

The following tables show the rate constant regression models generated using the four schemes for partitioning the data and the two criteria used for model selection. For each feature, absolute weights (W) and normalised weights (W_n), found after converting to z-scores, are shown. The term CONSTANT refers to the constant determined during regression.

Table 1: Rate constant models

Sch.	Sel.	$\log_{10} k_{\text{on}}$			$\log_{10} k_{\text{off}}$			ΔG_{sel}	ΔG_{val}	p
		Feat.	W	W_n	Feat.	W	W_n	Corr.	Corr.	
1	RMSE	CONSTANT	4.29	-	CONSTANT	-1.40	-	0.69	0.09	0.45
		NUM_HB	0.07	0.52	ROS_CG_BETA	-0.79	-0.85			
		DFIRE_EBU	-0.00	-0.50	TES_PP	0.10	0.35			
					ROS_FA_REP_UB	0.05	0.35			
				ACE19_HYDR_UB	0.00	0.43				
				OPUS_CA_ENS	0.03	0.57				
2	RMSE	CONSTANT	4.29	-	CONSTANT	-2.11	-	0.10	0.59	<0.01
		NUM_HB	0.07	0.52	ROS_CG_BETA	-0.68	-0.73			
		DFIRE_EBU	-0.00	-0.50	OPUS_CA_ENS	0.04	0.67			
3	RMSE	CONSTANT	6.13	-	CONSTANT	-6.32	-	0.60	0.19	0.14
		RES_C	-0.07	-0.51	ROS_CG_BETA	-0.49	-0.52			
		NUM_HB	0.08	0.44	NIP	8612.18	0.51			
		ACE22_ALL	0.00	0.21						
		ROS_FA_REP	0.04	0.23						
		ROS_CG_VDW	-0.76	-0.19						
		STC_H	-0.05	-0.24						
		GEN_4_BODY_UB	0.01	0.40						
		DFIRE_EBU	-0.00	-0.47						
4	RMSE	CONSTANT	4.18	-	CONSTANT	-6.32	-	0.17	0.51	<0.01
		NUM_HB	0.07	0.39	ROS_CG_BETA	-0.49	-0.52			
		DFIRE_EBU	-0.00	-0.47	NIP	8612.18	0.51			
1	Corr.	CONSTANT	4.29	-	CONSTANT	-5.51	-	0.69	0.12	0.29
		NUM_HB	0.07	0.52	ROS_CG_BETA	-0.78	-0.85			
		DFIRE_EBU	-0.00	-0.50	NIP	8744.08	0.50			
					OPUS_CA	-0.03	-0.59			
					TES_PP	0.13	0.46			
					MJPL_PP_UB	0.00	0.28			
					OPUS_CA_ENS	0.05	0.85			
2	Corr.	CONSTANT	4.84	-	CONSTANT	-1.32	-	0.22	0.39	0.03
		NUM_HB	0.09	0.61	ROS_CG_BETA	-0.77	-0.82			
		BIOSIMZ_KON	-0.02	-0.37	TES_PP	0.10	0.35			
		ROS_HBOND_UB	-0.04	-0.34	ACE19_HYDR_UB	0.00	0.30			
		TES_PP_UB	0.02	0.52	OPUS_CA_ENS	0.04	0.65			
		DFIRE_EBU	-0.00	-0.49						
3	Corr.	CONSTANT	5.17	-	CONSTANT	-2.65	-	0.72	0.03	0.85
		RES_C	-0.04	-0.32	PLANARITY	-1.11	-0.80			
		NUM_HB	0.08	0.44	ECCENTRIC	-1.64	-0.14			
		DFIRE_EBU	-0.00	-0.47	NUM_HB	0.03	0.14			
					ACE22_ALL	0.00	0.20			
					ROS_CG_BETA	-1.00	-1.07			
					MSBM_PP	-2.11	-0.56			
					ROS_CG_BETA_UB	0.41	0.51			
					ROS_HBOND_UB	0.09	0.62			
					DFIRE_UB	-0.09	-0.43			
					RF_PP_UB	0.04	0.53			
					QP_PP_UB	0.03	0.46			
					SKOB_PP_UB	-0.07	-0.98			
					MJPL_PP_UB	-0.00	-0.20			
					TD_PP_UB	0.09	0.95			

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Sch.	Sel.	$\log_{10} k_{\text{on}}$			$\log_{10} k_{\text{off}}$			ΔG_{sel}		ΔG_{val}
		Feat.	W	W_n	Feat.	W	W_n	Corr.	Corr.	p
					RO_PP_UB	-0.01	-0.33			
					ROS_FA_REP_ENS	0.06	0.43			
					ROS_HBOND_ENS	-0.35	-0.27			
					S_WLC_ALL2	-0.36	-0.72			
4	Corr.	CONSTANT	6.40	-	CONSTANT	-6.32	-	0.27	0.43	0.02
		RES_C	-0.07	-0.49	ROS_CG_BETA	-0.49	-0.52			
		NUM_HB	0.07	0.39	NIP	8612.18	0.51			
		ACE22_ALL	0.00	0.28						
		ROS_FA_REP	0.05	0.27						
		ROS_CG_VDW	-0.77	-0.20						
		STC_H	-0.06	-0.26						
		ROS_TOTAL_UB	0.01	0.13						
		GEN_4_BODY_UB	0.02	0.41						
		ROS_FA_PP_EBU	0.59	0.23						
		DFIRE_EBU	-0.00	-0.54						

Table 2: Rate constant models (2OZA omitted)

Sch.	Sel.	$\log_{10} k_{\text{on}}$			$\log_{10} k_{\text{off}}$			ΔG_{sel}		ΔG_{val}
		Feat.	W	W_n	Feat.	W	W_n	Corr.	Corr.	p
1	RMSE	CONSTANT	4.81	-	CONSTANT	1.02	-	0.51	0.08	0.48
		OPUS_PSP_EBU	-0.00	-0.56	CATION_PI	0.59	0.49			
					TD_PP	0.31	0.59			
					GEOMETRIC_EBU	0.05	0.71			
					RF_PP_EBU	-0.20	-0.43			
2	RMSE	CONSTANT	4.81	-	CONSTANT	-0.45	-	0.00	0.48	<0.01
		OPUS_PSP_EBU	-0.00	-0.56	TD_PP	0.28	0.52			
					ROS_CG_VDW_ENS	-4.55	-0.43			
3	RMSE	CONSTANT	4.44	-	CONSTANT	-0.45	-	0.72	0.25	0.05
		NUM_HB	0.07	0.37	ROS_CG_BETA	-0.45	-0.35			
		ROS_CG_BETA	0.45	0.44	MJ2H_PP	0.02	0.73			
		GEOMETRIC	-0.01	-0.30	SKOB_PP_UB	-0.05	-0.82			
		ROS_HBOND_UB	-0.12	-1.09	MJPL_PP_UB	0.00	0.15			
		DDFIRE_UB	0.06	0.96	TD_PP_UB	0.08	0.83			
		GEN_4_BODY_UB	0.01	0.33						
		RO_PP_UB	-0.00	-0.31						
		ROS_CG_VDW_ENS	-1.57	-0.23						
		DFIRE_EBU	-0.00	-0.28						
4	RMSE	CONSTANT	5.80	-	CONSTANT	-0.87	-	0.32	0.59	<0.01
		RES_C	-0.07	-0.53	MJ2H_PP	0.01	0.46			
		NUM_HB	0.08	0.42						
		ROS_CG_VDW	-1.01	-0.27						
		STC_H	-0.06	-0.28						
		GEN_4_BODY_UB	0.01	0.39						
		DFIRE_EBU	-0.00	-0.41						
		S_WLC_INT2	-0.28	-0.19						
1	Corr.	CONSTANT	4.81	-	CONSTANT	-0.50	-	0.52	0.09	0.43
		OPUS_PSP_EBU	-0.00	-0.56	RES_C	0.05	0.30			
					CATION_PI	0.59	0.49			
					TD_PP	0.27	0.52			
					GEOMETRIC_EBU	0.05	0.70			
					RF_PP_EBU	-0.16	-0.34			
2	Corr.	CONSTANT	4.30	-	CONSTANT	1.99	-	0.31	0.39	0.03
		NUM_HB	0.07	0.49	RES_NP	-0.03	-0.15			
		DFIRE_EBU	-0.00	-0.52	PLANARITY	0.02	0.01			
					NUM_SB	0.08	0.62			
					GAP_VOL	0.00	0.21			
					ROS_CG_VDW	-4.63	-0.42			

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Sch.	Sel.	$\log_{10} k_{\text{on}}$			$\log_{10} k_{\text{off}}$			ΔG_{sel}		ΔG_{val}
		Feat.	W	W_n	Feat.	W	W_n	Corr.	Corr.	p
					ROS_CG_ENV	-0.02	-0.13			
					ROS_HBOND	0.02	0.02			
					DELISLSOLV	-0.05	-0.20			
					CATION_PI	0.45	0.38			
					ALIPHATIC	0.07	0.09			
					TD_PP	0.39	0.73			
					TES_PP	-0.01	-0.03			
					ROS_CG_ENV_UB	-0.05	-0.24			
					INTERNAL_UB	0.00	0.01			
					ACE19_HYDR_UB	0.01	0.52			
					ROS_FA_REP_EBU	-0.02	-0.10			
					ROS_FA_PP_EBU	-0.21	-0.06			
					GEOMETRIC_EBU	0.05	0.73			
					RF_PP_EBU	-0.21	-0.46			
					S_GP_ALL2	0.00	0.00			
					S_WLC_INT2	0.64	0.30			
3	Corr.	CONSTANT	4.44	-	CONSTANT	-0.45	-	0.72	0.25	0.05
		NUM_HB	0.07	0.37	ROS_CG_BETA	-0.45	-0.35			
		ROS_CG_BETA	0.45	0.44	MJ2H_PP	0.02	0.73			
		GEOMETRIC	-0.01	-0.30	SKOB_PP_UB	-0.05	-0.82			
		ROS_HBOND_UB	-0.12	-1.09	MJPL_PP_UB	0.00	0.15			
		DDFIRE_UB	0.06	0.96	TD_PP_UB	0.08	0.83			
		GEN_4_BODY_UB	0.01	0.33						
		RO_PP_UB	-0.00	-0.31						
		ROS_CG_VDW_ENS	-1.57	-0.23						
		DFIRE_EBU	-0.00	-0.28						
4	Corr.	CONSTANT	5.80	-	CONSTANT	-0.67	-	0.33	0.60	<0.01
		RES_C	-0.07	-0.53	MJ2H_PP	0.01	0.53			
		NUM_HB	0.08	0.42	MJPL_PP_UB	0.00	0.40			
		ROS_CG_VDW	-1.01	-0.27						
		STC_H	-0.06	-0.28						
		GEN_4_BODY_UB	0.01	0.39						
		DFIRE_EBU	-0.00	-0.41						
		S_WLC_INT2	-0.28	-0.19						