**298 DPP-IV Inhibitors**

**1. Xanthine derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 1 |  | 5 | 8.301 | 8 |
| 2 |  | 3 | 8.523 | 8 |
| 3 |  | 2 | 8.699 | 8 |
| 4 |  | 4 | 8.398 | 8 |
| 5 |  | 4403.3 | 5.356 | 8 |
| 6 |  | 7500 | 5.125 | 8 |
| 7 |  | 800 | 6.097 | 8 |
| 8 |  | 3 | 8.523 | 8 |
| 9 |  | 3 | 8.523 | 8 |
| 10 |  | 57 | 7.244 | 8 |
| 11 |  | 1 | 9.000 | 8 |
| 12 |  | 2 | 8.699 | 8 |
| 13 |  | 47 | 7.328 | 8 |
| 14 |  | 2 | 8.699 | 8 |
| 15 |  | 1 | 9.000 | 8 |
| 16 |  | 3 | 8.523 | 8 |
| 17 |  | 400 | 6.398 | 8 |
| 18 |  | 1.6 | 8.796 | 8 |
| 19 |  | 7.2 | 8.143 | 8 |
| 20 |  | 4.5 | 8.347 | 8 |
| 21 |  | 7 | 8.155 | 8 |
| 22 |  | 1.7 | 8.770 | 8 |
| 23 |  | 72 | 7.143 | 8 |
| 24 |  | 1.255 | 8.921 | 9 |
| 25 |  | 29.67 | 7.828 | 9 |
| 26 |  | 8.853 | 8.053 | 9 |
| 27 |  | 1.98 | 8.703 | 10 |
| 28 |  | 10.21 | 7.991 | 10 |
| 29 |  | 2.35 | 8.629 | 10 |
| 30 |  | 3.90 | 8.409 | 10 |
| 31 |  | 0.18 | 9.745 | 10 |
| 32 |  | 0.10 | 10.000 | 10 |
| 33 |  | 1.05 | 8.979 | 10 |
| 34 |  | 0.72 | 9.143 | 10 |
| 35 |  | 0.22 | 9.658 | 10 |
| 36 |  | 5.99 | 8.223 | 10 |
| 37 |  | 0.44 | 9.357 | 10 |
| 38 |  | 2.43 | 8.614 | 10 |
| 39 |  | 2.91 | 8.536 | 10 |
| 40 |  | 5.06 | 8.296 | 10 |
| 41 |  | 50.9 | 7.293 | 10 |
| 42 |  | 5.61 | 8.251 | 10 |
| 43 |  | 20.48 | 7.689 | 10 |
| 44 |  | 74.43 | 7.128 | 10 |
| 45 |  | 22.09 | 7.656 | 10 |
| 46 |  | 85.48 | 7.068 | 10 |
| 47 |  | 87.41 | 7.058 | 11 |
| 48 |  | 67.98 | 7.168 | 11 |
| 49 |  | 16.34 | 7.787 | 11 |
| 50 |  | 29.87 | 7.525 | 11 |
| 51 |  | 1.32 | 8.879 | 11 |
| 52 |  | 2160 | 5.666 | 12 |
| 53 |  | 264 | 6.578 | 12 |
| 54 |  | 16 | 7.796 | 12 |
| 55 |  | 32 | 7.495 | 12 |
| 56 |  | 4 | 8.398 | 12 |
| 57 |  | 9 | 8.046 | 12 |
| 58 |  | 5 | 8.301 | 12 |
| 59 |  | 5 | 8.301 | 12 |
| 60 |  | 6 | 8.222 | 12 |
| 61 |  | 6 | 8.222 | 12 |
| 62 |  | 9 | 8.046 | 12 |
| 63 |  | 250 | 6.602 | 12 |
| 64 |  | 22 | 7.658 | 12 |
| 65 |  | 1 | 9.000 | 12 |
| 66 |  | 2 | 8.699 | 12 |
| 67 |  | 2 | 8.699 | 12 |
| 68 |  | 1 | 9.000 | 12 |
| 69 |  | 4 | 8.398 | 12 |
| 70 |  | 3 | 8.523 | 12 |
| 71 |  | 1 | 9.000 | 12 |
| 72 |  | 3 | 8.523 | 12 |
| 73 |  | 13 | 7.886 | 12 |
| 74 |  | 4 | 8.398 | 12 |
| 75 |  | 1 | 9.000 | 12 |
| 76 |  | 3 | 8.523 | 12 |
| 77 |  | 4 | 8.398 | 12 |
| 78 |  | 3 | 8.523 | 12 |
| 79 |  | 4 | 8.398 | 12 |
| 80 |  | 2 | 8.699 | 12 |
| 81 |  | 12 | 7.921 | 12 |
| 82 |  | 8 | 8.097 | 12 |
| 83 |  | 13 | 7.886 | 12 |
| 84 |  | 6 | 8.222 | 12 |
| 85 |  | 6 | 8.222 | 12 |
| 86 |  | 5 | 8.301 | 12 |
| 87 |  | 3 | 8.523 | 12 |
| 88 |  | 11 | 7.959 | 12 |
| 89 |  | 14 | 7.854 | 12 |
| 90 |  | 3 | 8.523 | 12 |

**2. Aminomethylpiperidone derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 91 |  | 1436 | 5.843 | 13 |
| 92 |  | 378 | 6.423 | 13 |
| 93 |  | 382 | 6.418 | 13 |
| 94 |  | 342 | 6.466 | 13 |
| 95 |  | 217 | 6.664 | 13 |
| 96 |  | 193 | 6.714 | 13 |
| 97 |  | 1388 | 5.858 | 13 |
| 98 |  | 452 | 6.345 | 13 |
| 99 |  | 443 | 6.354 | 13 |
| 100 |  | 404 | 6.394 | 13 |
| 101 |  | 885 | 6.053 | 13 |
| 102 |  | 910 | 6.041 | 13 |
| 103 |  | 1034 | 5.985 | 13 |
| 104 |  | 1023 | 5.990 | 13 |
| 105 |  | 997 | 6.001 | 13 |
| 106 |  | 119 | 6.924 | 13 |
| 107 |  | 84 | 7.706 | 13 |
| 108 |  | 77.6 | 7.110 | 13 |
| 109 |  | 122 | 6.914 | 13 |
| 110 |  | 79 | 7.102 | 13 |
| 111 |  | 74 | 7.131 | 13 |
| 112 |  | 8.5 | 8.071 | 13 |
| 113 |  | 157 | 6.804 | 13 |
| 114 |  | 119 | 6.924 | 13 |
| 115 |  | 125 | 6.903 | 13 |
| 116 |  | 111 | 6.955 | 13 |
| 117 |  | 19 | 7.721 | 13 |
| 118 |  | 197 | 6.706 | 13 |
| 119 |  | 148 | 6.830 | 13 |
| 120 |  | 134 | 6.873 | 13 |
| 121 |  | 137 | 6.863 | 13 |
| 122 |  | 43 | 7.367 | 13 |

**3.** **Pyridinepyrimidinedione derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 123 |  | 257 | 6.590 | 14 |
| 124 |  | 1070 | 5.971 | 14 |
| 125 |  | 128 | 6.893 | 14 |
| 126 |  | 2800 | 5.553 | 14 |
| 127 |  | 57 | 7.244 | 14 |
| 128 |  | 69 | 7.161 | 14 |
| 129 |  | 33 | 7.481 | 14 |
| 130 |  | 17 | 7.770 | 14 |
| 131 |  | 371 | 6.431 | 14 |
| 132 |  | 24 | 7.620 | 14 |
| 133 |  | 29 | 7.538 | 14 |
| 134 |  | 20 | 7.699 | 14 |
| 135 |  | 7.6 | 8.119 | 14 |
| 136 |  | 4.8 | 8.319 | 14 |
| 137 |  | 260 | 6.585 | 14 |
| 138 |  | 2.8 | 8.553 | 14 |
| 139 |  | 6.9 | 8.161 | 14 |
| 140 |  | 2.8 | 8.553 | 14 |
| 141 |  | 4.6 | 8.337 | 14 |
| 142 |  | 9.9 | 8.004 | 14 |

**4. β-phenylalanine derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 143 |  | 98 | 7.009 | 15 |
| 144 |  | 135 | 6.870 | 15 |
| 145 |  | 272 | 6.565 | 15 |
| 146 |  | 128 | 6.893 | 15 |
| 147 |  | 82 | 7.086 | 15 |
| 148 |  | 27 | 7.569 | 15 |
| 149 |  | 805 | 6.094 | 15 |
| 150 |  | 151 | 6.821 | 15 |
| 151 |  | 87 | 7.060 | 15 |
| 152 |  | 1018 | 5.992 | 15 |
| 153 |  | 486 | 6.313 | 15 |
| 154 |  | 366 | 6.437 | 15 |
| 155 |  | 511 | 6.292 | 15 |
| 156 |  | 145 | 6.839 | 15 |
| 157 |  | 59 | 7.229 | 15 |
| 158 |  | 264 | 6.578 | 15 |
| 159 |  | 1580 | 5.801 | 15 |
| 160 |  | 23 | 7.638 | 15 |
| 161 |  | 180 | 6.745 | 15 |
| 162 |  | 21 | 7.678 | 15 |
| 163 |  | 76 | 7.119 | 15 |
| 164 |  | 84 | 7.076 | 15 |
| 165 |  | 60 | 7.222 | 15 |
| 166 |  | 30 | 7.523 | 15 |
| 167 |  | 65 | 7.187 | 15 |
| 168 |  | 190 | 6.721 | 15 |
| 169 |  | 69 | 7.161 | 15 |
| 170 |  | 37 | 7.432 | 15 |
| 171 |  | 30 | 7.523 | 15 |
| 172 |  | 29 | 7.538 | 15 |
| 173 |  | 219 | 6.660 | 15 |
| 174 |  | 234 | 6.631 | 15 |
| 175 |  | 59 | 7.229 | 16 |
| 176 |  | 100 | 7.000 | 16 |
| 177 |  | 71 | 7.149 | 16 |
| 178 |  | 68 | 7.167 | 16 |
| 179 |  | 25 | 7.602 | 16 |
| 180 |  | 4 | 8.398 | 16 |
| 181 |  | 4 | 8.398 | 16 |
| 182 |  | 7 | 8.155 | 16 |
| 183 |  | 2 | 8.699 | 16 |
| 184 |  | 12 | 7.921 | 16 |
| 185 |  | 18 | 7.745 | 16 |
| 186 |  | 2 | 8.699 | 16 |
| 187 |  | 4 | 8.398 | 16 |
| 188 |  | 7800 | 5.108 | 17 |
| 189 |  | 1000 | 6.000 | 17 |
| 190 |  | 2200 | 5.658 | 17 |
| 191 |  | 870 | 6.060 | 17 |
| 192 |  | 2500 | 5.602 | 17 |
| 193 |  | 3300 | 5.481 | 17 |
| 194 |  | 570 | 6.244 | 17 |
| 195 |  | 470 | 6.328 | 17 |
| 196 |  | 190 | 6.721 | 17 |
| 197 |  | 64 | 7.194 | 17 |
| 198 |  | 13 | 7.886 | 17 |
| 199 |  | 12 | 7.921 | 17 |
| 200 |  | 2.7 | 8.569 | 17 |
| 201 |  | 3.3 | 8.481 | 17 |
| 202 |  | 270 | 6.569 | 17 |
| 203 |  | 35 | 7.456 | 17 |
| 204 |  | 130 | 6.886 | 17 |
| 205 |  | 70 | 7.155 | 17 |
| 206 |  | 350 | 6.456 | 17 |
| 207 |  | 1.0 | 9.000 | 17 |
| 208 |  | 3.6 | 8.444 | 17 |
| 209 |  | 0.64 | 9.194 | 17 |
| 210 |  | 1.9 | 8.721 | 17 |
| 211 |  | 0.79 | 9.102 | 17 |
| 212 |  | 83 | 7.081 | 18 |
| 213 |  | 12 | 7.921 | 18 |
| 214 |  | 490 | 6.310 | 18 |
| 215 |  | 390 | 6.409 | 18 |
| 216 |  | 41 | 7.387 | 18 |
| 217 |  | 7.8 | 8.108 | 18 |
| 218 |  | 330 | 6.481 | 18 |
| 219 |  | 84 | 7.076 | 18 |
| 220 |  | 280 | 6.553 | 18 |
| 221 |  | 250 | 6.602 | 18 |
| 222 |  | 60 | 7.222 | 18 |
| 223 |  | 16 | 7.796 | 18 |
| 224 |  | 24 | 7.620 | 18 |
| 225 |  | 670 | 6.172 | 18 |
| 226 |  | 59 | 7.229 | 18 |
| 227 |  | 1100 | 5.959 | 18 |
| 228 |  | 110 | 6.959 | 18 |
| 229 |  | 190 | 6.721 | 18 |
| 230 |  | 100 | 7.000 | 18 |
| 231 |  | 72 | 7.143 | 18 |
| 232 |  | 94 | 7.027 | 18 |
| 233 |  | 55 | 7.260 | 18 |
| 234 |  | 50 | 7.301 | 18 |
| 235 |  | 160 | 6.796 | 18 |

**5. Pyrrolidine derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 236 |  | 35 | 7.456 | 19 |
| 237 |  | 2 | 8.699 | 19 |
| 238 |  | 5 | 8.301 | 19 |
| 239 |  | 7 | 8.155 | 19 |
| 240 |  | 40 | 7.398 | 19 |
| 241 |  | 6 | 8.222 | 19 |
| 242 |  | 5 | 8.301 | 19 |
| 243 |  | 9 | 8.046 | 19 |
| 244 |  | 6 | 8.222 | 19 |
| 245 |  | 7 | 8.155 | 19 |
| 246 |  | 10 | 8.000 | 19 |
| 247 |  | 7 | 8.155 | 19 |
| 248 |  | 15 | 7.824 | 19 |
| 249 |  | 17 | 7.770 | 19 |
| 250 |  | 31 | 7.509 | 19 |
| 251 |  | 8 | 8.097 | 19 |
| 252 |  | 19 | 7.721 | 19 |
| 253 |  | 37 | 7.432 | 19 |
| 254 |  | 11 | 7.959 | 19 |
| 255 |  | 8 | 8.097 | 19 |
| 256 |  | 31 | 7.509 | 19 |
| 257 |  | 12 | 7.921 | 19 |
| 258 |  | 31 | 7.509 | 19 |
| 259 |  | 12 | 7.921 | 19 |
| 260 |  | 16 | 7.796 | 19 |
| 261 |  | 25 | 7.602 | 19 |
| 262 |  | 14 | 7.854 | 19 |
| 263 |  | 13 | 7.886 | 19 |
| 264 |  | 22 | 7.658 | 20 |
| 265 |  | 34 | 7.469 | 20 |
| 266 |  | 420 | 6.377 | 20 |
| 267 |  | 320 | 6.495 | 20 |
| 268 |  | 2700 | 5.569 | 20 |
| 269 |  | 23 | 7.638 | 20 |
| 270 |  | 22 | 7.658 | 20 |
| 271 |  | 24 | 7.620 | 20 |
| 272 |  | 24 | 7.620 | 20 |
| 273 |  | 18 | 7.745 | 20 |
| 274 |  | 7.5 | 8.125 | 20 |
| 275 |  | 33 | 7.481 | 20 |
| 276 |  | 33 | 7.481 | 20 |
| 277 |  | 53 | 7.276 | 20 |
| 278 |  | 38 | 7.420 | 20 |
| 279 |  | 15 | 7.824 | 20 |
| 280 |  | 21 | 7.678 | 20 |
| 281 |  | 9 | 8.046 | 20 |
| 282 |  | 25 | 7.602 | 20 |
| 283 |  | 29 | 7.538 | 20 |
| 284 |  | 17 | 7.770 | 20 |
| 285 |  | 20 | 7.699 | 20 |
| 286 |  | 10 | 8.000 | 20 |
| 287 |  | 55 | 7.260 | 20 |
| 288 |  | 17 | 7.770 | 20 |
| 289 |  | 35 | 7.456 | 20 |
| 290 |  | 89 | 7.051 | 20 |
| 291 |  | 88 | 7.056 | 20 |
| 292 |  | 98 | 7.009 | 20 |
| 293 |  | 26 | 7.585 | 20 |
| 294 |  | 2.6 | 8.585 | 20 |
| 295 |  | 190 | 6.721 | 20 |
| 296 |  | 46 | 7.337 | 20 |
| 297 |  | 64 | 7.194 | 20 |
| 298 |  | 94 | 7.027 | 20 |

**469 Non-DPP-IV Inhibitors**

**1. Xanthine derivatives**

|  |  |  |
| --- | --- | --- |
| **No.** | **Structure** | **Ref.** |
| 1 |  | 8 |
| 2 |  | 21 |
| 3 |  | 21 |
| 4 |  | 21 |
| 5 |  | 21 |
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| 8 |  | 22 |
| 9 |  | 22 |
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| 12 |  | 22 |
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| 25 |  | 22 |
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| 27 |  | 23 |
| 28 |  | 24 |
| 29 |  | 24 |
| 30 |  | 24 |
| 31 |  | 24 |
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| 93 |  | 26 |
| 94 |  | 26 |
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| 96 |  | 26 |
| 97 |  | 26 |
| 98 |  | 26 |
| 99 |  | 9 |
| 100 |  | 9 |
| 101 |  | 9 |
| 102 |  | 9 |
| 103 |  | 9 |
| 104 |  | 27 |
| 105 |  | 27 |
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| 171 |  | 27 |
| 172 |  | 27 |
| 173 |  | 27 |
| 174 |  | 27 |
| 175 |  | 27 |
| 176 |  | 27 |

**2. Aminomethylpiperidone derivatives**

|  |  |  |
| --- | --- | --- |
| **No.** | **Structure** | **Ref.** |
| 177 |  | 28 |
| 178 |  | 28 |
| 179 |  | 28 |
| 180 |  | 28 |
| 181 |  | 28 |
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| 240 |  | 31 |
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**3. Pyridinepyrimidinedione derivatives**

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| 242 |  | 33 |
| 243 |  | 34 |
| 244 |  | 34 |
| 245 |  | 34 |
| 246 |  | 34 |
| 247 |  | 34 |
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| 249 |  | 35 |
| 250 |  | 35 |
| 251 |  | 35 |
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| 254 |  | 35 |
| 255 |  | 35 |
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| 258 |  | 35 |
| 259 |  | 35 |

**4. β-phenylalanine derivatives**

|  |  |  |
| --- | --- | --- |
| **No.** | **Structure** | **Ref.** |
| 260 |  | 36 |
| 261 |  | 36 |
| 262 |  | 36 |
| 263 |  | 36 |
| 264 |  | 36 |
| 265 |  | 36 |
| 266 |  | 36 |
| 267 |  | 36 |
| 268 |  | 36 |
| 269 |  | 36 |
| 270 |  | 36 |
| 271 |  | 36 |
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| 273 |  | 36 |
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| 336 |  | 40 |
| 337 |  | 40 |
| 338 |  | 40 |
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| 359 |  | 42 |

**5. Pyrrolidine derivatives**

|  |  |  |
| --- | --- | --- |
| **No.** | **structure** | **Ref.** |
| 360 |  | 43 |
| 361 |  | 43 |
| 362 |  | 43 |
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**Activity Prediction**

**1.Xanthine Derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 1 |  | 1.255 | 8.921 | 9 |
| 2 |  | 8.853 | 8.053 | 9 |
| 3 |  | 1.98 | 8.903 | 10 |
| 4 |  | 10.21 | 7.991 | 10 |
| 5 |  | 2.35 | 8.629 | 10 |
| 6 |  | 3.90 | 8.409 | 10 |
| 7 |  | 0.18 | 9.945 | 10 |
| 8 |  | 0.10 | 10.000 | 10 |
| 9 |  | 1.05 | 8.979 | 10 |
| 10 |  | 0.72 | 9.343 | 10 |
| 11 |  | 0.22 | 9.758 | 10 |
| 12 |  | 5.99 | 8.523 | 10 |
| 13 |  | 0.44 | 9.357 | 10 |
| 14 |  | 2.43 | 8.814 | 10 |
| 15 |  | 2.91 | 8.536 | 10 |
| 16 |  | 5.06 | 8.296 | 10 |
| 17 |  | 50.90 | 7.293 | 10 |
| 18 |  | 5.61 | 8.251 | 10 |
| 19 |  | 20.48 | 7.689 | 10 |
| 20 |  | 74.43 | 7.128 | 10 |
| 21 |  | 22.09 | 7.656 | 10 |
| 22 |  | 85.48 | 7.068 | 10 |
| 23 |  | 87.41 | 7.058 | 11 |
| 24 |  | 67.98 | 7.168 | 11 |
| 25 |  | 16.34 | 7.787 | 11 |
| 26 |  | 29.87 | 7.525 | 11 |
| 27 |  | 1.32 | 8.879 | 11 |
| 28 |  | 3 | 8.523 | 12 |
| 29 |  | 1 | 9.000 | 12 |
| 30 |  | 2 | 8.699 | 12 |
| 31 |  | 1 | 9.000 | 12 |
| 32 |  | 4 | 8.398 | 12 |
| 33 |  | 3 | 8.523 | 12 |
| 34 |  | 3 | 8.523 | 12 |
| 35 |  | 3 | 8.523 | 12 |
| 36 |  | 1 | 9.000 | 12 |
| 37 |  | 3 | 8.523 | 12 |
| 38 |  | 13 | 7.886 | 12 |
| 39 |  | 8 | 8.097 | 12 |
| 40 |  | 4 | 8.398 | 12 |
| 41 |  | 1 | 9.000 | 12 |
| 42 |  | 1 | 9.000 | 12 |
| 43 |  | 3 | 8.523 | 12 |
| 44 |  | 4 | 8.398 | 12 |
| 45 |  | 3 | 8.523 | 12 |
| 46 |  | 4 | 8.398 | 12 |
| 47 |  | 2 | 8.699 | 12 |
| 48 |  | 12 | 7.921 | 12 |
| 49 |  | 8 | 8.097 | 12 |
| 50 |  | 13 | 7.886 | 12 |
| 51 |  | 6 | 8.222 | 12 |
| 52 |  | 6 | 8.222 | 12 |
| 53 |  | 5 | 8.301 | 12 |
| 54 |  | 3 | 8.523 | 12 |
| 55 |  | 11 | 7.959 | 12 |
| 56 |  | 14 | 7.854 | 12 |

**2. Aminomethylpiperidone Derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 57 |  | 1436 | 5.843 | 13 |
| 58 |  | 378 | 6.423 | 13 |
| 59 |  | 382 | 6.418 | 13 |
| 60 |  | 342 | 6.466 | 13 |
| 61 |  | 217 | 6.664 | 13 |
| 62 |  | 193 | 6.714 | 13 |
| 63 |  | 1388 | 5.858 | 13 |
| 64 |  | 452 | 6.345 | 13 |
| 65 |  | 443 | 6.354 | 13 |
| 66 |  | 404 | 6.394 | 13 |
| 67 |  | 885 | 6.053 | 13 |
| 68 |  | 910 | 6.041 | 13 |
| 69 |  | 1034 | 5.985 | 13 |
| 70 |  | 1023 | 5.990 | 13 |
| 71 |  | 997 | 6.001 | 13 |
| 72 |  | 119 | 6.924 | 13 |
| 73 |  | 84 | 7.706 | 13 |
| 74 |  | 77.6 | 7.110 | 13 |
| 75 |  | 122 | 6.914 | 13 |
| 76 |  | 79 | 7.102 | 13 |
| 77 |  | 74 | 7.131 | 13 |
| 78 |  | 8.5 | 8.071 | 13 |
| 79 |  | 157 | 6.804 | 13 |
| 80 |  | 119 | 6.924 | 13 |
| 81 |  | 125 | 6.903 | 13 |
| 82 |  | 111 | 6.955 | 13 |
| 83 |  | 19 | 7.721 | 13 |
| 84 |  | 197 | 6.706 | 13 |
| 85 |  | 148 | 6.830 | 13 |
| 86 |  | 134 | 6.873 | 13 |
| 87 |  | 137 | 6.863 | 13 |
| 88 |  | 43 | 7.367 | 13 |

**3.Pyridinepyrimidinedione Derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 89 |  | 257 | 6.590 | 14 |
| 90 |  | 1070 | 5.971 | 14 |
| 91 |  | 128 | 6.893 | 14 |
| 92 |  | 2800 | 5.553 | 14 |
| 93 |  | 57 | 7.244 | 14 |
| 94 |  | 69 | 7.161 | 14 |
| 95 |  | 33 | 7.481 | 14 |
| 96 |  | 17 | 7.770 | 14 |
| 97 |  | 371 | 6.431 | 14 |
| 98 |  | 24 | 7.620 | 14 |
| 99 |  | 29 | 7.538 | 14 |
| 100 |  | 20 | 7.699 | 14 |
| 101 |  | 7.6 | 8.119 | 14 |
| 102 |  | 4.8 | 8.319 | 14 |
| 103 |  | 260 | 6.585 | 14 |
| 104 |  | 2.8 | 8.553 | 14 |
| 105 |  | 6.9 | 8.161 | 14 |
| 106 |  | 2.8 | 8.553 | 14 |
| 107 |  | 4.6 | 8.337 | 14 |
| 108 |  | 9.9 | 8.004 | 14 |

**4. β-phenylalanine Derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 109 |  | 98 | 7.009 | 15 |
| 110 |  | 135 | 6.870 | 15 |
| 111 |  | 272 | 6.565 | 15 |
| 112 |  | 128 | 6.893 | 15 |
| 113 |  | 82 | 7.086 | 15 |
| 114 |  | 27 | 7.569 | 15 |
| 115 |  | 805 | 6.094 | 15 |
| 116 |  | 151 | 6.821 | 15 |
| 117 |  | 87 | 7.060 | 15 |
| 118 |  | 1018 | 5.992 | 15 |
| 119 |  | 486 | 6.313 | 15 |
| 120 |  | 366 | 6.437 | 15 |
| 121 |  | 511 | 6.292 | 15 |
| 122 |  | 145 | 6.839 | 15 |
| 123 |  | 59 | 7.229 | 15 |
| 124 |  | 264 | 6.578 | 15 |
| 125 |  | 1580 | 5.801 | 15 |
| 126 |  | 23 | 7.638 | 15 |
| 127 |  | 180 | 6.745 | 15 |
| 128 |  | 21 | 7.678 | 15 |
| 129 |  | 76 | 7.119 | 15 |
| 130 |  | 84 | 7.076 | 15 |
| 131 |  | 60 | 7.222 | 15 |
| 132 |  | 30 | 7.523 | 15 |
| 133 |  | 65 | 7.187 | 15 |
| 134 |  | 190 | 6.721 | 15 |
| 135 |  | 69 | 7.161 | 15 |
| 136 |  | 37 | 7.432 | 15 |
| 137 |  | 30 | 7.523 | 15 |
| 138 |  | 29 | 7.538 | 15 |
| 139 |  | 219 | 6.660 | 15 |
| 140 |  | 234 | 6.631 | 15 |
| 141 |  | 59 | 7.229 | 16 |
| 142 |  | 100 | 7.000 | 16 |
| 143 |  | 71 | 7.149 | 16 |
| 144 |  | 68 | 7.167 | 16 |
| 145 |  | 25 | 7.602 | 16 |
| 146 |  | 4 | 8.398 | 16 |
| 147 |  | 4 | 8.398 | 16 |
| 148 |  | 7 | 8.155 | 16 |
| 149 |  | 2 | 8.699 | 16 |
| 150 |  | 274 | 6.562 | 16 |
| 151 |  | 7800 | 5.108 | 17 |
| 152 |  | 1000 | 6.000 | 17 |
| 153 |  | 2200 | 5.658 | 17 |
| 154 |  | 870 | 6.060 | 17 |
| 155 |  | 2500 | 5.602 | 17 |
| 156 |  | 3300 | 5.481 | 17 |
| 157 |  | 570 | 6.244 | 17 |
| 158 |  | 470 | 6.328 | 17 |
| 159 |  | 190 | 6.721 | 17 |
| 160 |  | 64 | 7.194 | 17 |
| 161 |  | 13 | 7.886 | 17 |
| 162 |  | 12 | 7.921 | 17 |
| 163 |  | 2.7 | 8.569 | 17 |
| 164 |  | 3.3 | 8.481 | 17 |
| 165 |  | 270 | 6.569 | 17 |
| 166 |  | 35 | 7.456 | 17 |
| 167 |  | 130 | 6.886 | 17 |
| 168 |  | 70 | 7.155 | 17 |
| 169 |  | 350 | 6.456 | 17 |
| 170 |  | 1.0 | 9.000 | 17 |
| 171 |  | 3.6 | 8.444 | 17 |
| 172 |  | 0.64 | 9.194 | 17 |
| 173 |  | 1.9 | 8.721 | 17 |
| 174 |  | 0.79 | 9.102 | 17 |
| 175 |  | 83 | 7.081 | 18 |
| 176 |  | 12 | 7.921 | 18 |
| 177 |  | 490 | 6.310 | 18 |
| 178 |  | 390 | 6.409 | 18 |
| 179 |  | 41 | 7.387 | 18 |
| 180 |  | 7.8 | 8.108 | 18 |
| 181 |  | 330 | 6.481 | 18 |
| 182 |  | 84 | 7.076 | 18 |
| 183 |  | 280 | 6.553 | 18 |
| 184 |  | 250 | 6.602 | 18 |
| 185 |  | 60 | 7.222 | 18 |
| 186 |  | 16 | 7.796 | 18 |
| 187 |  | 24 | 7.620 | 18 |
| 188 |  | 670 | 6.172 | 18 |
| 189 |  | 59 | 7.229 | 18 |
| 190 |  | 1100 | 5.959 | 18 |
| 191 |  | 110 | 6.959 | 18 |
| 192 |  | 190 | 6.721 | 18 |
| 193 |  | 100 | 7.000 | 18 |
| 194 |  | 72 | 7.143 | 18 |
| 195 |  | 94 | 7.027 | 18 |
| 196 |  | 55 | 7.260 | 18 |
| 197 |  | 50 | 7.301 | 18 |
| 198 |  | 160 | 6.796 | 18 |

**5. Pyrrolidine Derivatives**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **Structure** | **IC50(nM)** | **pIC50** | **Ref.** |
| 199 |  | 2 | 8.699 | 19 |
| 200 |  | 5 | 8.301 | 19 |
| 201 |  | 7 | 8.155 | 19 |
| 202 |  | 40 | 7.398 | 19 |
| 203 |  | 6 | 8.222 | 19 |
| 204 |  | 5 | 8.301 | 19 |
| 205 |  | 9 | 8.046 | 19 |
| 206 |  | 6 | 8.222 | 19 |
| 207 |  | 7 | 8.155 | 19 |
| 208 |  | 10 | 8.000 | 19 |
| 209 |  | 22 | 7.658 | 19 |
| 210 |  | 7 | 8.155 | 19 |
| 211 |  | 15 | 7.824 | 19 |
| 212 |  | 17 | 7.770 | 19 |
| 213 |  | 31 | 7.509 | 19 |
| 214 |  | 8 | 8.097 | 19 |
| 215 |  | 19 | 7.721 | 19 |
| 216 |  | 37 | 7.432 | 19 |
| 217 |  | 11 | 7.959 | 19 |
| 218 |  | 8 | 8.097 | 19 |
| 219 |  | 31 | 7.509 | 19 |
| 220 |  | 12 | 7.921 | 19 |
| 221 |  | 31 | 7.509 | 19 |
| 222 |  | 12 | 7.921 | 19 |
| 223 |  | 16 | 7.796 | 19 |
| 224 |  | 25 | 7.602 | 19 |
| 225 |  | 14 | 7.854 | 19 |
| 226 |  | 13 | 7.886 | 19 |
| 227 |  | 22 | 7.658 | 20 |
| 228 |  | 34 | 7.469 | 20 |
| 229 |  | 420 | 6.377 | 20 |
| 230 |  | 320 | 6.495 | 20 |
| 231 |  | 2700 | 5.569 | 20 |
| 232 |  | 23 | 7.638 | 20 |
| 233 |  | 22 | 7.658 | 20 |
| 234 |  | 24 | 7.620 | 20 |
| 235 |  | 24 | 7.620 | 20 |
| 236 |  | 18 | 7.745 | 20 |
| 237 |  | 7.5 | 8.125 | 20 |
| 238 |  | 33 | 7.481 | 20 |
| 239 |  | 33 | 7.481 | 20 |
| 240 |  | 53 | 7.276 | 20 |
| 241 |  | 38 | 7.420 | 20 |
| 242 |  | 15 | 7.824 | 20 |
| 243 |  | 21 | 7.678 | 20 |
| 244 |  | 9 | 8.046 | 20 |
| 245 |  | 25 | 7.602 | 20 |
| 246 |  | 29 | 7.538 | 20 |
| 247 |  | 17 | 7.770 | 20 |
| 248 |  | 20 | 7.699 | 20 |
| 249 |  | 10 | 8.000 | 20 |
| 250 |  | 55 | 7.260 | 20 |
| 251 |  | 17 | 7.770 | 20 |
| 252 |  | 35 | 7.456 | 20 |
| 253 |  | 89 | 7.051 | 20 |
| 254 |  | 88 | 7.056 | 20 |
| 255 |  | 98 | 7.009 | 20 |
| 256 |  | 26 | 7.585 | 20 |
| 257 |  | 2.6 | 8.585 | 20 |
| 258 |  | 190 | 6.721 | 20 |
| 259 |  | 46 | 7.337 | 20 |
| 260 |  | 64 | 7.194 | 20 |
| 261 |  | 94 | 7.027 | 20 |