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| **S. No.** | **Name/Code** | **Structure** | **Binding Energy**  **Adrenergic β-2 Receptor**  **(5d5a)** | **Binding Energy Interleukin-13 (3bpl)** |
| 1 | 1H |  | -5.31 | -6.46 |
| 2 | AC |  | -5.21 | -4.84 |
| 3 | AG |  | -6.74 | -5.55 |
| 4 | ArT |  | -6.23 | -6.50 |
| 5 | AS |  | -6.01 | -4.23 |
| 6 | AT |  | -7.37 | -4.45 |
| 7 | AZ |  | -6.53 | -4.52 |
| 8 | AZb |  | -7.74 | -3.86 |
| 9 |  |  | -4.18 | -5.24 |
| 10 |  |  | -5.72 | -5.05 |
| 11 |  |  | -5.25 | -4.83 |
| 12 |  |  | -7.32 | -3.60 |
| 13 |  |  | -5.62 | -5.88 |
| 14 |  |  | -5.48 | -5.48 |
| 15 |  |  | -8.88 | -4.96 |
| 16 |  |  | -4.33 | -6.05 |
| 17 |  |  | -4.05 | -5.77 |
| 18 |  |  | -5.88 | -6.23 |
| 19 |  |  | -4.82 | -1.69 |
| 20 |  |  | -4.80 | -5.78 |
| 21 |  |  | -6.00 | -7.02 |
| 22 |  |  | -6.39 | -4.25 |
| 23 |  |  | -5.04 | -3.34 |
| 24 |  |  | -6.01 | -3.03 |
| 25 |  |  | -6.71 | -1.99 |
| 26 |  |  | -5.44 | -4.43 |
| 27 |  |  | -7.97 | -4.08 |
| 28 |  |  | -4.32 | -3.07 |
| 29 |  |  | -4.55 | -3.67 |
| 30 |  |  | -5.50 | -3.41 |
| 31 |  |  | -5.28 | -3.89 |
| 32 |  |  | -3.92 | -3.58 |
| 33 |  |  | -6.72 | -3.68 |
| 34 |  |  | -5.24 | -2.95 |
| 35 |  |  | -6.37 | -3.87 |
| 36 |  |  | -3.30 | -2.89 |
| 37 |  |  | -4.66 | -2.33 |
| 38 |  |  | -5.68 | -4.53 |
| 39 |  |  | -6.08 | -4.17 |
| 40 |  |  | -6.71 | -7.26 |
| 41 |  |  | -5.62 | -6.55 |
| 42 |  |  | -7.15 | -4.48 |
| 43 |  |  | -7.15 | -3.28 |
| 44 |  |  | -4.37 | -5.64 |
| 45 |  |  | -5.61 | -6.04 |
| 46 |  |  | -5.10 | -5.99 |
| 47 |  |  | -6.08 | -4.81 |
| 48 |  |  | -6.44 | -6.62 |
| 49 |  |  | -5.52 | -4.96 |
| 50 |  |  | -5.16 | -5.85 |
| 51 |  |  | -6.66 | -6.08 |
| 52 |  |  | -5.44 | -4.16 |
| 53 |  |  | -5.19 | -4.39 |
| 54 |  |  | -4.39 | -5.01 |
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