List of Selected PDB Structures

Target 1 - ACHE - 6O4W (Gerlits et al., 2019)

Target 2 - ADORA2A - 4EIY (Liu et al., 2012)

Target 2 - ADORA2A - 4UHR (Lebon et al., 2015)

Target 3 - ADRA1A - 7YM8 (Toyoda et al., 2023)

Target 3 - ADRA1A - 7YMJ (Toyoda et al., 2023)

Target 4 - ADRA2A - 6KUX (Qu et al., n.d.)

Target 4 - ADRA2A - 7EJ8 (Xu et al., 2022)

Target 5 - AR - 2AM9 (Pereira de Jésus-Tran et al., 2006)

Target 5 - AR - 2AX9 (Bohl et al., 2005)

Target 6 - ADRB1 - 7BU7 (X. Xu et al., 2021)

Target 6 - ADRB1 - 7BVQ (X. Xu et al., 2021)

Target 7 - ADRB2 - 4LDE (Ring et al., 2013)

Target 7 - ADRB2 - 6PS2 (Ishchenko et al., 2019)

Target 8 - BRD4 - 6FO5 (Hoffer et al., 2018)

Target 9 - CNR1 - 5U09 (Shao et al., 2016)

Target 9 - CNR1 - 5XRA (Hua et al., 2017)

Target 10 - CNR2 - 5ZTY (Li et al., 2019)

Target 10 - CNR2 - 8GUR (Li et al., 2023)

Target 11 - CTSD - 4OD9 (Grädler et al., 2014)

Target 12 - CCKAR - 7F8Y (X. Zhang et al., 2021)

Target 12 - CCKAR - 7MBX (Mobbs et al., 2021)

Target 13 - CCKAR - 7F8W (X. Zhang et al., 2021)

Target 14 - PTGS1 - 6Y3C (Miciaccia et al., 2021)

Target 15 - PTGS2 - 5IKR (Orlando & Malkowski, 2016)

Target 16 - CYP1A2 - 2HI4 (Sansen et al., 2007)

Target 17 - CYP2B6 - 3IBD (Gay et al., 2010)

Target 18 - CYP2C19 - 4GQS (Reynald et al., 2012)

Target 19 - CYP2C8 - 2NNJ (Schoch et al., 2008)

Target 20 - CYP2C9 - 5A5I (Skerratt et al., 2016a)

Target 21 - CYP2D6 - 3TBG (Wang et al., 2015)

Target 22 - CYP2E1 - 3E6I (Porubsky et al., 2008)

Target 23 - CYP3A4 - 3NXU (Sevrioukova & Poulos, 2010)

Target 24 - CYP3A5 - 5VEU (Hsu et al., 2018)

Target 25 - OPRD1 - 4N6H (Fenalti et al., 2014)

Target 25 - OPRD1 - 6PT3 (Claff et al., 2019)

Target 26 - DRD1 - 7JVP (Zhuang et al., 2021)

Target 27 - DRD1 - 7JVR (Zhuang et al., 2021)

Target 27 - DRD2 - 6CM4 (Wang et al., 2018)

Target 28 - DRD3 - 3PBL (Chien et al., 2010)

Target 28 - DRD3 - 7CMV (P. Xu et al., 2021)

Target 29 - SLC6A3 - 8Y2F (Li et al., 2024)

Target 29 - SLC6A3 - 9EO4 (Nielsen et al., 2024)

Target 30 - MAP2K7 - 6YG5 (Schröder et al., 2020)

Target 30 - MAP2K7 - 6YZ4 (Schröder et al., 2020)

Target 31 - EDNRA - 8HCQ (Ji et al., 2023)

Target 31 - EDNRA - 8XVK (Hou et al., 2024)

Target 32 - EGFR - 4WKQ (Yosaatmadja et al., n.d.)

Target 32 - EGFR - 8A27 (Obst-Sander et al., 2022)

Target 33 - ESR1 - 3ERD (Shiau et al., 1998)

Target 33 - ESR1 - 6IAR (Scott et al., 2019)

Target 34 - FGFR1 - 5EW8 (Patani et al., 2016)

Target 35 - PTK2 - 4EBV (Iwatani et al., 2013)

Target 35 - PTK2 - 6YOJ (Berger et al., 2021)

Target 36 - GPBAR1 - 9GYO (Castel et al., n.d.)

Target 37 - SLC6A1 - 7Y7Y (Zhu et al., 2023)

Target 37 - SLC6A1 - 7Y7Z (Zhu et al., 2023)

Target 38 - GABRA1/GABRB2/GABRG2 - 6X3X (Kim et al., 2020)

Target 39 - NR3C1 - 1M2Z (Bledsoe et al., 2002)

Target 39 - NR3C1 - 4LSJ (Carson et al., 2014)

Target 40 - GRIN1/GRIN2A - 5H8N (Hackos et al., 2016)

Target 40 - GRIN1/GRIN2A - 5H8Q (Hackos et al., 2016)

Target 40 - GRIN1/GRIN2A - 7EU7 (Y. Zhang et al., 2021)

Target 41 - GSK3B - 1Q5K (Bhat et al., 2003)

Target 42 - KCNH2 - 8ZYQ (Miyashita et al., 2024)

Target 43 - HRH1 - 3RZE (Shimamura et al., 2011)

Target 43 - HRH1 - 8YN2 (Zhang et al., 2024)

Target 44 - HRH2 - 7UL3 (Robertson et al., 2022)

Target 44 - HRH2 - 8YN3 (Zhang et al., 2024)

Target 45 - INSR - 5E1S (Sanderson et al., 2015)

Target 46 - OPRK1 - 4DJH (Wu et al., 2012)

Target 46 - OPRK1 - 8DZR (Han et al., 2023)

Target 47 - MRGPRX2 - 7S8O (Cao et al., 2021)

Target 48 - MAOA - 2Z5X (Son et al., 2008)

Target 49 - MAOB - 2V5Z (Binda et al., 2007)

Target 50 - OPRM1 - 8EFO (Zhuang et al., 2022)

Target 51 - MALT1 - 7AK0 (Pissot Soldermann et al., 2020)

Target 52 - CHRM1 - 6WJC (Maeda et al., 2020)

Target 52 - CHRM1 - 6ZFZ (Brown et al., 2021)

Target 53 - CHRM2 - 5ZKC (Suno et al., 2018)

Target 53 - CHRM2 - 7T8X (Xu et al., 2023)

Target 54 - CHRM3 - 8EA0 (Zhang et al., 2022)

Target 55 - NTRK1 - 5JFW (Skerratt et al., 2016b)

Target 56 - TACR3 - 8JBF (Sun et al., 2023)

Target 57 - CHRNA4/CHRNB2 - 8ST2 (Mazzaferro et al., 2024)

Target 58 - SLC6A2 - 8WGR (Tan et al., 2024)

Target 58 - SLC6A2 - 8ZP2 (Song & Wu, 2024)

Target 59 - RORA - 1N83 (Kallen et al., 2002)

Target 60 - ABCB1 - 8Y6H (Hamaguchi-Suzuki et al., 2024)

Target 61 - PDE3A - 7L28 (Garvie et al., 2021)

Target 62 - PDE4D - 1Y2K (Card et al., 2005)

Target 63 - PIK3CG - 3L54 (Knight et al., 2010)

Target 64 - PGR - 1SQN (Madauss et al., 2004)

Target 64 - PGR - 4OAR (Petit-Topin et al., 2014)

Target 65 - PDK1 - 2Q8G (Kato et al., 2007)

Target 66 - RARA - 5K13 (Hughes et al., 2016)

Target 66 - RARA - 9GFE (Perdriau et al., 2025)

Target 67 - ROCK1 - 3V8S (Li et al., 2012)

Target 68 - ROCK2 - 7JNT (Hu et al., 2020)

Target 69 - ATM - 7NI4 (Stakyte et al., 2021)

Target 70 - STK35 - Q8TDR2 (SWISS-MODEL, 2025a)

Target 71 - AURKA - 5OS5 (McIntyre et al., 2017)

Target 71 - AURKA - 5OSF (McIntyre et al., 2017)

Target 71 - AURKA - 8SSO (Kim et al., 2023)

Target 72 - AURKB - 4AF3 (Elkins et al., 2012)

Target 73 - HTR1A - 8PJK (Ullrich et al., 2023)

Target 74 - HTR1B - 4IAR (Wang et al., 2013)

Target 74 - HTR1B - 5V54 (Yin et al., 2018)

Target 75 - HTR2A - 7WC6 (Cao et al., 2022)

Target 75 - HTR2A - 7WC8 (Cao et al., 2022)

Target 76 - HTR2B - 4IB4 (Wacker et al., 2013)

Target 76 - HTR2B - 6DS0 (McCorvy et al., 2018)

Target 77 - HTR3A - 8BLB (López-Sánchez et al., 2024)

Target 78 - HTR6 - 8JLZ (Pei et al., 2023)

Target 79 - SLC6A4 - 5I73 (Coleman et al., 2016)

Target 79 - SLC6A4 - 6DZZ (Coleman et al., 2019)

Target 79 - SLC6A4 - 7TXT (Singh et al., 2023)

Target 80 - SCN5A - 7DTC (Li et al., 2021)

Target 81 - KIT - 4U0I (Garner et al., 2014)

Target 82 - LCK - 1QPJ (Zhu et al., 1999)

Target 82 - LCK - 2PL0 (Jacobs et al., 2008)

Target 83 - SRC - 1Y57 (Cowan-Jacob et al., 2005)

Target 83 - SRC - 7NG7 (Temps et al., 2021)

Target 84 - FLT1 - 3HNG (Tresaugues et al., n.d.)

Target 85 - KDR - 3VO3 (Miyamoto et al., 2013)

Target 86 - AVPR1A - P37288 (SWISS-MODEL, 2025b)

Target 87 - CACNA1C - 8FHS (Gao et al., 2023)

Target 87 - CACNA1C - 8WE8 (Gao et al., 2023)

Target 87 - CACNA1C - 8WEA (Gao et al., 2023)

Target 88 - KCNQ1 - 7XNN (Ma et al., 2022)

Target 88 - KCNQ1 - 7XNN additional 1 (Yang et al., 2013)

Target 88 - KCNQ1 - 7XNN additional 2 (Seebohm et al., 2003)

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