

Table S1. Non-redundant training and testing datasets used in TMSA.

| | |
|------------------|---|
| Training dataset | 2WJM_M 2JAF_A 3CN6_A 1KPL_A 3EFF_K 1M56_A 3M72_A 2WIE_A 1M56_B 2IC8_A 2NS1_A 2BG9_B 3EHZ_A 1OED_E 1Y5I_C 2FBW_C 1XME_A 3LNM_B 3KZI_C 2YXQ_A 3BHS_A 2J4Y_A 3A0B_A 2PNO_A 2J8S_A 3BA6_A 3B8C_A 3A0B_B 3D4S_A 2QTS_A 2ZIY_A 3GI9_C 2V8N_A 3FI1_A 2QI9_A 3H90_A 2ONK_C 2K4T_A 3KLY_A 1JB0_L 2F93_B 2DB4_A 1ZOY_D 3HFX_A 2JLN_A 1WP1_A 3I5D_A 3A2R_X 1XL4_A 1OKC_A 1ORQ_C 1FFT_C 2KSE_A 2OAR_A 2KSD_A 2KSF_A 1S5L_Z 1H2S_B |
| Testing dataset | 1EYS_M 3A7K_A 3CN5_A 1KPK_A 2A9H_A 1FFT_A 3M71_A 1YCE_A 1AR1_B 2NR9_A 2NUU_A 2BG9_A 3EAM_A 1OED_C 1Q16_C 1YQ3_C 3EH3_A 2R9R_B 1S5L_C 1RHZ_A 3B9W_A 1GZM_A 1S5L_A 2Q7M_A 2GIF_A 2ZXE_A 1IWO_A 1MHS_A 1S5L_B 2RH1_A 3HGC_A 2Z73_A 3GI8_C 2K9P_A 1VRY_A 3DIN_E 1PV6_A 1ZCD_A 1L7V_A 2QFI_A 3D31_C 3KCU_A 3CHX_B 2WSC_L 2F95_B 2BL2_A 1YQ3_D 2HYD_A 2QJU_A 2YVX_A 2ZJS_Y 1YEW_A 2GFP_A 2ZD9_A 2VL0_A 1FFT_B 2WCD_A 3CHX_C 3B4R_A 1KQF_C 3DHW_A 2K73_A 1C17_M 2KSR_A 3DWW_A 1ORS_C 1KF6_C 1NEK_C 2KDC_A 1KF6_D 1NEK_D 3DL8_E |