.921 |
| 112 |  | 6.309 |
| 113 |  | 6.409 |
| 114 |  | 7.387 |
| 115 |  | 8.108 |
| 116 |  | 6.481 |
| 117 |  | 7.075 |
| 118 |  | 6.553 |
| 119 |  | 6.602 |
| 120 |  | 6.721 |
| 121 |  | 7.221 |
| 122 |  | 7.796 |
| 123 |  | 7.619 |
| 124 |  | 6.173 |
| 125 |  | 7.229 |
| 126 |  | 5.958 |
| 127 |  | 6.958 |
| 128 |  | 6.721 |
| 129 |  | 7.000 |
| 130 |  | 7.142 |
| 131 |  | 7.026 |
| 132 |  | 7.259 |
| 133 |  | 7.301 |
| 134 |  | 6.796 |