

Table S1. Correlation-matrix for pMIC1119B, model 2. No descriptors correlated each other.

	pMI C111 9B	TS[1]_RA_B_AB_nCi_2_M8 _MP1_T_LGL[2-3]_c- s_MID	SD_B_AB_nCi_2_M5 _NS3_P_KA_v- h_MID	S_B_AB_nCi_2_M11_ NS4_T_KA_psa- r_MID	VC_B_AB_nCi_2_M15 _NS7_P_KA_v- m_MID
pMIC1119B	1.00				
TS[1]_RA_B_AB_nCi_2_M8 _MP1_T_LGL[2-3]_c- s_MID	0.80	1.00			
SD_B_AB_nCi_2_M5_NS3_ P_KA_v-h_MID	0.62	0.28	1.00		
SD_B_AB_nCi_2_M5_NS3_ P_KA_v-h_MID	-0.16	-0.20	-0.47	1.00	
VC_B_AB_nCi_2_M15_NS7 _P_KA_v-m_MID	-0.42	-0.08	-0.59	0.48	1.00

Table S2 Correlation-matrix for pMIC XU212, model 5. No descriptors correlated each other.

	pMIC XU21 2	TS[1]_RA_B_AB_nCi_2_ M8_MP1_T_LGL[2-3]_c- s_MID	Q1_Tr_AB_nCi_3_M26(M5)_NS3_P_KA_a-e- v_MID	Q1_Tr_AB_nCi_3_M26(M5)_NS3_P_KA_a-e- v_MID	AC[1]_RA_B_AB_nCi_ 2_M1_MP6_T_KA_h- s_MID
pMIC XU212	1.00				
TS[1]_RA_B_AB_nCi_2_ M8_MP1_T_LGL[2-3]_c- s_MID	0.79	1.00			
Q1_Tr_AB_nCi_3_M26(M5)_NS3_P_KA_a-e- v_MID	-0.69	-0.45	1.00		
Q1_Tr_AB_nCi_3_M26(M5)_NS3_P_KA_a-e- v_MID	0.33	0.19	0.03	1.00	
AC[1]_RA_B_AB_nCi_2_ M1_MP6_T_KA_h- s_MID	0.21	-0.06	-0.09	-0.11	1.00