

Panel 44 Datasheet

Moleculomics offer *in silico* screening platforms to enable analysis of the predicted interaction between any compound and panels of selected target proteins. These quantitative simulation methods offer significant savings as the first step in the drug discovery process for identification of the most problematic off-target interactions.

Panel 44: A target panel of 44 human receptors adopted as recommended by four major pharmaceutical companies (Joanne Bowes and colleagues)¹, including;

1. Bowes *et al* (2012), Nature reviews: Drug Discovery, 11: 909-922

G protein-coupled receptors

1. Adenosine receptor A2A (*ADORA2A*)
2. α 1A-adrenergic receptor (*ADRA1A*)
3. α 2A-adrenergic receptor (*ADRA2A*)
4. β 1-adrenergic receptor (*ADRB1*)
5. β 2-adrenergic receptor (*ADRB2*)
6. Cannabinoid receptor CB1 (*CNR1*)
7. Cannabinoid receptor CB2 (*CNR2*)
8. Cholecystokinin A receptor (*CCKAR*)
9. Dopamine receptor D1 (*DRD1*)
10. Dopamine receptor D2 (*DRD2*)
11. Endothelin receptor A (*EDNRA*)
12. Histamine H1 receptor (*HRH1*)
13. Histamine H2 receptor (*HRH2*)
14. δ -type opioid receptor (*OPRD1*)
15. κ -type opioid receptor (*OPRK1*)
16. μ -type opioid receptor (*OPRM1*)
17. Muscarinic acetylcholine receptor M1 (*CHRM1*)
18. Muscarinic acetylcholine receptor M2 (*CHRM2*)
19. Muscarinic acetylcholine receptor M3 (*CHRM3*)
20. 5-HT1A (*HTR1A*)
21. 5-HT1B (*HTR1B*)
22. 5-HT2A (*HTR2A*)[‡]
23. 5-HT2B (*HTR2B*) High
24. Vasopressin V1A receptor (*AVPR1A*)

Ion channels

25. Acetylcholine receptor subunit α 1 or α 4 (*CHRNA1* or *CHRNA4*)
26. Voltage-gated calcium channel subunit α Cav1.2 (*CACNA1C*)

27. GABAA receptor α 1 (*GABRA1*)
28. Potassium voltage-gated channel subfamily H member 2; hERG (*KCNH2*)
29. Potassium voltage gated channel KQT-like member 1 (*KCNQ1*) and minimal potassium channel MinK (*KCNE1*)
30. NMDA receptor subunit NR1 (*GRIN1*)
31. 5-HT3 (*HTR3A*)
32. Voltage-gated sodium channel subunit α

Enzymes

33. Acetylcholinesterase (*ACHE*)
34. Cyclooxygenase 1; COX1 (*PTGS1*)
35. Cyclooxygenase 2; COX2 (*PTGS2*)
36. Monoamine oxidase A (*MAOA*)
37. Phosphodiesterase 3A (*PDE3A*)
38. Phosphodiesterase 4D (*PDE4D*)
39. Lymphocyte-specific protein tyrosine kinase (*LCK*)

Transporters

40. Dopamine transporter (*SLC6A3*)
41. Noradrenaline transporter (*SLC6A2*)
42. Serotonin transporter (*SLC6A4*)

Nuclear receptors

43. Androgen receptor (*AR*)
44. Glucocorticoid receptor (*NR3C1*)